



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:44 AM EDT

PDB ID : 4V82 / pdb_00004v82
Title : Crystal structure of cyanobacterial Photosystem II in complex with terbutryn
Authors : Gabdulkhakov, A.; Broser, M.; Guskov, A.; Kern, J.; Glockner, C.; Muh, F.;
Saenger, W.; Zouni, A.
Deposited on : 2010-11-30
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

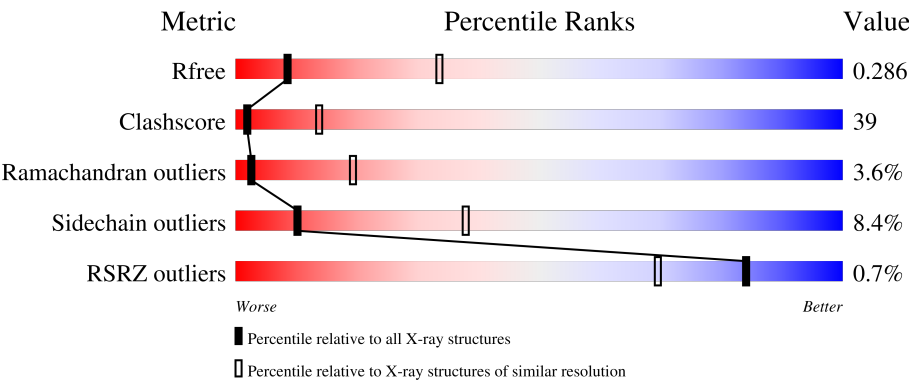
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



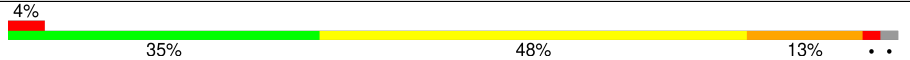
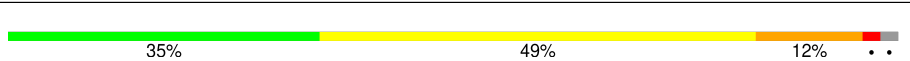
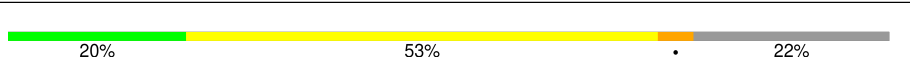
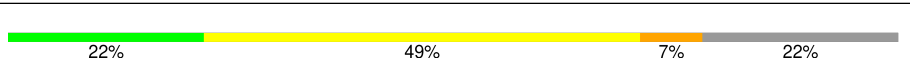
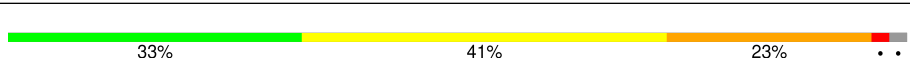
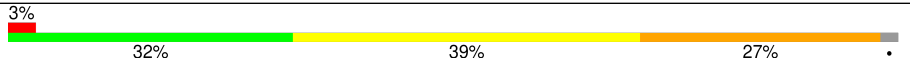
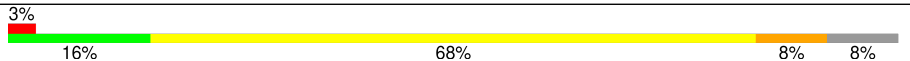
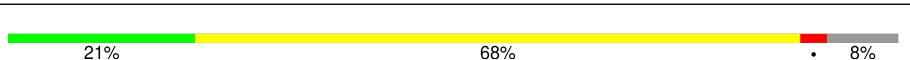
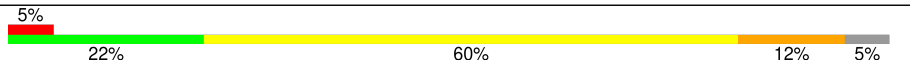
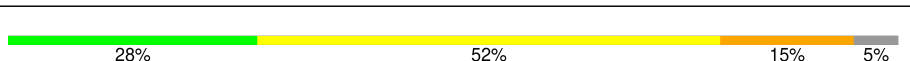
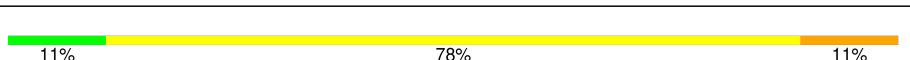
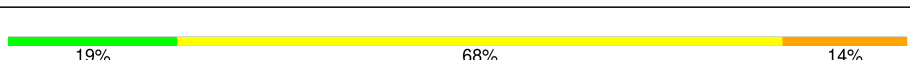
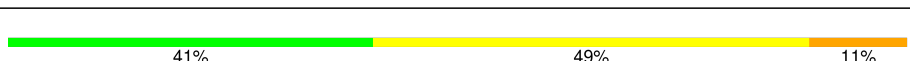
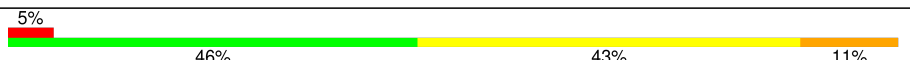
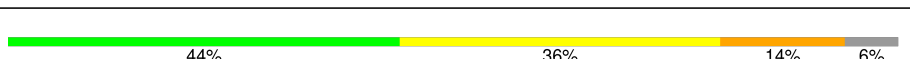
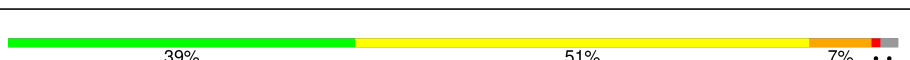
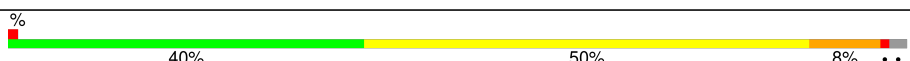
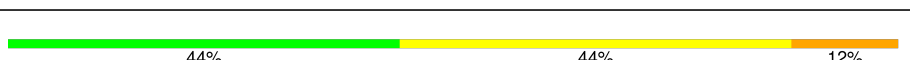
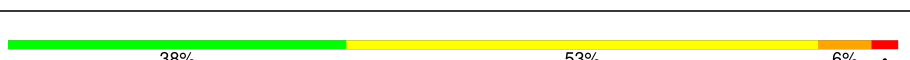
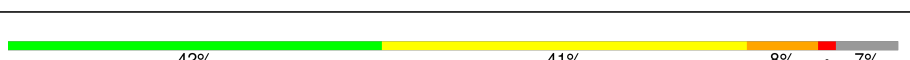
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	344	36%52%8% . .
1	BA	344	35%53%8% . .
2	AB	510	% 43%45%8% . .
2	BB	510	% 42%45%8% . .
3	AC	461	% 36%53%7% . .

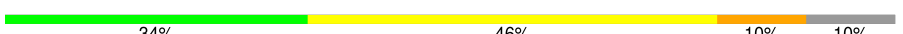
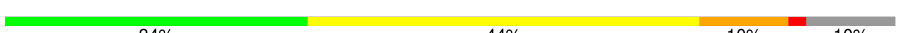
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Mol	Chain	Length	Quality of chain
3	BC	461	
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	BT	32	
15	AU	104	
15	BU	104	

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Mol	Chain	Length	Quality of chain
16	AV	137	
16	BV	137	
17	Ay	46	
17	By	46	
18	AX	41	
18	BX	41	
19	AY	28	
19	BY	28	
20	AZ	62	
20	BZ	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	AA	404	X	-	-	-
24	CLA	AA	405	X	-	-	-
24	CLA	AA	406	X	-	-	-
24	CLA	AA	407	X	-	-	-
24	CLA	AB	601	X	-	-	-
24	CLA	AB	602	X	-	-	-
24	CLA	AB	603	X	-	-	-
24	CLA	AB	604	X	-	-	-
24	CLA	AB	605	X	-	-	-
24	CLA	AB	606	X	-	-	-
24	CLA	AB	607	X	-	-	-
24	CLA	AB	608	X	-	-	-
24	CLA	AB	609	X	-	-	-
24	CLA	AB	610	X	-	-	-
24	CLA	AB	611	X	-	-	-
24	CLA	AB	612	X	-	-	-
24	CLA	AB	613	X	-	-	-
24	CLA	AB	614	X	-	-	-
24	CLA	AB	615	X	-	-	-
24	CLA	AB	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	AC	501	X	-	-	-
24	CLA	AC	502	X	-	-	-
24	CLA	AC	503	X	-	-	-
24	CLA	AC	504	X	-	-	-
24	CLA	AC	505	X	-	-	-
24	CLA	AC	506	X	-	-	-
24	CLA	AC	507	X	-	-	-
24	CLA	AC	508	X	-	-	-
24	CLA	AC	509	X	-	-	-
24	CLA	AC	510	X	-	-	-
24	CLA	AC	511	X	-	-	-
24	CLA	AC	512	X	-	-	-
24	CLA	AC	513	X	-	-	-
24	CLA	AD	401	X	-	-	-
24	CLA	AD	404	X	-	-	-
24	CLA	BA	5405	X	-	-	-
24	CLA	BA	5406	X	-	-	-
24	CLA	BA	5407	X	-	-	-
24	CLA	BA	5408	X	-	-	-
24	CLA	BB	5605	X	-	-	-
24	CLA	BB	5606	X	-	-	-
24	CLA	BB	5607	X	-	-	-
24	CLA	BB	5608	X	-	-	-
24	CLA	BB	5609	X	-	-	-
24	CLA	BB	5610	X	-	-	-
24	CLA	BB	5611	X	-	-	-
24	CLA	BB	5612	X	-	-	-
24	CLA	BB	5613	X	-	-	-
24	CLA	BB	5614	X	-	-	-
24	CLA	BB	5615	X	-	-	-
24	CLA	BB	5616	X	-	-	-
24	CLA	BB	5617	X	-	-	-
24	CLA	BB	5618	X	-	-	-
24	CLA	BB	5619	X	-	-	-
24	CLA	BB	5620	X	-	-	-
24	CLA	BC	5501	X	-	-	-
24	CLA	BC	5502	X	-	-	-
24	CLA	BC	5503	X	-	-	-
24	CLA	BC	5504	X	-	-	-
24	CLA	BC	5505	X	-	-	-
24	CLA	BC	5506	X	-	-	-
24	CLA	BC	5507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	BC	5508	X	-	-	-
24	CLA	BC	5509	X	-	-	-
24	CLA	BC	5510	X	-	-	-
24	CLA	BC	5511	X	-	-	-
24	CLA	BC	5512	X	-	-	-
24	CLA	BC	5513	X	-	-	-
24	CLA	BD	5402	X	-	-	-
24	CLA	BD	5405	X	-	-	-
25	MST	AA	408	-	-	X	-
25	MST	BA	5409	-	-	X	-
28	DGD	AC	518	X	-	-	-
28	DGD	AC	519	X	-	X	-
28	DGD	BC	5518	X	-	-	-
28	DGD	BC	5519	X	-	X	-
30	SQD	AA	413	-	X	-	-
34	PHO	AD	402	X	-	-	-
34	PHO	AD	403	X	-	-	-
34	PHO	BD	5403	X	-	-	-
34	PHO	BD	5404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50266 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	BA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	BB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

- Molecule 3 is a protein called Photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	BC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			
4	BD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AE	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	BE	82	Total	C	N	O	0	0	0
			666	434	108	124			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	BF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	BH	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	BI	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	38	Total	C	N	O	S	0	0	0
			271	182	42	46	1			
9	BJ	38	Total	C	N	O	S	0	0	0
			271	182	42	46	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AK	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	BK	37	Total	C	N	O	0	0	0
			293	204	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	BL	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	BM	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AO	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	BO	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	BT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AU	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	BU	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	BV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Ay	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	By	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AX	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	BX	37	Total	C	N	O		0	0	0
			270	182	41	47				

- Molecule 19 is a protein called PHOTOSYSTEM II PSBX PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AY	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	BY	28	Total	C	N	O		0	0	0
			140	84	28	28				

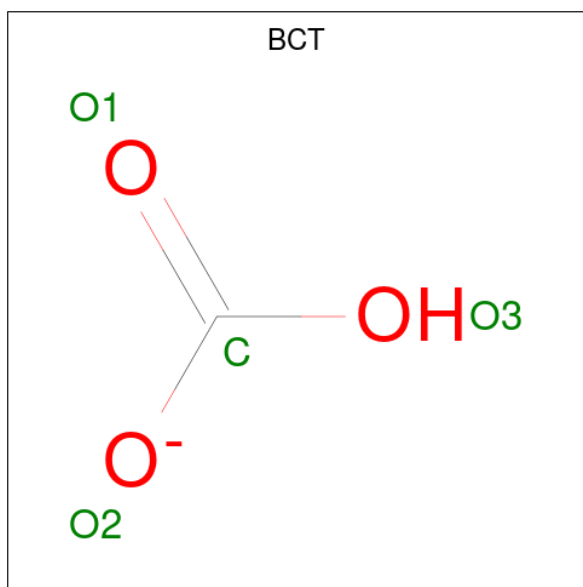
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	BZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	AA	1	Total	Fe	0	0
			1	1		
21	BD	1	Total	Fe	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).

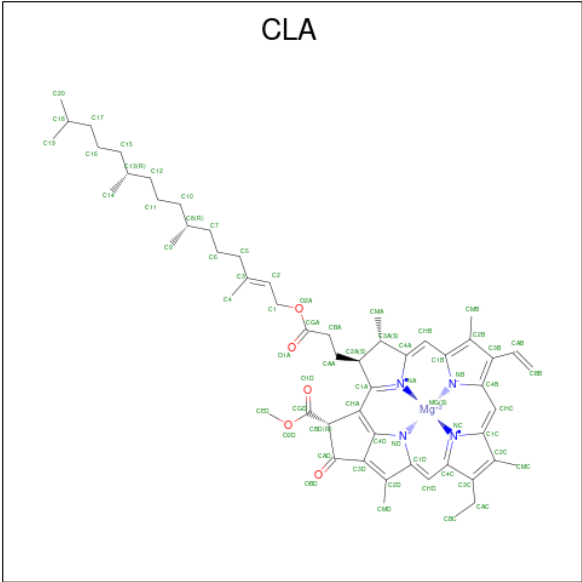


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	AA	1	Total	C	O	0	0
			4	1	3		
22	BA	1	Total	C	O	0	0
			4	1	3		

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	AA	1	Total	Cl	0	1
			2	2		
23	BA	1	Total	Cl	0	1
			2	2		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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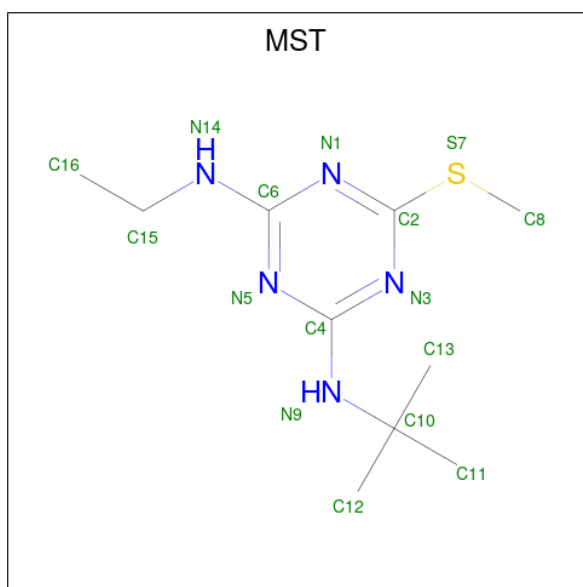
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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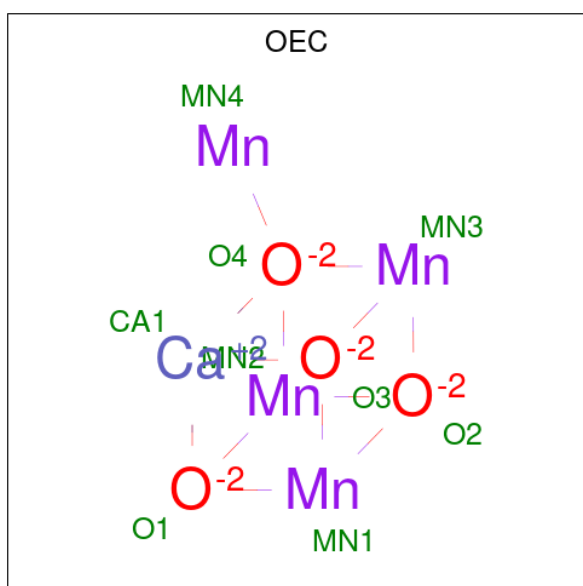
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (CCD ID: MST) (formula: C₁₀H₁₉N₅S).



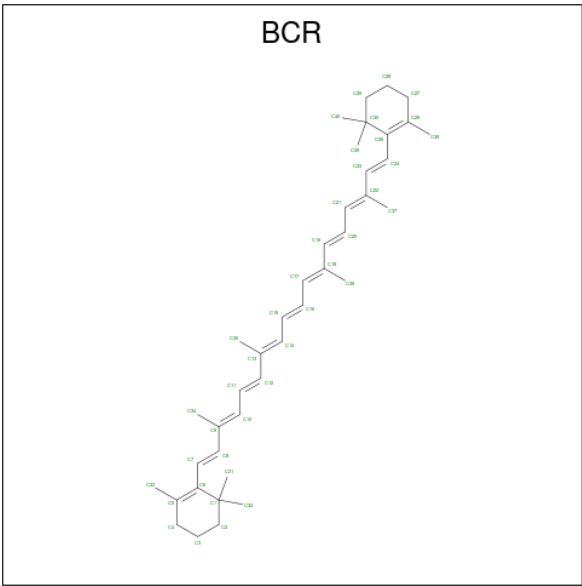
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	AA	1	Total	C	N	S	0	0
			16	10	5	1		
25	BA	1	Total	C	N	S	0	0
			16	10	5	1		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	AA	1	Total	Ca	Mn		
			5	1	4	0	0
26	BA	1	Total	Ca	Mn		
			5	1	4	0	0

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



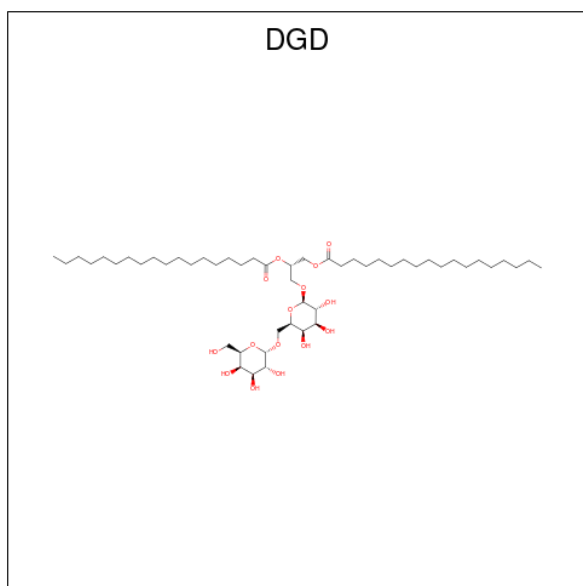
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AD	1	Total C 40 40	0	0
27	AJ	1	Total C 40 40	0	0
27	AK	1	Total C 40 40	0	0
27	AT	1	Total C 40 40	0	0
27	AX	1	Total C 40 40	0	0
27	BA	1	Total C 40 40	0	0

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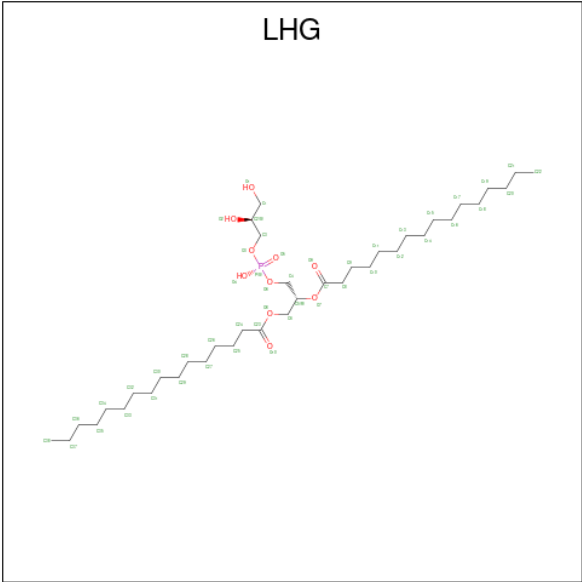
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BD	1	Total C 40 40	0	0
27	BJ	1	Total C 40 40	0	0
27	BK	1	Total C 40 40	0	0
27	BT	1	Total C 40 40	0	0
27	BX	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



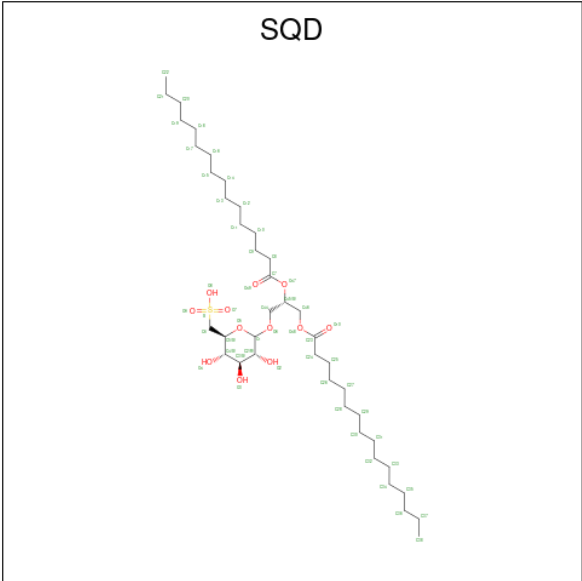
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	AA	1	Total	C	O	0	0
			56	41	15		
28	AB	1	Total	C	O	0	0
			52	37	15		
28	AC	1	Total	C	O	0	0
			53	38	15		
28	AC	1	Total	C	O	0	0
			62	47	15		
28	AC	1	Total	C	O	0	0
			66	51	15		
28	AE	1	Total	C	O	0	0
			63	48	15		
28	AH	1	Total	C	O	0	0
			58	43	15		
28	BA	1	Total	C	O	0	0
			56	41	15		
28	BB	1	Total	C	O	0	0
			52	37	15		
28	BC	1	Total	C	O	0	0
			53	38	15		
28	BC	1	Total	C	O	0	0
			62	47	15		
28	BC	1	Total	C	O	0	0
			66	51	15		
28	BE	1	Total	C	O	0	0
			63	48	15		
28	BH	1	Total	C	O	0	0
			58	43	15		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



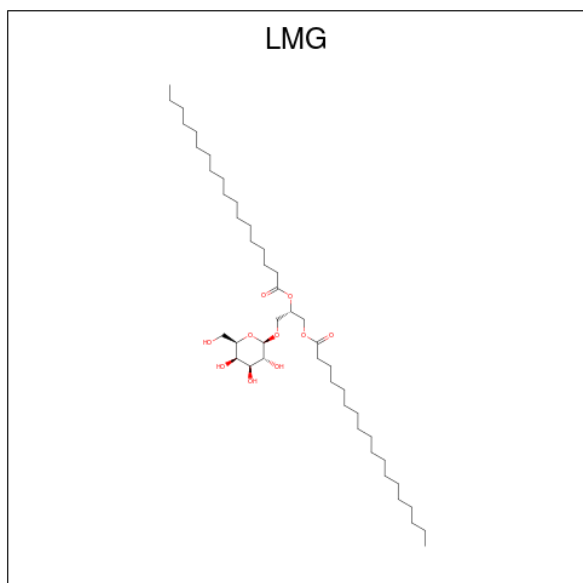
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	P	0	0
			39	28	10	1		
29	AA	1	Total	C	O	P	0	0
			37	26	10	1		
29	BA	1	Total	C	O	P	0	0
			39	28	10	1		
29	BA	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	AA	1	Total	C	O	S	0	0
			51	38	12	1		
30	AA	1	Total	C	O	S	0	0
			54	41	12	1		
30	AB	1	Total	C	O	S	0	0
			43	30	12	1		
30	AB	1	Total	C	O	S	0	0
			47	34	12	1		
30	AF	1	Total	C	O	S	0	0
			45	32	12	1		
30	BA	1	Total	C	O	S	0	0
			54	41	12	1		
30	BA	1	Total	C	O	S	0	0
			51	38	12	1		
30	BB	1	Total	C	O	S	0	0
			47	34	12	1		
30	BB	1	Total	C	O	S	0	0
			43	30	12	1		
30	BF	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



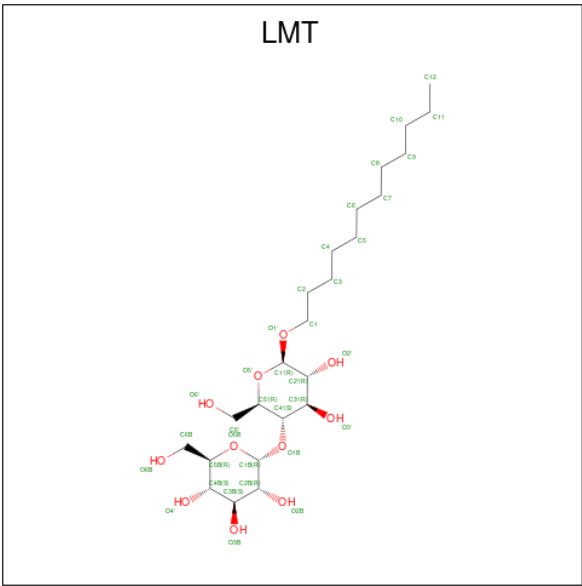
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			44	34	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			42	32	10		
31	AB	1	Total	C	O	0	0
			51	41	10		
31	AB	1	Total	C	O	0	0
			49	39	10		
31	AC	1	Total	C	O	0	0
			48	38	10		
31	AC	1	Total	C	O	0	0
			45	35	10		
31	AD	1	Total	C	O	0	0
			49	39	10		
31	AD	1	Total	C	O	0	0
			48	38	10		
31	AI	1	Total	C	O	0	0
			43	33	10		
31	AJ	1	Total	C	O	0	0
			46	36	10		
31	AM	1	Total	C	O	0	0
			42	32	10		
31	BA	1	Total	C	O	0	0
			42	32	10		
31	BB	1	Total	C	O	0	0
			49	39	10		
31	BC	1	Total	C	O	0	0
			48	38	10		
31	BC	1	Total	C	O	0	0
			45	35	10		
31	BD	1	Total	C	O	0	0
			46	36	10		
31	BD	1	Total	C	O	0	0
			49	39	10		
31	BD	1	Total	C	O	0	0
			48	38	10		
31	BE	1	Total	C	O	0	0
			44	34	10		
31	BI	1	Total	C	O	0	0
			43	33	10		
31	BL	1	Total	C	O	0	0
			51	41	10		
31	BM	1	Total	C	O	0	0
			42	32	10		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



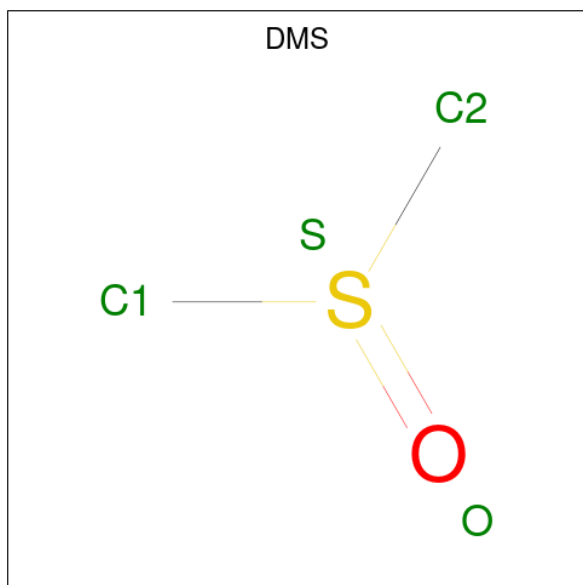
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BC	1	Total	C	O	0	0
			35	24	11		

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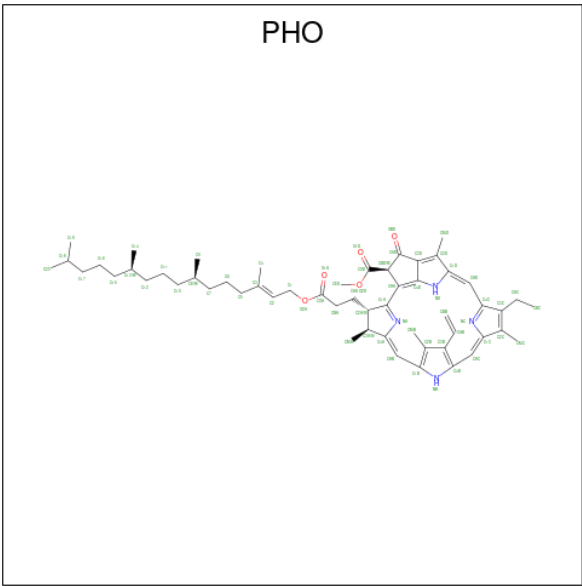
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	BD	1	Total	C	O	0	0
			31	20	11		
32	BI	1	Total	C	O	0	0
			35	24	11		
32	BM	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



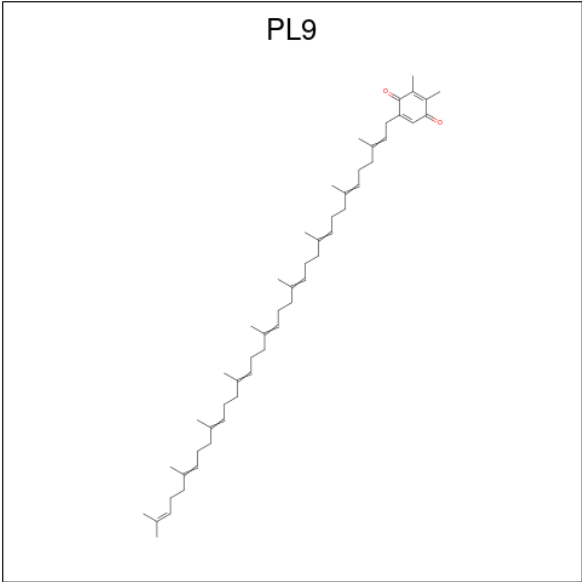
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AU	1	Total	C	O	S	0	0
			4	2	1	1		
33	AV	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



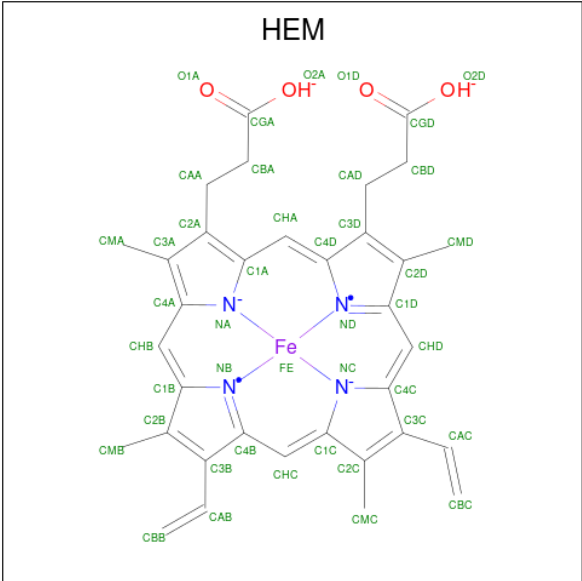
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 35 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	AD	1	Total	C	O	0	0
			55	53	2		
35	BD	1	Total	C	O	0	0
			55	53	2		

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	AF	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	BF	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	BV	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

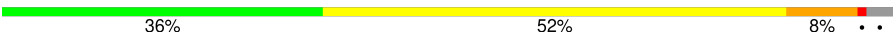
- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

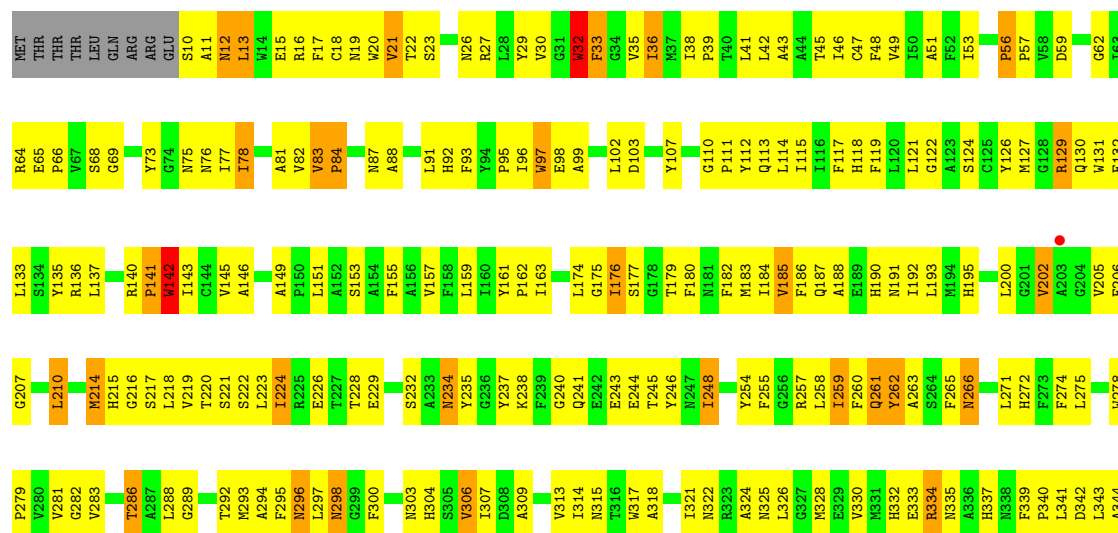
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	AF	1	Total 1	Ca 1	0	0
37	AK	1	Total 1	Ca 1	0	0
37	AO	1	Total 1	Ca 1	0	0
37	BF	1	Total 1	Ca 1	0	0
37	BK	1	Total 1	Ca 1	0	0
37	BO	1	Total 1	Ca 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

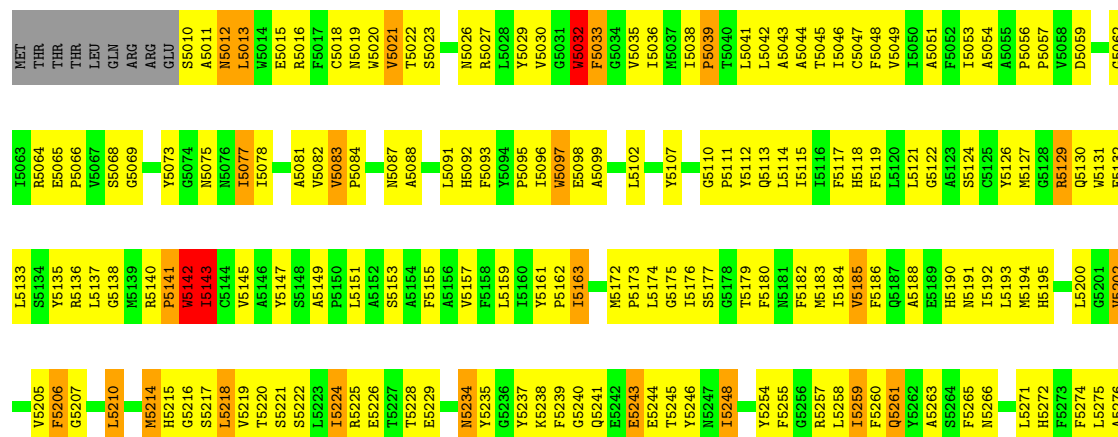
• Molecule 1: Photosystem Q(B) protein 1

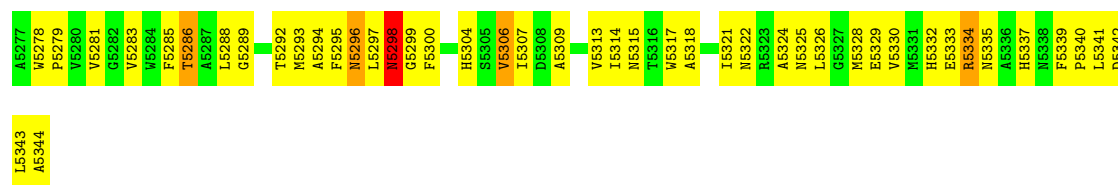
Chain AA: 



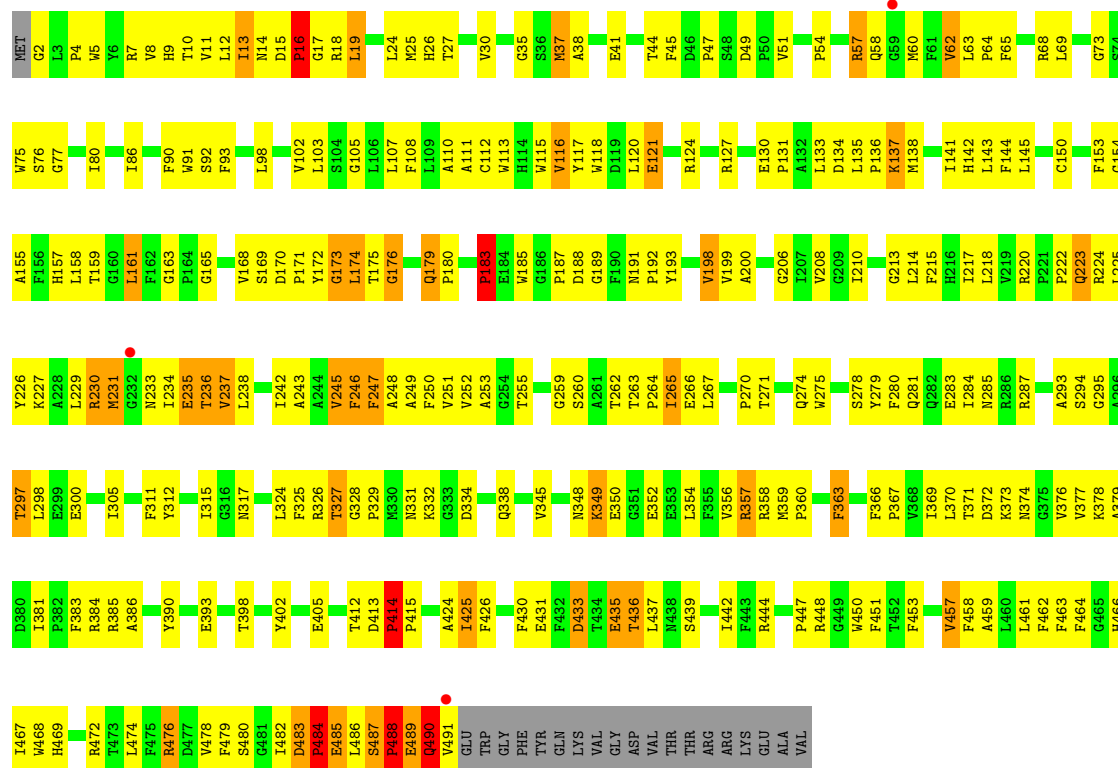
• Molecule 1: Photosystem Q(B) protein 1

Chain BA: 

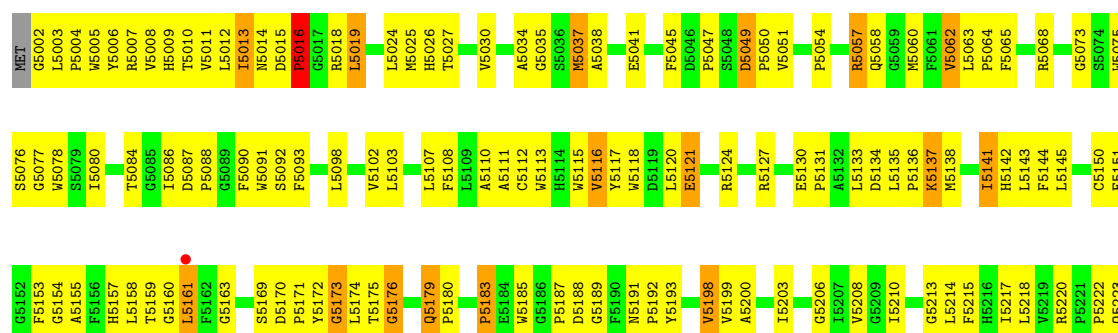


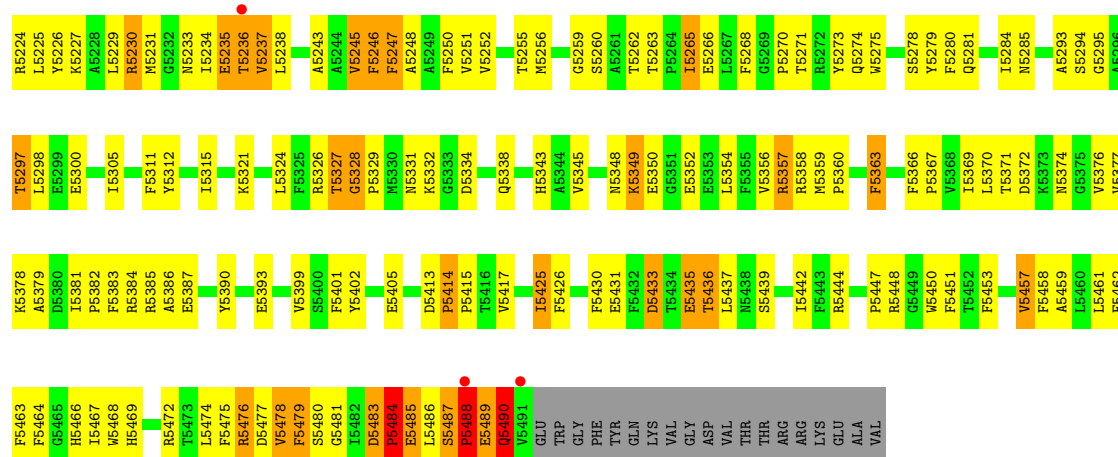


• Molecule 2: Photosystem II core light harvesting protein

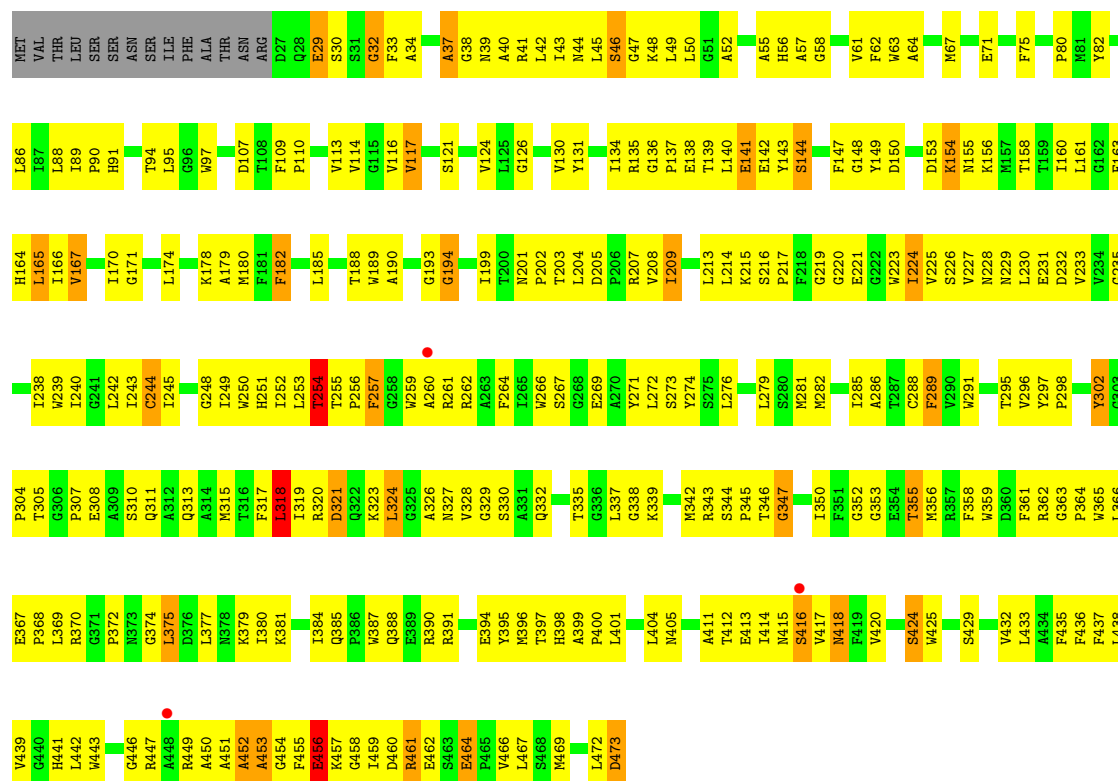


• Molecule 2: Photosystem II core light harvesting protein





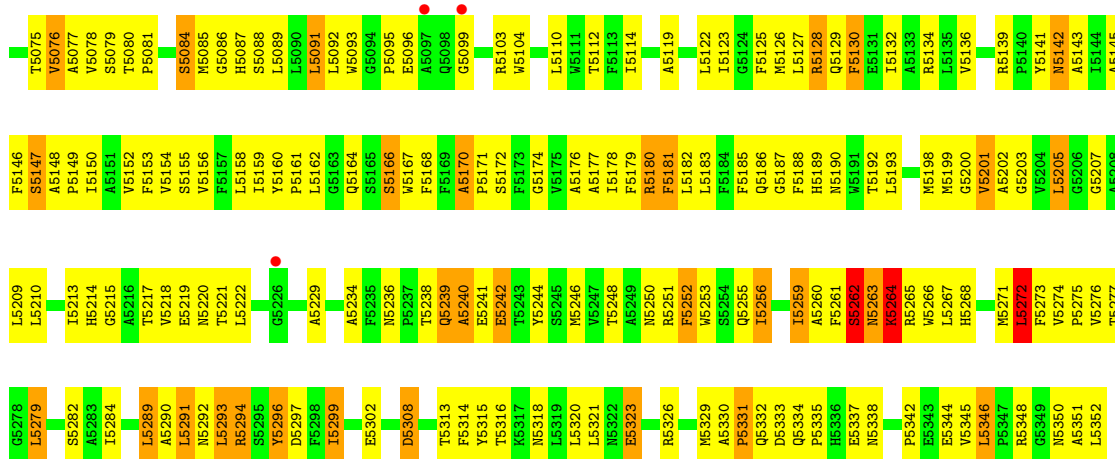
• Molecule 3: Photosystem II CP43 protein



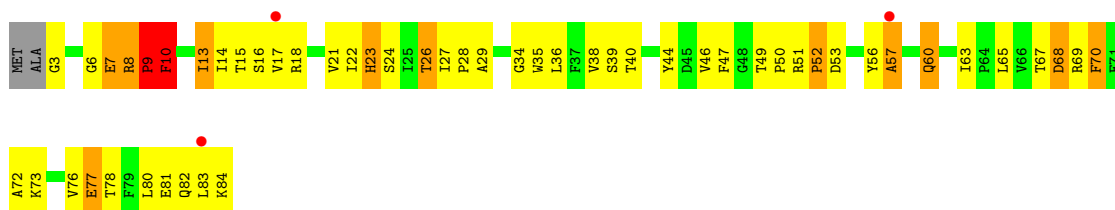
• Molecule 3: Photosystem II CP43 protein



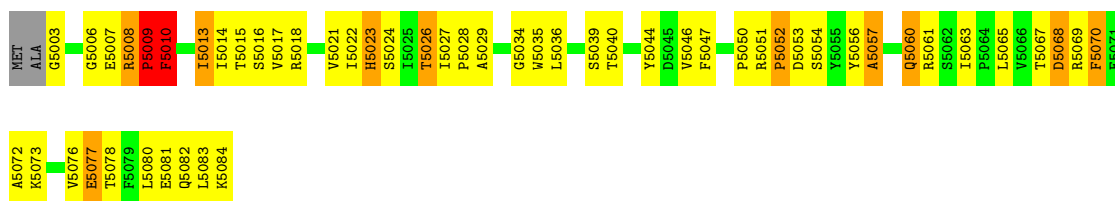




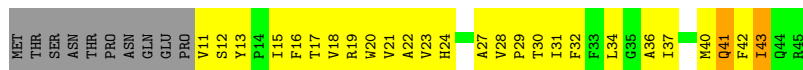
- Molecule 5: Cytochrome b559 subunit alpha



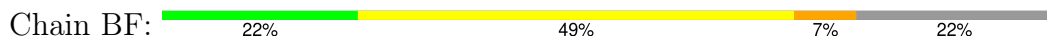
- Molecule 5: Cytochrome b559 subunit alpha



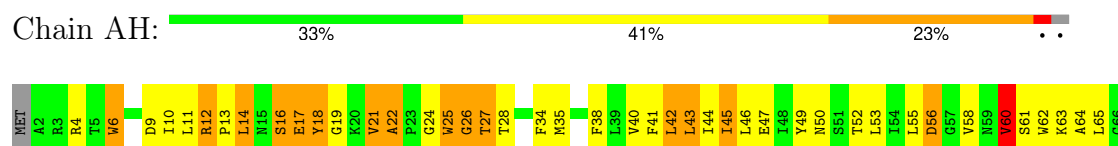
- Molecule 6: Cytochrome b559 subunit beta



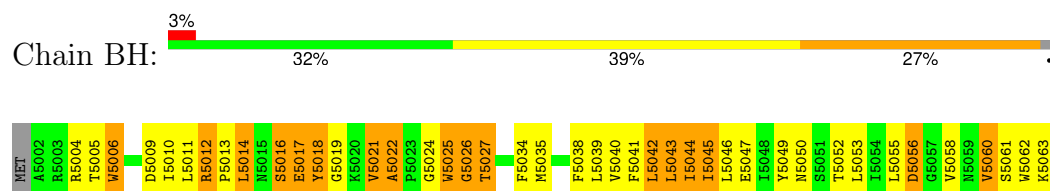
- Molecule 6: Cytochrome b559 subunit beta



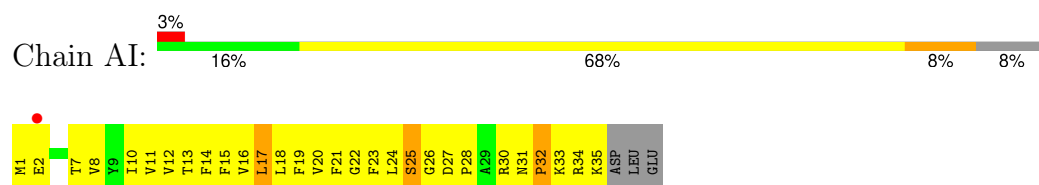
- Molecule 7: Photosystem II reaction center protein H



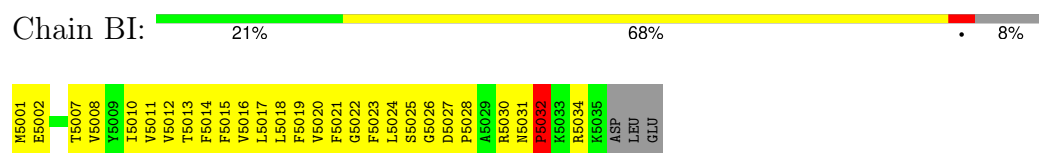
- Molecule 7: Photosystem II reaction center protein H



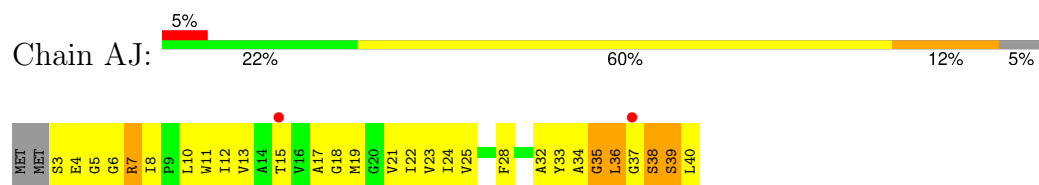
- Molecule 8: Photosystem II reaction center protein I



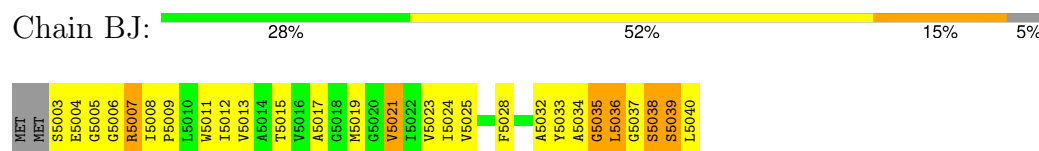
- Molecule 8: Photosystem II reaction center protein I



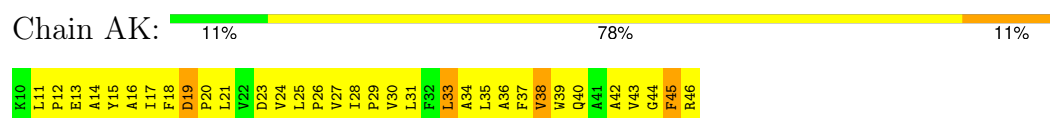
- Molecule 9: Photosystem II reaction center protein J



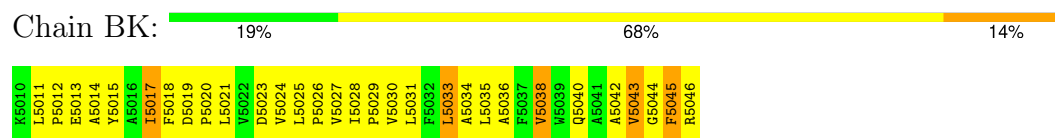
- Molecule 9: Photosystem II reaction center protein J



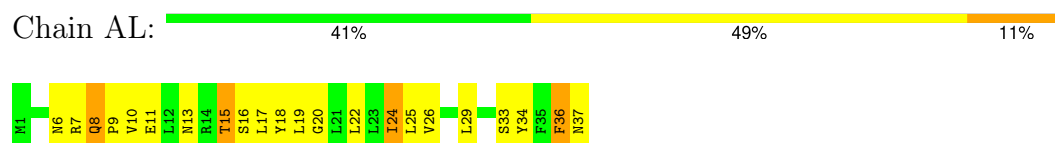
- Molecule 10: Photosystem II reaction center protein K



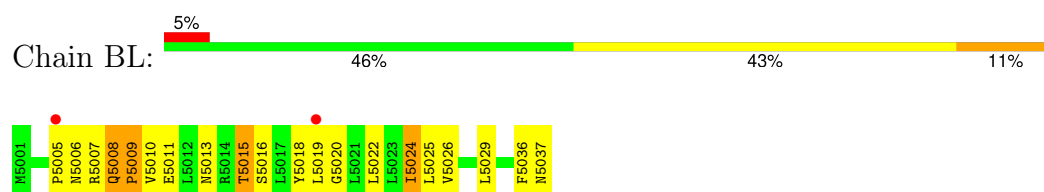
- Molecule 10: Photosystem II reaction center protein K



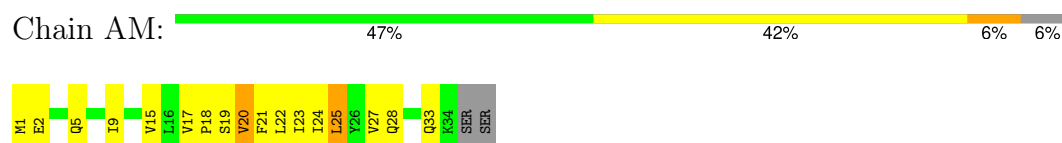
- Molecule 11: Photosystem II reaction center protein L



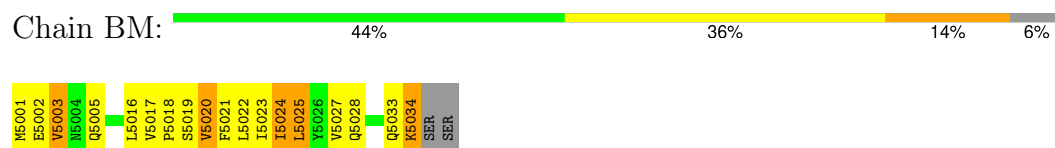
- Molecule 11: Photosystem II reaction center protein L



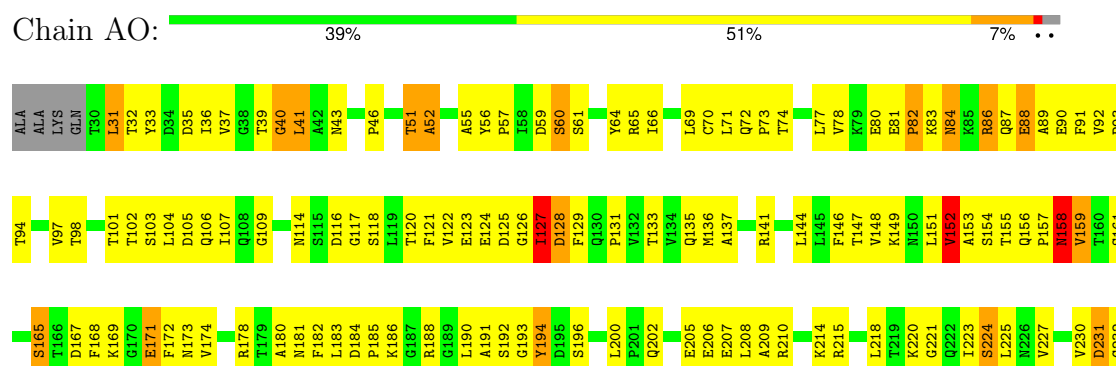
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

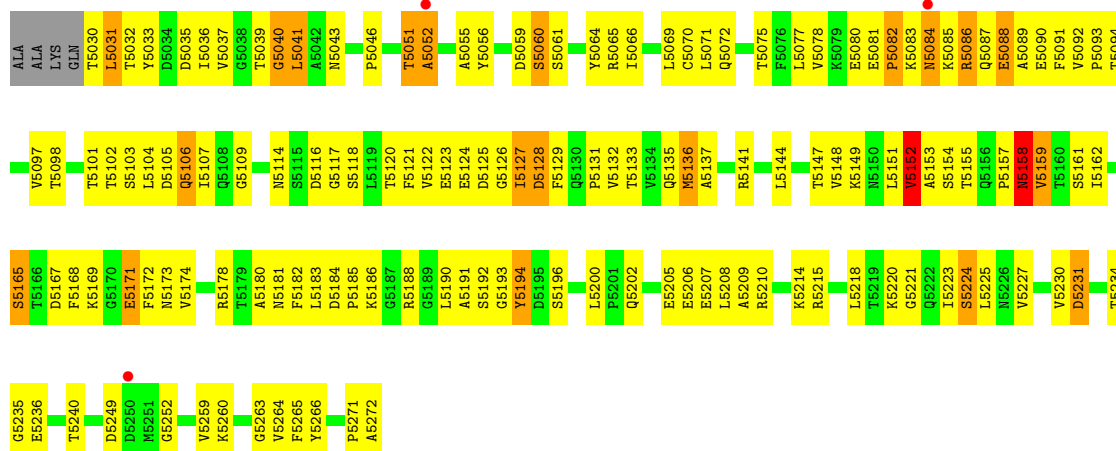


- Molecule 13: Photosystem II manganese-stabilizing polypeptide





- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

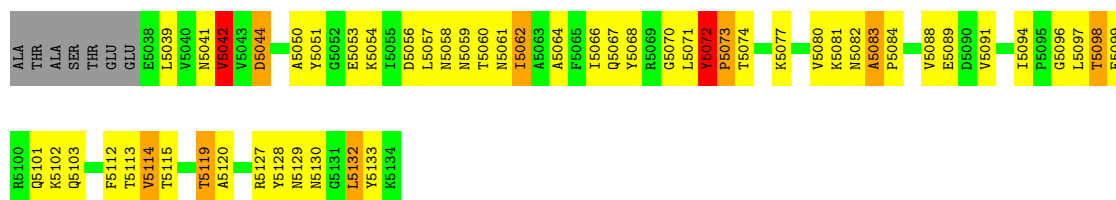


- Molecule 15: Photosystem II 12 kDa extrinsic protein



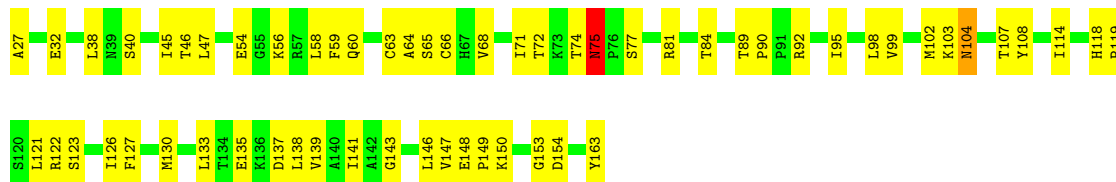
- Molecule 15: Photosystem II 12 kDa extrinsic protein





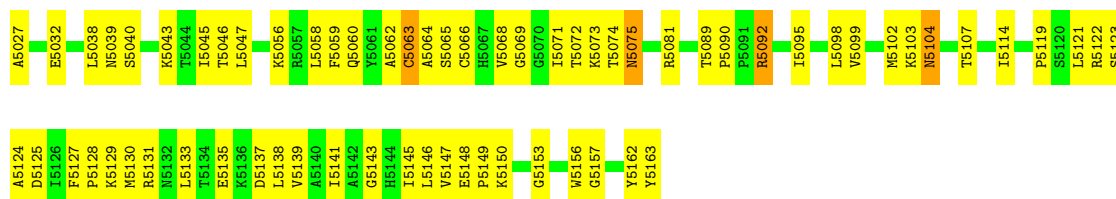
• Molecule 16: Cytochrome c-550

Chain AV: 57% 42% ..



• Molecule 16: Cytochrome c-550

Chain BV: 52% 45% .



• Molecule 17: Photosystem II reaction center protein ycf12

Chain Ay: 2% 9% 30% 15% 7% 39%



• Molecule 17: Photosystem II reaction center protein ycf12

Chain By: 9% 24% 26% . 39%

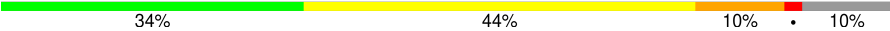


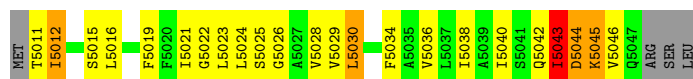
• Molecule 18: Photosystem II reaction center X protein

Chain AX: 34% 46% 10% 10%



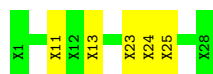
• Molecule 18: Photosystem II reaction center X protein

Chain BX:  34% 44% 10% 10%



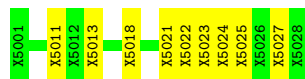
- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain AY:  82% 18%



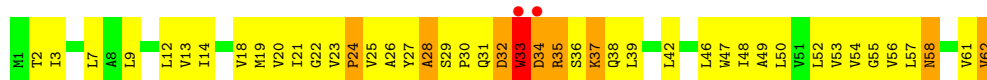
- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain BY:  68% 32%



- Molecule 20: Photosystem II reaction center protein Z

Chain AZ:  3% 29% 56% 13%



- Molecule 20: Photosystem II reaction center protein Z

Chain BZ:  2% 26% 60% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.08Å 225.37Å 305.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-3.20) 99.2 (20.00-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.12Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.269 , 0.299 0.264 , 0.286	Depositor DCC
R_{free} test set	3179 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	50266	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LHG, DMS, HEM, PHO, MST, OEC, LMG, PL9, BCT, BCR, CL, SQD, CLA, LMT, CA, FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.63	0/2713	1.11	21/3700 (0.6%)
1	BA	0.59	0/2713	1.10	22/3700 (0.6%)
2	AB	0.60	0/3986	1.09	31/5433 (0.6%)
2	BB	0.60	1/3986 (0.0%)	1.09	34/5433 (0.6%)
3	AC	0.55	0/3556	1.06	14/4842 (0.3%)
3	BC	0.52	0/3556	1.06	20/4842 (0.4%)
4	AD	0.63	0/2806	1.06	11/3825 (0.3%)
4	BD	0.60	0/2806	1.05	15/3825 (0.4%)
5	AE	0.60	0/685	1.23	11/933 (1.2%)
5	BE	0.60	0/685	1.23	10/933 (1.1%)
6	AF	0.89	1/291 (0.3%)	1.04	0/397
6	BF	0.90	1/291 (0.3%)	0.96	0/397
7	AH	0.54	0/520	1.08	3/709 (0.4%)
7	BH	0.57	0/520	1.09	4/709 (0.6%)
8	AI	0.61	0/293	1.17	2/395 (0.5%)
8	BI	0.67	0/293	1.17	2/395 (0.5%)
9	AJ	0.70	0/277	1.32	2/375 (0.5%)
9	BJ	0.73	0/277	1.27	3/375 (0.8%)
10	AK	0.61	0/303	1.02	1/416 (0.2%)
10	BK	0.74	1/303 (0.3%)	1.02	1/416 (0.2%)
11	AL	0.72	0/311	1.07	1/422 (0.2%)
11	BL	0.71	0/311	1.09	0/422
12	AM	0.79	0/270	1.07	1/367 (0.3%)
12	BM	0.88	2/270 (0.7%)	1.07	0/367
13	AO	0.59	0/1876	1.07	11/2548 (0.4%)
13	BO	0.57	0/1876	1.07	13/2548 (0.5%)
14	AT	0.92	1/284 (0.4%)	1.17	1/381 (0.3%)
14	BT	0.96	2/284 (0.7%)	1.25	3/381 (0.8%)
15	AU	0.67	0/785	1.19	6/1064 (0.6%)
15	BU	0.62	0/785	1.17	6/1064 (0.6%)
16	AV	0.59	0/1081	1.01	5/1468 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BV	0.54	0/1081	0.99	4/1468 (0.3%)
17	Ay	1.52	3/202 (1.5%)	1.52	3/272 (1.1%)
17	By	1.48	4/202 (2.0%)	1.60	2/272 (0.7%)
18	AX	0.69	0/273	1.10	1/370 (0.3%)
18	BX	0.84	2/273 (0.7%)	1.04	2/370 (0.5%)
20	AZ	0.62	0/490	1.14	4/669 (0.6%)
20	BZ	0.67	0/490	1.23	4/669 (0.6%)
All	All	0.63	18/42004 (0.0%)	1.09	274/57172 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
2	BB	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	By	5030	ILE	CA-CB	-11.38	1.41	1.54
17	Ay	35	ILE	CA-CB	-8.76	1.42	1.54
6	BF	5017	THR	CA-CB	8.33	1.66	1.53
14	BT	5029	ILE	CA-CB	7.72	1.65	1.54
17	Ay	31	ALA	CA-CB	-6.35	1.43	1.53
17	Ay	41	VAL	CA-CB	6.07	1.61	1.54
14	AT	32	LYS	CA-CB	5.96	1.65	1.53
18	BX	5043	ILE	CA-CB	5.68	1.62	1.54
10	BK	5043	VAL	CA-CB	5.61	1.62	1.54
17	By	5045	ASN	CA-CB	5.40	1.61	1.53
17	By	5039	LEU	CA-CB	5.34	1.62	1.53
12	BM	5024	ILE	CA-CB	-5.17	1.48	1.54
14	BT	5032	LYS	C-OXT	5.13	1.33	1.23
2	BB	5037	MET	SD-CE	5.11	1.92	1.79
18	BX	5046	VAL	CA-CB	5.09	1.59	1.54
12	BM	5003	VAL	CA-CB	-5.07	1.47	1.54
17	By	5026	ALA	CA-CB	-5.06	1.45	1.53
6	AF	43	ILE	CA-CB	-5.02	1.49	1.54

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	5489	GLU	N-CA-C	10.04	126.27	110.70
20	AZ	34	ASP	N-CA-C	-9.33	101.68	113.43
20	BZ	5034	ASP	N-CA-C	-9.08	101.99	113.43
17	By	5022	LEU	N-CA-C	-8.95	101.63	112.54
3	AC	182	PHE	N-CA-C	8.88	123.94	113.20
14	BT	5004	ILE	CB-CA-C	-8.77	100.31	112.14
13	AO	102	THR	N-CA-C	8.76	120.91	111.36
5	AE	57	ALA	N-CA-C	-8.64	99.39	110.53
15	AU	51	TYR	N-CA-C	-8.62	97.73	110.23
9	BJ	5036	LEU	N-CA-C	-8.58	102.94	113.41
3	AC	439	VAL	N-CA-C	-8.50	102.57	110.82
3	BC	5182	PHE	N-CA-C	8.44	123.41	113.20
5	BE	5057	ALA	N-CA-C	-8.43	99.17	110.55
2	AB	483	ASP	CA-C-N	8.42	130.37	119.84
2	AB	483	ASP	C-N-CA	8.42	130.37	119.84
9	AJ	36	LEU	N-CA-C	-8.33	103.25	113.41
3	BC	5318	LEU	N-CA-C	-8.24	102.37	111.36
15	BU	5051	TYR	N-CA-C	-8.24	98.27	110.23
2	BB	5328	GLY	CA-C-N	8.21	128.09	120.21
2	BB	5328	GLY	C-N-CA	8.21	128.09	120.21
2	BB	5483	ASP	CA-C-N	8.20	130.09	119.84
2	BB	5483	ASP	C-N-CA	8.20	130.09	119.84
13	BO	5102	THR	N-CA-C	8.17	120.27	111.36
15	AU	74	THR	N-CA-C	8.11	119.81	110.97
3	AC	318	LEU	N-CA-C	-8.05	102.59	111.36
3	BC	5439	VAL	N-CA-C	-8.01	103.00	110.53
15	BU	5074	THR	N-CA-C	7.96	119.65	110.97
13	BO	5103	SER	N-CA-C	7.91	121.69	110.23
13	AO	103	SER	N-CA-C	7.84	121.60	110.23
5	BE	5070	PHE	N-CA-C	7.72	119.33	111.07
18	BX	5046	VAL	N-CA-C	7.71	120.53	109.51
8	AI	2	GLU	N-CA-C	-7.63	103.43	112.89
18	AX	46	VAL	N-CA-C	7.55	120.30	109.51
5	AE	24	SER	N-CA-C	-7.54	103.34	112.54
2	BB	5141	ILE	CB-CA-C	-7.52	102.41	111.81
8	BI	5002	GLU	N-CA-C	-7.51	103.58	112.89
4	BD	5054	PHE	N-CA-C	7.50	122.32	112.72
2	AB	328	GLY	CA-C-N	7.48	127.39	120.21
2	AB	328	GLY	C-N-CA	7.48	127.39	120.21
5	AE	70	PHE	N-CA-C	7.42	119.01	111.07
2	AB	327	THR	N-CA-C	7.41	119.53	110.41
3	AC	347	GLY	N-CA-C	7.31	123.39	114.69
3	BC	5347	GLY	N-CA-C	7.26	123.33	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AD	54	PHE	N-CA-C	7.19	121.93	112.72
5	BE	5024	SER	N-CA-C	-7.19	103.77	112.54
2	BB	5236	THR	N-CA-C	-7.16	105.07	114.31
13	BO	5030	THR	N-CA-CB	-7.15	99.35	111.50
2	BB	5488	PRO	N-CA-C	7.04	126.97	112.47
2	BB	5327	THR	N-CA-C	7.02	119.04	110.41
2	AB	236	THR	N-CA-C	-6.99	105.30	114.31
4	AD	296	TYR	N-CA-C	6.98	118.67	111.14
10	AK	38	VAL	N-CA-C	-6.97	103.73	110.42
2	AB	363	PHE	N-CA-C	6.91	119.94	108.96
5	BE	5006	GLY	N-CA-C	6.90	121.24	112.83
2	BB	5363	PHE	N-CA-C	6.89	119.91	108.96
5	AE	6	GLY	N-CA-C	6.89	121.23	112.83
4	AD	156	VAL	N-CA-C	6.84	117.46	110.82
9	AJ	39	SER	N-CA-C	-6.84	104.04	114.16
3	AC	254	THR	N-CA-C	6.83	117.60	108.38
7	AH	64	ALA	N-CA-C	-6.78	105.45	113.38
1	BA	5339	PHE	CA-C-N	6.77	126.28	119.24
1	BA	5339	PHE	C-N-CA	6.77	126.28	119.24
15	AU	72	TYR	N-CA-C	6.74	124.71	109.81
17	By	5021	GLN	N-CA-CB	-6.69	100.87	110.57
14	AT	4	ILE	CB-CA-C	-6.67	103.14	112.14
4	BD	5296	TYR	N-CA-C	6.66	118.33	111.14
5	AE	67	THR	N-CA-C	6.65	122.21	113.30
13	AO	200	LEU	CA-C-N	6.63	128.13	119.84
13	AO	200	LEU	C-N-CA	6.63	128.13	119.84
20	BZ	5037	LYS	N-CA-C	-6.63	104.92	112.87
2	BB	5037	MET	N-CA-C	-6.62	104.14	111.82
1	AA	87	ASN	N-CA-C	-6.61	105.04	113.23
3	BC	5254	THR	N-CA-C	6.59	117.28	108.38
3	AC	37	ALA	N-CA-C	-6.57	103.36	112.30
20	AZ	37	LYS	N-CA-C	-6.57	104.99	112.87
13	BO	5200	LEU	CA-C-N	6.56	128.04	119.84
13	BO	5200	LEU	C-N-CA	6.56	128.04	119.84
15	AU	62	ILE	N-CA-C	6.54	118.07	110.62
2	BB	5381	ILE	CA-C-N	6.54	126.51	119.78
2	BB	5381	ILE	C-N-CA	6.54	126.51	119.78
15	BU	5062	ILE	N-CA-C	6.53	118.06	110.62
15	BU	5072	TYR	N-CA-C	6.51	124.20	109.81
5	BE	5067	THR	N-CA-C	6.48	121.98	113.30
16	AV	104	ASN	CA-C-N	6.41	126.17	119.76
16	AV	104	ASN	C-N-CA	6.41	126.17	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BC	5037	ALA	N-CA-C	-6.41	103.59	112.30
9	BJ	5039	SER	N-CA-C	-6.39	104.70	114.16
17	Ay	25	ILE	CB-CA-C	-6.37	100.84	111.29
2	AB	37	MET	N-CA-C	-6.35	104.45	111.82
1	BA	5142	TRP	N-CA-C	6.33	124.29	110.80
13	BO	5196	SER	N-CA-C	6.32	116.42	108.45
1	AA	36	ILE	N-CA-C	-6.32	106.38	111.81
4	AD	272	LEU	N-CA-C	-6.31	103.70	111.40
7	BH	5064	ALA	N-CA-C	-6.29	106.03	113.38
16	BV	5104	ASN	CA-C-N	6.28	126.04	119.76
16	BV	5104	ASN	C-N-CA	6.28	126.04	119.76
4	AD	142	ASN	N-CA-C	-6.28	105.45	113.23
1	BA	5032	TRP	N-CA-C	-6.28	103.97	111.69
10	BK	5038	VAL	N-CA-C	-6.27	104.40	110.42
4	AD	76	VAL	CB-CA-C	-6.22	104.48	111.45
2	AB	332	LYS	N-CA-C	-6.21	105.67	113.18
3	BC	5472	LEU	N-CA-C	-6.20	104.52	111.28
13	BO	5249	ASP	N-CA-C	-6.18	105.38	113.17
2	AB	381	ILE	CA-C-N	6.18	126.14	119.78
2	AB	381	ILE	C-N-CA	6.18	126.14	119.78
13	AO	40	GLY	N-CA-C	-6.14	107.22	115.21
1	AA	142	TRP	N-CA-C	6.13	123.86	110.80
3	AC	224	ILE	CB-CA-C	-6.09	104.07	112.04
2	BB	5484	PRO	N-CA-C	6.08	125.00	112.47
3	BC	5114	VAL	CB-CA-C	-6.03	104.14	112.04
1	BA	5087	ASN	N-CA-C	-6.02	105.76	113.23
13	AO	249	ASP	N-CA-C	-6.02	105.59	113.17
4	AD	147	SER	N-CA-C	-5.99	104.83	111.36
2	BB	5332	LYS	N-CA-C	-5.97	105.95	113.18
2	AB	484	PRO	N-CA-C	5.96	124.76	112.47
4	AD	273	PHE	N-CA-C	5.93	118.26	111.02
4	BD	5297	ASP	N-CA-C	5.93	118.42	109.41
2	BB	5051	VAL	CB-CA-C	-5.92	104.12	111.94
4	BD	5273	PHE	N-CA-C	5.92	118.24	111.02
3	AC	32	GLY	N-CA-C	-5.90	99.19	113.18
13	AO	196	SER	N-CA-C	5.90	116.02	108.24
1	BA	5036	ILE	N-CA-C	-5.90	106.74	111.81
2	AB	489	GLU	N-CA-C	5.87	118.33	108.23
3	BC	5302	TYR	N-CA-C	-5.86	100.99	109.31
2	AB	174	LEU	N-CA-C	-5.85	107.95	114.62
4	BD	5156	VAL	N-CA-C	5.84	117.36	111.00
1	AA	32	TRP	N-CA-C	-5.83	104.52	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BD	5076	VAL	CB-CA-C	-5.82	104.93	111.45
3	BC	5224	ILE	CB-CA-C	-5.80	104.44	112.04
16	AV	75	ASN	CA-C-N	5.79	125.50	119.82
16	AV	75	ASN	C-N-CA	5.79	125.50	119.82
4	BD	5272	LEU	N-CA-C	-5.79	103.70	112.04
2	BB	5163	GLY	CA-C-N	5.77	127.05	119.84
2	BB	5163	GLY	C-N-CA	5.77	127.05	119.84
2	BB	5077	GLY	N-CA-C	5.75	120.52	113.79
13	BO	5181	ASN	N-CA-C	5.75	119.91	113.01
1	AA	78	ILE	N-CA-C	5.73	116.51	110.72
5	AE	8	ARG	CA-C-N	5.73	127.00	119.84
5	AE	8	ARG	C-N-CA	5.73	127.00	119.84
2	AB	163	GLY	CA-C-N	5.73	127.00	119.84
2	AB	163	GLY	C-N-CA	5.73	127.00	119.84
14	BT	5029	ILE	N-CA-C	5.73	116.30	110.05
4	BD	5294	ARG	N-CA-C	5.72	118.25	110.35
5	BE	5008	ARG	CA-C-N	5.69	126.95	119.84
5	BE	5008	ARG	C-N-CA	5.69	126.95	119.84
3	AC	302	TYR	N-CA-C	-5.68	101.25	109.31
4	BD	5181	PHE	N-CA-C	-5.67	105.18	111.36
13	AO	128	ASP	N-CA-C	5.66	119.27	112.93
1	BA	5261	GLN	N-CA-C	5.62	122.76	110.80
4	AD	297	ASP	N-CA-C	5.60	117.92	109.41
1	AA	185	VAL	CB-CA-C	-5.57	104.72	112.02
4	BD	5147	SER	N-CA-C	-5.57	105.29	111.36
2	AB	49	ASP	CA-C-N	5.57	126.05	120.04
2	AB	49	ASP	C-N-CA	5.57	126.05	120.04
1	AA	261	GLN	N-CA-C	5.56	122.64	110.80
1	BA	5056	PRO	CA-C-N	5.55	125.56	119.90
1	BA	5056	PRO	C-N-CA	5.55	125.56	119.90
17	Ay	21	GLN	N-CA-C	5.55	119.67	113.01
4	BD	5142	ASN	N-CA-C	-5.54	106.03	112.89
2	AB	80	ILE	N-CA-C	5.53	116.92	110.62
1	AA	339	PHE	CA-C-N	5.52	126.74	119.84
1	AA	339	PHE	C-N-CA	5.52	126.74	119.84
13	BO	5128	ASP	N-CA-C	5.52	119.11	112.93
7	AH	34	PHE	N-CA-C	-5.51	105.28	111.28
5	AE	26	THR	N-CA-C	5.51	116.96	111.07
14	BT	5032	LYS	CB-CA-C	-5.51	99.64	110.10
1	BA	5083	VAL	CA-C-N	5.49	125.43	119.78
1	BA	5083	VAL	C-N-CA	5.49	125.43	119.78
1	BA	5185	VAL	CB-CA-C	-5.48	104.84	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	5120	LEU	N-CA-C	-5.48	102.78	110.50
1	BA	5195	HIS	CA-C-N	5.48	124.94	119.24
1	BA	5195	HIS	C-N-CA	5.48	124.94	119.24
8	BI	5017	LEU	N-CA-C	-5.48	104.95	111.03
5	AE	23	HIS	N-CA-C	5.47	119.22	112.54
2	BB	5049	ASP	CA-C-N	5.47	125.95	120.04
2	BB	5049	ASP	C-N-CA	5.47	125.95	120.04
1	AA	88	ALA	N-CA-C	-5.47	105.48	111.82
4	BD	5170	ALA	N-CA-C	-5.47	103.03	110.36
2	BB	5057	ARG	N-CA-C	-5.46	106.78	113.50
4	AD	170	ALA	N-CA-C	-5.46	103.05	110.36
5	BE	5023	HIS	N-CA-C	5.45	119.19	112.54
1	BA	5296	ASN	N-CA-C	5.45	119.22	112.24
4	AD	181	PHE	N-CA-C	-5.45	105.42	111.36
1	BA	5088	ALA	N-CA-C	-5.45	105.50	111.82
2	BB	5321	LYS	N-CA-C	-5.44	101.98	110.42
2	BB	5487	SER	N-CA-C	5.44	121.83	109.81
7	BH	5034	PHE	N-CA-C	-5.43	105.36	111.28
7	AH	22	ALA	N-CA-C	-5.41	102.27	110.39
5	AE	13	ILE	N-CA-C	5.41	115.61	110.42
1	AA	83	VAL	CA-C-N	5.40	125.34	119.78
1	AA	83	VAL	C-N-CA	5.40	125.34	119.78
3	BC	5032	GLY	N-CA-C	-5.40	100.39	113.18
2	AB	487	SER	N-CA-C	5.38	121.69	109.81
3	BC	5293	ASN	N-CA-C	5.37	118.02	110.23
4	BD	5299	ILE	N-CA-C	5.36	116.09	110.62
15	AU	70	GLY	N-CA-C	5.34	122.16	114.10
2	AB	247	PHE	N-CA-C	-5.34	105.38	111.14
3	AC	464	GLU	CA-C-N	5.33	126.50	119.84
3	AC	464	GLU	C-N-CA	5.33	126.50	119.84
2	AB	19	LEU	N-CA-C	-5.32	105.14	111.69
3	BC	5391	ARG	N-CA-C	-5.32	105.39	111.14
2	AB	77	GLY	N-CA-C	5.32	120.01	113.79
13	BO	5136	MET	N-CA-C	5.31	116.72	109.18
7	BH	5022	ALA	N-CA-C	-5.31	102.43	110.39
8	AI	17	LEU	N-CA-C	-5.31	105.14	111.03
13	AO	205	GLU	N-CA-C	5.31	120.03	113.50
20	BZ	5033	TRP	N-CA-C	-5.30	105.90	112.47
1	BA	5163	ILE	CB-CA-C	-5.29	105.19	111.97
1	BA	5077	ILE	N-CA-C	5.28	115.90	110.36
2	BB	5237	VAL	N-CA-C	-5.28	104.45	111.05
3	AC	228	ASN	N-CA-C	5.28	119.47	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AL	36	PHE	N-CA-C	-5.27	106.35	112.89
20	BZ	5035	ARG	N-CA-C	-5.27	105.59	112.23
3	AC	391	ARG	N-CA-C	-5.27	105.45	111.14
1	AA	56	PRO	CA-C-N	5.26	125.27	119.90
1	AA	56	PRO	C-N-CA	5.26	125.27	119.90
2	AB	51	VAL	CB-CA-C	-5.26	105.00	111.94
16	BV	5114	ILE	CB-CA-C	-5.23	105.19	112.36
1	BA	5298	ASN	N-CA-C	5.22	117.96	109.86
2	BB	5080	ILE	N-CA-C	5.22	116.57	110.62
20	AZ	35	ARG	N-CA-C	-5.21	105.66	112.23
7	BH	5044	ILE	CB-CA-C	-5.21	105.15	111.87
2	AB	488	PRO	N-CA-C	5.21	123.19	112.47
2	BB	5247	PHE	N-CA-C	-5.20	105.52	111.14
1	BA	5033	PHE	N-CA-C	-5.20	105.79	111.82
1	AA	146	ALA	N-CA-C	-5.19	105.31	111.69
4	BD	5187	GLY	N-CA-C	5.19	118.92	112.64
3	AC	418	ASN	N-CA-CB	-5.19	102.72	110.24
15	BU	5070	GLY	N-CA-C	5.18	121.92	114.10
16	BV	5073	LYS	N-CA-C	5.17	117.59	111.33
2	AB	237	VAL	N-CA-C	-5.17	104.58	111.05
3	BC	5431	PHE	N-CA-C	-5.17	105.33	111.69
13	BO	5040	GLY	N-CA-C	-5.17	108.49	115.21
16	AV	114	ILE	CB-CA-C	-5.16	105.29	112.36
13	AO	181	ASN	N-CA-C	5.14	119.40	113.18
1	AA	33	PHE	N-CA-C	-5.13	105.87	111.82
2	AB	57	ARG	N-CA-C	-5.13	107.19	113.50
1	AA	321	ILE	CB-CA-C	-5.13	103.95	112.26
18	BX	5030	LEU	N-CA-C	-5.13	105.69	111.28
9	BJ	5021	VAL	CB-CA-C	-5.12	105.37	112.24
13	AO	194	TYR	N-CA-C	5.11	117.71	110.50
2	AB	165	GLY	N-CA-C	-5.11	105.90	111.21
13	BO	5194	TYR	N-CA-C	5.11	117.70	110.50
1	BA	5143	ILE	N-CA-C	-5.10	105.52	110.42
1	AA	266	ASN	N-CA-C	-5.10	107.00	114.39
1	BA	5054	ALA	N-CA-C	5.10	121.26	113.61
2	AB	120	LEU	N-CA-C	-5.09	103.33	110.50
15	AU	75	LEU	N-CA-C	5.08	116.63	111.14
1	AA	296	ASN	N-CA-C	5.07	118.73	112.24
2	AB	317	ASN	N-CA-C	-5.07	105.88	113.89
3	BC	5464	GLU	CA-C-N	5.07	126.18	119.84
3	BC	5464	GLU	C-N-CA	5.07	126.18	119.84
3	BC	5252	ILE	N-CA-C	-5.07	105.56	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	5019	LEU	N-CA-C	-5.06	105.46	111.69
13	BO	5205	GLU	N-CA-C	5.05	119.72	113.50
15	BU	5082	ASN	N-CA-C	5.05	117.70	110.68
2	BB	5003	LEU	CA-C-N	-5.05	115.36	120.31
2	BB	5003	LEU	C-N-CA	-5.05	115.36	120.31
2	BB	5479	PHE	N-CA-C	-5.05	103.81	110.43
1	AA	195	HIS	CA-C-N	5.05	124.49	119.24
1	AA	195	HIS	C-N-CA	5.05	124.49	119.24
2	BB	5382	PRO	N-CA-C	5.04	119.23	111.21
5	BE	5026	THR	N-CA-C	5.04	116.47	111.07
3	BC	5406	SER	N-CA-C	5.04	116.81	110.91
17	Ay	21	GLN	N-CA-CB	5.03	119.19	110.39
20	AZ	33	TRP	N-CA-C	-5.03	106.24	112.47
3	BC	5190	ALA	CA-C-N	5.02	124.46	119.24
3	BC	5190	ALA	C-N-CA	5.02	124.46	119.24
4	BD	5064	ALA	N-CA-C	-5.02	101.77	109.76
5	AE	7	GLU	N-CA-C	5.02	117.32	110.24
2	BB	5265	ILE	CB-CA-C	-5.01	104.39	112.16
2	AB	265	ILE	CB-CA-C	-5.01	104.39	112.16
12	AM	15	VAL	CB-CA-C	-5.00	105.37	111.92
5	BE	5013	ILE	N-CA-C	5.00	115.77	110.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	262	TYR	Sidechain
2	BB	5273	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2628	0	2524	314	0
1	BA	2628	0	2524	330	0
2	AB	3850	0	3718	352	0
2	BB	3850	0	3718	359	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AC	3444	0	3365	365	0
3	BC	3444	0	3365	371	0
4	AD	2711	0	2610	262	0
4	BD	2711	0	2610	274	0
5	AE	666	0	651	70	0
5	BE	666	0	651	76	0
6	AF	282	0	291	40	0
6	BF	282	0	291	38	0
7	AH	507	0	521	71	0
7	BH	507	0	521	76	0
8	AI	286	0	308	40	0
8	BI	286	0	305	40	0
9	AJ	271	0	276	37	0
9	BJ	271	0	276	40	0
10	AK	293	0	305	56	0
10	BK	293	0	305	51	0
11	AL	304	0	316	35	0
11	BL	304	0	313	36	0
12	AM	267	0	289	27	0
12	BM	267	0	286	27	0
13	AO	1845	0	1801	144	0
13	BO	1845	0	1801	150	0
14	AT	275	0	288	30	0
14	BT	275	0	285	29	0
15	AU	774	0	773	53	0
15	BU	774	0	773	57	0
16	AV	1060	0	1068	55	0
16	BV	1060	0	1068	55	0
17	Ay	201	0	226	37	0
17	By	201	0	226	37	0
18	AX	270	0	299	32	0
18	BX	270	0	299	29	0
19	AY	140	0	32	3	0
19	BY	140	0	32	7	0
20	AZ	479	0	516	64	0
20	BZ	479	0	513	64	0
21	AA	1	0	0	0	0
21	BD	1	0	0	0	0
22	AA	4	0	0	0	0
22	BA	4	0	0	0	0
23	AA	2	0	0	1	0
23	BA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	AA	260	0	288	35	0
24	AB	1040	0	1152	115	0
24	AC	845	0	936	86	0
24	AD	130	0	144	15	0
24	BA	260	0	288	40	0
24	BB	1040	0	1152	124	0
24	BC	845	0	936	88	0
24	BD	130	0	144	16	0
25	AA	16	0	19	10	0
25	BA	16	0	19	11	0
26	AA	5	0	0	0	0
26	BA	5	0	0	0	0
27	AA	40	0	56	4	0
27	AB	120	0	168	9	0
27	AC	120	0	168	22	0
27	AD	40	0	56	2	0
27	AJ	40	0	56	4	0
27	AK	40	0	56	5	0
27	AT	40	0	56	9	0
27	AX	40	0	56	6	0
27	BA	40	0	56	3	0
27	BB	120	0	168	9	0
27	BC	120	0	168	24	0
27	BD	40	0	56	2	0
27	BJ	40	0	56	3	0
27	BK	40	0	56	5	0
27	BT	40	0	56	5	0
27	BX	40	0	56	2	0
28	AA	56	0	70	7	0
28	AB	52	0	62	0	0
28	AC	181	0	243	63	0
28	AE	63	0	87	1	0
28	AH	58	0	74	10	0
28	BA	56	0	70	7	0
28	BB	52	0	62	5	0
28	BC	181	0	243	63	0
28	BE	63	0	87	1	0
28	BH	58	0	74	10	0
29	AA	76	0	95	7	0
29	BA	76	0	95	9	0
30	AA	105	0	145	2	0
30	AB	90	0	109	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	AF	45	0	53	1	0
30	BA	105	0	145	3	0
30	BB	90	0	109	11	0
30	BF	45	0	53	1	0
31	AA	86	0	111	15	0
31	AB	100	0	139	21	0
31	AC	93	0	125	11	0
31	AD	97	0	134	14	0
31	AI	43	0	56	3	0
31	AJ	46	0	61	2	0
31	AM	42	0	54	6	0
31	BA	42	0	53	3	0
31	BB	49	0	68	4	0
31	BC	93	0	125	10	0
31	BD	143	0	195	15	0
31	BE	44	0	58	3	0
31	BI	43	0	56	4	0
31	BL	51	0	71	18	0
31	BM	42	0	54	4	0
32	AB	140	0	184	15	0
32	AD	31	0	35	0	0
32	AI	70	0	92	9	0
32	AM	35	0	46	2	0
32	BB	140	0	184	15	0
32	BC	35	0	46	3	0
32	BD	31	0	35	1	0
32	BI	35	0	46	5	0
32	BM	35	0	46	3	0
33	AB	8	0	12	1	0
33	AU	4	0	6	0	0
33	AV	4	0	6	1	0
33	BB	8	0	12	1	0
33	BV	8	0	12	1	0
34	AD	128	0	148	11	0
34	BD	128	0	148	13	0
35	AD	55	0	80	15	0
35	BD	55	0	80	15	0
36	AF	43	0	30	8	0
36	AV	43	0	30	5	0
36	BF	43	0	30	7	0
36	BV	43	0	30	7	0
37	AF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	AK	1	0	0	0	0
37	AO	1	0	0	0	0
37	BF	1	0	0	0	0
37	BK	1	0	0	0	0
37	BO	1	0	0	0	0
All	All	50266	0	51335	3946	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (3946) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG2	1.69	1.27
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG2	1.78	1.17
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.25	1.15
24:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.29	1.14
24:BB:5612:CLA:H42	4:BD:5127:LEU:HD11	1.29	1.14
15:BU:5083:ALA:HB1	15:BU:5084:PRO:HD2	1.29	1.09
10:AK:28:ILE:HA	10:AK:31:LEU:HD12	1.35	1.09
1:BA:5214:MET:HE2	1:BA:5214:MET:HA	1.34	1.08
1:AA:102:LEU:HB2	31:AA:417:LMG:H351	1.10	1.08
10:BK:5028:ILE:HA	10:BK:5031:LEU:HD12	1.35	1.08
2:BB:5027:THR:HG22	2:BB:5107:LEU:HD13	1.36	1.08
1:AA:278:TRP:CE3	28:AC:519:DGD:CIA	2.38	1.07
13:BO:5087:GLN:O	13:BO:5088:GLU:HG3	1.54	1.07
9:AJ:15:THR:HG21	10:AK:38:VAL:HG13	1.33	1.06
1:AA:214:MET:HE2	1:AA:214:MET:HA	1.33	1.06
16:AV:63:CYS:SG	36:AV:201:HEM:HAB	1.96	1.06
1:BA:5200:LEU:HD11	28:BC:5519:DGD:HAW2	1.38	1.05
1:BA:5325:ASN:HA	1:BA:5328:MET:HE3	1.37	1.05
13:AO:82:PRO:HG3	13:AO:89:ALA:HB2	1.35	1.04
17:Ay:22:LEU:HA	17:Ay:25:ILE:HD13	1.37	1.04
28:BA:5412:DGD:O2D	3:BC:5216:SER:HB2	1.57	1.04
9:BJ:5015:THR:HG21	10:BK:5038:VAL:HG13	1.35	1.04
14:AT:29:ILE:HD12	14:AT:29:ILE:H	1.22	1.04
13:BO:5082:PRO:HG3	13:BO:5089:ALA:HB2	1.34	1.04
1:AA:200:LEU:CD1	28:AC:519:DGD:HAW2	1.88	1.03
13:AO:87:GLN:O	13:AO:88:GLU:HG3	1.56	1.03
17:Ay:19:ILE:HG23	17:Ay:20:ALA:H	1.21	1.02
1:BA:5200:LEU:CD1	28:BC:5519:DGD:HAW2	1.89	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5260:SER:OG	2:BB:5262:THR:HG22	1.61	1.00
3:BC:5254:THR:HG22	3:BC:5255:THR:H	1.26	1.00
2:AB:27:THR:HG22	2:AB:107:LEU:HD13	1.40	1.00
28:AA:411:DGD:O2D	3:AC:216:SER:HB2	1.61	1.00
1:AA:200:LEU:HD11	28:AC:519:DGD:HAW2	1.42	0.99
2:AB:260:SER:OG	2:AB:262:THR:HG22	1.60	0.99
1:AA:325:ASN:HA	1:AA:328:MET:HE3	1.43	0.97
4:AD:14:TRP:HE1	7:AH:25:TRP:HH2	1.12	0.97
3:AC:254:THR:HG22	3:AC:255:THR:H	1.26	0.97
17:By:5034:MET:HA	17:By:5034:MET:CE	1.95	0.97
3:AC:305:THR:HG22	3:AC:308:GLU:HB2	1.47	0.97
5:BE:5056:TYR:O	16:BV:5027:ALA:HB2	1.64	0.96
1:BA:5278:TRP:CE3	28:BC:5519:DGD:CIA	2.48	0.96
1:BA:5190:HIS:HB3	1:BA:5293:MET:HE2	1.48	0.95
2:BB:5476:ARG:HB3	2:BB:5476:ARG:HH11	1.31	0.95
4:BD:5014:TRP:HE1	7:BH:5025:TRP:HH2	1.14	0.95
17:Ay:21:GLN:O	17:Ay:21:GLN:HG2	1.64	0.94
16:BV:5063:CYS:SG	36:BV:5201:HEM:HAB	2.07	0.94
2:AB:476:ARG:HB3	2:AB:476:ARG:HH11	1.32	0.94
13:BO:5069:LEU:HB3	13:BO:5107:ILE:HB	1.48	0.94
3:AC:305:THR:HG22	3:AC:308:GLU:CB	1.97	0.94
2:BB:5476:ARG:HB3	2:BB:5476:ARG:NH1	1.82	0.94
2:AB:248:ALA:HA	24:AB:603:CLA:H42	1.49	0.93
3:AC:29:GLU:HB3	10:AK:46:ARG:HH11	1.31	0.93
2:AB:16:PRO:HG3	2:AB:133:LEU:HD11	1.48	0.93
3:AC:461:ARG:HG3	3:AC:461:ARG:HH11	1.31	0.93
7:BH:5062:TRP:CD1	28:BH:5101:DGD:HO3E	1.87	0.93
3:BC:5461:ARG:HH11	3:BC:5461:ARG:HG3	1.33	0.93
4:BD:5274:VAL:HA	35:BD:5406:PL9:H253	1.51	0.93
1:BA:5341:LEU:HB2	3:BC:5313:GLN:HE22	1.30	0.92
13:AO:230:VAL:HG12	13:AO:231:ASP:H	1.35	0.92
17:By:5034:MET:HA	17:By:5034:MET:HE3	1.49	0.92
5:AE:15:THR:HG22	9:AJ:7:ARG:H	1.34	0.92
2:AB:476:ARG:HB3	2:AB:476:ARG:NH1	1.84	0.92
17:Ay:35:ILE:HG22	20:AZ:21:ILE:HG23	1.52	0.92
17:By:5035:ILE:HG22	20:BZ:5021:ILE:HG23	1.50	0.92
18:BX:5026:GLY:O	18:BX:5029:VAL:HG12	1.70	0.92
3:BC:5305:THR:HG22	3:BC:5308:GLU:CB	2.00	0.92
3:BC:5239:TRP:HE3	3:BC:5243:ILE:HD11	1.34	0.91
1:BA:5102:LEU:HB2	31:BA:5402:LMG:H351	1.51	0.91
2:BB:5248:ALA:HA	24:BB:5607:CLA:H42	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5305:THR:HG22	3:BC:5308:GLU:HB2	1.50	0.91
5:BE:5015:THR:HG22	9:BJ:5007:ARG:H	1.35	0.91
7:AH:62:TRP:CD1	28:AH:101:DGD:HO3E	1.86	0.91
4:BD:5103:ARG:HG3	5:BE:5073:LYS:HG3	1.52	0.91
24:BB:5607:CLA:HBB1	24:BB:5609:CLA:H171	1.52	0.91
24:AA:405:CLA:HED1	35:AD:405:PL9:H372	1.53	0.90
2:BB:5016:PRO:HG3	2:BB:5133:LEU:HD11	1.49	0.90
15:BU:5088:VAL:O	15:BU:5091:VAL:HG12	1.72	0.90
24:AB:603:CLA:HBB1	24:AB:605:CLA:H171	1.52	0.90
13:AO:69:LEU:HB3	13:AO:107:ILE:HB	1.51	0.90
1:AA:102:LEU:CB	31:AA:417:LMG:H351	2.00	0.90
2:AB:12:LEU:HD13	2:AB:19:LEU:HA	1.53	0.89
2:BB:5004:PRO:HG2	2:BB:5007:ARG:HD2	1.55	0.89
10:AK:24:VAL:HG11	17:Ay:25:ILE:HG13	1.55	0.89
15:AU:83:ALA:HB1	15:AU:84:PRO:CD	2.02	0.89
18:AX:26:GLY:O	18:AX:29:VAL:HG12	1.72	0.89
4:AD:87:HIS:CD2	4:AD:166:SER:HA	2.07	0.89
14:AT:18:PHE:HB2	27:AT:101:BCR:H10C	1.54	0.89
4:BD:5087:HIS:CD2	4:BD:5166:SER:HA	2.07	0.88
1:AA:271:LEU:HD21	25:AA:408:MST:H81	1.55	0.88
1:BA:5278:TRP:HH2	28:BC:5519:DGD:HBG1	1.38	0.88
24:BA:5406:CLA:HED1	35:BD:5406:PL9:H372	1.55	0.88
5:AE:46:VAL:HG13	28:AE:101:DGD:HG31	1.53	0.88
2:BB:5012:LEU:HD13	2:BB:5019:LEU:HA	1.56	0.88
3:AC:239:TRP:HE3	3:AC:243:ILE:HD11	1.35	0.88
3:BC:5451:ALA:HA	3:BC:5456:GLU:OE2	1.73	0.88
4:AD:103:ARG:HG3	5:AE:73:LYS:HG3	1.56	0.88
4:AD:88:SER:HB2	5:AE:69:ARG:NH2	1.88	0.87
7:BH:5061:SER:HA	28:BH:5101:DGD:HE4	1.54	0.87
3:AC:451:ALA:HA	3:AC:456:GLU:OE2	1.74	0.87
13:BO:5230:VAL:HG12	13:BO:5231:ASP:H	1.39	0.87
15:AU:88:VAL:O	15:AU:91:VAL:HG12	1.74	0.87
2:AB:414:PRO:HB2	2:AB:415:PRO:HD3	1.56	0.86
3:AC:29:GLU:HB3	10:AK:46:ARG:NH1	1.90	0.86
2:AB:226:TYR:HA	2:AB:231:MET:HE3	1.57	0.86
3:AC:52:ALA:HA	24:AC:511:CLA:HMB3	1.57	0.86
5:BE:5046:VAL:HG13	28:BE:5102:DGD:HG31	1.56	0.86
15:BU:5083:ALA:HB1	15:BU:5084:PRO:CD	2.04	0.86
3:BC:5052:ALA:HA	24:BC:5511:CLA:HMB3	1.58	0.86
5:AE:15:THR:HG23	9:AJ:8:ILE:O	1.75	0.85
2:BB:5179:GLN:HA	2:BB:5179:GLN:HE21	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5380:ILE:HA	3:BC:5384:ILE:HD11	1.55	0.85
3:BC:5117:VAL:HG11	31:BC:5521:LMG:H192	1.58	0.85
4:BD:5122:LEU:HD21	24:BD:5402:CLA:H92	1.58	0.85
3:AC:130:VAL:HG13	24:AC:511:CLA:H92	1.59	0.85
4:AD:148:ALA:HB2	4:AD:276:VAL:HG13	1.58	0.85
3:BC:5113:VAL:O	3:BC:5117:VAL:HG23	1.75	0.85
1:AA:341:LEU:HB2	3:AC:313:GLN:HE22	1.40	0.85
1:AA:190:HIS:HB3	1:AA:293:MET:HE2	1.56	0.85
3:AC:113:VAL:O	3:AC:117:VAL:HG23	1.75	0.85
1:BA:5271:LEU:HD21	25:BA:5409:MST:H81	1.59	0.85
4:BD:5148:ALA:HB3	4:BD:5149:PRO:HD3	1.59	0.84
2:AB:179:GLN:HA	2:AB:179:GLN:HE21	1.43	0.84
7:AH:61:SER:HA	28:AH:101:DGD:HE4	1.59	0.84
3:AC:380:ILE:HA	3:AC:384:ILE:HD11	1.58	0.84
4:AD:274:VAL:HA	35:AD:405:PL9:H253	1.57	0.84
1:BA:5033:PHE:HE1	24:BC:5505:CLA:H92	1.41	0.84
1:AA:177:SER:HA	1:AA:180:PHE:HD2	1.42	0.84
2:BB:5383:PHE:O	13:BO:5192:SER:HA	1.78	0.84
5:BE:5015:THR:HG22	9:BJ:5007:ARG:N	1.93	0.84
5:BE:5015:THR:HG23	9:BJ:5008:ILE:O	1.77	0.84
2:AB:223:GLN:HG3	2:AB:227:LYS:HE3	1.60	0.84
16:BV:5066:CYS:SG	36:BV:5201:HEM:HAC	2.18	0.84
2:BB:5226:TYR:HA	2:BB:5231:MET:HE3	1.60	0.83
5:AE:56:TYR:O	16:AV:27:ALA:HB2	1.78	0.83
17:Ay:33:PRO:O	17:Ay:36:ILE:HG23	1.78	0.83
1:AA:278:TRP:CZ3	28:AC:519:DGD:HAG2	2.12	0.83
1:BA:5289:GLY:O	1:BA:5292:THR:HG22	1.77	0.83
13:AO:32:THR:O	13:AO:36:ILE:HD12	1.79	0.83
2:BB:5464:PHE:HD2	24:BB:5615:CLA:HAC2	1.43	0.83
13:BO:5032:THR:O	13:BO:5036:ILE:HD12	1.77	0.83
1:AA:205:VAL:HG21	24:AA:404:CLA:HMA2	1.58	0.83
5:AE:15:THR:HG22	9:AJ:7:ARG:N	1.93	0.83
3:BC:5130:VAL:HG13	24:BC:5511:CLA:H92	1.60	0.83
4:BD:5148:ALA:HB2	4:BD:5276:VAL:HG13	1.58	0.83
13:BO:5031:LEU:H	13:BO:5031:LEU:HD12	1.44	0.83
31:AD:408:LMG:HC8	11:AL:19:LEU:HD23	1.60	0.83
3:AC:307:PRO:HB3	3:AC:358:PHE:CD1	2.14	0.83
24:BC:5504:CLA:C15	28:BC:5519:DGD:HA91	2.08	0.82
7:AH:55:LEU:HD21	18:AX:16:LEU:HD23	1.59	0.82
1:BA:5278:TRP:CH2	28:BC:5519:DGD:HBG1	2.13	0.82
4:BD:5088:SER:HB2	5:BE:5069:ARG:NH2	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AV:66:CYS:SG	36:AV:201:HEM:HAC	2.20	0.82
2:AB:464:PHE:HD2	24:AB:611:CLA:HAC2	1.45	0.82
32:AB:629:LMT:H51	14:BT:5004:ILE:HG13	1.60	0.82
20:BZ:5032:ASP:CG	20:BZ:5033:TRP:H	1.87	0.82
35:BD:5406:PL9:H201	31:BL:5101:LMG:H182	1.61	0.82
1:AA:278:TRP:HH2	28:AC:519:DGD:HGB1	1.42	0.82
2:AB:155:ALA:O	2:AB:161:LEU:HD22	1.79	0.82
3:BC:5116:VAL:HG21	27:BC:5515:BCR:H323	1.62	0.82
2:AB:121:GLU:HG3	7:AH:4:ARG:HA	1.60	0.81
2:BB:5357:ARG:HH11	2:BB:5357:ARG:HG3	1.45	0.81
3:AC:385:GLN:H	3:AC:388:GLN:NE2	1.79	0.81
2:BB:5155:ALA:O	2:BB:5161:LEU:HD22	1.80	0.81
1:BA:5214:MET:HA	1:BA:5214:MET:CE	2.10	0.81
4:AD:17:ILE:HG21	18:AX:42:GLN:HG2	1.63	0.81
10:AK:19:ASP:N	10:AK:20:PRO:HD2	1.96	0.81
2:BB:5354:LEU:HD23	2:BB:5378:LYS:HB2	1.62	0.81
5:AE:36:LEU:O	5:AE:40:THR:HG23	1.80	0.81
2:BB:5354:LEU:CD2	2:BB:5378:LYS:HB2	2.11	0.81
1:BA:5084:PRO:HA	1:BA:5112:TYR:CD2	2.15	0.81
3:BC:5029:GLU:HB3	10:BK:5046:ARG:HH11	1.46	0.81
31:BD:5410:LMG:HC8	11:BL:5019:LEU:HD23	1.61	0.81
1:BA:5205:VAL:HG21	24:BA:5405:CLA:HMA2	1.62	0.80
3:BC:5307:PRO:HB3	3:BC:5358:PHE:CD1	2.15	0.80
3:BC:5310:SER:OG	3:BC:5355:THR:HG23	1.82	0.80
5:BE:5036:LEU:O	5:BE:5040:THR:HG23	1.82	0.80
24:AB:603:CLA:HAC2	24:AB:606:CLA:HBB2	1.64	0.80
31:AB:620:LMG:H182	35:AD:405:PL9:H201	1.63	0.80
31:BI:5101:LMG:H152	32:BI:5102:LMT:H52	1.62	0.80
17:Ay:19:ILE:HG23	17:Ay:20:ALA:N	1.97	0.80
1:BA:5281:VAL:CG1	28:BC:5519:DGD:HAG3	2.11	0.80
1:AA:33:PHE:HE1	24:AC:505:CLA:H92	1.45	0.80
2:AB:354:LEU:CD2	2:AB:378:LYS:HB2	2.12	0.80
18:AX:34:PHE:O	18:AX:38:ILE:HG12	1.82	0.80
1:AA:179:THR:HG22	1:AA:183:MET:HE2	1.64	0.80
14:AT:4:ILE:HG13	32:BB:5603:LMT:H51	1.64	0.80
3:BC:5464:GLU:HB3	3:BC:5467:LEU:HD12	1.64	0.80
31:AA:414:LMG:O3	5:AE:9:PRO:HB3	1.81	0.80
2:AB:297:THR:HG23	2:AB:300:GLU:H	1.47	0.80
2:AB:357:ARG:HG3	2:AB:357:ARG:HH11	1.46	0.80
4:AD:122:LEU:HD21	24:AD:401:CLA:H92	1.64	0.80
4:BD:5221:THR:HG23	4:BD:5244:TYR:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BX:5034:PHE:O	18:BX:5038:ILE:HG12	1.82	0.79
2:BB:5135:LEU:HB2	2:BB:5136:PRO:HD3	1.62	0.79
2:AB:135:LEU:HB2	2:AB:136:PRO:HD3	1.63	0.79
2:AB:383:PHE:O	13:AO:192:SER:HA	1.82	0.79
24:BB:5607:CLA:HAC2	24:BB:5610:CLA:HBB2	1.65	0.79
3:BC:5155:ASN:HA	3:BC:5158:THR:HG22	1.65	0.79
3:AC:116:VAL:HG21	27:AC:515:BCR:H323	1.63	0.79
31:AI:101:LMG:H152	32:AI:102:LMT:H52	1.64	0.79
1:BA:5143:ILE:HD11	4:BD:5217:THR:HA	1.64	0.79
4:BD:5152:VAL:HG21	4:BD:5279:LEU:HD13	1.64	0.79
24:BD:5405:CLA:H41	18:BX:5023:LEU:HD12	1.64	0.79
5:BE:5009:PRO:HB3	31:BE:5101:LMG:O3	1.81	0.79
3:AC:372:PRO:O	13:AO:36:ILE:HD13	1.82	0.79
1:BA:5177:SER:HA	1:BA:5180:PHE:HD2	1.47	0.79
1:AA:84:PRO:HA	1:AA:112:TYR:CD2	2.16	0.79
17:Ay:25:ILE:H	17:Ay:25:ILE:HD12	1.48	0.79
1:AA:278:TRP:CH2	28:AC:519:DGD:HGB1	2.18	0.79
24:AA:407:CLA:H43	24:AC:505:CLA:H201	1.64	0.79
16:AV:63:CYS:SG	36:AV:201:HEM:CAB	2.71	0.79
2:BB:5173:GLY:HA3	2:BB:5265:ILE:HD11	1.64	0.79
1:AA:258:LEU:HB3	1:AA:259:ILE:HD13	1.63	0.78
7:AH:21:VAL:HG23	7:AH:22:ALA:O	1.83	0.78
1:BA:5258:LEU:HB3	1:BA:5259:ILE:HD13	1.65	0.78
2:AB:354:LEU:HD23	2:AB:378:LYS:HB2	1.63	0.78
20:AZ:19:MET:O	20:AZ:23:VAL:HG23	1.83	0.78
2:BB:5224:ARG:HG3	7:BH:5025:TRP:HD1	1.46	0.78
20:BZ:5036:SER:HA	20:BZ:5039:LEU:HG	1.65	0.78
24:BC:5504:CLA:H151	28:BC:5519:DGD:HA91	1.64	0.78
1:AA:214:MET:HE1	4:AD:142:ASN:OD1	1.83	0.78
1:BA:5179:THR:HG22	1:BA:5183:MET:HE2	1.64	0.78
4:BD:5017:ILE:HG21	18:BX:5042:GLN:HG2	1.63	0.78
31:BC:5520:LMG:O8	31:BC:5520:LMG:O9	2.01	0.78
15:BU:5072:TYR:HB3	15:BU:5073:PRO:HD3	1.66	0.78
1:BA:5214:MET:HE1	4:BD:5142:ASN:OD1	1.84	0.78
1:BA:5278:TRP:HB3	1:BA:5279:PRO:HD3	1.64	0.78
7:BH:5042:LEU:HD12	7:BH:5045:ILE:HD11	1.64	0.78
1:AA:289:GLY:O	1:AA:292:THR:HG22	1.82	0.78
31:AC:520:LMG:O9	31:AC:520:LMG:O8	2.01	0.78
3:AC:461:ARG:HH11	3:AC:461:ARG:CG	1.96	0.78
1:BA:5083:VAL:HG22	4:BD:5314:PHE:HE2	1.49	0.78
24:BA:5408:CLA:H43	24:BC:5505:CLA:H201	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:133:LEU:HB3	2:AB:138:MET:HE1	1.65	0.78
13:BO:5032:THR:HG22	13:BO:5035:ASP:OD2	1.83	0.77
4:AD:148:ALA:HB3	4:AD:149:PRO:HD3	1.65	0.77
1:AA:214:MET:HA	1:AA:214:MET:CE	2.11	0.77
1:BA:5133:LEU:HD23	4:BD:5252:PHE:CD1	2.18	0.77
2:BB:5489:GLU:HB2	5:BE:5003:GLY:N	1.98	0.77
17:Ay:19:ILE:CG2	17:Ay:20:ALA:H	1.97	0.77
28:BA:5412:DGD:O2D	3:BC:5216:SER:CB	2.32	0.77
7:BH:5055:LEU:HD21	18:BX:5016:LEU:HD23	1.64	0.77
3:AC:48:LYS:HE2	3:AC:138:GLU:HG3	1.67	0.77
3:AC:466:VAL:HA	3:AC:469:MET:HE3	1.67	0.77
10:AK:27:VAL:O	10:AK:30:VAL:HG12	1.82	0.77
20:AZ:36:SER:HA	20:AZ:39:LEU:HG	1.65	0.77
3:AC:415:ASN:O	3:AC:416:SER:HB3	1.85	0.77
3:AC:464:GLU:HB3	3:AC:467:LEU:HD12	1.65	0.77
4:AD:129:GLN:NE2	4:AD:143:ALA:HA	2.00	0.77
3:BC:5219:GLY:HA2	28:BC:5517:DGD:O3D	1.85	0.77
3:AC:117:VAL:HG11	31:AC:521:LMG:H192	1.67	0.77
3:AC:437:PHE:HA	24:AC:508:CLA:HMC2	1.67	0.77
24:AC:511:CLA:H202	20:AZ:20:VAL:HA	1.66	0.77
2:BB:5133:LEU:HB3	2:BB:5138:MET:HE1	1.67	0.77
2:AB:483:ASP:CB	2:AB:484:PRO:HD2	2.14	0.77
1:AA:127:MET:HE3	3:AC:442:LEU:HD21	1.67	0.77
2:BB:5068:ARG:HH22	24:BB:5608:CLA:HED1	1.49	0.77
2:BB:5223:GLN:HG3	2:BB:5227:LYS:HE3	1.66	0.76
3:AC:62:PHE:HE2	10:AK:29:PRO:HD3	1.51	0.76
13:AO:32:THR:HG22	13:AO:35:ASP:OD2	1.83	0.76
15:AU:72:TYR:HB3	15:AU:73:PRO:HD3	1.67	0.76
2:BB:5297:THR:HG23	2:BB:5300:GLU:H	1.50	0.76
24:AC:504:CLA:C15	28:AC:519:DGD:HA91	2.14	0.76
4:AD:221:THR:HG23	4:AD:244:TYR:HB2	1.67	0.76
24:BA:5405:CLA:H13	24:BA:5406:CLA:H91	1.67	0.76
3:BC:5062:PHE:HE2	10:BK:5029:PRO:HD3	1.50	0.76
28:AA:411:DGD:O2D	3:AC:216:SER:CB	2.33	0.76
3:AC:155:ASN:HA	3:AC:158:THR:HG22	1.66	0.76
24:AD:404:CLA:H41	18:AX:23:LEU:HD12	1.65	0.76
12:AM:33:GLN:HB3	12:BM:5033:GLN:HB3	1.65	0.76
2:BB:5461:LEU:HD11	31:BB:5624:LMG:H412	1.68	0.76
1:AA:262:TYR:CE1	31:AA:414:LMG:HC5	2.21	0.76
6:AF:11:VAL:HG12	6:AF:12:SER:H	1.49	0.76
1:BA:5259:ILE:HD13	1:BA:5259:ILE:N	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:121:GLU:CG	7:AH:4:ARG:HA	2.16	0.76
2:AB:4:PRO:HG2	2:AB:7:ARG:HD2	1.66	0.76
27:BC:5514:BCR:H353	27:BK:5102:BCR:H321	1.68	0.76
3:BC:5461:ARG:HH11	3:BC:5461:ARG:CG	1.97	0.76
5:BE:5078:THR:HA	5:BE:5081:GLU:HG2	1.68	0.76
12:BM:5001:MET:HG2	12:BM:5002:GLU:H	1.51	0.76
13:AO:128:ASP:OD2	13:AO:149:LYS:HG2	1.86	0.75
3:BC:5315:MET:HE1	3:BC:5369:LEU:HD12	1.68	0.75
7:AH:42:LEU:HD12	7:AH:45:ILE:HD11	1.67	0.75
17:By:5045:ASN:HB2	20:BZ:5028:ALA:O	1.86	0.75
2:AB:226:TYR:CA	2:AB:231:MET:HE3	2.16	0.75
2:BB:5016:PRO:CG	2:BB:5133:LEU:HD11	2.16	0.75
1:BA:5255:PHE:CE1	1:BA:5259:ILE:HD11	2.21	0.75
24:AB:604:CLA:H11	24:AB:612:CLA:H152	1.68	0.75
2:BB:5121:GLU:HG3	7:BH:5004:ARG:HA	1.67	0.75
3:BC:5372:PRO:O	13:BO:5036:ILE:HD13	1.86	0.75
27:AC:514:BCR:H353	27:AK:102:BCR:H321	1.68	0.75
4:AD:88:SER:HB2	5:AE:69:ARG:CZ	2.17	0.75
2:BB:5414:PRO:HB2	2:BB:5415:PRO:HD3	1.68	0.75
1:BA:5049:VAL:O	1:BA:5053:ILE:HG13	1.87	0.75
3:BC:5048:LYS:HE2	3:BC:5138:GLU:HG3	1.66	0.75
4:BD:5091:LEU:HD22	7:BH:5052:THR:HG21	1.69	0.75
10:BK:5024:VAL:HG11	17:By:5025:ILE:HG13	1.69	0.74
3:BC:5385:GLN:H	3:BC:5388:GLN:NE2	1.85	0.74
4:BD:5103:ARG:NH1	5:BE:5077:GLU:HG3	2.02	0.74
10:BK:5027:VAL:O	10:BK:5030:VAL:HG12	1.86	0.74
1:AA:330:VAL:HG11	4:AD:348:ARG:HG2	1.69	0.74
31:AA:417:LMG:H201	2:BB:5098:LEU:HD13	1.69	0.74
1:BA:5064:ARG:O	13:BO:5178:ARG:NH2	2.21	0.74
1:BA:5315:ASN:HD21	4:BD:5332:GLN:HE22	1.35	0.74
4:AD:152:VAL:HG21	4:AD:279:LEU:HD13	1.67	0.74
2:BB:5121:GLU:CG	7:BH:5004:ARG:HA	2.18	0.74
3:AC:219:GLY:HA2	28:AC:517:DGD:O3D	1.86	0.74
13:BO:5171:GLU:HG2	13:BO:5172:PHE:N	2.02	0.74
1:AA:13:LEU:HA	1:AA:16:ARG:HD3	1.69	0.74
13:AO:230:VAL:HG12	13:AO:231:ASP:N	2.03	0.74
10:AK:18:PHE:HE1	20:AZ:9:LEU:HG	1.51	0.74
13:AO:31:LEU:H	13:AO:31:LEU:HD12	1.51	0.74
13:BO:5178:ARG:HG3	13:BO:5178:ARG:HH11	1.53	0.74
13:AO:178:ARG:HH11	13:AO:178:ARG:HG3	1.53	0.74
2:AB:474:LEU:HD13	30:AB:622:SQD:H81	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5272:HIS:CD2	4:BD:5218:VAL:HG21	2.23	0.74
3:BC:5453:ALA:O	8:BI:5034:ARG:HB2	1.87	0.74
2:AB:222:PRO:HG3	7:AH:27:THR:H	1.53	0.73
24:AB:608:CLA:H52	24:AB:609:CLA:H8	1.70	0.73
3:BC:5209:ILE:HG23	27:BC:5516:BCR:H382	1.70	0.73
13:BO:5031:LEU:HD12	13:BO:5031:LEU:N	2.03	0.73
1:AA:64:ARG:O	13:AO:178:ARG:NH2	2.21	0.73
2:AB:16:PRO:CG	2:AB:133:LEU:HD11	2.17	0.73
13:AO:171:GLU:HG2	13:AO:172:PHE:N	2.02	0.73
1:BA:5127:MET:HE3	3:BC:5442:LEU:HD21	1.69	0.73
2:BB:5483:ASP:CB	2:BB:5484:PRO:HD2	2.16	0.73
2:AB:371:THR:HG22	2:AB:377:VAL:HA	1.70	0.73
5:AE:34:GLY:HA2	6:AF:32:PHE:CE1	2.22	0.73
1:AA:192:ILE:HA	1:AA:293:MET:HE1	1.70	0.73
2:AB:224:ARG:HG3	7:AH:25:TRP:HD1	1.51	0.73
4:AD:189:HIS:HA	4:AD:294:ARG:HD2	1.69	0.73
24:BB:5608:CLA:H11	24:BB:5616:CLA:H152	1.71	0.73
32:AB:624:LMT:H92	7:AH:35:MET:HE2	1.70	0.73
1:BA:5192:ILE:HA	1:BA:5293:MET:HE1	1.70	0.73
10:BK:5018:PHE:HE1	20:BZ:5009:LEU:HG	1.53	0.73
3:AC:397:THR:HG21	16:AV:66:CYS:SG	2.27	0.73
2:BB:5474:LEU:HD13	30:BB:5625:SQD:H81	1.68	0.73
2:BB:5324:LEU:HA	4:BD:5293:LEU:CD2	2.18	0.73
3:BC:5437:PHE:HA	24:BC:5508:CLA:HMC2	1.68	0.73
2:AB:248:ALA:HA	24:AB:603:CLA:C4	2.19	0.73
3:AC:55:ALA:HB1	27:AC:514:BCR:H373	1.69	0.73
3:AC:248:GLY:O	3:AC:252:ILE:HG12	1.89	0.73
24:BB:5612:CLA:H52	24:BB:5613:CLA:H8	1.71	0.73
1:AA:18:CYS:O	1:AA:22:THR:HG22	1.89	0.73
1:AA:300:PHE:HE2	28:AC:519:DGD:O1A	1.71	0.73
4:AD:103:ARG:NH1	5:AE:77:GLU:HG3	2.04	0.73
5:BE:5018:ARG:O	5:BE:5022:ILE:HG13	1.89	0.73
3:AC:315:MET:HE1	3:AC:369:LEU:HD12	1.71	0.72
8:AI:16:VAL:O	8:AI:20:VAL:HG23	1.87	0.72
14:AT:21:ILE:HD12	27:AT:101:BCR:H332	1.71	0.72
1:AA:259:ILE:HD13	1:AA:259:ILE:N	2.03	0.72
3:BC:5055:ALA:HB1	27:BC:5514:BCR:H373	1.68	0.72
24:BC:5509:CLA:HBD	24:BC:5509:CLA:H121	1.71	0.72
1:AA:278:TRP:HB3	1:AA:279:PRO:HD3	1.70	0.72
20:AZ:32:ASP:CG	20:AZ:33:TRP:H	1.96	0.72
3:BC:5029:GLU:HB3	10:BK:5046:ARG:NH1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:429:SER:O	3:AC:432:VAL:HG12	1.89	0.72
3:BC:5466:VAL:HA	3:BC:5469:MET:HE3	1.70	0.72
1:AA:260:PHE:CE1	1:AA:263:ALA:HB2	2.25	0.72
1:AA:315:ASN:HD21	4:AD:332:GLN:HE22	1.37	0.72
2:BB:5086:ILE:HD12	2:BB:5086:ILE:O	1.89	0.72
2:BB:5371:THR:HG22	2:BB:5377:VAL:HA	1.71	0.72
2:BB:5214:LEU:O	2:BB:5218:LEU:HG	1.89	0.72
3:BC:5117:VAL:CG1	31:BC:5521:LMG:H192	2.20	0.72
4:BD:5018:LEU:HD22	18:BX:5038:ILE:HD13	1.71	0.72
35:BD:5406:PL9:H23	35:BD:5406:PL9:H303	1.71	0.72
13:AO:120:THR:HG22	13:AO:154:SER:OG	1.90	0.72
7:BH:5021:VAL:HG23	7:BH:5022:ALA:O	1.88	0.72
8:BI:5016:VAL:O	8:BI:5020:VAL:HG23	1.90	0.72
2:AB:86:ILE:O	2:AB:86:ILE:HD12	1.90	0.72
1:BA:5013:LEU:HA	1:BA:5016:ARG:HD3	1.69	0.72
1:BA:5334:ARG:HD3	4:BD:5320:LEU:CD1	2.20	0.72
2:BB:5324:LEU:HA	4:BD:5293:LEU:HD23	1.72	0.72
32:BB:5627:LMT:H92	7:BH:5035:MET:HE2	1.71	0.72
3:BC:5254:THR:HG22	3:BC:5255:THR:N	2.04	0.72
13:BO:5120:THR:HG22	13:BO:5154:SER:OG	1.90	0.72
1:AA:83:VAL:HG22	4:AD:314:PHE:HE2	1.53	0.72
24:AC:504:CLA:H151	28:AC:519:DGD:HA91	1.69	0.72
3:BC:5318:LEU:HG	3:BC:5328:VAL:HG11	1.69	0.71
4:AD:91:LEU:HD22	7:AH:52:THR:HG21	1.70	0.71
3:BC:5418:ASN:CB	28:BC:5519:DGD:HE2	2.19	0.71
20:BZ:5002:THR:HG23	20:BZ:5003:ILE:N	2.06	0.71
2:AB:137:LYS:O	2:AB:141:ILE:HG13	1.90	0.71
35:AD:405:PL9:H303	35:AD:405:PL9:H23	1.70	0.71
2:BB:5425:ILE:HG22	2:BB:5426:PHE:CD2	2.25	0.71
4:BD:5053:THR:HG22	4:BD:5067:TYR:CE2	2.25	0.71
1:AA:57:PRO:HG3	1:AA:68:SER:HB3	1.72	0.71
1:AA:133:LEU:HD23	4:AD:252:PHE:CD1	2.26	0.71
13:AO:83:LYS:HG2	13:AO:84:ASN:H	1.55	0.71
3:BC:5397:THR:HG21	16:BV:5066:CYS:SG	2.30	0.71
1:AA:234:ASN:HD21	4:AD:266:TRP:HB2	1.56	0.71
32:AB:630:LMT:H41	8:BI:5001:MET:HE2	1.72	0.71
3:AC:254:THR:HG22	3:AC:255:THR:N	2.04	0.71
1:AA:255:PHE:CE1	1:AA:259:ILE:HD11	2.25	0.71
3:AC:344:SER:O	13:AO:101:THR:HG22	1.90	0.71
4:AD:134:ARG:HA	4:AD:134:ARG:HE	1.56	0.71
12:AM:20:VAL:HG21	12:BM:5020:VAL:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BZ:5019:MET:O	20:BZ:5023:VAL:HG23	1.90	0.71
2:AB:425:ILE:HG22	2:AB:426:PHE:CD2	2.26	0.71
4:AD:274:VAL:HB	4:AD:275:PRO:HD3	1.73	0.71
6:AF:28:VAL:HB	6:AF:29:PRO:HD3	1.73	0.71
15:AU:94:ILE:O	15:AU:97:LEU:HG	1.91	0.71
24:AC:509:CLA:HBD	24:AC:509:CLA:H121	1.71	0.71
7:AH:58:VAL:HG13	7:AH:58:VAL:O	1.91	0.71
20:AZ:52:LEU:O	20:AZ:56:VAL:HG23	1.91	0.71
24:BC:5501:CLA:HMB3	27:BC:5516:BCR:H403	1.72	0.71
11:BL:5013:ASN:HD21	11:BL:5015:THR:HG22	1.56	0.71
20:AZ:2:THR:HG23	20:AZ:3:ILE:N	2.06	0.71
3:BC:5344:SER:O	13:BO:5101:THR:HG22	1.91	0.71
2:AB:235:GLU:HG2	2:AB:235:GLU:O	1.91	0.70
3:AC:310:SER:OG	3:AC:355:THR:HG23	1.91	0.70
5:AE:18:ARG:O	5:AE:22:ILE:HG13	1.90	0.70
2:BB:5004:PRO:HD2	2:BB:5007:ARG:HB2	1.71	0.70
5:BE:5034:GLY:HA2	6:BF:5032:PHE:CE1	2.26	0.70
24:AA:404:CLA:H13	24:AA:405:CLA:H91	1.73	0.70
2:BB:5226:TYR:CA	2:BB:5231:MET:HE3	2.19	0.70
3:AC:44:ASN:C	3:AC:45:LEU:HD12	2.17	0.70
2:BB:5235:GLU:HG2	2:BB:5235:GLU:O	1.91	0.70
3:BC:5337:LEU:HD12	13:BO:5131:PRO:HG3	1.73	0.70
3:AC:305:THR:HG23	3:AC:308:GLU:H	1.55	0.70
2:BB:5130:GLU:HB2	2:BB:5131:PRO:HD2	1.73	0.70
10:BK:5028:ILE:HA	10:BK:5031:LEU:CD1	2.18	0.70
17:By:5021:GLN:O	17:By:5021:GLN:HG2	1.90	0.70
2:AB:461:LEU:HD11	31:AB:621:LMG:H412	1.71	0.70
2:BB:5121:GLU:HG2	7:BH:5004:ARG:HD2	1.73	0.70
1:AA:39:PRO:HB2	24:AA:407:CLA:HBB1	1.74	0.70
2:AB:98:LEU:HD13	31:BA:5402:LMG:H201	1.73	0.70
2:AB:116:VAL:HG21	27:AB:619:BCR:H271	1.73	0.70
24:AB:610:CLA:H111	24:AB:615:CLA:HAA1	1.74	0.70
17:Ay:31:ALA:O	17:Ay:35:ILE:HG23	1.91	0.70
24:BB:5618:CLA:OBD	11:BL:5010:VAL:HG21	1.90	0.70
1:AA:49:VAL:O	1:AA:53:ILE:HG13	1.92	0.70
17:Ay:45:ASN:HB2	20:AZ:28:ALA:O	1.92	0.70
2:BB:5116:VAL:HG21	27:BB:5623:BCR:H271	1.71	0.70
3:BC:5429:SER:O	3:BC:5432:VAL:HG12	1.90	0.70
2:AB:183:PRO:HG3	2:AB:199:VAL:CG1	2.21	0.70
3:AC:305:THR:CG2	3:AC:308:GLU:H	2.04	0.70
16:BV:5066:CYS:SG	36:BV:5201:HEM:CAC	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:288:LEU:HD13	3:AC:432:VAL:HG23	1.74	0.70
15:AU:58:ASN:OD1	15:AU:84:PRO:HA	1.92	0.70
1:BA:5260:PHE:CE1	1:BA:5263:ALA:HB2	2.27	0.70
2:BB:5068:ARG:HH12	24:BB:5608:CLA:HED1	1.56	0.70
3:BC:5416:SER:C	28:BC:5519:DGD:O3E	2.35	0.70
4:BD:5189:HIS:HA	4:BD:5294:ARG:HD2	1.74	0.70
2:BB:5191:ASN:HB2	7:BH:5058:VAL:CG2	2.20	0.70
24:BC:5511:CLA:H202	20:BZ:5020:VAL:HA	1.74	0.70
2:BB:5137:LYS:O	2:BB:5141:ILE:HG13	1.92	0.69
4:BD:5088:SER:HB2	5:BE:5069:ARG:CZ	2.22	0.69
16:BV:5135:GLU:O	16:BV:5139:VAL:HG23	1.91	0.69
1:BA:5032:TRP:HA	1:BA:5032:TRP:CE3	2.27	0.69
2:BB:5297:THR:HG22	2:BB:5300:GLU:OE1	1.92	0.69
7:BH:5058:VAL:O	7:BH:5058:VAL:HG13	1.92	0.69
20:BZ:5052:LEU:O	20:BZ:5056:VAL:HG23	1.93	0.69
3:AC:224:ILE:O	3:AC:227:VAL:HG23	1.93	0.69
11:AL:13:ASN:HD21	11:AL:15:THR:HG22	1.56	0.69
12:AM:33:GLN:CB	12:BM:5033:GLN:HB3	2.21	0.69
15:BU:5094:ILE:O	15:BU:5097:LEU:HG	1.92	0.69
1:AA:143:ILE:HD11	4:AD:217:THR:HA	1.75	0.69
1:AA:334:ARG:HD3	4:AD:320:LEU:CD1	2.23	0.69
2:AB:298:LEU:HD23	2:AB:402:TYR:CZ	2.28	0.69
3:BC:5259:TRP:H	3:BC:5259:TRP:CD1	2.09	0.69
4:BD:5018:LEU:HD22	18:BX:5038:ILE:CD1	2.22	0.69
5:AE:17:VAL:O	5:AE:21:VAL:HG23	1.93	0.69
1:BA:5261:GLN:NE2	2:BB:5489:GLU:HG3	2.07	0.69
24:BB:5614:CLA:H111	24:BB:5619:CLA:HAA1	1.75	0.69
3:BC:5154:LYS:HE2	3:BC:5261:ARG:HD2	1.74	0.69
4:AD:54:PHE:HB3	5:AE:47:PHE:CD2	2.27	0.69
6:AF:27:ALA:HB1	36:AF:101:HEM:HBC2	1.74	0.69
7:AH:55:LEU:O	7:AH:58:VAL:HG12	1.92	0.69
1:BA:5192:ILE:CA	1:BA:5293:MET:HE1	2.23	0.69
3:BC:5158:THR:O	3:BC:5251:HIS:HB3	1.92	0.69
4:BD:5274:VAL:HB	4:BD:5275:PRO:HD3	1.74	0.69
4:AD:122:LEU:HB3	4:AD:150:ILE:CD1	2.22	0.69
13:AO:92:VAL:CG1	13:AO:93:PRO:HD2	2.23	0.69
20:AZ:49:ALA:O	20:AZ:53:VAL:HG23	1.93	0.69
1:BA:5271:LEU:HD12	25:BA:5409:MST:H162	1.73	0.69
24:BA:5406:CLA:H92	34:BD:5403:PHO:HMB1	1.75	0.69
24:BB:5607:CLA:HMB2	24:BB:5607:CLA:H52	1.73	0.69
3:BC:5113:VAL:HG11	31:BC:5521:LMG:H132	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5103:ARG:HH12	5:BE:5077:GLU:HG3	1.58	0.69
1:AA:177:SER:HA	1:AA:180:PHE:CD2	2.28	0.69
1:AA:278:TRP:CD2	28:AC:519:DGD:HAG2	2.25	0.69
3:AC:318:LEU:HG	3:AC:328:VAL:HG11	1.75	0.69
1:BA:5300:PHE:HE2	28:BC:5519:DGD:O1A	1.75	0.69
24:BC:5502:CLA:HBB2	24:BC:5510:CLA:H152	1.74	0.69
4:BD:5054:PHE:HB3	5:BE:5047:PHE:CD2	2.28	0.69
30:BB:5625:SQD:H172	32:BB:5627:LMT:H101	1.74	0.69
13:BO:5230:VAL:HG12	13:BO:5231:ASP:N	2.08	0.69
1:AA:234:ASN:ND2	4:AD:266:TRP:HB2	2.08	0.68
2:BB:5246:PHE:CD1	2:BB:5246:PHE:C	2.71	0.68
3:BC:5415:ASN:O	3:BC:5416:SER:HB3	1.93	0.68
6:BF:5027:ALA:HB1	36:BF:5101:HEM:HBC2	1.73	0.68
3:AC:347:GLY:HA3	13:AO:43:ASN:HB2	1.74	0.68
1:BA:5018:CYS:O	1:BA:5022:THR:HG22	1.93	0.68
2:BB:5248:ALA:HA	24:BB:5607:CLA:C4	2.22	0.68
3:AC:259:TRP:CD1	3:AC:259:TRP:H	2.11	0.68
4:AD:192:THR:HG23	24:AD:401:CLA:HBC2	1.74	0.68
3:BC:5472:LEU:HG	4:BD:5251:ARG:NH1	2.08	0.68
27:AC:515:BCR:H312	20:AZ:55:GLY:HA2	1.74	0.68
4:AD:18:LEU:HD22	18:AX:38:ILE:HD13	1.75	0.68
1:BA:5038:ILE:HG23	30:BA:5401:SQD:H131	1.76	0.68
1:BA:5234:ASN:HD21	4:BD:5266:TRP:HB2	1.57	0.68
1:BA:5278:TRP:CZ3	28:BC:5519:DGD:HAG2	2.27	0.68
4:BD:5250:ASN:HD22	4:BD:5262:SER:HB3	1.57	0.68
1:AA:192:ILE:CA	1:AA:293:MET:HE1	2.23	0.68
2:AB:250:PHE:CD2	2:AB:459:ALA:HB1	2.29	0.68
2:AB:25:MET:HE1	2:AB:108:PHE:CE1	2.29	0.68
3:AC:215:LYS:HB3	3:AC:223:TRP:HA	1.76	0.68
3:AC:240:ILE:O	3:AC:244:CYS:HB2	1.93	0.68
5:AE:23:HIS:HA	5:AE:26:THR:OG1	1.93	0.68
8:AI:11:VAL:HG22	32:AI:102:LMT:H101	1.76	0.68
1:BA:5234:ASN:ND2	4:BD:5266:TRP:HB2	2.09	0.68
1:BA:5288:LEU:HD13	3:BC:5432:VAL:HG23	1.76	0.68
4:BD:5129:GLN:NE2	4:BD:5143:ALA:HA	2.08	0.68
4:BD:5192:THR:HG23	24:BD:5402:CLA:HBC2	1.75	0.68
2:AB:4:PRO:HD2	2:AB:7:ARG:HB2	1.76	0.68
3:AC:209:ILE:HG23	27:AC:516:BCR:H382	1.76	0.68
3:AC:385:GLN:H	3:AC:388:GLN:HE21	1.41	0.68
4:AD:53:THR:HG22	4:AD:67:TYR:CE2	2.29	0.68
18:AX:12:ILE:O	18:AX:12:ILE:HG13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:158:THR:O	3:AC:251:HIS:HB3	1.93	0.68
2:BB:5005:TRP:O	2:BB:5008:VAL:HG13	1.93	0.68
30:AB:622:SQD:H172	32:AB:624:LMT:H101	1.75	0.68
2:BB:5357:ARG:HG3	2:BB:5357:ARG:NH1	2.06	0.68
6:AF:17:THR:HG23	6:AF:20:TRP:H	1.59	0.68
15:AU:58:ASN:ND2	15:AU:114:VAL:HG13	2.08	0.68
16:AV:66:CYS:SG	36:AV:201:HEM:CAC	2.81	0.68
1:BA:5039:PRO:HB2	24:BA:5408:CLA:HBB1	1.74	0.68
3:BC:5062:PHE:HE2	10:BK:5028:ILE:HB	1.58	0.68
2:AB:188:ASP:OD1	7:AH:58:VAL:HA	1.94	0.67
3:AC:62:PHE:HE2	10:AK:28:ILE:HB	1.59	0.67
3:AC:262:ARG:HH21	32:AI:103:LMT:H5'	1.59	0.67
12:AM:33:GLN:HB3	12:BM:5033:GLN:CB	2.23	0.67
3:BC:5150:ASP:HB3	3:BC:5153:ASP:HB2	1.75	0.67
13:BO:5206:GLU:H	13:BO:5206:GLU:CD	2.01	0.67
2:AB:121:GLU:HG2	7:AH:4:ARG:HD2	1.74	0.67
2:BB:5065:PHE:O	24:BB:5609:CLA:HBA1	1.94	0.67
10:BK:5040:GLN:HA	10:BK:5043:VAL:HG12	1.74	0.67
3:AC:473:ASP:HB2	14:AT:26:PRO:HB3	1.76	0.67
4:AD:103:ARG:HH12	5:AE:77:GLU:HG3	1.60	0.67
1:BA:5239:PHE:O	14:BT:5029:ILE:HA	1.95	0.67
2:BB:5010:THR:O	2:BB:5013:ILE:HG13	1.94	0.67
3:BC:5305:THR:CG2	3:BC:5308:GLU:H	2.08	0.67
12:BM:5025:LEU:O	12:BM:5028:GLN:HG3	1.95	0.67
2:AB:297:THR:HG22	2:AB:300:GLU:OE1	1.94	0.67
27:AC:515:BCR:C31	20:AZ:55:GLY:HA2	2.24	0.67
13:AO:114:ASN:HD21	13:AO:120:THR:HG23	1.59	0.67
2:BB:5068:ARG:HH12	24:BB:5608:CLA:CED	2.07	0.67
13:BO:5092:VAL:CG1	13:BO:5093:PRO:HD2	2.24	0.67
1:AA:272:HIS:CD2	4:AD:218:VAL:HG21	2.30	0.67
2:AB:324:LEU:HA	4:AD:293:LEU:HD23	1.76	0.67
3:AC:52:ALA:HA	24:AC:511:CLA:CMB	2.23	0.67
2:BB:5250:PHE:CD2	2:BB:5459:ALA:HB1	2.30	0.67
24:AA:405:CLA:H92	34:AD:402:PHO:HMB1	1.77	0.67
2:AB:130:GLU:HB2	2:AB:131:PRO:HD2	1.76	0.67
2:AB:324:LEU:HA	4:AD:293:LEU:CD2	2.24	0.67
24:AC:502:CLA:HBB2	24:AC:510:CLA:H152	1.76	0.67
7:AH:9:ASP:O	7:AH:12:ARG:HB2	1.95	0.67
2:BB:5379:ALA:HA	2:BB:5390:TYR:HB3	1.76	0.67
14:BT:5029:ILE:H	14:BT:5029:ILE:HD12	1.58	0.67
2:AB:8:VAL:HB	24:AB:614:CLA:O1D	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5136:ARG:NH2	8:BI:5027:ASP:OD1	2.27	0.67
2:BB:5233:ASN:O	2:BB:5236:THR:HG22	1.95	0.67
4:BD:5241:GLU:H	4:BD:5241:GLU:CD	2.01	0.67
2:AB:234:ILE:HD12	2:AB:237:VAL:HG21	1.77	0.67
4:AD:56:THR:HG21	5:AE:50:PRO:HD3	1.77	0.67
24:BA:5406:CLA:H93	34:BD:5403:PHO:HMA3	1.75	0.67
3:BC:5215:LYS:HB3	3:BC:5223:TRP:HA	1.75	0.67
3:BC:5240:ILE:O	3:BC:5244:CYS:HB2	1.95	0.67
3:BC:5347:GLY:HA3	13:BO:5043:ASN:HB2	1.75	0.67
4:BD:5134:ARG:HA	4:BD:5134:ARG:HE	1.60	0.67
3:AC:150:ASP:HB3	3:AC:153:ASP:HB2	1.77	0.67
3:BC:5089:ILE:N	3:BC:5090:PRO:HD2	2.10	0.67
13:BO:5128:ASP:OD2	13:BO:5149:LYS:HG2	1.93	0.67
1:AA:93:PHE:CD2	1:AA:95:PRO:HD3	2.30	0.67
3:BC:5199:ILE:H	3:BC:5199:ILE:HD12	1.60	0.67
3:BC:5308:GLU:HB2	3:BC:5361:PHE:CE1	2.29	0.67
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CZ	2.29	0.67
16:BV:5063:CYS:SG	36:BV:5201:HEM:CAB	2.81	0.67
1:AA:33:PHE:CE1	24:AC:505:CLA:H92	2.29	0.66
2:AB:62:VAL:HG13	24:AB:605:CLA:HED3	1.77	0.66
3:AC:199:ILE:H	3:AC:199:ILE:HD12	1.60	0.66
3:AC:416:SER:C	28:AC:519:DGD:O3E	2.38	0.66
1:BA:5297:LEU:HD11	3:BC:5404:LEU:HD12	1.77	0.66
2:BB:5025:MET:HE1	2:BB:5108:PHE:CE1	2.29	0.66
13:BO:5169:LYS:HG2	13:BO:5224:SER:HB3	1.77	0.66
3:AC:134:ILE:HD11	24:AC:511:CLA:H93	1.77	0.66
15:AU:66:ILE:O	15:AU:66:ILE:HG22	1.95	0.66
2:BB:5222:PRO:HG3	7:BH:5027:THR:H	1.58	0.66
2:BB:5224:ARG:HG3	7:BH:5025:TRP:CD1	2.30	0.66
3:BC:5040:ALA:O	3:BC:5043:ILE:HG13	1.95	0.66
1:AA:161:TYR:HB3	1:AA:162:PRO:HD3	1.77	0.66
24:AB:603:CLA:HMB2	24:AB:603:CLA:H52	1.77	0.66
24:AB:613:CLA:H2	24:AB:613:CLA:HED3	1.76	0.66
10:AK:40:GLN:HA	10:AK:43:VAL:HG12	1.76	0.66
24:BB:5612:CLA:H18	24:BB:5613:CLA:H192	1.77	0.66
3:BC:5062:PHE:CE2	10:BK:5029:PRO:HD3	2.29	0.66
3:BC:5248:GLY:O	3:BC:5252:ILE:HG12	1.94	0.66
3:BC:5254:THR:CG2	3:BC:5255:THR:H	2.06	0.66
16:BV:5133:LEU:H	16:BV:5133:LEU:HD12	1.59	0.66
2:AB:173:GLY:HA3	2:AB:265:ILE:HD11	1.76	0.66
2:AB:233:ASN:O	2:AB:236:THR:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AB:608:CLA:H18	24:AB:609:CLA:H192	1.77	0.66
24:AC:501:CLA:HMB3	27:AC:516:BCR:H403	1.78	0.66
4:AD:250:ASN:HD22	4:AD:262:SER:HB3	1.60	0.66
10:AK:17:ILE:H	10:AK:17:ILE:HD12	1.59	0.66
10:AK:28:ILE:HA	10:AK:31:LEU:CD1	2.17	0.66
18:AX:36:VAL:O	18:AX:40:ILE:HG22	1.96	0.66
4:BD:5261:PHE:HA	31:BD:5410:LMG:O2	1.96	0.66
5:BE:5027:ILE:HB	5:BE:5028:PRO:HD3	1.78	0.66
1:AA:81:ALA:HB2	1:AA:175:GLY:HA3	1.77	0.66
2:AB:5:TRP:O	2:AB:8:VAL:HG13	1.95	0.66
2:AB:222:PRO:HG3	7:AH:26:GLY:HA3	1.76	0.66
2:AB:357:ARG:HG3	2:AB:357:ARG:NH1	2.06	0.66
20:AZ:32:ASP:HA	20:AZ:34:ASP:OD2	1.95	0.66
1:BA:5033:PHE:CE1	24:BC:5505:CLA:H92	2.27	0.66
1:BA:5190:HIS:CB	1:BA:5293:MET:HE2	2.24	0.66
24:AA:405:CLA:H93	34:AD:402:PHO:HMA3	1.76	0.66
3:AC:62:PHE:CE2	10:AK:29:PRO:HD3	2.29	0.66
3:AC:337:LEU:HD12	13:AO:131:PRO:HG3	1.77	0.66
13:AO:31:LEU:HD12	13:AO:31:LEU:N	2.11	0.66
13:AO:39:THR:OG1	13:AO:41:LEU:HB2	1.96	0.66
17:Ay:39:LEU:HD21	20:AZ:25:VAL:HA	1.77	0.66
1:BA:5330:VAL:HG11	4:BD:5348:ARG:HG2	1.77	0.66
24:BC:5504:CLA:H172	28:BC:5519:DGD:HAE1	1.76	0.66
10:BK:5019:ASP:N	10:BK:5020:PRO:HD2	2.10	0.66
17:By:5031:ALA:O	17:By:5035:ILE:HG23	1.95	0.66
4:AD:129:GLN:HE22	4:AD:143:ALA:HA	1.61	0.66
30:BB:5601:SQD:H242	30:BB:5601:SQD:H81	1.78	0.66
3:BC:5052:ALA:HA	24:BC:5511:CLA:CMB	2.24	0.66
3:BC:5453:ALA:HA	8:BI:5034:ARG:O	1.95	0.66
15:BU:5057:LEU:HD11	15:BU:5112:PHE:HB3	1.76	0.66
17:By:5021:GLN:HA	17:By:5023:THR:HG22	1.78	0.66
1:AA:102:LEU:HB2	31:AA:417:LMG:C35	2.06	0.66
1:BA:5221:SER:HB2	4:BD:5139:ARG:O	1.96	0.66
3:BC:5224:ILE:O	3:BC:5227:VAL:HG23	1.94	0.66
3:BC:5305:THR:HG23	3:BC:5308:GLU:H	1.59	0.66
3:BC:5342:MET:HE3	3:BC:5352:GLY:HA2	1.77	0.66
13:AO:87:GLN:O	13:AO:88:GLU:CG	2.41	0.66
2:BB:5008:VAL:HB	24:BB:5618:CLA:O1D	1.95	0.66
1:AA:39:PRO:HB2	24:AA:407:CLA:CBB	2.25	0.66
2:AB:75:TRP:CD1	2:AB:92:SER:HG	2.14	0.66
30:AB:627:SQD:H81	30:AB:627:SQD:H242	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:254:THR:CG2	3:AC:255:THR:H	2.07	0.66
16:AV:133:LEU:H	16:AV:133:LEU:HD12	1.61	0.66
1:BA:5081:ALA:HB2	1:BA:5175:GLY:HA3	1.77	0.66
1:BA:5176:ILE:HG22	1:BA:5180:PHE:CE2	2.30	0.66
24:BB:5617:CLA:H2	24:BB:5617:CLA:HED3	1.77	0.66
4:BD:5103:ARG:HG3	5:BE:5073:LYS:CG	2.26	0.66
13:BO:5114:ASN:HD21	13:BO:5120:THR:HG23	1.60	0.66
2:AB:191:ASN:HB2	7:AH:58:VAL:CG2	2.25	0.65
2:AB:246:PHE:C	2:AB:246:PHE:CD1	2.72	0.65
3:AC:405:ASN:HB2	28:AC:519:DGD:HG32	1.77	0.65
1:BA:5180:PHE:CD1	4:BD:5192:THR:HB	2.31	0.65
1:BA:5278:TRP:CD2	28:BC:5519:DGD:HAG2	2.29	0.65
4:BD:5122:LEU:HB3	4:BD:5150:ILE:CD1	2.26	0.65
15:BU:5068:TYR:HB2	15:BU:5071:LEU:HD12	1.77	0.65
1:AA:238:LYS:HD2	14:AT:32:LYS:HB3	1.79	0.65
2:AB:65:PHE:O	24:AB:605:CLA:HBA1	1.96	0.65
2:AB:489:GLU:HB2	5:AE:3:GLY:N	2.11	0.65
24:AB:614:CLA:OBD	11:AL:10:VAL:HG21	1.95	0.65
31:AI:101:LMG:O8	31:AI:101:LMG:O9	2.14	0.65
3:BC:5262:ARG:HH21	32:BC:5522:LMT:H5'	1.61	0.65
3:BC:5282:MET:HG2	24:BC:5501:CLA:H71	1.78	0.65
15:BU:5066:ILE:HG22	15:BU:5066:ILE:O	1.95	0.65
4:AD:261:PHE:HA	31:AD:408:LMG:O2	1.96	0.65
8:AI:1:MET:HE2	32:BB:5604:LMT:H41	1.78	0.65
11:AL:16:SER:HA	11:AL:19:LEU:HG	1.75	0.65
11:BL:5026:VAL:HG21	31:BL:5101:LMG:H202	1.78	0.65
1:AA:228:THR:HG22	1:AA:229:GLU:H	1.60	0.65
2:AB:468:TRP:HD1	2:AB:469:HIS:ND1	1.94	0.65
6:AF:11:VAL:HG12	6:AF:12:SER:N	2.10	0.65
8:AI:19:PHE:CE1	8:AI:23:PHE:HE2	2.14	0.65
20:AZ:2:THR:HG23	20:AZ:3:ILE:H	1.60	0.65
1:BA:5039:PRO:HB2	24:BA:5408:CLA:CBB	2.27	0.65
2:BB:5183:PRO:HG3	2:BB:5199:VAL:CG1	2.27	0.65
4:BD:5103:ARG:CG	5:BE:5073:LYS:HG3	2.26	0.65
5:BE:5017:VAL:O	5:BE:5021:VAL:HG23	1.95	0.65
13:BO:5087:GLN:O	13:BO:5088:GLU:CG	2.41	0.65
17:By:5025:ILE:H	17:By:5025:ILE:HD12	1.61	0.65
2:AB:134:ASP:OD2	2:AB:137:LYS:HB2	1.97	0.65
2:AB:183:PRO:HG3	2:AB:199:VAL:HG11	1.78	0.65
1:BA:5057:PRO:HG3	1:BA:5068:SER:HB3	1.77	0.65
1:BA:5093:PHE:CD2	1:BA:5095:PRO:HD3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5134:ILE:HD11	24:BC:5511:CLA:H93	1.79	0.65
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG1	2.30	0.65
3:AC:416:SER:N	28:AC:519:DGD:O3E	2.30	0.65
16:AV:71:ILE:HD12	16:AV:72:THR:N	2.11	0.65
3:BC:5405:ASN:HB2	28:BC:5519:DGD:HG32	1.77	0.65
5:BE:5023:HIS:HA	5:BE:5026:THR:OG1	1.96	0.65
31:BI:5101:LMG:O9	31:BI:5101:LMG:O8	2.15	0.65
1:AA:271:LEU:HD12	25:AA:408:MST:H162	1.78	0.65
2:AB:68:ARG:HH12	24:AB:604:CLA:CED	2.09	0.65
2:AB:213:GLY:O	2:AB:217:ILE:HG13	1.97	0.65
3:AC:89:ILE:N	3:AC:90:PRO:HD2	2.12	0.65
3:AC:110:PRO:O	3:AC:114:VAL:HG23	1.97	0.65
1:BA:5097:TRP:HA	8:BI:5001:MET:SD	2.36	0.65
2:BB:5062:VAL:HG13	24:BB:5609:CLA:HED3	1.78	0.65
3:BC:5062:PHE:CE2	10:BK:5028:ILE:HB	2.32	0.65
31:BD:5410:LMG:O6	11:BL:5015:THR:HG21	1.97	0.65
1:AA:32:TRP:HA	1:AA:32:TRP:CE3	2.32	0.65
2:AB:10:THR:O	2:AB:13:ILE:HG13	1.95	0.65
2:BB:5226:TYR:N	2:BB:5231:MET:HE3	2.12	0.65
3:BC:5320:ARG:O	3:BC:5324:LEU:HD23	1.96	0.65
16:BV:5071:ILE:HD12	16:BV:5072:THR:N	2.12	0.65
3:AC:179:ALA:HB1	3:AC:199:ILE:HD13	1.79	0.65
3:AC:282:MET:HG2	24:AC:501:CLA:H71	1.79	0.65
5:AE:51:ARG:HG3	5:AE:51:ARG:HH11	1.62	0.65
2:BB:5009:HIS:HB2	24:BB:5615:CLA:HBA2	1.79	0.65
2:BB:5222:PRO:HG3	7:BH:5026:GLY:HA3	1.78	0.65
2:BB:5234:ILE:HD12	2:BB:5237:VAL:HG21	1.78	0.65
3:BC:5044:ASN:C	3:BC:5045:LEU:HD12	2.21	0.65
3:BC:5223:TRP:CD2	3:BC:5224:ILE:HG13	2.32	0.65
4:BD:5153:PHE:HB2	24:BD:5402:CLA:H41	1.79	0.65
2:AB:224:ARG:HG2	7:AH:24:GLY:O	1.97	0.65
4:AD:153:PHE:HB2	24:AD:401:CLA:H41	1.79	0.65
5:AE:78:THR:HA	5:AE:81:GLU:HG2	1.78	0.65
1:AA:257:ARG:HH11	1:AA:257:ARG:HG3	1.62	0.64
3:AC:308:GLU:HB2	3:AC:361:PHE:CE1	2.32	0.64
3:AC:362:ARG:HE	3:AC:370:ARG:HH11	1.45	0.64
2:BB:5393:GLU:HG2	15:BU:5044:ASP:O	1.97	0.64
15:BU:5058:ASN:ND2	15:BU:5114:VAL:HG13	2.11	0.64
1:AA:288:LEU:HD22	3:AC:432:VAL:HG23	1.80	0.64
1:AA:300:PHE:CE2	28:AC:519:DGD:O1A	2.50	0.64
2:AB:226:TYR:N	2:AB:231:MET:HE3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:27:ILE:HB	5:AE:28:PRO:HD3	1.79	0.64
3:AC:320:ARG:O	3:AC:324:LEU:HD23	1.97	0.64
3:BC:5437:PHE:HA	24:BC:5508:CLA:CMC	2.27	0.64
20:BZ:5002:THR:HG23	20:BZ:5003:ILE:H	1.60	0.64
16:AV:135:GLU:O	16:AV:139:VAL:HG23	1.97	0.64
1:BA:5048:PHE:HB2	1:BA:5115:ILE:HD13	1.79	0.64
3:BC:5149:TYR:HA	3:BC:5156:LYS:HD3	1.77	0.64
2:AB:384:ARG:HD3	15:AU:132:LEU:CD1	2.28	0.64
24:AC:503:CLA:H171	24:AC:510:CLA:HBB2	1.79	0.64
10:AK:24:VAL:O	10:AK:27:VAL:HG12	1.98	0.64
13:AO:206:GLU:H	13:AO:206:GLU:CD	2.05	0.64
13:AO:234:THR:OG1	13:AO:236:GLU:HG2	1.98	0.64
2:BB:5213:GLY:O	2:BB:5217:ILE:HG13	1.96	0.64
10:BK:5017:ILE:H	10:BK:5017:ILE:HD12	1.62	0.64
3:AC:413:GLU:HG3	3:AC:414:ILE:H	1.62	0.64
31:AD:408:LMG:O6	11:AL:15:THR:HG21	1.98	0.64
1:BA:5228:THR:HG22	1:BA:5229:GLU:H	1.61	0.64
3:BC:5179:ALA:HB1	3:BC:5199:ILE:HD13	1.77	0.64
1:AA:136:ARG:NH2	8:AI:27:ASP:OD1	2.31	0.64
1:AA:228:THR:HG22	1:AA:229:GLU:N	2.12	0.64
1:BA:5010:SER:HB3	1:BA:5016:ARG:NH1	2.13	0.64
2:AB:9:HIS:HB2	24:AB:611:CLA:HBA2	1.79	0.64
2:AB:278:SER:HB3	2:AB:281:GLN:HE21	1.63	0.64
3:BC:5030:SER:HB3	10:BK:5046:ARG:O	1.98	0.64
3:BC:5037:ALA:C	24:BC:5508:CLA:HBA1	2.23	0.64
3:BC:5418:ASN:CA	28:BC:5519:DGD:HE2	2.27	0.64
1:AA:281:VAL:CG1	28:AC:519:DGD:HAG3	2.27	0.64
2:AB:68:ARG:HH22	24:AB:604:CLA:HED1	1.62	0.64
2:AB:214:LEU:O	2:AB:218:LEU:HG	1.97	0.64
2:AB:247:PHE:HB2	24:AB:608:CLA:HBC1	1.80	0.64
3:AC:42:LEU:HD23	24:AC:511:CLA:HED3	1.79	0.64
7:AH:38:PHE:HB2	27:AX:101:BCR:H10C	1.78	0.64
20:AZ:35:ARG:O	20:AZ:38:GLN:HB3	1.98	0.64
1:BA:5077:ILE:HD11	14:BT:5006:TYR:HB3	1.79	0.64
31:BB:5624:LMG:H411	4:BD:5284:ILE:HG12	1.80	0.63
4:BD:5261:PHE:CD2	4:BD:5267:LEU:HD12	2.33	0.63
13:BO:5039:THR:OG1	13:BO:5041:LEU:HB2	1.98	0.63
2:AB:25:MET:HE1	2:AB:108:PHE:CD1	2.33	0.63
31:AB:620:LMG:H202	11:AL:26:VAL:HG21	1.79	0.63
3:AC:154:LYS:HE2	3:AC:261:ARG:HD2	1.81	0.63
3:AC:437:PHE:HA	24:AC:508:CLA:CMC	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AH:101:DGD:O1B	28:AH:101:DGD:C1G	2.46	0.63
3:BC:5449:ARG:HG2	24:BC:5505:CLA:HED1	1.80	0.63
8:BI:5014:PHE:CZ	8:BI:5018:LEU:HD11	2.33	0.63
2:BB:5191:ASN:HB2	7:BH:5058:VAL:HG23	1.79	0.63
28:BC:5518:DGD:HG11	31:BC:5520:LMG:H301	1.81	0.63
4:BD:5236:ASN:ND2	4:BD:5239:GLN:O	2.29	0.63
8:BI:5011:VAL:HG22	32:BI:5102:LMT:H101	1.80	0.63
13:BO:5144:LEU:CD1	13:BO:5259:VAL:HG11	2.29	0.63
13:BO:5218:LEU:HD22	15:BU:5119:THR:HG21	1.80	0.63
14:BT:5022:PHE:C	14:BT:5023:PHE:HD2	2.06	0.63
1:AA:176:ILE:HG22	1:AA:180:PHE:CE2	2.34	0.63
3:AC:304:PRO:HB3	3:AC:395:TYR:CD1	2.33	0.63
4:AD:103:ARG:CG	5:AE:73:LYS:HG3	2.28	0.63
8:AI:8:VAL:O	8:AI:12:VAL:HG23	1.97	0.63
16:AV:95:ILE:O	16:AV:99:VAL:HG23	1.99	0.63
1:BA:5020:TRP:CD1	1:BA:5020:TRP:C	2.75	0.63
4:BD:5041:ALA:HB1	34:BD:5404:PHO:H42	1.81	0.63
17:By:5026:ALA:O	17:By:5030:ILE:HG12	1.98	0.63
2:AB:68:ARG:HH12	24:AB:604:CLA:HED1	1.64	0.63
3:AC:117:VAL:CG1	31:AC:521:LMG:H192	2.28	0.63
3:AC:288:CYS:SG	28:AC:517:DGD:HA21	2.39	0.63
28:AC:518:DGD:HG11	31:AC:520:LMG:H301	1.81	0.63
3:BC:5385:GLN:H	3:BC:5388:GLN:HE21	1.46	0.63
4:BD:5080:THR:HG23	4:BD:5172:SER:OG	1.99	0.63
28:BH:5101:DGD:C1G	28:BH:5101:DGD:O1B	2.45	0.63
15:BU:5058:ASN:OD1	15:BU:5084:PRO:HA	1.98	0.63
1:AA:271:LEU:C	1:AA:271:LEU:HD23	2.24	0.63
1:AA:274:PHE:CE2	25:AA:408:MST:H133	2.33	0.63
2:AB:124:ARG:HG3	2:AB:124:ARG:HH11	1.63	0.63
2:AB:191:ASN:HB2	7:AH:58:VAL:HG23	1.80	0.63
3:AC:461:ARG:CG	3:AC:461:ARG:NH1	2.60	0.63
5:AE:26:THR:O	5:AE:29:ALA:HB3	1.98	0.63
20:AZ:14:ILE:O	20:AZ:18:VAL:HG23	1.99	0.63
2:BB:5246:PHE:C	2:BB:5246:PHE:HD1	2.07	0.63
5:BE:5076:VAL:O	5:BE:5080:LEU:HD22	1.98	0.63
1:AA:221:SER:HB2	4:AD:139:ARG:O	1.99	0.63
1:BA:5343:LEU:O	1:BA:5344:ALA:HB2	1.99	0.63
11:BL:5016:SER:HA	11:BL:5019:LEU:HG	1.80	0.63
1:BA:5304:HIS:CE1	3:BC:5414:ILE:HD12	2.33	0.63
4:BD:5267:LEU:HD23	4:BD:5267:LEU:C	2.24	0.63
6:BF:5028:VAL:HB	6:BF:5029:PRO:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5234:THR:OG1	13:BO:5236:GLU:HG2	1.99	0.63
17:Ay:41:VAL:C	17:Ay:43:ARG:H	2.06	0.62
11:BL:5008:GLN:N	11:BL:5008:GLN:HE21	1.97	0.62
1:BA:5177:SER:HA	1:BA:5180:PHE:CD2	2.32	0.62
2:BB:5118:TRP:CH2	11:BL:5005:PRO:HD2	2.34	0.62
13:BO:5069:LEU:HD12	13:BO:5070:CYS:H	1.63	0.62
16:BV:5095:ILE:O	16:BV:5099:VAL:HG23	1.98	0.62
13:AO:144:LEU:CD1	13:AO:259:VAL:HG11	2.29	0.62
4:BD:5053:THR:HG22	4:BD:5067:TYR:CD2	2.34	0.62
7:BH:5038:PHE:HB2	27:BX:5101:BCR:H10C	1.81	0.62
3:AC:342:MET:HE3	3:AC:352:GLY:HA2	1.81	0.62
2:BB:5224:ARG:HG2	7:BH:5024:GLY:O	1.99	0.62
3:BC:5413:GLU:HG3	3:BC:5414:ILE:H	1.64	0.62
8:BI:5019:PHE:CE1	8:BI:5023:PHE:HE2	2.17	0.62
1:AA:45:THR:HG23	1:AA:46:ILE:N	2.14	0.62
1:AA:265:PHE:CD1	1:AA:271:LEU:HA	2.34	0.62
2:AB:379:ALA:HA	2:AB:390:TYR:HB3	1.80	0.62
3:AC:37:ALA:C	24:AC:508:CLA:HBA1	2.25	0.62
4:AD:207:GLY:HA3	4:AD:275:PRO:HG3	1.80	0.62
35:AD:405:PL9:H303	35:AD:405:PL9:C23	2.30	0.62
1:BA:5228:THR:HG22	1:BA:5229:GLU:N	2.15	0.62
2:BB:5008:VAL:HG23	2:BB:5009:HIS:CD2	2.34	0.62
11:BL:5018:TYR:CE2	14:BT:5020:ALA:HA	2.35	0.62
16:BV:5047:LEU:HD11	16:BV:5143:GLY:HA3	1.81	0.62
4:AD:68:LEU:HB2	6:AF:40:MET:HE2	1.82	0.62
4:AD:80:THR:HB	4:AD:81:PRO:HD2	1.80	0.62
4:AD:103:ARG:HG3	5:AE:73:LYS:CG	2.28	0.62
4:AD:185:PHE:CE2	4:AD:289:LEU:HD12	2.34	0.62
5:BE:5008:ARG:HH22	5:BE:5016:SER:HB3	1.64	0.62
3:AC:432:VAL:CG1	3:AC:433:LEU:N	2.63	0.62
4:AD:261:PHE:CD2	4:AD:267:LEU:HD12	2.35	0.62
5:AE:34:GLY:CA	6:AF:32:PHE:CE1	2.83	0.62
1:BA:5193:LEU:HD13	4:BD:5179:PHE:HB3	1.81	0.62
2:BB:5298:LEU:HD23	2:BB:5402:TYR:CZ	2.35	0.62
16:BV:5092:ARG:HH11	16:BV:5092:ARG:HG3	1.65	0.62
1:AA:48:PHE:HB2	1:AA:115:ILE:HD13	1.81	0.62
11:AL:13:ASN:ND2	11:AL:15:THR:HG22	2.15	0.62
3:BC:5039:ASN:HB3	24:BC:5509:CLA:CBB	2.30	0.62
3:BC:5062:PHE:HD2	10:BK:5029:PRO:HG3	1.65	0.62
17:By:5041:VAL:C	17:By:5043:ARG:H	2.07	0.62
2:AB:179:GLN:HE21	2:AB:180:PRO:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:246:PHE:C	2:AB:246:PHE:HD1	2.08	0.62
2:AB:483:ASP:CG	2:AB:484:PRO:HD2	2.24	0.62
4:AD:14:TRP:CD1	4:AD:15:PHE:N	2.68	0.62
15:AU:58:ASN:HD22	15:AU:114:VAL:HG13	1.64	0.62
1:BA:5296:ASN:HB2	3:BC:5400:PRO:O	2.00	0.62
1:BA:5306:VAL:HG13	1:BA:5314:ILE:O	2.00	0.62
2:BB:5025:MET:HE1	2:BB:5108:PHE:CD1	2.35	0.62
2:BB:5284:ILE:HG23	2:BB:5305:ILE:HD12	1.82	0.62
18:BX:5036:VAL:O	18:BX:5040:ILE:HG22	1.99	0.62
1:AA:200:LEU:HD13	28:AC:519:DGD:HAW2	1.76	0.62
2:AB:8:VAL:HG23	2:AB:9:HIS:CD2	2.34	0.62
2:AB:206:GLY:O	2:AB:210:ILE:HG13	2.00	0.62
2:AB:329:PRO:HD3	24:AB:607:CLA:HED1	1.82	0.62
3:AC:40:ALA:O	3:AC:43:ILE:HG13	2.00	0.62
3:AC:62:PHE:HD2	10:AK:29:PRO:HG3	1.65	0.62
1:BA:5161:TYR:HB3	1:BA:5162:PRO:HD3	1.82	0.62
3:BC:5288:CYS:SG	28:BC:5517:DGD:HA21	2.39	0.62
4:BD:5080:THR:HB	4:BD:5081:PRO:HD2	1.81	0.62
6:BF:5017:THR:HG23	6:BF:5020:TRP:H	1.65	0.62
2:AB:224:ARG:HG3	7:AH:25:TRP:CD1	2.34	0.61
5:AE:26:THR:HB	36:AF:101:HEM:HAB	1.81	0.61
13:AO:123:GLU:HG2	13:AO:124:GLU:N	2.15	0.61
3:BC:5041:ARG:NH1	24:BC:5511:CLA:OBD	2.33	0.61
3:BC:5047:GLY:O	3:BC:5050:LEU:HB3	2.00	0.61
4:BD:5086:GLY:C	4:BD:5166:SER:HB2	2.25	0.61
13:AO:69:LEU:HD12	13:AO:70:CYS:H	1.65	0.61
16:AV:99:VAL:O	16:AV:103:LYS:HG3	2.00	0.61
1:BA:5012:ASN:HD22	1:BA:5015:GLU:HB2	1.66	0.61
2:BB:5284:ILE:HG23	2:BB:5305:ILE:CD1	2.30	0.61
4:BD:5239:GLN:O	4:BD:5240:ALA:HB3	2.00	0.61
2:AB:453:PHE:HB2	4:AD:291:LEU:HD23	1.82	0.61
31:AB:621:LMG:H411	4:AD:284:ILE:HG12	1.82	0.61
2:BB:5027:THR:CG2	2:BB:5107:LEU:HD13	2.21	0.61
2:BB:5068:ARG:HH22	24:BB:5608:CLA:CED	2.12	0.61
2:BB:5134:ASP:OD2	2:BB:5137:LYS:HB2	2.00	0.61
11:BL:5007:ARG:HD2	11:BL:5007:ARG:O	2.00	0.61
2:AB:142:HIS:HA	2:AB:145:LEU:HD12	1.83	0.61
3:AC:62:PHE:CE2	10:AK:28:ILE:HB	2.34	0.61
1:BA:5064:ARG:HD3	1:BA:5064:ARG:N	2.14	0.61
5:BE:5051:ARG:HH11	5:BE:5051:ARG:HG3	1.65	0.61
13:BO:5151:LEU:HD12	13:BO:5152:VAL:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5247:PHE:HB2	24:BB:5612:CLA:HBC1	1.81	0.61
17:By:5019:ILE:HG23	17:By:5020:ALA:N	2.16	0.61
29:AA:412:LHG:HC11	3:AC:447:ARG:NH2	2.16	0.61
24:AB:611:CLA:H201	24:AB:613:CLA:H92	1.82	0.61
1:BA:5200:LEU:HD13	28:BC:5519:DGD:HAW2	1.78	0.61
2:BB:5468:TRP:HD1	2:BB:5469:HIS:ND1	1.98	0.61
3:BC:5033:PHE:CE1	4:BD:5229:ALA:CB	2.84	0.61
3:BC:5114:VAL:HG22	31:BC:5521:LMG:H141	1.81	0.61
3:BC:5324:LEU:HD22	3:BC:5324:LEU:N	2.15	0.61
4:BD:5207:GLY:HA3	4:BD:5275:PRO:HG3	1.83	0.61
1:AA:10:SER:HB3	1:AA:16:ARG:NH1	2.14	0.61
2:AB:179:GLN:NE2	2:AB:180:PRO:HD2	2.15	0.61
3:AC:324:LEU:HD22	3:AC:324:LEU:N	2.16	0.61
1:BA:5131:TRP:CE3	1:BA:5132:GLU:N	2.69	0.61
3:BC:5264:PHE:HE1	27:BC:5516:BCR:H321	1.66	0.61
1:AA:133:LEU:O	1:AA:137:LEU:HG	2.00	0.61
3:AC:472:LEU:HG	4:AD:251:ARG:NH1	2.16	0.61
27:AC:514:BCR:H391	10:AK:36:ALA:HB2	1.81	0.61
1:BA:5271:LEU:CD2	25:BA:5409:MST:H81	2.29	0.61
2:BB:5383:PHE:CZ	13:BO:5193:GLY:HA2	2.35	0.61
24:BC:5511:CLA:H151	20:BZ:5024:PRO:HG3	1.83	0.61
3:AC:223:TRP:CD2	3:AC:224:ILE:HG13	2.36	0.61
4:AD:18:LEU:HD22	18:AX:38:ILE:CD1	2.29	0.61
9:AJ:11:TRP:CE2	9:AJ:12:ILE:HG13	2.36	0.61
2:BB:5278:SER:HB3	2:BB:5281:GLN:HE21	1.65	0.61
7:BH:5009:ASP:O	7:BH:5012:ARG:HB2	2.01	0.61
1:AA:192:ILE:CB	1:AA:293:MET:HE1	2.31	0.61
1:AA:343:LEU:O	1:AA:344:ALA:HB2	2.01	0.61
3:AC:30:SER:HB3	10:AK:46:ARG:O	2.00	0.61
13:AO:151:LEU:HD12	13:AO:152:VAL:H	1.64	0.61
13:AO:169:LYS:HG2	13:AO:224:SER:HB3	1.82	0.61
2:BB:5173:GLY:CA	2:BB:5265:ILE:HD11	2.31	0.61
1:AA:262:TYR:CZ	31:AA:414:LMG:HC5	2.36	0.60
4:AD:241:GLU:H	4:AD:241:GLU:CD	2.08	0.60
2:BB:5183:PRO:HG3	2:BB:5199:VAL:HG11	1.83	0.60
6:BF:5017:THR:O	6:BF:5021:VAL:HG23	2.00	0.60
8:BI:5008:VAL:O	8:BI:5012:VAL:HG23	2.01	0.60
2:AB:222:PRO:HD2	2:AB:225:LEU:HD12	1.83	0.60
3:AC:113:VAL:HG11	31:AC:521:LMG:H132	1.83	0.60
2:BB:5133:LEU:HB3	2:BB:5138:MET:CE	2.30	0.60
1:AA:262:TYR:OH	31:AA:414:LMG:HC5	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:374:GLY:O	3:AC:375:LEU:C	2.44	0.60
16:AV:92:ARG:HH11	16:AV:92:ARG:HG3	1.66	0.60
1:BA:5300:PHE:CE2	28:BC:5519:DGD:O1A	2.54	0.60
7:BH:5006:TRP:CE2	7:BH:5010:ILE:HD11	2.36	0.60
1:AA:131:TRP:CE3	1:AA:132:GLU:N	2.70	0.60
2:AB:479:PHE:O	2:AB:480:SER:HB2	2.01	0.60
3:BC:5374:GLY:O	3:BC:5375:LEU:C	2.44	0.60
4:BD:5068:LEU:HB2	6:BF:5040:MET:HE2	1.83	0.60
4:BD:5253:TRP:HA	4:BD:5256:ILE:HG22	1.84	0.60
35:BD:5406:PL9:H303	35:BD:5406:PL9:C23	2.31	0.60
16:BV:5038:LEU:HD12	16:BV:5095:ILE:HB	1.83	0.60
1:AA:306:VAL:HG13	1:AA:314:ILE:O	2.02	0.60
1:AA:324:ALA:HB2	4:AD:329:MET:SD	2.42	0.60
24:AB:610:CLA:O1D	24:AB:610:CLA:H121	2.01	0.60
9:AJ:17:ALA:O	9:AJ:21:VAL:HG23	2.01	0.60
12:AM:19:SER:O	12:AM:23:ILE:HD13	2.01	0.60
24:BC:5504:CLA:H152	28:BC:5519:DGD:HA91	1.84	0.60
10:BK:5018:PHE:CE1	20:BZ:5009:LEU:HG	2.36	0.60
15:BU:5113:THR:O	15:BU:5114:VAL:HG23	2.01	0.60
4:AD:80:THR:HG23	4:AD:172:SER:OG	2.01	0.60
2:BB:5068:ARG:NH2	24:BB:5608:CLA:HED1	2.17	0.60
2:BB:5483:ASP:CG	2:BB:5484:PRO:HD2	2.26	0.60
1:AA:192:ILE:HB	1:AA:293:MET:HE1	1.84	0.60
1:AA:297:LEU:HD11	3:AC:404:LEU:HD12	1.84	0.60
29:AA:415:LHG:HC41	29:AA:415:LHG:O9	2.02	0.60
2:AB:133:LEU:HB3	2:AB:138:MET:CE	2.30	0.60
2:AB:284:ILE:HG23	2:AB:305:ILE:CD1	2.31	0.60
2:AB:284:ILE:HG23	2:AB:305:ILE:HD12	1.82	0.60
10:AK:18:PHE:CE1	20:AZ:9:LEU:HG	2.36	0.60
16:AV:104:ASN:HA	16:AV:122:ARG:HD3	1.83	0.60
2:BB:5384:ARG:HD3	15:BU:5132:LEU:CD1	2.32	0.60
24:BC:5503:CLA:H171	24:BC:5510:CLA:HBB2	1.83	0.60
12:BM:5001:MET:CG	12:BM:5002:GLU:H	2.13	0.60
1:AA:188:ALA:HB2	1:AA:328:MET:HB2	1.84	0.60
1:AA:271:LEU:CD2	25:AA:408:MST:H81	2.29	0.60
2:AB:113:TRP:CE2	2:AB:117:TYR:HD1	2.20	0.60
24:AB:603:CLA:H161	7:AH:38:PHE:HE2	1.65	0.60
3:AC:41:ARG:NH1	24:AC:511:CLA:OBD	2.34	0.60
3:AC:149:TYR:HA	3:AC:156:LYS:HD3	1.83	0.60
4:AD:86:GLY:C	4:AD:166:SER:HB2	2.26	0.60
1:BA:5289:GLY:O	1:BA:5292:THR:CG2	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5124:ARG:HH11	2:BB:5124:ARG:HG3	1.67	0.60
4:BD:5145:ALA:HB2	4:BD:5272:LEU:HD21	1.83	0.60
13:BO:5118:SER:HB3	13:BO:5157:PRO:HA	1.84	0.60
1:AA:326:LEU:HD21	3:AC:412:THR:HB	1.84	0.60
30:AB:622:SQD:H442	4:AD:23:LYS:HE2	1.82	0.60
13:AO:64:TYR:HD1	13:AO:271:PRO:HA	1.67	0.60
2:BB:5142:HIS:HA	2:BB:5145:LEU:HD12	1.83	0.60
3:BC:5156:LYS:O	3:BC:5160:ILE:HG13	2.02	0.60
20:BZ:5032:ASP:CG	20:BZ:5033:TRP:N	2.57	0.60
1:AA:20:TRP:CD1	1:AA:20:TRP:C	2.80	0.60
7:AH:6:TRP:CE2	7:AH:10:ILE:HD11	2.37	0.60
17:Ay:36:ILE:O	17:Ay:39:LEU:HB2	2.02	0.60
29:BA:5413:LHG:HC11	3:BC:5447:ARG:NH2	2.17	0.60
3:BC:5143:TYR:O	3:BC:5144:SER:HB2	2.02	0.60
3:BC:5216:SER:HB3	3:BC:5221:GLU:HB2	1.84	0.60
27:BC:5514:BCR:H391	10:BK:5036:ALA:HB2	1.83	0.60
27:BC:5516:BCR:HC41	8:BI:5020:VAL:HG13	1.82	0.60
3:AC:167:VAL:HG11	24:AC:512:CLA:H3A	1.84	0.59
3:AC:216:SER:HB3	3:AC:221:GLU:HB2	1.84	0.59
3:AC:233:VAL:HA	27:AC:516:BCR:H281	1.84	0.59
3:BC:5042:LEU:HD23	24:BC:5511:CLA:HED3	1.82	0.59
3:BC:5413:GLU:HG3	3:BC:5414:ILE:N	2.17	0.59
9:BJ:5017:ALA:O	9:BJ:5021:VAL:HG23	2.01	0.59
24:AA:405:CLA:HBA2	31:AB:620:LMG:C25	2.32	0.59
2:AB:27:THR:CG2	2:AB:107:LEU:HD13	2.25	0.59
2:AB:280:PHE:CE2	2:AB:312:TYR:HB3	2.36	0.59
2:AB:349:LYS:HG3	2:AB:350:GLU:OE1	2.02	0.59
2:AB:359:MET:HB2	2:AB:425:ILE:HG23	1.84	0.59
5:AE:8:ARG:HH22	5:AE:16:SER:HB3	1.67	0.59
16:AV:47:LEU:HD11	16:AV:143:GLY:HA3	1.83	0.59
1:BA:5265:PHE:CD1	1:BA:5271:LEU:HA	2.36	0.59
1:BA:5288:LEU:HD22	3:BC:5432:VAL:HG23	1.82	0.59
1:BA:5289:GLY:C	1:BA:5292:THR:HG22	2.27	0.59
2:BB:5265:ILE:HG13	2:BB:5266:GLU:N	2.17	0.59
3:BC:5178:LYS:HA	3:BC:5182:PHE:HB2	1.83	0.59
10:BK:5024:VAL:O	10:BK:5027:VAL:HG12	2.02	0.59
4:AD:14:TRP:CD1	4:AD:15:PHE:H	2.19	0.59
4:AD:53:THR:HG22	4:AD:67:TYR:CD2	2.38	0.59
13:AO:230:VAL:CG1	13:AO:231:ASP:H	2.13	0.59
2:BB:5188:ASP:OD1	7:BH:5058:VAL:HA	2.03	0.59
7:BH:5011:LEU:C	7:BH:5013:PRO:HD2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5083:LYS:HG2	13:BO:5084:ASN:H	1.66	0.59
3:AC:324:LEU:N	3:AC:324:LEU:CD2	2.66	0.59
6:AF:19:ARG:HH11	6:AF:19:ARG:HG3	1.67	0.59
1:BA:5257:ARG:HG3	1:BA:5257:ARG:HH11	1.66	0.59
3:BC:5415:ASN:HB3	9:BJ:5039:SER:OG	2.03	0.59
3:BC:5453:ALA:C	8:BI:5034:ARG:HB2	2.27	0.59
4:BD:5014:TRP:CD1	4:BD:5015:PHE:N	2.70	0.59
10:BK:5017:ILE:HD12	10:BK:5017:ILE:N	2.17	0.59
24:AB:604:CLA:H121	24:AB:615:CLA:HBA1	1.83	0.59
3:AC:362:ARG:HE	3:AC:370:ARG:NH1	1.99	0.59
13:AO:116:ASP:OD2	13:AO:116:ASP:C	2.46	0.59
1:BA:5220:THR:HG23	4:BD:5141:TYR:HD1	1.68	0.59
2:BB:5487:SER:N	2:BB:5488:PRO:HD2	2.17	0.59
17:By:5034:MET:HE3	17:By:5034:MET:CA	2.27	0.59
3:AC:305:THR:HG22	3:AC:308:GLU:HB3	1.81	0.59
13:AO:218:LEU:HD22	15:AU:119:THR:HG21	1.84	0.59
1:BA:5083:VAL:HG22	4:BD:5314:PHE:CE2	2.36	0.59
24:BB:5609:CLA:HMA2	24:BB:5610:CLA:HMA2	1.84	0.59
35:BD:5406:PL9:C30	35:BD:5406:PL9:H262	2.32	0.59
11:BL:5013:ASN:ND2	11:BL:5015:THR:HG22	2.18	0.59
16:BV:5099:VAL:O	16:BV:5103:LYS:HG3	2.02	0.59
1:AA:97:TRP:HA	8:AI:1:MET:SD	2.43	0.59
1:AA:296:ASN:HB2	3:AC:400:PRO:O	2.02	0.59
3:AC:178:LYS:HA	3:AC:182:PHE:HB2	1.84	0.59
24:AC:511:CLA:H151	20:AZ:24:PRO:HG3	1.84	0.59
4:AD:299:ILE:HG13	11:AL:37:ASN:HD21	1.67	0.59
5:AE:51:ARG:HG3	5:AE:51:ARG:NH1	2.15	0.59
8:AI:14:PHE:CZ	8:AI:18:LEU:HD11	2.38	0.59
24:BB:5607:CLA:H161	7:BH:5038:PHE:HE2	1.68	0.59
24:BC:5504:CLA:H151	28:BC:5519:DGD:C9A	2.31	0.59
5:BE:5026:THR:HB	36:BF:5101:HEM:HAB	1.85	0.59
6:BF:5037:ILE:HA	6:BF:5040:MET:SD	2.43	0.59
17:By:5019:ILE:HG23	17:By:5020:ALA:H	1.67	0.59
2:AB:483:ASP:HB3	2:AB:484:PRO:HD2	1.85	0.59
1:BA:5032:TRP:HA	1:BA:5032:TRP:HE3	1.67	0.59
3:BC:5033:PHE:CE1	4:BD:5229:ALA:HB3	2.38	0.59
3:BC:5170:ILE:HG22	3:BC:5174:LEU:CD2	2.33	0.59
2:AB:384:ARG:HD3	15:AU:132:LEU:HD11	1.85	0.59
35:AD:405:PL9:C30	35:AD:405:PL9:H262	2.33	0.59
15:AU:68:TYR:HB2	15:AU:71:LEU:HD12	1.84	0.59
16:AV:71:ILE:HD12	16:AV:71:ILE:C	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Ay:22:LEU:H	17:Ay:22:LEU:HD12	1.67	0.59
1:BA:5188:ALA:HB2	1:BA:5328:MET:HB2	1.85	0.59
3:BC:5405:ASN:HB2	28:BC:5519:DGD:C3G	2.32	0.59
7:BH:5055:LEU:O	7:BH:5058:VAL:HG12	2.02	0.59
10:BK:5031:LEU:O	10:BK:5034:ALA:HB3	2.03	0.59
1:AA:64:ARG:HD3	1:AA:64:ARG:N	2.17	0.59
2:AB:356:VAL:HG22	2:AB:370:LEU:HD21	1.85	0.59
3:AC:413:GLU:HG3	3:AC:414:ILE:N	2.18	0.59
3:AC:418:ASN:CB	28:AC:519:DGD:HE2	2.32	0.59
4:AD:150:ILE:O	4:AD:154:VAL:HG23	2.03	0.59
6:AF:15:ILE:HG22	6:AF:16:PHE:HD1	1.68	0.59
15:AU:98:THR:HG23	15:AU:101:GLN:OE1	2.03	0.59
24:BB:5612:CLA:H202	7:BH:5043:LEU:HD11	1.83	0.59
4:BD:5023:LYS:HZ2	4:BD:5032:TRP:CD1	2.21	0.59
1:AA:180:PHE:CD1	4:AD:192:THR:HB	2.38	0.58
3:AC:33:PHE:CE1	4:AD:229:ALA:CB	2.85	0.58
3:AC:156:LYS:O	3:AC:160:ILE:HG13	2.03	0.58
4:AD:49:LEU:O	4:AD:53:THR:HG23	2.03	0.58
12:AM:25:LEU:O	12:AM:28:GLN:HG3	2.03	0.58
1:BA:5013:LEU:CA	1:BA:5016:ARG:HD3	2.33	0.58
2:BB:5458:PHE:HB3	24:BB:5608:CLA:HBC2	1.84	0.58
3:BC:5324:LEU:N	3:BC:5324:LEU:CD2	2.65	0.58
7:BH:5017:GLU:CD	7:BH:5017:GLU:H	2.10	0.58
3:AC:264:PHE:HE1	27:AC:516:BCR:H321	1.67	0.58
20:AZ:31:GLN:O	20:AZ:32:ASP:HB3	2.02	0.58
1:BA:5275:LEU:HD13	25:BA:5409:MST:H83	1.85	0.58
4:BD:5299:ILE:HG13	11:BL:5037:ASN:HD21	1.68	0.58
6:BF:5015:ILE:HG22	6:BF:5016:PHE:HD1	1.68	0.58
7:BH:5012:ARG:N	7:BH:5013:PRO:HD2	2.18	0.58
10:BK:5026:PRO:O	10:BK:5029:PRO:HD2	2.02	0.58
10:AK:39:TRP:HE1	17:Ay:46:LEU:C	2.11	0.58
2:BB:5075:TRP:CD1	2:BB:5092:SER:HG	2.22	0.58
28:BC:5519:DGD:HG2	9:BJ:5033:TYR:OH	2.03	0.58
9:BJ:5011:TRP:CE3	10:BK:5042:ALA:HB2	2.39	0.58
1:AA:333:GLU:HB2	1:AA:337:HIS:HE1	1.68	0.58
2:AB:144:PHE:CE1	2:AB:210:ILE:HG23	2.39	0.58
2:AB:490:GLN:OE1	2:AB:490:GLN:O	2.21	0.58
3:AC:453:ALA:O	8:AI:34:ARG:HB2	2.03	0.58
15:AU:54:LYS:HD2	15:AU:113:THR:HG23	1.86	0.58
1:BA:5163:ILE:HG12	28:BC:5517:DGD:HB31	1.85	0.58
1:BA:5271:LEU:HD23	1:BA:5271:LEU:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BB:5615:CLA:H201	24:BB:5617:CLA:H92	1.84	0.58
3:BC:5167:VAL:HG11	24:BC:5512:CLA:H3A	1.83	0.58
3:BC:5250:TRP:CD1	3:BC:5250:TRP:C	2.81	0.58
35:BD:5406:PL9:H301	35:BD:5406:PL9:C33	2.34	0.58
5:BE:5026:THR:O	5:BE:5029:ALA:HB3	2.02	0.58
2:BB:5359:MET:HB2	2:BB:5425:ILE:HG23	1.85	0.58
3:BC:5110:PRO:O	3:BC:5114:VAL:HG23	2.02	0.58
3:BC:5116:VAL:HG23	3:BC:5117:VAL:N	2.19	0.58
24:BC:5507:CLA:H2	24:BC:5507:CLA:HMA3	1.86	0.58
16:BV:5056:LYS:O	16:BV:5060:GLN:HG3	2.03	0.58
4:AD:41:ALA:HB1	34:AD:403:PHO:H42	1.85	0.58
2:BB:5349:LYS:HG3	2:BB:5350:GLU:OE1	2.03	0.58
3:BC:5432:VAL:CG1	3:BC:5433:LEU:N	2.65	0.58
6:BF:5011:VAL:HG12	6:BF:5012:SER:H	1.69	0.58
14:BT:5018:PHE:HB2	27:BT:5101:BCR:HC8	1.84	0.58
20:BZ:5033:TRP:HD1	20:BZ:5033:TRP:O	1.87	0.58
2:AB:215:PHE:C	2:AB:215:PHE:CD2	2.82	0.58
2:AB:230:ARG:O	2:AB:233:ASN:HB3	2.04	0.58
3:AC:39:ASN:HB3	24:AC:509:CLA:CBB	2.33	0.58
3:AC:257:PHE:O	3:AC:261:ARG:HG3	2.03	0.58
14:AT:18:PHE:HB2	27:AT:101:BCR:HC8	1.84	0.58
1:BA:5192:ILE:CB	1:BA:5293:MET:HE1	2.33	0.58
1:BA:5274:PHE:CE2	25:BA:5409:MST:H133	2.37	0.58
2:BB:5170:ASP:HB2	2:BB:5171:PRO:CD	2.32	0.58
1:AA:332:HIS:CD2	1:AA:333:GLU:HG3	2.38	0.58
24:AB:605:CLA:HMA2	24:AB:606:CLA:HMA2	1.86	0.58
3:AC:39:ASN:HB2	24:AC:508:CLA:HBA2	1.84	0.58
3:AC:279:LEU:HA	3:AC:282:MET:HE3	1.86	0.58
4:AD:244:TYR:OH	4:AD:264:LYS:HD2	2.03	0.58
16:AV:74:THR:O	16:AV:75:ASN:HB2	2.03	0.58
1:BA:5272:HIS:HD2	4:BD:5218:VAL:HG21	1.68	0.58
2:BB:5479:PHE:O	2:BB:5480:SER:HB2	2.03	0.58
24:BB:5608:CLA:H121	24:BB:5619:CLA:HBA1	1.85	0.58
3:BC:5279:LEU:HD12	3:BC:5437:PHE:HE1	1.69	0.58
4:BD:5086:GLY:CA	4:BD:5166:SER:HB2	2.34	0.58
6:BF:5018:VAL:HG12	6:BF:5019:ARG:N	2.19	0.58
16:BV:5133:LEU:H	16:BV:5133:LEU:CD1	2.16	0.58
1:AA:219:VAL:HG11	4:AD:268:HIS:CD2	2.38	0.58
3:AC:47:GLY:O	3:AC:50:LEU:HB3	2.03	0.58
4:AD:171:PRO:HG3	4:AD:181:PHE:CZ	2.39	0.58
2:BB:5179:GLN:NE2	2:BB:5180:PRO:HD2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BB:5618:CLA:H202	31:BL:5101:LMG:H422	1.86	0.58
3:BC:5367:GLU:HB2	3:BC:5368:PRO:HD3	1.86	0.58
4:BD:5014:TRP:CD1	4:BD:5015:PHE:H	2.22	0.58
4:BD:5244:TYR:OH	4:BD:5264:LYS:HD2	2.04	0.58
8:BI:5027:ASP:N	8:BI:5028:PRO:CD	2.66	0.58
2:AB:383:PHE:CZ	13:AO:193:GLY:HA2	2.39	0.58
1:BA:5219:VAL:HG11	4:BD:5268:HIS:CD2	2.38	0.58
1:BA:5307:ILE:HG22	1:BA:5313:VAL:HA	1.86	0.58
24:BA:5406:CLA:HBA2	31:BL:5101:LMG:C25	2.33	0.58
2:BB:5113:TRP:CE2	2:BB:5117:TYR:HD1	2.22	0.58
1:AA:330:VAL:CG1	4:AD:348:ARG:HG2	2.34	0.57
18:AX:16:LEU:O	18:AX:16:LEU:HD13	2.04	0.57
1:BA:5341:LEU:HB2	3:BC:5313:GLN:NE2	2.10	0.57
3:BC:5226:SER:O	28:BC:5517:DGD:HE62	2.04	0.57
3:BC:5377:LEU:O	3:BC:5381:LYS:HB2	2.04	0.57
6:BF:5037:ILE:HG22	9:BJ:5028:PHE:CE1	2.38	0.57
13:BO:5123:GLU:HG2	13:BO:5124:GLU:N	2.17	0.57
1:AA:260:PHE:CZ	1:AA:263:ALA:HB2	2.39	0.57
3:AC:38:GLY:HA3	24:AC:511:CLA:HMD2	1.86	0.57
1:BA:5283:VAL:HG21	34:BD:5403:PHO:HBC3	1.86	0.57
24:BC:5505:CLA:O1A	8:BI:5023:PHE:CE1	2.57	0.57
3:AC:449:ARG:HG2	24:AC:505:CLA:HED1	1.86	0.57
6:AF:37:ILE:HA	6:AF:40:MET:SD	2.44	0.57
8:AI:13:THR:HA	8:AI:16:VAL:HG12	1.86	0.57
24:BB:5606:CLA:H11	7:BH:5049:TYR:HD2	1.69	0.57
30:BB:5625:SQD:H442	4:BD:5023:LYS:HE2	1.85	0.57
3:BC:5279:LEU:HD23	3:BC:5282:MET:HE3	1.85	0.57
3:BC:5297:TYR:HA	3:BC:5302:TYR:HE2	1.69	0.57
24:AB:602:CLA:HBD	24:AB:602:CLA:H43	1.86	0.57
13:AO:32:THR:O	13:AO:36:ILE:CD1	2.52	0.57
20:AZ:23:VAL:O	20:AZ:26:ALA:HB3	2.05	0.57
1:BA:5045:THR:HG23	1:BA:5046:ILE:N	2.18	0.57
1:BA:5192:ILE:HB	1:BA:5293:MET:HE1	1.87	0.57
24:BC:5512:CLA:H203	31:BC:5521:LMG:H381	1.86	0.57
11:BL:5008:GLN:N	11:BL:5008:GLN:NE2	2.52	0.57
2:AB:270:PRO:HG3	2:AB:312:TYR:HD2	1.69	0.57
2:AB:458:PHE:HB3	24:AB:604:CLA:HBC2	1.86	0.57
3:AC:226:SER:O	28:AC:517:DGD:HE62	2.04	0.57
7:AH:58:VAL:O	7:AH:58:VAL:CG1	2.52	0.57
2:BB:5262:THR:HG23	2:BB:5263:THR:HG23	1.86	0.57
1:AA:13:LEU:CA	1:AA:16:ARG:HD3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:57:PRO:HD3	1:AA:73:TYR:CD2	2.40	0.57
4:AD:267:LEU:HD23	4:AD:267:LEU:C	2.30	0.57
1:BA:5317:TRP:CD1	4:BD:5177:ALA:HB2	2.38	0.57
3:BC:5220:GLY:N	28:BC:5517:DGD:O3D	2.35	0.57
17:By:5039:LEU:HD21	20:BZ:5025:VAL:HA	1.85	0.57
3:AC:199:ILE:HD12	3:AC:199:ILE:N	2.18	0.57
3:AC:279:LEU:HD23	3:AC:282:MET:HE3	1.86	0.57
4:AD:335:PRO:HB2	5:AE:65:LEU:HD21	1.86	0.57
13:AO:92:VAL:HG13	13:AO:93:PRO:HD2	1.87	0.57
20:AZ:30:PRO:C	20:AZ:32:ASP:H	2.12	0.57
20:AZ:33:TRP:O	20:AZ:37:LYS:HB2	2.05	0.57
1:BA:5315:ASN:HD21	4:BD:5332:GLN:NE2	2.02	0.57
2:BB:5483:ASP:HB3	2:BB:5484:PRO:HD2	1.85	0.57
3:BC:5039:ASN:HB2	24:BC:5508:CLA:HBA2	1.85	0.57
4:BD:5056:THR:HG21	5:BE:5050:PRO:HD3	1.87	0.57
14:BT:5022:PHE:C	14:BT:5023:PHE:CD2	2.83	0.57
1:BA:5289:GLY:HA2	1:BA:5292:THR:HG22	1.86	0.57
2:BB:5237:VAL:HG22	24:BB:5614:CLA:HBC2	1.86	0.57
5:BE:5015:THR:HB	9:BJ:5006:GLY:HA2	1.87	0.57
3:AC:33:PHE:CE1	4:AD:229:ALA:HB3	2.38	0.57
24:AC:504:CLA:H2	28:AC:518:DGD:HA21	1.87	0.57
4:AD:308:ASP:C	4:AD:308:ASP:OD1	2.47	0.57
2:BB:5462:PHE:HA	24:BB:5615:CLA:CMC	2.35	0.57
24:BB:5614:CLA:O1D	24:BB:5614:CLA:H121	2.04	0.57
3:BC:5405:ASN:HA	28:BC:5519:DGD:HG11	1.87	0.57
28:BC:5519:DGD:O3D	9:BJ:5037:GLY:O	2.20	0.57
13:BO:5114:ASN:ND2	13:BO:5120:THR:HG23	2.20	0.57
1:AA:99:ALA:O	8:AI:1:MET:HE3	2.04	0.57
2:AB:327:THR:O	2:AB:444:ARG:NE	2.36	0.57
24:AC:504:CLA:H172	28:AC:519:DGD:HAE1	1.85	0.57
1:BA:5191:ASN:HB2	3:BC:5411:ALA:HB1	1.85	0.57
3:BC:5233:VAL:HA	27:BC:5516:BCR:H281	1.87	0.57
5:BE:5017:VAL:HG22	9:BJ:5008:ILE:HD11	1.87	0.57
13:BO:5218:LEU:CD2	15:BU:5119:THR:HG21	2.35	0.57
18:BX:5045:LYS:HD3	18:BX:5045:LYS:N	2.19	0.57
25:AA:408:MST:N3	25:AA:408:MST:H122	2.20	0.56
2:AB:170:ASP:HB2	2:AB:171:PRO:CD	2.35	0.56
2:AB:280:PHE:O	2:AB:284:ILE:HG13	2.05	0.56
3:AC:250:TRP:CD1	3:AC:250:TRP:C	2.82	0.56
3:AC:367:GLU:HB2	3:AC:368:PRO:HD3	1.87	0.56
4:AD:239:GLN:O	4:AD:240:ALA:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5278:TRP:O	1:BA:5281:VAL:HG12	2.05	0.56
2:BB:5010:THR:C	2:BB:5012:LEU:H	2.11	0.56
24:BB:5606:CLA:HBD	24:BB:5606:CLA:H43	1.86	0.56
32:BB:5627:LMT:H92	7:BH:5035:MET:CE	2.35	0.56
3:BC:5057:ALA:HB1	24:BC:5512:CLA:HED2	1.85	0.56
3:BC:5062:PHE:HZ	10:BK:5028:ILE:HD12	1.69	0.56
4:BD:5150:ILE:O	4:BD:5154:VAL:HG23	2.06	0.56
5:BE:5077:GLU:HA	5:BE:5080:LEU:HD23	1.87	0.56
13:BO:5098:THR:HG23	13:BO:5133:THR:HB	1.87	0.56
28:AA:411:DGD:C1G	28:AA:411:DGD:O1B	2.53	0.56
2:AB:10:THR:C	2:AB:12:LEU:H	2.11	0.56
3:AC:366:LEU:HD23	3:AC:366:LEU:C	2.29	0.56
24:AC:507:CLA:H2	24:AC:507:CLA:HMA3	1.86	0.56
13:AO:114:ASN:ND2	13:AO:120:THR:HG23	2.19	0.56
1:BA:5180:PHE:CE1	4:BD:5192:THR:HB	2.40	0.56
2:BB:5025:MET:HE3	27:BB:5621:BCR:H23C	1.87	0.56
7:BH:5058:VAL:O	7:BH:5058:VAL:CG1	2.53	0.56
1:AA:15:GLU:O	1:AA:19:ASN:OD1	2.23	0.56
1:AA:262:TYR:CE1	31:AA:414:LMG:C5	2.89	0.56
3:AC:116:VAL:HG23	3:AC:117:VAL:N	2.20	0.56
3:AC:193:GLY:O	3:AC:194:GLY:C	2.49	0.56
3:AC:343:ARG:NH1	3:AC:347:GLY:O	2.38	0.56
27:AC:516:BCR:HC41	8:AI:20:VAL:HG13	1.86	0.56
5:AE:56:TYR:HE1	5:AE:63:ILE:HD12	1.69	0.56
8:AI:27:ASP:N	8:AI:28:PRO:CD	2.68	0.56
10:AK:26:PRO:O	10:AK:29:PRO:HD2	2.06	0.56
13:AO:80:GLU:O	13:AO:89:ALA:HB1	2.06	0.56
20:AZ:32:ASP:C	20:AZ:34:ASP:N	2.60	0.56
2:BB:5271:THR:OG1	2:BB:5274:GLN:HG3	2.05	0.56
2:BB:5453:PHE:HB2	4:BD:5291:LEU:HD23	1.87	0.56
3:BC:5141:GLU:CD	3:BC:5141:GLU:H	2.13	0.56
3:BC:5199:ILE:HD12	3:BC:5199:ILE:N	2.20	0.56
3:BC:5304:PRO:HB3	3:BC:5395:TYR:CD1	2.40	0.56
3:BC:5362:ARG:HE	3:BC:5370:ARG:HH11	1.52	0.56
3:BC:5375:LEU:HB3	3:BC:5380:ILE:HD11	1.87	0.56
4:BD:5158:LEU:O	4:BD:5162:LEU:HG	2.06	0.56
4:BD:5221:THR:CG2	4:BD:5244:TYR:HB2	2.35	0.56
20:BZ:5014:ILE:O	20:BZ:5018:VAL:HG23	2.05	0.56
1:AA:126:TYR:O	1:AA:130:GLN:HG3	2.06	0.56
1:AA:278:TRP:O	1:AA:281:VAL:HG12	2.04	0.56
2:AB:462:PHE:HA	24:AB:611:CLA:HMC2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:69:ARG:HG3	5:AE:70:PHE:N	2.21	0.56
10:AK:18:PHE:C	10:AK:20:PRO:HD2	2.29	0.56
10:AK:31:LEU:O	10:AK:34:ALA:HB3	2.05	0.56
1:BA:5326:LEU:HD21	3:BC:5412:THR:HB	1.87	0.56
2:BB:5027:THR:HG22	2:BB:5107:LEU:CD1	2.24	0.56
3:BC:5297:TYR:HA	3:BC:5302:TYR:CE2	2.40	0.56
5:BE:5014:ILE:CG2	9:BJ:5013:VAL:HG11	2.35	0.56
5:BE:5051:ARG:HG3	5:BE:5051:ARG:NH1	2.19	0.56
8:BI:5013:THR:HA	8:BI:5016:VAL:HG12	1.85	0.56
13:BO:5154:SER:O	13:BO:5168:PHE:HA	2.05	0.56
2:AB:262:THR:HG23	2:AB:263:THR:HG23	1.88	0.56
2:AB:271:THR:OG1	2:AB:274:GLN:HG3	2.05	0.56
24:AB:611:CLA:C5	24:AB:614:CLA:HBC2	2.36	0.56
16:AV:133:LEU:H	16:AV:133:LEU:CD1	2.18	0.56
3:BC:5149:TYR:HA	3:BC:5156:LYS:CD	2.35	0.56
13:BO:5173:ASN:ND2	13:BO:5220:LYS:HD3	2.20	0.56
1:AA:142:TRP:HB2	4:AD:220:ASN:OD1	2.05	0.56
1:AA:289:GLY:C	1:AA:292:THR:HG22	2.31	0.56
2:AB:235:GLU:OE1	2:AB:472:ARG:NH1	2.39	0.56
2:AB:293:ALA:C	2:AB:295:GLY:H	2.14	0.56
3:AC:114:VAL:HG22	31:AC:521:LMG:H141	1.87	0.56
24:AC:505:CLA:O1A	8:AI:23:PHE:CE1	2.59	0.56
4:AD:145:ALA:HB2	4:AD:272:LEU:HD21	1.86	0.56
8:AI:13:THR:O	8:AI:16:VAL:HG12	2.06	0.56
13:AO:148:VAL:HA	13:AO:172:PHE:CD2	2.40	0.56
1:BA:5221:SER:HB3	4:BD:5141:TYR:HB2	1.86	0.56
2:BB:5206:GLY:O	2:BB:5210:ILE:HG13	2.05	0.56
2:BB:5270:PRO:HG3	2:BB:5312:TYR:HD2	1.70	0.56
2:BB:5280:PHE:CE2	2:BB:5312:TYR:HB3	2.40	0.56
3:BC:5038:GLY:HA3	24:BC:5511:CLA:HMD2	1.88	0.56
3:BC:5158:THR:HG21	3:BC:5254:THR:O	2.06	0.56
3:BC:5461:ARG:NH2	4:BD:5242:GLU:O	2.38	0.56
13:BO:5215:ARG:NH1	13:BO:5252:GLY:O	2.38	0.56
15:BU:5083:ALA:CB	15:BU:5084:PRO:CD	2.82	0.56
1:AA:221:SER:HB3	4:AD:141:TYR:HB2	1.88	0.56
2:AB:250:PHE:CE2	2:AB:459:ALA:HB1	2.41	0.56
3:AC:42:LEU:CD2	24:AC:511:CLA:HED3	2.36	0.56
3:AC:143:TYR:O	3:AC:144:SER:HB2	2.05	0.56
3:AC:170:ILE:HG22	3:AC:174:LEU:CD2	2.36	0.56
4:AD:330:ALA:HB3	4:AD:331:PRO:HD3	1.88	0.56
5:AE:57:ALA:H	5:AE:60:GLN:NE2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AT:22:PHE:C	14:AT:23:PHE:HD2	2.14	0.56
1:BA:5020:TRP:O	1:BA:5021:VAL:C	2.49	0.56
1:BA:5092:HIS:HD2	3:BC:5219:GLY:HA3	1.71	0.56
1:BA:5124:SER:O	1:BA:5127:MET:HB3	2.06	0.56
1:BA:5133:LEU:O	1:BA:5137:LEU:HG	2.06	0.56
2:BB:5179:GLN:HE21	2:BB:5180:PRO:HD2	1.71	0.56
2:BB:5329:PRO:HD3	24:BB:5611:CLA:HED1	1.86	0.56
2:BB:5433:ASP:C	2:BB:5433:ASP:OD1	2.47	0.56
4:BD:5129:GLN:HE22	4:BD:5143:ALA:HA	1.70	0.56
5:BE:5056:TYR:HE1	5:BE:5063:ILE:HD12	1.71	0.56
10:BK:5035:LEU:HA	10:BK:5038:VAL:HG23	1.88	0.56
13:BO:5080:GLU:O	13:BO:5089:ALA:HB1	2.05	0.56
20:BZ:5030:PRO:C	20:BZ:5032:ASP:H	2.12	0.56
20:BZ:5032:ASP:C	20:BZ:5034:ASP:N	2.60	0.56
1:AA:157:VAL:HG21	24:AA:405:CLA:CMC	2.36	0.56
1:AA:180:PHE:CE1	4:AD:192:THR:HB	2.41	0.56
3:AC:57:ALA:HB1	24:AC:512:CLA:HED2	1.88	0.56
5:AE:15:THR:HB	9:AJ:6:GLY:HA2	1.87	0.56
15:AU:66:ILE:HG12	15:AU:72:TYR:CG	2.41	0.56
2:BB:5369:ILE:O	2:BB:5370:LEU:HD23	2.04	0.56
3:BC:5305:THR:HG22	3:BC:5308:GLU:HB3	1.83	0.56
5:BE:5069:ARG:HG3	5:BE:5070:PHE:N	2.20	0.56
1:AA:183:MET:HE1	24:AA:405:CLA:HMD3	1.87	0.56
3:AC:44:ASN:O	3:AC:45:LEU:HD12	2.05	0.56
1:BA:5057:PRO:HD3	1:BA:5073:TYR:CD2	2.41	0.56
3:BC:5343:ARG:NH1	3:BC:5347:GLY:O	2.39	0.56
4:BD:5092:LEU:HA	4:BD:5104:TRP:CD1	2.41	0.56
1:AA:77:ILE:HD11	14:AT:6:TYR:HB3	1.87	0.56
24:AB:608:CLA:H203	24:AD:404:CLA:HBA2	1.89	0.56
24:BA:5406:CLA:H93	34:BD:5403:PHO:HHB	1.88	0.56
3:BC:5366:LEU:HD23	3:BC:5366:LEU:C	2.30	0.56
4:BD:5346:LEU:O	4:BD:5348:ARG:HG3	2.06	0.56
15:BU:5058:ASN:HD22	15:BU:5114:VAL:HG13	1.69	0.56
3:AC:95:LEU:HD13	24:AC:502:CLA:H143	1.89	0.55
3:AC:233:VAL:HA	27:AC:516:BCR:C28	2.36	0.55
3:AC:405:ASN:HA	28:AC:519:DGD:HG11	1.88	0.55
24:AC:513:CLA:HAA1	24:AC:513:CLA:H42	1.88	0.55
35:AD:405:PL9:H301	35:AD:405:PL9:C33	2.34	0.55
14:AT:29:ILE:HD12	14:AT:29:ILE:N	2.06	0.55
18:AX:12:ILE:HA	27:AX:101:BCR:H401	1.88	0.55
1:BA:5048:PHE:HA	1:BA:5115:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5124:VAL:HB	27:BC:5515:BCR:H362	1.88	0.55
28:BC:5518:DGD:HB22	28:BC:5519:DGD:HA21	1.88	0.55
16:AV:81:ARG:HG2	16:AV:81:ARG:HH11	1.70	0.55
2:BB:5144:PHE:CE1	2:BB:5210:ILE:HG23	2.41	0.55
3:BC:5033:PHE:HE1	4:BD:5229:ALA:CB	2.19	0.55
3:BC:5416:SER:N	28:BC:5519:DGD:O3E	2.37	0.55
5:BE:5076:VAL:O	5:BE:5080:LEU:CD2	2.54	0.55
17:By:5034:MET:CE	17:By:5034:MET:CA	2.80	0.55
1:AA:304:HIS:CE1	3:AC:414:ILE:HD12	2.41	0.55
1:AA:330:VAL:HG12	4:AD:348:ARG:HA	1.89	0.55
1:BA:5281:VAL:HG11	28:BC:5519:DGD:CIA	2.36	0.55
25:BA:5409:MST:N3	25:BA:5409:MST:H131	2.20	0.55
8:BI:5013:THR:O	8:BI:5016:VAL:HG12	2.06	0.55
13:BO:5059:ASP:C	13:BO:5061:SER:H	2.13	0.55
1:AA:217:SER:HA	1:AA:220:THR:HG22	1.88	0.55
24:AA:405:CLA:H201	14:AT:14:ILE:HD11	1.86	0.55
2:BB:5154:GLY:O	2:BB:5159:THR:HG23	2.06	0.55
2:BB:5384:ARG:HD3	15:BU:5132:LEU:HD11	1.89	0.55
3:BC:5170:ILE:HG22	3:BC:5174:LEU:HD23	1.88	0.55
3:BC:5225:VAL:HG22	3:BC:5289:PHE:CD1	2.42	0.55
4:BD:5014:TRP:NE1	7:BH:5025:TRP:HH2	1.95	0.55
4:BD:5239:GLN:O	4:BD:5240:ALA:CB	2.54	0.55
9:BJ:5011:TRP:CG	10:BK:5042:ALA:HA	2.41	0.55
12:BM:5005:GLN:HE22	32:BM:5101:LMT:H3'	1.71	0.55
13:BO:5092:VAL:HG13	13:BO:5093:PRO:HD2	1.87	0.55
15:BU:5098:THR:HG23	15:BU:5101:GLN:OE1	2.07	0.55
4:AD:253:TRP:HA	4:AD:256:ILE:HG22	1.89	0.55
3:BC:5155:ASN:O	3:BC:5158:THR:HG22	2.07	0.55
4:BD:5266:TRP:CD1	31:BD:5410:LMG:HC1	2.42	0.55
15:BU:5066:ILE:HG12	15:BU:5072:TYR:CG	2.42	0.55
17:By:5039:LEU:HD21	20:BZ:5028:ALA:HB3	1.88	0.55
20:BZ:5033:TRP:O	20:BZ:5033:TRP:CD1	2.60	0.55
1:AA:124:SER:O	1:AA:127:MET:HB3	2.07	0.55
1:AA:191:ASN:HB2	3:AC:411:ALA:HB1	1.89	0.55
1:AA:340:PRO:HG2	3:AC:317:PHE:CZ	2.42	0.55
2:AB:121:GLU:HG3	7:AH:4:ARG:CA	2.36	0.55
2:AB:133:LEU:CB	2:AB:138:MET:HE1	2.36	0.55
24:AB:602:CLA:H11	7:AH:49:TYR:HD2	1.71	0.55
4:AD:201:VAL:O	4:AD:205:LEU:HB2	2.07	0.55
4:AD:221:THR:CG2	4:AD:244:TYR:HB2	2.36	0.55
5:AE:76:VAL:O	5:AE:80:LEU:HD22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5176:ILE:HG22	1:BA:5180:PHE:HE2	1.71	0.55
2:BB:5176:GLY:HA3	2:BB:5266:GLU:OE1	2.06	0.55
2:BB:5275:TRP:CH2	2:BB:5358:ARG:HD3	2.41	0.55
3:BC:5461:ARG:CG	3:BC:5461:ARG:NH1	2.61	0.55
24:BC:5501:CLA:HMB3	27:BC:5516:BCR:C40	2.35	0.55
27:BC:5515:BCR:H312	20:BZ:5055:GLY:HA2	1.88	0.55
4:BD:5049:LEU:O	4:BD:5053:THR:HG23	2.06	0.55
31:AB:620:LMG:H191	11:AL:22:LEU:HG	1.88	0.55
32:AB:630:LMT:H41	8:BI:5001:MET:CE	2.36	0.55
12:AM:20:VAL:HG22	12:BM:5020:VAL:HG11	1.89	0.55
1:BA:5325:ASN:HA	1:BA:5328:MET:CE	2.26	0.55
29:BA:5415:LHG:HC41	29:BA:5415:LHG:O9	2.05	0.55
2:BB:5215:PHE:C	2:BB:5215:PHE:CD2	2.85	0.55
2:BB:5348:ASN:OD1	2:BB:5352:GLU:HB2	2.06	0.55
3:BC:5257:PHE:O	3:BC:5261:ARG:HG3	2.06	0.55
7:BH:5055:LEU:HB2	7:BH:5058:VAL:HG12	1.89	0.55
1:AA:341:LEU:HB2	3:AC:313:GLN:NE2	2.17	0.55
2:AB:90:PHE:CE2	2:AB:91:TRP:CZ3	2.94	0.55
4:AD:201:VAL:HB	24:AD:401:CLA:HMB2	1.89	0.55
4:AD:259:ILE:HG12	31:AD:408:LMG:H301	1.89	0.55
12:AM:23:ILE:HG12	31:AM:101:LMG:H212	1.89	0.55
13:AO:64:TYR:CD1	13:AO:271:PRO:HA	2.41	0.55
1:BA:5157:VAL:HG21	24:BA:5406:CLA:CMC	2.36	0.55
1:BA:5217:SER:HA	1:BA:5220:THR:HG22	1.89	0.55
2:BB:5354:LEU:HD21	2:BB:5378:LYS:HB2	1.89	0.55
3:BC:5193:GLY:O	3:BC:5194:GLY:C	2.48	0.55
3:BC:5281:MET:O	3:BC:5285:ILE:HG13	2.06	0.55
24:BC:5513:CLA:HAA1	24:BC:5513:CLA:H42	1.88	0.55
4:BD:5313:THR:OG1	4:BD:5315:TYR:HB3	2.07	0.55
13:BO:5064:TYR:HD1	13:BO:5271:PRO:HA	1.72	0.55
25:AA:408:MST:N3	25:AA:408:MST:H131	2.21	0.55
3:AC:62:PHE:HZ	10:AK:28:ILE:HD12	1.71	0.55
13:AO:173:ASN:ND2	13:AO:220:LYS:HD3	2.22	0.55
2:BB:5230:ARG:O	2:BB:5233:ASN:HB3	2.07	0.55
30:BB:5625:SQD:H152	32:BB:5627:LMT:H81	1.89	0.55
18:BX:5022:GLY:HA2	18:BX:5025:SER:HG	1.71	0.55
1:AA:20:TRP:O	1:AA:21:VAL:C	2.50	0.55
1:AA:288:LEU:HD13	3:AC:432:VAL:CG2	2.37	0.55
2:AB:76:SER:HB3	31:BA:5402:LMG:H301	1.88	0.55
2:AB:487:SER:N	2:AB:488:PRO:HD2	2.22	0.55
24:AB:613:CLA:H203	31:AD:407:LMG:H401	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AB:624:LMT:H92	7:AH:35:MET:CE	2.35	0.55
24:AC:512:CLA:H203	31:AC:521:LMG:H381	1.88	0.55
28:AC:519:DGD:O3D	9:AJ:37:GLY:O	2.25	0.55
13:AO:92:VAL:HG12	13:AO:93:PRO:HD2	1.88	0.55
1:BA:5064:ARG:HD3	1:BA:5064:ARG:H	1.72	0.55
1:BA:5281:VAL:CG1	28:BC:5519:DGD:CIA	2.84	0.55
1:BA:5330:VAL:HG12	4:BD:5348:ARG:HA	1.87	0.55
28:BA:5412:DGD:O1B	28:BA:5412:DGD:C1G	2.55	0.55
3:BC:5326:ALA:HB2	15:BU:5128:TYR:CG	2.42	0.55
27:BC:5515:BCR:C31	20:BZ:5055:GLY:HA2	2.37	0.55
4:BD:5053:THR:HG22	4:BD:5067:TYR:HE2	1.72	0.55
4:BD:5077:ALA:HB2	4:BD:5174:GLY:HA3	1.88	0.55
1:AA:38:ILE:HB	1:AA:39:PRO:HD3	1.89	0.54
30:AA:416:SQD:H302	24:BB:5620:CLA:H51	1.88	0.54
2:AB:18:ARG:HD3	2:AB:118:TRP:HB3	1.87	0.54
2:AB:462:PHE:HA	24:AB:611:CLA:CMC	2.37	0.54
28:AC:519:DGD:HE62	9:AJ:40:LEU:HD11	1.89	0.54
15:AU:57:LEU:HD11	15:AU:112:PHE:HB3	1.89	0.54
1:BA:5234:ASN:HB2	31:BL:5101:LMG:O3	2.05	0.54
3:BC:5095:LEU:HD13	24:BC:5502:CLA:H143	1.87	0.54
3:BC:5259:TRP:H	3:BC:5259:TRP:HD1	1.55	0.54
3:BC:5399:ALA:HB3	33:BV:5202:DMS:H11	1.87	0.54
4:BD:5086:GLY:HA2	4:BD:5166:SER:HB2	1.88	0.54
13:BO:5086:ARG:NE	13:BO:5086:ARG:O	2.40	0.54
1:AA:32:TRP:HA	1:AA:32:TRP:HE3	1.72	0.54
1:AA:235:TYR:C	1:AA:237:TYR:H	2.16	0.54
1:AA:289:GLY:HA2	1:AA:292:THR:HG22	1.90	0.54
2:AB:222:PRO:CG	7:AH:27:THR:H	2.20	0.54
3:AC:279:LEU:HD12	3:AC:437:PHE:HE1	1.73	0.54
13:AO:59:ASP:C	13:AO:61:SER:H	2.14	0.54
2:BB:5068:ARG:NH1	24:BB:5608:CLA:HED1	2.22	0.54
2:BB:5222:PRO:HD2	2:BB:5225:LEU:HD12	1.88	0.54
24:BB:5617:CLA:H203	31:BD:5409:LMG:H401	1.88	0.54
8:BI:5010:ILE:HG21	32:BI:5102:LMT:H82	1.88	0.54
20:BZ:5012:LEU:HD12	20:BZ:5012:LEU:O	2.08	0.54
24:AB:609:CLA:OBD	7:AH:27:THR:HB	2.06	0.54
1:BA:5099:ALA:O	8:BI:5001:MET:HE3	2.07	0.54
24:BB:5615:CLA:C5	24:BB:5618:CLA:HBC2	2.38	0.54
3:BC:5223:TRP:CG	3:BC:5224:ILE:H	2.26	0.54
3:BC:5279:LEU:HD22	24:BC:5503:CLA:H143	1.89	0.54
4:BD:5330:ALA:HB3	4:BD:5331:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BU:5064:ALA:O	15:BU:5067:GLN:HG2	2.06	0.54
20:BZ:5023:VAL:O	20:BZ:5026:ALA:HB3	2.08	0.54
24:AB:610:CLA:HHC	24:AB:610:CLA:HBB1	1.89	0.54
4:AD:14:TRP:NE1	7:AH:25:TRP:HH2	1.93	0.54
7:AH:55:LEU:HB2	7:AH:58:VAL:HG12	1.88	0.54
13:AO:117:GLY:O	13:AO:159:VAL:HG12	2.07	0.54
13:AO:154:SER:O	13:AO:168:PHE:HA	2.07	0.54
1:BA:5069:GLY:HA2	1:BA:5075:ASN:ND2	2.22	0.54
2:BB:5183:PRO:HB2	2:BB:5185:TRP:CH2	2.42	0.54
5:BE:5034:GLY:CA	6:BF:5032:PHE:CE1	2.90	0.54
16:BV:5102:MET:HE2	16:BV:5138:LEU:HD22	1.89	0.54
17:By:5022:LEU:HA	17:By:5025:ILE:HD13	1.90	0.54
1:AA:261:GLN:NE2	2:AB:489:GLU:HG3	2.22	0.54
2:AB:27:THR:HG22	2:AB:107:LEU:CD1	2.28	0.54
2:AB:103:LEU:HD21	24:AB:605:CLA:HMC2	1.90	0.54
24:AB:603:CLA:H161	7:AH:38:PHE:CE2	2.43	0.54
3:AC:126:GLY:O	3:AC:130:VAL:HG23	2.07	0.54
3:AC:281:MET:O	3:AC:285:ILE:HG13	2.07	0.54
4:AD:128:ARG:HG2	4:AD:129:GLN:N	2.22	0.54
4:AD:152:VAL:HG11	24:AD:401:CLA:H11	1.88	0.54
1:BA:5193:LEU:HD11	24:BA:5405:CLA:HMC2	1.90	0.54
2:BB:5018:ARG:HD3	2:BB:5118:TRP:HB3	1.89	0.54
27:BD:5407:BCR:H321	27:BD:5407:BCR:H343	1.89	0.54
31:BD:5410:LMG:H192	31:BL:5101:LMG:H201	1.89	0.54
13:BO:5180:ALA:HB1	13:BO:5191:ALA:HB2	1.90	0.54
14:BT:5025:GLU:O	14:BT:5026:PRO:C	2.50	0.54
20:BZ:5029:SER:C	20:BZ:5031:GLN:H	2.16	0.54
28:AA:411:DGD:O1B	28:AA:411:DGD:HG12	2.07	0.54
24:AB:614:CLA:H202	31:AB:620:LMG:H422	1.90	0.54
12:AM:33:GLN:HA	31:AM:101:LMG:HC62	1.90	0.54
15:AU:72:TYR:O	15:AU:73:PRO:C	2.48	0.54
20:AZ:33:TRP:O	20:AZ:33:TRP:HD1	1.90	0.54
2:BB:5058:GLN:O	24:BB:5611:CLA:HED3	2.07	0.54
4:BD:5185:PHE:CE2	4:BD:5289:LEU:HD12	2.42	0.54
2:AB:12:LEU:CD1	2:AB:19:LEU:HD12	2.38	0.54
2:AB:26:HIS:CE1	24:AB:612:CLA:HMA2	2.43	0.54
24:AC:511:CLA:H143	17:Ay:35:ILE:HD13	1.90	0.54
1:BA:5064:ARG:HH11	1:BA:5064:ARG:HG3	1.71	0.54
1:BA:5240:GLY:HA3	14:BT:5029:ILE:HG22	1.88	0.54
1:BA:5315:ASN:ND2	4:BD:5332:GLN:NE2	2.56	0.54
2:BB:5293:ALA:C	2:BB:5295:GLY:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5042:LEU:CD2	24:BC:5511:CLA:HED3	2.37	0.54
35:BD:5406:PL9:H401	11:BL:5029:LEU:HD23	1.90	0.54
24:AA:405:CLA:H93	34:AD:402:PHO:HHB	1.89	0.54
2:AB:237:VAL:HG22	24:AB:610:CLA:HBC2	1.88	0.54
3:AC:166:ILE:HG23	3:AC:245:ILE:HG23	1.90	0.54
35:AD:405:PL9:H401	11:AL:29:LEU:HD23	1.90	0.54
11:AL:18:TYR:CE2	14:AT:20:ALA:HA	2.43	0.54
1:BA:5013:LEU:N	1:BA:5016:ARG:HH11	2.06	0.54
1:BA:5081:ALA:CB	1:BA:5175:GLY:HA3	2.37	0.54
24:BA:5406:CLA:C9	34:BD:5403:PHO:HHB	2.37	0.54
2:BB:5011:VAL:HG23	11:BL:5006:ASN:O	2.07	0.54
3:BC:5155:ASN:CA	3:BC:5158:THR:HG22	2.36	0.54
3:BC:5311:GLN:OE1	3:BC:5355:THR:HG22	2.08	0.54
4:BD:5259:ILE:HG12	31:BD:5410:LMG:H301	1.89	0.54
4:BD:5335:PRO:HB2	5:BE:5065:LEU:HD21	1.89	0.54
6:BF:5011:VAL:HG12	6:BF:5012:SER:N	2.23	0.54
1:AA:12:ASN:HD22	1:AA:15:GLU:HB2	1.73	0.54
2:AB:393:GLU:HG2	15:AU:44:ASP:O	2.08	0.54
4:AD:23:LYS:HZ2	4:AD:32:TRP:CD1	2.25	0.54
5:AE:76:VAL:O	5:AE:80:LEU:CD2	2.56	0.54
1:BA:5012:ASN:ND2	1:BA:5015:GLU:HB2	2.22	0.54
1:BA:5119:PHE:HZ	24:BA:5405:CLA:H101	1.72	0.54
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG1	2.41	0.54
2:BB:5246:PHE:CE2	2:BB:5463:PHE:HA	2.43	0.54
3:BC:5223:TRP:CE3	3:BC:5224:ILE:HG13	2.43	0.54
16:BV:5071:ILE:HD12	16:BV:5071:ILE:C	2.33	0.54
1:AA:64:ARG:HH11	1:AA:64:ARG:HG3	1.73	0.54
1:AA:275:LEU:HD13	25:AA:408:MST:H83	1.89	0.54
2:AB:265:ILE:HG13	2:AB:266:GLU:N	2.21	0.54
3:AC:259:TRP:H	3:AC:259:TRP:HD1	1.56	0.54
10:AK:43:VAL:HG21	10:AK:46:ARG:HE	1.72	0.54
1:BA:5260:PHE:CZ	1:BA:5263:ALA:HB2	2.43	0.54
1:BA:5340:PRO:HG2	3:BC:5317:PHE:CZ	2.43	0.54
2:BB:5331:ASN:HB3	2:BB:5437:LEU:HD22	1.88	0.54
2:BB:5356:VAL:HA	2:BB:5370:LEU:HD22	1.90	0.54
3:BC:5472:LEU:HG	4:BD:5251:ARG:HH12	1.72	0.54
4:BD:5238:THR:O	4:BD:5239:GLN:O	2.26	0.54
12:BM:5023:ILE:HG12	31:BM:5102:LMG:H212	1.90	0.54
16:BV:5104:ASN:HA	16:BV:5122:ARG:HD3	1.90	0.54
18:BX:5022:GLY:HA2	18:BX:5025:SER:OG	2.08	0.54
1:AA:81:ALA:CB	1:AA:175:GLY:HA3	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:192:PRO:HD2	7:AH:60:VAL:HG12	1.91	0.53
15:AU:50:ALA:HB1	15:AU:113:THR:HG21	1.90	0.53
15:AU:113:THR:O	15:AU:114:VAL:HG23	2.08	0.53
16:AV:38:LEU:HD12	16:AV:95:ILE:HB	1.89	0.53
1:BA:5126:TYR:O	1:BA:5130:GLN:HG3	2.07	0.53
1:BA:5244:GLU:OE2	4:BD:5264:LYS:NZ	2.41	0.53
2:BB:5135:LEU:HA	2:BB:5138:MET:HE3	1.89	0.53
2:BB:5462:PHE:HA	24:BB:5615:CLA:HMC2	1.88	0.53
17:By:5024:MET:O	17:By:5027:MET:HG3	2.08	0.53
1:AA:262:TYR:HE1	31:AA:414:LMG:HC5	1.72	0.53
2:AB:157:HIS:HD2	2:AB:158:LEU:HD23	1.73	0.53
3:AC:163:PHE:O	3:AC:167:VAL:HG23	2.09	0.53
3:AC:170:ILE:HG22	3:AC:174:LEU:HD23	1.91	0.53
10:AK:19:ASP:N	10:AK:20:PRO:CD	2.70	0.53
2:BB:5250:PHE:CE2	2:BB:5459:ALA:HB1	2.43	0.53
24:BB:5609:CLA:H141	24:BB:5614:CLA:HED2	1.88	0.53
24:BB:5612:CLA:H203	24:BD:5405:CLA:HBA2	1.89	0.53
16:BV:5146:LEU:O	16:BV:5150:LYS:HG3	2.08	0.53
1:AA:119:PHE:HZ	24:AA:404:CLA:H101	1.74	0.53
1:AA:315:ASN:HD21	4:AD:332:GLN:NE2	2.05	0.53
9:AJ:19:MET:O	9:AJ:23:VAL:HG23	2.07	0.53
1:BA:5159:LEU:C	1:BA:5162:PRO:HD2	2.34	0.53
1:BA:5332:HIS:HB3	4:BD:5321:LEU:HD21	1.90	0.53
3:BC:5044:ASN:O	3:BC:5045:LEU:HD12	2.08	0.53
3:BC:5155:ASN:HA	3:BC:5158:THR:CG2	2.34	0.53
4:BD:5068:LEU:HD11	5:BE:5044:TYR:CE1	2.43	0.53
4:BD:5308:ASP:C	4:BD:5308:ASP:OD1	2.49	0.53
9:BJ:5011:TRP:CE2	9:BJ:5012:ILE:HG13	2.42	0.53
13:BO:5116:ASP:OD2	13:BO:5116:ASP:C	2.50	0.53
1:AA:92:HIS:HD2	3:AC:219:GLY:HA3	1.72	0.53
3:AC:311:GLN:OE1	3:AC:355:THR:HG22	2.08	0.53
3:AC:415:ASN:O	3:AC:416:SER:CB	2.55	0.53
4:AD:26:ARG:HG3	4:AD:26:ARG:HH11	1.72	0.53
4:AD:86:GLY:CA	4:AD:166:SER:HB2	2.38	0.53
24:BA:5406:CLA:H201	14:BT:5014:ILE:HD11	1.90	0.53
24:BB:5612:CLA:H171	24:BD:5405:CLA:HMA2	1.89	0.53
20:BZ:5049:ALA:O	20:BZ:5053:VAL:HG23	2.07	0.53
2:AB:348:ASN:OD1	2:AB:352:GLU:HB2	2.08	0.53
24:AB:608:CLA:H202	7:AH:43:LEU:HD11	1.90	0.53
3:AC:124:VAL:HB	27:AC:515:BCR:H362	1.89	0.53
4:AD:337:GLU:O	4:AD:338:ASN:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AD:408:LMG:H392	27:AT:101:BCR:HC32	1.91	0.53
13:AO:98:THR:HG23	13:AO:133:THR:HB	1.89	0.53
15:AU:64:ALA:O	15:AU:67:GLN:HG2	2.08	0.53
17:Ay:34:MET:HE2	17:Ay:37:PHE:CD2	2.44	0.53
18:AX:12:ILE:O	18:AX:12:ILE:HG23	2.09	0.53
1:BA:5190:HIS:O	1:BA:5298:ASN:HB3	2.09	0.53
1:BA:5324:ALA:HB2	4:BD:5329:MET:SD	2.49	0.53
2:BB:5327:THR:O	2:BB:5444:ARG:NE	2.39	0.53
24:BC:5504:CLA:H2	28:BC:5518:DGD:HA21	1.89	0.53
4:BD:5088:SER:CB	5:BE:5069:ARG:NH2	2.69	0.53
5:BE:5010:PHE:HD2	31:BE:5101:LMG:O2	1.92	0.53
1:AA:193:LEU:HD11	24:AA:404:CLA:HMC2	1.91	0.53
3:AC:33:PHE:CD1	4:AD:229:ALA:HB3	2.43	0.53
2:BB:5133:LEU:CB	2:BB:5138:MET:HE1	2.36	0.53
11:BL:5022:LEU:HG	31:BL:5101:LMG:H191	1.89	0.53
11:BL:5022:LEU:O	11:BL:5026:VAL:HG22	2.08	0.53
1:AA:190:HIS:CB	1:AA:293:MET:HE2	2.32	0.53
3:AC:279:LEU:HD22	24:AC:503:CLA:H143	1.90	0.53
3:AC:405:ASN:HB2	28:AC:519:DGD:C3G	2.38	0.53
3:AC:432:VAL:HG13	3:AC:433:LEU:N	2.23	0.53
4:AD:160:TYR:HB3	4:AD:161:PRO:CD	2.39	0.53
27:AD:406:BCR:H343	27:AD:406:BCR:H321	1.91	0.53
7:AH:11:LEU:C	7:AH:13:PRO:HD2	2.34	0.53
8:AI:1:MET:CE	32:BB:5604:LMT:H41	2.39	0.53
13:AO:144:LEU:HD13	13:AO:259:VAL:HG11	1.90	0.53
1:BA:5155:PHE:CE1	28:BA:5412:DGD:HBE1	2.44	0.53
1:BA:5254:TYR:CD1	4:BD:5132:ILE:HG22	2.43	0.53
2:BB:5030:VAL:HG12	24:BB:5609:CLA:HHD	1.91	0.53
2:BB:5087:ASP:OD1	28:BB:5602:DGD:HD62	2.08	0.53
2:BB:5363:PHE:HD1	4:BD:5326:ARG:HD2	1.74	0.53
3:BC:5149:TYR:CA	3:BC:5156:LYS:HD3	2.38	0.53
3:BC:5368:PRO:O	3:BC:5379:LYS:HE2	2.08	0.53
4:BD:5037:LEU:HD13	4:BD:5125:PHE:N	2.24	0.53
16:BV:5074:THR:O	16:BV:5075:ASN:HB2	2.08	0.53
1:AA:307:ILE:HG22	1:AA:313:VAL:HA	1.89	0.53
1:AA:332:HIS:HB3	4:AD:321:LEU:HD21	1.91	0.53
2:AB:154:GLY:O	2:AB:159:THR:HG23	2.08	0.53
2:AB:183:PRO:HG3	2:AB:199:VAL:HG12	1.90	0.53
2:AB:183:PRO:HB2	2:AB:185:TRP:CH2	2.44	0.53
24:AB:616:CLA:H51	30:BA:5401:SQD:H302	1.90	0.53
13:AO:118:SER:HB3	13:AO:157:PRO:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:218:LEU:CD2	15:AU:119:THR:HG21	2.39	0.53
20:AZ:12:LEU:O	20:AZ:12:LEU:HD12	2.08	0.53
1:BA:5333:GLU:HB2	1:BA:5337:HIS:HE1	1.74	0.53
2:BB:5062:VAL:CG1	24:BB:5609:CLA:HED3	2.39	0.53
3:BC:5387:TRP:CE2	3:BC:5388:GLN:HG3	2.44	0.53
1:AA:220:THR:HG23	4:AD:141:TYR:HD1	1.73	0.53
1:AA:234:ASN:HB2	31:AB:620:LMG:O3	2.09	0.53
1:AA:289:GLY:O	1:AA:292:THR:CG2	2.53	0.53
2:AB:68:ARG:HH22	24:AB:604:CLA:CED	2.21	0.53
24:AC:504:CLA:H151	28:AC:519:DGD:C9A	2.36	0.53
4:AD:313:THR:OG1	4:AD:315:TYR:HB3	2.09	0.53
10:AK:35:LEU:HA	10:AK:38:VAL:HG23	1.89	0.53
17:Ay:24:MET:O	17:Ay:28:ILE:HG23	2.09	0.53
4:BD:5076:VAL:O	4:BD:5077:ALA:HB2	2.09	0.53
2:AB:91:TRP:CD1	24:AB:606:CLA:HBD	2.43	0.53
2:AB:135:LEU:HD13	2:AB:237:VAL:CG2	2.39	0.53
2:AB:172:TYR:O	2:AB:173:GLY:C	2.52	0.53
2:AB:225:LEU:HD23	32:AB:624:LMT:H42	1.91	0.53
3:AC:399:ALA:HB3	33:AV:202:DMS:H11	1.90	0.53
12:AM:20:VAL:O	12:AM:24:ILE:HG13	2.07	0.53
20:AZ:21:ILE:O	20:AZ:25:VAL:HG22	2.09	0.53
20:AZ:47:TRP:O	20:AZ:50:LEU:HB2	2.09	0.53
1:BA:5142:TRP:HB2	4:BD:5220:ASN:OD1	2.09	0.53
24:BA:5406:CLA:H102	24:BA:5406:CLA:H152	1.91	0.53
3:BC:5166:ILE:HG23	3:BC:5245:ILE:HG23	1.91	0.53
3:BC:5233:VAL:HA	27:BC:5516:BCR:C28	2.38	0.53
4:BD:5134:ARG:HE	4:BD:5134:ARG:CA	2.21	0.53
5:BE:5008:ARG:HD3	5:BE:5013:ILE:HG12	1.91	0.53
5:BE:5017:VAL:HG22	9:BJ:5008:ILE:CD1	2.38	0.53
24:AA:405:CLA:C9	34:AD:402:PHO:HHB	2.39	0.52
4:AD:239:GLN:O	4:AD:240:ALA:CB	2.56	0.52
2:BB:5005:TRP:CH2	31:BL:5101:LMG:H291	2.44	0.52
24:BB:5614:CLA:HHC	24:BB:5614:CLA:HBB1	1.89	0.52
3:BC:5137:PRO:HB2	3:BC:5139:THR:O	2.09	0.52
4:BD:5209:LEU:HD23	4:BD:5209:LEU:C	2.34	0.52
6:BF:5041:GLN:N	6:BF:5041:GLN:HE21	2.07	0.52
20:BZ:5035:ARG:O	20:BZ:5038:GLN:HB3	2.09	0.52
1:AA:234:ASN:HD21	4:AD:266:TRP:CB	2.21	0.52
24:AA:405:CLA:H102	24:AA:405:CLA:H152	1.91	0.52
2:AB:246:PHE:CE2	2:AB:463:PHE:HA	2.44	0.52
24:AB:608:CLA:H171	24:AD:404:CLA:HMA2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AB:622:SQD:H152	32:AB:624:LMT:H81	1.90	0.52
3:AC:141:GLU:CD	3:AC:141:GLU:H	2.16	0.52
4:AD:238:THR:O	4:AD:239:GLN:O	2.28	0.52
20:AZ:34:ASP:OD1	20:AZ:35:ARG:N	2.42	0.52
1:BA:5202:VAL:HG11	24:BA:5407:CLA:OBD	2.10	0.52
1:BA:5254:TYR:OH	4:BD:5129:GLN:HB3	2.09	0.52
3:BC:5113:VAL:CG1	31:BC:5521:LMG:H132	2.40	0.52
3:BC:5126:GLY:O	3:BC:5130:VAL:HG23	2.09	0.52
3:BC:5279:LEU:HD23	3:BC:5282:MET:CE	2.39	0.52
3:BC:5337:LEU:HD12	13:BO:5131:PRO:CG	2.39	0.52
20:BZ:5002:THR:CG2	20:BZ:5003:ILE:N	2.72	0.52
1:AA:215:HIS:O	1:AA:216:GLY:C	2.53	0.52
24:AB:611:CLA:H51	24:AB:614:CLA:HBC2	1.92	0.52
3:AC:33:PHE:HE1	4:AD:229:ALA:CB	2.21	0.52
3:AC:149:TYR:HA	3:AC:156:LYS:CD	2.40	0.52
3:AC:259:TRP:CD1	3:AC:259:TRP:N	2.78	0.52
24:AC:504:CLA:H61	28:AC:518:DGD:HA61	1.89	0.52
24:AC:504:CLA:H152	28:AC:519:DGD:HA91	1.90	0.52
16:AV:56:LYS:O	16:AV:60:GLN:HG3	2.09	0.52
16:AV:90:PRO:O	16:AV:92:ARG:HD3	2.10	0.52
1:BA:5035:VAL:HA	27:BA:5411:BCR:H333	1.90	0.52
2:BB:5026:HIS:CE1	24:BB:5616:CLA:HMA2	2.44	0.52
2:BB:5030:VAL:HG22	24:BB:5617:CLA:C3C	2.39	0.52
2:BB:5143:LEU:HD12	2:BB:5143:LEU:O	2.10	0.52
2:BB:5324:LEU:HA	4:BD:5293:LEU:HD21	1.91	0.52
24:BB:5613:CLA:OBD	7:BH:5027:THR:HB	2.10	0.52
4:BD:5096:GLU:H	4:BD:5096:GLU:CD	2.17	0.52
13:BO:5144:LEU:HD13	13:BO:5259:VAL:HG11	1.90	0.52
31:AA:414:LMG:O2	5:AE:10:PHE:HD2	1.92	0.52
2:AB:62:VAL:CG1	24:AB:605:CLA:HED3	2.39	0.52
4:AD:334:GLN:N	4:AD:335:PRO:HD3	2.25	0.52
16:AV:133:LEU:HD12	16:AV:133:LEU:N	2.24	0.52
20:AZ:32:ASP:C	20:AZ:34:ASP:H	2.17	0.52
13:BO:5210:ARG:HA	15:BU:5039:LEU:CD1	2.40	0.52
15:BU:5054:LYS:HD2	15:BU:5113:THR:HG23	1.90	0.52
16:BV:5081:ARG:HG2	16:BV:5081:ARG:HH11	1.73	0.52
1:AA:29:TYR:CD2	1:AA:133:LEU:HD13	2.45	0.52
1:AA:155:PHE:CE1	28:AA:411:DGD:HBE1	2.44	0.52
2:AB:25:MET:HE3	27:AB:617:BCR:H23C	1.92	0.52
24:AB:615:CLA:H142	24:AB:616:CLA:H151	1.91	0.52
3:AC:220:GLY:N	28:AC:517:DGD:O3D	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:452:ALA:O	3:AC:454:GLY:N	2.42	0.52
10:AK:17:ILE:HD12	10:AK:17:ILE:N	2.23	0.52
12:AM:27:VAL:HG12	12:BM:5028:GLN:HB3	1.90	0.52
16:AV:119:PRO:HA	16:AV:127:PHE:CD2	2.44	0.52
1:BA:5220:THR:CG2	4:BD:5141:TYR:HD1	2.23	0.52
2:BB:5010:THR:HG22	2:BB:5013:ILE:HD11	1.92	0.52
2:BB:5090:PHE:CE2	2:BB:5091:TRP:CZ3	2.97	0.52
2:BB:5157:HIS:HD2	2:BB:5158:LEU:HD23	1.75	0.52
24:BB:5612:CLA:C4	4:BD:5127:LEU:HD11	2.20	0.52
3:BC:5279:LEU:HA	3:BC:5282:MET:HE3	1.91	0.52
17:By:5030:ILE:HG22	17:By:5030:ILE:O	2.10	0.52
1:AA:10:SER:C	1:AA:12:ASN:H	2.16	0.52
2:AB:331:ASN:HB3	2:AB:437:LEU:HD22	1.92	0.52
31:AB:620:LMG:H201	31:AD:408:LMG:H192	1.90	0.52
11:AL:22:LEU:O	11:AL:26:VAL:HG22	2.10	0.52
13:AO:215:ARG:NH1	13:AO:252:GLY:O	2.43	0.52
1:BA:5183:MET:HE1	24:BA:5406:CLA:HMD3	1.92	0.52
3:BC:5140:LEU:HB2	3:BC:5148:GLY:HA2	1.91	0.52
17:By:5023:THR:HG23	17:By:5024:MET:N	2.25	0.52
20:BZ:5002:THR:CG2	20:BZ:5003:ILE:H	2.22	0.52
3:AC:140:LEU:HB2	3:AC:148:GLY:HA2	1.92	0.52
3:AC:279:LEU:HD23	3:AC:282:MET:CE	2.39	0.52
3:AC:466:VAL:CA	3:AC:469:MET:HE3	2.38	0.52
4:AD:96:GLU:CD	4:AD:96:GLU:H	2.18	0.52
20:AZ:32:ASP:OD1	20:AZ:36:SER:HB2	2.10	0.52
1:BA:5289:GLY:CA	1:BA:5292:THR:HG22	2.38	0.52
3:BC:5418:ASN:HA	28:BC:5519:DGD:HE2	1.91	0.52
4:BD:5128:ARG:HG2	4:BD:5129:GLN:N	2.24	0.52
31:BL:5101:LMG:H302	12:BM:5022:LEU:HD21	1.91	0.52
17:By:5045:ASN:CB	20:BZ:5028:ALA:O	2.55	0.52
1:AA:193:LEU:HD13	4:AD:179:PHE:HB3	1.91	0.52
2:AB:30:VAL:HG22	24:AB:613:CLA:C3C	2.40	0.52
2:AB:354:LEU:HD21	2:AB:378:LYS:HB2	1.90	0.52
2:AB:356:VAL:HG22	2:AB:370:LEU:CD2	2.40	0.52
24:AB:601:CLA:HBB1	24:AB:601:CLA:HHC	1.91	0.52
3:AC:223:TRP:CG	3:AC:224:ILE:H	2.26	0.52
4:AD:236:ASN:ND2	4:AD:239:GLN:O	2.37	0.52
5:AE:9:PRO:O	5:AE:10:PHE:C	2.53	0.52
7:AH:17:GLU:H	7:AH:17:GLU:CD	2.16	0.52
13:AO:46:PRO:HD2	13:AO:266:TYR:HD2	1.74	0.52
13:AO:91:PHE:CE1	13:AO:260:LYS:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:180:ALA:HB1	13:AO:191:ALA:HB2	1.92	0.52
20:AZ:32:ASP:CG	20:AZ:33:TRP:N	2.68	0.52
1:BA:5093:PHE:CZ	24:BA:5408:CLA:HBA1	2.45	0.52
3:BC:5149:TYR:CB	3:BC:5156:LYS:HD3	2.40	0.52
4:BD:5154:VAL:O	4:BD:5158:LEU:HB2	2.10	0.52
13:BO:5223:ILE:HG12	13:BO:5224:SER:N	2.25	0.52
17:By:5039:LEU:HD21	20:BZ:5028:ALA:CB	2.40	0.52
20:BZ:5042:LEU:O	20:BZ:5046:LEU:HB2	2.10	0.52
1:AA:176:ILE:HG22	1:AA:180:PHE:HE2	1.73	0.52
1:AA:216:GLY:O	1:AA:220:THR:HG22	2.10	0.52
3:AC:149:TYR:CB	3:AC:156:LYS:HD3	2.40	0.52
3:AC:252:ILE:HG22	3:AC:253:LEU:HD23	1.91	0.52
4:AD:88:SER:CB	5:AE:69:ARG:NH2	2.69	0.52
4:AD:158:LEU:O	4:AD:162:LEU:HG	2.09	0.52
5:AE:8:ARG:HD3	5:AE:13:ILE:HG12	1.92	0.52
5:AE:17:VAL:HG22	9:AJ:8:ILE:HD11	1.92	0.52
5:AE:26:THR:HB	36:AF:101:HEM:CAB	2.40	0.52
7:AH:12:ARG:N	7:AH:13:PRO:HD2	2.25	0.52
1:BA:5064:ARG:HG3	1:BA:5064:ARG:NH1	2.25	0.52
1:BA:5315:ASN:ND2	4:BD:5332:GLN:HE22	2.06	0.52
25:BA:5409:MST:N3	25:BA:5409:MST:H122	2.24	0.52
3:BC:5037:ALA:O	24:BC:5508:CLA:HBA1	2.10	0.52
3:BC:5362:ARG:HE	3:BC:5370:ARG:NH1	2.07	0.52
4:BD:5072:ASN:HA	31:BD:5408:LMG:HC72	1.92	0.52
7:BH:5025:TRP:O	7:BH:5026:GLY:C	2.53	0.52
2:AB:135:LEU:HA	2:AB:138:MET:HE3	1.91	0.52
2:AB:369:ILE:O	2:AB:370:LEU:HD23	2.09	0.52
27:AT:101:BCR:H19C	27:BB:5622:BCR:H363	1.91	0.52
17:Ay:22:LEU:HA	17:Ay:25:ILE:CD1	2.25	0.52
17:Ay:28:ILE:O	17:Ay:28:ILE:HD12	2.11	0.52
1:BA:5027:ARG:NH1	1:BA:5027:ARG:O	2.43	0.52
2:BB:5091:TRP:CD1	24:BB:5610:CLA:HBD	2.45	0.52
2:BB:5461:LEU:HD21	31:BB:5624:LMG:C43	2.39	0.52
3:BC:5214:LEU:HD22	3:BC:5214:LEU:N	2.24	0.52
4:BD:5026:ARG:HH11	4:BD:5026:ARG:HG3	1.75	0.52
4:BD:5201:VAL:O	4:BD:5205:LEU:HB2	2.09	0.52
4:BD:5201:VAL:HB	24:BD:5402:CLA:HMB2	1.91	0.52
13:BO:5230:VAL:CG1	13:BO:5231:ASP:H	2.17	0.52
20:BZ:5032:ASP:C	20:BZ:5034:ASP:H	2.17	0.52
1:AA:159:LEU:C	1:AA:162:PRO:HD2	2.35	0.51
1:AA:315:ASN:ND2	4:AD:332:GLN:NE2	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:11:VAL:CG1	6:AF:12:SER:H	2.20	0.51
13:AO:84:ASN:ND2	2:BB:5431:GLU:OE2	2.43	0.51
1:BA:5082:VAL:HB	1:BA:5174:LEU:HB2	1.91	0.51
1:BA:5159:LEU:HD11	28:BC:5517:DGD:HB51	1.92	0.51
2:BB:5121:GLU:HG3	7:BH:5004:ARG:CA	2.39	0.51
2:BB:5192:PRO:HD2	7:BH:5060:VAL:HG12	1.93	0.51
28:BC:5519:DGD:HE62	9:BJ:5040:LEU:HD11	1.93	0.51
4:BD:5274:VAL:HA	35:BD:5406:PL9:C25	2.34	0.51
4:BD:5350:ASN:O	4:BD:5352:LEU:N	2.42	0.51
15:BU:5072:TYR:O	15:BU:5073:PRO:C	2.51	0.51
20:BZ:5031:GLN:O	20:BZ:5032:ASP:HB3	2.11	0.51
1:AA:283:VAL:HG21	34:AD:402:PHO:HBC3	1.91	0.51
4:AD:35:ILE:O	24:AD:404:CLA:HBB2	2.11	0.51
4:AD:77:ALA:HB2	4:AD:174:GLY:HA3	1.91	0.51
4:AD:92:LEU:HA	4:AD:104:TRP:CD1	2.45	0.51
17:Ay:24:MET:O	17:Ay:27:MET:HG3	2.09	0.51
20:AZ:42:LEU:O	20:AZ:46:LEU:HB2	2.09	0.51
1:BA:5011:ALA:O	1:BA:5012:ASN:CB	2.58	0.51
1:BA:5288:LEU:HD13	3:BC:5432:VAL:CG2	2.37	0.51
2:BB:5369:ILE:C	2:BB:5370:LEU:HD23	2.35	0.51
3:BC:5342:MET:HE1	3:BC:5356:MET:HE2	1.92	0.51
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CE2	2.46	0.51
4:BD:5188:PHE:CZ	4:BD:5326:ARG:HG2	2.46	0.51
10:BK:5020:PRO:O	10:BK:5023:ASP:HB2	2.11	0.51
27:BK:5102:BCR:H331	27:BK:5102:BCR:HC8	1.92	0.51
11:BL:5008:GLN:HB3	11:BL:5009:PRO:HD2	1.93	0.51
12:BM:5020:VAL:O	12:BM:5024:ILE:HG13	2.11	0.51
13:BO:5046:PRO:HD2	13:BO:5266:TYR:HD2	1.75	0.51
13:BO:5180:ALA:HB2	15:BU:5120:ALA:O	2.09	0.51
1:AA:38:ILE:HG23	30:AA:416:SQD:H131	1.93	0.51
1:AA:93:PHE:CZ	24:AA:407:CLA:HBA1	2.44	0.51
2:AB:10:THR:HG22	2:AB:13:ILE:HD11	1.92	0.51
2:AB:58:GLN:O	24:AB:607:CLA:HED3	2.10	0.51
3:AC:297:TYR:HA	3:AC:302:TYR:CE2	2.46	0.51
3:AC:415:ASN:HB3	9:AJ:39:SER:OG	2.08	0.51
9:AJ:15:THR:O	9:AJ:19:MET:HG3	2.09	0.51
20:AZ:29:SER:C	20:AZ:31:GLN:H	2.17	0.51
2:BB:5012:LEU:CD1	2:BB:5019:LEU:HD12	2.40	0.51
2:BB:5135:LEU:HD13	2:BB:5237:VAL:CG2	2.41	0.51
3:BC:5163:PHE:O	3:BC:5167:VAL:HG23	2.09	0.51
3:BC:5259:TRP:CD1	3:BC:5259:TRP:N	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5259:ILE:HD13	14:BT:5021:ILE:HG12	1.93	0.51
24:BD:5405:CLA:H42	18:BX:5023:LEU:HA	1.92	0.51
9:BJ:5019:MET:O	9:BJ:5023:VAL:HG23	2.10	0.51
3:AC:377:LEU:O	3:AC:381:LYS:HB2	2.10	0.51
4:AD:161:PRO:HB3	4:AD:170:ALA:HB2	1.93	0.51
7:AH:25:TRP:O	7:AH:26:GLY:C	2.53	0.51
24:BB:5607:CLA:H161	7:BH:5038:PHE:CE2	2.45	0.51
3:BC:5204:LEU:HD21	3:BC:5238:ILE:HG21	1.92	0.51
24:BC:5504:CLA:H61	28:BC:5518:DGD:HA61	1.92	0.51
4:BD:5334:GLN:N	4:BD:5335:PRO:HD3	2.24	0.51
15:BU:5050:ALA:HB1	15:BU:5113:THR:HG21	1.93	0.51
16:BV:5058:LEU:HD13	16:BV:5137:ASP:HB3	1.92	0.51
1:AA:64:ARG:HD3	1:AA:64:ARG:H	1.75	0.51
1:AA:83:VAL:HG22	4:AD:314:PHE:CE2	2.41	0.51
1:AA:210:LEU:HD23	1:AA:210:LEU:C	2.36	0.51
2:AB:461:LEU:HD21	31:AB:621:LMG:C43	2.41	0.51
2:AB:489:GLU:C	2:AB:490:GLN:HG3	2.36	0.51
3:AC:453:ALA:HA	8:AI:34:ARG:O	2.10	0.51
5:AE:8:ARG:HB2	6:AF:13:TYR:CB	2.41	0.51
6:AF:23:VAL:O	6:AF:27:ALA:CB	2.59	0.51
7:AH:13:PRO:HG2	7:AH:14:LEU:H	1.75	0.51
1:BA:5129:ARG:NH2	4:BD:5256:ILE:HA	2.26	0.51
28:BA:5412:DGD:O1B	28:BA:5412:DGD:HG12	2.11	0.51
24:BB:5619:CLA:H142	24:BB:5620:CLA:H151	1.92	0.51
3:BC:5458:GLY:HA2	4:BD:5222:LEU:O	2.11	0.51
4:BD:5266:TRP:HE1	31:BD:5410:LMG:HC72	1.74	0.51
17:By:5020:ALA:C	17:By:5022:LEU:H	2.18	0.51
1:AA:82:VAL:HB	1:AA:174:LEU:HB2	1.92	0.51
2:AB:229:LEU:O	2:AB:231:MET:N	2.43	0.51
3:AC:158:THR:HG21	3:AC:254:THR:O	2.09	0.51
4:AD:302:GLU:HA	4:AD:302:GLU:OE2	2.11	0.51
5:BE:5072:ALA:O	5:BE:5076:VAL:HG23	2.10	0.51
1:AA:214:MET:O	1:AA:215:HIS:C	2.54	0.51
2:AB:173:GLY:CA	2:AB:265:ILE:HD11	2.41	0.51
2:AB:377:VAL:HG11	4:AD:342:PRO:HG2	1.93	0.51
24:AB:611:CLA:H142	31:AB:620:LMG:H371	1.92	0.51
3:AC:321:ASP:OD2	15:AU:129:ASN:HB2	2.11	0.51
2:BB:5187:PRO:HB3	24:BB:5605:CLA:CMB	2.41	0.51
2:BB:5280:PHE:O	2:BB:5284:ILE:HG13	2.10	0.51
2:BB:5315:ILE:HG22	2:BB:5426:PHE:HB3	1.92	0.51
3:BC:5297:TYR:HD1	3:BC:5302:TYR:CE2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5071:LEU:HD23	13:BO:5265:PHE:HB3	1.91	0.51
15:BU:5080:VAL:HG22	15:BU:5127:ARG:HH21	1.76	0.51
18:BX:5024:LEU:O	18:BX:5028:VAL:HG23	2.10	0.51
1:AA:210:LEU:C	1:AA:210:LEU:CD2	2.84	0.51
1:AA:244:GLU:OE2	4:AD:264:LYS:NZ	2.43	0.51
2:AB:356:VAL:HA	2:AB:370:LEU:HD22	1.93	0.51
2:AB:383:PHE:HE1	13:AO:194:TYR:CE2	2.29	0.51
3:AC:37:ALA:O	24:AC:508:CLA:HBA1	2.11	0.51
3:AC:171:GLY:O	3:AC:174:LEU:HB2	2.11	0.51
3:AC:327:ASN:HB3	13:AO:125:ASP:OD1	2.11	0.51
4:AD:86:GLY:HA2	4:AD:166:SER:HB2	1.93	0.51
5:AE:8:ARG:HB2	6:AF:13:TYR:HB3	1.93	0.51
7:AH:55:LEU:HB2	7:AH:58:VAL:CG1	2.41	0.51
11:AL:8:GLN:N	11:AL:8:GLN:HE21	2.08	0.51
20:AZ:2:THR:CG2	20:AZ:3:ILE:H	2.23	0.51
24:BB:5615:CLA:H142	31:BL:5101:LMG:H371	1.92	0.51
32:BB:5627:LMT:H112	7:BH:5035:MET:HE2	1.93	0.51
1:AA:129:ARG:NH2	4:AD:256:ILE:HA	2.26	0.51
2:AB:383:PHE:HE1	13:AO:194:TYR:CD2	2.29	0.51
3:AC:264:PHE:HE1	27:AC:516:BCR:C32	2.24	0.51
31:AC:520:LMG:H292	27:AJ:101:BCR:H363	1.93	0.51
4:AD:134:ARG:HE	4:AD:134:ARG:CA	2.20	0.51
4:AD:209:LEU:HD23	4:AD:209:LEU:C	2.35	0.51
1:BA:5010:SER:C	1:BA:5012:ASN:H	2.19	0.51
1:BA:5261:GLN:CD	2:BB:5489:GLU:HG3	2.36	0.51
2:BB:5015:ASP:N	2:BB:5016:PRO:HD3	2.26	0.51
2:BB:5063:LEU:N	2:BB:5064:PRO:HD2	2.26	0.51
2:BB:5091:TRP:CZ3	24:BB:5610:CLA:O1A	2.64	0.51
2:BB:5225:LEU:HD23	32:BB:5627:LMT:H42	1.92	0.51
2:BB:5251:VAL:O	2:BB:5255:THR:HG23	2.11	0.51
2:BB:5366:PHE:CD1	2:BB:5367:PRO:HD2	2.46	0.51
2:BB:5383:PHE:HE1	13:BO:5194:TYR:CE2	2.29	0.51
3:BC:5028:GLN:HB2	24:BC:5511:CLA:CED	2.41	0.51
3:BC:5094:THR:HG22	3:BC:5298:PRO:HD2	1.93	0.51
4:BD:5218:VAL:HG22	4:BD:5244:TYR:CE2	2.45	0.51
10:BK:5020:PRO:HB2	17:By:5021:GLN:HB2	1.93	0.51
14:BT:5018:PHE:HB2	27:BT:5101:BCR:H10C	1.93	0.51
20:BZ:5034:ASP:OD1	20:BZ:5035:ARG:N	2.44	0.51
1:AA:317:TRP:CD1	4:AD:177:ALA:HB2	2.46	0.51
2:AB:30:VAL:HG12	24:AB:605:CLA:HHD	1.93	0.51
2:AB:243:ALA:HB2	2:AB:466:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:414:PRO:HB2	2:AB:415:PRO:CD	2.35	0.51
3:AC:452:ALA:C	3:AC:454:GLY:N	2.68	0.51
4:AD:53:THR:HG22	4:AD:67:TYR:HE2	1.75	0.51
6:AF:23:VAL:O	6:AF:27:ALA:HB2	2.10	0.51
15:AU:66:ILE:CG1	15:AU:72:TYR:CD1	2.94	0.51
1:BA:5180:PHE:HA	1:BA:5183:MET:HE3	1.92	0.51
3:BC:5288:CYS:HB3	28:BC:5517:DGD:HG2	1.92	0.51
4:BD:5302:GLU:OE2	4:BD:5302:GLU:HA	2.10	0.51
13:BO:5092:VAL:HG12	13:BO:5093:PRO:HD2	1.91	0.51
1:AA:262:TYR:HE1	31:AA:414:LMG:C5	2.24	0.50
2:AB:2:GLY:HA3	11:AL:9:PRO:HG2	1.93	0.50
2:AB:176:GLY:HA3	2:AB:266:GLU:OE1	2.12	0.50
31:AB:620:LMG:HC91	11:AL:19:LEU:CD1	2.41	0.50
3:AC:458:GLY:HA2	4:AD:222:LEU:O	2.10	0.50
4:AD:87:HIS:HB2	28:AH:101:DGD:O2D	2.11	0.50
18:AX:43:ILE:O	18:AX:43:ILE:HG22	2.10	0.50
3:BC:5264:PHE:HE1	27:BC:5516:BCR:C32	2.25	0.50
18:BX:5044:ASP:O	18:BX:5045:LYS:HB3	2.11	0.50
27:AB:618:BCR:H363	27:BT:5101:BCR:H19C	1.92	0.50
5:AE:14:ILE:CG2	9:AJ:13:VAL:HG11	2.41	0.50
31:AM:101:LMG:O2	11:BL:5009:PRO:HB3	2.11	0.50
13:AO:240:THR:HA	13:AO:264:VAL:HA	1.92	0.50
29:BA:5413:LHG:HC11	3:BC:5447:ARG:CZ	2.41	0.50
2:BB:5172:TYR:OH	7:BH:5063:LYS:HE2	2.11	0.50
2:BB:5354:LEU:HD12	2:BB:5354:LEU:N	2.26	0.50
3:BC:5460:ASP:O	3:BC:5461:ARG:C	2.54	0.50
4:BD:5253:TRP:HB2	4:BD:5260:ALA:HB2	1.93	0.50
1:AA:92:HIS:CD2	3:AC:219:GLY:HA3	2.45	0.50
3:AC:321:ASP:OD1	3:AC:321:ASP:N	2.42	0.50
4:AD:37:LEU:HD13	4:AD:125:PHE:N	2.26	0.50
20:AZ:23:VAL:HG12	20:AZ:27:TYR:CE2	2.46	0.50
1:BA:5057:PRO:HD3	1:BA:5073:TYR:CE2	2.47	0.50
2:BB:5103:LEU:HD21	24:BB:5609:CLA:HMC2	1.93	0.50
3:BC:5033:PHE:CD1	4:BD:5229:ALA:HB3	2.45	0.50
24:BC:5505:CLA:H2	24:BC:5505:CLA:HAA1	1.94	0.50
16:BV:5133:LEU:HD12	16:BV:5133:LEU:N	2.24	0.50
1:AA:11:ALA:O	1:AA:12:ASN:CB	2.60	0.50
1:AA:48:PHE:HA	1:AA:115:ILE:HD11	1.92	0.50
1:AA:200:LEU:HD11	28:AC:519:DGD:CCA	2.29	0.50
2:AB:260:SER:HG	2:AB:262:THR:HG22	1.72	0.50
24:AB:612:CLA:H171	24:AB:613:CLA:HBB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:262:ARG:HH21	32:AI:103:LMT:C5'	2.25	0.50
4:AD:76:VAL:O	4:AD:77:ALA:HB2	2.10	0.50
7:AH:50:ASN:HD22	28:AH:101:DGD:HA21	1.76	0.50
8:AI:19:PHE:CZ	8:AI:23:PHE:HE2	2.29	0.50
8:AI:21:PHE:HE1	32:AI:103:LMT:H41	1.75	0.50
10:AK:14:ALA:O	10:AK:17:ILE:HD13	2.10	0.50
13:AO:46:PRO:HD2	13:AO:266:TYR:CD2	2.45	0.50
1:BA:5114:LEU:HD23	1:BA:5114:LEU:C	2.37	0.50
2:BB:5405:GLU:OE1	2:BB:5405:GLU:HA	2.10	0.50
3:BC:5415:ASN:CB	9:BJ:5039:SER:OG	2.60	0.50
11:BL:5019:LEU:CD1	31:BL:5101:LMG:HC91	2.42	0.50
13:BO:5046:PRO:HD2	13:BO:5266:TYR:CD2	2.46	0.50
16:BV:5119:PRO:HA	16:BV:5127:PHE:CD2	2.46	0.50
1:AA:10:SER:C	1:AA:12:ASN:N	2.69	0.50
3:AC:235:GLY:O	3:AC:238:ILE:HB	2.12	0.50
3:AC:326:ALA:HB2	15:AU:128:TYR:CG	2.46	0.50
3:AC:350:ILE:HG21	3:AC:359:TRP:HB2	1.93	0.50
24:AC:501:CLA:CAD	24:AC:503:CLA:H12	2.42	0.50
24:AD:401:CLA:H2	34:AD:403:PHO:HBB1	1.92	0.50
6:AF:19:ARG:O	6:AF:23:VAL:HG23	2.11	0.50
24:BB:5616:CLA:H171	24:BB:5617:CLA:HBB2	1.93	0.50
3:BC:5321:ASP:OD1	3:BC:5321:ASP:N	2.44	0.50
3:BC:5377:LEU:CD2	13:BO:5126:GLY:HA2	2.41	0.50
4:BD:5068:LEU:CA	6:BF:5040:MET:HE2	2.42	0.50
13:BO:5032:THR:O	13:BO:5036:ILE:CD1	2.54	0.50
18:BX:5012:ILE:O	18:BX:5012:ILE:HG13	2.11	0.50
20:BZ:5033:TRP:O	20:BZ:5037:LYS:HB2	2.12	0.50
1:AA:57:PRO:HG3	1:AA:68:SER:CB	2.39	0.50
13:AO:155:THR:HG23	13:AO:168:PHE:CE2	2.47	0.50
16:AV:102:MET:HE2	16:AV:138:LEU:HD22	1.94	0.50
1:BA:5182:PHE:O	1:BA:5186:PHE:HB2	2.12	0.50
1:BA:5234:ASN:HD21	4:BD:5266:TRP:CB	2.23	0.50
1:BA:5235:TYR:C	1:BA:5237:TYR:H	2.20	0.50
2:BB:5377:VAL:HG11	4:BD:5342:PRO:HG2	1.93	0.50
13:BO:5091:PHE:CE1	13:BO:5260:LYS:HB2	2.47	0.50
14:BT:5022:PHE:O	14:BT:5023:PHE:CD2	2.64	0.50
17:By:5028:ILE:O	17:By:5028:ILE:HG13	2.01	0.50
2:AB:5:TRP:CH2	31:AB:620:LMG:H291	2.47	0.50
3:AC:225:VAL:CG2	28:AC:517:DGD:HG11	2.41	0.50
3:AC:368:PRO:O	3:AC:379:LYS:HE2	2.12	0.50
24:AC:501:CLA:HMB3	27:AC:516:BCR:C40	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:190:ASN:HB2	4:AD:296:TYR:CE1	2.47	0.50
7:AH:11:LEU:HA	7:AH:14:LEU:HD12	1.93	0.50
10:AK:43:VAL:CG2	10:AK:46:ARG:HE	2.24	0.50
27:AK:102:BCR:HC8	27:AK:102:BCR:H331	1.93	0.50
13:AO:223:ILE:HG12	13:AO:224:SER:N	2.25	0.50
3:BC:5335:THR:HA	13:BO:5178:ARG:HD3	1.94	0.50
10:BK:5017:ILE:H	10:BK:5017:ILE:CD1	2.25	0.50
1:AA:214:MET:HE2	1:AA:214:MET:CA	2.24	0.50
33:AB:625:DMS:H22	16:AV:77:SER:HA	1.92	0.50
3:AC:418:ASN:CA	28:AC:519:DGD:HE2	2.42	0.50
4:AD:19:ASP:O	4:AD:20:ASP:C	2.55	0.50
4:AD:86:GLY:O	4:AD:166:SER:HB2	2.12	0.50
13:AO:78:VAL:HB	13:AO:136:MET:HE3	1.94	0.50
14:AT:29:ILE:N	14:AT:29:ILE:CD1	2.71	0.50
1:BA:5258:LEU:HB3	1:BA:5259:ILE:CD1	2.40	0.50
2:BB:5172:TYR:O	2:BB:5173:GLY:C	2.52	0.50
3:BC:5055:ALA:CB	27:BC:5514:BCR:H373	2.38	0.50
27:BC:5516:BCR:HC41	8:BI:5020:VAL:CG1	2.41	0.50
12:BM:5025:LEU:HD23	12:BM:5025:LEU:N	2.27	0.50
13:BO:5225:LEU:HD12	13:BO:5225:LEU:N	2.27	0.50
2:AB:229:LEU:O	2:AB:230:ARG:C	2.54	0.50
31:AB:620:LMG:H302	12:AM:22:LEU:HD21	1.93	0.50
3:AC:89:ILE:N	3:AC:90:PRO:CD	2.75	0.50
3:AC:109:PHE:O	3:AC:113:VAL:HG23	2.11	0.50
10:AK:17:ILE:H	10:AK:17:ILE:CD1	2.23	0.50
13:AO:86:ARG:NE	13:AO:86:ARG:O	2.45	0.50
1:BA:5275:LEU:HD13	25:BA:5409:MST:C8	2.42	0.50
24:BB:5615:CLA:H51	24:BB:5618:CLA:HBC2	1.94	0.50
3:BC:5276:LEU:HD21	24:BC:5508:CLA:HBB1	1.93	0.50
6:BF:5018:VAL:CG1	6:BF:5019:ARG:N	2.74	0.50
11:BL:5022:LEU:HD13	14:BT:5016:LEU:HD23	1.94	0.50
13:BO:5064:TYR:CD1	13:BO:5271:PRO:HA	2.47	0.50
1:AA:258:LEU:HB3	1:AA:259:ILE:CD1	2.39	0.49
29:AA:412:LHG:HC11	3:AC:447:ARG:CZ	2.41	0.49
3:AC:29:GLU:CB	10:AK:46:ARG:NH1	2.71	0.49
3:AC:223:TRP:CE3	3:AC:224:ILE:HG13	2.46	0.49
2:BB:5010:THR:C	2:BB:5012:LEU:N	2.70	0.49
3:BC:5171:GLY:O	3:BC:5174:LEU:HB2	2.12	0.49
4:BD:5337:GLU:O	4:BD:5338:ASN:C	2.55	0.49
13:BO:5117:GLY:O	13:BO:5159:VAL:HG12	2.11	0.49
1:AA:69:GLY:HA2	1:AA:75:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:200:LEU:HD21	28:AC:519:DGD:HAW1	1.94	0.49
1:AA:289:GLY:CA	1:AA:292:THR:HG22	2.42	0.49
2:AB:311:PHE:HA	2:AB:430:PHE:CZ	2.47	0.49
28:AC:519:DGD:HG2	9:AJ:33:TYR:OH	2.12	0.49
4:AD:141:TYR:OH	31:AD:407:LMG:HC2	2.11	0.49
4:AD:154:VAL:O	4:AD:158:LEU:HB2	2.12	0.49
4:AD:193:LEU:HG	4:AD:193:LEU:O	2.11	0.49
4:AD:350:ASN:O	4:AD:352:LEU:N	2.42	0.49
9:AJ:18:GLY:HA3	27:AK:102:BCR:H371	1.94	0.49
17:AY:24:MET:O	17:AY:25:ILE:C	2.55	0.49
1:BA:5043:ALA:HB3	1:BA:5118:HIS:HD2	1.77	0.49
1:BA:5257:ARG:HG3	1:BA:5257:ARG:NH1	2.26	0.49
2:BB:5235:GLU:OE1	2:BB:5472:ARG:NH1	2.44	0.49
2:BB:5311:PHE:HA	2:BB:5430:PHE:CZ	2.47	0.49
3:BC:5225:VAL:CG2	28:BC:5517:DGD:HG11	2.42	0.49
4:BD:5053:THR:HA	4:BD:5067:TYR:CD2	2.47	0.49
4:BD:5141:TYR:OH	31:BD:5409:LMG:HC2	2.13	0.49
13:BO:5186:LYS:HE2	13:BO:5186:LYS:HA	1.92	0.49
15:BU:5080:VAL:HG22	15:BU:5127:ARG:NH2	2.27	0.49
2:AB:91:TRP:CZ3	24:AB:606:CLA:O1A	2.65	0.49
2:AB:371:THR:HG22	2:AB:377:VAL:CA	2.41	0.49
24:AB:608:CLA:C4	4:AD:127:LEU:HD11	2.21	0.49
3:AC:56:HIS:C	3:AC:58:GLY:N	2.68	0.49
3:AC:137:PRO:HB2	3:AC:139:THR:O	2.12	0.49
3:AC:225:VAL:HG22	3:AC:289:PHE:CD1	2.47	0.49
5:AE:7:GLU:O	5:AE:9:PRO:HD3	2.12	0.49
5:AE:36:LEU:HA	5:AE:39:SER:HG	1.77	0.49
7:AH:18:TYR:C	7:AH:18:TYR:CD1	2.89	0.49
24:BB:5605:CLA:HBC3	7:BH:5041:PHE:CE1	2.47	0.49
3:BC:5109:PHE:O	3:BC:5113:VAL:HG23	2.12	0.49
2:AB:243:ALA:HB2	2:AB:466:HIS:ND1	2.27	0.49
2:AB:384:ARG:HD3	15:AU:132:LEU:HD13	1.94	0.49
3:AC:55:ALA:CB	27:AC:514:BCR:H373	2.40	0.49
3:AC:453:ALA:C	8:AI:34:ARG:HB2	2.38	0.49
4:AD:57:SER:HA	4:AD:60:THR:HG22	1.95	0.49
6:AF:41:GLN:N	6:AF:41:GLN:HE21	2.10	0.49
13:AO:225:LEU:HD12	13:AO:225:LEU:N	2.28	0.49
15:AU:83:ALA:CB	15:AU:84:PRO:CD	2.80	0.49
16:AV:63:CYS:O	16:AV:64:ALA:C	2.55	0.49
17:AY:39:LEU:HD21	20:AZ:28:ALA:HB3	1.94	0.49
20:AZ:2:THR:CG2	20:AZ:3:ILE:N	2.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5224:ARG:HG3	7:BH:5025:TRP:HA	1.94	0.49
2:BB:5372:ASP:OD1	2:BB:5374:ASN:N	2.44	0.49
3:BC:5114:VAL:CG2	31:BC:5521:LMG:H141	2.41	0.49
3:BC:5332:GLN:HG3	13:BO:5129:PHE:CE2	2.47	0.49
31:BC:5520:LMG:H292	27:BJ:5101:BCR:H363	1.93	0.49
12:BM:5017:VAL:HG12	12:BM:5018:PRO:N	2.26	0.49
1:AA:57:PRO:HD3	1:AA:73:TYR:CE2	2.48	0.49
1:AA:163:ILE:HG12	28:AC:517:DGD:HB31	1.93	0.49
1:AA:257:ARG:HG3	1:AA:257:ARG:NH1	2.24	0.49
3:AC:452:ALA:O	3:AC:453:ALA:C	2.56	0.49
6:AF:19:ARG:HG3	6:AF:19:ARG:NH1	2.28	0.49
13:AO:147:THR:OG1	13:AO:148:VAL:N	2.46	0.49
13:AO:186:LYS:HE2	13:AO:186:LYS:HA	1.95	0.49
2:BB:5435:GLU:O	2:BB:5436:THR:C	2.56	0.49
3:BC:5252:ILE:HG22	3:BC:5253:LEU:HD23	1.95	0.49
3:BC:5452:ALA:O	3:BC:5454:GLY:N	2.44	0.49
11:BL:5020:GLY:HA3	12:BM:5022:LEU:CD1	2.43	0.49
13:BO:5178:ARG:HD2	13:BO:5182:PHE:CD1	2.46	0.49
16:BV:5090:PRO:O	16:BV:5092:ARG:HD3	2.13	0.49
2:AB:41:GLU:HB3	2:AB:60:MET:SD	2.52	0.49
2:AB:44:THR:HB	32:AB:629:LMT:O6'	2.13	0.49
3:AC:155:ASN:CA	3:AC:158:THR:HG22	2.39	0.49
3:AC:276:LEU:HD21	24:AC:508:CLA:HBB1	1.94	0.49
28:AH:101:DGD:O1B	28:AH:101:DGD:HG12	2.12	0.49
13:AO:178:ARG:HD2	13:AO:182:PHE:CD1	2.48	0.49
15:AU:89:GLU:H	15:AU:89:GLU:CD	2.21	0.49
18:AX:24:LEU:O	18:AX:28:VAL:HG23	2.12	0.49
20:AZ:23:VAL:HB	20:AZ:24:PRO:HD3	1.95	0.49
1:BA:5077:ILE:HG12	14:BT:5006:TYR:CD1	2.47	0.49
2:BB:5252:VAL:HG12	24:BB:5607:CLA:O1A	2.13	0.49
4:BD:5161:PRO:HB3	4:BD:5170:ALA:HB2	1.94	0.49
1:AA:207:GLY:O	1:AA:210:LEU:HB3	2.12	0.49
24:AA:405:CLA:H92	34:AD:402:PHO:CMB	2.41	0.49
2:AB:251:VAL:O	2:AB:255:THR:HG23	2.12	0.49
24:AB:605:CLA:H141	24:AB:610:CLA:HED2	1.94	0.49
3:AC:346:THR:O	13:AO:40:GLY:HA2	2.13	0.49
13:AO:126:GLY:O	13:AO:128:ASP:N	2.45	0.49
14:AT:22:PHE:C	14:AT:23:PHE:CD2	2.91	0.49
1:BA:5038:ILE:HB	1:BA:5039:PRO:HD3	1.93	0.49
24:BA:5406:CLA:H92	34:BD:5403:PHO:CMB	2.41	0.49
29:BA:5413:LHG:HC11	3:BC:5447:ARG:NE	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5337:LEU:CD1	13:BO:5131:PRO:HG3	2.41	0.49
5:BE:5009:PRO:O	5:BE:5010:PHE:C	2.55	0.49
9:BJ:5024:ILE:HG23	9:BJ:5025:VAL:N	2.27	0.49
13:BO:5148:VAL:HA	13:BO:5172:PHE:CD2	2.47	0.49
15:BU:5072:TYR:CB	15:BU:5073:PRO:HD3	2.40	0.49
20:BZ:5036:SER:C	20:BZ:5038:GLN:N	2.70	0.49
1:AA:205:VAL:HG21	24:AA:404:CLA:CMA	2.37	0.49
3:AC:297:TYR:HA	3:AC:302:TYR:HE2	1.77	0.49
4:AD:52:THR:HG22	4:AD:67:TYR:CE2	2.48	0.49
7:AH:44:ILE:HG12	18:AX:19:PHE:CE2	2.48	0.49
10:AK:12:PRO:HB3	20:AZ:62:VAL:HG11	1.93	0.49
10:AK:24:VAL:CG1	17:Ay:25:ILE:HG13	2.36	0.49
13:AO:83:LYS:HE2	2:BB:5338:GLN:HA	1.94	0.49
2:BB:5008:VAL:HG23	2:BB:5009:HIS:HD2	1.76	0.49
2:BB:5115:TRP:CZ2	24:BB:5618:CLA:HBA2	2.47	0.49
3:BC:5049:LEU:HD23	3:BC:5149:TYR:OH	2.12	0.49
3:BC:5056:HIS:C	3:BC:5058:GLY:N	2.70	0.49
3:BC:5089:ILE:N	3:BC:5090:PRO:CD	2.74	0.49
4:BD:5186:GLN:HB2	24:BD:5402:CLA:HBC1	1.95	0.49
9:BJ:5034:ALA:O	9:BJ:5035:GLY:O	2.31	0.49
1:AA:22:THR:HG21	8:AI:30:ARG:HE	1.78	0.49
3:AC:155:ASN:O	3:AC:158:THR:HG22	2.12	0.49
28:AC:518:DGD:HB22	28:AC:519:DGD:HA21	1.95	0.49
4:AD:57:SER:CA	4:AD:60:THR:HG22	2.43	0.49
24:AD:404:CLA:C4	18:AX:23:LEU:HA	2.43	0.49
13:AO:66:ILE:HD12	13:AO:121:PHE:CD1	2.48	0.49
13:AO:71:LEU:HD23	13:AO:265:PHE:HB3	1.94	0.49
17:Ay:45:ASN:CB	20:AZ:28:ALA:O	2.60	0.49
1:BA:5215:HIS:O	1:BA:5216:GLY:C	2.56	0.49
2:BB:5002:GLY:HA3	11:BL:5009:PRO:HG2	1.94	0.49
2:BB:5413:ASP:O	2:BB:5414:PRO:C	2.55	0.49
4:BD:5052:THR:HG22	4:BD:5067:TYR:CE2	2.48	0.49
28:BH:5101:DGD:O1B	28:BH:5101:DGD:HG12	2.12	0.49
13:BO:5155:THR:HG23	13:BO:5168:PHE:CE2	2.48	0.49
13:BO:5240:THR:HA	13:BO:5264:VAL:HA	1.95	0.49
1:AA:59:ASP:OD1	1:AA:64:ARG:N	2.46	0.49
2:AB:8:VAL:HG23	2:AB:9:HIS:HD2	1.77	0.49
2:AB:187:PRO:HB3	24:AB:601:CLA:CMB	2.42	0.49
3:AC:149:TYR:CA	3:AC:156:LYS:HD3	2.42	0.49
3:AC:337:LEU:CD1	13:AO:131:PRO:HG3	2.43	0.49
3:AC:363:GLY:O	3:AC:364:PRO:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:210:ARG:HA	15:AU:39:LEU:CD1	2.43	0.49
15:AU:66:ILE:O	15:AU:66:ILE:CG2	2.61	0.49
16:AV:45:ILE:HG12	16:AV:46:THR:N	2.27	0.49
2:BB:5305:ILE:O	2:BB:5305:ILE:HG22	2.11	0.49
3:BC:5271:TYR:CE1	24:BC:5507:CLA:HAC2	2.48	0.49
3:BC:5346:THR:O	13:BO:5040:GLY:HA2	2.13	0.49
24:BC:5501:CLA:CMB	27:BC:5516:BCR:H403	2.42	0.49
18:BX:5043:ILE:O	18:BX:5043:ILE:HG22	2.13	0.49
1:AA:64:ARG:HG3	1:AA:64:ARG:NH1	2.27	0.48
2:AB:224:ARG:HG3	7:AH:25:TRP:HA	1.94	0.48
2:AB:435:GLU:O	2:AB:436:THR:C	2.56	0.48
24:AC:505:CLA:H2	24:AC:505:CLA:HAA1	1.95	0.48
15:AU:80:VAL:HG22	15:AU:127:ARG:HH21	1.78	0.48
20:AZ:48:ILE:O	20:AZ:52:LEU:HG	2.13	0.48
1:BA:5210:LEU:HD23	1:BA:5210:LEU:C	2.38	0.48
24:BA:5408:CLA:HBA2	28:BA:5412:DGD:HB22	1.95	0.48
2:BB:5270:PRO:HG3	2:BB:5312:TYR:CD2	2.48	0.48
2:BB:5384:ARG:HH11	15:BU:5132:LEU:HD13	1.77	0.48
24:BB:5606:CLA:H191	4:BD:5158:LEU:HB3	1.96	0.48
3:BC:5296:VAL:HG23	3:BC:5297:TYR:CD2	2.48	0.48
3:BC:5380:ILE:CA	3:BC:5384:ILE:HD11	2.37	0.48
5:BE:5026:THR:HB	36:BF:5101:HEM:CAB	2.43	0.48
20:BZ:5023:VAL:HB	20:BZ:5024:PRO:HD3	1.95	0.48
20:BZ:5032:ASP:OD1	20:BZ:5036:SER:HB2	2.13	0.48
20:BZ:5048:ILE:O	20:BZ:5052:LEU:HG	2.13	0.48
1:AA:190:HIS:O	1:AA:298:ASN:HB3	2.13	0.48
2:AB:384:ARG:NH1	15:AU:132:LEU:HD13	2.28	0.48
3:AC:49:LEU:HD23	3:AC:149:TYR:OH	2.13	0.48
3:AC:208:VAL:O	3:AC:209:ILE:C	2.56	0.48
4:AD:266:TRP:CD1	31:AD:408:LMG:HC1	2.47	0.48
13:AO:71:LEU:HD12	13:AO:104:LEU:HD12	1.95	0.48
16:AV:146:LEU:O	16:AV:150:LYS:HG3	2.13	0.48
1:BA:5057:PRO:HG3	1:BA:5068:SER:CB	2.43	0.48
1:BA:5210:LEU:C	1:BA:5210:LEU:CD2	2.86	0.48
2:BB:5324:LEU:CA	4:BD:5293:LEU:HD23	2.38	0.48
3:BC:5235:GLY:O	3:BC:5238:ILE:HB	2.13	0.48
3:BC:5249:ILE:O	3:BC:5253:LEU:HG	2.13	0.48
4:BD:5266:TRP:NE1	31:BD:5410:LMG:HC72	2.28	0.48
10:BK:5044:GLY:O	10:BK:5045:PHE:C	2.56	0.48
13:BO:5066:ILE:HD12	13:BO:5121:PHE:CD1	2.48	0.48
15:BU:5057:LEU:HD11	15:BU:5112:PHE:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:By:5024:MET:O	17:By:5027:MET:CG	2.62	0.48
1:AA:131:TRP:CE3	1:AA:132:GLU:CA	2.97	0.48
2:AB:175:THR:O	2:AB:176:GLY:O	2.31	0.48
13:AO:159:VAL:HG13	13:AO:159:VAL:O	2.13	0.48
15:AU:73:PRO:HG2	16:AV:107:THR:HB	1.95	0.48
1:BA:5092:HIS:CD2	3:BC:5219:GLY:HA3	2.48	0.48
29:BA:5413:LHG:HC11	3:BC:5447:ARG:HH21	1.78	0.48
29:BA:5413:LHG:C1	3:BC:5447:ARG:HE	2.26	0.48
24:BB:5605:CLA:HBB1	24:BB:5605:CLA:HHC	1.94	0.48
13:BO:5065:ARG:HB2	13:BO:5065:ARG:NH1	2.28	0.48
13:BO:5147:THR:OG1	13:BO:5148:VAL:N	2.47	0.48
1:AA:27:ARG:NH1	1:AA:27:ARG:O	2.47	0.48
1:AA:254:TYR:CD1	4:AD:132:ILE:HG22	2.48	0.48
1:AA:318:ALA:HB2	4:AD:75:THR:HG22	1.95	0.48
2:AB:354:LEU:HD12	2:AB:354:LEU:N	2.28	0.48
2:AB:433:ASP:C	2:AB:433:ASP:OD1	2.55	0.48
24:AB:611:CLA:H92	31:AD:407:LMG:H232	1.95	0.48
7:AH:35:MET:SD	27:AX:101:BCR:H322	2.53	0.48
10:AK:20:PRO:HB2	17:Ay:21:GLN:HB2	1.95	0.48
1:BA:5214:MET:O	1:BA:5215:HIS:C	2.54	0.48
1:BA:5330:VAL:CG1	4:BD:5348:ARG:HG2	2.42	0.48
2:BB:5383:PHE:HE1	13:BO:5194:TYR:CD2	2.30	0.48
8:BI:5019:PHE:CZ	8:BI:5023:PHE:HE2	2.30	0.48
17:By:5034:MET:O	17:By:5038:LEU:HG	2.14	0.48
20:BZ:5032:ASP:OD1	20:BZ:5033:TRP:N	2.41	0.48
1:AA:45:THR:CG2	1:AA:46:ILE:N	2.76	0.48
32:AB:624:LMT:H112	7:AH:35:MET:HE2	1.95	0.48
3:AC:94:THR:CG2	3:AC:298:PRO:HD2	2.44	0.48
3:AC:155:ASN:HA	3:AC:158:THR:CG2	2.38	0.48
3:AC:337:LEU:HD12	13:AO:131:PRO:CG	2.44	0.48
2:BB:5004:PRO:CG	2:BB:5007:ARG:HD2	2.35	0.48
3:BC:5452:ALA:C	3:BC:5454:GLY:N	2.68	0.48
4:BD:5068:LEU:CB	6:BF:5040:MET:HE2	2.43	0.48
4:BD:5087:HIS:HB2	28:BH:5101:DGD:O2D	2.12	0.48
4:BD:5210:LEU:HA	4:BD:5213:ILE:HG22	1.95	0.48
5:BE:5061:ARG:NH2	16:BV:5153:GLY:HA3	2.28	0.48
7:BH:5011:LEU:HA	7:BH:5014:LEU:HD12	1.94	0.48
13:BO:5135:GLN:HG2	13:BO:5141:ARG:HG3	1.96	0.48
1:AA:182:PHE:O	1:AA:186:PHE:HB2	2.14	0.48
2:AB:372:ASP:OD1	2:AB:374:ASN:N	2.46	0.48
3:AC:80:PRO:HB3	3:AC:82:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AJ:34:ALA:O	9:AJ:35:GLY:O	2.31	0.48
32:AM:102:LMT:H11	14:BT:5001:MET:HE3	1.96	0.48
16:AV:64:ALA:O	16:AV:65:SER:C	2.56	0.48
17:Ay:41:VAL:C	17:Ay:43:ARG:N	2.71	0.48
1:BA:5220:THR:HG23	4:BD:5141:TYR:CD1	2.49	0.48
2:BB:5012:LEU:HD12	2:BB:5019:LEU:HD12	1.96	0.48
2:BB:5222:PRO:O	2:BB:5223:GLN:C	2.56	0.48
24:BC:5511:CLA:H143	20:BZ:5024:PRO:HG2	1.96	0.48
5:BE:5014:ILE:HG22	5:BE:5014:ILE:O	2.12	0.48
5:BE:5078:THR:O	5:BE:5081:GLU:HB2	2.14	0.48
6:BF:5015:ILE:HG22	6:BF:5016:PHE:CD1	2.47	0.48
13:BO:5120:THR:HA	13:BO:5153:ALA:O	2.14	0.48
3:AC:147:PHE:CD2	24:AC:513:CLA:H3A	2.49	0.48
13:AO:155:THR:HG22	13:AO:167:ASP:O	2.14	0.48
14:AT:25:GLU:O	14:AT:26:PRO:C	2.54	0.48
1:BA:5022:THR:HG21	8:BI:5030:ARG:HE	1.78	0.48
1:BA:5278:TRP:HA	28:BC:5519:DGD:HAG1	1.96	0.48
2:AB:245:VAL:HG22	24:AB:612:CLA:H192	1.95	0.48
24:AB:608:CLA:HMB1	4:AD:126:MET:SD	2.53	0.48
3:AC:214:LEU:HD22	3:AC:214:LEU:N	2.28	0.48
3:AC:271:TYR:CE1	24:AC:507:CLA:HAC2	2.49	0.48
3:AC:461:ARG:NH2	4:AD:242:GLU:O	2.46	0.48
4:AD:188:PHE:CZ	4:AD:326:ARG:HG2	2.49	0.48
10:AK:25:LEU:HB2	10:AK:26:PRO:HD3	1.96	0.48
16:AV:143:GLY:O	16:AV:147:VAL:HG23	2.14	0.48
1:BA:5281:VAL:HG13	28:BC:5519:DGD:HAG3	1.93	0.48
3:BC:5350:ILE:HG21	3:BC:5359:TRP:HB2	1.96	0.48
3:BC:5418:ASN:HB2	28:BC:5519:DGD:HE2	1.92	0.48
24:BC:5501:CLA:CAD	24:BC:5503:CLA:H12	2.44	0.48
24:BC:5511:CLA:H143	17:By:5035:ILE:HD13	1.95	0.48
7:BH:5013:PRO:HG2	7:BH:5014:LEU:H	1.78	0.48
1:AA:205:VAL:CG2	24:AA:404:CLA:HMA2	2.37	0.48
1:AA:315:ASN:ND2	4:AD:332:GLN:HE22	2.07	0.48
3:AC:29:GLU:CD	3:AC:29:GLU:N	2.72	0.48
12:AM:1:MET:HG2	12:AM:2:GLU:H	1.79	0.48
16:AV:58:LEU:HD13	16:AV:137:ASP:HB3	1.95	0.48
1:BA:5047:CYS:SG	1:BA:5114:LEU:HD22	2.53	0.48
1:BA:5131:TRP:CE3	1:BA:5132:GLU:CA	2.97	0.48
1:BA:5214:MET:HE3	34:BD:5404:PHO:HMD2	1.95	0.48
2:BB:5107:LEU:HD21	24:BB:5619:CLA:H42	1.95	0.48
2:BB:5208:VAL:HG21	24:BB:5606:CLA:HMC3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5436:PHE:O	24:BC:5508:CLA:HAC1	2.14	0.48
24:BC:5507:CLA:HHC	24:BC:5507:CLA:HBB1	1.96	0.48
5:BE:5069:ARG:HG3	5:BE:5070:PHE:H	1.79	0.48
11:BL:5016:SER:HA	11:BL:5019:LEU:CG	2.44	0.48
15:BU:5066:ILE:O	15:BU:5066:ILE:CG2	2.61	0.48
2:AB:222:PRO:HG3	7:AH:27:THR:N	2.25	0.48
2:AB:234:ILE:HD12	2:AB:237:VAL:CG2	2.43	0.48
2:AB:326:ARG:HD3	2:AB:442:ILE:HG22	1.95	0.48
4:AD:68:LEU:CB	6:AF:40:MET:HE2	2.42	0.48
4:AD:218:VAL:HG22	4:AD:244:TYR:CE2	2.49	0.48
18:AX:44:ASP:N	18:AX:44:ASP:OD1	2.46	0.48
2:BB:5329:PRO:HD2	31:BB:5624:LMG:O4	2.14	0.48
24:BB:5610:CLA:H52	27:BB:5623:BCR:H321	1.96	0.48
3:BC:5452:ALA:O	3:BC:5453:ALA:C	2.57	0.48
3:BC:5466:VAL:CA	3:BC:5469:MET:HE3	2.39	0.48
4:BD:5152:VAL:HG11	24:BD:5402:CLA:H11	1.94	0.48
5:BE:5082:GLN:O	5:BE:5083:LEU:C	2.56	0.48
16:BV:5121:LEU:CD2	16:BV:5138:LEU:HD11	2.44	0.48
1:AA:180:PHE:HA	1:AA:183:MET:HE3	1.96	0.47
1:AA:202:VAL:O	1:AA:206:PHE:HB2	2.14	0.47
2:AB:12:LEU:HD12	2:AB:19:LEU:HD12	1.94	0.47
2:AB:15:ASP:N	2:AB:16:PRO:HD3	2.29	0.47
3:AC:256:PRO:HG2	3:AC:266:TRP:CH2	2.49	0.47
5:AE:69:ARG:HG3	5:AE:70:PHE:H	1.78	0.47
10:AK:44:GLY:O	10:AK:45:PHE:C	2.57	0.47
11:AL:20:GLY:HA3	12:AM:22:LEU:CD1	2.44	0.47
15:AU:38:GLU:O	15:AU:39:LEU:O	2.32	0.47
16:AV:81:ARG:HG2	16:AV:81:ARG:NH1	2.29	0.47
1:BA:5048:PHE:CA	1:BA:5115:ILE:HD11	2.44	0.47
1:BA:5322:ASN:OD1	3:BC:5412:THR:HA	2.14	0.47
24:BA:5406:CLA:HED2	4:BD:5198:MET:SD	2.54	0.47
2:BB:5229:LEU:O	2:BB:5230:ARG:C	2.56	0.47
3:BC:5365:TRP:HA	3:BC:5387:TRP:CH2	2.49	0.47
5:BE:5051:ARG:O	5:BE:5053:ASP:N	2.47	0.47
13:BO:5071:LEU:HD12	13:BO:5104:LEU:HD12	1.96	0.47
13:BO:5157:PRO:O	13:BO:5158:ASN:O	2.32	0.47
1:AA:21:VAL:HG11	1:AA:32:TRP:CE3	2.49	0.47
1:AA:295:PHE:O	3:AC:424:SER:OG	2.32	0.47
2:AB:24:LEU:HD13	2:AB:111:ALA:N	2.29	0.47
3:AC:460:ASP:O	3:AC:461:ARG:C	2.55	0.47
24:AC:507:CLA:HBB1	24:AC:507:CLA:HHC	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:221:THR:HG23	4:AD:221:THR:O	2.13	0.47
4:AD:261:PHE:HE1	4:AD:266:TRP:CD1	2.33	0.47
5:AE:14:ILE:HG22	5:AE:14:ILE:O	2.13	0.47
5:AE:77:GLU:HA	5:AE:80:LEU:HD23	1.96	0.47
19:AY:11:UNK:C	19:AY:13:UNK:N	2.75	0.47
20:AZ:30:PRO:C	20:AZ:32:ASP:N	2.73	0.47
1:BA:5281:VAL:HG11	28:BC:5519:DGD:HAV1	1.96	0.47
2:BB:5012:LEU:HD22	2:BB:5018:ARG:HB2	1.95	0.47
3:BC:5286:ALA:HB2	24:BC:5502:CLA:HMD1	1.96	0.47
3:BC:5441:HIS:HD2	3:BC:5442:LEU:HD12	1.78	0.47
24:BC:5504:CLA:H192	28:BC:5518:DGD:HBN2	1.96	0.47
4:BD:5160:TYR:HB3	4:BD:5161:PRO:CD	2.44	0.47
11:BL:5026:VAL:HG11	31:BL:5101:LMG:H202	1.96	0.47
17:By:5034:MET:HA	17:By:5034:MET:HE2	1.89	0.47
20:BZ:5036:SER:HA	20:BZ:5039:LEU:CG	2.40	0.47
20:BZ:5047:TRP:O	20:BZ:5050:LEU:HB2	2.14	0.47
1:AA:127:MET:HE3	24:AC:505:CLA:HMB2	1.96	0.47
1:AA:275:LEU:HD13	25:AA:408:MST:C8	2.44	0.47
24:AA:407:CLA:HBA2	28:AA:411:DGD:HB22	1.96	0.47
2:AB:10:THR:C	2:AB:12:LEU:N	2.71	0.47
2:AB:457:VAL:HG12	2:AB:458:PHE:N	2.29	0.47
3:AC:297:TYR:HD1	3:AC:302:TYR:CE2	2.33	0.47
3:AC:330:SER:HB2	13:AO:149:LYS:NZ	2.29	0.47
3:AC:450:ALA:HA	3:AC:455:PHE:CE2	2.49	0.47
4:BD:5084:SER:HB3	5:BE:5068:ASP:HA	1.95	0.47
5:BE:5035:TRP:CD1	5:BE:5035:TRP:C	2.92	0.47
6:BF:5016:PHE:CD1	6:BF:5016:PHE:N	2.82	0.47
6:BF:5019:ARG:HG3	6:BF:5019:ARG:HH11	1.78	0.47
7:BH:5017:GLU:CD	7:BH:5017:GLU:N	2.72	0.47
1:AA:153:SER:CB	24:AA:404:CLA:H11	2.45	0.47
2:AB:35:GLY:O	2:AB:38:ALA:HB3	2.14	0.47
24:AB:603:CLA:H2	24:AB:605:CLA:H91	1.96	0.47
24:AB:608:CLA:C1	24:AB:608:CLA:HAA1	2.44	0.47
24:AC:504:CLA:H192	28:AC:518:DGD:HBN2	1.96	0.47
13:AO:155:THR:HG23	13:AO:168:PHE:CD2	2.50	0.47
1:BA:5091:LEU:HD11	1:BA:5163:ILE:HA	1.94	0.47
1:BA:5119:PHE:HD1	34:BD:5403:PHO:H92	1.78	0.47
1:BA:5288:LEU:HD22	3:BC:5432:VAL:HA	1.95	0.47
3:BC:5147:PHE:CD2	24:BC:5513:CLA:H3A	2.49	0.47
7:BH:5050:ASN:HD22	28:BH:5101:DGD:HA21	1.79	0.47
8:BI:5014:PHE:CE2	8:BI:5018:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5039:THR:HB	13:BO:5041:LEU:HD22	1.95	0.47
1:AA:272:HIS:HD2	4:AD:218:VAL:HG21	1.76	0.47
1:AA:326:LEU:CD2	3:AC:412:THR:HB	2.44	0.47
29:AA:412:LHG:HC11	3:AC:447:ARG:HH21	1.78	0.47
2:AB:54:PRO:HD2	2:AB:57:ARG:HG3	1.95	0.47
3:AC:131:TYR:HE1	3:AC:135:ARG:HD2	1.79	0.47
3:AC:267:SER:O	3:AC:271:TYR:CD2	2.67	0.47
28:AC:519:DGD:HE62	9:AJ:40:LEU:CD1	2.45	0.47
4:AD:253:TRP:HB2	4:AD:260:ALA:HB2	1.96	0.47
4:AD:274:VAL:HA	35:AD:405:PL9:C25	2.37	0.47
4:AD:299:ILE:HG13	11:AL:37:ASN:ND2	2.29	0.47
12:AM:24:ILE:HD13	31:BM:5102:LMG:H351	1.96	0.47
20:AZ:53:VAL:O	20:AZ:57:LEU:HB2	2.14	0.47
1:BA:5029:TYR:CD2	1:BA:5133:LEU:HD13	2.49	0.47
1:BA:5039:PRO:CB	24:BA:5408:CLA:HBB1	2.44	0.47
2:BB:5198:VAL:HG11	24:BB:5607:CLA:HED2	1.97	0.47
2:BB:5348:ASN:O	2:BB:5349:LYS:C	2.56	0.47
3:BC:5131:TYR:HE1	3:BC:5135:ARG:HD2	1.80	0.47
3:BC:5327:ASN:HB3	13:BO:5125:ASP:OD1	2.14	0.47
5:BE:5027:ILE:CB	5:BE:5028:PRO:HD3	2.43	0.47
11:BL:5024:ILE:HG21	12:BM:5019:SER:OG	2.14	0.47
16:BV:5045:ILE:HG12	16:BV:5046:THR:N	2.29	0.47
19:BY:5011:UNK:C	19:BY:5013:UNK:N	2.76	0.47
1:AA:13:LEU:N	1:AA:16:ARG:HH11	2.13	0.47
1:AA:43:ALA:HB3	1:AA:118:HIS:HD2	1.80	0.47
1:AA:223:LEU:O	2:AB:482:ILE:HG12	2.13	0.47
1:AA:238:LYS:O	1:AA:241:GLN:HG3	2.14	0.47
2:AB:25:MET:HE2	27:AB:617:BCR:H393	1.95	0.47
2:AB:405:GLU:HA	2:AB:405:GLU:OE1	2.14	0.47
31:AB:620:LMG:H202	11:AL:26:VAL:HG11	1.95	0.47
5:AE:27:ILE:CB	5:AE:28:PRO:HD3	2.44	0.47
13:AO:36:ILE:HG23	13:AO:41:LEU:CB	2.44	0.47
13:AO:39:THR:HB	13:AO:41:LEU:HD22	1.96	0.47
2:BB:5234:ILE:C	2:BB:5236:THR:H	2.23	0.47
3:BC:5330:SER:HB2	13:BO:5149:LYS:NZ	2.29	0.47
4:BD:5087:HIS:HD2	4:BD:5166:SER:HA	1.72	0.47
4:BD:5180:ARG:HG3	4:BD:5181:PHE:N	2.29	0.47
15:BU:5099:GLU:HA	15:BU:5102:LYS:HE3	1.97	0.47
16:BV:5063:CYS:O	16:BV:5064:ALA:C	2.56	0.47
1:AA:32:TRP:HB2	8:AI:23:PHE:CZ	2.49	0.47
1:AA:47:CYS:SG	1:AA:114:LEU:HD22	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:64:ARG:NH1	13:AO:98:THR:HG21	2.29	0.47
1:AA:119:PHE:HD1	34:AD:402:PHO:H92	1.79	0.47
1:AA:248:ILE:O	1:AA:248:ILE:CG1	2.61	0.47
1:AA:288:LEU:HD22	3:AC:432:VAL:HA	1.96	0.47
2:AB:9:HIS:HB2	24:AB:611:CLA:CBA	2.44	0.47
2:AB:143:LEU:HD12	2:AB:143:LEU:O	2.14	0.47
2:AB:275:TRP:CH2	2:AB:358:ARG:HD3	2.50	0.47
2:AB:279:TYR:HE1	7:AH:63:LYS:HE3	1.80	0.47
2:AB:324:LEU:CA	4:AD:293:LEU:HD23	2.43	0.47
2:AB:325:PHE:CD1	11:AL:34:TYR:HB3	2.49	0.47
24:AB:602:CLA:H93	7:AH:46:LEU:HD13	1.96	0.47
3:AC:94:THR:HG22	3:AC:298:PRO:HD2	1.95	0.47
3:AC:416:SER:CA	28:AC:519:DGD:O3E	2.62	0.47
3:AC:472:LEU:O	3:AC:473:ASP:O	2.32	0.47
4:AD:274:VAL:CB	4:AD:275:PRO:HD3	2.44	0.47
24:AD:404:CLA:H42	18:AX:23:LEU:HA	1.96	0.47
13:AO:65:ARG:NH1	13:AO:65:ARG:HB2	2.29	0.47
13:AO:236:GLU:HG3	13:AO:236:GLU:O	2.14	0.47
16:AV:148:GLU:OE1	16:AV:148:GLU:HA	2.15	0.47
1:BA:5015:GLU:O	1:BA:5019:ASN:OD1	2.32	0.47
1:BA:5059:ASP:OD2	1:BA:5062:GLY:HA2	2.15	0.47
1:BA:5153:SER:HB2	24:BA:5405:CLA:H11	1.97	0.47
1:BA:5183:MET:HG3	24:BA:5406:CLA:HBC1	1.96	0.47
1:BA:5248:ILE:O	1:BA:5248:ILE:CG1	2.62	0.47
2:BB:5187:PRO:HG2	2:BB:5188:ASP:H	1.80	0.47
2:BB:5250:PHE:O	28:BH:5101:DGD:HB82	2.15	0.47
24:BB:5611:CLA:H61	24:BB:5611:CLA:H41	1.74	0.47
24:BB:5615:CLA:H92	31:BD:5409:LMG:H232	1.95	0.47
3:BC:5075:PHE:CD1	3:BC:5086:LEU:HD21	2.50	0.47
3:BC:5262:ARG:HH21	32:BC:5522:LMT:C5'	2.26	0.47
3:BC:5271:TYR:HA	3:BC:5274:TYR:CD2	2.49	0.47
3:BC:5318:LEU:HD21	3:BC:5380:ILE:HG23	1.97	0.47
3:BC:5394:GLU:OE2	3:BC:5398:HIS:CD2	2.68	0.47
24:BC:5510:CLA:H161	24:BC:5510:CLA:H122	1.81	0.47
4:BD:5263:ASN:O	4:BD:5266:TRP:N	2.47	0.47
5:BE:5015:THR:O	9:BJ:5008:ILE:CD1	2.63	0.47
9:BJ:5036:LEU:C	9:BJ:5038:SER:H	2.22	0.47
10:BK:5018:PHE:O	10:BK:5019:ASP:C	2.57	0.47
13:BO:5236:GLU:O	13:BO:5236:GLU:HG3	2.14	0.47
17:By:5024:MET:O	17:By:5025:ILE:C	2.58	0.47
1:AA:39:PRO:CB	24:AA:407:CLA:HBB1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:208:VAL:HG21	24:AB:602:CLA:HMC3	1.95	0.47
2:AB:250:PHE:O	28:AH:101:DGD:HB82	2.15	0.47
2:AB:329:PRO:HD2	31:AB:621:LMG:O4	2.15	0.47
2:AB:356:VAL:HA	2:AB:370:LEU:CD2	2.45	0.47
2:AB:384:ARG:HH11	15:AU:132:LEU:HD13	1.79	0.47
3:AC:319:ILE:O	3:AC:323:LYS:HG3	2.15	0.47
3:AC:387:TRP:CE2	3:AC:388:GLN:HG3	2.49	0.47
4:AD:68:LEU:HD11	5:AE:44:TYR:CE1	2.49	0.47
11:AL:8:GLN:N	11:AL:8:GLN:NE2	2.62	0.47
11:AL:17:LEU:HD11	12:AM:23:ILE:HD12	1.97	0.47
13:AO:271:PRO:HG2	13:AO:272:ALA:H	1.79	0.47
15:AU:58:ASN:OD1	15:AU:84:PRO:CA	2.61	0.47
1:BA:5135:TYR:HE1	3:BC:5449:ARG:O	1.97	0.47
29:BA:5415:LHG:H102	31:BE:5101:LMG:H142	1.97	0.47
2:BB:5250:PHE:HD1	28:BH:5101:DGD:HB92	1.80	0.47
24:BB:5618:CLA:H162	31:BL:5101:LMG:H422	1.96	0.47
4:BD:5086:GLY:O	4:BD:5166:SER:HB2	2.15	0.47
16:BV:5143:GLY:O	16:BV:5147:VAL:HG23	2.14	0.47
20:BZ:5030:PRO:C	20:BZ:5032:ASP:N	2.72	0.47
2:AB:234:ILE:C	2:AB:236:THR:H	2.23	0.47
2:AB:329:PRO:HD3	24:AB:607:CLA:CED	2.44	0.47
2:AB:425:ILE:HG22	2:AB:426:PHE:HD2	1.75	0.47
2:AB:485:GLU:HG2	2:AB:486:LEU:N	2.29	0.47
3:AC:193:GLY:O	3:AC:194:GLY:O	2.33	0.47
3:AC:436:PHE:O	24:AC:508:CLA:HAC1	2.15	0.47
8:AI:11:VAL:CG2	32:AI:102:LMT:H101	2.44	0.47
1:BA:5329:GLU:O	1:BA:5332:HIS:ND1	2.45	0.47
24:BB:5614:CLA:H111	24:BB:5619:CLA:CAA	2.44	0.47
3:BC:5281:MET:HE3	3:BC:5285:ILE:HD11	1.97	0.47
3:BC:5342:MET:HE3	3:BC:5352:GLY:CA	2.44	0.47
5:BE:5014:ILE:HG22	9:BJ:5013:VAL:HG11	1.96	0.47
10:BK:5015:TYR:OH	20:BZ:5058:ASN:ND2	2.48	0.47
13:BO:5031:LEU:N	13:BO:5031:LEU:CD1	2.72	0.47
13:BO:5070:CYS:SG	13:BO:5105:ASP:OD1	2.72	0.47
13:BO:5171:GLU:HA	13:BO:5221:GLY:O	2.15	0.47
1:AA:13:LEU:HD12	1:AA:16:ARG:NH1	2.29	0.47
1:AA:96:ILE:C	1:AA:98:GLU:H	2.23	0.47
1:AA:202:VAL:HG11	24:AA:406:CLA:OBD	2.14	0.47
2:AB:24:LEU:HB3	2:AB:111:ALA:HB2	1.97	0.47
2:AB:115:TRP:CZ2	24:AB:614:CLA:HBA2	2.50	0.47
2:AB:413:ASP:O	2:AB:414:PRO:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AB:601:CLA:HBC3	7:AH:41:PHE:CE1	2.50	0.47
3:AC:204:LEU:HD21	3:AC:238:ILE:HG21	1.97	0.47
3:AC:375:LEU:HB3	3:AC:380:ILE:HD11	1.96	0.47
3:AC:394:GLU:OE2	3:AC:398:HIS:CD2	2.68	0.47
15:AU:80:VAL:HG22	15:AU:127:ARG:NH2	2.30	0.47
2:BB:5009:HIS:HB2	24:BB:5615:CLA:CBA	2.45	0.47
2:BB:5175:THR:O	2:BB:5176:GLY:O	2.33	0.47
2:BB:5183:PRO:HG3	2:BB:5199:VAL:HG12	1.95	0.47
3:BC:5042:LEU:HD21	24:BC:5511:CLA:H2A	1.97	0.47
3:BC:5143:TYR:O	3:BC:5144:SER:CB	2.62	0.47
3:BC:5318:LEU:HD23	3:BC:5318:LEU:C	2.40	0.47
3:BC:5473:ASP:HB2	14:BT:5026:PRO:HB3	1.96	0.47
28:BC:5518:DGD:O3D	27:BJ:5101:BCR:H382	2.14	0.47
5:BE:5078:THR:HA	5:BE:5081:GLU:CG	2.43	0.47
13:BO:5077:LEU:HB3	13:BO:5091:PHE:HB3	1.97	0.47
16:BV:5081:ARG:CZ	16:BV:5157:GLY:HA3	2.45	0.47
1:AA:78:ILE:O	1:AA:176:ILE:HB	2.15	0.46
3:AC:264:PHE:CE1	27:AC:516:BCR:H321	2.50	0.46
10:AK:20:PRO:O	10:AK:23:ASP:HB2	2.15	0.46
13:AO:36:ILE:HG23	13:AO:41:LEU:HB2	1.97	0.46
1:BA:5222:SER:O	1:BA:5246:TYR:HB2	2.14	0.46
2:BB:5112:CYS:HB3	27:BB:5623:BCR:H393	1.96	0.46
2:BB:5193:TYR:CD1	2:BB:5260:SER:HA	2.50	0.46
3:BC:5038:GLY:HA3	24:BC:5511:CLA:C2D	2.45	0.46
3:BC:5420:VAL:HB	3:BC:5425:TRP:HE1	1.80	0.46
3:BC:5432:VAL:HG13	3:BC:5433:LEU:N	2.29	0.46
24:BC:5510:CLA:HHC	24:BC:5510:CLA:HBB1	1.96	0.46
24:BD:5405:CLA:C4	18:BX:5023:LEU:HA	2.45	0.46
5:BE:5036:LEU:HA	5:BE:5039:SER:OG	2.15	0.46
8:BI:5027:ASP:O	8:BI:5028:PRO:C	2.56	0.46
11:BL:5016:SER:O	11:BL:5019:LEU:HD12	2.14	0.46
20:BZ:5023:VAL:HG12	20:BZ:5027:TYR:CE2	2.49	0.46
1:AA:12:ASN:ND2	1:AA:15:GLU:HB2	2.29	0.46
1:AA:240:GLY:HA3	14:AT:29:ILE:HG22	1.98	0.46
24:AB:602:CLA:H191	4:AD:158:LEU:HB3	1.97	0.46
3:AC:45:LEU:O	3:AC:46:SER:C	2.58	0.46
5:AE:78:THR:O	5:AE:81:GLU:HB2	2.15	0.46
6:AF:24:HIS:HA	6:AF:27:ALA:HB3	1.97	0.46
8:AI:33:LYS:O	8:AI:35:LYS:HG2	2.14	0.46
1:BA:5131:TRP:CE3	1:BA:5132:GLU:HA	2.51	0.46
1:BA:5140:ARG:HB2	4:BD:5220:ASN:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5007:ARG:HA	24:BB:5615:CLA:HBA1	1.97	0.46
2:BB:5153:PHE:CZ	2:BB:5158:LEU:HD21	2.50	0.46
4:BD:5093:TRP:HA	4:BD:5099:GLY:H	1.81	0.46
10:BK:5043:VAL:HG21	10:BK:5046:ARG:HE	1.80	0.46
15:BU:5073:PRO:HG2	16:BV:5107:THR:HB	1.97	0.46
16:BV:5098:LEU:O	16:BV:5102:MET:HG3	2.14	0.46
18:BX:5012:ILE:CD1	18:BX:5016:LEU:HD12	2.44	0.46
18:BX:5024:LEU:HD12	18:BX:5024:LEU:HA	1.74	0.46
1:AA:11:ALA:HB1	1:AA:15:GLU:OE1	2.15	0.46
1:AA:35:VAL:HA	27:AA:410:BCR:H333	1.95	0.46
24:AB:608:CLA:CAB	4:AD:123:ILE:HG23	2.45	0.46
3:AC:328:VAL:HG23	3:AC:329:GLY:N	2.30	0.46
4:AD:36:LEU:O	4:AD:39:PRO:HD2	2.16	0.46
6:AF:15:ILE:HG22	6:AF:16:PHE:N	2.29	0.46
7:AH:43:LEU:O	7:AH:47:GLU:HG3	2.14	0.46
15:AU:89:GLU:CD	15:AU:89:GLU:N	2.74	0.46
18:AX:16:LEU:HD13	18:AX:16:LEU:C	2.39	0.46
1:BA:5021:VAL:HG12	1:BA:5022:THR:N	2.30	0.46
1:BA:5138:GLY:HA3	8:BI:5032:PRO:HG2	1.98	0.46
1:BA:5326:LEU:CD2	3:BC:5412:THR:HB	2.46	0.46
2:BB:5005:TRP:CZ2	31:BL:5101:LMG:H291	2.50	0.46
2:BB:5025:MET:HE2	27:BB:5621:BCR:H393	1.98	0.46
2:BB:5243:ALA:HB2	2:BB:5466:HIS:ND1	2.30	0.46
2:BB:5245:VAL:HG22	24:BB:5616:CLA:H192	1.96	0.46
2:BB:5384:ARG:NH1	15:BU:5132:LEU:HD13	2.30	0.46
4:BD:5036:LEU:O	4:BD:5039:PRO:HD2	2.15	0.46
4:BD:5299:ILE:HG13	11:BL:5037:ASN:ND2	2.30	0.46
5:BE:5017:VAL:HA	9:BJ:5008:ILE:HD11	1.96	0.46
6:BF:5023:VAL:O	6:BF:5027:ALA:CB	2.63	0.46
13:BO:5086:ARG:O	13:BO:5086:ARG:CG	2.63	0.46
13:BO:5120:THR:HG22	13:BO:5154:SER:HG	1.81	0.46
13:BO:5206:GLU:CD	13:BO:5206:GLU:N	2.73	0.46
1:AA:21:VAL:HG12	1:AA:22:THR:N	2.29	0.46
1:AA:48:PHE:CA	1:AA:115:ILE:HD11	2.45	0.46
31:AA:417:LMG:H301	2:BB:5076:SER:HB3	1.96	0.46
2:AB:112:CYS:HB3	27:AB:619:BCR:H393	1.98	0.46
2:AB:242:ILE:HG22	2:AB:466:HIS:HB2	1.96	0.46
2:AB:298:LEU:HD23	2:AB:402:TYR:CE1	2.51	0.46
3:AC:420:VAL:HB	3:AC:425:TRP:HE1	1.79	0.46
4:AD:251:ARG:HG2	4:AD:255:GLN:OE1	2.16	0.46
8:AI:30:ARG:O	8:AI:31:ASN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5064:ARG:NH1	13:BO:5098:THR:HG21	2.31	0.46
1:BA:5244:GLU:HG3	1:BA:5246:TYR:H	1.80	0.46
1:BA:5275:LEU:CD1	25:BA:5409:MST:H83	2.45	0.46
2:BB:5030:VAL:HG13	24:BB:5617:CLA:HMC2	1.96	0.46
2:BB:5225:LEU:O	2:BB:5226:TYR:C	2.59	0.46
3:BC:5057:ALA:O	3:BC:5061:VAL:HG23	2.15	0.46
3:BC:5094:THR:CG2	3:BC:5298:PRO:HD2	2.44	0.46
24:BC:5511:CLA:H141	20:BZ:5020:VAL:O	2.16	0.46
4:BD:5136:VAL:O	4:BD:5136:VAL:HG12	2.15	0.46
16:BV:5148:GLU:OE1	16:BV:5148:GLU:HA	2.15	0.46
1:AA:131:TRP:CE3	1:AA:132:GLU:HA	2.50	0.46
1:AA:220:THR:CG2	4:AD:141:TYR:HD1	2.29	0.46
29:AA:412:LHG:HC11	3:AC:447:ARG:NE	2.31	0.46
2:AB:179:GLN:HE21	2:AB:179:GLN:CA	2.18	0.46
2:AB:237:VAL:HB	24:AB:612:CLA:CMD	2.46	0.46
2:AB:348:ASN:O	2:AB:349:LYS:C	2.58	0.46
2:BB:5243:ALA:HB2	2:BB:5466:HIS:CE1	2.50	0.46
3:BC:5029:GLU:HA	10:BK:5046:ARG:HH12	1.80	0.46
3:BC:5142:GLU:C	3:BC:5144:SER:H	2.22	0.46
3:BC:5380:ILE:HA	3:BC:5384:ILE:CD1	2.37	0.46
4:BD:5250:ASN:ND2	4:BD:5262:SER:HB3	2.28	0.46
6:BF:5021:VAL:HG21	30:BF:5102:SQD:H101	1.97	0.46
13:BO:5072:GLN:O	13:BO:5263:GLY:HA3	2.14	0.46
20:BZ:5021:ILE:O	20:BZ:5025:VAL:HG22	2.16	0.46
20:BZ:5022:GLY:O	20:BZ:5023:VAL:C	2.58	0.46
1:AA:84:PRO:HA	1:AA:112:TYR:CG	2.50	0.46
2:AB:334:ASP:HB3	13:AO:202:GLN:HG3	1.98	0.46
24:AB:610:CLA:H111	24:AB:615:CLA:CAA	2.43	0.46
3:AC:239:TRP:CE3	3:AC:243:ILE:HD11	2.28	0.46
3:AC:288:CYS:HB3	28:AC:517:DGD:HG2	1.98	0.46
4:AD:67:TYR:CE1	4:AD:76:VAL:HG11	2.51	0.46
4:AD:72:ASN:HA	31:AJ:102:LMG:HC72	1.97	0.46
4:AD:88:SER:HA	7:AH:50:ASN:OD1	2.15	0.46
4:AD:155:SER:HA	4:AD:159:ILE:HG13	1.98	0.46
4:AD:210:LEU:HA	4:AD:213:ILE:HG22	1.97	0.46
1:BA:5140:ARG:HD3	4:BD:5219:GLU:O	2.15	0.46
2:BB:5124:ARG:HD3	2:BB:5131:PRO:N	2.30	0.46
30:BB:5601:SQD:H141	24:BB:5618:CLA:H143	1.97	0.46
24:BB:5609:CLA:HMA2	24:BB:5610:CLA:CMA	2.45	0.46
3:BC:5266:TRP:HZ3	24:BC:5507:CLA:HBC2	1.80	0.46
4:BD:5253:TRP:HA	4:BD:5256:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5071:LEU:HD23	13:BO:5265:PHE:CB	2.45	0.46
1:AA:32:TRP:CB	8:AI:23:PHE:CZ	2.98	0.46
1:AA:153:SER:HB2	24:AA:404:CLA:H11	1.98	0.46
24:AA:405:CLA:H72	31:AB:620:LMG:C25	2.46	0.46
2:AB:135:LEU:HD21	2:AB:234:ILE:HD13	1.98	0.46
3:AC:57:ALA:O	3:AC:61:VAL:HG23	2.16	0.46
3:AC:418:ASN:HB2	28:AC:519:DGD:HE2	1.98	0.46
4:AD:119:ALA:O	4:AD:123:ILE:HG13	2.16	0.46
5:AE:26:THR:HB	36:AF:101:HEM:C3B	2.51	0.46
10:AK:11:LEU:O	10:AK:12:PRO:C	2.59	0.46
1:BA:5010:SER:C	1:BA:5012:ASN:N	2.71	0.46
1:BA:5096:ILE:C	1:BA:5098:GLU:H	2.24	0.46
1:BA:5149:ALA:HB1	1:BA:5283:VAL:CG1	2.45	0.46
2:BB:5371:THR:HG22	2:BB:5377:VAL:CA	2.42	0.46
2:BB:5490:GLN:OE1	2:BB:5490:GLN:O	2.33	0.46
3:BC:5213:LEU:HD21	27:BC:5516:BCR:C19	2.46	0.46
3:BC:5267:SER:O	3:BC:5271:TYR:CD2	2.69	0.46
3:BC:5319:ILE:O	3:BC:5323:LYS:HG3	2.15	0.46
4:BD:5057:SER:HA	4:BD:5060:THR:HG22	1.97	0.46
4:BD:5210:LEU:HD13	4:BD:5271:MET:HG2	1.98	0.46
6:BF:5031:ILE:HG12	36:BF:5101:HEM:HMC2	1.97	0.46
7:BH:5016:SER:C	7:BH:5018:TYR:H	2.23	0.46
16:BV:5059:PHE:HA	16:BV:5063:CYS:SG	2.56	0.46
1:AA:135:TYR:HE1	3:AC:449:ARG:O	1.99	0.46
2:AB:12:LEU:HD22	2:AB:18:ARG:HB2	1.96	0.46
2:AB:107:LEU:HD21	24:AB:615:CLA:H42	1.97	0.46
2:AB:363:PHE:HD1	4:AD:326:ARG:HD2	1.80	0.46
3:AC:62:PHE:HZ	10:AK:28:ILE:CD1	2.29	0.46
3:AC:164:HIS:HA	3:AC:167:VAL:HG23	1.97	0.46
3:AC:286:ALA:HB2	24:AC:502:CLA:HMD1	1.96	0.46
4:AD:30:VAL:HG12	4:AD:31:GLY:N	2.30	0.46
4:AD:162:LEU:HD21	4:AD:167:TRP:CH2	2.50	0.46
4:AD:180:ARG:HG3	4:AD:181:PHE:N	2.31	0.46
8:AI:24:LEU:O	8:AI:26:GLY:N	2.41	0.46
9:AJ:36:LEU:C	9:AJ:38:SER:H	2.24	0.46
14:AT:1:MET:HE3	32:BM:5101:LMT:H11	1.98	0.46
17:Ay:38:LEU:HB2	20:AZ:25:VAL:HG11	1.97	0.46
20:AZ:36:SER:C	20:AZ:38:GLN:H	2.24	0.46
2:BB:5179:GLN:HE21	2:BB:5179:GLN:CA	2.17	0.46
2:BB:5356:VAL:HG22	2:BB:5370:LEU:HD21	1.97	0.46
2:BB:5384:ARG:HD3	15:BU:5132:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BB:5612:CLA:CAB	4:BD:5123:ILE:HG23	2.46	0.46
4:BD:5019:ASP:O	4:BD:5020:ASP:C	2.57	0.46
4:BD:5217:THR:O	4:BD:5221:THR:HB	2.15	0.46
1:AA:107:TYR:CD1	13:AO:141:ARG:NH1	2.84	0.46
2:AB:30:VAL:HG13	24:AB:613:CLA:HMC2	1.96	0.46
2:AB:121:GLU:HG2	7:AH:4:ARG:CD	2.43	0.46
2:AB:187:PRO:HG2	2:AB:188:ASP:H	1.80	0.46
3:AC:189:TRP:O	3:AC:190:ALA:C	2.59	0.46
3:AC:215:LYS:HZ3	3:AC:226:SER:CB	2.28	0.46
3:AC:271:TYR:HA	3:AC:274:TYR:CD2	2.50	0.46
4:AD:128:ARG:O	4:AD:129:GLN:C	2.59	0.46
9:AJ:11:TRP:CE3	10:AK:42:ALA:HB2	2.51	0.46
11:AL:22:LEU:HD13	14:AT:16:LEU:HD23	1.98	0.46
20:AZ:33:TRP:O	20:AZ:33:TRP:CD1	2.67	0.46
1:BA:5151:LEU:HD21	1:BA:5155:PHE:HE2	1.81	0.46
2:BB:5012:LEU:O	2:BB:5014:ASN:N	2.49	0.46
2:BB:5121:GLU:HG2	7:BH:5004:ARG:CD	2.42	0.46
2:BB:5425:ILE:HG22	2:BB:5426:PHE:HD2	1.78	0.46
30:BB:5601:SQD:H92	24:BB:5618:CLA:H42	1.98	0.46
3:BC:5310:SER:HG	3:BC:5355:THR:HG23	1.78	0.46
3:BC:5335:THR:HA	13:BO:5178:ARG:CD	2.46	0.46
4:BD:5128:ARG:O	4:BD:5129:GLN:C	2.59	0.46
4:BD:5193:LEU:O	4:BD:5193:LEU:HG	2.16	0.46
4:BD:5323:GLU:HG2	13:BO:5194:TYR:OH	2.16	0.46
9:BJ:5003:SER:CA	9:BJ:5007:ARG:HH22	2.29	0.46
13:BO:5086:ARG:O	13:BO:5086:ARG:CD	2.64	0.46
13:BO:5159:VAL:HG13	13:BO:5159:VAL:O	2.16	0.46
18:BX:5044:ASP:C	18:BX:5045:LYS:HD3	2.41	0.46
1:AA:159:LEU:HD11	28:AC:517:DGD:HB51	1.97	0.46
2:AB:9:HIS:HB2	24:AB:611:CLA:CGA	2.46	0.46
2:AB:485:GLU:CG	2:AB:486:LEU:N	2.78	0.46
3:AC:107:ASP:OD2	3:AC:110:PRO:HD3	2.16	0.46
4:AD:93:TRP:HA	4:AD:99:GLY:H	1.81	0.46
1:BA:5020:TRP:CD1	1:BA:5026:ASN:HD21	2.34	0.46
1:BA:5021:VAL:HG11	1:BA:5032:TRP:CE3	2.51	0.46
1:BA:5318:ALA:HB2	4:BD:5075:THR:HG22	1.97	0.46
2:BB:5285:ASN:N	2:BB:5285:ASN:HD22	2.14	0.46
2:BB:5354:LEU:HD21	2:BB:5378:LYS:CB	2.46	0.46
2:BB:5485:GLU:CG	2:BB:5486:LEU:N	2.79	0.46
3:BC:5185:LEU:HD12	3:BC:5230:LEU:HD12	1.97	0.46
4:BD:5084:SER:HB3	5:BE:5068:ASP:CA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BD:5406:PL9:H303	35:BD:5406:PL9:H262	1.97	0.46
7:BH:5006:TRP:O	7:BH:5010:ILE:HG13	2.16	0.46
12:BM:5019:SER:O	12:BM:5023:ILE:HD13	2.16	0.46
13:BO:5036:ILE:HG23	13:BO:5041:LEU:CB	2.46	0.46
13:BO:5271:PRO:HG2	13:BO:5272:ALA:H	1.81	0.46
1:AA:244:GLU:HG3	1:AA:246:TYR:H	1.80	0.45
2:AB:16:PRO:HB3	2:AB:133:LEU:HD21	1.99	0.45
2:AB:398:THR:HG22	2:AB:412:THR:HG22	1.96	0.45
24:AB:604:CLA:H111	24:AB:615:CLA:H2	1.97	0.45
3:AC:142:GLU:C	3:AC:144:SER:H	2.24	0.45
31:AC:520:LMG:H202	9:AJ:22:ILE:HG21	1.97	0.45
11:AL:7:ARG:O	11:AL:7:ARG:HD2	2.16	0.45
16:AV:102:MET:HE3	36:AV:201:HEM:HMB3	1.99	0.45
20:AZ:36:SER:C	20:AZ:38:GLN:N	2.69	0.45
1:BA:5084:PRO:HA	1:BA:5112:TYR:CG	2.49	0.45
2:BB:5356:VAL:HA	2:BB:5370:LEU:CD2	2.45	0.45
3:BC:5229:ASN:ND2	3:BC:5231:GLU:HB2	2.31	0.45
3:BC:5315:MET:HE1	3:BC:5369:LEU:CD1	2.43	0.45
13:BO:5215:ARG:HD2	15:BU:5039:LEU:HD22	1.98	0.45
14:BT:5014:ILE:HD13	14:BT:5017:PHE:CD2	2.52	0.45
1:AA:29:TYR:HD2	1:AA:133:LEU:HB2	1.80	0.45
2:AB:144:PHE:CE1	2:AB:210:ILE:CG2	2.99	0.45
2:AB:366:PHE:CD1	2:AB:367:PRO:HD2	2.52	0.45
3:AC:55:ALA:HB1	27:AC:514:BCR:C37	2.43	0.45
3:AC:75:PHE:CD1	3:AC:86:LEU:HD21	2.51	0.45
3:AC:244:CYS:HA	24:AC:506:CLA:HMC2	1.97	0.45
1:BA:5042:LEU:HD21	30:BA:5401:SQD:H152	1.97	0.45
2:BB:5016:PRO:HB3	2:BB:5133:LEU:HD21	1.97	0.45
2:BB:5329:PRO:HD3	24:BB:5611:CLA:CED	2.46	0.45
3:BC:5414:ILE:HG22	3:BC:5415:ASN:N	2.32	0.45
3:BC:5435:PHE:O	3:BC:5438:LEU:N	2.47	0.45
3:BC:5450:ALA:HA	3:BC:5455:PHE:CE2	2.51	0.45
3:BC:5455:PHE:C	3:BC:5457:LYS:H	2.24	0.45
4:BD:5119:ALA:O	4:BD:5123:ILE:HG13	2.16	0.45
6:BF:5016:PHE:HD1	6:BF:5016:PHE:N	2.14	0.45
16:BV:5141:ILE:O	16:BV:5145:ILE:HG13	2.16	0.45
2:AB:179:GLN:HA	2:AB:179:GLN:NE2	2.22	0.45
2:AB:447:PRO:O	2:AB:448:ARG:C	2.60	0.45
3:AC:318:LEU:HD21	3:AC:380:ILE:HG23	1.97	0.45
4:AD:68:LEU:CA	6:AF:40:MET:HE2	2.46	0.45
14:AT:18:PHE:CB	27:AT:101:BCR:HC8	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5102:VAL:HB	24:BB:5610:CLA:H91	1.98	0.45
2:BB:5187:PRO:C	2:BB:5189:GLY:H	2.24	0.45
3:BC:5055:ALA:HB1	27:BC:5514:BCR:C37	2.41	0.45
3:BC:5202:PRO:HB2	3:BC:5235:GLY:HA2	1.98	0.45
3:BC:5438:LEU:HD23	28:BC:5517:DGD:HAW2	1.97	0.45
4:BD:5079:SER:HA	4:BD:5172:SER:HB3	1.97	0.45
7:BH:5044:ILE:HG12	18:BX:5019:PHE:CE2	2.51	0.45
11:BL:5022:LEU:HG	31:BL:5101:LMG:C19	2.46	0.45
13:BO:5114:ASN:HD21	13:BO:5120:THR:CG2	2.29	0.45
16:BV:5130:MET:SD	16:BV:5133:LEU:HD22	2.56	0.45
1:AA:342:ASP:HB2	4:AD:352:LEU:HD21	1.98	0.45
2:AB:112:CYS:O	2:AB:116:VAL:HG23	2.16	0.45
24:AC:510:CLA:HHC	24:AC:510:CLA:HBB1	1.98	0.45
4:AD:291:LEU:O	4:AD:292:ASN:HB2	2.16	0.45
35:AD:405:PL9:H303	35:AD:405:PL9:H262	1.98	0.45
6:AF:24:HIS:NE2	36:AF:101:HEM:NB	2.65	0.45
13:AO:135:GLN:HE21	13:AO:135:GLN:HB3	1.48	0.45
16:AV:118:HIS:ND1	16:AV:119:PRO:HD2	2.31	0.45
1:BA:5041:LEU:HD21	1:BA:5122:GLY:HA3	1.99	0.45
1:BA:5292:THR:HB	28:BC:5518:DGD:HAH2	1.99	0.45
2:BB:5041:GLU:HB3	2:BB:5060:MET:SD	2.55	0.45
24:BB:5612:CLA:C1	24:BB:5612:CLA:HAA1	2.45	0.45
3:BC:5472:LEU:HD11	4:BD:5255:GLN:CD	2.40	0.45
4:BD:5057:SER:CA	4:BD:5060:THR:HG22	2.46	0.45
4:BD:5088:SER:HA	7:BH:5050:ASN:OD1	2.16	0.45
8:BI:5024:LEU:O	8:BI:5026:GLY:N	2.41	0.45
1:AA:65:GLU:N	1:AA:66:PRO:HD3	2.32	0.45
1:AA:234:ASN:HD21	4:AD:266:TRP:CA	2.30	0.45
2:AB:153:PHE:O	2:AB:157:HIS:HB3	2.17	0.45
24:AB:612:CLA:H13	24:AB:613:CLA:CBB	2.47	0.45
3:AC:213:LEU:HD21	27:AC:516:BCR:C19	2.47	0.45
24:AC:507:CLA:O1D	24:AC:509:CLA:H101	2.17	0.45
5:AE:17:VAL:HG22	9:AJ:8:ILE:CD1	2.47	0.45
5:AE:36:LEU:HA	5:AE:39:SER:OG	2.16	0.45
13:AO:215:ARG:HD2	15:AU:39:LEU:HD22	1.97	0.45
18:AX:43:ILE:O	18:AX:43:ILE:CG2	2.64	0.45
1:BA:5045:THR:CG2	1:BA:5046:ILE:N	2.79	0.45
1:BA:5216:GLY:O	1:BA:5220:THR:HG22	2.17	0.45
2:BB:5007:ARG:HG2	24:BB:5615:CLA:HED1	1.97	0.45
24:BB:5608:CLA:H111	24:BB:5619:CLA:H2	1.99	0.45
10:BK:5021:LEU:HD11	27:BK:5102:BCR:HC42	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:29:TYR:CD2	1:AA:133:LEU:HB2	2.51	0.45
1:AA:129:ARG:C	1:AA:131:TRP:H	2.23	0.45
3:AC:365:TRP:HA	3:AC:387:TRP:CH2	2.51	0.45
5:AE:14:ILE:HG22	9:AJ:13:VAL:HG11	1.99	0.45
5:AE:51:ARG:O	5:AE:53:ASP:N	2.49	0.45
16:AV:103:LYS:O	16:AV:122:ARG:HG2	2.17	0.45
20:AZ:30:PRO:HA	20:AZ:33:TRP:CE3	2.51	0.45
24:BA:5408:CLA:HBC1	31:BI:5101:LMG:H361	1.98	0.45
2:BB:5153:PHE:O	2:BB:5157:HIS:HB3	2.17	0.45
2:BB:5200:ALA:HB3	24:BB:5606:CLA:HMB1	1.98	0.45
2:BB:5234:ILE:HD12	2:BB:5237:VAL:CG2	2.45	0.45
2:BB:5278:SER:HB3	2:BB:5281:GLN:NE2	2.31	0.45
2:BB:5279:TYR:HE1	7:BH:5063:LYS:HE3	1.80	0.45
2:BB:5385:ARG:O	2:BB:5386:ALA:C	2.60	0.45
2:BB:5390:TYR:HD2	4:BD:5344:GLU:OE1	2.00	0.45
3:BC:5193:GLY:O	3:BC:5194:GLY:O	2.34	0.45
4:BD:5038:PHE:CE2	4:BD:5128:ARG:NH2	2.85	0.45
4:BD:5176:ALA:HA	4:BD:5179:PHE:CD2	2.52	0.45
4:BD:5251:ARG:HG2	4:BD:5255:GLN:OE1	2.17	0.45
32:BD:5411:LMT:O2'	18:BX:5021:ILE:HG21	2.15	0.45
6:BF:5030:THR:HG22	6:BF:5034:LEU:CD1	2.47	0.45
9:BJ:5003:SER:CB	9:BJ:5007:ARG:HH22	2.30	0.45
12:BM:5003:VAL:HG11	14:BT:5002:GLU:HG2	1.99	0.45
13:BO:5184:ASP:HB2	13:BO:5185:PRO:HD2	1.99	0.45
13:BO:5210:ARG:HA	15:BU:5039:LEU:HD13	1.97	0.45
15:BU:5056:ASP:OD2	15:BU:5115:THR:OG1	2.34	0.45
16:BV:5081:ARG:HG2	16:BV:5081:ARG:NH1	2.31	0.45
27:AB:617:BCR:HC41	12:AM:9:ILE:HG23	1.98	0.45
3:AC:38:GLY:HA3	24:AC:511:CLA:C2D	2.46	0.45
28:AC:518:DGD:O3D	27:AJ:101:BCR:H382	2.16	0.45
8:AI:10:ILE:HG21	32:AI:102:LMT:H82	1.98	0.45
8:AI:14:PHE:CE2	8:AI:18:LEU:HD11	2.52	0.45
13:AO:171:GLU:HA	13:AO:221:GLY:O	2.17	0.45
20:AZ:9:LEU:HD13	20:AZ:54:VAL:HG11	1.97	0.45
1:BA:5013:LEU:CA	1:BA:5016:ARG:HH11	2.30	0.45
1:BA:5180:PHE:O	1:BA:5184:ILE:HG13	2.17	0.45
1:BA:5295:PHE:O	3:BC:5424:SER:OG	2.31	0.45
2:BB:5112:CYS:O	2:BB:5116:VAL:HG23	2.16	0.45
3:BC:5276:LEU:HD23	3:BC:5276:LEU:HA	1.75	0.45
4:BD:5035:ILE:O	24:BD:5405:CLA:HBB2	2.16	0.45
8:BI:5007:THR:O	8:BI:5008:VAL:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BK:5011:LEU:HD12	10:BK:5019:ASP:HA	1.98	0.45
12:BM:5033:GLN:HG2	12:BM:5034:LYS:N	2.32	0.45
13:BO:5081:GLU:C	13:BO:5083:LYS:H	2.25	0.45
13:BO:5126:GLY:O	13:BO:5128:ASP:N	2.50	0.45
15:BU:5066:ILE:CG1	15:BU:5072:TYR:CD1	3.00	0.45
16:BV:5124:ALA:HB1	16:BV:5131:ARG:CG	2.47	0.45
20:BZ:5009:LEU:HD13	20:BZ:5054:VAL:HG11	1.98	0.45
1:AA:103:ASP:OD1	31:AA:417:LMG:H342	2.16	0.45
3:AC:249:ILE:O	3:AC:253:LEU:HG	2.17	0.45
3:AC:435:PHE:O	3:AC:438:LEU:N	2.49	0.45
3:AC:472:LEU:HG	4:AD:251:ARG:HH12	1.80	0.45
4:AD:277:THR:HG22	35:AD:405:PL9:H272	1.98	0.45
6:AF:37:ILE:HG22	9:AJ:28:PHE:CE1	2.52	0.45
13:AO:56:TYR:O	13:AO:161:SER:HA	2.17	0.45
13:AO:71:LEU:HD23	13:AO:265:PHE:CB	2.47	0.45
13:AO:83:LYS:HG2	13:AO:84:ASN:N	2.28	0.45
13:AO:91:PHE:CD1	13:AO:260:LYS:HB2	2.51	0.45
13:AO:120:THR:HG22	13:AO:154:SER:HG	1.81	0.45
13:AO:147:THR:O	13:AO:172:PHE:CE2	2.70	0.45
2:BB:5088:PRO:HD2	28:BB:5602:DGD:O4D	2.17	0.45
2:BB:5229:LEU:O	2:BB:5231:MET:N	2.50	0.45
2:BB:5357:ARG:NH2	4:BD:5337:GLU:OE1	2.50	0.45
24:BB:5612:CLA:HBA1	30:BB:5625:SQD:H102	1.98	0.45
3:BC:5095:LEU:HD21	24:BC:5501:CLA:OBD	2.16	0.45
3:BC:5208:VAL:O	3:BC:5209:ILE:C	2.60	0.45
3:BC:5239:TRP:CE3	3:BC:5243:ILE:HD11	2.27	0.45
3:BC:5425:TRP:CD1	24:BC:5504:CLA:HMA2	2.51	0.45
4:BD:5067:TYR:CE1	4:BD:5076:VAL:HG11	2.51	0.45
7:BH:5055:LEU:HB2	7:BH:5058:VAL:CG1	2.46	0.45
13:BO:5056:TYR:O	13:BO:5161:SER:HA	2.17	0.45
17:By:5041:VAL:C	17:By:5043:ARG:N	2.72	0.45
1:AA:176:ILE:HD12	24:AA:405:CLA:HED3	1.98	0.45
2:AB:69:LEU:HD21	24:AB:603:CLA:OBD	2.17	0.45
2:AB:112:CYS:HA	27:AB:617:BCR:H282	1.98	0.45
2:AB:345:VAL:HG21	2:AB:402:TYR:HE2	1.82	0.45
3:AC:180:MET:HE3	3:AC:202:PRO:HD3	1.98	0.45
3:AC:347:GLY:CA	13:AO:43:ASN:HB2	2.45	0.45
24:AC:511:CLA:H2	24:AC:511:CLA:H61	1.86	0.45
4:AD:199:MET:O	4:AD:200:GLY:C	2.59	0.45
8:AI:19:PHE:CE1	8:AI:23:PHE:CE2	3.00	0.45
12:AM:5:GLN:HE22	32:AM:102:LMT:H3'	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:168:PHE:O	13:AO:224:SER:HA	2.17	0.45
17:Ay:26:ALA:O	17:Ay:30:ILE:HG12	2.17	0.45
17:Ay:39:LEU:HG	20:AZ:25:VAL:HG12	1.99	0.45
18:AX:24:LEU:HD12	18:AX:24:LEU:HA	1.69	0.45
1:BA:5129:ARG:C	1:BA:5131:TRP:H	2.25	0.45
1:BA:5172:MET:HE1	24:BA:5406:CLA:CHC	2.47	0.45
2:BB:5008:VAL:HG22	24:BB:5615:CLA:O1A	2.17	0.45
24:BB:5620:CLA:HHC	24:BB:5620:CLA:HBB1	1.99	0.45
3:BC:5256:PRO:HG2	3:BC:5266:TRP:CH2	2.51	0.45
3:BC:5328:VAL:HG23	3:BC:5329:GLY:N	2.31	0.45
7:BH:5018:TYR:CD1	7:BH:5018:TYR:C	2.94	0.45
18:BX:5043:ILE:O	18:BX:5043:ILE:CG2	2.64	0.45
1:AA:224:ILE:H	1:AA:224:ILE:HG13	1.55	0.45
2:AB:124:ARG:HD3	2:AB:131:PRO:N	2.32	0.45
2:AB:172:TYR:O	2:AB:174:LEU:HG	2.17	0.45
2:AB:476:ARG:HB3	2:AB:476:ARG:CZ	2.46	0.45
24:AB:611:CLA:H52	24:AB:614:CLA:HBC2	1.99	0.45
3:AC:414:ILE:HG22	3:AC:415:ASN:N	2.31	0.45
3:AC:437:PHE:CD2	24:AC:508:CLA:HMC1	2.51	0.45
24:AC:501:CLA:HMB2	24:AC:501:CLA:H61	1.97	0.45
2:BB:5009:HIS:HB2	24:BB:5615:CLA:CGA	2.47	0.45
2:BB:5073:GLY:O	2:BB:5093:PHE:CD1	2.70	0.45
3:BC:5164:HIS:HA	3:BC:5167:VAL:HG23	1.98	0.45
3:BC:5472:LEU:O	3:BC:5473:ASP:O	2.35	0.45
24:BC:5511:CLA:H151	20:BZ:5024:PRO:CG	2.45	0.45
4:BD:5238:THR:O	4:BD:5239:GLN:C	2.59	0.45
24:BD:5405:CLA:H41	18:BX:5023:LEU:CD1	2.42	0.45
31:BM:5102:LMG:O8	31:BM:5102:LMG:O9	2.35	0.45
16:BV:5064:ALA:O	16:BV:5065:SER:C	2.60	0.45
20:BZ:5030:PRO:HB3	20:BZ:5033:TRP:CZ3	2.51	0.45
1:AA:93:PHE:CE2	24:AA:407:CLA:HBA1	2.52	0.44
1:AA:187:GLN:HG2	4:AD:183:LEU:HD21	2.00	0.44
2:AB:193:TYR:CD1	2:AB:260:SER:HA	2.52	0.44
2:AB:223:GLN:HG3	2:AB:227:LYS:CE	2.41	0.44
31:AB:620:LMG:C19	11:AL:22:LEU:HG	2.46	0.44
3:AC:342:MET:HE1	3:AC:356:MET:HE2	2.00	0.44
4:AD:70:GLY:O	9:AJ:37:GLY:CA	2.64	0.44
6:AF:31:ILE:HG12	36:AF:101:HEM:HMC2	1.99	0.44
18:AX:12:ILE:CD1	18:AX:16:LEU:HD12	2.47	0.44
1:BA:5271:LEU:CD1	25:BA:5409:MST:H162	2.45	0.44
2:BB:5035:GLY:O	2:BB:5038:ALA:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5076:SER:HG	2:BB:5078:TRP:CD1	2.35	0.44
30:BB:5625:SQD:H281	32:BB:5627:LMT:H82	1.98	0.44
4:BD:5052:THR:HG22	4:BD:5067:TYR:CZ	2.53	0.44
4:BD:5053:THR:CB	4:BD:5067:TYR:HD2	2.30	0.44
4:BD:5096:GLU:CD	4:BD:5096:GLU:N	2.75	0.44
5:BE:5051:ARG:O	5:BE:5054:SER:N	2.50	0.44
7:BH:5062:TRP:CD1	28:BH:5101:DGD:O3E	2.61	0.44
13:BO:5155:THR:HG23	13:BO:5168:PHE:CD2	2.52	0.44
16:BV:5092:ARG:HG3	16:BV:5092:ARG:NH1	2.31	0.44
1:AA:12:ASN:O	1:AA:13:LEU:C	2.60	0.44
2:AB:15:ASP:O	2:AB:17:GLY:N	2.50	0.44
4:AD:87:HIS:HD2	4:AD:166:SER:HA	1.74	0.44
4:AD:136:VAL:HG12	4:AD:136:VAL:O	2.16	0.44
6:AF:15:ILE:HG23	36:AF:101:HEM:HAA1	1.98	0.44
13:AO:72:GLN:O	13:AO:263:GLY:HA3	2.17	0.44
16:AV:121:LEU:CD2	16:AV:138:LEU:HD11	2.47	0.44
1:BA:5011:ALA:O	1:BA:5012:ASN:HB3	2.17	0.44
1:BA:5032:TRP:CZ2	8:BI:5022:GLY:HA2	2.52	0.44
1:BA:5343:LEU:O	1:BA:5344:ALA:CB	2.64	0.44
2:BB:5173:GLY:N	2:BB:5265:ILE:HD11	2.33	0.44
2:BB:5399:VAL:HG12	2:BB:5417:VAL:HG22	1.99	0.44
24:BC:5511:CLA:C14	20:BZ:5024:PRO:HG2	2.47	0.44
4:BD:5218:VAL:HG22	4:BD:5244:TYR:CD2	2.53	0.44
4:BD:5261:PHE:CG	4:BD:5267:LEU:HD12	2.53	0.44
13:BO:5184:ASP:OD2	13:BO:5188:ARG:HB2	2.17	0.44
15:BU:5089:GLU:C	15:BU:5091:VAL:N	2.75	0.44
31:AA:414:LMG:H142	29:AA:415:LHG:H102	1.99	0.44
2:AB:225:LEU:O	2:AB:226:TYR:C	2.60	0.44
2:AB:248:ALA:CA	24:AB:603:CLA:H42	2.32	0.44
4:AD:78:VAL:HG11	4:AD:114:ILE:HD12	1.98	0.44
31:AD:408:LMG:HC71	11:AL:15:THR:HG23	1.98	0.44
9:AJ:24:ILE:HG23	9:AJ:25:VAL:N	2.32	0.44
12:AM:28:GLN:HB3	12:BM:5027:VAL:HG12	1.99	0.44
18:AX:12:ILE:H	27:AX:101:BCR:C29	2.30	0.44
1:BA:5042:LEU:HD23	1:BA:5042:LEU:HA	1.76	0.44
1:BA:5051:ALA:HA	27:BA:5411:BCR:H381	1.99	0.44
1:BA:5292:THR:C	1:BA:5294:ALA:H	2.24	0.44
2:BB:5045:PHE:HE2	2:BB:5047:PRO:HB3	1.83	0.44
2:BB:5485:GLU:HG2	2:BB:5486:LEU:N	2.31	0.44
24:BC:5507:CLA:O1D	24:BC:5509:CLA:H101	2.17	0.44
5:BE:5078:THR:O	5:BE:5082:GLN:OE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BI:5030:ARG:O	8:BI:5031:ASN:HB3	2.17	0.44
31:BI:5101:LMG:H132	32:BI:5102:LMT:H42	1.98	0.44
12:BM:5001:MET:CG	12:BM:5002:GLU:N	2.81	0.44
13:BO:5055:ALA:HA	13:BO:5230:VAL:HG11	1.99	0.44
14:BT:5016:LEU:O	14:BT:5017:PHE:C	2.60	0.44
18:BX:5030:LEU:HD23	18:BX:5030:LEU:HA	1.87	0.44
2:AB:222:PRO:O	2:AB:223:GLN:C	2.58	0.44
4:AD:127:LEU:HD23	4:AD:127:LEU:HA	1.80	0.44
10:AK:18:PHE:O	10:AK:19:ASP:C	2.60	0.44
11:AL:24:ILE:HG21	12:AM:19:SER:OG	2.17	0.44
1:BA:5153:SER:CB	24:BA:5405:CLA:H11	2.47	0.44
2:BB:5334:ASP:HB3	13:BO:5202:GLN:HG3	2.00	0.44
3:BC:5166:ILE:HG13	3:BC:5248:GLY:HA3	1.99	0.44
3:BC:5205:ASP:OD1	3:BC:5207:ARG:HB3	2.17	0.44
4:BD:5068:LEU:HA	6:BF:5040:MET:HE2	1.99	0.44
4:BD:5176:ALA:C	4:BD:5178:ILE:H	2.25	0.44
4:BD:5291:LEU:O	4:BD:5292:ASN:HB2	2.17	0.44
5:BE:5015:THR:CG2	9:BJ:5006:GLY:HA2	2.47	0.44
5:BE:5026:THR:HB	36:BF:5101:HEM:C3B	2.53	0.44
6:BF:5030:THR:HG22	6:BF:5034:LEU:HD12	1.99	0.44
7:BH:5019:GLY:O	7:BH:5021:VAL:CG1	2.66	0.44
13:BO:5080:GLU:O	13:BO:5089:ALA:CB	2.65	0.44
13:BO:5109:GLY:HA3	13:BO:5122:VAL:O	2.16	0.44
20:BZ:5024:PRO:C	20:BZ:5026:ALA:N	2.75	0.44
1:AA:59:ASP:OD2	1:AA:62:GLY:HA2	2.17	0.44
1:AA:91:LEU:HD11	1:AA:163:ILE:HA	1.99	0.44
1:AA:110:GLY:O	1:AA:111:PRO:C	2.60	0.44
1:AA:113:GLN:HB3	1:AA:117:PHE:CE2	2.52	0.44
2:AB:11:VAL:HG23	11:AL:6:ASN:O	2.18	0.44
2:AB:252:VAL:HG12	24:AB:603:CLA:O1A	2.17	0.44
3:AC:42:LEU:HD21	24:AC:511:CLA:H2A	1.98	0.44
3:AC:165:LEU:HD11	24:AC:506:CLA:CHC	2.47	0.44
3:AC:414:ILE:HD11	16:AV:163:TYR:CG	2.53	0.44
3:AC:438:LEU:HD23	28:AC:517:DGD:HAW2	1.99	0.44
4:AD:195:PRO:HD3	11:AL:34:TYR:CE1	2.52	0.44
4:AD:279:LEU:CD2	24:AD:401:CLA:HMA2	2.47	0.44
5:AE:49:THR:HA	5:AE:50:PRO:HD3	1.86	0.44
11:AL:17:LEU:HD12	12:AM:22:LEU:HB3	2.00	0.44
13:AO:210:ARG:HA	15:AU:39:LEU:HD13	1.99	0.44
15:AU:56:ASP:OD2	15:AU:115:THR:OG1	2.36	0.44
1:BA:5185:VAL:O	1:BA:5186:PHE:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5222:PRO:HG3	7:BH:5027:THR:N	2.30	0.44
3:BC:5045:LEU:O	3:BC:5046:SER:C	2.60	0.44
24:BD:5402:CLA:H2	34:BD:5404:PHO:HBB1	2.00	0.44
11:BL:5016:SER:HA	11:BL:5019:LEU:CD1	2.48	0.44
15:BU:5058:ASN:OD1	15:BU:5084:PRO:CA	2.65	0.44
17:By:5034:MET:HE2	17:By:5037:PHE:HB3	2.00	0.44
18:BX:5012:ILE:HD13	18:BX:5016:LEU:HD12	1.98	0.44
20:BZ:5036:SER:C	20:BZ:5038:GLN:H	2.25	0.44
1:AA:12:ASN:O	1:AA:15:GLU:HB3	2.17	0.44
1:AA:20:TRP:CD1	1:AA:26:ASN:HD21	2.36	0.44
1:AA:41:LEU:HD21	1:AA:122:GLY:HA3	2.00	0.44
1:AA:141:PRO:HG3	3:AC:446:GLY:C	2.43	0.44
24:AB:606:CLA:H52	27:AB:619:BCR:H321	2.00	0.44
3:AC:205:ASP:OD1	3:AC:207:ARG:HB3	2.18	0.44
3:AC:338:GLY:O	3:AC:339:LYS:C	2.60	0.44
3:AC:344:SER:HB2	3:AC:345:PRO:CD	2.48	0.44
4:AD:122:LEU:HB3	4:AD:150:ILE:HD11	1.99	0.44
4:AD:186:GLN:HB2	24:AD:401:CLA:HBC1	2.00	0.44
4:AD:323:GLU:HG2	13:AO:194:TYR:OH	2.18	0.44
4:AD:346:LEU:O	4:AD:348:ARG:HG3	2.18	0.44
6:AF:17:THR:O	6:AF:21:VAL:HG23	2.18	0.44
7:AH:16:SER:C	7:AH:18:TYR:H	2.25	0.44
11:AL:36:PHE:O	11:AL:37:ASN:C	2.61	0.44
12:AM:20:VAL:HG11	12:BM:5020:VAL:HG22	2.00	0.44
13:AO:184:ASP:HB2	13:AO:185:PRO:HD2	1.99	0.44
18:AX:22:GLY:HA2	18:AX:25:SER:OG	2.18	0.44
2:BB:5054:PRO:HD2	2:BB:5057:ARG:HG3	2.00	0.44
2:BB:5466:HIS:HE1	24:BB:5612:CLA:C4D	2.30	0.44
28:BB:5602:DGD:C6E	32:BB:5626:LMT:H2'	2.47	0.44
24:BB:5607:CLA:H2	24:BB:5609:CLA:H91	2.00	0.44
3:BC:5057:ALA:CB	24:BC:5512:CLA:HED2	2.48	0.44
3:BC:5176:VAL:O	3:BC:5180:MET:HG3	2.17	0.44
4:BD:5221:THR:HG23	4:BD:5221:THR:O	2.16	0.44
16:BV:5102:MET:HE3	36:BV:5201:HEM:HMB3	1.99	0.44
1:AA:129:ARG:C	1:AA:131:TRP:N	2.76	0.44
2:AB:63:LEU:N	2:AB:64:PRO:HD2	2.32	0.44
2:AB:369:ILE:C	2:AB:370:LEU:HD23	2.41	0.44
2:AB:483:ASP:OD2	2:AB:484:PRO:HD2	2.18	0.44
3:AC:217:PRO:O	28:AC:517:DGD:HB21	2.17	0.44
3:AC:296:VAL:HG23	3:AC:297:TYR:CD2	2.53	0.44
3:AC:425:TRP:CD1	24:AC:504:CLA:HMA2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:333:ASP:C	4:AD:335:PRO:HD3	2.42	0.44
10:AK:12:PRO:CB	20:AZ:62:VAL:HG11	2.48	0.44
13:AO:94:THR:HB	13:AO:135:GLN:O	2.18	0.44
1:BA:5135:TYR:HD2	1:BA:5136:ARG:HH11	1.64	0.44
2:BB:5150:CYS:HB2	24:BB:5607:CLA:CMC	2.47	0.44
2:BB:5387:GLU:OE2	33:BB:5628:DMS:H13	2.17	0.44
24:BB:5612:CLA:HMA1	4:BD:5130:PHE:CE1	2.53	0.44
3:BC:5053:HIS:ND1	24:BC:5509:CLA:H141	2.33	0.44
3:BC:5053:HIS:HB3	24:BC:5512:CLA:OBD	2.17	0.44
3:BC:5116:VAL:CG2	3:BC:5117:VAL:N	2.81	0.44
4:BD:5145:ALA:HB2	4:BD:5272:LEU:CD2	2.47	0.44
31:BD:5410:LMG:HC71	11:BL:5015:THR:HG23	1.99	0.44
8:BI:5011:VAL:CG2	32:BI:5102:LMT:H101	2.46	0.44
8:BI:5028:PRO:O	8:BI:5031:ASN:ND2	2.51	0.44
10:BK:5025:LEU:HB2	10:BK:5026:PRO:HD3	2.00	0.44
13:BO:5036:ILE:HG23	13:BO:5041:LEU:HB2	2.00	0.44
20:BZ:5002:THR:O	20:BZ:5005:PHE:HB3	2.18	0.44
1:AA:292:THR:HB	28:AC:518:DGD:HAH2	1.99	0.44
2:AB:15:ASP:O	2:AB:16:PRO:C	2.61	0.44
24:AB:614:CLA:H162	31:AB:620:LMG:H422	1.98	0.44
4:AD:14:TRP:CG	4:AD:15:PHE:N	2.85	0.44
4:AD:161:PRO:CB	4:AD:170:ALA:HB2	2.47	0.44
10:AK:33:LEU:C	10:AK:33:LEU:HD13	2.43	0.44
11:AL:16:SER:O	11:AL:19:LEU:HD12	2.17	0.44
12:AM:18:PRO:O	12:AM:21:PHE:HB3	2.18	0.44
13:AO:141:ARG:HG2	13:AO:141:ARG:HH11	1.83	0.44
1:BA:5059:ASP:OD1	1:BA:5064:ARG:N	2.50	0.44
1:BA:5272:HIS:CD2	4:BD:5218:VAL:HG11	2.53	0.44
1:BA:5304:HIS:CD2	1:BA:5313:VAL:HG11	2.52	0.44
2:BB:5144:PHE:CE1	2:BB:5210:ILE:CG2	3.01	0.44
2:BB:5326:ARG:HD3	2:BB:5442:ILE:HG22	1.98	0.44
2:BB:5363:PHE:CD1	4:BD:5326:ARG:HD2	2.52	0.44
3:BC:5264:PHE:CE1	27:BC:5516:BCR:H321	2.49	0.44
4:BD:5176:ALA:C	4:BD:5178:ILE:N	2.76	0.44
35:BD:5406:PL9:H103	35:BD:5406:PL9:HC72	1.77	0.44
18:BX:5044:ASP:C	18:BX:5045:LYS:CD	2.91	0.44
28:AA:411:DGD:HA82	3:AC:223:TRP:CH2	2.53	0.44
2:AB:7:ARG:HG2	24:AB:611:CLA:HED1	1.99	0.44
2:AB:153:PHE:CZ	2:AB:158:LEU:HD21	2.53	0.44
2:AB:187:PRO:C	2:AB:189:GLY:H	2.26	0.44
3:AC:455:PHE:C	3:AC:457:LYS:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:472:LEU:HD11	4:AD:255:GLN:CD	2.43	0.44
4:AD:126:MET:HE1	4:AD:147:SER:HA	2.00	0.44
4:AD:253:TRP:HA	4:AD:256:ILE:CG2	2.48	0.44
7:AH:19:GLY:O	7:AH:21:VAL:CG1	2.66	0.44
1:BA:5107:TYR:CD1	13:BO:5141:ARG:NH1	2.86	0.44
1:BA:5131:TRP:HZ3	1:BA:5132:GLU:HG3	1.83	0.44
1:BA:5141:PRO:HG3	3:BC:5446:GLY:C	2.43	0.44
1:BA:5276:ALA:HB2	4:BD:5215:GLY:HA3	2.00	0.44
24:BA:5406:CLA:H72	31:BL:5101:LMG:C25	2.47	0.44
2:BB:5049:ASP:HA	2:BB:5050:PRO:HD2	1.81	0.44
3:BC:5028:GLN:HB2	24:BC:5511:CLA:HED1	1.99	0.44
3:BC:5029:GLU:CB	10:BK:5046:ARG:NH1	2.79	0.44
3:BC:5080:PRO:HB3	3:BC:5082:TYR:CE1	2.53	0.44
3:BC:5244:CYS:HA	24:BC:5506:CLA:HMC2	2.00	0.44
3:BC:5416:SER:CA	28:BC:5519:DGD:O3E	2.66	0.44
2:AB:169:SER:O	7:AH:65:LEU:HG	2.18	0.43
2:AB:246:PHE:CD2	2:AB:463:PHE:HA	2.53	0.43
24:AB:608:CLA:HMA1	4:AD:130:PHE:CE1	2.53	0.43
30:AB:627:SQD:H45	14:BT:5023:PHE:CD1	2.52	0.43
3:AC:311:GLN:OE1	3:AC:355:THR:CG2	2.66	0.43
4:AD:128:ARG:CG	4:AD:129:GLN:N	2.81	0.43
13:AO:51:THR:OG1	13:AO:52:ALA:N	2.50	0.43
2:BB:5091:TRP:CE3	24:BB:5610:CLA:O1A	2.71	0.43
2:BB:5137:LYS:HG3	2:BB:5220:ARG:NH2	2.32	0.43
24:BB:5607:CLA:H3A	24:BB:5607:CLA:CGA	2.48	0.43
3:BC:5347:GLY:CA	13:BO:5043:ASN:HB2	2.47	0.43
4:BD:5183:LEU:HD23	4:BD:5183:LEU:HA	1.87	0.43
4:BD:5246:MET:HE2	4:BD:5264:LYS:H	1.83	0.43
4:BD:5253:TRP:HB2	4:BD:5260:ALA:CB	2.48	0.43
5:BE:5008:ARG:HB2	6:BF:5013:TYR:CB	2.47	0.43
13:BO:5190:LEU:HB2	13:BO:5214:LYS:HB2	2.00	0.43
1:AA:309:ALA:HB3	16:AV:27:ALA:O	2.17	0.43
2:AB:24:LEU:HD13	2:AB:110:ALA:C	2.43	0.43
2:AB:137:LYS:HG3	2:AB:220:ARG:NH2	2.33	0.43
2:AB:250:PHE:HB3	28:AH:101:DGD:HB82	2.00	0.43
24:AB:608:CLA:HBA1	30:AB:622:SQD:H102	2.00	0.43
3:AC:116:VAL:CG2	3:AC:117:VAL:N	2.81	0.43
3:AC:143:TYR:O	3:AC:144:SER:CB	2.65	0.43
3:AC:318:LEU:HD23	3:AC:318:LEU:C	2.44	0.43
4:AD:266:TRP:HE1	31:AD:408:LMG:HC72	1.82	0.43
4:AD:329:MET:O	4:AD:330:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:82:GLN:O	5:AE:83:LEU:C	2.60	0.43
9:AJ:3:SER:CA	9:AJ:7:ARG:HH22	2.32	0.43
11:AL:9:PRO:HB3	31:BM:5102:LMG:O2	2.18	0.43
13:AO:59:ASP:C	13:AO:61:SER:N	2.76	0.43
14:AT:23:PHE:CD1	30:BB:5601:SQD:H45	2.53	0.43
15:AU:72:TYR:CB	15:AU:73:PRO:HD3	2.40	0.43
1:BA:5093:PHE:CE2	24:BA:5408:CLA:HBA1	2.52	0.43
24:BB:5614:CLA:H2	24:BB:5614:CLA:H61	1.88	0.43
24:BB:5616:CLA:H13	24:BB:5617:CLA:CBB	2.47	0.43
4:BD:5060:THR:C	4:BD:5061:HIS:HD2	2.26	0.43
4:BD:5081:PRO:HB2	4:BD:5085:MET:HG3	1.99	0.43
4:BD:5190:ASN:HB2	4:BD:5296:TYR:CE1	2.53	0.43
5:BE:5008:ARG:NH2	9:BJ:5004:GLU:HB2	2.34	0.43
17:By:5042:ARG:O	17:By:5043:ARG:C	2.60	0.43
2:AB:247:PHE:O	2:AB:251:VAL:HG23	2.19	0.43
2:AB:260:SER:C	2:AB:262:THR:N	2.76	0.43
3:AC:166:ILE:HG13	3:AC:248:GLY:HA3	2.01	0.43
3:AC:185:LEU:HD12	3:AC:230:LEU:HD12	2.00	0.43
4:AD:238:THR:O	4:AD:239:GLN:C	2.60	0.43
7:AH:63:LYS:C	7:AH:65:LEU:N	2.73	0.43
31:AM:101:LMG:H132	24:BB:5618:CLA:H12	2.00	0.43
16:AV:54:GLU:O	16:AV:58:LEU:HG	2.18	0.43
17:Ay:42:ARG:O	17:Ay:43:ARG:C	2.61	0.43
18:AX:20:PHE:HZ	27:AX:101:BCR:H371	1.84	0.43
1:BA:5193:LEU:CD1	4:BD:5179:PHE:HB3	2.47	0.43
1:BA:5234:ASN:HD21	4:BD:5266:TRP:CA	2.30	0.43
2:BB:5024:LEU:HD13	2:BB:5111:ALA:N	2.34	0.43
2:BB:5222:PRO:CG	7:BH:5027:THR:H	2.26	0.43
2:BB:5447:PRO:O	2:BB:5448:ARG:C	2.60	0.43
3:BC:5161:LEU:HD23	3:BC:5251:HIS:HD2	1.84	0.43
3:BC:5224:ILE:HG22	3:BC:5289:PHE:CZ	2.53	0.43
4:BD:5279:LEU:CD2	24:BD:5402:CLA:HMA2	2.48	0.43
12:BM:5021:PHE:CD2	12:BM:5022:LEU:HD23	2.53	0.43
13:BO:5155:THR:HG22	13:BO:5167:ASP:O	2.18	0.43
2:AB:413:ASP:O	2:AB:413:ASP:CG	2.62	0.43
3:AC:342:MET:HE3	3:AC:352:GLY:CA	2.46	0.43
3:AC:438:LEU:HD12	3:AC:438:LEU:O	2.18	0.43
31:AI:101:LMG:H132	32:AI:102:LMT:H42	2.00	0.43
13:AO:184:ASP:OD2	13:AO:188:ARG:HB2	2.17	0.43
1:BA:5309:ALA:HB3	5:BE:5053:ASP:HA	2.01	0.43
2:BB:5075:TRP:CZ3	28:BB:5602:DGD:HB32	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5179:GLN:HA	2:BB:5179:GLN:NE2	2.22	0.43
2:BB:5343:HIS:O	2:BB:5401:PHE:HA	2.18	0.43
2:BB:5356:VAL:HG22	2:BB:5370:LEU:CD2	2.48	0.43
2:BB:5476:ARG:HB3	2:BB:5476:ARG:CZ	2.44	0.43
3:BC:5407:VAL:HA	28:BC:5519:DGD:O2E	2.18	0.43
4:BD:5126:MET:HE2	4:BD:5146:PHE:HB3	2.01	0.43
5:BE:5007:GLU:O	5:BE:5009:PRO:HD3	2.17	0.43
10:BK:5033:LEU:C	10:BK:5033:LEU:HD13	2.44	0.43
13:BO:5135:GLN:HE21	13:BO:5135:GLN:HB3	1.53	0.43
13:BO:5168:PHE:O	13:BO:5224:SER:HA	2.18	0.43
17:By:5032:GLY:N	17:By:5033:PRO:HD2	2.32	0.43
2:AB:37:MET:O	2:AB:41:GLU:HG3	2.18	0.43
27:AC:514:BCR:H11C	27:AK:102:BCR:H322	2.00	0.43
4:AD:17:ILE:CG2	18:AX:42:GLN:HG2	2.42	0.43
7:AH:17:GLU:CD	7:AH:17:GLU:N	2.77	0.43
14:AT:18:PHE:CD1	27:AT:101:BCR:HC8	2.54	0.43
16:AV:148:GLU:N	16:AV:149:PRO:HD2	2.34	0.43
3:BC:5266:TRP:HB3	3:BC:5271:TYR:OH	2.17	0.43
28:BC:5519:DGD:HE62	9:BJ:5040:LEU:CD1	2.48	0.43
4:BD:5078:VAL:HG11	4:BD:5114:ILE:HD12	2.01	0.43
9:BJ:5008:ILE:O	9:BJ:5009:PRO:C	2.60	0.43
13:BO:5059:ASP:C	13:BO:5061:SER:N	2.74	0.43
1:AA:222:SER:O	1:AA:246:TYR:HB2	2.19	0.43
1:AA:281:VAL:HG13	1:AA:282:GLY:N	2.33	0.43
2:AB:5:TRP:CZ2	31:AB:620:LMG:H291	2.53	0.43
2:AB:68:ARG:NH1	24:AB:604:CLA:HED1	2.30	0.43
2:AB:90:PHE:HE2	2:AB:91:TRP:CZ3	2.35	0.43
2:AB:230:ARG:H	2:AB:230:ARG:HD2	1.84	0.43
3:AC:353:GLY:C	3:AC:355:THR:N	2.76	0.43
3:AC:377:LEU:CD2	13:AO:126:GLY:HA2	2.48	0.43
3:AC:380:ILE:CA	3:AC:384:ILE:HD11	2.40	0.43
24:AC:510:CLA:H161	24:AC:510:CLA:H122	1.85	0.43
4:AD:246:MET:HE3	4:AD:262:SER:HA	2.00	0.43
6:AF:15:ILE:HG22	6:AF:16:PHE:CD1	2.50	0.43
8:AI:17:LEU:O	8:AI:18:LEU:C	2.61	0.43
10:AK:28:ILE:O	10:AK:29:PRO:C	2.61	0.43
13:AO:180:ALA:HB2	15:AU:120:ALA:O	2.18	0.43
14:AT:31:LYS:O	14:AT:32:LYS:HB2	2.18	0.43
15:AU:89:GLU:C	15:AU:91:VAL:N	2.76	0.43
16:AV:84:THR:O	16:AV:108:TYR:OH	2.35	0.43
20:AZ:22:GLY:O	20:AZ:23:VAL:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AZ:24:PRO:C	20:AZ:26:ALA:N	2.76	0.43
1:BA:5013:LEU:HA	1:BA:5016:ARG:NH1	2.33	0.43
1:BA:5078:ILE:O	1:BA:5176:ILE:HB	2.18	0.43
1:BA:5149:ALA:HB1	1:BA:5283:VAL:HG12	2.00	0.43
2:BB:5159:THR:OG1	2:BB:5161:LEU:HD13	2.19	0.43
3:BC:5203:THR:O	3:BC:5235:GLY:HA3	2.19	0.43
24:BC:5502:CLA:HHC	24:BC:5502:CLA:HBB1	2.01	0.43
24:BC:5505:CLA:HAA2	24:BC:5505:CLA:HBD	2.00	0.43
24:BC:5507:CLA:O1A	24:BC:5509:CLA:H2	2.19	0.43
4:BD:5333:ASP:C	4:BD:5335:PRO:HD3	2.43	0.43
7:BH:5043:LEU:O	7:BH:5047:GLU:HG3	2.17	0.43
19:BY:5023:UNK:O	19:BY:5024:UNK:C	2.67	0.43
1:AA:228:THR:CG2	1:AA:229:GLU:N	2.81	0.43
24:AA:405:CLA:HED2	4:AD:198:MET:SD	2.58	0.43
27:AA:410:BCR:H312	8:AI:15:PHE:CE1	2.54	0.43
2:AB:12:LEU:CD1	2:AB:19:LEU:HA	2.36	0.43
2:AB:358:ARG:O	2:AB:360:PRO:HD3	2.18	0.43
30:AB:622:SQD:H281	32:AB:624:LMT:H82	2.00	0.43
3:AC:95:LEU:HD21	24:AC:501:CLA:OBD	2.18	0.43
24:AC:511:CLA:H141	20:AZ:20:VAL:O	2.18	0.43
4:AD:52:THR:HG22	4:AD:67:TYR:CZ	2.53	0.43
4:AD:253:TRP:HB2	4:AD:260:ALA:CB	2.49	0.43
13:AO:81:GLU:C	13:AO:83:LYS:H	2.26	0.43
13:AO:127:ILE:H	13:AO:127:ILE:HG12	1.64	0.43
15:AU:66:ILE:HG12	15:AU:72:TYR:CD1	2.54	0.43
1:BA:5342:ASP:HB2	4:BD:5352:LEU:HD21	1.99	0.43
2:BB:5098:LEU:O	2:BB:5102:VAL:HG23	2.18	0.43
2:BB:5457:VAL:HG12	2:BB:5458:PHE:N	2.33	0.43
3:BC:5071:GLU:OE2	3:BC:5088:LEU:HG	2.19	0.43
3:BC:5324:LEU:HB3	15:BU:5062:ILE:HD13	2.01	0.43
3:BC:5404:LEU:HD12	3:BC:5404:LEU:HA	1.73	0.43
3:BC:5437:PHE:CD2	24:BC:5508:CLA:HMC1	2.53	0.43
24:BC:5501:CLA:H61	24:BC:5501:CLA:HMB2	2.01	0.43
4:BD:5189:HIS:O	4:BD:5190:ASN:C	2.61	0.43
4:BD:5261:PHE:HE1	4:BD:5266:TRP:CD1	2.37	0.43
6:BF:5040:MET:C	6:BF:5042:PHE:H	2.26	0.43
7:BH:5063:LYS:C	7:BH:5065:LEU:N	2.75	0.43
8:BI:5027:ASP:N	8:BI:5028:PRO:HD3	2.33	0.43
11:BL:5024:ILE:HG22	11:BL:5025:LEU:N	2.33	0.43
13:BO:5208:LEU:O	13:BO:5209:ALA:C	2.61	0.43
14:BT:5029:ILE:O	14:BT:5031:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:248:ILE:O	1:AA:248:ILE:HG12	2.18	0.43
1:AA:281:VAL:HG11	28:AC:519:DGD:CIA	2.49	0.43
1:AA:325:ASN:HA	1:AA:328:MET:CE	2.31	0.43
1:AA:341:LEU:HD12	3:AC:396:MET:HE3	2.01	0.43
2:AB:249:ALA:O	2:AB:252:VAL:HG22	2.19	0.43
2:AB:271:THR:N	2:AB:274:GLN:OE1	2.47	0.43
3:AC:259:TRP:C	3:AC:261:ARG:N	2.74	0.43
4:AD:43:LEU:HD23	4:AD:117:HIS:CE1	2.53	0.43
4:AD:203:GLY:O	4:AD:207:GLY:N	2.52	0.43
4:AD:263:ASN:O	4:AD:265:ARG:N	2.52	0.43
5:AE:15:THR:CG2	9:AJ:6:GLY:HA2	2.49	0.43
6:AF:30:THR:HG22	6:AF:34:LEU:CD1	2.48	0.43
1:BA:5013:LEU:HD12	1:BA:5016:ARG:NH1	2.33	0.43
1:BA:5065:GLU:N	1:BA:5066:PRO:HD3	2.34	0.43
1:BA:5299:GLY:O	3:BC:5403:SER:HB2	2.18	0.43
2:BB:5011:VAL:CG2	11:BL:5007:ARG:HA	2.49	0.43
2:BB:5024:LEU:HB3	2:BB:5111:ALA:HB2	2.00	0.43
2:BB:5092:SER:O	2:BB:5093:PHE:C	2.62	0.43
2:BB:5260:SER:C	2:BB:5262:THR:N	2.76	0.43
24:BB:5616:CLA:H12	24:BB:5619:CLA:HAA2	2.01	0.43
3:BC:5259:TRP:C	3:BC:5261:ARG:N	2.76	0.43
3:BC:5465:PRO:C	3:BC:5469:MET:HE3	2.44	0.43
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CE1	2.53	0.43
5:BE:5057:ALA:H	5:BE:5060:GLN:NE2	2.17	0.43
7:BH:5055:LEU:O	7:BH:5056:ASP:C	2.59	0.43
1:AA:42:LEU:HA	1:AA:45:THR:HG22	2.00	0.43
1:AA:51:ALA:HA	27:AA:410:BCR:H381	2.01	0.43
1:AA:77:ILE:HG12	14:AT:6:TYR:CD1	2.54	0.43
1:AA:185:VAL:O	1:AA:186:PHE:C	2.61	0.43
2:AB:68:ARG:NH2	24:AB:604:CLA:HED1	2.29	0.43
2:AB:102:VAL:HG13	27:AB:618:BCR:H401	2.00	0.43
2:AB:354:LEU:HD21	2:AB:378:LYS:CB	2.49	0.43
3:AC:259:TRP:O	3:AC:260:ALA:C	2.62	0.43
24:AC:504:CLA:H141	28:AC:518:DGD:HBT1	2.01	0.43
24:AC:512:CLA:H162	24:AC:512:CLA:H122	1.87	0.43
4:AD:36:LEU:C	4:AD:39:PRO:HD2	2.44	0.43
4:AD:217:THR:O	4:AD:221:THR:HB	2.18	0.43
5:AE:16:SER:HB2	9:AJ:3:SER:O	2.18	0.43
13:AO:120:THR:HA	13:AO:153:ALA:O	2.19	0.43
16:AV:130:MET:SD	16:AV:133:LEU:HD22	2.58	0.43
1:BA:5113:GLN:HB3	1:BA:5117:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5176:ILE:HD12	24:BA:5406:CLA:HED3	2.01	0.43
2:BB:5011:VAL:HG23	11:BL:5007:ARG:HA	2.01	0.43
3:BC:5062:PHE:HZ	10:BK:5028:ILE:CD1	2.29	0.43
3:BC:5155:ASN:C	3:BC:5158:THR:HG22	2.44	0.43
3:BC:5313:GLN:HE21	3:BC:5313:GLN:HB2	1.54	0.43
3:BC:5415:ASN:O	3:BC:5416:SER:CB	2.63	0.43
3:BC:5438:LEU:HD12	3:BC:5438:LEU:O	2.19	0.43
27:BC:5514:BCR:H11C	27:BK:5102:BCR:H322	2.00	0.43
13:BO:5147:THR:O	13:BO:5172:PHE:CE2	2.71	0.43
15:BU:5130:ASN:O	15:BU:5132:LEU:HD23	2.18	0.43
16:BV:5071:ILE:CD1	16:BV:5072:THR:N	2.81	0.43
1:AA:11:ALA:O	1:AA:12:ASN:HB3	2.18	0.43
1:AA:18:CYS:O	1:AA:22:THR:CG2	2.65	0.43
1:AA:286:THR:HG23	24:AA:404:CLA:HED3	2.01	0.43
1:AA:295:PHE:HD2	3:AC:291:TRP:CD2	2.37	0.43
2:AB:222:PRO:HB3	7:AH:26:GLY:N	2.34	0.43
2:AB:315:ILE:HG22	2:AB:426:PHE:HB3	2.00	0.43
2:AB:345:VAL:HG21	2:AB:402:TYR:CE2	2.53	0.43
24:AB:603:CLA:H3A	24:AB:603:CLA:CGA	2.49	0.43
3:AC:232:ASP:OD2	3:AC:232:ASP:N	2.52	0.43
3:AC:417:VAL:O	3:AC:417:VAL:HG13	2.19	0.43
4:AD:171:PRO:HG3	4:AD:181:PHE:CE2	2.54	0.43
11:AL:16:SER:HA	11:AL:19:LEU:CG	2.45	0.43
13:AO:32:THR:OG1	13:AO:33:TYR:N	2.52	0.43
13:AO:92:VAL:HG12	13:AO:93:PRO:CD	2.49	0.43
13:AO:109:GLY:HA3	13:AO:122:VAL:O	2.18	0.43
18:AX:44:ASP:O	18:AX:45:LYS:HB3	2.18	0.43
20:AZ:31:GLN:HG3	20:AZ:32:ASP:OD2	2.19	0.43
1:BA:5032:TRP:HB2	8:BI:5023:PHE:CZ	2.54	0.43
1:BA:5207:GLY:HA3	1:BA:5278:TRP:HE1	1.84	0.43
1:BA:5239:PHE:HB3	14:BT:5028:ARG:O	2.18	0.43
2:BB:5037:MET:O	2:BB:5041:GLU:HG3	2.19	0.43
24:BB:5609:CLA:H143	24:BB:5614:CLA:HBA1	2.01	0.43
3:BC:5366:LEU:HD21	3:BC:5370:ARG:NH2	2.34	0.43
4:BD:5126:MET:HE1	4:BD:5147:SER:HA	2.01	0.43
4:BD:5272:LEU:O	4:BD:5276:VAL:HG23	2.19	0.43
5:BE:5008:ARG:HB2	6:BF:5013:TYR:HB3	2.00	0.43
10:BK:5014:ALA:HB2	20:BZ:5061:VAL:HG12	2.00	0.43
19:BY:5023:UNK:O	19:BY:5025:UNK:N	2.52	0.43
1:AA:114:LEU:C	1:AA:114:LEU:HD23	2.43	0.42
23:AA:403[A]:CL:CL	4:AD:317:LYS:HD3	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:102:VAL:HB	24:AB:606:CLA:H91	2.00	0.42
2:AB:144:PHE:HE1	2:AB:210:ILE:CG2	2.31	0.42
2:AB:200:ALA:HB3	24:AB:602:CLA:HMB1	2.01	0.42
2:AB:250:PHE:HD1	28:AH:101:DGD:HB92	1.83	0.42
2:AB:490:GLN:O	2:AB:491:VAL:O	2.37	0.42
3:AC:404:LEU:HD12	3:AC:404:LEU:HA	1.69	0.42
4:AD:176:ALA:C	4:AD:178:ILE:N	2.77	0.42
4:AD:250:ASN:OD1	4:AD:250:ASN:C	2.62	0.42
24:AD:404:CLA:H41	18:AX:23:LEU:CD1	2.43	0.42
7:AH:55:LEU:O	7:AH:56:ASP:C	2.62	0.42
16:AV:92:ARG:HG3	16:AV:92:ARG:NH1	2.33	0.42
1:BA:5205:VAL:HG21	24:BA:5405:CLA:CMA	2.41	0.42
1:BA:5281:VAL:HG11	28:BC:5519:DGD:CHA	2.48	0.42
2:BB:5135:LEU:HD21	2:BB:5234:ILE:HD13	2.01	0.42
2:BB:5169:SER:O	7:BH:5065:LEU:HG	2.19	0.42
2:BB:5437:LEU:N	2:BB:5437:LEU:HD12	2.34	0.42
24:BB:5609:CLA:H41	24:BB:5609:CLA:H61	1.83	0.42
3:BC:5239:TRP:O	3:BC:5243:ILE:HD12	2.19	0.42
4:BD:5036:LEU:C	4:BD:5039:PRO:HD2	2.44	0.42
6:BF:5025:THR:O	6:BF:5029:PRO:HG2	2.18	0.42
7:BH:5040:VAL:O	7:BH:5044:ILE:HG13	2.19	0.42
13:BO:5069:LEU:HD12	13:BO:5070:CYS:N	2.33	0.42
13:BO:5127:ILE:H	13:BO:5127:ILE:HG12	1.65	0.42
15:BU:5059:ASN:O	15:BU:5060:THR:C	2.62	0.42
15:BU:5096:GLY:O	15:BU:5097:LEU:C	2.62	0.42
16:BV:5121:LEU:HD21	16:BV:5138:LEU:HD11	2.01	0.42
19:BY:5021:UNK:O	19:BY:5022:UNK:C	2.66	0.42
1:AA:303:ASN:O	1:AA:304:HIS:HB2	2.20	0.42
3:AC:242:LEU:O	3:AC:243:ILE:C	2.61	0.42
4:AD:96:GLU:CD	4:AD:96:GLU:N	2.76	0.42
4:AD:266:TRP:NE1	31:AD:408:LMG:HC72	2.34	0.42
10:AK:14:ALA:HB2	20:AZ:61:VAL:HG12	2.01	0.42
16:AV:90:PRO:O	16:AV:92:ARG:CD	2.67	0.42
17:Ay:39:LEU:HD21	20:AZ:28:ALA:CB	2.49	0.42
1:BA:5259:ILE:N	1:BA:5259:ILE:CD1	2.69	0.42
29:BA:5413:LHG:HC62	3:BC:5443:TRP:HH2	1.85	0.42
2:BB:5015:ASP:N	2:BB:5016:PRO:CD	2.81	0.42
2:BB:5137:LYS:HE2	7:BH:5017:GLU:CG	2.49	0.42
2:BB:5358:ARG:O	2:BB:5360:PRO:HD3	2.19	0.42
3:BC:5165:LEU:HD11	24:BC:5506:CLA:CHC	2.48	0.42
3:BC:5426:LEU:HD23	3:BC:5426:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:5518:DGD:HBT2	27:BJ:5101:BCR:H342	2.01	0.42
4:BD:5089:LEU:HD12	7:BH:5050:ASN:CG	2.44	0.42
4:BD:5210:LEU:HD21	35:BD:5406:PL9:H13	2.00	0.42
10:BK:5028:ILE:O	10:BK:5029:PRO:C	2.60	0.42
13:BO:5051:THR:OG1	13:BO:5052:ALA:N	2.52	0.42
13:BO:5075:THR:HG21	13:BO:5077:LEU:HD21	2.01	0.42
15:BU:5072:TYR:CG	15:BU:5073:PRO:N	2.84	0.42
1:AA:20:TRP:O	1:AA:23:SER:HB3	2.18	0.42
1:AA:157:VAL:HG21	24:AA:405:CLA:HMC1	2.01	0.42
1:AA:288:LEU:CD1	3:AC:432:VAL:HG23	2.44	0.42
2:AB:193:TYR:HE1	2:AB:259:GLY:C	2.27	0.42
30:AB:627:SQD:H45	14:BT:5023:PHE:HD1	1.85	0.42
3:AC:304:PRO:HB3	3:AC:395:TYR:CG	2.54	0.42
3:AC:369:LEU:HD21	3:AC:384:ILE:HD13	2.01	0.42
3:AC:385:GLN:O	3:AC:388:GLN:HB2	2.19	0.42
3:AC:415:ASN:CB	9:AJ:39:SER:OG	2.67	0.42
24:AC:503:CLA:H191	24:AC:503:CLA:HMD1	2.02	0.42
4:AD:181:PHE:CZ	4:AD:185:PHE:CE1	3.07	0.42
31:AM:101:LMG:O8	31:AM:101:LMG:O9	2.37	0.42
13:AO:135:GLN:HG2	13:AO:141:ARG:HG3	2.00	0.42
1:BA:5127:MET:HE3	24:BC:5505:CLA:HMB2	2.01	0.42
2:BB:5141:ILE:O	2:BB:5144:PHE:HB3	2.20	0.42
2:BB:5345:VAL:HG21	2:BB:5402:TYR:CE2	2.54	0.42
2:BB:5477:ASP:OD2	2:BB:5478:VAL:HG13	2.19	0.42
24:BB:5607:CLA:H203	24:BB:5613:CLA:H92	2.00	0.42
3:BC:5321:ASP:OD2	15:BU:5129:ASN:HB2	2.19	0.42
4:BD:5122:LEU:HD21	24:BD:5402:CLA:C9	2.41	0.42
4:BD:5125:PHE:CD2	4:BD:5125:PHE:C	2.97	0.42
4:BD:5155:SER:HA	4:BD:5159:ILE:HG13	2.01	0.42
4:BD:5164:GLN:NE2	4:BD:5290:ALA:O	2.53	0.42
16:BV:5121:LEU:C	16:BV:5123:SER:H	2.27	0.42
1:AA:322:ASN:OD1	3:AC:412:THR:HA	2.19	0.42
2:AB:385:ARG:O	2:AB:386:ALA:C	2.60	0.42
2:AB:457:VAL:O	2:AB:458:PHE:C	2.62	0.42
2:AB:466:HIS:CE1	24:AB:608:CLA:ND	2.87	0.42
24:AB:613:CLA:H61	24:AB:613:CLA:H41	1.63	0.42
27:AC:516:BCR:HC41	8:AI:20:VAL:CG1	2.48	0.42
28:AC:518:DGD:HBT2	27:AJ:101:BCR:H342	2.02	0.42
6:AF:40:MET:C	6:AF:42:PHE:H	2.28	0.42
9:AJ:3:SER:CB	9:AJ:7:ARG:HH22	2.32	0.42
13:AO:57:PRO:HA	13:AO:161:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5042:LEU:HA	1:BA:5045:THR:HG22	2.01	0.42
1:BA:5131:TRP:CZ3	1:BA:5132:GLU:HG3	2.53	0.42
2:BB:5144:PHE:HE1	2:BB:5210:ILE:CG2	2.33	0.42
2:BB:5225:LEU:C	2:BB:5227:LYS:N	2.77	0.42
2:BB:5230:ARG:HD2	2:BB:5230:ARG:H	1.84	0.42
2:BB:5298:LEU:HD23	2:BB:5402:TYR:CE1	2.54	0.42
24:BB:5618:CLA:HAA2	24:BB:5618:CLA:HBD	2.01	0.42
32:BC:5522:LMT:H41	8:BI:5021:PHE:HE1	1.84	0.42
11:BL:5036:PHE:O	11:BL:5037:ASN:C	2.62	0.42
13:BO:5141:ARG:HG2	13:BO:5141:ARG:HH11	1.83	0.42
13:BO:5178:ARG:HG3	13:BO:5178:ARG:NH1	2.28	0.42
15:BU:5056:ASP:HB3	15:BU:5060:THR:H	1.84	0.42
1:AA:257:ARG:NH1	2:AB:489:GLU:OE2	2.52	0.42
2:AB:12:LEU:HD13	2:AB:19:LEU:CA	2.38	0.42
2:AB:124:ARG:HG3	2:AB:124:ARG:NH1	2.33	0.42
2:AB:357:ARG:NH2	4:AD:337:GLU:OE1	2.53	0.42
3:AC:229:ASN:O	3:AC:233:VAL:HG23	2.18	0.42
3:AC:390:ARG:CZ	16:AV:126:ILE:HG21	2.50	0.42
24:AC:506:CLA:HMC1	24:AC:507:CLA:H8	2.01	0.42
4:AD:57:SER:C	4:AD:60:THR:HG22	2.44	0.42
5:AE:35:TRP:CD1	5:AE:35:TRP:C	2.98	0.42
8:AI:20:VAL:C	8:AI:22:GLY:N	2.77	0.42
10:AK:16:ALA:O	10:AK:19:ASP:HB2	2.19	0.42
13:AO:70:CYS:SG	13:AO:105:ASP:OD1	2.77	0.42
13:AO:73:PRO:HG3	13:AO:146:PHE:CE2	2.54	0.42
15:AU:56:ASP:HB3	15:AU:60:THR:H	1.85	0.42
1:BA:5217:SER:HB2	4:BD:5141:TYR:O	2.19	0.42
2:BB:5274:GLN:HG2	2:BB:5279:TYR:CD2	2.54	0.42
3:BC:5189:TRP:O	3:BC:5190:ALA:C	2.61	0.42
3:BC:5217:PRO:O	28:BC:5517:DGD:HB21	2.20	0.42
24:BC:5506:CLA:HMC1	24:BC:5507:CLA:H8	2.02	0.42
5:BE:5069:ARG:CG	5:BE:5070:PHE:N	2.82	0.42
13:BO:5081:GLU:HA	13:BO:5082:PRO:HD3	1.88	0.42
13:BO:5091:PHE:CD1	13:BO:5260:LYS:HB2	2.55	0.42
16:BV:5062:ALA:O	36:BV:5201:HEM:HAB	2.20	0.42
19:BY:5018:UNK:O	19:BY:5022:UNK:N	2.52	0.42
2:AB:224:ARG:CZ	32:AB:624:LMT:H2'	2.50	0.42
2:AB:450:TRP:NE1	24:AB:607:CLA:HBA2	2.34	0.42
2:AB:466:HIS:HE1	24:AB:608:CLA:C4D	2.31	0.42
3:AC:266:TRP:HB3	3:AC:271:TYR:OH	2.20	0.42
3:AC:337:LEU:HA	13:AO:131:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:164:GLN:NE2	4:AD:290:ALA:O	2.53	0.42
4:AD:263:ASN:O	4:AD:266:TRP:N	2.50	0.42
6:AF:27:ALA:CB	36:AF:101:HEM:HBC2	2.46	0.42
8:AI:21:PHE:HD1	8:AI:21:PHE:HA	1.76	0.42
10:AK:43:VAL:O	10:AK:46:ARG:HG3	2.20	0.42
14:AT:14:ILE:HD13	14:AT:17:PHE:CD2	2.55	0.42
1:BA:5069:GLY:HA2	1:BA:5075:ASN:HD21	1.83	0.42
1:BA:5190:HIS:HB3	1:BA:5293:MET:CE	2.34	0.42
1:BA:5214:MET:HE3	34:BD:5404:PHO:CMD	2.49	0.42
2:BB:5112:CYS:HA	27:BB:5621:BCR:H282	2.01	0.42
2:BB:5238:LEU:CD2	2:BB:5469:HIS:CD2	3.03	0.42
2:BB:5246:PHE:CD2	2:BB:5463:PHE:HA	2.54	0.42
8:BI:5019:PHE:CE1	8:BI:5023:PHE:CE2	3.02	0.42
10:BK:5018:PHE:C	10:BK:5020:PRO:HD2	2.45	0.42
13:BO:5078:VAL:HB	13:BO:5136:MET:HE3	2.02	0.42
13:BO:5094:THR:HB	13:BO:5135:GLN:O	2.20	0.42
1:AA:259:ILE:N	1:AA:259:ILE:CD1	2.71	0.42
2:AB:91:TRP:CE3	24:AB:606:CLA:O1A	2.73	0.42
3:AC:63:TRP:O	3:AC:64:ALA:C	2.62	0.42
3:AC:269:GLU:O	3:AC:272:LEU:HB3	2.19	0.42
3:AC:324:LEU:HB3	15:AU:62:ILE:HD13	2.01	0.42
4:AD:79:SER:HA	4:AD:172:SER:HB3	2.02	0.42
8:AI:20:VAL:C	8:AI:22:GLY:H	2.26	0.42
10:AK:34:ALA:O	10:AK:37:PHE:HB2	2.19	0.42
13:AO:56:TYR:CD1	13:AO:235:GLY:HA2	2.55	0.42
13:AO:190:LEU:HB2	13:AO:214:LYS:HB2	2.02	0.42
1:BA:5118:HIS:HE1	24:BA:5408:CLA:C1A	2.32	0.42
1:BA:5157:VAL:HG13	1:BA:5172:MET:HB2	2.00	0.42
1:BA:5205:VAL:CG2	24:BA:5405:CLA:HMA2	2.41	0.42
1:BA:5207:GLY:O	1:BA:5210:LEU:HB3	2.19	0.42
2:BB:5188:ASP:HA	7:BH:5058:VAL:HG23	2.02	0.42
2:BB:5256:MET:HE1	2:BB:5268:PHE:CE1	2.55	0.42
3:BC:5223:TRP:CH2	3:BC:5224:ILE:HD11	2.54	0.42
10:BK:5011:LEU:O	10:BK:5012:PRO:C	2.60	0.42
13:BO:5059:ASP:O	13:BO:5061:SER:N	2.53	0.42
1:AA:149:ALA:HB1	1:AA:283:VAL:CG1	2.49	0.42
1:AA:288:LEU:CD2	3:AC:432:VAL:HG23	2.49	0.42
2:AB:270:PRO:HG3	2:AB:312:TYR:CD2	2.51	0.42
2:AB:372:ASP:OD1	2:AB:372:ASP:C	2.62	0.42
2:AB:451:PHE:CD2	2:AB:451:PHE:C	2.98	0.42
3:AC:67:MET:HE1	24:AC:504:CLA:ND	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:276:LEU:HD23	3:AC:276:LEU:HA	1.76	0.42
3:AC:366:LEU:HD23	3:AC:366:LEU:O	2.20	0.42
3:AC:443:TRP:CE2	24:AC:508:CLA:HMD2	2.55	0.42
28:AC:518:DGD:O1B	28:AC:518:DGD:C1G	2.68	0.42
4:AD:176:ALA:C	4:AD:178:ILE:H	2.26	0.42
6:AF:20:TRP:NE1	6:AF:24:HIS:CE1	2.88	0.42
13:AO:141:ARG:NH1	13:AO:141:ARG:HG2	2.35	0.42
15:AU:41:ASN:O	15:AU:42:VAL:C	2.63	0.42
1:BA:5225:ARG:CA	2:BB:5481:GLY:HA3	2.50	0.42
1:BA:5240:GLY:HA3	14:BT:5029:ILE:CG2	2.48	0.42
1:BA:5271:LEU:HD21	25:BA:5409:MST:C8	2.40	0.42
2:BB:5475:PHE:HB3	2:BB:5478:VAL:HG22	2.02	0.42
3:BC:5418:ASN:HB2	28:BC:5519:DGD:O4E	2.20	0.42
4:BD:5014:TRP:CG	4:BD:5015:PHE:N	2.88	0.42
6:BF:5022:ALA:O	6:BF:5023:VAL:C	2.62	0.42
6:BF:5023:VAL:O	6:BF:5027:ALA:HB2	2.20	0.42
7:BH:5019:GLY:O	7:BH:5021:VAL:HG13	2.20	0.42
9:BJ:5021:VAL:HA	9:BJ:5024:ILE:HG22	2.02	0.42
1:AA:254:TYR:OH	4:AD:129:GLN:HB3	2.20	0.42
1:AA:292:THR:HB	28:AC:518:DGD:CDA	2.49	0.42
2:AB:19:LEU:HA	2:AB:19:LEU:HD12	1.80	0.42
2:AB:260:SER:C	2:AB:262:THR:H	2.28	0.42
2:AB:264:PRO:HG2	2:AB:267:LEU:HB2	2.02	0.42
2:AB:356:VAL:HG21	2:AB:424:ALA:CB	2.50	0.42
4:AD:128:ARG:HE	4:AD:128:ARG:HB2	1.66	0.42
4:AD:303:ILE:HG21	12:AM:2:GLU:HG2	2.02	0.42
6:AF:22:ALA:O	6:AF:23:VAL:C	2.62	0.42
6:AF:30:THR:HG22	6:AF:34:LEU:HD12	2.01	0.42
20:AZ:30:PRO:HB3	20:AZ:33:TRP:CZ3	2.54	0.42
1:BA:5200:LEU:HD12	1:BA:5285:PHE:CG	2.54	0.42
1:BA:5286:THR:HG23	24:BA:5405:CLA:HED3	2.02	0.42
24:BA:5405:CLA:H111	34:BD:5403:PHO:H3A	2.00	0.42
2:BB:5260:SER:C	2:BB:5262:THR:H	2.28	0.42
2:BB:5260:SER:HG	2:BB:5262:THR:HG22	1.79	0.42
32:BB:5603:LMT:H5'	32:BB:5603:LMT:H1B	1.79	0.42
4:BD:5161:PRO:HG3	4:BD:5170:ALA:HB2	2.02	0.42
4:BD:5203:GLY:O	4:BD:5207:GLY:N	2.51	0.42
4:BD:5274:VAL:CB	4:BD:5275:PRO:HD3	2.47	0.42
8:BI:5020:VAL:C	8:BI:5022:GLY:H	2.27	0.42
13:BO:5036:ILE:O	13:BO:5037:VAL:C	2.62	0.42
20:BZ:5031:GLN:HG3	20:BZ:5032:ASP:OD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:13:LEU:CA	1:AA:16:ARG:HH11	2.33	0.42
1:AA:275:LEU:CD1	25:AA:408:MST:H83	2.49	0.42
1:AA:281:VAL:HG11	28:AC:519:DGD:HAG3	2.01	0.42
2:AB:175:THR:O	2:AB:176:GLY:C	2.63	0.42
2:AB:450:TRP:CZ3	24:AB:607:CLA:H2	2.55	0.42
3:AC:243:ILE:O	24:AC:506:CLA:HAC1	2.20	0.42
3:AC:335:THR:HA	13:AO:178:ARG:HD3	2.02	0.42
5:AE:72:ALA:O	5:AE:76:VAL:HG23	2.20	0.42
5:AE:78:THR:HA	5:AE:81:GLU:CG	2.49	0.42
9:AJ:11:TRP:CZ3	17:AY:36:ILE:HD11	2.54	0.42
13:AO:59:ASP:O	13:AO:61:SER:N	2.53	0.42
14:AT:14:ILE:HD13	14:AT:14:ILE:HA	1.88	0.42
20:AZ:38:GLN:O	20:AZ:42:LEU:HG	2.19	0.42
1:BA:5133:LEU:HD23	4:BD:5252:PHE:HD1	1.81	0.42
1:BA:5147:TYR:O	1:BA:5147:TYR:CG	2.73	0.42
1:BA:5183:MET:HG3	24:BA:5406:CLA:CBC	2.50	0.42
2:BB:5135:LEU:HB2	2:BB:5136:PRO:CD	2.41	0.42
2:BB:5224:ARG:NH1	32:BB:5627:LMT:H2'	2.35	0.42
2:BB:5237:VAL:HB	24:BB:5616:CLA:CMD	2.50	0.42
2:BB:5450:TRP:NE1	24:BB:5611:CLA:HBA2	2.35	0.42
3:BC:5128:GLY:HA3	24:BC:5513:CLA:C3C	2.50	0.42
3:BC:5141:GLU:HA	3:BC:5148:GLY:HA3	2.02	0.42
3:BC:5160:ILE:HA	3:BC:5163:PHE:CD2	2.54	0.42
3:BC:5269:GLU:OE1	3:BC:5447:ARG:HD3	2.20	0.42
3:BC:5335:THR:C	13:BO:5178:ARG:HD3	2.45	0.42
3:BC:5363:GLY:O	3:BC:5364:PRO:C	2.62	0.42
24:BC:5509:CLA:HBB1	24:BC:5509:CLA:HHC	2.02	0.42
5:BE:5015:THR:O	9:BJ:5008:ILE:HD13	2.19	0.42
8:BI:5020:VAL:C	8:BI:5022:GLY:N	2.78	0.42
1:AA:220:THR:HG23	4:AD:141:TYR:CD1	2.54	0.41
1:AA:232:SER:HB3	1:AA:235:TYR:CD2	2.55	0.41
1:AA:317:TRP:HZ3	4:AD:180:ARG:HD3	1.85	0.41
1:AA:343:LEU:O	1:AA:344:ALA:CB	2.66	0.41
2:AB:187:PRO:HG2	2:AB:188:ASP:N	2.35	0.41
2:AB:363:PHE:CD1	4:AD:326:ARG:HD2	2.55	0.41
2:AB:390:TYR:HD2	4:AD:344:GLU:OE1	2.02	0.41
24:AB:616:CLA:HHC	24:AB:616:CLA:HBB1	2.01	0.41
32:AB:629:LMT:H51	14:BT:5004:ILE:CG1	2.42	0.41
3:AC:160:ILE:HA	3:AC:163:PHE:CD2	2.55	0.41
4:AD:60:THR:C	4:AD:61:HIS:HD2	2.28	0.41
1:BA:5032:TRP:CB	8:BI:5023:PHE:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5191:ASN:ND2	1:BA:5194:MET:HB2	2.35	0.41
27:BA:5411:BCR:H312	8:BI:5015:PHE:CE1	2.54	0.41
2:BB:5324:LEU:HD13	4:BD:5293:LEU:CD2	2.50	0.41
2:BB:5466:HIS:CE1	24:BB:5612:CLA:ND	2.87	0.41
24:BB:5606:CLA:H93	7:BH:5046:LEU:HD13	2.02	0.41
24:BB:5615:CLA:H52	24:BB:5618:CLA:HBC2	2.01	0.41
3:BC:5229:ASN:O	3:BC:5233:VAL:HG23	2.19	0.41
3:BC:5307:PRO:O	3:BC:5311:GLN:HG2	2.20	0.41
4:BD:5318:ASN:O	4:BD:5321:LEU:HB2	2.20	0.41
13:BO:5065:ARG:CB	13:BO:5065:ARG:HH11	2.33	0.41
13:BO:5141:ARG:NH1	13:BO:5141:ARG:HG2	2.35	0.41
16:BV:5090:PRO:O	16:BV:5092:ARG:CD	2.67	0.41
20:BZ:5005:PHE:HA	20:BZ:5057:LEU:CD2	2.50	0.41
1:AA:140:ARG:HB2	4:AD:220:ASN:HA	2.01	0.41
1:AA:278:TRP:HB3	1:AA:279:PRO:CD	2.46	0.41
1:AA:306:VAL:HG22	1:AA:314:ILE:HB	2.03	0.41
2:AB:12:LEU:O	2:AB:14:ASN:N	2.53	0.41
2:AB:198:VAL:HG11	24:AB:603:CLA:HED2	2.02	0.41
2:AB:338:GLN:HB2	2:AB:431:GLU:O	2.21	0.41
24:AB:603:CLA:H203	24:AB:609:CLA:H92	2.02	0.41
24:AB:605:CLA:HMA2	24:AB:606:CLA:CMA	2.49	0.41
3:AC:29:GLU:CD	3:AC:29:GLU:H	2.27	0.41
3:AC:225:VAL:O	3:AC:225:VAL:HG12	2.20	0.41
3:AC:441:HIS:HD2	3:AC:442:LEU:HD12	1.85	0.41
24:AC:502:CLA:HAA2	24:AC:502:CLA:HBD	2.01	0.41
24:AC:511:CLA:H143	20:AZ:24:PRO:HG2	2.02	0.41
4:AD:53:THR:HA	4:AD:67:TYR:CD2	2.56	0.41
9:AJ:32:ALA:HA	31:AJ:102:LMG:O3	2.20	0.41
12:AM:17:VAL:HG12	12:AM:18:PRO:N	2.34	0.41
31:AM:101:LMG:H132	24:BB:5618:CLA:C1	2.51	0.41
13:AO:46:PRO:HB2	13:AO:266:TYR:CD2	2.55	0.41
13:AO:114:ASN:HD21	13:AO:120:THR:CG2	2.29	0.41
16:AV:121:LEU:C	16:AV:123:SER:H	2.28	0.41
18:AX:42:GLN:O	18:AX:43:ILE:HG13	2.20	0.41
1:BA:5239:PHE:O	14:BT:5030:THR:N	2.53	0.41
1:BA:5243:GLU:HA	4:BD:5240:ALA:O	2.20	0.41
2:BB:5185:TRP:HD1	24:BB:5606:CLA:HBB2	1.85	0.41
24:BB:5618:CLA:H162	31:BL:5101:LMG:C42	2.50	0.41
3:BC:5062:PHE:CD2	10:BK:5029:PRO:HG3	2.50	0.41
3:BC:5215:LYS:HZ3	3:BC:5226:SER:CB	2.32	0.41
3:BC:5337:LEU:HA	13:BO:5131:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5161:PRO:CB	4:BD:5170:ALA:HB2	2.50	0.41
12:BM:5018:PRO:O	12:BM:5021:PHE:HB3	2.20	0.41
13:BO:5106:GLN:HE21	13:BO:5106:GLN:HB3	1.68	0.41
16:BV:5062:ALA:O	36:BV:5201:HEM:CAB	2.68	0.41
2:AB:373:LYS:HG3	2:AB:374:ASN:N	2.35	0.41
24:AB:614:CLA:HAA2	24:AB:614:CLA:HBD	2.01	0.41
24:AB:615:CLA:HBB1	24:AB:615:CLA:HHC	2.02	0.41
3:AC:204:LEU:HA	3:AC:204:LEU:HD23	1.79	0.41
4:AD:199:MET:HG2	35:AD:405:PL9:H312	2.03	0.41
5:AE:8:ARG:NH2	9:AJ:4:GLU:HB2	2.35	0.41
8:AI:27:ASP:O	8:AI:28:PRO:C	2.59	0.41
13:AO:77:LEU:HB3	13:AO:91:PHE:HB3	2.02	0.41
13:AO:156:GLN:OE1	13:AO:156:GLN:HA	2.20	0.41
13:AO:157:PRO:O	13:AO:158:ASN:O	2.38	0.41
14:AT:23:PHE:HD1	30:BB:5601:SQD:H45	1.85	0.41
17:Ay:35:ILE:HD12	17:Ay:35:ILE:O	2.20	0.41
1:BA:5048:PHE:HA	1:BA:5115:ILE:CD1	2.48	0.41
1:BA:5135:TYR:CE1	3:BC:5449:ARG:HB3	2.55	0.41
1:BA:5321:ILE:HG22	1:BA:5325:ASN:ND2	2.35	0.41
24:BA:5406:CLA:H72	31:BL:5101:LMG:H241	2.02	0.41
2:BB:5224:ARG:CZ	32:BB:5627:LMT:H2'	2.50	0.41
3:BC:5417:VAL:O	3:BC:5417:VAL:HG13	2.19	0.41
3:BC:5466:VAL:HG21	4:BD:5248:THR:OG1	2.20	0.41
28:BC:5519:DGD:HD3	9:BJ:5032:ALA:O	2.20	0.41
7:BH:5035:MET:SD	27:BX:5101:BCR:H322	2.61	0.41
9:BJ:5003:SER:CB	9:BJ:5007:ARG:NH2	2.83	0.41
16:BV:5069:GLY:O	16:BV:5156:TRP:O	2.38	0.41
16:BV:5128:PRO:C	16:BV:5130:MET:N	2.78	0.41
1:AA:36:ILE:HD13	1:AA:36:ILE:HA	1.89	0.41
1:AA:57:PRO:HA	1:AA:68:SER:HA	2.03	0.41
1:AA:296:ASN:HB3	3:AC:401:LEU:HD13	2.02	0.41
2:AB:297:THR:HG22	2:AB:300:GLU:CD	2.45	0.41
3:AC:272:LEU:O	3:AC:273:SER:C	2.63	0.41
3:AC:367:GLU:OE1	3:AC:367:GLU:HA	2.18	0.41
28:AC:519:DGD:HD3	9:AJ:32:ALA:O	2.20	0.41
4:AD:53:THR:CB	4:AD:67:TYR:HD2	2.34	0.41
7:AH:63:LYS:C	7:AH:65:LEU:H	2.28	0.41
12:AM:21:PHE:CD2	12:AM:22:LEU:HD23	2.55	0.41
1:BA:5119:PHE:CZ	24:BA:5405:CLA:H101	2.52	0.41
1:BA:5138:GLY:CA	8:BI:5032:PRO:HG2	2.51	0.41
1:BA:5278:TRP:HB3	1:BA:5279:PRO:CD	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5306:VAL:HG22	1:BA:5314:ILE:HB	2.02	0.41
2:BB:5034:ALA:HB2	24:BB:5609:CLA:C2D	2.51	0.41
4:BD:5329:MET:O	4:BD:5330:ALA:C	2.63	0.41
5:BE:5069:ARG:HG3	5:BE:5070:PHE:CD1	2.55	0.41
6:BF:5024:HIS:NE2	36:BF:5101:HEM:NB	2.67	0.41
7:BH:5063:LYS:O	7:BH:5064:ALA:HB3	2.20	0.41
13:BO:5120:THR:HG22	13:BO:5154:SER:CB	2.50	0.41
15:BU:5077:LYS:O	15:BU:5081:LYS:HB2	2.21	0.41
17:By:5039:LEU:CD1	20:BZ:5028:ALA:HB1	2.50	0.41
1:AA:200:LEU:HD21	28:AC:519:DGD:CCA	2.50	0.41
2:AB:150:CYS:HB2	24:AB:603:CLA:CMC	2.51	0.41
2:AB:252:VAL:HG23	2:AB:253:ALA:N	2.35	0.41
2:AB:297:THR:OG1	2:AB:298:LEU:N	2.52	0.41
2:AB:483:ASP:CB	2:AB:484:PRO:CD	2.94	0.41
3:AC:62:PHE:CD2	10:AK:29:PRO:HG3	2.50	0.41
3:AC:244:CYS:HA	24:AC:506:CLA:CMC	2.51	0.41
3:AC:449:ARG:HE	24:AC:505:CLA:HED1	1.86	0.41
4:AD:218:VAL:HG22	4:AD:244:TYR:CD2	2.54	0.41
4:AD:259:ILE:HD13	14:AT:21:ILE:HG12	2.02	0.41
7:AH:42:LEU:HD12	7:AH:42:LEU:HA	1.83	0.41
8:AI:7:THR:O	8:AI:8:VAL:C	2.63	0.41
10:AK:21:LEU:HD11	27:AK:102:BCR:HC42	2.03	0.41
10:AK:24:VAL:HG21	17:Ay:25:ILE:CD1	2.51	0.41
13:AO:36:ILE:O	13:AO:37:VAL:C	2.64	0.41
18:AX:12:ILE:CA	27:AX:101:BCR:H401	2.48	0.41
1:BA:5092:HIS:HE1	3:BC:5359:TRP:CZ2	2.38	0.41
1:BA:5172:MET:HA	1:BA:5173:PRO:HD3	1.97	0.41
1:BA:5292:THR:HB	28:BC:5518:DGD:CDA	2.50	0.41
1:BA:5340:PRO:HG3	15:BU:5133:TYR:CD1	2.55	0.41
2:BB:5271:THR:N	2:BB:5274:GLN:OE1	2.45	0.41
2:BB:5298:LEU:HD12	2:BB:5298:LEU:HA	1.89	0.41
3:BC:5244:CYS:HA	24:BC:5506:CLA:CMC	2.51	0.41
4:BD:5272:LEU:HD22	4:BD:5276:VAL:HG21	2.03	0.41
9:BJ:5038:SER:OG	9:BJ:5039:SER:N	2.53	0.41
17:By:5019:ILE:CG2	17:By:5020:ALA:N	2.83	0.41
19:BY:5025:UNK:C	19:BY:5027:UNK:N	2.82	0.41
1:AA:184:ILE:CD1	4:AD:186:GLN:HG2	2.51	0.41
24:AA:405:CLA:H72	31:AB:620:LMG:H241	2.01	0.41
2:AB:4:PRO:CG	2:AB:7:ARG:HD2	2.42	0.41
2:AB:105:GLY:O	2:AB:108:PHE:HB3	2.20	0.41
2:AB:278:SER:HB3	2:AB:281:GLN:NE2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AB:605:CLA:H143	24:AB:610:CLA:HBA1	2.02	0.41
3:AC:71:GLU:OE2	3:AC:88:LEU:HG	2.21	0.41
3:AC:149:TYR:HB3	3:AC:156:LYS:HD3	2.02	0.41
3:AC:437:PHE:CD2	24:AC:508:CLA:CMC	3.04	0.41
3:AC:459:ILE:HG21	3:AC:464:GLU:HG3	2.02	0.41
3:AC:466:VAL:HG13	4:AD:251:ARG:CD	2.50	0.41
24:AC:505:CLA:HBD	24:AC:505:CLA:HAA2	2.02	0.41
4:AD:84:SER:HB3	5:AE:68:ASP:HA	2.03	0.41
4:AD:189:HIS:O	4:AD:190:ASN:C	2.63	0.41
4:AD:202:ALA:HB3	35:AD:405:PL9:C30	2.49	0.41
7:AH:27:THR:O	7:AH:28:THR:C	2.63	0.41
13:AO:168:PHE:HB2	13:AO:225:LEU:HB2	2.03	0.41
13:AO:206:GLU:CD	13:AO:206:GLU:N	2.77	0.41
1:BA:5020:TRP:O	1:BA:5023:SER:HB3	2.19	0.41
1:BA:5044:ALA:HB1	34:BD:5403:PHO:H91	2.02	0.41
1:BA:5129:ARG:C	1:BA:5131:TRP:N	2.78	0.41
2:BB:5112:CYS:CB	27:BB:5623:BCR:H393	2.51	0.41
2:BB:5135:LEU:HD23	2:BB:5138:MET:CE	2.50	0.41
2:BB:5187:PRO:C	2:BB:5189:GLY:N	2.79	0.41
2:BB:5193:TYR:CE1	2:BB:5260:SER:HA	2.55	0.41
2:BB:5489:GLU:CB	5:BE:5003:GLY:N	2.76	0.41
24:BB:5615:CLA:HHC	24:BB:5615:CLA:HBB1	2.03	0.41
3:BC:5250:TRP:O	3:BC:5254:THR:OG1	2.38	0.41
4:BD:5199:MET:O	4:BD:5200:GLY:C	2.61	0.41
4:BD:5262:SER:HG	31:BD:5410:LMG:HO3	1.58	0.41
15:BU:5072:TYR:CB	15:BU:5073:PRO:CD	2.98	0.41
15:BU:5089:GLU:C	15:BU:5091:VAL:H	2.29	0.41
16:BV:5162:TYR:O	16:BV:5163:TYR:C	2.63	0.41
20:BZ:5032:ASP:HA	20:BZ:5034:ASP:OD2	2.21	0.41
1:AA:119:PHE:CZ	24:AA:404:CLA:H101	2.53	0.41
1:AA:278:TRP:CD2	28:AC:519:DGD:CIA	2.96	0.41
29:AA:412:LHG:C1	3:AC:447:ARG:HE	2.34	0.41
2:AB:12:LEU:HD13	2:AB:19:LEU:HD12	2.03	0.41
2:AB:369:ILE:HD13	4:AD:340:VAL:O	2.21	0.41
24:AB:612:CLA:H12	24:AB:615:CLA:HAA2	2.03	0.41
3:AC:48:LYS:HE2	3:AC:138:GLU:OE2	2.20	0.41
3:AC:229:ASN:ND2	3:AC:231:GLU:HB2	2.36	0.41
4:AD:261:PHE:CG	4:AD:267:LEU:HD12	2.56	0.41
7:AH:40:VAL:O	7:AH:44:ILE:HG13	2.21	0.41
27:AJ:101:BCR:H361	27:AJ:101:BCR:H20C	1.91	0.41
16:AV:59:PHE:HA	16:AV:63:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Ay:27:MET:C	17:Ay:29:GLY:N	2.79	0.41
1:BA:5129:ARG:NH2	4:BD:5256:ILE:O	2.54	0.41
1:BA:5224:ILE:H	1:BA:5224:ILE:HG13	1.57	0.41
2:BB:5175:THR:O	2:BB:5176:GLY:C	2.63	0.41
2:BB:5464:PHE:HE2	24:BB:5615:CLA:HMD3	1.85	0.41
3:BC:5067:MET:HE1	24:BC:5504:CLA:ND	2.35	0.41
3:BC:5242:LEU:O	3:BC:5243:ILE:C	2.63	0.41
3:BC:5311:GLN:OE1	3:BC:5355:THR:CG2	2.68	0.41
3:BC:5384:ILE:H	3:BC:5384:ILE:HG12	1.75	0.41
4:BD:5030:VAL:HG12	4:BD:5031:GLY:N	2.35	0.41
6:BF:5015:ILE:HG23	36:BF:5101:HEM:HAA1	2.03	0.41
10:BK:5019:ASP:N	10:BK:5020:PRO:CD	2.81	0.41
13:BO:5136:MET:O	13:BO:5137:ALA:C	2.62	0.41
15:BU:5041:ASN:O	15:BU:5042:VAL:C	2.64	0.41
1:AA:292:THR:C	1:AA:294:ALA:H	2.28	0.41
24:AA:404:CLA:H111	34:AD:402:PHO:H3A	2.02	0.41
2:AB:73:GLY:O	2:AB:93:PHE:CD1	2.74	0.41
2:AB:113:TRP:NE1	2:AB:117:TYR:CD1	2.89	0.41
2:AB:324:LEU:HA	4:AD:293:LEU:HD21	1.99	0.41
3:AC:332:GLN:HG3	13:AO:129:PHE:CE2	2.56	0.41
27:AC:515:BCR:H342	27:AC:515:BCR:H331	2.02	0.41
4:AD:168:PHE:CD2	4:AD:168:PHE:O	2.74	0.41
4:AD:272:LEU:O	4:AD:276:VAL:HG23	2.21	0.41
5:AE:10:PHE:CD2	5:AE:10:PHE:N	2.89	0.41
13:AO:86:ARG:O	13:AO:86:ARG:CG	2.69	0.41
14:AT:16:LEU:O	14:AT:17:PHE:C	2.63	0.41
19:AY:23:UNK:O	19:AY:24:UNK:C	2.68	0.41
28:BA:5412:DGD:HA82	3:BC:5223:TRP:CH2	2.56	0.41
2:BB:5103:LEU:O	2:BB:5107:LEU:HG	2.20	0.41
2:BB:5160:GLY:O	2:BB:5161:LEU:C	2.64	0.41
3:BC:5038:GLY:HA3	24:BC:5511:CLA:CMD	2.51	0.41
3:BC:5466:VAL:HG13	4:BD:5251:ARG:CD	2.51	0.41
24:BC:5513:CLA:NB	27:BC:5515:BCR:H383	2.36	0.41
4:BD:5056:THR:OG1	4:BD:5057:SER:N	2.53	0.41
4:BD:5162:LEU:HD21	4:BD:5167:TRP:CH2	2.56	0.41
7:BH:5018:TYR:CG	7:BH:5019:GLY:N	2.89	0.41
10:BK:5030:VAL:CG1	10:BK:5031:LEU:N	2.84	0.41
15:BU:5089:GLU:H	15:BU:5089:GLU:CD	2.28	0.41
1:AA:38:ILE:O	1:AA:42:LEU:HG	2.20	0.41
1:AA:151:LEU:HD21	1:AA:155:PHE:HE2	1.85	0.41
2:AB:168:VAL:O	2:AB:176:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:173:GLY:N	2:AB:265:ILE:HD11	2.36	0.41
2:AB:224:ARG:NH1	32:AB:624:LMT:H2'	2.35	0.41
2:AB:329:PRO:CD	24:AB:607:CLA:HED1	2.49	0.41
24:AB:602:CLA:C9	7:AH:46:LEU:HD22	2.51	0.41
24:AB:607:CLA:HAC2	27:BT:5101:BCR:H393	2.02	0.41
3:AC:56:HIS:C	3:AC:58:GLY:H	2.27	0.41
3:AC:114:VAL:CG2	31:AC:521:LMG:H141	2.50	0.41
3:AC:315:MET:HE1	3:AC:369:LEU:CD1	2.45	0.41
4:AD:162:LEU:HD22	28:AH:101:DGD:O1A	2.21	0.41
6:AF:40:MET:O	6:AF:43:ILE:HG13	2.21	0.41
11:AL:24:ILE:HG22	11:AL:25:LEU:N	2.35	0.41
13:AO:136:MET:O	13:AO:137:ALA:C	2.63	0.41
13:AO:208:LEU:O	13:AO:209:ALA:C	2.63	0.41
27:AT:101:BCR:H372	27:BB:5621:BCR:H353	2.03	0.41
16:AV:98:LEU:O	16:AV:102:MET:HG3	2.20	0.41
16:AV:102:MET:HE1	16:AV:141:ILE:HD12	2.03	0.41
16:AV:153:GLY:O	16:AV:154:ASP:C	2.62	0.41
1:BA:5092:HIS:HE1	3:BC:5359:TRP:HZ2	1.68	0.41
1:BA:5278:TRP:HA	28:BC:5519:DGD:CIA	2.51	0.41
1:BA:5289:GLY:HA2	1:BA:5292:THR:CG2	2.51	0.41
2:BB:5024:LEU:HD13	2:BB:5110:ALA:C	2.46	0.41
2:BB:5137:LYS:HE3	7:BH:5014:LEU:O	2.21	0.41
3:BC:5063:TRP:O	3:BC:5064:ALA:C	2.63	0.41
3:BC:5441:HIS:O	3:BC:5442:LEU:C	2.64	0.41
4:BD:5145:ALA:CB	4:BD:5272:LEU:HD21	2.51	0.41
4:BD:5179:PHE:HA	4:BD:5182:LEU:HD12	2.03	0.41
4:BD:5214:HIS:HA	35:BD:5406:PL9:O2	2.21	0.41
27:BD:5407:BCR:H392	9:BJ:5025:VAL:HG21	2.03	0.41
10:BK:5014:ALA:HB2	20:BZ:5061:VAL:CG1	2.51	0.41
10:BK:5043:VAL:CG2	10:BK:5046:ARG:HE	2.34	0.41
13:BO:5078:VAL:HG22	13:BO:5259:VAL:HG22	2.03	0.41
13:BO:5162:ILE:O	13:BO:5230:VAL:HG11	2.20	0.41
14:BT:5018:PHE:CD1	27:BT:5101:BCR:HC8	2.56	0.41
16:BV:5039:ASN:HD21	16:BV:5043:LYS:HB3	1.86	0.41
16:BV:5148:GLU:N	16:BV:5149:PRO:HD2	2.36	0.41
19:BY:5021:UNK:HA	19:BY:5024:UNK:CB	2.51	0.41
1:AA:29:TYR:CG	1:AA:133:LEU:HD13	2.56	0.41
2:AB:45:PHE:HE2	2:AB:47:PRO:HB3	1.86	0.41
2:AB:464:PHE:HE2	24:AB:611:CLA:HMD3	1.86	0.41
3:AC:203:THR:O	3:AC:235:GLY:HA3	2.20	0.41
3:AC:266:TRP:HZ3	24:AC:507:CLA:HBC2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:390:ARG:NE	16:AV:126:ILE:CG2	2.84	0.41
24:AC:504:CLA:H2	28:AC:518:DGD:C2A	2.51	0.41
4:AD:250:ASN:ND2	4:AD:262:SER:HB3	2.33	0.41
8:AI:25:SER:HA	32:AI:103:LMT:H6D	2.02	0.41
10:AK:30:VAL:CG1	10:AK:31:LEU:N	2.84	0.41
13:AO:55:ALA:HA	13:AO:230:VAL:HG11	2.03	0.41
19:AY:23:UNK:O	19:AY:25:UNK:N	2.54	0.41
20:AZ:33:TRP:CD1	20:AZ:33:TRP:C	2.99	0.41
1:BA:5258:LEU:HD12	4:BD:5128:ARG:CG	2.51	0.41
29:BA:5415:LHG:H272	10:BK:5045:PHE:CE2	2.56	0.41
2:BB:5005:TRP:CE3	24:BB:5615:CLA:H42	2.56	0.41
2:BB:5193:TYR:HE1	2:BB:5259:GLY:C	2.29	0.41
2:BB:5297:THR:OG1	2:BB:5298:LEU:N	2.54	0.41
2:BB:5328:GLY:O	24:BB:5611:CLA:HBA1	2.21	0.41
2:BB:5348:ASN:O	2:BB:5350:GLU:N	2.54	0.41
2:BB:5377:VAL:HG11	4:BD:5342:PRO:CG	2.51	0.41
24:BB:5606:CLA:H161	28:BH:5101:DGD:HAW1	2.02	0.41
24:BB:5608:CLA:H143	24:BB:5619:CLA:HMA2	2.02	0.41
3:BC:5172:ALA:O	3:BC:5176:VAL:HG23	2.21	0.41
3:BC:5305:THR:HG23	3:BC:5307:PRO:HG2	2.03	0.41
3:BC:5338:GLY:O	3:BC:5339:LYS:C	2.62	0.41
28:BC:5518:DGD:O1B	28:BC:5518:DGD:C1G	2.69	0.41
4:BD:5070:GLY:O	9:BJ:5037:GLY:CA	2.69	0.41
4:BD:5202:ALA:HB3	35:BD:5406:PL9:C30	2.51	0.41
6:BF:5024:HIS:HA	6:BF:5027:ALA:HB3	2.03	0.41
32:BM:5101:LMT:H5'	32:BM:5101:LMT:H1B	1.97	0.41
13:BO:5056:TYR:CD1	13:BO:5235:GLY:HA2	2.55	0.41
1:AA:76:ASN:ND2	11:AL:33:SER:HB3	2.37	0.40
1:AA:333:GLU:HB2	1:AA:337:HIS:CE1	2.53	0.40
1:AA:340:PRO:HG3	15:AU:133:TYR:CD1	2.56	0.40
2:AB:431:GLU:OE2	13:BO:5084:ASN:ND2	2.54	0.40
24:AB:602:CLA:H93	7:AH:46:LEU:HD22	2.02	0.40
3:AC:269:GLU:OE1	3:AC:447:ARG:HD3	2.21	0.40
3:AC:282:MET:SD	24:AC:503:CLA:H142	2.61	0.40
24:AC:509:CLA:HBB1	24:AC:509:CLA:HHC	2.03	0.40
6:AF:29:PRO:O	6:AF:32:PHE:HB3	2.21	0.40
8:AI:11:VAL:O	8:AI:15:PHE:HD2	2.04	0.40
9:AJ:10:LEU:HD12	9:AJ:10:LEU:HA	1.86	0.40
16:AV:71:ILE:CD1	16:AV:72:THR:N	2.82	0.40
1:BA:5012:ASN:O	1:BA:5013:LEU:C	2.64	0.40
1:BA:5012:ASN:O	1:BA:5015:GLU:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5110:GLY:O	1:BA:5111:PRO:C	2.62	0.40
1:BA:5184:ILE:CD1	4:BD:5186:GLN:HG2	2.51	0.40
1:BA:5206:PHE:HD2	1:BA:5206:PHE:HA	1.77	0.40
1:BA:5295:PHE:HD2	3:BC:5291:TRP:CD2	2.39	0.40
2:BB:5004:PRO:HB2	2:BB:5006:TYR:CE1	2.56	0.40
2:BB:5172:TYR:O	2:BB:5174:LEU:HG	2.21	0.40
2:BB:5238:LEU:CD2	2:BB:5469:HIS:HD2	2.34	0.40
2:BB:5328:GLY:N	24:BB:5611:CLA:O1A	2.49	0.40
3:BC:5081:MET:HE1	3:BC:5090:PRO:N	2.36	0.40
4:BD:5263:ASN:O	4:BD:5265:ARG:N	2.54	0.40
12:BM:5021:PHE:O	12:BM:5022:LEU:C	2.63	0.40
1:AA:278:TRP:HA	28:AC:519:DGD:HAG1	2.02	0.40
2:AB:121:GLU:CG	7:AH:4:ARG:CA	2.94	0.40
3:AC:34:ALA:HB2	4:AD:230:SER:CB	2.51	0.40
3:AC:113:VAL:CG1	31:AC:521:LMG:H132	2.49	0.40
27:AD:406:BCR:H392	9:AJ:25:VAL:HG21	2.03	0.40
6:AF:15:ILE:CG2	6:AF:16:PHE:HD1	2.33	0.40
10:AK:15:TYR:OH	20:AZ:58:ASN:ND2	2.52	0.40
13:AO:83:LYS:CG	13:AO:84:ASN:H	2.29	0.40
14:AT:29:ILE:HG22	14:AT:30:THR:H	1.86	0.40
15:AU:72:TYR:CG	15:AU:73:PRO:N	2.89	0.40
15:AU:75:LEU:HD23	15:AU:75:LEU:HA	1.85	0.40
16:AV:121:LEU:HD21	16:AV:138:LEU:HD11	2.02	0.40
1:BA:5029:TYR:HD2	1:BA:5133:LEU:HB2	1.87	0.40
1:BA:5157:VAL:HG21	24:BA:5406:CLA:HMC1	2.03	0.40
2:BB:5161:LEU:N	2:BB:5161:LEU:CD1	2.84	0.40
28:BB:5602:DGD:HE61	32:BB:5626:LMT:H2'	2.02	0.40
3:BC:5272:LEU:O	3:BC:5273:SER:C	2.64	0.40
4:BD:5277:THR:HG22	35:BD:5406:PL9:H272	2.02	0.40
5:BE:5015:THR:HG23	9:BJ:5008:ILE:C	2.43	0.40
7:BH:5005:THR:O	7:BH:5006:TRP:C	2.64	0.40
9:BJ:5008:ILE:HD12	9:BJ:5008:ILE:H	1.85	0.40
11:BL:5008:GLN:HE21	11:BL:5008:GLN:H	1.68	0.40
13:BO:5032:THR:OG1	13:BO:5033:TYR:N	2.54	0.40
18:BX:5011:THR:O	18:BX:5012:ILE:C	2.64	0.40
1:AA:214:MET:HE3	34:AD:403:PHO:HMD2	2.04	0.40
1:AA:217:SER:O	1:AA:220:THR:HG22	2.22	0.40
2:AB:238:LEU:CD2	2:AB:469:HIS:CD2	3.05	0.40
32:AB:629:LMT:H5'	32:AB:629:LMT:H1B	1.80	0.40
3:AC:161:LEU:HD23	3:AC:251:HIS:HD2	1.85	0.40
4:AD:180:ARG:NH1	4:AD:333:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AD:405:PL9:H103	35:AD:405:PL9:HC72	1.74	0.40
5:AE:69:ARG:CG	5:AE:70:PHE:N	2.83	0.40
10:AK:46:ARG:NH1	10:AK:46:ARG:HB2	2.36	0.40
12:AM:21:PHE:O	12:AM:22:LEU:C	2.64	0.40
1:BA:5069:GLY:CA	1:BA:5075:ASN:ND2	2.84	0.40
1:BA:5200:LEU:HD11	28:BC:5519:DGD:CCA	2.27	0.40
2:BB:5151:PHE:CE1	2:BB:5203:ILE:HG23	2.57	0.40
2:BB:5451:PHE:CD2	2:BB:5451:PHE:C	2.99	0.40
24:BC:5502:CLA:HAA2	24:BC:5502:CLA:HBD	2.03	0.40
24:BC:5505:CLA:HAA1	24:BC:5505:CLA:C2	2.51	0.40
24:BC:5507:CLA:H122	27:BC:5516:BCR:H362	2.03	0.40
4:BD:5148:ALA:HB3	4:BD:5149:PRO:CD	2.41	0.40
4:BD:5168:PHE:CD2	4:BD:5168:PHE:C	3.00	0.40
7:BH:5039:LEU:C	7:BH:5039:LEU:HD23	2.46	0.40
15:BU:5072:TYR:CD2	15:BU:5073:PRO:N	2.90	0.40
1:AA:16:ARG:O	1:AA:17:PHE:C	2.64	0.40
1:AA:39:PRO:HG3	27:AA:410:BCR:HC8	2.04	0.40
1:AA:200:LEU:CD2	28:AC:519:DGD:CCA	2.99	0.40
1:AA:278:TRP:HE3	28:AC:519:DGD:HAG1	1.83	0.40
2:AB:86:ILE:HD12	2:AB:86:ILE:C	2.46	0.40
2:AB:135:LEU:HD23	2:AB:138:MET:CE	2.51	0.40
2:AB:285:ASN:N	2:AB:285:ASN:HD22	2.18	0.40
3:AC:38:GLY:HA3	24:AC:511:CLA:CMD	2.50	0.40
3:AC:134:ILE:HD11	24:AC:511:CLA:C9	2.49	0.40
24:AC:502:CLA:HHC	24:AC:502:CLA:HBB1	2.03	0.40
4:AD:210:LEU:HD21	35:AD:405:PL9:H13	2.03	0.40
4:AD:262:SER:N	31:AD:408:LMG:O3	2.55	0.40
4:AD:313:THR:H	4:AD:316:THR:HG23	1.86	0.40
13:AO:230:VAL:CG1	13:AO:231:ASP:N	2.73	0.40
14:AT:30:THR:HB	14:AT:31:LYS:NZ	2.35	0.40
27:AT:101:BCR:H393	24:BB:5611:CLA:HAC2	2.03	0.40
15:AU:83:ALA:CB	15:AU:84:PRO:HD2	2.17	0.40
18:AX:30:LEU:HA	18:AX:30:LEU:HD23	1.88	0.40
1:BA:5238:LYS:O	1:BA:5241:GLN:HG3	2.21	0.40
3:BC:5278:ALA:HB1	24:BC:5501:CLA:H142	2.03	0.40
3:BC:5447:ARG:HH11	3:BC:5447:ARG:HG2	1.86	0.40
7:BH:5063:LYS:C	7:BH:5065:LEU:H	2.29	0.40
27:BK:5102:BCR:H332	20:BZ:5017:PHE:CD1	2.56	0.40
16:BV:5128:PRO:O	16:BV:5129:LYS:C	2.64	0.40
1:AA:271:LEU:CD1	25:AA:408:MST:H162	2.48	0.40
2:AB:243:ALA:O	24:AB:608:CLA:HBC3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:283:GLU:O	2:AB:287:ARG:HG3	2.21	0.40
3:AC:202:PRO:HB2	3:AC:235:GLY:HA2	2.02	0.40
3:AC:307:PRO:O	3:AC:311:GLN:HG2	2.21	0.40
24:AC:511:CLA:H151	20:AZ:24:PRO:CG	2.50	0.40
4:AD:24:ARG:NH2	18:AX:44:ASP:O	2.55	0.40
4:AD:126:MET:HE2	4:AD:146:PHE:HB3	2.02	0.40
5:AE:38:VAL:HG21	6:AF:36:ALA:O	2.21	0.40
6:AF:21:VAL:HG21	30:AF:102:SQD:H101	2.02	0.40
7:AH:41:PHE:O	7:AH:45:ILE:HG12	2.21	0.40
1:BA:5011:ALA:HB1	1:BA:5015:GLU:OE1	2.21	0.40
1:BA:5217:SER:O	1:BA:5218:LEU:C	2.65	0.40
1:BA:5296:ASN:HB3	3:BC:5401:LEU:HD13	2.04	0.40
2:BB:5012:LEU:O	2:BB:5013:ILE:C	2.65	0.40
2:BB:5170:ASP:CB	2:BB:5171:PRO:CD	2.97	0.40
2:BB:5297:THR:HG22	2:BB:5300:GLU:CD	2.45	0.40
24:BB:5619:CLA:HBB1	24:BB:5619:CLA:HHC	2.03	0.40
4:BD:5095:PRO:HG3	18:BX:5015:SER:HB3	2.03	0.40
4:BD:5262:SER:N	31:BD:5410:LMG:O3	2.54	0.40
6:BF:5020:TRP:NE1	6:BF:5024:HIS:CE1	2.89	0.40
6:BF:5029:PRO:O	6:BF:5032:PHE:HB3	2.22	0.40
12:BM:5016:LEU:HA	12:BM:5016:LEU:HD23	1.78	0.40
13:BO:5065:ARG:NH1	13:BO:5065:ARG:CB	2.85	0.40
13:BO:5132:VAL:HG12	13:BO:5133:THR:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	333/344 (97%)	284 (85%)	42 (13%)	7 (2%)	5	31
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	488/510 (96%)	418 (86%)	54 (11%)	16 (3%)	3	21
2	BB	488/510 (96%)	422 (86%)	51 (10%)	15 (3%)	3	22
3	AC	445/461 (96%)	371 (83%)	58 (13%)	16 (4%)	2	19
3	BC	445/461 (96%)	372 (84%)	56 (13%)	17 (4%)	2	18
4	AD	339/352 (96%)	286 (84%)	44 (13%)	9 (3%)	4	25
4	BD	339/352 (96%)	288 (85%)	43 (13%)	8 (2%)	4	28
5	AE	80/84 (95%)	71 (89%)	6 (8%)	3 (4%)	2	18
5	BE	80/84 (95%)	70 (88%)	7 (9%)	3 (4%)	2	18
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	3	23
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	3	23
7	AH	63/66 (96%)	47 (75%)	11 (18%)	5 (8%)	1	5
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	1	8
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1	9
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	1	9
9	AJ	36/40 (90%)	27 (75%)	6 (17%)	3 (8%)	0	4
9	BJ	36/40 (90%)	25 (69%)	8 (22%)	3 (8%)	0	4
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	11
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	11
11	AL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	BL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	AM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
13	AO	241/247 (98%)	198 (82%)	31 (13%)	12 (5%)	1	13
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	2	15
14	AT	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	3	21
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3	21
15	AU	95/104 (91%)	78 (82%)	12 (13%)	5 (5%)	1	12
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	2	16
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	18	52
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	18	52
17	Ay	26/46 (56%)	15 (58%)	7 (27%)	4 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	By	26/46 (56%)	14 (54%)	9 (35%)	3 (12%)	0	1
18	AX	35/41 (85%)	26 (74%)	5 (14%)	4 (11%)	0	2
18	BX	35/41 (85%)	27 (77%)	4 (11%)	4 (11%)	0	2
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1	13
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1	13
All	All	5148/5438 (95%)	4279 (83%)	686 (13%)	183 (4%)	2	19

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP
2	AB	176	GLY
2	AB	230	ARG
2	AB	484	PRO
2	AB	488	PRO
2	AB	490	GLN
3	AC	144	SER
3	AC	257	PHE
3	AC	416	SER
3	AC	452	ALA
4	AD	239	GLN
4	AD	240	ALA
4	AD	262	SER
7	AH	18	TYR
8	AI	25	SER
9	AJ	35	GLY
13	AO	52	ALA
14	AT	30	THR
15	AU	72	TYR
15	AU	83	ALA
16	AV	75	ASN
17	Ay	43	ARG
18	AX	45	LYS
20	AZ	32	ASP
1	BA	5012	ASN
1	BA	5141	PRO
1	BA	5142	TRP
2	BB	5176	GLY

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Mol	Chain	Res	Type
2	BB	5230	ARG
2	BB	5484	PRO
2	BB	5488	PRO
3	BC	5144	SER
3	BC	5257	PHE
3	BC	5416	SER
3	BC	5452	ALA
4	BD	5239	GLN
4	BD	5240	ALA
4	BD	5262	SER
7	BH	5018	TYR
8	BI	5025	SER
9	BJ	5035	GLY
13	BO	5052	ALA
14	BT	5030	THR
15	BU	5072	TYR
15	BU	5083	ALA
17	By	5043	ARG
18	BX	5045	LYS
20	BZ	5032	ASP
2	AB	349	LYS
3	AC	46	SER
3	AC	136	GLY
3	AC	194	GLY
3	AC	209	ILE
3	AC	456	GLU
4	AD	234	ALA
4	AD	264	LYS
7	AH	26	GLY
9	AJ	38	SER
13	AO	231	ASP
15	AU	39	LEU
15	AU	73	PRO
17	Ay	25	ILE
18	AX	43	ILE
2	BB	5349	LYS
2	BB	5436	THR
3	BC	5136	GLY
3	BC	5141	GLU
3	BC	5194	GLY
4	BD	5234	ALA
7	BH	5026	GLY

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Mol	Chain	Res	Type
9	BJ	5038	SER
13	BO	5158	ASN
13	BO	5231	ASP
15	BU	5073	PRO
16	BV	5075	ASN
18	BX	5043	ILE
2	AB	13	ILE
2	AB	127	ARG
2	AB	183	PRO
2	AB	414	PRO
2	AB	436	THR
3	AC	32	GLY
3	AC	141	GLU
3	AC	375	LEU
3	AC	453	ALA
4	AD	263	ASN
5	AE	9	PRO
7	AH	16	SER
10	AK	13	GLU
10	AK	45	PHE
13	AO	60	SER
13	AO	158	ASN
13	AO	165	SER
20	AZ	24	PRO
20	AZ	28	ALA
2	BB	5013	ILE
2	BB	5127	ARG
2	BB	5183	PRO
2	BB	5414	PRO
3	BC	5032	GLY
3	BC	5046	SER
3	BC	5209	ILE
3	BC	5375	LEU
3	BC	5411	ALA
3	BC	5456	GLU
4	BD	5263	ASN
4	BD	5264	LYS
5	BE	5009	PRO
7	BH	5016	SER
10	BK	5013	GLU
10	BK	5045	PHE
13	BO	5165	SER

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Mol	Chain	Res	Type
17	By	5025	ILE
20	BZ	5024	PRO
20	BZ	5028	ALA
2	AB	173	GLY
2	AB	231	MET
3	AC	154	LYS
4	AD	73	PHE
5	AE	10	PHE
13	AO	51	THR
13	AO	82	PRO
17	Ay	24	MET
18	AX	44	ASP
2	BB	5235	GLU
5	BE	5010	PHE
13	BO	5060	SER
13	BO	5082	PRO
1	AA	97	TRP
2	AB	235	GLU
3	AC	462	GLU
6	AF	41	GLN
7	AH	6	TRP
15	AU	42	VAL
2	BB	5435	GLU
2	BB	5490	GLN
3	BC	5453	ALA
3	BC	5462	GLU
4	BD	5252	PHE
6	BF	5041	GLN
7	BH	5006	TRP
13	BO	5085	LYS
13	BO	5088	GLU
15	BU	5042	VAL
17	By	5024	MET
18	BX	5044	ASP
1	AA	334	ARG
2	AB	435	GLU
4	AD	351	ALA
13	AO	88	GLU
18	AX	12	ILE
1	BA	5097	TRP
1	BA	5334	ARG
2	BB	5173	GLY

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Mol	Chain	Res	Type
3	BC	5382	ASN
4	BD	5351	ALA
5	BE	5052	PRO
13	BO	5051	THR
13	BO	5159	VAL
18	BX	5012	ILE
1	AA	21	VAL
2	AB	16	PRO
9	AJ	5	GLY
13	AO	159	VAL
1	BA	5021	VAL
3	AC	201	ASN
17	Ay	35	ILE
3	BC	5201	ASN
5	AE	52	PRO
7	AH	60	VAL
8	AI	32	PRO
13	AO	232	GLY
2	BB	5016	PRO
8	BI	5032	PRO
1	AA	176	ILE
4	AD	160	TYR
13	AO	127	ILE
1	BA	5039	PRO
13	AO	152	VAL
9	BJ	5005	GLY
13	BO	5152	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	271/280 (97%)	247 (91%)	24 (9%)	9	34
1	BA	271/280 (97%)	247 (91%)	24 (9%)	9	34
2	AB	390/407 (96%)	362 (93%)	28 (7%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BB	390/407 (96%)	364 (93%)	26 (7%)	15	47
3	AC	347/362 (96%)	327 (94%)	20 (6%)	18	51
3	BC	347/362 (96%)	325 (94%)	22 (6%)	16	48
4	AD	275/283 (97%)	248 (90%)	27 (10%)	7	31
4	BD	275/283 (97%)	247 (90%)	28 (10%)	7	29
5	AE	72/73 (99%)	65 (90%)	7 (10%)	8	32
5	BE	72/73 (99%)	65 (90%)	7 (10%)	8	32
6	AF	29/39 (74%)	28 (97%)	1 (3%)	32	64
6	BF	29/39 (74%)	28 (97%)	1 (3%)	32	64
7	AH	53/55 (96%)	41 (77%)	12 (23%)	1	5
7	BH	53/55 (96%)	41 (77%)	12 (23%)	1	5
8	AI	32/35 (91%)	31 (97%)	1 (3%)	35	66
8	BI	32/35 (91%)	31 (97%)	1 (3%)	35	66
9	AJ	25/28 (89%)	24 (96%)	1 (4%)	28	61
9	BJ	25/28 (89%)	24 (96%)	1 (4%)	28	61
10	AK	30/30 (100%)	28 (93%)	2 (7%)	15	47
10	BK	30/30 (100%)	28 (93%)	2 (7%)	15	47
11	AL	35/35 (100%)	31 (89%)	4 (11%)	5	24
11	BL	35/35 (100%)	30 (86%)	5 (14%)	3	16
12	AM	31/33 (94%)	29 (94%)	2 (6%)	15	47
12	BM	31/33 (94%)	28 (90%)	3 (10%)	8	32
13	AO	202/208 (97%)	183 (91%)	19 (9%)	8	33
13	BO	202/208 (97%)	184 (91%)	18 (9%)	9	34
14	AT	29/29 (100%)	27 (93%)	2 (7%)	14	45
14	BT	29/29 (100%)	27 (93%)	2 (7%)	14	45
15	AU	84/89 (94%)	75 (89%)	9 (11%)	6	27
15	BU	84/89 (94%)	75 (89%)	9 (11%)	6	27
16	AV	116/117 (99%)	112 (97%)	4 (3%)	32	64
16	BV	116/117 (99%)	109 (94%)	7 (6%)	17	50
17	Ay	20/37 (54%)	15 (75%)	5 (25%)	0	3
17	By	20/37 (54%)	14 (70%)	6 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AX	30/34 (88%)	28 (93%)	2 (7%)	15	47
18	BX	30/34 (88%)	30 (100%)	0	100	100
20	AZ	52/52 (100%)	47 (90%)	5 (10%)	8	32
20	BZ	52/52 (100%)	46 (88%)	6 (12%)	5	24
All	All	4246/4452 (95%)	3891 (92%)	355 (8%)	10	38

All (355) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	13	LEU
1	AA	30	VAL
1	AA	32	TRP
1	AA	56	PRO
1	AA	84	PRO
1	AA	121	LEU
1	AA	129	ARG
1	AA	145	VAL
1	AA	202	VAL
1	AA	210	LEU
1	AA	214	MET
1	AA	218	LEU
1	AA	224	ILE
1	AA	226	GLU
1	AA	234	ASN
1	AA	243	GLU
1	AA	245	THR
1	AA	248	ILE
1	AA	259	ILE
1	AA	266	ASN
1	AA	286	THR
1	AA	298	ASN
1	AA	306	VAL
1	AA	335	ASN
2	AB	16	PRO
2	AB	62	VAL
2	AB	116	VAL
2	AB	121	GLU
2	AB	137	LYS
2	AB	161	LEU
2	AB	179	GLN
2	AB	183	PRO

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Mol	Chain	Res	Type
2	AB	198	VAL
2	AB	223	GLN
2	AB	245	VAL
2	AB	246	PHE
2	AB	294	SER
2	AB	297	THR
2	AB	357	ARG
2	AB	376	VAL
2	AB	414	PRO
2	AB	425	ILE
2	AB	433	ASP
2	AB	439	SER
2	AB	457	VAL
2	AB	467	ILE
2	AB	476	ARG
2	AB	478	VAL
2	AB	484	PRO
2	AB	485	GLU
2	AB	488	PRO
2	AB	490	GLN
3	AC	29	GLU
3	AC	91	HIS
3	AC	97	TRP
3	AC	117	VAL
3	AC	121	SER
3	AC	165	LEU
3	AC	167	VAL
3	AC	188	THR
3	AC	244	CYS
3	AC	254	THR
3	AC	289	PHE
3	AC	295	THR
3	AC	318	LEU
3	AC	321	ASP
3	AC	324	LEU
3	AC	355	THR
3	AC	424	SER
3	AC	456	GLU
3	AC	461	ARG
3	AC	473	ASP
4	AD	43	LEU
4	AD	84	SER

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Mol	Chain	Res	Type
4	AD	91	LEU
4	AD	110	LEU
4	AD	112	THR
4	AD	128	ARG
4	AD	130	PHE
4	AD	166	SER
4	AD	180	ARG
4	AD	201	VAL
4	AD	205	LEU
4	AD	242	GLU
4	AD	256	ILE
4	AD	259	ILE
4	AD	262	SER
4	AD	264	LYS
4	AD	272	LEU
4	AD	279	LEU
4	AD	282	SER
4	AD	291	LEU
4	AD	293	LEU
4	AD	308	ASP
4	AD	316	THR
4	AD	323	GLU
4	AD	331	PRO
4	AD	345	VAL
4	AD	346	LEU
5	AE	9	PRO
5	AE	10	PHE
5	AE	52	PRO
5	AE	60	GLN
5	AE	68	ASP
5	AE	77	GLU
5	AE	84	LYS
6	AF	18	VAL
7	AH	12	ARG
7	AH	14	LEU
7	AH	17	GLU
7	AH	21	VAL
7	AH	25	TRP
7	AH	27	THR
7	AH	42	LEU
7	AH	43	LEU
7	AH	45	ILE

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Mol	Chain	Res	Type
7	AH	53	LEU
7	AH	56	ASP
7	AH	60	VAL
8	AI	32	PRO
9	AJ	7	ARG
10	AK	19	ASP
10	AK	33	LEU
11	AL	8	GLN
11	AL	11	GLU
11	AL	15	THR
11	AL	24	ILE
12	AM	20	VAL
12	AM	25	LEU
13	AO	31	LEU
13	AO	41	LEU
13	AO	60	SER
13	AO	74	THR
13	AO	84	ASN
13	AO	86	ARG
13	AO	90	GLU
13	AO	97	VAL
13	AO	106	GLN
13	AO	127	ILE
13	AO	152	VAL
13	AO	158	ASN
13	AO	165	SER
13	AO	171	GLU
13	AO	174	VAL
13	AO	183	LEU
13	AO	207	GLU
13	AO	224	SER
13	AO	227	VAL
14	AT	7	VAL
14	AT	29	ILE
15	AU	42	VAL
15	AU	44	ASP
15	AU	53	GLU
15	AU	61	ASN
15	AU	98	THR
15	AU	103	GLN
15	AU	114	VAL
15	AU	119	THR

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Mol	Chain	Res	Type
15	AU	132	LEU
16	AV	32	GLU
16	AV	40	SER
16	AV	68	VAL
16	AV	89	THR
17	Ay	21	GLN
17	Ay	28	ILE
17	Ay	34	MET
17	Ay	35	ILE
17	Ay	36	ILE
18	AX	14	PRO
18	AX	33	THR
20	AZ	7	LEU
20	AZ	13	VAL
20	AZ	33	TRP
20	AZ	58	ASN
20	AZ	62	VAL
1	BA	5013	LEU
1	BA	5030	VAL
1	BA	5032	TRP
1	BA	5121	LEU
1	BA	5129	ARG
1	BA	5143	ILE
1	BA	5145	VAL
1	BA	5202	VAL
1	BA	5206	PHE
1	BA	5210	LEU
1	BA	5214	MET
1	BA	5218	LEU
1	BA	5224	ILE
1	BA	5226	GLU
1	BA	5234	ASN
1	BA	5243	GLU
1	BA	5245	THR
1	BA	5248	ILE
1	BA	5259	ILE
1	BA	5266	ASN
1	BA	5286	THR
1	BA	5298	ASN
1	BA	5306	VAL
1	BA	5335	ASN
2	BB	5016	PRO

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Mol	Chain	Res	Type
2	BB	5062	VAL
2	BB	5084	THR
2	BB	5116	VAL
2	BB	5121	GLU
2	BB	5137	LYS
2	BB	5161	LEU
2	BB	5179	GLN
2	BB	5198	VAL
2	BB	5245	VAL
2	BB	5246	PHE
2	BB	5294	SER
2	BB	5297	THR
2	BB	5357	ARG
2	BB	5376	VAL
2	BB	5425	ILE
2	BB	5433	ASP
2	BB	5439	SER
2	BB	5457	VAL
2	BB	5467	ILE
2	BB	5476	ARG
2	BB	5478	VAL
2	BB	5484	PRO
2	BB	5485	GLU
2	BB	5488	PRO
2	BB	5490	GLN
3	BC	5027	ASP
3	BC	5029	GLU
3	BC	5091	HIS
3	BC	5097	TRP
3	BC	5117	VAL
3	BC	5121	SER
3	BC	5165	LEU
3	BC	5167	VAL
3	BC	5188	THR
3	BC	5244	CYS
3	BC	5254	THR
3	BC	5289	PHE
3	BC	5295	THR
3	BC	5313	GLN
3	BC	5318	LEU
3	BC	5324	LEU
3	BC	5355	THR

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Mol	Chain	Res	Type
3	BC	5424	SER
3	BC	5432	VAL
3	BC	5456	GLU
3	BC	5461	ARG
3	BC	5473	ASP
4	BD	5043	LEU
4	BD	5084	SER
4	BD	5091	LEU
4	BD	5110	LEU
4	BD	5112	THR
4	BD	5128	ARG
4	BD	5130	PHE
4	BD	5166	SER
4	BD	5180	ARG
4	BD	5201	VAL
4	BD	5205	LEU
4	BD	5242	GLU
4	BD	5256	ILE
4	BD	5259	ILE
4	BD	5262	SER
4	BD	5264	LYS
4	BD	5272	LEU
4	BD	5279	LEU
4	BD	5282	SER
4	BD	5289	LEU
4	BD	5291	LEU
4	BD	5293	LEU
4	BD	5308	ASP
4	BD	5316	THR
4	BD	5323	GLU
4	BD	5331	PRO
4	BD	5345	VAL
4	BD	5346	LEU
5	BE	5009	PRO
5	BE	5010	PHE
5	BE	5052	PRO
5	BE	5060	GLN
5	BE	5068	ASP
5	BE	5077	GLU
5	BE	5084	LYS
6	BF	5018	VAL
7	BH	5012	ARG

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Mol	Chain	Res	Type
7	BH	5014	LEU
7	BH	5017	GLU
7	BH	5021	VAL
7	BH	5025	TRP
7	BH	5027	THR
7	BH	5042	LEU
7	BH	5043	LEU
7	BH	5045	ILE
7	BH	5053	LEU
7	BH	5056	ASP
7	BH	5060	VAL
8	BI	5032	PRO
9	BJ	5007	ARG
10	BK	5017	ILE
10	BK	5033	LEU
11	BL	5008	GLN
11	BL	5009	PRO
11	BL	5011	GLU
11	BL	5015	THR
11	BL	5024	ILE
12	BM	5020	VAL
12	BM	5025	LEU
12	BM	5034	LYS
13	BO	5031	LEU
13	BO	5041	LEU
13	BO	5060	SER
13	BO	5084	ASN
13	BO	5086	ARG
13	BO	5090	GLU
13	BO	5097	VAL
13	BO	5106	GLN
13	BO	5127	ILE
13	BO	5152	VAL
13	BO	5158	ASN
13	BO	5165	SER
13	BO	5171	GLU
13	BO	5174	VAL
13	BO	5183	LEU
13	BO	5207	GLU
13	BO	5224	SER
13	BO	5227	VAL
14	BT	5007	VAL

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Mol	Chain	Res	Type
14	BT	5029	ILE
15	BU	5042	VAL
15	BU	5044	ASP
15	BU	5053	GLU
15	BU	5061	ASN
15	BU	5098	THR
15	BU	5103	GLN
15	BU	5114	VAL
15	BU	5119	THR
15	BU	5132	LEU
16	BV	5032	GLU
16	BV	5040	SER
16	BV	5063	CYS
16	BV	5068	VAL
16	BV	5089	THR
16	BV	5092	ARG
16	BV	5125	ASP
17	By	5021	GLN
17	By	5027	MET
17	By	5028	ILE
17	By	5034	MET
17	By	5035	ILE
17	By	5036	ILE
20	BZ	5007	LEU
20	BZ	5013	VAL
20	BZ	5023	VAL
20	BZ	5025	VAL
20	BZ	5033	TRP
20	BZ	5062	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	19	ASN
1	AA	92	HIS
1	AA	118	HIS
1	AA	199	GLN
1	AA	234	ASN
1	AA	241	GLN
1	AA	247	ASN
1	AA	272	HIS

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Mol	Chain	Res	Type
1	AA	315	ASN
1	AA	338	ASN
2	AB	26	HIS
2	AB	53	ASN
2	AB	157	HIS
2	AB	179	GLN
2	AB	201	HIS
2	AB	216	HIS
2	AB	281	GLN
2	AB	282	GLN
2	AB	285	ASN
2	AB	331	ASN
2	AB	343	HIS
2	AB	374	ASN
2	AB	438	ASN
2	AB	469	HIS
2	AB	490	GLN
3	AC	56	HIS
3	AC	155	ASN
3	AC	228	ASN
3	AC	251	HIS
3	AC	388	GLN
3	AC	398	HIS
3	AC	415	ASN
3	AC	418	ASN
4	AD	83	ASN
4	AD	98	GLN
4	AD	129	GLN
4	AD	186	GLN
4	AD	250	ASN
4	AD	332	GLN
5	AE	60	GLN
5	AE	75	GLN
6	AF	41	GLN
11	AL	8	GLN
11	AL	37	ASN
12	AM	5	GLN
12	AM	32	GLN
13	AO	62	GLN
13	AO	84	ASN
13	AO	87	GLN
13	AO	106	GLN

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Mol	Chain	Res	Type
13	AO	114	ASN
13	AO	135	GLN
13	AO	150	ASN
13	AO	173	ASN
13	AO	181	ASN
13	AO	202	GLN
13	AO	222	GLN
13	AO	226	ASN
16	AV	104	ASN
18	AX	47	GLN
20	AZ	58	ASN
1	BA	5012	ASN
1	BA	5019	ASN
1	BA	5092	HIS
1	BA	5118	HIS
1	BA	5199	GLN
1	BA	5234	ASN
1	BA	5241	GLN
1	BA	5247	ASN
1	BA	5272	HIS
1	BA	5315	ASN
1	BA	5338	ASN
2	BB	5026	HIS
2	BB	5053	ASN
2	BB	5157	HIS
2	BB	5179	GLN
2	BB	5201	HIS
2	BB	5216	HIS
2	BB	5281	GLN
2	BB	5282	GLN
2	BB	5285	ASN
2	BB	5331	ASN
2	BB	5338	GLN
2	BB	5343	HIS
2	BB	5374	ASN
2	BB	5469	HIS
2	BB	5490	GLN
3	BC	5056	HIS
3	BC	5155	ASN
3	BC	5228	ASN
3	BC	5251	HIS
3	BC	5388	GLN

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Mol	Chain	Res	Type
3	BC	5398	HIS
3	BC	5415	ASN
3	BC	5418	ASN
4	BD	5083	ASN
4	BD	5129	GLN
4	BD	5186	GLN
4	BD	5250	ASN
4	BD	5332	GLN
5	BE	5060	GLN
5	BE	5075	GLN
11	BL	5008	GLN
11	BL	5037	ASN
12	BM	5005	GLN
12	BM	5028	GLN
12	BM	5032	GLN
13	BO	5062	GLN
13	BO	5084	ASN
13	BO	5087	GLN
13	BO	5106	GLN
13	BO	5114	ASN
13	BO	5150	ASN
13	BO	5173	ASN
13	BO	5181	ASN
13	BO	5202	GLN
13	BO	5222	GLN
16	BV	5060	GLN
16	BV	5104	ASN
16	BV	5144	HIS
18	BX	5047	GLN
20	BZ	5058	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 196 ligands modelled in this entry, 12 are monoatomic - leaving 184 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
29	LHG	AA	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.14	3 (7%)
27	BCR	BB	5621	-	41,41,41	1.52	7 (17%)	56,56,56	2.15	21 (37%)
30	SQD	AA	413	-	49,51,54	2.55	28 (57%)	59,62,65	2.70	20 (33%)
34	PHO	BD	5404	-	58,69,69	3.07	16 (27%)	55,99,99	2.25	13 (23%)
30	SQD	AA	416	-	52,54,54	2.57	30 (57%)	62,65,65	2.68	20 (32%)
32	LMT	AI	103	-	36,36,36	1.46	7 (19%)	47,47,47	1.81	9 (19%)
27	BCR	BD	5407	-	41,41,41	1.85	8 (19%)	56,56,56	2.38	24 (42%)
31	LMG	BM	5102	-	42,42,55	1.02	3 (7%)	50,50,63	1.65	8 (16%)
27	BCR	BB	5622	-	41,41,41	1.92	7 (17%)	56,56,56	2.11	17 (30%)
32	LMT	BI	5102	-	36,36,36	1.66	8 (22%)	47,47,47	1.01	2 (4%)
24	CLA	AC	503	3	69,73,73	2.23	17 (24%)	82,113,113	2.32	16 (19%)
27	BCR	BB	5623	-	41,41,41	1.78	8 (19%)	56,56,56	1.99	18 (32%)
30	SQD	BB	5625	-	41,43,54	2.68	20 (48%)	51,54,65	2.74	15 (29%)
32	LMT	AM	102	-	36,36,36	1.76	10 (27%)	47,47,47	0.91	2 (4%)
24	CLA	BB	5607	2	69,73,73	2.54	19 (27%)	82,113,113	2.18	22 (26%)
27	BCR	AD	406	-	41,41,41	1.68	7 (17%)	56,56,56	2.40	25 (44%)
24	CLA	AB	602	2	69,73,73	2.21	16 (23%)	82,113,113	2.08	13 (15%)
24	CLA	AB	615	2	69,73,73	2.21	16 (23%)	82,113,113	2.18	13 (15%)
24	CLA	AC	504	-	69,73,73	2.20	18 (26%)	82,113,113	2.16	15 (18%)
24	CLA	BA	5407	-	69,73,73	2.32	20 (28%)	82,113,113	2.23	14 (17%)
31	LMG	BL	5101	-	51,51,55	1.43	3 (5%)	59,59,63	1.96	13 (22%)
31	LMG	AD	408	-	48,48,55	0.97	4 (8%)	56,56,63	2.08	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	AI	102	-	36,36,36	1.62	7 (19%)	47,47,47	1.02	2 (4%)
27	BCR	BJ	5101	-	41,41,41	2.34	10 (24%)	56,56,56	3.33	24 (42%)
27	BCR	BC	5515	-	41,41,41	1.97	8 (19%)	56,56,56	2.29	25 (44%)
24	CLA	BB	5617	2	69,73,73	2.12	16 (23%)	82,113,113	2.00	12 (14%)
24	CLA	BB	5612	2	69,73,73	2.39	20 (28%)	82,113,113	2.32	15 (18%)
32	LMT	BB	5604	-	36,36,36	1.72	10 (27%)	47,47,47	1.01	1 (2%)
27	BCR	AC	515	-	41,41,41	1.81	7 (17%)	56,56,56	2.29	23 (41%)
33	DMS	BV	5203	-	3,3,3	0.85	0	3,3,3	1.24	0
24	CLA	AC	502	3	69,73,73	2.23	17 (24%)	82,113,113	2.11	14 (17%)
34	PHO	AD	402	-	58,69,69	2.97	16 (27%)	55,99,99	2.08	12 (21%)
33	DMS	BV	5202	-	3,3,3	0.88	0	3,3,3	1.03	0
24	CLA	BB	5608	2	69,73,73	2.20	16 (23%)	82,113,113	2.10	16 (19%)
31	LMG	AD	407	-	49,49,55	0.77	1 (2%)	57,57,63	2.74	19 (33%)
28	DGD	BC	5518	-	63,63,67	1.29	6 (9%)	77,77,81	2.72	24 (31%)
36	HEM	BF	5101	6,5	50,50,50	3.08	23 (46%)	67,82,82	2.52	19 (28%)
24	CLA	AB	613	2	69,73,73	2.09	14 (20%)	82,113,113	2.00	12 (14%)
24	CLA	BB	5620	2	69,73,73	2.28	15 (21%)	82,113,113	2.09	10 (12%)
24	CLA	AB	607	-	69,73,73	2.29	16 (23%)	82,113,113	2.22	17 (20%)
24	CLA	AC	512	3	69,73,73	2.31	19 (27%)	82,113,113	2.19	13 (15%)
24	CLA	AD	404	-	69,73,73	2.31	18 (26%)	82,113,113	2.20	14 (17%)
24	CLA	BB	5606	2	69,73,73	2.21	16 (23%)	82,113,113	2.11	15 (18%)
24	CLA	BB	5618	2	69,73,73	2.73	20 (28%)	82,113,113	2.14	15 (18%)
29	LHG	BA	5415	-	36,36,48	1.09	2 (5%)	39,42,54	1.14	3 (7%)
30	SQD	BF	5102	-	43,45,54	2.61	22 (51%)	53,56,65	2.82	20 (37%)
31	LMG	BB	5624	-	49,49,55	0.81	1 (2%)	57,57,63	1.93	14 (24%)
28	DGD	BA	5412	-	57,57,67	1.85	12 (21%)	71,71,81	3.54	23 (32%)
33	DMS	BB	5629	-	3,3,3	0.69	0	3,3,3	1.27	0
24	CLA	BB	5615	-	69,73,73	2.20	16 (23%)	82,113,113	2.22	20 (24%)
31	LMG	AM	101	-	42,42,55	0.97	2 (4%)	50,50,63	1.65	8 (16%)
27	BCR	BC	5514	-	41,41,41	1.89	6 (14%)	56,56,56	2.15	25 (44%)
28	DGD	AE	101	-	64,64,67	1.58	13 (20%)	78,78,81	1.43	11 (14%)
28	DGD	BE	5102	-	64,64,67	1.55	14 (21%)	78,78,81	1.41	10 (12%)
27	BCR	BC	5516	-	41,41,41	1.84	7 (17%)	56,56,56	2.27	20 (35%)
24	CLA	AB	604	2	69,73,73	2.21	17 (24%)	82,113,113	2.06	15 (18%)
24	CLA	BB	5610	2	69,73,73	2.39	17 (24%)	82,113,113	2.13	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PHO	AD	403	-	58,69,69	2.99	17 (29%)	55,99,99	2.21	13 (23%)
35	PL9	BD	5406	-	55,55,55	4.08	19 (34%)	68,69,69	2.77	22 (32%)
28	DGD	BC	5517	-	54,54,67	1.45	8 (14%)	68,68,81	2.70	22 (32%)
24	CLA	AC	507	-	69,73,73	2.13	16 (23%)	82,113,113	2.12	12 (14%)
24	CLA	BA	5406	-	69,73,73	2.20	19 (27%)	82,113,113	2.37	19 (23%)
24	CLA	AB	608	2	69,73,73	2.38	20 (28%)	82,113,113	2.31	16 (19%)
24	CLA	BC	5504	-	69,73,73	2.30	18 (26%)	82,113,113	2.15	12 (14%)
27	BCR	AB	618	-	41,41,41	1.96	7 (17%)	56,56,56	2.12	17 (30%)
28	DGD	AB	628	-	53,53,67	1.47	7 (13%)	67,67,81	2.04	13 (19%)
32	LMT	BB	5603	-	36,36,36	1.59	7 (19%)	47,47,47	1.41	7 (14%)
28	DGD	BH	5101	-	59,59,67	1.33	8 (13%)	73,73,81	2.07	18 (24%)
35	PL9	AD	405	-	55,55,55	3.97	18 (32%)	68,69,69	2.77	23 (33%)
30	SQD	BA	5401	-	52,54,54	2.60	30 (57%)	62,65,65	2.68	22 (35%)
31	LMG	BD	5409	-	49,49,55	0.74	1 (2%)	57,57,63	2.75	20 (35%)
24	CLA	BB	5613	2	69,73,73	2.31	20 (28%)	82,113,113	2.06	14 (17%)
31	LMG	AB	621	-	49,49,55	0.79	1 (2%)	57,57,63	1.93	14 (24%)
24	CLA	BB	5605	-	69,73,73	2.56	20 (28%)	82,113,113	2.19	12 (14%)
24	CLA	BC	5503	3	69,73,73	2.27	17 (24%)	82,113,113	2.25	16 (19%)
32	LMT	AD	409	-	32,32,36	1.74	7 (21%)	43,43,47	1.29	2 (4%)
31	LMG	BC	5520	-	48,48,55	1.11	3 (6%)	56,56,63	1.90	18 (32%)
29	LHG	BA	5413	-	38,38,48	2.05	5 (13%)	41,44,54	1.45	5 (12%)
30	SQD	BA	5414	-	49,51,54	2.62	27 (55%)	59,62,65	2.68	19 (32%)
24	CLA	BC	5513	3	69,73,73	2.81	23 (33%)	82,113,113	1.99	13 (15%)
32	LMT	AB	629	-	36,36,36	1.59	7 (19%)	47,47,47	1.41	6 (12%)
31	LMG	BD	5410	-	48,48,55	0.95	3 (6%)	56,56,63	2.08	11 (19%)
33	DMS	BB	5628	-	3,3,3	0.72	0	3,3,3	1.19	0
24	CLA	BB	5611	-	69,73,73	2.25	19 (27%)	82,113,113	2.26	17 (20%)
29	LHG	AA	412	-	38,38,48	2.06	5 (13%)	41,44,54	1.48	5 (12%)
24	CLA	AB	609	2	69,73,73	2.29	17 (24%)	82,113,113	2.04	14 (17%)
31	LMG	BE	5101	-	44,44,55	1.10	2 (4%)	52,52,63	1.52	6 (11%)
27	BCR	AK	102	-	41,41,41	1.83	7 (17%)	56,56,56	2.53	25 (44%)
25	MST	BA	5409	-	16,16,16	0.48	0	22,22,22	3.70	9 (40%)
22	BCT	AA	402	21	3,3,3	1.92	1 (33%)	2,3,3	0.09	0
27	BCR	AB	617	-	41,41,41	1.59	7 (17%)	56,56,56	2.16	21 (37%)
31	LMG	AA	417	-	42,42,55	1.09	5 (11%)	50,50,63	2.31	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	BC	5508	3	69,73,73	2.27	18 (26%)	82,113,113	2.29	15 (18%)
27	BCR	AB	619	-	41,41,41	1.92	8 (19%)	56,56,56	2.01	20 (35%)
27	BCR	AT	101	-	41,41,41	1.69	7 (17%)	56,56,56	2.29	24 (42%)
24	CLA	BC	5506	-	69,73,73	2.37	21 (30%)	82,113,113	2.14	14 (17%)
30	SQD	AF	102	-	43,45,54	2.61	22 (51%)	53,56,65	2.81	18 (33%)
24	CLA	BC	5512	3	69,73,73	2.38	18 (26%)	82,113,113	2.18	11 (13%)
22	BCT	BA	5403	21	3,3,3	2.30	1 (33%)	2,3,3	0.38	0
24	CLA	AC	501	3	69,73,73	2.28	18 (26%)	82,113,113	2.28	15 (18%)
27	BCR	AJ	101	-	41,41,41	2.38	11 (26%)	56,56,56	3.35	24 (42%)
24	CLA	AB	605	2	69,73,73	2.36	21 (30%)	82,113,113	2.11	16 (19%)
31	LMG	BA	5402	-	42,42,55	1.09	3 (7%)	50,50,63	2.32	11 (22%)
32	LMT	BB	5627	-	36,36,36	1.64	8 (22%)	47,47,47	0.93	2 (4%)
24	CLA	AB	612	2	69,73,73	2.43	19 (27%)	82,113,113	2.00	13 (15%)
24	CLA	BB	5614	-	69,73,73	2.15	15 (21%)	82,113,113	2.06	14 (17%)
28	DGD	BB	5602	-	53,53,67	1.52	7 (13%)	67,67,81	2.06	13 (19%)
24	CLA	AA	405	-	69,73,73	2.20	19 (27%)	82,113,113	2.32	18 (21%)
24	CLA	BC	5502	3	69,73,73	2.30	17 (24%)	82,113,113	2.21	15 (18%)
32	LMT	AB	630	-	36,36,36	1.74	9 (25%)	47,47,47	1.02	1 (2%)
30	SQD	BB	5601	-	45,47,54	2.59	23 (51%)	55,58,65	2.62	16 (29%)
31	LMG	AI	101	-	43,43,55	1.04	3 (6%)	51,51,63	1.69	8 (15%)
31	LMG	BI	5101	-	43,43,55	1.03	3 (6%)	51,51,63	1.68	8 (15%)
27	BCR	AA	410	-	41,41,41	1.67	8 (19%)	56,56,56	2.11	22 (39%)
24	CLA	AC	506	-	69,73,73	2.36	21 (30%)	82,113,113	2.12	13 (15%)
24	CLA	AC	510	3	69,73,73	2.17	16 (23%)	82,113,113	2.08	13 (15%)
24	CLA	BB	5616	2	69,73,73	2.50	21 (30%)	82,113,113	2.06	13 (15%)
24	CLA	BC	5507	-	69,73,73	2.19	17 (24%)	82,113,113	2.12	14 (17%)
24	CLA	BA	5405	1	69,73,73	2.17	15 (21%)	82,113,113	1.97	15 (18%)
24	CLA	BC	5511	3	69,73,73	2.79	23 (33%)	82,113,113	2.14	17 (20%)
25	MST	AA	408	-	16,16,16	0.51	0	22,22,22	3.77	9 (40%)
28	DGD	AH	101	-	59,59,67	1.35	9 (15%)	73,73,81	2.06	18 (24%)
33	DMS	AB	626	-	3,3,3	0.69	0	3,3,3	1.10	0
28	DGD	AC	519	-	67,67,67	1.52	12 (17%)	81,81,81	3.23	30 (37%)
32	LMT	BD	5411	-	32,32,36	1.73	8 (25%)	43,43,47	1.30	2 (4%)
24	CLA	AB	601	-	69,73,73	2.57	22 (31%)	82,113,113	2.23	11 (13%)
24	CLA	BC	5505	3	69,73,73	2.50	20 (28%)	82,113,113	2.25	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AA	406	-	69,73,73	2.21	18 (26%)	82,113,113	2.18	15 (18%)
28	DGD	AA	411	-	57,57,67	1.82	12 (21%)	71,71,81	3.53	24 (33%)
31	LMG	AB	620	-	51,51,55	1.38	3 (5%)	59,59,63	1.98	12 (20%)
30	SQD	AB	627	-	45,47,54	2.60	24 (53%)	55,58,65	2.61	15 (27%)
34	PHO	BD	5403	-	58,69,69	3.11	17 (29%)	55,99,99	2.09	12 (21%)
27	BCR	BA	5411	-	41,41,41	1.74	7 (17%)	56,56,56	2.13	22 (39%)
24	CLA	AA	407	1	69,73,73	2.19	16 (23%)	82,113,113	2.20	15 (18%)
36	HEM	AV	201	16	50,50,50	2.84	20 (40%)	67,82,82	2.40	18 (26%)
24	CLA	BA	5408	1	69,73,73	2.27	18 (26%)	82,113,113	2.15	15 (18%)
24	CLA	AA	404	1	69,73,73	2.22	15 (21%)	82,113,113	1.96	15 (18%)
24	CLA	BB	5619	2	69,73,73	2.19	15 (21%)	82,113,113	2.22	12 (14%)
31	LMG	BC	5521	-	45,45,55	1.04	2 (4%)	53,53,63	1.91	13 (24%)
27	BCR	BT	5101	-	41,41,41	1.83	7 (17%)	56,56,56	2.28	24 (42%)
33	DMS	AU	201	-	3,3,3	0.94	0	3,3,3	1.17	0
24	CLA	BC	5510	3	69,73,73	2.20	17 (24%)	82,113,113	2.09	12 (14%)
24	CLA	AC	513	3	69,73,73	2.73	20 (28%)	82,113,113	1.97	13 (15%)
24	CLA	BD	5402	4	69,73,73	2.23	16 (23%)	82,113,113	2.14	17 (20%)
24	CLA	BB	5609	2	69,73,73	2.28	19 (27%)	82,113,113	2.11	16 (19%)
27	BCR	AX	101	-	41,41,41	1.90	7 (17%)	56,56,56	2.27	23 (41%)
28	DGD	BC	5519	-	67,67,67	1.55	12 (17%)	81,81,81	3.23	30 (37%)
30	SQD	AB	622	-	41,43,54	2.66	19 (46%)	51,54,65	2.73	15 (29%)
24	CLA	AB	614	2	69,73,73	2.80	22 (31%)	82,113,113	2.17	15 (18%)
24	CLA	AB	606	2	69,73,73	2.38	18 (26%)	82,113,113	2.11	15 (18%)
28	DGD	AC	517	-	54,54,67	1.37	7 (12%)	68,68,81	2.70	22 (32%)
24	CLA	AC	508	3	69,73,73	2.19	17 (24%)	82,113,113	2.21	14 (17%)
31	LMG	AC	520	-	48,48,55	1.07	5 (10%)	56,56,63	1.93	18 (32%)
36	HEM	AF	101	6,5	50,50,50	3.00	23 (46%)	67,82,82	2.49	20 (29%)
24	CLA	AB	610	-	69,73,73	2.18	15 (21%)	82,113,113	2.07	13 (15%)
24	CLA	AB	603	2	69,73,73	2.56	18 (26%)	82,113,113	2.20	22 (26%)
27	BCR	BK	5102	-	41,41,41	1.95	8 (19%)	56,56,56	2.48	26 (46%)
24	CLA	AC	511	3	69,73,73	2.68	20 (28%)	82,113,113	2.12	17 (20%)
24	CLA	AB	611	-	69,73,73	2.17	16 (23%)	82,113,113	2.22	18 (21%)
32	LMT	BB	5626	-	36,36,36	1.78	9 (25%)	47,47,47	1.03	2 (4%)
31	LMG	AJ	102	-	46,46,55	1.00	3 (6%)	54,54,63	2.58	16 (29%)
32	LMT	AB	624	-	36,36,36	1.67	8 (22%)	47,47,47	0.94	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BM	5101	-	36,36,36	1.77	9 (25%)	47,47,47	0.90	2 (4%)
24	CLA	AD	401	4	69,73,73	2.16	17 (24%)	82,113,113	2.12	17 (20%)
31	LMG	AA	414	-	44,44,55	1.12	3 (6%)	52,52,63	1.51	6 (11%)
31	LMG	AC	521	-	45,45,55	1.09	2 (4%)	53,53,63	1.91	14 (26%)
28	DGD	AC	518	-	63,63,67	1.26	6 (9%)	77,77,81	2.74	23 (29%)
24	CLA	BC	5509	3	69,73,73	2.59	21 (30%)	82,113,113	2.12	12 (14%)
33	DMS	AB	625	-	3,3,3	0.74	0	3,3,3	1.51	1 (33%)
32	LMT	AB	623	-	36,36,36	1.78	8 (22%)	47,47,47	1.01	2 (4%)
27	BCR	BX	5101	-	41,41,41	1.92	7 (17%)	56,56,56	2.30	22 (39%)
27	BCR	AC	516	-	41,41,41	1.68	9 (21%)	56,56,56	2.31	22 (39%)
31	LMG	BD	5408	-	46,46,55	1.00	3 (6%)	54,54,63	2.57	16 (29%)
24	CLA	AB	616	2	69,73,73	2.26	15 (21%)	82,113,113	2.09	12 (14%)
24	CLA	AC	509	3	69,73,73	2.48	13 (18%)	82,113,113	2.13	14 (17%)
27	BCR	AC	514	-	41,41,41	1.67	7 (17%)	56,56,56	2.19	24 (42%)
24	CLA	AC	505	3	69,73,73	2.51	20 (28%)	82,113,113	2.25	13 (15%)
33	DMS	AV	202	-	3,3,3	0.77	0	3,3,3	1.10	0
24	CLA	BD	5405	-	69,73,73	2.34	16 (23%)	82,113,113	2.19	15 (18%)
32	LMT	BC	5522	-	36,36,36	1.53	7 (19%)	47,47,47	1.80	10 (21%)
24	CLA	BC	5501	3	69,73,73	2.33	20 (28%)	82,113,113	2.31	15 (18%)
36	HEM	BV	5201	16	50,50,50	2.95	25 (50%)	67,82,82	2.39	18 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	AA	415	-	-	21/41/41/53	-
34	PHO	BD	5404	-	1/1/17/22	10/37/103/103	0/5/6/6
27	BCR	BB	5621	-	-	1/29/63/63	0/2/2/2
30	SQD	AA	413	-	-	24/46/66/69	0/1/1/1
30	SQD	AA	416	-	-	20/49/69/69	0/1/1/1
32	LMT	AI	103	-	-	1/21/61/61	0/2/2/2
27	BCR	BD	5407	-	-	5/29/63/63	0/2/2/2
31	LMG	BM	5102	-	-	3/37/57/70	0/1/1/1
27	BCR	BB	5622	-	-	1/29/63/63	0/2/2/2
32	LMT	BI	5102	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AC	503	3	1/1/15/20	15/39/115/115	-
27	BCR	BB	5623	-	-	4/29/63/63	0/2/2/2
30	SQD	BB	5625	-	-	18/38/58/69	0/1/1/1
32	LMT	AM	102	-	-	3/21/61/61	0/2/2/2
24	CLA	BB	5607	2	1/1/15/20	11/39/115/115	-
27	BCR	AD	406	-	-	5/29/63/63	0/2/2/2
24	CLA	AB	602	2	1/1/15/20	7/39/115/115	-
24	CLA	AB	615	2	1/1/15/20	5/39/115/115	-
24	CLA	AC	504	-	1/1/15/20	8/39/115/115	-
24	CLA	BA	5407	-	1/1/15/20	3/39/115/115	-
31	LMG	BL	5101	-	-	5/46/66/70	0/1/1/1
31	LMG	AD	408	-	-	5/43/63/70	0/1/1/1
32	LMT	AI	102	-	-	3/21/61/61	0/2/2/2
27	BCR	BJ	5101	-	-	1/29/63/63	0/2/2/2
27	BCR	BC	5515	-	-	3/29/63/63	0/2/2/2
24	CLA	BB	5617	2	1/1/15/20	10/39/115/115	-
24	CLA	BB	5612	2	1/1/15/20	10/39/115/115	-
32	LMT	BB	5604	-	-	3/21/61/61	0/2/2/2
27	BCR	AC	515	-	-	3/29/63/63	0/2/2/2
24	CLA	AC	502	3	1/1/15/20	7/39/115/115	-
34	PHO	AD	402	-	1/1/17/22	10/37/103/103	0/5/6/6
24	CLA	BB	5608	2	1/1/15/20	10/39/115/115	-
31	LMG	AD	407	-	-	7/44/64/70	0/1/1/1
28	DGD	BC	5518	-	1/1/13/13	8/51/91/95	0/2/2/2
36	HEM	BF	5101	6,5	-	8/14/54/54	-
24	CLA	AB	613	2	1/1/15/20	9/39/115/115	-
24	CLA	BB	5620	2	1/1/15/20	11/39/115/115	-
24	CLA	AB	607	-	1/1/15/20	5/39/115/115	-
24	CLA	AC	512	3	1/1/15/20	11/39/115/115	-
24	CLA	AD	404	-	1/1/15/20	10/39/115/115	-
24	CLA	BB	5606	2	1/1/15/20	7/39/115/115	-
24	CLA	BB	5618	2	1/1/15/20	7/39/115/115	-
29	LHG	BA	5415	-	-	21/41/41/53	-
30	SQD	BF	5102	-	-	22/40/60/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	BB	5624	-	-	4/44/64/70	0/1/1/1
28	DGD	BA	5412	-	-	8/45/85/95	0/2/2/2
24	CLA	BB	5615	-	1/1/15/20	8/39/115/115	-
31	LMG	AM	101	-	-	3/37/57/70	0/1/1/1
27	BCR	BC	5514	-	-	5/29/63/63	0/2/2/2
28	DGD	AE	101	-	-	5/52/92/95	0/2/2/2
28	DGD	BE	5102	-	-	6/52/92/95	0/2/2/2
27	BCR	BC	5516	-	-	4/29/63/63	0/2/2/2
24	CLA	AB	604	2	1/1/15/20	9/39/115/115	-
24	CLA	BB	5610	2	1/1/15/20	10/39/115/115	-
34	PHO	AD	403	-	1/1/17/22	10/37/103/103	0/5/6/6
35	PL9	BD	5406	-	-	17/53/73/73	0/1/1/1
28	DGD	BC	5517	-	-	4/42/82/95	0/2/2/2
24	CLA	AC	507	-	1/1/15/20	6/39/115/115	-
24	CLA	BA	5406	-	1/1/15/20	14/39/115/115	-
24	CLA	AB	608	2	1/1/15/20	10/39/115/115	-
24	CLA	BC	5504	-	1/1/15/20	9/39/115/115	-
27	BCR	AB	618	-	-	1/29/63/63	0/2/2/2
28	DGD	AB	628	-	-	7/41/81/95	0/2/2/2
32	LMT	BB	5603	-	-	3/21/61/61	0/2/2/2
28	DGD	BH	5101	-	-	3/47/87/95	0/2/2/2
35	PL9	AD	405	-	-	16/53/73/73	0/1/1/1
30	SQD	BA	5401	-	-	21/49/69/69	0/1/1/1
31	LMG	BD	5409	-	-	7/44/64/70	0/1/1/1
24	CLA	BB	5613	2	1/1/15/20	7/39/115/115	-
31	LMG	AB	621	-	-	4/44/64/70	0/1/1/1
24	CLA	BB	5605	-	1/1/15/20	13/39/115/115	-
24	CLA	BC	5503	3	1/1/15/20	15/39/115/115	-
32	LMT	AD	409	-	-	1/17/57/61	0/2/2/2
31	LMG	BC	5520	-	-	5/43/63/70	0/1/1/1
29	LHG	BA	5413	-	-	19/43/43/53	-
30	SQD	BA	5414	-	-	24/46/66/69	0/1/1/1
24	CLA	BC	5513	3	1/1/15/20	7/39/115/115	-
32	LMT	AB	629	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	BD	5410	-	-	5/43/63/70	0/1/1/1
24	CLA	BB	5611	-	1/1/15/20	5/39/115/115	-
29	LHG	AA	412	-	-	18/43/43/53	-
24	CLA	AB	609	2	1/1/15/20	6/39/115/115	-
31	LMG	BE	5101	-	-	5/39/59/70	0/1/1/1
27	BCR	AK	102	-	-	2/29/63/63	0/2/2/2
25	MST	BA	5409	-	-	2/10/10/10	0/1/1/1
27	BCR	AB	617	-	-	1/29/63/63	0/2/2/2
31	LMG	AA	417	-	-	3/37/57/70	0/1/1/1
24	CLA	BC	5508	3	1/1/15/20	8/39/115/115	-
27	BCR	AB	619	-	-	4/29/63/63	0/2/2/2
27	BCR	AT	101	-	-	4/29/63/63	0/2/2/2
24	CLA	BC	5506	-	1/1/15/20	4/39/115/115	-
30	SQD	AF	102	-	-	21/40/60/69	0/1/1/1
24	CLA	BC	5512	3	1/1/15/20	10/39/115/115	-
24	CLA	AC	501	3	1/1/15/20	11/39/115/115	-
27	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
24	CLA	AB	605	2	1/1/15/20	8/39/115/115	-
31	LMG	BA	5402	-	-	3/37/57/70	0/1/1/1
32	LMT	BB	5627	-	-	3/21/61/61	0/2/2/2
24	CLA	AB	612	2	1/1/15/20	10/39/115/115	-
24	CLA	BB	5614	-	1/1/15/20	10/39/115/115	-
28	DGD	BB	5602	-	-	6/41/81/95	0/2/2/2
24	CLA	AA	405	-	1/1/15/20	13/39/115/115	-
24	CLA	BC	5502	3	1/1/15/20	8/39/115/115	-
32	LMT	AB	630	-	-	3/21/61/61	0/2/2/2
30	SQD	BB	5601	-	-	23/42/62/69	0/1/1/1
31	LMG	AI	101	-	-	2/38/58/70	0/1/1/1
31	LMG	BI	5101	-	-	2/38/58/70	0/1/1/1
25	MST	AA	408	-	-	2/10/10/10	0/1/1/1
24	CLA	AC	506	-	1/1/15/20	5/39/115/115	-
24	CLA	AC	510	3	1/1/15/20	10/39/115/115	-
24	CLA	BB	5616	2	1/1/15/20	9/39/115/115	-
24	CLA	BC	5507	-	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BA	5405	1	1/1/15/20	14/39/115/115	-
24	CLA	BC	5511	3	1/1/15/20	15/39/115/115	-
27	BCR	AA	410	-	-	5/29/63/63	0/2/2/2
28	DGD	AH	101	-	-	3/47/87/95	0/2/2/2
28	DGD	AC	519	-	1/1/13/13	9/55/95/95	0/2/2/2
32	LMT	BD	5411	-	-	1/17/57/61	0/2/2/2
24	CLA	AB	601	-	1/1/15/20	13/39/115/115	-
24	CLA	BC	5505	3	1/1/15/20	9/39/115/115	-
24	CLA	AA	406	-	1/1/15/20	3/39/115/115	-
28	DGD	AA	411	-	-	7/45/85/95	0/2/2/2
31	LMG	AB	620	-	-	5/46/66/70	0/1/1/1
34	PHO	BD	5403	-	1/1/17/22	10/37/103/103	0/5/6/6
30	SQD	AB	627	-	-	24/42/62/69	0/1/1/1
27	BCR	BA	5411	-	-	5/29/63/63	0/2/2/2
24	CLA	AA	407	1	1/1/15/20	11/39/115/115	-
36	HEM	AV	201	16	-	6/14/54/54	-
24	CLA	BA	5408	1	1/1/15/20	11/39/115/115	-
24	CLA	AA	404	1	1/1/15/20	13/39/115/115	-
24	CLA	BB	5619	2	1/1/15/20	5/39/115/115	-
31	LMG	BC	5521	-	-	6/40/60/70	0/1/1/1
27	BCR	BT	5101	-	-	4/29/63/63	0/2/2/2
24	CLA	BC	5510	3	1/1/15/20	10/39/115/115	-
24	CLA	AC	513	3	1/1/15/20	8/39/115/115	-
24	CLA	BD	5402	4	1/1/15/20	10/39/115/115	-
24	CLA	BB	5609	2	1/1/15/20	8/39/115/115	-
27	BCR	AX	101	-	-	1/29/63/63	0/2/2/2
28	DGD	BC	5519	-	1/1/13/13	7/55/95/95	0/2/2/2
30	SQD	AB	622	-	-	20/38/58/69	0/1/1/1
24	CLA	AB	614	2	1/1/15/20	7/39/115/115	-
24	CLA	AB	606	2	1/1/15/20	11/39/115/115	-
28	DGD	AC	517	-	-	4/42/82/95	0/2/2/2
24	CLA	AC	508	3	1/1/15/20	7/39/115/115	-
31	LMG	AC	520	-	-	5/43/63/70	0/1/1/1
36	HEM	AF	101	6,5	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AB	610	-	1/1/15/20	10/39/115/115	-
24	CLA	AB	603	2	1/1/15/20	10/39/115/115	-
27	BCR	BK	5102	-	-	2/29/63/63	0/2/2/2
24	CLA	AC	511	3	1/1/15/20	15/39/115/115	-
24	CLA	AB	611	-	1/1/15/20	9/39/115/115	-
32	LMT	BB	5626	-	-	1/21/61/61	0/2/2/2
31	LMG	AJ	102	-	-	5/41/61/70	0/1/1/1
32	LMT	AB	624	-	-	3/21/61/61	0/2/2/2
32	LMT	BM	5101	-	-	3/21/61/61	0/2/2/2
24	CLA	AD	401	4	1/1/15/20	10/39/115/115	-
31	LMG	AA	414	-	-	5/39/59/70	0/1/1/1
31	LMG	AC	521	-	-	6/40/60/70	0/1/1/1
28	DGD	AC	518	-	1/1/13/13	8/51/91/95	0/2/2/2
24	CLA	BC	5509	3	1/1/15/20	3/39/115/115	-
32	LMT	AB	623	-	-	1/21/61/61	0/2/2/2
27	BCR	BX	5101	-	-	1/29/63/63	0/2/2/2
27	BCR	AC	516	-	-	4/29/63/63	0/2/2/2
31	LMG	BD	5408	-	-	5/41/61/70	0/1/1/1
24	CLA	AB	616	2	1/1/15/20	10/39/115/115	-
24	CLA	AC	509	3	1/1/15/20	5/39/115/115	-
27	BCR	AC	514	-	-	5/29/63/63	0/2/2/2
24	CLA	AC	505	3	1/1/15/20	8/39/115/115	-
24	CLA	BD	5405	-	1/1/15/20	10/39/115/115	-
32	LMT	BC	5522	-	-	1/21/61/61	0/2/2/2
24	CLA	BC	5501	3	1/1/15/20	11/39/115/115	-
36	HEM	BV	5201	16	-	6/14/54/54	-

All (2213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	614	CLA	MG-NA	12.11	2.35	2.06
24	BC	5513	CLA	MG-NA	12.03	2.34	2.06
24	BC	5511	CLA	MG-NA	11.84	2.34	2.06
24	AC	513	CLA	MG-NA	11.69	2.34	2.06
24	AC	511	CLA	MG-NA	11.67	2.34	2.06
24	BB	5618	CLA	MG-NA	11.37	2.33	2.06
24	AB	608	CLA	C2-C3	10.90	1.58	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5612	CLA	C2-C3	10.89	1.58	1.33
24	AB	606	CLA	C2-C3	10.89	1.58	1.33
24	BB	5610	CLA	C2-C3	10.87	1.58	1.33
24	AC	509	CLA	MG-NA	10.83	2.32	2.06
24	AB	607	CLA	C2-C3	10.57	1.57	1.33
24	BB	5620	CLA	C2-C3	10.56	1.57	1.33
24	BC	5511	CLA	C2-C3	10.55	1.57	1.33
24	BC	5509	CLA	MG-NA	10.38	2.30	2.06
24	AB	614	CLA	C2-C3	10.34	1.56	1.33
24	BB	5613	CLA	C2-C3	10.34	1.56	1.33
24	AB	616	CLA	C2-C3	10.33	1.56	1.33
24	AC	511	CLA	C2-C3	10.33	1.56	1.33
24	AB	603	CLA	C2-C3	10.27	1.56	1.33
24	BC	5505	CLA	C2-C3	10.16	1.56	1.33
35	AD	405	PL9	C28-C29	10.13	1.56	1.33
24	AB	609	CLA	C2-C3	10.12	1.56	1.33
24	BC	5506	CLA	C2-C3	10.09	1.56	1.33
24	BB	5607	CLA	C2-C3	10.09	1.56	1.33
35	BD	5406	PL9	C13-C14	10.06	1.56	1.33
34	AD	403	PHO	C2-C3	10.03	1.56	1.33
24	AC	506	CLA	C2-C3	10.00	1.56	1.33
24	BB	5615	CLA	C2-C3	10.00	1.56	1.33
24	BB	5611	CLA	C2-C3	9.99	1.56	1.33
24	BB	5605	CLA	C2-C3	9.99	1.56	1.33
35	BD	5406	PL9	C28-C29	9.98	1.56	1.33
24	BB	5618	CLA	C2-C3	9.97	1.56	1.33
35	BD	5406	PL9	C23-C24	9.96	1.56	1.33
35	AD	405	PL9	C13-C14	9.94	1.55	1.33
34	BD	5404	PHO	C2-C3	9.93	1.55	1.33
24	AC	505	CLA	C2-C3	9.92	1.55	1.33
34	BD	5403	PHO	C2-C3	9.92	1.55	1.33
24	AB	605	CLA	C2-C3	9.88	1.55	1.33
24	AC	513	CLA	C2-C3	9.88	1.55	1.33
24	BC	5513	CLA	C2-C3	9.86	1.55	1.33
24	AC	501	CLA	C2-C3	9.85	1.55	1.33
35	BD	5406	PL9	C33-C34	9.83	1.55	1.33
24	BD	5405	CLA	C2-C3	9.82	1.55	1.33
24	AC	502	CLA	C2-C3	9.81	1.55	1.33
24	BB	5609	CLA	C2-C3	9.80	1.55	1.33
24	AB	601	CLA	C2-C3	9.78	1.55	1.33
24	BC	5501	CLA	C2-C3	9.76	1.55	1.33
24	BA	5408	CLA	C2-C3	9.71	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5509	CLA	C2-C3	9.69	1.55	1.33
24	BC	5508	CLA	C2-C3	9.68	1.55	1.33
24	AA	405	CLA	C2-C3	9.67	1.55	1.33
24	BA	5406	CLA	C2-C3	9.64	1.55	1.33
24	AB	611	CLA	C2-C3	9.64	1.55	1.33
34	AD	402	PHO	C2-C3	9.63	1.55	1.33
35	BD	5406	PL9	C43-C44	9.59	1.55	1.33
24	AC	508	CLA	C2-C3	9.54	1.55	1.33
35	AD	405	PL9	C33-C34	9.53	1.55	1.33
24	AA	406	CLA	C2-C3	9.53	1.55	1.33
24	BC	5502	CLA	C2-C3	9.53	1.55	1.33
24	AB	612	CLA	C2-C3	9.51	1.55	1.33
24	BC	5504	CLA	C2-C3	9.46	1.54	1.33
24	BB	5606	CLA	C2-C3	9.44	1.54	1.33
34	BD	5403	PHO	C1D-C2D	9.42	1.49	1.39
24	AA	407	CLA	C2-C3	9.41	1.54	1.33
24	BC	5503	CLA	C2-C3	9.40	1.54	1.33
35	BD	5406	PL9	C8-C9	9.40	1.54	1.33
24	BB	5616	CLA	C2-C3	9.40	1.54	1.33
24	AC	503	CLA	C2-C3	9.37	1.54	1.33
24	BD	5402	CLA	C2-C3	9.37	1.54	1.33
24	BC	5507	CLA	C2-C3	9.36	1.54	1.33
24	AD	404	CLA	C2-C3	9.35	1.54	1.33
24	BC	5512	CLA	C2-C3	9.34	1.54	1.33
24	BA	5407	CLA	C2-C3	9.33	1.54	1.33
24	AC	510	CLA	C2-C3	9.33	1.54	1.33
35	BD	5406	PL9	C2-C3	9.32	1.57	1.34
35	AD	405	PL9	C8-C9	9.30	1.54	1.33
24	AB	602	CLA	C2-C3	9.29	1.54	1.33
24	AB	604	CLA	C2-C3	9.28	1.54	1.33
24	AC	512	CLA	C2-C3	9.27	1.54	1.33
35	AD	405	PL9	C43-C44	9.27	1.54	1.33
24	BC	5510	CLA	C2-C3	9.24	1.54	1.33
35	AD	405	PL9	C2-C3	9.21	1.57	1.34
24	BB	5617	CLA	C2-C3	9.20	1.54	1.33
24	AD	401	CLA	C2-C3	9.19	1.54	1.33
24	BB	5608	CLA	C2-C3	9.19	1.54	1.33
24	AC	504	CLA	C2-C3	9.16	1.54	1.33
24	AB	613	CLA	C2-C3	9.15	1.54	1.33
24	AA	404	CLA	C2-C3	9.10	1.54	1.33
24	AB	610	CLA	C2-C3	9.09	1.54	1.33
24	BB	5616	CLA	MG-NA	9.09	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	509	CLA	C2-C3	9.08	1.54	1.33
34	AD	402	PHO	C1D-C2D	9.06	1.49	1.39
24	AC	507	CLA	C2-C3	9.00	1.53	1.33
24	BB	5607	CLA	MG-NA	9.00	2.27	2.06
24	AB	615	CLA	C2-C3	8.96	1.53	1.33
24	BB	5614	CLA	C2-C3	8.95	1.53	1.33
24	BB	5619	CLA	C2-C3	8.90	1.53	1.33
35	AD	405	PL9	C23-C24	8.89	1.53	1.33
24	AB	603	CLA	MG-NA	8.82	2.27	2.06
34	BD	5404	PHO	C3B-C2B	8.78	1.52	1.40
34	BD	5404	PHO	C3D-C4D	8.71	1.53	1.41
34	BD	5403	PHO	C3D-C4D	8.68	1.53	1.41
34	AD	403	PHO	C3D-C4D	8.62	1.52	1.41
34	AD	402	PHO	C3D-C4D	8.56	1.52	1.41
34	BD	5404	PHO	C1D-C2D	8.49	1.48	1.39
30	BB	5625	SQD	C4-C3	8.39	1.74	1.52
34	AD	403	PHO	C1D-C2D	8.35	1.48	1.39
24	AB	612	CLA	MG-NA	8.31	2.26	2.06
29	AA	412	LHG	P-O5	8.24	1.79	1.50
34	BD	5403	PHO	C3B-C2B	8.20	1.51	1.40
30	AB	622	SQD	C4-C3	8.20	1.73	1.52
29	BA	5413	LHG	P-O5	8.17	1.79	1.50
34	BD	5403	PHO	CHA-CBD	8.10	1.61	1.51
24	BA	5405	CLA	C2-C3	8.09	1.51	1.33
30	AB	627	SQD	C4-C3	7.83	1.72	1.52
30	BA	5401	SQD	C4-C3	7.77	1.72	1.52
35	BD	5406	PL9	C48-C49	7.76	1.55	1.32
34	AD	403	PHO	C3B-C2B	7.74	1.50	1.40
30	BA	5414	SQD	C4-C3	7.68	1.72	1.52
27	AJ	101	BCR	C30-C25	7.64	1.63	1.53
30	BB	5601	SQD	C4-C3	7.62	1.72	1.52
30	AA	416	SQD	C4-C3	7.58	1.72	1.52
35	AD	405	PL9	C48-C49	7.56	1.55	1.32
34	AD	402	PHO	CHA-CBD	7.46	1.60	1.51
30	BF	5102	SQD	C4-C3	7.44	1.71	1.52
34	BD	5404	PHO	CHA-CBD	7.37	1.60	1.51
36	AF	101	HEM	O1D-CGD	7.31	1.46	1.22
30	AF	102	SQD	C4-C3	7.30	1.71	1.52
36	BF	5101	HEM	O1D-CGD	7.26	1.45	1.22
27	BJ	5101	BCR	C30-C25	7.24	1.63	1.53
24	BB	5605	CLA	MG-NA	7.23	2.23	2.06
34	AD	402	PHO	C3B-C2B	7.21	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BF	5101	HEM	C3C-C2C	7.18	1.51	1.37
35	BD	5406	PL9	O2-C1	7.12	1.43	1.24
35	AD	405	PL9	O2-C1	7.09	1.43	1.24
36	BV	5201	HEM	O1D-CGD	7.09	1.45	1.22
34	AD	403	PHO	CHA-CBD	7.08	1.59	1.51
30	AA	413	SQD	C4-C3	7.07	1.70	1.52
24	AB	601	CLA	C3C-C2C	7.02	1.51	1.36
24	BB	5605	CLA	C3C-C2C	6.94	1.51	1.36
36	BF	5101	HEM	C3B-C2B	6.93	1.51	1.37
24	AD	404	CLA	C3C-C2C	6.82	1.51	1.36
24	BC	5504	CLA	C3C-C2C	6.81	1.51	1.36
36	AV	201	HEM	O1D-CGD	6.77	1.44	1.22
24	BC	5513	CLA	C3C-C2C	6.72	1.51	1.36
24	AB	603	CLA	C3C-C2C	6.70	1.51	1.36
24	BC	5511	CLA	C3C-C2C	6.67	1.51	1.36
36	AF	101	HEM	C3B-C2B	6.66	1.50	1.37
24	AB	601	CLA	MG-NA	6.64	2.22	2.06
36	BV	5201	HEM	C3B-C2B	6.60	1.50	1.37
24	AC	513	CLA	C3C-C2C	6.59	1.51	1.36
24	BD	5405	CLA	C3C-C2C	6.57	1.50	1.36
24	AB	604	CLA	C3C-C2C	6.51	1.50	1.36
36	AF	101	HEM	C3C-C2C	6.49	1.50	1.37
24	BC	5509	CLA	C3C-C2C	6.48	1.50	1.36
24	AC	511	CLA	C3C-C2C	6.48	1.50	1.36
24	BA	5405	CLA	C3C-C2C	6.41	1.50	1.36
24	BC	5512	CLA	C3C-C2C	6.40	1.50	1.36
36	AV	201	HEM	C3C-C2C	6.39	1.50	1.37
24	BA	5408	CLA	C3C-C2C	6.39	1.50	1.36
24	AA	404	CLA	C3C-C2C	6.39	1.50	1.36
24	BB	5612	CLA	C3C-C2C	6.37	1.50	1.36
24	BC	5502	CLA	C3C-C2C	6.37	1.50	1.36
24	BB	5616	CLA	C3C-C2C	6.36	1.50	1.36
27	BC	5514	BCR	C1-C6	6.35	1.61	1.53
28	BA	5412	DGD	O5D-C1E	6.35	1.50	1.40
24	BC	5505	CLA	C3C-C2C	6.34	1.50	1.36
36	BV	5201	HEM	C3C-C2C	6.34	1.50	1.37
24	AC	505	CLA	C3C-C2C	6.31	1.50	1.36
36	AV	201	HEM	C3B-C2B	6.30	1.50	1.37
34	BD	5404	PHO	C3B-C4B	6.28	1.47	1.41
24	AC	505	CLA	CAA-C2A	-6.25	1.42	1.54
24	BB	5607	CLA	C3C-C2C	6.24	1.50	1.36
27	AB	619	BCR	C30-C25	6.23	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	615	CLA	C3C-C2C	6.21	1.50	1.36
24	BB	5618	CLA	C3C-C2C	6.19	1.50	1.36
24	BC	5506	CLA	C3C-C2C	6.19	1.50	1.36
24	AC	504	CLA	C3C-C2C	6.19	1.50	1.36
27	BB	5622	BCR	C1-C6	6.17	1.61	1.53
27	BK	5102	BCR	C30-C25	6.17	1.61	1.53
24	AB	608	CLA	C3C-C2C	6.17	1.50	1.36
24	AB	612	CLA	C3C-C2C	6.16	1.50	1.36
28	AA	411	DGD	O5D-C1E	6.16	1.50	1.40
24	BD	5402	CLA	C3C-C2C	6.15	1.50	1.36
24	AA	407	CLA	C3C-C2C	6.14	1.50	1.36
24	BA	5407	CLA	C3C-C2C	6.13	1.50	1.36
24	BB	5614	CLA	C3C-C2C	6.13	1.50	1.36
24	BB	5610	CLA	C3C-C2C	6.12	1.50	1.36
24	BC	5501	CLA	C3C-C2C	6.12	1.50	1.36
24	AB	610	CLA	C3C-C2C	6.12	1.50	1.36
24	BB	5606	CLA	C3C-C2C	6.06	1.49	1.36
24	AD	401	CLA	C3C-C2C	6.05	1.49	1.36
24	AC	512	CLA	C3C-C2C	6.04	1.49	1.36
31	BL	5101	LMG	O7-C8	-6.04	1.32	1.46
27	BC	5514	BCR	C30-C25	6.01	1.61	1.53
27	AB	618	BCR	C1-C6	6.00	1.61	1.53
27	BT	5101	BCR	C1-C6	5.96	1.61	1.53
24	BC	5510	CLA	C3C-C2C	5.95	1.49	1.36
24	AB	602	CLA	C3C-C2C	5.94	1.49	1.36
24	BC	5503	CLA	C3C-C2C	5.94	1.49	1.36
24	AC	509	CLA	C3C-C2C	5.93	1.49	1.36
24	AC	506	CLA	C3C-C2C	5.93	1.49	1.36
24	AC	505	CLA	MG-NA	5.92	2.20	2.06
27	BC	5515	BCR	C30-C25	5.91	1.61	1.53
27	AK	102	BCR	C30-C25	5.90	1.61	1.53
24	AB	606	CLA	C3C-C2C	5.90	1.49	1.36
24	AC	503	CLA	C3C-C2C	5.89	1.49	1.36
24	AB	601	CLA	O2D-CGD	5.89	1.47	1.33
27	BD	5407	BCR	C30-C25	5.86	1.61	1.53
27	AB	619	BCR	C1-C6	5.86	1.61	1.53
24	AC	508	CLA	C3C-C2C	5.85	1.49	1.36
24	AB	614	CLA	C3C-C2C	5.84	1.49	1.36
31	BL	5101	LMG	O1-C1	5.83	1.49	1.40
24	AC	501	CLA	C3C-C2C	5.82	1.49	1.36
24	BA	5406	CLA	C3C-C2C	5.82	1.49	1.36
27	AC	515	BCR	C30-C25	5.82	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5608	CLA	C3C-C2C	5.79	1.49	1.36
24	BC	5508	CLA	C3C-C2C	5.74	1.49	1.36
24	AB	607	CLA	C3C-C2C	5.73	1.49	1.36
24	AB	609	CLA	C3C-C2C	5.72	1.49	1.36
27	BA	5411	BCR	C1-C6	5.71	1.61	1.53
24	BC	5508	CLA	O2D-CGD	5.69	1.47	1.33
27	AJ	101	BCR	C1-C6	5.69	1.61	1.53
24	BB	5619	CLA	C3C-C2C	5.67	1.49	1.36
24	BB	5605	CLA	O2D-CGD	5.66	1.47	1.33
24	BB	5615	CLA	C3C-C2C	5.66	1.49	1.36
27	BC	5515	BCR	C1-C6	5.65	1.61	1.53
34	AD	403	PHO	C3B-C4B	5.64	1.47	1.41
31	AB	620	LMG	O7-C8	-5.64	1.33	1.46
31	AB	620	LMG	O1-C1	5.64	1.49	1.40
27	BX	5101	BCR	C30-C25	5.62	1.61	1.53
24	AC	510	CLA	C3C-C2C	5.56	1.48	1.36
24	BB	5619	CLA	MG-NA	5.55	2.19	2.06
24	BB	5617	CLA	C3C-C2C	5.55	1.48	1.36
24	AB	613	CLA	C3C-C2C	5.53	1.48	1.36
27	AC	514	BCR	C30-C25	5.53	1.60	1.53
24	AA	406	CLA	C3C-C2C	5.49	1.48	1.36
24	BB	5620	CLA	C3C-C2C	5.48	1.48	1.36
24	BB	5613	CLA	C3C-C2C	5.47	1.48	1.36
24	AB	605	CLA	C3C-C2C	5.46	1.48	1.36
24	AB	605	CLA	O2D-CGD	5.45	1.46	1.33
27	AB	618	BCR	C30-C25	5.45	1.60	1.53
27	BB	5622	BCR	C30-C25	5.44	1.60	1.53
24	BC	5513	CLA	O2D-CGD	5.44	1.46	1.33
36	BF	5101	HEM	C4A-C3A	5.44	1.55	1.43
24	AC	502	CLA	C3C-C2C	5.43	1.48	1.36
27	BB	5623	BCR	C1-C6	5.42	1.60	1.53
27	BJ	5101	BCR	C5-C6	5.42	1.43	1.34
35	BD	5406	PL9	C6-C1	-5.37	1.39	1.48
27	BJ	5101	BCR	C1-C6	5.37	1.60	1.53
27	AX	101	BCR	C30-C25	5.36	1.60	1.53
24	AB	611	CLA	C3C-C2C	5.35	1.48	1.36
27	BC	5516	BCR	C1-C6	5.33	1.60	1.53
24	AC	507	CLA	C3C-C2C	5.31	1.48	1.36
27	AJ	101	BCR	C5-C6	5.30	1.43	1.34
35	AD	405	PL9	C6-C1	-5.29	1.39	1.48
24	BC	5506	CLA	O2D-CGD	5.28	1.46	1.33
24	BC	5507	CLA	C3C-C2C	5.25	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	512	CLA	MG-NA	5.25	2.18	2.06
27	AT	101	BCR	C1-C6	5.25	1.60	1.53
24	BB	5609	CLA	C3C-C2C	5.23	1.48	1.36
24	BC	5505	CLA	CAA-C2A	-5.23	1.44	1.54
24	AC	506	CLA	O2D-CGD	5.22	1.46	1.33
24	AC	509	CLA	O2D-CGD	5.22	1.46	1.33
24	AC	513	CLA	O2D-CGD	5.21	1.46	1.33
24	AA	404	CLA	MG-NA	5.20	2.18	2.06
24	AB	616	CLA	C3C-C2C	5.20	1.48	1.36
27	AA	410	BCR	C1-C6	5.17	1.60	1.53
36	AV	201	HEM	C4D-C3D	5.16	1.53	1.45
24	AA	405	CLA	C3C-C2C	5.16	1.47	1.36
28	BB	5602	DGD	O5D-C1E	5.15	1.48	1.40
28	BC	5517	DGD	O5D-C1E	5.11	1.48	1.40
29	BA	5413	LHG	P-O3	5.10	1.79	1.59
36	AF	101	HEM	C4D-C3D	5.09	1.53	1.45
36	AF	101	HEM	C4A-C3A	5.08	1.55	1.43
24	BB	5618	CLA	O2D-CGD	5.08	1.45	1.33
27	AX	101	BCR	C1-C6	5.08	1.60	1.53
36	BV	5201	HEM	C4D-C3D	5.07	1.53	1.45
24	BB	5609	CLA	O2D-CGD	5.06	1.45	1.33
27	BX	5101	BCR	C26-C25	5.05	1.43	1.34
24	BB	5620	CLA	O2D-CGD	5.05	1.45	1.33
24	BD	5405	CLA	MG-NA	5.04	2.18	2.06
24	AC	507	CLA	C4C-C3C	5.03	1.53	1.45
24	BC	5505	CLA	CBB-CAB	5.03	1.54	1.30
24	BC	5507	CLA	O2D-CGD	5.03	1.45	1.33
24	AC	505	CLA	CBB-CAB	5.02	1.54	1.30
24	BC	5502	CLA	MG-NA	5.01	2.18	2.06
24	AB	606	CLA	O2D-CGD	5.01	1.45	1.33
24	AB	601	CLA	CBB-CAB	5.01	1.54	1.30
36	AV	201	HEM	CBC-CAC	4.99	1.54	1.30
24	AA	404	CLA	O2D-CGD	4.99	1.45	1.33
27	AX	101	BCR	C26-C25	4.99	1.42	1.34
36	BV	5201	HEM	CBC-CAC	4.99	1.54	1.30
36	BF	5101	HEM	C4D-C3D	4.98	1.53	1.45
29	AA	412	LHG	P-O3	4.97	1.78	1.59
34	BD	5403	PHO	O2D-CGD	4.96	1.45	1.33
24	AB	610	CLA	O2D-CGD	4.95	1.45	1.33
28	BA	5412	DGD	O6D-C1D	4.94	1.54	1.41
24	AB	609	CLA	O2D-CGD	4.94	1.45	1.33
24	AA	405	CLA	CBB-CAB	4.94	1.54	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5501	CLA	CBB-CAB	4.92	1.54	1.30
24	AD	404	CLA	MG-NA	4.92	2.18	2.06
24	AB	605	CLA	CBB-CAB	4.91	1.54	1.30
36	BF	5101	HEM	CBB-CAB	4.90	1.53	1.30
24	AB	616	CLA	O2D-CGD	4.90	1.45	1.33
24	BB	5605	CLA	CBB-CAB	4.90	1.53	1.30
24	BC	5501	CLA	O2D-CGD	4.89	1.45	1.33
24	BB	5607	CLA	O2D-CGD	4.88	1.45	1.33
24	BB	5612	CLA	O2A-CGA	4.88	1.47	1.33
24	BB	5613	CLA	O2D-CGD	4.87	1.45	1.33
24	BB	5609	CLA	CBB-CAB	4.87	1.53	1.30
24	BB	5614	CLA	C4C-C3C	4.87	1.53	1.45
27	BB	5623	BCR	C30-C25	4.87	1.60	1.53
24	BB	5613	CLA	CBB-CAB	4.87	1.53	1.30
36	BF	5101	HEM	CBC-CAC	4.87	1.53	1.30
28	AC	519	DGD	O6D-C1D	4.86	1.54	1.41
27	BA	5411	BCR	C30-C25	4.86	1.60	1.53
24	AB	604	CLA	CBB-CAB	4.86	1.53	1.30
24	AB	613	CLA	MG-NA	4.85	2.17	2.06
24	AB	608	CLA	O2A-CGA	4.85	1.47	1.33
24	BA	5407	CLA	CBB-CAB	4.85	1.53	1.30
24	AC	501	CLA	CBB-CAB	4.83	1.53	1.30
36	AF	101	HEM	CBB-CAB	4.82	1.53	1.30
24	BC	5512	CLA	MG-NA	4.82	2.17	2.06
24	BB	5615	CLA	O2D-CGD	4.81	1.45	1.33
36	BV	5201	HEM	CBB-CAB	4.81	1.53	1.30
24	BB	5619	CLA	CBB-CAB	4.81	1.53	1.30
24	AB	614	CLA	O2D-CGD	4.80	1.45	1.33
24	AB	615	CLA	CBB-CAB	4.79	1.53	1.30
28	BE	5102	DGD	O3G-C1D	4.79	1.48	1.40
24	BB	5611	CLA	C3C-C2C	4.79	1.47	1.36
24	BA	5406	CLA	CBB-CAB	4.79	1.53	1.30
24	BC	5513	CLA	CBB-CAB	4.79	1.53	1.30
24	BC	5502	CLA	O2D-CGD	4.78	1.45	1.33
28	BC	5519	DGD	O6D-C1D	4.77	1.54	1.41
24	BC	5512	CLA	C4C-C3C	4.77	1.53	1.45
27	AC	514	BCR	C1-C6	4.76	1.59	1.53
24	AA	406	CLA	CBB-CAB	4.75	1.53	1.30
24	AB	616	CLA	CBB-CAB	4.75	1.53	1.30
24	BB	5612	CLA	CBB-CAB	4.75	1.53	1.30
24	BB	5610	CLA	O2D-CGD	4.75	1.44	1.33
24	BC	5510	CLA	O2D-CGD	4.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5509	CLA	O2D-CGD	4.74	1.44	1.33
30	BB	5625	SQD	O47-C7	4.73	1.47	1.34
24	BC	5511	CLA	O2D-CGD	4.73	1.44	1.33
24	AB	602	CLA	CBB-CAB	4.72	1.53	1.30
24	BC	5503	CLA	CBB-CAB	4.70	1.53	1.30
27	BT	5101	BCR	C30-C25	4.70	1.59	1.53
24	AC	513	CLA	CBB-CAB	4.70	1.53	1.30
27	BX	5101	BCR	C1-C6	4.70	1.59	1.53
24	BD	5405	CLA	O2D-CGD	4.70	1.44	1.33
27	BD	5407	BCR	C26-C25	4.70	1.42	1.34
24	AB	608	CLA	CBB-CAB	4.69	1.52	1.30
27	AD	406	BCR	C30-C25	4.69	1.59	1.53
24	AB	610	CLA	C4C-C3C	4.69	1.53	1.45
24	BA	5405	CLA	C4C-C3C	4.69	1.53	1.45
36	AF	101	HEM	CBC-CAC	4.69	1.52	1.30
24	AB	609	CLA	CBB-CAB	4.68	1.52	1.30
27	BK	5102	BCR	C5-C6	4.68	1.42	1.34
24	AC	506	CLA	CBB-CAB	4.68	1.52	1.30
24	BC	5502	CLA	CBB-CAB	4.67	1.52	1.30
34	AD	403	PHO	O2D-CGD	4.67	1.44	1.33
24	AB	602	CLA	C4C-C3C	4.67	1.53	1.45
24	BD	5402	CLA	C4C-C3C	4.67	1.53	1.45
24	BC	5506	CLA	CBB-CAB	4.66	1.52	1.30
24	BB	5608	CLA	CBB-CAB	4.66	1.52	1.30
24	AC	510	CLA	CBB-CAB	4.66	1.52	1.30
24	BA	5405	CLA	O2D-CGD	4.65	1.44	1.33
24	BB	5616	CLA	C4C-C3C	4.65	1.52	1.45
24	BC	5510	CLA	CBB-CAB	4.65	1.52	1.30
24	AC	508	CLA	O2D-CGD	4.65	1.44	1.33
28	BC	5518	DGD	O6D-C1D	4.65	1.53	1.41
24	BB	5606	CLA	CBB-CAB	4.65	1.52	1.30
24	BC	5512	CLA	CBB-CAB	4.65	1.52	1.30
24	AC	512	CLA	CBB-CAB	4.65	1.52	1.30
34	BD	5403	PHO	C3A-C2A	-4.64	1.50	1.54
24	BA	5405	CLA	CBB-CAB	4.63	1.52	1.30
24	AB	610	CLA	MG-NA	4.62	2.17	2.06
36	AV	201	HEM	C4A-C3A	4.62	1.54	1.43
24	BB	5620	CLA	CBB-CAB	4.62	1.52	1.30
28	BC	5517	DGD	O6D-C1D	4.61	1.53	1.41
24	BB	5614	CLA	CBB-CAB	4.60	1.52	1.30
36	BF	5101	HEM	C4D-ND	-4.60	1.32	1.40
27	AA	410	BCR	C30-C25	4.60	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BF	5102	SQD	O47-C7	4.60	1.47	1.34
27	AB	618	BCR	C26-C25	4.60	1.42	1.34
30	BA	5414	SQD	O47-C7	4.59	1.47	1.34
24	AD	401	CLA	CBB-CAB	4.59	1.52	1.30
24	AC	507	CLA	CBB-CAB	4.59	1.52	1.30
24	BC	5507	CLA	CBB-CAB	4.59	1.52	1.30
24	AB	610	CLA	CBB-CAB	4.58	1.52	1.30
24	AC	502	CLA	O2D-CGD	4.57	1.44	1.33
29	AA	412	LHG	P-O6	4.57	1.77	1.59
24	AB	606	CLA	CBB-CAB	4.56	1.52	1.30
24	AB	601	CLA	C4C-C3C	4.56	1.52	1.45
24	BB	5610	CLA	C4C-C3C	4.56	1.52	1.45
24	BC	5507	CLA	C4C-C3C	4.55	1.52	1.45
27	BT	5101	BCR	C5-C6	4.55	1.42	1.34
24	AC	512	CLA	C4C-C3C	4.55	1.52	1.45
34	BD	5404	PHO	O2D-CGD	4.54	1.44	1.33
24	AB	606	CLA	C4C-C3C	4.54	1.52	1.45
24	AC	503	CLA	CBB-CAB	4.54	1.52	1.30
34	AD	402	PHO	C3A-C2A	-4.53	1.50	1.54
24	BB	5618	CLA	C4C-C3C	4.53	1.52	1.45
24	AC	508	CLA	CBB-CAB	4.52	1.52	1.30
24	BA	5407	CLA	MG-NA	4.52	2.17	2.06
24	AC	510	CLA	C4C-C3C	4.52	1.52	1.45
30	BF	5102	SQD	O5-C5	4.52	1.55	1.44
24	BC	5513	CLA	C4C-C3C	4.52	1.52	1.45
24	AC	509	CLA	CBB-CAB	4.51	1.52	1.30
24	BD	5402	CLA	C1C-C2C	4.51	1.53	1.44
24	BC	5504	CLA	O2D-CGD	4.51	1.44	1.33
30	BA	5401	SQD	O47-C7	4.51	1.47	1.34
24	AC	502	CLA	CBB-CAB	4.51	1.52	1.30
24	BB	5610	CLA	CBB-CAB	4.50	1.52	1.30
30	BA	5401	SQD	O5-C5	4.49	1.55	1.44
24	BB	5606	CLA	O2D-CGD	4.49	1.44	1.33
24	AB	603	CLA	O2A-CGA	4.49	1.46	1.33
24	BD	5402	CLA	CBB-CAB	4.49	1.51	1.30
36	AV	201	HEM	CBB-CAB	4.48	1.51	1.30
30	AF	102	SQD	O5-C5	4.48	1.55	1.44
24	BD	5402	CLA	O2D-CGD	4.48	1.44	1.33
24	AD	401	CLA	C1C-C2C	4.48	1.53	1.44
24	AA	404	CLA	CBB-CAB	4.48	1.51	1.30
24	BC	5505	CLA	MG-NA	4.48	2.16	2.06
24	AC	505	CLA	C1C-C2C	4.46	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5611	CLA	MG-NA	4.46	2.16	2.06
27	AD	406	BCR	C26-C25	4.46	1.42	1.34
24	BA	5405	CLA	C1C-C2C	4.46	1.53	1.44
24	BB	5618	CLA	C1C-C2C	4.45	1.53	1.44
24	BC	5505	CLA	O2D-CGD	4.45	1.44	1.33
24	BC	5508	CLA	CBB-CAB	4.45	1.51	1.30
30	AA	413	SQD	O47-C7	4.45	1.46	1.34
24	BC	5512	CLA	O2D-CGD	4.44	1.44	1.33
24	BA	5406	CLA	C1C-C2C	4.44	1.53	1.44
24	AC	507	CLA	O2D-CGD	4.44	1.44	1.33
24	AC	510	CLA	O2D-CGD	4.44	1.44	1.33
27	BC	5516	BCR	C5-C6	4.44	1.42	1.34
24	AB	614	CLA	C1C-C2C	4.44	1.53	1.44
24	BC	5513	CLA	C1C-C2C	4.44	1.53	1.44
28	AC	518	DGD	O6D-C1D	4.44	1.53	1.41
24	AB	613	CLA	C4C-C3C	4.44	1.52	1.45
24	BA	5408	CLA	C1C-C2C	4.43	1.53	1.44
24	AB	602	CLA	O2D-CGD	4.43	1.44	1.33
24	BC	5506	CLA	C1C-C2C	4.43	1.53	1.44
24	AB	614	CLA	C4C-C3C	4.42	1.52	1.45
24	AC	506	CLA	C1C-C2C	4.42	1.53	1.44
24	BC	5503	CLA	O2D-CGD	4.42	1.44	1.33
24	BB	5615	CLA	CBB-CAB	4.42	1.51	1.30
24	AA	405	CLA	C1C-C2C	4.42	1.53	1.44
24	BD	5405	CLA	CBB-CAB	4.42	1.51	1.30
28	AC	519	DGD	O5D-C6D	-4.41	1.36	1.43
24	BB	5606	CLA	C4C-C3C	4.41	1.52	1.45
24	BC	5505	CLA	C1C-C2C	4.41	1.53	1.44
24	AB	611	CLA	O2D-CGD	4.41	1.44	1.33
24	BC	5510	CLA	C1C-C2C	4.41	1.53	1.44
24	AD	404	CLA	CBB-CAB	4.41	1.51	1.30
24	AB	604	CLA	C1C-C2C	4.41	1.53	1.44
27	AT	101	BCR	C30-C25	4.40	1.59	1.53
24	AC	506	CLA	C4C-C3C	4.40	1.52	1.45
24	BC	5511	CLA	C1C-C2C	4.40	1.53	1.44
24	AC	513	CLA	C1C-C2C	4.40	1.53	1.44
24	BB	5616	CLA	CBB-CAB	4.39	1.51	1.30
24	BB	5611	CLA	C1C-C2C	4.39	1.53	1.44
24	AC	509	CLA	C1C-C2C	4.39	1.53	1.44
24	AB	608	CLA	C1C-C2C	4.39	1.53	1.44
24	BC	5509	CLA	CBB-CAB	4.39	1.51	1.30
24	AB	607	CLA	C1C-C2C	4.38	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	5603	LMT	C1B-C2B	-4.38	1.39	1.52
24	BC	5504	CLA	C1C-C2C	4.38	1.53	1.44
24	AA	406	CLA	MG-NA	4.38	2.16	2.06
32	BD	5411	LMT	C1B-C2B	-4.38	1.39	1.52
24	AA	407	CLA	C1C-C2C	4.38	1.53	1.44
24	AC	512	CLA	O2D-CGD	4.38	1.44	1.33
24	AA	404	CLA	C1C-C2C	4.38	1.53	1.44
32	AB	624	LMT	C1B-C2B	-4.38	1.39	1.52
32	AB	629	LMT	C1B-C2B	-4.38	1.39	1.52
24	AC	511	CLA	C1C-C2C	4.37	1.53	1.44
24	AB	605	CLA	C1C-C2C	4.37	1.53	1.44
24	BC	5508	CLA	C1C-C2C	4.37	1.53	1.44
24	AD	404	CLA	C1C-C2C	4.37	1.53	1.44
24	AC	503	CLA	C1C-C2C	4.37	1.53	1.44
24	AA	404	CLA	C4C-C3C	4.37	1.52	1.45
30	AF	102	SQD	C1-C2	4.37	1.65	1.52
24	AB	613	CLA	C1C-C2C	4.37	1.53	1.44
24	BB	5613	CLA	C1C-C2C	4.37	1.53	1.44
32	AD	409	LMT	C1B-C2B	-4.36	1.39	1.52
24	AA	406	CLA	C1C-C2C	4.36	1.53	1.44
24	AB	603	CLA	C1C-C2C	4.36	1.53	1.44
24	BB	5616	CLA	C1C-C2C	4.36	1.53	1.44
24	BC	5502	CLA	C1C-C2C	4.36	1.53	1.44
24	AB	602	CLA	C1C-C2C	4.36	1.53	1.44
32	AI	103	LMT	C1B-C2B	-4.36	1.39	1.52
24	AB	611	CLA	C1C-C2C	4.36	1.53	1.44
24	BB	5613	CLA	MG-NA	4.36	2.16	2.06
24	BB	5612	CLA	C1C-C2C	4.36	1.53	1.44
24	BB	5608	CLA	O2D-CGD	4.36	1.43	1.33
24	AB	609	CLA	C1C-C2C	4.36	1.53	1.44
24	AC	508	CLA	C1C-C2C	4.36	1.53	1.44
32	BB	5604	LMT	C1B-C2B	-4.36	1.39	1.52
32	BB	5627	LMT	C1B-C2B	-4.36	1.39	1.52
24	BB	5607	CLA	C1C-C2C	4.36	1.53	1.44
24	BC	5507	CLA	C1C-C2C	4.36	1.53	1.44
24	AC	510	CLA	C1C-C2C	4.36	1.53	1.44
24	BC	5509	CLA	C1C-C2C	4.35	1.53	1.44
24	AB	612	CLA	C1C-C2C	4.35	1.53	1.44
24	AC	507	CLA	C1C-C2C	4.35	1.53	1.44
24	AC	513	CLA	C4C-C3C	4.35	1.52	1.45
24	BC	5503	CLA	C1C-C2C	4.35	1.53	1.44
27	AC	515	BCR	C1-C6	4.35	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	601	CLA	C1C-C2C	4.35	1.53	1.44
36	BF	5101	HEM	FE-NB	4.35	2.08	1.94
24	AB	603	CLA	CBB-CAB	4.35	1.51	1.30
24	AC	511	CLA	O2D-CGD	4.35	1.43	1.33
24	AB	610	CLA	C1C-C2C	4.35	1.53	1.44
32	AI	102	LMT	C1B-C2B	-4.35	1.39	1.52
32	BM	5101	LMT	C1B-C2B	-4.35	1.39	1.52
32	AB	630	LMT	C1B-C2B	-4.34	1.39	1.52
24	AB	616	CLA	C1C-C2C	4.34	1.53	1.44
24	BB	5617	CLA	C1C-C2C	4.34	1.53	1.44
24	BC	5512	CLA	C1C-C2C	4.34	1.53	1.44
32	BI	5102	LMT	C1B-C2B	-4.34	1.39	1.52
24	AB	615	CLA	C1C-C2C	4.34	1.53	1.44
24	BB	5620	CLA	C4C-C3C	4.34	1.52	1.45
24	BA	5407	CLA	C1C-C2C	4.34	1.53	1.44
24	BB	5608	CLA	C1C-C2C	4.34	1.53	1.44
24	AB	603	CLA	O2D-CGD	4.33	1.43	1.33
24	BB	5606	CLA	C1C-C2C	4.33	1.53	1.44
32	AM	102	LMT	C1B-C2B	-4.33	1.39	1.52
24	AC	512	CLA	C1C-C2C	4.33	1.53	1.44
24	AC	501	CLA	C1C-C2C	4.33	1.53	1.44
24	BB	5614	CLA	C1C-C2C	4.33	1.53	1.44
32	BB	5626	LMT	C1B-C2B	-4.33	1.39	1.52
24	BB	5609	CLA	C1C-C2C	4.33	1.53	1.44
27	BK	5102	BCR	C1-C6	4.33	1.59	1.53
28	AA	411	DGD	O6D-C1D	4.32	1.53	1.41
24	BB	5619	CLA	C1C-C2C	4.32	1.53	1.44
32	BC	5522	LMT	C1B-C2B	-4.32	1.39	1.52
24	BD	5405	CLA	C1C-C2C	4.32	1.53	1.44
36	AF	101	HEM	C4D-ND	-4.32	1.32	1.40
24	BC	5501	CLA	C1C-C2C	4.32	1.53	1.44
24	AC	504	CLA	C1C-C2C	4.31	1.53	1.44
24	BB	5619	CLA	O2D-CGD	4.31	1.43	1.33
30	AB	622	SQD	O47-C7	4.31	1.46	1.34
24	BB	5605	CLA	C1C-C2C	4.31	1.53	1.44
32	AB	623	LMT	C1B-C2B	-4.31	1.39	1.52
29	AA	415	LHG	O8-C23	4.31	1.45	1.33
24	AA	407	CLA	O2D-CGD	4.31	1.43	1.33
24	AB	611	CLA	CBB-CAB	4.31	1.51	1.30
24	AB	606	CLA	C1C-C2C	4.30	1.53	1.44
24	AB	612	CLA	CBB-CAB	4.30	1.51	1.30
24	BB	5616	CLA	O2D-CGD	4.30	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BH	5101	DGD	O5D-C1E	4.30	1.47	1.40
24	AD	404	CLA	C4C-C3C	4.30	1.52	1.45
24	BC	5501	CLA	C4C-C3C	4.30	1.52	1.45
24	BB	5615	CLA	C1C-C2C	4.30	1.53	1.44
24	AC	501	CLA	MG-NA	4.30	2.16	2.06
24	BB	5610	CLA	C1C-C2C	4.29	1.53	1.44
34	AD	402	PHO	CMC-C2C	4.29	1.57	1.50
24	BB	5605	CLA	C4C-C3C	4.29	1.52	1.45
24	BA	5408	CLA	O2D-CGD	4.29	1.43	1.33
27	BC	5516	BCR	C30-C25	4.29	1.59	1.53
30	BB	5601	SQD	O7-S	4.29	1.57	1.45
24	BB	5607	CLA	O2A-CGA	4.28	1.45	1.33
30	BA	5414	SQD	O7-S	4.28	1.57	1.45
36	BF	5101	HEM	FE-NA	4.28	2.09	1.95
28	AC	517	DGD	O6D-C1D	4.28	1.52	1.41
29	BA	5415	LHG	O8-C23	4.28	1.45	1.33
24	AC	502	CLA	C1C-C2C	4.28	1.53	1.44
24	AC	501	CLA	O2D-CGD	4.28	1.43	1.33
24	BB	5620	CLA	C1C-C2C	4.27	1.53	1.44
30	BB	5625	SQD	O5-C5	4.26	1.54	1.44
24	AB	615	CLA	O2D-CGD	4.26	1.43	1.33
24	AD	401	CLA	C4C-C3C	4.26	1.52	1.45
30	AB	622	SQD	O5-C5	4.26	1.54	1.44
30	AA	416	SQD	O47-C7	4.26	1.46	1.34
28	AE	101	DGD	O3G-C1D	4.25	1.47	1.40
30	AF	102	SQD	O47-C7	4.25	1.46	1.34
24	BC	5503	CLA	C4C-C3C	4.25	1.52	1.45
30	AB	622	SQD	O7-S	4.25	1.57	1.45
24	BC	5504	CLA	CBB-CAB	4.25	1.50	1.30
24	AB	609	CLA	MG-NA	4.24	2.16	2.06
24	AB	615	CLA	MG-NA	4.24	2.16	2.06
34	AD	402	PHO	O2D-CGD	4.23	1.43	1.33
30	AA	416	SQD	O5-C5	4.23	1.54	1.44
24	AC	504	CLA	CBB-CAB	4.23	1.50	1.30
24	AB	607	CLA	MG-NA	4.22	2.16	2.06
24	BC	5509	CLA	C4C-C3C	4.22	1.52	1.45
24	BA	5408	CLA	CBB-CAB	4.21	1.50	1.30
30	BB	5601	SQD	O5-C5	4.21	1.54	1.44
36	BF	5101	HEM	O2D-CGD	4.21	1.44	1.30
27	AJ	101	BCR	C29-C30	4.20	1.63	1.54
24	AC	505	CLA	O2A-CGA	4.19	1.45	1.33
30	AF	102	SQD	O48-C23	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AB	627	SQD	O7-S	4.18	1.56	1.45
36	AV	201	HEM	C1C-C2C	4.17	1.53	1.45
24	BB	5618	CLA	CBB-CAB	4.17	1.50	1.30
27	AJ	101	BCR	C26-C25	4.17	1.41	1.34
24	AB	616	CLA	C4C-C3C	4.17	1.52	1.45
24	BC	5511	CLA	CBB-CAB	4.17	1.50	1.30
24	BB	5607	CLA	CBB-CAB	4.17	1.50	1.30
24	BC	5504	CLA	C4C-C3C	4.17	1.52	1.45
24	AB	604	CLA	C4C-C3C	4.17	1.52	1.45
24	BB	5613	CLA	C4C-C3C	4.17	1.52	1.45
36	AF	101	HEM	FE-NC	4.16	2.08	1.95
24	AB	615	CLA	C4C-C3C	4.16	1.52	1.45
27	BJ	5101	BCR	C26-C25	4.16	1.41	1.34
30	BB	5625	SQD	C1-C2	4.16	1.64	1.52
28	AH	101	DGD	O5D-C1E	4.15	1.47	1.40
24	AC	503	CLA	C4C-C3C	4.15	1.52	1.45
36	AF	101	HEM	C1C-C2C	4.14	1.53	1.45
24	AA	407	CLA	CBB-CAB	4.14	1.50	1.30
24	BB	5610	CLA	MG-NA	4.14	2.16	2.06
24	BC	5506	CLA	C4C-C3C	4.14	1.52	1.45
24	AC	503	CLA	O2D-CGD	4.13	1.43	1.33
24	AB	614	CLA	CBB-CAB	4.13	1.50	1.30
28	AE	101	DGD	O5D-C1E	4.13	1.47	1.40
24	BD	5405	CLA	C4C-C3C	4.13	1.52	1.45
29	BA	5415	LHG	O7-C7	4.13	1.45	1.34
27	AX	101	BCR	C29-C30	4.12	1.63	1.54
30	AF	102	SQD	O6-C1	4.12	1.47	1.40
28	AB	628	DGD	O5D-C1E	4.12	1.47	1.40
36	BF	5101	HEM	C1C-C2C	4.12	1.53	1.45
24	AB	616	CLA	MG-NA	4.12	2.16	2.06
30	AB	622	SQD	O48-C23	4.12	1.45	1.33
36	BV	5201	HEM	C4A-C3A	4.12	1.52	1.43
24	BC	5510	CLA	C4C-C3C	4.11	1.52	1.45
24	AC	511	CLA	CBB-CAB	4.11	1.50	1.30
24	AB	606	CLA	MG-NA	4.11	2.16	2.06
24	BB	5611	CLA	C4C-C3C	4.10	1.52	1.45
24	AC	504	CLA	O2D-CGD	4.10	1.43	1.33
24	AD	404	CLA	O2D-CGD	4.10	1.43	1.33
24	BB	5617	CLA	O2D-CGD	4.09	1.43	1.33
27	AC	516	BCR	C1-C6	4.09	1.59	1.53
27	BC	5515	BCR	C26-C25	4.08	1.41	1.34
36	AF	101	HEM	FE-NA	4.08	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BF	5102	SQD	C1-C2	4.08	1.64	1.52
24	BA	5405	CLA	MG-NA	4.08	2.16	2.06
29	AA	415	LHG	O7-C7	4.07	1.45	1.34
24	AD	401	CLA	O2D-CGD	4.07	1.43	1.33
28	AB	628	DGD	O3G-C1D	4.07	1.47	1.40
24	BC	5512	CLA	MG-NC	4.07	2.15	2.06
30	BB	5601	SQD	C1-C2	4.06	1.64	1.52
27	BJ	5101	BCR	C29-C30	4.06	1.63	1.54
24	AB	609	CLA	C4C-C3C	4.05	1.51	1.45
24	AB	603	CLA	C4C-C3C	4.05	1.51	1.45
36	BV	5201	HEM	C1C-C2C	4.05	1.53	1.45
30	AB	622	SQD	C1-C2	4.05	1.64	1.52
27	AC	515	BCR	C26-C25	4.04	1.41	1.34
30	AB	627	SQD	O5-C5	4.04	1.54	1.44
24	BC	5505	CLA	O2A-CGA	4.04	1.45	1.33
24	AB	613	CLA	CBB-CAB	4.03	1.49	1.30
27	AK	102	BCR	C5-C6	4.03	1.41	1.34
24	AC	505	CLA	O2D-CGD	4.03	1.43	1.33
36	BV	5201	HEM	O2D-CGD	4.03	1.44	1.30
24	BC	5508	CLA	MG-NB	4.02	2.13	2.05
24	BC	5511	CLA	C4C-C3C	4.02	1.51	1.45
30	BF	5102	SQD	O6-C1	4.02	1.46	1.40
24	BB	5608	CLA	MG-NA	4.02	2.15	2.06
29	BA	5413	LHG	P-O6	4.02	1.75	1.59
24	AB	612	CLA	C4C-C3C	4.02	1.51	1.45
24	AC	504	CLA	MG-NA	4.01	2.15	2.06
24	BB	5609	CLA	MG-NA	4.01	2.15	2.06
27	BC	5515	BCR	C5-C6	4.01	1.41	1.34
24	AA	405	CLA	O2D-CGD	4.01	1.43	1.33
30	AB	627	SQD	C1-C2	4.01	1.64	1.52
28	AA	411	DGD	O6E-C1E	4.00	1.52	1.41
24	BB	5614	CLA	O2D-CGD	4.00	1.43	1.33
24	AA	406	CLA	C4C-C3C	3.99	1.51	1.45
28	AC	517	DGD	O5D-C1E	3.99	1.46	1.40
24	BB	5617	CLA	CBB-CAB	3.99	1.49	1.30
24	AC	509	CLA	C4C-C3C	3.98	1.51	1.45
32	AB	623	LMT	O5B-C1B	3.98	1.52	1.41
30	BF	5102	SQD	O48-C23	3.98	1.44	1.33
24	BB	5614	CLA	MG-NA	3.97	2.15	2.06
27	BB	5622	BCR	C26-C25	3.96	1.41	1.34
36	AV	201	HEM	FE-NA	3.96	2.08	1.95
24	AB	608	CLA	O2D-CGD	3.96	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BV	5201	HEM	CAC-C3C	3.96	1.58	1.47
24	AB	612	CLA	O2D-CGD	3.96	1.43	1.33
27	BX	5101	BCR	C29-C30	3.96	1.63	1.54
24	AB	606	CLA	C3D-C4D	3.95	1.53	1.44
36	AF	101	HEM	O2D-CGD	3.95	1.43	1.30
27	BD	5407	BCR	C29-C30	3.95	1.63	1.54
24	BC	5510	CLA	C3D-C4D	3.95	1.53	1.44
28	AC	518	DGD	C2A-C1A	-3.95	1.39	1.50
22	BA	5403	BCT	O1-C	3.95	1.39	1.25
32	AB	623	LMT	O1'-C1'	3.95	1.46	1.40
24	BC	5503	CLA	C3D-C4D	3.95	1.53	1.44
24	BB	5615	CLA	C3D-C4D	3.94	1.53	1.44
28	BC	5518	DGD	C2A-C1A	-3.94	1.39	1.50
24	AC	512	CLA	C3D-C4D	3.94	1.53	1.44
24	AB	601	CLA	C3D-C4D	3.94	1.53	1.44
30	BA	5414	SQD	O5-C5	3.94	1.54	1.44
36	AF	101	HEM	C3C-C4C	3.94	1.52	1.46
27	AT	101	BCR	C5-C6	3.93	1.41	1.34
24	BB	5618	CLA	C3D-C4D	3.93	1.53	1.44
24	AA	407	CLA	C3D-C4D	3.93	1.53	1.44
24	BC	5512	CLA	C3D-C4D	3.93	1.53	1.44
24	BC	5509	CLA	C3D-C4D	3.93	1.53	1.44
24	BB	5608	CLA	C4C-C3C	3.93	1.51	1.45
24	BB	5611	CLA	CBB-CAB	3.93	1.49	1.30
24	AB	601	CLA	MG-NC	3.93	2.15	2.06
24	AC	513	CLA	C3D-C4D	3.92	1.53	1.44
24	BB	5605	CLA	C3D-C4D	3.92	1.53	1.44
24	BB	5606	CLA	C3D-C4D	3.92	1.53	1.44
24	BB	5610	CLA	C3D-C4D	3.92	1.53	1.44
24	AC	502	CLA	C3D-C4D	3.92	1.53	1.44
24	BC	5513	CLA	C3D-C4D	3.91	1.53	1.44
24	AC	508	CLA	C3D-C4D	3.91	1.53	1.44
24	AB	614	CLA	C3D-C4D	3.91	1.53	1.44
24	AC	501	CLA	C4C-C3C	3.91	1.51	1.45
24	AC	506	CLA	C3D-C4D	3.91	1.53	1.44
24	AB	607	CLA	O2D-CGD	3.91	1.42	1.33
34	BD	5403	PHO	CMC-C2C	3.91	1.56	1.50
32	AB	630	LMT	O5B-C1B	3.91	1.51	1.41
24	AB	602	CLA	C3D-C4D	3.91	1.53	1.44
24	AB	616	CLA	C3D-C4D	3.91	1.53	1.44
24	AC	507	CLA	C3D-C4D	3.90	1.53	1.44
24	AC	503	CLA	MG-NA	3.90	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	608	CLA	C3D-C4D	3.90	1.53	1.44
28	BC	5517	DGD	C2A-C1A	-3.90	1.39	1.50
24	BC	5503	CLA	MG-NC	3.90	2.15	2.06
30	BB	5625	SQD	O48-C23	3.90	1.44	1.33
24	AC	504	CLA	C3D-C4D	3.90	1.53	1.44
24	BC	5507	CLA	C3D-C4D	3.90	1.53	1.44
24	BB	5614	CLA	C3D-C4D	3.90	1.53	1.44
24	BD	5405	CLA	C3D-C4D	3.90	1.53	1.44
24	AB	607	CLA	C3D-C4D	3.90	1.53	1.44
24	AC	511	CLA	C3D-C4D	3.89	1.53	1.44
28	BE	5102	DGD	O5D-C1E	3.89	1.46	1.40
24	BB	5607	CLA	C4C-C3C	3.89	1.51	1.45
24	AB	605	CLA	C3D-C4D	3.89	1.52	1.44
24	AD	404	CLA	C3D-C4D	3.89	1.52	1.44
24	BC	5505	CLA	C3D-C4D	3.89	1.52	1.44
24	BA	5405	CLA	C3D-C4D	3.89	1.52	1.44
24	AB	612	CLA	C3D-C4D	3.89	1.52	1.44
28	AC	519	DGD	C2A-C1A	-3.89	1.39	1.50
30	AF	102	SQD	O7-S	3.89	1.56	1.45
24	BC	5511	CLA	C3D-C4D	3.89	1.52	1.44
24	AA	404	CLA	C3D-C4D	3.89	1.52	1.44
30	BB	5625	SQD	O7-S	3.89	1.56	1.45
24	BB	5617	CLA	C3D-C4D	3.89	1.52	1.44
24	AC	509	CLA	C3D-C4D	3.89	1.52	1.44
24	AB	614	CLA	CHC-C1C	3.88	1.46	1.38
24	AC	505	CLA	C3D-C4D	3.88	1.52	1.44
24	AB	615	CLA	C3D-C4D	3.88	1.52	1.44
24	BC	5508	CLA	C3D-C4D	3.88	1.52	1.44
24	AB	610	CLA	C3D-C4D	3.88	1.52	1.44
24	BB	5612	CLA	C3D-C4D	3.88	1.52	1.44
28	BH	5101	DGD	C2A-C1A	-3.88	1.39	1.50
36	BF	5101	HEM	FE-NC	3.88	2.08	1.95
24	BB	5611	CLA	C3D-C4D	3.88	1.52	1.44
24	BB	5619	CLA	C3D-C4D	3.88	1.52	1.44
24	BB	5608	CLA	C3D-C4D	3.87	1.52	1.44
30	BA	5401	SQD	O7-S	3.87	1.56	1.45
24	AC	510	CLA	C3D-C4D	3.87	1.52	1.44
24	BA	5408	CLA	C3D-C4D	3.87	1.52	1.44
24	BB	5609	CLA	C3D-C4D	3.87	1.52	1.44
24	AB	603	CLA	C3D-C4D	3.87	1.52	1.44
24	AB	611	CLA	C3D-C4D	3.87	1.52	1.44
24	AB	607	CLA	CBB-CAB	3.87	1.49	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	5407	CLA	C4C-C3C	3.87	1.51	1.45
24	BB	5613	CLA	C3D-C4D	3.86	1.52	1.44
24	BC	5504	CLA	C3D-C4D	3.86	1.52	1.44
24	BC	5506	CLA	C3D-C4D	3.86	1.52	1.44
28	AC	517	DGD	C2A-C1A	-3.86	1.39	1.50
24	AC	503	CLA	C3D-C4D	3.86	1.52	1.44
24	AC	502	CLA	MG-NA	3.86	2.15	2.06
24	BA	5406	CLA	C3D-C4D	3.86	1.52	1.44
24	BD	5402	CLA	C1C-NC	3.86	1.44	1.37
24	BB	5620	CLA	C3D-C4D	3.86	1.52	1.44
24	AB	613	CLA	C3D-C4D	3.85	1.52	1.44
24	BC	5502	CLA	C3D-C4D	3.85	1.52	1.44
24	AC	511	CLA	C4C-C3C	3.85	1.51	1.45
36	BV	5201	HEM	FE-NA	3.85	2.07	1.95
28	BC	5519	DGD	C2A-C1A	-3.85	1.39	1.50
24	BB	5618	CLA	CHC-C1C	3.85	1.46	1.38
24	BB	5616	CLA	C3D-C4D	3.85	1.52	1.44
24	AC	501	CLA	C3D-C4D	3.85	1.52	1.44
36	BF	5101	HEM	C3C-C4C	3.84	1.52	1.46
24	BC	5507	CLA	MG-NC	3.84	2.15	2.06
24	BD	5402	CLA	C3D-C4D	3.84	1.52	1.44
24	BC	5501	CLA	C3D-C4D	3.84	1.52	1.44
27	BK	5102	BCR	C26-C25	3.84	1.41	1.34
34	BD	5404	PHO	CBB-CAB	3.84	1.53	1.29
27	AB	617	BCR	C26-C25	3.84	1.41	1.34
36	BV	5201	HEM	FE-NC	3.84	2.07	1.95
24	BB	5607	CLA	C3D-C4D	3.84	1.52	1.44
36	AF	101	HEM	FE-NB	3.84	2.06	1.94
28	AB	628	DGD	C2A-C1A	-3.84	1.39	1.50
27	BB	5622	BCR	C2-C1	3.84	1.62	1.54
28	AH	101	DGD	C2A-C1A	-3.83	1.39	1.50
24	AB	613	CLA	O2D-CGD	3.83	1.42	1.33
24	AB	607	CLA	C4C-C3C	3.83	1.51	1.45
24	AB	609	CLA	C3D-C4D	3.83	1.52	1.44
24	BB	5612	CLA	O2D-CGD	3.83	1.42	1.33
24	AA	406	CLA	C3D-C4D	3.82	1.52	1.44
24	AB	604	CLA	C3D-C4D	3.82	1.52	1.44
24	AB	604	CLA	O2D-CGD	3.82	1.42	1.33
24	BA	5407	CLA	C3D-C4D	3.82	1.52	1.44
24	AB	605	CLA	MG-NB	3.81	2.13	2.05
29	AA	412	LHG	O8-C23	3.81	1.44	1.33
24	AC	505	CLA	C4C-C3C	3.81	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AE	101	DGD	C2A-C1A	-3.81	1.39	1.50
24	AA	405	CLA	C3D-C4D	3.81	1.52	1.44
34	BD	5404	PHO	CMC-C2C	3.81	1.56	1.50
29	BA	5413	LHG	O7-C7	3.80	1.45	1.34
28	BA	5412	DGD	O6E-C1E	3.80	1.51	1.41
28	BB	5602	DGD	C2A-C1A	-3.80	1.39	1.50
36	AV	201	HEM	O2D-CGD	3.80	1.43	1.30
30	AA	416	SQD	C1-C2	3.79	1.63	1.52
27	AK	102	BCR	C26-C25	3.79	1.40	1.34
28	BE	5102	DGD	C2A-C1A	-3.79	1.39	1.50
24	AD	401	CLA	C3D-C4D	3.79	1.52	1.44
28	AA	411	DGD	C2A-C1A	-3.79	1.39	1.50
36	BV	5201	HEM	FE-NB	3.79	2.06	1.94
24	AB	614	CLA	O2A-CGA	3.79	1.44	1.33
24	BA	5408	CLA	C4C-C3C	3.78	1.51	1.45
24	BC	5501	CLA	MG-NA	3.78	2.15	2.06
27	BC	5516	BCR	C2-C1	3.78	1.62	1.54
24	AB	605	CLA	MG-NA	3.77	2.15	2.06
30	BF	5102	SQD	O7-S	3.77	1.55	1.45
32	BB	5626	LMT	O5B-C1B	3.76	1.51	1.41
28	AC	518	DGD	O5D-C1E	3.76	1.46	1.40
30	AB	627	SQD	O48-C23	3.76	1.44	1.33
28	BA	5412	DGD	C2A-C1A	-3.76	1.39	1.50
24	BA	5408	CLA	MG-NB	3.76	2.13	2.05
24	BB	5617	CLA	C4C-C3C	3.76	1.51	1.45
24	BB	5606	CLA	MG-NC	3.76	2.15	2.06
34	BD	5403	PHO	CBB-CAB	3.75	1.52	1.29
34	AD	402	PHO	CBB-CAB	3.75	1.52	1.29
28	BC	5518	DGD	O5D-C1E	3.75	1.46	1.40
30	BA	5401	SQD	C1-C2	3.75	1.63	1.52
24	BC	5505	CLA	MG-NC	3.74	2.15	2.06
27	AK	102	BCR	C1-C6	3.74	1.58	1.53
34	AD	403	PHO	CBB-CAB	3.74	1.52	1.29
31	AJ	102	LMG	O1-C1	3.74	1.46	1.40
27	AC	516	BCR	C5-C6	3.73	1.40	1.34
28	BC	5519	DGD	C3E-C2E	3.73	1.62	1.52
30	BA	5401	SQD	O48-C23	3.72	1.44	1.33
30	BA	5414	SQD	C1-C2	3.72	1.63	1.52
24	AC	502	CLA	O2A-CGA	3.72	1.44	1.33
27	AK	102	BCR	C29-C30	3.71	1.62	1.54
30	AB	627	SQD	O47-C7	3.71	1.44	1.34
24	BA	5408	CLA	C1C-NC	3.71	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	5621	BCR	C26-C25	3.71	1.40	1.34
24	BC	5506	CLA	MG-NC	3.70	2.15	2.06
24	BB	5611	CLA	O2D-CGD	3.70	1.42	1.33
24	AB	611	CLA	C4C-C3C	3.70	1.51	1.45
30	BB	5601	SQD	O47-C7	3.69	1.44	1.34
27	AB	618	BCR	C2-C1	3.69	1.62	1.54
32	AM	102	LMT	C6B-C5B	-3.69	1.39	1.51
24	BB	5618	CLA	O2A-CGA	3.68	1.44	1.33
24	AC	512	CLA	MG-NC	3.68	2.15	2.06
32	AD	409	LMT	C6B-C5B	-3.68	1.39	1.51
24	BC	5505	CLA	CMC-C2C	3.68	1.58	1.50
32	BB	5626	LMT	O1'-C1'	3.68	1.46	1.40
24	AB	601	CLA	O1D-CGD	3.67	1.30	1.21
32	BD	5411	LMT	C6B-C5B	-3.67	1.39	1.51
32	AB	623	LMT	C6B-C5B	-3.67	1.39	1.51
32	BB	5604	LMT	C6B-C5B	-3.67	1.39	1.51
32	AI	103	LMT	C6B-C5B	-3.66	1.39	1.51
24	AD	404	CLA	CMC-C2C	3.66	1.58	1.50
30	AB	622	SQD	O6-C1	3.66	1.46	1.40
34	BD	5404	PHO	C3A-C2A	-3.65	1.51	1.54
32	AB	624	LMT	C6B-C5B	-3.65	1.39	1.51
36	AF	101	HEM	CAC-C3C	3.65	1.57	1.47
32	BC	5522	LMT	C6B-C5B	-3.65	1.39	1.51
32	AI	102	LMT	C6B-C5B	-3.65	1.39	1.51
32	BB	5603	LMT	C6B-C5B	-3.65	1.39	1.51
24	AC	508	CLA	MG-NB	3.65	2.13	2.05
32	AB	630	LMT	C6B-C5B	-3.65	1.39	1.51
24	BC	5502	CLA	C4C-C3C	3.65	1.51	1.45
32	BM	5101	LMT	C6B-C5B	-3.65	1.39	1.51
32	BB	5627	LMT	C6B-C5B	-3.65	1.39	1.51
32	AI	102	LMT	O5B-C1B	3.64	1.51	1.41
24	BC	5510	CLA	MG-NA	3.64	2.14	2.06
32	BI	5102	LMT	C6B-C5B	-3.64	1.39	1.51
28	AA	411	DGD	O2G-C1B	3.64	1.44	1.34
32	BB	5626	LMT	C6B-C5B	-3.64	1.39	1.51
34	AD	403	PHO	CMC-C2C	3.63	1.56	1.50
36	AV	201	HEM	FE-NC	3.63	2.07	1.95
35	BD	5406	PL9	C37-C38	-3.63	1.39	1.50
30	AA	416	SQD	O7-S	3.63	1.55	1.45
27	AC	516	BCR	C30-C25	3.63	1.58	1.53
32	AB	629	LMT	C6B-C5B	-3.62	1.39	1.51
28	BA	5412	DGD	O2G-C1B	3.62	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	506	CLA	MG-NC	3.62	2.14	2.06
24	BA	5407	CLA	O2D-CGD	3.61	1.42	1.33
24	BA	5407	CLA	MG-NB	3.61	2.12	2.05
28	AH	101	DGD	O2G-C2G	3.61	1.55	1.46
24	BB	5620	CLA	MG-NA	3.61	2.14	2.06
24	AC	504	CLA	C4C-C3C	3.60	1.51	1.45
32	AD	409	LMT	O5B-C1B	3.60	1.51	1.41
30	AA	413	SQD	C1-C2	3.60	1.63	1.52
24	BB	5620	CLA	MG-NC	3.60	2.14	2.06
27	BC	5515	BCR	C29-C30	3.60	1.62	1.54
24	BB	5605	CLA	O2A-CGA	3.60	1.43	1.33
35	BD	5406	PL9	C32-C33	-3.59	1.39	1.50
30	AA	413	SQD	O5-C5	3.59	1.53	1.44
27	BB	5623	BCR	C2-C1	3.59	1.62	1.54
35	AD	405	PL9	C32-C33	-3.57	1.39	1.50
32	BB	5604	LMT	O5B-C1B	3.57	1.51	1.41
30	BA	5401	SQD	O6-C1	3.57	1.46	1.40
28	BH	5101	DGD	O2G-C2G	3.57	1.55	1.46
27	AB	619	BCR	C29-C30	3.56	1.62	1.54
24	BA	5406	CLA	O2D-CGD	3.56	1.42	1.33
36	AV	201	HEM	FE-ND	3.56	2.05	1.94
24	AB	611	CLA	MG-NB	3.56	2.12	2.05
28	AB	628	DGD	O6D-C1D	3.56	1.51	1.41
24	BB	5605	CLA	C3B-C2B	3.56	1.53	1.41
27	AA	410	BCR	C26-C25	3.55	1.40	1.34
24	BC	5505	CLA	C4C-C3C	3.55	1.51	1.45
36	BV	5201	HEM	FE-ND	3.55	2.05	1.94
36	BF	5101	HEM	CAC-C3C	3.55	1.56	1.47
28	BB	5602	DGD	O3G-C1D	3.55	1.46	1.40
27	AB	617	BCR	C5-C6	3.55	1.40	1.34
24	BB	5610	CLA	MG-NB	3.55	2.12	2.05
27	AB	618	BCR	C29-C30	3.54	1.62	1.54
24	AA	407	CLA	MG-NA	3.54	2.14	2.06
32	BM	5101	LMT	O5B-C1B	3.54	1.50	1.41
24	AC	505	CLA	CMC-C2C	3.53	1.58	1.50
24	BC	5506	CLA	O2A-CGA	3.53	1.43	1.33
28	BB	5602	DGD	O6D-C1D	3.53	1.50	1.41
32	BI	5102	LMT	O5B-C1B	3.53	1.50	1.41
34	AD	402	PHO	C3B-C4B	3.52	1.45	1.41
30	AA	416	SQD	O6-C1	3.52	1.46	1.40
34	BD	5403	PHO	C3B-C4B	3.52	1.45	1.41
27	AD	406	BCR	C29-C30	3.51	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	AF	101	HEM	FE-ND	3.51	2.05	1.94
24	AD	401	CLA	MG-NA	3.51	2.14	2.06
27	BT	5101	BCR	C2-C1	3.51	1.62	1.54
30	AA	416	SQD	O48-C23	3.51	1.43	1.33
24	BB	5619	CLA	C4C-C3C	3.50	1.51	1.45
27	BB	5623	BCR	C29-C30	3.50	1.62	1.54
27	AB	619	BCR	C2-C1	3.50	1.62	1.54
24	BA	5407	CLA	O1D-CGD	3.50	1.30	1.21
24	BC	5508	CLA	MG-NC	3.49	2.14	2.06
24	BA	5406	CLA	CBA-CGA	3.49	1.60	1.50
24	BB	5609	CLA	MG-NB	3.49	2.12	2.05
27	BB	5621	BCR	C2-C1	3.48	1.62	1.54
24	AB	601	CLA	O2A-CGA	3.48	1.43	1.33
24	BB	5605	CLA	O1D-CGD	3.47	1.30	1.21
32	AB	629	LMT	O5B-C1B	3.46	1.50	1.41
24	BC	5504	CLA	MG-NB	3.46	2.12	2.05
24	BD	5402	CLA	MG-NA	3.46	2.14	2.06
35	AD	405	PL9	C37-C38	-3.45	1.40	1.50
24	AB	602	CLA	MG-NB	3.45	2.12	2.05
30	AA	413	SQD	O7-S	3.45	1.54	1.45
27	AJ	101	BCR	C2-C1	3.45	1.62	1.54
24	AB	605	CLA	C4C-C3C	3.45	1.50	1.45
24	AD	401	CLA	CMC-C2C	3.45	1.57	1.50
24	AC	507	CLA	MG-NC	3.45	2.14	2.06
24	BC	5505	CLA	C3B-C2B	3.44	1.52	1.41
30	BA	5414	SQD	O48-C23	3.44	1.43	1.33
27	BC	5514	BCR	C29-C30	3.44	1.61	1.54
27	AT	101	BCR	C29-C30	3.43	1.61	1.54
27	BB	5622	BCR	C29-C30	3.43	1.61	1.54
30	BB	5601	SQD	O48-C23	3.43	1.43	1.33
24	BB	5615	CLA	MG-NB	3.43	2.12	2.05
24	AB	607	CLA	C5-C3	3.43	1.58	1.51
32	BC	5522	LMT	O5B-C1B	3.43	1.50	1.41
27	AB	617	BCR	C30-C25	3.42	1.58	1.53
36	AV	201	HEM	CAC-C3C	3.42	1.56	1.47
24	AB	609	CLA	O2A-CGA	3.42	1.43	1.33
32	AB	624	LMT	O1'-C1'	3.42	1.45	1.40
27	AB	617	BCR	C2-C1	3.42	1.61	1.54
27	BX	5101	BCR	C2-C1	3.41	1.61	1.54
24	AA	406	CLA	O2D-CGD	3.41	1.41	1.33
30	AF	102	SQD	O5-C1	3.41	1.50	1.41
24	AC	504	CLA	MG-NB	3.40	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	510	CLA	MG-NC	3.40	2.14	2.06
24	AA	405	CLA	CBA-CGA	3.40	1.60	1.50
24	AA	405	CLA	MG-NB	3.40	2.12	2.05
24	AC	509	CLA	O1D-CGD	3.40	1.29	1.21
24	BB	5609	CLA	C4C-C3C	3.40	1.50	1.45
24	AB	605	CLA	O2A-CGA	3.40	1.43	1.33
36	AV	201	HEM	FE-NB	3.40	2.05	1.94
24	AC	505	CLA	CAA-CBA	-3.40	1.42	1.52
27	AC	515	BCR	C5-C6	3.39	1.40	1.34
24	BC	5501	CLA	O2A-CGA	3.39	1.43	1.33
27	BJ	5101	BCR	C2-C1	3.39	1.61	1.54
27	BK	5102	BCR	C29-C30	3.39	1.61	1.54
24	AB	602	CLA	MG-NC	3.39	2.14	2.06
32	BB	5603	LMT	O5B-C1B	3.39	1.50	1.41
27	AC	515	BCR	C29-C30	3.39	1.61	1.54
31	AC	521	LMG	O1-C1	3.39	1.45	1.40
34	AD	403	PHO	C3D-CAD	-3.38	1.41	1.47
32	BD	5411	LMT	O5B-C1B	3.38	1.50	1.41
27	BD	5407	BCR	C1-C6	3.37	1.58	1.53
24	BD	5405	CLA	CMC-C2C	3.37	1.57	1.50
24	AB	601	CLA	C3B-C2B	3.36	1.52	1.41
24	BC	5504	CLA	MG-NA	3.36	2.14	2.06
24	BB	5609	CLA	O2A-CGA	3.36	1.43	1.33
24	BB	5605	CLA	MG-NC	3.36	2.14	2.06
30	AA	413	SQD	O6-C44	-3.35	1.37	1.43
24	AA	405	CLA	CMC-C2C	3.35	1.57	1.50
24	BC	5511	CLA	O1D-CGD	3.34	1.29	1.21
24	AC	510	CLA	MG-NA	3.34	2.14	2.06
27	AC	516	BCR	C2-C1	3.34	1.61	1.54
32	AM	102	LMT	O5B-C1B	3.34	1.50	1.41
24	BB	5606	CLA	MG-NA	3.34	2.14	2.06
24	BA	5406	CLA	CMC-C2C	3.34	1.57	1.50
24	AC	506	CLA	O2A-CGA	3.33	1.43	1.33
24	BA	5407	CLA	CBA-CGA	3.33	1.60	1.50
24	BC	5511	CLA	CHC-C1C	3.33	1.45	1.38
30	BB	5625	SQD	C12-C11	-3.33	1.35	1.51
24	AC	505	CLA	C3B-C2B	3.33	1.52	1.41
24	BC	5506	CLA	MG-NB	3.32	2.12	2.05
36	BV	5201	HEM	C4D-ND	-3.32	1.34	1.40
30	BB	5625	SQD	O6-C1	3.32	1.45	1.40
24	BC	5502	CLA	O2A-CGA	3.31	1.43	1.33
27	BT	5101	BCR	C29-C30	3.31	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5612	CLA	C4C-C3C	3.31	1.50	1.45
24	BB	5620	CLA	O1D-CGD	3.31	1.29	1.21
27	AB	618	BCR	C5-C6	3.31	1.40	1.34
31	AA	414	LMG	O1-C1	3.31	1.45	1.40
27	BC	5514	BCR	C2-C1	3.30	1.61	1.54
24	AA	407	CLA	C4C-C3C	3.30	1.50	1.45
24	AA	404	CLA	CMC-C2C	3.30	1.57	1.50
22	AA	402	BCT	O1-C	3.30	1.37	1.25
27	AC	514	BCR	C29-C30	3.29	1.61	1.54
24	AB	607	CLA	O2A-CGA	3.29	1.42	1.33
27	BD	5407	BCR	C2-C1	3.29	1.61	1.54
27	BA	5411	BCR	C26-C25	3.29	1.40	1.34
27	AT	101	BCR	C2-C1	3.28	1.61	1.54
24	BC	5507	CLA	MG-NA	3.28	2.14	2.06
30	AB	622	SQD	C12-C11	-3.28	1.35	1.51
30	AA	413	SQD	O48-C23	3.28	1.42	1.33
24	BB	5611	CLA	C5-C3	3.28	1.58	1.51
34	BD	5404	PHO	C3D-CAD	-3.28	1.41	1.47
24	AB	616	CLA	O1D-CGD	3.28	1.29	1.21
24	AB	606	CLA	MG-NB	3.27	2.12	2.05
27	AC	515	BCR	C2-C1	3.27	1.61	1.54
30	BB	5625	SQD	O3-C3	3.26	1.51	1.43
24	AB	604	CLA	CMC-C2C	3.26	1.57	1.50
24	BC	5501	CLA	MG-NC	3.26	2.14	2.06
24	BC	5513	CLA	O1D-CGD	3.26	1.29	1.21
31	BD	5408	LMG	O1-C1	3.26	1.45	1.40
24	AB	608	CLA	C4C-C3C	3.26	1.50	1.45
24	AC	511	CLA	CHC-C1C	3.26	1.45	1.38
27	AB	619	BCR	C5-C6	3.26	1.40	1.34
24	BC	5503	CLA	O2A-CGA	3.26	1.42	1.33
24	BC	5511	CLA	MG-NB	3.26	2.12	2.05
30	AA	413	SQD	C17-C16	-3.26	1.35	1.51
24	BA	5408	CLA	CMC-C2C	3.25	1.57	1.50
30	BB	5625	SQD	C11-C10	-3.25	1.35	1.51
30	BB	5601	SQD	C12-C11	-3.25	1.35	1.51
24	BB	5614	CLA	CMC-C2C	3.25	1.57	1.50
27	BK	5102	BCR	C2-C1	3.24	1.61	1.54
32	AI	103	LMT	O5B-C1B	3.24	1.50	1.41
24	BB	5608	CLA	MG-NB	3.23	2.12	2.05
36	BV	5201	HEM	O2A-CGA	-3.23	1.20	1.30
29	AA	412	LHG	O7-C7	3.23	1.43	1.34
24	AB	614	CLA	MG-NB	3.23	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	5621	BCR	C5-C6	3.23	1.39	1.34
36	BF	5101	HEM	CMC-C2C	3.23	1.57	1.50
24	AA	406	CLA	MG-NB	3.23	2.12	2.05
24	BC	5512	CLA	MG-NB	3.23	2.12	2.05
29	BA	5413	LHG	O8-C23	3.23	1.42	1.33
27	AC	514	BCR	C26-C25	3.23	1.39	1.34
24	BC	5511	CLA	C1B-NB	3.23	1.42	1.37
31	AC	521	LMG	O6-C1	3.23	1.50	1.41
32	BM	5101	LMT	O1B-C4'	3.22	1.52	1.43
27	AB	617	BCR	C29-C30	3.22	1.61	1.54
24	BB	5617	CLA	MG-NA	3.22	2.13	2.06
36	BF	5101	HEM	FE-ND	3.22	2.04	1.94
30	BF	5102	SQD	O5-C1	3.22	1.50	1.41
30	AB	627	SQD	C15-C14	-3.22	1.35	1.51
32	BB	5604	LMT	O1B-C4'	3.22	1.52	1.43
24	AA	406	CLA	CBA-CGA	3.22	1.60	1.50
24	BD	5402	CLA	MG-NC	3.21	2.13	2.06
32	AD	409	LMT	O1'-C1'	3.21	1.45	1.40
24	AC	501	CLA	CMC-C2C	3.21	1.57	1.50
30	BB	5601	SQD	C15-C14	-3.21	1.35	1.51
24	AB	602	CLA	MG-NA	3.21	2.13	2.06
36	BV	5201	HEM	C3C-C4C	3.21	1.51	1.46
24	AC	503	CLA	O2A-CGA	3.21	1.42	1.33
34	BD	5403	PHO	O1D-CGD	3.20	1.29	1.21
28	BC	5519	DGD	O5D-C6D	-3.20	1.38	1.43
30	BB	5601	SQD	C16-C15	-3.20	1.35	1.51
24	BA	5406	CLA	C3B-C2B	3.20	1.51	1.41
30	AB	627	SQD	C20-C19	-3.19	1.35	1.51
32	BB	5627	LMT	O1'-C1'	3.19	1.45	1.40
30	BA	5414	SQD	C17-C16	-3.19	1.35	1.51
24	AB	610	CLA	CMC-C2C	3.19	1.57	1.50
36	AV	201	HEM	C3C-C4C	3.19	1.51	1.46
30	AA	413	SQD	C15-C14	-3.19	1.35	1.51
24	BC	5512	CLA	C1C-NC	3.19	1.43	1.37
27	AD	406	BCR	C1-C6	3.19	1.57	1.53
30	AB	622	SQD	C11-C10	-3.18	1.35	1.51
24	AC	502	CLA	C4C-C3C	3.18	1.50	1.45
30	AB	627	SQD	C16-C15	-3.18	1.36	1.51
24	BC	5513	CLA	O2A-CGA	3.18	1.42	1.33
24	AC	501	CLA	O2A-CGA	3.18	1.42	1.33
27	AD	406	BCR	C2-C1	3.18	1.61	1.54
30	AB	622	SQD	O3-C3	3.18	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AA	411	DGD	O1G-C1A	3.18	1.42	1.33
27	BA	5411	BCR	C29-C30	3.18	1.61	1.54
24	AC	507	CLA	MG-NA	3.17	2.13	2.06
24	BB	5617	CLA	MG-NC	3.17	2.13	2.06
24	BC	5505	CLA	O1D-CGD	3.17	1.29	1.21
30	AB	627	SQD	C12-C11	-3.17	1.36	1.51
24	BB	5616	CLA	O2A-CGA	3.17	1.42	1.33
24	BC	5512	CLA	C3B-C2B	3.17	1.51	1.41
24	BB	5617	CLA	C1C-NC	3.17	1.43	1.37
32	BM	5101	LMT	O1'-C1'	3.17	1.45	1.40
30	BA	5401	SQD	O5-C1	3.17	1.50	1.41
24	BB	5616	CLA	O1D-CGD	3.17	1.29	1.21
36	AV	201	HEM	O2A-CGA	-3.17	1.20	1.30
27	AA	410	BCR	C29-C30	3.16	1.61	1.54
30	BF	5102	SQD	C17-C16	-3.16	1.36	1.51
30	BA	5414	SQD	C33-C32	-3.16	1.36	1.51
28	BA	5412	DGD	O5D-C6D	-3.16	1.38	1.43
30	BA	5414	SQD	C15-C14	-3.16	1.36	1.51
24	BC	5513	CLA	C3B-C2B	3.16	1.51	1.41
24	BB	5611	CLA	O2A-CGA	3.16	1.42	1.33
24	AC	508	CLA	MG-NC	3.16	2.13	2.06
32	AM	102	LMT	O1'-C1'	3.15	1.45	1.40
30	BB	5601	SQD	C20-C19	-3.15	1.36	1.51
24	AC	503	CLA	MG-NB	3.15	2.12	2.05
36	BV	5201	HEM	CMC-C2C	3.15	1.57	1.50
32	AM	102	LMT	O1B-C4'	3.15	1.51	1.43
36	AV	201	HEM	C4D-ND	-3.14	1.34	1.40
24	BC	5505	CLA	CAA-CBA	-3.14	1.43	1.52
24	BB	5613	CLA	O2A-CGA	3.14	1.42	1.33
30	AB	627	SQD	C19-C18	-3.14	1.36	1.51
24	BD	5405	CLA	O1D-CGD	3.14	1.29	1.21
24	BC	5512	CLA	CMC-C2C	3.14	1.57	1.50
24	BA	5408	CLA	MG-NC	3.14	2.13	2.06
24	BC	5508	CLA	C4C-C3C	3.14	1.50	1.45
24	AC	502	CLA	MG-NC	3.14	2.13	2.06
24	AC	506	CLA	MG-NB	3.14	2.12	2.05
30	BB	5601	SQD	C11-C10	-3.14	1.36	1.51
30	AB	627	SQD	C14-C13	-3.14	1.36	1.51
24	BB	5618	CLA	MG-NB	3.13	2.12	2.05
24	BC	5509	CLA	C3B-C2B	3.13	1.51	1.41
30	AA	413	SQD	C16-C15	-3.13	1.36	1.51
24	BB	5612	CLA	CMC-C2C	3.13	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	5603	LMT	O1B-C1B	3.13	1.50	1.41
24	AB	616	CLA	MG-NC	3.13	2.13	2.06
27	BB	5621	BCR	C29-C30	3.12	1.61	1.54
30	BB	5601	SQD	C14-C13	-3.12	1.36	1.51
24	AC	508	CLA	C4C-C3C	3.12	1.50	1.45
24	BB	5615	CLA	MG-NC	3.11	2.13	2.06
30	BA	5414	SQD	C16-C15	-3.11	1.36	1.51
27	AA	410	BCR	C2-C1	3.11	1.61	1.54
30	AA	413	SQD	C33-C32	-3.11	1.36	1.51
31	BC	5521	LMG	O1-C1	3.11	1.45	1.40
24	BD	5402	CLA	CMC-C2C	3.11	1.57	1.50
24	AD	401	CLA	C1C-NC	3.11	1.42	1.37
24	BC	5501	CLA	CMC-C2C	3.10	1.57	1.50
31	AJ	102	LMG	O7-C8	-3.10	1.39	1.46
24	BC	5511	CLA	O2A-CGA	3.10	1.42	1.33
24	BC	5512	CLA	O1D-CGD	3.09	1.29	1.21
30	BF	5102	SQD	C11-C10	-3.09	1.36	1.51
32	AB	629	LMT	O1B-C1B	3.09	1.50	1.41
24	AC	512	CLA	C3B-C2B	3.09	1.51	1.41
30	AB	627	SQD	C11-C10	-3.09	1.36	1.51
30	BB	5601	SQD	C17-C16	-3.09	1.36	1.51
30	BF	5102	SQD	C16-C15	-3.09	1.36	1.51
31	BD	5408	LMG	O7-C8	-3.09	1.39	1.46
24	BA	5407	CLA	CMC-C2C	3.08	1.57	1.50
24	AB	604	CLA	MG-NB	3.08	2.11	2.05
24	BC	5509	CLA	O1D-CGD	3.08	1.29	1.21
27	BX	5101	BCR	C5-C6	3.08	1.39	1.34
24	AD	401	CLA	MG-NC	3.08	2.13	2.06
24	BC	5510	CLA	MG-NC	3.08	2.13	2.06
24	BC	5502	CLA	C1B-NB	3.08	1.41	1.37
27	BB	5623	BCR	C5-C6	3.08	1.39	1.34
24	AA	405	CLA	C4C-C3C	3.08	1.50	1.45
24	BB	5614	CLA	MG-NC	3.08	2.13	2.06
31	BL	5101	LMG	O6-C1	3.08	1.49	1.41
28	BA	5412	DGD	O1G-C1A	3.07	1.42	1.33
24	AC	511	CLA	O2A-CGA	3.07	1.42	1.33
24	BB	5620	CLA	MG-NB	3.07	2.11	2.05
24	AC	509	CLA	CMC-C2C	3.07	1.57	1.50
24	AC	506	CLA	C1B-NB	3.07	1.41	1.37
24	BA	5405	CLA	C1C-NC	3.07	1.42	1.37
24	AC	513	CLA	O2A-CGA	3.07	1.42	1.33
24	AC	503	CLA	CMC-C2C	3.07	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	5405	CLA	CMC-C2C	3.07	1.57	1.50
24	BC	5509	CLA	CMC-C2C	3.07	1.57	1.50
24	AB	605	CLA	C3B-C2B	3.07	1.51	1.41
28	BB	5602	DGD	O6E-C1E	3.07	1.49	1.41
24	AC	502	CLA	MG-NB	3.06	2.11	2.05
30	AB	627	SQD	C13-C12	-3.06	1.36	1.51
30	AF	102	SQD	C17-C16	-3.06	1.36	1.51
30	BB	5601	SQD	C19-C18	-3.06	1.36	1.51
24	AC	512	CLA	MG-NB	3.06	2.11	2.05
30	AF	102	SQD	C11-C10	-3.06	1.36	1.51
30	BA	5414	SQD	C11-C10	-3.06	1.36	1.51
24	BB	5606	CLA	CMC-C2C	3.05	1.57	1.50
30	AA	416	SQD	C17-C16	-3.05	1.36	1.51
28	AA	411	DGD	O5D-C6D	-3.05	1.38	1.43
24	BB	5615	CLA	C4C-C3C	3.05	1.50	1.45
24	BC	5503	CLA	C3B-C2B	3.04	1.51	1.41
30	AA	416	SQD	O5-C1	3.04	1.49	1.41
30	BA	5414	SQD	O5-C1	3.04	1.49	1.41
24	AB	605	CLA	O1D-CGD	3.04	1.28	1.21
28	AB	628	DGD	O6E-C1E	3.04	1.49	1.41
30	BB	5601	SQD	C13-C12	-3.04	1.36	1.51
24	AB	606	CLA	O2A-CGA	3.04	1.42	1.33
30	BA	5414	SQD	C12-C11	-3.04	1.36	1.51
30	AA	416	SQD	O3-C3	3.04	1.50	1.43
24	BC	5501	CLA	C3B-C2B	3.04	1.51	1.41
27	AB	619	BCR	C26-C25	3.03	1.39	1.34
24	BC	5507	CLA	O2A-CGA	3.03	1.42	1.33
24	AB	616	CLA	O2A-CGA	3.03	1.42	1.33
30	BA	5414	SQD	C19-C18	-3.03	1.36	1.51
24	AB	606	CLA	O1D-CGD	3.02	1.28	1.21
24	BC	5506	CLA	CMC-C2C	3.02	1.57	1.50
24	BC	5504	CLA	O2A-CGA	3.02	1.42	1.33
24	BC	5501	CLA	O1D-CGD	3.02	1.28	1.21
24	AB	609	CLA	O1D-CGD	3.02	1.28	1.21
30	BF	5102	SQD	C15-C14	-3.02	1.36	1.51
27	BC	5515	BCR	C2-C1	3.01	1.61	1.54
24	AB	605	CLA	CMC-C2C	3.01	1.56	1.50
30	AB	627	SQD	C17-C16	-3.01	1.36	1.51
28	BC	5519	DGD	C4E-C3E	3.01	1.60	1.52
34	AD	403	PHO	C4D-ND	-3.01	1.34	1.38
24	AC	506	CLA	C3B-C2B	3.01	1.51	1.41
32	BB	5627	LMT	O5B-C1B	3.01	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AA	413	SQD	C19-C18	-3.01	1.36	1.51
27	BA	5411	BCR	C2-C1	3.01	1.60	1.54
34	BD	5403	PHO	C4D-ND	-3.01	1.34	1.38
24	AB	606	CLA	C1D-C2D	3.01	1.51	1.45
30	BB	5625	SQD	C16-C15	-3.00	1.36	1.51
24	AB	604	CLA	MG-NA	3.00	2.13	2.06
24	BB	5619	CLA	MG-NB	3.00	2.11	2.05
27	BC	5516	BCR	C29-C30	3.00	1.60	1.54
30	BA	5414	SQD	O6-C44	-3.00	1.38	1.43
27	BB	5621	BCR	C1-C6	3.00	1.57	1.53
30	AF	102	SQD	C12-C11	-3.00	1.36	1.51
30	AA	416	SQD	C16-C15	-3.00	1.36	1.51
30	BF	5102	SQD	C12-C11	-3.00	1.36	1.51
24	AA	404	CLA	O1D-CGD	3.00	1.28	1.21
24	BB	5609	CLA	C3B-C2B	3.00	1.51	1.41
30	BA	5401	SQD	C36-C35	-2.99	1.36	1.51
34	AD	403	PHO	C3A-C2A	-2.99	1.52	1.54
30	AA	413	SQD	C12-C11	-2.99	1.36	1.51
24	BB	5619	CLA	C3B-C2B	2.99	1.51	1.41
24	BB	5617	CLA	O1D-CGD	2.99	1.28	1.21
24	AB	611	CLA	O2A-CGA	2.98	1.42	1.33
27	AX	101	BCR	C2-C1	2.98	1.60	1.54
24	AC	507	CLA	O2A-CGA	2.98	1.42	1.33
24	AB	615	CLA	MG-NC	2.98	2.13	2.06
24	BB	5613	CLA	MG-NB	2.98	2.11	2.05
30	AB	622	SQD	O8-S	2.98	1.58	1.47
24	AC	505	CLA	MG-NC	2.98	2.13	2.06
34	AD	402	PHO	O1D-CGD	2.98	1.28	1.21
27	BB	5621	BCR	C30-C25	2.98	1.57	1.53
27	BC	5516	BCR	C26-C25	2.97	1.39	1.34
27	AC	514	BCR	C2-C1	2.97	1.60	1.54
24	BB	5605	CLA	C1B-NB	2.97	1.41	1.37
24	BC	5511	CLA	C3B-C2B	2.97	1.51	1.41
24	BB	5615	CLA	O1D-CGD	2.97	1.28	1.21
24	BB	5613	CLA	C3B-C2B	2.97	1.51	1.41
30	AB	622	SQD	C16-C15	-2.97	1.37	1.51
28	AH	101	DGD	O6D-C1D	2.97	1.49	1.41
32	BD	5411	LMT	O1'-C1'	2.97	1.45	1.40
24	AC	513	CLA	O1D-CGD	2.96	1.28	1.21
27	AB	617	BCR	C1-C6	2.96	1.57	1.53
34	AD	402	PHO	C4D-ND	-2.96	1.34	1.38
30	AA	416	SQD	C19-C18	-2.96	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	513	CLA	C3B-C2B	2.96	1.51	1.41
24	BC	5502	CLA	MG-NB	2.96	2.11	2.05
24	AB	615	CLA	MG-NB	2.96	2.11	2.05
30	AA	416	SQD	C12-C11	-2.96	1.37	1.51
24	BC	5510	CLA	O1D-CGD	2.96	1.28	1.21
35	BD	5406	PL9	C3-C4	2.96	1.54	1.49
24	BB	5613	CLA	O1D-CGD	2.96	1.28	1.21
27	BC	5514	BCR	C26-C25	2.96	1.39	1.34
31	AA	414	LMG	O6-C1	2.96	1.49	1.41
24	BA	5407	CLA	C3B-C2B	2.96	1.51	1.41
24	BC	5506	CLA	C3B-C2B	2.95	1.51	1.41
24	AB	608	CLA	CMC-C2C	2.95	1.56	1.50
24	BC	5504	CLA	CMC-C2C	2.95	1.56	1.50
30	BB	5601	SQD	O6-C1	2.95	1.45	1.40
32	AM	102	LMT	C4'-C5'	2.95	1.60	1.52
24	AB	609	CLA	C3B-C2B	2.95	1.51	1.41
24	AB	611	CLA	MG-NC	2.95	2.13	2.06
30	AF	102	SQD	C15-C14	-2.95	1.37	1.51
24	AC	503	CLA	MG-NC	2.95	2.13	2.06
30	BA	5401	SQD	C12-C11	-2.95	1.37	1.51
24	AA	407	CLA	C1C-NC	2.95	1.42	1.37
31	BE	5101	LMG	O6-C1	2.94	1.49	1.41
24	AB	604	CLA	MG-NC	2.94	2.13	2.06
27	BD	5407	BCR	C5-C6	2.94	1.39	1.34
30	AA	413	SQD	C32-C31	-2.94	1.37	1.51
24	AC	512	CLA	CMC-C2C	2.94	1.56	1.50
24	BD	5405	CLA	MG-NC	2.94	2.13	2.06
24	AB	615	CLA	CMC-C2C	2.94	1.56	1.50
30	AB	622	SQD	C13-C12	-2.94	1.37	1.51
24	BD	5405	CLA	C1D-C2D	2.93	1.51	1.45
30	AF	102	SQD	C16-C15	-2.93	1.37	1.51
30	BA	5401	SQD	C33-C32	-2.93	1.37	1.51
30	BB	5625	SQD	C13-C12	-2.93	1.37	1.51
30	AA	416	SQD	C36-C35	-2.93	1.37	1.51
24	BB	5607	CLA	CHC-C1C	2.93	1.44	1.38
32	AB	624	LMT	O5B-C1B	2.93	1.49	1.41
24	AC	506	CLA	MG-NA	2.93	2.13	2.06
24	BC	5502	CLA	O1D-CGD	2.93	1.28	1.21
30	BA	5414	SQD	C14-C13	-2.93	1.37	1.51
30	AA	413	SQD	O3-C3	2.92	1.50	1.43
27	AK	102	BCR	C2-C1	2.92	1.60	1.54
24	BC	5503	CLA	CMC-C2C	2.92	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	609	CLA	MG-NC	2.92	2.13	2.06
27	BA	5411	BCR	C5-C6	2.92	1.39	1.34
24	AC	510	CLA	MG-NB	2.92	2.11	2.05
24	AA	405	CLA	O2A-CGA	2.92	1.41	1.33
24	BC	5510	CLA	C3B-C2B	2.92	1.51	1.41
24	AB	616	CLA	C3B-C2B	2.92	1.51	1.41
24	BB	5608	CLA	MG-NC	2.92	2.13	2.06
30	BA	5401	SQD	O3-C3	2.91	1.50	1.43
24	BB	5612	CLA	MG-NB	2.91	2.11	2.05
30	BA	5401	SQD	C17-C16	-2.91	1.37	1.51
30	BA	5401	SQD	C15-C14	-2.91	1.37	1.51
30	AA	413	SQD	C14-C13	-2.91	1.37	1.51
28	BC	5519	DGD	O5D-C1E	2.91	1.45	1.40
24	AB	602	CLA	CMC-C2C	2.91	1.56	1.50
30	AA	413	SQD	C11-C10	-2.90	1.37	1.51
24	BB	5618	CLA	CMC-C2C	2.90	1.56	1.50
28	AC	517	DGD	O3G-C3G	-2.90	1.38	1.43
24	BA	5405	CLA	O1D-CGD	2.90	1.28	1.21
30	BA	5401	SQD	C16-C15	-2.90	1.37	1.51
34	AD	402	PHO	O2A-CGA	2.90	1.41	1.33
24	AA	407	CLA	C1D-C2D	2.90	1.51	1.45
27	AC	516	BCR	C26-C25	2.89	1.39	1.34
36	AF	101	HEM	CMC-C2C	2.89	1.56	1.50
32	BB	5603	LMT	O5'-C1'	2.89	1.49	1.41
24	BB	5619	CLA	O2A-CGA	2.89	1.41	1.33
24	BB	5605	CLA	CMC-C2C	2.89	1.56	1.50
30	AA	413	SQD	C18-C17	-2.89	1.37	1.51
32	AB	630	LMT	O1B-C4'	2.89	1.51	1.43
30	AA	413	SQD	C20-C19	-2.89	1.37	1.51
30	BB	5601	SQD	C18-C17	-2.89	1.37	1.51
28	AE	101	DGD	O6E-C1E	2.89	1.49	1.41
24	BB	5614	CLA	C3B-C2B	2.89	1.50	1.41
24	AB	603	CLA	CHD-C1D	2.89	1.44	1.38
31	BA	5402	LMG	O1-C1	2.89	1.45	1.40
24	AC	502	CLA	O1D-CGD	2.89	1.28	1.21
30	AA	413	SQD	O5-C1	2.88	1.49	1.41
32	BI	5102	LMT	O1'-C1'	2.88	1.45	1.40
24	AA	407	CLA	MG-NC	2.88	2.13	2.06
30	BB	5625	SQD	O8-S	2.88	1.58	1.47
30	BA	5414	SQD	C20-C19	-2.88	1.37	1.51
28	BH	5101	DGD	O6D-C1D	2.88	1.49	1.41
24	AD	404	CLA	O1D-CGD	2.87	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	601	CLA	CMC-C2C	2.87	1.56	1.50
36	AF	101	HEM	O2A-CGA	-2.87	1.21	1.30
24	BB	5610	CLA	C1D-C2D	2.87	1.51	1.45
30	AA	416	SQD	C15-C14	-2.87	1.37	1.51
30	AA	416	SQD	C33-C32	-2.86	1.37	1.51
30	BA	5414	SQD	C32-C31	-2.86	1.37	1.51
24	AB	615	CLA	C3B-C2B	2.86	1.50	1.41
35	BD	5406	PL9	C38-C39	2.86	1.39	1.33
24	BC	5509	CLA	C1B-NB	2.86	1.41	1.37
24	AB	615	CLA	C1C-NC	2.86	1.42	1.37
24	BB	5607	CLA	CHD-C1D	2.86	1.44	1.38
30	BA	5414	SQD	O3-C3	2.86	1.50	1.43
30	AB	627	SQD	O3-C3	2.86	1.50	1.43
24	AA	405	CLA	O1D-CGD	2.85	1.28	1.21
24	AB	612	CLA	CMC-C2C	2.85	1.56	1.50
24	AD	404	CLA	C1D-C2D	2.85	1.51	1.45
24	AC	503	CLA	C3B-C2B	2.85	1.50	1.41
24	BB	5607	CLA	CBA-CGA	2.85	1.59	1.50
31	AB	620	LMG	O6-C1	2.85	1.49	1.41
30	BB	5625	SQD	C15-C14	-2.85	1.37	1.51
24	AB	602	CLA	C1C-NC	2.84	1.42	1.37
24	BC	5506	CLA	O1D-CGD	2.84	1.28	1.21
30	AB	622	SQD	C15-C14	-2.84	1.37	1.51
30	BA	5401	SQD	C13-C12	-2.84	1.37	1.51
24	BB	5606	CLA	MG-NB	2.84	2.11	2.05
24	BC	5504	CLA	C1C-NC	2.84	1.42	1.37
24	AB	612	CLA	MG-NB	2.84	2.11	2.05
24	AC	513	CLA	CHC-C1C	2.84	1.44	1.38
24	BC	5509	CLA	MG-NB	2.84	2.11	2.05
24	AC	506	CLA	O1D-CGD	2.84	1.28	1.21
24	BC	5502	CLA	C3B-C2B	2.84	1.50	1.41
31	BE	5101	LMG	O1-C1	2.84	1.44	1.40
24	AC	510	CLA	O1D-CGD	2.83	1.28	1.21
36	BF	5101	HEM	O2A-CGA	-2.83	1.21	1.30
24	AB	603	CLA	CBA-CGA	2.83	1.58	1.50
30	BA	5401	SQD	C32-C31	-2.83	1.37	1.51
24	BC	5509	CLA	O2A-CGA	2.83	1.41	1.33
31	BC	5521	LMG	O6-C1	2.83	1.49	1.41
24	AB	601	CLA	MG-NB	2.83	2.11	2.05
24	BC	5503	CLA	C1D-C2D	2.82	1.50	1.45
24	AB	605	CLA	C1B-NB	2.82	1.41	1.37
24	BA	5406	CLA	C4C-C3C	2.82	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	601	CLA	C1C-NC	2.82	1.42	1.37
30	BB	5625	SQD	C14-C13	-2.82	1.37	1.51
30	BA	5414	SQD	C13-C12	-2.82	1.37	1.51
24	AC	511	CLA	O1D-CGD	2.82	1.28	1.21
30	BA	5414	SQD	C18-C17	-2.81	1.37	1.51
24	BB	5609	CLA	O1D-CGD	2.81	1.28	1.21
24	AB	615	CLA	O2A-CGA	2.81	1.41	1.33
24	AC	511	CLA	C3B-C2B	2.81	1.50	1.41
30	AB	627	SQD	C18-C17	-2.81	1.37	1.51
30	AA	416	SQD	C11-C10	-2.81	1.37	1.51
24	AA	407	CLA	CMC-C2C	2.81	1.56	1.50
24	BC	5510	CLA	CMC-C2C	2.81	1.56	1.50
24	AA	407	CLA	MG-NB	2.80	2.11	2.05
35	BD	5406	PL9	C18-C19	2.80	1.39	1.33
24	BB	5619	CLA	CMC-C2C	2.80	1.56	1.50
30	AF	102	SQD	O3-C3	2.80	1.49	1.43
24	AA	406	CLA	C3B-C2B	2.80	1.50	1.41
32	BM	5101	LMT	C4'-C5'	2.80	1.60	1.52
24	BB	5609	CLA	CMC-C2C	2.80	1.56	1.50
24	BB	5620	CLA	O2A-CGA	2.80	1.41	1.33
24	BB	5610	CLA	O1D-CGD	2.80	1.28	1.21
24	AD	404	CLA	MG-NC	2.79	2.12	2.06
32	AB	630	LMT	O1'-C1'	2.79	1.44	1.40
30	AF	102	SQD	C14-C13	-2.79	1.37	1.51
35	AD	405	PL9	C18-C19	2.79	1.39	1.33
24	AB	601	CLA	C1B-NB	2.79	1.41	1.37
28	AA	411	DGD	O6D-C5D	2.79	1.51	1.44
27	BB	5622	BCR	C5-C6	2.79	1.39	1.34
30	BA	5401	SQD	C34-C33	-2.79	1.37	1.51
30	AA	413	SQD	C8-C7	2.79	1.58	1.50
24	AB	608	CLA	MG-NB	2.79	2.11	2.05
24	AC	501	CLA	MG-NB	2.79	2.11	2.05
31	BA	5402	LMG	O6-C1	2.79	1.49	1.41
24	BB	5615	CLA	O2A-CGA	2.79	1.41	1.33
24	AC	510	CLA	C3B-C2B	2.79	1.50	1.41
24	AB	607	CLA	C1C-NC	2.78	1.42	1.37
31	AD	408	LMG	O1-C1	2.78	1.44	1.40
30	AB	622	SQD	C14-C13	-2.78	1.37	1.51
31	BC	5520	LMG	O6-C1	2.78	1.49	1.41
30	AA	416	SQD	C20-C19	-2.78	1.37	1.51
24	BD	5405	CLA	O2A-CGA	2.78	1.41	1.33
30	BA	5401	SQD	C14-C13	-2.78	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	608	CLA	CBA-CGA	2.78	1.58	1.50
24	AC	511	CLA	MG-NB	2.78	2.11	2.05
28	BE	5102	DGD	O6E-C1E	2.78	1.49	1.41
30	AA	413	SQD	C13-C12	-2.78	1.38	1.51
30	AA	416	SQD	C32-C31	-2.78	1.38	1.51
32	BB	5604	LMT	O1'-C1'	2.77	1.44	1.40
30	BB	5601	SQD	O8-S	2.77	1.57	1.47
24	AB	603	CLA	O1D-CGD	2.77	1.28	1.21
30	AF	102	SQD	C13-C12	-2.77	1.38	1.51
30	BA	5401	SQD	C35-C34	-2.77	1.38	1.51
24	AB	614	CLA	C3B-C2B	2.76	1.50	1.41
24	AB	604	CLA	O2A-CGA	2.76	1.41	1.33
24	AC	510	CLA	C1C-NC	2.76	1.42	1.37
24	BB	5612	CLA	CBA-CGA	2.76	1.58	1.50
24	AB	604	CLA	C3B-C2B	2.76	1.50	1.41
24	BB	5618	CLA	C3B-C2B	2.75	1.50	1.41
24	BB	5607	CLA	O1D-CGD	2.75	1.28	1.21
35	AD	405	PL9	C38-C39	2.75	1.39	1.33
24	BB	5615	CLA	C3B-C2B	2.75	1.50	1.41
24	BC	5507	CLA	C3B-C2B	2.75	1.50	1.41
24	BB	5608	CLA	O1D-CGD	2.75	1.28	1.21
24	BC	5513	CLA	CHD-C4C	2.75	1.45	1.39
24	BC	5501	CLA	MG-NB	2.75	2.11	2.05
24	BB	5619	CLA	O1D-CGD	2.75	1.28	1.21
30	AA	416	SQD	C13-C12	-2.75	1.38	1.51
24	AB	610	CLA	C3B-C2B	2.75	1.50	1.41
24	AB	612	CLA	CHC-C1C	2.75	1.44	1.38
24	BC	5503	CLA	O1D-CGD	2.75	1.28	1.21
31	BC	5520	LMG	O1-C1	2.74	1.44	1.40
32	AB	629	LMT	O5'-C1'	2.74	1.48	1.41
24	AB	609	CLA	MG-NB	2.74	2.11	2.05
28	BC	5519	DGD	O6E-C1E	2.74	1.48	1.41
24	AB	608	CLA	CAA-C2A	-2.74	1.49	1.54
24	AD	404	CLA	C3B-C2B	2.74	1.50	1.41
35	AD	405	PL9	C3-C4	2.73	1.53	1.49
24	BB	5608	CLA	C3B-C2B	2.73	1.50	1.41
24	BA	5408	CLA	O1D-CGD	2.73	1.28	1.21
24	BC	5506	CLA	C1B-NB	2.73	1.41	1.37
24	AA	405	CLA	C1C-NC	2.73	1.42	1.37
24	BB	5613	CLA	CMC-C2C	2.73	1.56	1.50
30	BF	5102	SQD	C14-C13	-2.73	1.38	1.51
24	AB	612	CLA	O2A-CGA	2.73	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BA	5401	SQD	C19-C18	-2.73	1.38	1.51
30	BA	5401	SQD	C20-C19	-2.73	1.38	1.51
30	AA	416	SQD	C35-C34	-2.73	1.38	1.51
24	AC	501	CLA	MG-NC	2.73	2.12	2.06
24	AC	512	CLA	O1D-CGD	2.73	1.28	1.21
24	BB	5619	CLA	MG-NC	2.72	2.12	2.06
24	BC	5510	CLA	C1B-NB	2.72	1.41	1.37
24	BC	5506	CLA	C1C-NC	2.72	1.42	1.37
31	AA	417	LMG	O6-C1	2.72	1.48	1.41
27	AC	516	BCR	C29-C30	2.72	1.60	1.54
24	BD	5405	CLA	C3B-C2B	2.72	1.50	1.41
24	BC	5501	CLA	CBA-CGA	2.72	1.58	1.50
27	BT	5101	BCR	C26-C25	2.72	1.39	1.34
24	AB	612	CLA	C2A-C1A	-2.72	1.46	1.52
24	BB	5616	CLA	C2A-C1A	-2.72	1.46	1.52
24	BB	5606	CLA	C1C-NC	2.72	1.42	1.37
27	BB	5621	BCR	C23-C22	-2.71	1.40	1.46
24	BB	5607	CLA	CHD-C4C	2.71	1.45	1.39
28	AE	101	DGD	O6E-C5E	2.71	1.51	1.44
27	AJ	101	BCR	C14-C13	2.71	1.42	1.35
24	AB	608	CLA	C1C-NC	2.71	1.42	1.37
24	AB	607	CLA	CBA-CGA	2.71	1.58	1.50
30	BF	5102	SQD	O3-C3	2.71	1.49	1.43
31	BI	5101	LMG	O6-C1	2.71	1.48	1.41
30	BF	5102	SQD	C13-C12	-2.71	1.38	1.51
24	AB	604	CLA	C1C-NC	2.71	1.42	1.37
24	BB	5610	CLA	CMC-C2C	2.71	1.56	1.50
27	BC	5516	BCR	C19-C18	-2.71	1.40	1.46
24	AA	407	CLA	O1D-CGD	2.71	1.28	1.21
30	BA	5401	SQD	C11-C10	-2.70	1.38	1.51
24	AC	501	CLA	C3B-C2B	2.70	1.50	1.41
24	AD	404	CLA	MG-NB	2.70	2.11	2.05
24	BC	5502	CLA	CMC-C2C	2.70	1.56	1.50
24	AB	603	CLA	CHC-C1C	2.69	1.43	1.38
30	AA	416	SQD	C34-C33	-2.69	1.38	1.51
24	AB	613	CLA	O1D-CGD	2.69	1.28	1.21
24	BC	5513	CLA	C1B-NB	2.69	1.41	1.37
24	BA	5406	CLA	C1C-NC	2.69	1.42	1.37
24	BC	5503	CLA	MG-NB	2.69	2.11	2.05
30	AA	416	SQD	C18-C17	-2.69	1.38	1.51
30	AA	413	SQD	O8-S	2.69	1.57	1.47
30	AA	416	SQD	C14-C13	-2.69	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AC	519	DGD	O3G-C3G	2.68	1.48	1.43
24	BA	5405	CLA	C3B-C2B	2.68	1.50	1.41
24	BB	5620	CLA	C3B-C2B	2.68	1.50	1.41
30	AB	627	SQD	O8-S	2.68	1.57	1.47
30	BA	5414	SQD	O8-S	2.68	1.57	1.47
27	BB	5623	BCR	C26-C25	2.68	1.39	1.34
24	BB	5607	CLA	CMC-C2C	2.68	1.56	1.50
28	BE	5102	DGD	O6D-C1D	2.68	1.48	1.41
28	AC	517	DGD	O6D-C5D	2.68	1.50	1.44
36	BF	5101	HEM	CBA-CGA	2.67	1.56	1.50
24	AB	612	CLA	C3B-C2B	2.67	1.50	1.41
24	BC	5511	CLA	CHC-C4B	2.67	1.45	1.39
31	BB	5624	LMG	O6-C1	2.67	1.48	1.41
24	BB	5608	CLA	CMC-C2C	2.67	1.56	1.50
24	AB	603	CLA	CHD-C4C	2.67	1.45	1.39
24	AB	603	CLA	CMC-C2C	2.67	1.56	1.50
24	BB	5608	CLA	O2A-CGA	2.67	1.41	1.33
24	AB	608	CLA	C3B-C2B	2.66	1.50	1.41
24	BD	5402	CLA	O2A-CGA	2.66	1.41	1.33
24	BC	5508	CLA	CHC-C1C	2.66	1.43	1.38
24	AB	611	CLA	C3B-C2B	2.66	1.50	1.41
35	BD	5406	PL9	C27-C28	2.66	1.58	1.50
24	BB	5611	CLA	CBA-CGA	2.66	1.58	1.50
24	AC	501	CLA	C5-C3	2.66	1.56	1.51
24	AB	614	CLA	C1B-NB	2.66	1.41	1.37
24	AC	504	CLA	CMC-C2C	2.66	1.56	1.50
32	BB	5604	LMT	O1B-C1B	2.66	1.49	1.41
30	BB	5601	SQD	O3-C3	2.66	1.49	1.43
24	AB	605	CLA	C1C-NC	2.66	1.42	1.37
24	BC	5513	CLA	CHC-C1C	2.65	1.43	1.38
24	AB	607	CLA	CMC-C2C	2.65	1.56	1.50
24	BB	5617	CLA	CMC-C2C	2.65	1.56	1.50
28	AE	101	DGD	O6D-C1D	2.65	1.48	1.41
24	BD	5402	CLA	C3B-C2B	2.65	1.50	1.41
32	AB	623	LMT	O5'-C1'	2.65	1.48	1.41
31	BM	5102	LMG	O1-C1	2.64	1.44	1.40
24	BA	5406	CLA	C1D-C2D	2.64	1.50	1.45
24	BA	5408	CLA	C1D-C2D	2.64	1.50	1.45
24	BB	5613	CLA	MG-NC	2.64	2.12	2.06
24	AC	506	CLA	CMC-C2C	2.64	1.56	1.50
31	BD	5410	LMG	O6-C1	2.64	1.48	1.41
31	AI	101	LMG	O6-C1	2.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AD	409	LMT	O1B-C1B	2.64	1.49	1.41
24	BB	5610	CLA	O2A-CGA	2.63	1.41	1.33
32	AI	102	LMT	O1'-C1'	2.63	1.44	1.40
24	BB	5606	CLA	O2A-CGA	2.63	1.41	1.33
24	BB	5616	CLA	C3B-C2B	2.63	1.50	1.41
30	AB	627	SQD	O6-C1	2.63	1.44	1.40
28	AE	101	DGD	O2G-C2G	2.63	1.52	1.46
28	BA	5412	DGD	O6D-C5D	2.63	1.50	1.44
24	BB	5612	CLA	O1D-CGD	2.63	1.27	1.21
24	BA	5408	CLA	C3B-C2B	2.63	1.50	1.41
24	BA	5405	CLA	MG-NC	2.62	2.12	2.06
30	BB	5625	SQD	O5-C1	2.62	1.48	1.41
31	AM	101	LMG	O1-C1	2.62	1.44	1.40
32	AB	624	LMT	O5'-C1'	2.62	1.48	1.41
24	BA	5406	CLA	OBD-CAD	2.62	1.27	1.22
24	BB	5618	CLA	O1D-CGD	2.62	1.27	1.21
24	AC	509	CLA	C3B-C2B	2.62	1.50	1.41
24	AB	611	CLA	O1D-CGD	2.62	1.27	1.21
24	AC	512	CLA	C1C-NC	2.62	1.42	1.37
24	BC	5507	CLA	CMC-C2C	2.62	1.56	1.50
24	BA	5406	CLA	O1D-CGD	2.62	1.27	1.21
24	AC	513	CLA	CMC-C2C	2.61	1.56	1.50
27	AX	101	BCR	C5-C6	2.61	1.38	1.34
24	AB	612	CLA	C1D-C2D	2.61	1.50	1.45
30	BF	5102	SQD	O8-S	2.61	1.57	1.47
30	AB	622	SQD	O5-C1	2.61	1.48	1.41
30	BB	5625	SQD	C17-C16	-2.61	1.35	1.51
24	BB	5616	CLA	CMC-C2C	2.61	1.56	1.50
24	BB	5606	CLA	C3B-C2B	2.61	1.50	1.41
24	BB	5612	CLA	CAA-C2A	-2.61	1.49	1.54
24	AB	614	CLA	CMC-C2C	2.61	1.56	1.50
24	BB	5610	CLA	C3B-C2B	2.61	1.50	1.41
28	AE	101	DGD	O6D-C5D	2.60	1.50	1.44
24	AB	608	CLA	MG-NC	2.60	2.12	2.06
24	AA	406	CLA	CHC-C1C	2.60	1.43	1.38
24	BB	5609	CLA	C1B-NB	2.60	1.41	1.37
24	BA	5407	CLA	C1D-C2D	2.60	1.50	1.45
24	BD	5405	CLA	MG-NB	2.59	2.10	2.05
24	AC	504	CLA	O2A-CGA	2.59	1.40	1.33
30	AB	622	SQD	C17-C16	-2.59	1.35	1.51
36	AV	201	HEM	CMC-C2C	2.59	1.56	1.50
24	BB	5613	CLA	C1B-NB	2.59	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5508	CLA	C3B-C2B	2.59	1.49	1.41
35	AD	405	PL9	C27-C28	2.59	1.58	1.50
24	BC	5512	CLA	O2A-CGA	2.58	1.40	1.33
24	BC	5505	CLA	C1B-NB	2.58	1.41	1.37
24	BB	5611	CLA	CMC-C2C	2.58	1.56	1.50
24	AD	404	CLA	C1C-NC	2.58	1.42	1.37
24	BB	5617	CLA	C1D-C2D	2.58	1.50	1.45
24	AB	614	CLA	CHC-C4B	2.58	1.45	1.39
28	BE	5102	DGD	O2G-C2G	2.58	1.52	1.46
24	AC	502	CLA	C3B-C2B	2.58	1.49	1.41
24	AA	407	CLA	C3B-C2B	2.58	1.49	1.41
24	BC	5508	CLA	O1D-CGD	2.58	1.27	1.21
24	AB	615	CLA	O1D-CGD	2.58	1.27	1.21
32	AB	630	LMT	O1B-C1B	2.58	1.49	1.41
24	AC	503	CLA	O1D-CGD	2.58	1.27	1.21
24	AB	612	CLA	O1D-CGD	2.58	1.27	1.21
24	BA	5406	CLA	O2A-CGA	2.57	1.40	1.33
24	AB	605	CLA	MG-NC	2.57	2.12	2.06
30	AB	627	SQD	O5-C1	2.57	1.48	1.41
27	AC	516	BCR	C19-C18	-2.57	1.40	1.46
31	AB	621	LMG	O6-C1	2.57	1.48	1.41
28	AH	101	DGD	O6E-C1E	2.57	1.48	1.41
24	AD	404	CLA	O2A-CGA	2.57	1.40	1.33
24	BB	5615	CLA	C2A-C1A	-2.56	1.46	1.52
24	BC	5513	CLA	CHC-C4B	2.56	1.45	1.39
24	BA	5407	CLA	O2A-CGA	2.56	1.40	1.33
30	AB	627	SQD	C21-C20	-2.56	1.35	1.51
30	BA	5401	SQD	C8-C7	2.56	1.58	1.50
24	BC	5513	CLA	CHD-C1D	2.56	1.43	1.38
28	BE	5102	DGD	C3G-C2G	2.56	1.58	1.50
32	BI	5102	LMT	O1B-C1B	2.56	1.49	1.41
24	BC	5503	CLA	C1C-NC	2.56	1.42	1.37
24	AC	510	CLA	CMC-C2C	2.56	1.56	1.50
24	BC	5513	CLA	MG-NB	2.56	2.10	2.05
24	BC	5511	CLA	CHD-C4C	2.56	1.45	1.39
24	AB	608	CLA	O1D-CGD	2.55	1.27	1.21
30	BB	5601	SQD	O5-C1	2.55	1.48	1.41
24	AC	502	CLA	C1B-NB	2.55	1.41	1.37
24	AC	504	CLA	C3B-C2B	2.55	1.49	1.41
24	AD	401	CLA	O1D-CGD	2.55	1.27	1.21
32	AB	630	LMT	O5'-C1'	2.55	1.48	1.41
27	AB	619	BCR	C23-C22	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BD	5402	CLA	MG-NB	2.55	2.10	2.05
31	AD	408	LMG	O6-C1	2.55	1.48	1.41
24	AB	606	CLA	MG-NC	2.55	2.12	2.06
24	AA	404	CLA	C3B-C2B	2.55	1.49	1.41
24	AC	502	CLA	C1D-C2D	2.55	1.50	1.45
24	AB	609	CLA	CMC-C2C	2.55	1.56	1.50
24	AA	406	CLA	CMC-C2C	2.54	1.56	1.50
24	AB	607	CLA	O1D-CGD	2.54	1.27	1.21
24	AC	513	CLA	MG-NB	2.54	2.10	2.05
24	AC	508	CLA	O2A-CGA	2.54	1.40	1.33
32	BD	5411	LMT	C4'-C5'	2.54	1.59	1.52
24	BC	5507	CLA	O1D-CGD	2.54	1.27	1.21
24	BB	5614	CLA	MG-NB	2.54	2.10	2.05
30	BB	5601	SQD	C21-C20	-2.54	1.36	1.51
27	AX	101	BCR	C38-C26	2.54	1.55	1.50
36	AV	201	HEM	C1B-C2B	-2.53	1.39	1.44
32	BM	5101	LMT	O1B-C1B	2.53	1.48	1.41
24	BC	5504	CLA	C3B-C2B	2.53	1.49	1.41
24	BB	5617	CLA	O2A-CGA	2.53	1.40	1.33
30	BA	5414	SQD	C8-C7	2.53	1.58	1.50
32	BB	5626	LMT	O5'-C1'	2.53	1.48	1.41
24	BC	5504	CLA	CHC-C1C	2.53	1.43	1.38
27	BC	5515	BCR	C19-C18	-2.53	1.40	1.46
24	BC	5507	CLA	C1D-C2D	2.53	1.50	1.45
24	BC	5513	CLA	CMC-C2C	2.52	1.55	1.50
24	AA	405	CLA	MG-NC	2.52	2.12	2.06
24	BC	5511	CLA	CMC-C2C	2.52	1.55	1.50
24	AD	401	CLA	C3B-C2B	2.52	1.49	1.41
24	AB	606	CLA	C1C-NC	2.52	1.42	1.37
32	BB	5603	LMT	O1B-C4'	2.52	1.50	1.43
28	BH	5101	DGD	O6E-C1E	2.51	1.48	1.41
24	AB	602	CLA	O1D-CGD	2.51	1.27	1.21
30	AA	416	SQD	O8-S	2.51	1.56	1.47
24	AB	602	CLA	O2A-CGA	2.51	1.40	1.33
24	AC	507	CLA	CMC-C2C	2.51	1.55	1.50
34	AD	403	PHO	C1C-C2C	2.51	1.53	1.45
24	BB	5611	CLA	C1D-C2D	2.51	1.50	1.45
32	BB	5626	LMT	C4'-C5'	2.51	1.59	1.52
28	BC	5519	DGD	C6A-C5A	-2.50	1.39	1.51
28	BC	5517	DGD	O3G-C1D	2.50	1.44	1.40
24	BB	5610	CLA	MG-NC	2.50	2.12	2.06
28	AC	519	DGD	C6A-C5A	-2.50	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AA	411	DGD	C3G-C2G	2.50	1.58	1.50
24	AB	616	CLA	MG-NB	2.50	2.10	2.05
30	BA	5401	SQD	C18-C17	-2.50	1.39	1.51
24	AC	501	CLA	C1D-C2D	2.50	1.50	1.45
32	BD	5411	LMT	O1B-C1B	2.49	1.48	1.41
32	BB	5603	LMT	C10-C9	-2.49	1.39	1.51
28	AC	518	DGD	C6A-C5A	-2.49	1.39	1.51
28	BC	5518	DGD	C6A-C5A	-2.49	1.39	1.51
32	BB	5604	LMT	C10-C9	-2.49	1.39	1.51
24	BC	5508	CLA	C1B-NB	2.49	1.41	1.37
24	BB	5617	CLA	MG-NB	2.49	2.10	2.05
32	BC	5522	LMT	C4'-C5'	2.49	1.59	1.52
28	BC	5518	DGD	O2G-C1B	2.49	1.41	1.34
32	AI	102	LMT	C10-C9	-2.49	1.39	1.51
32	AB	629	LMT	C10-C9	-2.49	1.39	1.51
24	AB	602	CLA	C3B-C2B	2.49	1.49	1.41
32	BB	5627	LMT	C4'-C5'	2.49	1.59	1.52
28	BC	5518	DGD	CEB-CDB	-2.49	1.39	1.51
24	AC	501	CLA	O1D-CGD	2.49	1.27	1.21
34	BD	5404	PHO	C1C-C2C	2.49	1.53	1.45
34	BD	5403	PHO	C1C-C2C	2.49	1.53	1.45
28	AA	411	DGD	C6A-C5A	-2.48	1.39	1.51
28	AH	101	DGD	C6A-C5A	-2.48	1.39	1.51
28	BH	5101	DGD	C1G-C2G	2.48	1.58	1.50
28	AC	518	DGD	CEB-CDB	-2.48	1.39	1.51
31	AC	520	LMG	O6-C1	2.48	1.48	1.41
31	BM	5102	LMG	O7-C10	2.48	1.41	1.34
28	BA	5412	DGD	C6A-C5A	-2.48	1.39	1.51
24	AC	513	CLA	CHC-C4B	2.48	1.45	1.39
28	BC	5517	DGD	C6A-C5A	-2.48	1.39	1.51
36	AF	101	HEM	C1B-C2B	-2.48	1.39	1.44
24	BC	5504	CLA	O1D-CGD	2.48	1.27	1.21
24	BD	5402	CLA	O1D-CGD	2.48	1.27	1.21
27	AJ	101	BCR	C24-C23	2.48	1.40	1.33
32	AI	103	LMT	C10-C9	-2.48	1.39	1.51
24	BA	5407	CLA	C1C-NC	2.48	1.41	1.37
32	BC	5522	LMT	C10-C9	-2.48	1.39	1.51
28	AC	517	DGD	C6A-C5A	-2.48	1.39	1.51
28	AE	101	DGD	CEB-CDB	-2.48	1.39	1.51
24	BB	5616	CLA	MG-NB	2.48	2.10	2.05
28	BH	5101	DGD	C6A-C5A	-2.47	1.39	1.51
28	AB	628	DGD	C6A-C5A	-2.47	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BE	5102	DGD	CEB-CDB	-2.47	1.39	1.51
32	AB	630	LMT	C10-C9	-2.47	1.39	1.51
32	AB	623	LMT	C10-C9	-2.47	1.39	1.51
31	AA	417	LMG	O7-C8	-2.47	1.40	1.46
24	BC	5502	CLA	C1D-C2D	2.47	1.50	1.45
32	BI	5102	LMT	C10-C9	-2.47	1.39	1.51
28	BB	5602	DGD	C6A-C5A	-2.47	1.39	1.51
24	BC	5512	CLA	C1B-NB	2.47	1.41	1.37
32	AB	624	LMT	C10-C9	-2.47	1.39	1.51
32	BB	5626	LMT	C10-C9	-2.46	1.39	1.51
27	BJ	5101	BCR	C24-C23	2.46	1.40	1.33
30	BF	5102	SQD	C24-C23	2.46	1.57	1.50
32	BM	5101	LMT	C10-C9	-2.46	1.39	1.51
24	AC	508	CLA	C3B-C4B	2.46	1.49	1.42
24	BB	5612	CLA	C1C-NC	2.46	1.41	1.37
32	AM	102	LMT	C10-C9	-2.46	1.39	1.51
28	AE	101	DGD	C6A-C5A	-2.46	1.39	1.51
34	BD	5403	PHO	O2A-CGA	2.46	1.40	1.33
28	BC	5519	DGD	CEB-CDB	-2.46	1.39	1.51
24	AC	513	CLA	C1D-C2D	2.46	1.50	1.45
28	AC	519	DGD	CEB-CDB	-2.46	1.39	1.51
27	AJ	101	BCR	C7-C6	2.46	1.53	1.45
24	AB	613	CLA	C1C-NC	2.46	1.41	1.37
34	BD	5403	PHO	CBD-CGD	2.46	1.55	1.52
31	BD	5408	LMG	O6-C1	2.46	1.48	1.41
24	BC	5508	CLA	C3B-C4B	2.46	1.49	1.42
36	BF	5101	HEM	C1B-C2B	-2.46	1.39	1.44
30	AA	416	SQD	C37-C36	-2.45	1.36	1.51
28	BE	5102	DGD	C6A-C5A	-2.45	1.39	1.51
27	BJ	5101	BCR	C7-C6	2.45	1.53	1.45
28	AE	101	DGD	C3G-C2G	2.45	1.58	1.50
28	AA	411	DGD	C4E-C3E	2.45	1.58	1.52
24	AB	608	CLA	C1D-C2D	2.45	1.50	1.45
24	AB	610	CLA	MG-NB	2.45	2.10	2.05
31	AA	417	LMG	O1-C1	2.45	1.44	1.40
30	AF	102	SQD	C24-C23	2.45	1.57	1.50
24	AC	506	CLA	C1C-NC	2.45	1.41	1.37
34	AD	402	PHO	C1C-C2C	2.45	1.53	1.45
24	AC	513	CLA	CHD-C1D	2.45	1.43	1.38
32	BB	5627	LMT	C10-C9	-2.45	1.39	1.51
36	BV	5201	HEM	C1B-C2B	-2.45	1.39	1.44
24	BB	5612	CLA	C1D-C2D	2.45	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	508	CLA	C3B-C2B	2.45	1.49	1.41
24	AB	603	CLA	C3B-C4B	2.44	1.49	1.42
24	AB	602	CLA	C1D-C2D	2.44	1.50	1.45
24	AD	401	CLA	CHC-C1C	2.44	1.43	1.38
24	AC	509	CLA	O2A-CGA	2.44	1.40	1.33
24	AB	614	CLA	O1D-CGD	2.44	1.27	1.21
31	AC	520	LMG	O1-C1	2.44	1.44	1.40
24	BC	5504	CLA	MG-NC	2.44	2.12	2.06
30	AA	416	SQD	C8-C7	2.44	1.57	1.50
24	AB	605	CLA	C1D-C2D	2.44	1.50	1.45
24	BC	5503	CLA	MG-NA	2.44	2.12	2.06
28	BA	5412	DGD	O3G-C1D	2.44	1.44	1.40
24	BB	5612	CLA	C3B-C2B	2.44	1.49	1.41
27	BJ	5101	BCR	C14-C13	2.43	1.41	1.35
28	BE	5102	DGD	O6E-C5E	2.43	1.50	1.44
24	BA	5405	CLA	MG-NB	2.43	2.10	2.05
27	AD	406	BCR	C5-C6	2.43	1.38	1.34
24	AB	613	CLA	C1D-C2D	2.43	1.50	1.45
24	BC	5502	CLA	MG-NC	2.43	2.12	2.06
24	AA	406	CLA	C1D-C2D	2.43	1.50	1.45
27	BB	5623	BCR	C33-C5	2.43	1.54	1.50
24	AB	610	CLA	O1D-CGD	2.43	1.27	1.21
30	BA	5414	SQD	C34-C33	-2.42	1.36	1.51
24	BB	5612	CLA	MG-NA	2.42	2.12	2.06
32	AB	630	LMT	C4'-C5'	2.42	1.59	1.52
28	AH	101	DGD	C1G-C2G	2.42	1.58	1.50
27	AC	514	BCR	C5-C6	2.42	1.38	1.34
24	AC	504	CLA	C1D-C2D	2.41	1.50	1.45
24	BB	5611	CLA	MG-NB	2.41	2.10	2.05
24	BB	5613	CLA	MG-ND	-2.41	2.01	2.05
32	AB	624	LMT	C4'-C5'	2.41	1.59	1.52
24	AB	604	CLA	O1D-CGD	2.41	1.27	1.21
24	BC	5506	CLA	CBA-CGA	2.41	1.57	1.50
28	BH	5101	DGD	O3G-C1D	2.41	1.44	1.40
28	AC	519	DGD	C4E-C3E	2.41	1.58	1.52
24	BA	5406	CLA	MG-NC	2.41	2.12	2.06
24	AC	506	CLA	CBA-CGA	2.41	1.57	1.50
24	AC	507	CLA	O1D-CGD	2.41	1.27	1.21
30	AB	622	SQD	C44-C45	2.41	1.58	1.50
24	BC	5513	CLA	C1D-C2D	2.41	1.50	1.45
24	AC	511	CLA	C1B-NB	2.40	1.41	1.37
24	BC	5510	CLA	C1C-NC	2.40	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5610	CLA	C1C-NC	2.40	1.41	1.37
24	AC	507	CLA	C3B-C2B	2.40	1.49	1.41
28	BA	5412	DGD	C3G-C2G	2.40	1.58	1.50
24	AA	407	CLA	O2A-CGA	2.40	1.40	1.33
24	AB	614	CLA	C1C-NC	2.40	1.41	1.37
24	BC	5508	CLA	O2A-CGA	2.40	1.40	1.33
30	BA	5401	SQD	O8-S	2.39	1.56	1.47
32	BI	5102	LMT	O5'-C1'	2.39	1.48	1.41
24	BB	5606	CLA	O1D-CGD	2.39	1.27	1.21
34	BD	5404	PHO	C4D-ND	-2.39	1.35	1.38
24	AC	501	CLA	CBA-CGA	2.39	1.57	1.50
31	AD	407	LMG	O7-C8	-2.39	1.41	1.46
24	BB	5617	CLA	MG-ND	-2.39	2.01	2.05
31	BI	5101	LMG	O1-C1	2.39	1.44	1.40
32	BB	5604	LMT	C4'-C5'	2.39	1.59	1.52
27	BB	5623	BCR	C23-C22	-2.39	1.40	1.46
32	AB	623	LMT	O1B-C1B	2.39	1.48	1.41
28	AC	519	DGD	C6E-C5E	2.39	1.59	1.51
24	AC	513	CLA	CHD-C4C	2.39	1.44	1.39
24	AC	511	CLA	CHC-C4B	2.39	1.44	1.39
24	BB	5618	CLA	CHC-C4B	2.39	1.44	1.39
24	AC	503	CLA	C1C-NC	2.39	1.41	1.37
24	AC	511	CLA	CMC-C2C	2.39	1.55	1.50
28	AH	101	DGD	O3G-C1D	2.38	1.44	1.40
24	AC	504	CLA	MG-NC	2.38	2.11	2.06
24	BD	5402	CLA	CHC-C1C	2.38	1.43	1.38
30	AA	413	SQD	C34-C33	-2.38	1.36	1.51
24	AB	611	CLA	C2A-C1A	-2.38	1.46	1.52
35	BD	5406	PL9	C11-C9	2.37	1.56	1.51
24	AA	405	CLA	C3B-C2B	2.37	1.49	1.41
24	AC	508	CLA	CHC-C1C	2.37	1.43	1.38
34	AD	403	PHO	O1D-CGD	2.37	1.27	1.21
32	AD	409	LMT	C4'-C5'	2.37	1.59	1.52
24	AC	512	CLA	C1B-NB	2.37	1.41	1.37
27	BK	5102	BCR	C38-C26	2.37	1.54	1.50
24	BC	5505	CLA	MG-NB	2.37	2.10	2.05
24	AB	610	CLA	MG-NC	2.37	2.11	2.06
24	BC	5504	CLA	C5-C3	2.37	1.56	1.51
24	AA	406	CLA	MG-ND	-2.36	2.01	2.05
24	AB	606	CLA	CMC-C2C	2.36	1.55	1.50
27	BC	5514	BCR	C5-C6	2.36	1.38	1.34
34	AD	403	PHO	C4C-C3C	2.36	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5612	CLA	C3B-C4B	2.36	1.49	1.42
28	AC	519	DGD	O5D-C1E	2.35	1.44	1.40
27	BD	5407	BCR	C38-C26	2.35	1.54	1.50
24	BD	5405	CLA	C1C-NC	2.35	1.41	1.37
24	AC	503	CLA	C1B-NB	2.35	1.41	1.37
30	AA	413	SQD	O6-C1	2.35	1.44	1.40
24	AC	504	CLA	C5-C3	2.35	1.56	1.51
24	BA	5408	CLA	O2A-CGA	2.35	1.40	1.33
24	AC	504	CLA	O1D-CGD	2.35	1.27	1.21
24	AC	512	CLA	O2A-CGA	2.35	1.40	1.33
24	AC	505	CLA	O1D-CGD	2.35	1.27	1.21
24	BC	5507	CLA	C1C-NC	2.35	1.41	1.37
31	BA	5402	LMG	O7-C8	-2.35	1.41	1.46
24	AB	607	CLA	MG-NB	2.34	2.10	2.05
34	BD	5404	PHO	CAC-C3C	2.34	1.56	1.51
24	BC	5501	CLA	C1C-NC	2.34	1.41	1.37
28	BC	5519	DGD	C6E-C5E	2.33	1.59	1.51
31	AD	408	LMG	O7-C8	-2.33	1.41	1.46
24	AC	508	CLA	O1D-CGD	2.33	1.27	1.21
30	BA	5401	SQD	C37-C36	-2.33	1.37	1.51
32	BC	5522	LMT	O1'-C1'	2.33	1.44	1.40
30	BA	5414	SQD	C21-C20	-2.33	1.37	1.51
32	BB	5604	LMT	O5'-C1'	2.33	1.47	1.41
24	AB	613	CLA	MG-NC	2.33	2.11	2.06
24	AD	401	CLA	MG-NB	2.33	2.10	2.05
27	BX	5101	BCR	C38-C26	2.33	1.54	1.50
24	AB	614	CLA	C4B-NB	2.33	1.40	1.37
27	AD	406	BCR	C38-C26	2.33	1.54	1.50
34	AD	403	PHO	O2A-CGA	2.33	1.40	1.33
36	AF	101	HEM	CMA-C3A	2.33	1.55	1.50
24	BA	5408	CLA	CHC-C1C	2.32	1.43	1.38
24	AC	506	CLA	C3B-C4B	2.32	1.49	1.42
24	BA	5408	CLA	MG-NA	2.32	2.11	2.06
30	AA	416	SQD	O6-C44	-2.32	1.39	1.43
24	AD	404	CLA	CAC-C3C	2.32	1.57	1.51
24	AC	504	CLA	CHC-C1C	2.32	1.43	1.38
24	BB	5612	CLA	MG-NC	2.32	2.11	2.06
28	BE	5102	DGD	C1G-C2G	2.32	1.58	1.50
24	AB	601	CLA	CBD-CGD	2.32	1.59	1.52
24	AB	608	CLA	C2A-C1A	-2.31	1.47	1.52
24	AC	503	CLA	C1D-C2D	2.31	1.49	1.45
24	AB	601	CLA	MG-ND	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5509	CLA	CHC-C1C	2.31	1.43	1.38
36	AF	101	HEM	CBA-CGA	2.31	1.55	1.50
24	BB	5616	CLA	CHC-C1C	2.31	1.43	1.38
27	BJ	5101	BCR	C4-C5	2.30	1.55	1.51
24	BC	5504	CLA	C1D-C2D	2.30	1.49	1.45
28	BC	5517	DGD	O6D-C5D	2.30	1.50	1.44
24	BB	5605	CLA	MG-NB	2.30	2.10	2.05
24	AB	606	CLA	C3B-C2B	2.30	1.48	1.41
27	AT	101	BCR	C26-C25	2.30	1.38	1.34
24	AB	612	CLA	CHD-C1D	2.30	1.42	1.38
32	BB	5627	LMT	O5'-C1'	2.30	1.47	1.41
31	AI	101	LMG	O1-C1	2.30	1.44	1.40
30	AA	413	SQD	C21-C20	-2.30	1.37	1.51
34	BD	5404	PHO	O1D-CGD	2.30	1.27	1.21
24	AB	613	CLA	CMC-C2C	2.30	1.55	1.50
30	BF	5102	SQD	C8-C7	2.30	1.57	1.50
24	BC	5511	CLA	C5-C3	2.29	1.56	1.51
30	BB	5601	SQD	C24-C23	2.29	1.57	1.50
24	BB	5620	CLA	C5-C3	2.29	1.56	1.51
24	AB	605	CLA	CHC-C1C	2.29	1.43	1.38
34	BD	5403	PHO	C3D-CAD	-2.29	1.43	1.47
30	BF	5102	SQD	C18-C17	-2.29	1.37	1.51
28	AC	519	DGD	C1E-C2E	-2.29	1.45	1.52
24	BB	5605	CLA	C1C-NC	2.29	1.41	1.37
24	BC	5508	CLA	C1C-NC	2.29	1.41	1.37
24	BB	5605	CLA	CAC-C3C	2.29	1.56	1.51
28	BC	5519	DGD	O3E-C3E	-2.29	1.37	1.43
24	BB	5605	CLA	CBD-CHA	2.28	1.63	1.51
24	BB	5611	CLA	C3B-C2B	2.28	1.48	1.41
24	BB	5618	CLA	C4B-NB	2.28	1.40	1.37
24	AB	607	CLA	CHC-C1C	2.28	1.43	1.38
24	AA	406	CLA	C1C-NC	2.28	1.41	1.37
34	AD	402	PHO	CBD-CGD	2.28	1.55	1.52
24	BC	5506	CLA	C3B-C4B	2.27	1.49	1.42
34	BD	5403	PHO	C4C-C3C	2.27	1.52	1.45
24	BC	5501	CLA	C1B-NB	2.27	1.40	1.37
34	AD	402	PHO	C3D-CAD	-2.27	1.43	1.47
24	BC	5511	CLA	C4B-NB	2.27	1.40	1.37
24	BB	5607	CLA	C1D-C2D	2.27	1.49	1.45
24	AB	609	CLA	C1B-NB	2.27	1.40	1.37
24	AB	601	CLA	CAC-C3C	2.27	1.56	1.51
28	AE	101	DGD	C1G-C2G	2.27	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	610	CLA	C1D-C2D	2.27	1.49	1.45
31	BM	5102	LMG	O6-C1	2.27	1.47	1.41
24	BB	5613	CLA	C1D-C2D	2.27	1.49	1.45
27	AA	410	BCR	C5-C6	2.27	1.38	1.34
24	AC	508	CLA	C1B-NB	2.27	1.40	1.37
28	AC	518	DGD	O2G-C1B	2.27	1.40	1.34
27	AJ	101	BCR	C4-C5	2.26	1.55	1.51
24	BB	5618	CLA	C1B-NB	2.26	1.40	1.37
24	BC	5511	CLA	CHD-C1D	2.26	1.42	1.38
32	AB	623	LMT	C4'-C5'	2.25	1.59	1.52
31	BC	5520	LMG	O7-C8	2.25	1.51	1.46
24	BB	5614	CLA	MG-ND	-2.25	2.01	2.05
32	AI	102	LMT	O5'-C1'	2.25	1.47	1.41
24	BB	5609	CLA	C1C-NC	2.24	1.41	1.37
24	BC	5512	CLA	C1D-C2D	2.24	1.49	1.45
24	AB	616	CLA	C5-C3	2.24	1.55	1.51
24	AC	511	CLA	CHD-C4C	2.24	1.44	1.39
27	AC	514	BCR	C23-C22	-2.24	1.41	1.46
24	BC	5510	CLA	C1D-C2D	2.24	1.49	1.45
24	BC	5506	CLA	CMD-C2D	2.24	1.55	1.50
24	BB	5606	CLA	C1D-C2D	2.23	1.49	1.45
24	BB	5613	CLA	CBA-CGA	2.23	1.57	1.50
27	AB	618	BCR	C33-C5	2.23	1.54	1.50
32	AI	103	LMT	O1B-C1B	2.23	1.48	1.41
24	BC	5507	CLA	MG-NB	2.23	2.10	2.05
30	BA	5401	SQD	O6-C44	-2.23	1.39	1.43
24	BC	5509	CLA	MG-ND	-2.23	2.01	2.05
32	AB	629	LMT	O1B-C4'	2.23	1.49	1.43
24	AC	506	CLA	C1D-C2D	2.23	1.49	1.45
24	BA	5407	CLA	CHC-C1C	2.23	1.42	1.38
36	AV	201	HEM	CMA-C3A	2.23	1.55	1.50
31	AC	520	LMG	O7-C8	2.22	1.51	1.46
32	BD	5411	LMT	O5'-C1'	2.22	1.47	1.41
27	AB	619	BCR	C33-C5	2.22	1.54	1.50
30	AF	102	SQD	C18-C17	-2.22	1.37	1.51
31	AM	101	LMG	O7-C10	2.22	1.40	1.34
31	BD	5410	LMG	O7-C8	-2.22	1.41	1.46
24	BB	5614	CLA	O1D-CGD	2.22	1.26	1.21
31	AA	417	LMG	O8-C9	2.22	1.50	1.45
24	AC	507	CLA	C1C-NC	2.22	1.41	1.37
24	BC	5511	CLA	C1D-C2D	2.21	1.49	1.45
24	BB	5611	CLA	C1C-NC	2.21	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BA	5414	SQD	O6-C1	2.21	1.43	1.40
27	AC	515	BCR	C19-C18	-2.21	1.41	1.46
24	BC	5513	CLA	CMD-C2D	2.21	1.55	1.50
31	AA	417	LMG	C4-C5	2.21	1.57	1.53
36	AF	101	HEM	CMD-C2D	2.21	1.55	1.50
24	BB	5609	CLA	C1D-C2D	2.21	1.49	1.45
24	BC	5513	CLA	CAC-C3C	2.21	1.56	1.51
27	AC	516	BCR	C33-C5	2.20	1.54	1.50
24	BB	5620	CLA	C1C-NC	2.20	1.41	1.37
24	AC	504	CLA	C1C-NC	2.20	1.41	1.37
24	AC	510	CLA	C1D-C2D	2.20	1.49	1.45
24	BB	5611	CLA	O1D-CGD	2.20	1.26	1.21
24	BC	5505	CLA	CBD-CHA	2.20	1.62	1.51
32	BB	5626	LMT	O1B-C1B	2.20	1.48	1.41
24	BB	5605	CLA	CBD-CGD	2.20	1.59	1.52
30	AF	102	SQD	O8-S	2.20	1.55	1.47
24	AC	505	CLA	MG-NB	2.19	2.10	2.05
24	AA	406	CLA	O2A-CGA	2.19	1.39	1.33
32	AM	102	LMT	O5'-C1'	2.19	1.47	1.41
24	BB	5614	CLA	C1C-NC	2.19	1.41	1.37
31	AJ	102	LMG	O6-C1	2.19	1.47	1.41
24	AC	505	CLA	CBD-CHA	2.19	1.62	1.51
24	AB	609	CLA	C1D-C2D	2.19	1.49	1.45
30	AA	416	SQD	C38-C37	-2.18	1.34	1.50
24	BB	5608	CLA	C2A-C1A	-2.18	1.47	1.52
24	AA	406	CLA	O1D-CGD	2.18	1.26	1.21
24	BB	5615	CLA	C1D-C2D	2.18	1.49	1.45
24	AC	507	CLA	MG-NB	2.18	2.10	2.05
34	BD	5404	PHO	C4C-C3C	2.18	1.52	1.45
32	AM	102	LMT	O1B-C1B	2.18	1.47	1.41
24	BC	5503	CLA	C1B-NB	2.18	1.40	1.37
24	BB	5607	CLA	C3B-C4B	2.18	1.49	1.42
24	BB	5616	CLA	MG-ND	-2.18	2.01	2.05
32	AI	103	LMT	C4'-C5'	2.18	1.58	1.52
24	AB	611	CLA	MG-NA	2.17	2.11	2.06
30	AF	102	SQD	C8-C7	2.17	1.57	1.50
24	AC	506	CLA	CMD-C2D	2.17	1.55	1.50
24	BB	5605	CLA	MG-ND	-2.17	2.01	2.05
27	AA	410	BCR	C19-C18	-2.17	1.41	1.46
24	AB	601	CLA	CBD-CHA	2.17	1.62	1.51
24	AB	611	CLA	C1C-NC	2.17	1.41	1.37
28	BE	5102	DGD	O6D-C5D	2.17	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5611	CLA	CBD-CHA	2.16	1.62	1.51
36	BV	5201	HEM	CMD-C2D	2.16	1.55	1.50
24	BB	5618	CLA	C1C-NC	2.16	1.41	1.37
36	BF	5101	HEM	CAD-C3D	-2.16	1.45	1.51
24	BB	5611	CLA	MG-NC	2.16	2.11	2.06
24	BA	5406	CLA	C1B-NB	2.16	1.40	1.37
27	AJ	101	BCR	C10-C9	2.15	1.40	1.35
24	BB	5609	CLA	MG-NC	2.15	2.11	2.06
24	BB	5608	CLA	C1D-C2D	2.15	1.49	1.45
24	AD	401	CLA	O2A-CGA	2.14	1.39	1.33
30	AB	627	SQD	C24-C23	2.14	1.56	1.50
24	BC	5509	CLA	C1C-NC	2.14	1.41	1.37
32	AI	102	LMT	O1B-C1B	2.14	1.47	1.41
24	AC	509	CLA	MG-NB	2.14	2.10	2.05
24	BC	5507	CLA	CMD-C2D	2.14	1.55	1.50
24	BA	5406	CLA	MG-NB	2.14	2.10	2.05
31	AC	520	LMG	O7-C10	2.14	1.40	1.34
27	BC	5515	BCR	C38-C26	2.14	1.54	1.50
24	BC	5502	CLA	CMD-C2D	2.14	1.55	1.50
30	BB	5625	SQD	C44-C45	2.14	1.57	1.50
24	AC	502	CLA	CMC-C2C	2.14	1.55	1.50
24	BC	5506	CLA	C1D-C2D	2.13	1.49	1.45
24	AB	604	CLA	CHC-C1C	2.13	1.42	1.38
24	AC	511	CLA	C1D-C2D	2.13	1.49	1.45
24	AA	404	CLA	MG-NB	2.13	2.10	2.05
32	BC	5522	LMT	O1B-C1B	2.13	1.47	1.41
28	AC	519	DGD	O4D-C4D	2.13	1.48	1.43
32	BI	5102	LMT	O1B-C4'	2.13	1.49	1.43
24	BA	5407	CLA	MG-ND	-2.12	2.01	2.05
24	AB	611	CLA	C1D-C2D	2.12	1.49	1.45
24	BC	5505	CLA	CAC-C3C	2.12	1.56	1.51
24	AC	511	CLA	C4B-NB	2.12	1.40	1.37
24	BA	5405	CLA	CHC-C1C	2.12	1.42	1.38
28	BB	5602	DGD	C3E-C2E	2.12	1.57	1.52
36	AF	101	HEM	CAA-C2A	2.12	1.56	1.51
24	AB	614	CLA	C3B-C4B	2.11	1.48	1.42
24	BC	5501	CLA	C5-C3	2.11	1.55	1.51
28	AE	101	DGD	C4E-C5E	2.11	1.57	1.53
36	BV	5201	HEM	C4A-NA	-2.11	1.35	1.39
24	AB	614	CLA	CAA-C2A	-2.11	1.50	1.54
30	BA	5401	SQD	C21-C20	-2.11	1.38	1.51
30	AB	627	SQD	C22-C21	-2.11	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	601	CLA	CBA-CGA	2.11	1.56	1.50
30	BA	5414	SQD	C22-C21	-2.11	1.35	1.50
28	AH	101	DGD	O6D-C5D	2.11	1.49	1.44
24	AB	606	CLA	OBD-CAD	2.11	1.26	1.22
24	BB	5616	CLA	CHD-C1D	2.11	1.42	1.38
34	AD	403	PHO	CAC-C3C	2.11	1.55	1.51
24	BC	5511	CLA	C3B-C4B	2.11	1.48	1.42
24	BB	5610	CLA	CBA-CGA	2.11	1.56	1.50
24	BB	5615	CLA	C1C-NC	2.11	1.41	1.37
31	BD	5409	LMG	O7-C8	-2.11	1.41	1.46
24	AC	511	CLA	C5-C3	2.11	1.55	1.51
36	BF	5101	HEM	CMA-C3A	2.11	1.55	1.50
27	BD	5407	BCR	C23-C22	-2.11	1.41	1.46
36	BV	5201	HEM	CBD-CAD	2.10	1.59	1.51
24	AA	405	CLA	C3D-C2D	-2.10	1.33	1.39
30	BB	5601	SQD	C22-C21	-2.10	1.35	1.50
27	BA	5411	BCR	C19-C18	-2.10	1.41	1.46
24	BB	5612	CLA	C2A-C1A	-2.10	1.47	1.52
31	BD	5410	LMG	O1-C1	2.10	1.43	1.40
24	AB	605	CLA	C5-C3	2.10	1.55	1.51
24	AC	501	CLA	C1C-NC	2.10	1.41	1.37
24	BC	5512	CLA	CAC-C3C	2.10	1.56	1.51
24	BC	5506	CLA	MG-ND	-2.10	2.01	2.05
24	BB	5609	CLA	CAA-C2A	-2.10	1.50	1.54
24	BC	5506	CLA	MG-NA	2.10	2.11	2.06
24	BC	5509	CLA	CHC-C4B	2.10	1.44	1.39
24	BC	5508	CLA	MG-NA	2.10	2.11	2.06
24	AB	614	CLA	C1D-C2D	2.10	1.49	1.45
28	BE	5102	DGD	O2G-C1B	2.10	1.40	1.34
24	AB	616	CLA	MG-ND	-2.09	2.01	2.05
24	BB	5613	CLA	C1C-NC	2.09	1.41	1.37
24	AC	505	CLA	MG-ND	-2.09	2.01	2.05
24	BB	5613	CLA	CMD-C2D	2.09	1.55	1.50
24	AB	601	CLA	CMD-C2D	2.09	1.55	1.50
31	AD	408	LMG	O3-C3	-2.08	1.37	1.43
24	AB	608	CLA	C5-C3	2.08	1.55	1.51
30	AA	416	SQD	C21-C20	-2.08	1.38	1.51
27	AT	101	BCR	C19-C18	-2.08	1.41	1.46
24	BC	5513	CLA	C5-C3	2.08	1.55	1.51
28	BC	5517	DGD	O6E-C1E	2.08	1.47	1.41
30	AA	413	SQD	C22-C21	-2.08	1.35	1.50
24	BC	5505	CLA	MG-ND	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5510	CLA	CMD-C2D	2.08	1.55	1.50
24	AC	512	CLA	C1D-C2D	2.08	1.49	1.45
35	BD	5406	PL9	C47-C48	2.08	1.56	1.50
24	BC	5511	CLA	CBA-CGA	2.07	1.56	1.50
24	AC	508	CLA	CAC-C3C	2.07	1.56	1.51
27	BB	5622	BCR	C33-C5	2.07	1.54	1.50
30	BA	5401	SQD	C38-C37	-2.07	1.35	1.50
35	BD	5406	PL9	C10-C9	2.07	1.55	1.50
27	AB	617	BCR	C19-C18	-2.07	1.41	1.46
28	BA	5412	DGD	C1G-C2G	2.07	1.57	1.50
31	AC	520	LMG	C4-C5	2.07	1.57	1.53
24	AD	404	CLA	CBA-CGA	2.07	1.56	1.50
24	AB	610	CLA	O2A-CGA	2.07	1.39	1.33
28	BE	5102	DGD	C4D-C5D	2.07	1.57	1.53
24	AC	505	CLA	C1C-NC	2.07	1.41	1.37
24	BC	5501	CLA	C1D-C2D	2.07	1.49	1.45
24	AA	404	CLA	MG-ND	-2.07	2.01	2.05
24	AB	609	CLA	CBA-CGA	2.06	1.56	1.50
24	AB	612	CLA	CHC-C4B	2.06	1.44	1.39
24	BB	5616	CLA	CHD-C4C	2.06	1.43	1.39
24	AB	603	CLA	CHC-C4B	2.06	1.44	1.39
32	BM	5101	LMT	O5'-C1'	2.06	1.47	1.41
30	BB	5625	SQD	C24-C23	2.06	1.56	1.50
24	AA	404	CLA	C1C-NC	2.06	1.41	1.37
24	AC	508	CLA	C1C-NC	2.06	1.41	1.37
24	BB	5616	CLA	C5-C3	2.06	1.55	1.51
30	AB	622	SQD	C24-C23	2.06	1.56	1.50
36	BV	5201	HEM	CHC-C1C	2.06	1.42	1.38
32	AM	102	LMT	O5'-C5'	2.06	1.49	1.44
32	BD	5411	LMT	C3'-C4'	2.06	1.57	1.52
24	BA	5408	CLA	CBD-CHA	2.06	1.61	1.51
24	AB	612	CLA	MG-ND	-2.05	2.01	2.05
24	AB	605	CLA	C3B-C4B	2.05	1.48	1.42
24	AC	502	CLA	MG-ND	-2.05	2.01	2.05
24	AA	404	CLA	CHC-C1C	2.05	1.42	1.38
24	AB	608	CLA	C3B-C4B	2.05	1.48	1.42
24	BA	5407	CLA	C1B-NB	2.05	1.40	1.37
32	BB	5626	LMT	O5B-C5B	2.05	1.49	1.44
24	AD	401	CLA	C3B-C4B	2.05	1.48	1.42
24	BB	5607	CLA	CHB-C1B	-2.05	1.34	1.39
32	BB	5627	LMT	O1B-C4'	2.05	1.49	1.43
27	BK	5102	BCR	C19-C18	-2.04	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	614	CLA	C5-C3	2.04	1.55	1.51
24	BB	5618	CLA	C1D-C2D	2.04	1.49	1.45
31	BI	5101	LMG	C4-C5	2.04	1.57	1.53
24	AC	506	CLA	CAC-C3C	2.04	1.56	1.51
24	AB	603	CLA	C1D-C2D	2.04	1.49	1.45
24	BB	5607	CLA	CHC-C4B	2.04	1.44	1.39
27	BT	5101	BCR	C19-C18	-2.04	1.41	1.46
30	BF	5102	SQD	C19-C18	-2.04	1.35	1.50
24	BB	5615	CLA	C1B-NB	2.04	1.40	1.37
24	AB	605	CLA	CAA-C2A	-2.04	1.50	1.54
28	AB	628	DGD	O6D-C5D	2.04	1.49	1.44
36	BF	5101	HEM	CMD-C2D	2.04	1.54	1.50
30	BB	5625	SQD	C8-C7	2.04	1.56	1.50
24	BB	5618	CLA	CHD-C4C	2.03	1.43	1.39
24	BC	5509	CLA	C4B-NB	2.03	1.40	1.37
24	BA	5406	CLA	C3D-C2D	-2.03	1.33	1.39
24	AA	405	CLA	CHC-C1C	2.03	1.42	1.38
24	BB	5616	CLA	CHC-C4B	2.03	1.44	1.39
30	AF	102	SQD	C32-C31	-2.03	1.35	1.50
24	AB	606	CLA	CBA-CGA	2.03	1.56	1.50
32	AI	103	LMT	O1'-C1'	2.03	1.43	1.40
24	AC	513	CLA	CMD-C2D	2.03	1.54	1.50
24	BB	5609	CLA	C3B-C4B	2.03	1.48	1.42
28	AC	519	DGD	C3E-C2E	2.03	1.57	1.52
24	AC	510	CLA	C1B-NB	2.03	1.40	1.37
28	AA	411	DGD	C4D-C3D	-2.03	1.47	1.52
24	AC	512	CLA	CAC-C3C	2.03	1.56	1.51
30	AF	102	SQD	C19-C18	-2.03	1.35	1.50
24	BC	5510	CLA	MG-NB	2.03	2.09	2.05
32	AD	409	LMT	O5'-C1'	2.02	1.47	1.41
35	AD	405	PL9	C11-C9	2.02	1.55	1.51
24	BA	5407	CLA	C3B-C4B	2.02	1.48	1.42
24	BC	5508	CLA	C1D-C2D	2.02	1.49	1.45
36	BV	5201	HEM	CAB-C3B	-2.02	1.42	1.47
28	BC	5517	DGD	O3G-C3G	-2.02	1.40	1.43
32	BB	5604	LMT	O5B-C5B	2.02	1.49	1.44
24	AC	512	CLA	C3B-C4B	2.02	1.48	1.42
24	BC	5501	CLA	CBD-CHA	2.02	1.61	1.51
28	AC	517	DGD	C2B-C1B	-2.02	1.44	1.50
31	AI	101	LMG	C4-C3	2.02	1.57	1.52
27	AK	102	BCR	C19-C18	-2.02	1.41	1.46
24	AB	604	CLA	C1D-C2D	2.02	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	405	CLA	OBD-CAD	2.02	1.26	1.22
35	AD	405	PL9	C47-C48	2.01	1.56	1.50
24	AC	505	CLA	CAC-C3C	2.01	1.56	1.51
24	AC	513	CLA	C5-C3	2.01	1.55	1.51
30	AB	627	SQD	C8-C7	2.01	1.56	1.50
27	AC	516	BCR	C40-C30	-2.01	1.50	1.53
28	BC	5519	DGD	O3G-C3G	2.01	1.47	1.43
24	BC	5509	CLA	C3B-C4B	2.01	1.48	1.42
30	BF	5102	SQD	C32-C31	-2.01	1.36	1.50
24	AA	405	CLA	C1D-C2D	2.01	1.49	1.45
24	BC	5509	CLA	C1D-C2D	2.01	1.49	1.45
27	AA	410	BCR	C23-C22	-2.01	1.41	1.46
32	AB	624	LMT	C1'-C2'	2.01	1.58	1.52
24	BC	5513	CLA	C4-C3	2.01	1.55	1.50
24	AC	507	CLA	C1D-C2D	2.00	1.49	1.45
24	AB	613	CLA	C3B-C2B	2.00	1.47	1.41
24	BB	5616	CLA	C1D-C2D	2.00	1.49	1.45
24	BB	5619	CLA	C1C-NC	2.00	1.41	1.37
36	BV	5201	HEM	C2A-C3A	2.00	1.44	1.38
30	AA	413	SQD	C35-C34	-2.00	1.36	1.50
24	AB	615	CLA	CBD-CHA	2.00	1.61	1.51
31	AA	414	LMG	O8-C9	2.00	1.49	1.45

All (2556) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	601	CLA	C4A-NA-C1A	14.17	113.14	106.68
24	BB	5605	CLA	C4A-NA-C1A	13.73	112.94	106.68
24	AC	512	CLA	C4A-NA-C1A	13.38	112.78	106.68
24	BC	5512	CLA	C4A-NA-C1A	13.37	112.78	106.68
24	BB	5619	CLA	C4A-NA-C1A	13.28	112.74	106.68
24	BC	5501	CLA	C4A-NA-C1A	13.08	112.65	106.68
24	BC	5508	CLA	C4A-NA-C1A	12.97	112.59	106.68
24	BC	5502	CLA	C4A-NA-C1A	12.96	112.59	106.68
24	AB	615	CLA	C4A-NA-C1A	12.75	112.50	106.68
24	AC	501	CLA	C4A-NA-C1A	12.63	112.44	106.68
24	BD	5405	CLA	C4A-NA-C1A	12.62	112.44	106.68
24	AC	503	CLA	C4A-NA-C1A	12.53	112.40	106.68
24	AB	616	CLA	C4A-NA-C1A	12.47	112.37	106.68
24	AD	404	CLA	C4A-NA-C1A	12.45	112.36	106.68
24	AC	507	CLA	C4A-NA-C1A	12.44	112.36	106.68
24	BB	5620	CLA	C4A-NA-C1A	12.44	112.35	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5507	CLA	C4A-NA-C1A	12.26	112.27	106.68
24	BC	5505	CLA	C4A-NA-C1A	12.20	112.24	106.68
24	AA	407	CLA	C4A-NA-C1A	12.13	112.21	106.68
24	AC	505	CLA	C4A-NA-C1A	11.99	112.15	106.68
24	BB	5606	CLA	C4A-NA-C1A	11.96	112.13	106.68
24	BC	5510	CLA	C4A-NA-C1A	11.95	112.13	106.68
24	AC	510	CLA	C4A-NA-C1A	11.90	112.11	106.68
24	BC	5509	CLA	C4A-NA-C1A	11.88	112.10	106.68
24	BC	5503	CLA	C4A-NA-C1A	11.87	112.09	106.68
24	BC	5506	CLA	C4A-NA-C1A	11.85	112.08	106.68
24	AC	502	CLA	C4A-NA-C1A	11.84	112.08	106.68
24	AC	508	CLA	C4A-NA-C1A	11.81	112.07	106.68
24	AC	509	CLA	C4A-NA-C1A	11.70	112.02	106.68
24	BB	5610	CLA	C4A-NA-C1A	11.65	112.00	106.68
24	AC	506	CLA	C4A-NA-C1A	11.64	111.99	106.68
24	BB	5608	CLA	C4A-NA-C1A	11.64	111.99	106.68
24	AB	611	CLA	C4A-NA-C1A	11.64	111.99	106.68
24	AB	602	CLA	C4A-NA-C1A	11.62	111.98	106.68
24	BB	5612	CLA	C4A-NA-C1A	11.60	111.97	106.68
24	BB	5615	CLA	C4A-NA-C1A	11.58	111.96	106.68
24	AB	608	CLA	C4A-NA-C1A	11.54	111.95	106.68
24	AB	606	CLA	C4A-NA-C1A	11.51	111.93	106.68
24	AB	610	CLA	C4A-NA-C1A	11.51	111.93	106.68
28	AC	518	DGD	O5D-C1E-C2E	11.51	125.75	108.27
24	AD	401	CLA	C4A-NA-C1A	11.47	111.91	106.68
24	BB	5614	CLA	C4A-NA-C1A	11.47	111.91	106.68
24	BD	5402	CLA	C4A-NA-C1A	11.43	111.89	106.68
24	BA	5408	CLA	C4A-NA-C1A	11.40	111.88	106.68
24	AB	613	CLA	C4A-NA-C1A	11.37	111.86	106.68
24	BB	5617	CLA	C4A-NA-C1A	11.33	111.85	106.68
28	BC	5518	DGD	O5D-C1E-C2E	11.30	125.43	108.27
24	AB	614	CLA	C4A-NA-C1A	11.26	111.81	106.68
24	BB	5611	CLA	C4A-NA-C1A	11.11	111.75	106.68
24	AB	604	CLA	C4A-NA-C1A	11.08	111.73	106.68
24	BC	5511	CLA	C4A-NA-C1A	11.03	111.71	106.68
24	AC	504	CLA	C4A-NA-C1A	11.00	111.70	106.68
24	BB	5618	CLA	C4A-NA-C1A	10.97	111.68	106.68
24	BC	5504	CLA	C4A-NA-C1A	10.96	111.68	106.68
24	AB	607	CLA	C4A-NA-C1A	10.95	111.67	106.68
24	BB	5613	CLA	C4A-NA-C1A	10.84	111.62	106.68
24	AB	609	CLA	C4A-NA-C1A	10.84	111.62	106.68
24	BA	5407	CLA	C4A-NA-C1A	10.83	111.62	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	5406	CLA	C4A-NA-C1A	10.82	111.61	106.68
24	AC	511	CLA	C4A-NA-C1A	10.76	111.59	106.68
24	BB	5609	CLA	C4A-NA-C1A	10.69	111.56	106.68
24	AB	605	CLA	C4A-NA-C1A	10.64	111.53	106.68
24	BB	5616	CLA	C4A-NA-C1A	10.61	111.52	106.68
24	BC	5513	CLA	C4A-NA-C1A	10.48	111.46	106.68
36	BF	5101	HEM	CMA-C3A-C4A	10.47	141.36	125.42
24	AA	405	CLA	C4A-NA-C1A	10.38	111.41	106.68
36	AF	101	HEM	CMA-C3A-C4A	10.35	141.18	125.42
27	BJ	5101	BCR	C32-C1-C6	-10.29	94.11	110.24
27	AJ	101	BCR	C32-C1-C6	-10.23	94.20	110.24
24	AB	603	CLA	C4A-NA-C1A	10.17	111.32	106.68
27	BJ	5101	BCR	C32-C1-C31	-10.13	79.64	108.63
24	AC	513	CLA	C4A-NA-C1A	10.10	111.29	106.68
27	AJ	101	BCR	C32-C1-C31	-10.08	79.78	108.63
24	BB	5607	CLA	C4A-NA-C1A	10.00	111.24	106.68
24	AB	612	CLA	C4A-NA-C1A	9.96	111.22	106.68
24	AA	406	CLA	C4A-NA-C1A	9.92	111.21	106.68
36	AV	201	HEM	CMA-C3A-C4A	9.92	140.52	125.42
36	BV	5201	HEM	CMA-C3A-C4A	9.90	140.50	125.42
24	AC	503	CLA	C1-C2-C3	-9.84	110.08	126.20
28	BB	5602	DGD	C2G-O2G-C1B	9.79	141.23	117.80
28	AC	519	DGD	O5D-C6D-C5D	9.77	131.44	109.42
24	BA	5405	CLA	C4A-NA-C1A	9.76	111.13	106.68
28	BC	5519	DGD	O5D-C6D-C5D	9.71	131.30	109.42
25	AA	408	MST	C2-N1-C6	9.70	120.12	113.42
31	AJ	102	LMG	C8-O7-C10	9.69	140.99	117.80
24	BC	5503	CLA	C1-C2-C3	-9.65	110.38	126.20
24	AA	404	CLA	C4A-NA-C1A	9.62	111.07	106.68
25	BA	5409	MST	C2-N1-C6	9.61	120.06	113.42
28	AC	519	DGD	C3G-O3G-C1D	-9.58	93.25	113.80
28	AB	628	DGD	C2G-O2G-C1B	9.56	140.68	117.80
28	BC	5519	DGD	O5D-C1E-C2E	9.50	122.70	108.27
31	BD	5408	LMG	C8-O7-C10	9.47	140.46	117.80
28	BC	5519	DGD	C3G-O3G-C1D	-9.42	93.61	113.80
28	AC	519	DGD	O5D-C1E-C2E	9.34	122.46	108.27
28	BC	5517	DGD	C2G-O2G-C1B	9.32	140.10	117.80
28	BA	5412	DGD	O1G-C1G-C2G	9.21	134.96	108.40
25	AA	408	MST	C2-N3-C4	9.20	119.78	113.42
28	AA	411	DGD	O1G-C1G-C2G	9.20	134.92	108.40
24	AB	611	CLA	C1-C2-C3	-9.13	111.24	126.20
24	BB	5615	CLA	C1-C2-C3	-9.12	111.26	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AC	517	DGD	C2G-O2G-C1B	9.09	139.56	117.80
30	AA	413	SQD	O5-C1-O6	9.08	131.51	110.04
30	AA	416	SQD	O5-C1-O6	9.03	131.39	110.04
30	BA	5401	SQD	O5-C1-O6	8.99	131.28	110.04
30	BA	5414	SQD	O5-C1-O6	8.96	131.22	110.04
35	AD	405	PL9	C7-C3-C4	8.90	124.24	116.91
25	BA	5409	MST	C2-N3-C4	8.89	119.56	113.42
24	BC	5501	CLA	C1-C2-C3	-8.88	111.64	126.20
24	BB	5619	CLA	C1-C2-C3	-8.86	111.68	126.20
28	BA	5412	DGD	O5D-C1E-C2E	8.86	121.73	108.27
24	BA	5405	CLA	C1-C2-C3	-8.83	111.74	126.20
24	AC	501	CLA	C1-C2-C3	-8.81	111.77	126.20
28	AA	411	DGD	O5D-C6D-C5D	8.77	129.19	109.42
30	BF	5102	SQD	O5-C1-O6	8.77	130.76	110.04
24	AB	615	CLA	C1-C2-C3	-8.77	111.83	126.20
24	BB	5608	CLA	C1-C2-C3	-8.75	111.86	126.20
28	AA	411	DGD	C6D-C5D-C4D	-8.75	93.70	112.07
28	BA	5412	DGD	O5D-C6D-C5D	8.74	129.13	109.42
35	BD	5406	PL9	C7-C3-C4	8.74	124.11	116.91
28	AC	519	DGD	O6D-C5D-C6D	8.73	124.01	106.69
30	AF	102	SQD	O5-C1-O6	8.73	130.67	110.04
28	BA	5412	DGD	O6D-C5D-C6D	8.67	123.89	106.69
24	AB	604	CLA	C1-C2-C3	-8.67	111.99	126.20
28	AA	411	DGD	O5D-C1E-C2E	8.67	121.44	108.27
28	BA	5412	DGD	C6D-C5D-C4D	-8.64	93.92	112.07
24	BB	5614	CLA	C1-C2-C3	-8.64	112.05	126.20
24	BC	5512	CLA	C1-C2-C3	-8.64	112.05	126.20
28	AA	411	DGD	O6D-C5D-C6D	8.63	123.81	106.69
36	BF	5101	HEM	CMA-C3A-C2A	-8.62	107.34	125.62
24	AA	404	CLA	C1-C2-C3	-8.62	112.08	126.20
24	BD	5402	CLA	C1-C2-C3	-8.60	112.11	126.20
24	AC	512	CLA	C1-C2-C3	-8.51	112.25	126.20
24	AC	508	CLA	C1-C2-C3	-8.51	112.26	126.20
34	BD	5403	PHO	C1-C2-C3	-8.46	112.33	126.20
36	AF	101	HEM	CMA-C3A-C2A	-8.45	107.71	125.62
24	AB	610	CLA	C1-C2-C3	-8.43	112.39	126.20
24	BC	5510	CLA	C1-C2-C3	-8.43	112.39	126.20
28	AC	519	DGD	C2G-O2G-C1B	8.42	137.95	117.80
24	BC	5508	CLA	C1-C2-C3	-8.39	112.45	126.20
35	AD	405	PL9	C7-C8-C9	-8.39	112.38	126.83
24	AC	509	CLA	C1-C2-C3	-8.38	112.46	126.20
24	AC	510	CLA	C1-C2-C3	-8.38	112.46	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AD	401	CLA	C1-C2-C3	-8.37	112.48	126.20
34	AD	403	PHO	C1-C2-C3	-8.33	112.55	126.20
36	AV	201	HEM	CMA-C3A-C2A	-8.32	107.97	125.62
35	BD	5406	PL9	C7-C8-C9	-8.32	112.50	126.83
28	AA	411	DGD	O3G-C3G-C2G	-8.30	90.62	110.82
28	BA	5412	DGD	O3G-C1D-C2D	-8.30	95.67	108.27
28	BA	5412	DGD	O3G-C3G-C2G	-8.30	90.63	110.82
34	AD	402	PHO	C1-C2-C3	-8.30	112.60	126.20
36	BV	5201	HEM	CMA-C3A-C2A	-8.30	108.03	125.62
24	BA	5408	CLA	C1-C2-C3	-8.29	112.62	126.20
24	BC	5504	CLA	C1-C2-C3	-8.28	112.62	126.20
24	BA	5407	CLA	C1-C2-C3	-8.28	112.63	126.20
24	AB	612	CLA	C1-C2-C3	-8.27	112.65	126.20
24	BB	5616	CLA	C1-C2-C3	-8.26	112.67	126.20
24	AA	407	CLA	C1-C2-C3	-8.25	112.67	126.20
30	AB	622	SQD	O5-C1-O6	8.25	129.55	110.04
24	AC	504	CLA	C1-C2-C3	-8.22	112.73	126.20
28	AA	411	DGD	O3G-C1D-C2D	-8.21	95.80	108.27
24	AC	506	CLA	C1-C2-C3	-8.21	112.75	126.20
28	BC	5519	DGD	C2G-O2G-C1B	8.20	137.41	117.80
34	BD	5404	PHO	C1-C2-C3	-8.20	112.77	126.20
30	BB	5601	SQD	O5-C1-O6	8.19	129.41	110.04
30	AB	627	SQD	O5-C1-O6	8.16	129.33	110.04
24	BC	5509	CLA	C1-C2-C3	-8.16	112.83	126.20
24	BB	5606	CLA	C1-C2-C3	-8.15	112.84	126.20
28	BC	5519	DGD	O6D-C5D-C6D	8.13	122.82	106.69
30	BB	5625	SQD	O5-C1-O6	8.13	129.25	110.04
24	BB	5609	CLA	C1-C2-C3	-8.13	112.88	126.20
24	AA	406	CLA	C1-C2-C3	-8.11	112.91	126.20
24	BC	5506	CLA	C1-C2-C3	-8.11	112.91	126.20
24	BB	5617	CLA	C1-C2-C3	-8.09	112.94	126.20
24	AB	613	CLA	C1-C2-C3	-8.09	112.94	126.20
24	BC	5502	CLA	C1-C2-C3	-8.09	112.95	126.20
24	AD	404	CLA	C1-C2-C3	-8.08	112.96	126.20
24	BB	5612	CLA	C1-C2-C3	-8.08	112.96	126.20
24	BC	5505	CLA	C1-C2-C3	-8.08	112.96	126.20
24	AB	601	CLA	C1-C2-C3	-8.07	112.97	126.20
24	BC	5513	CLA	C1-C2-C3	-8.05	113.00	126.20
24	AB	608	CLA	C1-C2-C3	-8.05	113.01	126.20
24	AC	505	CLA	C1-C2-C3	-8.00	113.09	126.20
24	AB	616	CLA	C1-C2-C3	-7.99	113.11	126.20
24	AB	602	CLA	C1-C2-C3	-7.99	113.11	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	513	CLA	C1-C2-C3	-7.98	113.13	126.20
24	BD	5405	CLA	C1-C2-C3	-7.96	113.15	126.20
24	AB	605	CLA	C1-C2-C3	-7.94	113.19	126.20
24	BB	5605	CLA	C1-C2-C3	-7.90	113.26	126.20
24	BB	5613	CLA	C1-C2-C3	-7.88	113.28	126.20
24	BB	5620	CLA	C1-C2-C3	-7.86	113.31	126.20
24	AB	609	CLA	C1-C2-C3	-7.86	113.32	126.20
24	AA	405	CLA	C1-C2-C3	-7.85	113.34	126.20
24	BA	5406	CLA	C1-C2-C3	-7.84	113.36	126.20
24	AC	502	CLA	C1-C2-C3	-7.83	113.36	126.20
31	BA	5402	LMG	C8-O7-C10	7.79	136.44	117.80
30	BB	5601	SQD	O6-C1-C2	7.78	120.09	108.27
24	AC	507	CLA	C1-C2-C3	-7.76	113.48	126.20
30	BB	5625	SQD	O6-C1-C2	7.75	120.05	108.27
24	BC	5507	CLA	C1-C2-C3	-7.74	113.51	126.20
30	AB	622	SQD	O6-C1-C2	7.73	120.01	108.27
24	BB	5618	CLA	C1-C2-C3	-7.69	113.60	126.20
28	AC	518	DGD	O6D-C5D-C6D	7.67	121.89	106.69
24	BB	5607	CLA	C1-C2-C3	-7.64	113.68	126.20
30	AB	627	SQD	O6-C1-C2	7.64	119.87	108.27
31	AD	407	LMG	C19-C18-C17	-7.64	75.76	114.37
24	AB	614	CLA	C1-C2-C3	-7.63	113.70	126.20
31	AD	407	LMG	C8-O7-C10	7.62	136.04	117.80
31	BD	5409	LMG	C19-C18-C17	-7.61	75.90	114.37
31	AA	417	LMG	C8-O7-C10	7.61	136.00	117.80
30	BF	5102	SQD	O7-S-C6	7.58	118.07	106.76
24	AB	606	CLA	C1-C2-C3	-7.57	113.79	126.20
31	BD	5409	LMG	C8-O7-C10	7.56	135.90	117.80
24	BB	5610	CLA	C1-C2-C3	-7.56	113.82	126.20
24	AB	603	CLA	C1-C2-C3	-7.55	113.83	126.20
30	AF	102	SQD	O7-S-C6	7.54	118.01	106.76
30	BF	5102	SQD	O6-C1-C2	7.54	119.72	108.27
30	AF	102	SQD	O6-C1-C2	7.49	119.64	108.27
28	BC	5518	DGD	O6D-C5D-C6D	7.46	121.48	106.69
31	AC	520	LMG	O7-C10-C11	7.45	127.60	111.48
34	BD	5404	PHO	C4D-CHA-CBD	-7.40	104.91	108.45
28	BC	5519	DGD	C6D-O5D-C1E	-7.36	98.02	113.80
27	AD	406	BCR	C38-C26-C25	7.32	132.47	124.48
31	BC	5520	LMG	O7-C10-C11	7.25	127.16	111.48
27	AJ	101	BCR	C32-C1-C2	-7.24	81.14	108.95
27	BJ	5101	BCR	C32-C1-C2	-7.12	81.62	108.95
27	AJ	101	BCR	C2-C1-C6	7.10	120.75	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BD	5407	BCR	C38-C26-C25	7.03	132.16	124.48
27	BJ	5101	BCR	C2-C1-C6	7.02	120.64	110.44
31	AD	408	LMG	C8-O7-C10	7.00	134.55	117.80
30	AA	413	SQD	O7-S-C6	7.00	117.20	106.76
31	BD	5410	LMG	C8-O7-C10	6.97	134.47	117.80
24	BC	5511	CLA	C1-C2-C3	-6.96	114.80	126.20
24	BB	5611	CLA	C1-C2-C3	-6.94	114.83	126.20
28	AC	519	DGD	C6D-O5D-C1E	-6.91	98.99	113.80
24	AC	511	CLA	C1-C2-C3	-6.90	114.89	126.20
28	AH	101	DGD	O2G-C1B-C2B	6.88	126.36	111.48
24	AB	607	CLA	C1-C2-C3	-6.86	114.96	126.20
30	BB	5625	SQD	O7-S-C6	6.85	116.99	106.76
30	BA	5401	SQD	O6-C1-C2	6.85	118.68	108.27
28	BH	5101	DGD	O2G-C1B-C2B	6.85	126.30	111.48
24	BA	5406	CLA	CBA-CAA-C2A	6.81	134.05	113.79
30	BA	5414	SQD	O7-S-C6	6.80	116.91	106.76
30	AA	416	SQD	O7-S-C6	6.74	116.82	106.76
34	AD	403	PHO	C4D-CHA-CBD	-6.74	105.22	108.45
35	BD	5406	PL9	C32-C33-C34	-6.73	112.22	127.62
24	AA	405	CLA	CBA-CAA-C2A	6.73	133.82	113.79
27	AK	102	BCR	C33-C5-C6	6.73	131.82	124.48
28	BA	5412	DGD	C6D-O5D-C1E	-6.71	99.41	113.80
31	AD	408	LMG	C13-C12-C11	-6.70	88.49	113.13
31	BD	5410	LMG	C13-C12-C11	-6.70	88.49	113.13
31	BM	5102	LMG	O7-C10-C11	6.70	125.98	111.48
30	AA	416	SQD	O6-C1-C2	6.70	118.44	108.27
31	AM	101	LMG	O7-C10-C11	6.63	125.83	111.48
35	AD	405	PL9	C32-C33-C34	-6.63	112.45	127.62
28	AA	411	DGD	C6D-O5D-C1E	-6.62	99.60	113.80
28	AC	518	DGD	O5D-C6D-C5D	6.61	124.33	109.42
31	BB	5624	LMG	O7-C10-C11	6.60	125.77	111.48
27	AB	618	BCR	C38-C26-C25	6.60	131.69	124.48
31	AC	521	LMG	C8-O7-C10	6.59	133.57	117.80
28	AC	517	DGD	O6D-C5D-C6D	6.58	119.75	106.69
31	AB	621	LMG	O7-C10-C11	6.58	125.72	111.48
28	BC	5518	DGD	O5D-C6D-C5D	6.58	124.25	109.42
30	BA	5401	SQD	O7-S-C6	6.58	116.58	106.76
31	BL	5101	LMG	C7-O1-C1	-6.54	99.77	113.80
30	AB	622	SQD	O7-S-C6	6.53	116.51	106.76
31	BC	5521	LMG	C8-O7-C10	6.52	133.41	117.80
32	BC	5522	LMT	C1B-O1B-C4'	-6.51	102.55	117.98
27	BK	5102	BCR	C33-C5-C6	6.47	131.54	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	516	BCR	C33-C5-C6	6.46	131.53	124.48
30	AA	413	SQD	O6-C1-C2	6.45	118.06	108.27
31	AB	620	LMG	C7-O1-C1	-6.44	99.99	113.80
27	BB	5622	BCR	C38-C26-C25	6.44	131.51	124.48
27	BC	5516	BCR	C33-C5-C6	6.43	131.50	124.48
31	AJ	102	LMG	C13-C12-C11	-6.41	89.56	113.13
30	BA	5414	SQD	O6-C1-C2	6.40	117.99	108.27
31	AB	620	LMG	C13-C12-C11	-6.38	89.70	113.13
31	BD	5408	LMG	C13-C12-C11	-6.37	89.73	113.13
30	AB	627	SQD	O7-S-C6	6.35	116.23	106.76
28	AC	519	DGD	C6D-C5D-C4D	-6.35	98.75	112.07
31	BL	5101	LMG	C13-C12-C11	-6.32	89.90	113.13
31	AA	417	LMG	C7-O1-C1	-6.32	100.25	113.80
27	BX	5101	BCR	C38-C26-C25	6.31	131.37	124.48
29	AA	412	LHG	C25-C24-C23	6.30	136.79	113.69
34	BD	5404	PHO	O2D-CGD-CBD	6.30	117.87	110.95
27	BC	5515	BCR	C33-C5-C6	6.29	131.35	124.48
32	AI	103	LMT	C1B-O1B-C4'	-6.29	103.06	117.98
31	BD	5408	LMG	C7-O1-C1	-6.29	100.31	113.80
28	BA	5412	DGD	C3G-O3G-C1D	6.28	127.27	113.80
28	AA	411	DGD	C3G-O3G-C1D	6.27	127.24	113.80
28	BC	5517	DGD	O6D-C5D-C6D	6.27	119.12	106.69
24	AA	406	CLA	CBA-CAA-C2A	6.26	132.42	113.79
27	AJ	101	BCR	C38-C26-C25	6.26	131.31	124.48
27	AC	515	BCR	C38-C26-C25	6.24	131.29	124.48
31	BA	5402	LMG	C13-C12-C11	-6.24	90.20	113.13
34	BD	5403	PHO	O2D-CGD-CBD	6.23	117.80	110.95
34	AD	402	PHO	O2D-CGD-CBD	6.23	117.79	110.95
31	AA	417	LMG	C13-C12-C11	-6.22	90.26	113.13
27	AT	101	BCR	C33-C5-C6	6.20	131.25	124.48
29	BA	5413	LHG	C25-C24-C23	6.19	136.39	113.69
31	BA	5402	LMG	C7-O1-C1	-6.18	100.56	113.80
27	BJ	5101	BCR	C38-C26-C25	6.16	131.21	124.48
27	BT	5101	BCR	C33-C5-C6	6.15	131.20	124.48
27	AC	515	BCR	C33-C5-C6	6.15	131.19	124.48
28	BC	5519	DGD	C4B-C3B-C2B	-6.14	90.56	113.13
31	AJ	102	LMG	C7-O1-C1	-6.14	100.63	113.80
30	BB	5601	SQD	C10-C9-C8	6.12	135.62	113.13
27	BC	5515	BCR	C38-C26-C25	6.12	131.16	124.48
30	BA	5401	SQD	C10-C9-C8	6.11	135.57	113.13
28	AC	518	DGD	C4A-C3A-C2A	-6.10	90.70	113.13
34	AD	403	PHO	O2D-CGD-CBD	6.10	117.65	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BB	5621	BCR	C38-C26-C25	6.10	131.14	124.48
27	AX	101	BCR	C38-C26-C25	6.10	131.14	124.48
30	AA	413	SQD	C10-C9-C8	6.08	135.49	113.13
27	AB	617	BCR	C38-C26-C25	6.08	131.12	124.48
30	BB	5601	SQD	O7-S-C6	6.08	115.83	106.76
36	BF	5101	HEM	CHA-C4D-ND	6.07	131.88	124.37
30	AA	416	SQD	C10-C9-C8	6.06	135.38	113.13
30	BA	5414	SQD	C10-C9-C8	6.04	135.31	113.13
24	BA	5407	CLA	CBA-CAA-C2A	6.02	131.72	113.79
27	BJ	5101	BCR	C31-C1-C6	6.00	119.65	110.24
30	AB	627	SQD	C10-C9-C8	5.98	135.12	113.13
28	AA	411	DGD	C1D-O6D-C5D	-5.98	102.04	113.72
30	BB	5625	SQD	C10-C9-C8	5.96	135.04	113.13
28	AC	519	DGD	C4B-C3B-C2B	-5.96	91.23	113.13
30	BF	5102	SQD	C25-C24-C23	5.95	135.51	113.69
28	BA	5412	DGD	O1G-C1A-C2A	5.95	129.97	111.83
31	BD	5409	LMG	C13-C12-C11	-5.93	91.32	113.13
28	AC	517	DGD	C4B-C3B-C2B	-5.93	91.35	113.13
28	BC	5518	DGD	C4A-C3A-C2A	-5.92	91.37	113.13
28	BC	5517	DGD	C4B-C3B-C2B	-5.92	91.39	113.13
30	AF	102	SQD	C10-C9-C8	5.91	134.85	113.13
30	AF	102	SQD	C25-C24-C23	5.91	135.35	113.69
30	BF	5102	SQD	C10-C9-C8	5.91	134.84	113.13
30	AB	622	SQD	C10-C9-C8	5.90	134.82	113.13
35	AD	405	PL9	C10-C9-C8	-5.88	108.51	123.63
28	BA	5412	DGD	C1D-O6D-C5D	-5.88	102.23	113.72
27	AC	516	BCR	C38-C26-C25	5.88	130.90	124.48
28	AA	411	DGD	O1G-C1A-C2A	5.88	129.76	111.83
28	BC	5518	DGD	O2G-C1B-C2B	5.88	124.20	111.48
31	AD	407	LMG	C13-C12-C11	-5.88	91.53	113.13
32	BD	5411	LMT	C1B-O1B-C4'	-5.87	104.06	117.98
28	BA	5412	DGD	O6D-C1D-O3G	5.87	123.91	110.04
28	AC	518	DGD	O2G-C1B-C2B	5.87	124.18	111.48
28	BB	5602	DGD	C3G-O3G-C1D	-5.87	101.22	113.80
27	AJ	101	BCR	C31-C1-C6	5.87	119.44	110.24
30	BA	5414	SQD	C25-C24-C23	5.86	135.16	113.69
27	BK	5102	BCR	C38-C26-C25	5.86	130.87	124.48
36	AF	101	HEM	CHA-C4D-ND	5.85	131.61	124.37
24	AA	405	CLA	CAA-C2A-C1A	-5.85	92.81	111.97
31	AI	101	LMG	O7-C10-C11	5.85	124.13	111.48
28	BC	5517	DGD	C6D-O5D-C1E	-5.83	101.29	113.80
31	AD	407	LMG	O7-C8-C7	5.83	129.26	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AA	413	SQD	C25-C24-C23	5.83	135.05	113.69
27	AK	102	BCR	C38-C26-C25	5.82	130.83	124.48
24	BA	5406	CLA	CAA-C2A-C1A	-5.82	92.90	111.97
35	AD	405	PL9	C22-C23-C24	-5.81	114.33	127.62
28	AC	517	DGD	O1G-C1G-C2G	-5.80	91.68	108.40
27	BT	5101	BCR	C38-C26-C25	5.79	130.80	124.48
28	BC	5519	DGD	C6D-C5D-C4D	-5.79	99.91	112.07
28	AB	628	DGD	C3G-O3G-C1D	-5.78	101.39	113.80
31	BD	5409	LMG	O7-C8-C7	5.77	129.03	108.34
31	BI	5101	LMG	O7-C10-C11	5.76	123.95	111.48
31	BD	5409	LMG	C17-C16-C15	-5.76	85.27	114.37
28	AA	411	DGD	O6D-C1D-O3G	5.75	123.63	110.04
30	BB	5601	SQD	C25-C24-C23	5.75	134.76	113.69
28	AC	517	DGD	C6D-C5D-C4D	-5.73	100.05	112.07
30	AB	627	SQD	C25-C24-C23	5.72	134.67	113.69
31	AJ	102	LMG	O7-C8-C7	5.70	128.79	108.34
27	AC	514	BCR	C38-C26-C25	5.70	130.70	124.48
32	AD	409	LMT	C1B-O1B-C4'	-5.68	104.52	117.98
27	BC	5516	BCR	C38-C26-C25	5.68	130.68	124.48
31	AD	407	LMG	C17-C16-C15	-5.68	85.67	114.37
28	AC	518	DGD	C3G-O3G-C1D	-5.66	101.66	113.80
28	BC	5517	DGD	C6D-C5D-C4D	-5.65	100.20	112.07
35	BD	5406	PL9	C10-C9-C8	-5.65	109.11	123.63
31	BD	5408	LMG	O7-C8-C7	5.65	128.61	108.34
28	BC	5517	DGD	O1G-C1G-C2G	-5.64	92.14	108.40
25	AA	408	MST	C10-N9-C4	-5.64	120.93	128.06
28	BC	5518	DGD	C6D-O5D-C1E	-5.63	101.72	113.80
35	BD	5406	PL9	C22-C23-C24	-5.62	114.77	127.62
30	BA	5401	SQD	C25-C24-C23	5.60	134.22	113.69
27	AT	101	BCR	C38-C26-C25	5.59	130.58	124.48
27	BA	5411	BCR	C33-C5-C6	5.58	130.57	124.48
28	BC	5517	DGD	C1G-O1G-C1A	5.58	137.50	117.12
28	BC	5518	DGD	C3G-O3G-C1D	-5.57	101.84	113.80
30	AA	416	SQD	C25-C24-C23	5.57	134.10	113.69
27	BA	5411	BCR	C38-C26-C25	5.56	130.55	124.48
28	AC	517	DGD	C6D-O5D-C1E	-5.55	101.91	113.80
27	BC	5514	BCR	C38-C26-C25	5.50	130.48	124.48
27	BB	5621	BCR	C33-C5-C6	5.49	130.48	124.48
24	AC	505	CLA	CAA-CBA-CGA	-5.48	97.64	113.21
28	AC	517	DGD	C1G-O1G-C1A	5.48	137.16	117.12
24	BC	5505	CLA	CAA-CBA-CGA	-5.47	97.68	113.21
27	AB	617	BCR	C33-C5-C6	5.45	130.44	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BJ	5101	BCR	C33-C5-C6	5.45	130.43	124.48
24	BB	5612	CLA	CAA-C2A-C1A	-5.45	94.13	111.97
36	AV	201	HEM	CHA-C4D-ND	5.44	131.10	124.37
27	AA	410	BCR	C33-C5-C6	5.44	130.42	124.48
27	AJ	101	BCR	C33-C5-C6	5.44	130.42	124.48
27	AA	410	BCR	C38-C26-C25	5.44	130.42	124.48
24	AB	608	CLA	CAA-C2A-C1A	-5.42	94.20	111.97
30	AB	622	SQD	C25-C24-C23	5.38	133.39	113.69
36	BV	5201	HEM	CHA-C4D-ND	5.37	131.01	124.37
30	BB	5625	SQD	C25-C24-C23	5.36	133.35	113.69
28	AC	518	DGD	C6D-O5D-C1E	-5.35	102.33	113.80
28	BA	5412	DGD	O2G-C1B-C2B	5.33	123.02	111.48
25	BA	5409	MST	C10-N9-C4	-5.32	121.33	128.06
28	AA	411	DGD	O2G-C1B-C2B	5.30	122.96	111.48
31	BL	5101	LMG	O7-C8-C7	5.30	127.36	108.34
27	AB	619	BCR	C33-C5-C6	5.30	130.27	124.48
24	BB	5612	CLA	CBA-CAA-C2A	5.29	129.52	113.79
31	AB	620	LMG	O7-C8-C7	5.27	127.26	108.34
24	BA	5407	CLA	CAA-C2A-C1A	-5.27	94.72	111.97
24	AB	607	CLA	CBA-CAA-C2A	5.26	129.45	113.79
27	BD	5407	BCR	C33-C5-C6	5.25	130.22	124.48
25	AA	408	MST	C8-S7-C2	5.24	106.18	102.25
25	BA	5409	MST	C8-S7-C2	5.23	106.17	102.25
27	AB	619	BCR	C38-C26-C25	5.22	130.18	124.48
27	BB	5623	BCR	C38-C26-C25	5.22	130.18	124.48
28	BH	5101	DGD	C6D-C5D-C4D	-5.21	101.12	112.07
27	BX	5101	BCR	C33-C5-C6	5.21	130.17	124.48
35	BD	5406	PL9	C12-C13-C14	-5.20	115.73	127.62
28	BC	5519	DGD	O6D-C5D-C4D	5.18	119.03	109.70
27	AX	101	BCR	C33-C5-C6	5.17	130.13	124.48
24	AB	608	CLA	CBA-CAA-C2A	5.16	129.16	113.79
28	AC	518	DGD	C6D-C5D-C4D	-5.16	101.24	112.07
28	AH	101	DGD	C6D-C5D-C4D	-5.15	101.26	112.07
24	BB	5611	CLA	CAA-C2A-C1A	-5.14	95.14	111.97
27	AD	406	BCR	C33-C5-C6	5.07	130.02	124.48
24	AB	607	CLA	CAA-C2A-C1A	-5.07	95.36	111.97
24	BB	5611	CLA	CBA-CAA-C2A	5.06	128.83	113.79
28	AC	517	DGD	O5D-C6D-C5D	5.05	120.81	109.42
35	AD	405	PL9	C12-C13-C14	-5.05	116.06	127.62
28	BC	5517	DGD	O5D-C6D-C5D	5.04	120.78	109.42
27	AJ	101	BCR	C1-C6-C5	-5.04	115.75	122.64
24	AA	406	CLA	CAA-C2A-C1A	-5.03	95.48	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BB	5623	BCR	C33-C5-C6	5.02	129.96	124.48
28	BC	5518	DGD	C6D-C5D-C4D	-5.00	101.56	112.07
27	AB	618	BCR	C33-C5-C6	5.00	129.94	124.48
28	BC	5519	DGD	O2G-C2G-C1G	-5.00	90.41	108.34
27	BJ	5101	BCR	C1-C6-C5	-5.00	115.81	122.64
28	BH	5101	DGD	C6D-O5D-C1E	-4.92	103.26	113.80
30	BF	5102	SQD	C44-O6-C1	4.88	124.26	113.80
31	BD	5409	LMG	C20-C19-C18	4.87	139.00	114.37
31	BD	5409	LMG	C9-C8-C7	-4.83	100.51	111.78
31	AD	407	LMG	C20-C19-C18	4.82	138.73	114.37
31	AD	407	LMG	C9-C8-C7	-4.80	100.58	111.78
27	AC	514	BCR	C33-C5-C6	4.79	129.71	124.48
27	AC	516	BCR	C29-C30-C25	4.77	117.36	110.44
28	BC	5517	DGD	O5D-C1E-C2E	4.75	115.49	108.27
35	AD	405	PL9	C20-C19-C21	4.75	123.47	115.23
31	BC	5521	LMG	C13-C12-C11	-4.75	95.69	113.13
31	AC	521	LMG	C13-C12-C11	-4.74	95.72	113.13
34	AD	402	PHO	C4D-CHA-CBD	-4.73	106.19	108.45
30	AF	102	SQD	C44-O6-C1	4.73	123.94	113.80
27	AK	102	BCR	C11-C10-C9	4.73	133.91	127.28
28	AC	519	DGD	O6D-C5D-C4D	4.73	118.22	109.70
34	BD	5403	PHO	C4D-CHA-CBD	-4.72	106.19	108.45
24	BB	5618	CLA	CBA-CAA-C2A	4.71	127.82	113.79
24	BA	5406	CLA	C4D-C3D-CAD	4.70	113.21	108.11
28	AH	101	DGD	C6D-O5D-C1E	-4.70	103.73	113.80
28	AC	519	DGD	O2G-C2G-C1G	-4.69	91.50	108.34
36	AF	101	HEM	CAD-C3D-C2D	4.68	136.62	127.87
28	BC	5519	DGD	C1D-O6D-C5D	-4.68	104.59	113.72
24	AB	614	CLA	CBA-CAA-C2A	4.68	127.70	113.79
28	AC	517	DGD	O5D-C1E-C2E	4.67	115.36	108.27
24	AB	608	CLA	CAA-CBA-CGA	-4.67	99.96	113.21
28	AH	101	DGD	O3G-C3G-C2G	-4.66	99.50	110.82
28	AC	519	DGD	O6E-C1E-O5D	4.64	121.00	110.04
28	BC	5519	DGD	O6E-C1E-O5D	4.64	121.00	110.04
31	AC	521	LMG	C7-O1-C1	-4.63	103.86	113.80
28	BC	5517	DGD	C4A-C3A-C2A	-4.63	96.12	113.13
31	BE	5101	LMG	C8-O7-C10	4.62	128.86	117.80
31	BC	5521	LMG	C7-O1-C1	-4.62	103.90	113.80
36	BF	5101	HEM	CAD-C3D-C2D	4.61	136.50	127.87
24	BC	5505	CLA	CBA-CAA-C2A	4.60	127.48	113.79
35	BD	5406	PL9	C20-C19-C21	4.59	123.19	115.23
32	AI	103	LMT	O1B-C1B-C2B	4.59	119.38	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BD	5409	LMG	C18-C17-C16	4.58	137.54	114.37
31	AA	414	LMG	C8-O7-C10	4.58	128.76	117.80
27	AK	102	BCR	C2-C1-C6	4.57	117.07	110.44
28	BB	5602	DGD	C1G-O1G-C1A	4.56	133.80	117.12
28	AB	628	DGD	C1G-O1G-C1A	4.56	133.79	117.12
31	BE	5101	LMG	C7-O1-C1	-4.54	104.06	113.80
31	AA	414	LMG	C7-O1-C1	-4.53	104.08	113.80
28	BC	5518	DGD	C1D-O6D-C5D	-4.53	104.88	113.72
27	BB	5622	BCR	C33-C5-C6	4.53	129.42	124.48
32	AI	103	LMT	C1-O1'-C1'	4.51	121.39	113.68
31	AD	407	LMG	C18-C17-C16	4.50	137.13	114.37
27	BC	5516	BCR	C29-C30-C25	4.50	116.97	110.44
28	AC	519	DGD	C1D-O6D-C5D	-4.49	104.95	113.72
27	BK	5102	BCR	C11-C10-C9	4.49	133.57	127.28
24	BB	5610	CLA	O2A-CGA-CBA	4.48	125.50	111.83
24	AC	505	CLA	CBA-CAA-C2A	4.48	127.12	113.79
27	BC	5514	BCR	C33-C5-C6	4.48	129.37	124.48
27	AC	516	BCR	C2-C1-C6	4.48	116.94	110.44
28	BH	5101	DGD	O3G-C1D-C2D	-4.47	101.48	108.27
28	AC	517	DGD	C4A-C3A-C2A	-4.46	96.74	113.13
24	BB	5612	CLA	CAA-CBA-CGA	-4.45	100.59	113.21
28	BH	5101	DGD	O3G-C3G-C2G	-4.44	100.01	110.82
27	BD	5407	BCR	C29-C30-C25	4.44	116.89	110.44
30	AA	413	SQD	O8-S-C6	-4.42	97.44	105.97
30	AA	416	SQD	O8-S-C6	-4.42	97.45	105.97
36	BF	5101	HEM	CHA-C4D-C3D	-4.41	117.09	125.23
24	AC	504	CLA	CAA-C2A-C1A	-4.40	97.56	111.97
35	BD	5406	PL9	C35-C34-C36	4.40	122.86	115.23
27	AT	101	BCR	C29-C30-C25	4.39	116.82	110.44
28	AH	101	DGD	O3G-C1D-C2D	-4.39	101.60	108.27
30	AF	102	SQD	O8-S-C6	-4.39	97.50	105.97
36	AF	101	HEM	C4A-C3A-C2A	-4.39	101.79	106.82
24	AA	405	CLA	C4D-C3D-CAD	4.39	112.87	108.11
28	AC	518	DGD	C1D-O6D-C5D	-4.39	105.16	113.72
24	AB	606	CLA	O2A-CGA-CBA	4.38	125.20	111.83
24	BB	5611	CLA	O2A-CGA-CBA	4.38	125.20	111.83
31	AA	417	LMG	C9-C8-C7	4.38	122.00	111.78
32	BC	5522	LMT	C1-O1'-C1'	4.38	121.17	113.68
31	BA	5402	LMG	C9-C8-C7	4.38	122.00	111.78
24	BC	5504	CLA	CBA-CAA-C2A	4.37	126.81	113.79
32	BC	5522	LMT	O1B-C1B-C2B	4.37	118.83	108.09
24	AB	612	CLA	O2D-CGD-CBD	4.36	118.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BK	5102	BCR	C2-C1-C6	4.35	116.76	110.44
27	BC	5514	BCR	C24-C23-C22	4.35	132.67	126.23
24	BA	5406	CLA	O2A-CGA-CBA	4.34	125.08	111.83
24	AC	504	CLA	CBA-CAA-C2A	4.34	126.70	113.79
30	BF	5102	SQD	O8-S-C6	-4.34	97.60	105.97
24	BC	5505	CLA	C4D-C3D-CAD	4.33	112.81	108.11
36	AF	101	HEM	CHA-C4D-C3D	-4.33	117.24	125.23
27	BX	5101	BCR	C29-C30-C25	4.33	116.73	110.44
31	AD	407	LMG	C15-C14-C13	-4.33	92.47	114.37
31	BD	5409	LMG	C15-C14-C13	-4.32	92.55	114.37
24	AA	405	CLA	O2D-CGD-CBD	4.31	118.77	111.23
30	BA	5401	SQD	O8-S-C6	-4.31	97.65	105.97
24	BA	5406	CLA	O2D-CGD-CBD	4.31	118.76	111.23
24	AB	607	CLA	O2A-CGA-CBA	4.30	124.95	111.83
35	AD	405	PL9	C35-C34-C36	4.30	122.68	115.23
24	BC	5504	CLA	CAA-C2A-C1A	-4.29	97.90	111.97
36	BF	5101	HEM	C4A-C3A-C2A	-4.29	101.90	106.82
28	AH	101	DGD	C5B-C4B-C3B	-4.29	92.68	114.37
24	AA	406	CLA	O2D-CGD-CBD	4.29	118.72	111.23
31	BC	5521	LMG	C9-O8-C28	4.29	132.78	117.12
32	BB	5626	LMT	C1B-O1B-C4'	-4.27	107.85	117.98
27	AK	102	BCR	C7-C8-C9	4.27	132.55	126.23
28	AE	101	DGD	O2G-C1B-C2B	4.26	120.70	111.48
28	BH	5101	DGD	C5B-C4B-C3B	-4.26	92.85	114.37
27	AJ	101	BCR	C23-C24-C25	4.25	138.36	127.00
27	AX	101	BCR	C29-C30-C25	4.25	116.62	110.44
27	BT	5101	BCR	C29-C30-C25	4.25	116.61	110.44
28	BE	5102	DGD	O2G-C1B-C2B	4.24	120.66	111.48
30	AA	413	SQD	C44-O6-C1	4.24	122.89	113.80
24	AD	404	CLA	O2D-CGD-CBD	4.24	118.64	111.23
31	BM	5102	LMG	C9-O8-C28	4.22	132.54	117.12
28	AC	517	DGD	O3G-C1D-C2D	-4.22	101.87	108.27
28	BC	5519	DGD	C1E-C2E-C3E	-4.21	101.15	110.01
31	AC	521	LMG	C9-O8-C28	4.21	132.49	117.12
31	AM	101	LMG	C9-O8-C28	4.20	132.46	117.12
24	BA	5407	CLA	O2A-CGA-CBA	4.19	124.62	111.83
24	AB	603	CLA	C3A-C2A-C1A	4.19	107.61	101.34
24	BC	5504	CLA	O2D-CGD-CBD	4.19	118.55	111.23
28	AC	519	DGD	C8A-C7A-C6A	-4.19	93.20	114.37
31	AB	620	LMG	C8-O7-C10	4.18	127.81	117.80
24	AA	405	CLA	O2A-CGA-CBA	4.18	124.59	111.83
27	AC	514	BCR	C24-C23-C22	4.18	132.41	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BA	5414	SQD	C44-O6-C1	4.16	122.71	113.80
24	AA	407	CLA	O2D-CGD-CBD	4.15	118.48	111.23
28	BC	5519	DGD	C8A-C7A-C6A	-4.15	93.40	114.37
24	BB	5607	CLA	C3A-C2A-C1A	4.15	107.55	101.34
24	AA	406	CLA	O2A-CGA-CBA	4.15	124.48	111.83
27	AD	406	BCR	C29-C30-C25	4.15	116.46	110.44
24	AC	505	CLA	C4D-C3D-CAD	4.15	112.61	108.11
24	BB	5616	CLA	O2D-CGD-CBD	4.14	118.48	111.23
31	AB	620	LMG	O1-C7-C8	4.14	120.90	110.82
27	BK	5102	BCR	C7-C8-C9	4.14	132.36	126.23
24	AB	603	CLA	C2A-C1A-CHA	4.14	131.05	123.87
24	BC	5511	CLA	CBA-CAA-C2A	4.14	126.10	113.79
24	BA	5407	CLA	O2D-CGD-CBD	4.13	118.45	111.23
27	BX	5101	BCR	C2-C1-C6	4.13	116.43	110.44
35	BD	5406	PL9	C2-C1-C6	4.12	123.90	119.00
27	AJ	101	BCR	C30-C25-C26	-4.12	117.00	122.64
31	AD	407	LMG	C21-C20-C19	4.11	135.14	114.37
27	BJ	5101	BCR	C23-C24-C25	4.11	137.97	127.00
32	AB	623	LMT	C1B-O1B-C4'	-4.10	108.26	117.98
27	BC	5515	BCR	C23-C24-C25	4.10	137.95	127.00
31	BD	5408	LMG	O8-C9-C8	-4.10	96.59	108.40
24	AC	511	CLA	CBA-CAA-C2A	4.09	125.98	113.79
27	AD	406	BCR	C38-C26-C27	-4.09	104.87	113.60
28	AB	628	DGD	C4B-C3B-C2B	-4.09	98.10	113.13
24	BB	5607	CLA	C2A-C1A-CHA	4.09	130.97	123.87
31	BD	5410	LMG	C19-C18-C17	-4.09	93.72	114.37
30	AB	622	SQD	O48-C23-C24	4.08	124.29	111.83
28	AH	101	DGD	C3B-C2B-C1B	-4.08	98.73	113.69
24	AB	614	CLA	C3B-C4B-NB	-4.08	106.89	110.53
25	AA	408	MST	N5-C6-N1	-4.08	119.57	126.26
27	AC	515	BCR	C23-C24-C25	4.08	137.89	127.00
24	BA	5408	CLA	O2D-CGD-CBD	4.08	118.36	111.23
35	AD	405	PL9	C2-C1-C6	4.08	123.84	119.00
30	BA	5401	SQD	C44-O6-C1	4.08	122.53	113.80
24	BB	5610	CLA	C4D-C3D-CAD	4.07	112.53	108.11
24	AC	511	CLA	O2D-CGD-CBD	4.07	118.34	111.23
24	BD	5405	CLA	O2D-CGD-CBD	4.07	118.34	111.23
24	BC	5503	CLA	C4D-C3D-CAD	4.06	112.52	108.11
28	BC	5518	DGD	C8A-C7A-C6A	-4.06	93.86	114.37
25	BA	5409	MST	N5-C6-N1	-4.06	119.61	126.26
28	BH	5101	DGD	C3B-C2B-C1B	-4.05	98.84	113.69
27	BA	5411	BCR	C7-C8-C9	4.05	132.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BJ	5101	BCR	C30-C25-C26	-4.05	117.11	122.64
31	BC	5520	LMG	C12-C11-C10	-4.05	98.87	113.69
24	AC	509	CLA	C4D-C3D-CAD	4.05	112.50	108.11
28	BB	5602	DGD	C4B-C3B-C2B	-4.05	98.26	113.13
31	AD	408	LMG	C19-C18-C17	-4.04	93.94	114.37
27	BB	5621	BCR	C29-C30-C25	4.04	116.31	110.44
28	AC	518	DGD	C8A-C7A-C6A	-4.04	93.96	114.37
24	AC	504	CLA	O2D-CGD-CBD	4.03	118.27	111.23
30	BA	5401	SQD	C31-C30-C29	4.02	134.68	114.37
28	BC	5517	DGD	O3G-C1D-C2D	-4.02	102.17	108.27
29	AA	415	LHG	O7-C7-C8	4.01	120.16	111.48
30	AA	416	SQD	C31-C30-C29	4.01	134.63	114.37
30	BA	5401	SQD	O48-C23-C24	4.01	124.05	111.83
24	BD	5402	CLA	C4D-C3D-CAD	4.01	112.46	108.11
29	BA	5415	LHG	O7-C7-C8	4.01	120.15	111.48
31	BL	5101	LMG	O1-C7-C8	4.00	120.56	110.82
30	AA	416	SQD	O48-C23-C24	4.00	124.04	111.83
24	AB	603	CLA	C4D-C3D-CAD	4.00	112.45	108.11
31	AA	417	LMG	O7-C8-C7	3.99	122.67	108.34
31	BL	5101	LMG	C8-O7-C10	3.99	127.36	117.80
30	AB	627	SQD	O8-S-C6	-3.99	98.26	105.97
28	BE	5102	DGD	C6D-O5D-C1E	-3.99	105.25	113.80
30	AA	416	SQD	C44-O6-C1	3.99	122.34	113.80
31	AI	101	LMG	C9-C8-C7	-3.98	102.50	111.78
31	AJ	102	LMG	O8-C9-C8	-3.98	96.92	108.40
31	AC	520	LMG	C12-C11-C10	-3.98	99.12	113.69
24	BB	5613	CLA	O2A-CGA-CBA	3.98	123.96	111.83
24	AB	615	CLA	C4D-C3D-CAD	3.98	112.42	108.11
27	AJ	101	BCR	C29-C30-C25	3.97	116.21	110.44
24	AC	501	CLA	C3A-C2A-C1A	3.97	107.29	101.34
24	BA	5407	CLA	C4D-C3D-CAD	3.97	112.42	108.11
27	AB	617	BCR	C23-C24-C25	3.97	137.59	127.00
28	BH	5101	DGD	O6D-C5D-C6D	3.96	114.56	106.69
27	AJ	101	BCR	C38-C26-C27	-3.96	105.14	113.60
24	BC	5512	CLA	C4D-C3D-CAD	3.96	112.41	108.11
31	BD	5409	LMG	C21-C20-C19	3.96	134.40	114.37
28	AC	519	DGD	C1E-C2E-C3E	-3.96	101.68	110.01
24	AB	604	CLA	O2A-CGA-CBA	3.96	123.91	111.83
24	BC	5511	CLA	C4D-C3D-CAD	3.96	112.41	108.11
24	BB	5608	CLA	O2A-CGA-CBA	3.95	123.89	111.83
27	AD	406	BCR	C24-C23-C22	3.95	132.08	126.23
24	BB	5618	CLA	C3B-C4B-NB	-3.95	107.00	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5609	CLA	CBA-CAA-C2A	3.94	125.53	113.79
24	BC	5509	CLA	C4D-C3D-CAD	3.94	112.38	108.11
31	AB	621	LMG	C34-C33-C32	3.94	134.27	114.37
31	AC	521	LMG	O7-C8-C7	3.93	122.46	108.34
24	BC	5508	CLA	CAA-C2A-C1A	-3.93	99.09	111.97
32	AB	629	LMT	C1-O1'-C1'	-3.93	106.96	113.68
27	AK	102	BCR	C33-C5-C4	-3.93	105.21	113.60
24	AB	603	CLA	C3B-C4B-NB	-3.93	107.02	110.53
27	AJ	101	BCR	C7-C8-C9	3.93	132.05	126.23
36	BV	5201	HEM	C4A-C3A-C2A	-3.92	102.32	106.82
24	BB	5612	CLA	C3A-C2A-C1A	3.92	107.22	101.34
24	AC	503	CLA	C4D-C3D-CAD	3.92	112.37	108.11
24	BB	5619	CLA	C4D-C3D-CAD	3.92	112.37	108.11
24	BC	5505	CLA	CAA-C2A-C1A	-3.92	99.12	111.97
28	AC	517	DGD	C1D-O6D-C5D	-3.92	106.07	113.72
24	AB	609	CLA	O2A-CGA-CBA	3.91	123.77	111.83
24	AB	606	CLA	C4D-C3D-CAD	3.91	112.36	108.11
30	BA	5401	SQD	C11-C10-C9	3.91	134.14	114.37
28	AH	101	DGD	O6D-C5D-C6D	3.91	114.44	106.69
31	BB	5624	LMG	C34-C33-C32	3.91	134.12	114.37
30	AA	416	SQD	C11-C10-C9	3.91	134.12	114.37
24	AC	510	CLA	O2D-CGD-CBD	3.90	118.05	111.23
27	BD	5407	BCR	C38-C26-C27	-3.90	105.28	113.60
27	BJ	5101	BCR	C29-C30-C25	3.90	116.11	110.44
24	BC	5501	CLA	C4D-C3D-CAD	3.90	112.34	108.11
24	AB	606	CLA	C3A-C2A-C1A	3.90	107.18	101.34
31	BC	5521	LMG	O7-C8-C7	3.90	122.32	108.34
24	AC	503	CLA	O2D-CGD-CBD	3.89	118.03	111.23
32	BC	5522	LMT	O1'-C1-C2	-3.89	96.18	109.37
28	BC	5517	DGD	C1D-O6D-C5D	-3.89	106.13	113.72
28	AC	519	DGD	C6B-C5B-C4B	-3.89	94.73	114.37
24	AB	605	CLA	CBA-CAA-C2A	3.88	125.35	113.79
34	BD	5404	PHO	C1A-C2A-C3A	3.88	106.53	102.84
24	AC	505	CLA	O2D-CGD-CBD	3.88	118.01	111.23
24	BC	5503	CLA	O2D-CGD-CBD	3.88	118.01	111.23
27	AB	617	BCR	C29-C30-C25	3.87	116.06	110.44
24	AB	605	CLA	C4D-C3D-CAD	3.87	112.31	108.11
27	BC	5515	BCR	C29-C30-C25	3.87	116.06	110.44
24	AC	505	CLA	CAA-C2A-C1A	-3.87	99.30	111.97
31	BA	5402	LMG	O7-C8-C7	3.87	122.22	108.34
24	BB	5616	CLA	C4D-C3D-CAD	3.87	112.30	108.11
32	AI	103	LMT	O1'-C1-C2	-3.86	96.26	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	508	CLA	CBA-CAA-C2A	3.86	125.28	113.79
27	AX	101	BCR	C2-C1-C6	3.86	116.04	110.44
36	AV	201	HEM	C4A-C3A-C2A	-3.86	102.40	106.82
27	BK	5102	BCR	C23-C24-C25	3.85	137.30	127.00
24	AB	608	CLA	C3A-C2A-C1A	3.85	107.11	101.34
27	AD	406	BCR	C23-C24-C25	3.85	137.29	127.00
24	AC	508	CLA	C4D-C3D-CAD	3.85	112.29	108.11
24	BB	5615	CLA	O2A-CGA-CBA	3.85	123.58	111.83
30	BB	5601	SQD	O48-C23-C24	3.85	123.57	111.83
24	BC	5507	CLA	O2D-CGD-CBD	3.85	117.96	111.23
27	AK	102	BCR	C23-C24-C25	3.85	137.28	127.00
24	BD	5402	CLA	O2A-CGA-CBA	3.85	123.56	111.83
35	BD	5406	PL9	C15-C14-C16	3.85	121.90	115.23
36	AV	201	HEM	CHA-C4D-C3D	-3.84	118.14	125.23
24	AB	601	CLA	C4D-C3D-CAD	3.84	112.28	108.11
28	AE	101	DGD	C6D-O5D-C1E	-3.84	105.56	113.80
27	AB	619	BCR	C29-C30-C25	3.84	116.02	110.44
24	BB	5607	CLA	C3B-C4B-NB	-3.84	107.10	110.53
35	AD	405	PL9	C20-C19-C18	-3.84	113.77	123.63
31	AI	101	LMG	C9-O8-C28	3.84	131.14	117.12
24	BB	5611	CLA	C4D-C3D-CAD	3.84	112.27	108.11
28	BA	5412	DGD	O6E-C1E-O5D	3.84	119.11	110.04
30	AF	102	SQD	O48-C23-C24	3.83	123.53	111.83
30	AB	622	SQD	C11-C10-C9	3.83	133.75	114.37
28	AA	411	DGD	O6E-C1E-O5D	3.83	119.10	110.04
24	AC	502	CLA	CBA-CAA-C2A	3.83	125.19	113.79
24	AC	501	CLA	C4D-C3D-CAD	3.83	112.27	108.11
24	AC	511	CLA	C4D-C3D-CAD	3.83	112.27	108.11
31	AB	621	LMG	C14-C13-C12	-3.83	95.02	114.37
30	AA	413	SQD	C31-C30-C29	3.82	133.70	114.37
27	AA	410	BCR	C7-C8-C9	3.82	131.89	126.23
27	BJ	5101	BCR	C38-C26-C27	-3.82	105.45	113.60
24	BB	5610	CLA	C3A-C2A-C1A	3.82	107.06	101.34
27	AK	102	BCR	C29-C30-C25	3.82	115.99	110.44
24	AB	611	CLA	O2A-CGA-CBA	3.82	123.48	111.83
31	AD	408	LMG	C7-O1-C1	-3.82	105.61	113.80
24	BB	5605	CLA	C4D-C3D-CAD	3.82	112.25	108.11
30	AB	627	SQD	O48-C23-C24	3.82	123.47	111.83
27	AD	406	BCR	C30-C25-C26	-3.82	117.42	122.64
31	BI	5101	LMG	C9-C8-C7	-3.81	102.89	111.78
24	AD	404	CLA	C4D-C3D-CAD	3.81	112.25	108.11
30	BB	5625	SQD	C11-C10-C9	3.81	133.64	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BD	5407	BCR	C30-C25-C26	-3.81	117.43	122.64
27	AB	618	BCR	C38-C26-C27	-3.81	105.47	113.60
28	BC	5519	DGD	C6B-C5B-C4B	-3.81	95.10	114.37
31	BB	5624	LMG	C14-C13-C12	-3.81	95.11	114.37
30	BA	5414	SQD	O8-S-C6	-3.81	98.61	105.97
30	BF	5102	SQD	O48-C23-C24	3.81	123.45	111.83
30	AA	413	SQD	C45-O47-C7	3.81	126.92	117.80
24	AB	614	CLA	C4D-C3D-CAD	3.81	112.24	108.11
32	BB	5603	LMT	C1-O1'-C1'	-3.81	107.17	113.68
27	AC	515	BCR	C2-C1-C6	3.80	115.97	110.44
30	BA	5414	SQD	C31-C30-C29	3.80	133.59	114.37
31	BA	5402	LMG	C9-O8-C28	3.80	131.02	117.12
31	BI	5101	LMG	C9-O8-C28	3.80	131.01	117.12
30	BA	5414	SQD	C45-O47-C7	3.80	126.89	117.80
24	AC	508	CLA	CAA-C2A-C1A	-3.80	99.52	111.97
24	BB	5608	CLA	C4D-C3D-CAD	3.80	112.23	108.11
25	AA	408	MST	N5-C4-N3	-3.80	120.03	126.26
27	AC	516	BCR	C23-C24-C25	3.80	137.14	127.00
24	BC	5510	CLA	O2D-CGD-CBD	3.79	117.86	111.23
24	BC	5501	CLA	C3A-C2A-C1A	3.79	107.02	101.34
24	BC	5508	CLA	C4D-C3D-CAD	3.79	112.22	108.11
27	BB	5621	BCR	C23-C24-C25	3.79	137.12	127.00
30	AF	102	SQD	C11-C10-C9	3.79	133.51	114.37
31	AB	621	LMG	C37-C36-C35	-3.79	95.23	114.37
31	BD	5410	LMG	C7-O1-C1	-3.79	105.68	113.80
24	BB	5611	CLA	C3B-C4B-NB	-3.79	107.15	110.53
27	BD	5407	BCR	C23-C24-C25	3.79	137.11	127.00
30	AB	622	SQD	O8-S-C6	-3.79	98.66	105.97
24	AC	513	CLA	O2A-CGA-CBA	3.78	123.37	111.83
24	BB	5618	CLA	C4D-C3D-CAD	3.78	112.22	108.11
24	AB	602	CLA	O2A-CGA-CBA	3.78	123.37	111.83
24	BC	5511	CLA	C3B-C4B-NB	-3.78	107.16	110.53
30	BF	5102	SQD	C11-C10-C9	3.78	133.46	114.37
30	BB	5625	SQD	O48-C23-C24	3.78	123.35	111.83
31	BB	5624	LMG	C37-C36-C35	-3.78	95.28	114.37
24	BC	5510	CLA	C4D-C3D-CAD	3.77	112.21	108.11
24	AC	511	CLA	C3B-C4B-NB	-3.77	107.16	110.53
24	BD	5405	CLA	C4D-C3D-CAD	3.77	112.20	108.11
28	AC	518	DGD	C3G-C2G-C1G	-3.77	103.00	111.78
27	BB	5622	BCR	C38-C26-C27	-3.77	105.56	113.60
24	BB	5619	CLA	C2A-C1A-CHA	3.77	130.40	123.87
30	AA	413	SQD	C11-C10-C9	3.76	133.38	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BD	5408	LMG	O1-C7-C8	3.76	119.96	110.82
24	BA	5408	CLA	C4D-C3D-CAD	3.76	112.19	108.11
27	BK	5102	BCR	C29-C30-C25	3.76	115.90	110.44
27	AX	101	BCR	C30-C25-C26	-3.76	117.50	122.64
30	BA	5414	SQD	C11-C10-C9	3.76	133.37	114.37
24	AB	601	CLA	O2D-CGD-CBD	3.76	117.80	111.23
27	BD	5407	BCR	C24-C23-C22	3.75	131.79	126.23
27	BC	5516	BCR	C2-C1-C6	3.75	115.89	110.44
25	AA	408	MST	N3-C2-N1	-3.75	120.15	127.00
24	AC	512	CLA	C4D-C3D-CAD	3.75	112.17	108.11
27	BA	5411	BCR	C29-C30-C25	3.74	115.88	110.44
28	BC	5518	DGD	C3G-C2G-C1G	-3.74	103.06	111.78
30	BB	5601	SQD	C11-C10-C9	3.74	133.29	114.37
24	BC	5502	CLA	C4D-C3D-CAD	3.74	112.17	108.11
24	BC	5507	CLA	C4D-C3D-CAD	3.74	112.17	108.11
27	BC	5515	BCR	C2-C1-C6	3.74	115.86	110.44
24	BC	5508	CLA	CBA-CAA-C2A	3.73	124.90	113.79
24	AC	507	CLA	O2D-CGD-CBD	3.73	117.75	111.23
24	AB	615	CLA	C2A-C1A-CHA	3.73	130.34	123.87
27	BC	5516	BCR	C23-C24-C25	3.73	136.96	127.00
24	AC	505	CLA	C3A-C2A-C1A	3.73	106.92	101.34
24	BB	5614	CLA	O2D-CGD-CBD	3.72	117.74	111.23
24	AB	604	CLA	C4D-C3D-CAD	3.72	112.15	108.11
30	AB	622	SQD	C44-O6-C1	3.72	121.78	113.80
27	AC	516	BCR	C8-C7-C6	3.72	136.94	127.00
27	BX	5101	BCR	C38-C26-C27	-3.72	105.66	113.60
24	AD	401	CLA	O2A-CGA-CBA	3.72	123.18	111.83
24	BC	5506	CLA	O2A-CGA-CBA	3.72	123.18	111.83
27	BK	5102	BCR	C33-C5-C4	-3.72	105.67	113.60
27	AC	516	BCR	C1-C6-C5	-3.72	117.56	122.64
24	AB	607	CLA	C3B-C4B-NB	-3.72	107.21	110.53
24	BC	5502	CLA	CBA-CAA-C2A	3.72	124.85	113.79
27	BT	5101	BCR	C30-C25-C26	-3.71	117.56	122.64
31	AA	417	LMG	C9-O8-C28	3.71	130.69	117.12
32	BB	5603	LMT	C1B-O1B-C4'	-3.71	109.18	117.98
24	BB	5620	CLA	O2D-CGD-CBD	3.71	117.72	111.23
24	BB	5609	CLA	C4D-C3D-CAD	3.71	112.14	108.11
24	AB	603	CLA	O2A-CGA-CBA	3.71	123.14	111.83
30	BB	5601	SQD	O8-S-C6	-3.71	98.81	105.97
27	BC	5516	BCR	C33-C5-C4	-3.71	105.69	113.60
24	AC	509	CLA	C2A-C1A-CHA	3.71	130.30	123.87
24	BB	5607	CLA	C4D-C3D-CAD	3.71	112.13	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	5409	MST	N5-C4-N3	-3.71	120.19	126.26
24	BB	5611	CLA	C3A-C2A-C1A	3.70	106.89	101.34
35	AD	405	PL9	C15-C14-C16	3.70	121.66	115.23
24	BB	5609	CLA	C3A-C2A-C1A	3.70	106.88	101.34
27	AK	102	BCR	C1-C6-C5	-3.70	117.58	122.64
24	BC	5512	CLA	C2A-C1A-CHA	3.70	130.29	123.87
27	AB	618	BCR	C29-C30-C25	3.70	115.81	110.44
27	BB	5621	BCR	C38-C26-C27	-3.70	105.71	113.60
32	AB	629	LMT	C1B-O1B-C4'	-3.69	109.23	117.98
27	AT	101	BCR	C30-C25-C26	-3.69	117.59	122.64
24	BC	5508	CLA	O2D-CGD-CBD	3.69	117.68	111.23
27	AC	515	BCR	C29-C30-C25	3.69	115.80	110.44
24	AC	508	CLA	O2A-CGA-CBA	3.69	123.08	111.83
24	AB	612	CLA	C4D-C3D-CAD	3.69	112.11	108.11
27	BB	5622	BCR	C2-C1-C6	3.68	115.79	110.44
30	AB	627	SQD	C11-C10-C9	3.68	132.99	114.37
27	BB	5623	BCR	C29-C30-C25	3.68	115.79	110.44
35	AD	405	PL9	C25-C24-C26	3.68	121.62	115.23
36	BV	5201	HEM	CHA-C4D-C3D	-3.68	118.44	125.23
27	BJ	5101	BCR	C7-C8-C9	3.68	131.68	126.23
24	BC	5505	CLA	C3A-C2A-C1A	3.68	106.85	101.34
28	AH	101	DGD	O5D-C6D-C5D	3.67	117.70	109.42
27	BB	5622	BCR	C23-C24-C25	3.67	136.80	127.00
36	AF	101	HEM	C1B-NB-C4B	3.67	109.55	105.21
30	BB	5625	SQD	O8-S-C6	-3.66	98.90	105.97
24	AC	509	CLA	O2A-CGA-CBA	3.66	123.01	111.83
27	BK	5102	BCR	C1-C6-C5	-3.66	117.63	122.64
27	BT	5101	BCR	C33-C5-C4	-3.66	105.79	113.60
31	AJ	102	LMG	C12-C11-C10	3.66	127.11	113.69
25	BA	5409	MST	N3-C2-N1	-3.66	120.32	127.00
27	BB	5622	BCR	C29-C30-C25	3.66	115.76	110.44
24	AB	610	CLA	O2D-CGD-CBD	3.66	117.63	111.23
24	BB	5606	CLA	O2A-CGA-CBA	3.66	122.99	111.83
27	AX	101	BCR	C38-C26-C27	-3.66	105.80	113.60
24	AC	503	CLA	O2A-CGA-CBA	3.66	122.98	111.83
24	BC	5501	CLA	O2A-CGA-CBA	3.66	122.98	111.83
24	BC	5507	CLA	O2A-CGA-CBA	3.65	122.98	111.83
36	BV	5201	HEM	C1B-NB-C4B	3.65	109.53	105.21
24	AA	406	CLA	C4D-C3D-CAD	3.65	112.07	108.11
24	BC	5506	CLA	C4D-C3D-CAD	3.65	112.07	108.11
24	AC	512	CLA	C2A-C1A-CHA	3.65	130.20	123.87
27	AT	101	BCR	C33-C5-C4	-3.65	105.81	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	514	BCR	C29-C30-C25	3.65	115.73	110.44
24	AC	507	CLA	O2A-CGA-CBA	3.64	122.95	111.83
24	BB	5605	CLA	O2D-CGD-CBD	3.64	117.60	111.23
24	BC	5513	CLA	O2A-CGA-CBA	3.64	122.94	111.83
31	AJ	102	LMG	O1-C7-C8	3.64	119.67	110.82
32	BD	5411	LMT	O1B-C1B-C2B	3.64	117.04	108.09
24	BD	5402	CLA	O2D-CGD-CBD	3.64	117.59	111.23
35	BD	5406	PL9	C20-C19-C18	-3.64	114.29	123.63
24	AB	607	CLA	C3A-C2A-C1A	3.64	106.78	101.34
24	BC	5513	CLA	C3B-C4B-NB	-3.64	107.28	110.53
24	BB	5612	CLA	O2D-CGD-CBD	3.63	117.58	111.23
31	BD	5408	LMG	C9-C8-C7	3.63	120.26	111.78
24	AB	602	CLA	C4D-C3D-CAD	3.63	112.05	108.11
28	BA	5412	DGD	C3A-C2A-C1A	-3.63	100.38	113.69
31	AJ	102	LMG	C9-C8-C7	3.63	120.25	111.78
24	BC	5511	CLA	O2D-CGD-CBD	3.63	117.58	111.23
27	AK	102	BCR	C30-C25-C26	-3.62	117.68	122.64
25	AA	408	MST	C6-N5-C4	3.62	120.34	113.85
24	AC	506	CLA	O2A-CGA-CBA	3.62	122.88	111.83
27	AD	406	BCR	C8-C7-C6	3.62	136.68	127.00
27	AB	618	BCR	C2-C1-C6	3.62	115.70	110.44
31	BA	5402	LMG	O8-C9-C8	-3.62	97.96	108.40
24	AA	407	CLA	C4D-C3D-CAD	3.62	112.04	108.11
24	AB	610	CLA	C4D-C3D-CAD	3.62	112.04	108.11
24	AC	507	CLA	C4D-C3D-CAD	3.61	112.03	108.11
27	BB	5623	BCR	C2-C1-C6	3.61	115.69	110.44
27	BX	5101	BCR	C30-C25-C26	-3.61	117.70	122.64
24	BC	5503	CLA	O2A-CGA-CBA	3.61	122.85	111.83
32	AD	409	LMT	O1B-C1B-C2B	3.61	116.97	108.09
27	BD	5407	BCR	C8-C7-C6	3.61	136.64	127.00
24	BB	5607	CLA	O2A-CGA-CBA	3.61	122.84	111.83
24	BC	5509	CLA	C2A-C1A-CHA	3.61	130.13	123.87
36	BV	5201	HEM	CBD-CAD-C3D	-3.60	102.58	112.53
27	BC	5516	BCR	C8-C7-C6	3.60	136.61	127.00
27	AC	514	BCR	C38-C26-C27	-3.60	105.93	113.60
24	AB	612	CLA	C3A-C2A-C1A	3.60	106.73	101.34
27	AB	618	BCR	C30-C25-C26	-3.59	117.72	122.64
24	AC	501	CLA	CAA-C2A-C1A	-3.59	100.20	111.97
27	AB	617	BCR	C38-C26-C27	-3.59	105.94	113.60
28	AA	411	DGD	C3A-C2A-C1A	-3.59	100.54	113.69
27	AA	410	BCR	C29-C30-C25	3.59	115.65	110.44
24	BB	5612	CLA	C4D-C3D-CAD	3.59	112.00	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BX	5101	BCR	C23-C24-C25	3.59	136.58	127.00
24	AB	607	CLA	C4D-C3D-CAD	3.58	112.00	108.11
24	AD	404	CLA	CBA-CAA-C2A	3.58	124.45	113.79
24	AC	504	CLA	C4D-C3D-CAD	3.58	112.00	108.11
24	BC	5501	CLA	CAA-C2A-C1A	-3.58	100.24	111.97
27	AX	101	BCR	C23-C24-C25	3.58	136.56	127.00
27	AC	515	BCR	C38-C26-C27	-3.58	105.96	113.60
25	BA	5409	MST	C6-N5-C4	3.58	120.26	113.85
24	BC	5506	CLA	CBA-CAA-C2A	3.58	124.44	113.79
24	BC	5513	CLA	C4D-C3D-CAD	3.58	111.99	108.11
24	AC	506	CLA	C4D-C3D-CAD	3.57	111.98	108.11
28	BH	5101	DGD	O5D-C6D-C5D	3.57	117.47	109.42
24	AB	608	CLA	O2D-CGD-CBD	3.57	117.47	111.23
27	AC	516	BCR	C33-C5-C4	-3.57	105.99	113.60
27	BB	5622	BCR	C30-C25-C26	-3.56	117.77	122.64
24	AB	616	CLA	O2D-CGD-CBD	3.56	117.46	111.23
31	BD	5408	LMG	C12-C11-C10	3.56	126.75	113.69
24	BC	5508	CLA	O2A-CGA-CBA	3.56	122.69	111.83
27	AD	406	BCR	C2-C1-C6	3.56	115.61	110.44
24	BA	5408	CLA	O2A-CGA-CBA	3.56	122.67	111.83
27	BC	5515	BCR	C33-C5-C4	-3.55	106.02	113.60
24	BC	5504	CLA	C4D-C3D-CAD	3.55	111.96	108.11
34	AD	403	PHO	O2A-CGA-CBA	3.55	122.66	111.83
36	AV	201	HEM	C1B-NB-C4B	3.55	109.41	105.21
28	BA	5412	DGD	O1G-C1A-O1A	-3.55	114.75	123.63
24	AC	502	CLA	O2A-CGA-CBA	3.55	122.66	111.83
27	BB	5622	BCR	C8-C7-C6	3.55	136.47	127.00
27	BB	5621	BCR	C33-C5-C4	-3.54	106.04	113.60
24	BB	5618	CLA	CAA-CBA-CGA	-3.54	103.15	113.21
24	BA	5405	CLA	C4D-C3D-CAD	3.54	111.95	108.11
27	AC	515	BCR	C33-C5-C4	-3.54	106.05	113.60
28	AA	411	DGD	O1G-C1A-O1A	-3.54	114.78	123.63
24	AC	510	CLA	C4D-C3D-CAD	3.54	111.95	108.11
24	BB	5617	CLA	C3B-C4B-NB	-3.54	107.37	110.53
24	AC	512	CLA	O2A-CGA-CBA	3.53	122.61	111.83
30	BB	5625	SQD	C44-O6-C1	3.53	121.37	113.80
24	AC	510	CLA	O2A-CGA-CBA	3.53	122.61	111.83
24	AC	513	CLA	C4D-C3D-CAD	3.53	111.94	108.11
24	BC	5508	CLA	C3A-C2A-C1A	3.53	106.63	101.34
35	BD	5406	PL9	C25-C24-C26	3.53	121.36	115.23
24	AC	513	CLA	C3B-C4B-NB	-3.53	107.38	110.53
24	BB	5606	CLA	O2D-CGD-CBD	3.53	117.39	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5501	CLA	C2A-C1A-CHA	3.52	129.98	123.87
24	AB	615	CLA	O2D-CGD-CBD	3.52	117.39	111.23
27	AC	516	BCR	C30-C25-C26	-3.52	117.82	122.64
24	BC	5502	CLA	O2A-CGA-CBA	3.52	122.58	111.83
24	BB	5616	CLA	C3A-C2A-C1A	3.52	106.61	101.34
31	AB	621	LMG	C12-C11-C10	-3.52	100.80	113.69
24	AC	501	CLA	C2A-C1A-CHA	3.52	129.97	123.87
30	BA	5414	SQD	O48-C23-C24	3.51	122.54	111.83
27	BC	5514	BCR	C2-C1-C6	3.51	115.54	110.44
24	BB	5613	CLA	C4D-C3D-CAD	3.51	111.92	108.11
31	BB	5624	LMG	C33-C32-C31	-3.51	96.64	114.37
27	BT	5101	BCR	C38-C26-C27	-3.51	106.12	113.60
34	BD	5404	PHO	O2A-CGA-CBA	3.51	122.52	111.83
34	AD	403	PHO	C1A-C2A-C3A	3.50	106.17	102.84
24	AA	407	CLA	O2A-CGA-CBA	3.50	122.52	111.83
24	AB	605	CLA	C3A-C2A-C1A	3.50	106.59	101.34
27	AB	618	BCR	C23-C24-C25	3.50	136.35	127.00
24	BB	5615	CLA	C3A-C2A-C1A	3.50	106.58	101.34
27	AC	516	BCR	C38-C26-C27	-3.50	106.13	113.60
36	AV	201	HEM	CBD-CAD-C3D	-3.50	102.86	112.53
24	AC	506	CLA	CBA-CAA-C2A	3.50	124.20	113.79
30	AA	413	SQD	O48-C23-C24	3.49	122.49	111.83
31	BB	5624	LMG	C39-C38-C37	3.49	132.03	114.37
24	AB	611	CLA	O2D-CGD-CBD	3.49	117.33	111.23
28	AE	101	DGD	O5D-C1E-C2E	3.49	113.58	108.27
27	BC	5516	BCR	C1-C6-C5	-3.49	117.86	122.64
31	AJ	102	LMG	C9-O8-C28	3.49	129.86	117.12
24	AC	508	CLA	O2D-CGD-CBD	3.48	117.32	111.23
27	BJ	5101	BCR	C33-C5-C4	-3.48	106.17	113.60
24	AB	605	CLA	O2A-CGA-CBA	3.48	122.45	111.83
31	BD	5410	LMG	C9-O8-C28	3.48	129.84	117.12
36	BF	5101	HEM	C1B-NB-C4B	3.48	109.33	105.21
31	AD	408	LMG	C9-O8-C28	3.48	129.82	117.12
28	AA	411	DGD	C1G-O1G-C1A	-3.47	104.42	117.12
24	AB	614	CLA	CAA-CBA-CGA	-3.47	103.35	113.21
28	BA	5412	DGD	C1G-O1G-C1A	-3.47	104.43	117.12
29	AA	412	LHG	O8-C23-C24	3.47	122.42	111.83
24	BB	5620	CLA	C4D-C3D-CAD	3.47	111.87	108.11
24	BA	5408	CLA	C3A-C2A-C1A	3.47	106.53	101.34
24	AC	504	CLA	O2A-CGA-CBA	3.47	122.41	111.83
27	AB	618	BCR	C8-C7-C6	3.47	136.26	127.00
28	BC	5519	DGD	C3B-C2B-C1B	3.47	126.39	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	5405	CLA	O2A-CGA-CBA	3.47	122.40	111.83
24	BC	5509	CLA	O2A-CGA-CBA	3.47	122.40	111.83
31	BB	5624	LMG	C12-C11-C10	-3.46	101.01	113.69
24	AB	616	CLA	C4D-C3D-CAD	3.46	111.86	108.11
24	BB	5606	CLA	C4D-C3D-CAD	3.46	111.86	108.11
27	BC	5514	BCR	C29-C30-C25	3.46	115.47	110.44
27	AT	101	BCR	C38-C26-C27	-3.46	106.22	113.60
24	AA	404	CLA	O2A-CGA-CBA	3.46	122.38	111.83
24	BC	5511	CLA	O2A-CGA-CBA	3.46	122.37	111.83
24	BC	5513	CLA	O2D-CGD-CBD	3.45	117.27	111.23
27	AC	515	BCR	C30-C25-C26	-3.45	117.92	122.64
31	AD	408	LMG	C12-C11-C10	3.45	126.33	113.69
31	AI	101	LMG	C12-C11-C10	-3.45	101.06	113.69
27	AK	102	BCR	C38-C26-C27	-3.45	106.25	113.60
27	BC	5515	BCR	C38-C26-C27	-3.45	106.25	113.60
28	BB	5602	DGD	O1G-C1G-C2G	-3.45	98.46	108.40
24	BC	5511	CLA	CAA-C2A-C1A	-3.44	100.70	111.97
27	AJ	101	BCR	C33-C5-C4	-3.44	106.26	113.60
31	BI	5101	LMG	C12-C11-C10	-3.44	101.09	113.69
31	AB	621	LMG	C39-C38-C37	3.44	131.74	114.37
27	BC	5515	BCR	C1-C6-C5	-3.44	117.94	122.64
28	AE	101	DGD	C2G-O2G-C1B	3.44	126.02	117.80
24	AB	613	CLA	C3B-C4B-NB	-3.43	107.46	110.53
24	AC	502	CLA	C4D-C3D-CAD	3.43	111.83	108.11
24	AB	605	CLA	CAA-C2A-C1A	-3.43	100.74	111.97
24	AC	501	CLA	O2A-CGA-CBA	3.43	122.28	111.83
24	AB	613	CLA	C4D-C3D-CAD	3.43	111.83	108.11
24	AC	508	CLA	C3A-C2A-C1A	3.42	106.47	101.34
28	AB	628	DGD	O3G-C3G-C2G	3.42	119.14	110.82
35	BD	5406	PL9	C11-C9-C8	-3.42	113.48	121.17
24	BC	5501	CLA	CBA-CAA-C2A	3.42	123.97	113.79
24	AC	503	CLA	C7-C6-C5	-3.42	104.15	113.26
24	BB	5620	CLA	C2A-C1A-CHA	3.42	129.80	123.87
31	AB	621	LMG	C33-C32-C31	-3.42	97.09	114.37
30	AA	416	SQD	C32-C31-C30	3.42	131.63	114.37
24	AC	504	CLA	C3A-C2A-C1A	3.41	106.45	101.34
24	AB	601	CLA	O2A-CGA-CBA	3.41	122.24	111.83
27	BD	5407	BCR	C2-C1-C6	3.41	115.40	110.44
24	BD	5405	CLA	CBA-CAA-C2A	3.41	123.94	113.79
24	AC	511	CLA	O2A-CGA-CBA	3.41	122.23	111.83
27	BX	5101	BCR	C24-C23-C22	3.41	131.28	126.23
27	BK	5102	BCR	C8-C9-C10	-3.41	113.64	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5618	CLA	O2D-CGD-CBD	3.41	117.19	111.23
35	BD	5406	PL9	C7-C3-C2	-3.41	119.37	123.39
24	AC	501	CLA	CAA-CBA-CGA	-3.41	103.53	113.21
27	BB	5621	BCR	C30-C25-C26	-3.41	117.98	122.64
31	AA	417	LMG	O8-C9-C8	-3.40	98.58	108.40
24	BC	5504	CLA	C3A-C2A-C1A	3.40	106.44	101.34
28	BC	5517	DGD	C3B-C2B-C1B	3.40	126.16	113.69
24	BB	5614	CLA	C4D-C3D-CAD	3.40	111.80	108.11
28	BC	5518	DGD	O6E-C1E-O5D	3.40	118.08	110.04
31	BI	5101	LMG	C8-O7-C10	3.40	125.93	117.80
31	BD	5410	LMG	C12-C11-C10	3.40	126.15	113.69
28	BE	5102	DGD	C2G-O2G-C1B	3.40	125.93	117.80
24	AB	616	CLA	C2A-C1A-CHA	3.40	129.76	123.87
36	AV	201	HEM	CBC-CAC-C3C	-3.40	110.55	127.53
27	BT	5101	BCR	C16-C17-C18	3.40	132.04	127.28
28	BC	5517	DGD	C6B-C5B-C4B	-3.40	97.20	114.37
24	AB	608	CLA	C4D-C3D-CAD	3.40	111.79	108.11
28	AC	517	DGD	C6B-C5B-C4B	-3.39	97.22	114.37
24	BC	5508	CLA	C3B-C4B-NB	-3.39	107.50	110.53
24	BB	5615	CLA	C4D-C3D-CAD	3.39	111.79	108.11
28	AB	628	DGD	O1G-C1G-C2G	-3.39	98.63	108.40
24	BC	5510	CLA	O2A-CGA-CBA	3.39	122.16	111.83
24	BB	5609	CLA	O2A-CGA-CBA	3.39	122.16	111.83
27	BK	5102	BCR	C30-C25-C26	-3.39	118.01	122.64
24	BB	5607	CLA	O2D-CGD-CBD	3.38	117.14	111.23
27	AC	515	BCR	C1-C6-C5	-3.38	118.01	122.64
35	BD	5406	PL9	C50-C49-C48	-3.38	112.51	122.66
30	BA	5401	SQD	C32-C31-C30	3.38	131.44	114.37
27	BC	5516	BCR	C38-C26-C27	-3.38	106.40	113.60
24	AC	511	CLA	CAA-C2A-C1A	-3.37	100.92	111.97
24	BB	5609	CLA	CAA-C2A-C1A	-3.37	100.93	111.97
24	AD	401	CLA	C4D-C3D-CAD	3.37	111.77	108.11
27	AC	514	BCR	C1-C6-C5	-3.37	118.03	122.64
24	BB	5611	CLA	CAA-CBA-CGA	-3.37	103.64	113.21
31	BD	5408	LMG	C9-O8-C28	3.37	129.43	117.12
34	AD	402	PHO	CBC-CAC-C3C	-3.37	108.05	112.87
24	AB	605	CLA	O2D-CGD-CBD	3.37	117.11	111.23
27	BK	5102	BCR	C38-C26-C27	-3.36	106.43	113.60
24	AC	503	CLA	C3A-C2A-C1A	3.36	106.37	101.34
27	BX	5101	BCR	C1-C6-C5	-3.36	118.04	122.64
24	AD	401	CLA	C3B-C4B-NB	-3.36	107.53	110.53
36	BF	5101	HEM	O1D-CGD-CBD	-3.36	112.44	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5512	CLA	O2A-CGA-CBA	3.36	122.08	111.83
24	AB	603	CLA	O2D-CGD-CBD	3.36	117.10	111.23
24	BC	5502	CLA	CAA-C2A-C1A	-3.36	100.97	111.97
24	AC	502	CLA	O2D-CGD-CBD	3.35	117.09	111.23
35	AD	405	PL9	C51-C49-C50	3.35	122.30	114.59
24	BB	5614	CLA	O2A-CGA-CBA	3.35	122.05	111.83
27	BX	5101	BCR	C8-C7-C6	3.35	135.95	127.00
27	AT	101	BCR	C24-C23-C22	3.35	131.19	126.23
36	AV	201	HEM	CAD-C3D-C2D	3.35	134.13	127.87
27	AX	101	BCR	C8-C7-C6	3.34	135.93	127.00
24	AC	513	CLA	O2D-CGD-CBD	3.34	117.08	111.23
27	BC	5516	BCR	C30-C25-C26	-3.34	118.07	122.64
24	AD	401	CLA	O2D-CGD-CBD	3.34	117.06	111.23
24	AA	407	CLA	C3B-C4B-NB	-3.34	107.55	110.53
24	AB	606	CLA	C2A-C1A-CHA	3.34	129.66	123.87
27	AB	617	BCR	C30-C25-C26	-3.33	118.08	122.64
24	BB	5610	CLA	C2A-C1A-CHA	3.33	129.65	123.87
27	BC	5515	BCR	C30-C25-C26	-3.33	118.09	122.64
27	AC	514	BCR	C2-C1-C6	3.33	115.28	110.44
36	BV	5201	HEM	CBC-CAC-C3C	-3.33	110.90	127.53
24	BB	5605	CLA	O2A-CGA-CBA	3.33	121.98	111.83
27	AX	101	BCR	C24-C23-C22	3.32	131.15	126.23
27	AB	617	BCR	C33-C5-C4	-3.32	106.52	113.60
28	AC	518	DGD	O6E-C1E-O5D	3.32	117.88	110.04
24	BC	5501	CLA	CAA-CBA-CGA	-3.32	103.79	113.21
24	BB	5619	CLA	O2D-CGD-CBD	3.31	117.02	111.23
28	BC	5519	DGD	O1G-C1G-C2G	-3.31	98.84	108.40
24	AA	404	CLA	C4D-C3D-CAD	3.31	111.70	108.11
24	BB	5617	CLA	C4D-C3D-CAD	3.31	111.70	108.11
31	AD	408	LMG	C17-C16-C15	-3.31	97.65	114.37
24	BC	5502	CLA	O2D-CGD-CBD	3.31	117.01	111.23
34	BD	5404	PHO	O1D-CGD-CBD	-3.31	119.71	124.72
35	AD	405	PL9	C50-C49-C48	-3.30	112.74	122.66
27	BA	5411	BCR	C38-C26-C27	-3.30	106.56	113.60
24	AB	610	CLA	O2A-CGA-CBA	3.30	121.89	111.83
24	AA	407	CLA	C3A-C2A-C1A	3.30	106.28	101.34
24	BA	5405	CLA	C3B-C4B-NB	-3.30	107.59	110.53
31	BB	5624	LMG	O7-C10-O9	-3.30	116.00	123.70
27	AK	102	BCR	C8-C7-C6	3.29	135.80	127.00
34	AD	403	PHO	O1D-CGD-CBD	-3.29	119.73	124.72
31	AI	101	LMG	C7-O1-C1	-3.29	106.74	113.80
28	AB	628	DGD	O6D-C5D-C6D	3.29	113.22	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	611	CLA	C3A-C2A-C1A	3.29	106.26	101.34
28	BE	5102	DGD	O5D-C1E-C2E	3.29	113.27	108.27
27	AC	514	BCR	C33-C5-C4	-3.28	106.59	113.60
31	AI	101	LMG	C8-O7-C10	3.28	125.65	117.80
27	BB	5623	BCR	C38-C26-C27	-3.28	106.60	113.60
27	AJ	101	BCR	C8-C7-C6	3.28	135.76	127.00
24	AB	612	CLA	C3B-C4B-NB	-3.28	107.60	110.53
31	AC	520	LMG	C8-O7-C10	3.28	125.64	117.80
27	BC	5514	BCR	C38-C26-C27	-3.28	106.61	113.60
24	AB	602	CLA	O2D-CGD-CBD	3.28	116.96	111.23
24	BB	5615	CLA	CAA-C2A-C1A	-3.28	101.23	111.97
35	AD	405	PL9	C11-C9-C8	-3.28	113.81	121.17
36	AV	201	HEM	CAB-C3B-C2B	-3.28	117.78	128.43
24	AB	609	CLA	C4D-C3D-CAD	3.28	111.66	108.11
27	AC	515	BCR	C8-C7-C6	3.27	135.75	127.00
31	AM	101	LMG	C12-C11-C10	-3.27	101.71	113.69
34	BD	5403	PHO	C3D-C4D-ND	3.27	111.90	107.71
27	BA	5411	BCR	C23-C24-C25	3.27	135.74	127.00
27	AB	617	BCR	C2-C1-C6	3.27	115.19	110.44
24	AC	501	CLA	CBA-CAA-C2A	3.27	123.52	113.79
27	AK	102	BCR	C8-C9-C10	-3.27	113.87	119.01
28	BH	5101	DGD	C4B-C3B-C2B	3.27	125.12	113.13
24	BC	5505	CLA	O2D-CGD-CBD	3.27	116.94	111.23
36	BV	5201	HEM	CAD-C3D-C2D	3.26	133.98	127.87
24	BB	5613	CLA	O2D-CGD-CBD	3.26	116.94	111.23
27	AB	619	BCR	C2-C1-C6	3.26	115.18	110.44
27	BC	5515	BCR	C8-C7-C6	3.26	135.71	127.00
35	BD	5406	PL9	C35-C34-C33	-3.26	115.25	123.63
24	BA	5408	CLA	C3B-C4B-NB	-3.26	107.62	110.53
35	BD	5406	PL9	C51-C49-C50	3.25	122.08	114.59
27	AA	410	BCR	C38-C26-C27	-3.25	106.66	113.60
27	BA	5411	BCR	C33-C5-C4	-3.25	106.66	113.60
31	AC	520	LMG	C14-C13-C12	-3.25	97.94	114.37
31	AA	417	LMG	O1-C7-C8	3.25	118.72	110.82
24	BC	5503	CLA	C7-C6-C5	-3.25	104.61	113.26
24	AB	614	CLA	CAA-C2A-C1A	-3.25	101.34	111.97
27	BB	5621	BCR	C2-C1-C6	3.25	115.15	110.44
31	BI	5101	LMG	C7-O1-C1	-3.24	106.84	113.80
27	AA	410	BCR	C23-C24-C25	3.24	135.66	127.00
24	BC	5509	CLA	C3B-C4B-NB	-3.24	107.64	110.53
24	BB	5619	CLA	C3A-C2A-C1A	3.24	106.20	101.34
24	BC	5504	CLA	O2A-CGA-CBA	3.24	121.72	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	406	CLA	O2A-CGA-O1A	-3.24	115.52	123.63
31	BD	5410	LMG	C17-C16-C15	-3.24	97.98	114.37
27	BT	5101	BCR	C24-C23-C22	3.24	131.03	126.23
34	AD	402	PHO	C3D-C4D-ND	3.24	111.86	107.71
24	BC	5503	CLA	C3A-C2A-C1A	3.24	106.19	101.34
27	BC	5515	BCR	C35-C13-C12	3.24	123.03	118.09
28	BH	5101	DGD	C1D-O6D-C5D	-3.24	107.40	113.72
27	AK	102	BCR	C24-C23-C22	3.24	131.02	126.23
27	BK	5102	BCR	C24-C23-C22	3.23	131.02	126.23
28	BB	5602	DGD	O6D-C5D-C6D	3.23	113.10	106.69
28	AE	101	DGD	C1G-O1G-C1A	3.23	128.93	117.12
28	AC	518	DGD	O2G-C2G-C3G	3.23	119.92	108.34
24	BC	5504	CLA	C3B-C4B-NB	-3.23	107.65	110.53
28	BB	5602	DGD	O3G-C3G-C2G	3.23	118.66	110.82
27	AT	101	BCR	C7-C8-C9	3.22	131.01	126.23
35	AD	405	PL9	C35-C34-C33	-3.22	115.35	123.63
31	AB	621	LMG	O7-C10-O9	-3.22	116.17	123.70
24	AA	405	CLA	CAA-CBA-CGA	-3.22	104.07	113.21
34	AD	402	PHO	OBD-CAD-C3D	3.22	132.91	127.89
24	BB	5616	CLA	C3B-C4B-NB	-3.22	107.66	110.53
28	AC	519	DGD	C3B-C2B-C1B	3.22	125.48	113.69
29	BA	5413	LHG	O8-C23-C24	3.22	121.64	111.83
28	BC	5518	DGD	O2G-C2G-C3G	3.22	119.88	108.34
27	AA	410	BCR	C30-C25-C26	-3.22	118.24	122.64
24	BB	5618	CLA	CAA-C2A-C1A	-3.21	101.44	111.97
27	AA	410	BCR	C2-C1-C6	3.21	115.11	110.44
36	AF	101	HEM	O1D-CGD-CBD	-3.21	112.90	123.09
24	BB	5612	CLA	O2A-CGA-CBA	3.21	121.63	111.83
27	AD	406	BCR	C16-C17-C18	3.21	131.78	127.28
27	AB	618	BCR	C24-C23-C22	3.21	130.98	126.23
27	AB	619	BCR	C23-C24-C25	3.21	135.57	127.00
28	AC	517	DGD	C3B-C2B-C1B	3.21	125.45	113.69
31	BD	5409	LMG	O1-C7-C8	-3.21	103.02	110.82
24	BD	5402	CLA	C3B-C4B-NB	-3.21	107.67	110.53
24	AC	502	CLA	CAA-C2A-C1A	-3.21	101.47	111.97
24	AC	508	CLA	C3B-C4B-NB	-3.20	107.67	110.53
27	BK	5102	BCR	C12-C13-C14	-3.20	113.98	119.01
36	AF	101	HEM	CBD-CAD-C3D	-3.20	103.69	112.53
24	AB	615	CLA	C3A-C2A-C1A	3.20	106.13	101.34
28	BE	5102	DGD	C1G-O1G-C1A	3.20	128.80	117.12
24	BC	5506	CLA	C3A-C2A-C1A	3.19	106.12	101.34
35	AD	405	PL9	C7-C3-C2	-3.19	119.63	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5615	CLA	O2D-CGD-CBD	3.19	116.81	111.23
24	AC	505	CLA	O2A-CGA-CBA	3.19	121.56	111.83
30	BB	5625	SQD	C45-O47-C7	3.19	125.43	117.80
31	BM	5102	LMG	O7-C8-C7	3.19	119.78	108.34
28	AH	101	DGD	C4B-C3B-C2B	3.19	124.84	113.13
24	BB	5616	CLA	O2A-CGA-CBA	3.19	121.55	111.83
31	BC	5520	LMG	C14-C13-C12	-3.19	98.27	114.37
24	BB	5612	CLA	C3B-C4B-NB	-3.18	107.69	110.53
24	AB	607	CLA	C2A-C1A-CHA	3.18	129.39	123.87
30	BA	5414	SQD	C32-C31-C30	3.18	130.46	114.37
27	BC	5514	BCR	C1-C6-C5	-3.18	118.29	122.64
31	BC	5520	LMG	C8-O7-C10	3.18	125.41	117.80
36	BF	5101	HEM	CBD-CAD-C3D	-3.18	103.74	112.53
27	BJ	5101	BCR	C8-C7-C6	3.18	135.49	127.00
24	AC	506	CLA	C3A-C2A-C1A	3.18	106.10	101.34
24	AB	608	CLA	O2A-CGA-CBA	3.18	121.53	111.83
28	AA	411	DGD	O2G-C2G-C3G	3.17	119.72	108.34
24	BA	5407	CLA	O2A-CGA-O1A	-3.17	115.70	123.63
31	BD	5408	LMG	C15-C14-C13	-3.17	98.37	114.37
27	BD	5407	BCR	C7-C8-C9	3.16	130.91	126.23
27	BK	5102	BCR	C8-C7-C6	3.16	135.44	127.00
27	BA	5411	BCR	C30-C25-C26	-3.16	118.32	122.64
27	AB	619	BCR	C38-C26-C27	-3.16	106.86	113.60
24	BC	5507	CLA	C7-C6-C5	-3.16	104.84	113.26
24	BA	5406	CLA	O2A-CGA-O1A	-3.16	115.73	123.63
31	AJ	102	LMG	C15-C14-C13	-3.16	98.41	114.37
27	BX	5101	BCR	C33-C5-C4	-3.16	106.86	113.60
36	BF	5101	HEM	C4C-NC-C1C	3.16	110.97	105.82
31	BD	5408	LMG	O7-C10-C11	-3.16	104.65	111.48
31	AD	407	LMG	C16-C15-C14	3.15	130.31	114.37
27	BD	5407	BCR	C33-C5-C4	-3.15	106.87	113.60
24	AD	404	CLA	O2A-CGA-CBA	3.15	121.45	111.83
24	BB	5613	CLA	CBA-CAA-C2A	3.15	123.17	113.79
28	BA	5412	DGD	O2G-C2G-C3G	3.15	119.64	108.34
27	AA	410	BCR	C33-C5-C4	-3.15	106.89	113.60
27	AT	101	BCR	C2-C1-C6	3.15	115.01	110.44
24	BA	5406	CLA	CAA-CBA-CGA	-3.15	104.28	113.21
34	BD	5403	PHO	O1D-CGD-CBD	-3.14	119.95	124.72
28	BC	5519	DGD	CBA-CAA-C9A	-3.14	98.49	114.37
31	AM	101	LMG	O7-C8-C7	3.14	119.61	108.34
27	BB	5623	BCR	C30-C25-C26	-3.14	118.35	122.64
28	AB	628	DGD	C3B-C2B-C1B	3.14	125.19	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5609	CLA	CED-O2D-CGD	3.14	123.03	115.92
24	BC	5512	CLA	C3B-C4B-NB	-3.14	107.73	110.53
28	BB	5602	DGD	C3B-C2B-C1B	3.13	125.18	113.69
31	BM	5102	LMG	C12-C11-C10	-3.13	102.21	113.69
36	BV	5201	HEM	CAB-C3B-C2B	-3.13	118.25	128.43
27	BB	5622	BCR	C24-C23-C22	3.13	130.87	126.23
24	AA	405	CLA	C3A-C2A-C1A	3.12	106.02	101.34
36	BF	5101	HEM	CBC-CAC-C3C	-3.12	111.92	127.53
24	AB	609	CLA	CBA-CAA-C2A	3.12	123.08	113.79
31	BA	5402	LMG	O1-C7-C8	3.12	118.41	110.82
24	BC	5505	CLA	O2A-CGA-CBA	3.12	121.36	111.83
27	AB	619	BCR	C30-C25-C26	-3.12	118.37	122.64
27	AT	101	BCR	C16-C17-C18	3.12	131.66	127.28
27	BT	5101	BCR	C2-C1-C6	3.12	114.97	110.44
31	AD	407	LMG	C12-C11-C10	3.12	125.13	113.69
31	BD	5409	LMG	C16-C15-C14	3.12	130.13	114.37
27	AB	619	BCR	C8-C7-C6	3.12	135.33	127.00
24	AC	506	CLA	C3B-C4B-NB	-3.12	107.75	110.53
27	AC	514	BCR	C30-C25-C26	-3.11	118.38	122.64
27	BB	5623	BCR	C8-C7-C6	3.11	135.32	127.00
28	AC	519	DGD	O1G-C1G-C2G	-3.11	99.42	108.40
24	BB	5611	CLA	C2A-C1A-CHA	3.11	129.27	123.87
24	AC	509	CLA	C3B-C4B-NB	-3.11	107.75	110.53
24	AC	507	CLA	C2A-C1A-CHA	3.11	129.26	123.87
27	AX	101	BCR	C33-C5-C4	-3.11	106.97	113.60
31	BD	5408	LMG	O7-C8-C9	-3.11	97.20	108.34
30	AA	413	SQD	C32-C31-C30	3.11	130.06	114.37
24	AB	603	CLA	C7-C6-C5	-3.10	105.00	113.26
28	AH	101	DGD	C1D-O6D-C5D	-3.10	107.66	113.72
24	AB	607	CLA	CAA-CBA-CGA	-3.10	104.41	113.21
27	AT	101	BCR	C1-C6-C5	-3.10	118.40	122.64
31	BA	5402	LMG	C12-C11-C10	3.10	125.05	113.69
24	AC	501	CLA	O2D-CGD-CBD	3.10	116.64	111.23
31	BD	5409	LMG	C12-C11-C10	3.09	125.03	113.69
27	AC	515	BCR	C16-C17-C18	3.09	131.62	127.28
24	AC	504	CLA	C3B-C4B-NB	-3.09	107.77	110.53
27	BD	5407	BCR	C16-C17-C18	3.09	131.61	127.28
24	AC	511	CLA	C6-C7-C8	-3.09	105.70	115.97
32	BC	5522	LMT	C4-C3-C2	-3.09	98.77	114.37
27	AX	101	BCR	C1-C6-C5	-3.08	118.42	122.64
27	BT	5101	BCR	C1-C6-C5	-3.08	118.42	122.64
27	BC	5514	BCR	C35-C13-C12	3.08	122.80	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	609	CLA	O2D-CGD-CBD	3.08	116.62	111.23
24	AC	504	CLA	CAA-CBA-CGA	-3.08	104.47	113.21
24	AB	601	CLA	C2A-C1A-CHA	3.08	129.20	123.87
24	AB	614	CLA	O2D-CGD-CBD	3.07	116.61	111.23
36	AF	101	HEM	CBC-CAC-C3C	-3.07	112.17	127.53
24	BC	5507	CLA	C2A-C1A-CHA	3.07	129.20	123.87
27	AB	618	BCR	C33-C5-C4	-3.07	107.05	113.60
24	AA	404	CLA	C3B-C4B-NB	-3.07	107.79	110.53
32	AI	103	LMT	C4-C3-C2	-3.07	98.87	114.37
24	BC	5504	CLA	CAA-CBA-CGA	-3.07	104.50	113.21
24	BD	5405	CLA	CAA-C2A-C1A	-3.06	101.94	111.97
24	AB	611	CLA	CAA-C2A-C1A	-3.06	101.94	111.97
27	BX	5101	BCR	C12-C13-C14	-3.06	114.20	119.01
24	BD	5402	CLA	C2A-C1A-CHA	3.06	129.18	123.87
28	BH	5101	DGD	C3G-C2G-C1G	-3.06	104.65	111.78
31	AJ	102	LMG	O7-C8-C9	-3.06	97.37	108.34
24	BD	5405	CLA	C3A-C2A-C1A	3.06	105.92	101.34
24	AB	605	CLA	CED-O2D-CGD	3.05	122.84	115.92
24	BC	5506	CLA	C3B-C4B-NB	-3.05	107.81	110.53
24	AB	610	CLA	C2A-C1A-CHA	3.05	129.16	123.87
27	AD	406	BCR	C33-C5-C4	-3.05	107.09	113.60
24	AC	507	CLA	C7-C6-C5	-3.05	105.14	113.26
31	AD	407	LMG	O1-C7-C8	-3.05	103.41	110.82
27	BX	5101	BCR	C35-C13-C12	3.05	122.74	118.09
24	AD	404	CLA	CAA-C2A-C1A	-3.04	102.00	111.97
31	AA	417	LMG	C12-C11-C10	3.04	124.84	113.69
24	AC	513	CLA	CED-O2D-CGD	3.04	122.82	115.92
32	BB	5603	LMT	C9-C8-C7	-3.04	98.99	114.37
28	AC	519	DGD	CBA-CAA-C9A	-3.04	99.00	114.37
24	AB	609	CLA	C3B-C4B-NB	-3.04	107.82	110.53
27	AB	619	BCR	C33-C5-C4	-3.04	107.12	113.60
35	BD	5406	PL9	C15-C14-C13	-3.03	115.83	123.63
36	BF	5101	HEM	CAB-C3B-C2B	-3.03	118.58	128.43
24	BA	5408	CLA	CBA-CAA-C2A	3.03	122.81	113.79
32	AB	629	LMT	C9-C8-C7	-3.03	99.06	114.37
24	BB	5609	CLA	O2D-CGD-CBD	3.03	116.52	111.23
24	BC	5508	CLA	CED-O2D-CGD	3.03	122.78	115.92
24	AB	610	CLA	C3A-C2A-C1A	3.03	105.87	101.34
24	AB	613	CLA	C2A-C1A-CHA	3.03	129.12	123.87
27	BB	5623	BCR	C23-C24-C25	3.03	135.08	127.00
24	AC	508	CLA	CED-O2D-CGD	3.02	122.78	115.92
24	BB	5614	CLA	C2A-C1A-CHA	3.02	129.11	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5510	CLA	C3B-C4B-NB	-3.02	107.83	110.53
34	BD	5403	PHO	OBD-CAD-C3D	3.02	132.61	127.89
24	AB	611	CLA	C4D-C3D-CAD	3.02	111.39	108.11
24	AB	607	CLA	CAA-C2A-C3A	-3.02	104.84	113.00
36	AF	101	HEM	CAB-C3B-C2B	-3.02	118.61	128.43
27	AK	102	BCR	C12-C13-C14	-3.02	114.26	119.01
24	AC	512	CLA	C3B-C4B-NB	-3.02	107.84	110.53
34	BD	5403	PHO	CBC-CAC-C3C	-3.02	108.56	112.87
24	BC	5511	CLA	C6-C7-C8	-3.01	105.95	115.97
24	BB	5608	CLA	C3A-C2A-C1A	3.01	105.85	101.34
28	BA	5412	DGD	C4A-C3A-C2A	3.01	124.19	113.13
27	BC	5515	BCR	C12-C13-C14	-3.01	114.28	119.01
32	BB	5604	LMT	C4-C3-C2	-3.01	99.16	114.37
27	AX	101	BCR	C12-C13-C14	-3.01	114.28	119.01
24	AA	405	CLA	O2A-CGA-O1A	-3.01	116.11	123.63
27	BD	5407	BCR	C11-C10-C9	3.00	131.49	127.28
27	AD	406	BCR	C11-C10-C9	3.00	131.49	127.28
28	BC	5519	DGD	O6E-C5E-C4E	3.00	115.11	109.70
24	AA	407	CLA	C2A-C1A-CHA	3.00	129.08	123.87
27	BJ	5101	BCR	C21-C20-C19	3.00	131.90	123.20
24	BC	5505	CLA	C3B-C4B-NB	-3.00	107.85	110.53
28	BC	5519	DGD	C8B-C7B-C6B	-3.00	99.21	114.37
24	BB	5619	CLA	O2A-CGA-CBA	3.00	120.97	111.83
36	AV	201	HEM	CAD-CBD-CGD	2.99	121.59	113.67
32	AB	630	LMT	C4-C3-C2	-2.99	99.27	114.37
31	AC	520	LMG	C9-C8-C7	-2.99	104.82	111.78
28	AH	101	DGD	C7B-C6B-C5B	-2.99	99.28	114.37
24	AB	616	CLA	C3A-C2A-C1A	2.99	105.81	101.34
24	BB	5616	CLA	C2A-C1A-CHA	2.99	129.05	123.87
27	AK	102	BCR	C35-C13-C12	2.98	122.65	118.09
24	AB	606	CLA	CED-O2D-CGD	2.98	122.68	115.92
24	AB	609	CLA	C3A-C2A-C1A	2.98	105.81	101.34
30	BB	5625	SQD	C31-C30-C29	2.98	133.50	113.36
24	AC	510	CLA	C3B-C4B-NB	-2.98	107.87	110.53
28	AA	411	DGD	C4A-C3A-C2A	2.98	124.07	113.13
24	BB	5614	CLA	C3A-C2A-C1A	2.98	105.80	101.34
28	AC	517	DGD	C3G-O3G-C1D	-2.98	107.41	113.80
31	BE	5101	LMG	O7-C10-C11	2.98	117.92	111.48
27	BT	5101	BCR	C32-C1-C6	2.97	114.91	110.24
24	BC	5510	CLA	C2A-C1A-CHA	2.97	129.03	123.87
27	BC	5514	BCR	C33-C5-C4	-2.97	107.26	113.60
28	AC	519	DGD	C8B-C7B-C6B	-2.97	99.34	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	615	CLA	O2A-CGA-CBA	2.97	120.90	111.83
24	BC	5509	CLA	C3A-C2A-C1A	2.97	105.79	101.34
27	AB	617	BCR	C35-C13-C12	2.97	122.63	118.09
27	BK	5102	BCR	C16-C17-C18	2.97	131.44	127.28
24	AD	404	CLA	C3A-C2A-C1A	2.97	105.79	101.34
36	BV	5201	HEM	CAD-CBD-CGD	2.97	121.54	113.67
24	BB	5618	CLA	CED-O2D-CGD	2.97	122.64	115.92
24	AB	603	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
24	BC	5506	CLA	CED-O2D-CGD	2.97	122.64	115.92
24	AC	506	CLA	CAA-C2A-C1A	-2.97	102.26	111.97
35	AD	405	PL9	C25-C24-C23	-2.97	116.01	123.63
24	AB	612	CLA	O2A-CGA-CBA	2.96	120.87	111.83
30	BB	5625	SQD	O9-S-C6	-2.96	102.33	106.76
24	AA	404	CLA	CED-O2D-CGD	2.96	122.63	115.92
30	AB	622	SQD	C3-C4-C5	-2.96	104.87	110.23
24	BA	5406	CLA	C3A-C2A-C1A	2.96	105.77	101.34
27	AB	617	BCR	C36-C18-C19	2.96	122.61	118.09
24	BD	5405	CLA	O2A-CGA-CBA	2.95	120.84	111.83
24	BA	5406	CLA	C3B-C4B-NB	-2.95	107.89	110.53
24	AC	506	CLA	CED-O2D-CGD	2.95	122.61	115.92
30	AB	622	SQD	C31-C30-C29	2.95	133.28	113.36
28	AH	101	DGD	C3G-C2G-C1G	-2.95	104.91	111.78
27	BK	5102	BCR	C35-C13-C12	2.95	122.59	118.09
24	BA	5407	CLA	C3B-C4B-NB	-2.95	107.90	110.53
27	BB	5623	BCR	C33-C5-C4	-2.95	107.31	113.60
24	AB	605	CLA	C3B-C4B-NB	-2.95	107.90	110.53
34	AD	402	PHO	O1D-CGD-CBD	-2.95	120.25	124.72
27	AD	406	BCR	C12-C13-C14	-2.95	114.38	119.01
27	AC	515	BCR	C12-C13-C14	-2.94	114.38	119.01
31	BC	5520	LMG	C9-C8-C7	-2.94	104.93	111.78
24	BB	5605	CLA	C2A-C1A-CHA	2.94	128.97	123.87
24	BB	5615	CLA	CBA-CAA-C2A	2.94	122.54	113.79
32	BB	5603	LMT	C4-C3-C2	-2.94	99.51	114.37
30	AB	627	SQD	C31-C30-C29	2.94	133.21	113.36
27	BT	5101	BCR	C7-C8-C9	2.94	130.58	126.23
24	AB	604	CLA	C3B-C4B-NB	-2.94	107.91	110.53
27	AT	101	BCR	C23-C24-C25	2.94	134.84	127.00
28	BH	5101	DGD	C7B-C6B-C5B	-2.93	99.53	114.37
30	AB	627	SQD	C44-O6-C1	2.93	120.08	113.80
31	BC	5520	LMG	O8-C9-C8	2.93	116.85	108.40
24	BB	5620	CLA	C3A-C2A-C1A	2.93	105.73	101.34
24	BB	5607	CLA	C7-C6-C5	-2.93	105.45	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BB	5622	BCR	C1-C6-C5	-2.93	118.63	122.64
24	BB	5613	CLA	C3A-C2A-C1A	2.93	105.73	101.34
31	AA	414	LMG	O7-C10-C11	2.93	117.82	111.48
31	BI	5101	LMG	C14-C13-C12	-2.93	99.56	114.37
24	AB	603	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
30	BB	5601	SQD	C44-O6-C1	2.93	120.08	113.80
31	BD	5410	LMG	C32-C31-C30	-2.93	99.56	114.37
24	BC	5510	CLA	C3A-C2A-C1A	2.93	105.73	101.34
24	BC	5506	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
25	BA	5409	MST	C15-N14-C6	-2.93	120.03	124.35
24	AB	614	CLA	O2A-CGA-CBA	2.93	120.76	111.83
24	BB	5615	CLA	C3B-C4B-NB	-2.93	107.92	110.53
27	AX	101	BCR	C35-C13-C12	2.93	122.56	118.09
30	BB	5601	SQD	C31-C30-C29	2.93	133.12	113.36
27	AK	102	BCR	C16-C17-C18	2.92	131.38	127.28
24	BC	5502	CLA	C3A-C2A-C1A	2.92	105.71	101.34
24	BB	5613	CLA	C3B-C4B-NB	-2.92	107.92	110.53
27	AD	406	BCR	C1-C6-C5	-2.92	118.65	122.64
36	BV	5201	HEM	C4C-NC-C1C	2.92	110.58	105.82
27	AK	102	BCR	C34-C9-C8	2.91	122.54	118.09
24	AB	608	CLA	C3B-C4B-NB	-2.91	107.93	110.53
24	AB	603	CLA	CHA-C4D-ND	2.91	138.56	132.55
24	AA	407	CLA	CAA-C2A-C1A	-2.91	102.44	111.97
24	AD	401	CLA	C2A-C1A-CHA	2.91	128.92	123.87
28	BC	5517	DGD	O6D-C1D-O3G	2.91	116.92	110.04
31	AJ	102	LMG	O7-C10-C11	-2.91	105.19	111.48
24	AA	406	CLA	C3B-C4B-NB	-2.91	107.94	110.53
36	AF	101	HEM	C4C-NC-C1C	2.91	110.56	105.82
31	AA	414	LMG	C34-C33-C32	2.91	129.06	114.37
27	AJ	101	BCR	C16-C15-C14	2.90	129.46	123.52
27	AC	514	BCR	C35-C13-C12	2.90	122.52	118.09
24	AC	502	CLA	C3B-C4B-NB	-2.90	107.94	110.53
28	BC	5517	DGD	C3G-O3G-C1D	-2.90	107.57	113.80
28	AC	519	DGD	O6E-C1E-C2E	2.90	116.33	110.37
27	AA	410	BCR	C1-C6-C5	-2.90	118.67	122.64
24	BB	5619	CLA	C3B-C4B-NB	-2.90	107.94	110.53
31	AC	520	LMG	O8-C9-C8	2.90	116.76	108.40
27	BD	5407	BCR	C1-C6-C5	-2.90	118.68	122.64
30	BB	5625	SQD	C3-C4-C5	-2.90	104.98	110.23
31	AD	408	LMG	C32-C31-C30	-2.90	99.73	114.37
27	BC	5516	BCR	C35-C13-C12	2.89	122.51	118.09
24	AB	604	CLA	C3A-C2A-C1A	2.89	105.67	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5501	CLA	O2D-CGD-CBD	2.89	116.29	111.23
24	BB	5607	CLA	CAA-C2A-C3A	-2.89	105.18	113.00
35	AD	405	PL9	C15-C14-C13	-2.89	116.20	123.63
27	AJ	101	BCR	C21-C20-C19	2.89	131.58	123.20
24	BB	5611	CLA	CAA-C2A-C3A	-2.89	105.19	113.00
31	AD	408	LMG	O7-C8-C7	2.89	118.71	108.34
24	BC	5508	CLA	O1D-CGD-CBD	-2.89	118.82	124.52
27	BB	5623	BCR	C1-C6-C5	-2.89	118.69	122.64
24	BB	5617	CLA	C2A-C1A-CHA	2.88	128.87	123.87
27	AD	406	BCR	C23-C22-C21	-2.88	114.48	119.01
24	AC	503	CLA	C3B-C4B-NB	-2.88	107.96	110.53
27	BB	5622	BCR	C33-C5-C4	-2.88	107.46	113.60
27	BB	5621	BCR	C35-C13-C12	2.88	122.49	118.09
24	AB	614	CLA	CED-O2D-CGD	2.88	122.44	115.92
27	AD	406	BCR	C7-C8-C9	2.88	130.49	126.23
24	AB	611	CLA	CBA-CAA-C2A	2.88	122.35	113.79
28	AC	517	DGD	O6D-C1D-O3G	2.88	116.84	110.04
31	BE	5101	LMG	C34-C33-C32	2.88	128.90	114.37
24	BC	5509	CLA	O2D-CGD-CBD	2.87	116.26	111.23
31	BB	5624	LMG	C16-C15-C14	-2.87	99.86	114.37
24	BC	5506	CLA	O2D-CGD-CBD	2.87	116.25	111.23
27	BJ	5101	BCR	C16-C15-C14	2.87	129.39	123.52
24	BB	5611	CLA	O2A-CGA-O1A	-2.87	116.45	123.63
27	AC	515	BCR	C35-C13-C12	2.87	122.47	118.09
24	BB	5610	CLA	O2A-CGA-O1A	-2.87	116.46	123.63
27	BC	5514	BCR	C23-C22-C21	-2.87	114.50	119.01
28	AC	519	DGD	C1D-C2D-C3D	-2.87	103.98	110.01
27	BC	5515	BCR	C16-C17-C18	2.86	131.29	127.28
24	BA	5408	CLA	C2A-C1A-CHA	2.86	128.83	123.87
24	BB	5609	CLA	C3B-C4B-NB	-2.86	107.98	110.53
29	BA	5413	LHG	O7-C7-C8	2.86	117.66	111.48
30	AB	622	SQD	C45-O47-C7	2.86	124.63	117.80
27	BA	5411	BCR	C2-C1-C6	2.85	114.58	110.44
28	AA	411	DGD	O6D-C1D-C2D	-2.85	104.51	110.37
24	AC	510	CLA	C2A-C1A-CHA	2.85	128.82	123.87
31	BL	5101	LMG	C15-C14-C13	-2.85	99.95	114.37
31	AI	101	LMG	C14-C13-C12	-2.85	99.95	114.37
24	BC	5509	CLA	CHA-C4D-ND	2.85	138.43	132.55
24	BB	5616	CLA	CHA-C4D-ND	2.85	138.43	132.55
24	BB	5620	CLA	CED-O2D-CGD	2.85	122.37	115.92
27	BC	5516	BCR	C40-C30-C29	-2.85	98.02	108.95
29	AA	412	LHG	O7-C7-C8	2.85	117.64	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	5411	BCR	C35-C13-C12	2.84	122.43	118.09
24	BC	5513	CLA	CED-O2D-CGD	2.84	122.37	115.92
24	AB	614	CLA	CHA-C4D-ND	2.84	138.42	132.55
27	BT	5101	BCR	C23-C24-C25	2.84	134.59	127.00
24	BB	5607	CLA	CHA-C4D-ND	2.84	138.41	132.55
30	BB	5601	SQD	O9-S-C6	-2.84	102.52	106.76
24	BB	5610	CLA	CAA-C2A-C1A	-2.84	102.67	111.97
24	BB	5605	CLA	CED-O2D-CGD	2.84	122.36	115.92
31	AB	621	LMG	C16-C15-C14	-2.84	100.03	114.37
24	BB	5620	CLA	O2A-CGA-CBA	2.83	120.48	111.83
24	AC	509	CLA	CED-O2D-CGD	2.83	122.34	115.92
24	BB	5617	CLA	O2A-CGA-CBA	2.83	120.47	111.83
24	AB	612	CLA	C2A-C1A-CHA	2.83	128.78	123.87
35	AD	405	PL9	C30-C29-C31	2.83	120.14	115.23
24	BB	5608	CLA	C3B-C4B-NB	-2.83	108.00	110.53
24	BC	5503	CLA	C3B-C4B-NB	-2.83	108.00	110.53
24	AD	404	CLA	C3B-C4B-NB	-2.83	108.00	110.53
31	BD	5410	LMG	O7-C8-C7	2.83	118.49	108.34
24	AC	509	CLA	O2D-CGD-CBD	2.83	116.17	111.23
27	AX	101	BCR	C11-C10-C9	2.82	131.24	127.28
31	AA	414	LMG	O8-C28-C29	2.82	120.44	111.83
35	BD	5406	PL9	C25-C24-C23	-2.82	116.38	123.63
27	BA	5411	BCR	C24-C23-C22	2.82	130.41	126.23
31	AM	101	LMG	O7-C10-O9	-2.82	117.11	123.70
24	AA	404	CLA	C3A-C2A-C1A	2.82	105.56	101.34
31	BE	5101	LMG	O8-C28-C29	2.82	120.43	111.83
24	BA	5407	CLA	C3A-C2A-C1A	2.82	105.56	101.34
30	AA	416	SQD	C3-C4-C5	-2.82	105.13	110.23
32	AB	629	LMT	C4-C3-C2	-2.82	100.14	114.37
27	AJ	101	BCR	C11-C10-C9	2.82	131.23	127.28
36	AV	201	HEM	CAB-C3B-C4B	2.81	136.83	124.39
28	AC	519	DGD	O1G-C1A-C2A	2.81	120.42	111.83
31	AB	620	LMG	C15-C14-C13	-2.81	100.14	114.37
24	BB	5610	CLA	CED-O2D-CGD	2.81	122.30	115.92
36	BV	5201	HEM	O1D-CGD-CBD	-2.81	114.17	123.09
27	BC	5514	BCR	C8-C7-C6	2.81	134.51	127.00
34	AD	403	PHO	OBD-CAD-C3D	2.81	132.28	127.89
24	AB	615	CLA	C3B-C4B-NB	-2.81	108.02	110.53
28	BA	5412	DGD	O6D-C1D-C2D	-2.81	104.60	110.37
36	AV	201	HEM	O1D-CGD-CBD	-2.81	114.19	123.09
24	AB	611	CLA	C7-C6-C5	-2.81	105.78	113.26
24	BB	5607	CLA	CAA-C2A-C1A	-2.81	102.78	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	407	CLA	CBA-CAA-C2A	2.81	122.14	113.79
28	BC	5518	DGD	O6D-C5D-C4D	2.80	114.75	109.70
27	AT	101	BCR	C32-C1-C6	2.80	114.64	110.24
28	BC	5519	DGD	O6E-C1E-C2E	2.80	116.13	110.37
24	AB	602	CLA	C3B-C4B-NB	-2.80	108.03	110.53
24	AC	509	CLA	CHA-C4D-ND	2.80	138.33	132.55
35	BD	5406	PL9	C30-C29-C31	2.80	120.09	115.23
24	BB	5618	CLA	O2A-CGA-CBA	2.79	120.35	111.83
31	AC	521	LMG	O8-C9-C8	-2.79	100.35	108.40
30	BA	5401	SQD	C3-C4-C5	-2.79	105.17	110.23
27	BC	5514	BCR	C1-C6-C7	2.79	123.22	115.65
28	AC	517	DGD	C3G-C2G-C1G	2.79	118.29	111.78
24	AC	507	CLA	C3B-C4B-NB	-2.79	108.04	110.53
24	BB	5606	CLA	C3B-C4B-NB	-2.79	108.04	110.53
27	AC	516	BCR	C40-C30-C29	-2.79	98.25	108.95
27	BC	5514	BCR	C30-C25-C26	-2.79	118.83	122.64
24	BB	5615	CLA	C7-C6-C5	-2.79	105.84	113.26
28	BC	5517	DGD	C3G-C2G-C1G	2.78	118.28	111.78
27	AB	618	BCR	C1-C6-C5	-2.78	118.83	122.64
24	AB	607	CLA	O2D-CGD-CBD	2.78	116.09	111.23
24	BC	5507	CLA	C3B-C4B-NB	-2.78	108.05	110.53
31	AB	621	LMG	O8-C28-C29	2.78	120.30	111.83
27	AB	619	BCR	C1-C6-C5	-2.78	118.84	122.64
28	BB	5602	DGD	O6E-C1E-O5D	2.78	116.60	110.04
28	AH	101	DGD	C3G-O3G-C1D	2.78	119.75	113.80
27	AC	514	BCR	C8-C7-C6	2.77	134.41	127.00
24	AB	601	CLA	CED-O2D-CGD	2.77	122.20	115.92
27	BB	5621	BCR	C36-C18-C19	2.77	122.32	118.09
24	BB	5610	CLA	C3B-C4B-NB	-2.77	108.06	110.53
29	AA	412	LHG	O8-C6-C5	2.77	116.38	108.40
36	AV	201	HEM	C4C-NC-C1C	2.77	110.33	105.82
27	AC	514	BCR	C23-C22-C21	-2.77	114.66	119.01
28	AH	101	DGD	O6D-C1D-O3G	2.77	116.58	110.04
27	BB	5621	BCR	C1-C6-C5	-2.76	118.86	122.64
27	BX	5101	BCR	C15-C14-C13	2.76	131.15	127.28
27	AT	101	BCR	C36-C18-C19	2.76	122.31	118.09
31	BM	5102	LMG	O7-C10-O9	-2.76	117.25	123.70
28	BC	5519	DGD	O1G-C1A-C2A	2.76	120.25	111.83
27	BC	5514	BCR	C37-C22-C23	2.76	122.30	118.09
28	BH	5101	DGD	C3G-O3G-C1D	2.76	119.71	113.80
31	BD	5410	LMG	C15-C14-C13	-2.76	100.43	114.37
24	BC	5501	CLA	O2A-CGA-O1A	-2.76	116.73	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	616	CLA	O2A-CGA-CBA	2.75	120.23	111.83
24	BA	5408	CLA	CAA-C2A-C1A	-2.75	102.96	111.97
24	BB	5618	CLA	CHA-C4D-ND	2.75	138.22	132.55
27	BB	5621	BCR	C16-C17-C18	2.75	131.14	127.28
24	AB	602	CLA	C3A-C2A-C1A	2.75	105.46	101.34
24	AC	505	CLA	C3B-C4B-NB	-2.75	108.08	110.53
27	BX	5101	BCR	C11-C10-C9	2.75	131.13	127.28
27	AC	514	BCR	C37-C22-C23	2.75	122.29	118.09
27	AD	406	BCR	C35-C13-C12	2.75	122.28	118.09
24	AD	401	CLA	CHA-C4D-ND	2.75	138.22	132.55
29	BA	5415	LHG	O8-C23-C24	2.75	120.21	111.83
27	AD	406	BCR	C37-C22-C23	2.74	122.28	118.09
24	BC	5503	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
24	AB	614	CLA	C2C-C1C-NC	-2.74	107.10	109.98
24	BB	5611	CLA	O2D-CGD-CBD	2.74	116.03	111.23
36	BV	5201	HEM	CAB-C3B-C4B	2.74	136.50	124.39
24	AB	604	CLA	O2D-CGD-CBD	2.74	116.02	111.23
24	BC	5511	CLA	C2C-C1C-NC	-2.74	107.10	109.98
32	BI	5102	LMT	C4-C3-C2	-2.74	100.52	114.37
34	BD	5403	PHO	C3D-CAD-CBD	-2.74	104.00	107.61
31	BC	5521	LMG	O8-C9-C8	-2.74	100.50	108.40
24	BC	5512	CLA	C3A-C2A-C1A	2.74	105.44	101.34
28	AC	519	DGD	O6E-C5E-C4E	2.74	114.63	109.70
29	AA	415	LHG	O8-C23-C24	2.73	120.16	111.83
31	BB	5624	LMG	O7-C8-C7	2.73	118.13	108.34
24	BB	5605	CLA	CHA-C4D-ND	2.73	138.17	132.55
32	AI	102	LMT	C4-C3-C2	-2.73	100.59	114.37
28	BH	5101	DGD	O6D-C1D-O3G	2.73	116.48	110.04
34	AD	403	PHO	C3D-C4D-ND	2.73	111.20	107.71
27	BD	5407	BCR	C23-C22-C21	-2.72	114.72	119.01
27	AC	514	BCR	C40-C30-C25	2.72	114.51	110.24
24	AB	607	CLA	O2A-CGA-O1A	-2.72	116.82	123.63
24	AC	509	CLA	C3A-C2A-C1A	2.72	105.41	101.34
27	BC	5516	BCR	C37-C22-C23	2.72	122.24	118.09
24	AB	606	CLA	CAA-C2A-C1A	-2.72	103.06	111.97
24	AB	614	CLA	C3A-C2A-C1A	2.72	105.41	101.34
24	BC	5512	CLA	CED-O2D-CGD	2.72	122.08	115.92
24	AC	506	CLA	C2A-C1A-CHA	2.72	128.58	123.87
24	BA	5405	CLA	C3A-C2A-C1A	2.72	105.41	101.34
27	AA	410	BCR	C16-C17-C18	2.71	131.09	127.28
34	AD	402	PHO	C3D-CAD-CBD	-2.71	104.03	107.61
24	AC	506	CLA	O2D-CGD-CBD	2.71	115.97	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AC	520	LMG	O7-C8-C7	2.71	118.07	108.34
24	BB	5607	CLA	CAA-CBA-CGA	-2.71	105.51	113.21
36	AF	101	HEM	CAB-C3B-C4B	2.71	136.36	124.39
27	BD	5407	BCR	C37-C22-C23	2.71	122.22	118.09
24	BC	5510	CLA	O1D-CGD-CBD	-2.71	119.18	124.52
32	BB	5603	LMT	O1B-C1B-C2B	2.71	114.75	108.09
24	BC	5501	CLA	C3B-C4B-NB	-2.71	108.11	110.53
36	AF	101	HEM	CAD-C3D-C4D	-2.70	119.98	124.70
24	AB	606	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	AC	511	CLA	C2C-C1C-NC	-2.70	107.14	109.98
30	BF	5102	SQD	O9-S-C6	-2.70	102.72	106.76
34	BD	5404	PHO	OBD-CAD-C3D	2.70	132.11	127.89
24	BB	5607	CLA	CED-O2D-CGD	2.70	122.05	115.92
24	AB	613	CLA	C3A-C2A-C1A	2.70	105.39	101.34
32	AB	629	LMT	O1B-C1B-C2B	2.70	114.73	108.09
36	BF	5101	HEM	CAB-C3B-C4B	2.70	136.32	124.39
24	AB	609	CLA	CED-O2D-CGD	2.70	122.04	115.92
24	BC	5501	CLA	CED-O2D-CGD	2.70	122.03	115.92
27	AC	514	BCR	C7-C8-C9	2.70	130.23	126.23
31	BC	5520	LMG	O7-C8-C7	2.70	118.02	108.34
24	AC	501	CLA	CED-O2D-CGD	2.69	122.03	115.92
24	BC	5511	CLA	CHA-C4D-ND	2.69	138.10	132.55
27	AX	101	BCR	C16-C17-C18	2.69	131.05	127.28
24	AB	611	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	BB	5613	CLA	C2A-C1A-CHA	2.69	128.53	123.87
27	BK	5102	BCR	C34-C9-C8	2.69	122.19	118.09
27	BD	5407	BCR	C35-C13-C12	2.68	122.19	118.09
24	AB	613	CLA	O2A-CGA-CBA	2.68	120.02	111.83
36	AV	201	HEM	C4D-C3D-C2D	-2.68	102.99	106.89
24	AC	511	CLA	CHA-C4D-ND	2.68	138.08	132.55
27	AB	617	BCR	C16-C17-C18	2.68	131.04	127.28
30	AF	102	SQD	O9-S-C6	-2.68	102.75	106.76
32	BC	5522	LMT	O1'-C1'-C2'	-2.68	104.20	108.27
27	BJ	5101	BCR	C1-C6-C7	2.68	122.92	115.65
24	BC	5506	CLA	C2A-C1A-CHA	2.68	128.51	123.87
24	AB	601	CLA	CHA-C4D-ND	2.68	138.07	132.55
27	AC	516	BCR	C35-C13-C12	2.67	122.17	118.09
27	AX	101	BCR	C15-C14-C13	2.67	131.03	127.28
28	AB	628	DGD	O6E-C1E-O5D	2.67	116.36	110.04
31	AB	621	LMG	O7-C8-C7	2.67	117.93	108.34
27	AT	101	BCR	C20-C21-C22	2.67	131.03	127.28
24	AB	608	CLA	C11-C12-C13	2.67	124.84	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	405	CLA	C3B-C4B-NB	-2.67	108.15	110.53
34	BD	5403	PHO	C1A-C2A-C3A	2.67	105.38	102.84
24	AB	616	CLA	CED-O2D-CGD	2.67	121.97	115.92
24	BC	5502	CLA	C3B-C4B-NB	-2.67	108.15	110.53
27	AJ	101	BCR	C1-C6-C7	2.67	122.88	115.65
24	AC	502	CLA	CED-O2D-CGD	2.67	121.96	115.92
24	AB	615	CLA	CHA-C4D-ND	2.66	138.04	132.55
24	BB	5608	CLA	O2D-CGD-CBD	2.66	115.88	111.23
31	AC	520	LMG	C9-O8-C28	2.66	126.84	117.12
27	AK	102	BCR	C37-C22-C23	2.66	122.15	118.09
30	AB	622	SQD	O9-S-C6	-2.66	102.79	106.76
31	BL	5101	LMG	C12-C11-C10	2.66	123.43	113.69
27	BT	5101	BCR	C8-C9-C10	-2.66	114.83	119.01
27	BK	5102	BCR	C30-C25-C24	2.66	122.85	115.65
30	AB	627	SQD	O9-S-C6	-2.66	102.79	106.76
24	AC	512	CLA	CED-O2D-CGD	2.65	121.93	115.92
24	BC	5509	CLA	CED-O2D-CGD	2.65	121.93	115.92
28	AC	517	DGD	C8A-C7A-C6A	-2.65	100.97	114.37
24	AB	611	CLA	CED-O2D-CGD	2.65	121.93	115.92
24	AA	404	CLA	C2A-C1A-CHA	2.65	128.46	123.87
27	BK	5102	BCR	C37-C22-C23	2.65	122.13	118.09
31	AA	417	LMG	C15-C14-C13	-2.65	101.00	114.37
24	BB	5613	CLA	CED-O2D-CGD	2.64	121.91	115.92
30	BA	5414	SQD	O9-S-C6	-2.64	102.81	106.76
27	AB	619	BCR	C35-C13-C12	2.64	122.12	118.09
30	AA	416	SQD	O9-S-C6	-2.64	102.81	106.76
24	BB	5612	CLA	C11-C12-C13	2.64	124.74	115.97
24	AC	501	CLA	CHA-C4D-ND	2.64	138.00	132.55
24	BB	5618	CLA	C3A-C2A-C1A	2.64	105.29	101.34
31	AD	408	LMG	C15-C14-C13	-2.64	101.05	114.37
32	AI	103	LMT	O1'-C1'-C2'	-2.63	104.27	108.27
24	BB	5606	CLA	C3A-C2A-C1A	2.63	105.28	101.34
27	AC	514	BCR	C1-C6-C7	2.63	122.80	115.65
30	BA	5401	SQD	C45-O47-C7	2.63	124.10	117.80
31	BC	5520	LMG	C9-O8-C28	2.63	126.74	117.12
28	BC	5518	DGD	C3A-C2A-C1A	2.63	123.33	113.69
24	AB	606	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
24	AB	609	CLA	C2A-C1A-CHA	2.63	128.43	123.87
31	BB	5624	LMG	O8-C28-C29	2.63	119.84	111.83
28	AC	518	DGD	C3A-C2A-C1A	2.62	123.31	113.69
27	BA	5411	BCR	C1-C6-C5	-2.62	119.05	122.64
24	AC	512	CLA	O2D-CGD-CBD	2.62	115.81	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	613	CLA	CHA-C4D-ND	2.62	137.96	132.55
28	AC	518	DGD	O6D-C5D-C4D	2.62	114.42	109.70
31	BA	5402	LMG	C15-C14-C13	-2.62	101.12	114.37
30	AF	102	SQD	C45-O47-C7	2.62	124.07	117.80
31	AB	620	LMG	C12-C11-C10	2.62	123.29	113.69
27	BT	5101	BCR	C36-C18-C19	2.62	122.09	118.09
24	AA	406	CLA	CAA-CBA-CGA	-2.62	105.77	113.21
31	AC	520	LMG	C32-C31-C30	-2.62	101.14	114.37
28	AC	519	DGD	C3G-C2G-C1G	2.62	117.89	111.78
27	BC	5514	BCR	C40-C30-C25	2.62	114.34	110.24
34	AD	403	PHO	C6-C7-C8	-2.62	107.27	115.97
24	BC	5507	CLA	CED-O2D-CGD	2.61	121.84	115.92
27	AA	410	BCR	C35-C13-C12	2.61	122.08	118.09
24	BB	5618	CLA	C2C-C1C-NC	-2.61	107.24	109.98
30	BA	5401	SQD	O9-S-C6	-2.61	102.86	106.76
28	AC	517	DGD	C3A-C2A-C1A	2.61	123.25	113.69
30	AA	416	SQD	C36-C35-C34	2.61	127.54	114.37
27	BT	5101	BCR	C19-C18-C17	-2.60	114.92	119.01
24	AC	512	CLA	CHA-C4D-ND	2.60	137.92	132.55
27	AK	102	BCR	C30-C25-C24	2.60	122.71	115.65
24	BB	5615	CLA	CED-O2D-CGD	2.60	121.81	115.92
24	AB	616	CLA	CHA-C4D-ND	2.60	137.91	132.55
27	AT	101	BCR	C8-C9-C10	-2.60	114.92	119.01
27	AT	101	BCR	C19-C18-C17	-2.60	114.92	119.01
24	BB	5620	CLA	C3B-C4B-NB	-2.60	108.21	110.53
27	AC	516	BCR	C37-C22-C23	2.60	122.06	118.09
27	BC	5516	BCR	C24-C23-C22	2.60	130.08	126.23
27	AT	101	BCR	C23-C22-C21	-2.60	114.92	119.01
24	AB	603	CLA	C6-C5-C3	2.59	119.79	113.47
24	BC	5501	CLA	CHA-C4D-ND	2.59	137.90	132.55
24	AC	505	CLA	C2A-C1A-CHA	2.59	128.37	123.87
24	AC	502	CLA	C3A-C2A-C1A	2.59	105.22	101.34
24	BB	5608	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
27	AC	516	BCR	C16-C17-C18	2.59	130.91	127.28
24	AB	605	CLA	CAA-CBA-CGA	-2.59	105.86	113.21
24	AC	510	CLA	CED-O2D-CGD	2.58	121.78	115.92
24	BD	5402	CLA	CHA-C4D-ND	2.58	137.88	132.55
24	AC	505	CLA	CHA-C4D-ND	2.58	137.88	132.55
30	AA	416	SQD	C45-O47-C7	2.58	123.97	117.80
28	BH	5101	DGD	O2G-C1B-O1B	-2.58	117.67	123.70
27	BC	5514	BCR	C32-C1-C6	2.58	114.29	110.24
27	BC	5515	BCR	C19-C18-C17	-2.58	114.95	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	617	BCR	C1-C6-C5	-2.58	119.11	122.64
24	BC	5502	CLA	CED-O2D-CGD	2.58	121.77	115.92
27	AB	617	BCR	C24-C23-C22	2.58	130.05	126.23
31	BC	5521	LMG	C9-C8-C7	2.58	117.80	111.78
27	BJ	5101	BCR	C11-C10-C9	2.58	130.89	127.28
27	AC	514	BCR	C32-C1-C6	2.58	114.28	110.24
27	AC	515	BCR	C19-C18-C17	-2.58	114.96	119.01
24	AC	513	CLA	CHA-C4D-ND	2.58	137.86	132.55
27	BT	5101	BCR	C8-C7-C6	2.57	133.88	127.00
27	AC	515	BCR	C36-C18-C19	2.57	122.02	118.09
30	BB	5625	SQD	C15-C14-C13	2.57	127.36	114.37
24	BB	5608	CLA	CBA-CAA-C2A	2.57	121.44	113.79
24	AD	401	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
24	BB	5617	CLA	CED-O2D-CGD	2.57	121.74	115.92
24	AB	613	CLA	C6-C7-C8	-2.57	107.43	115.97
24	BC	5510	CLA	CED-O2D-CGD	2.57	121.74	115.92
31	AC	520	LMG	O7-C10-O9	-2.57	117.70	123.70
27	AB	617	BCR	C8-C9-C10	-2.57	114.97	119.01
24	BB	5619	CLA	CHA-C4D-ND	2.57	137.84	132.55
27	BB	5622	BCR	C32-C1-C6	2.57	114.27	110.24
34	BD	5403	PHO	CED-O2D-CGD	2.56	121.73	115.92
28	AC	518	DGD	C5A-C4A-C3A	2.56	127.32	114.37
24	AB	612	CLA	CHA-C4D-ND	2.56	137.84	132.55
31	AA	417	LMG	C32-C31-C30	-2.56	101.42	114.37
31	BC	5520	LMG	C32-C31-C30	-2.56	101.42	114.37
24	BA	5405	CLA	CED-O2D-CGD	2.56	121.72	115.92
28	BC	5518	DGD	C5A-C4A-C3A	2.56	127.31	114.37
24	AC	507	CLA	CED-O2D-CGD	2.56	121.72	115.92
30	AB	622	SQD	C15-C14-C13	2.55	127.27	114.37
27	AT	101	BCR	C8-C7-C6	2.55	133.82	127.00
24	AB	603	CLA	CAA-CBA-CGA	-2.55	105.97	113.21
24	BB	5616	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
27	BB	5622	BCR	C1-C6-C7	2.55	122.56	115.65
27	AB	617	BCR	C8-C7-C6	2.55	133.80	127.00
24	BC	5508	CLA	CAA-CBA-CGA	-2.54	105.98	113.21
24	AC	508	CLA	O2A-CGA-O1A	-2.54	117.26	123.63
27	BD	5407	BCR	C12-C13-C14	-2.54	115.01	119.01
28	AA	411	DGD	C5A-C4A-C3A	-2.54	101.53	114.37
27	AB	617	BCR	C37-C22-C23	2.54	121.97	118.09
28	BC	5519	DGD	C3G-C2G-C1G	2.54	117.70	111.78
36	BF	5101	HEM	CAD-C3D-C4D	-2.54	120.27	124.70
24	AA	406	CLA	C3A-C2A-C1A	2.54	105.14	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5620	CLA	CHA-C4D-ND	2.54	137.78	132.55
24	BC	5513	CLA	CHA-C4D-ND	2.54	137.78	132.55
24	AB	603	CLA	CHB-C1B-NB	2.54	127.86	124.05
30	BB	5601	SQD	C3-C4-C5	-2.54	105.63	110.23
24	AB	610	CLA	CED-O2D-CGD	2.53	121.66	115.92
24	BD	5405	CLA	C3B-C4B-NB	-2.53	108.27	110.53
31	AC	521	LMG	C12-C11-C10	2.53	122.98	113.69
31	BA	5402	LMG	C32-C31-C30	-2.53	101.56	114.37
27	AA	410	BCR	C24-C23-C22	2.53	129.98	126.23
30	BA	5401	SQD	C36-C35-C34	2.53	127.17	114.37
31	AJ	102	LMG	C32-C31-C30	-2.53	101.58	114.37
24	BC	5511	CLA	C3A-C2A-C1A	2.53	105.13	101.34
24	BB	5609	CLA	C2A-C1A-CHA	2.53	128.25	123.87
28	BC	5517	DGD	C8A-C7A-C6A	-2.53	101.60	114.37
24	AC	501	CLA	C3B-C4B-NB	-2.52	108.28	110.53
36	BF	5101	HEM	C4D-C3D-C2D	-2.52	103.22	106.89
28	BC	5517	DGD	C3A-C2A-C1A	2.52	122.94	113.69
24	AC	503	CLA	CAA-C2A-C1A	-2.52	103.71	111.97
28	BA	5412	DGD	C5A-C4A-C3A	-2.52	101.62	114.37
27	BC	5515	BCR	C36-C18-C19	2.52	121.94	118.09
27	BD	5407	BCR	C34-C9-C8	2.52	121.94	118.09
27	BC	5514	BCR	C7-C8-C9	2.52	129.97	126.23
24	AB	606	CLA	O2D-CGD-CBD	2.52	115.63	111.23
27	AD	406	BCR	C36-C18-C19	2.52	121.93	118.09
24	BB	5617	CLA	CHA-C4D-ND	2.52	137.74	132.55
24	BC	5512	CLA	CHA-C4D-ND	2.52	137.74	132.55
32	AB	623	LMT	O1B-C1B-C2B	2.51	114.28	108.09
30	BF	5102	SQD	O47-C7-C8	2.51	116.92	111.48
25	AA	408	MST	C15-N14-C6	-2.51	120.65	124.35
24	AC	503	CLA	CBA-CAA-C2A	2.51	121.27	113.79
27	BB	5621	BCR	C8-C7-C6	2.51	133.71	127.00
27	BC	5514	BCR	C12-C13-C14	-2.51	115.06	119.01
24	AD	401	CLA	C3A-C2A-C1A	2.51	105.10	101.34
24	AA	404	CLA	CHA-C4D-ND	2.51	137.73	132.55
24	BB	5609	CLA	CAA-CBA-CGA	-2.51	106.09	113.21
34	BD	5404	PHO	C3D-C4D-ND	2.51	110.92	107.71
24	BB	5612	CLA	C2A-C1A-CHA	2.51	128.22	123.87
24	AB	601	CLA	C3A-C2A-C1A	2.51	105.09	101.34
24	BD	5402	CLA	C3A-C2A-C1A	2.51	105.09	101.34
27	BB	5623	BCR	C1-C6-C7	2.51	122.45	115.65
27	AB	618	BCR	C32-C1-C6	2.51	114.17	110.24
24	AC	501	CLA	O2A-CGA-O1A	-2.51	117.36	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BD	5405	CLA	C2A-C1A-CHA	2.50	128.21	123.87
24	AC	507	CLA	C3A-C2A-C1A	2.50	105.09	101.34
28	BC	5519	DGD	O3D-C3D-C2D	2.50	116.28	110.38
31	AB	620	LMG	C9-O8-C28	2.50	126.27	117.12
24	AB	615	CLA	CED-O2D-CGD	2.50	121.59	115.92
29	BA	5415	LHG	C5-O7-C7	-2.50	111.81	117.80
24	BB	5607	CLA	CHB-C1B-NB	2.50	127.80	124.05
34	BD	5403	PHO	O2A-CGA-CBA	2.50	119.45	111.83
31	BE	5101	LMG	O8-C9-C8	2.50	115.60	108.40
28	BC	5519	DGD	O1G-C1A-O1A	-2.50	117.38	123.63
24	BC	5513	CLA	C3A-C2A-C1A	2.50	105.08	101.34
28	AH	101	DGD	O2G-C1B-O1B	-2.49	117.87	123.70
24	AB	605	CLA	C2A-C1A-CHA	2.49	128.19	123.87
29	AA	415	LHG	C5-O7-C7	-2.49	111.83	117.80
27	BX	5101	BCR	C16-C17-C18	2.49	130.78	127.28
24	BB	5608	CLA	C6-C7-C8	-2.49	107.68	115.97
27	AB	617	BCR	C11-C10-C9	2.49	130.77	127.28
35	BD	5406	PL9	C45-C44-C46	2.49	119.55	115.23
31	BD	5408	LMG	C36-C35-C34	-2.49	101.78	114.37
28	AC	519	DGD	O6D-C1D-C2D	-2.49	105.25	110.37
27	BT	5101	BCR	C37-C22-C23	2.49	121.89	118.09
24	BC	5503	CLA	CAA-C2A-C1A	-2.49	103.82	111.97
24	BC	5503	CLA	CBA-CAA-C2A	2.49	121.20	113.79
24	BB	5607	CLA	C4B-C3B-C2B	-2.49	104.21	107.30
24	AB	616	CLA	C3B-C4B-NB	-2.49	108.31	110.53
34	BD	5404	PHO	C3D-CAD-CBD	-2.49	104.33	107.61
24	AB	613	CLA	O2D-CGD-CBD	2.49	115.58	111.23
24	BC	5508	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
24	BB	5607	CLA	C6-C5-C3	2.48	119.52	113.47
24	AC	510	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
24	BB	5607	CLA	C2C-C1C-NC	-2.48	107.38	109.98
24	BA	5406	CLA	C12-C11-C10	-2.48	102.16	113.28
24	AC	508	CLA	CAA-CBA-CGA	-2.48	106.17	113.21
31	AD	407	LMG	C39-C38-C37	2.48	126.90	114.37
27	BB	5621	BCR	C12-C13-C14	-2.48	115.11	119.01
24	AB	611	CLA	CAA-CBA-CGA	-2.48	106.17	113.21
31	AD	407	LMG	O1-C1-C2	-2.48	104.51	108.27
31	BL	5101	LMG	C9-O8-C28	2.48	126.17	117.12
24	BC	5512	CLA	O2D-CGD-CBD	2.48	115.56	111.23
27	BB	5623	BCR	C24-C23-C22	2.48	129.90	126.23
31	AC	520	LMG	C13-C12-C11	2.48	122.22	113.13
27	BT	5101	BCR	C23-C22-C21	-2.47	115.12	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	513	CLA	C3A-C2A-C1A	2.47	105.05	101.34
24	AD	404	CLA	C2A-C1A-CHA	2.47	128.16	123.87
27	BC	5516	BCR	C30-C25-C24	2.47	122.36	115.65
24	AC	511	CLA	C3A-C2A-C1A	2.47	105.04	101.34
28	AB	628	DGD	O2G-C2G-C3G	2.47	117.21	108.34
30	BA	5414	SQD	C15-C14-C13	2.47	126.86	114.37
24	BB	5613	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
24	AB	612	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
24	AD	401	CLA	C6-C7-C8	-2.47	107.76	115.97
24	AC	503	CLA	C2A-C1A-CHA	2.47	128.15	123.87
24	AC	512	CLA	C3A-C2A-C1A	2.46	105.03	101.34
31	BD	5408	LMG	C32-C31-C30	-2.46	101.92	114.37
27	AC	515	BCR	C24-C23-C22	2.46	129.87	126.23
24	AC	510	CLA	C3A-C2A-C1A	2.46	105.02	101.34
24	AB	604	CLA	CBA-CAA-C2A	2.46	121.11	113.79
27	BA	5411	BCR	C36-C18-C19	2.46	121.84	118.09
24	BC	5505	CLA	C2A-C1A-CHA	2.46	128.13	123.87
31	AC	521	LMG	C15-C14-C13	-2.46	101.95	114.37
31	BC	5521	LMG	C12-C11-C10	2.46	122.69	113.69
24	AB	601	CLA	C3B-C4B-NB	-2.46	108.34	110.53
31	BC	5521	LMG	C34-C33-C32	2.46	126.78	114.37
24	AC	510	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	BD	5409	LMG	C39-C38-C37	2.45	126.77	114.37
24	BC	5505	CLA	CHA-C4D-ND	2.45	137.61	132.55
27	BB	5621	BCR	C19-C18-C17	-2.45	115.15	119.01
24	AB	608	CLA	C2A-C1A-CHA	2.45	128.12	123.87
24	BB	5616	CLA	CAA-CBA-CGA	-2.45	106.25	113.21
27	AC	516	BCR	C30-C25-C24	2.45	122.30	115.65
32	BB	5627	LMT	C4-C3-C2	-2.45	101.98	114.37
36	AF	101	HEM	C4B-C3B-C2B	-2.45	105.03	107.28
34	AD	402	PHO	O2A-CGA-CBA	2.45	119.30	111.83
27	BD	5407	BCR	C8-C9-C10	-2.45	115.16	119.01
28	AC	519	DGD	O3D-C3D-C2D	2.45	116.14	110.38
30	BF	5102	SQD	C45-O47-C7	2.45	123.65	117.80
24	AD	401	CLA	CED-O2D-CGD	2.45	121.46	115.92
30	AB	627	SQD	C3-C4-C5	-2.44	105.80	110.23
31	AA	414	LMG	O8-C9-C8	2.44	115.44	108.40
28	AC	518	DGD	O6D-C1D-O3G	2.44	115.82	110.04
27	BA	5411	BCR	C12-C13-C14	-2.44	115.17	119.01
27	BA	5411	BCR	C37-C22-C23	2.44	121.82	118.09
30	AA	413	SQD	C15-C14-C13	2.44	126.72	114.37
36	BF	5101	HEM	O2D-CGD-CBD	2.44	121.72	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5610	CLA	CBA-CAA-C2A	2.44	121.06	113.79
36	BV	5201	HEM	C4D-C3D-C2D	-2.44	103.34	106.89
31	BB	5624	LMG	C13-C12-C11	2.44	122.10	113.13
28	AC	518	DGD	CBA-CAA-C9A	-2.44	102.03	114.37
24	BA	5407	CLA	CAA-CBA-CGA	-2.44	106.29	113.21
24	AB	612	CLA	CAA-CBA-CGA	-2.44	106.29	113.21
28	BC	5518	DGD	CBA-CAA-C9A	-2.44	102.05	114.37
31	BC	5521	LMG	C15-C14-C13	-2.44	102.05	114.37
27	AB	619	BCR	C1-C6-C7	2.44	122.26	115.65
30	BF	5102	SQD	C32-C31-C30	2.44	129.81	113.36
24	AB	603	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
27	AT	101	BCR	C37-C22-C23	2.44	121.81	118.09
28	AC	517	DGD	O2G-C2G-C1G	-2.43	99.61	108.34
31	BD	5409	LMG	O1-C1-C2	-2.43	104.58	108.27
24	AC	503	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
30	AF	102	SQD	O47-C7-C8	2.43	116.75	111.48
27	BC	5516	BCR	C23-C22-C21	-2.43	115.18	119.01
24	BC	5507	CLA	C3A-C2A-C1A	2.43	104.98	101.34
24	BD	5402	CLA	C6-C7-C8	-2.43	107.88	115.97
34	AD	403	PHO	C3D-CAD-CBD	-2.43	104.41	107.61
27	AX	101	BCR	C36-C18-C19	2.43	121.80	118.09
27	BT	5101	BCR	C40-C30-C25	2.43	114.05	110.24
31	BB	5624	LMG	C40-C39-C38	-2.43	102.10	114.37
24	AB	611	CLA	C6-C5-C3	2.43	119.38	113.47
27	BC	5515	BCR	C34-C9-C8	2.43	121.80	118.09
24	BD	5402	CLA	CBA-CAA-C2A	2.43	121.02	113.79
27	AC	514	BCR	C12-C13-C14	-2.43	115.19	119.01
24	AC	503	CLA	CED-O2D-CGD	2.43	121.42	115.92
24	AC	511	CLA	CED-O2D-CGD	2.42	121.42	115.92
31	AC	521	LMG	C34-C33-C32	2.42	126.62	114.37
27	AC	516	BCR	C24-C23-C22	2.42	129.82	126.23
27	AJ	101	BCR	C40-C30-C25	2.42	114.04	110.24
29	BA	5413	LHG	O8-C6-C5	2.42	115.37	108.40
27	BK	5102	BCR	C15-C14-C13	2.42	130.67	127.28
32	BB	5626	LMT	O1B-C1B-C2B	2.42	114.04	108.09
24	BB	5606	CLA	C2A-C1A-CHA	2.42	128.06	123.87
32	AB	624	LMT	C4-C3-C2	-2.42	102.15	114.37
30	AF	102	SQD	C32-C31-C30	2.42	129.67	113.36
31	AB	621	LMG	C13-C12-C11	2.41	122.00	113.13
24	BA	5405	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
24	AB	611	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
24	AB	602	CLA	C2A-C1A-CHA	2.41	128.05	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BB	5623	BCR	C35-C13-C12	2.41	121.77	118.09
31	AB	621	LMG	C40-C39-C38	-2.41	102.18	114.37
36	AF	101	HEM	C4D-C3D-C2D	-2.41	103.38	106.89
27	AB	617	BCR	C12-C13-C14	-2.41	115.22	119.01
27	BA	5411	BCR	C16-C17-C18	2.41	130.66	127.28
31	AD	408	LMG	O7-C8-C9	-2.41	99.70	108.34
24	AA	406	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
27	BC	5515	BCR	C37-C22-C23	2.41	121.76	118.09
28	BC	5517	DGD	CBA-CAA-C9A	-2.41	102.21	114.37
24	AC	508	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
30	BA	5414	SQD	O8-S-O9	-2.40	105.38	111.40
27	AA	410	BCR	C37-C22-C23	2.40	121.76	118.09
28	AB	628	DGD	C4A-C3A-C2A	-2.40	104.30	113.13
24	AB	604	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
28	BB	5602	DGD	O2G-C2G-C3G	2.40	116.96	108.34
27	AC	515	BCR	C34-C9-C8	2.40	121.76	118.09
24	BB	5610	CLA	O2D-CGD-CBD	2.40	115.42	111.23
24	AA	407	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
27	BA	5411	BCR	C30-C25-C24	2.40	122.15	115.65
30	BA	5401	SQD	O47-C7-C8	2.40	116.67	111.48
27	BC	5516	BCR	C36-C18-C19	2.40	121.75	118.09
24	BA	5406	CLA	CMD-C2D-C1D	2.40	128.95	124.73
24	AC	510	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
24	BC	5510	CLA	CHA-C4D-ND	2.40	137.49	132.55
24	AB	604	CLA	C6-C7-C8	-2.39	108.00	115.97
27	AA	410	BCR	C36-C18-C19	2.39	121.75	118.09
27	AA	410	BCR	C30-C25-C24	2.39	122.14	115.65
24	BA	5405	CLA	C2A-C1A-CHA	2.39	128.02	123.87
27	BJ	5101	BCR	C16-C17-C18	2.39	130.63	127.28
24	BC	5508	CLA	C2A-C1A-CHA	2.39	128.02	123.87
24	BD	5405	CLA	CHA-C4D-ND	2.39	137.48	132.55
27	AB	619	BCR	C37-C22-C23	2.39	121.74	118.09
28	BC	5519	DGD	C1D-C2D-C3D	-2.39	104.98	110.01
28	AC	517	DGD	CBA-CAA-C9A	-2.39	102.29	114.37
27	AK	102	BCR	C32-C1-C2	-2.39	99.78	108.95
24	AA	406	CLA	CHA-C4D-ND	2.39	137.48	132.55
30	AA	416	SQD	C15-C14-C13	2.39	126.44	114.37
27	BD	5407	BCR	C36-C18-C19	2.39	121.74	118.09
24	AB	606	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
31	AC	521	LMG	C9-C8-C7	2.39	117.35	111.78
31	AB	621	LMG	C7-O1-C1	-2.38	108.68	113.80
24	AB	608	CLA	CED-O2D-CGD	2.38	121.32	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5619	CLA	CED-O2D-CGD	2.38	121.32	115.92
24	BC	5511	CLA	CED-O2D-CGD	2.38	121.32	115.92
31	BM	5102	LMG	C14-C13-C12	-2.38	102.33	114.37
31	BC	5520	LMG	O7-C10-O9	-2.38	118.14	123.70
31	AB	620	LMG	O7-C8-C9	-2.38	99.81	108.34
24	BB	5613	CLA	CHA-C4D-ND	2.38	137.45	132.55
24	AA	404	CLA	CAA-C2A-C3A	-2.38	106.58	113.00
24	BA	5408	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
24	AC	508	CLA	C2A-C1A-CHA	2.38	127.99	123.87
36	BF	5101	HEM	C4B-C3B-C2B	-2.37	105.10	107.28
24	BB	5605	CLA	C3A-C2A-C1A	2.37	104.90	101.34
30	BF	5102	SQD	C3-C4-C5	-2.37	105.93	110.23
24	BB	5614	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	BC	5520	LMG	C13-C12-C11	2.37	121.84	113.13
24	AA	404	CLA	C4B-C3B-C2B	-2.37	104.36	107.30
24	BC	5503	CLA	CED-O2D-CGD	2.37	121.29	115.92
31	BD	5409	LMG	O8-C28-C29	2.37	119.05	111.83
27	AX	101	BCR	C1-C6-C7	2.37	122.07	115.65
24	AC	513	CLA	C2C-C1C-NC	-2.37	107.50	109.98
24	AC	507	CLA	CHA-C4D-ND	2.36	137.43	132.55
24	BB	5617	CLA	C3A-C2A-C1A	2.36	104.88	101.34
24	BA	5408	CLA	CED-O2D-CGD	2.36	121.27	115.92
24	BB	5608	CLA	CAA-C2A-C1A	-2.36	104.24	111.97
24	AB	603	CLA	C2C-C1C-NC	-2.36	107.50	109.98
28	AB	628	DGD	C6B-C5B-C4B	-2.36	102.44	114.37
24	BA	5408	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
31	AM	101	LMG	C14-C13-C12	-2.36	102.44	114.37
24	AB	603	CLA	CED-O2D-CGD	2.36	121.26	115.92
35	BD	5406	PL9	C42-C41-C39	-2.36	105.38	113.19
28	BE	5102	DGD	C3G-C2G-C1G	2.36	117.28	111.78
28	BB	5602	DGD	O5D-C1E-C2E	2.36	111.85	108.27
24	AD	401	CLA	CBA-CAA-C2A	2.35	120.80	113.79
31	AJ	102	LMG	C36-C35-C34	-2.35	102.47	114.37
31	AC	520	LMG	C39-C38-C37	2.35	126.26	114.37
34	BD	5404	PHO	C6-C7-C8	-2.35	108.14	115.97
24	BC	5511	CLA	CAA-CBA-CGA	-2.35	106.53	113.21
31	AC	521	LMG	C19-C18-C17	-2.35	102.48	114.37
24	AB	609	CLA	CHA-C4D-ND	2.35	137.40	132.55
28	BC	5519	DGD	C1E-O6E-C5E	2.35	118.31	113.72
31	BL	5101	LMG	O7-C8-C9	-2.35	99.92	108.34
27	BC	5514	BCR	C23-C24-C25	2.35	133.27	127.00
28	AC	519	DGD	O3G-C3G-C2G	2.35	116.53	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	515	BCR	C15-C14-C13	2.35	130.57	127.28
24	BD	5402	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
27	AB	617	BCR	C19-C18-C17	-2.35	115.32	119.01
28	BE	5102	DGD	C5B-C4B-C3B	-2.34	102.52	114.37
29	BA	5413	LHG	P-O6-C4	-2.34	107.92	121.35
27	AC	514	BCR	C23-C24-C25	2.34	133.26	127.00
24	BA	5405	CLA	C7-C6-C5	-2.34	107.02	113.26
24	AC	503	CLA	CHA-C4D-ND	2.34	137.38	132.55
24	AC	511	CLA	CAA-CBA-CGA	-2.34	106.56	113.21
24	AA	405	CLA	C12-C11-C10	-2.34	102.80	113.28
28	AC	519	DGD	C5B-C4B-C3B	2.34	126.19	114.37
24	AD	404	CLA	CHA-C4D-ND	2.34	137.38	132.55
24	AB	602	CLA	CED-O2D-CGD	2.34	121.22	115.92
24	AB	604	CLA	CAA-C2A-C1A	-2.34	104.31	111.97
27	BB	5621	BCR	C8-C9-C10	-2.34	115.33	119.01
30	AA	416	SQD	O47-C7-C8	2.34	116.53	111.48
27	AC	515	BCR	C37-C22-C23	2.33	121.65	118.09
24	BD	5402	CLA	CED-O2D-CGD	2.33	121.21	115.92
24	BB	5610	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
27	AK	102	BCR	C15-C14-C13	2.33	130.55	127.28
24	BB	5615	CLA	C6-C5-C3	2.33	119.14	113.47
24	BC	5510	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
27	AA	410	BCR	C1-C6-C7	2.33	121.97	115.65
31	BD	5410	LMG	O7-C8-C9	-2.33	99.99	108.34
27	BT	5101	BCR	C40-C30-C29	-2.33	100.02	108.95
24	BA	5407	CLA	CHA-C4D-ND	2.33	137.35	132.55
28	BB	5602	DGD	C4A-C3A-C2A	-2.32	104.59	113.13
31	AC	520	LMG	O9-C10-C11	-2.32	114.69	123.78
31	BC	5520	LMG	O9-C10-C11	-2.32	114.70	123.78
36	AF	101	HEM	O2D-CGD-CBD	2.32	121.34	114.00
27	AB	618	BCR	C1-C6-C7	2.32	121.95	115.65
24	BD	5405	CLA	CAA-CBA-CGA	-2.32	106.62	113.21
24	AB	610	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
27	BK	5102	BCR	C32-C1-C2	-2.32	100.04	108.95
28	BB	5602	DGD	C6B-C5B-C4B	-2.32	102.64	114.37
27	BT	5101	BCR	C20-C21-C22	2.32	130.53	127.28
31	AB	620	LMG	C34-C33-C32	2.32	126.07	114.37
24	AA	407	CLA	CED-O2D-CGD	2.32	121.17	115.92
27	AC	514	BCR	C15-C14-C13	2.32	130.53	127.28
24	AB	606	CLA	CBA-CAA-C2A	2.31	120.68	113.79
24	AC	513	CLA	CHB-C1B-NB	2.31	127.52	124.05
24	BB	5607	CLA	O1D-CGD-CBD	-2.31	119.96	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AD	403	PHO	CED-O2D-CGD	2.31	121.16	115.92
24	AB	607	CLA	CHA-C4D-ND	2.31	137.32	132.55
27	BX	5101	BCR	C36-C18-C19	2.31	121.62	118.09
24	BB	5608	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
27	BJ	5101	BCR	C40-C30-C25	2.31	113.86	110.24
31	BD	5409	LMG	C32-C31-C30	-2.31	102.70	114.37
24	BB	5611	CLA	CHA-C4D-ND	2.31	137.31	132.55
34	AD	402	PHO	C1A-C2A-C3A	2.31	105.03	102.84
28	AE	101	DGD	C5B-C4B-C3B	-2.31	102.71	114.37
30	BA	5401	SQD	C15-C14-C13	2.31	126.02	114.37
24	AC	511	CLA	CHB-C1B-NB	2.31	127.51	124.05
31	AD	407	LMG	O8-C28-C29	2.30	118.86	111.83
24	BA	5405	CLA	CHA-C4D-ND	2.30	137.30	132.55
30	AF	102	SQD	C15-C14-C13	2.30	126.01	114.37
24	BC	5502	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
35	AD	405	PL9	C45-C44-C46	2.30	119.22	115.23
24	BB	5615	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
28	BC	5517	DGD	O2G-C2G-C1G	-2.30	100.10	108.34
27	BB	5622	BCR	C37-C22-C23	2.30	121.60	118.09
24	BC	5507	CLA	CHA-C4D-ND	2.30	137.29	132.55
24	AC	512	CLA	CHA-C1A-NA	-2.30	121.19	126.39
30	BF	5102	SQD	C15-C14-C13	2.30	125.97	114.37
24	BB	5612	CLA	CED-O2D-CGD	2.29	121.12	115.92
34	BD	5404	PHO	CED-O2D-CGD	2.29	121.12	115.92
24	BA	5408	CLA	CHA-C4D-ND	2.29	137.28	132.55
24	BC	5504	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
27	AD	406	BCR	C15-C14-C13	2.29	130.49	127.28
27	AC	516	BCR	C36-C18-C19	2.29	121.58	118.09
28	BC	5519	DGD	C5B-C4B-C3B	2.29	125.94	114.37
24	BB	5606	CLA	CED-O2D-CGD	2.29	121.11	115.92
27	AA	410	BCR	C34-C9-C8	2.29	121.58	118.09
24	AD	401	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
27	BX	5101	BCR	C1-C6-C7	2.29	121.85	115.65
24	BC	5513	CLA	C2C-C1C-NC	-2.29	107.58	109.98
24	AC	509	CLA	CHA-C1A-NA	-2.28	121.22	126.39
24	AB	614	CLA	CHB-C1B-NB	2.28	127.47	124.05
27	BC	5516	BCR	C19-C18-C17	-2.28	115.42	119.01
31	BL	5101	LMG	C19-C18-C17	-2.28	102.83	114.37
35	AD	405	PL9	C42-C41-C39	-2.28	105.62	113.19
30	AA	416	SQD	C34-C33-C32	2.28	125.90	114.37
28	BC	5518	DGD	O2G-C2G-C1G	2.28	116.53	108.34
27	AA	410	BCR	C8-C9-C10	-2.28	115.42	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BC	5518	DGD	C7A-C6A-C5A	2.28	125.89	114.37
24	AA	405	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
24	AC	505	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
24	BB	5617	CLA	C6-C7-C8	-2.28	108.40	115.97
24	BB	5609	CLA	CHA-C4D-ND	2.28	137.25	132.55
24	AB	602	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
24	BB	5605	CLA	C4B-C3B-C2B	-2.27	104.48	107.30
31	AD	407	LMG	C14-C13-C12	2.27	125.84	114.37
31	AD	407	LMG	C32-C31-C30	-2.27	102.89	114.37
31	BC	5520	LMG	C39-C38-C37	2.27	125.84	114.37
24	AB	609	CLA	C6-C7-C8	-2.27	108.43	115.97
27	AB	618	BCR	C16-C17-C18	2.27	130.46	127.28
27	BC	5516	BCR	C16-C17-C18	2.27	130.46	127.28
24	BC	5503	CLA	CAA-CBA-CGA	-2.26	106.78	113.21
24	AB	603	CLA	CBA-CAA-C2A	2.26	120.53	113.79
32	BC	5522	LMT	C1B-C2B-C3B	2.26	114.77	110.01
27	AB	619	BCR	C24-C23-C22	2.26	129.58	126.23
31	BB	5624	LMG	C7-O1-C1	-2.26	108.95	113.80
30	AF	102	SQD	C3-C4-C5	-2.26	106.13	110.23
27	AC	516	BCR	C23-C22-C21	-2.26	115.45	119.01
27	BB	5622	BCR	C16-C17-C18	2.26	130.45	127.28
24	AA	404	CLA	C6-C7-C8	-2.26	108.45	115.97
27	BA	5411	BCR	C34-C9-C8	2.26	121.54	118.09
27	AJ	101	BCR	C31-C1-C2	2.26	117.62	108.95
30	AB	627	SQD	O47-C7-C8	2.26	116.36	111.48
27	BA	5411	BCR	C8-C9-C10	-2.26	115.46	119.01
30	AB	622	SQD	O8-S-O9	-2.25	105.76	111.40
27	AC	514	BCR	C36-C18-C19	2.25	121.53	118.09
27	BJ	5101	BCR	C31-C1-C2	2.25	117.60	108.95
24	BB	5615	CLA	CAA-CBA-CGA	-2.25	106.81	113.21
30	BB	5625	SQD	O8-S-O9	-2.25	105.77	111.40
24	BB	5605	CLA	C3B-C4B-NB	-2.25	108.52	110.53
27	AB	618	BCR	C23-C22-C21	-2.25	115.47	119.01
31	BL	5101	LMG	C34-C33-C32	2.25	125.75	114.37
24	AC	511	CLA	C12-C11-C10	-2.25	103.20	113.28
30	BA	5401	SQD	C34-C33-C32	2.25	125.74	114.37
24	AC	502	CLA	CAA-CBA-CGA	-2.25	106.82	113.21
28	AC	518	DGD	CDB-CCB-CBB	-2.25	103.01	114.37
27	AB	619	BCR	C12-C13-C14	-2.25	115.48	119.01
27	AX	101	BCR	C28-C27-C26	2.24	118.06	114.06
24	BD	5402	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
36	AV	201	HEM	O2D-CGD-CBD	2.24	121.09	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	404	CLA	C7-C6-C5	-2.24	107.29	113.26
24	AB	614	CLA	C2A-C1A-CHA	2.24	127.75	123.87
24	AB	604	CLA	CHA-C4D-ND	2.24	137.17	132.55
34	AD	402	PHO	CED-O2D-CGD	2.24	121.00	115.92
27	AT	101	BCR	C40-C30-C25	2.24	113.75	110.24
27	BB	5623	BCR	C37-C22-C23	2.24	121.50	118.09
27	AD	406	BCR	C8-C9-C10	-2.24	115.49	119.01
28	BC	5518	DGD	O6D-C1D-O3G	2.24	115.33	110.04
31	BC	5521	LMG	C19-C18-C17	-2.23	103.07	114.37
31	AB	620	LMG	C19-C18-C17	-2.23	103.08	114.37
24	BB	5610	CLA	CHA-C4D-ND	2.23	137.16	132.55
31	BD	5409	LMG	C14-C13-C12	2.23	125.65	114.37
28	BC	5518	DGD	CDB-CCB-CBB	-2.23	103.09	114.37
27	BA	5411	BCR	C1-C6-C7	2.23	121.70	115.65
24	BB	5619	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
30	BB	5601	SQD	O47-C7-C8	2.23	116.31	111.48
24	BA	5406	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
24	AA	407	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
29	AA	412	LHG	P-O6-C4	-2.23	108.57	121.35
32	AI	103	LMT	C1B-C2B-C3B	2.23	114.70	110.01
28	AC	518	DGD	C7A-C6A-C5A	2.23	125.64	114.37
24	AB	605	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
31	BC	5520	LMG	O1-C7-C8	-2.23	105.40	110.82
36	BF	5101	HEM	C2A-C1A-NA	2.23	112.62	110.15
28	AC	518	DGD	C8B-C7B-C6B	-2.23	103.11	114.37
28	AC	517	DGD	O2G-C2G-C3G	2.23	116.34	108.34
24	BB	5613	CLA	C6-C7-C8	-2.23	108.56	115.97
27	BB	5621	BCR	C34-C9-C8	2.23	121.49	118.09
24	BA	5405	CLA	O2D-CGD-CBD	2.23	115.12	111.23
28	AH	101	DGD	O2G-C2G-C3G	2.23	116.33	108.34
30	BA	5401	SQD	C17-C16-C15	2.22	125.61	114.37
27	BT	5101	BCR	C34-C9-C8	2.22	121.49	118.09
27	AT	101	BCR	C40-C30-C29	-2.22	100.41	108.95
28	AB	628	DGD	O5D-C1E-C2E	2.22	111.65	108.27
27	BC	5514	BCR	C30-C25-C24	2.22	121.68	115.65
34	BD	5404	PHO	C12-C11-C10	-2.22	103.32	113.28
24	AB	609	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
24	BB	5609	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
27	AD	406	BCR	C19-C18-C17	-2.22	115.51	119.01
27	BX	5101	BCR	C7-C8-C9	2.22	129.52	126.23
27	AA	410	BCR	C12-C13-C14	-2.22	115.52	119.01
24	BB	5617	CLA	O2D-CGD-CBD	2.22	115.11	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BH	5101	DGD	O2G-C2G-C3G	2.22	116.31	108.34
24	AA	407	CLA	CHA-C4D-ND	2.22	137.13	132.55
31	AB	620	LMG	C17-C16-C15	-2.22	103.15	114.37
24	AB	611	CLA	C12-C11-C10	-2.22	103.34	113.28
27	BX	5101	BCR	C37-C22-C23	2.22	121.48	118.09
24	AA	405	CLA	C2A-C1A-CHA	2.22	127.72	123.87
28	AE	101	DGD	C6D-C5D-C4D	-2.22	107.41	112.07
31	AC	520	LMG	O7-C8-C9	2.22	116.30	108.34
24	BB	5605	CLA	CHB-C1B-NB	2.22	127.37	124.05
24	AB	611	CLA	C4B-C3B-C2B	-2.22	104.55	107.30
27	BX	5101	BCR	C34-C9-C8	2.22	121.47	118.09
28	BC	5518	DGD	C8B-C7B-C6B	-2.22	103.17	114.37
24	AB	611	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
24	BB	5606	CLA	CHA-C4D-ND	2.21	137.12	132.55
24	BC	5506	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
24	BC	5513	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
24	AC	503	CLA	CAA-CBA-CGA	-2.21	106.93	113.21
24	BB	5614	CLA	CED-O2D-CGD	2.21	120.93	115.92
24	BC	5503	CLA	C2A-C1A-CHA	2.21	127.70	123.87
27	BC	5514	BCR	C36-C18-C19	2.21	121.46	118.09
24	AB	605	CLA	CHA-C4D-ND	2.21	137.10	132.55
27	AB	618	BCR	C37-C22-C23	2.21	121.46	118.09
36	BV	5201	HEM	C4B-C3B-C2B	-2.21	105.25	107.28
24	BC	5509	CLA	CHA-C1A-NA	-2.21	121.40	126.39
27	BB	5621	BCR	C11-C10-C9	2.20	130.37	127.28
24	BB	5606	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
24	BC	5512	CLA	CHA-C1A-NA	-2.20	121.40	126.39
24	AA	405	CLA	CBC-CAC-C3C	-2.20	106.45	112.42
24	BD	5405	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
24	BB	5615	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
36	AF	101	HEM	CAD-CBD-CGD	2.20	119.50	113.67
24	BC	5507	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
24	AC	513	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
31	BL	5101	LMG	C17-C16-C15	-2.20	103.25	114.37
31	BC	5520	LMG	O7-C8-C9	2.20	116.23	108.34
27	AT	101	BCR	C34-C9-C8	2.20	121.45	118.09
24	BB	5608	CLA	CHA-C4D-ND	2.20	137.08	132.55
24	AB	610	CLA	CHA-C4D-ND	2.20	137.08	132.55
24	AC	502	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
24	BC	5505	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
24	BC	5507	CLA	C11-C12-C13	2.19	123.25	115.97
30	BA	5414	SQD	C17-C16-C15	2.19	125.44	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BD	5407	BCR	C19-C18-C17	-2.19	115.56	119.01
24	AB	615	CLA	CHA-C1A-NA	-2.19	121.43	126.39
27	AB	619	BCR	C30-C25-C24	2.19	121.59	115.65
34	AD	403	PHO	C12-C11-C10	-2.19	103.47	113.28
31	BD	5409	LMG	C1-O6-C5	-2.19	109.45	113.72
24	BB	5606	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
31	BC	5521	LMG	C17-C16-C15	-2.19	103.31	114.37
27	AX	101	BCR	C7-C8-C9	2.19	129.47	126.23
36	BV	5201	HEM	O2D-CGD-CBD	2.19	120.90	114.00
24	BC	5511	CLA	CHB-C1B-NB	2.18	127.32	124.05
24	BB	5607	CLA	CBA-CAA-C2A	2.18	120.29	113.79
28	BA	5412	DGD	O1A-C1A-C2A	-2.18	115.25	123.78
24	BC	5511	CLA	C12-C11-C10	-2.18	103.52	113.28
36	AF	101	HEM	C2A-C1A-NA	2.18	112.57	110.15
28	AE	101	DGD	C3G-C2G-C1G	2.18	116.86	111.78
28	AC	518	DGD	O2G-C2G-C1G	2.18	116.16	108.34
27	AB	617	BCR	C34-C9-C8	2.18	121.42	118.09
24	BB	5614	CLA	C3B-C4B-NB	-2.18	108.59	110.53
27	BC	5514	BCR	C34-C9-C8	2.18	121.41	118.09
32	AI	103	LMT	C3'-C4'-C5'	-2.18	106.11	110.93
24	BB	5613	CLA	CAA-C2A-C1A	-2.18	104.85	111.97
24	AB	605	CLA	CAA-C2A-C3A	-2.17	107.12	113.00
24	AA	405	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
27	AB	619	BCR	C40-C30-C25	2.17	113.65	110.24
24	AC	506	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
27	AD	406	BCR	C34-C9-C8	2.17	121.40	118.09
27	BC	5514	BCR	C32-C1-C2	-2.17	100.62	108.95
24	AB	606	CLA	CHA-C4D-ND	2.17	137.03	132.55
24	AB	613	CLA	CED-O2D-CGD	2.17	120.84	115.92
24	BC	5502	CLA	C4D-CHA-C1A	2.17	123.83	121.24
34	BD	5404	PHO	O2A-CGA-O1A	-2.17	118.20	123.63
31	BD	5409	LMG	C6-C5-C4	-2.17	107.70	113.02
27	BK	5102	BCR	C23-C22-C21	-2.17	115.60	119.01
31	AJ	102	LMG	C35-C34-C33	2.16	125.29	114.37
24	AB	609	CLA	CAA-C2A-C1A	-2.16	104.90	111.97
24	BC	5513	CLA	CHB-C1B-NB	2.16	127.29	124.05
30	BB	5601	SQD	O48-C23-O10	-2.16	118.23	123.63
31	BD	5408	LMG	C35-C34-C33	2.16	125.28	114.37
27	AX	101	BCR	C34-C9-C8	2.16	121.39	118.09
24	AA	406	CLA	CED-O2D-CGD	2.16	120.81	115.92
33	AB	625	DMS	O-S-C1	2.16	117.29	106.49
24	BB	5609	CLA	CAA-C2A-C3A	-2.15	107.18	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5618	CLA	CHB-C1B-NB	2.15	127.28	124.05
24	AC	511	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
27	AJ	101	BCR	C30-C25-C24	2.15	121.49	115.65
27	AB	619	BCR	C23-C22-C21	-2.15	115.62	119.01
27	BC	5515	BCR	C24-C23-C22	2.15	129.42	126.23
24	BB	5615	CLA	C4-C3-C5	-2.15	111.50	115.23
30	BB	5601	SQD	C15-C14-C13	2.15	125.23	114.37
24	AB	602	CLA	C12-C11-C10	-2.15	103.65	113.28
28	AA	411	DGD	C3G-C2G-C1G	2.15	116.79	111.78
24	AB	610	CLA	C4B-C3B-C2B	-2.15	104.63	107.30
27	AJ	101	BCR	C16-C17-C18	2.15	130.29	127.28
24	AD	401	CLA	C4B-C3B-C2B	-2.15	104.63	107.30
24	AC	502	CLA	CHA-C4D-ND	2.15	136.98	132.55
27	AK	102	BCR	C11-C12-C13	2.15	132.25	126.36
24	BB	5606	CLA	C12-C11-C10	-2.15	103.67	113.28
30	AA	413	SQD	C17-C16-C15	2.14	125.21	114.37
28	AC	518	DGD	O6E-C5E-C4E	2.14	113.56	109.70
24	BB	5611	CLA	CED-O2D-CGD	2.14	120.78	115.92
36	AF	101	HEM	C4C-C3C-C2C	-2.14	104.96	106.81
27	BA	5411	BCR	C32-C1-C6	2.14	113.60	110.24
24	BC	5506	CLA	CHA-C4D-ND	2.14	136.96	132.55
27	BB	5622	BCR	C23-C22-C21	-2.14	115.64	119.01
24	AB	602	CLA	CHA-C4D-ND	2.14	136.96	132.55
24	BC	5502	CLA	CHA-C4D-ND	2.14	136.96	132.55
30	AA	413	SQD	O47-C7-C8	2.14	116.11	111.48
27	AC	514	BCR	C30-C25-C24	2.14	121.45	115.65
28	BC	5519	DGD	O3G-C3G-C2G	2.14	116.02	110.82
27	BB	5623	BCR	C30-C25-C24	2.14	121.45	115.65
27	BB	5623	BCR	C36-C18-C19	2.14	121.35	118.09
24	AC	513	CLA	C2A-C1A-CHA	2.14	127.58	123.87
24	AD	401	CLA	C7-C6-C5	-2.14	107.57	113.26
24	BB	5614	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
24	BA	5406	CLA	O1D-CGD-CBD	-2.14	120.31	124.52
28	AA	411	DGD	O1A-C1A-C2A	-2.14	115.43	123.78
24	AB	612	CLA	C2C-C1C-NC	-2.14	107.74	109.98
30	AF	102	SQD	C17-C16-C15	2.13	125.16	114.37
30	AA	416	SQD	C17-C16-C15	2.13	125.15	114.37
24	AB	608	CLA	C4-C3-C5	-2.13	111.53	115.23
24	BB	5617	CLA	CHA-C1A-NA	-2.13	121.56	126.39
24	AC	504	CLA	CED-O2D-CGD	2.13	120.75	115.92
24	BB	5609	CLA	CBC-CAC-C3C	-2.13	106.64	112.42
24	BC	5503	CLA	C4B-C3B-C2B	-2.13	104.66	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AC	520	LMG	O1-C7-C8	-2.13	105.64	110.82
36	BV	5201	HEM	C3B-C4B-NB	-2.13	107.94	109.47
24	AA	405	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
24	BB	5608	CLA	C2A-C1A-CHA	2.13	127.56	123.87
28	AC	519	DGD	O1G-C1A-O1A	-2.13	118.31	123.63
27	AK	102	BCR	C36-C18-C19	2.13	121.33	118.09
24	AB	612	CLA	CED-O2D-CGD	2.12	120.73	115.92
27	BC	5515	BCR	C7-C8-C9	2.12	129.38	126.23
27	BB	5621	BCR	C24-C23-C22	2.12	129.38	126.23
36	BF	5101	HEM	CAD-CBD-CGD	2.12	119.30	113.67
24	BB	5615	CLA	C12-C11-C10	-2.12	103.77	113.28
27	BD	5407	BCR	C28-C27-C26	2.12	117.84	114.06
24	AB	604	CLA	OBD-CAD-C3D	2.12	133.38	128.42
24	AB	603	CLA	CHA-C1A-NA	-2.12	121.59	126.39
24	AB	605	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
24	AD	404	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
24	AC	506	CLA	CHA-C4D-ND	2.12	136.92	132.55
30	AB	627	SQD	C15-C14-C13	2.12	125.07	114.37
27	BX	5101	BCR	C28-C27-C26	2.12	117.83	114.06
24	AB	613	CLA	CHA-C1A-NA	-2.12	121.60	126.39
31	AC	520	LMG	O8-C28-C29	2.12	118.29	111.83
24	AC	509	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
27	AX	101	BCR	C37-C22-C23	2.12	121.32	118.09
24	AA	404	CLA	O2D-CGD-CBD	2.11	114.93	111.23
24	BC	5511	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
28	BA	5412	DGD	O1B-C1B-C2B	-2.11	115.52	123.78
24	AD	404	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
24	BC	5513	CLA	C2A-C1A-CHA	2.11	127.53	123.87
27	BJ	5101	BCR	C30-C25-C24	2.11	121.38	115.65
32	AI	103	LMT	C3-C2-C1	2.11	122.64	113.47
27	BC	5516	BCR	C32-C1-C2	-2.11	100.84	108.95
31	AC	521	LMG	C17-C16-C15	-2.11	103.69	114.37
27	AC	516	BCR	C19-C18-C17	-2.11	115.69	119.01
31	AI	101	LMG	O7-C10-O9	-2.11	118.77	123.70
24	AC	507	CLA	C11-C12-C13	2.11	122.98	115.97
24	AD	401	CLA	C12-C11-C10	-2.11	103.82	113.28
24	BC	5503	CLA	CHA-C4D-ND	2.11	136.90	132.55
24	AB	610	CLA	C7-C6-C5	-2.11	107.64	113.26
28	AC	519	DGD	C4D-C3D-C2D	2.11	114.53	110.83
31	AC	521	LMG	O1-C7-C8	2.11	115.94	110.82
27	AC	515	BCR	C32-C1-C6	2.11	113.55	110.24
24	BC	5502	CLA	CHB-C1B-NB	2.11	127.21	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BD	5408	LMG	C17-C16-C15	-2.10	103.73	114.37
27	BC	5514	BCR	C8-C9-C10	-2.10	115.70	119.01
24	AB	608	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
27	BD	5407	BCR	C15-C14-C13	2.10	130.23	127.28
24	AB	604	CLA	C2A-C1A-CHA	2.10	127.52	123.87
32	AB	629	LMT	C6'-C5'-C4'	-2.10	107.47	113.38
24	BD	5402	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
24	AB	616	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
24	BB	5611	CLA	C11-C12-C13	2.10	122.94	115.97
24	AB	607	CLA	CED-O2D-CGD	2.10	120.68	115.92
24	AB	607	CLA	C11-C12-C13	2.10	122.94	115.97
27	BC	5515	BCR	C8-C9-C10	-2.10	115.71	119.01
24	AC	504	CLA	CHA-C4D-ND	2.10	136.88	132.55
24	AB	601	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
24	BB	5606	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
30	BF	5102	SQD	C17-C16-C15	2.10	124.96	114.37
30	BF	5102	SQD	O48-C23-O10	-2.09	118.39	123.63
24	BB	5612	CLA	C4-C3-C5	-2.09	111.59	115.23
24	AB	602	CLA	CAA-CBA-CGA	-2.09	107.26	113.21
24	BC	5502	CLA	CAA-CBA-CGA	-2.09	107.26	113.21
24	BB	5608	CLA	CAA-CBA-CGA	-2.09	107.26	113.21
24	BA	5406	CLA	C2A-C1A-CHA	2.09	127.50	123.87
24	BB	5618	CLA	C2A-C1A-CHA	2.09	127.50	123.87
27	BC	5515	BCR	C1-C6-C7	2.09	121.33	115.65
32	AM	102	LMT	O1B-C1B-C2B	2.09	113.23	108.09
24	AC	512	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
24	BA	5406	CLA	C4-C3-C5	-2.09	111.60	115.23
24	AD	404	CLA	CED-O2D-CGD	2.09	120.66	115.92
30	BF	5102	SQD	O8-S-O9	-2.09	106.17	111.40
31	BM	5102	LMG	C34-C33-C32	2.09	124.93	114.37
30	AF	102	SQD	C31-C30-C29	2.09	133.58	115.25
24	BA	5407	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
30	BA	5414	SQD	C13-C12-C11	2.09	124.93	114.37
28	BC	5519	DGD	O2E-C2E-C3E	2.09	115.30	110.38
27	AD	406	BCR	C1-C6-C7	2.09	121.31	115.65
27	BB	5621	BCR	C37-C22-C23	2.09	121.28	118.09
28	AA	411	DGD	O1B-C1B-C2B	-2.09	115.62	123.78
30	AA	413	SQD	O8-S-O7	2.09	116.62	111.40
24	BB	5615	CLA	CHC-C1C-NC	2.09	127.45	124.31
24	BC	5505	CLA	CED-O2D-CGD	2.09	120.64	115.92
30	BF	5102	SQD	C31-C30-C29	2.08	133.54	115.25
24	AC	501	CLA	C4B-C3B-C2B	-2.08	104.71	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BD	5403	PHO	C6-C7-C8	-2.08	109.04	115.97
32	AB	624	LMT	C1'-O5'-C5'	-2.08	109.65	113.72
27	BK	5102	BCR	C40-C30-C29	-2.08	100.97	108.95
27	AC	516	BCR	C12-C13-C14	-2.08	115.74	119.01
27	BC	5515	BCR	C32-C1-C6	2.08	113.50	110.24
24	AB	615	CLA	C4B-C3B-C2B	-2.08	104.72	107.30
24	BB	5614	CLA	C7-C6-C5	-2.08	107.72	113.26
27	AC	515	BCR	C30-C25-C24	2.08	121.29	115.65
24	BC	5504	CLA	C6-C7-C8	-2.08	109.06	115.97
31	AC	521	LMG	O7-C8-C9	-2.08	100.89	108.34
27	AA	410	BCR	C19-C18-C17	-2.08	115.74	119.01
24	BC	5508	CLA	C2C-C1C-NC	-2.08	107.80	109.98
24	BB	5612	CLA	CHA-C4D-ND	2.08	136.83	132.55
24	BD	5405	CLA	CED-O2D-CGD	2.07	120.62	115.92
30	AA	416	SQD	C13-C12-C11	2.07	124.85	114.37
27	BJ	5101	BCR	C34-C9-C8	2.07	121.25	118.09
27	BC	5515	BCR	C30-C25-C24	2.07	121.27	115.65
31	BM	5102	LMG	C6-C5-C4	-2.07	107.93	113.02
32	BC	5522	LMT	C6B-C5B-C4B	2.07	118.11	113.02
24	AC	509	CLA	C12-C11-C10	-2.07	104.00	113.28
27	BB	5623	BCR	C23-C22-C21	-2.07	115.75	119.01
24	AC	504	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
27	BK	5102	BCR	C11-C12-C13	2.07	132.04	126.36
24	AA	404	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
27	BB	5622	BCR	C30-C25-C24	2.07	121.26	115.65
24	BB	5611	CLA	OBD-CAD-C3D	2.07	133.25	128.42
31	AM	101	LMG	C6-C5-C4	-2.07	107.94	113.02
30	BA	5401	SQD	C13-C12-C11	2.07	124.83	114.37
28	AH	101	DGD	O1B-C1B-C2B	-2.07	115.69	123.78
32	BI	5102	LMT	C9-C8-C7	-2.07	103.92	114.37
24	AC	503	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
27	AA	410	BCR	C32-C1-C6	2.07	113.48	110.24
27	AB	619	BCR	C36-C18-C19	2.07	121.24	118.09
24	AC	510	CLA	C2A-C3A-C4A	2.06	105.20	101.87
31	AC	520	LMG	C36-C35-C34	-2.06	103.94	114.37
24	BB	5614	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
24	AB	608	CLA	CHA-C4D-ND	2.06	136.80	132.55
27	AK	102	BCR	C19-C18-C17	-2.06	115.77	119.01
24	AC	504	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
24	BA	5406	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
24	BC	5506	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
30	AB	627	SQD	C17-C16-C15	2.06	124.79	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AA	413	SQD	C13-C12-C11	2.06	124.79	114.37
24	AB	603	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
24	BD	5402	CLA	C12-C11-C10	-2.06	104.05	113.28
27	AC	515	BCR	C1-C6-C7	2.06	121.23	115.65
24	AB	611	CLA	CHA-C4D-ND	2.06	136.79	132.55
27	AB	619	BCR	C16-C17-C18	2.06	130.16	127.28
24	AA	406	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
32	BB	5603	LMT	C6'-C5'-C4'	-2.06	107.59	113.38
27	AC	516	BCR	C32-C1-C2	-2.06	101.05	108.95
24	BA	5405	CLA	C6-C7-C8	-2.06	109.13	115.97
30	AA	413	SQD	O47-C45-C44	2.06	115.72	108.34
24	AA	407	CLA	CAA-CBA-CGA	-2.05	107.38	113.21
24	BD	5405	CLA	C4B-C3B-C2B	-2.05	104.75	107.30
24	AB	616	CLA	C4B-C3B-C2B	-2.05	104.75	107.30
32	BM	5101	LMT	C6B-C5B-C4B	2.05	118.06	113.02
31	AC	520	LMG	C35-C34-C33	2.05	124.75	114.37
36	AV	201	HEM	C4B-C3B-C2B	-2.05	105.39	107.28
24	AC	504	CLA	C6-C7-C8	-2.05	109.14	115.97
27	AX	101	BCR	C32-C1-C6	2.05	113.46	110.24
31	BC	5520	LMG	C6-C5-C4	-2.05	107.98	113.02
27	AC	514	BCR	C32-C1-C2	-2.05	101.07	108.95
35	AD	405	PL9	C2-C3-C4	-2.05	116.02	118.78
28	BH	5101	DGD	O1G-C1A-C2A	2.05	118.09	111.83
30	AA	413	SQD	O9-S-C6	-2.05	103.69	106.76
30	AF	102	SQD	C13-C12-C11	2.05	124.73	114.37
32	BM	5101	LMT	O1B-C1B-C2B	2.05	113.13	108.09
27	AT	101	BCR	C30-C25-C24	2.05	121.21	115.65
27	BB	5621	BCR	C15-C16-C17	-2.05	119.33	123.52
24	AC	509	CLA	CHB-C1B-NB	2.05	127.12	124.05
28	BC	5517	DGD	C4E-C3E-C2E	-2.05	107.23	110.83
24	BA	5405	CLA	CAA-CBA-CGA	-2.05	107.39	113.21
28	BC	5518	DGD	O6E-C1E-C2E	2.05	114.58	110.37
27	AD	406	BCR	C20-C21-C22	2.05	130.15	127.28
24	BC	5501	CLA	C4B-C3B-C2B	-2.05	104.76	107.30
30	BA	5414	SQD	C3-C4-C5	-2.05	106.52	110.23
24	AB	615	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
24	BB	5619	CLA	CHA-C1A-NA	-2.04	121.77	126.39
24	BB	5616	CLA	CED-O2D-CGD	2.04	120.55	115.92
32	BC	5522	LMT	C3'-C4'-C5'	-2.04	106.41	110.93
27	AC	516	BCR	C7-C8-C9	2.04	129.25	126.23
30	BF	5102	SQD	C13-C12-C11	2.04	124.68	114.37
30	BB	5601	SQD	C17-C16-C15	2.04	124.68	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	604	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
27	BK	5102	BCR	C19-C18-C17	-2.04	115.80	119.01
30	BA	5401	SQD	O48-C23-O10	-2.04	118.53	123.63
31	BC	5520	LMG	C35-C34-C33	2.04	124.67	114.37
31	AM	101	LMG	C34-C33-C32	2.04	124.67	114.37
24	BD	5402	CLA	C7-C6-C5	-2.04	107.83	113.26
32	BB	5603	LMT	C6-C5-C4	2.04	124.66	114.37
24	BA	5408	CLA	CAA-CBA-CGA	-2.03	107.43	113.21
27	AC	515	BCR	C11-C10-C9	2.03	130.13	127.28
31	BI	5101	LMG	O7-C10-O9	-2.03	118.95	123.70
30	BA	5414	SQD	O47-C7-C8	2.03	115.88	111.48
24	AC	512	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
24	BB	5615	CLA	C5-C3-C2	2.03	125.73	121.17
24	BB	5606	CLA	C7-C6-C5	-2.03	107.85	113.26
24	BB	5614	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
31	BC	5521	LMG	O7-C8-C9	-2.03	101.06	108.34
24	BA	5406	CLA	CHD-C4C-NC	2.03	127.38	124.23
24	AB	606	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
24	BB	5616	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
24	BC	5507	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
27	BA	5411	BCR	C19-C18-C17	-2.03	115.82	119.01
27	BB	5623	BCR	C16-C17-C18	2.03	130.12	127.28
27	BC	5515	BCR	C11-C10-C9	2.03	130.12	127.28
32	AI	102	LMT	C9-C8-C7	-2.02	104.14	114.37
27	BC	5515	BCR	C32-C1-C2	-2.02	101.18	108.95
31	AJ	102	LMG	C17-C16-C15	-2.02	104.15	114.37
24	BA	5405	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
24	AA	405	CLA	CMD-C2D-C1D	2.02	128.29	124.73
24	BC	5509	CLA	C12-C11-C10	-2.02	104.23	113.28
27	BC	5514	BCR	C20-C21-C22	2.02	130.11	127.28
32	BB	5627	LMT	C1'-O5'-C5'	-2.02	109.78	113.72
28	BE	5102	DGD	O5D-C6D-C5D	2.02	113.97	109.42
28	BE	5102	DGD	C6D-C5D-C4D	-2.02	107.83	112.07
24	BB	5607	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
27	AB	617	BCR	C7-C8-C9	2.02	129.22	126.23
27	AC	514	BCR	C20-C21-C22	2.02	130.11	127.28
30	BA	5401	SQD	C19-C18-C17	2.02	124.56	114.37
28	BE	5102	DGD	C6E-C5E-C4E	-2.02	108.07	113.02
34	AD	403	PHO	O2A-CGA-O1A	-2.01	118.59	123.63
28	AE	101	DGD	O5D-C6D-C5D	2.01	113.96	109.42
36	AV	201	HEM	C3B-C4B-NB	-2.01	108.02	109.47
34	AD	402	PHO	C6-C7-C8	-2.01	109.27	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	618	BCR	C35-C13-C12	2.01	121.16	118.09
28	BC	5518	DGD	O6E-C5E-C4E	2.01	113.33	109.70
24	AB	610	CLA	C3B-C4B-NB	-2.01	108.73	110.53
31	AD	407	LMG	C1-O6-C5	-2.01	109.79	113.72
30	AA	413	SQD	C3-C4-C5	-2.01	106.59	110.23
27	AJ	101	BCR	C3-C4-C5	2.01	117.64	114.06
24	BB	5607	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
28	AE	101	DGD	O6E-C1E-O5D	-2.01	105.30	110.04
32	BC	5522	LMT	C3-C2-C1	2.01	122.19	113.47
28	AE	101	DGD	C4A-C3A-C2A	-2.01	105.75	113.13
24	BB	5608	CLA	OBD-CAD-C3D	2.01	133.11	128.42
24	BA	5407	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
24	AB	603	CLA	CMA-C3A-C4A	2.01	117.16	111.77
32	AM	102	LMT	C6B-C5B-C4B	2.01	117.94	113.02
24	BB	5615	CLA	C4B-C3B-C2B	-2.00	104.81	107.30
24	AB	607	CLA	OBD-CAD-C3D	2.00	133.10	128.42
31	BL	5101	LMG	O1-C1-C2	2.00	111.31	108.27
27	BT	5101	BCR	C1-C6-C7	2.00	121.08	115.65
24	AC	502	CLA	C4D-CHA-C1A	2.00	123.63	121.24
31	BC	5520	LMG	O8-C28-C29	2.00	117.94	111.83

All (78) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	AA	404	CLA	C8
24	AA	405	CLA	C8
24	AA	406	CLA	C8
24	AA	407	CLA	C8
24	AB	601	CLA	C8
24	AB	602	CLA	C8
24	AB	603	CLA	C8
24	AB	604	CLA	C8
24	AB	605	CLA	C8
24	AB	606	CLA	C8
24	AB	607	CLA	C8
24	AB	608	CLA	C8
24	AB	609	CLA	C8
24	AB	610	CLA	C8
24	AB	611	CLA	C8
24	AB	612	CLA	C8
24	AB	613	CLA	C8
24	AB	614	CLA	C8

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Mol	Chain	Res	Type	Atom
24	AB	615	CLA	C8
24	AB	616	CLA	C8
24	AC	501	CLA	C8
24	AC	502	CLA	C8
24	AC	503	CLA	C8
24	AC	504	CLA	C8
24	AC	505	CLA	C8
24	AC	506	CLA	C8
24	AC	507	CLA	C8
24	AC	508	CLA	C8
24	AC	509	CLA	C8
24	AC	510	CLA	C8
24	AC	511	CLA	C8
24	AC	512	CLA	C8
24	AC	513	CLA	C8
24	AD	401	CLA	C8
24	AD	404	CLA	C8
24	BA	5405	CLA	C8
24	BA	5406	CLA	C8
24	BA	5407	CLA	C8
24	BA	5408	CLA	C8
24	BB	5605	CLA	C8
24	BB	5606	CLA	C8
24	BB	5607	CLA	C8
24	BB	5608	CLA	C8
24	BB	5609	CLA	C8
24	BB	5610	CLA	C8
24	BB	5611	CLA	C8
24	BB	5612	CLA	C8
24	BB	5613	CLA	C8
24	BB	5614	CLA	C8
24	BB	5615	CLA	C8
24	BB	5616	CLA	C8
24	BB	5617	CLA	C8
24	BB	5618	CLA	C8
24	BB	5619	CLA	C8
24	BB	5620	CLA	C8
24	BC	5501	CLA	C8
24	BC	5502	CLA	C8
24	BC	5503	CLA	C8
24	BC	5504	CLA	C8
24	BC	5505	CLA	C8

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Mol	Chain	Res	Type	Atom
24	BC	5506	CLA	C8
24	BC	5507	CLA	C8
24	BC	5508	CLA	C8
24	BC	5509	CLA	C8
24	BC	5510	CLA	C8
24	BC	5511	CLA	C8
24	BC	5512	CLA	C8
24	BC	5513	CLA	C8
24	BD	5402	CLA	C8
24	BD	5405	CLA	C8
28	AC	518	DGD	C1E
28	AC	519	DGD	C1E
28	BC	5518	DGD	C1E
28	BC	5519	DGD	C1E
34	AD	402	PHO	C8
34	AD	403	PHO	C8
34	BD	5403	PHO	C8
34	BD	5404	PHO	C8

All (1327) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AA	405	CLA	C6-C7-C8-C9
24	AB	607	CLA	C4-C3-C5-C6
24	AB	610	CLA	CHA-CBD-CGD-O2D
24	AB	610	CLA	C14-C13-C15-C16
24	AC	503	CLA	CHA-CBD-CGD-O2D
24	AC	508	CLA	CHA-CBD-CGD-O1D
24	AC	508	CLA	CHA-CBD-CGD-O2D
24	BA	5406	CLA	C6-C7-C8-C9
24	BB	5611	CLA	C4-C3-C5-C6
24	BB	5614	CLA	CHA-CBD-CGD-O2D
24	BB	5614	CLA	C14-C13-C15-C16
24	BC	5508	CLA	CHA-CBD-CGD-O1D
24	BC	5508	CLA	CHA-CBD-CGD-O2D
25	AA	408	MST	N1-C2-S7-C8
25	AA	408	MST	N3-C2-S7-C8
25	BA	5409	MST	N1-C2-S7-C8
25	BA	5409	MST	N3-C2-S7-C8
27	AB	618	BCR	C6-C7-C8-C9
27	AB	619	BCR	C23-C24-C25-C26
27	AB	619	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
27	AC	514	BCR	C1-C6-C7-C8
27	AC	514	BCR	C5-C6-C7-C8
27	AC	514	BCR	C6-C7-C8-C9
27	AC	515	BCR	C6-C7-C8-C9
27	AC	516	BCR	C6-C7-C8-C9
27	AC	516	BCR	C23-C24-C25-C26
27	AC	516	BCR	C23-C24-C25-C30
27	AD	406	BCR	C6-C7-C8-C9
27	AD	406	BCR	C23-C24-C25-C26
27	AJ	101	BCR	C6-C7-C8-C9
27	AT	101	BCR	C6-C7-C8-C9
27	AT	101	BCR	C22-C23-C24-C25
27	AX	101	BCR	C6-C7-C8-C9
27	BB	5622	BCR	C6-C7-C8-C9
27	BB	5623	BCR	C23-C24-C25-C26
27	BB	5623	BCR	C23-C24-C25-C30
27	BC	5514	BCR	C1-C6-C7-C8
27	BC	5514	BCR	C5-C6-C7-C8
27	BC	5514	BCR	C6-C7-C8-C9
27	BC	5515	BCR	C6-C7-C8-C9
27	BC	5516	BCR	C6-C7-C8-C9
27	BC	5516	BCR	C23-C24-C25-C26
27	BC	5516	BCR	C23-C24-C25-C30
27	BD	5407	BCR	C6-C7-C8-C9
27	BD	5407	BCR	C23-C24-C25-C26
27	BJ	5101	BCR	C6-C7-C8-C9
27	BT	5101	BCR	C6-C7-C8-C9
27	BT	5101	BCR	C22-C23-C24-C25
27	BX	5101	BCR	C6-C7-C8-C9
28	AA	411	DGD	O6E-C1E-O5D-C6D
28	AC	518	DGD	O6E-C1E-O5D-C6D
28	BA	5412	DGD	O6E-C1E-O5D-C6D
28	BC	5518	DGD	O6E-C1E-O5D-C6D
29	AA	412	LHG	O2-C2-C3-O3
29	AA	415	LHG	C1-C2-C3-O3
29	BA	5413	LHG	O2-C2-C3-O3
29	BA	5415	LHG	C1-C2-C3-O3
30	AA	413	SQD	O5-C1-O6-C44
30	AA	413	SQD	C8-C7-O47-C45
30	AA	413	SQD	O5-C5-C6-S
30	AA	413	SQD	C5-C6-S-O7
30	AA	413	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
30	AA	413	SQD	C5-C6-S-O9
30	AA	416	SQD	O6-C44-C45-O47
30	AA	416	SQD	O5-C5-C6-S
30	AA	416	SQD	C5-C6-S-O7
30	AA	416	SQD	C5-C6-S-O8
30	AA	416	SQD	C5-C6-S-O9
30	AB	622	SQD	O5-C1-O6-C44
30	AB	622	SQD	O5-C5-C6-S
30	AB	622	SQD	C5-C6-S-O7
30	AB	622	SQD	C5-C6-S-O8
30	AB	627	SQD	O49-C7-O47-C45
30	AB	627	SQD	C8-C7-O47-C45
30	AB	627	SQD	O5-C5-C6-S
30	AB	627	SQD	C5-C6-S-O7
30	AB	627	SQD	C5-C6-S-O8
30	AB	627	SQD	C5-C6-S-O9
30	AF	102	SQD	C8-C7-O47-C45
30	AF	102	SQD	O5-C5-C6-S
30	AF	102	SQD	C5-C6-S-O7
30	AF	102	SQD	C5-C6-S-O8
30	AF	102	SQD	C5-C6-S-O9
30	BA	5401	SQD	O6-C44-C45-O47
30	BA	5401	SQD	O5-C5-C6-S
30	BA	5401	SQD	C5-C6-S-O7
30	BA	5401	SQD	C5-C6-S-O8
30	BA	5401	SQD	C5-C6-S-O9
30	BA	5414	SQD	O5-C1-O6-C44
30	BA	5414	SQD	C8-C7-O47-C45
30	BA	5414	SQD	O5-C5-C6-S
30	BA	5414	SQD	C5-C6-S-O7
30	BA	5414	SQD	C5-C6-S-O8
30	BB	5601	SQD	O49-C7-O47-C45
30	BB	5601	SQD	C8-C7-O47-C45
30	BB	5601	SQD	O5-C5-C6-S
30	BB	5601	SQD	C5-C6-S-O7
30	BB	5601	SQD	C5-C6-S-O8
30	BB	5601	SQD	C5-C6-S-O9
30	BB	5625	SQD	O5-C1-O6-C44
30	BB	5625	SQD	O5-C5-C6-S
30	BB	5625	SQD	C5-C6-S-O7
30	BB	5625	SQD	C5-C6-S-O8
30	BF	5102	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
30	BF	5102	SQD	O5-C5-C6-S
30	BF	5102	SQD	C5-C6-S-O7
30	BF	5102	SQD	C5-C6-S-O8
30	BF	5102	SQD	C5-C6-S-O9
31	AB	620	LMG	O1-C7-C8-O7
31	AC	520	LMG	O7-C8-C9-O8
31	BC	5520	LMG	O7-C8-C9-O8
31	BL	5101	LMG	O1-C7-C8-O7
34	AD	403	PHO	CBD-CGD-O2D-CED
34	BD	5404	PHO	CBD-CGD-O2D-CED
35	AD	405	PL9	C7-C8-C9-C10
35	AD	405	PL9	C26-C27-C28-C29
35	AD	405	PL9	C46-C47-C48-C49
35	BD	5406	PL9	C7-C8-C9-C10
35	BD	5406	PL9	C26-C27-C28-C29
35	BD	5406	PL9	C46-C47-C48-C49
36	AF	101	HEM	C2B-C3B-CAB-CBB
36	AF	101	HEM	C4B-C3B-CAB-CBB
36	AF	101	HEM	C2C-C3C-CAC-CBC
36	AV	201	HEM	C2B-C3B-CAB-CBB
36	AV	201	HEM	C4B-C3B-CAB-CBB
36	AV	201	HEM	C2C-C3C-CAC-CBC
36	AV	201	HEM	C4C-C3C-CAC-CBC
36	BF	5101	HEM	C2B-C3B-CAB-CBB
36	BF	5101	HEM	C4B-C3B-CAB-CBB
36	BF	5101	HEM	C2C-C3C-CAC-CBC
36	BV	5201	HEM	C2B-C3B-CAB-CBB
36	BV	5201	HEM	C4B-C3B-CAB-CBB
36	BV	5201	HEM	C2C-C3C-CAC-CBC
36	BV	5201	HEM	C4C-C3C-CAC-CBC
30	AA	416	SQD	O10-C23-O48-C46
30	BA	5401	SQD	O10-C23-O48-C46
28	AC	519	DGD	O6D-C5D-C6D-O5D
28	BC	5519	DGD	O6D-C5D-C6D-O5D
24	BB	5606	CLA	CBA-CGA-O2A-C1
24	AB	602	CLA	O1A-CGA-O2A-C1
24	AC	513	CLA	O1A-CGA-O2A-C1
24	AD	401	CLA	O1A-CGA-O2A-C1
24	BB	5606	CLA	O1A-CGA-O2A-C1
24	BC	5513	CLA	O1A-CGA-O2A-C1
24	BD	5402	CLA	O1A-CGA-O2A-C1
29	AA	412	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
29	AA	415	LHG	O10-C23-O8-C6
29	BA	5413	LHG	O10-C23-O8-C6
29	BA	5415	LHG	O10-C23-O8-C6
30	AF	102	SQD	O10-C23-O48-C46
30	BF	5102	SQD	O10-C23-O48-C46
34	AD	403	PHO	O1D-CGD-O2D-CED
34	BD	5404	PHO	O1D-CGD-O2D-CED
24	AB	612	CLA	C10-C11-C12-C13
24	BB	5616	CLA	C10-C11-C12-C13
30	AA	413	SQD	O49-C7-O47-C45
30	AF	102	SQD	O49-C7-O47-C45
30	BA	5414	SQD	O49-C7-O47-C45
30	BF	5102	SQD	O49-C7-O47-C45
24	AA	405	CLA	C3-C5-C6-C7
24	AA	406	CLA	C3-C5-C6-C7
24	AA	407	CLA	C3-C5-C6-C7
24	AB	613	CLA	C3-C5-C6-C7
24	AB	614	CLA	C3-C5-C6-C7
24	AC	501	CLA	C3-C5-C6-C7
24	AC	504	CLA	C3-C5-C6-C7
24	AC	506	CLA	C3-C5-C6-C7
24	AC	511	CLA	C3-C5-C6-C7
24	AC	513	CLA	C3-C5-C6-C7
24	BA	5408	CLA	C3-C5-C6-C7
24	BB	5617	CLA	C3-C5-C6-C7
24	BB	5618	CLA	C3-C5-C6-C7
24	BC	5501	CLA	C3-C5-C6-C7
24	BC	5504	CLA	C3-C5-C6-C7
24	BC	5506	CLA	C3-C5-C6-C7
24	BC	5511	CLA	C3-C5-C6-C7
24	BC	5513	CLA	C3-C5-C6-C7
24	AB	602	CLA	CBA-CGA-O2A-C1
24	AB	608	CLA	CBA-CGA-O2A-C1
24	AC	513	CLA	CBA-CGA-O2A-C1
24	BB	5612	CLA	CBA-CGA-O2A-C1
24	BC	5513	CLA	CBA-CGA-O2A-C1
29	AA	415	LHG	C24-C23-O8-C6
30	AA	416	SQD	C24-C23-O48-C46
30	BA	5401	SQD	C24-C23-O48-C46
32	AI	102	LMT	C3'-C4'-O1B-C1B
32	BI	5102	LMT	C3'-C4'-O1B-C1B
24	AA	407	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	BA	5408	CLA	O1A-CGA-O2A-C1
24	AB	613	CLA	C4-C3-C5-C6
24	BB	5617	CLA	C4-C3-C5-C6
24	AB	607	CLA	C2-C3-C5-C6
24	AB	613	CLA	C2-C3-C5-C6
24	BB	5611	CLA	C2-C3-C5-C6
24	BB	5617	CLA	C2-C3-C5-C6
35	AD	405	PL9	C28-C29-C31-C32
35	BD	5406	PL9	C28-C29-C31-C32
24	AB	601	CLA	C2A-CAA-CBA-CGA
24	BB	5605	CLA	C2A-CAA-CBA-CGA
24	AB	604	CLA	C3-C5-C6-C7
24	AB	607	CLA	C3-C5-C6-C7
24	BA	5406	CLA	C3-C5-C6-C7
24	BA	5407	CLA	C3-C5-C6-C7
24	BB	5608	CLA	C3-C5-C6-C7
24	BB	5611	CLA	C3-C5-C6-C7
24	AC	501	CLA	CBA-CGA-O2A-C1
24	AD	401	CLA	CBA-CGA-O2A-C1
24	BC	5501	CLA	CBA-CGA-O2A-C1
24	BD	5402	CLA	CBA-CGA-O2A-C1
29	AA	412	LHG	C24-C23-O8-C6
29	BA	5413	LHG	C24-C23-O8-C6
29	BA	5415	LHG	C24-C23-O8-C6
30	AF	102	SQD	C24-C23-O48-C46
30	BF	5102	SQD	C24-C23-O48-C46
31	BB	5624	LMG	C36-C37-C38-C39
31	BM	5102	LMG	C18-C19-C20-C21
31	AC	521	LMG	C36-C37-C38-C39
31	AB	621	LMG	C36-C37-C38-C39
31	AM	101	LMG	C18-C19-C20-C21
31	BC	5521	LMG	C36-C37-C38-C39
32	BD	5411	LMT	C3-C4-C5-C6
24	AB	612	CLA	O1A-CGA-O2A-C1
24	AC	501	CLA	O1A-CGA-O2A-C1
24	AC	510	CLA	O1A-CGA-O2A-C1
24	BB	5612	CLA	O1A-CGA-O2A-C1
24	BB	5616	CLA	O1A-CGA-O2A-C1
24	BC	5501	CLA	O1A-CGA-O2A-C1
24	BC	5510	CLA	O1A-CGA-O2A-C1
28	AC	519	DGD	C7B-C8B-C9B-CAB
32	BB	5604	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
28	AC	517	DGD	C7A-C8A-C9A-CAA
28	BC	5517	DGD	C7A-C8A-C9A-CAA
28	BC	5519	DGD	C7B-C8B-C9B-CAB
31	AA	414	LMG	C18-C19-C20-C21
31	AA	417	LMG	C18-C19-C20-C21
31	AD	407	LMG	C18-C19-C20-C21
31	AD	407	LMG	C36-C37-C38-C39
31	BA	5402	LMG	C18-C19-C20-C21
31	BB	5624	LMG	C18-C19-C20-C21
31	BC	5520	LMG	C36-C37-C38-C39
31	BD	5409	LMG	C36-C37-C38-C39
31	BE	5101	LMG	C18-C19-C20-C21
32	AB	623	LMT	C3-C4-C5-C6
32	AB	630	LMT	C3-C4-C5-C6
32	AD	409	LMT	C3-C4-C5-C6
32	AI	102	LMT	C3-C4-C5-C6
32	BB	5626	LMT	C3-C4-C5-C6
32	BI	5102	LMT	C3-C4-C5-C6
24	AB	606	CLA	C3-C5-C6-C7
24	AC	502	CLA	C3-C5-C6-C7
24	AC	508	CLA	C3-C5-C6-C7
24	AD	404	CLA	C3-C5-C6-C7
24	BB	5610	CLA	C3-C5-C6-C7
24	BC	5502	CLA	C3-C5-C6-C7
24	BC	5512	CLA	C3-C5-C6-C7
24	BD	5405	CLA	C3-C5-C6-C7
28	AA	411	DGD	C7A-C8A-C9A-CAA
28	AE	101	DGD	C7B-C8B-C9B-CAB
28	BA	5412	DGD	C7A-C8A-C9A-CAA
28	BE	5102	DGD	C7B-C8B-C9B-CAB
31	AB	620	LMG	C18-C19-C20-C21
31	AB	620	LMG	C36-C37-C38-C39
31	AB	621	LMG	C18-C19-C20-C21
31	AC	520	LMG	C36-C37-C38-C39
31	AC	521	LMG	C18-C19-C20-C21
31	AD	408	LMG	C36-C37-C38-C39
31	AI	101	LMG	C18-C19-C20-C21
31	AJ	102	LMG	C36-C37-C38-C39
31	BC	5521	LMG	C18-C19-C20-C21
31	BD	5408	LMG	C36-C37-C38-C39
31	BD	5409	LMG	C18-C19-C20-C21
31	BD	5410	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
31	BI	5101	LMG	C18-C19-C20-C21
31	BL	5101	LMG	C18-C19-C20-C21
31	BL	5101	LMG	C36-C37-C38-C39
32	AB	629	LMT	C3-C4-C5-C6
32	BB	5603	LMT	C3-C4-C5-C6
29	AA	415	LHG	O2-C2-C3-O3
29	BA	5415	LHG	O2-C2-C3-O3
31	AJ	102	LMG	C18-C19-C20-C21
31	BD	5408	LMG	C18-C19-C20-C21
32	AM	102	LMT	C3-C4-C5-C6
32	BB	5627	LMT	C3-C4-C5-C6
32	BC	5522	LMT	C3-C4-C5-C6
32	BM	5101	LMT	C3-C4-C5-C6
24	AB	608	CLA	O1A-CGA-O2A-C1
28	BE	5102	DGD	C7A-C8A-C9A-CAA
31	BD	5410	LMG	C18-C19-C20-C21
32	AB	624	LMT	C3-C4-C5-C6
32	AI	103	LMT	C3-C4-C5-C6
28	BC	5518	DGD	C7B-C8B-C9B-CAB
28	AB	628	DGD	C7B-C8B-C9B-CAB
28	AC	518	DGD	C7A-C8A-C9A-CAA
28	AC	518	DGD	C7B-C8B-C9B-CAB
28	AE	101	DGD	C7A-C8A-C9A-CAA
28	BB	5602	DGD	C7B-C8B-C9B-CAB
28	BC	5518	DGD	C7A-C8A-C9A-CAA
31	AC	520	LMG	C18-C19-C20-C21
31	AD	408	LMG	C18-C19-C20-C21
31	BC	5520	LMG	C18-C19-C20-C21
24	AA	404	CLA	C3-C5-C6-C7
24	AC	512	CLA	C3-C5-C6-C7
24	BA	5405	CLA	C3-C5-C6-C7
24	BC	5508	CLA	C3-C5-C6-C7
28	AA	411	DGD	C7B-C8B-C9B-CAB
28	BA	5412	DGD	C7B-C8B-C9B-CAB
24	AA	407	CLA	CBA-CGA-O2A-C1
24	AB	612	CLA	CBA-CGA-O2A-C1
24	AC	510	CLA	CBA-CGA-O2A-C1
24	BA	5408	CLA	CBA-CGA-O2A-C1
24	BB	5616	CLA	CBA-CGA-O2A-C1
24	BC	5510	CLA	CBA-CGA-O2A-C1
28	AH	101	DGD	C7A-C8A-C9A-CAA
28	BH	5101	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
24	BB	5610	CLA	C2A-CAA-CBA-CGA
28	AH	101	DGD	C7B-C8B-C9B-CAB
28	BH	5101	DGD	C7B-C8B-C9B-CAB
24	BB	5614	CLA	O1A-CGA-O2A-C1
28	AC	519	DGD	O6E-C1E-O5D-C6D
28	BC	5519	DGD	O6E-C1E-O5D-C6D
30	AA	416	SQD	O5-C1-O6-C44
30	AB	627	SQD	O5-C1-O6-C44
30	BA	5401	SQD	O5-C1-O6-C44
30	BB	5601	SQD	O5-C1-O6-C44
28	AC	519	DGD	C7A-C8A-C9A-CAA
28	BC	5519	DGD	C7A-C8A-C9A-CAA
24	AB	610	CLA	CBA-CGA-O2A-C1
24	AB	614	CLA	CBA-CGA-O2A-C1
24	BB	5614	CLA	CBA-CGA-O2A-C1
24	BB	5618	CLA	CBA-CGA-O2A-C1
24	BC	5505	CLA	CBA-CGA-O2A-C1
30	AA	413	SQD	C24-C23-O48-C46
30	AA	416	SQD	C29-C30-C31-C32
30	BA	5401	SQD	C29-C30-C31-C32
24	AB	610	CLA	O1A-CGA-O2A-C1
24	AB	614	CLA	O1A-CGA-O2A-C1
24	BB	5618	CLA	O1A-CGA-O2A-C1
24	AC	505	CLA	CBA-CGA-O2A-C1
24	AC	508	CLA	CBA-CGA-O2A-C1
24	AC	512	CLA	CBA-CGA-O2A-C1
24	BC	5508	CLA	CBA-CGA-O2A-C1
24	BC	5512	CLA	CBA-CGA-O2A-C1
30	AB	627	SQD	C24-C23-O48-C46
30	BA	5414	SQD	C24-C23-O48-C46
30	BB	5601	SQD	C24-C23-O48-C46
24	AB	603	CLA	C11-C12-C13-C14
24	AC	504	CLA	C11-C12-C13-C14
24	BB	5607	CLA	C11-C12-C13-C14
24	BC	5504	CLA	C11-C12-C13-C14
24	AD	404	CLA	C2C-C3C-CAC-CBC
32	BM	5101	LMT	C5'-C4'-O1B-C1B
24	BC	5512	CLA	O1A-CGA-O2A-C1
24	AB	606	CLA	C2A-CAA-CBA-CGA
32	AM	102	LMT	C5'-C4'-O1B-C1B
24	AC	508	CLA	O1A-CGA-O2A-C1
24	AC	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	BC	5508	CLA	O1A-CGA-O2A-C1
30	AB	627	SQD	O10-C23-O48-C46
30	BB	5601	SQD	O10-C23-O48-C46
32	BB	5604	LMT	C5'-C4'-O1B-C1B
28	AE	101	DGD	O1G-C1G-C2G-O2G
28	BE	5102	DGD	O1G-C1G-C2G-O2G
31	BB	5624	LMG	O1-C7-C8-O7
24	BA	5405	CLA	CBA-CGA-O2A-C1
34	BD	5403	PHO	C15-C16-C17-C18
32	AB	630	LMT	C5'-C4'-O1B-C1B
24	AC	512	CLA	C10-C11-C12-C13
24	BC	5512	CLA	C10-C11-C12-C13
34	BD	5404	PHO	C5-C6-C7-C8
24	BD	5405	CLA	C2C-C3C-CAC-CBC
24	AB	611	CLA	C12-C13-C15-C16
24	BB	5615	CLA	C12-C13-C15-C16
24	BA	5408	CLA	C10-C11-C12-C13
34	AD	403	PHO	C5-C6-C7-C8
35	AD	405	PL9	C39-C41-C42-C43
35	BD	5406	PL9	C39-C41-C42-C43
24	BB	5613	CLA	C3-C5-C6-C7
34	AD	402	PHO	C15-C16-C17-C18
24	AA	407	CLA	C10-C11-C12-C13
24	AB	602	CLA	C10-C11-C12-C13
24	AB	614	CLA	C13-C15-C16-C17
24	AC	503	CLA	C13-C15-C16-C17
24	AC	504	CLA	C13-C15-C16-C17
24	BA	5405	CLA	C10-C11-C12-C13
24	BB	5618	CLA	C13-C15-C16-C17
24	BC	5504	CLA	C13-C15-C16-C17
24	AB	608	CLA	C2A-CAA-CBA-CGA
24	AB	612	CLA	C2A-CAA-CBA-CGA
24	AC	501	CLA	C2A-CAA-CBA-CGA
24	BB	5612	CLA	C2A-CAA-CBA-CGA
24	BC	5501	CLA	C2A-CAA-CBA-CGA
24	AA	404	CLA	C10-C11-C12-C13
24	AB	602	CLA	C13-C15-C16-C17
24	AB	607	CLA	C13-C15-C16-C17
24	AB	614	CLA	C10-C11-C12-C13
24	BB	5606	CLA	C10-C11-C12-C13
24	BB	5606	CLA	C13-C15-C16-C17
24	BC	5505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	AB	610	CLA	C3-C5-C6-C7
27	AB	617	BCR	C6-C7-C8-C9
27	BB	5621	BCR	C6-C7-C8-C9
30	AF	102	SQD	O5-C1-O6-C44
30	BF	5102	SQD	O5-C1-O6-C44
24	BB	5618	CLA	C10-C11-C12-C13
24	BC	5503	CLA	C13-C15-C16-C17
24	BD	5402	CLA	C13-C15-C16-C17
24	AC	507	CLA	CBA-CGA-O2A-C1
32	AB	629	LMT	C3'-C4'-O1B-C1B
31	BE	5101	LMG	C36-C37-C38-C39
24	AC	505	CLA	O1A-CGA-O2A-C1
30	AA	413	SQD	O10-C23-O48-C46
30	BA	5414	SQD	O10-C23-O48-C46
24	AD	401	CLA	C13-C15-C16-C17
24	BB	5611	CLA	C13-C15-C16-C17
28	AE	101	DGD	CFB-CGB-CHB-CIB
28	BE	5102	DGD	CFB-CGB-CHB-CIB
31	AA	414	LMG	C36-C37-C38-C39
28	AC	518	DGD	CFB-CGB-CHB-CIB
28	BC	5518	DGD	CFB-CGB-CHB-CIB
35	AD	405	PL9	C30-C29-C31-C32
24	BA	5405	CLA	O1A-CGA-O2A-C1
29	BA	5415	LHG	C23-C24-C25-C26
24	AA	404	CLA	CBA-CGA-O2A-C1
24	AB	604	CLA	CBA-CGA-O2A-C1
28	BC	5519	DGD	CFB-CGB-CHB-CIB
28	AC	519	DGD	CFB-CGB-CHB-CIB
32	BB	5603	LMT	C3'-C4'-O1B-C1B
24	AA	405	CLA	C10-C11-C12-C13
24	BA	5406	CLA	C10-C11-C12-C13
29	AA	415	LHG	C23-C24-C25-C26
29	AA	412	LHG	C1-C2-C3-O3
29	BA	5413	LHG	C1-C2-C3-O3
24	BB	5616	CLA	C2A-CAA-CBA-CGA
24	BB	5608	CLA	CBA-CGA-O2A-C1
24	BC	5507	CLA	CBA-CGA-O2A-C1
24	AA	405	CLA	C13-C15-C16-C17
24	AB	601	CLA	C10-C11-C12-C13
24	AC	513	CLA	C13-C15-C16-C17
24	AD	404	CLA	C13-C15-C16-C17
24	BA	5406	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	BB	5605	CLA	C10-C11-C12-C13
24	BD	5405	CLA	C13-C15-C16-C17
34	AD	403	PHO	C15-C16-C17-C18
24	AB	609	CLA	C3-C5-C6-C7
24	BB	5614	CLA	C3-C5-C6-C7
32	BB	5603	LMT	C5'-C4'-O1B-C1B
24	BC	5513	CLA	C13-C15-C16-C17
35	BD	5406	PL9	C30-C29-C31-C32
34	BD	5404	PHO	C15-C16-C17-C18
32	AB	629	LMT	C5'-C4'-O1B-C1B
24	AD	404	CLA	CBA-CGA-O2A-C1
24	BC	5503	CLA	CBA-CGA-O2A-C1
24	BA	5408	CLA	C13-C15-C16-C17
24	AA	404	CLA	O1A-CGA-O2A-C1
24	AB	604	CLA	O1A-CGA-O2A-C1
24	BB	5608	CLA	O1A-CGA-O2A-C1
24	BC	5507	CLA	O1A-CGA-O2A-C1
24	AD	404	CLA	C2A-CAA-CBA-CGA
24	BD	5405	CLA	C2A-CAA-CBA-CGA
29	AA	415	LHG	O1-C1-C2-C3
29	BA	5415	LHG	O1-C1-C2-C3
28	AB	628	DGD	C3G-C2G-O2G-C1B
28	BB	5602	DGD	C3G-C2G-O2G-C1B
31	AD	408	LMG	C7-C8-O7-C10
31	AJ	102	LMG	C7-C8-O7-C10
31	BD	5408	LMG	C7-C8-O7-C10
31	BD	5410	LMG	C7-C8-O7-C10
24	AB	616	CLA	C3-C5-C6-C7
24	BB	5620	CLA	C3-C5-C6-C7
31	AB	621	LMG	O1-C7-C8-O7
24	AC	503	CLA	CBA-CGA-O2A-C1
24	BD	5405	CLA	CBA-CGA-O2A-C1
24	AB	612	CLA	C2-C1-O2A-CGA
24	BB	5616	CLA	C2-C1-O2A-CGA
24	AC	507	CLA	O1A-CGA-O2A-C1
24	AA	407	CLA	C13-C15-C16-C17
24	AB	616	CLA	C13-C15-C16-C17
24	BB	5620	CLA	C13-C15-C16-C17
30	AA	413	SQD	C24-C25-C26-C27
30	AA	416	SQD	C15-C16-C17-C18
30	AA	416	SQD	C27-C28-C29-C30
30	BA	5401	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	BA	5401	SQD	C27-C28-C29-C30
30	BA	5414	SQD	C24-C25-C26-C27
30	BB	5601	SQD	C26-C27-C28-C29
30	AB	627	SQD	C26-C27-C28-C29
30	AF	102	SQD	C11-C12-C13-C14
30	BB	5601	SQD	C15-C16-C17-C18
29	AA	415	LHG	C11-C10-C9-C8
30	AB	627	SQD	C15-C16-C17-C18
30	BB	5601	SQD	C17-C18-C19-C20
30	BF	5102	SQD	C11-C12-C13-C14
24	AB	603	CLA	C2A-CAA-CBA-CGA
29	BA	5415	LHG	C11-C10-C9-C8
24	AC	509	CLA	C10-C11-C12-C13
30	AB	627	SQD	C17-C18-C19-C20
24	AC	512	CLA	C12-C13-C15-C16
24	BC	5512	CLA	C12-C13-C15-C16
24	AB	601	CLA	C13-C15-C16-C17
24	AC	511	CLA	C10-C11-C12-C13
24	BC	5511	CLA	C10-C11-C12-C13
30	AB	622	SQD	C12-C13-C14-C15
32	AB	630	LMT	C3'-C4'-O1B-C1B
30	AA	413	SQD	C18-C19-C20-C21
30	BA	5414	SQD	C18-C19-C20-C21
30	BB	5625	SQD	C12-C13-C14-C15
24	BC	5509	CLA	C10-C11-C12-C13
32	AM	102	LMT	C3'-C4'-O1B-C1B
30	AB	622	SQD	C11-C12-C13-C14
30	BB	5625	SQD	C11-C12-C13-C14
24	AC	510	CLA	C3-C5-C6-C7
24	BB	5605	CLA	C13-C15-C16-C17
30	BB	5601	SQD	C9-C10-C11-C12
24	AD	404	CLA	O1A-CGA-O2A-C1
24	BC	5503	CLA	O1A-CGA-O2A-C1
32	BB	5604	LMT	C3'-C4'-O1B-C1B
32	BM	5101	LMT	C3'-C4'-O1B-C1B
27	AA	410	BCR	C1-C6-C7-C8
27	AA	410	BCR	C5-C6-C7-C8
27	AB	619	BCR	C1-C6-C7-C8
27	AB	619	BCR	C5-C6-C7-C8
27	AC	514	BCR	C23-C24-C25-C26
27	AC	514	BCR	C23-C24-C25-C30
27	AD	406	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
27	AK	102	BCR	C5-C6-C7-C8
27	AT	101	BCR	C23-C24-C25-C26
27	AT	101	BCR	C23-C24-C25-C30
27	BA	5411	BCR	C1-C6-C7-C8
27	BA	5411	BCR	C5-C6-C7-C8
27	BB	5623	BCR	C1-C6-C7-C8
27	BB	5623	BCR	C5-C6-C7-C8
27	BC	5514	BCR	C23-C24-C25-C26
27	BC	5514	BCR	C23-C24-C25-C30
27	BD	5407	BCR	C23-C24-C25-C30
27	BK	5102	BCR	C5-C6-C7-C8
27	BT	5101	BCR	C23-C24-C25-C26
27	BT	5101	BCR	C23-C24-C25-C30
24	BC	5510	CLA	C3-C5-C6-C7
24	BB	5607	CLA	C2A-CAA-CBA-CGA
30	AB	627	SQD	C9-C10-C11-C12
24	AC	503	CLA	O1A-CGA-O2A-C1
24	BD	5405	CLA	O1A-CGA-O2A-C1
35	BD	5406	PL9	C4-C3-C7-C8
24	AC	507	CLA	C10-C11-C12-C13
24	BA	5407	CLA	CBA-CGA-O2A-C1
24	BB	5615	CLA	CBA-CGA-O2A-C1
24	AB	611	CLA	C11-C12-C13-C14
24	BB	5612	CLA	C11-C12-C13-C14
29	BA	5413	LHG	C11-C10-C9-C8
24	BB	5605	CLA	C2C-C3C-CAC-CBC
29	AA	412	LHG	C11-C10-C9-C8
30	BB	5625	SQD	C25-C26-C27-C28
30	AB	622	SQD	C8-C7-O47-C45
30	BB	5625	SQD	C8-C7-O47-C45
30	BF	5102	SQD	C24-C25-C26-C27
24	BC	5507	CLA	C10-C11-C12-C13
24	BC	5513	CLA	C10-C11-C12-C13
30	AB	622	SQD	O49-C7-O47-C45
30	AF	102	SQD	C24-C25-C26-C27
24	AB	601	CLA	C2C-C3C-CAC-CBC
24	BC	5501	CLA	C10-C11-C12-C13
24	AD	404	CLA	C4C-C3C-CAC-CBC
34	BD	5403	PHO	CBD-CGD-O2D-CED
30	AB	622	SQD	C25-C26-C27-C28
35	BD	5406	PL9	C15-C14-C16-C17
24	AC	504	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	AC	513	CLA	C10-C11-C12-C13
24	BC	5504	CLA	C10-C11-C12-C13
30	AB	627	SQD	C10-C11-C12-C13
30	BB	5625	SQD	C27-C28-C29-C30
24	AC	501	CLA	C13-C15-C16-C17
24	BC	5501	CLA	C13-C15-C16-C17
30	AB	622	SQD	C27-C28-C29-C30
30	BB	5625	SQD	O49-C7-O47-C45
34	AD	402	PHO	CBD-CGD-O2D-CED
24	AC	501	CLA	C10-C11-C12-C13
24	BB	5609	CLA	C10-C11-C12-C13
36	AF	101	HEM	C4C-C3C-CAC-CBC
36	BF	5101	HEM	C4C-C3C-CAC-CBC
24	AC	502	CLA	O1A-CGA-O2A-C1
30	AA	413	SQD	C15-C16-C17-C18
30	BA	5414	SQD	C17-C18-C19-C20
30	BB	5601	SQD	C10-C11-C12-C13
28	AC	519	DGD	O2G-C2G-C3G-O3G
28	BC	5519	DGD	O2G-C2G-C3G-O3G
31	AJ	102	LMG	O1-C7-C8-O7
31	BD	5408	LMG	O1-C7-C8-O7
24	AC	502	CLA	CBA-CGA-O2A-C1
30	AA	413	SQD	C11-C10-C9-C8
30	AA	413	SQD	C17-C18-C19-C20
30	BA	5414	SQD	C15-C16-C17-C18
24	AB	605	CLA	C10-C11-C12-C13
30	BF	5102	SQD	C12-C13-C14-C15
30	AF	102	SQD	C12-C13-C14-C15
28	AC	518	DGD	O6D-C5D-C6D-O5D
28	BC	5518	DGD	O6D-C5D-C6D-O5D
24	AA	405	CLA	C2-C3-C5-C6
24	BA	5406	CLA	C2-C3-C5-C6
35	BD	5406	PL9	C13-C14-C16-C17
29	AA	415	LHG	C9-C10-C11-C12
24	AA	405	CLA	C2A-CAA-CBA-CGA
24	AB	602	CLA	C2A-CAA-CBA-CGA
24	BB	5606	CLA	C2A-CAA-CBA-CGA
24	AB	611	CLA	CBA-CGA-O2A-C1
24	BC	5502	CLA	CBA-CGA-O2A-C1
29	BA	5415	LHG	C9-C10-C11-C12
29	AA	415	LHG	O1-C1-C2-O2
29	BA	5415	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
24	BC	5502	CLA	O1A-CGA-O2A-C1
30	BA	5414	SQD	C11-C10-C9-C8
29	AA	412	LHG	C25-C26-C27-C28
29	BA	5413	LHG	C25-C26-C27-C28
24	AA	405	CLA	C6-C7-C8-C10
24	AA	405	CLA	C12-C13-C15-C16
24	AA	407	CLA	C12-C13-C15-C16
24	AB	612	CLA	C11-C12-C13-C15
24	AC	501	CLA	C11-C12-C13-C15
24	AC	504	CLA	C6-C7-C8-C10
24	AC	504	CLA	C11-C12-C13-C15
24	AC	510	CLA	C11-C12-C13-C15
24	BA	5406	CLA	C6-C7-C8-C10
24	BA	5406	CLA	C12-C13-C15-C16
24	BA	5408	CLA	C12-C13-C15-C16
24	BC	5501	CLA	C11-C12-C13-C15
24	BC	5504	CLA	C6-C7-C8-C10
24	BC	5504	CLA	C11-C12-C13-C15
24	BC	5510	CLA	C11-C12-C13-C15
34	AD	402	PHO	C12-C13-C15-C16
34	AD	403	PHO	C6-C7-C8-C10
34	BD	5403	PHO	C12-C13-C15-C16
34	BD	5404	PHO	C6-C7-C8-C10
24	BB	5615	CLA	O1A-CGA-O2A-C1
24	AB	603	CLA	C10-C11-C12-C13
24	AD	401	CLA	C10-C11-C12-C13
35	AD	405	PL9	C15-C14-C16-C17
35	AD	405	PL9	C13-C14-C16-C17
29	BA	5415	LHG	C13-C14-C15-C16
24	BA	5407	CLA	O1A-CGA-O2A-C1
24	BA	5406	CLA	C2A-CAA-CBA-CGA
24	AA	405	CLA	C14-C13-C15-C16
24	AA	407	CLA	C14-C13-C15-C16
24	AB	608	CLA	C11-C12-C13-C14
24	AB	611	CLA	C6-C7-C8-C9
24	AB	613	CLA	C6-C7-C8-C9
24	AC	502	CLA	C14-C13-C15-C16
24	AC	504	CLA	C6-C7-C8-C9
24	AC	510	CLA	C11-C12-C13-C14
24	BA	5406	CLA	C14-C13-C15-C16
24	BA	5408	CLA	C14-C13-C15-C16
24	BB	5615	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	BB	5617	CLA	C6-C7-C8-C9
24	BC	5502	CLA	C14-C13-C15-C16
24	BC	5504	CLA	C6-C7-C8-C9
24	BC	5510	CLA	C11-C12-C13-C14
24	BD	5402	CLA	C11-C12-C13-C14
24	AA	406	CLA	CBA-CGA-O2A-C1
24	BC	5509	CLA	CBA-CGA-O2A-C1
24	BD	5405	CLA	C4C-C3C-CAC-CBC
28	AA	411	DGD	C1G-C2G-C3G-O3G
28	AE	101	DGD	O1G-C1G-C2G-C3G
28	BA	5412	DGD	C1G-C2G-C3G-O3G
28	BC	5518	DGD	C1G-C2G-C3G-O3G
28	BE	5102	DGD	O1G-C1G-C2G-C3G
30	AA	413	SQD	O6-C44-C45-C46
30	AB	622	SQD	O6-C44-C45-C46
30	BA	5414	SQD	O6-C44-C45-C46
30	BB	5625	SQD	O6-C44-C45-C46
31	AJ	102	LMG	O1-C7-C8-C9
31	BD	5408	LMG	O1-C7-C8-C9
30	AA	416	SQD	C9-C10-C11-C12
29	AA	415	LHG	C13-C14-C15-C16
24	AB	615	CLA	CBA-CGA-O2A-C1
24	BB	5619	CLA	CBA-CGA-O2A-C1
24	BD	5402	CLA	C10-C11-C12-C13
24	AA	405	CLA	C4-C3-C5-C6
24	BA	5406	CLA	C4-C3-C5-C6
24	BB	5607	CLA	C10-C11-C12-C13
30	AF	102	SQD	C25-C26-C27-C28
24	AB	611	CLA	O1A-CGA-O2A-C1
24	BB	5619	CLA	O1A-CGA-O2A-C1
24	BA	5406	CLA	O2A-C1-C2-C3
28	AA	411	DGD	C1G-C2G-O2G-C1B
28	AC	517	DGD	C3G-C2G-O2G-C1B
28	AH	101	DGD	C1G-C2G-O2G-C1B
28	BA	5412	DGD	C1G-C2G-O2G-C1B
28	BC	5517	DGD	C3G-C2G-O2G-C1B
28	BH	5101	DGD	C1G-C2G-O2G-C1B
29	BA	5415	LHG	C4-C5-O7-C7
30	AA	413	SQD	C44-C45-O47-C7
30	BA	5414	SQD	C44-C45-O47-C7
31	AA	417	LMG	C7-C8-O7-C10
31	AC	520	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
31	AC	521	LMG	C7-C8-O7-C10
31	BA	5402	LMG	C7-C8-O7-C10
31	BC	5520	LMG	C9-C8-O7-C10
31	BC	5521	LMG	C7-C8-O7-C10
34	AD	403	PHO	O2A-C1-C2-C3
34	BD	5404	PHO	O2A-C1-C2-C3
29	AA	412	LHG	C26-C27-C28-C29
30	AA	416	SQD	C24-C25-C26-C27
30	BF	5102	SQD	C25-C26-C27-C28
24	AC	509	CLA	CBA-CGA-O2A-C1
24	BC	5509	CLA	O1A-CGA-O2A-C1
30	BA	5401	SQD	C24-C25-C26-C27
30	BA	5401	SQD	C9-C10-C11-C12
30	AA	416	SQD	C10-C11-C12-C13
29	BA	5413	LHG	C26-C27-C28-C29
30	BA	5414	SQD	C11-C12-C13-C14
30	BF	5102	SQD	C10-C11-C12-C13
30	AF	102	SQD	C10-C11-C12-C13
30	BA	5401	SQD	C10-C11-C12-C13
30	BF	5102	SQD	C11-C10-C9-C8
28	AB	628	DGD	O1G-C1G-C2G-O2G
28	BB	5602	DGD	O1G-C1G-C2G-O2G
31	AC	521	LMG	O7-C8-C9-O8
31	BC	5521	LMG	O7-C8-C9-O8
30	AF	102	SQD	C11-C10-C9-C8
30	AB	627	SQD	C19-C20-C21-C22
30	BB	5601	SQD	C19-C20-C21-C22
29	AA	412	LHG	C9-C10-C11-C12
29	BA	5413	LHG	C9-C10-C11-C12
29	AA	415	LHG	C8-C7-O7-C5
29	BA	5415	LHG	C8-C7-O7-C5
24	AB	616	CLA	C10-C11-C12-C13
24	AB	613	CLA	C13-C15-C16-C17
24	AC	508	CLA	C13-C15-C16-C17
24	BB	5617	CLA	C13-C15-C16-C17
24	AB	611	CLA	C4-C3-C5-C6
30	AA	413	SQD	C11-C12-C13-C14
24	AA	404	CLA	C6-C7-C8-C9
24	AB	612	CLA	C11-C12-C13-C14
24	AB	616	CLA	C6-C7-C8-C9
24	AC	503	CLA	C6-C7-C8-C9
24	AC	506	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	AD	401	CLA	C11-C12-C13-C14
24	BA	5405	CLA	C6-C7-C8-C9
24	BB	5615	CLA	C6-C7-C8-C9
24	BB	5616	CLA	C11-C12-C13-C14
24	BB	5620	CLA	C6-C7-C8-C9
24	BC	5501	CLA	C11-C12-C13-C14
24	BC	5503	CLA	C6-C7-C8-C9
24	BC	5506	CLA	C6-C7-C8-C9
34	AD	402	PHO	C14-C13-C15-C16
34	BD	5403	PHO	C14-C13-C15-C16
24	AB	615	CLA	O1A-CGA-O2A-C1
30	AA	413	SQD	C10-C11-C12-C13
24	BB	5620	CLA	C10-C11-C12-C13
30	AF	102	SQD	C2-C1-O6-C44
30	BF	5102	SQD	C2-C1-O6-C44
34	AD	403	PHO	C3-C5-C6-C7
30	BA	5401	SQD	C8-C7-O47-C45
24	AA	404	CLA	C6-C7-C8-C10
24	AA	407	CLA	C6-C7-C8-C10
24	AB	601	CLA	C12-C13-C15-C16
24	AB	610	CLA	C12-C13-C15-C16
24	AB	613	CLA	C6-C7-C8-C10
24	AB	616	CLA	C6-C7-C8-C10
24	AC	502	CLA	C12-C13-C15-C16
24	AC	506	CLA	C6-C7-C8-C10
24	BA	5405	CLA	C6-C7-C8-C10
24	BA	5408	CLA	C6-C7-C8-C10
24	BB	5605	CLA	C12-C13-C15-C16
24	BB	5610	CLA	C11-C12-C13-C15
24	BB	5614	CLA	C11-C12-C13-C15
24	BB	5614	CLA	C12-C13-C15-C16
24	BB	5616	CLA	C11-C12-C13-C15
24	BB	5617	CLA	C6-C7-C8-C10
24	BB	5620	CLA	C6-C7-C8-C10
24	BC	5502	CLA	C12-C13-C15-C16
24	BC	5503	CLA	C6-C7-C8-C10
24	BC	5506	CLA	C6-C7-C8-C10
24	BC	5511	CLA	C6-C7-C8-C10
24	AA	406	CLA	O1A-CGA-O2A-C1
30	AA	413	SQD	C23-C24-C25-C26
30	BA	5401	SQD	C17-C18-C19-C20
30	AB	622	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	AB	601	CLA	C4-C3-C5-C6
24	BB	5605	CLA	C4-C3-C5-C6
24	BB	5615	CLA	C4-C3-C5-C6
24	BC	5503	CLA	C4-C3-C5-C6
24	BC	5508	CLA	C13-C15-C16-C17
29	AA	415	LHG	C25-C26-C27-C28
34	BD	5404	PHO	C3-C5-C6-C7
24	BB	5611	CLA	C10-C11-C12-C13
29	BA	5415	LHG	C15-C16-C17-C18
30	AA	416	SQD	C17-C18-C19-C20
30	BB	5625	SQD	C10-C11-C12-C13
30	BA	5414	SQD	C23-C24-C25-C26
29	AA	415	LHG	C15-C16-C17-C18
24	AB	610	CLA	C2A-CAA-CBA-CGA
28	AC	518	DGD	C1G-C2G-C3G-O3G
30	AA	413	SQD	C44-C45-C46-O48
30	AB	622	SQD	C44-C45-C46-O48
30	AB	627	SQD	C44-C45-C46-O48
30	BA	5414	SQD	C44-C45-C46-O48
30	BB	5601	SQD	C44-C45-C46-O48
30	BB	5625	SQD	C44-C45-C46-O48
31	AB	620	LMG	O1-C7-C8-C9
31	AB	620	LMG	C7-C8-C9-O8
31	AB	621	LMG	O1-C7-C8-C9
31	AC	520	LMG	C7-C8-C9-O8
31	AC	521	LMG	O1-C7-C8-C9
31	AD	407	LMG	C7-C8-C9-O8
31	BC	5520	LMG	C7-C8-C9-O8
31	BC	5521	LMG	O1-C7-C8-C9
31	BD	5409	LMG	C7-C8-C9-O8
31	BL	5101	LMG	O1-C7-C8-C9
31	BL	5101	LMG	C7-C8-C9-O8
24	AB	607	CLA	C10-C11-C12-C13
30	BA	5414	SQD	C10-C11-C12-C13
24	AC	503	CLA	C4-C3-C5-C6
24	BC	5511	CLA	C4-C3-C5-C6
30	BF	5102	SQD	C27-C28-C29-C30
27	AA	410	BCR	C23-C24-C25-C30
27	AC	515	BCR	C23-C24-C25-C30
27	AD	406	BCR	C1-C6-C7-C8
27	BA	5411	BCR	C23-C24-C25-C30
27	BC	5515	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
27	BD	5407	BCR	C1-C6-C7-C8
30	AA	416	SQD	C8-C7-O47-C45
29	AA	412	LHG	C2-C3-O3-P
29	BA	5413	LHG	C2-C3-O3-P
24	BB	5613	CLA	C10-C11-C12-C13
28	AC	517	DGD	O2G-C2G-C3G-O3G
28	BC	5517	DGD	O2G-C2G-C3G-O3G
30	AB	622	SQD	O6-C44-C45-O47
30	AB	627	SQD	O47-C45-C46-O48
30	BB	5601	SQD	O47-C45-C46-O48
30	BB	5625	SQD	O6-C44-C45-O47
31	AD	407	LMG	O1-C7-C8-O7
31	AD	407	LMG	O7-C8-C9-O8
31	AD	408	LMG	O7-C8-C9-O8
31	BD	5409	LMG	O1-C7-C8-O7
31	BD	5409	LMG	O7-C8-C9-O8
31	BD	5410	LMG	O7-C8-C9-O8
35	AD	405	PL9	C4-C3-C7-C8
30	AF	102	SQD	C27-C28-C29-C30
24	AC	511	CLA	C4-C3-C5-C6
24	AB	609	CLA	C10-C11-C12-C13
24	AC	511	CLA	C2-C3-C5-C6
24	BB	5605	CLA	C2-C3-C5-C6
24	BC	5511	CLA	C2-C3-C5-C6
29	BA	5415	LHG	C25-C26-C27-C28
24	AB	601	CLA	C14-C13-C15-C16
24	AC	501	CLA	C11-C12-C13-C14
24	BB	5605	CLA	C14-C13-C15-C16
34	AD	403	PHO	C11-C10-C8-C9
34	BD	5404	PHO	C6-C7-C8-C9
34	BD	5404	PHO	C11-C10-C8-C9
27	AA	410	BCR	C6-C7-C8-C9
27	BA	5411	BCR	C6-C7-C8-C9
24	AC	509	CLA	O1A-CGA-O2A-C1
24	AB	601	CLA	C3-C5-C6-C7
34	AD	402	PHO	C3-C5-C6-C7
34	BD	5403	PHO	C3-C5-C6-C7
24	AB	601	CLA	C2-C3-C5-C6
24	AC	503	CLA	C2-C3-C5-C6
24	BC	5503	CLA	C2-C3-C5-C6
24	AB	608	CLA	C10-C11-C12-C13
30	AB	627	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	BB	5601	SQD	C25-C26-C27-C28
24	AB	604	CLA	C11-C12-C13-C15
24	AB	606	CLA	C11-C12-C13-C15
24	AB	610	CLA	C11-C12-C13-C15
24	AB	615	CLA	C11-C12-C13-C15
24	AC	503	CLA	C6-C7-C8-C10
24	AC	511	CLA	C12-C13-C15-C16
24	BB	5608	CLA	C11-C12-C13-C15
24	BB	5619	CLA	C11-C12-C13-C15
24	BC	5511	CLA	C12-C13-C15-C16
34	AD	403	PHO	C11-C10-C8-C7
34	BD	5404	PHO	C11-C10-C8-C7
24	BB	5605	CLA	C3-C5-C6-C7
24	BB	5613	CLA	O1A-CGA-O2A-C1
24	BB	5605	CLA	C4C-C3C-CAC-CBC
30	AF	102	SQD	C45-C44-O6-C1
30	BF	5102	SQD	C45-C44-O6-C1
24	BB	5612	CLA	C10-C11-C12-C13
24	BB	5614	CLA	C2A-CAA-CBA-CGA
30	AA	416	SQD	O49-C7-O47-C45
30	BA	5401	SQD	O49-C7-O47-C45
34	AD	402	PHO	C4-C3-C5-C6
24	AB	611	CLA	C2-C3-C5-C6
24	BB	5615	CLA	C2-C3-C5-C6
24	AA	405	CLA	O2A-C1-C2-C3
28	AC	519	DGD	C3G-C2G-O2G-C1B
28	BC	5519	DGD	C3G-C2G-O2G-C1B
31	AD	407	LMG	C7-C8-O7-C10
31	BD	5409	LMG	C7-C8-O7-C10
32	BI	5102	LMT	C5'-C4'-O1B-C1B
24	AB	609	CLA	C13-C15-C16-C17
32	AI	102	LMT	C5'-C4'-O1B-C1B
24	BB	5613	CLA	C13-C15-C16-C17
29	AA	415	LHG	O9-C7-O7-C5
29	BA	5415	LHG	O9-C7-O7-C5
28	AA	411	DGD	O1G-C1G-C2G-C3G
28	BA	5412	DGD	O1G-C1G-C2G-C3G
29	AA	412	LHG	C4-C5-C6-O8
29	BA	5413	LHG	C4-C5-C6-O8
30	AA	416	SQD	O6-C44-C45-C46
30	BA	5401	SQD	O6-C44-C45-C46
31	AD	407	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	BB	5624	LMG	O1-C7-C8-C9
31	BD	5409	LMG	O1-C7-C8-C9
24	AB	601	CLA	C4C-C3C-CAC-CBC
28	AA	411	DGD	O2G-C2G-C3G-O3G
28	AB	628	DGD	O2G-C2G-C3G-O3G
28	BA	5412	DGD	O2G-C2G-C3G-O3G
28	BB	5602	DGD	O2G-C2G-C3G-O3G
29	AA	412	LHG	O7-C5-C6-O8
29	BA	5413	LHG	O7-C5-C6-O8
30	AA	413	SQD	O6-C44-C45-O47
30	AB	622	SQD	O47-C45-C46-O48
30	BA	5414	SQD	O6-C44-C45-O47
30	BA	5414	SQD	O47-C45-C46-O48
30	BB	5625	SQD	O47-C45-C46-O48
31	AM	101	LMG	O1-C7-C8-O7
31	BM	5102	LMG	O1-C7-C8-O7
24	AB	605	CLA	C11-C12-C13-C14
24	AB	606	CLA	C11-C12-C13-C14
24	BB	5609	CLA	C11-C12-C13-C14
24	BB	5610	CLA	C11-C12-C13-C14
34	AD	402	PHO	C11-C10-C8-C9
34	AD	403	PHO	C6-C7-C8-C9
34	BD	5403	PHO	C11-C10-C8-C9
24	AB	603	CLA	CAA-CBA-CGA-O2A
24	BB	5613	CLA	CBA-CGA-O2A-C1
24	AB	609	CLA	O1A-CGA-O2A-C1
24	BC	5503	CLA	C10-C11-C12-C13
24	AB	609	CLA	CBA-CGA-O2A-C1
34	BD	5403	PHO	C4-C3-C5-C6
24	AC	503	CLA	CAA-CBA-CGA-O2A
24	BB	5607	CLA	CAA-CBA-CGA-O2A
29	BA	5413	LHG	C30-C31-C32-C33
30	BA	5414	SQD	C5-C6-S-O9
24	AC	503	CLA	C10-C11-C12-C13
24	AB	603	CLA	C6-C7-C8-C10
24	AB	603	CLA	C11-C12-C13-C15
24	AB	613	CLA	C12-C13-C15-C16
24	AC	501	CLA	C6-C7-C8-C10
24	AC	505	CLA	C11-C12-C13-C15
24	AC	511	CLA	C6-C7-C8-C10
24	BB	5607	CLA	C6-C7-C8-C10
24	BB	5607	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	BB	5617	CLA	C12-C13-C15-C16
24	BC	5501	CLA	C6-C7-C8-C10
24	BC	5505	CLA	C11-C12-C13-C15
24	AC	511	CLA	CBA-CGA-O2A-C1
24	AA	407	CLA	C6-C7-C8-C9
24	AB	604	CLA	C11-C12-C13-C14
24	AB	610	CLA	C11-C12-C13-C14
24	AB	615	CLA	C11-C12-C13-C14
24	AC	511	CLA	C6-C7-C8-C9
24	BB	5607	CLA	C6-C7-C8-C9
24	BB	5608	CLA	C11-C12-C13-C14
24	BB	5614	CLA	C11-C12-C13-C14
24	BC	5511	CLA	C6-C7-C8-C9
24	BC	5503	CLA	CAA-CBA-CGA-O2A
29	BA	5413	LHG	C23-C24-C25-C26
29	AA	412	LHG	C30-C31-C32-C33
24	AC	502	CLA	C10-C11-C12-C13
30	AA	413	SQD	O47-C45-C46-O48
31	AM	101	LMG	O1-C7-C8-C9
31	BM	5102	LMG	O1-C7-C8-C9
24	AB	603	CLA	CAD-CBD-CGD-O2D
24	BB	5607	CLA	CAD-CBD-CGD-O2D
24	BC	5511	CLA	CBA-CGA-O2A-C1
30	BF	5102	SQD	C15-C16-C17-C18
24	AB	603	CLA	CAD-CBD-CGD-O1D
24	AB	610	CLA	CHA-CBD-CGD-O1D
24	AC	503	CLA	CHA-CBD-CGD-O1D
24	AC	507	CLA	CHA-CBD-CGD-O1D
24	AC	507	CLA	CHA-CBD-CGD-O2D
24	BB	5607	CLA	CAD-CBD-CGD-O1D
24	BB	5614	CLA	CHA-CBD-CGD-O1D
24	BC	5503	CLA	CHA-CBD-CGD-O1D
24	BC	5503	CLA	CHA-CBD-CGD-O2D
24	BC	5507	CLA	CHA-CBD-CGD-O1D
24	BC	5507	CLA	CHA-CBD-CGD-O2D
29	AA	415	LHG	C3-O3-P-O4
24	AB	605	CLA	C4-C3-C5-C6
27	AC	516	BCR	C5-C6-C7-C8
27	AK	102	BCR	C1-C6-C7-C8
27	BK	5102	BCR	C1-C6-C7-C8
24	BB	5608	CLA	C10-C11-C12-C13
28	AC	518	DGD	C1G-C2G-O2G-C1B

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Mol	Chain	Res	Type	Atoms
28	BC	5518	DGD	C1G-C2G-O2G-C1B
29	AA	415	LHG	C4-C5-O7-C7
31	AA	414	LMG	C9-C8-O7-C10
31	AI	101	LMG	C9-C8-O7-C10
31	BE	5101	LMG	C9-C8-O7-C10
24	AC	510	CLA	C10-C11-C12-C13
34	AD	402	PHO	C2-C3-C5-C6
24	AC	511	CLA	O1A-CGA-O2A-C1
24	AB	603	CLA	C6-C7-C8-C9
24	AC	501	CLA	C6-C7-C8-C9
24	AC	511	CLA	C14-C13-C15-C16
24	BA	5408	CLA	C6-C7-C8-C9
24	BB	5619	CLA	C11-C12-C13-C14
24	BC	5501	CLA	C6-C7-C8-C9
24	BC	5511	CLA	C14-C13-C15-C16
24	AB	605	CLA	C11-C12-C13-C15
24	BB	5609	CLA	C11-C12-C13-C15
29	AA	412	LHG	C23-C24-C25-C26
32	BB	5627	LMT	C3'-C4'-O1B-C1B
31	AC	521	LMG	O1-C7-C8-O7
31	BC	5521	LMG	O1-C7-C8-O7
24	BA	5406	CLA	O1A-CGA-O2A-C1
24	BC	5511	CLA	O1A-CGA-O2A-C1
24	BC	5502	CLA	C10-C11-C12-C13
24	AB	604	CLA	C10-C11-C12-C13
29	BA	5415	LHG	C27-C28-C29-C30
32	AB	624	LMT	C3'-C4'-O1B-C1B
34	AD	402	PHO	C2A-CAA-CBA-CGA
34	BD	5403	PHO	C2A-CAA-CBA-CGA
24	BD	5402	CLA	C4-C3-C5-C6
24	BB	5612	CLA	C13-C15-C16-C17
34	BD	5403	PHO	C2-C3-C5-C6
30	BA	5414	SQD	C19-C20-C21-C22
29	AA	415	LHG	C27-C28-C29-C30
24	AB	602	CLA	C14-C13-C15-C16
24	AC	503	CLA	C11-C12-C13-C14
24	AC	512	CLA	C14-C13-C15-C16
24	BC	5503	CLA	C11-C12-C13-C14
34	BD	5403	PHO	O1D-CGD-O2D-CED
24	BA	5406	CLA	CBA-CGA-O2A-C1
30	AF	102	SQD	C15-C16-C17-C18
24	AB	608	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	AA	413	SQD	C19-C20-C21-C22
24	AB	606	CLA	CBA-CGA-O2A-C1
24	AD	401	CLA	C4-C3-C5-C6
24	BB	5620	CLA	C4-C3-C5-C6
24	AA	404	CLA	C12-C13-C15-C16
24	AC	510	CLA	C12-C13-C15-C16
24	BC	5503	CLA	C11-C12-C13-C15
24	BC	5510	CLA	C12-C13-C15-C16
34	AD	402	PHO	O1D-CGD-O2D-CED
24	AB	606	CLA	O1A-CGA-O2A-C1
24	BB	5609	CLA	C4-C3-C5-C6
29	AA	412	LHG	C24-C25-C26-C27
24	BD	5402	CLA	C2-C3-C5-C6
24	AB	616	CLA	C2C-C3C-CAC-CBC
29	BA	5413	LHG	O9-C7-O7-C5
29	BA	5413	LHG	C24-C25-C26-C27
24	AB	606	CLA	C4-C3-C5-C6
24	AB	616	CLA	C4-C3-C5-C6
29	AA	412	LHG	O9-C7-O7-C5
24	BC	5510	CLA	C10-C11-C12-C13
24	AB	606	CLA	C14-C13-C15-C16
24	AC	511	CLA	C11-C12-C13-C14
24	BB	5606	CLA	C14-C13-C15-C16
24	BC	5512	CLA	C14-C13-C15-C16
31	BI	5101	LMG	C9-C8-O7-C10
24	AB	616	CLA	C2-C3-C5-C6
36	AF	101	HEM	CAD-CBD-CGD-O2D
36	BF	5101	HEM	CAD-CBD-CGD-O2D
27	AA	410	BCR	C23-C24-C25-C26
27	AC	515	BCR	C23-C24-C25-C26
27	AD	406	BCR	C5-C6-C7-C8
27	BA	5411	BCR	C23-C24-C25-C26
27	BC	5515	BCR	C23-C24-C25-C26
27	BC	5516	BCR	C5-C6-C7-C8
27	BD	5407	BCR	C5-C6-C7-C8
29	AA	412	LHG	C8-C7-O7-C5
29	BA	5413	LHG	C8-C7-O7-C5
36	AF	101	HEM	CAD-CBD-CGD-O1D
36	BF	5101	HEM	CAD-CBD-CGD-O1D
24	BB	5619	CLA	C13-C15-C16-C17
24	AA	404	CLA	C4-C3-C5-C6
24	AC	505	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	BC	5505	CLA	C4-C3-C5-C6
35	AD	405	PL9	C45-C44-C46-C47
24	AD	401	CLA	C2-C3-C5-C6
24	BB	5620	CLA	C2-C3-C5-C6
24	AC	503	CLA	C11-C12-C13-C15
24	AC	507	CLA	C12-C13-C15-C16
24	BC	5507	CLA	C12-C13-C15-C16
31	AA	414	LMG	O7-C8-C9-O8
31	BE	5101	LMG	O7-C8-C9-O8
30	BB	5601	SQD	C12-C13-C14-C15
24	BB	5612	CLA	CAA-CBA-CGA-O2A
29	AA	415	LHG	C26-C27-C28-C29
24	BB	5610	CLA	C4-C3-C5-C6
35	BD	5406	PL9	C45-C44-C46-C47
24	AB	608	CLA	CAA-CBA-CGA-O2A
24	AB	615	CLA	C13-C15-C16-C17
24	AD	401	CLA	C2-C1-O2A-CGA
24	BC	5501	CLA	CAA-CBA-CGA-O2A
24	AA	405	CLA	O1A-CGA-O2A-C1
24	BB	5610	CLA	C14-C13-C15-C16
30	AB	627	SQD	C11-C10-C9-C8
24	AC	510	CLA	C4-C3-C5-C6
24	AC	501	CLA	CAA-CBA-CGA-O2A
30	AB	622	SQD	C11-C10-C9-C8
30	AB	622	SQD	O10-C23-O48-C46
36	AV	201	HEM	CAD-CBD-CGD-O2D
36	BV	5201	HEM	CAD-CBD-CGD-O2D
30	AB	627	SQD	C2-C1-O6-C44
30	BB	5601	SQD	C2-C1-O6-C44
24	BC	5511	CLA	C13-C15-C16-C17
28	AC	518	DGD	O1G-C1G-C2G-C3G
31	BA	5402	LMG	O1-C7-C8-C9
31	BD	5410	LMG	C7-C8-C9-O8
35	AD	405	PL9	C34-C36-C37-C38
35	BD	5406	PL9	C34-C36-C37-C38
30	BF	5102	SQD	C29-C30-C31-C32
24	BC	5510	CLA	C4-C3-C5-C6
24	AC	510	CLA	C2-C3-C5-C6
24	BC	5510	CLA	C2-C3-C5-C6
24	BB	5610	CLA	O1A-CGA-O2A-C1
30	BB	5625	SQD	C11-C10-C9-C8
24	AB	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	BB	5615	CLA	CAA-CBA-CGA-O2A
24	AC	512	CLA	C13-C15-C16-C17
29	BA	5415	LHG	C26-C27-C28-C29
24	BB	5608	CLA	CAA-CBA-CGA-O2A
24	BC	5502	CLA	CAA-CBA-CGA-O2A
30	AB	622	SQD	C24-C23-O48-C46
24	BB	5620	CLA	C12-C13-C15-C16
24	BC	5505	CLA	C12-C13-C15-C16
24	AB	604	CLA	CAA-CBA-CGA-O2A
24	AC	502	CLA	CAA-CBA-CGA-O2A
24	AB	608	CLA	C14-C13-C15-C16
24	AC	510	CLA	C6-C7-C8-C9
24	BB	5612	CLA	C14-C13-C15-C16
24	BC	5505	CLA	C11-C12-C13-C14
24	AC	504	CLA	O1A-CGA-O2A-C1
30	AB	627	SQD	C12-C13-C14-C15
30	BA	5414	SQD	C45-C44-O6-C1
24	AA	404	CLA	C2-C1-O2A-CGA
24	AC	513	CLA	C2-C1-O2A-CGA
24	BA	5405	CLA	C2-C1-O2A-CGA
24	BC	5513	CLA	C2-C1-O2A-CGA
24	BC	5512	CLA	C13-C15-C16-C17
24	AA	405	CLA	CBA-CGA-O2A-C1
24	BB	5610	CLA	CBA-CGA-O2A-C1
24	BC	5508	CLA	CAA-CBA-CGA-O2A
30	BB	5625	SQD	O10-C23-O48-C46
24	AB	605	CLA	C2-C3-C5-C6
24	AC	508	CLA	CAA-CBA-CGA-O2A
36	AV	201	HEM	CAD-CBD-CGD-O1D
32	BB	5627	LMT	C5'-C4'-O1B-C1B
32	AB	624	LMT	C5'-C4'-O1B-C1B
30	AF	102	SQD	C29-C30-C31-C32
28	AB	628	DGD	C1G-C2G-C3G-O3G
28	AC	517	DGD	C1G-C2G-C3G-O3G
28	BB	5602	DGD	C1G-C2G-C3G-O3G
28	BC	5517	DGD	C1G-C2G-C3G-O3G
28	BC	5518	DGD	O1G-C1G-C2G-C3G
31	AA	414	LMG	C7-C8-C9-O8
31	AA	417	LMG	O1-C7-C8-C9
31	AD	408	LMG	C7-C8-C9-O8
31	BE	5101	LMG	C7-C8-C9-O8
24	AC	511	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	BA	5405	CLA	C4-C3-C5-C6
24	BB	5616	CLA	C4-C3-C5-C6
36	BV	5201	HEM	CAD-CBD-CGD-O1D
24	AB	601	CLA	CAA-CBA-CGA-O2A
24	AB	605	CLA	C3-C5-C6-C7
24	AC	505	CLA	C11-C12-C13-C14
24	AD	404	CLA	C6-C7-C8-C9
24	BC	5503	CLA	C14-C13-C15-C16
24	BC	5511	CLA	C11-C12-C13-C14
24	AB	612	CLA	C4-C3-C5-C6
24	BB	5613	CLA	C4-C3-C5-C6
24	AD	401	CLA	CAA-CBA-CGA-O2A
24	BC	5505	CLA	C2-C3-C5-C6
24	AA	407	CLA	C11-C12-C13-C15
24	AB	602	CLA	C12-C13-C15-C16
24	AB	606	CLA	C12-C13-C15-C16
24	AB	608	CLA	C11-C12-C13-C15
24	AB	616	CLA	C12-C13-C15-C16
24	AC	505	CLA	C12-C13-C15-C16
24	AD	404	CLA	C6-C7-C8-C10
24	BA	5405	CLA	C12-C13-C15-C16
24	BA	5408	CLA	C11-C12-C13-C15
24	BB	5606	CLA	C12-C13-C15-C16
24	BB	5610	CLA	C12-C13-C15-C16
24	BB	5612	CLA	C11-C12-C13-C15
24	AC	505	CLA	CAA-CBA-CGA-O2A
24	BB	5605	CLA	CAA-CBA-CGA-O2A
24	AA	407	CLA	C2-C1-O2A-CGA
24	BD	5402	CLA	C2-C1-O2A-CGA
24	BD	5402	CLA	CAA-CBA-CGA-O2A
30	BB	5625	SQD	C24-C23-O48-C46
30	BB	5601	SQD	C11-C10-C9-C8
24	AB	606	CLA	C2-C3-C5-C6
24	AC	505	CLA	C2-C3-C5-C6
24	BB	5609	CLA	C2-C3-C5-C6
35	AD	405	PL9	C43-C44-C46-C47
35	BD	5406	PL9	C43-C44-C46-C47
29	AA	412	LHG	C31-C32-C33-C34
36	BF	5101	HEM	CAA-CBA-CGA-O2A
24	AB	603	CLA	CAA-CBA-CGA-O1A
24	AB	613	CLA	C14-C13-C15-C16
24	AD	404	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	BB	5620	CLA	C14-C13-C15-C16
24	BD	5405	CLA	C6-C7-C8-C9
24	AA	404	CLA	CAA-CBA-CGA-O2A
24	BC	5511	CLA	CAA-CBA-CGA-O2A
29	AA	415	LHG	O7-C7-C8-C9
28	AC	519	DGD	C1G-C2G-C3G-O3G
24	AB	601	CLA	C4B-C3B-CAB-CBB
24	AB	605	CLA	C4B-C3B-CAB-CBB
24	AB	606	CLA	C4B-C3B-CAB-CBB
24	AB	608	CLA	C4B-C3B-CAB-CBB
24	AB	613	CLA	C4B-C3B-CAB-CBB
24	AC	503	CLA	C4B-C3B-CAB-CBB
24	AC	506	CLA	C4B-C3B-CAB-CBB
24	AC	511	CLA	C4B-C3B-CAB-CBB
24	AC	512	CLA	C4B-C3B-CAB-CBB
24	BA	5406	CLA	C4B-C3B-CAB-CBB
24	BB	5605	CLA	C4B-C3B-CAB-CBB
24	BB	5607	CLA	C4B-C3B-CAB-CBB
24	BB	5608	CLA	C4B-C3B-CAB-CBB
24	BB	5609	CLA	C4B-C3B-CAB-CBB
24	BB	5612	CLA	C4B-C3B-CAB-CBB
24	BB	5617	CLA	C4B-C3B-CAB-CBB
24	BB	5620	CLA	C4B-C3B-CAB-CBB
24	BC	5502	CLA	C4B-C3B-CAB-CBB
24	BC	5503	CLA	C4B-C3B-CAB-CBB
24	BC	5505	CLA	C4B-C3B-CAB-CBB
24	BC	5506	CLA	C4B-C3B-CAB-CBB
24	BC	5508	CLA	C4B-C3B-CAB-CBB
24	BC	5510	CLA	C4B-C3B-CAB-CBB
24	BC	5511	CLA	C4B-C3B-CAB-CBB
36	BF	5101	HEM	CAA-CBA-CGA-O1A
24	AB	609	CLA	C4-C3-C5-C6
24	AC	512	CLA	CAA-CBA-CGA-O2A
24	BC	5512	CLA	CAA-CBA-CGA-O2A
35	AD	405	PL9	C31-C32-C33-C34
35	BD	5406	PL9	C31-C32-C33-C34
35	BD	5406	PL9	C41-C42-C43-C44
36	AF	101	HEM	CAA-CBA-CGA-O1A
30	BA	5401	SQD	C12-C13-C14-C15
24	AC	511	CLA	CAA-CBA-CGA-O2A
24	BB	5620	CLA	C2C-C3C-CAC-CBC
24	AB	616	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
36	AF	101	HEM	CAA-CBA-CGA-O2A
24	BA	5405	CLA	CAA-CBA-CGA-O2A
29	BA	5415	LHG	O7-C7-C8-C9
28	AC	519	DGD	C4D-C5D-C6D-O5D
24	AB	604	CLA	C2-C1-O2A-CGA
24	BA	5408	CLA	C2-C1-O2A-CGA
24	BB	5608	CLA	C2-C1-O2A-CGA
24	BC	5512	CLA	C2-C1-O2A-CGA
24	AB	604	CLA	C12-C13-C15-C16
24	AC	513	CLA	C12-C13-C15-C16
24	BB	5608	CLA	C12-C13-C15-C16
24	BC	5513	CLA	C12-C13-C15-C16
24	BD	5405	CLA	C6-C7-C8-C10
30	AB	627	SQD	C27-C28-C29-C30
28	BE	5102	DGD	C1G-C2G-O2G-C1B
29	AA	412	LHG	C4-C5-O7-C7
29	BA	5413	LHG	C4-C5-O7-C7
30	BA	5401	SQD	C30-C31-C32-C33
24	BA	5405	CLA	C13-C15-C16-C17
35	AD	405	PL9	C41-C42-C43-C44
35	BD	5406	PL9	C21-C22-C23-C24
29	AA	415	LHG	O8-C23-C24-C25
29	BA	5415	LHG	O8-C23-C24-C25
24	BB	5610	CLA	C2-C3-C5-C6
30	AA	416	SQD	C12-C13-C14-C15
24	AC	512	CLA	CAA-CBA-CGA-O1A
24	BB	5607	CLA	CAA-CBA-CGA-O1A
28	AB	628	DGD	O6E-C1E-O5D-C6D
28	BB	5602	DGD	O6E-C1E-O5D-C6D
35	AD	405	PL9	C11-C12-C13-C14
35	AD	405	PL9	C21-C22-C23-C24
35	BD	5406	PL9	C11-C12-C13-C14
24	BC	5512	CLA	CAA-CBA-CGA-O1A
24	AA	404	CLA	C2A-CAA-CBA-CGA
24	AB	612	CLA	C14-C13-C15-C16
24	AB	614	CLA	C14-C13-C15-C16
24	AC	503	CLA	C14-C13-C15-C16
24	BB	5616	CLA	C14-C13-C15-C16
24	BB	5617	CLA	C14-C13-C15-C16
24	BB	5618	CLA	C14-C13-C15-C16
24	BB	5605	CLA	CAA-CBA-CGA-O1A
30	BB	5601	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	BD	5402	CLA	CAA-CBA-CGA-O1A
30	BF	5102	SQD	C26-C27-C28-C29
24	BC	5505	CLA	CAA-CBA-CGA-O2A
24	BC	5504	CLA	O1A-CGA-O2A-C1
24	AB	601	CLA	CAA-CBA-CGA-O1A
29	AA	415	LHG	O9-C7-C8-C9
29	BA	5415	LHG	O9-C7-C8-C9
30	AA	416	SQD	C30-C31-C32-C33
30	AA	413	SQD	C45-C44-O6-C1
30	AB	627	SQD	C45-C44-O6-C1
30	BB	5601	SQD	C45-C44-O6-C1
28	BA	5412	DGD	O1G-C1G-C2G-O2G
29	BA	5413	LHG	C31-C32-C33-C34
24	AD	401	CLA	CAA-CBA-CGA-O1A
28	AB	628	DGD	O1G-C1G-C2G-C3G
35	BD	5406	PL9	C24-C26-C27-C28
24	AC	506	CLA	C10-C11-C12-C13
24	AB	614	CLA	CAA-CBA-CGA-O2A
24	AC	513	CLA	CAA-CBA-CGA-O2A
24	BB	5609	CLA	CAA-CBA-CGA-O2A
24	BB	5617	CLA	CAA-CBA-CGA-O2A
24	BB	5618	CLA	CAA-CBA-CGA-O2A
30	AB	622	SQD	O47-C7-C8-C9
24	BC	5511	CLA	CAA-CBA-CGA-O1A
24	AA	404	CLA	CAD-CBD-CGD-O2D
24	AB	611	CLA	CAD-CBD-CGD-O2D
24	BA	5405	CLA	CAD-CBD-CGD-O2D
24	BD	5405	CLA	CAD-CBD-CGD-O2D
30	AB	627	SQD	O47-C7-C8-C9
24	BB	5609	CLA	C3-C5-C6-C7
24	AC	512	CLA	C2-C1-O2A-CGA
24	BC	5504	CLA	C2-C1-O2A-CGA
24	AC	511	CLA	CAA-CBA-CGA-O1A
24	BA	5405	CLA	C2A-CAA-CBA-CGA
29	BA	5413	LHG	C29-C30-C31-C32
30	AB	622	SQD	C24-C25-C26-C27
24	AC	509	CLA	C13-C15-C16-C17
30	BA	5401	SQD	O47-C7-C8-C9
30	BF	5102	SQD	O47-C7-C8-C9
29	BA	5415	LHG	O10-C23-C24-C25
24	AB	612	CLA	C3-C5-C6-C7
24	AB	605	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	AC	509	CLA	CAA-CBA-CGA-O2A
24	BB	5613	CLA	CAA-CBA-CGA-O2A
30	AF	102	SQD	O47-C7-C8-C9
24	AA	404	CLA	CAA-CBA-CGA-O1A
24	BA	5405	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

171 monomers are involved in 1019 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	AA	415	LHG	2	0
27	BB	5621	BCR	4	0
34	BD	5404	PHO	4	0
30	AA	416	SQD	2	0
32	AI	103	LMT	4	0
27	BD	5407	BCR	2	0
31	BM	5102	LMG	4	0
27	BB	5622	BCR	1	0
32	BI	5102	LMT	5	0
24	AC	503	CLA	5	0
27	BB	5623	BCR	4	0
30	BB	5625	SQD	6	0
32	AM	102	LMT	2	0
24	BB	5607	CLA	13	0
27	AD	406	BCR	2	0
24	AB	602	CLA	8	0
24	AB	615	CLA	8	0
24	AC	504	CLA	12	0
24	BA	5407	CLA	1	0
31	BL	5101	LMG	18	0
31	AD	408	LMG	11	0
32	AI	102	LMT	5	0
27	BJ	5101	BCR	3	0
27	BC	5515	BCR	5	0
24	BB	5617	CLA	7	0
24	BB	5612	CLA	14	0
32	BB	5604	LMT	2	0
27	AC	515	BCR	5	0
24	AC	502	CLA	5	0
34	AD	402	PHO	8	0
33	BV	5202	DMS	1	0
24	BB	5608	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	AD	407	LMG	3	0
28	BC	5518	DGD	10	0
36	BF	5101	HEM	7	0
24	AB	613	CLA	8	0
24	BB	5620	CLA	3	0
24	AB	607	CLA	7	0
24	AC	512	CLA	4	0
24	AD	404	CLA	7	0
24	BB	5606	CLA	8	0
24	BB	5618	CLA	14	0
29	BA	5415	LHG	3	0
30	BF	5102	SQD	1	0
31	BB	5624	LMG	4	0
28	BA	5412	DGD	7	0
24	BB	5615	CLA	18	0
31	AM	101	LMG	6	0
27	BC	5514	BCR	6	0
28	AE	101	DGD	1	0
28	BE	5102	DGD	1	0
27	BC	5516	BCR	13	0
24	AB	604	CLA	10	0
24	BB	5610	CLA	8	0
34	AD	403	PHO	3	0
35	BD	5406	PL9	15	0
28	BC	5517	DGD	10	0
24	AC	507	CLA	6	0
24	BA	5406	CLA	20	0
24	AB	608	CLA	16	0
24	BC	5504	CLA	10	0
27	AB	618	BCR	2	0
32	BB	5603	LMT	2	0
28	BH	5101	DGD	10	0
35	AD	405	PL9	15	0
30	BA	5401	SQD	3	0
31	BD	5409	LMG	3	0
24	BB	5613	CLA	4	0
31	AB	621	LMG	4	0
24	BB	5605	CLA	3	0
24	BC	5503	CLA	3	0
31	BC	5520	LMG	3	0
29	BA	5413	LHG	6	0
24	BC	5513	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	AB	629	LMT	4	0
31	BD	5410	LMG	11	0
33	BB	5628	DMS	1	0
24	BB	5611	CLA	8	0
29	AA	412	LHG	5	0
24	AB	609	CLA	4	0
31	BE	5101	LMG	3	0
27	AK	102	BCR	5	0
25	BA	5409	MST	11	0
27	AB	617	BCR	4	0
31	AA	417	LMG	6	0
24	BC	5508	CLA	8	0
27	AB	619	BCR	3	0
27	AT	101	BCR	9	0
24	BC	5506	CLA	4	0
30	AF	102	SQD	1	0
24	BC	5512	CLA	5	0
24	AC	501	CLA	6	0
27	AJ	101	BCR	4	0
24	AB	605	CLA	11	0
31	BA	5402	LMG	3	0
32	BB	5627	LMT	9	0
24	AB	612	CLA	7	0
24	BB	5614	CLA	8	0
28	BB	5602	DGD	5	0
24	AA	405	CLA	17	0
24	BC	5502	CLA	5	0
32	AB	630	LMT	2	0
30	BB	5601	SQD	5	0
31	AI	101	LMG	3	0
31	BI	5101	LMG	4	0
27	AA	410	BCR	4	0
24	AC	506	CLA	5	0
24	AC	510	CLA	4	0
24	BB	5616	CLA	7	0
24	BC	5507	CLA	8	0
24	BA	5405	CLA	11	0
24	BC	5511	CLA	20	0
25	AA	408	MST	10	0
28	AH	101	DGD	10	0
28	AC	519	DGD	42	0
32	BD	5411	LMT	1	0

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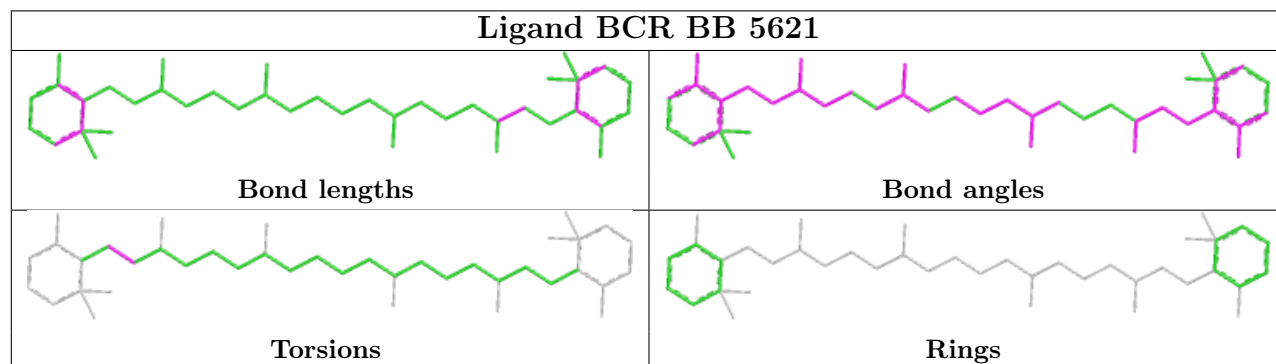
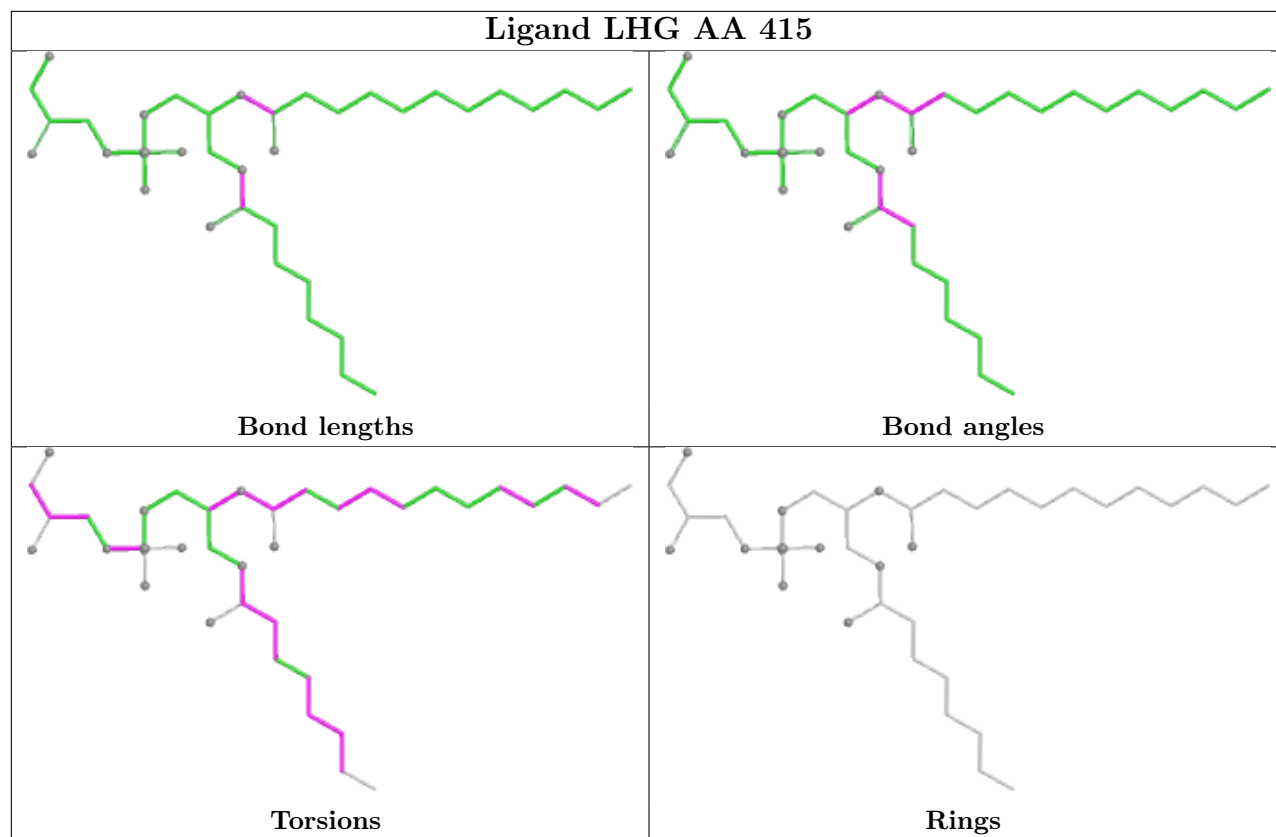
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AB	601	CLA	3	0
24	BC	5505	CLA	9	0
24	AA	406	CLA	1	0
28	AA	411	DGD	7	0
31	AB	620	LMG	17	0
30	AB	627	SQD	3	0
34	BD	5403	PHO	9	0
27	BA	5411	BCR	3	0
24	AA	407	CLA	7	0
36	AV	201	HEM	5	0
24	BA	5408	CLA	9	0
24	AA	404	CLA	11	0
24	BB	5619	CLA	9	0
31	BC	5521	LMG	7	0
27	BT	5101	BCR	5	0
24	BC	5510	CLA	4	0
24	AC	513	CLA	2	0
24	BD	5402	CLA	9	0
24	BB	5609	CLA	13	0
27	AX	101	BCR	6	0
28	BC	5519	DGD	44	0
30	AB	622	SQD	6	0
24	AB	614	CLA	9	0
24	AB	606	CLA	8	0
28	AC	517	DGD	10	0
24	AC	508	CLA	10	0
31	AC	520	LMG	4	0
36	AF	101	HEM	8	0
24	AB	610	CLA	7	0
24	AB	603	CLA	15	0
27	BK	5102	BCR	5	0
24	AC	511	CLA	19	0
24	AB	611	CLA	14	0
32	BB	5626	LMT	2	0
31	AJ	102	LMG	2	0
32	AB	624	LMT	9	0
32	BM	5101	LMT	3	0
24	AD	401	CLA	8	0
31	AA	414	LMG	9	0
31	AC	521	LMG	7	0
28	AC	518	DGD	12	0
24	BC	5509	CLA	6	0

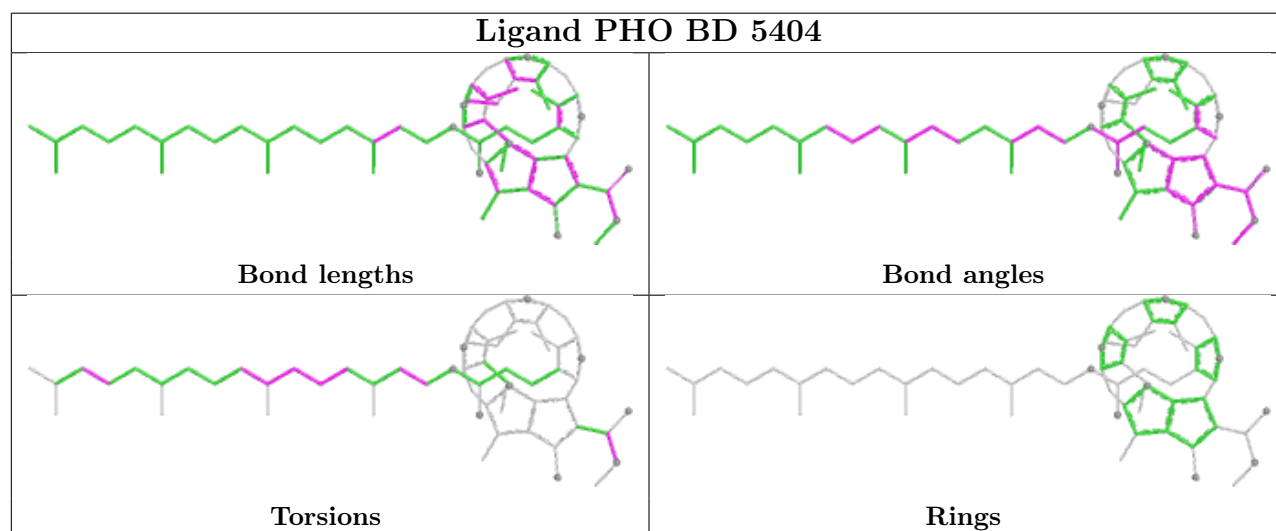
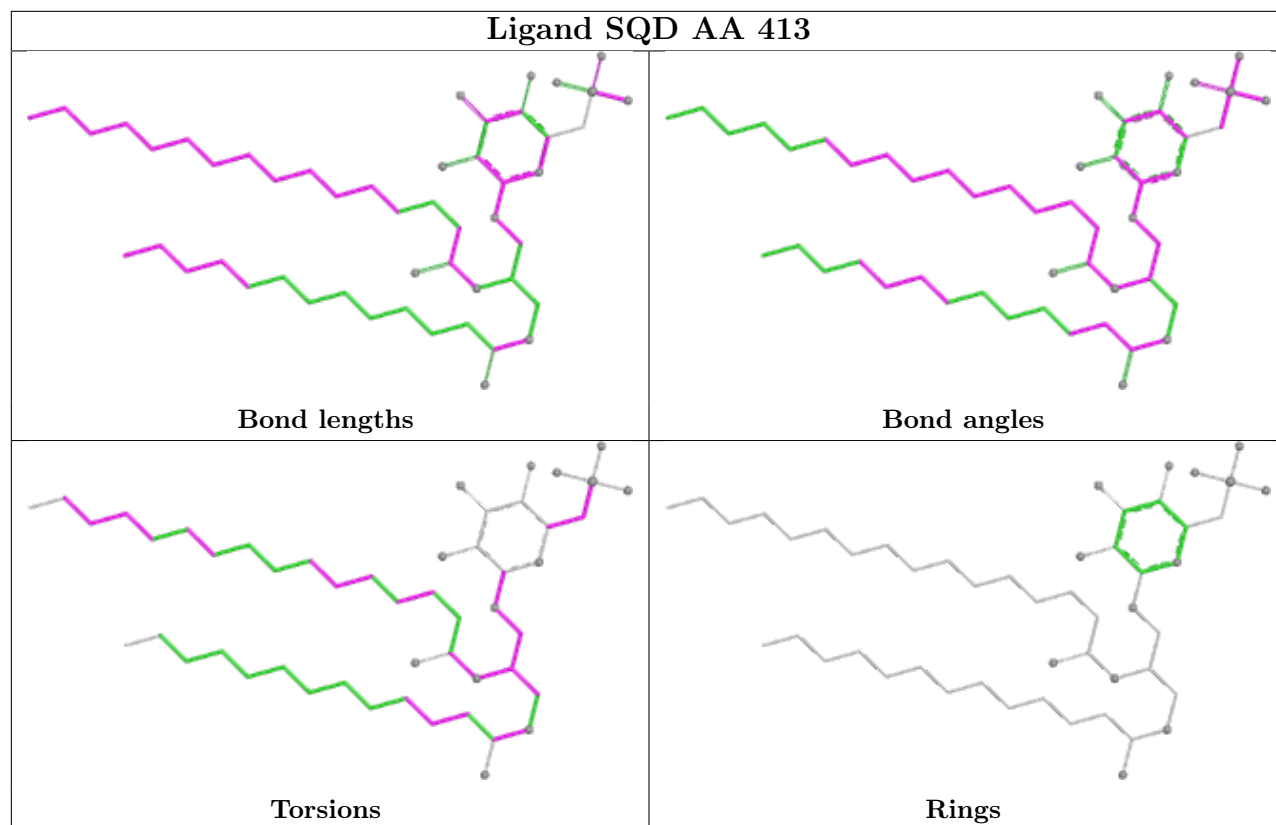
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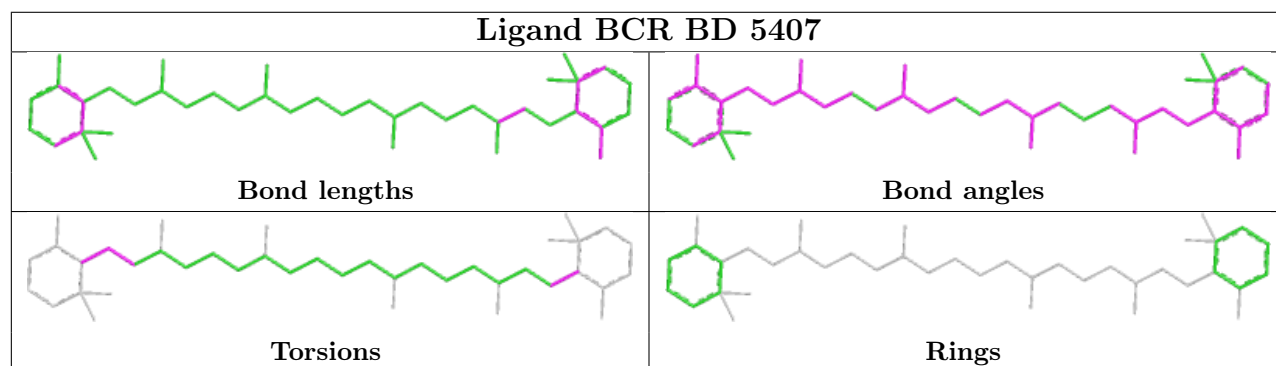
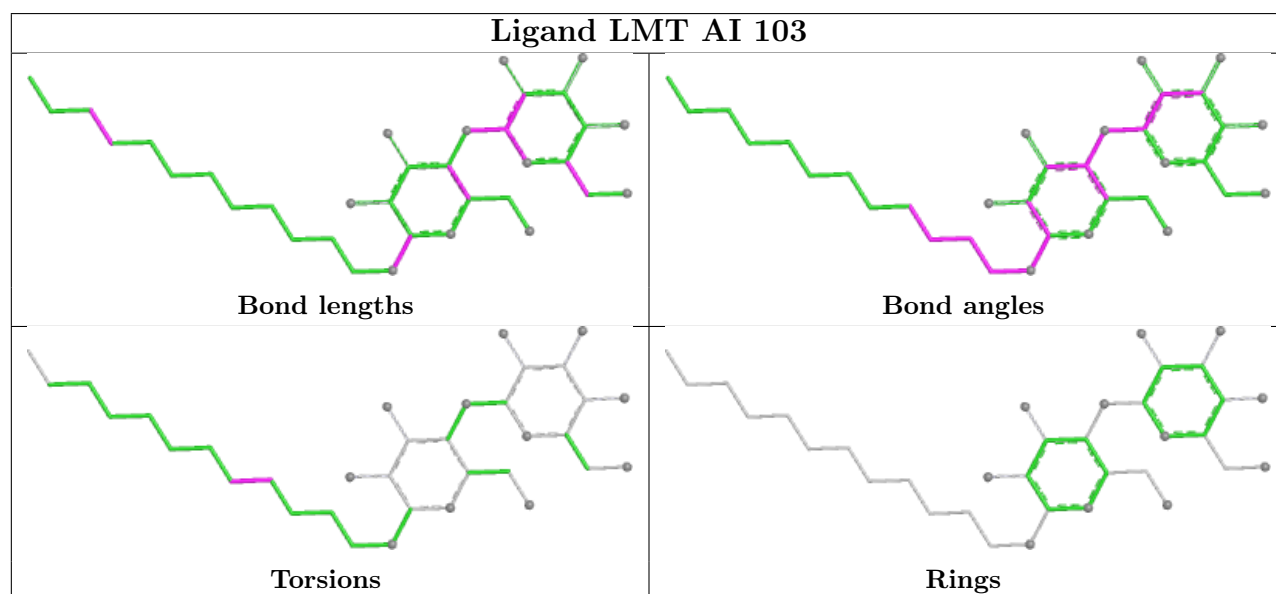
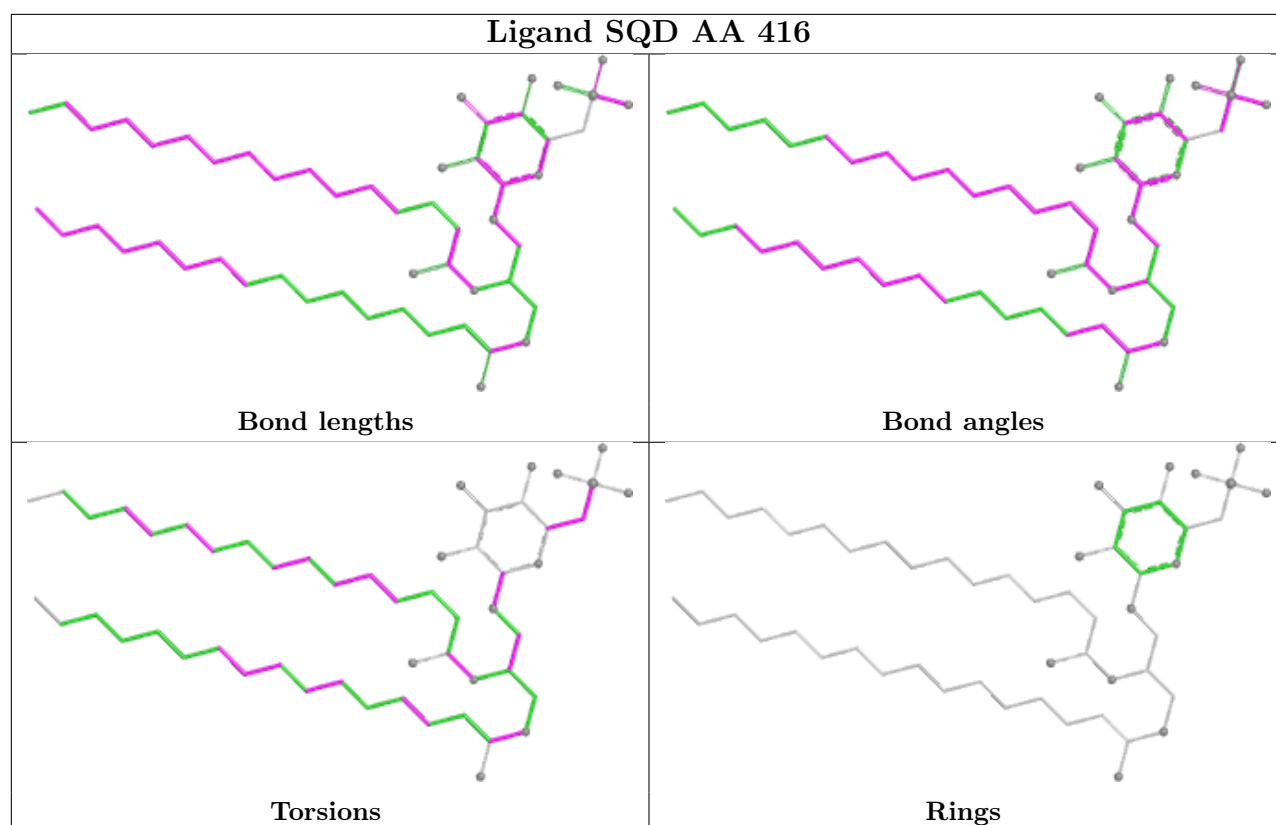
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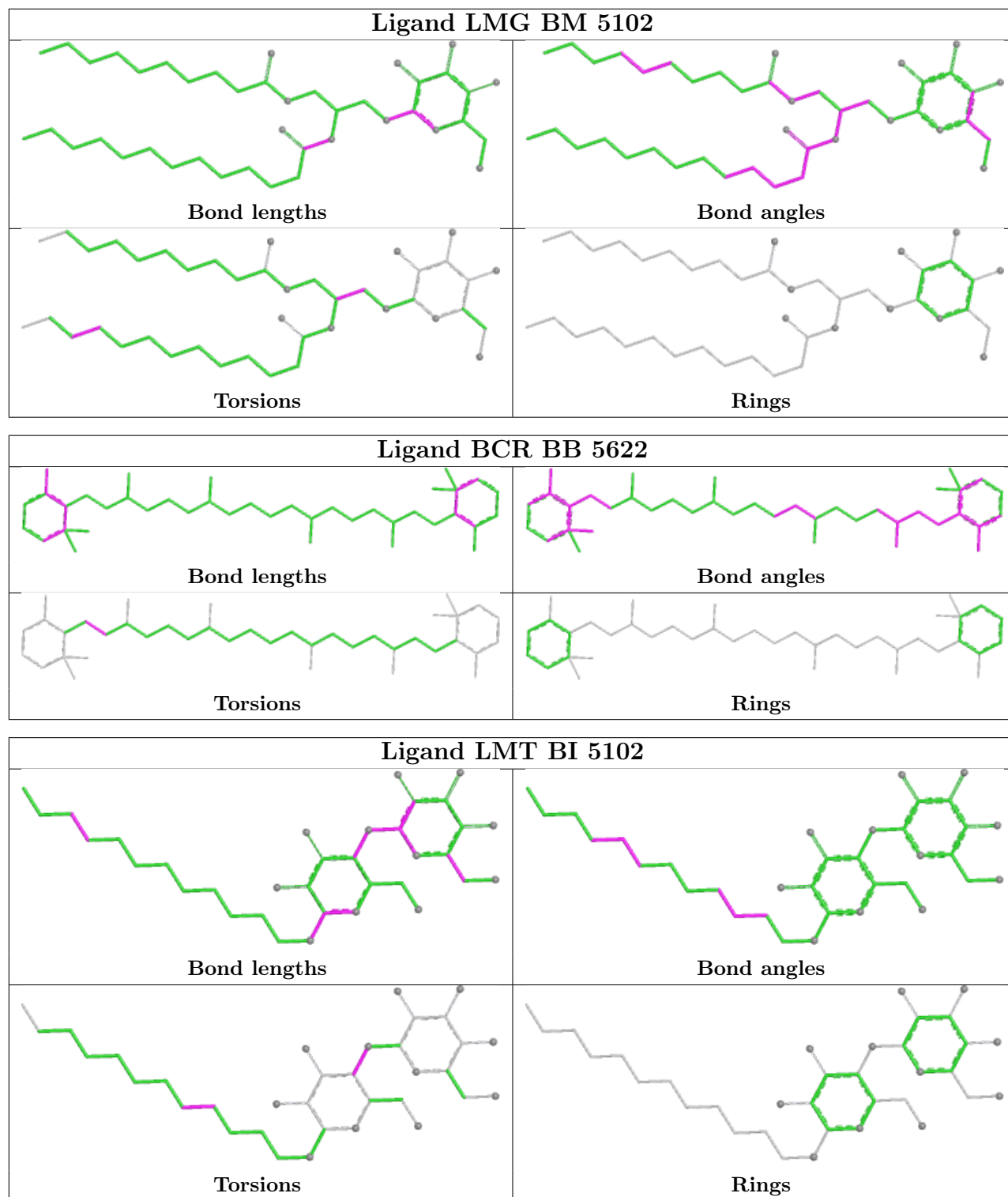
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	AB	625	DMS	1	0
27	BX	5101	BCR	2	0
27	AC	516	BCR	11	0
31	BD	5408	LMG	1	0
24	AB	616	CLA	3	0
24	AC	509	CLA	4	0
27	AC	514	BCR	6	0
24	AC	505	CLA	9	0
33	AV	202	DMS	1	0
24	BD	5405	CLA	7	0
32	BC	5522	LMT	3	0
24	BC	5501	CLA	8	0
36	BV	5201	HEM	7	0

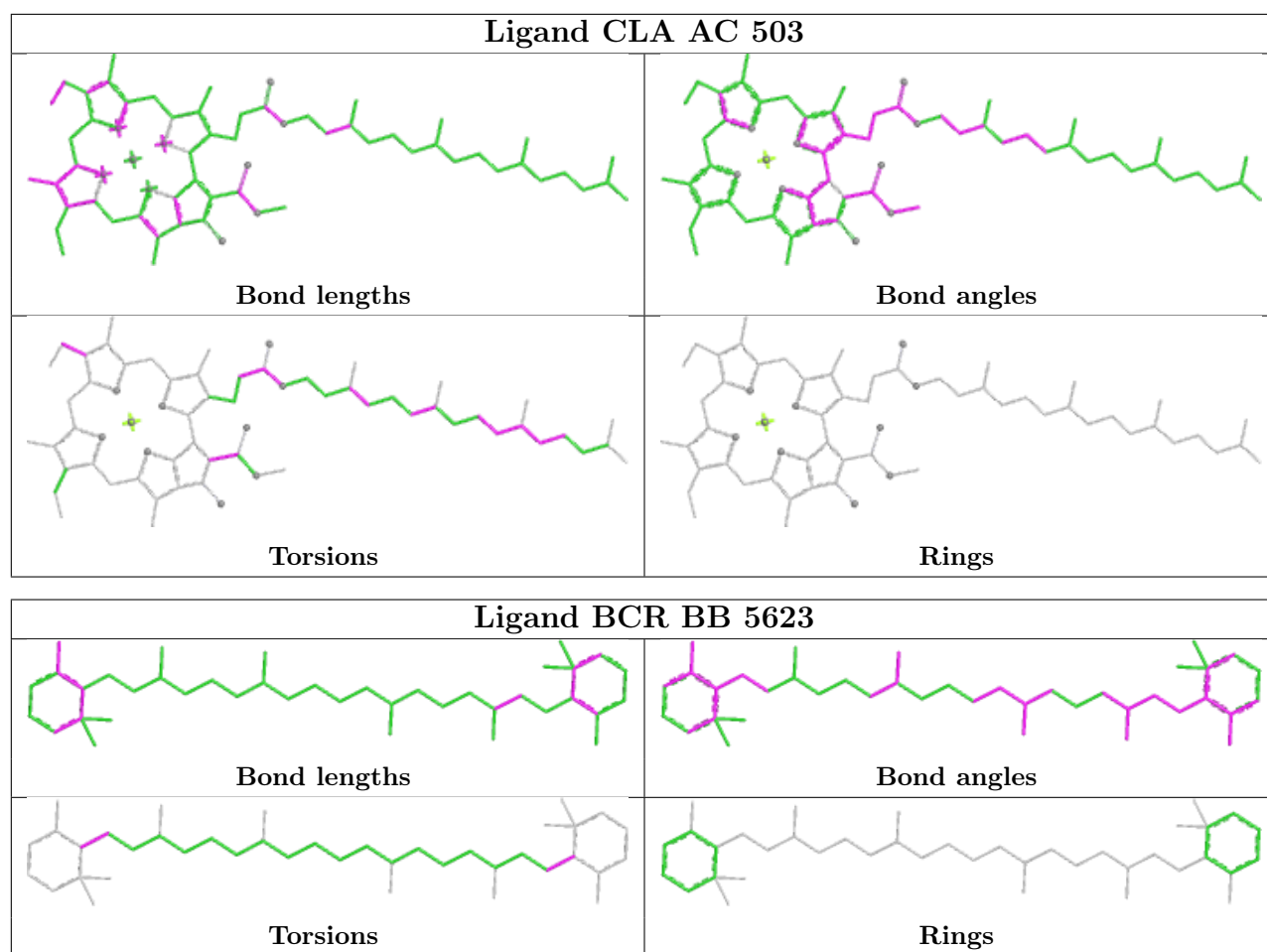
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

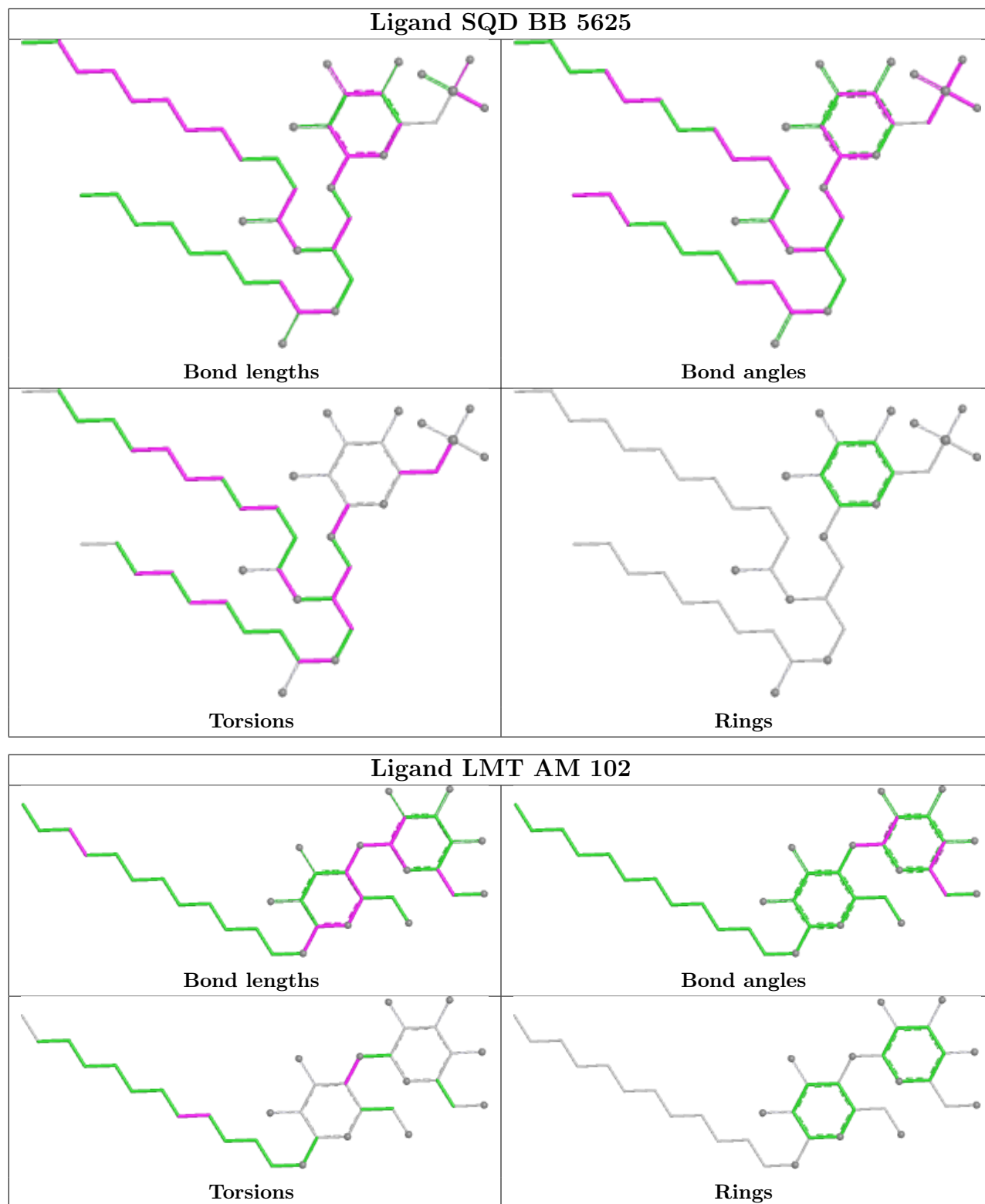


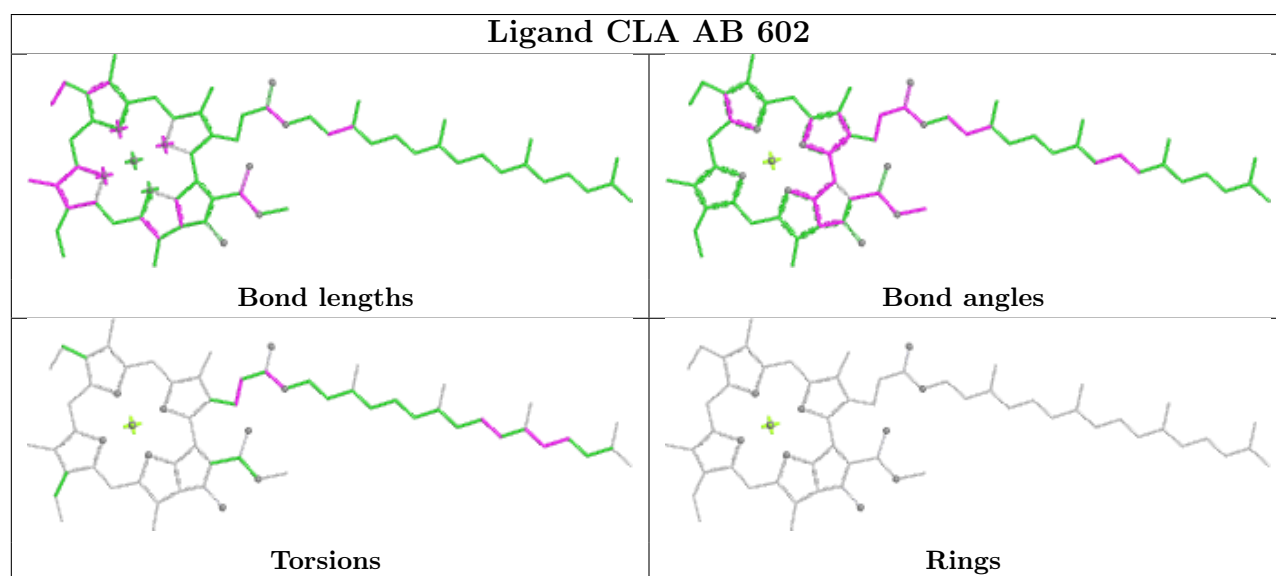
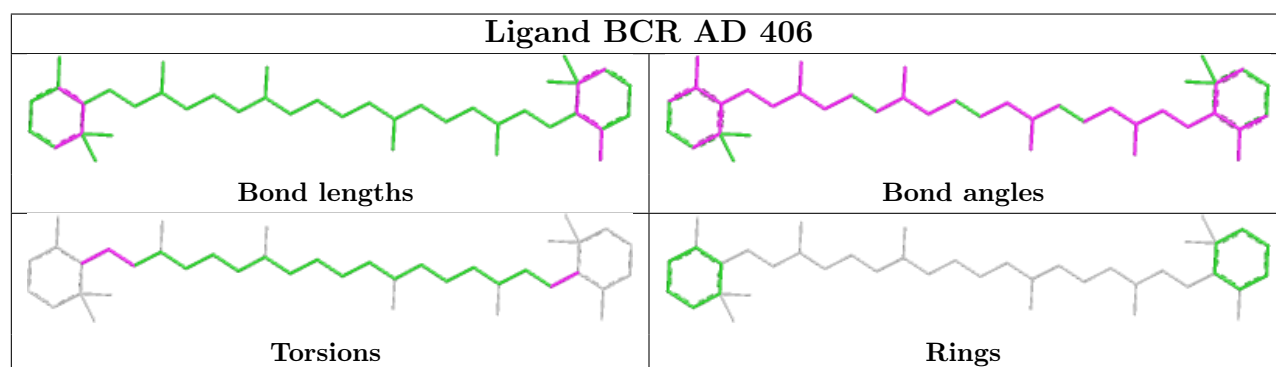
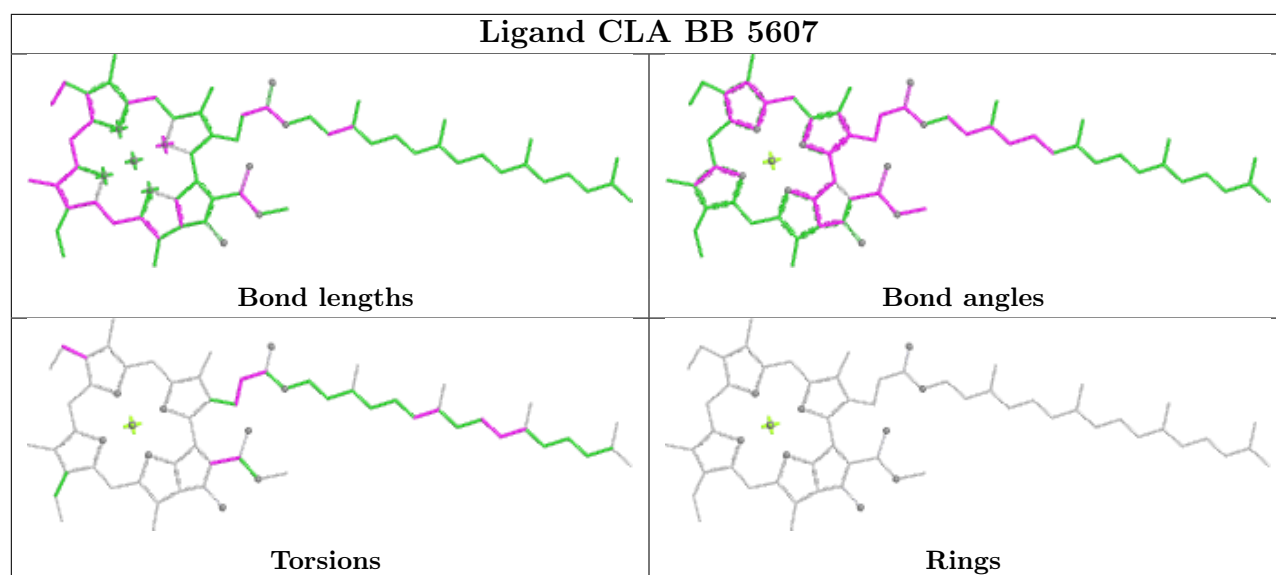




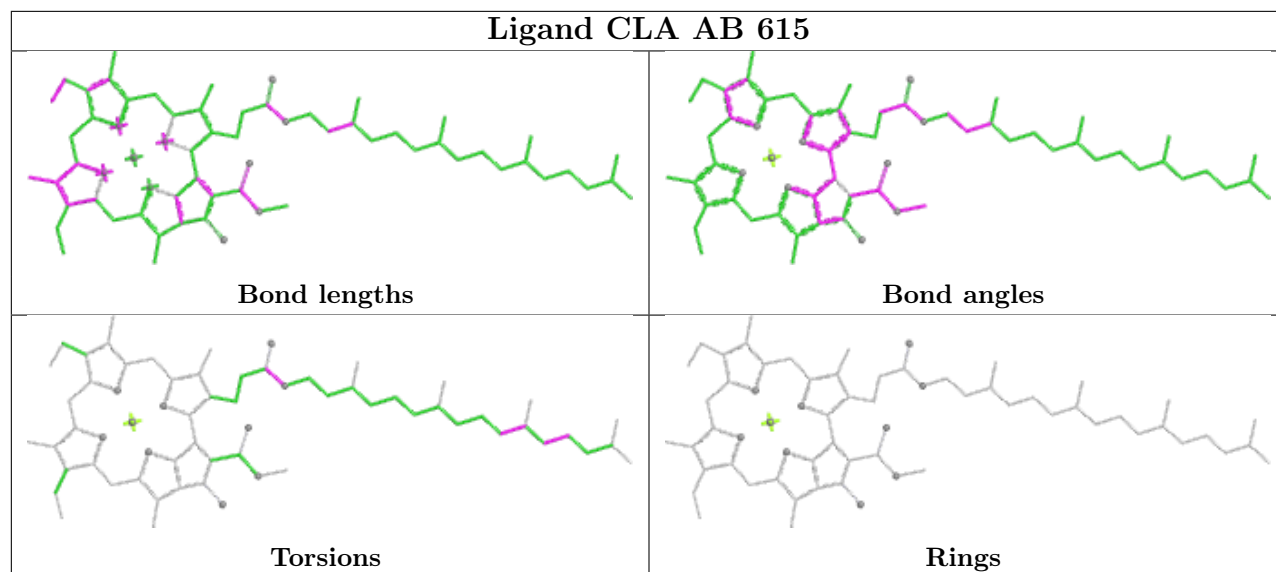




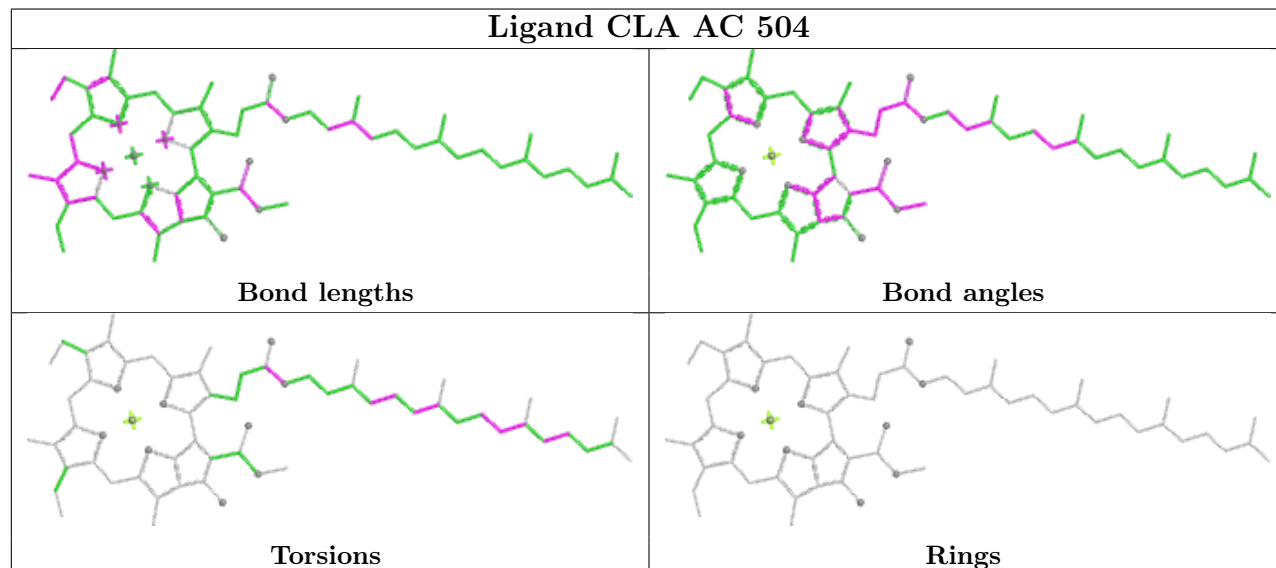




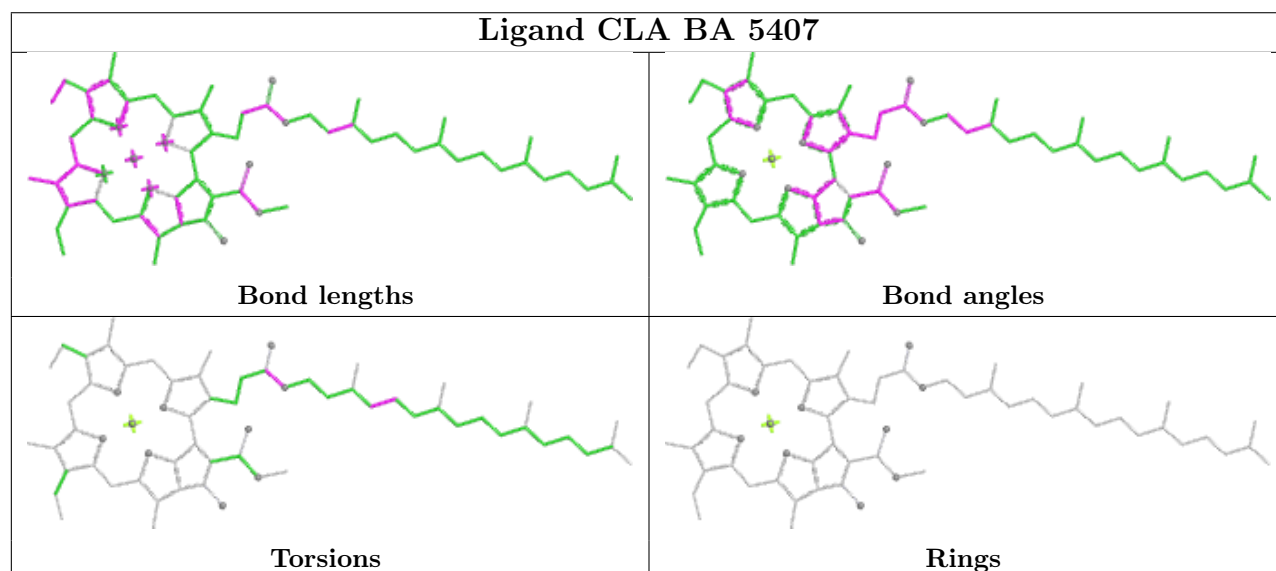
Ligand CLA AB 615

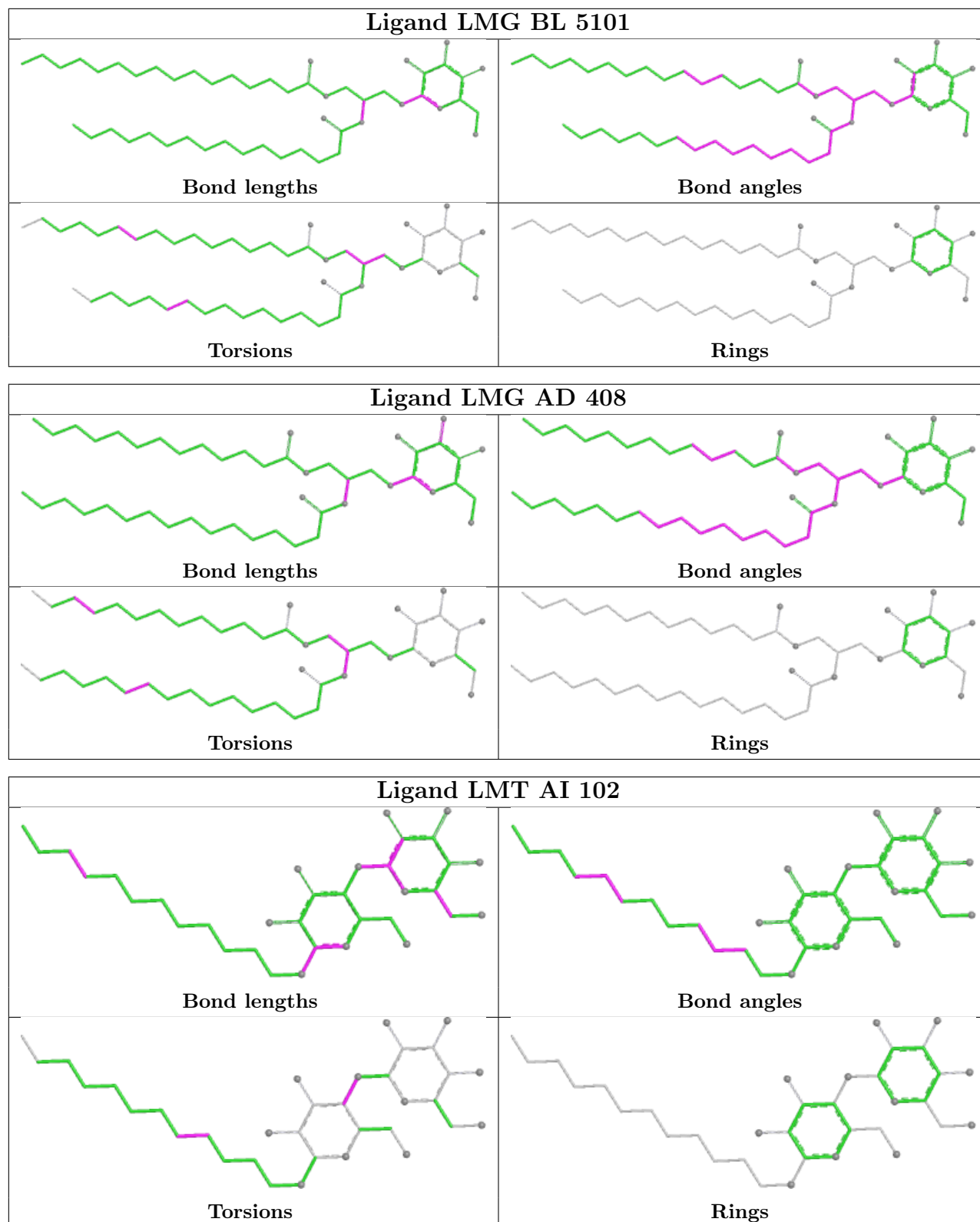


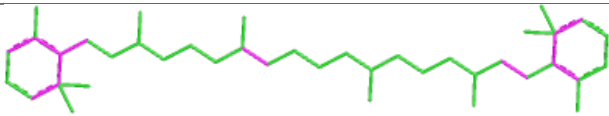
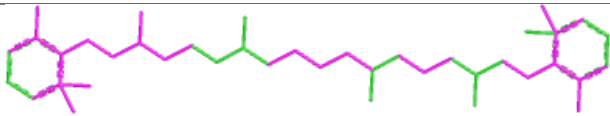
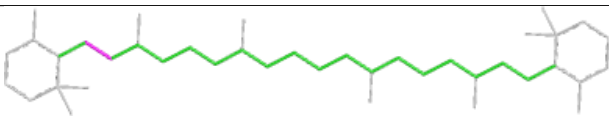
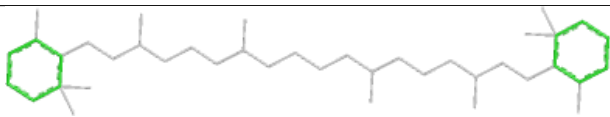
Ligand CLA AC 504

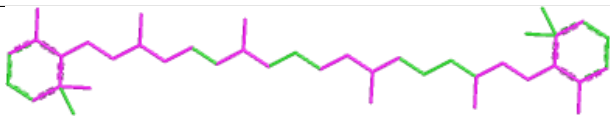
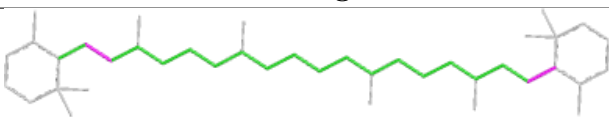
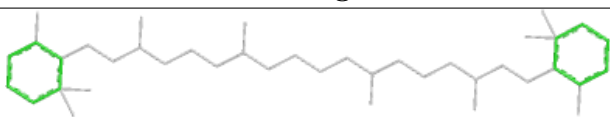


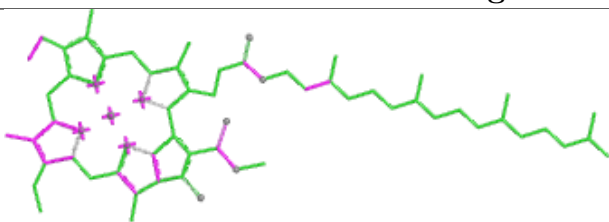
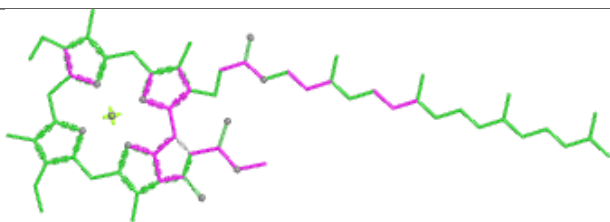
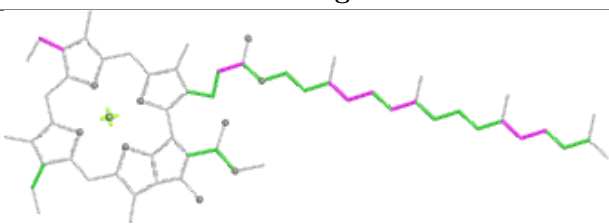
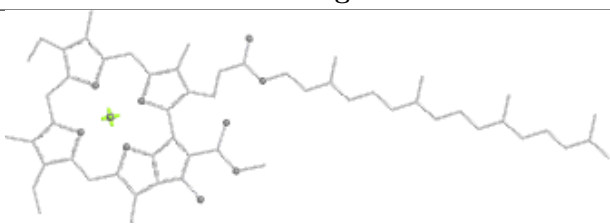
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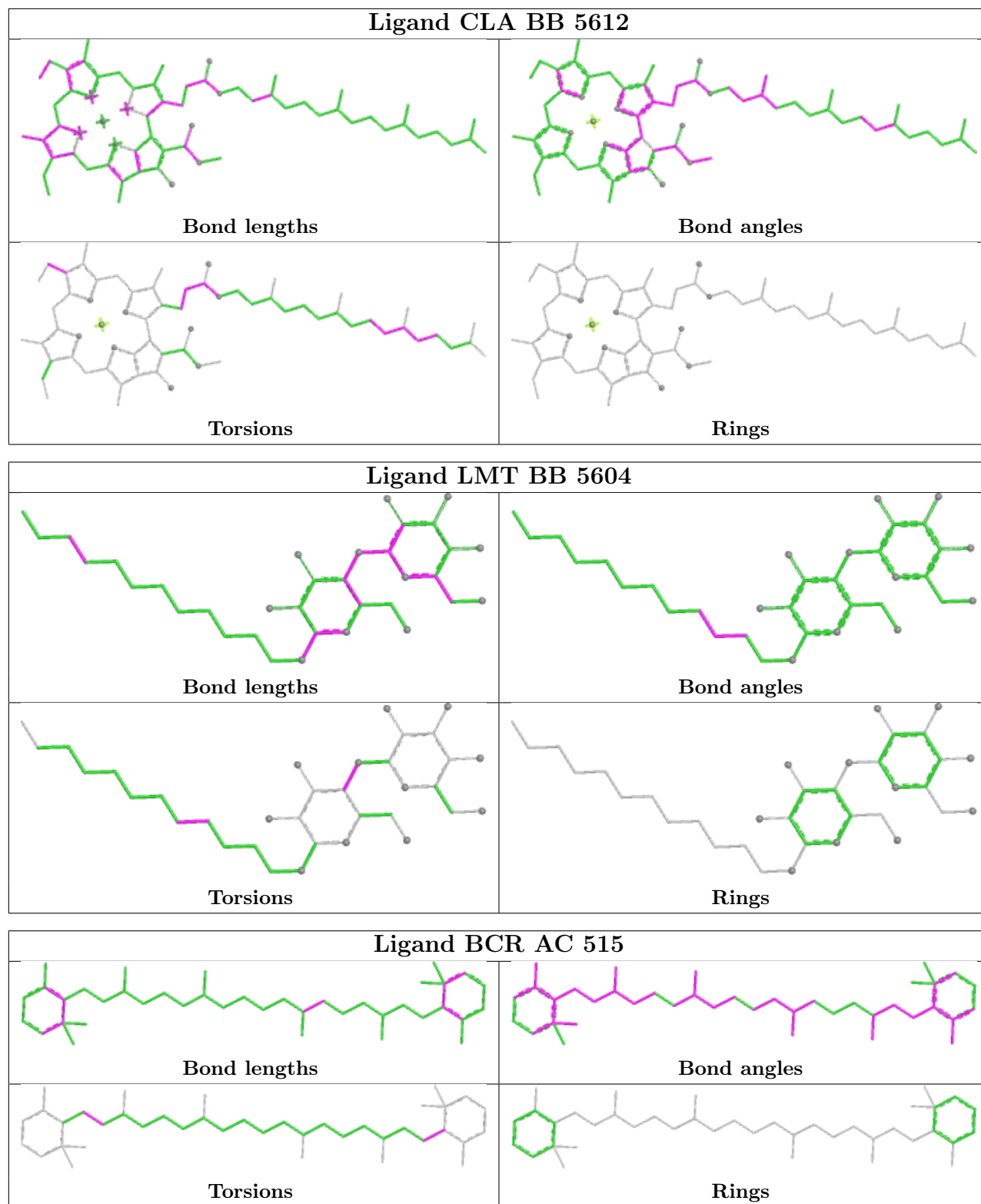




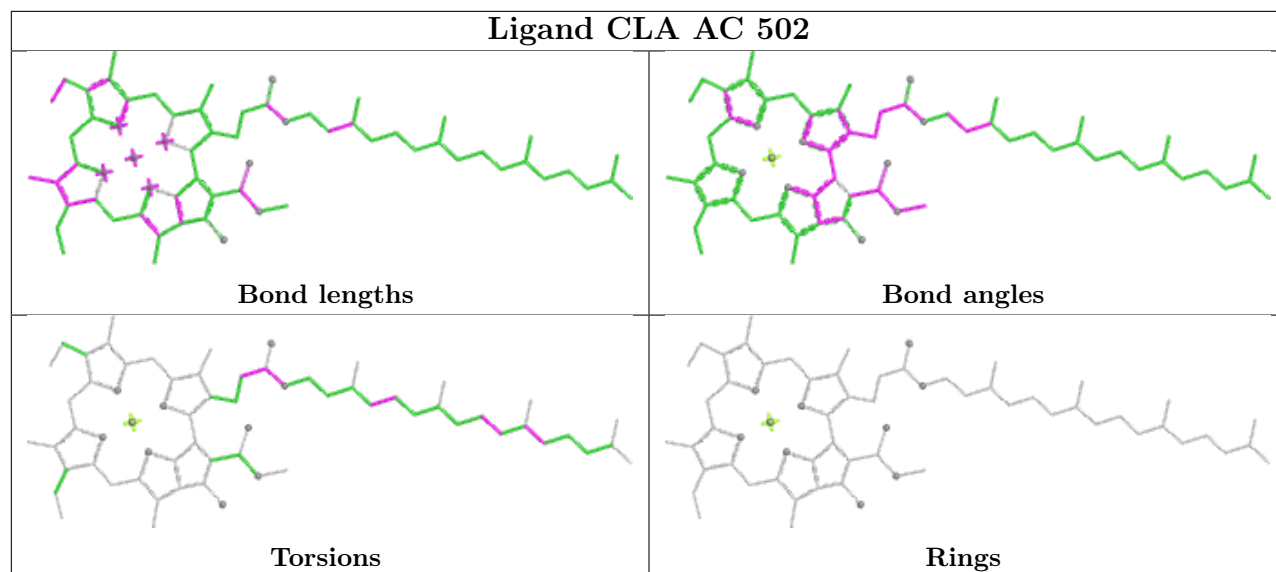
Ligand BCR BJ 5101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR BC 5515	
	
Bond lengths	Bond angles
	
Torsions	Rings

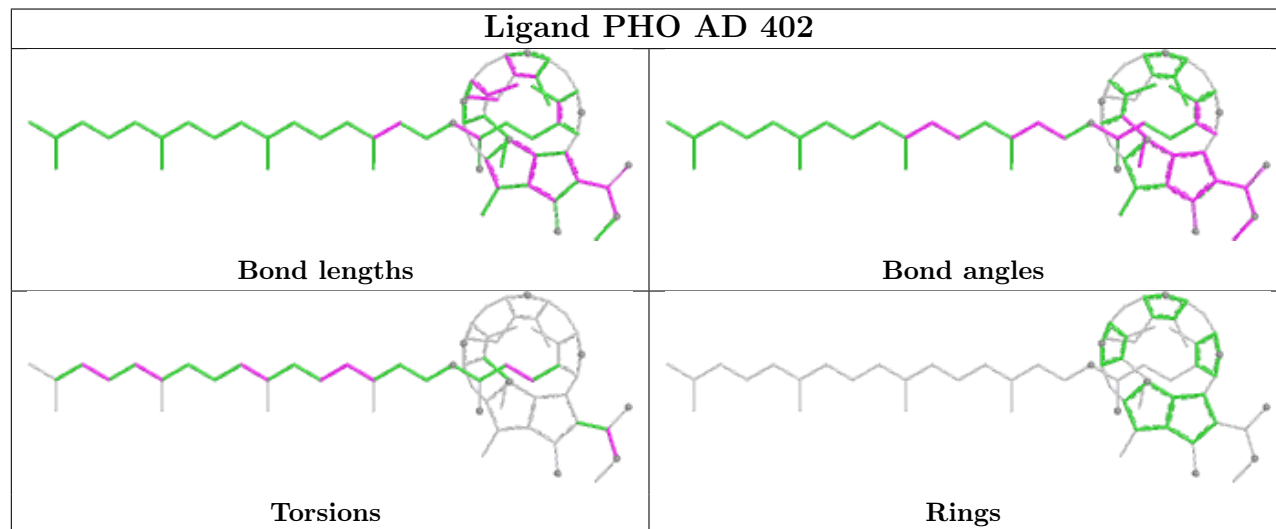
Ligand CLA BB 5617	
	
Bond lengths	Bond angles
	
Torsions	Rings



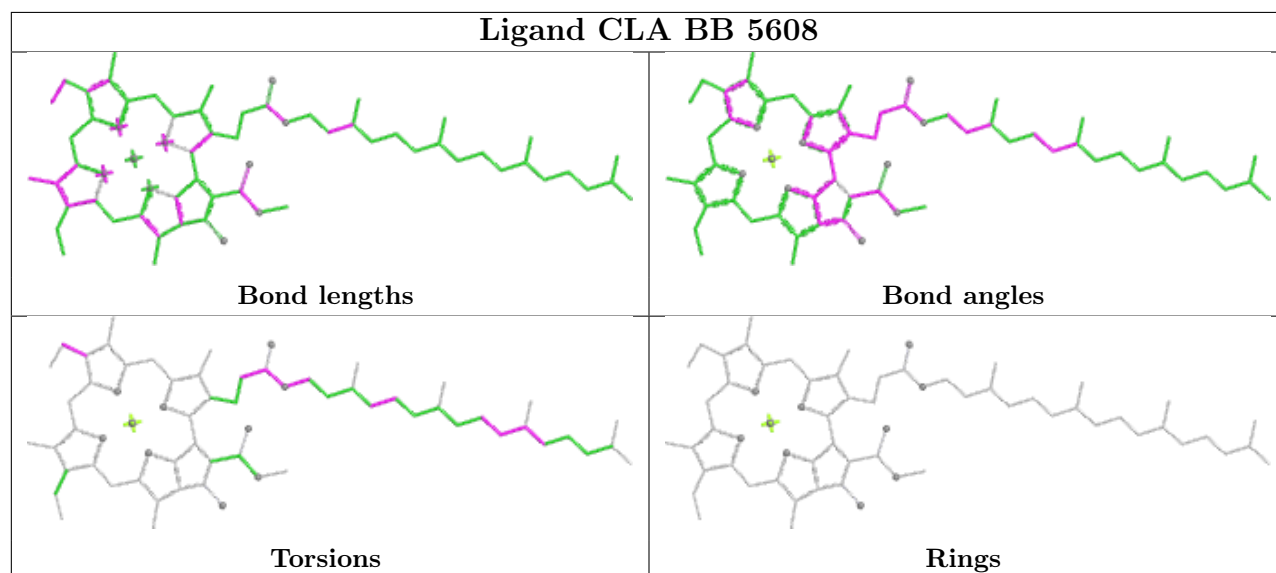
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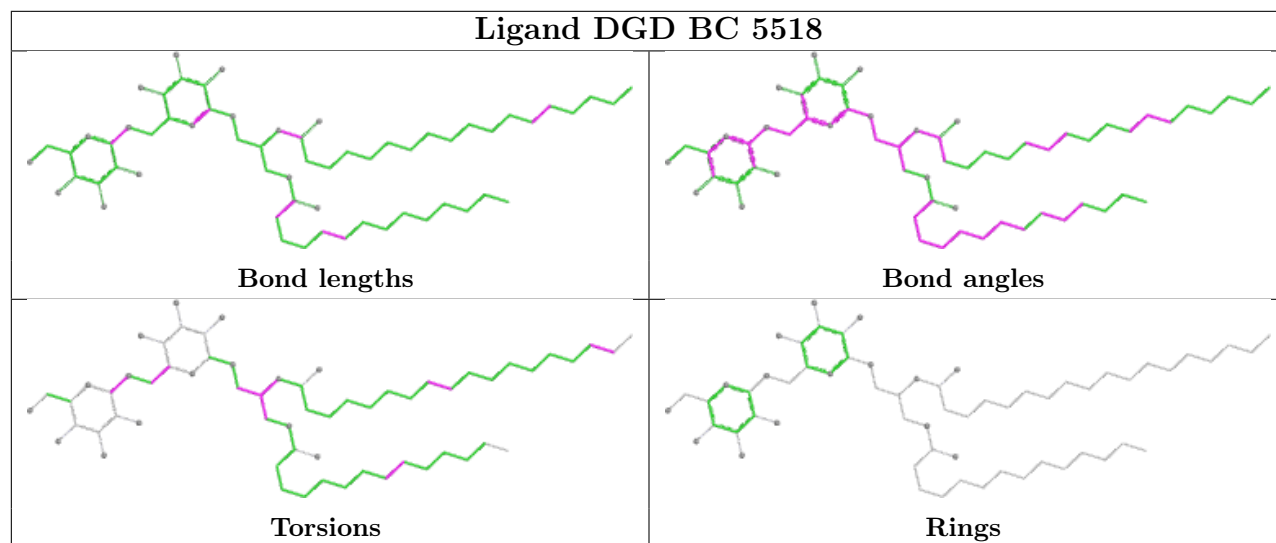
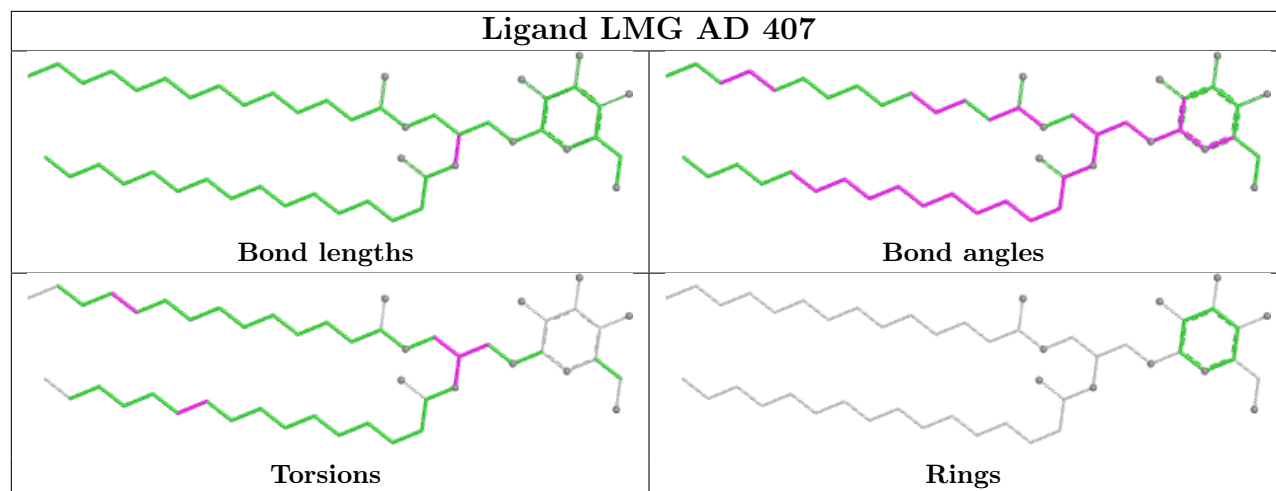


Ligand PHO AD 402

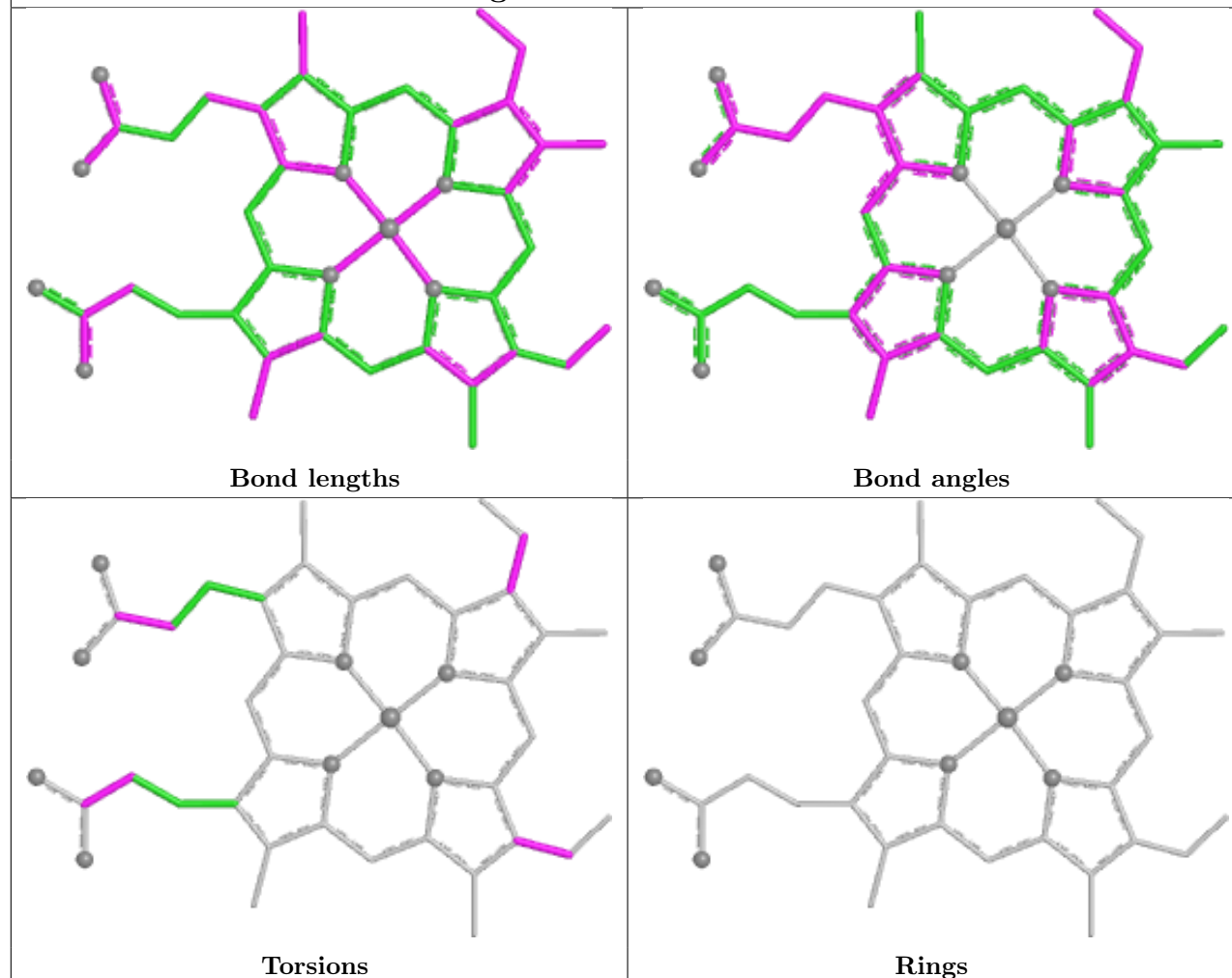


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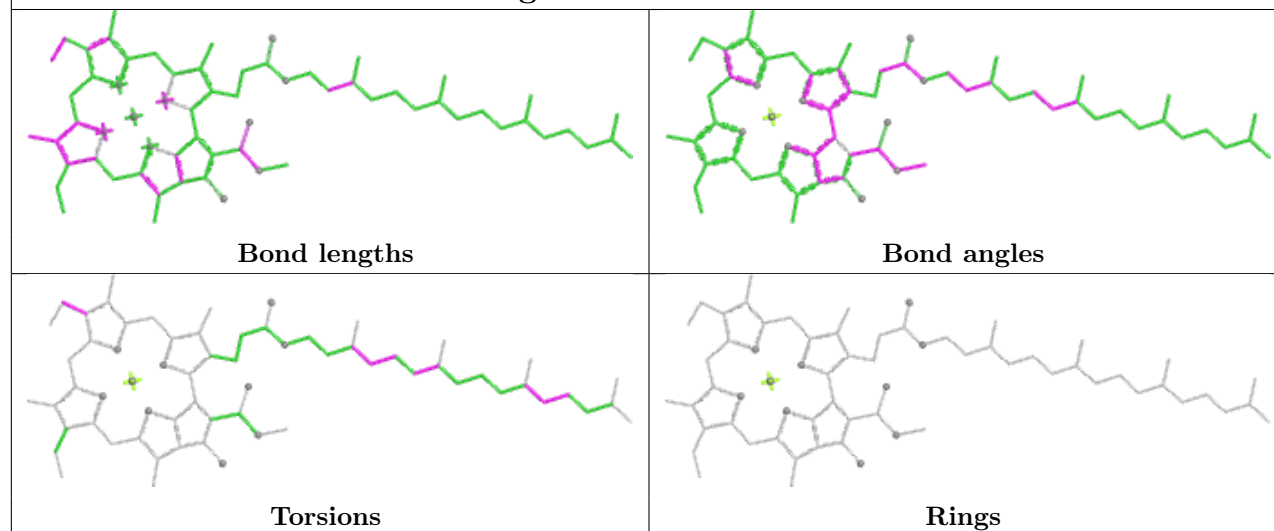




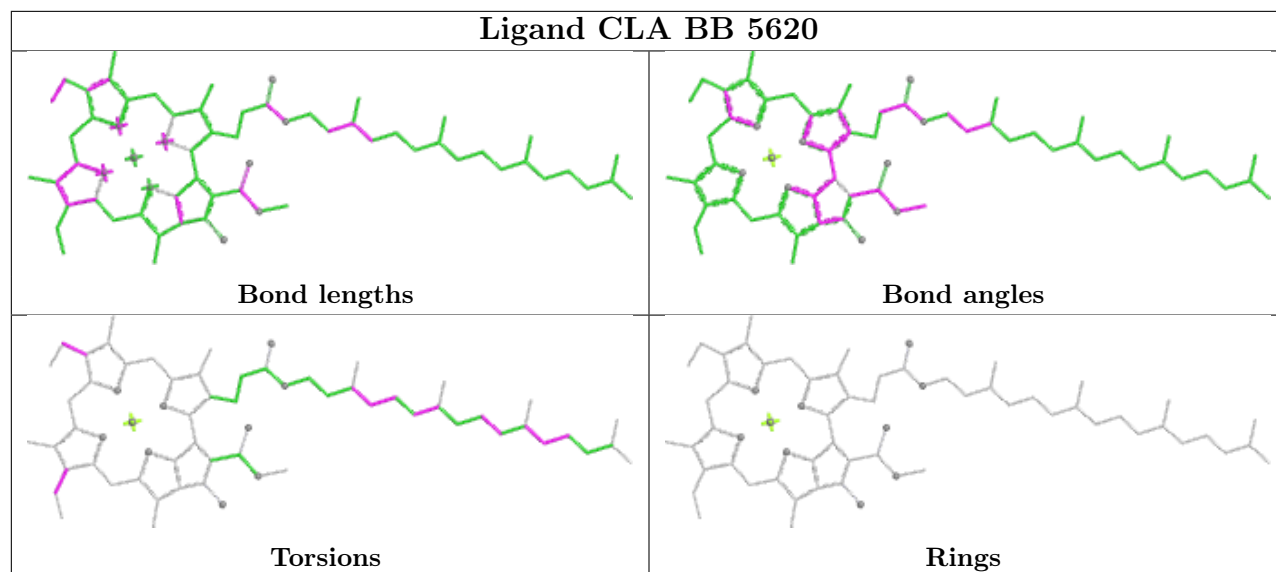
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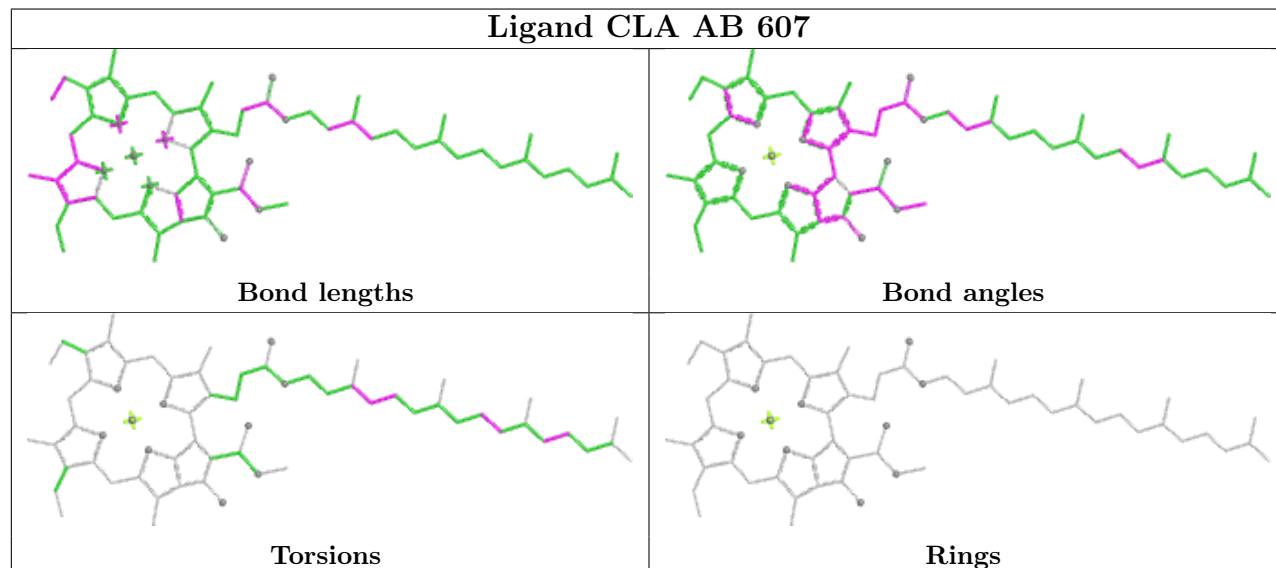
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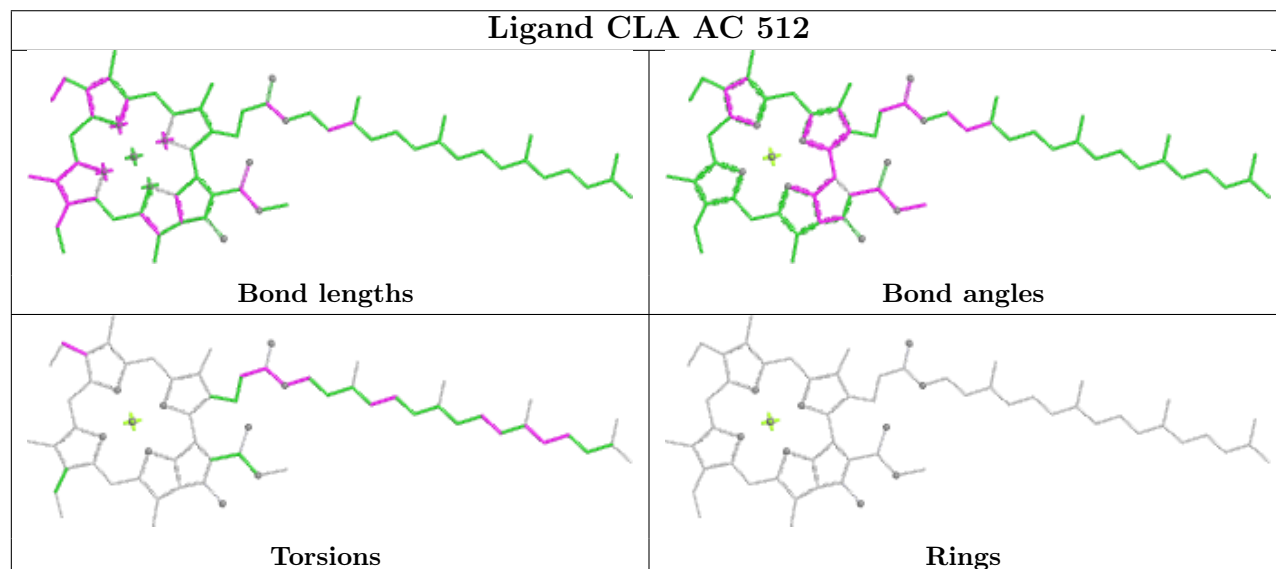
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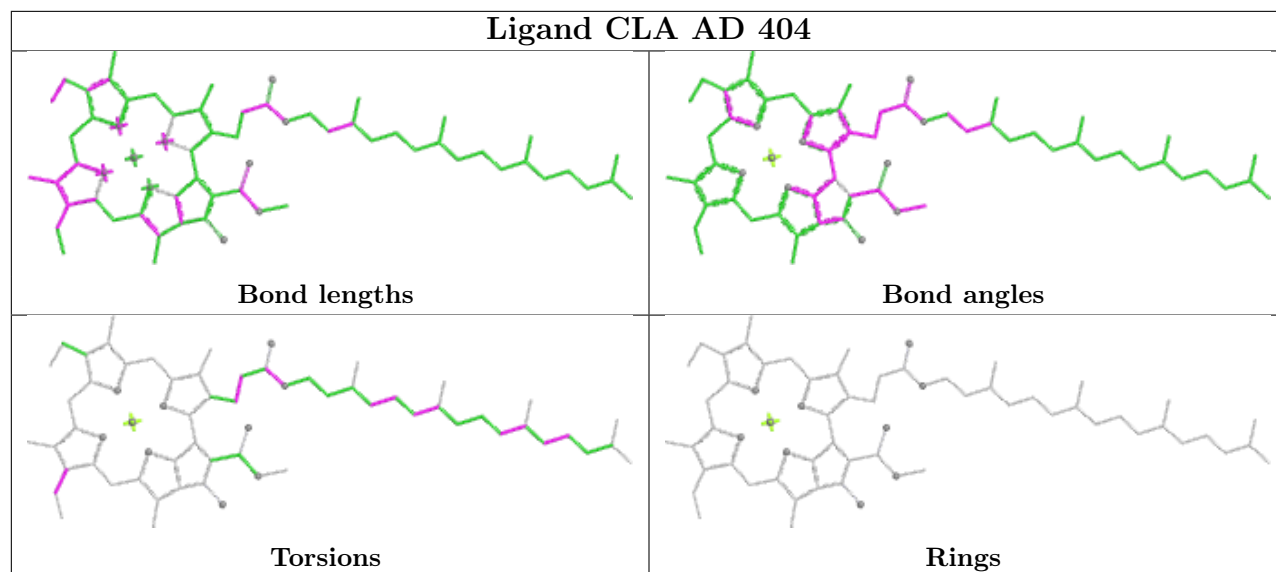
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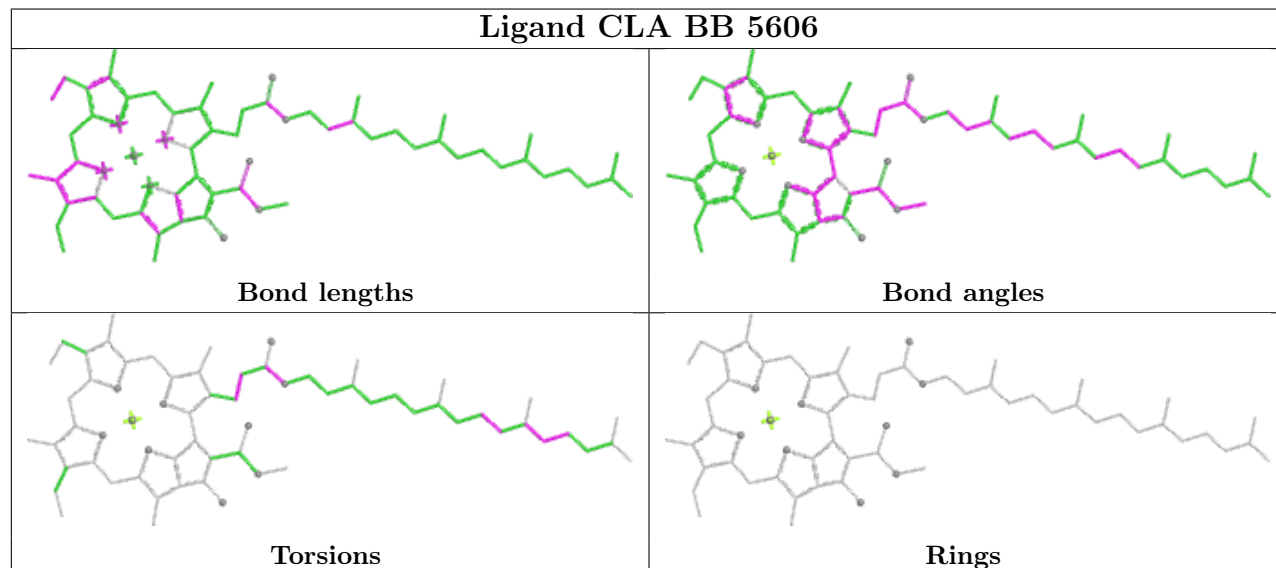
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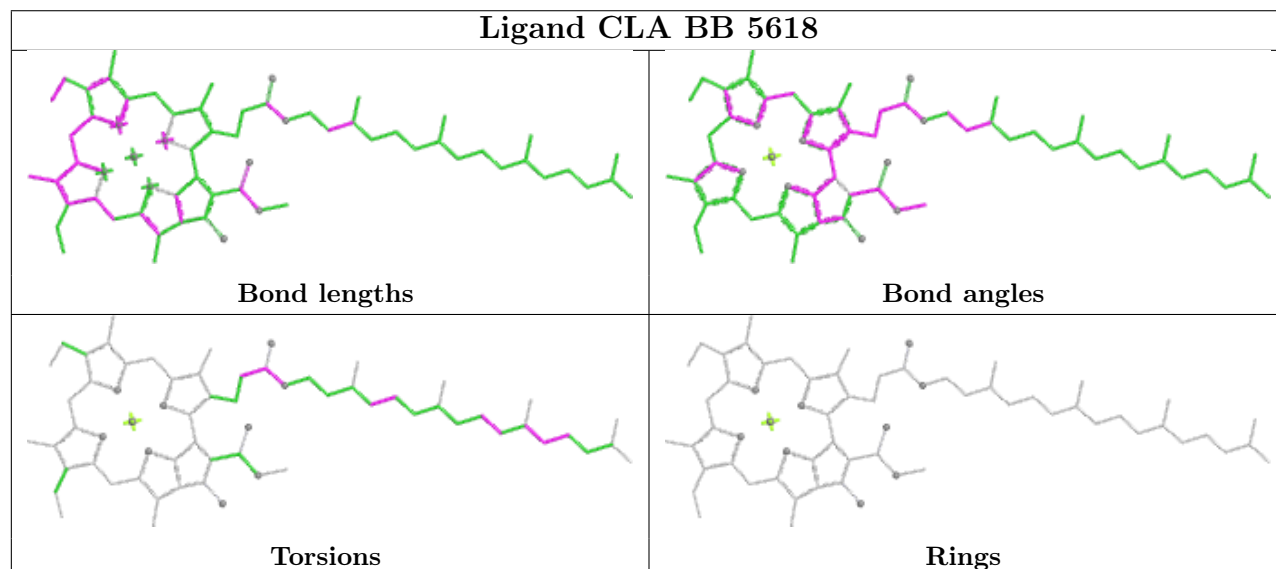
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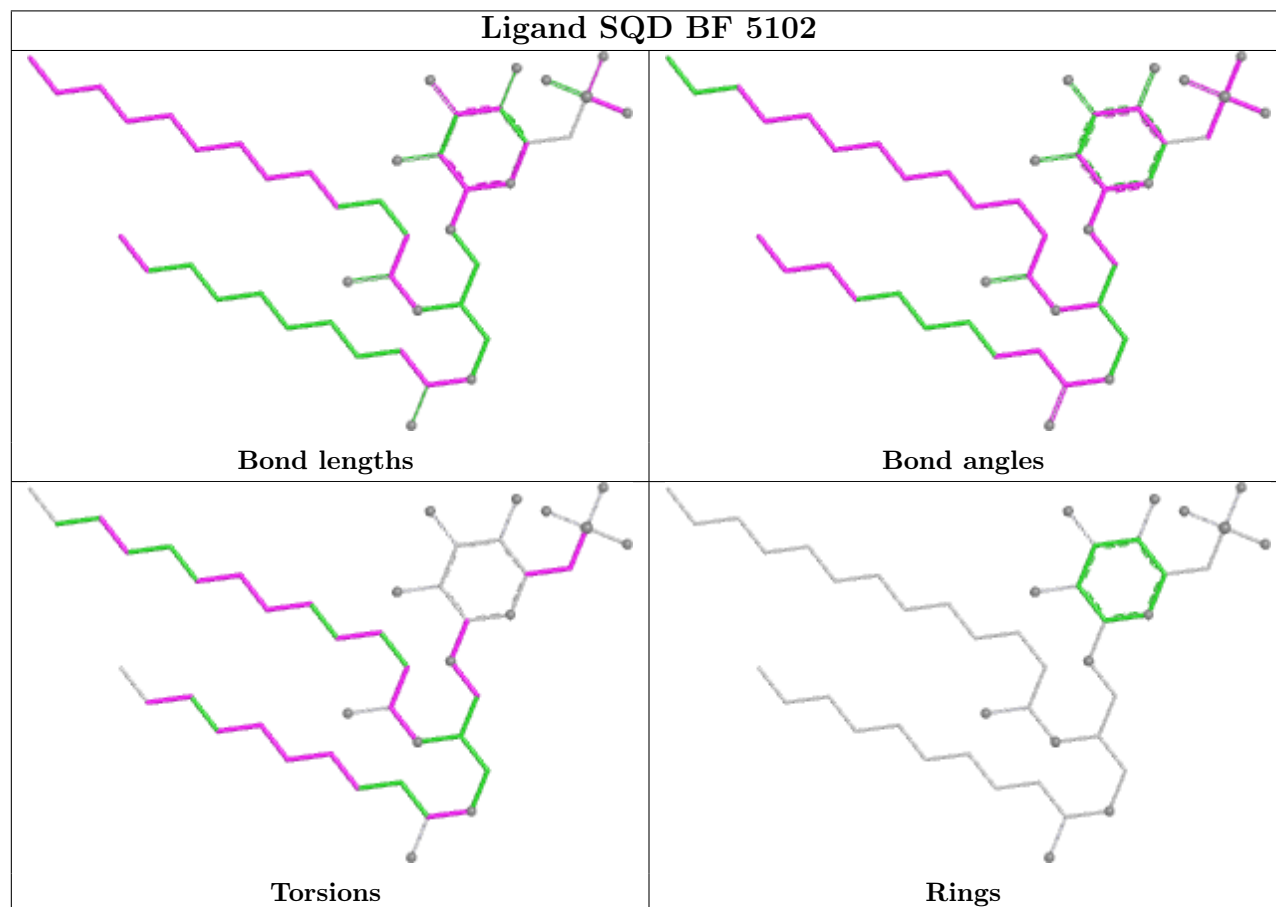
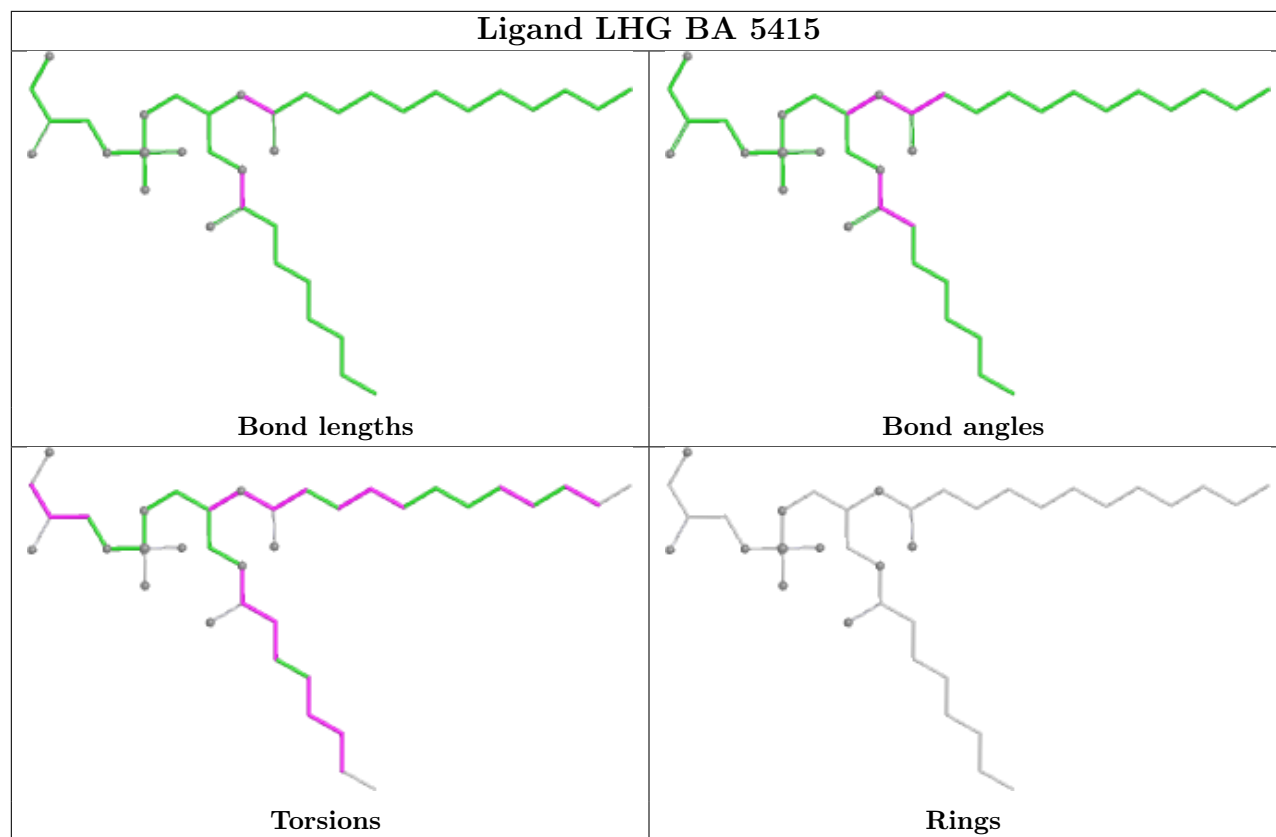


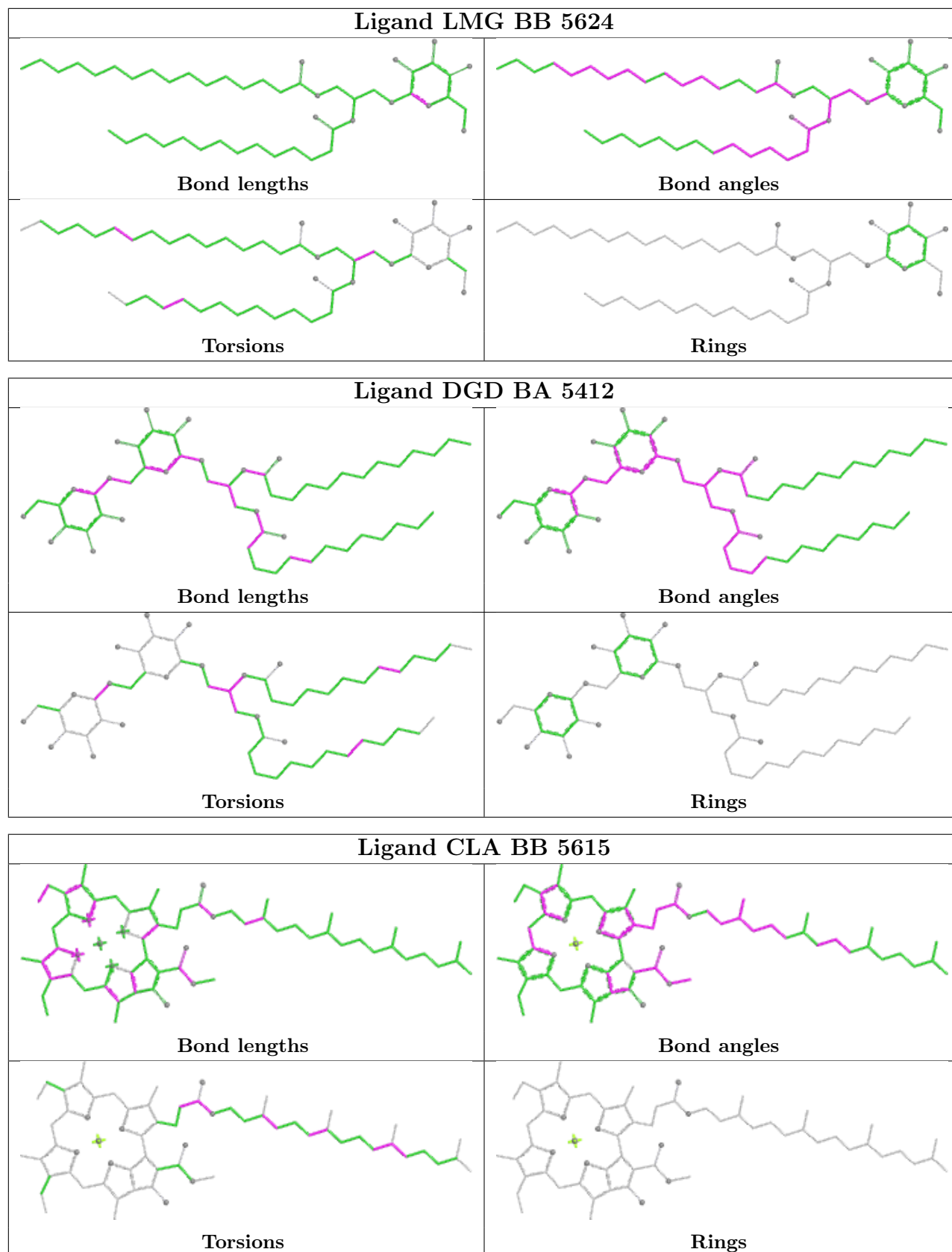
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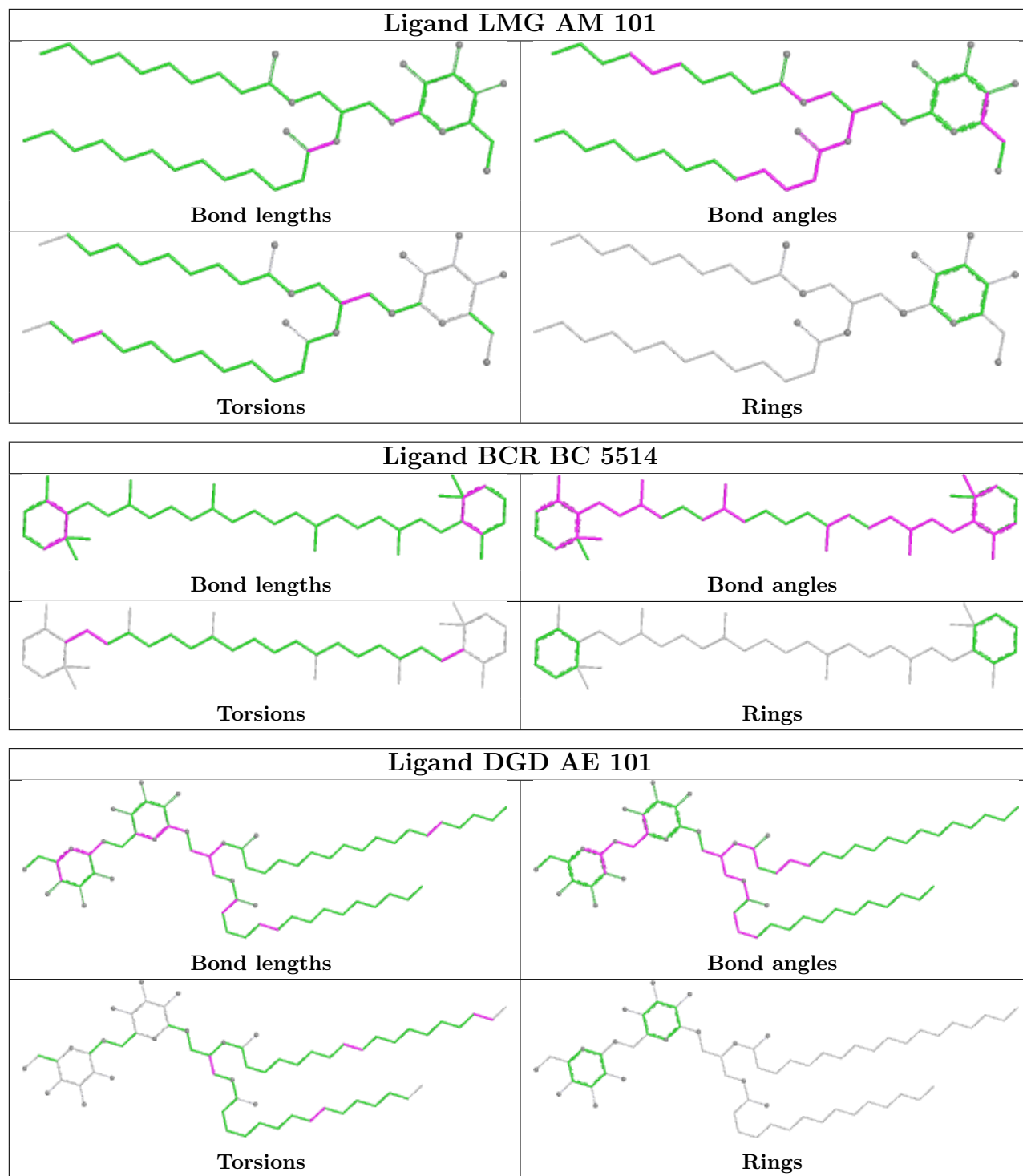


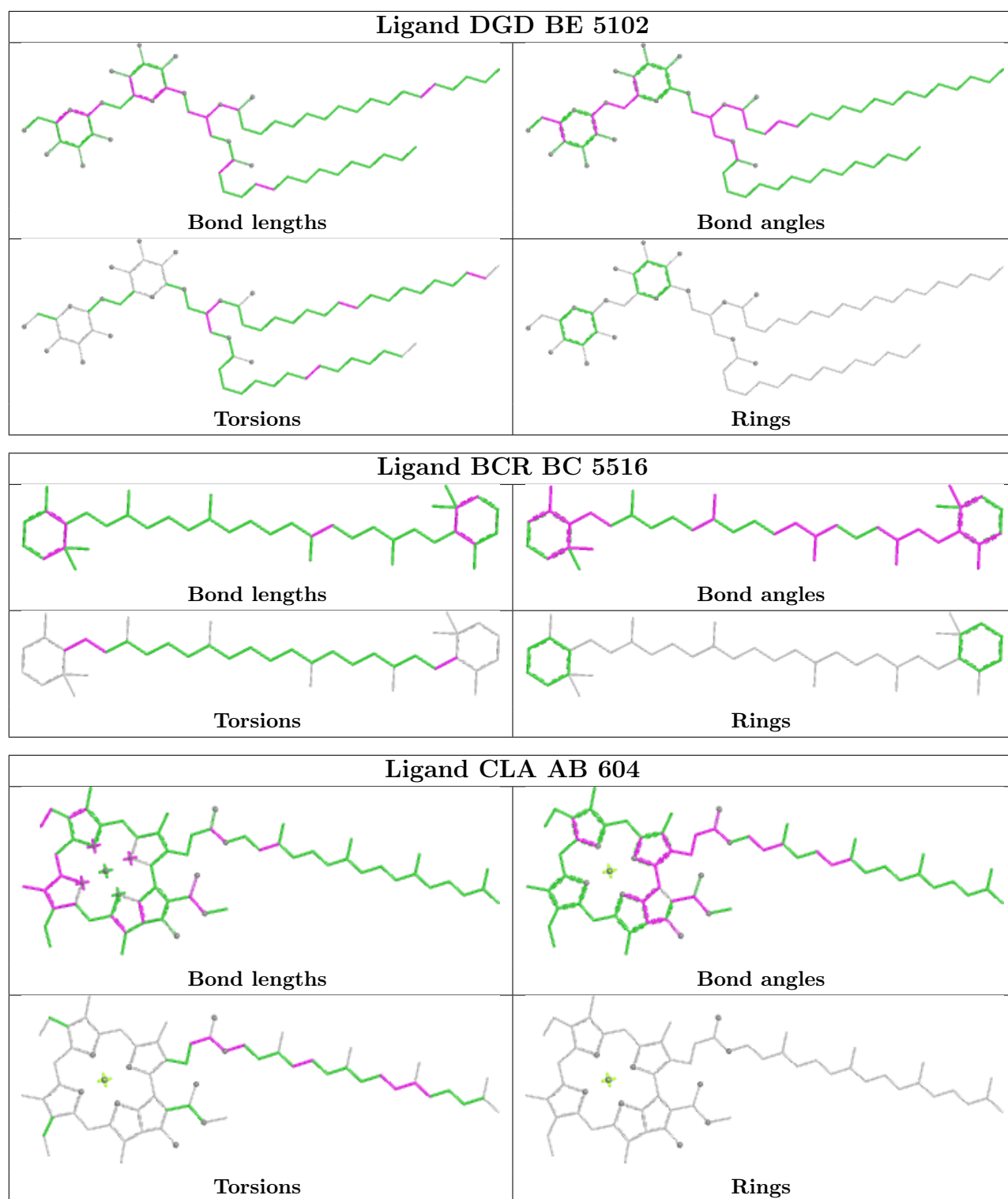
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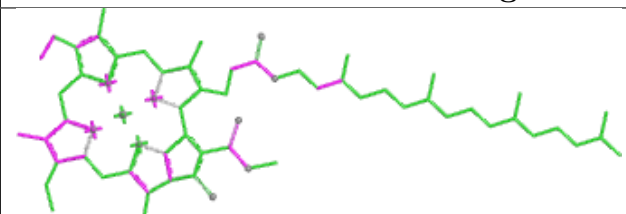
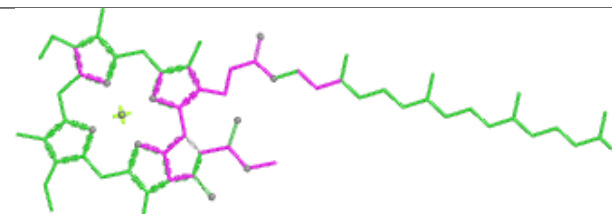
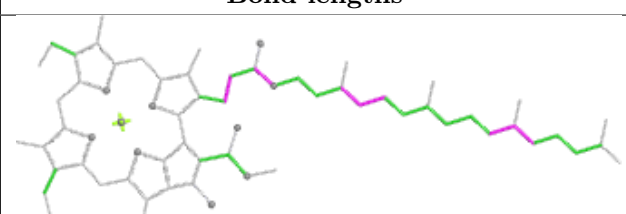
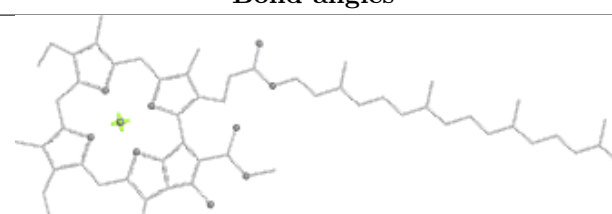


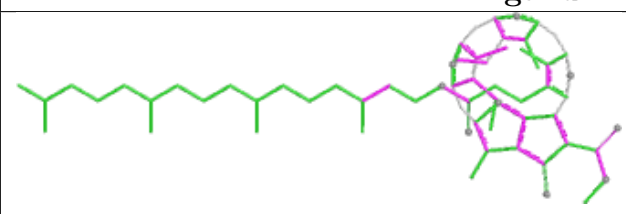
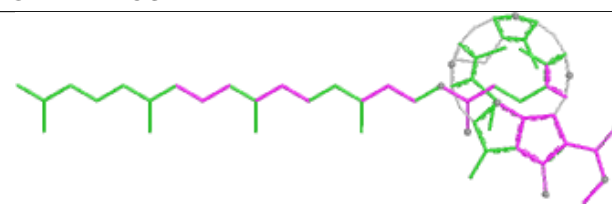
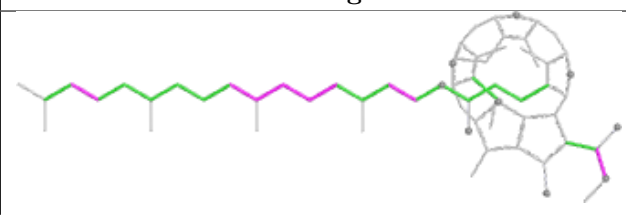
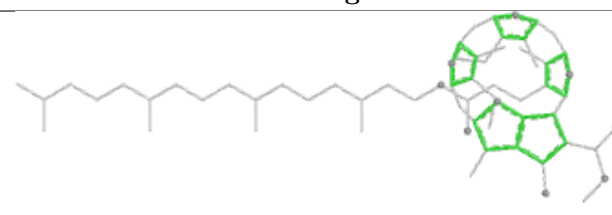


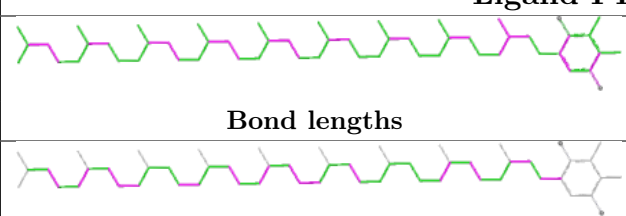
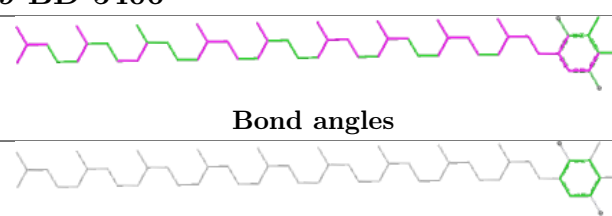




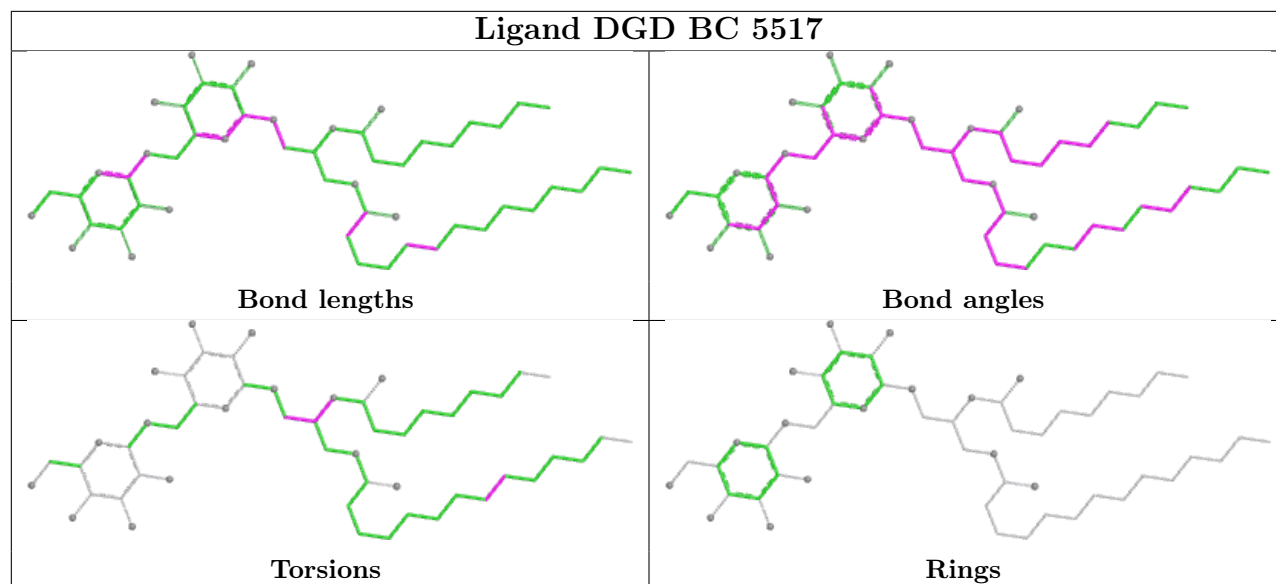


Ligand CLA BB 5610	
	
Bond lengths	Bond angles
	
Torsions	Rings

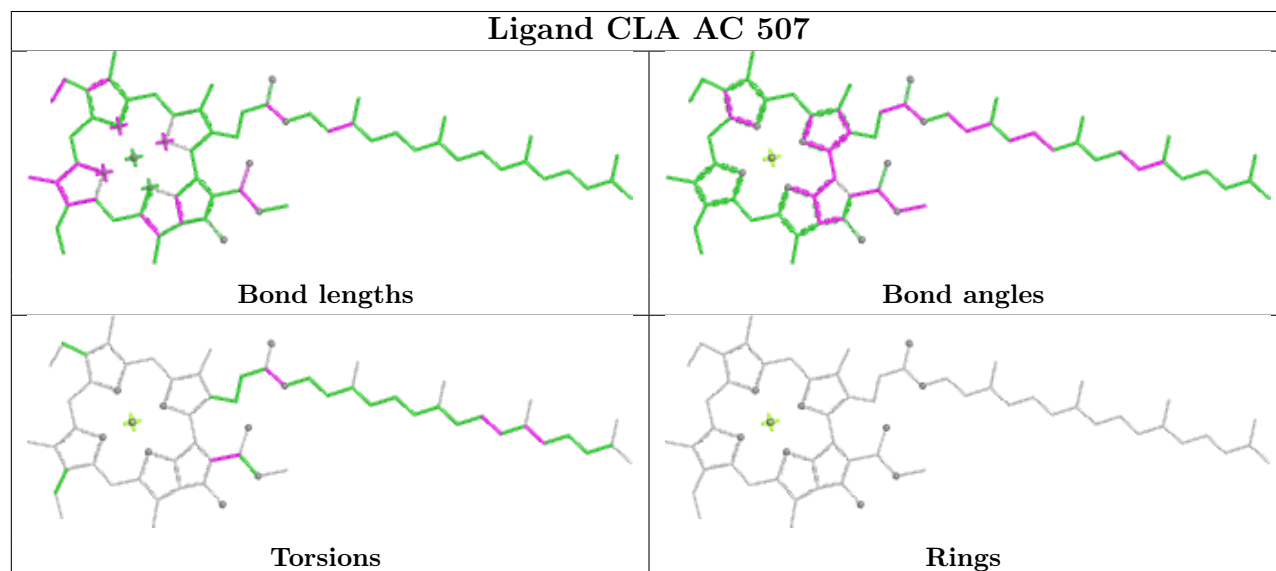
Ligand PHO AD 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 BD 5406	
	
Bond lengths	Bond angles
	
Torsions	Rings

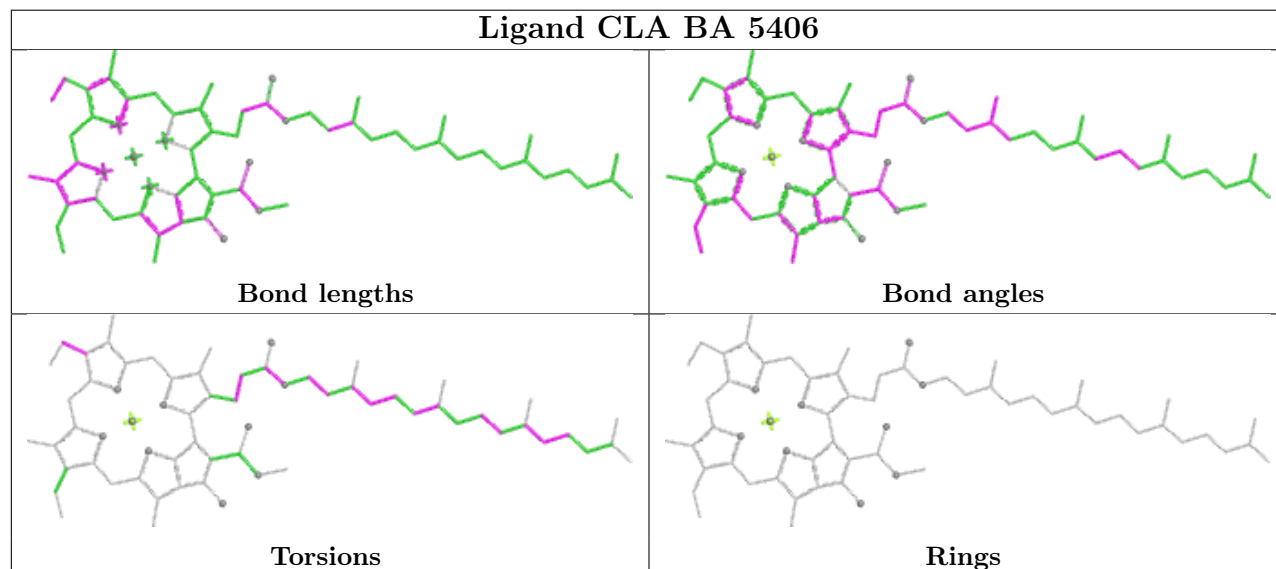
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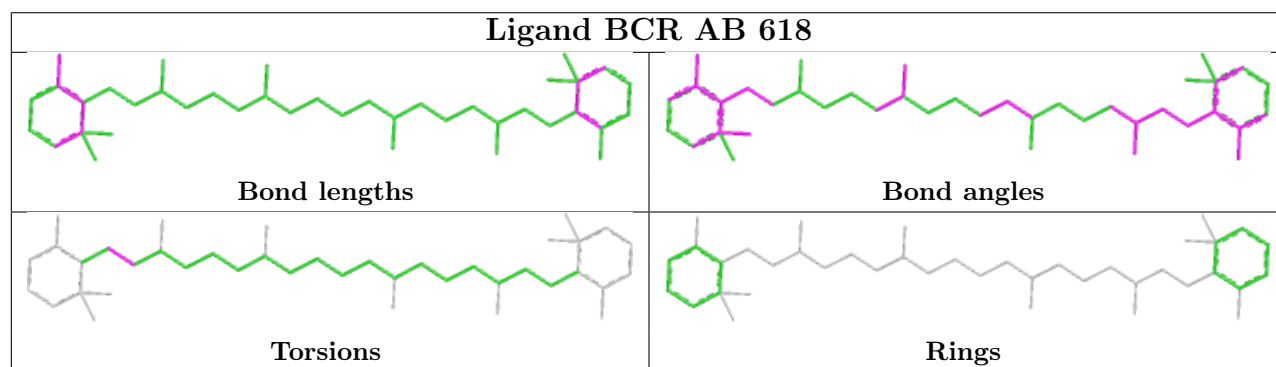
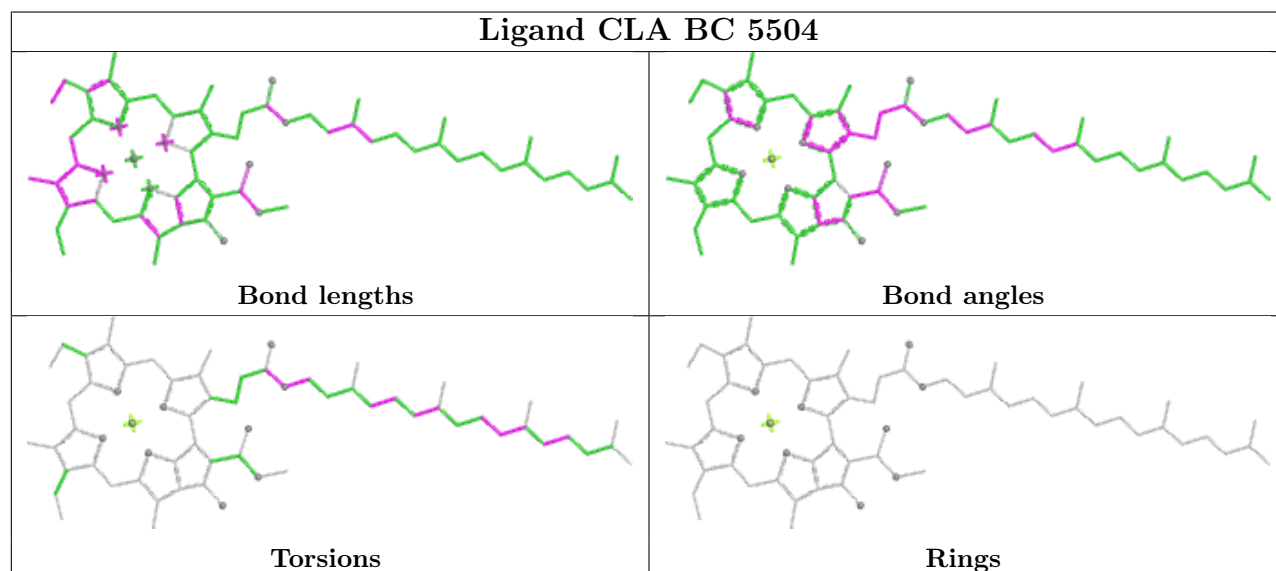
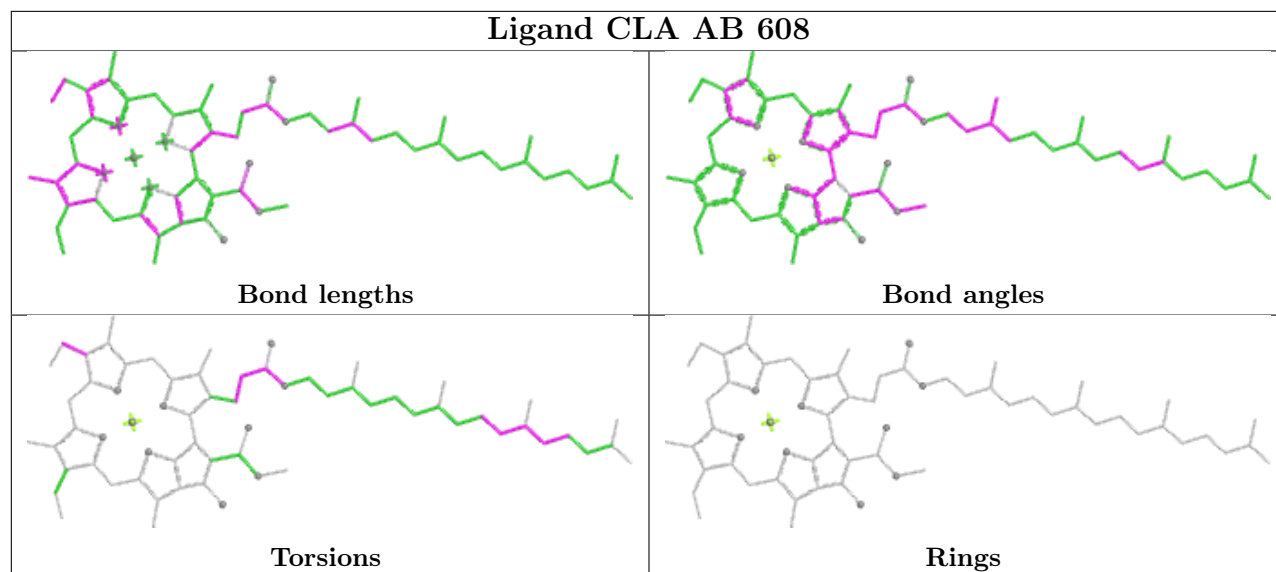


Ligand CLA AC 507

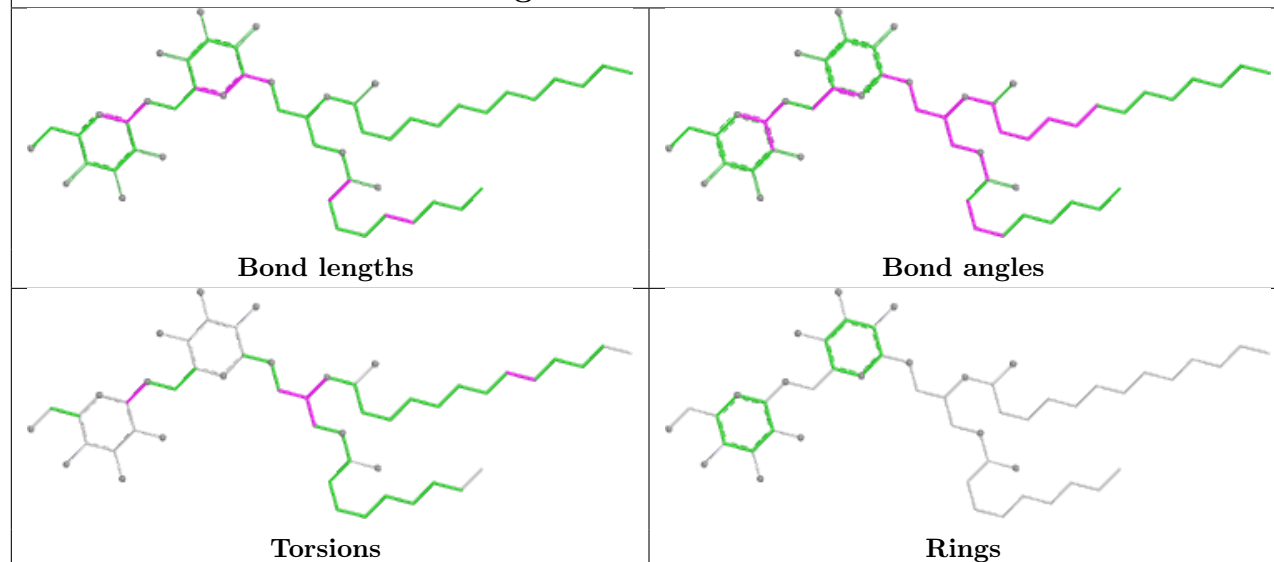


Ligand CLA BA 5406

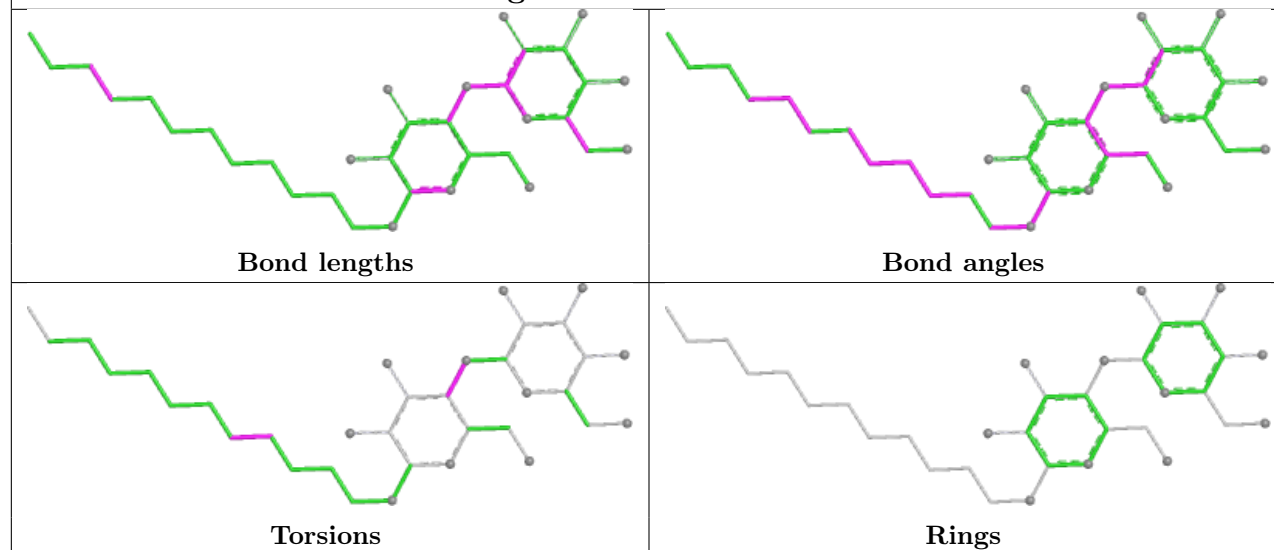


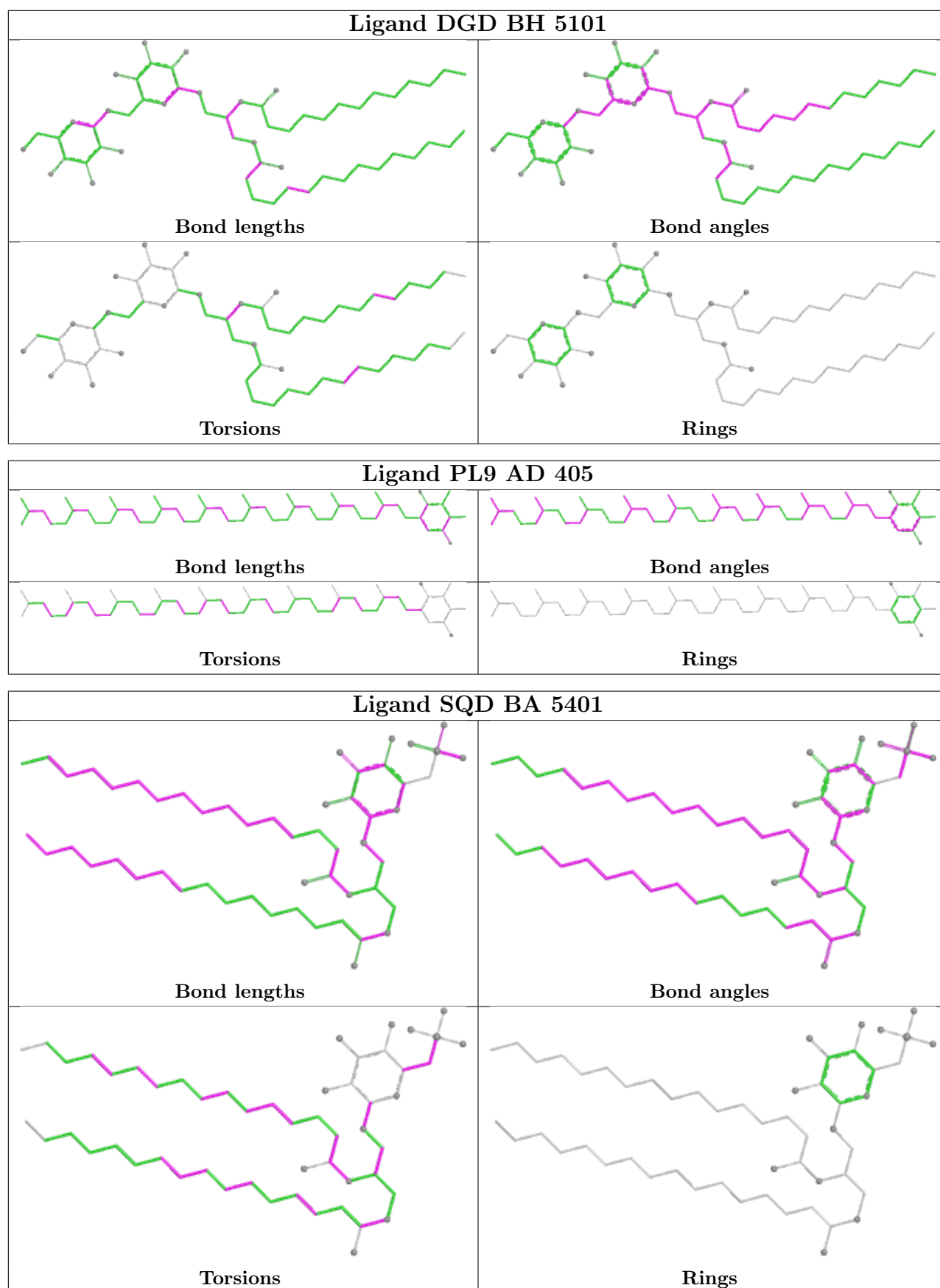


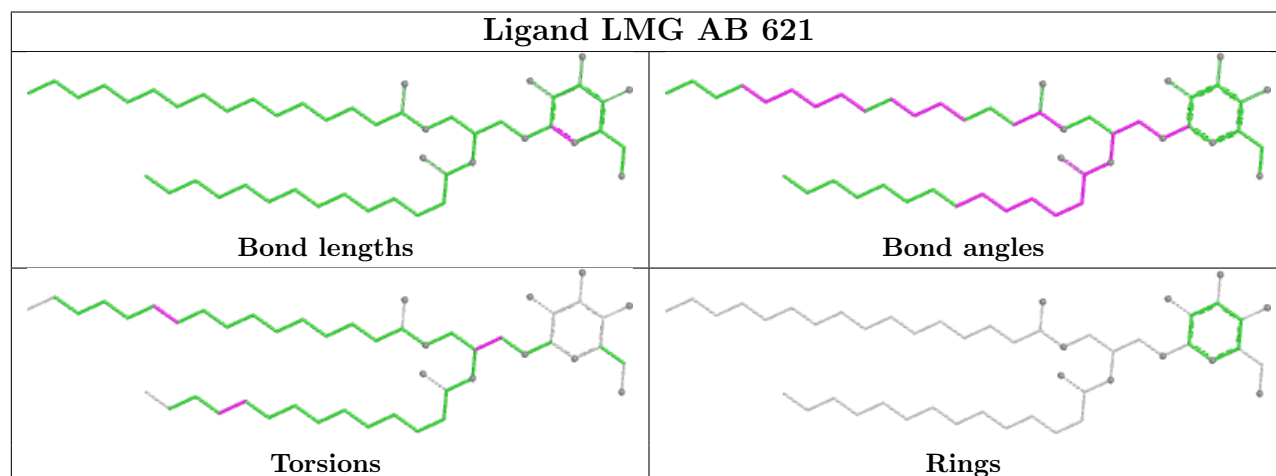
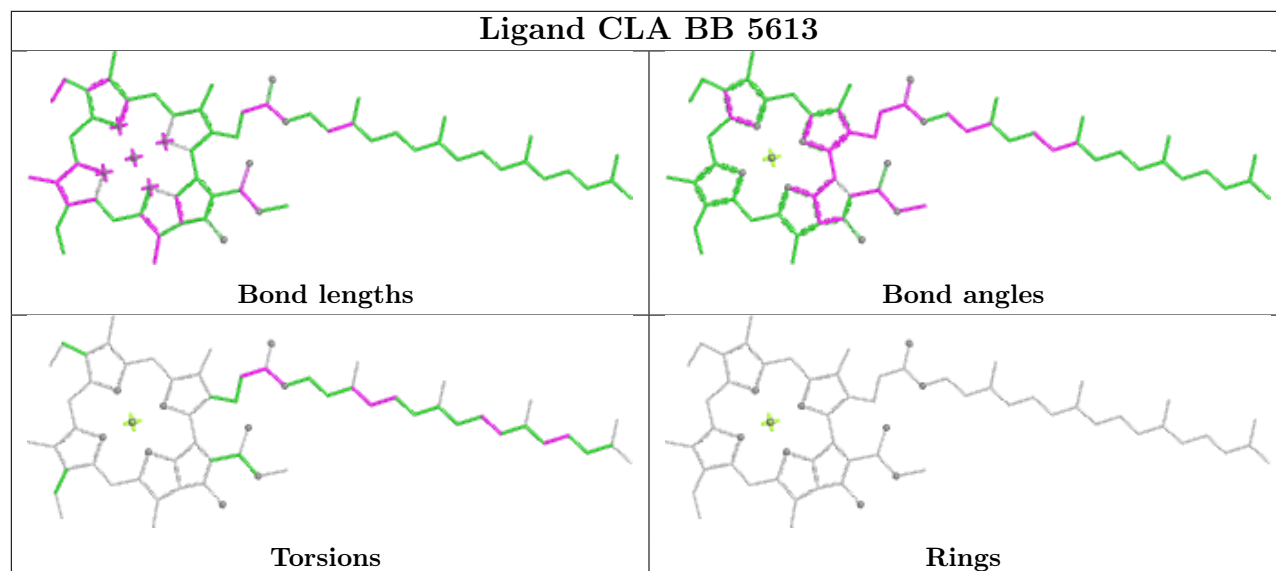
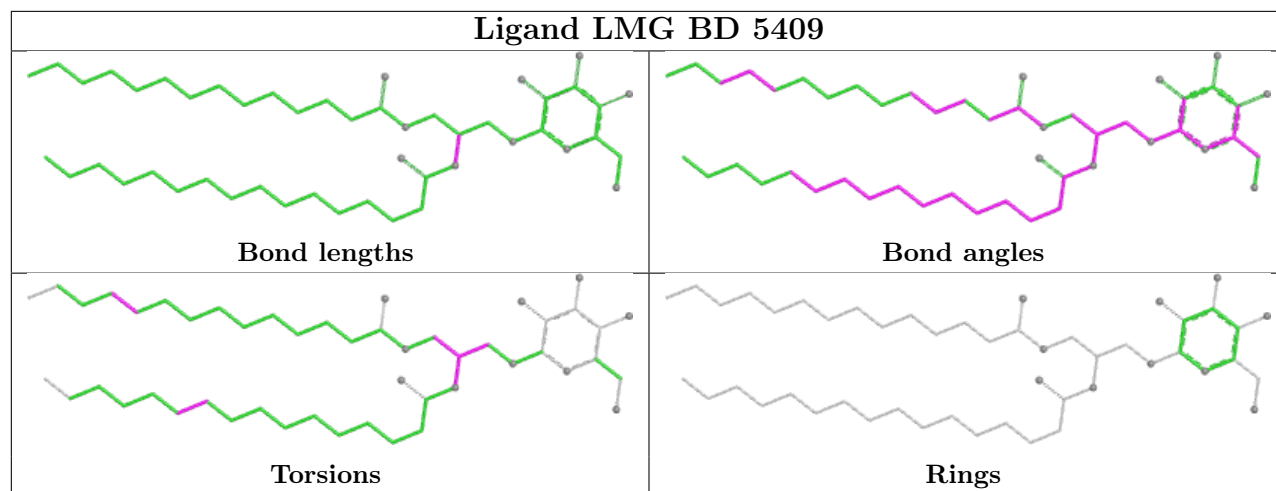
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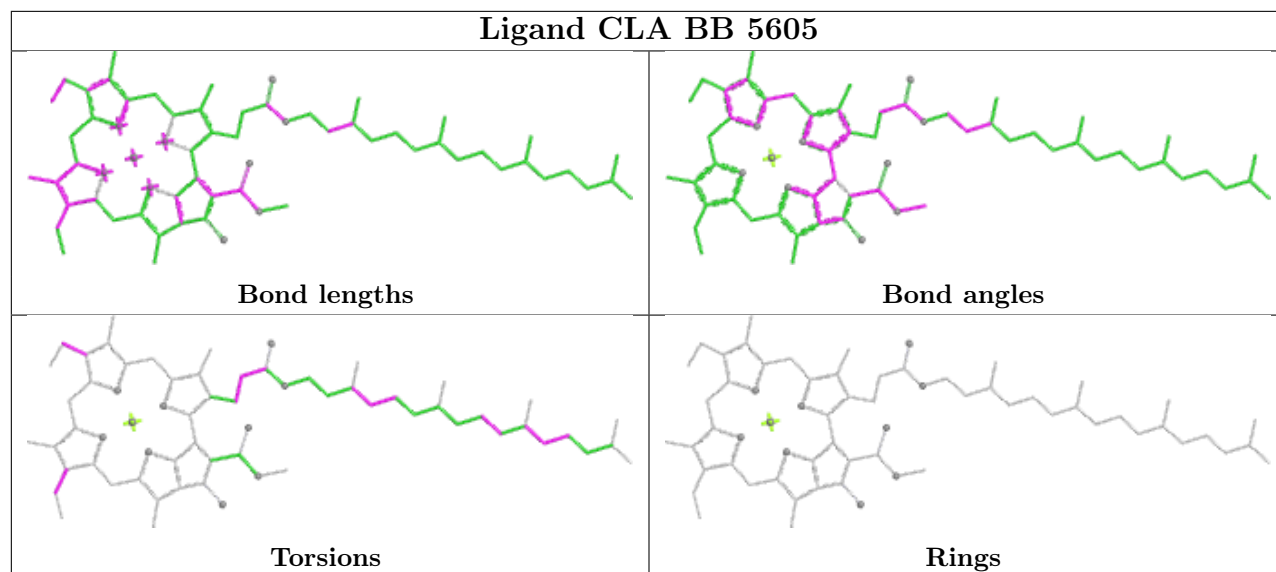
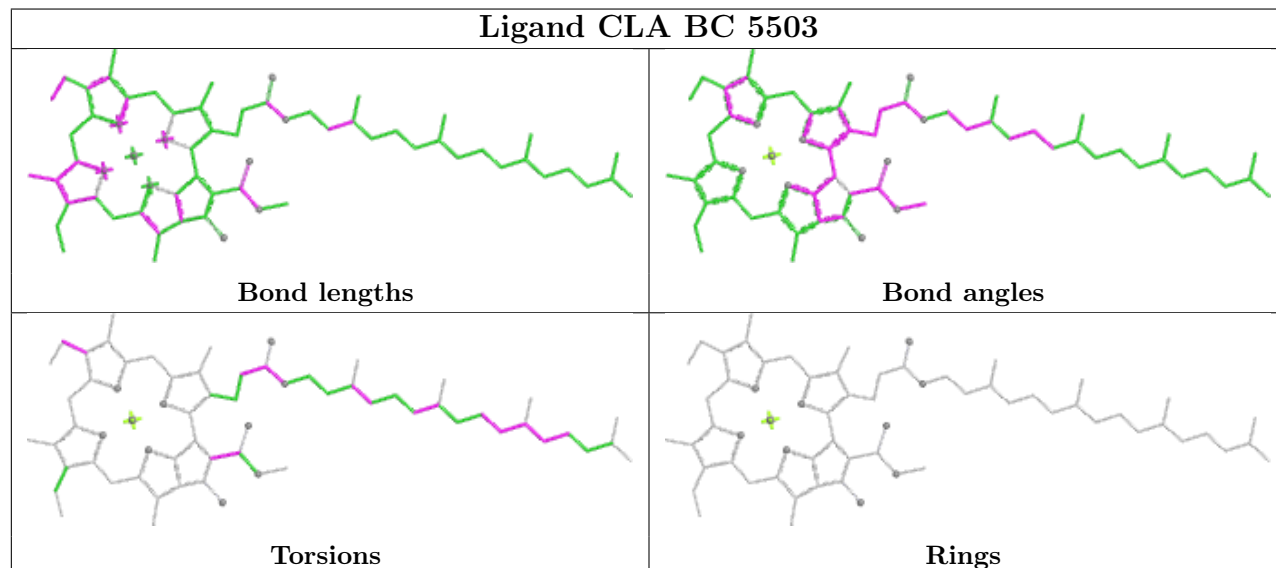


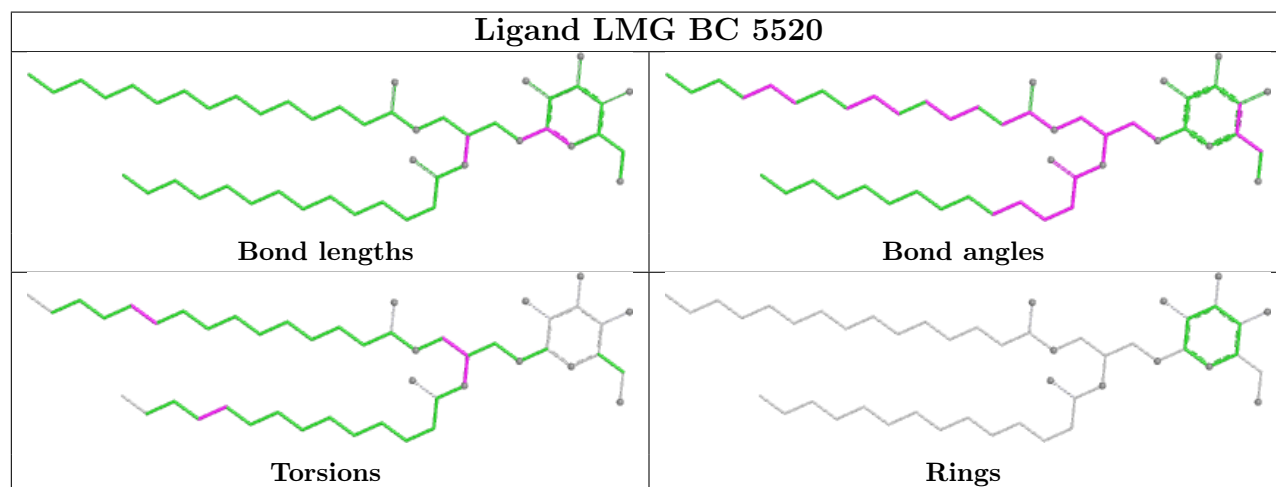
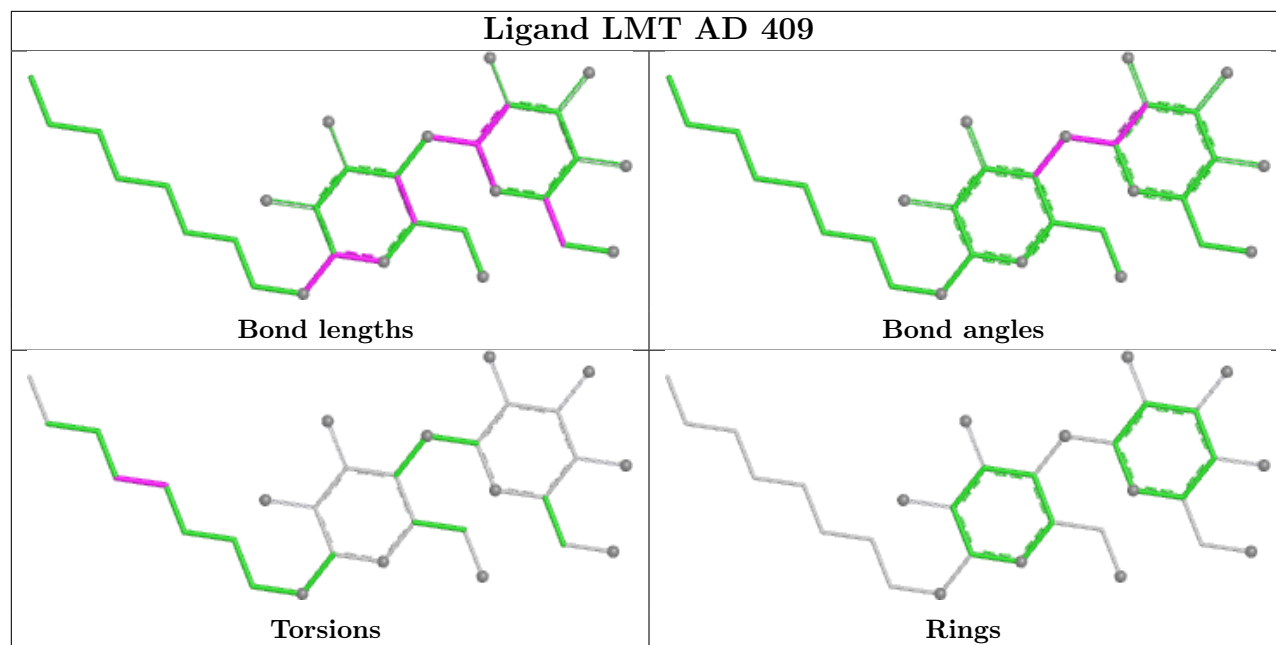
Ligand LMT BB 5603

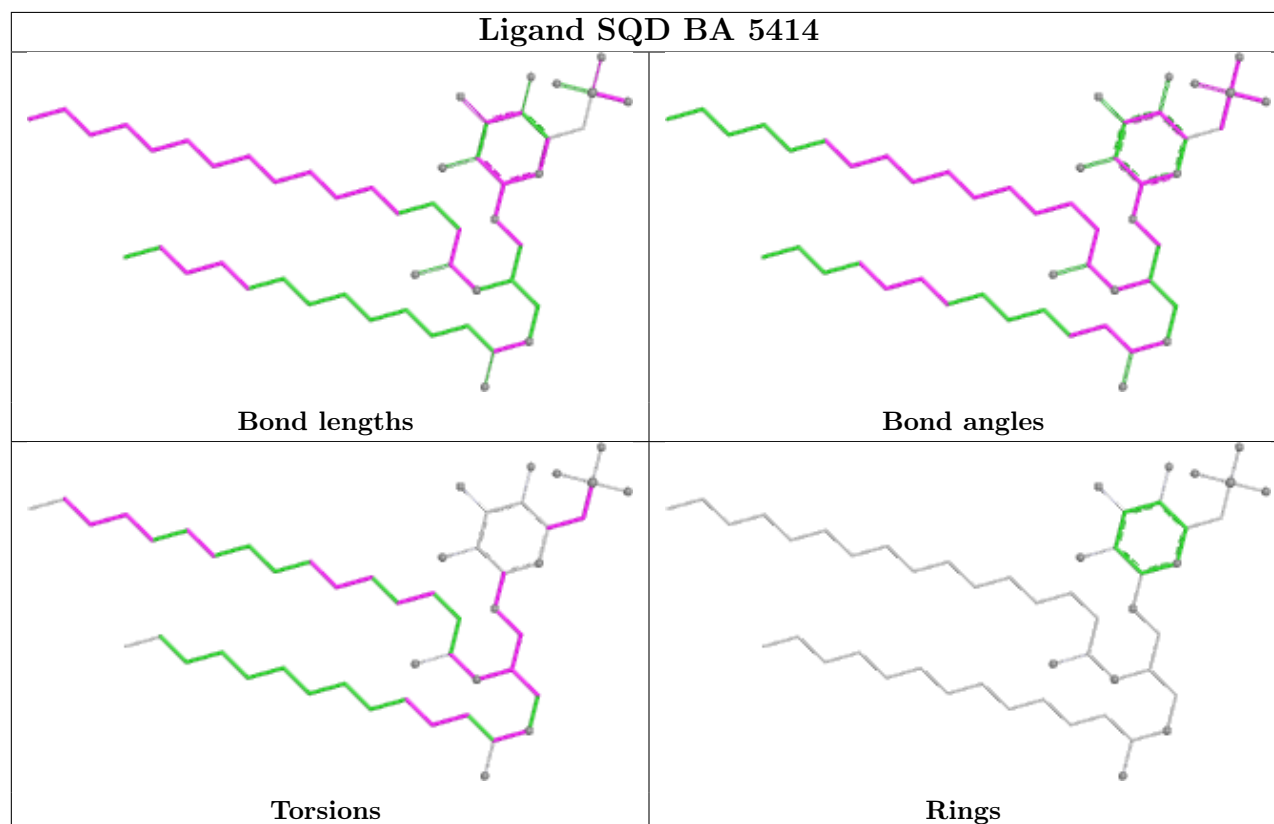
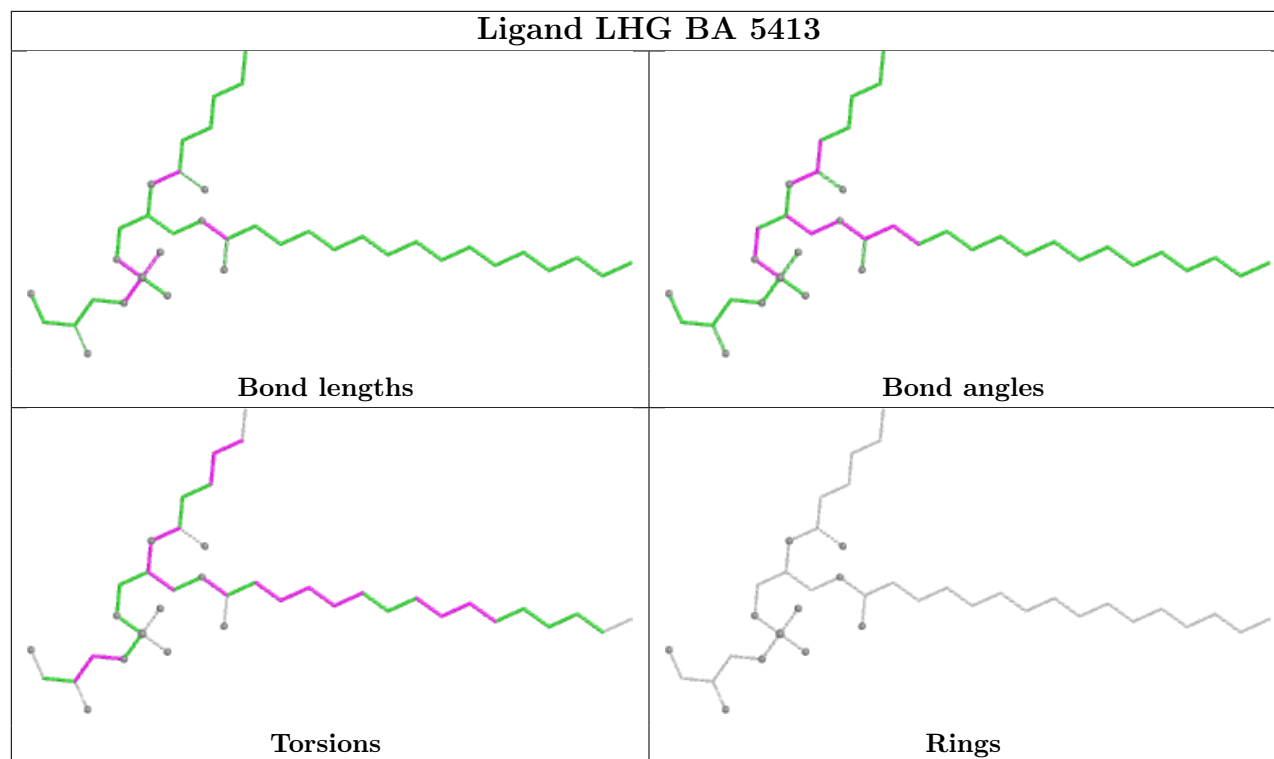


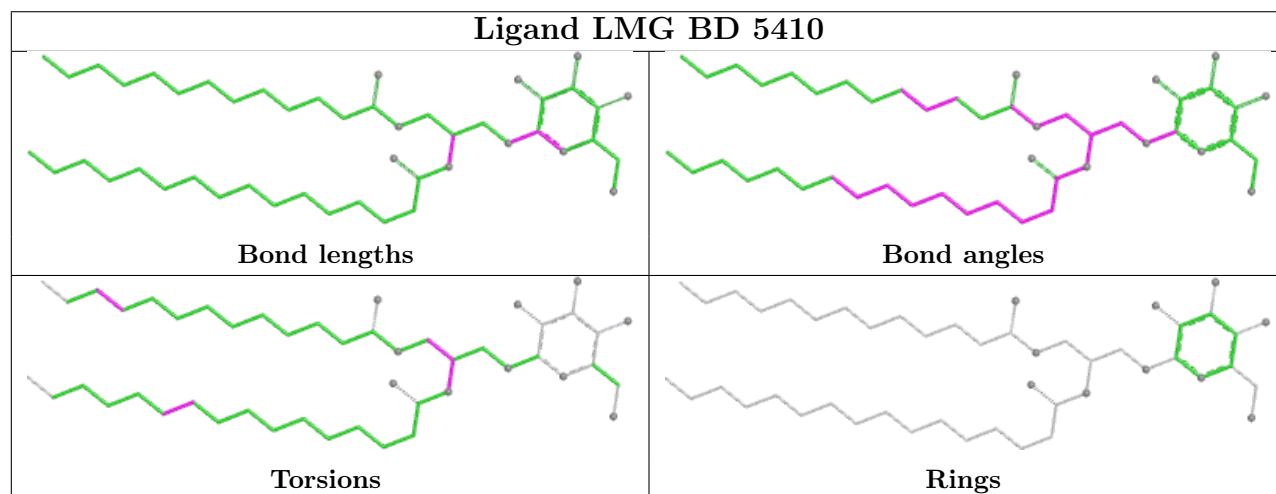
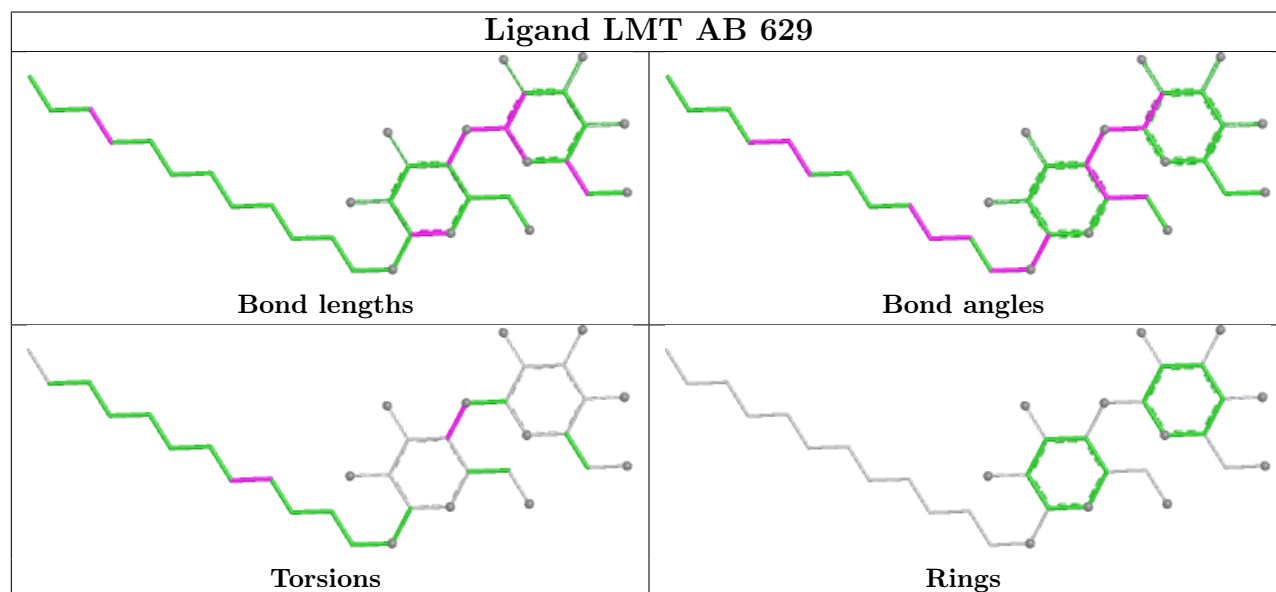
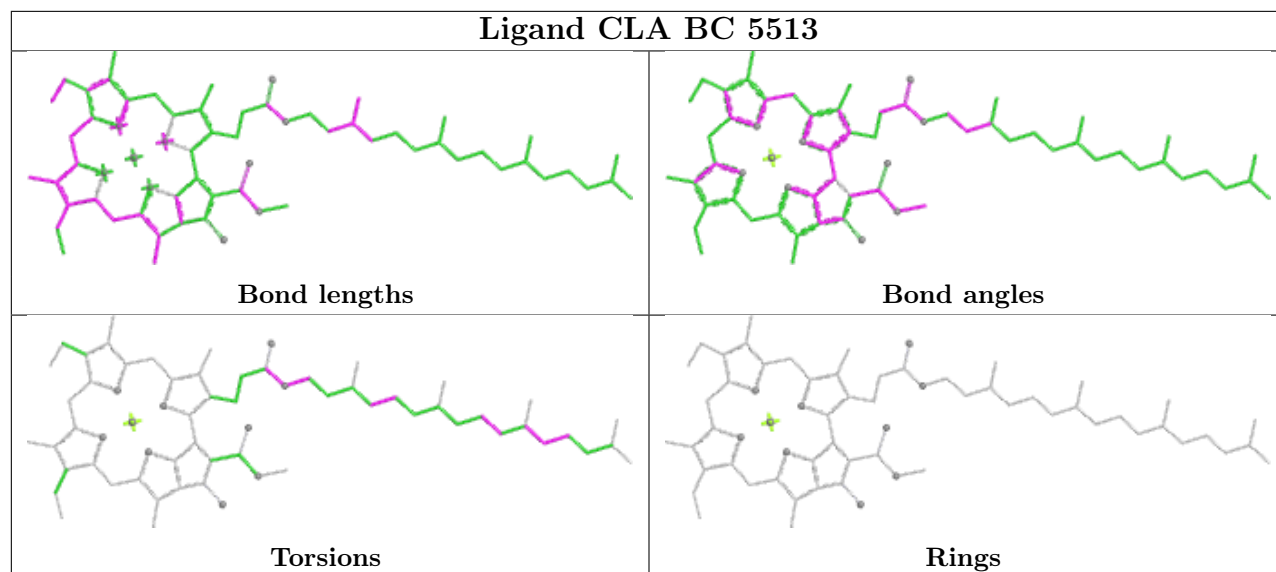




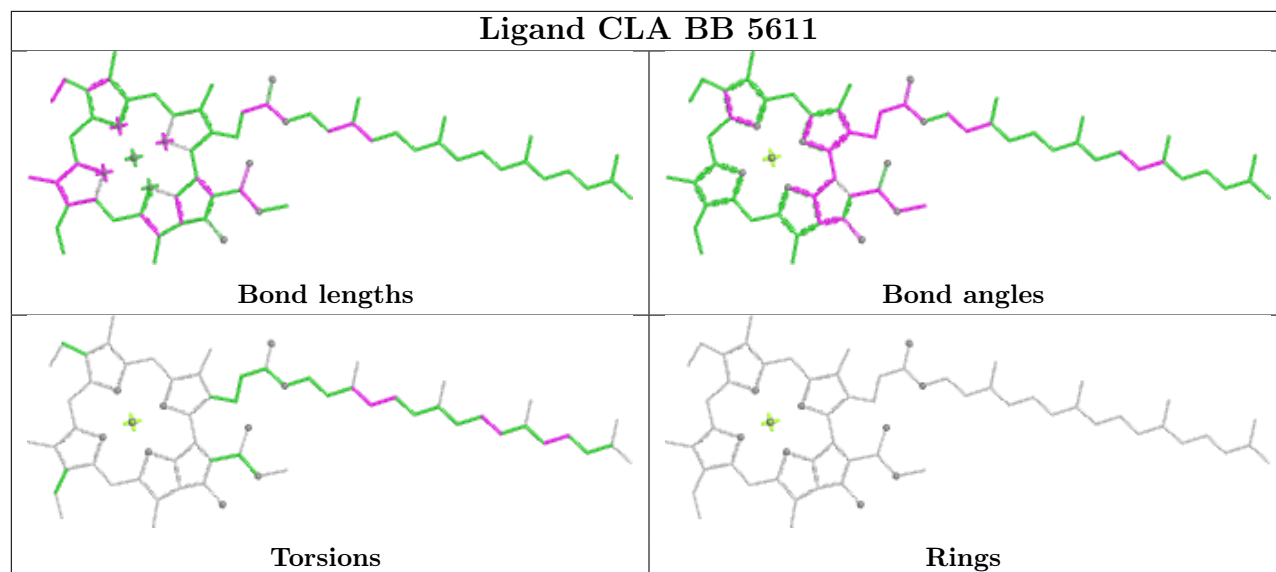
Ligand CLA BB 5605**Ligand CLA BC 5503**



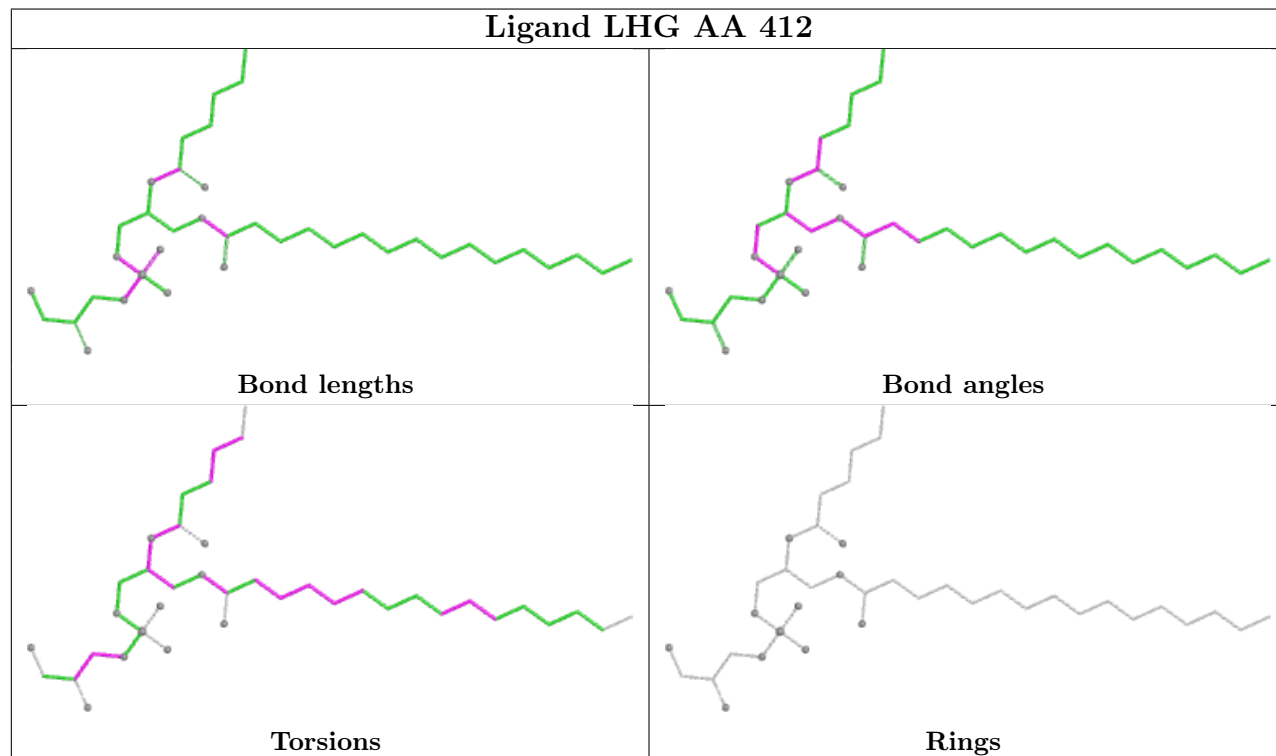


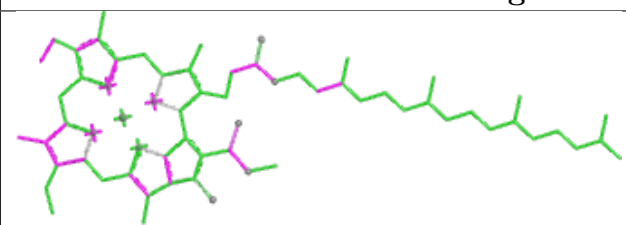
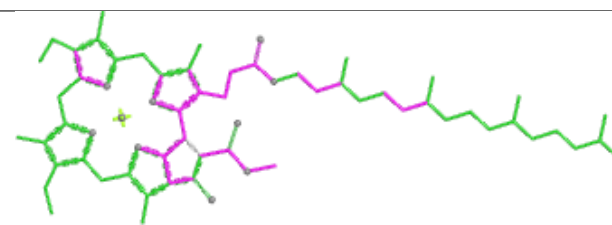
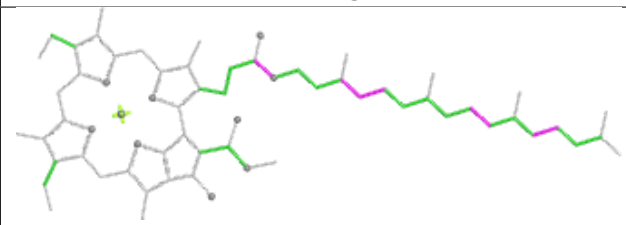
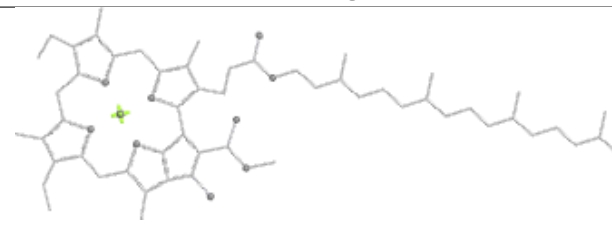


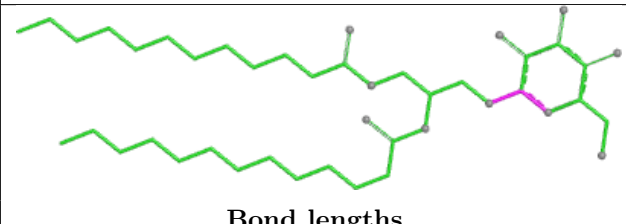
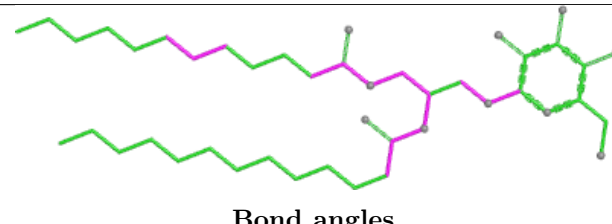
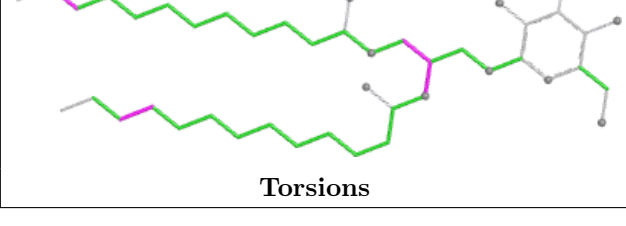
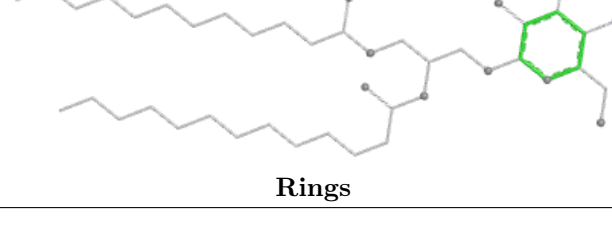
Ligand CLA BB 5611

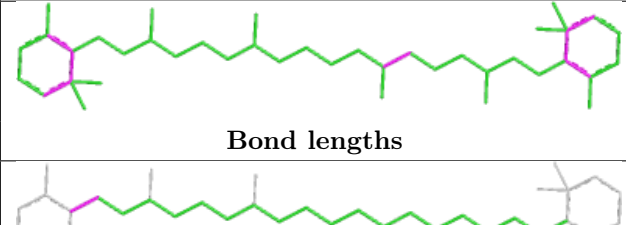
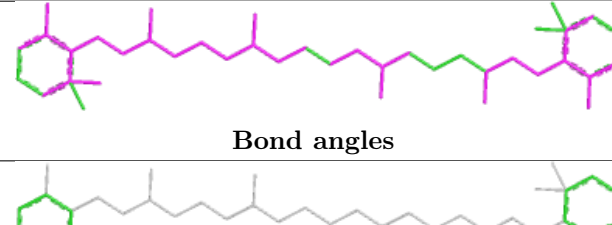
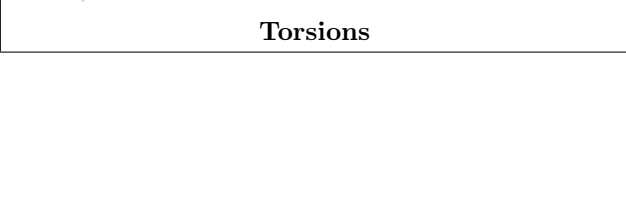
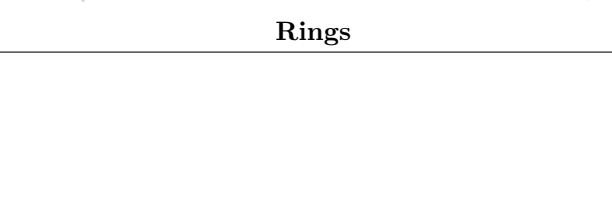


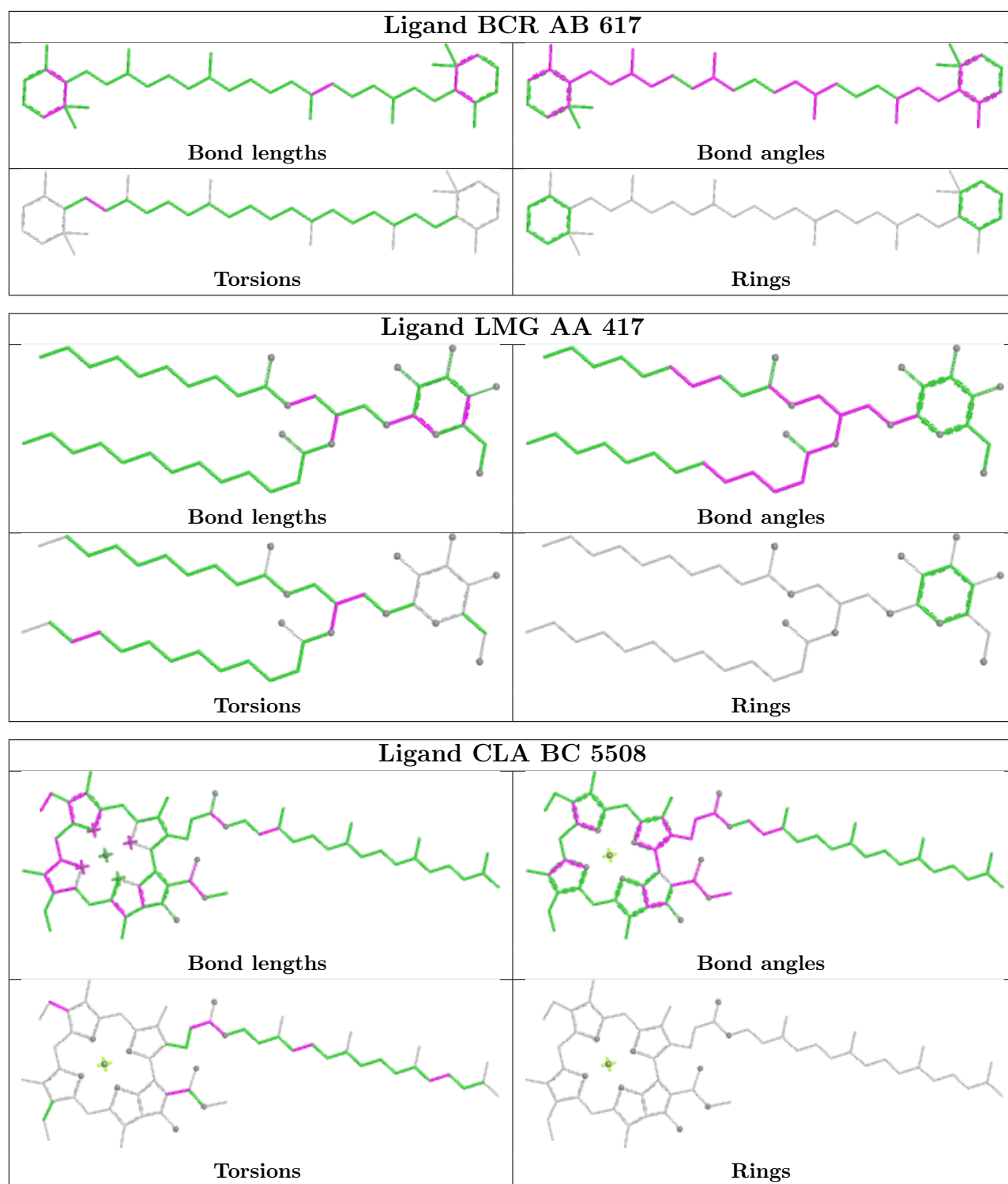
Ligand LHG AA 412

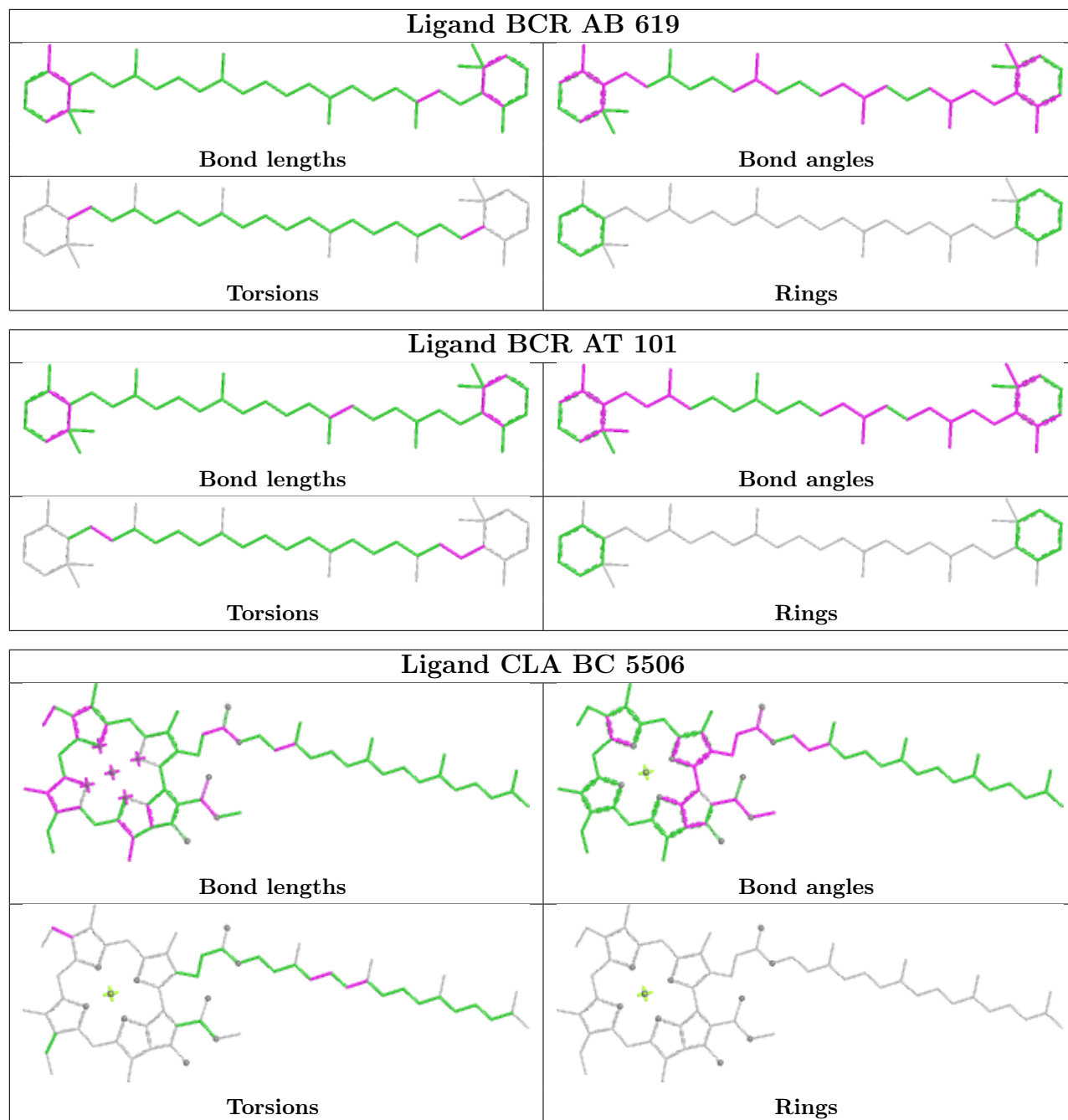


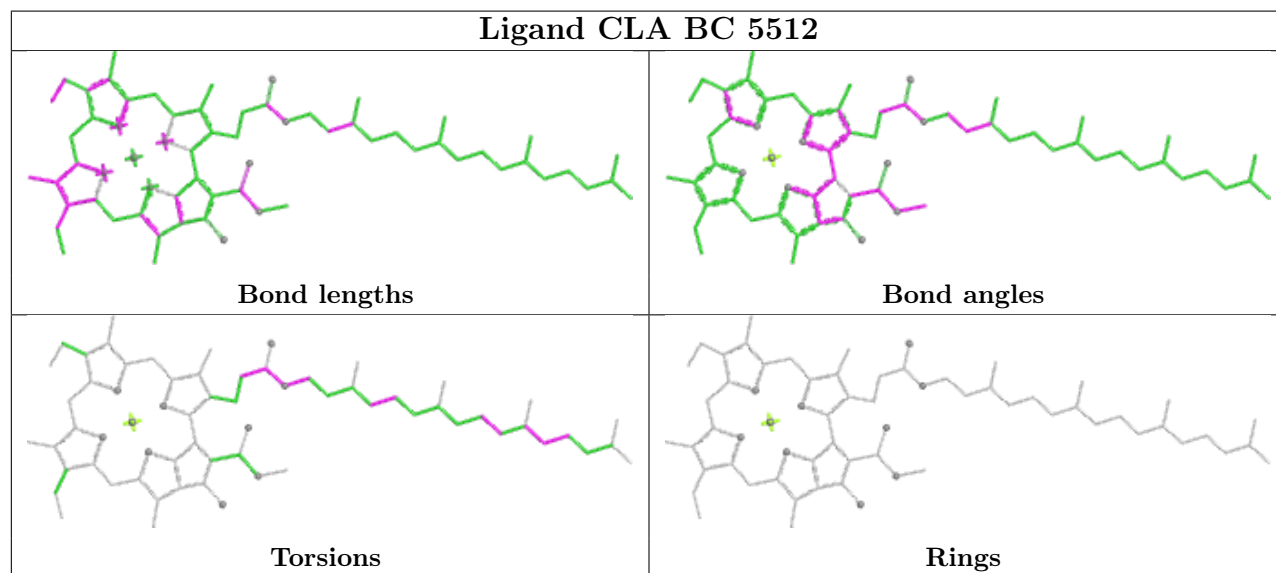
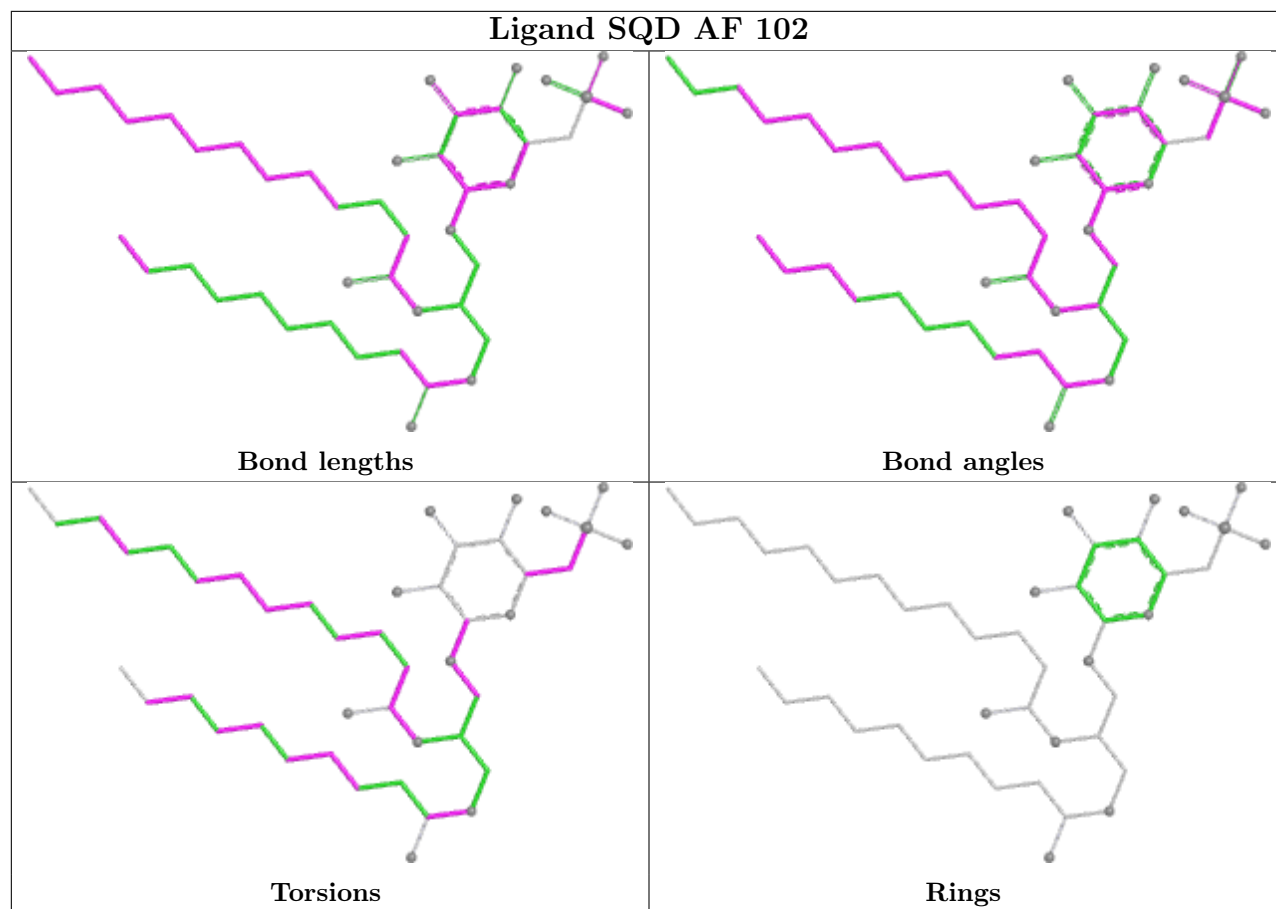
Ligand CLA AB 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

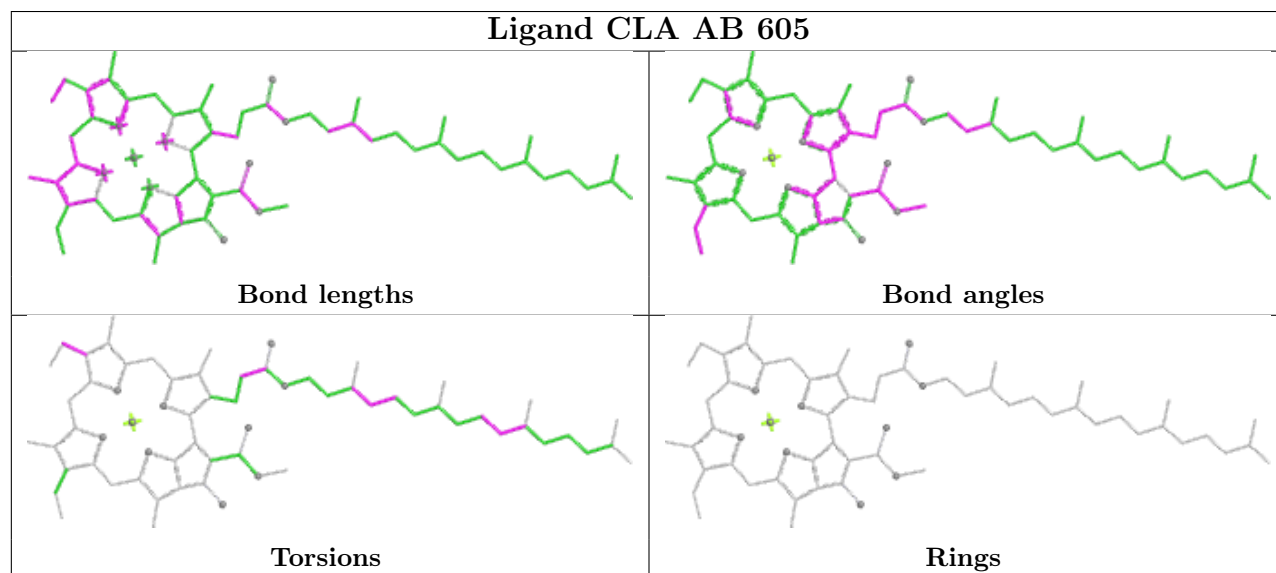
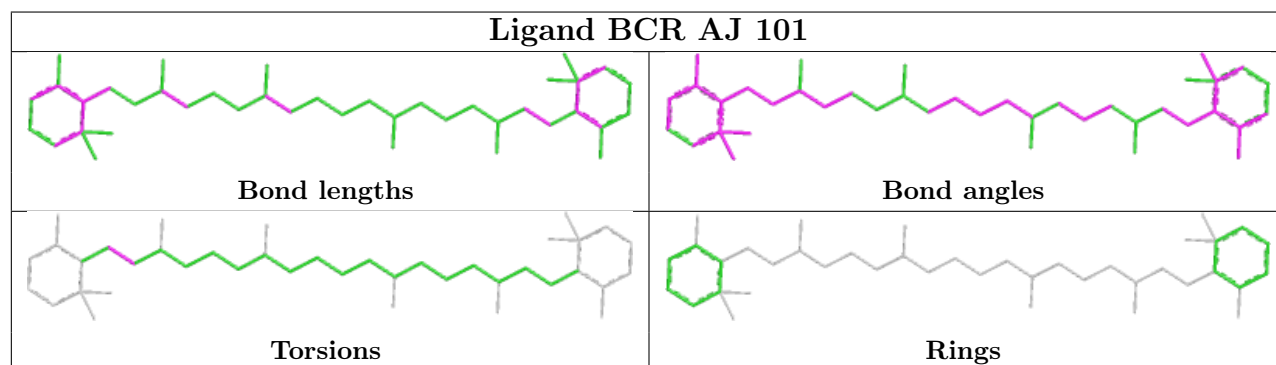
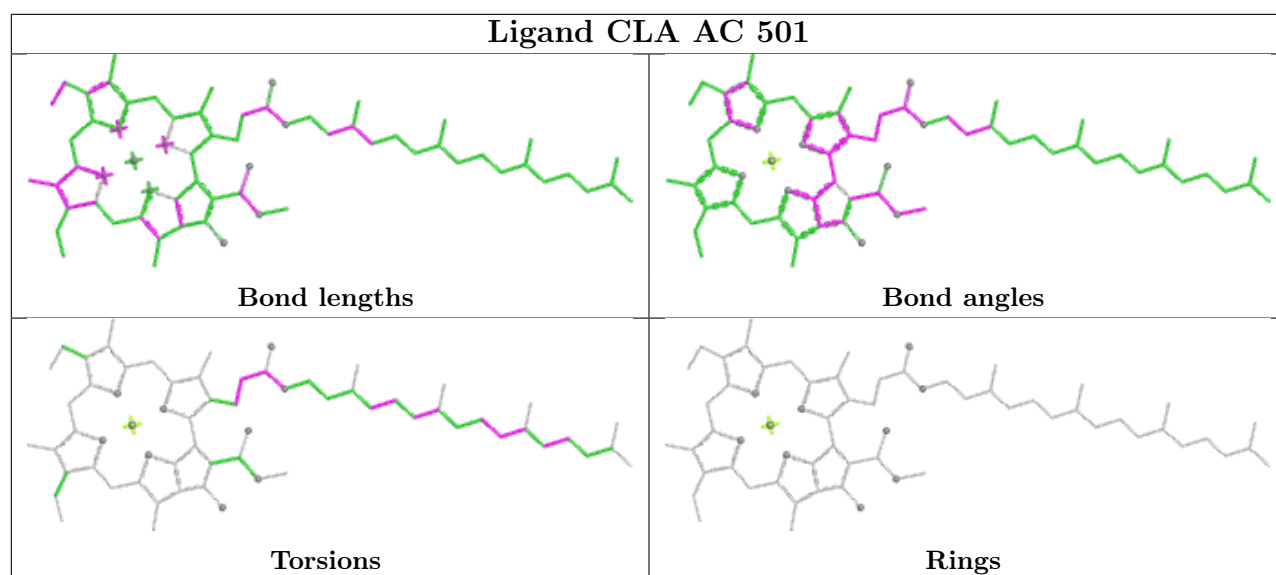
Ligand LMG BE 5101	
	
Bond lengths	Bond angles
	
Torsions	Rings

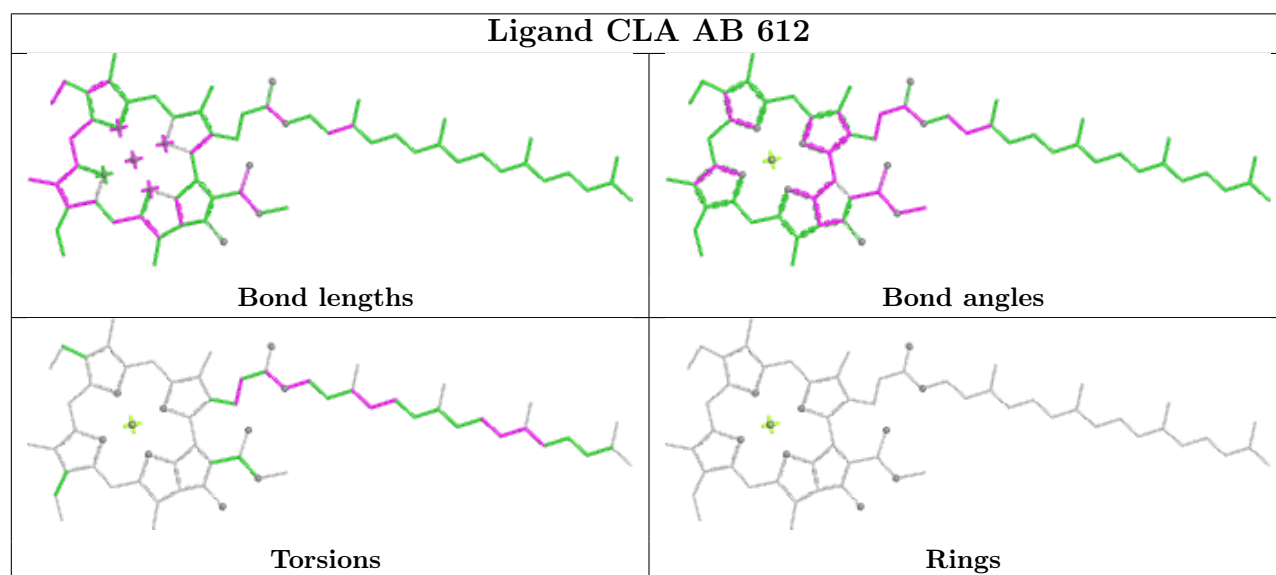
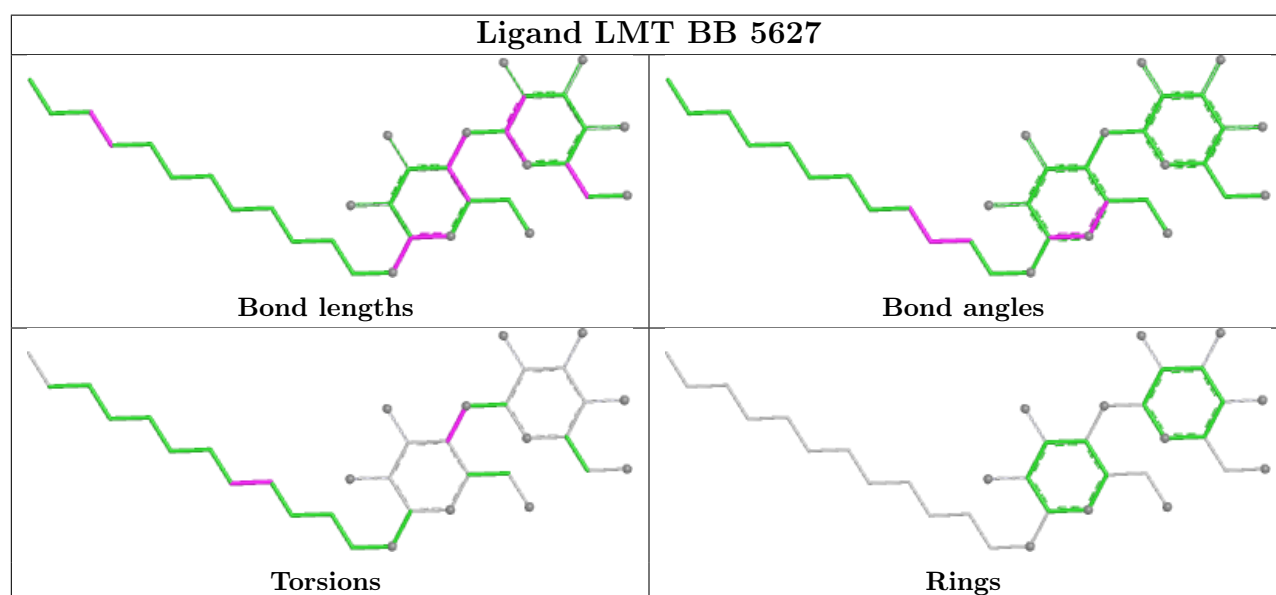
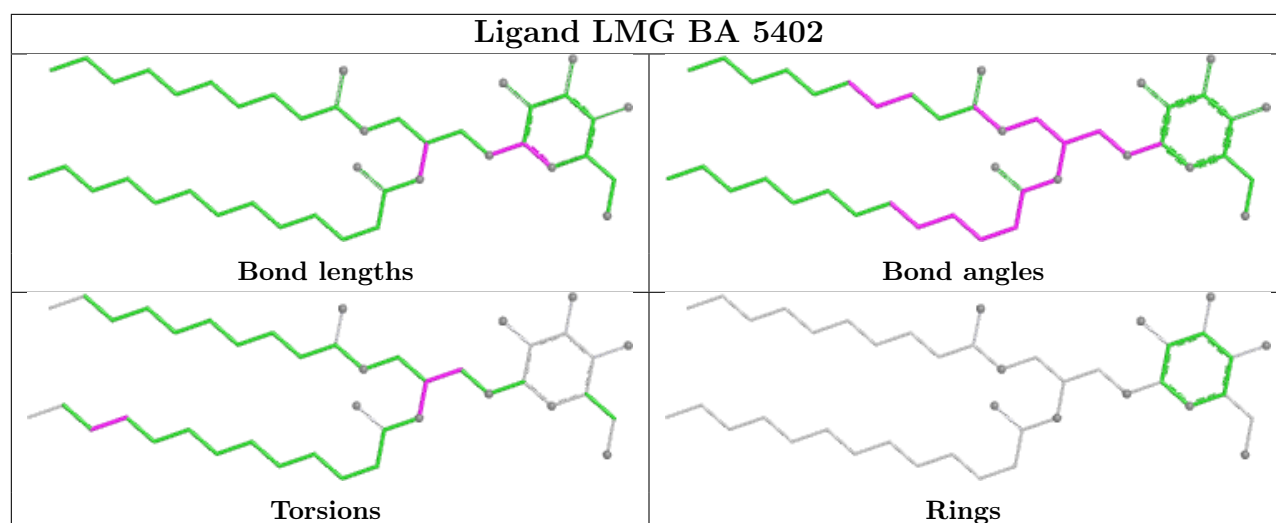
Ligand BCR AK 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



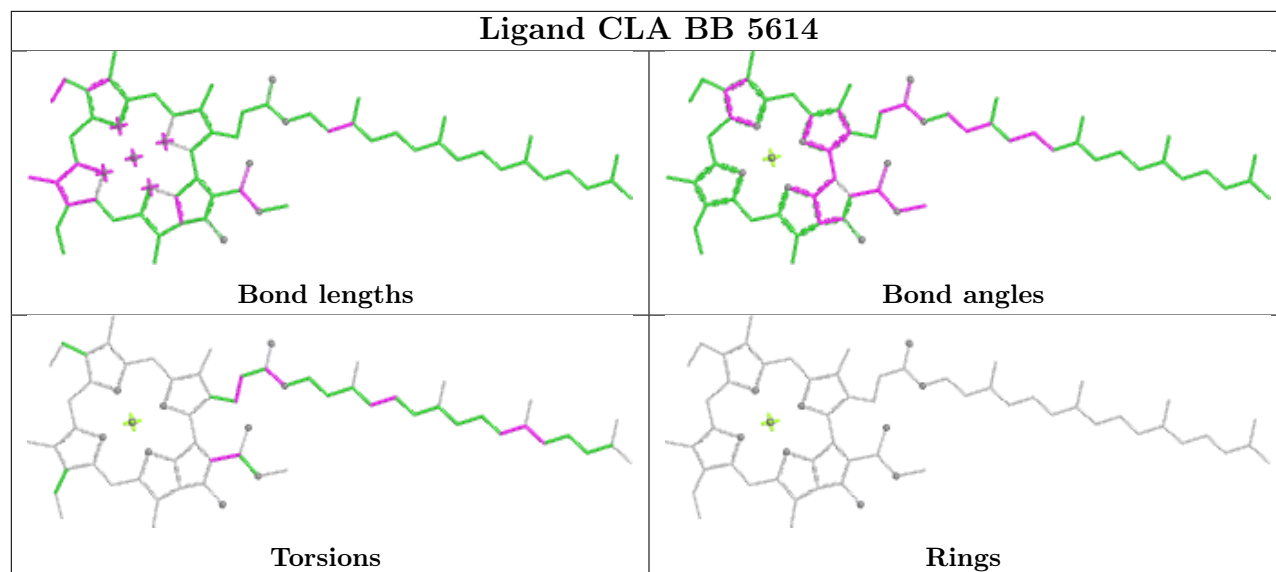




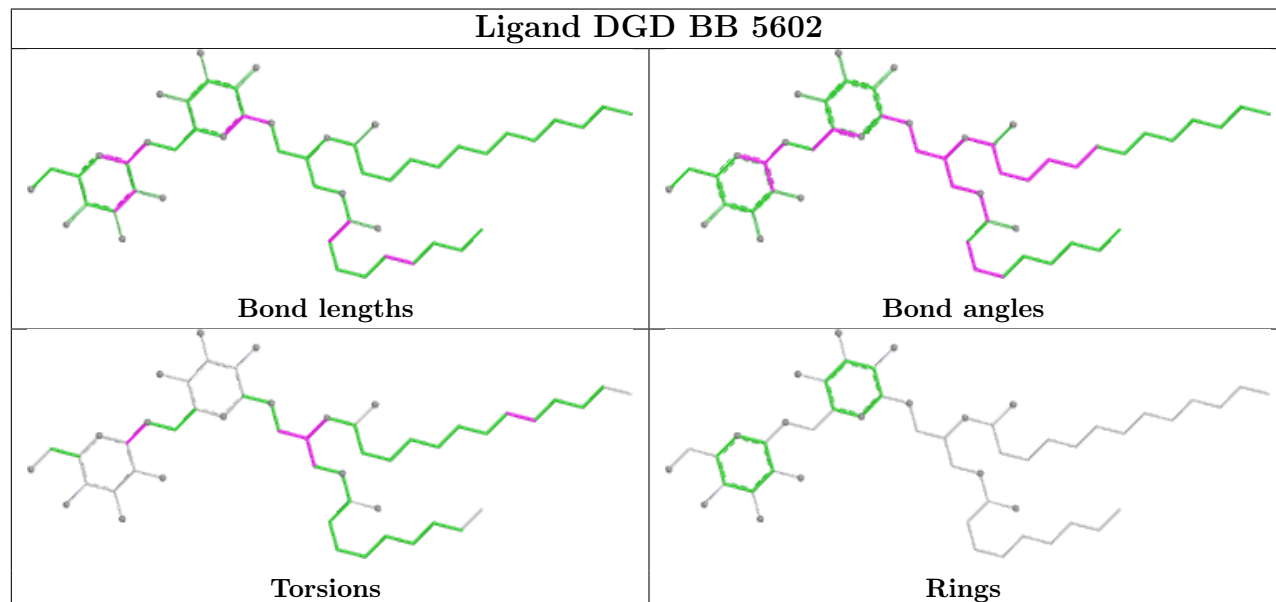




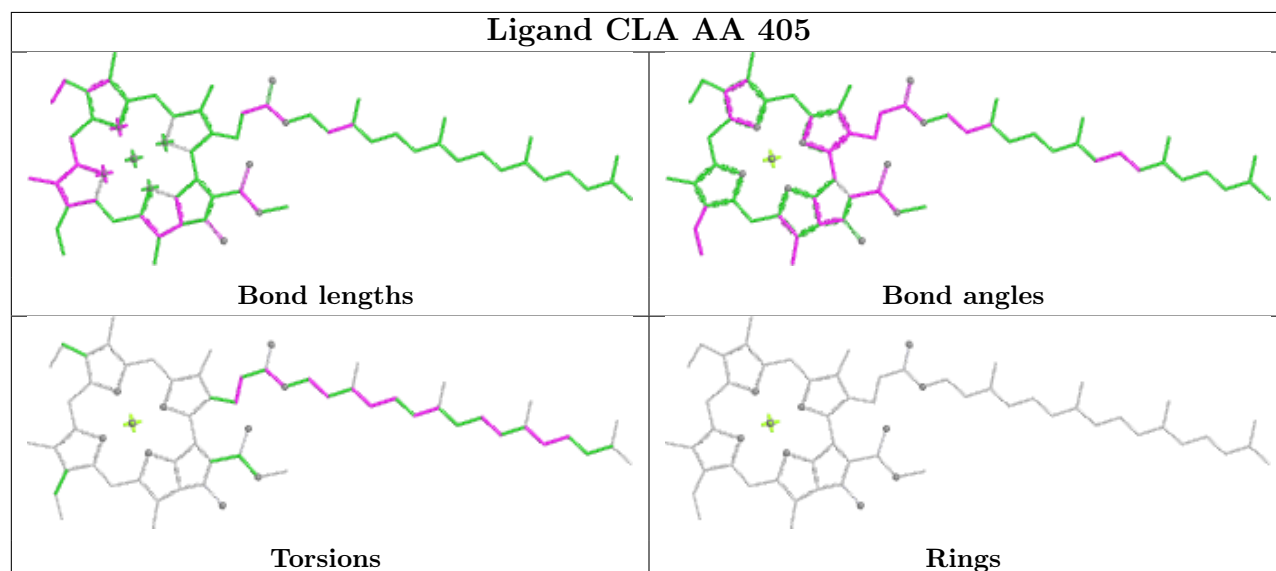
Ligand CLA BB 5614

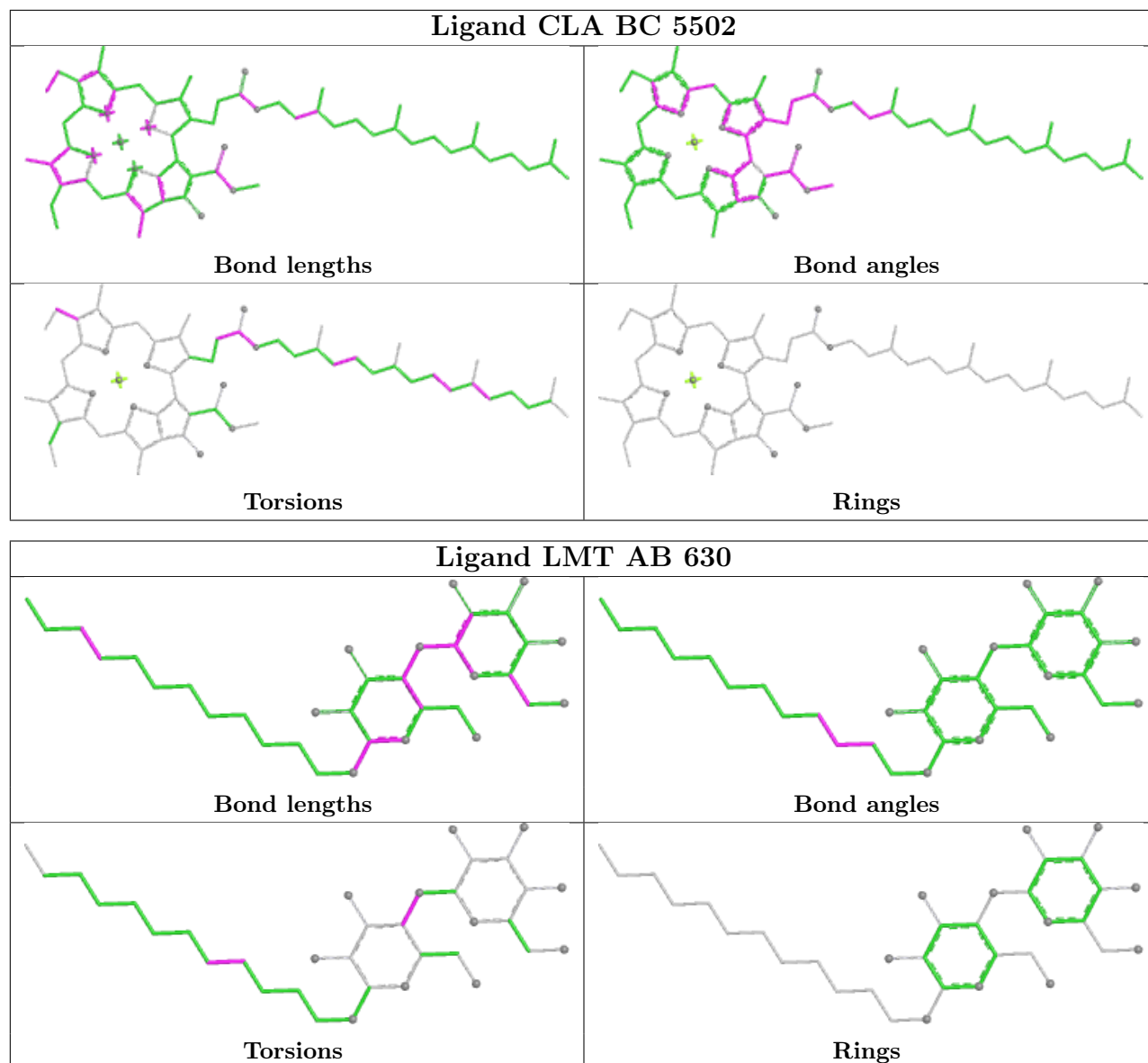


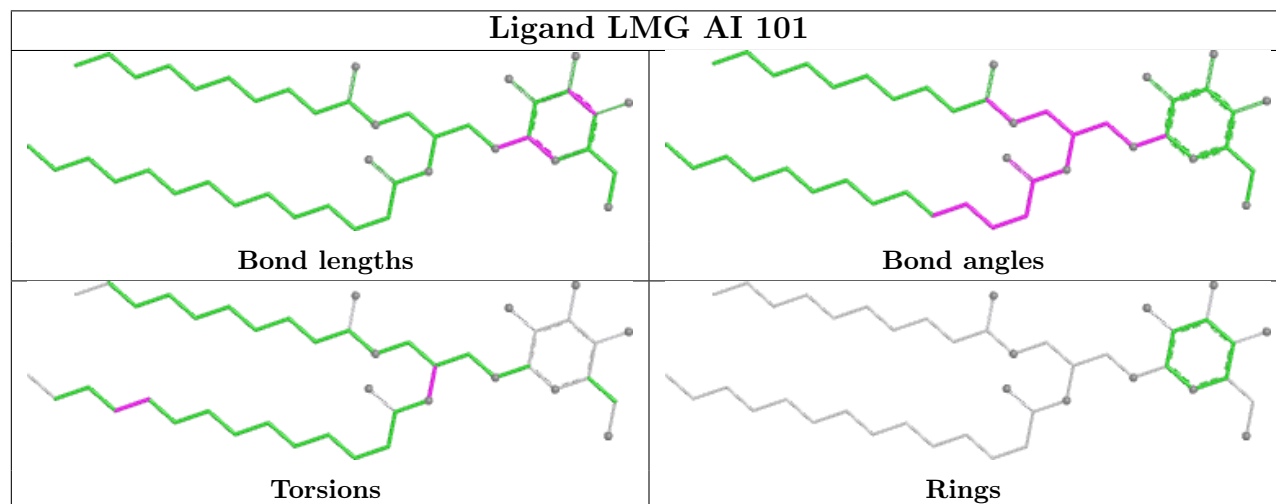
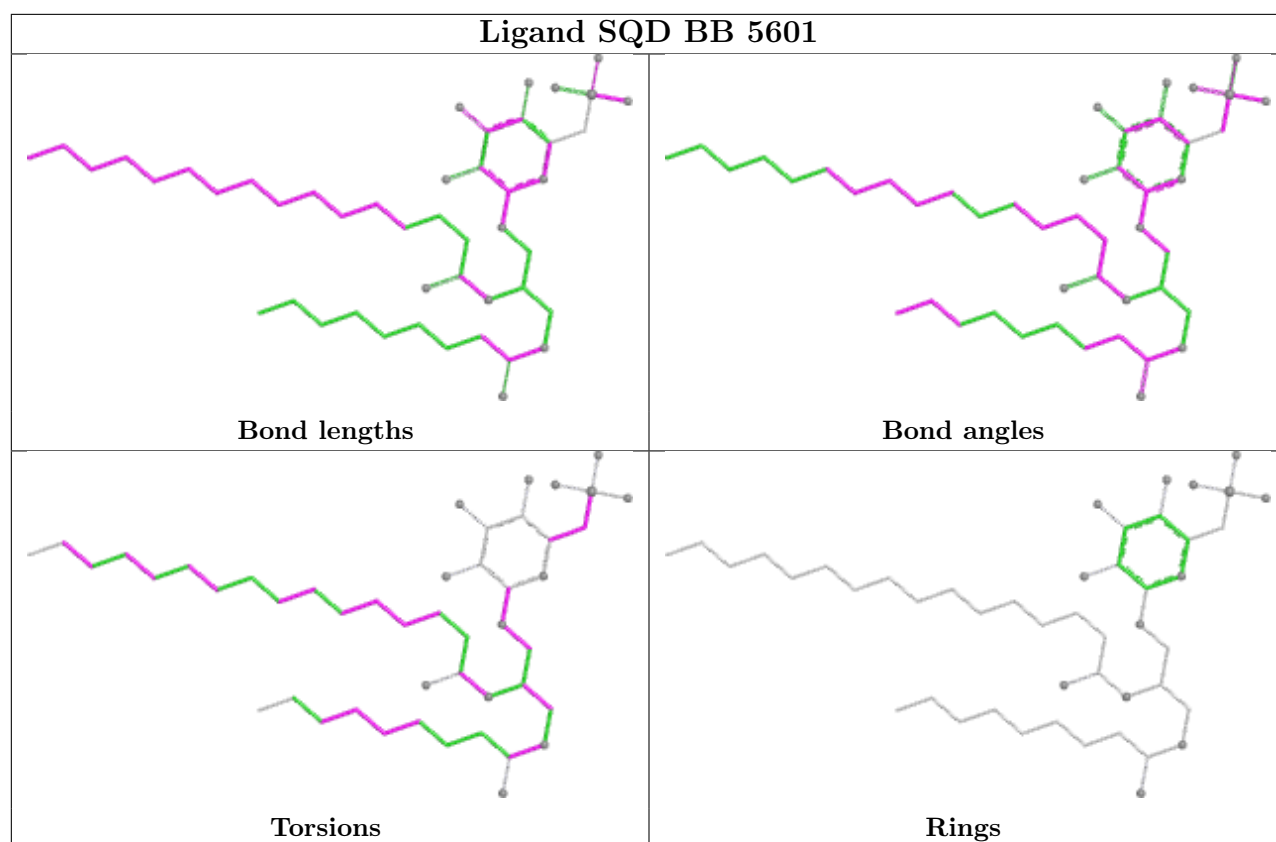
Ligand DGD BB 5602

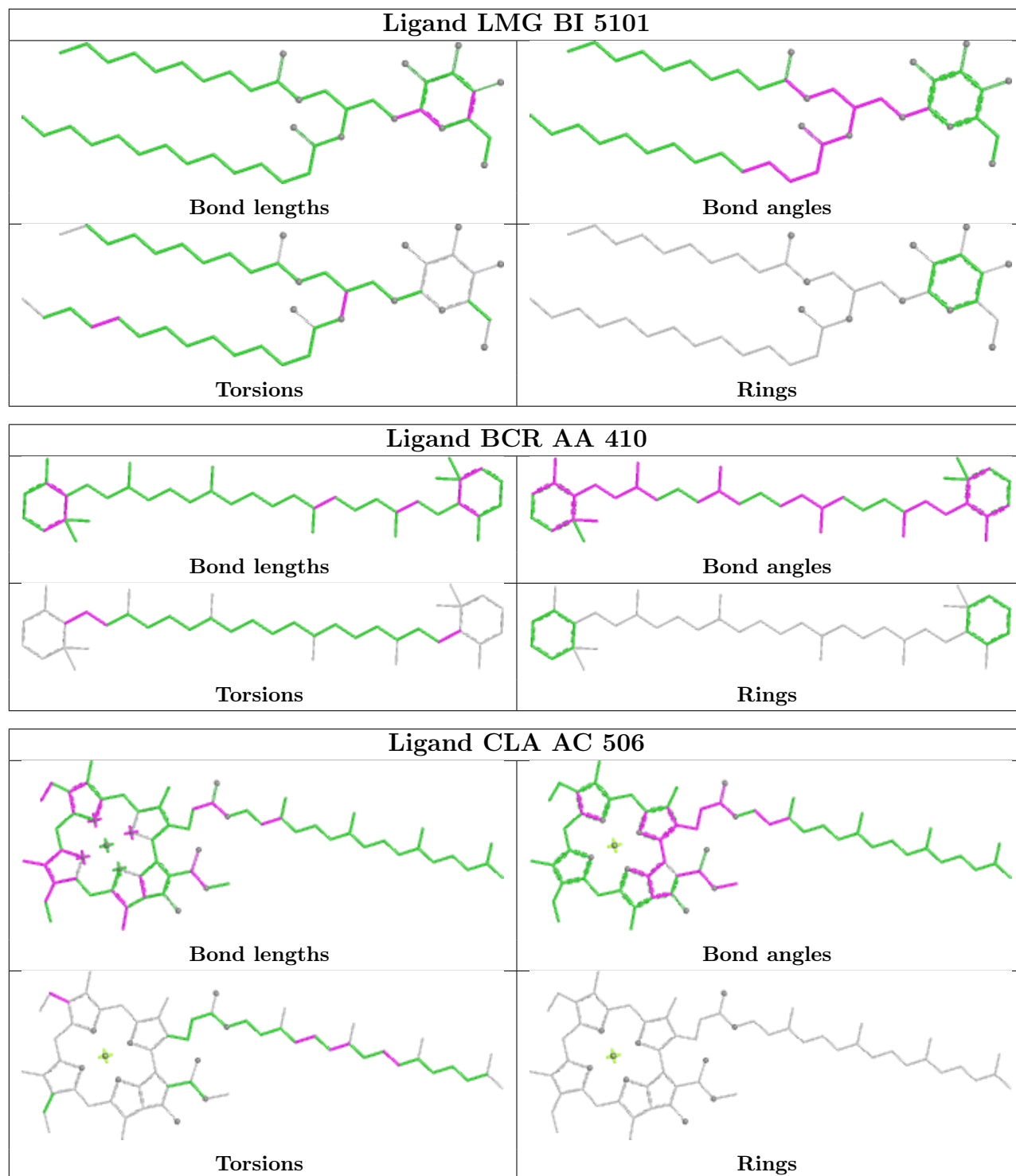


Ligand CLA AA 405

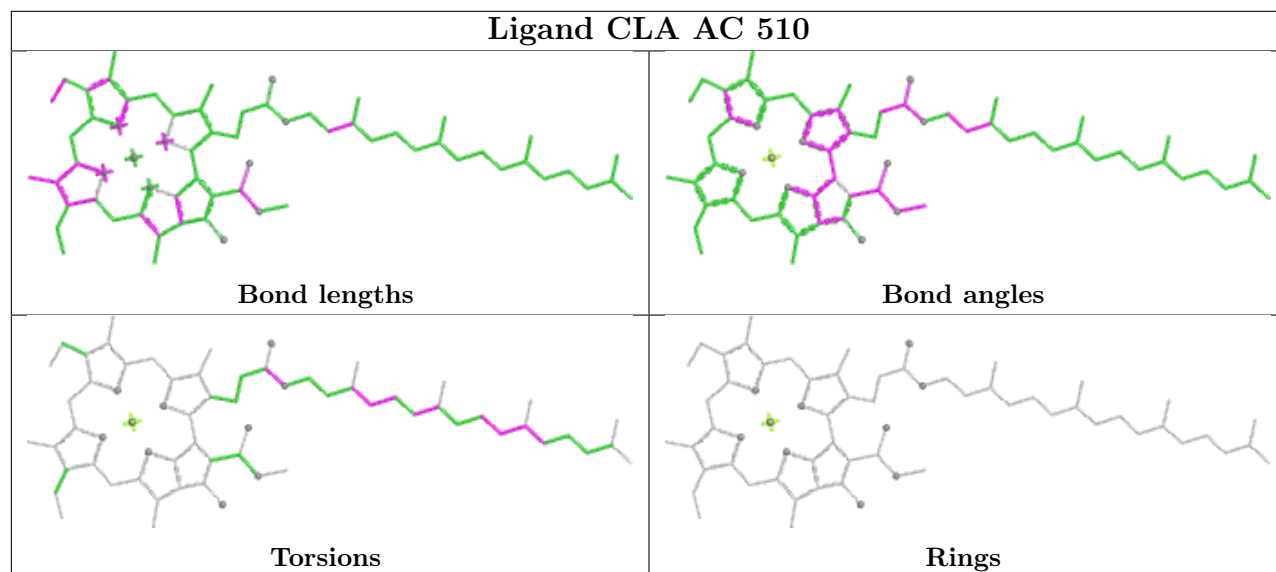




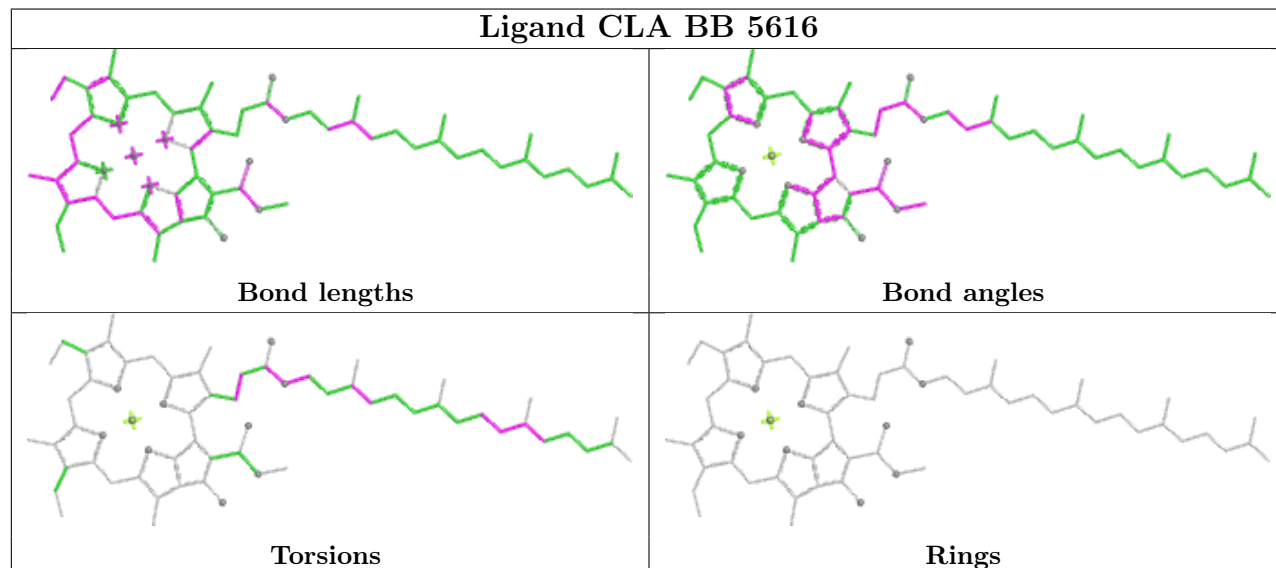




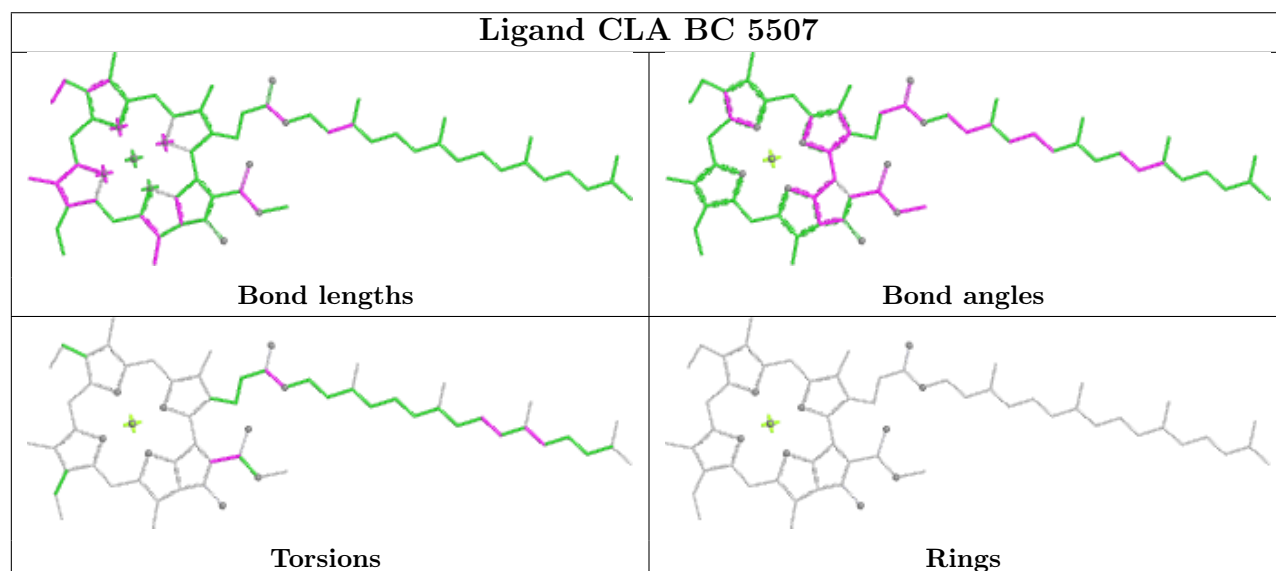
Ligand CLA AC 510



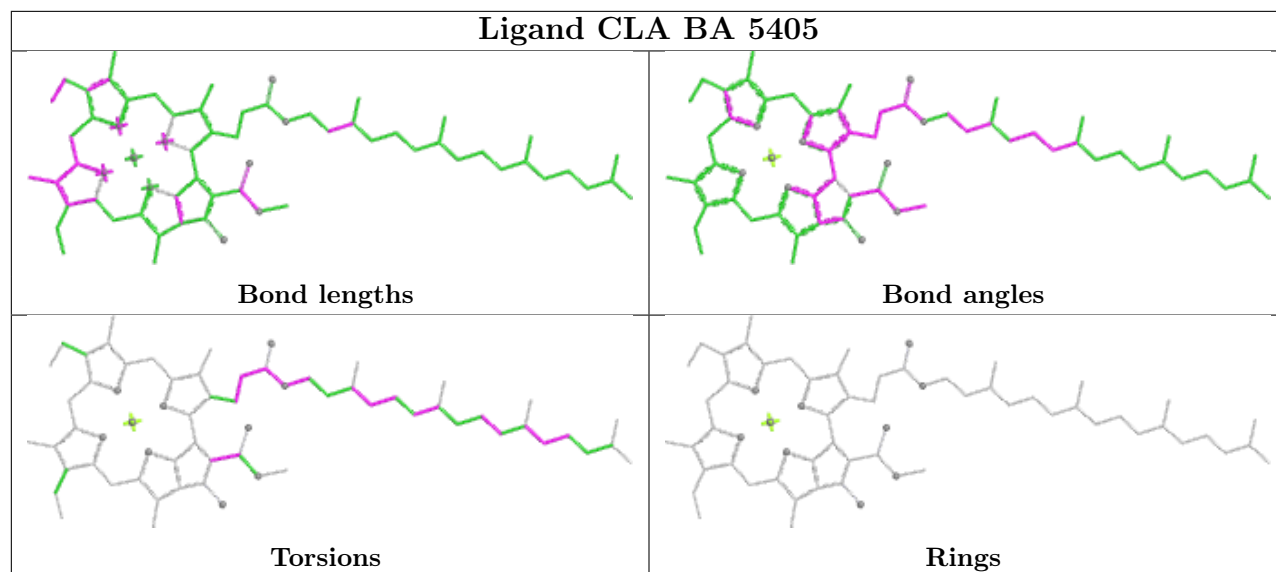
Ligand CLA BB 5616



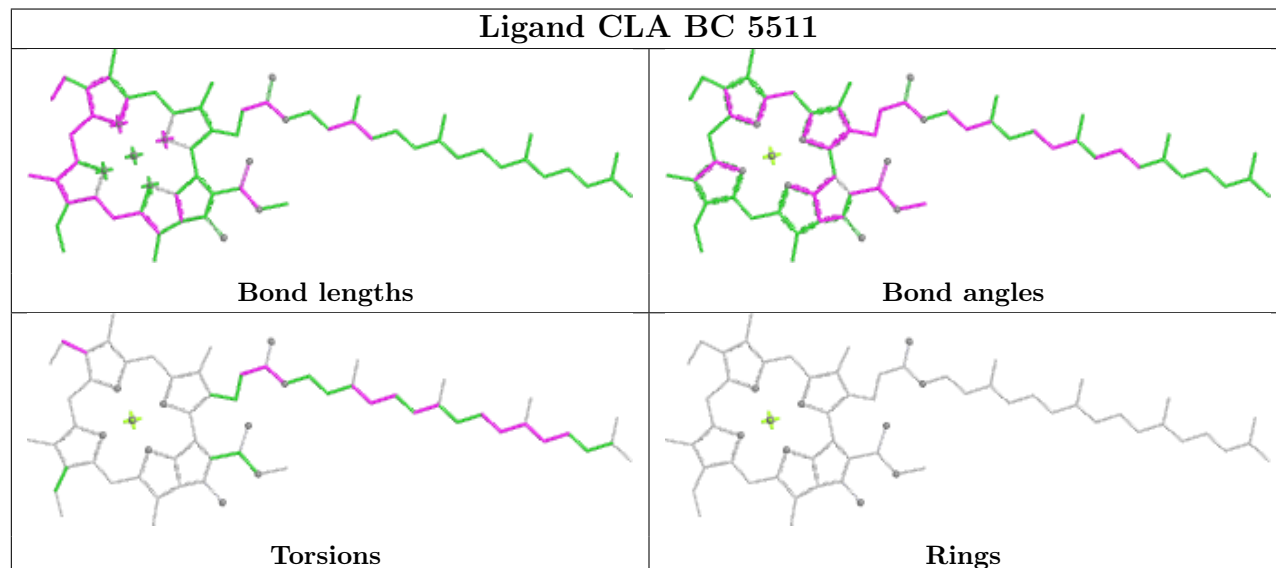
Ligand CLA BC 5507



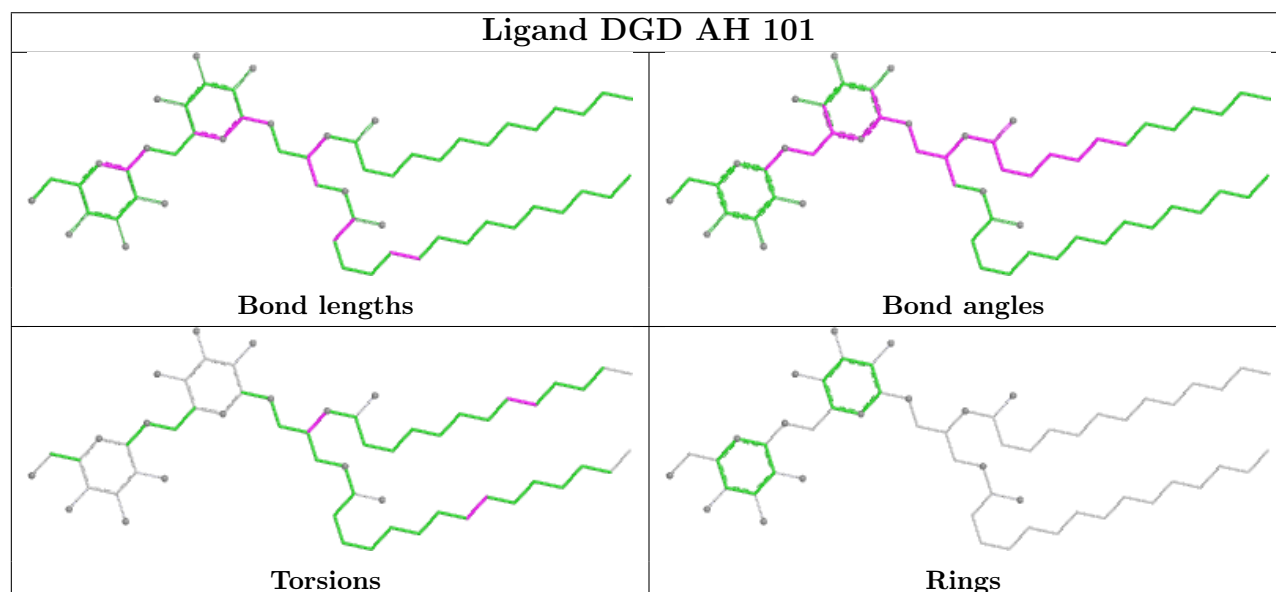
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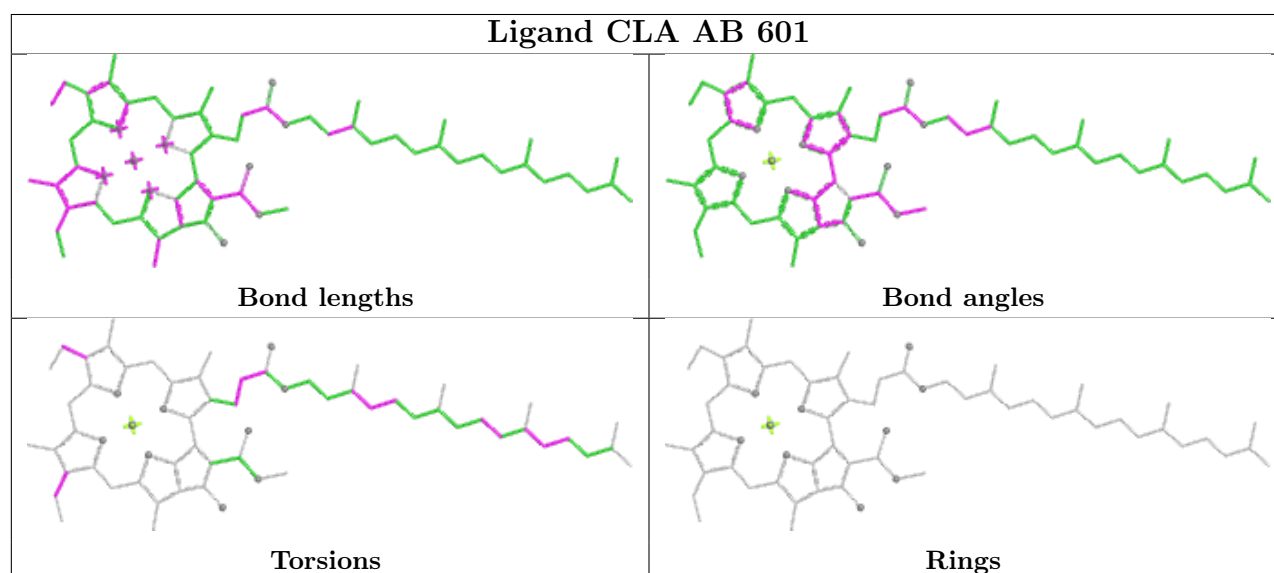
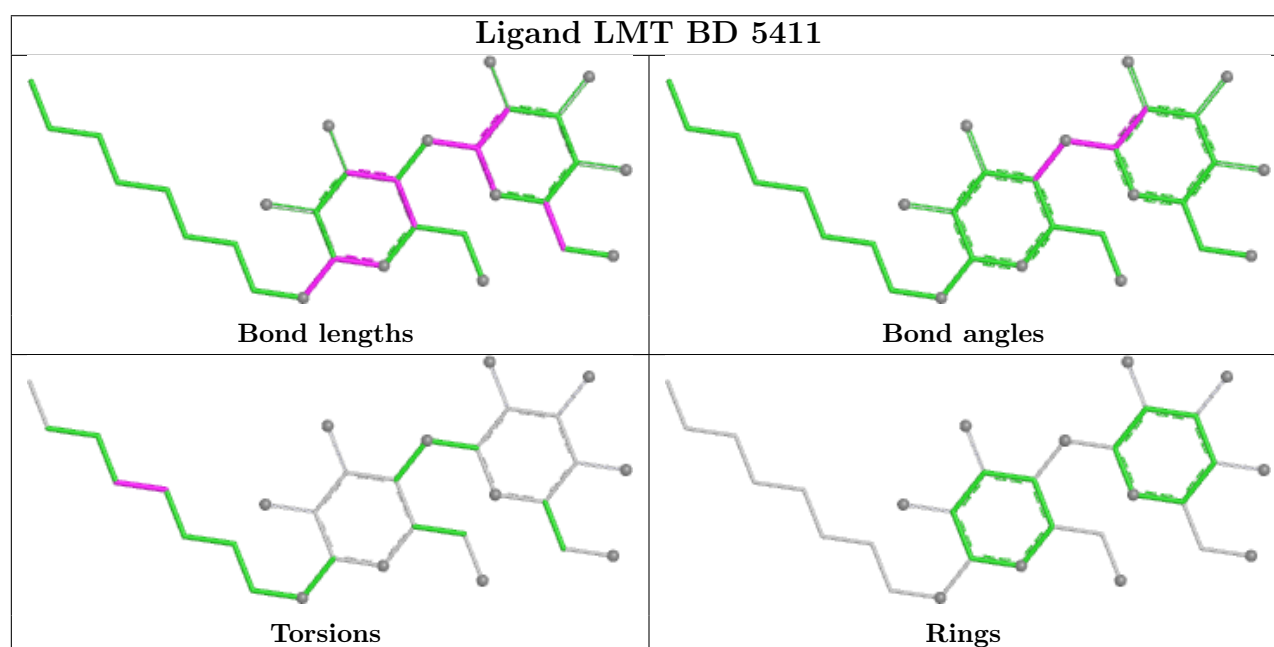
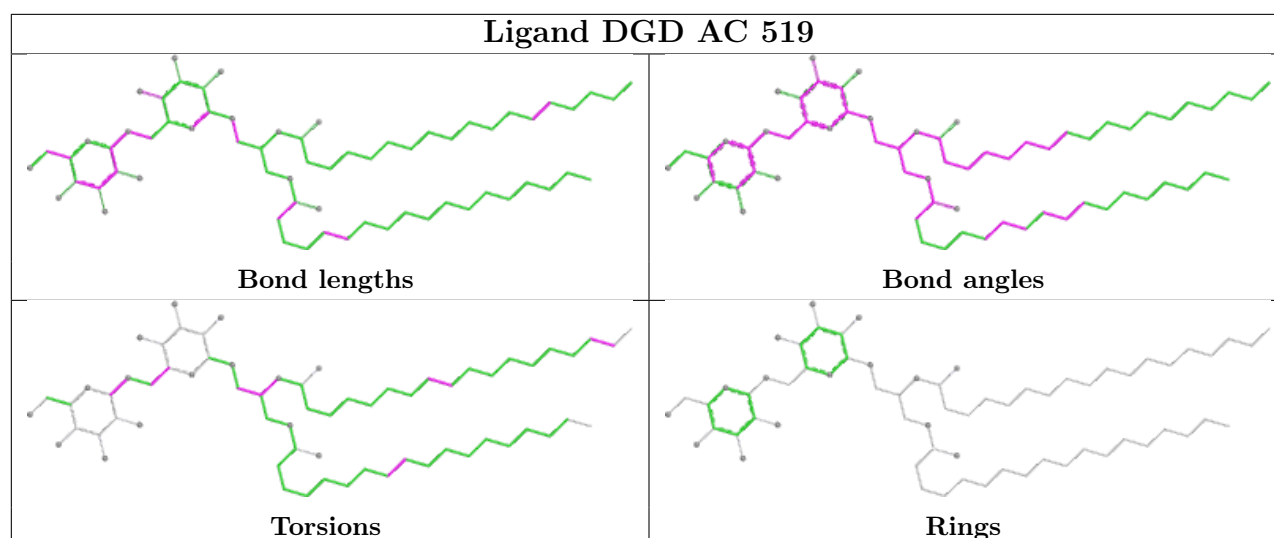


Ligand CLA BC 5511

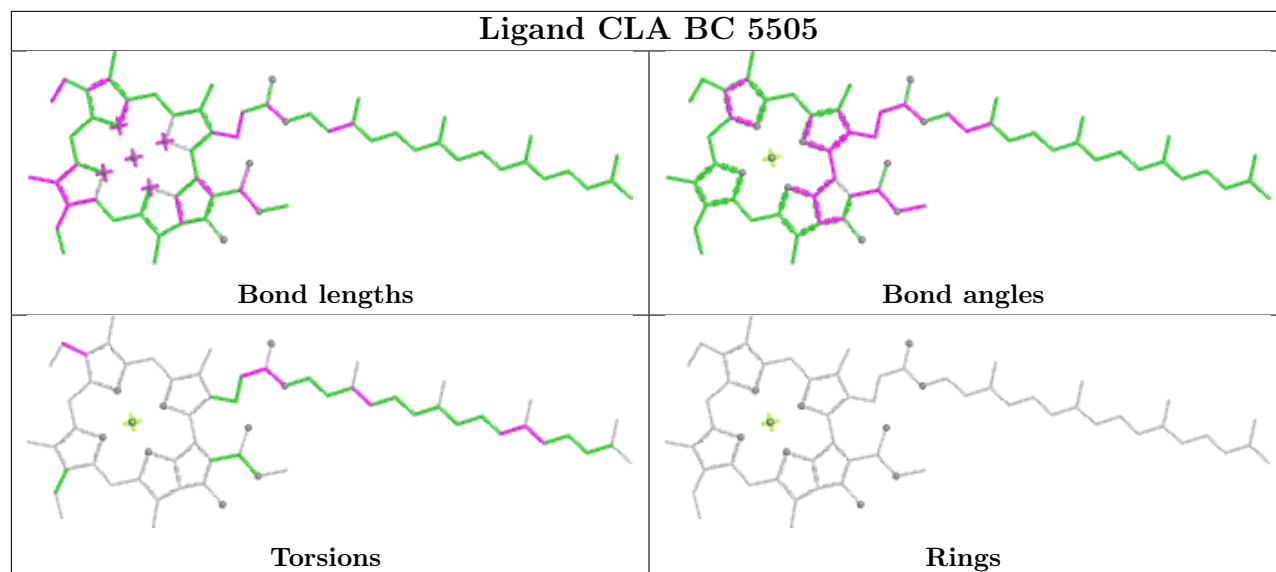


Ligand DGD AH 101

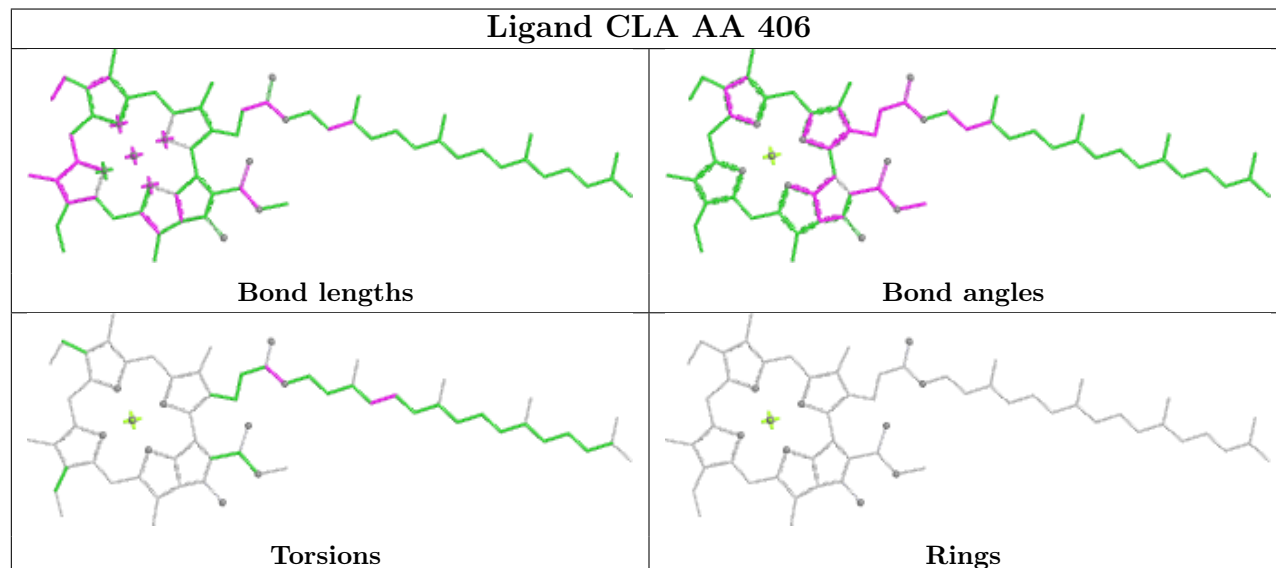




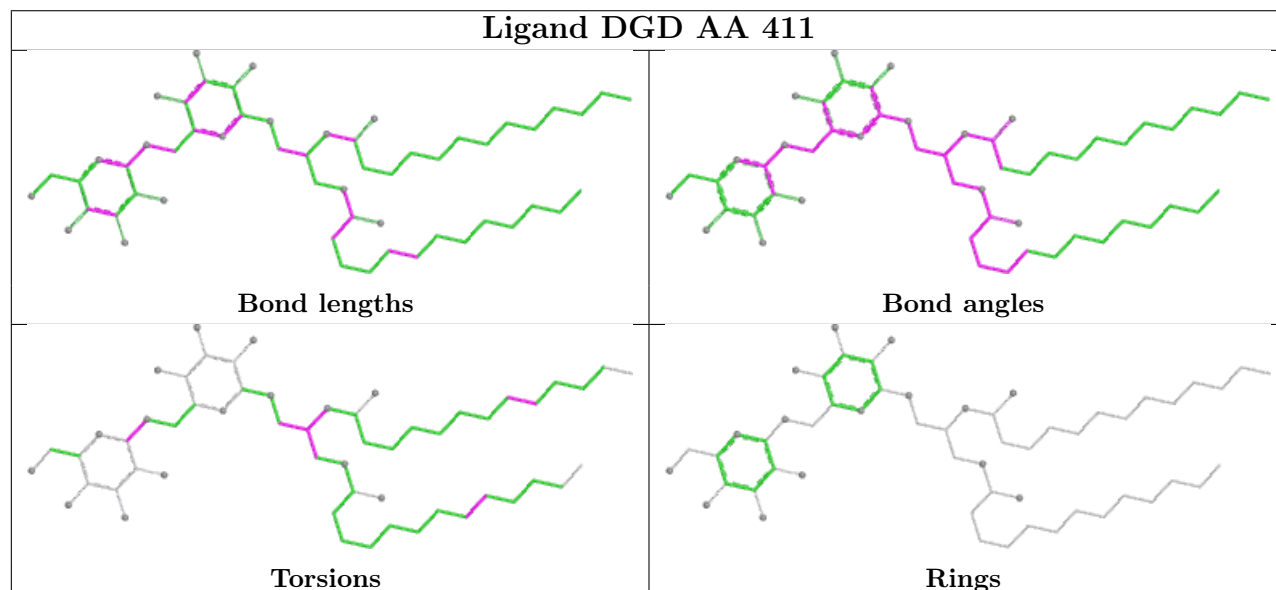
Ligand CLA BC 5505

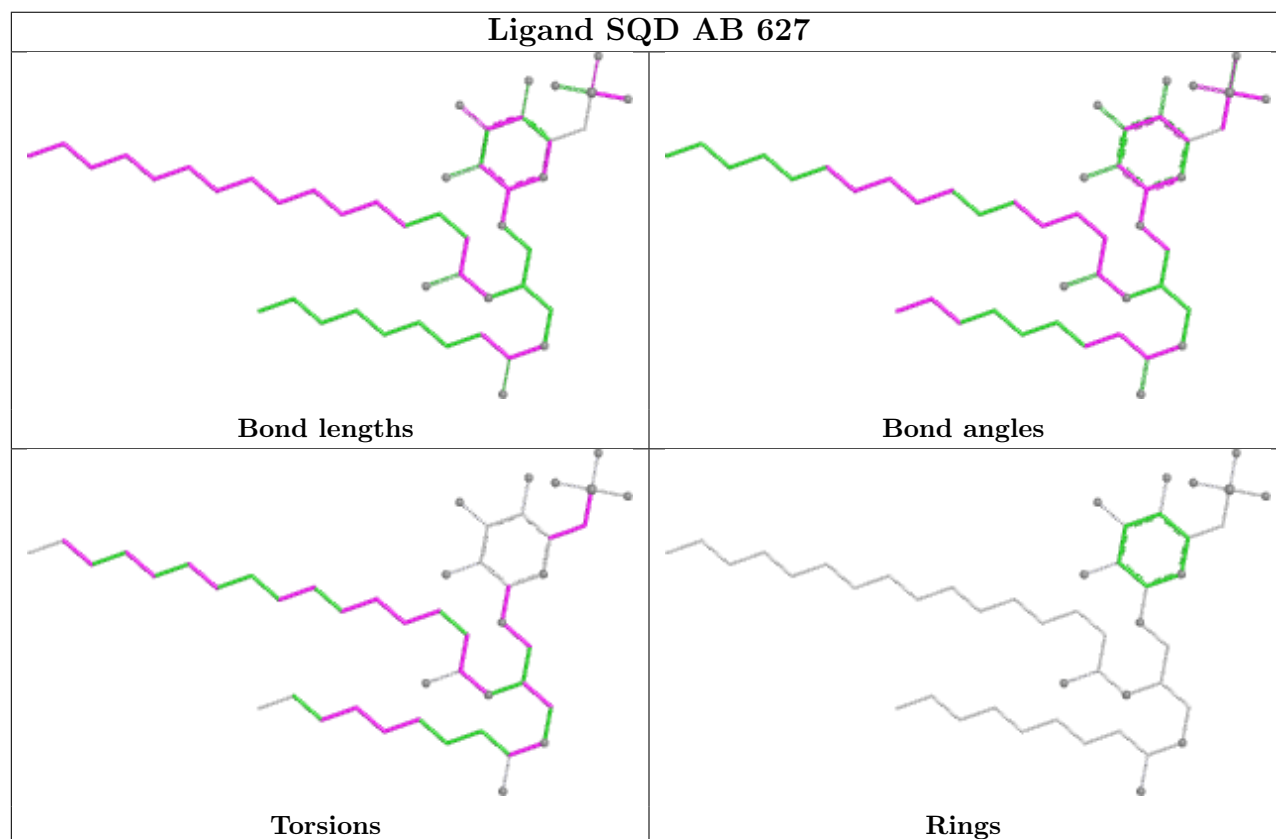
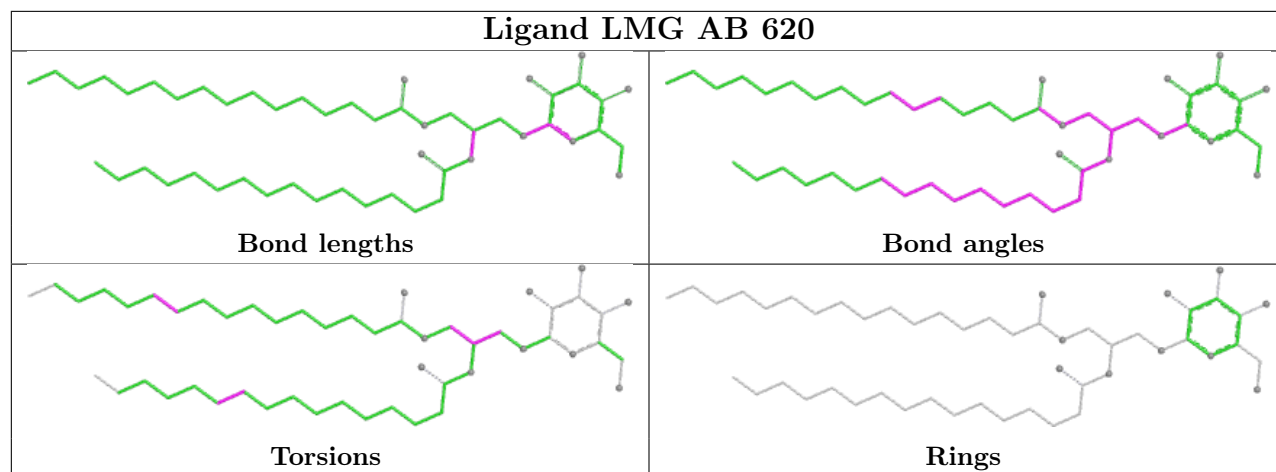


Ligand CLA AA 406

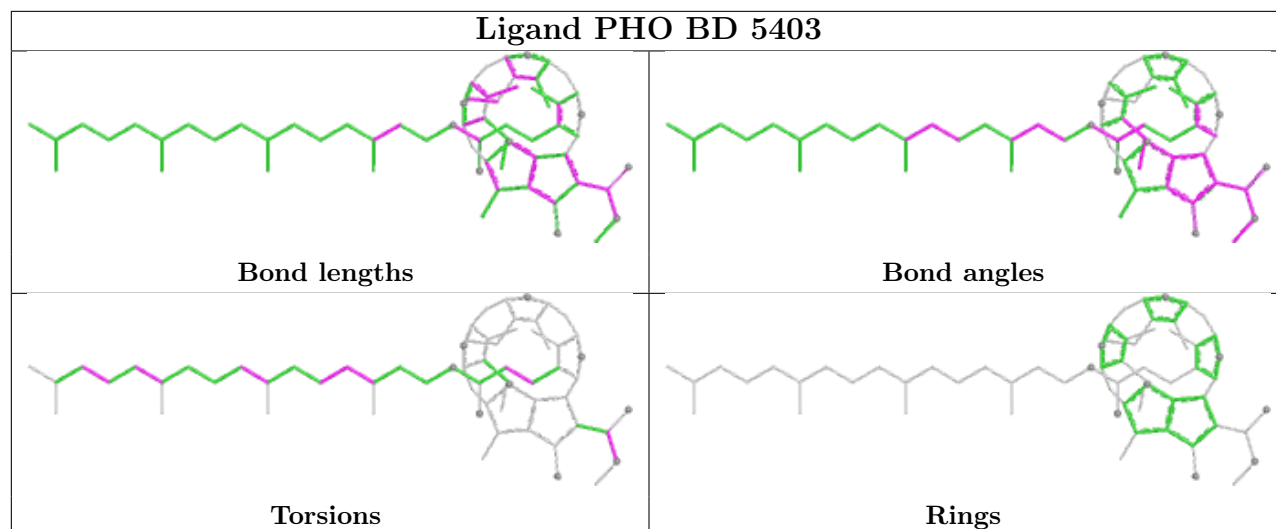


Ligand DGD AA 411

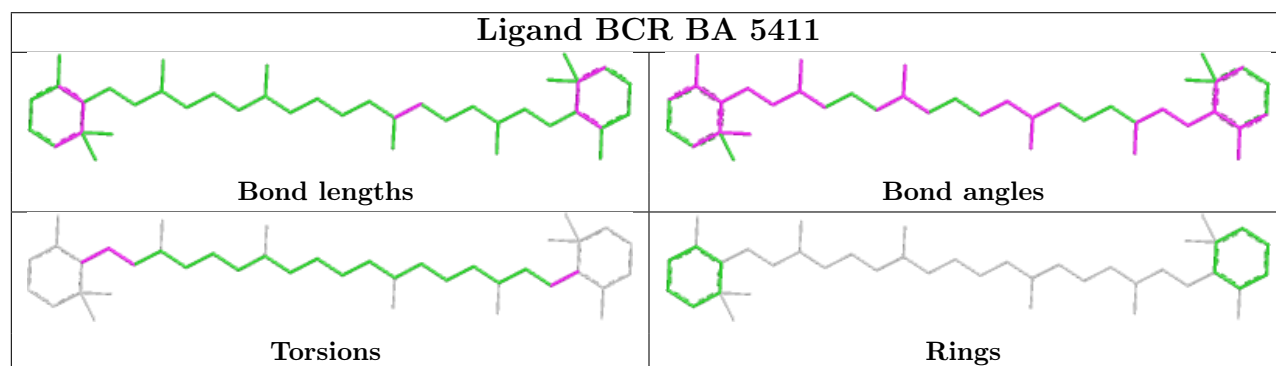




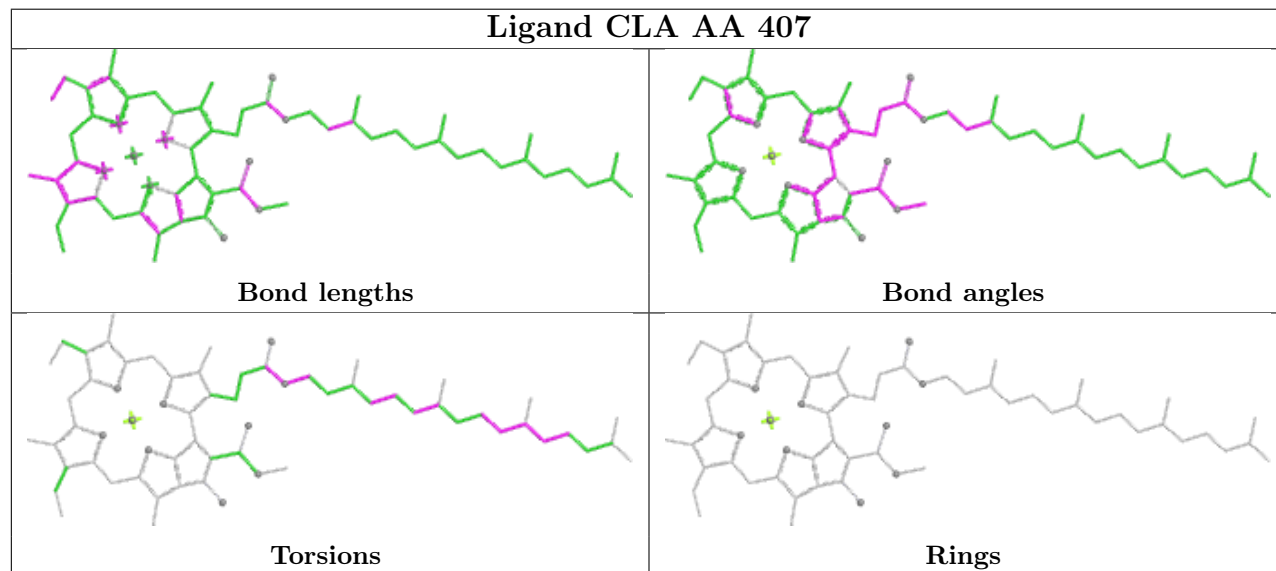
Ligand PHO BD 5403



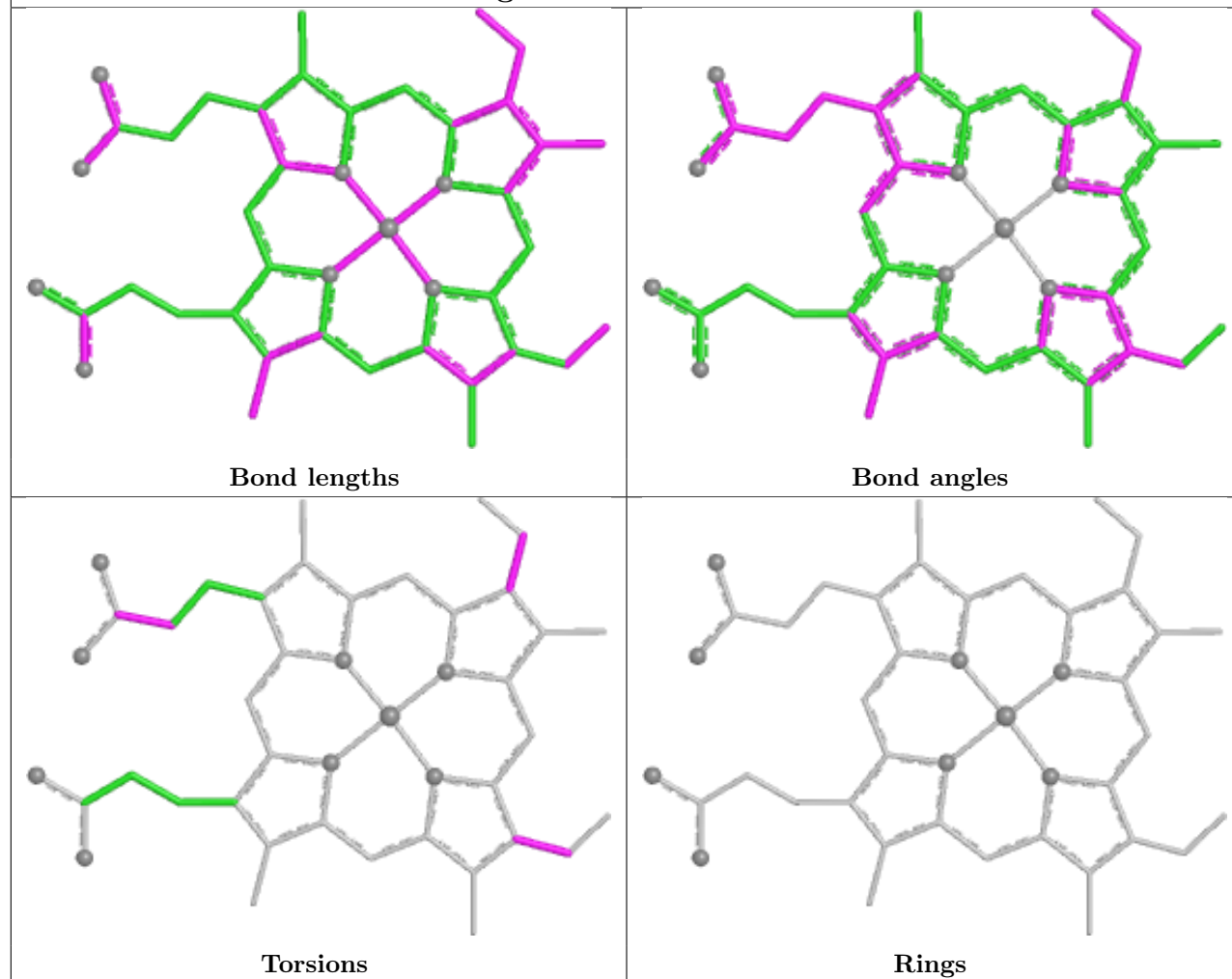
Ligand BCR BA 5411



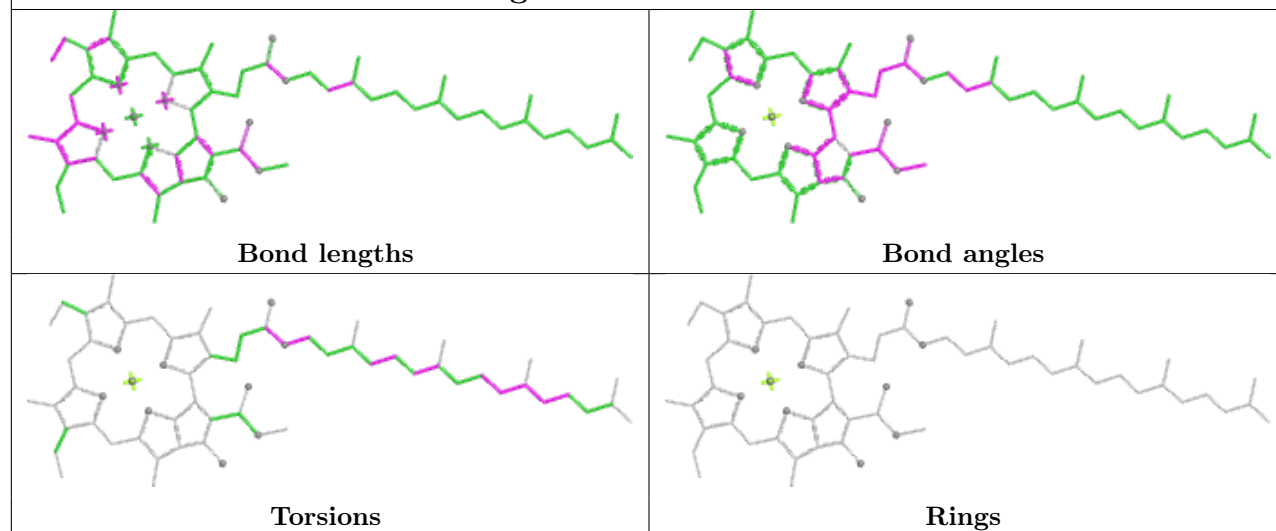
Ligand CLA AA 407

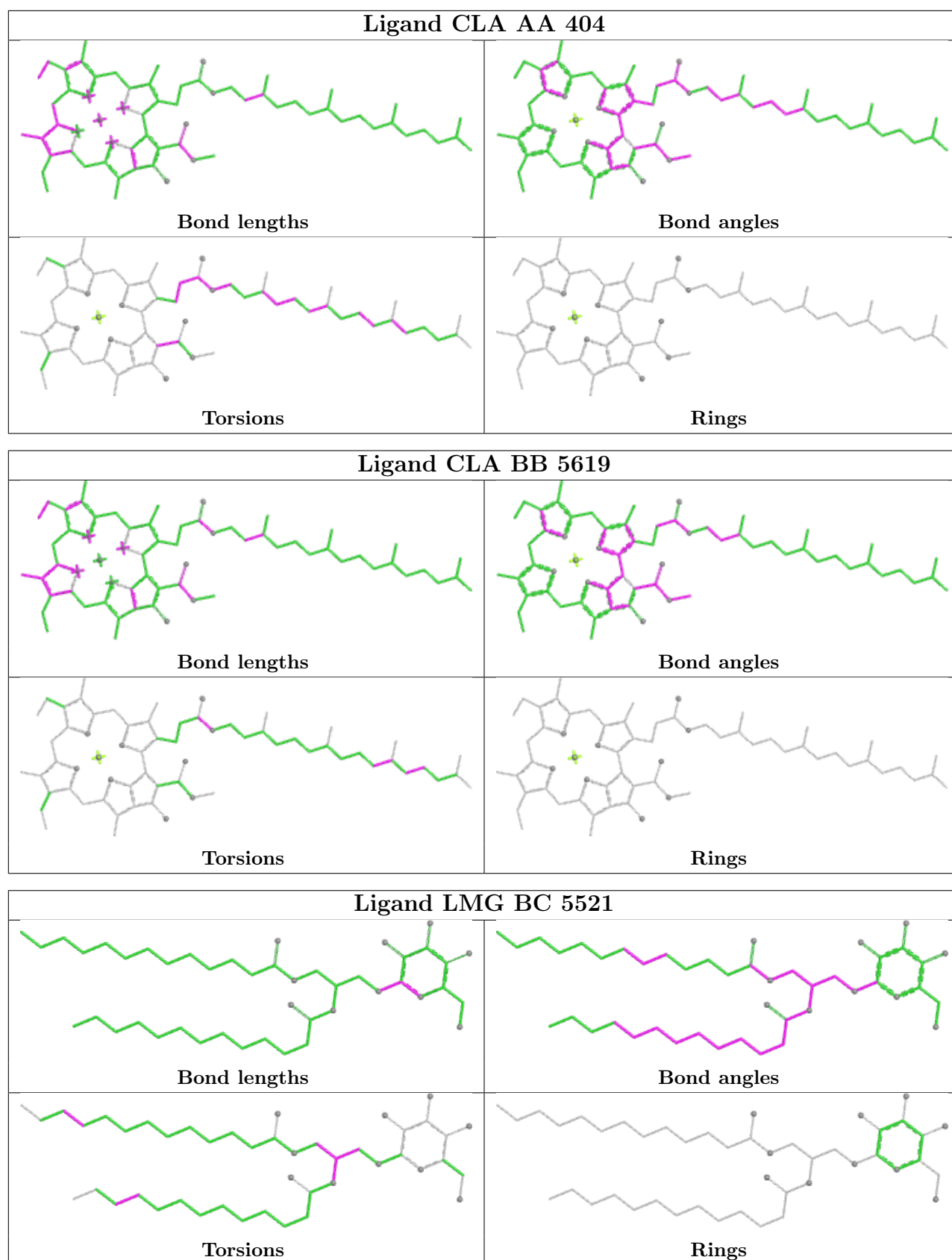


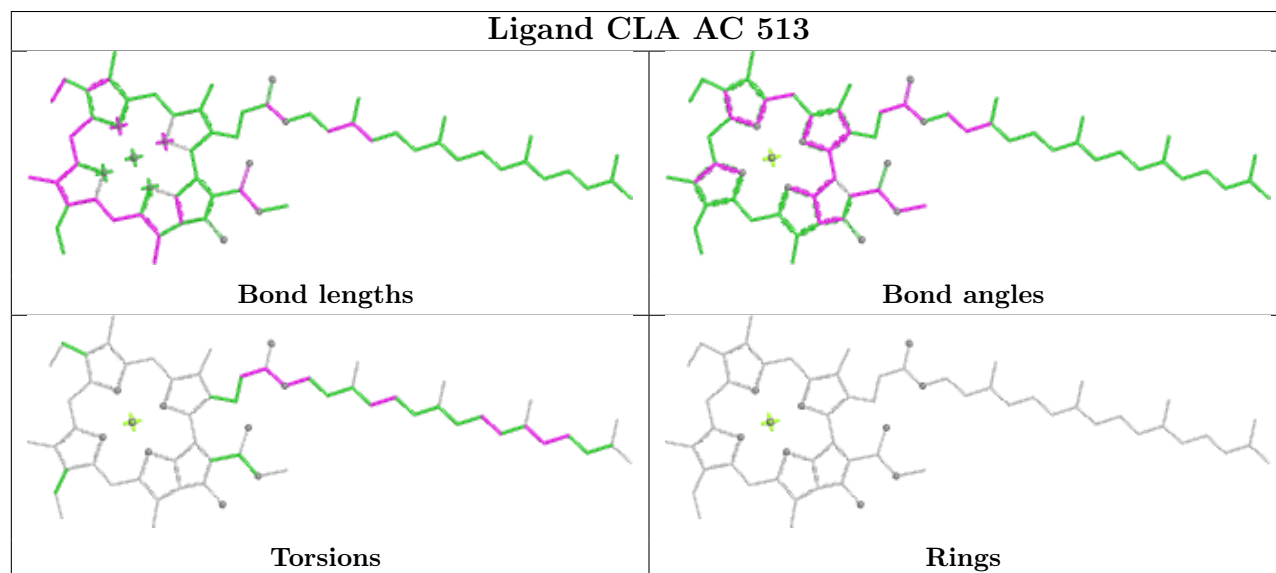
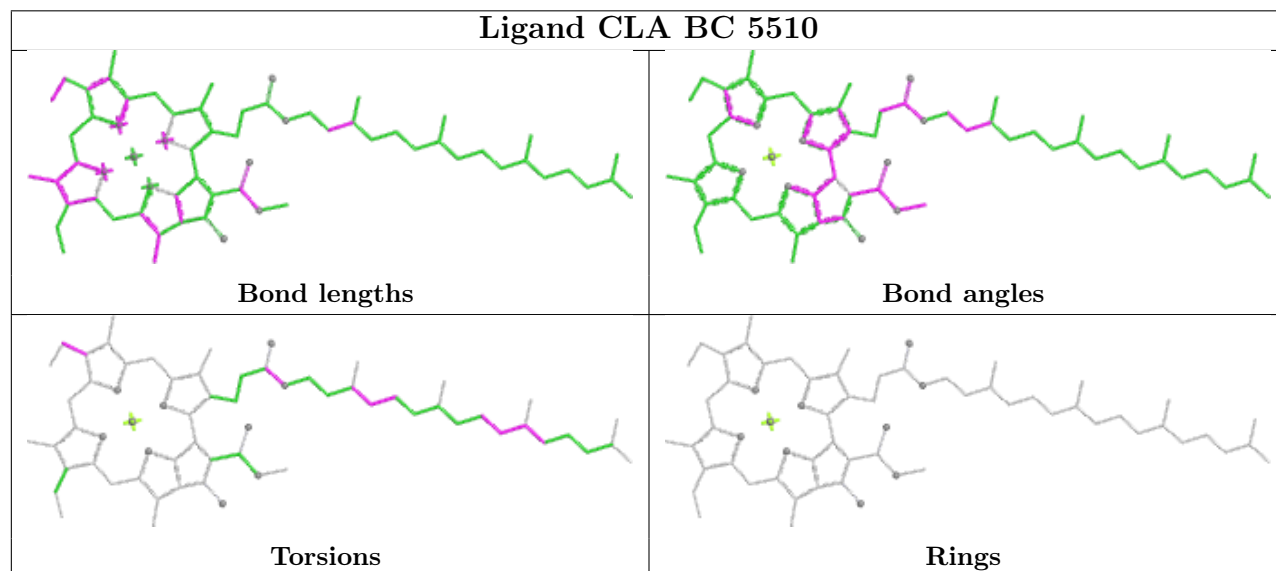
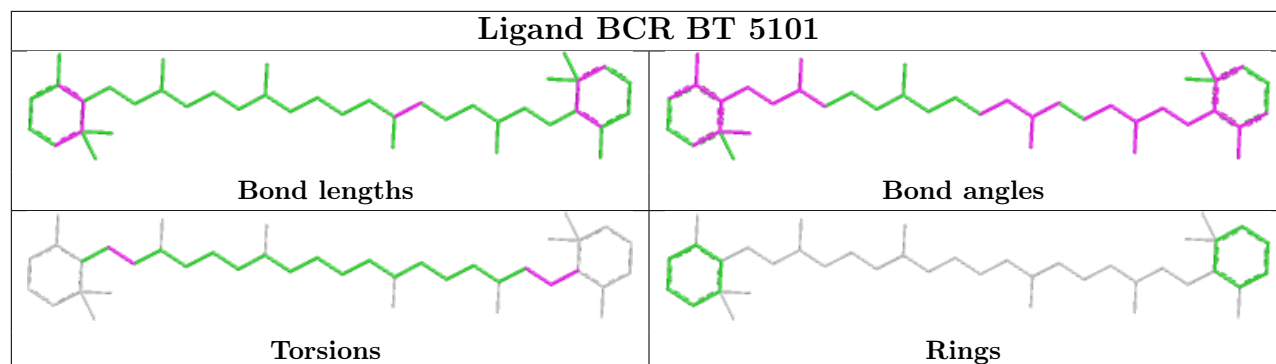
Ligand HEM AV 201



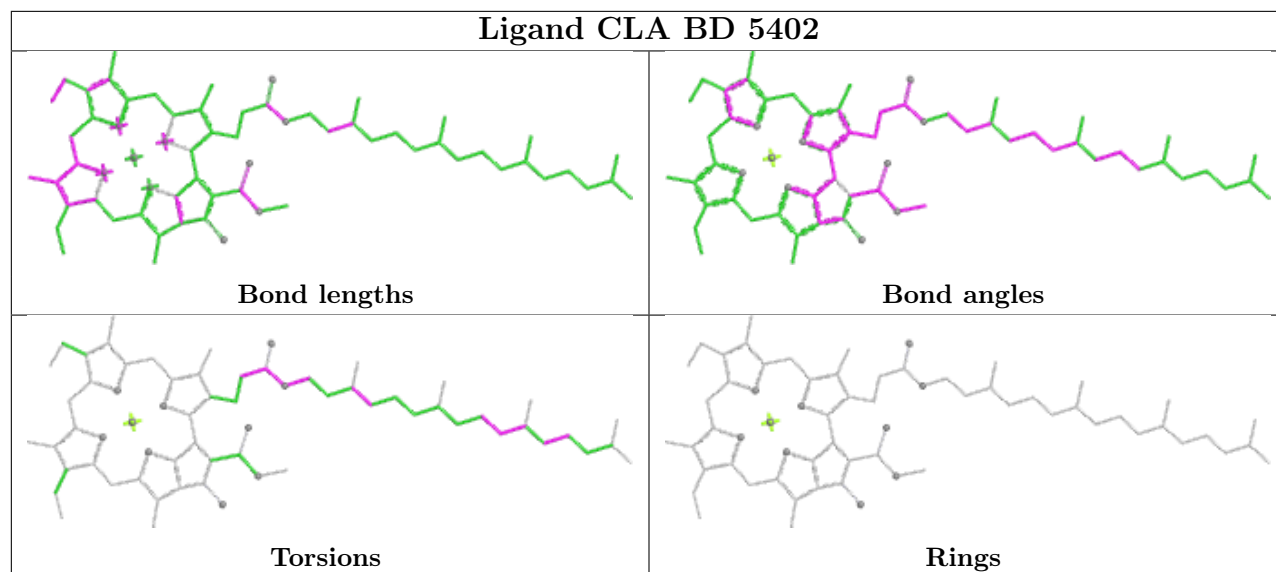
Ligand CLA BA 5408



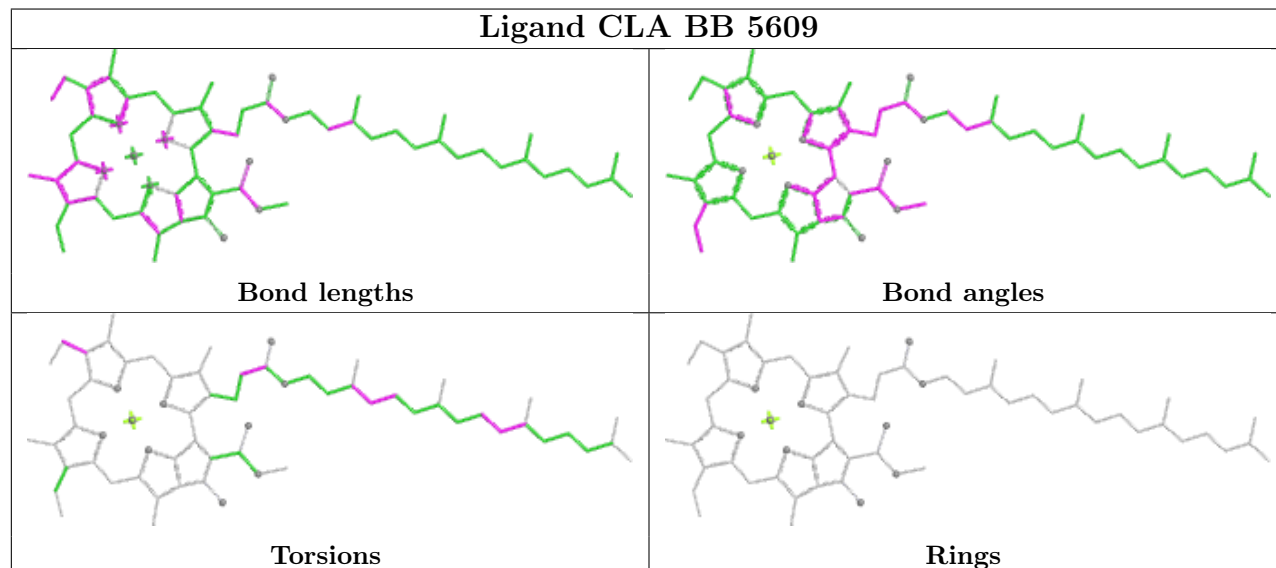




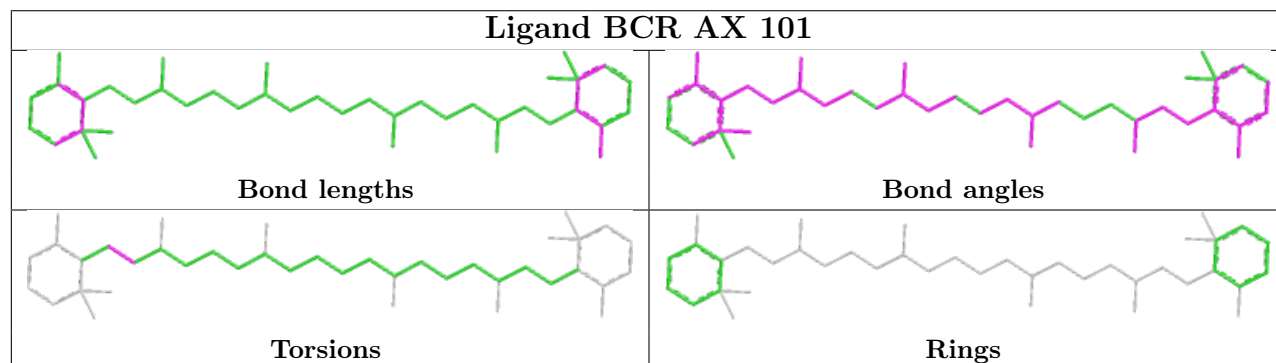
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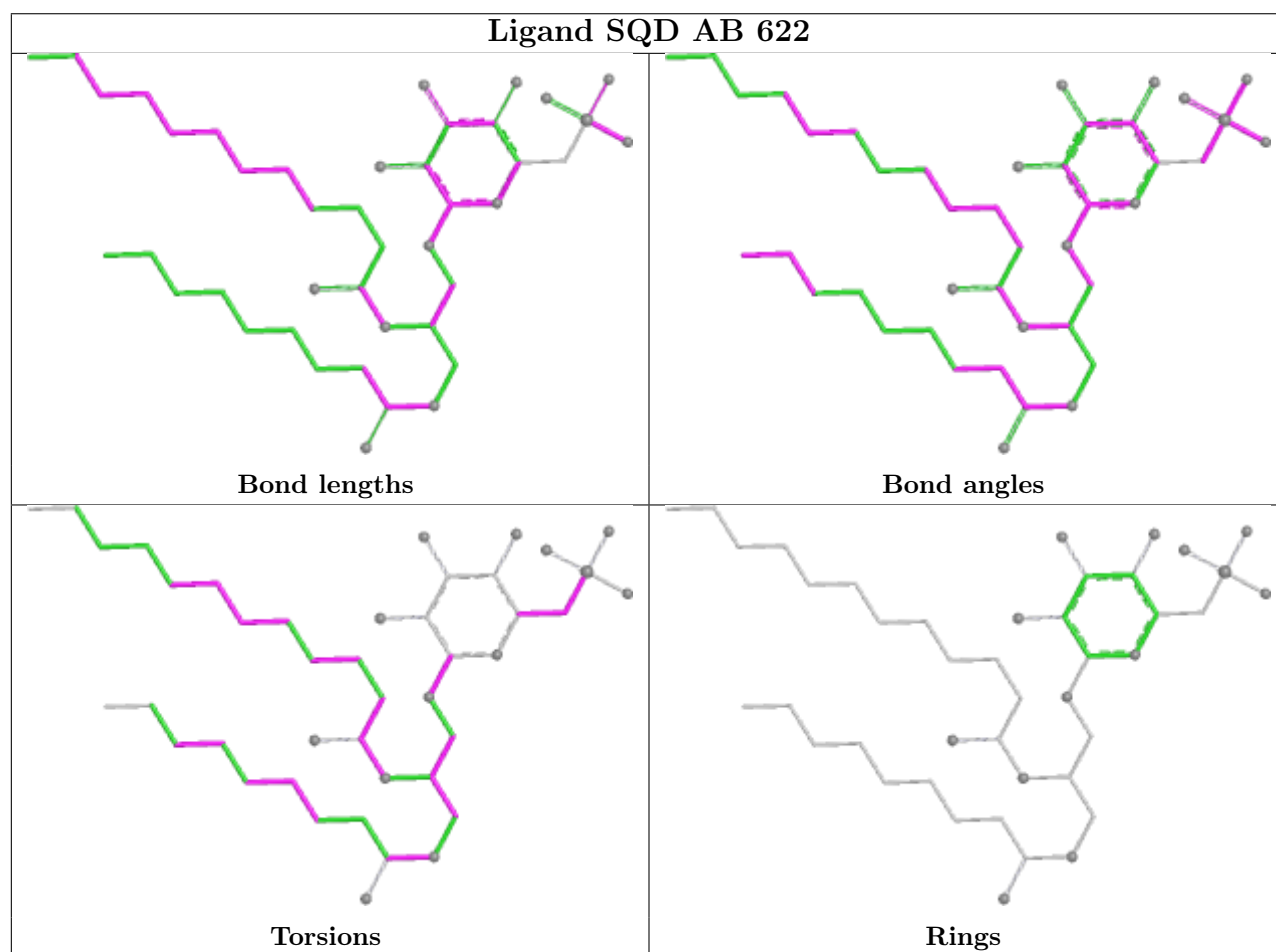
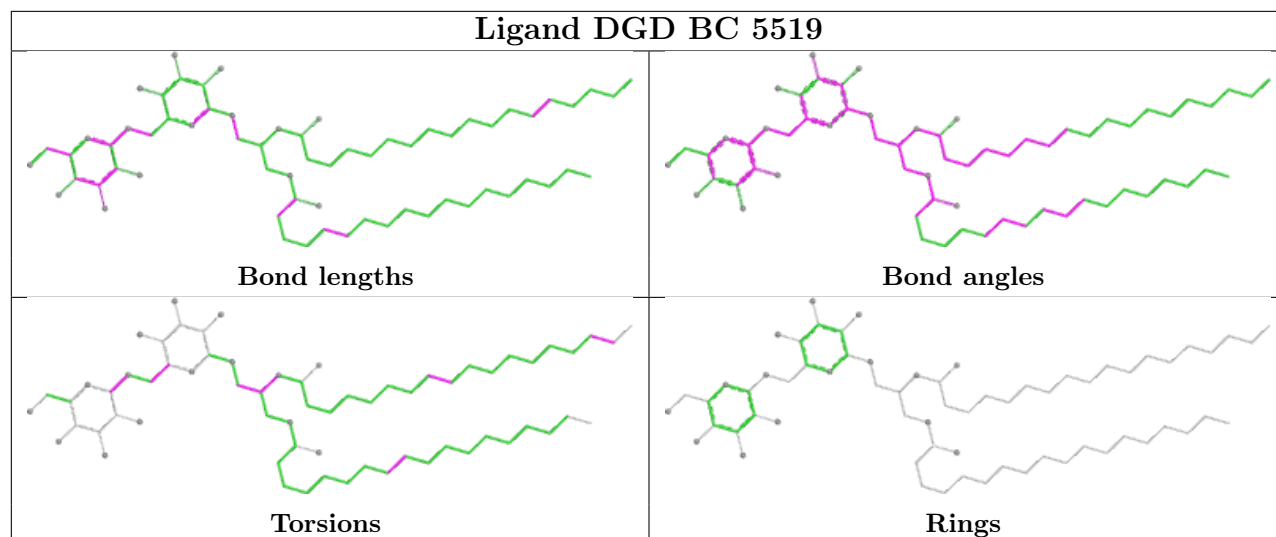


Ligand CLA BB 5609

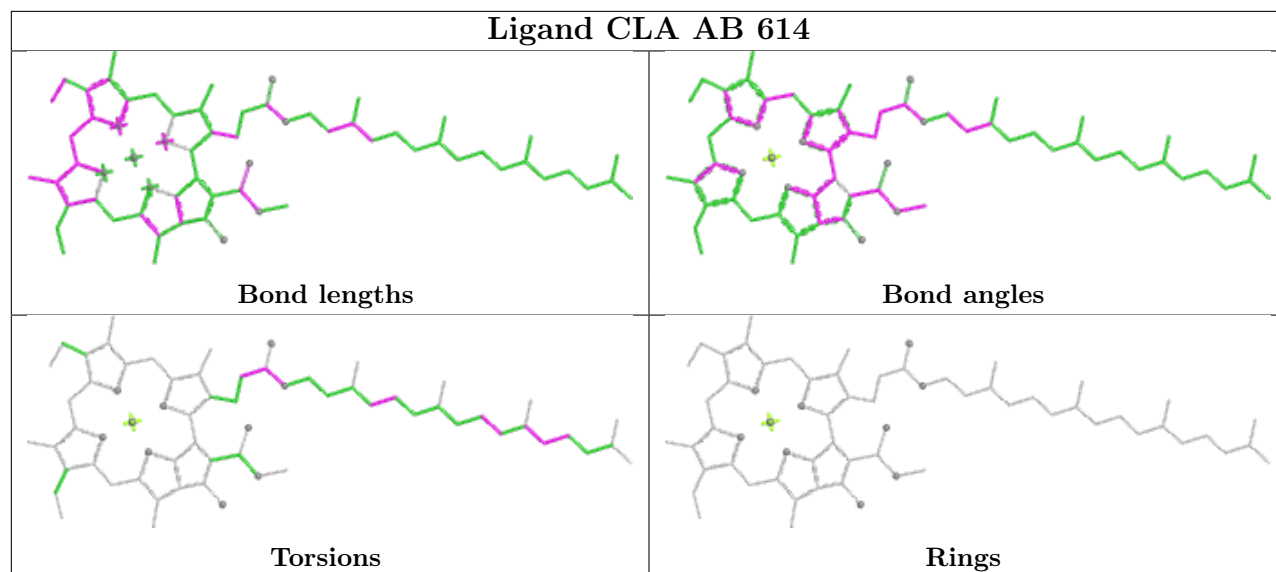


Ligand BCR AX 101

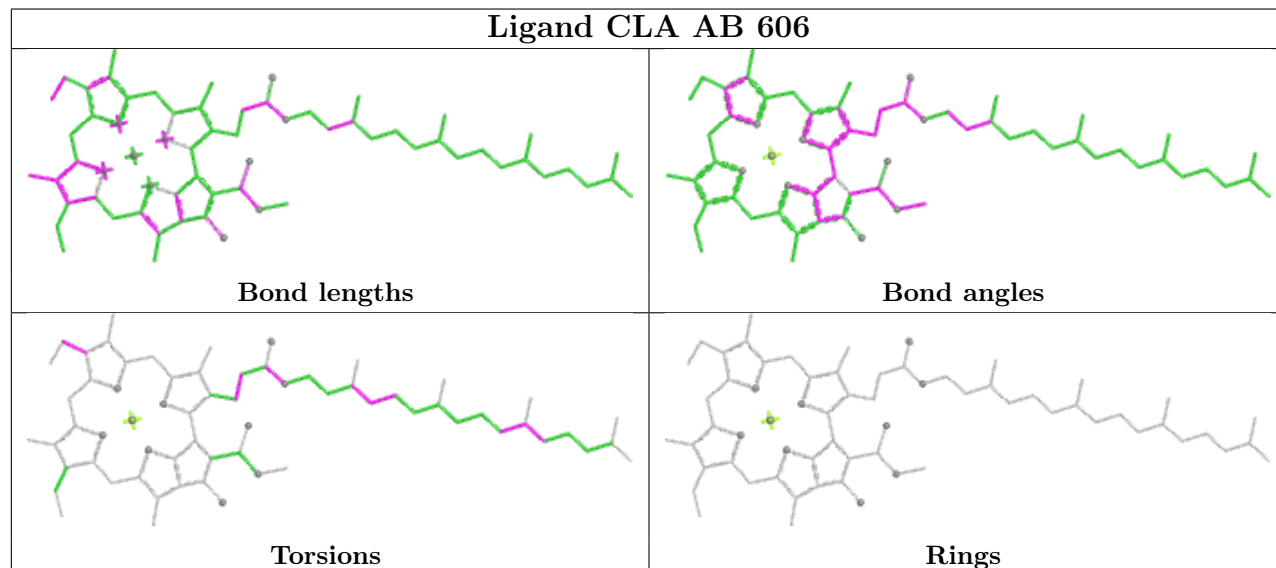




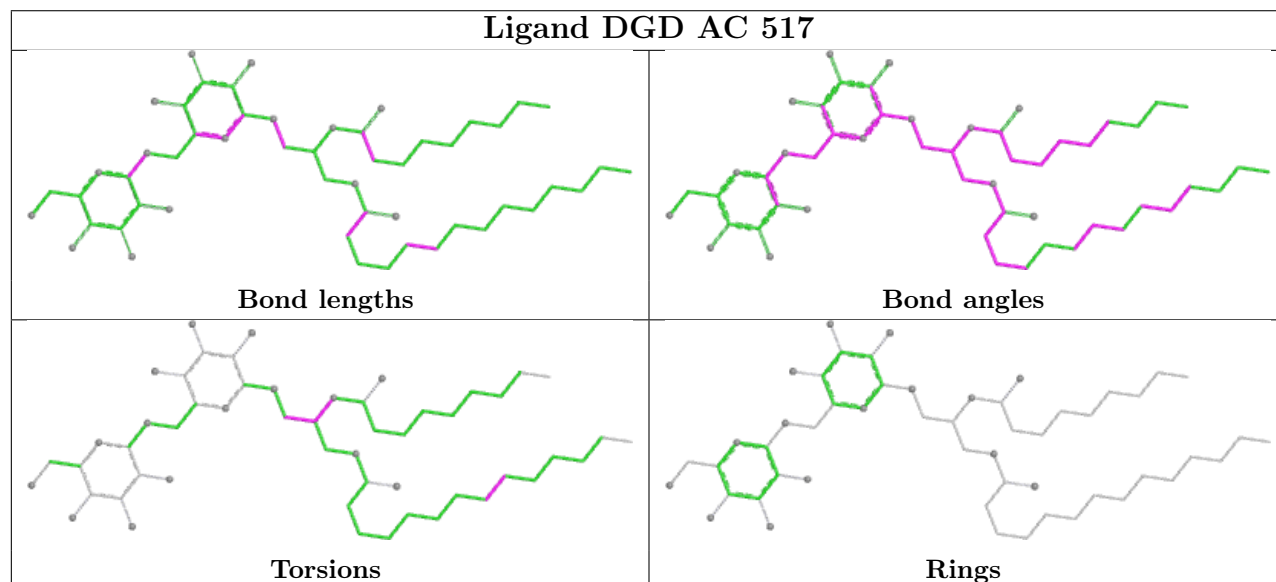
Ligand CLA AB 614



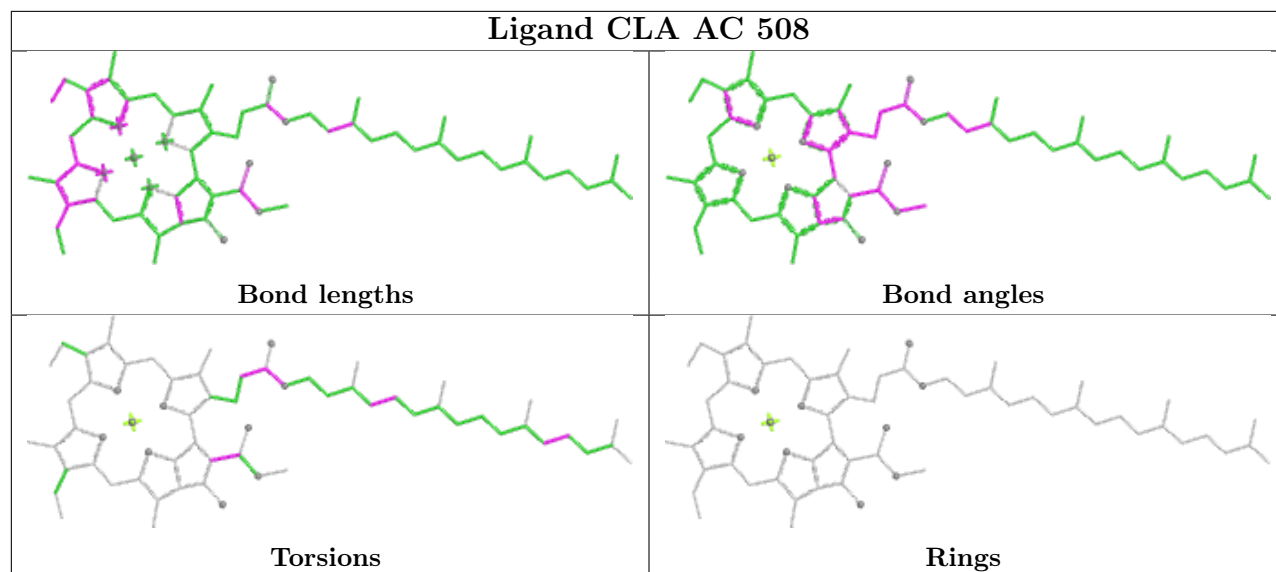
Ligand CLA AB 606



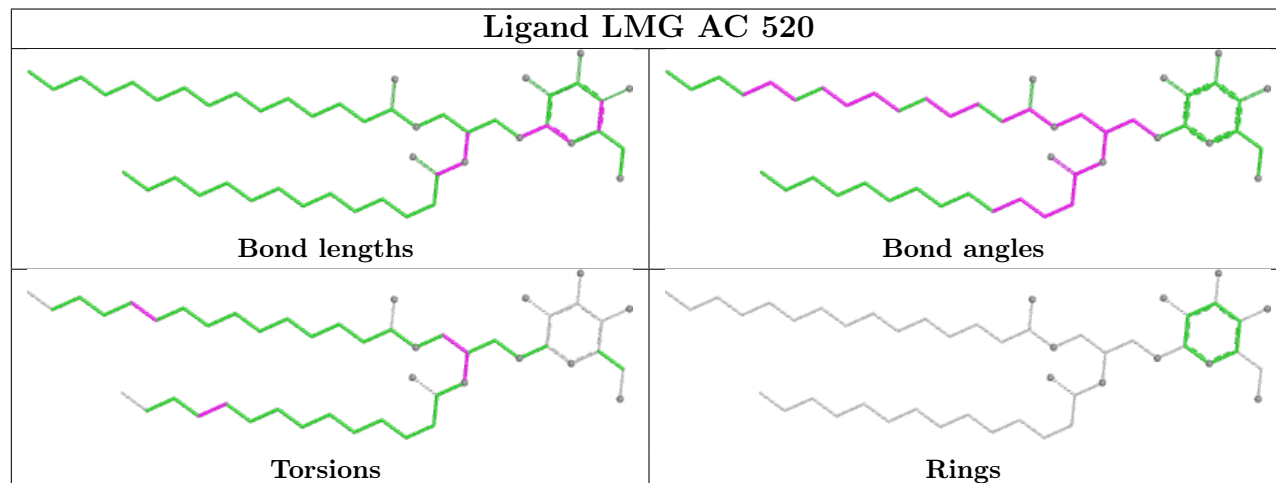
Ligand DGD AC 517



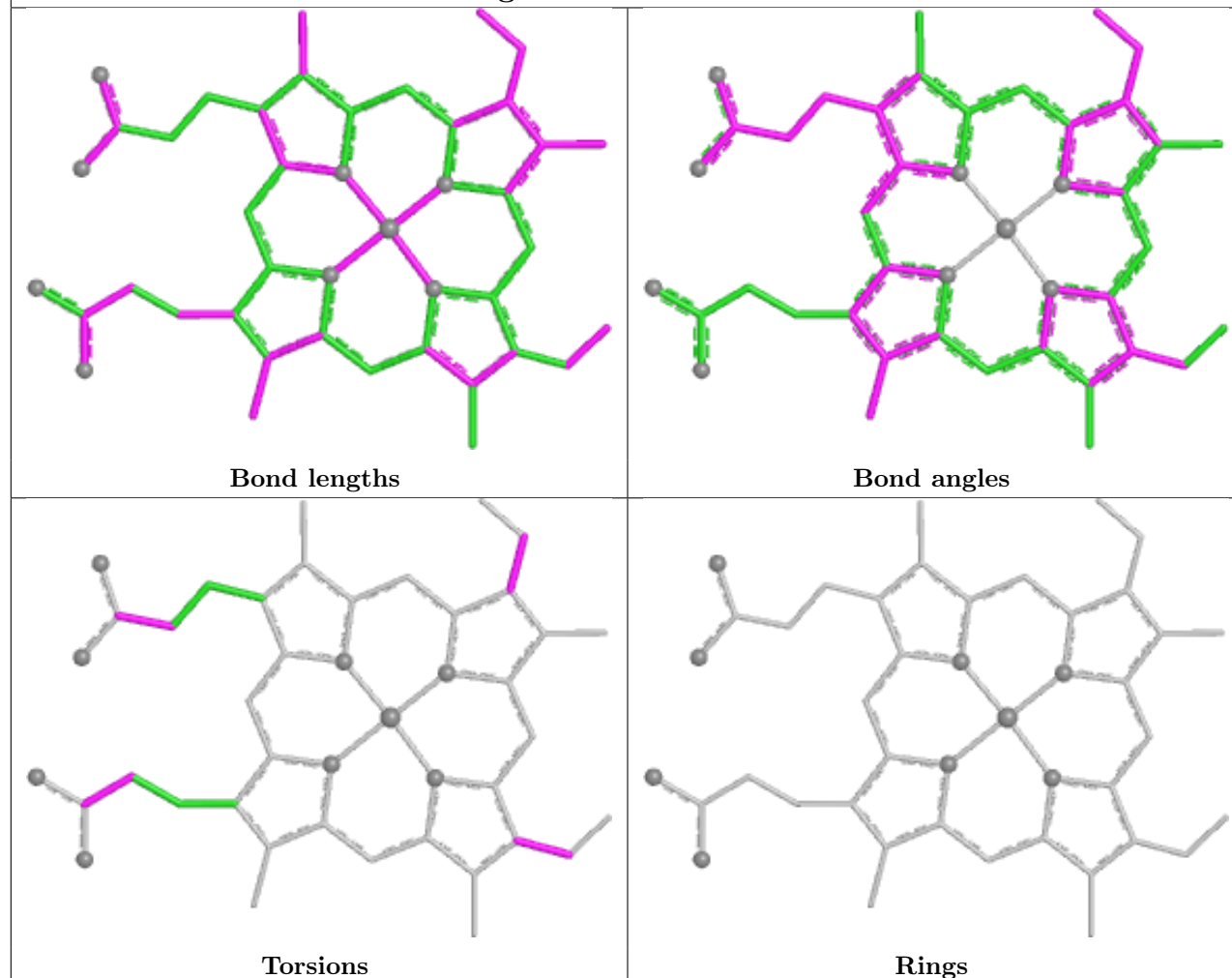
Ligand CLA AC 508



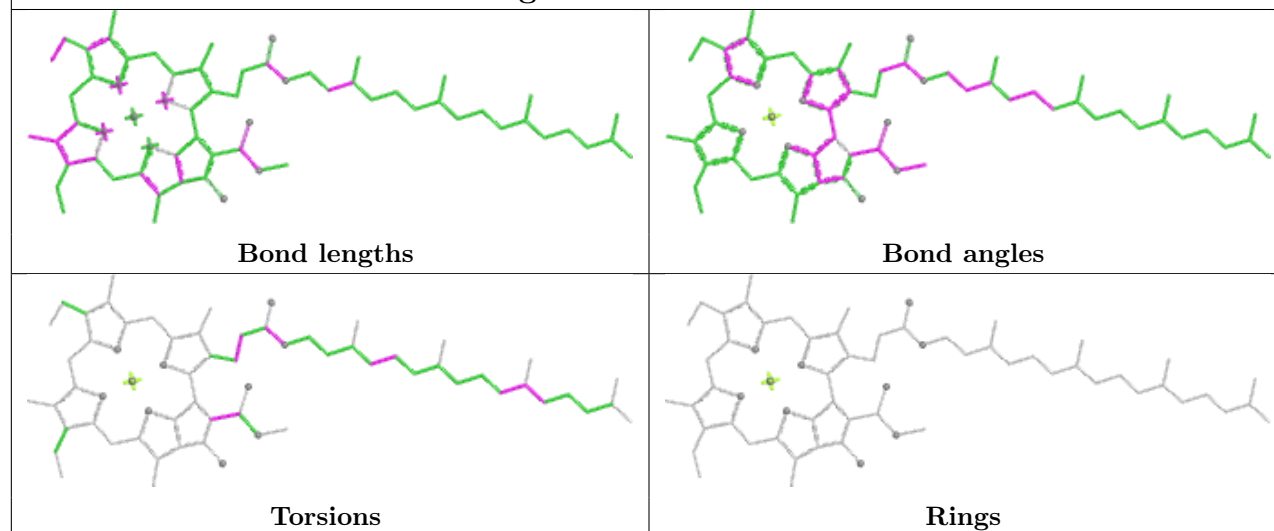
Ligand LMG AC 520

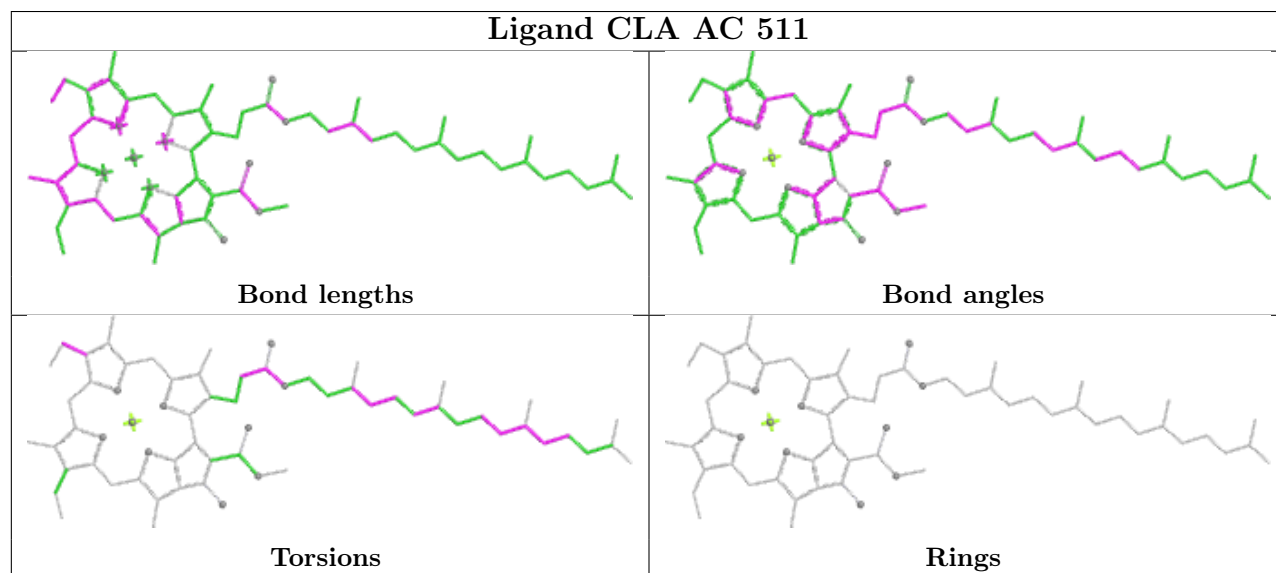
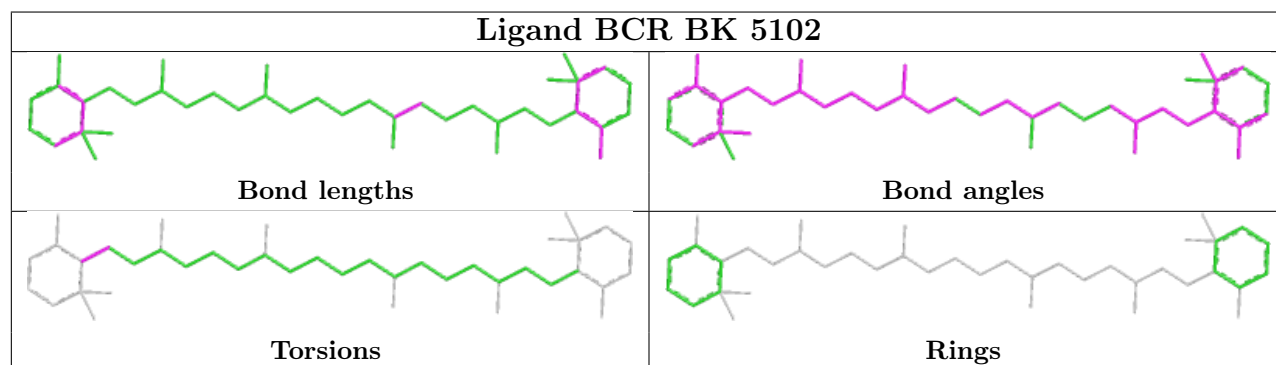
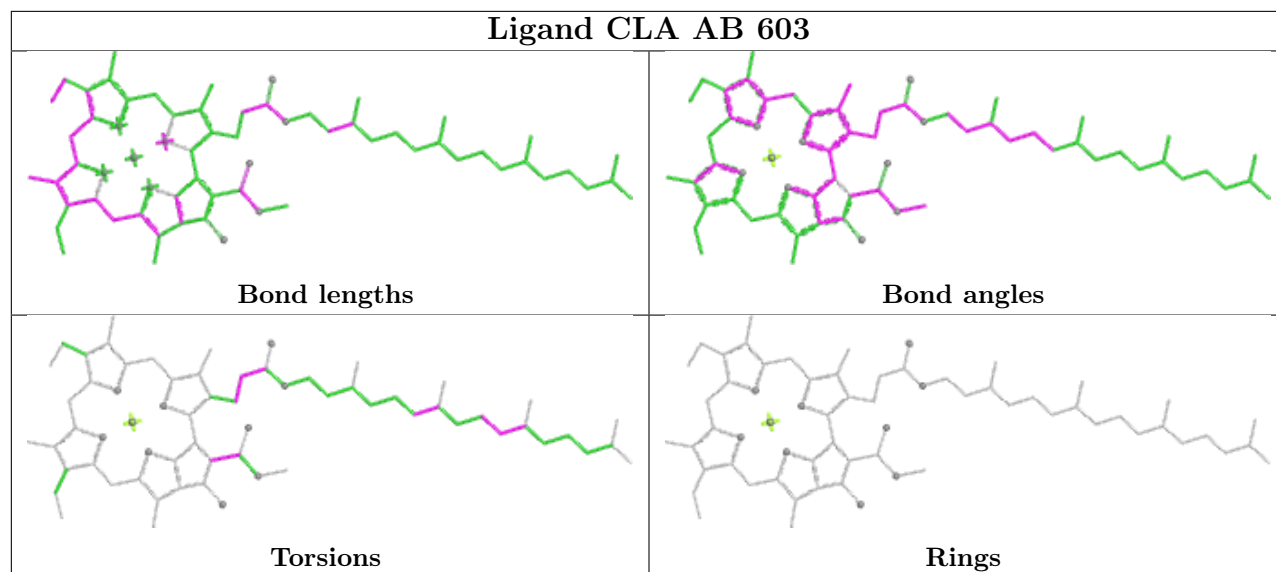


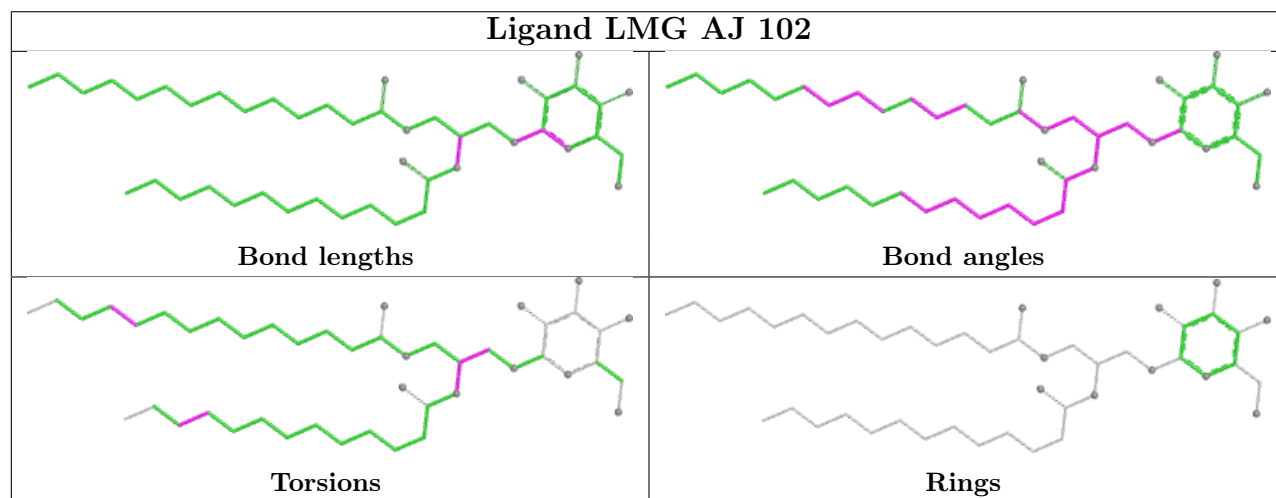
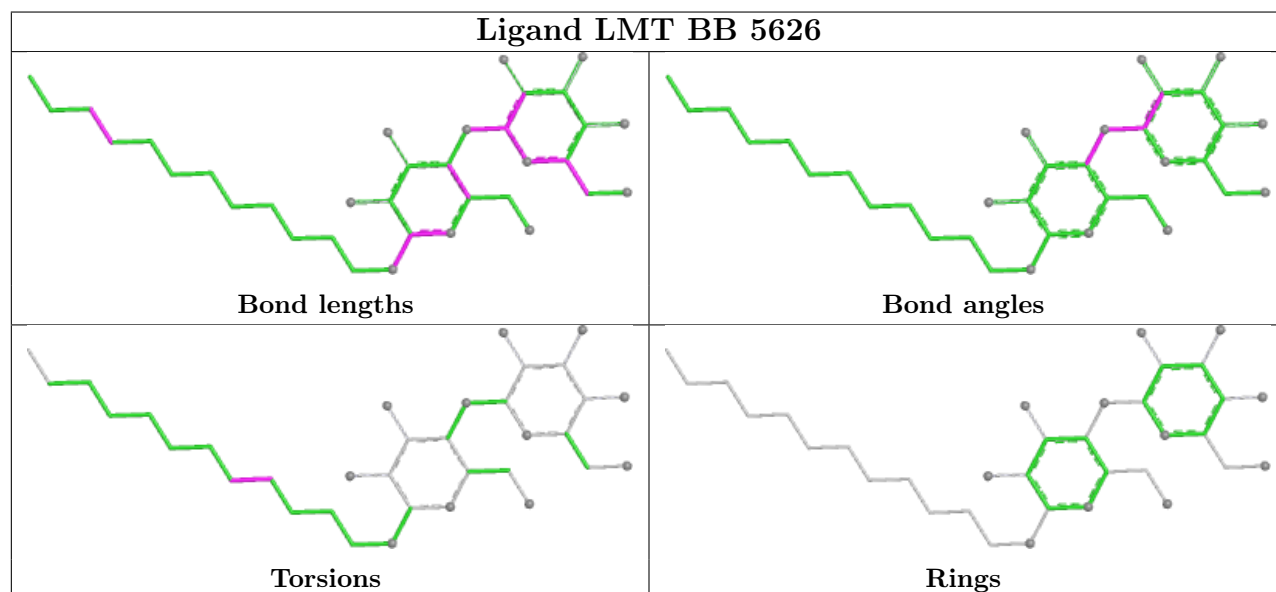
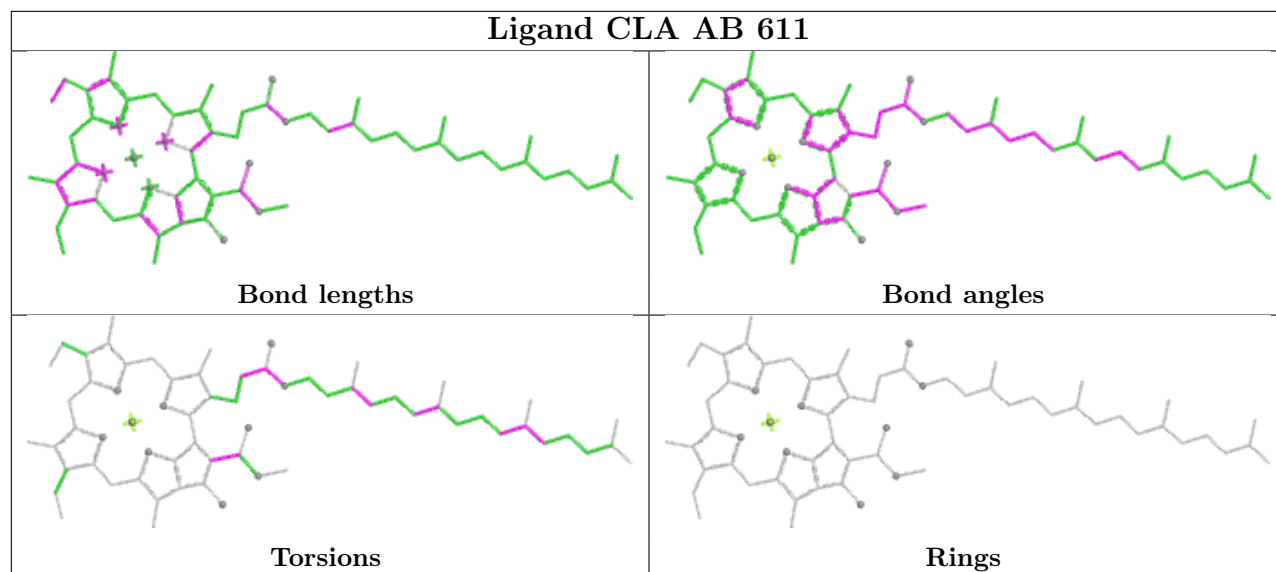
Ligand HEM AF 101

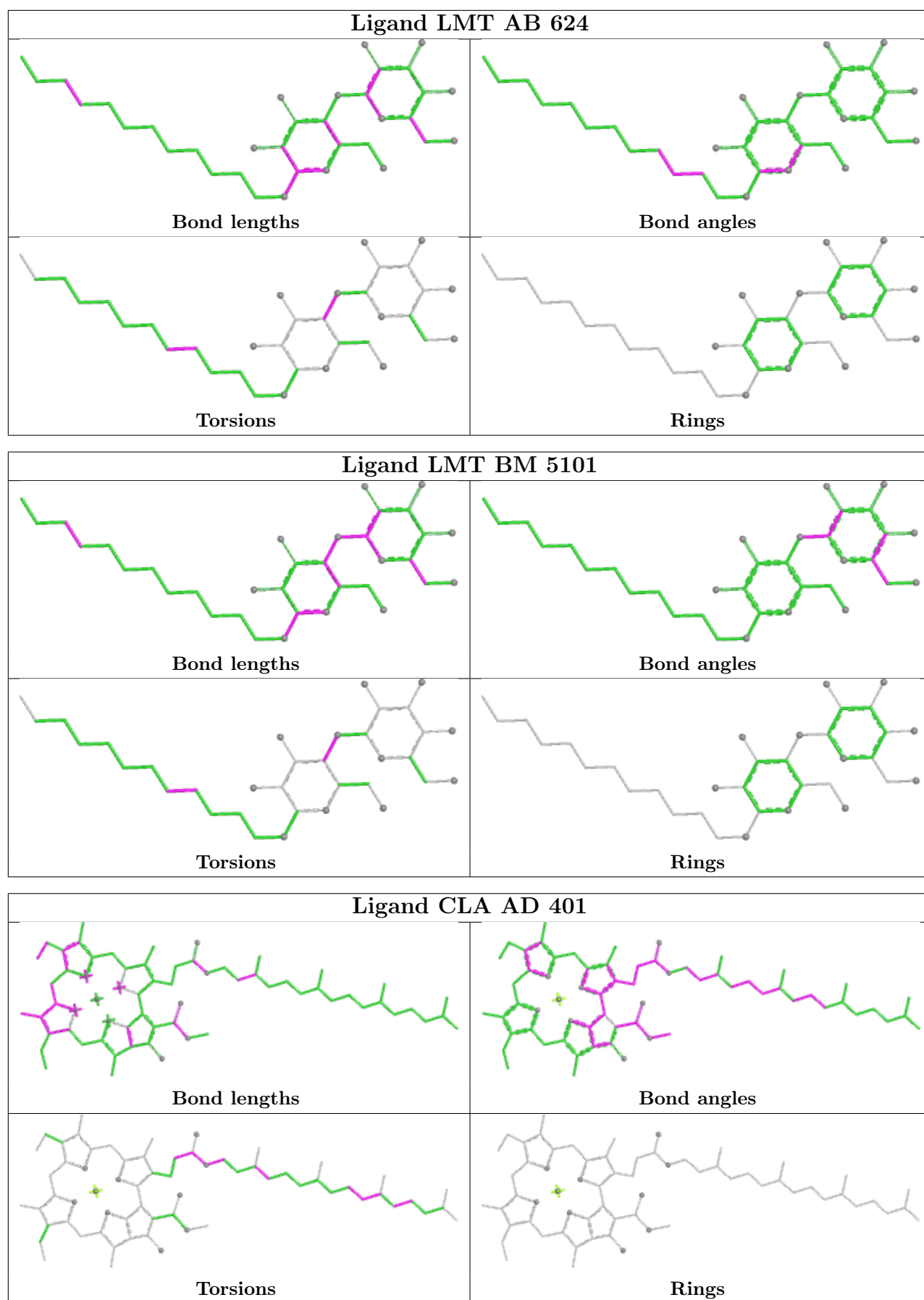


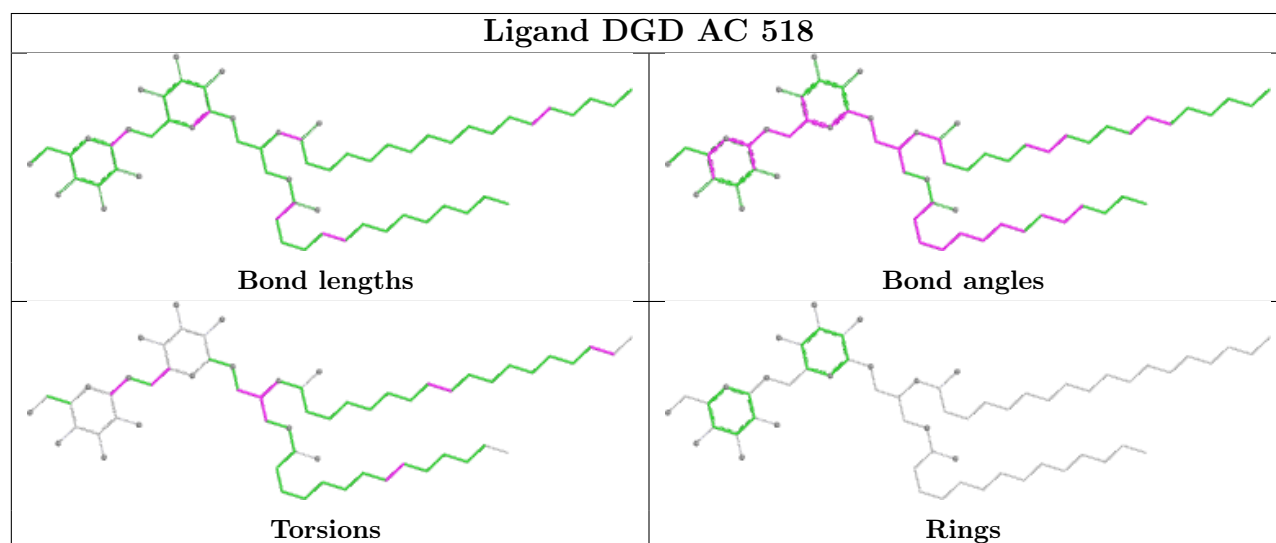
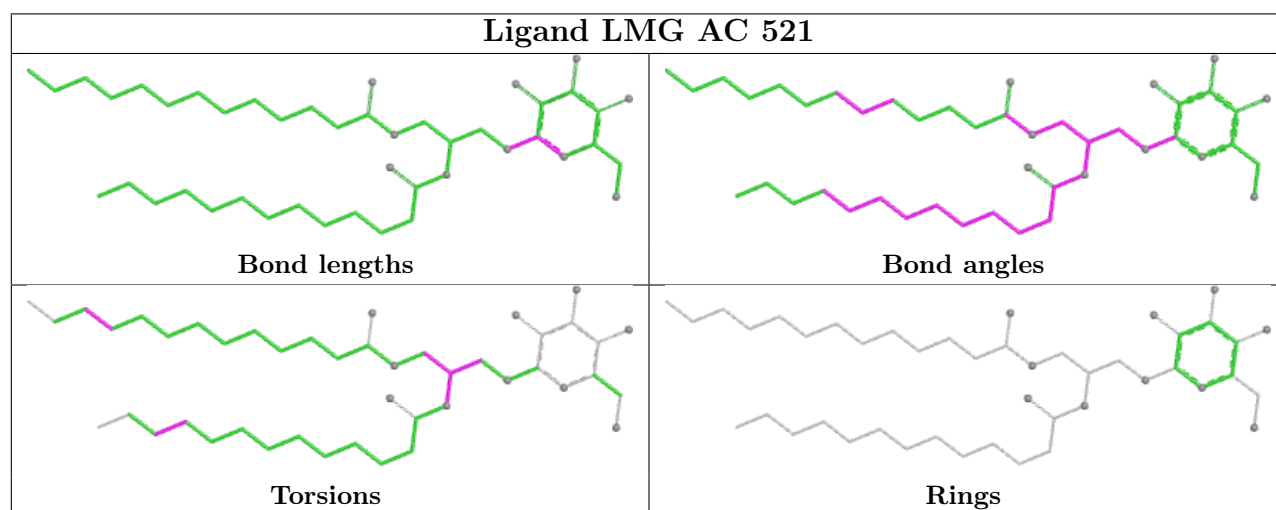
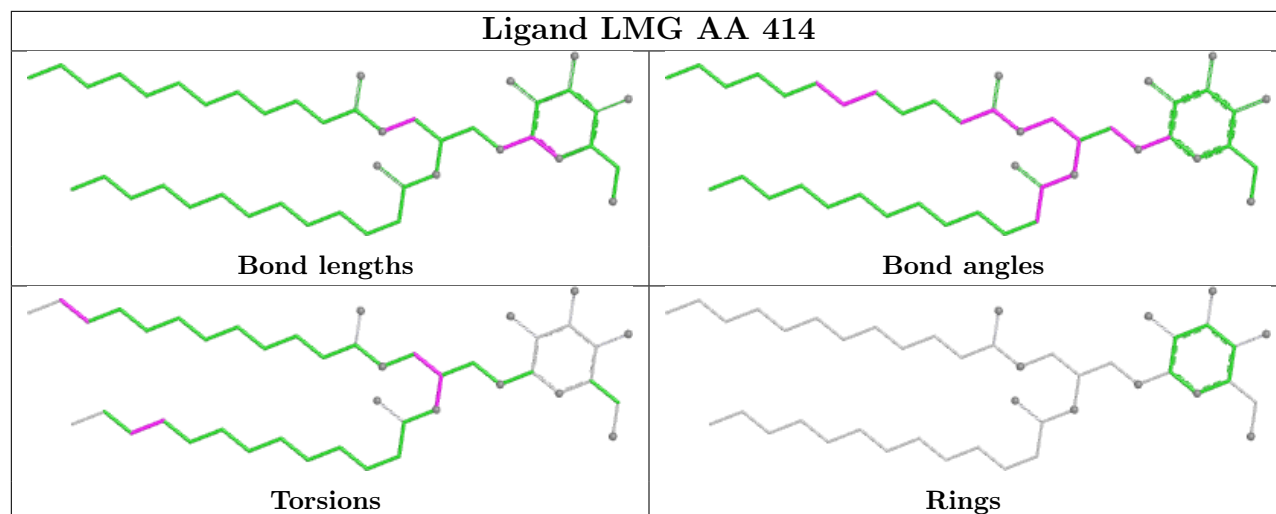
Ligand CLA AB 610

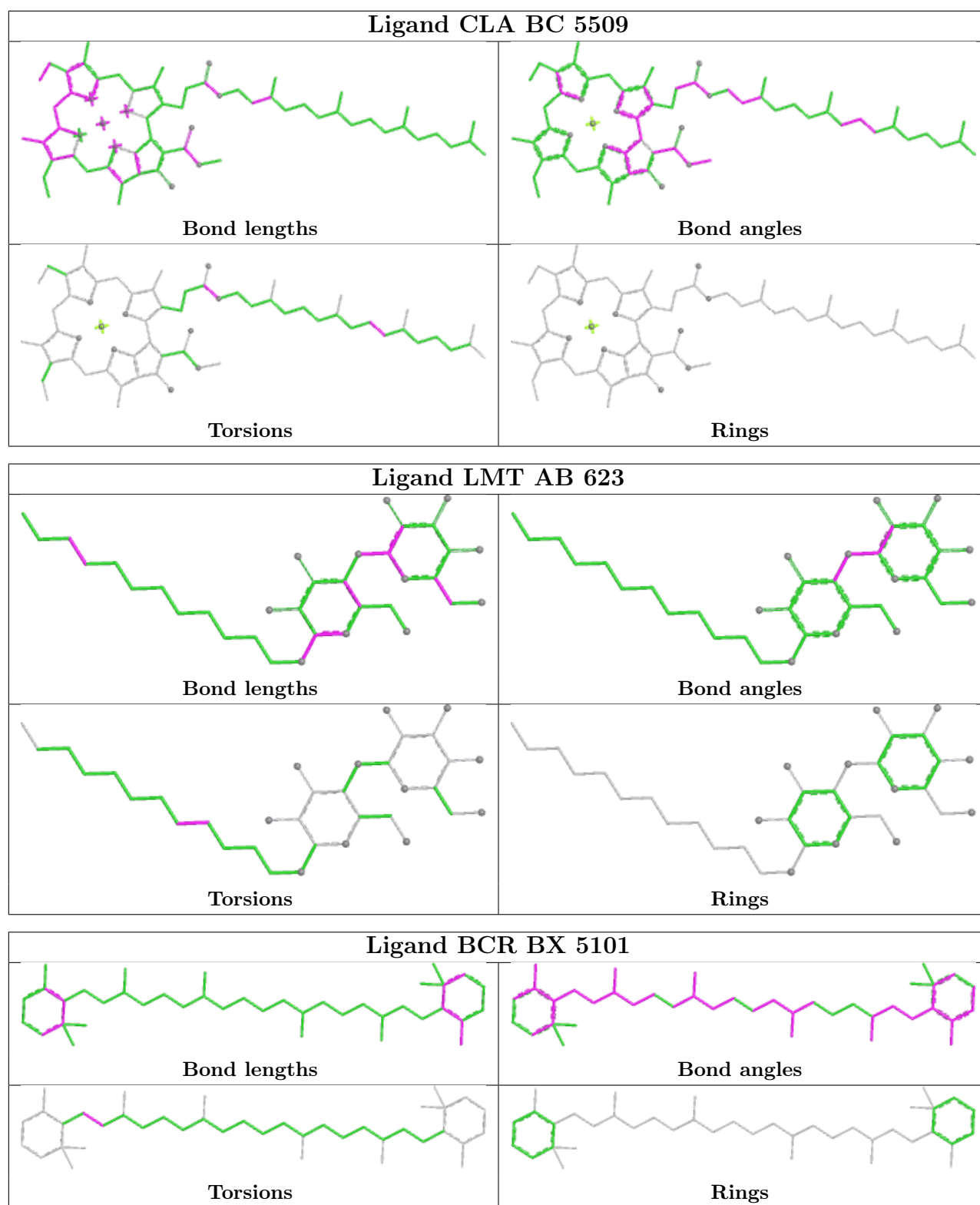


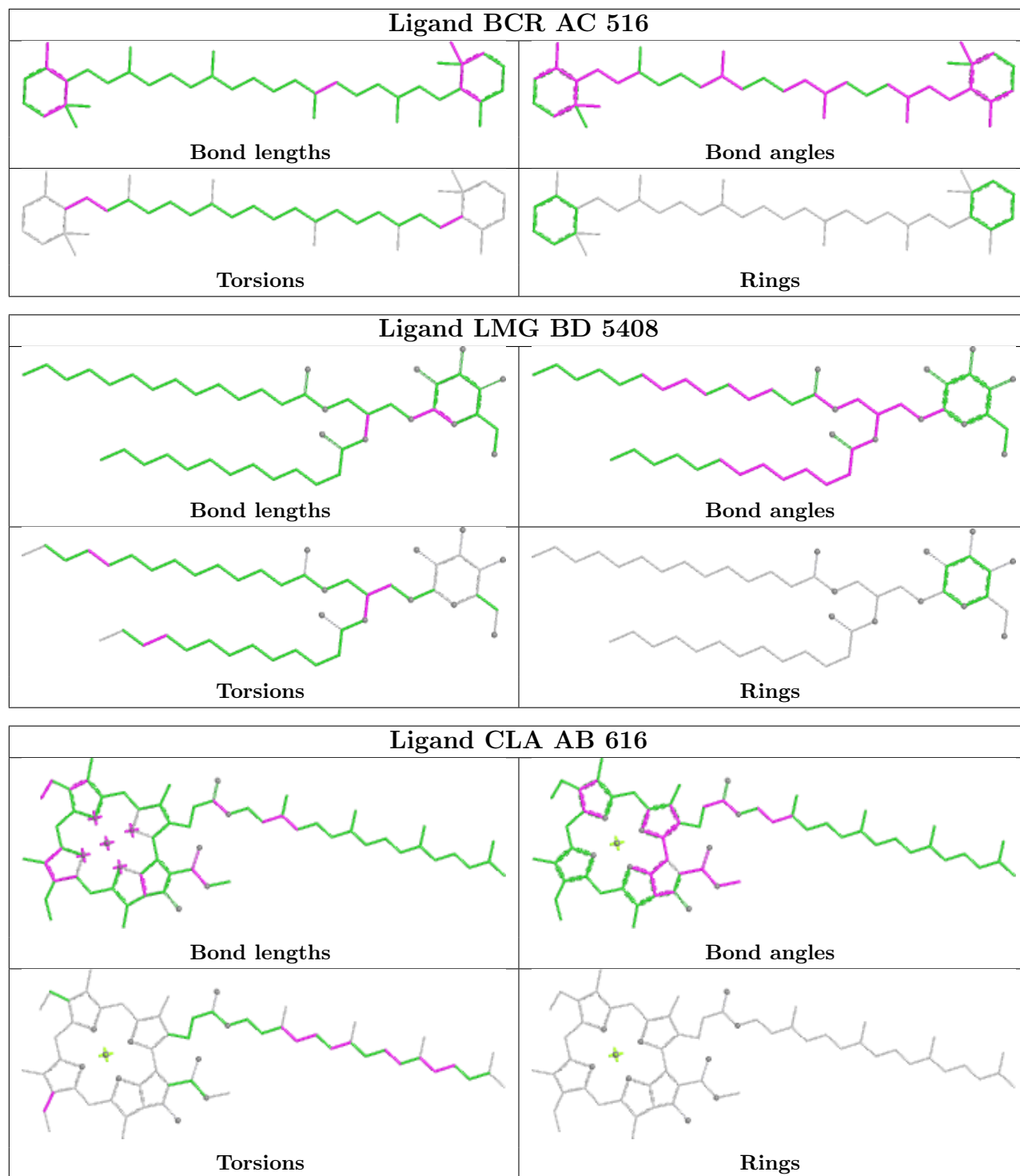


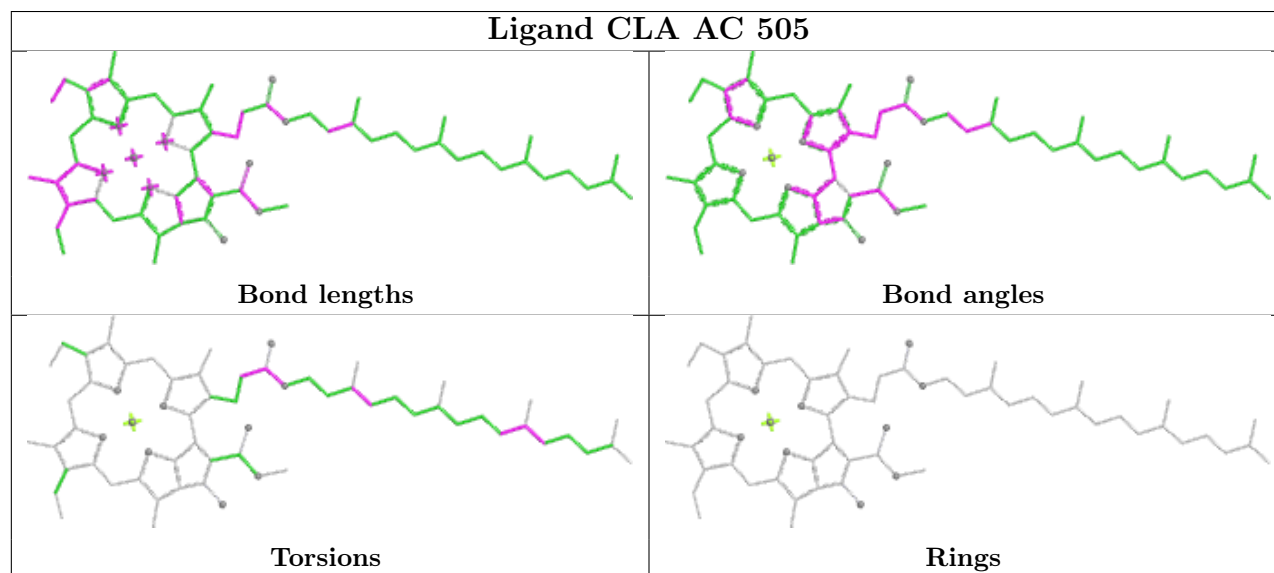
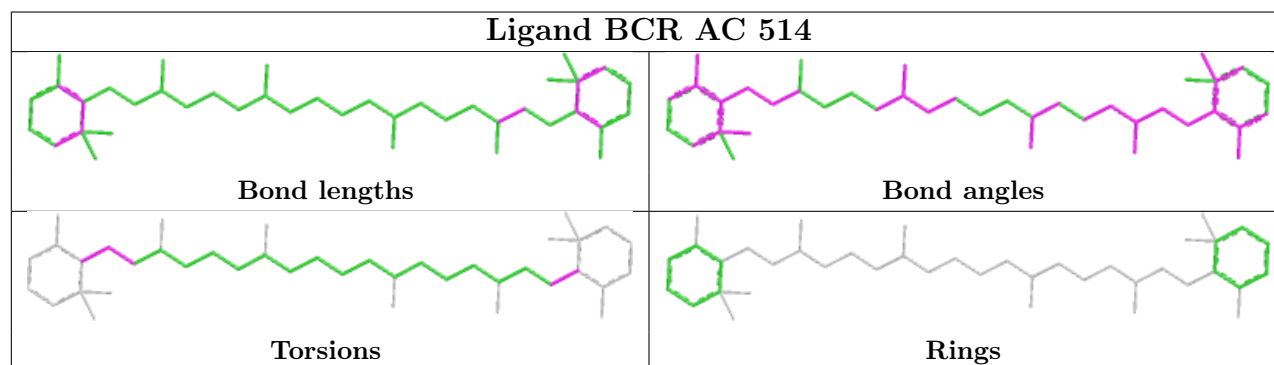
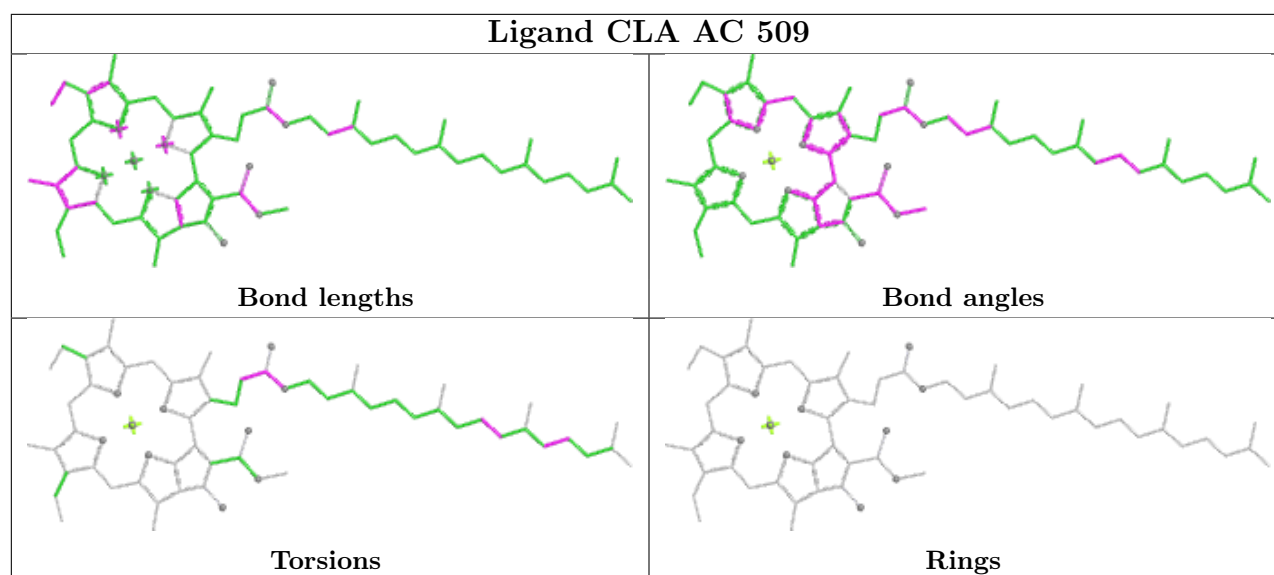




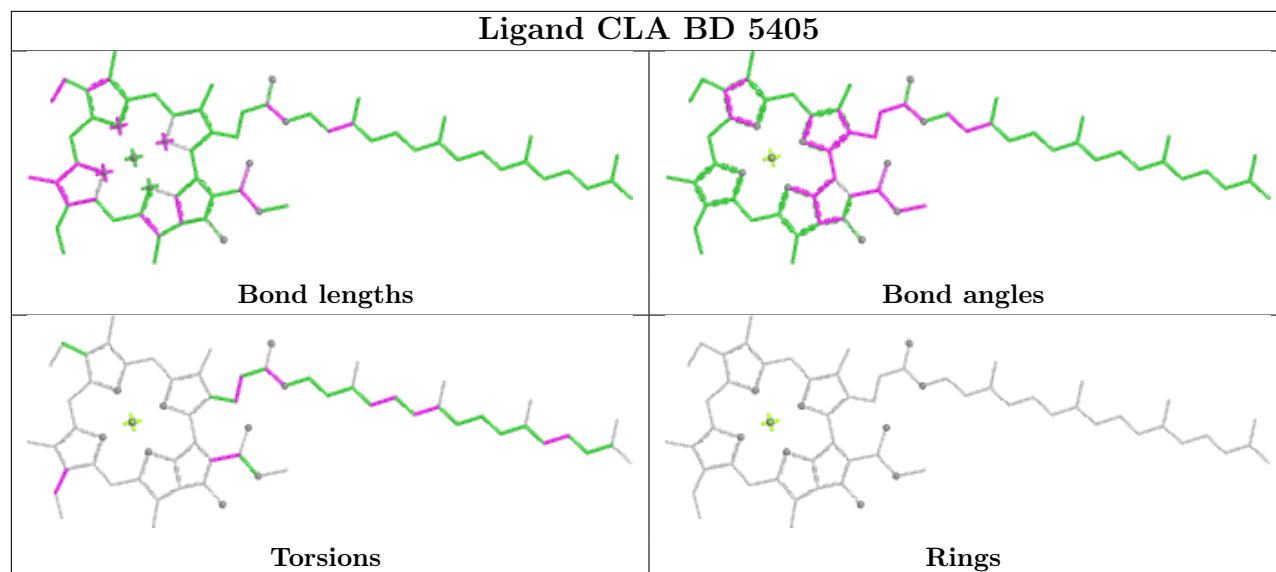




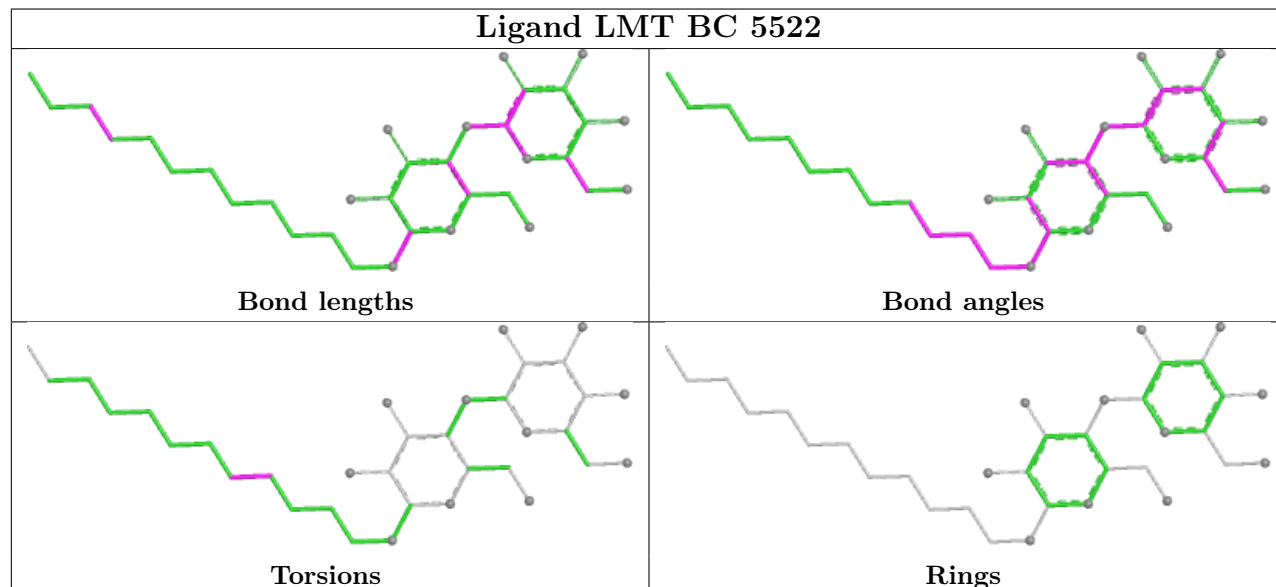




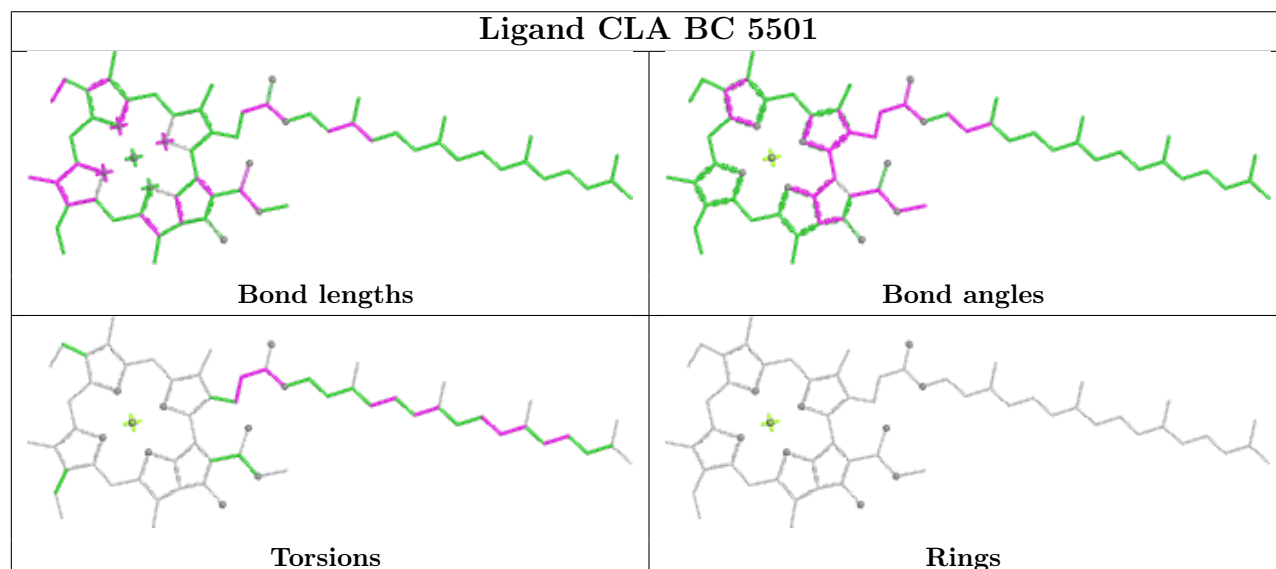
Ligand CLA BD 5405

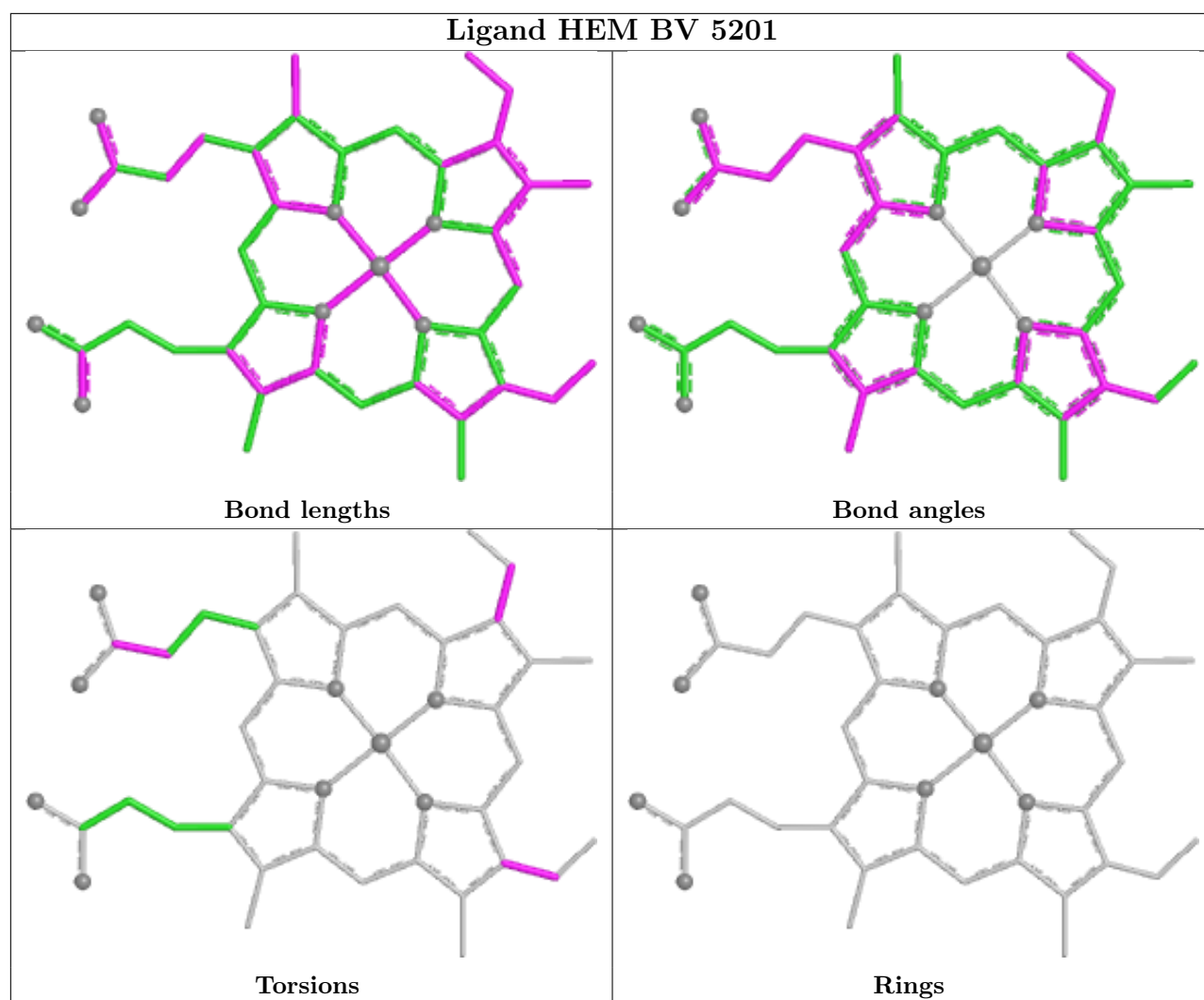


Ligand LMT BC 5522



Ligand CLA BC 5501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	335/344 (97%)	-0.02	1 (0%) 90 81	82, 104, 147, 160	0
1	BA	335/344 (97%)	-0.05	0 100 100	86, 106, 148, 160	0
2	AB	490/510 (96%)	-0.18	3 (0%) 85 73	81, 103, 136, 152	0
2	BB	490/510 (96%)	-0.13	4 (0%) 82 67	81, 103, 137, 152	0
3	AC	447/461 (96%)	0.09	3 (0%) 84 69	88, 122, 148, 158	0
3	BC	447/461 (96%)	0.06	4 (0%) 81 64	91, 124, 149, 159	0
4	AD	341/352 (96%)	-0.07	2 (0%) 85 73	81, 105, 139, 153	0
4	BD	341/352 (96%)	-0.15	5 (1%) 72 52	84, 106, 140, 154	0
5	AE	82/84 (97%)	0.15	3 (3%) 45 28	104, 126, 151, 155	0
5	BE	82/84 (97%)	-0.09	0 100 100	106, 127, 152, 156	0
6	AF	35/45 (77%)	0.04	0 100 100	107, 122, 157, 160	0
6	BF	35/45 (77%)	0.16	0 100 100	110, 123, 157, 160	0
7	AH	65/66 (98%)	0.03	0 100 100	113, 124, 140, 147	0
7	BH	65/66 (98%)	-0.05	2 (3%) 51 32	114, 124, 140, 148	0
8	AI	35/38 (92%)	0.10	1 (2%) 53 35	108, 115, 141, 147	0
8	BI	35/38 (92%)	0.09	0 100 100	108, 116, 142, 147	0
9	AJ	38/40 (95%)	0.04	2 (5%) 32 20	109, 122, 157, 159	0
9	BJ	38/40 (95%)	-0.10	0 100 100	111, 125, 158, 159	0
10	AK	37/37 (100%)	-0.17	0 100 100	121, 135, 145, 147	0
10	BK	37/37 (100%)	-0.11	0 100 100	123, 136, 147, 148	0
11	AL	37/37 (100%)	-0.15	0 100 100	88, 104, 159, 160	0
11	BL	37/37 (100%)	0.02	2 (5%) 31 20	90, 104, 158, 160	0
12	AM	34/36 (94%)	-0.36	0 100 100	89, 99, 142, 153	0
12	BM	34/36 (94%)	-0.34	0 100 100	90, 99, 140, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	0.04	0 100 100	83, 116, 148, 160	0
13	BO	243/247 (98%)	-0.11	3 (1%) 76 58	85, 117, 147, 160	0
14	AT	32/32 (100%)	-0.09	0 100 100	92, 106, 158, 160	0
14	BT	32/32 (100%)	-0.27	0 100 100	93, 106, 158, 160	0
15	AU	97/104 (93%)	-0.24	0 100 100	93, 105, 116, 125	0
15	BU	97/104 (93%)	-0.29	0 100 100	94, 106, 116, 127	0
16	AV	137/137 (100%)	-0.02	0 100 100	96, 112, 128, 132	0
16	BV	137/137 (100%)	-0.24	0 100 100	99, 114, 130, 134	0
17	Ay	28/46 (60%)	0.31	1 (3%) 46 28	141, 154, 160, 160	0
17	By	28/46 (60%)	0.33	0 100 100	143, 154, 160, 160	0
18	AX	37/41 (90%)	0.01	0 100 100	121, 129, 147, 150	0
18	BX	37/41 (90%)	-0.13	0 100 100	120, 130, 146, 149	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	-0.04	2 (3%) 50 31	134, 148, 160, 160	0
20	BZ	62/62 (100%)	0.36	1 (1%) 70 51	135, 150, 160, 160	0
All	All	5224/5494 (95%)	-0.06	39 (0%) 84 69	81, 113, 149, 160	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BH	5065	LEU	4.6
3	AC	260	ALA	4.5
2	BB	5491	VAL	3.3
9	AJ	15	THR	3.0
4	AD	241	GLU	2.9
4	AD	234	ALA	2.9
3	AC	416	SER	2.8
2	AB	491	VAL	2.8
4	BD	5099	GLY	2.7
2	BB	5236	THR	2.7
5	AE	83	LEU	2.7
13	BO	5084	ASN	2.7
4	BD	5097	ALA	2.6
1	AA	203	ALA	2.4
2	BB	5488	PRO	2.3
4	BD	5064	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
13	BO	5250	ASP	2.3
2	AB	232	GLY	2.3
7	BH	5066	GLY	2.2
11	BL	5005	PRO	2.2
3	BC	5264	PHE	2.2
20	BZ	5062	VAL	2.2
4	BD	5059	TYR	2.2
3	BC	5032	GLY	2.2
4	BD	5226	GLY	2.2
8	AI	2	GLU	2.1
11	BL	5019	LEU	2.1
9	AJ	37	GLY	2.1
20	AZ	33	TRP	2.1
13	BO	5052	ALA	2.1
2	AB	59	GLY	2.1
5	AE	17	VAL	2.0
3	AC	448	ALA	2.0
17	Ay	35	ILE	2.0
3	BC	5057	ALA	2.0
3	BC	5260	ALA	2.0
5	AE	57	ALA	2.0
20	AZ	34	ASP	2.0
2	BB	5161	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	LMG	AI	101	43/55	0.35	0.18	159,160,160,160	0
28	DGD	BE	5102	63/66	0.44	0.18	145,160,160,160	0
28	DGD	AE	101	63/66	0.47	0.19	146,160,160,160	0
29	LHG	BA	5415	37/49	0.48	0.17	151,160,160,160	0
31	LMG	BI	5101	43/55	0.49	0.13	160,160,160,160	0
28	DGD	AA	411	56/66	0.52	0.18	148,158,160,160	0
28	DGD	BA	5412	56/66	0.52	0.15	150,160,160,160	0
28	DGD	BB	5602	52/66	0.53	0.16	152,160,160,160	0
32	LMT	AB	623	35/35	0.53	0.15	135,160,160,160	0
28	DGD	AB	628	52/66	0.55	0.15	154,160,160,160	0
32	LMT	BI	5102	35/35	0.55	0.16	151,160,160,160	0
32	LMT	BB	5626	35/35	0.57	0.20	131,160,160,160	0
31	LMG	AA	414	44/55	0.57	0.15	140,160,160,160	0
30	SQD	BA	5401	54/54	0.58	0.14	136,160,160,160	0
31	LMG	BC	5521	45/55	0.60	0.13	154,160,160,160	0
27	BCR	BJ	5101	40/40	0.62	0.15	160,160,160,160	0
32	LMT	BB	5604	35/35	0.62	0.15	131,160,160,160	0
31	LMG	AC	520	48/55	0.63	0.17	136,157,160,160	0
31	LMG	BE	5101	44/55	0.64	0.16	140,160,160,160	0
32	LMT	BC	5522	35/35	0.64	0.11	157,160,160,160	0
30	SQD	BB	5625	43/54	0.64	0.13	132,148,160,160	0
37	CA	AF	103	1/1	0.64	0.08	150,150,150,150	0
32	LMT	AI	103	35/35	0.67	0.17	156,158,160,160	0
30	SQD	AB	622	43/54	0.68	0.13	133,149,160,160	0
30	SQD	BF	5102	45/54	0.68	0.13	154,160,160,160	0
30	SQD	AF	102	45/54	0.68	0.15	154,160,160,160	0
24	CLA	AB	601	65/65	0.68	0.17	146,159,160,160	0
31	LMG	AC	521	45/55	0.68	0.14	154,160,160,160	0
32	LMT	AB	624	35/35	0.68	0.14	156,160,160,160	0
32	LMT	AB	630	35/35	0.69	0.14	132,160,160,160	0
32	LMT	AI	102	35/35	0.69	0.14	149,158,160,160	0
32	LMT	BD	5411	31/35	0.69	0.16	140,152,160,160	0
31	LMG	BC	5520	48/55	0.69	0.15	138,159,160,160	0
30	SQD	BA	5414	51/54	0.69	0.14	145,150,160,160	0
28	DGD	BC	5518	62/66	0.70	0.17	147,156,160,160	0
27	BCR	AJ	101	40/40	0.70	0.20	158,160,160,160	0
32	LMT	BB	5603	35/35	0.70	0.17	132,160,160,160	0
37	CA	AO	301	1/1	0.70	0.07	152,152,152,152	0
31	LMG	BA	5402	42/55	0.71	0.20	144,157,160,160	0
31	LMG	AB	620	51/55	0.71	0.20	125,139,150,151	0
23	CL	AA	403[B]	1/1	0.72	0.33	108,108,108,108	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMT	AD	409	31/35	0.72	0.13	139,154,160,160	0
29	LHG	AA	415	37/49	0.72	0.14	149,160,160,160	0
23	CL	AA	403[A]	1/1	0.72	0.33	33,33,33,33	1
31	LMG	BL	5101	51/55	0.73	0.18	122,138,151,152	0
33	DMS	AV	202	4/4	0.73	0.22	148,148,148,149	0
28	DGD	BC	5519	66/66	0.74	0.16	112,121,158,159	0
24	CLA	BB	5605	65/65	0.74	0.20	146,159,160,160	0
32	LMT	AB	629	35/35	0.74	0.17	133,160,160,160	0
31	LMG	BD	5410	48/55	0.74	0.20	126,131,141,141	0
28	DGD	AC	518	62/66	0.75	0.16	146,155,160,160	0
28	DGD	AC	519	66/66	0.75	0.16	110,120,157,158	0
31	LMG	BD	5408	46/55	0.76	0.17	139,145,160,160	0
30	SQD	BB	5601	47/54	0.76	0.14	137,156,160,160	0
33	DMS	AU	201	4/4	0.76	0.23	160,160,160,160	0
30	SQD	AA	416	54/54	0.76	0.12	136,160,160,160	0
32	LMT	BB	5627	35/35	0.76	0.12	156,160,160,160	0
31	LMG	AM	101	42/55	0.76	0.17	136,158,160,160	0
31	LMG	AA	417	42/55	0.77	0.20	145,157,160,160	0
31	LMG	AB	621	49/55	0.77	0.17	145,150,157,160	0
24	CLA	BC	5513	65/65	0.78	0.14	158,160,160,160	0
33	DMS	BB	5629	4/4	0.78	0.18	125,126,127,127	0
31	LMG	AD	408	48/55	0.78	0.18	121,130,139,139	0
31	LMG	BM	5102	42/55	0.78	0.18	136,160,160,160	0
30	SQD	AA	413	51/54	0.79	0.12	143,150,160,160	0
32	LMT	AM	102	35/35	0.79	0.11	126,149,154,154	0
32	LMT	BM	5101	35/35	0.80	0.13	126,149,154,155	0
30	SQD	AB	627	47/54	0.80	0.12	138,157,160,160	0
27	BCR	BC	5516	40/40	0.80	0.14	136,140,145,145	0
27	BCR	BK	5102	40/40	0.81	0.16	136,140,152,152	0
24	CLA	AC	506	65/65	0.81	0.15	136,143,160,160	0
31	LMG	BB	5624	49/55	0.82	0.15	145,150,157,160	0
24	CLA	BC	5512	65/65	0.82	0.13	157,160,160,160	0
31	LMG	AJ	102	46/55	0.82	0.18	139,144,160,160	0
37	CA	BO	5301	1/1	0.82	0.10	160,160,160,160	0
24	CLA	BC	5511	65/65	0.83	0.16	154,158,159,160	0
33	DMS	BB	5628	4/4	0.83	0.14	156,157,157,157	0
27	BCR	AX	101	40/40	0.83	0.15	135,143,158,159	0
28	DGD	BC	5517	53/66	0.83	0.15	124,130,136,139	0
27	BCR	BT	5101	40/40	0.83	0.14	124,143,147,147	0
26	OEC	BA	5410	5/9	0.83	0.10	23,88,99,134	0
24	CLA	BD	5405	65/65	0.84	0.15	125,131,148,149	0
28	DGD	BH	5101	58/66	0.84	0.15	107,118,156,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	BCR	AC	515	40/40	0.84	0.14	149,152,155,155	0
28	DGD	AC	517	53/66	0.85	0.20	121,128,135,140	0
22	BCT	AA	402	4/4	0.85	0.10	135,136,137,137	0
27	BCR	BC	5515	40/40	0.85	0.13	150,152,155,156	0
24	CLA	BC	5505	65/65	0.85	0.14	123,148,152,153	0
31	LMG	AD	407	49/55	0.85	0.14	126,133,143,145	0
24	CLA	AD	404	65/65	0.85	0.14	126,130,148,149	0
27	BCR	AT	101	40/40	0.86	0.15	126,140,146,147	0
31	LMG	BD	5409	49/55	0.86	0.15	128,133,144,146	0
27	BCR	BX	5101	40/40	0.86	0.14	136,143,157,158	0
33	DMS	AB	625	4/4	0.86	0.14	156,157,157,157	0
33	DMS	AB	626	4/4	0.86	0.15	129,130,130,130	0
37	CA	BF	5103	1/1	0.86	0.07	146,146,146,146	0
24	CLA	BC	5503	65/65	0.86	0.15	137,147,148,152	0
27	BCR	BD	5407	40/40	0.87	0.12	112,127,132,132	0
24	CLA	BC	5504	65/65	0.87	0.12	132,135,160,160	0
24	CLA	AC	513	65/65	0.87	0.14	158,160,160,160	0
29	LHG	BA	5413	39/49	0.87	0.11	113,122,128,129	0
24	CLA	BC	5506	65/65	0.87	0.13	136,143,160,160	0
24	CLA	AB	608	65/65	0.87	0.15	123,127,135,140	0
24	CLA	AB	616	65/65	0.87	0.12	143,147,160,160	0
24	CLA	BB	5618	65/65	0.87	0.13	128,133,160,160	0
37	CA	BK	5101	1/1	0.87	0.09	145,145,145,145	0
24	CLA	AB	606	65/65	0.87	0.16	120,133,140,141	0
29	LHG	AA	412	39/49	0.88	0.13	110,118,128,132	0
28	DGD	AH	101	58/66	0.88	0.14	108,120,155,157	0
24	CLA	BA	5407	65/65	0.88	0.12	110,114,138,139	0
27	BCR	AB	617	40/40	0.88	0.10	112,121,125,125	0
27	BCR	AB	618	40/40	0.88	0.11	109,117,122,122	0
22	BCT	BA	5403	4/4	0.88	0.10	135,136,136,137	0
27	BCR	AD	406	40/40	0.88	0.13	110,126,131,131	0
24	CLA	AC	512	65/65	0.88	0.15	154,158,160,160	0
24	CLA	BB	5620	65/65	0.88	0.13	143,147,160,160	0
27	BCR	AB	619	40/40	0.89	0.12	111,117,131,131	0
24	CLA	AB	609	65/65	0.89	0.14	126,136,141,143	0
24	CLA	BB	5610	65/65	0.89	0.14	121,132,140,141	0
24	CLA	AA	407	65/65	0.89	0.12	93,101,150,151	0
24	CLA	AC	505	65/65	0.89	0.16	121,146,150,151	0
24	CLA	AA	406	65/65	0.89	0.15	105,112,138,139	0
27	BCR	BC	5514	40/40	0.89	0.12	123,126,129,129	0
24	CLA	BC	5501	65/65	0.90	0.13	134,137,141,144	0
27	BCR	AK	102	40/40	0.90	0.16	133,139,151,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	CLA	BB	5607	65/65	0.90	0.11	108,111,120,123	0
25	MST	BA	5409	16/16	0.90	0.12	124,129,131,132	0
27	BCR	BA	5411	40/40	0.90	0.12	94,122,132,132	0
27	BCR	BB	5623	40/40	0.90	0.14	111,116,131,131	0
24	CLA	AB	603	65/65	0.90	0.14	107,109,119,121	0
24	CLA	BB	5612	65/65	0.90	0.12	122,127,136,139	0
35	PL9	BD	5406	55/55	0.90	0.14	103,110,115,116	0
24	CLA	BB	5613	65/65	0.90	0.13	127,135,140,142	0
37	CA	AK	101	1/1	0.90	0.07	146,146,146,146	0
24	CLA	BC	5510	65/65	0.90	0.11	113,116,130,131	0
24	CLA	AC	504	65/65	0.90	0.14	129,134,160,160	0
27	BCR	AC	516	40/40	0.90	0.15	135,138,143,143	0
24	CLA	AB	614	65/65	0.90	0.13	129,133,160,160	0
24	CLA	AB	615	65/65	0.91	0.12	134,139,155,157	0
24	CLA	BC	5502	65/65	0.91	0.11	108,111,143,144	0
27	BCR	BB	5621	40/40	0.91	0.10	112,120,124,125	0
24	CLA	BC	5507	65/65	0.91	0.12	136,150,153,154	0
33	DMS	BV	5202	4/4	0.91	0.14	148,149,149,150	0
24	CLA	BC	5508	65/65	0.91	0.12	142,146,157,159	0
24	CLA	BB	5611	65/65	0.92	0.10	95,102,132,136	0
24	CLA	BC	5509	65/65	0.92	0.12	116,128,138,138	0
24	CLA	AB	611	65/65	0.92	0.12	99,113,116,122	0
24	CLA	AB	613	65/65	0.92	0.10	99,102,136,140	0
24	CLA	BB	5617	65/65	0.92	0.10	98,102,138,141	0
24	CLA	AB	604	65/65	0.92	0.10	96,104,125,127	0
27	BCR	BB	5622	40/40	0.92	0.10	110,117,120,121	0
24	CLA	BB	5619	65/65	0.92	0.12	135,137,155,157	0
24	CLA	BA	5406	65/65	0.92	0.11	89,94,108,112	0
33	DMS	BV	5203	4/4	0.92	0.16	160,160,160,160	0
34	PHO	BD	5404	64/64	0.92	0.13	123,125,129,130	0
24	CLA	AB	607	65/65	0.92	0.11	94,100,132,135	0
24	CLA	BA	5408	65/65	0.92	0.11	95,103,150,150	0
24	CLA	AC	507	65/65	0.92	0.14	137,149,152,153	0
24	CLA	BB	5606	65/65	0.92	0.13	124,127,130,131	0
24	CLA	AC	508	65/65	0.92	0.13	140,144,157,158	0
24	CLA	BB	5609	65/65	0.92	0.14	103,110,124,124	0
24	CLA	AC	510	65/65	0.92	0.11	110,113,129,130	0
24	CLA	AC	501	65/65	0.93	0.13	133,136,139,143	0
24	CLA	AC	503	65/65	0.93	0.16	137,144,147,152	0
34	PHO	AD	403	64/64	0.93	0.14	119,123,128,129	0
34	PHO	BD	5403	64/64	0.93	0.12	102,109,118,118	0
24	CLA	AA	405	65/65	0.93	0.11	88,93,108,111	0

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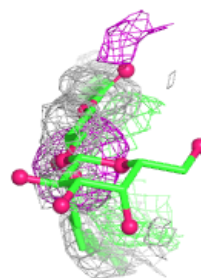
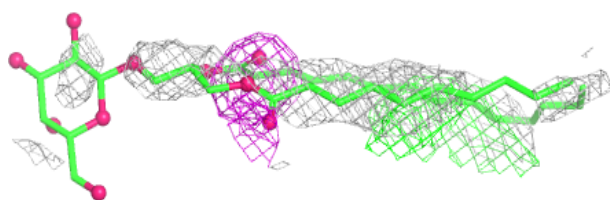
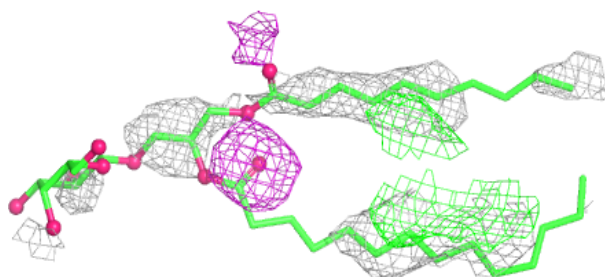
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	PL9	AD	405	55/55	0.93	0.16	99,109,113,113	0
26	OEC	AA	409	5/9	0.93	0.10	82,83,90,110	0
36	HEM	AF	101	43/43	0.93	0.19	148,152,159,160	0
36	HEM	BF	5101	43/43	0.93	0.18	148,152,160,160	0
24	CLA	AC	511	65/65	0.93	0.16	152,155,157,158	0
27	BCR	AA	410	40/40	0.93	0.11	91,122,130,130	0
24	CLA	AB	602	65/65	0.93	0.12	124,127,129,132	0
24	CLA	AB	605	65/65	0.93	0.12	105,113,122,124	0
24	CLA	BB	5614	65/65	0.93	0.13	117,123,124,128	0
24	CLA	BB	5615	65/65	0.93	0.10	101,113,117,120	0
24	CLA	AD	401	65/65	0.94	0.13	93,100,115,119	0
24	CLA	AA	404	65/65	0.94	0.12	89,99,106,108	0
24	CLA	BA	5405	65/65	0.94	0.11	90,101,105,109	0
24	CLA	BD	5402	65/65	0.94	0.13	97,101,117,119	0
27	BCR	AC	514	40/40	0.94	0.12	120,123,127,128	0
24	CLA	AC	509	65/65	0.94	0.12	115,128,135,137	0
25	MST	AA	408	16/16	0.94	0.13	123,126,129,130	0
24	CLA	BB	5608	65/65	0.94	0.10	96,103,124,125	0
34	PHO	AD	402	64/64	0.94	0.12	99,109,116,117	0
24	CLA	AB	612	65/65	0.94	0.12	107,111,120,121	0
24	CLA	BB	5616	65/65	0.94	0.14	108,110,120,122	0
23	CL	BA	5404[A]	1/1	0.95	0.60	29,29,29,29	1
24	CLA	AB	610	65/65	0.95	0.12	117,121,123,127	0
23	CL	BA	5404[B]	1/1	0.95	0.60	115,115,115,115	1
24	CLA	AC	502	65/65	0.95	0.11	103,109,142,143	0
36	HEM	BV	5201	43/43	0.96	0.12	97,102,106,109	0
36	HEM	AV	201	43/43	0.98	0.13	94,100,102,103	0
21	FE2	AA	401	1/1	0.99	0.06	115,115,115,115	0
21	FE2	BD	5401	1/1	0.99	0.03	119,119,119,119	0

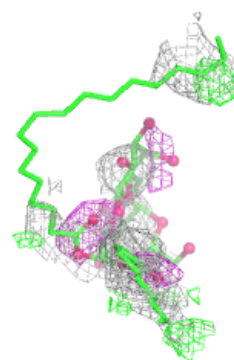
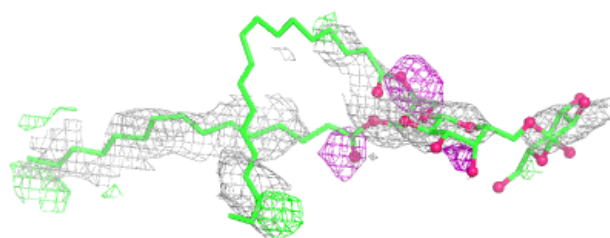
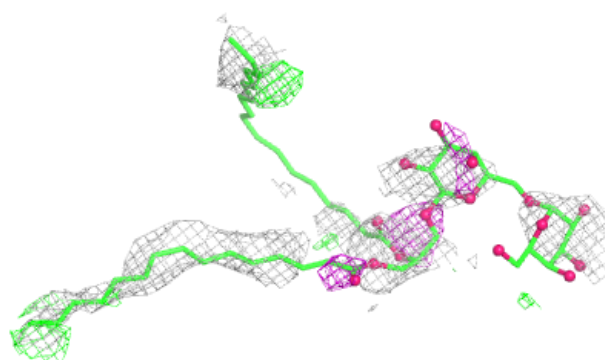
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMG AI 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

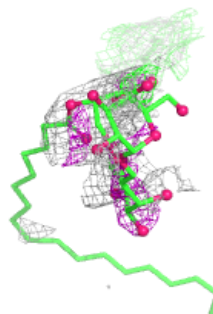
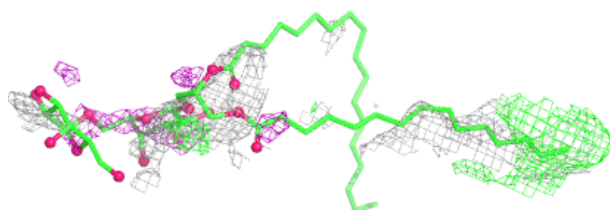
**Electron density around DGD BE 5102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

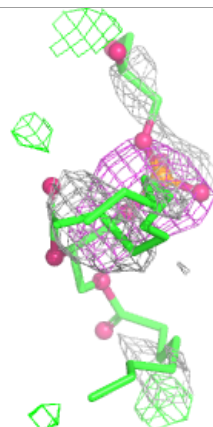
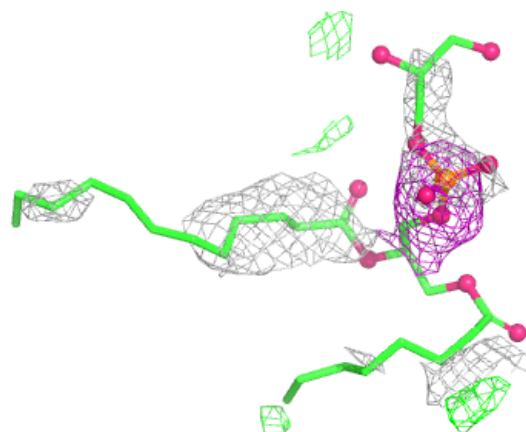


Electron density around DGD AE 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

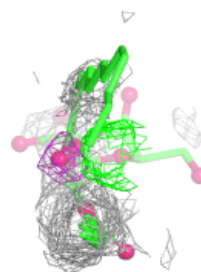
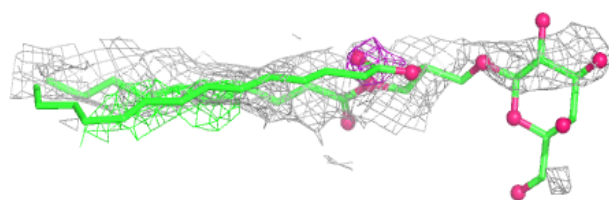
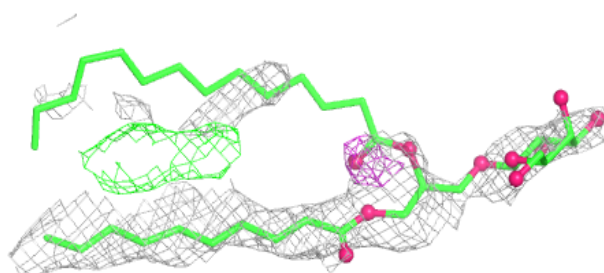
**Electron density around LHG BA 5415:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

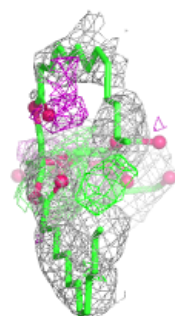
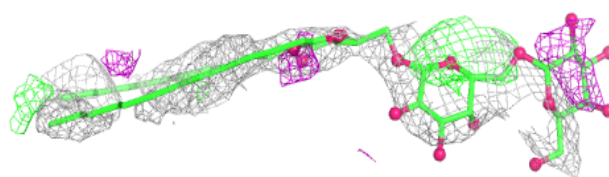
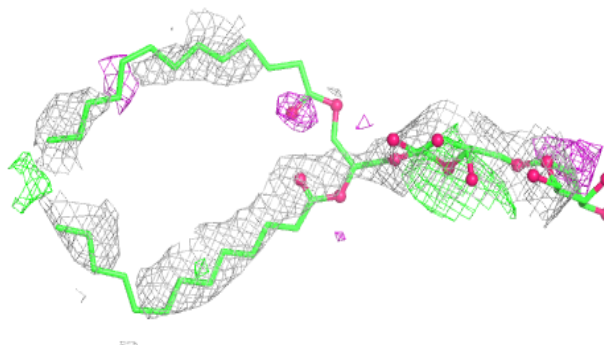


Electron density around LMG BI 5101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

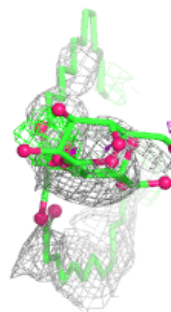
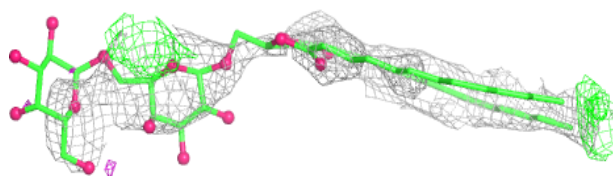
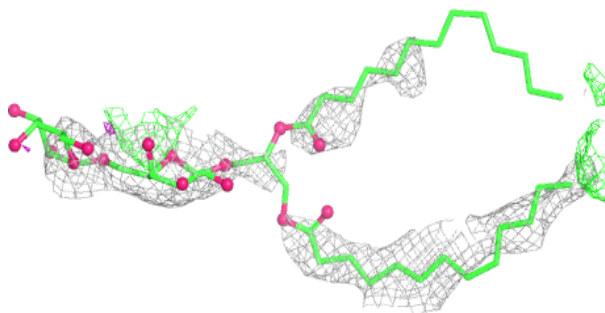
**Electron density around DGD AA 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

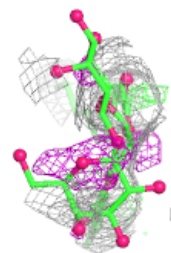
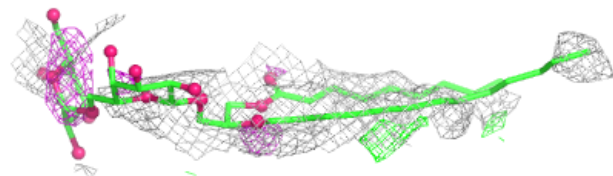
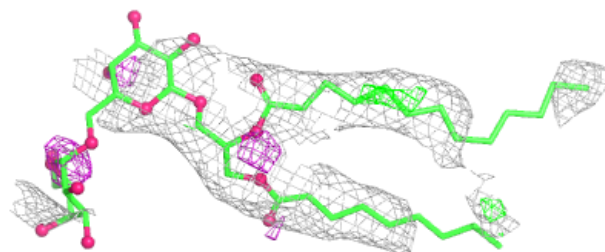


Electron density around DGD BA 5412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

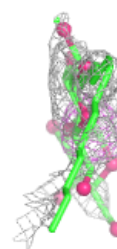
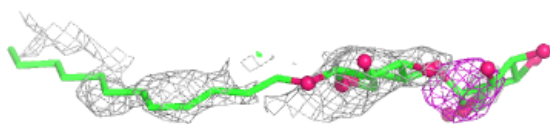
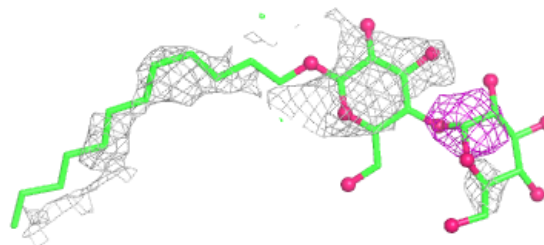
**Electron density around DGD BB 5602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

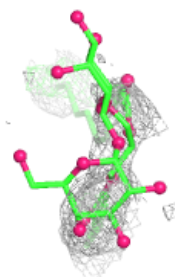
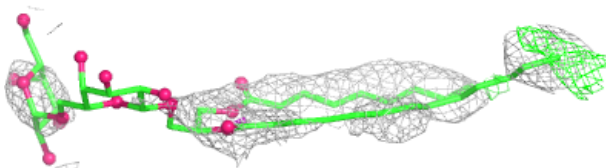
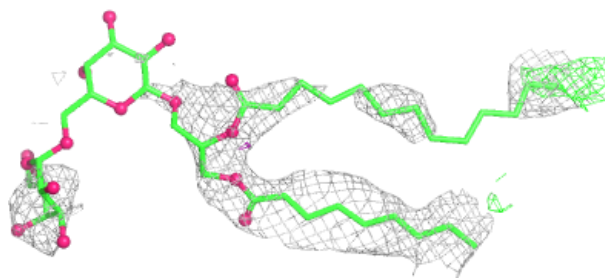


Electron density around LMT AB 623:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

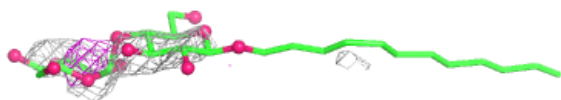
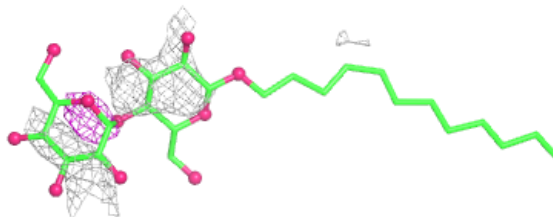
**Electron density around DGD AB 628:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

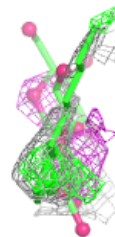
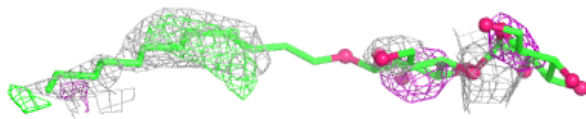
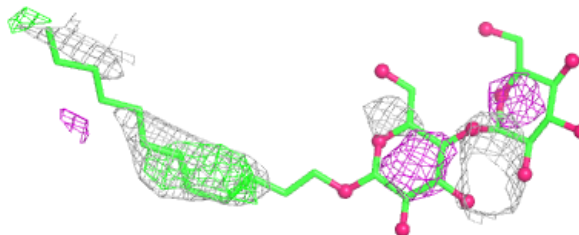


Electron density around LMT BI 5102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

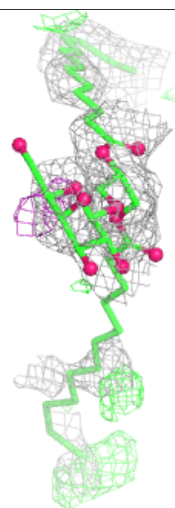
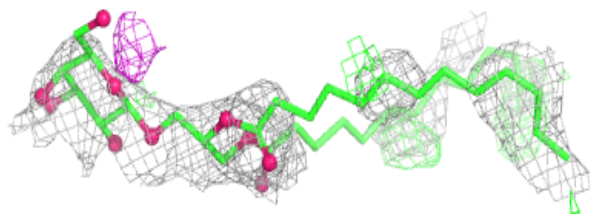
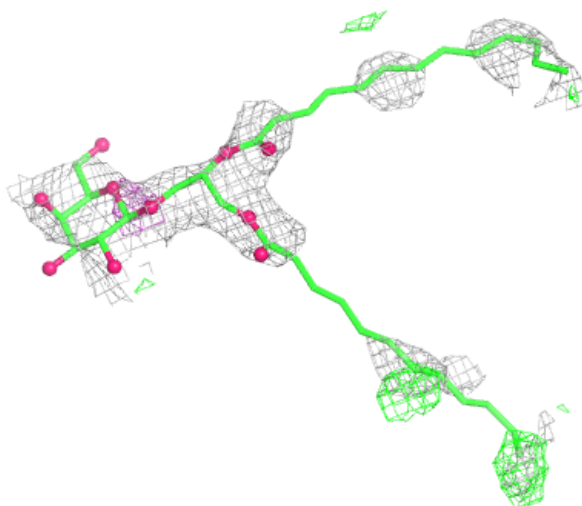
**Electron density around LMT BB 5626:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



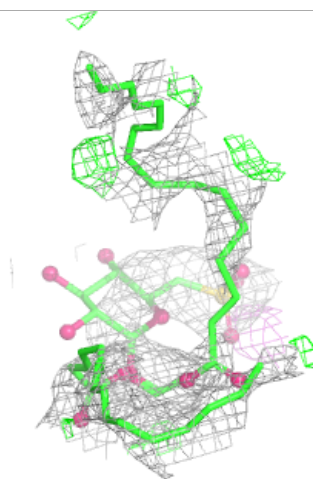
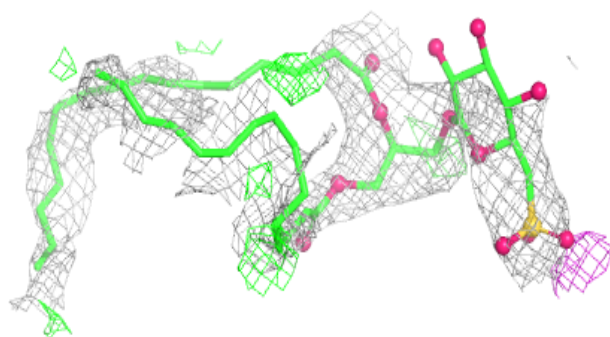
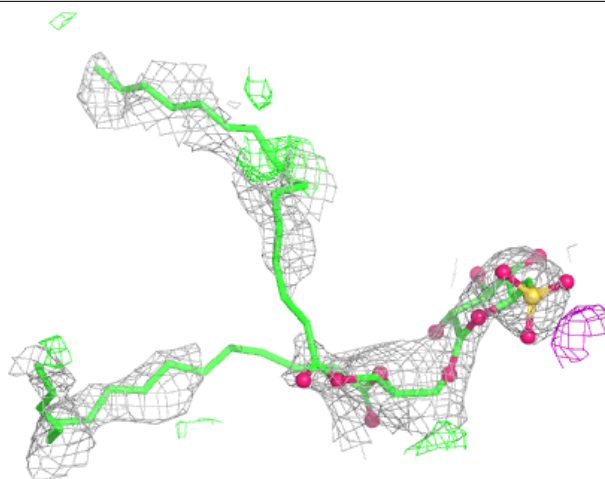
Electron density around LMG AA 414:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



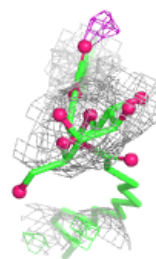
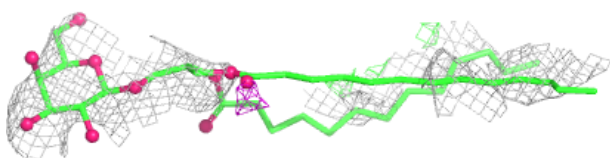
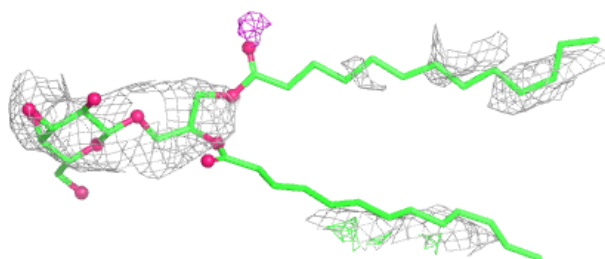
Electron density around SQD BA 5401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

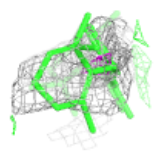
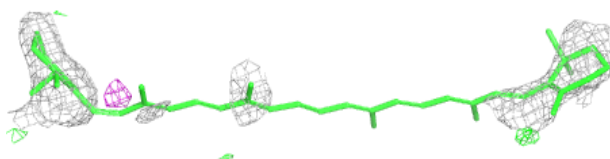
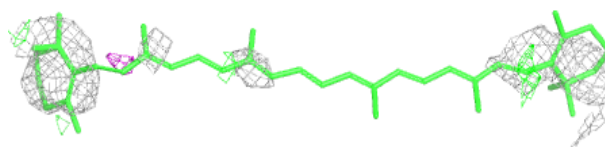


Electron density around LMG BC 5521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

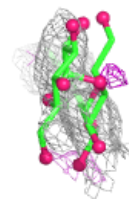
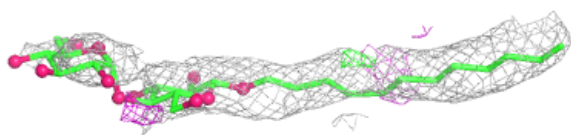
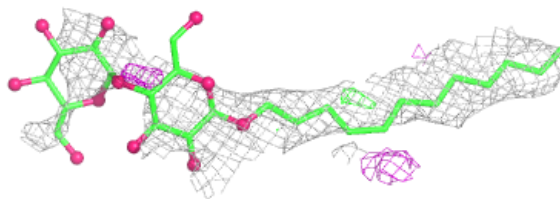
**Electron density around BCR BJ 5101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



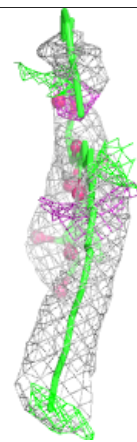
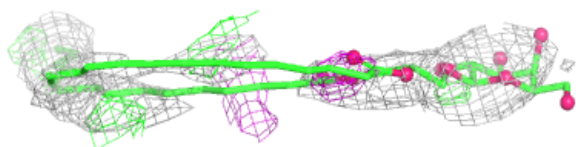
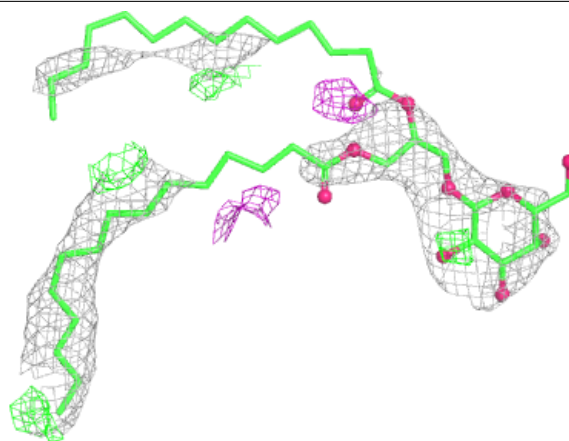
Electron density around LMT BB 5604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



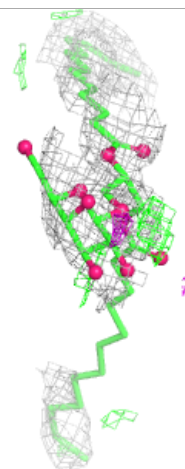
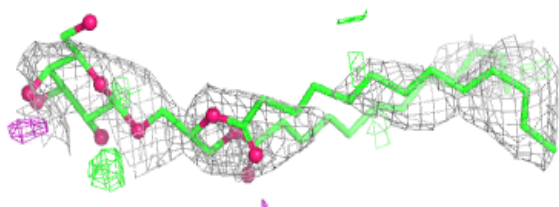
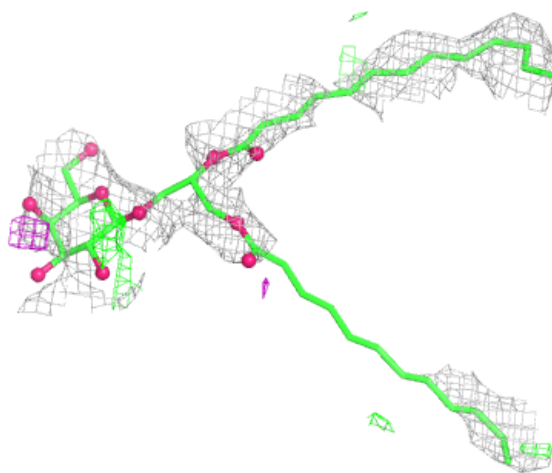
Electron density around LMG AC 520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



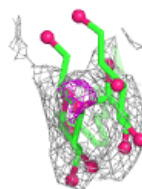
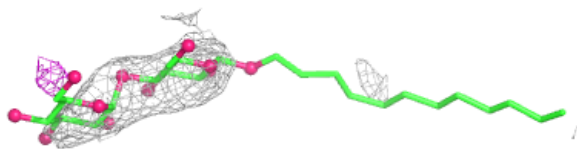
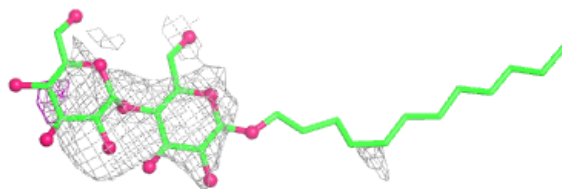
Electron density around LMG BE 5101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

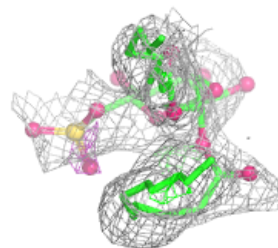
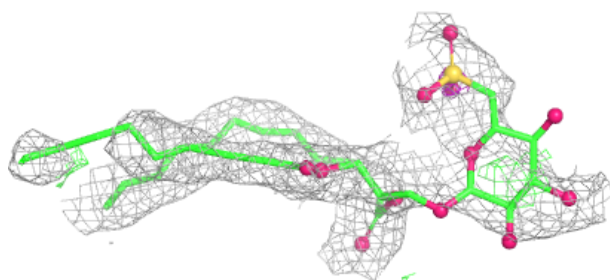
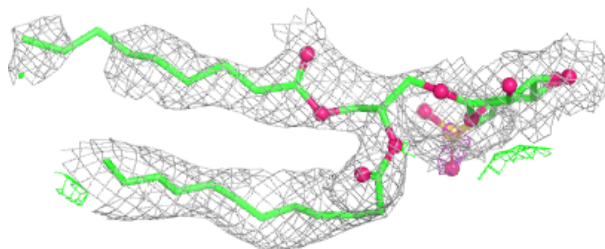


Electron density around LMT BC 5522:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

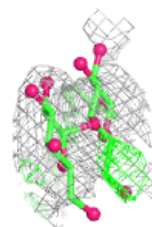
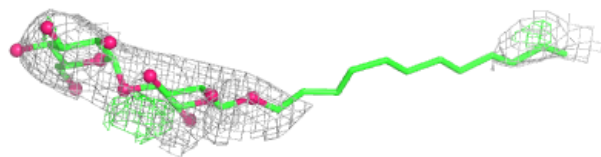
**Electron density around SQD BB 5625:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

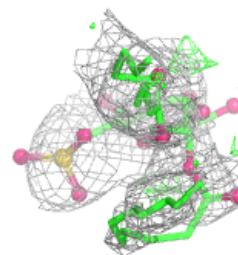
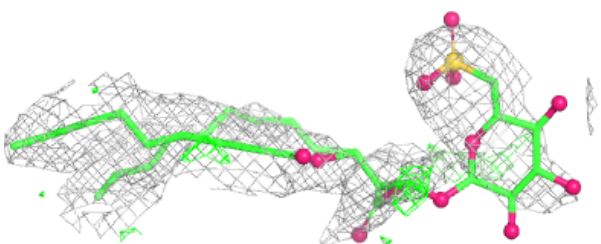
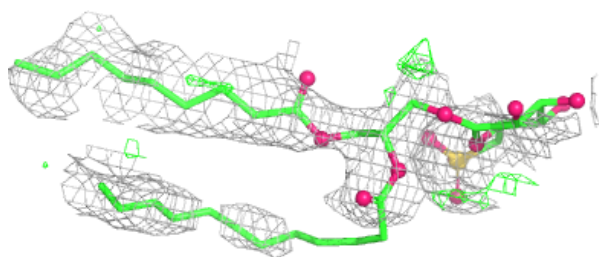


Electron density around LMT AI 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

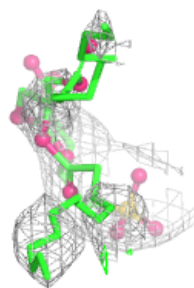
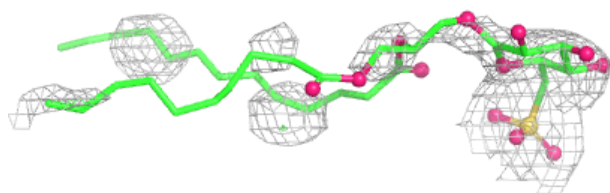
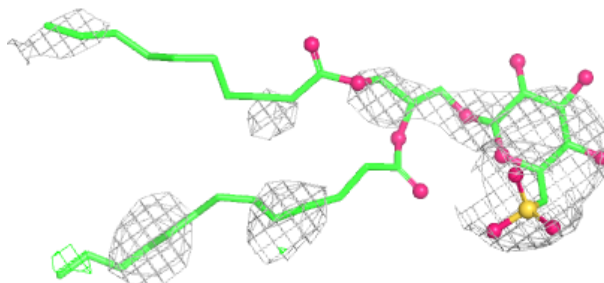
**Electron density around SQD AB 622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

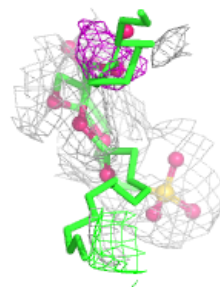
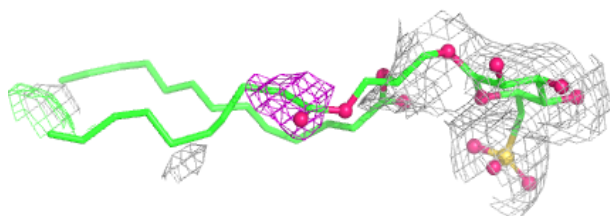
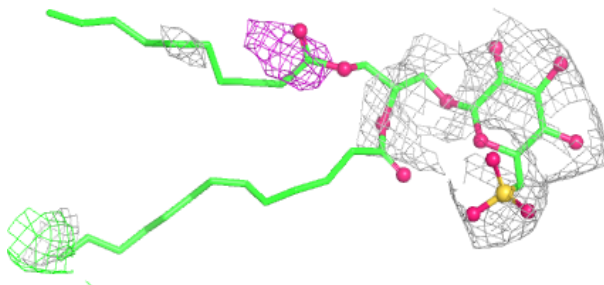


Electron density around SQD BF 5102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

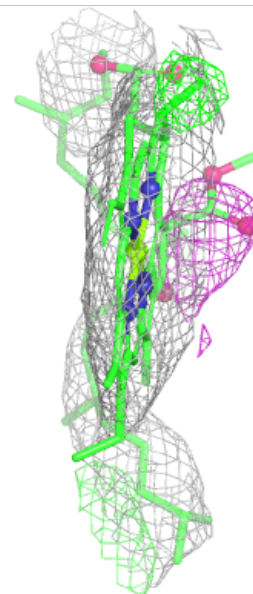
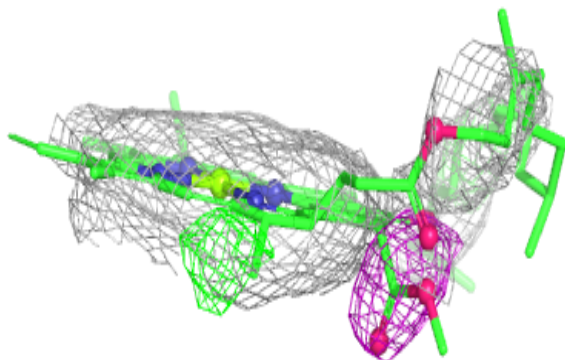
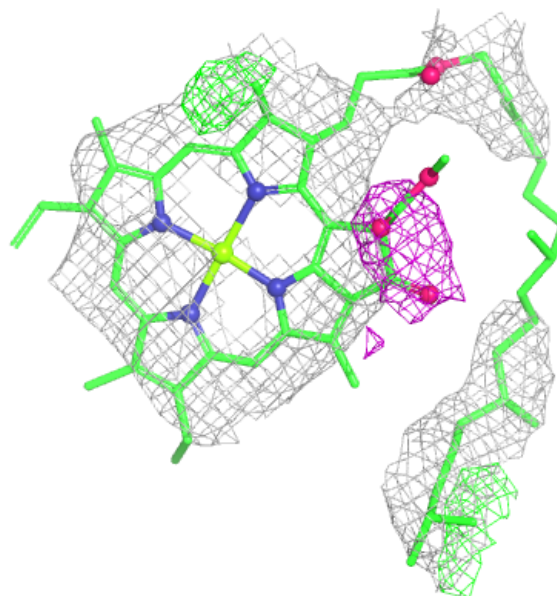
**Electron density around SQD AF 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



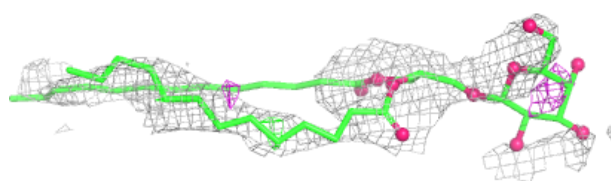
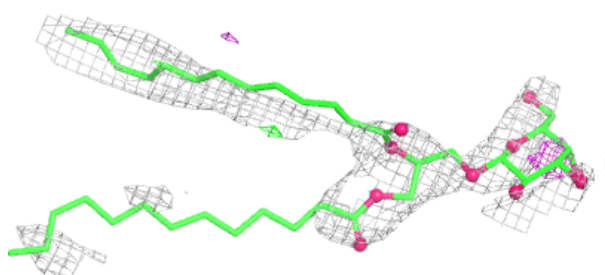
Electron density around CLA AB 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

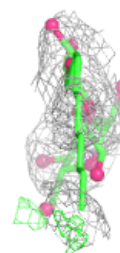
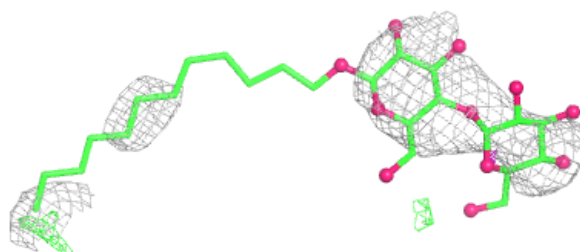


Electron density around LMG AC 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

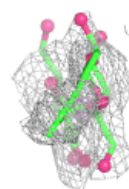
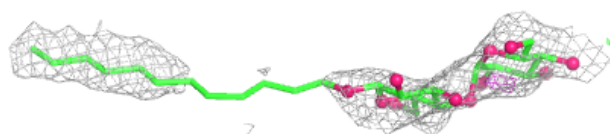
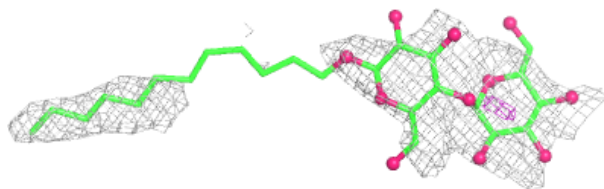
**Electron density around LMT AB 624:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

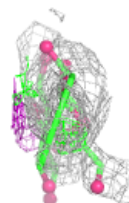
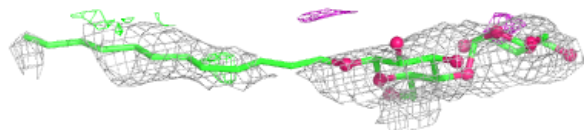
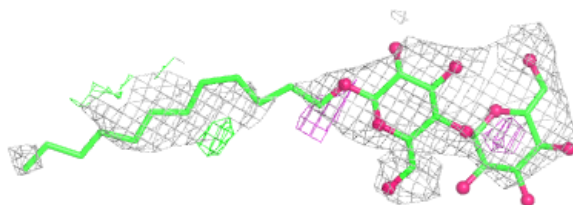


Electron density around LMT AB 630:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

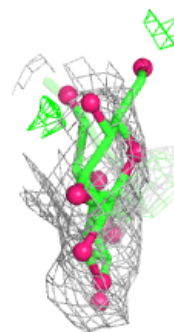
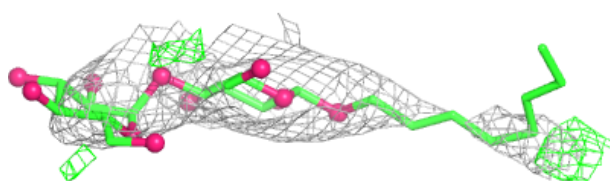
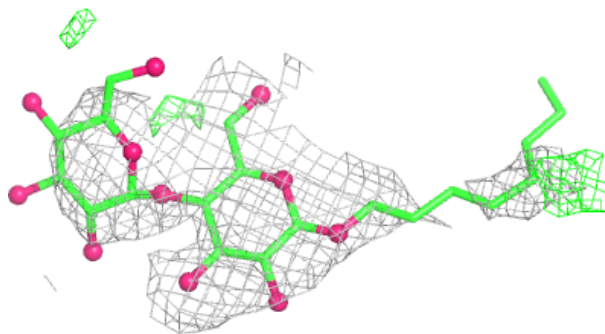
**Electron density around LMT AI 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

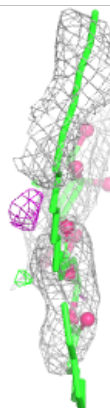
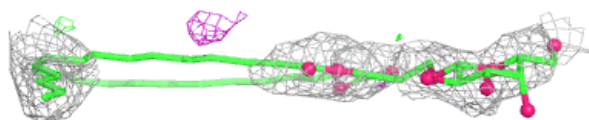
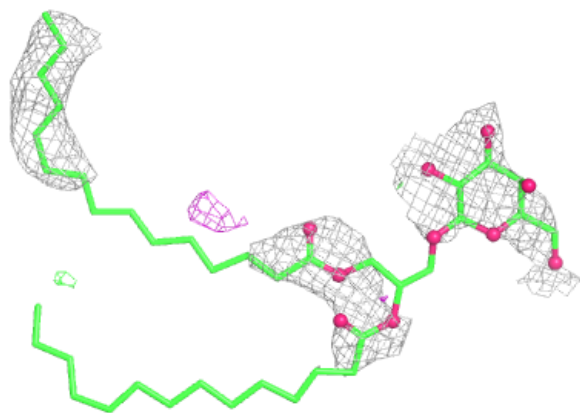


Electron density around LMT BD 5411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

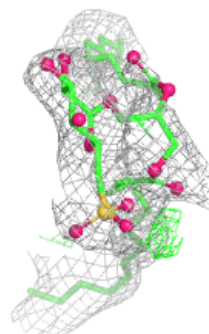
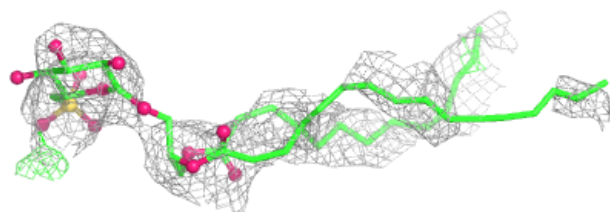
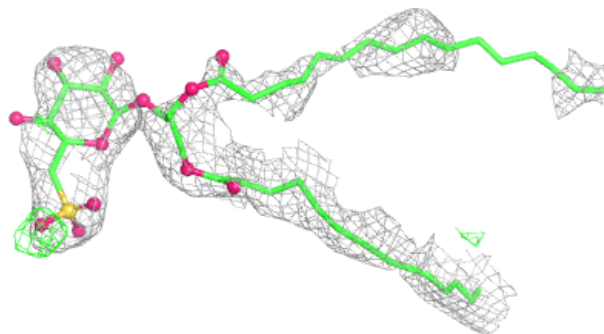
**Electron density around LMG BC 5520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

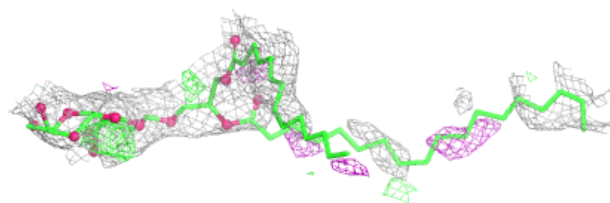
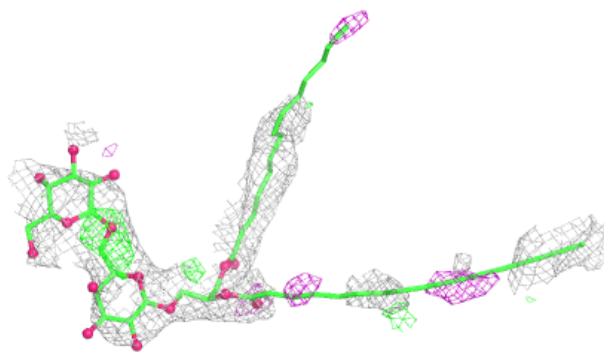


Electron density around SQD BA 5414:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

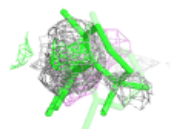
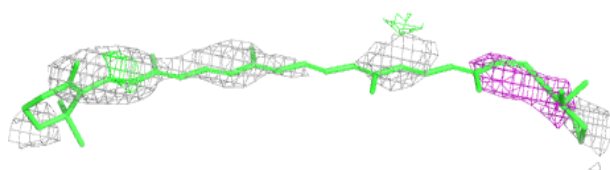
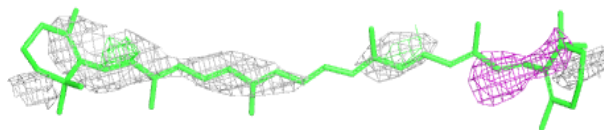
**Electron density around DGD BC 5518:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

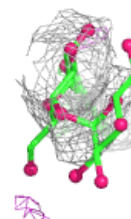
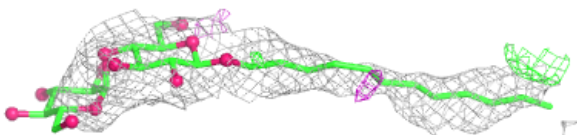
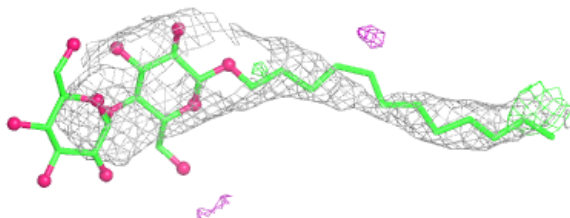


Electron density around BCR AJ 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

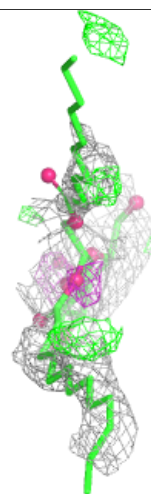
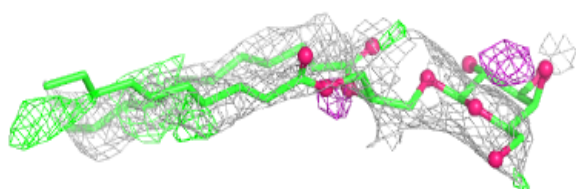
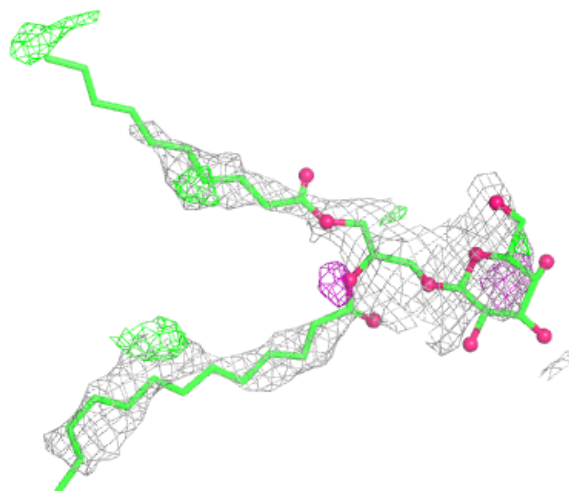
**Electron density around LMT BB 5603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



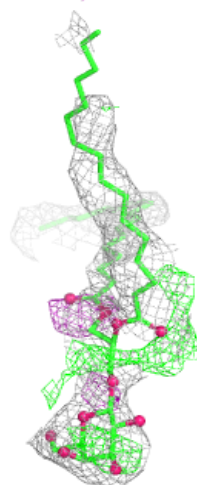
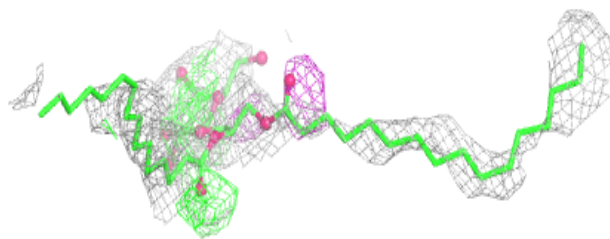
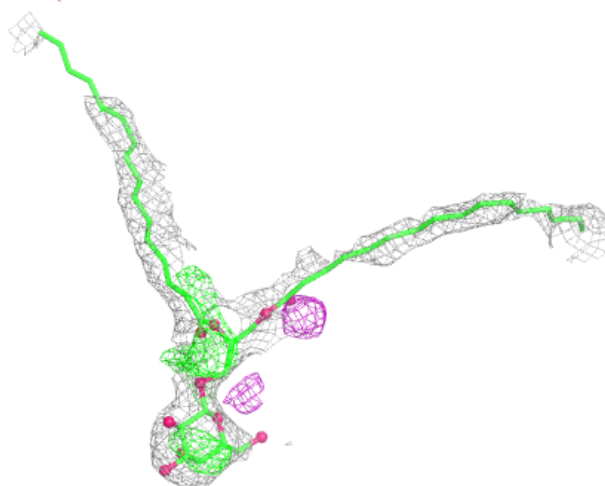
Electron density around LMG BA 5402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



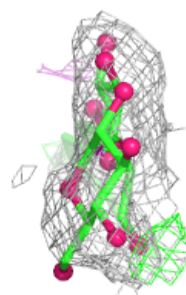
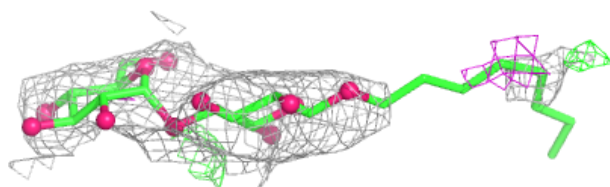
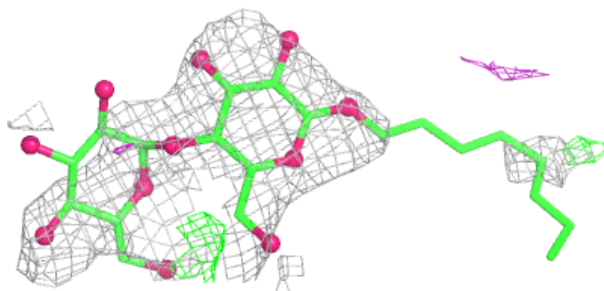
Electron density around LMG AB 620:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

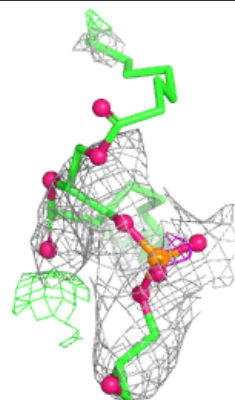
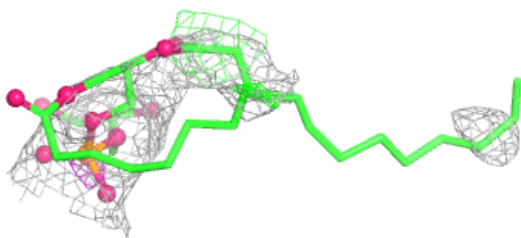
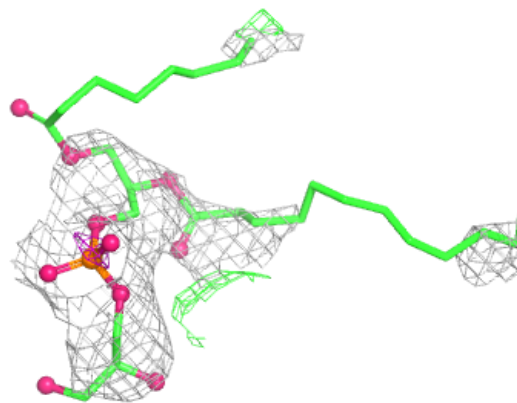


Electron density around LMT AD 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

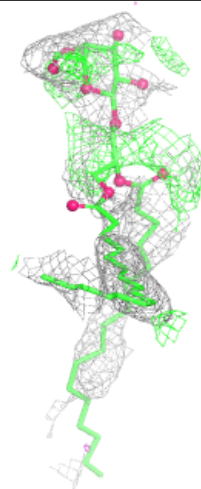
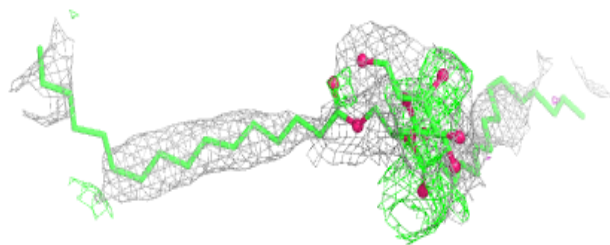
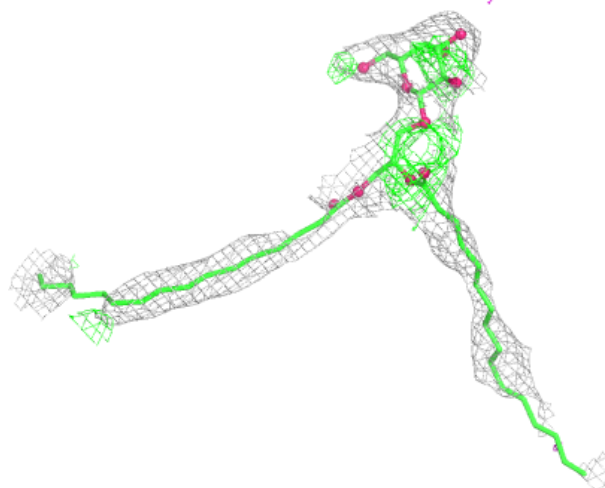
**Electron density around LHG AA 415:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



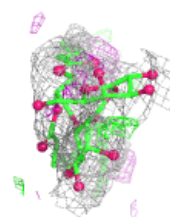
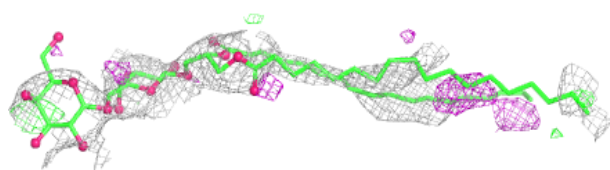
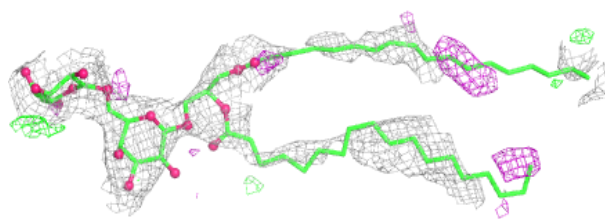
Electron density around LMG BL 5101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



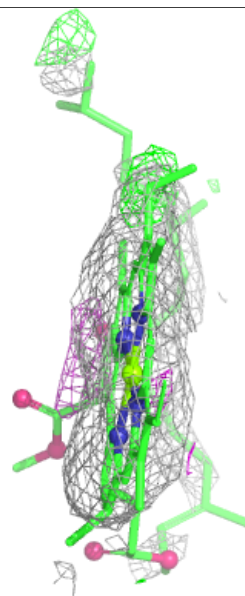
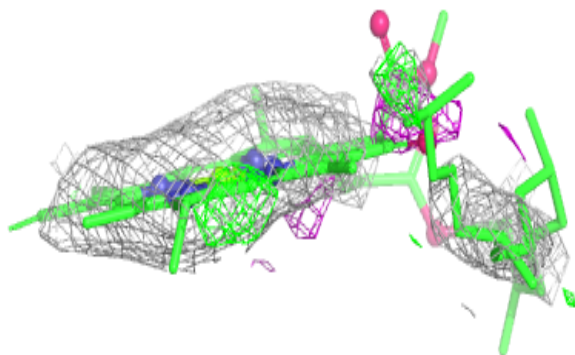
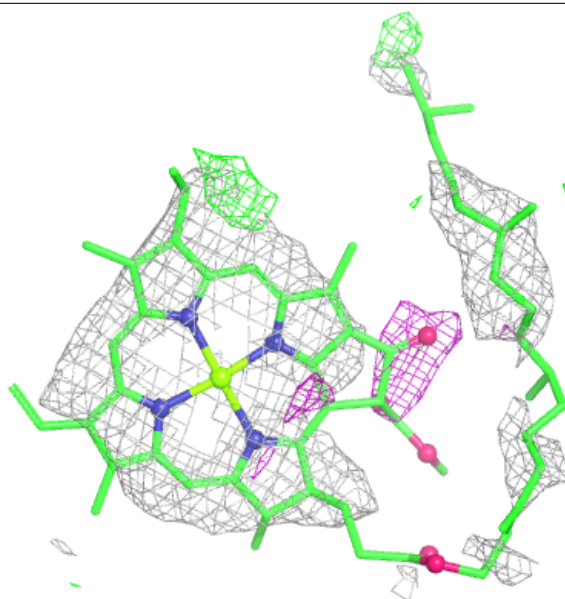
Electron density around DGD BC 5519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



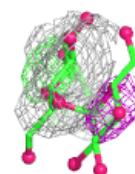
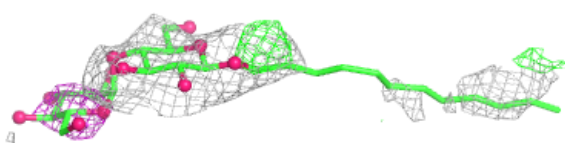
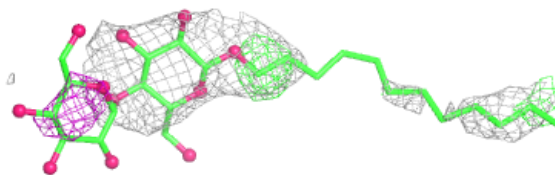
Electron density around CLA BB 5605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

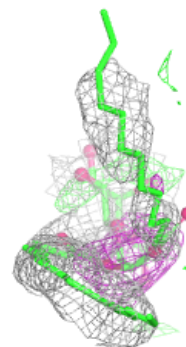
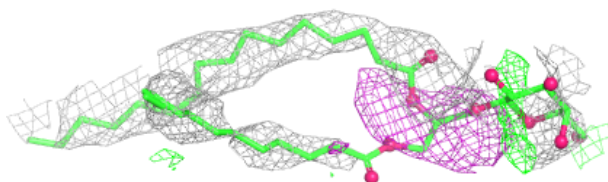
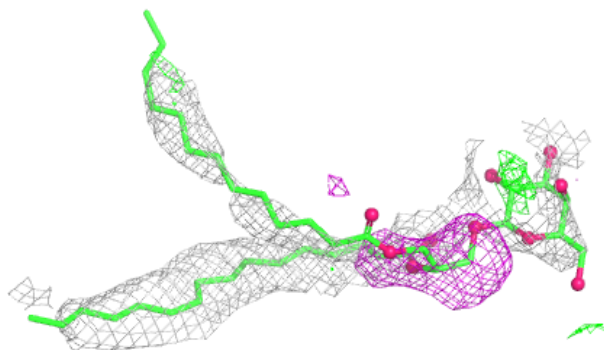


Electron density around LMT AB 629:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

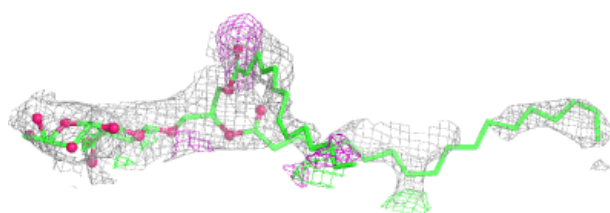
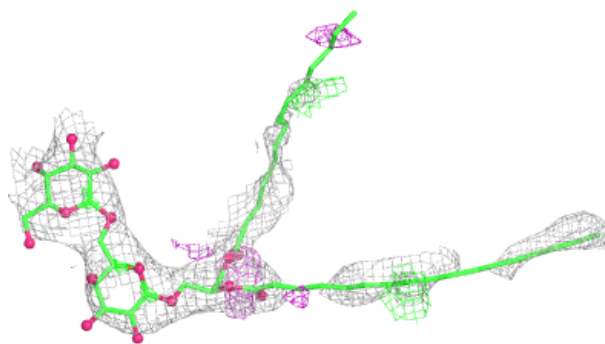
**Electron density around LMG BD 5410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

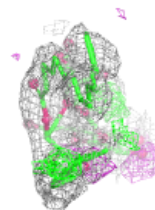
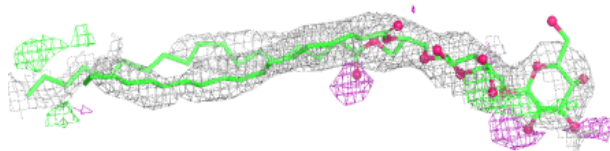
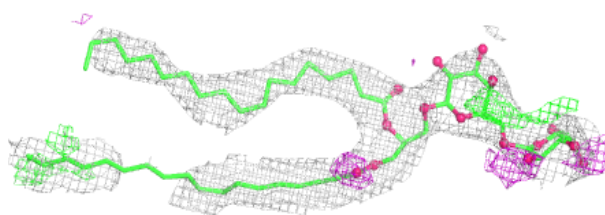


Electron density around DGD AC 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

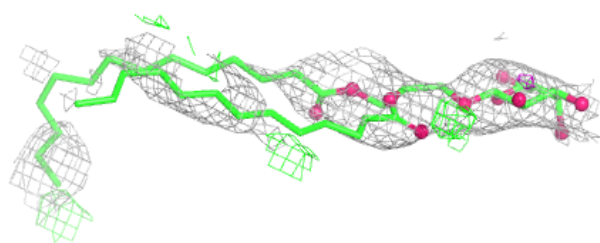
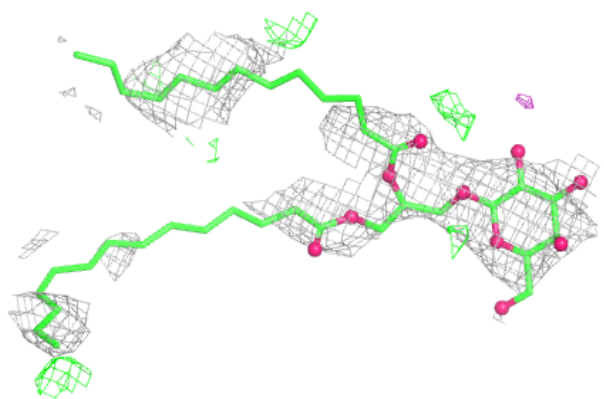
**Electron density around DGD AC 519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

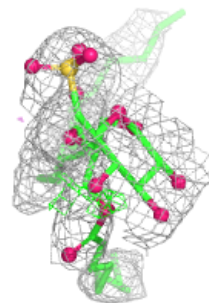
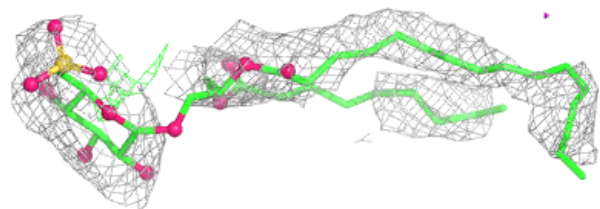
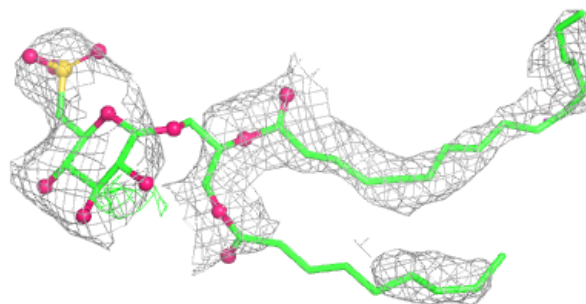


Electron density around LMG BD 5408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

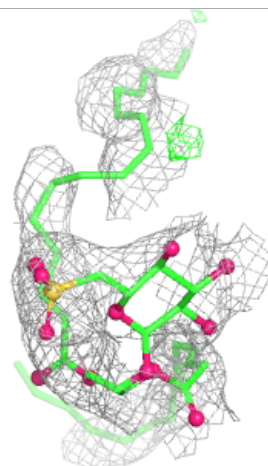
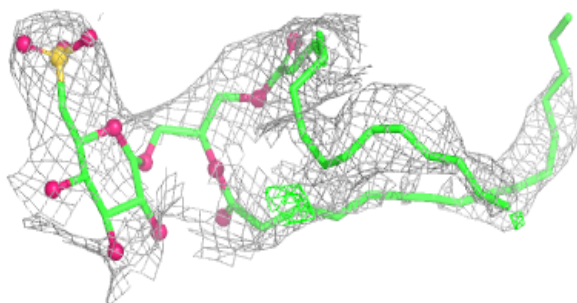
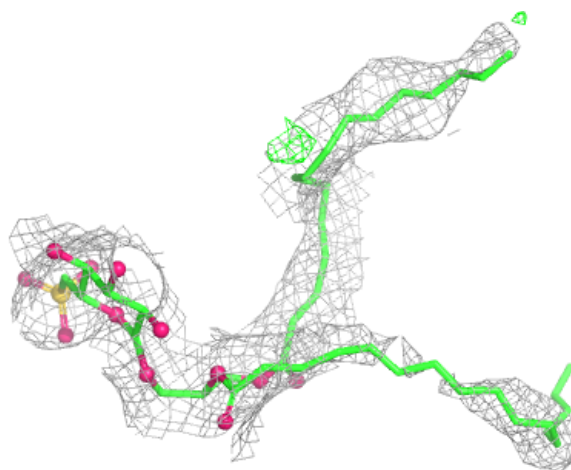
**Electron density around SQD BB 5601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



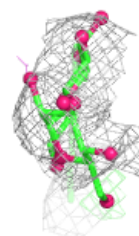
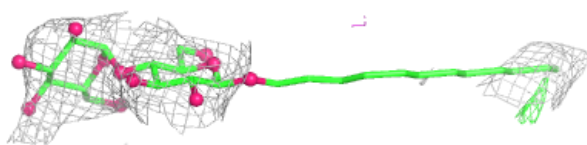
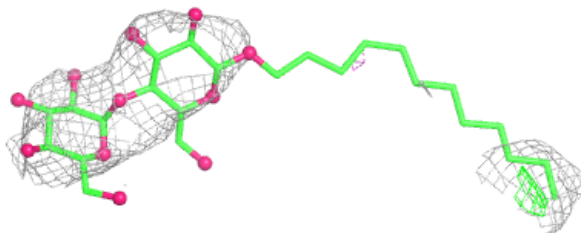
Electron density around SQD AA 416:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

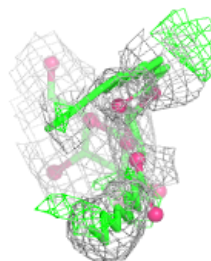
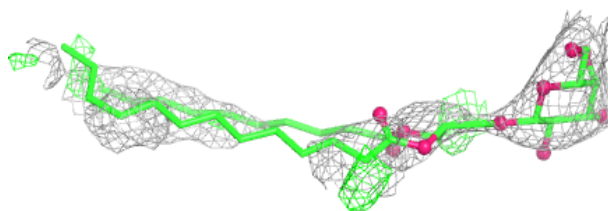
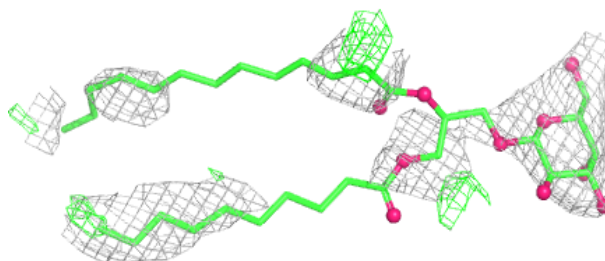


Electron density around LMT BB 5627:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

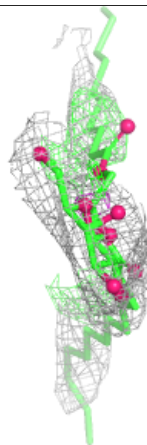
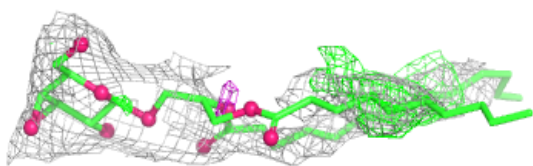
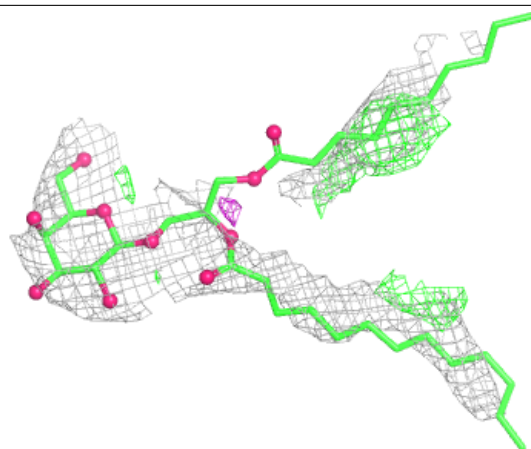
**Electron density around LMG AM 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



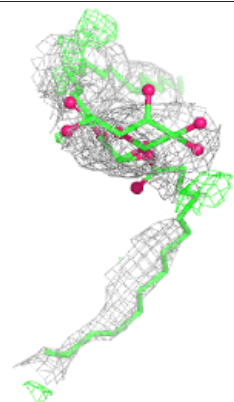
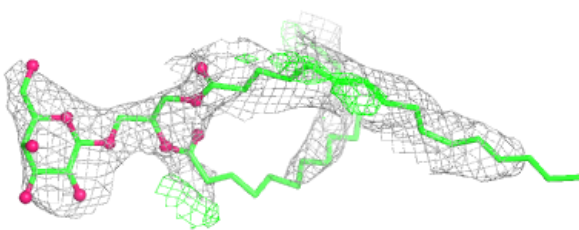
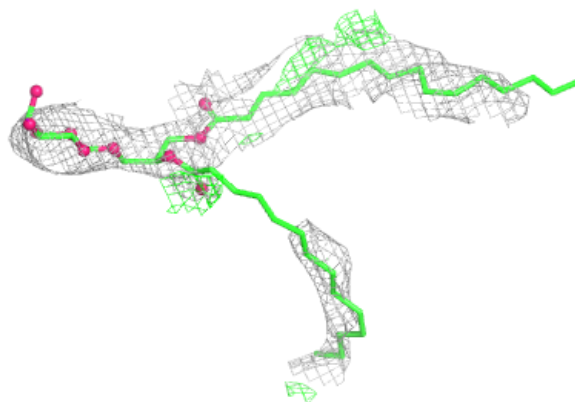
Electron density around LMG AA 417:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

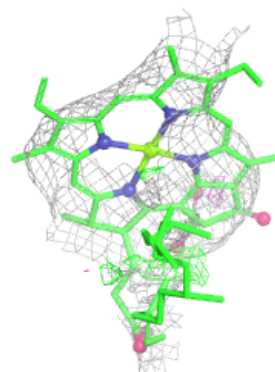
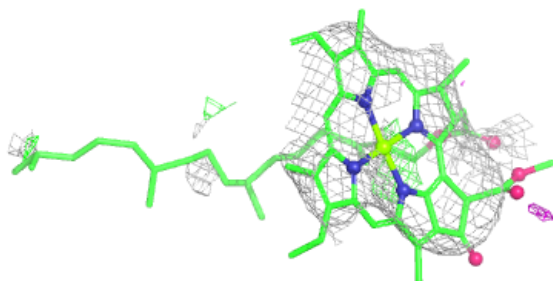
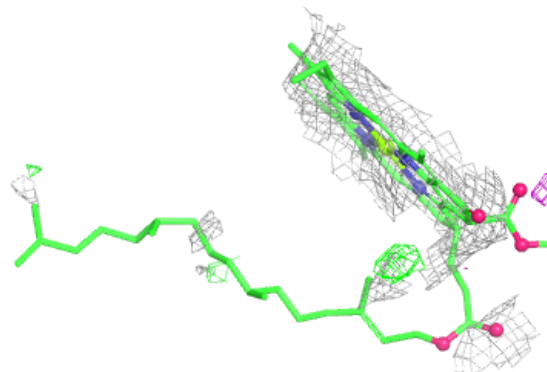


Electron density around LMG AB 621:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

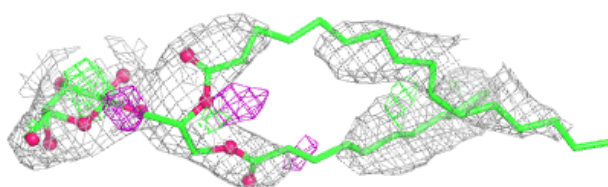
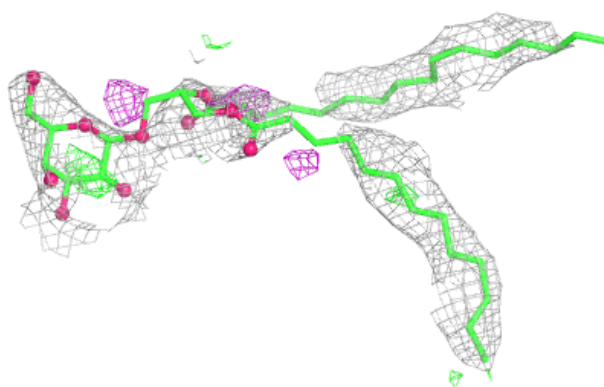
**Electron density around CLA BC 5513:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

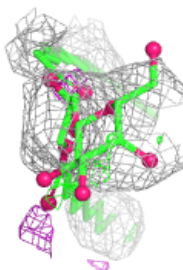
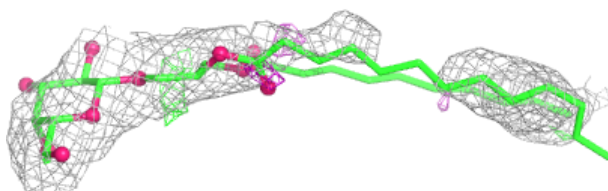
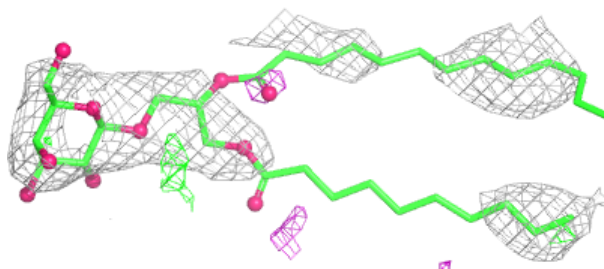


Electron density around LMG AD 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

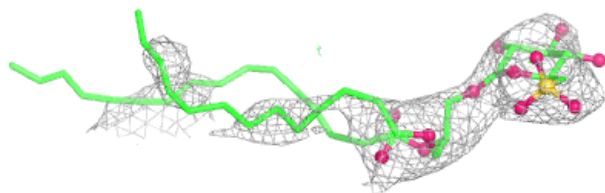
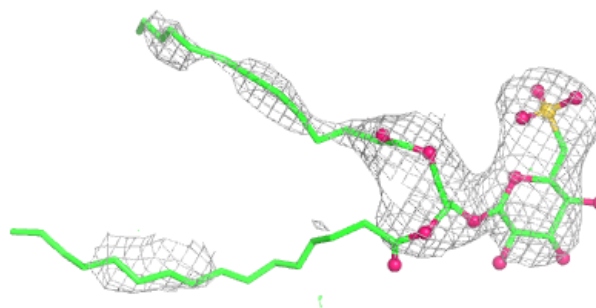
**Electron density around LMG BM 5102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

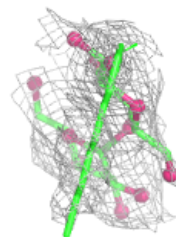
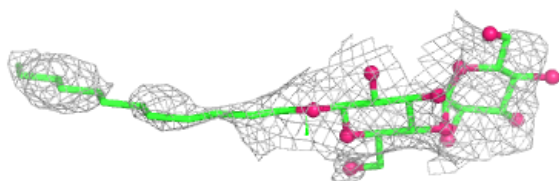
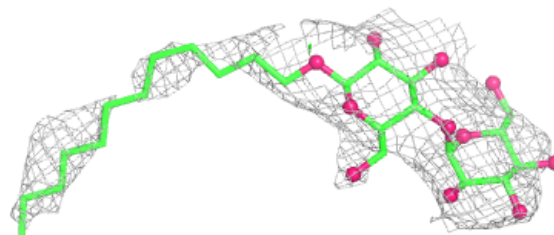


Electron density around SQD AA 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

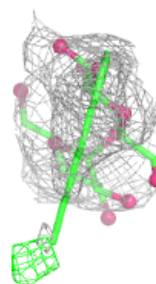
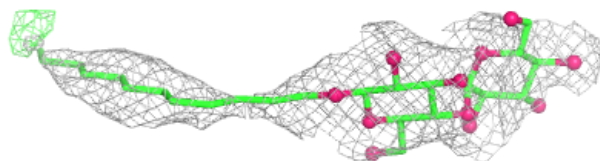
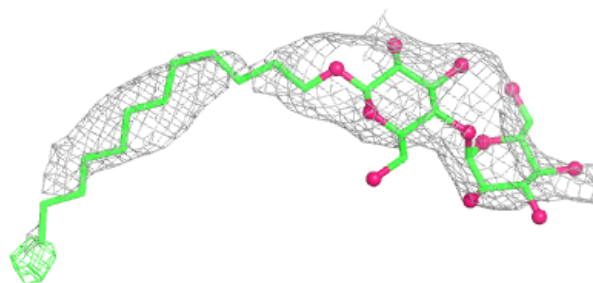
**Electron density around LMT AM 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

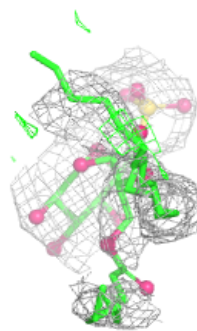
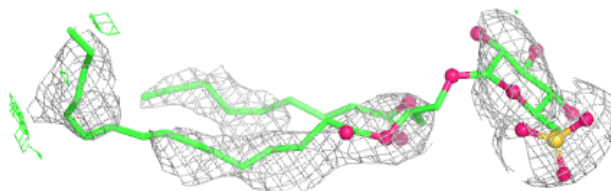
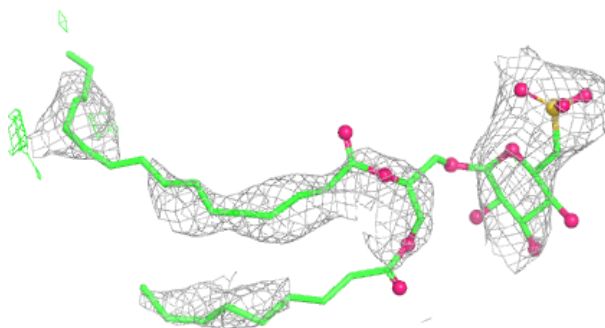


Electron density around LMT BM 5101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

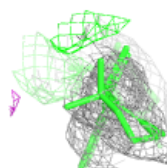
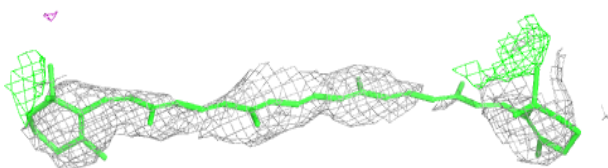
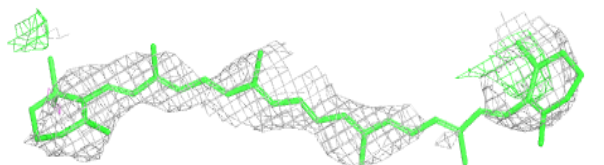
**Electron density around SQD AB 627:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

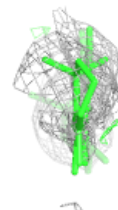
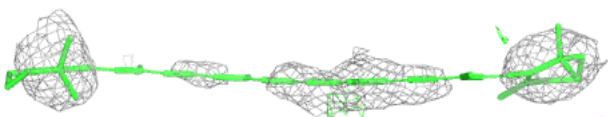
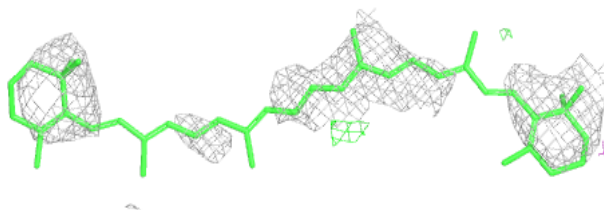


Electron density around BCR BC 5516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

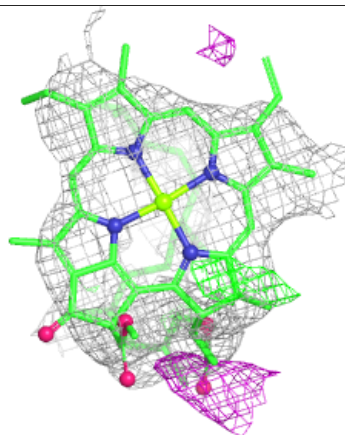
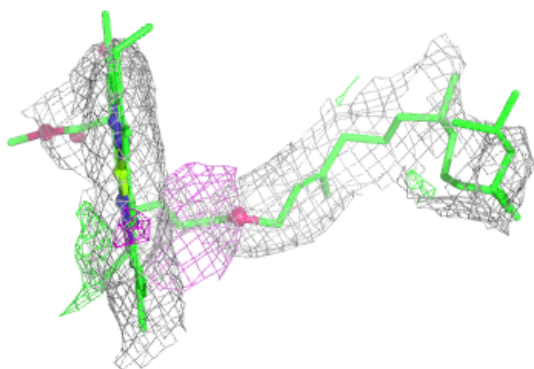
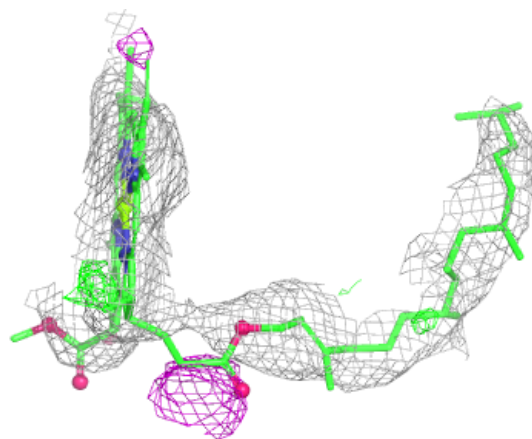
**Electron density around BCR BK 5102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



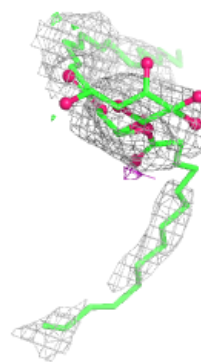
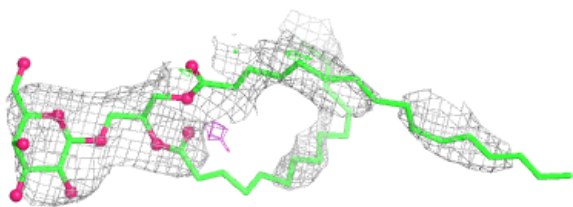
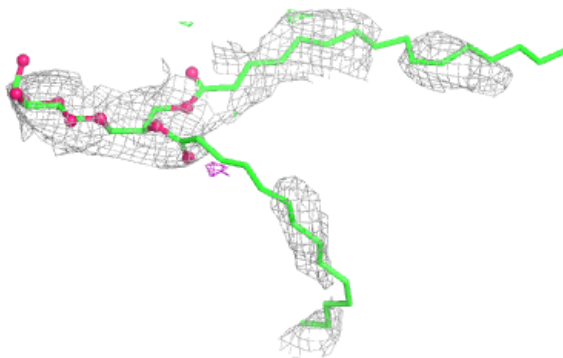
Electron density around CLA AC 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

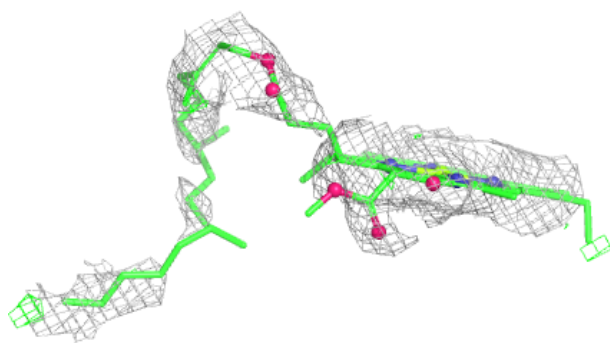
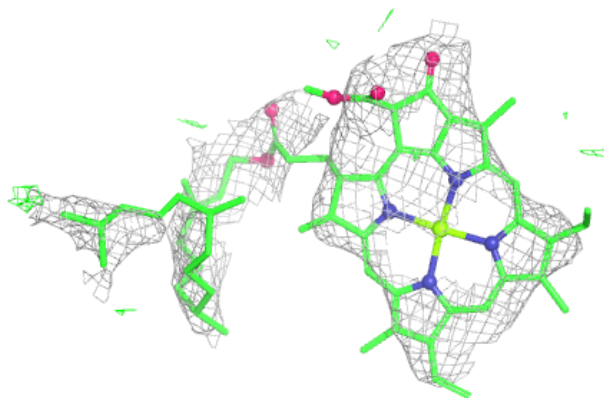


Electron density around LMG BB 5624:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

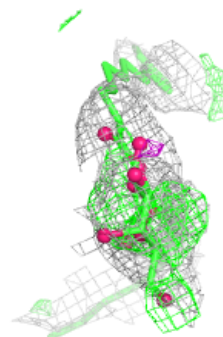
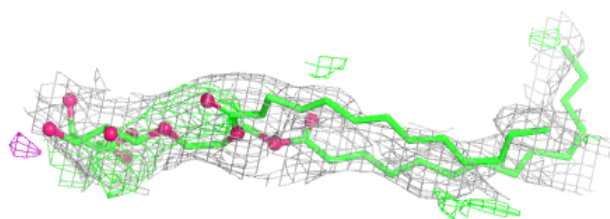
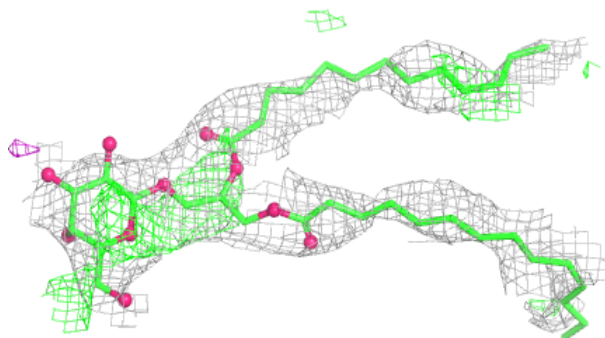
**Electron density around CLA BC 5512:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

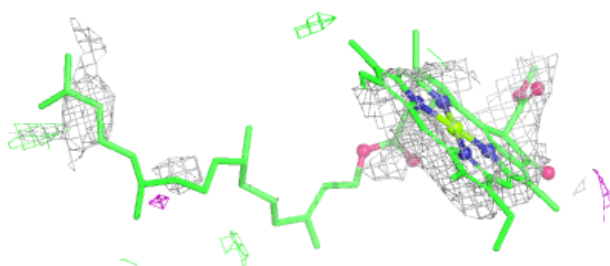
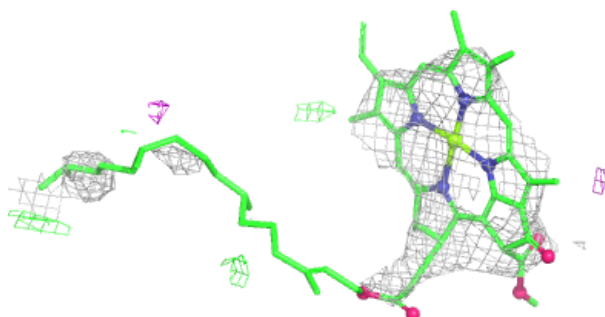


Electron density around LMG AJ 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

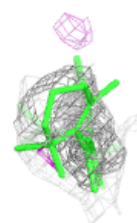
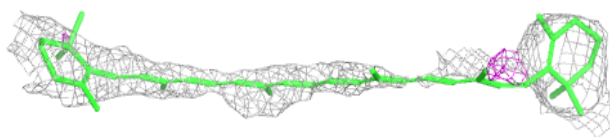
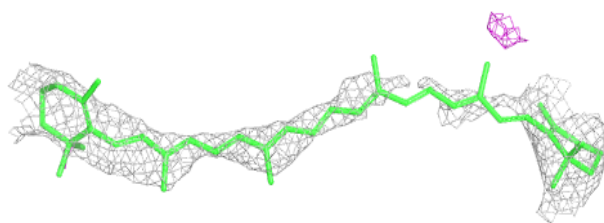
**Electron density around CLA BC 5511:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

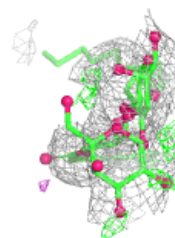
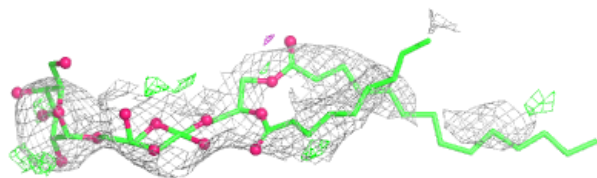
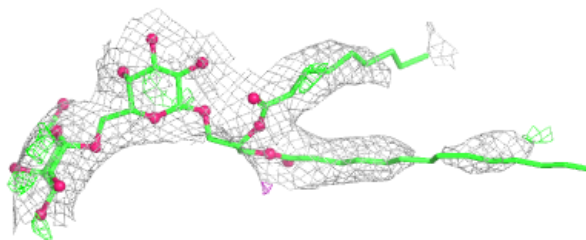


Electron density around BCR AX 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

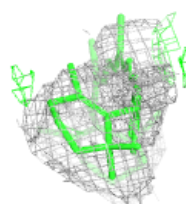
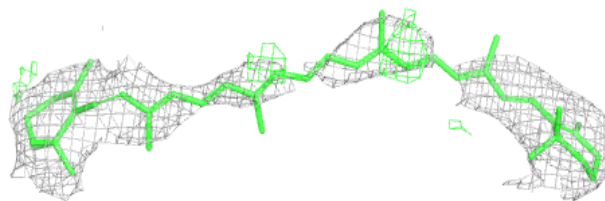
**Electron density around DGD BC 5517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

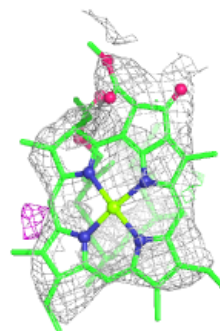
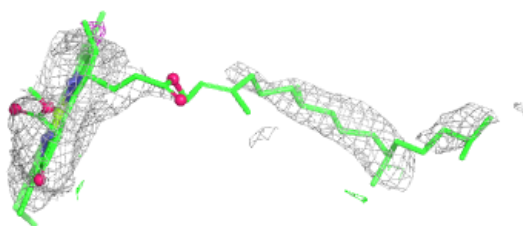
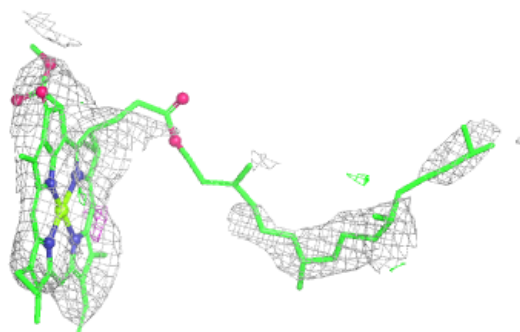


Electron density around BCR BT 5101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

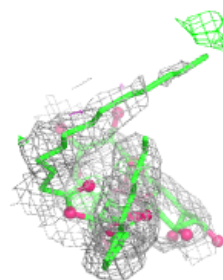
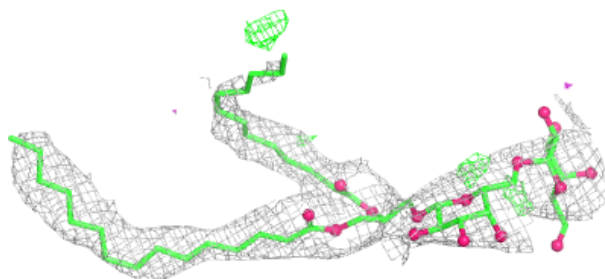
**Electron density around CLA BD 5405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

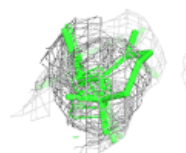
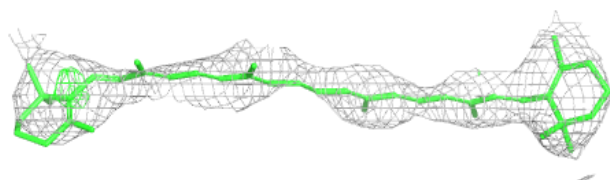
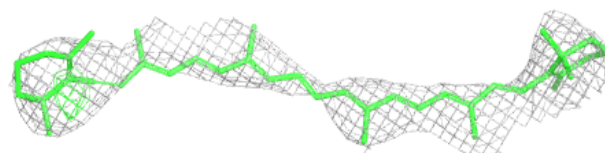


Electron density around DGD BH 5101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

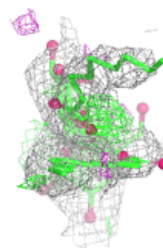
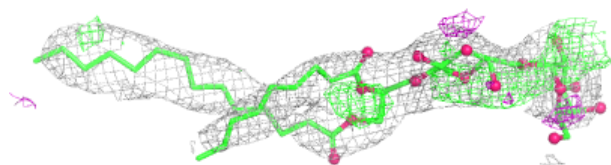
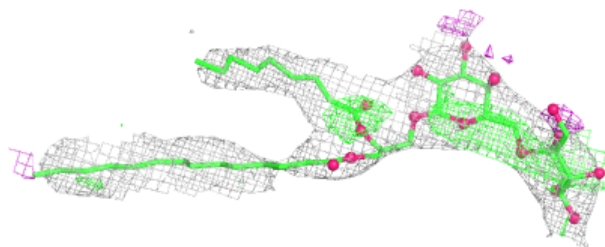
**Electron density around BCR AC 515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

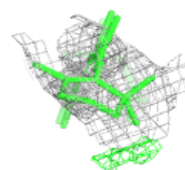
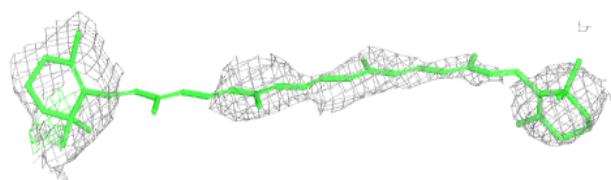
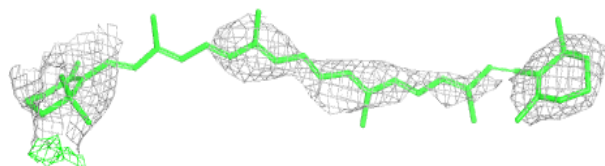


Electron density around DGD AC 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

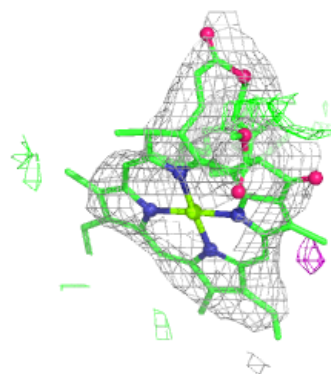
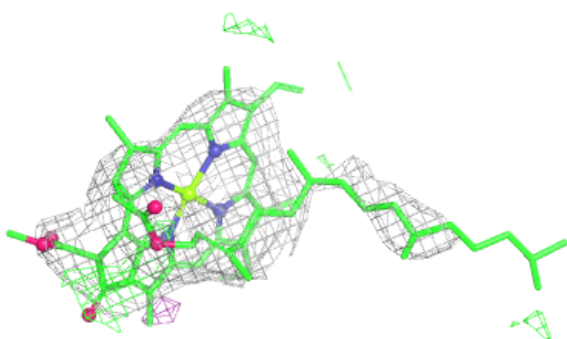
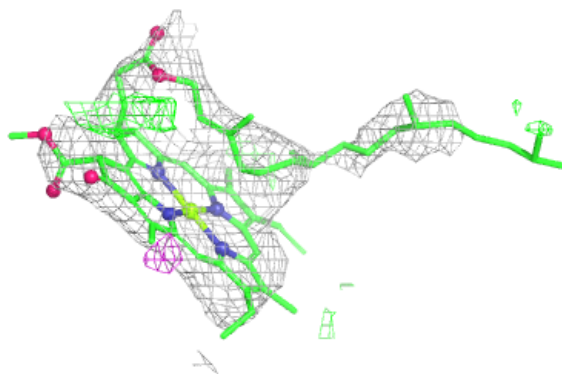
**Electron density around BCR BC 5515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

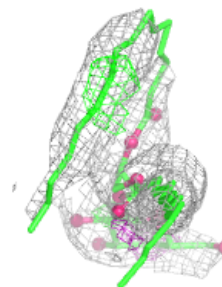
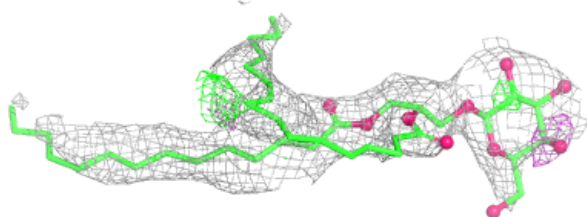
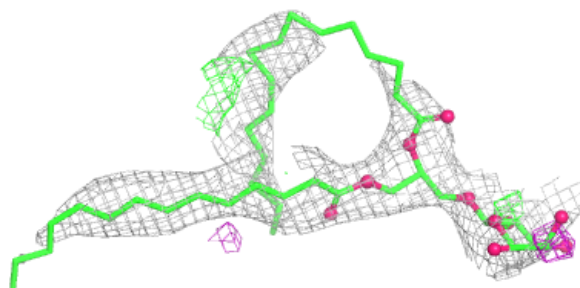


Electron density around CLA BC 5505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

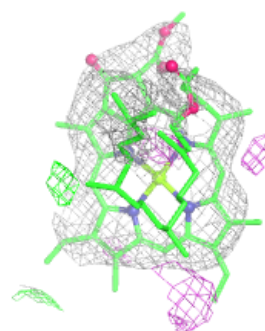
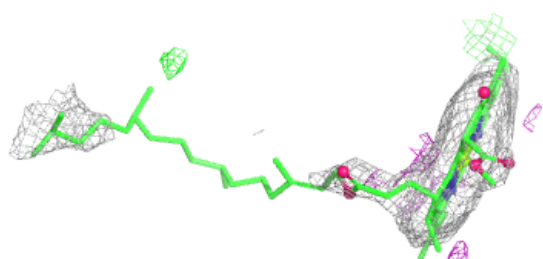
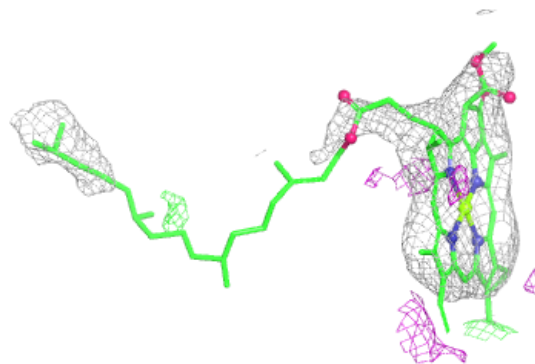
**Electron density around LMG AD 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

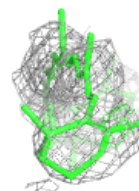
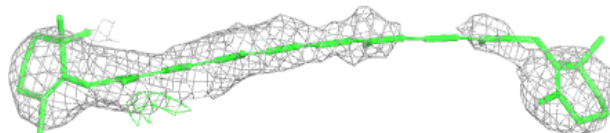
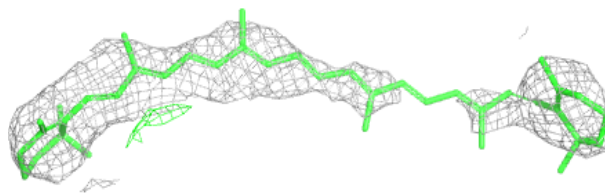


Electron density around CLA AD 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

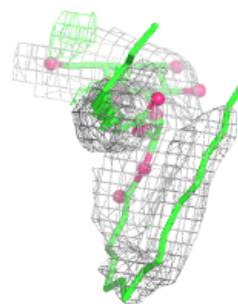
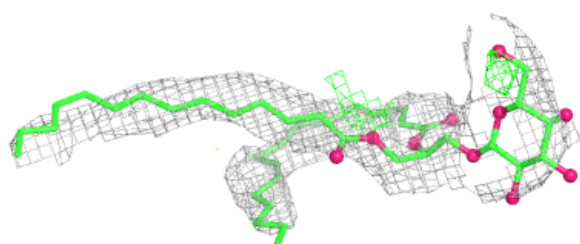
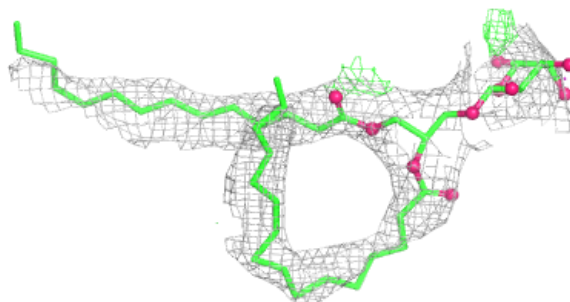
**Electron density around BCR AT 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

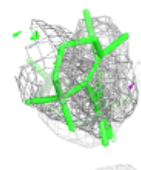
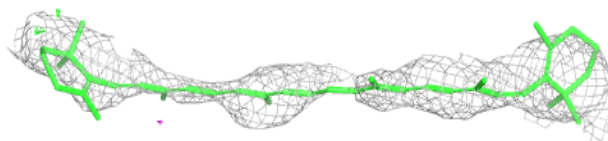
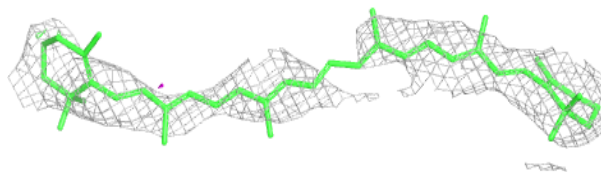


Electron density around LMG BD 5409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

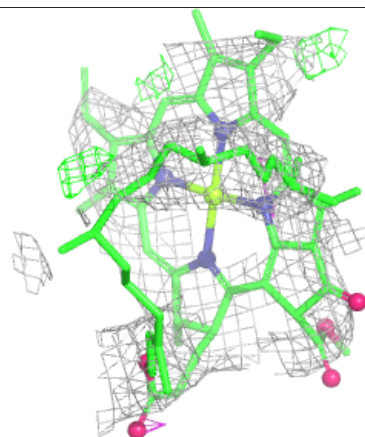
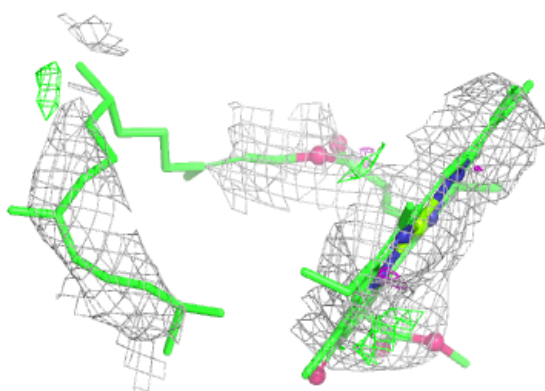
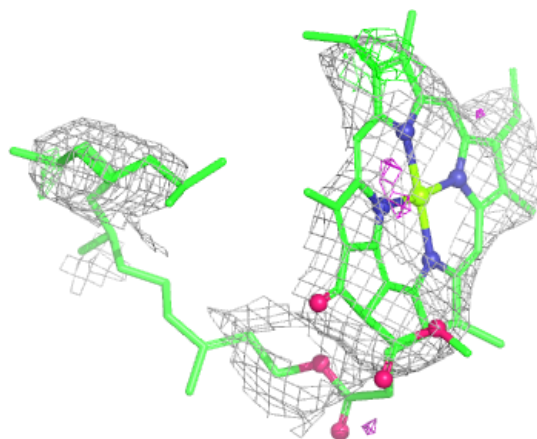
**Electron density around BCR BX 5101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

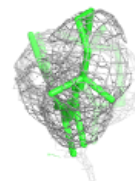
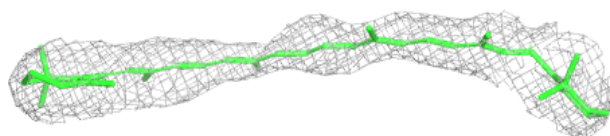
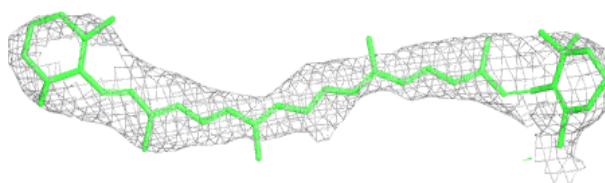


Electron density around CLA BC 5503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

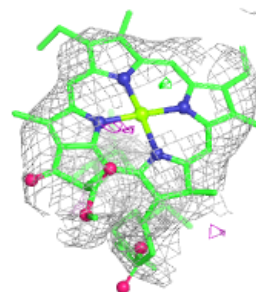
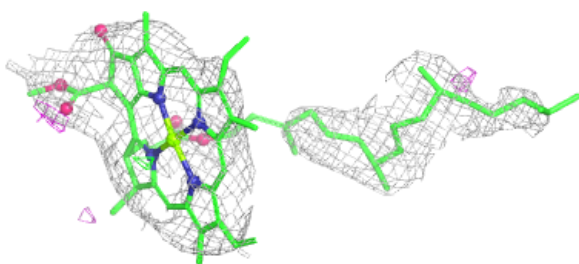
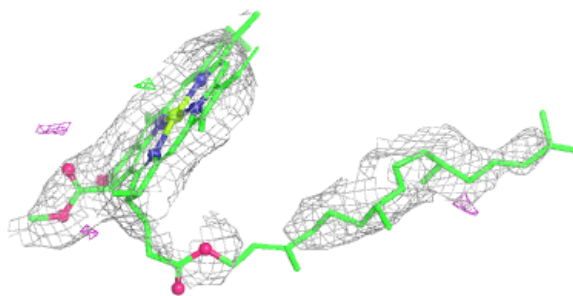
**Electron density around BCR BD 5407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

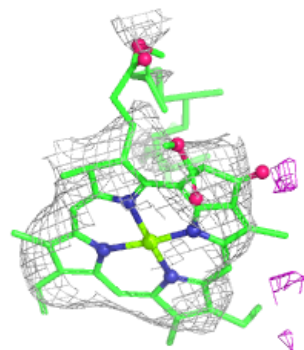
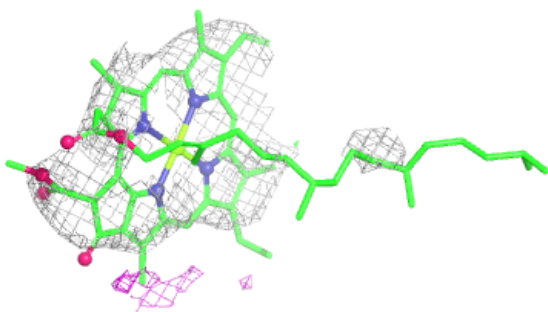
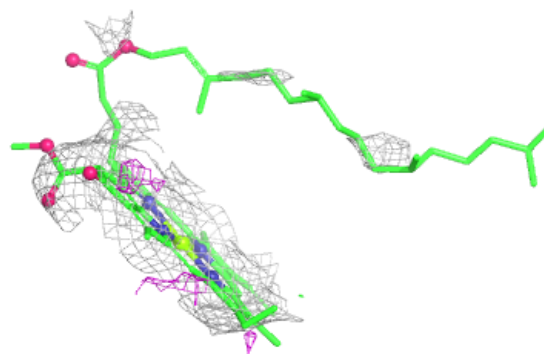


Electron density around CLA BC 5504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

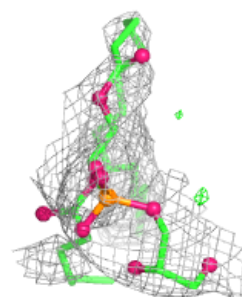
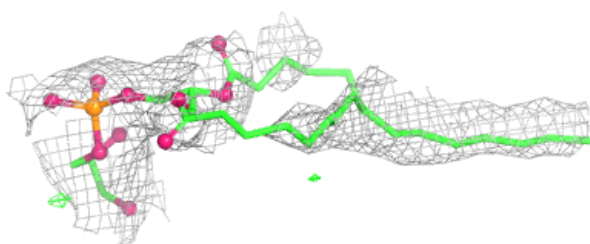
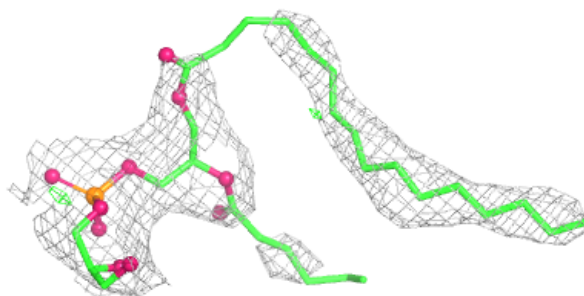
**Electron density around CLA AC 513:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

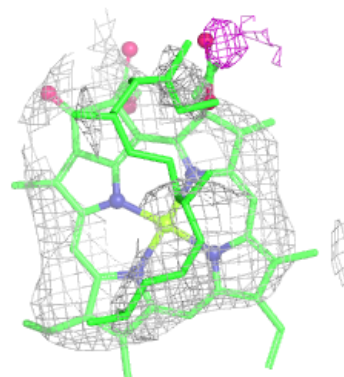
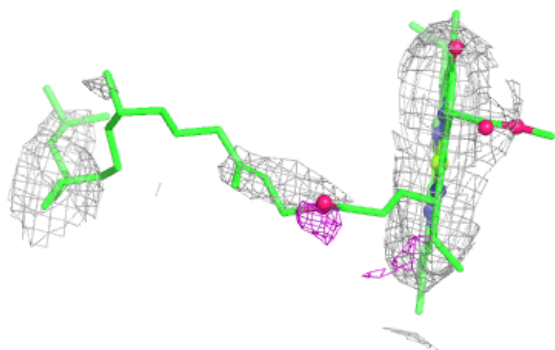
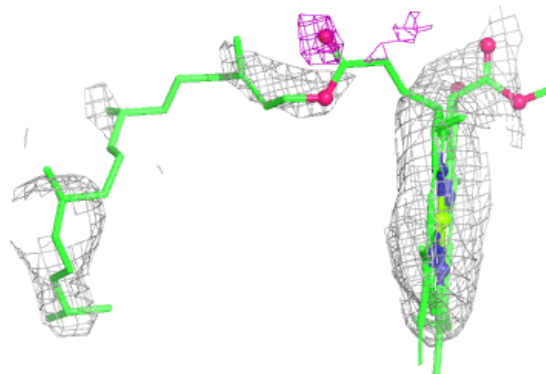


Electron density around LHG BA 5413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

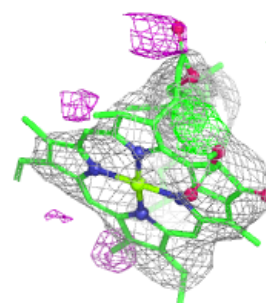
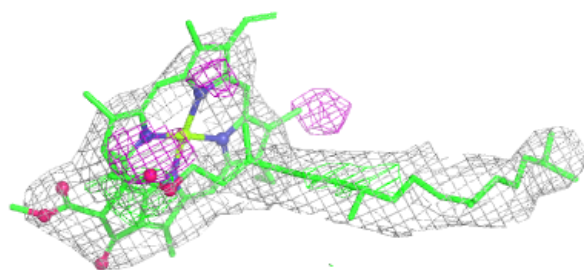
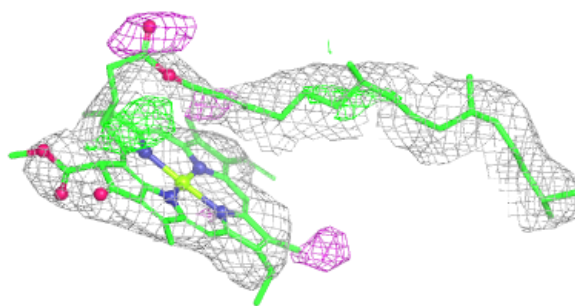
**Electron density around CLA BC 5506:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



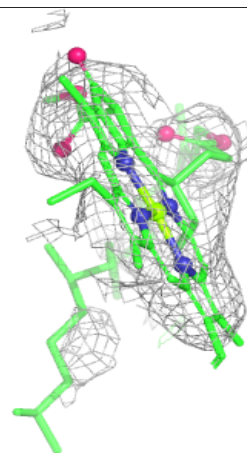
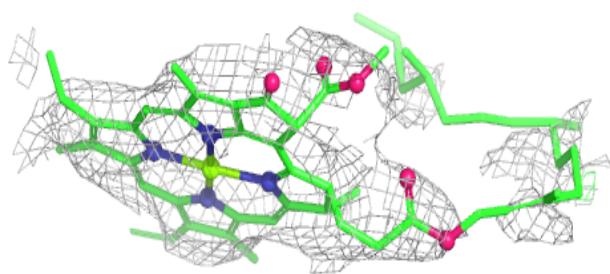
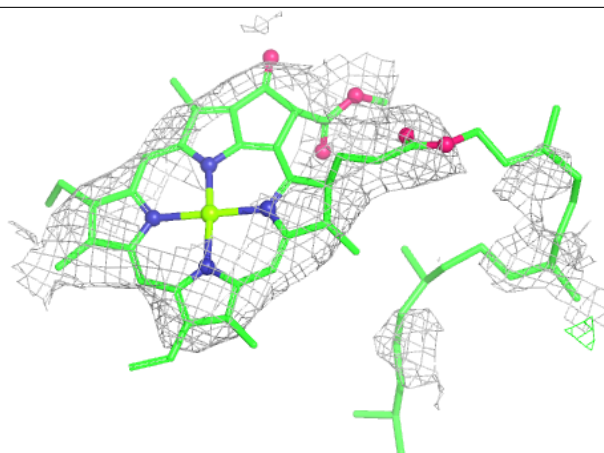
Electron density around CLA AB 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

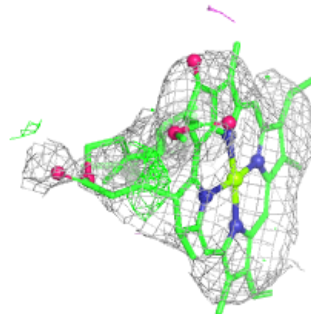
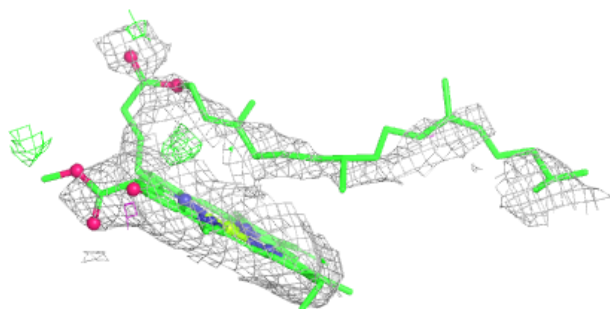
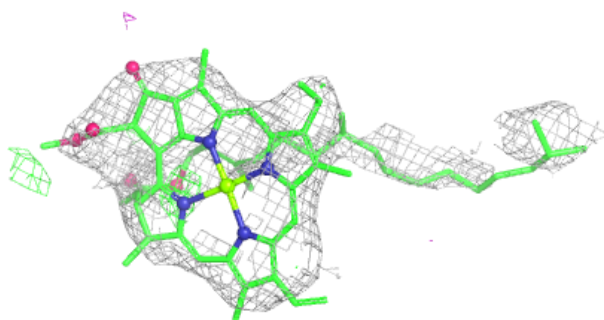


Electron density around CLA AB 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA BB 5618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

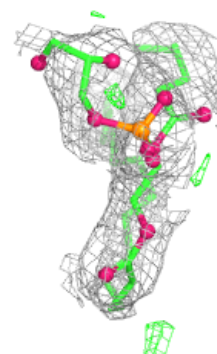
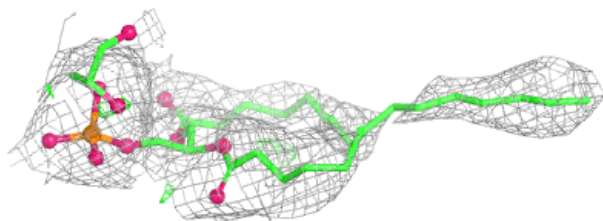


Electron density around CLA AB 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

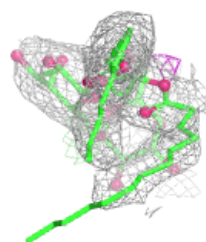
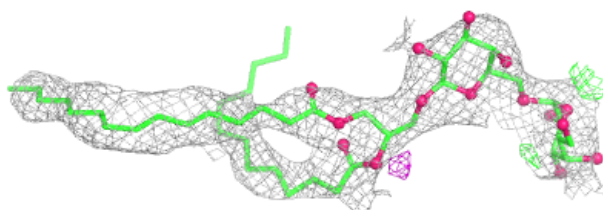
**Electron density around LHG AA 412:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

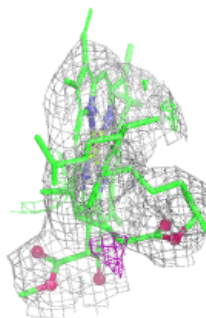
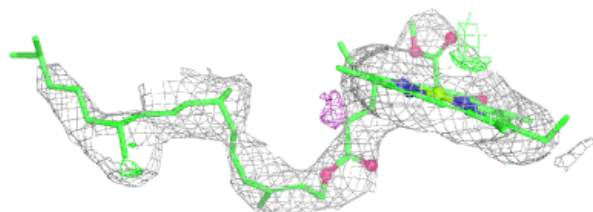
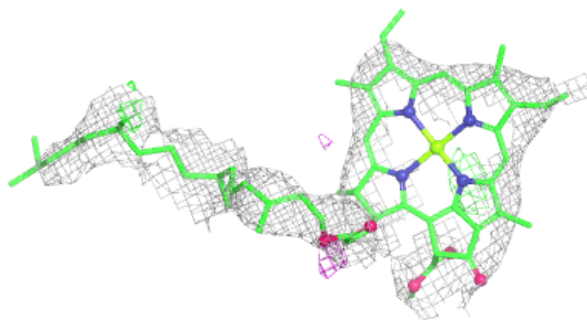


Electron density around DGD AH 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

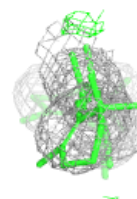
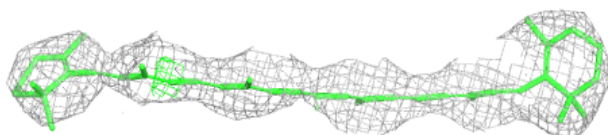
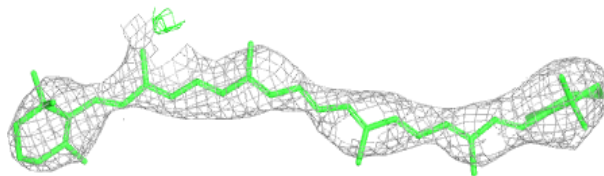
**Electron density around CLA BA 5407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

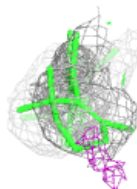
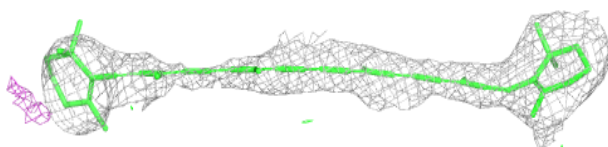
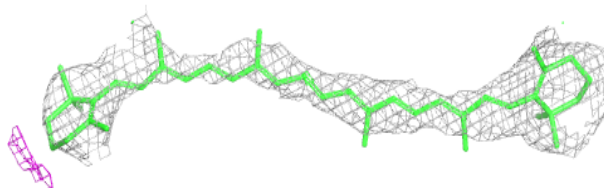


Electron density around BCR AB 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

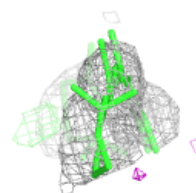
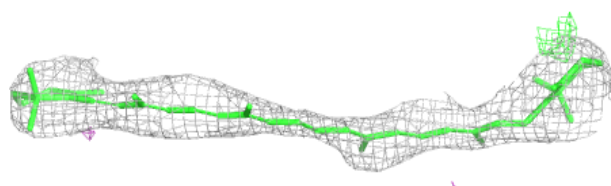
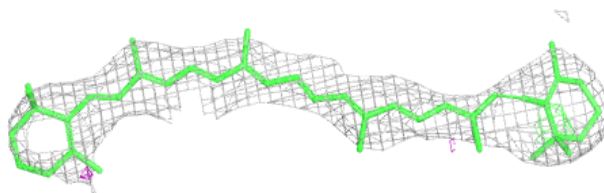
**Electron density around BCR AB 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

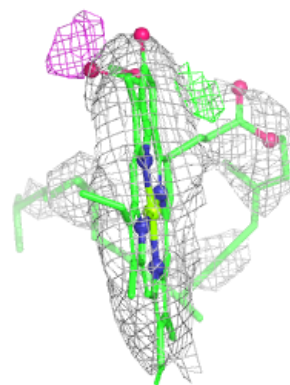
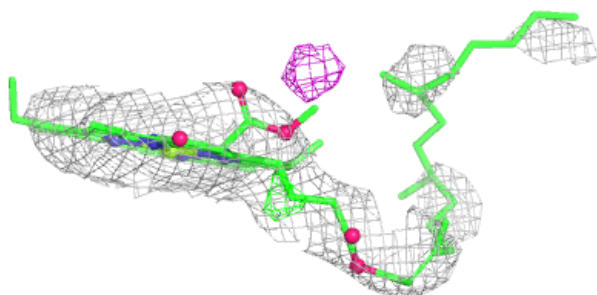
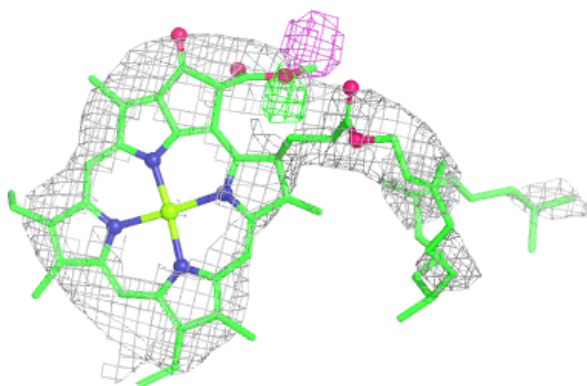


Electron density around BCR AD 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

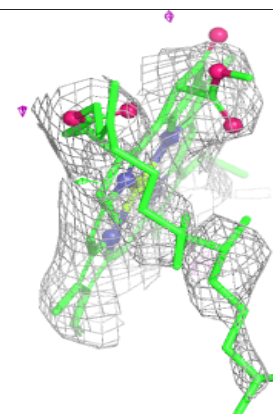
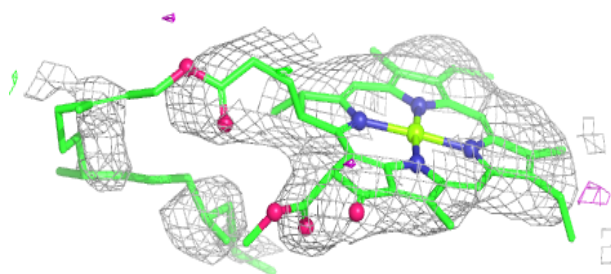
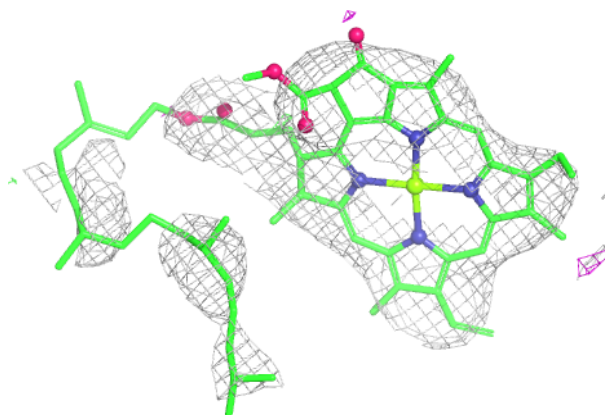
**Electron density around CLA AC 512:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

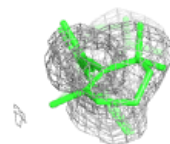
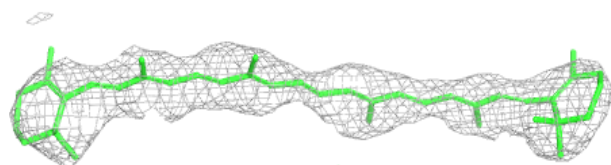
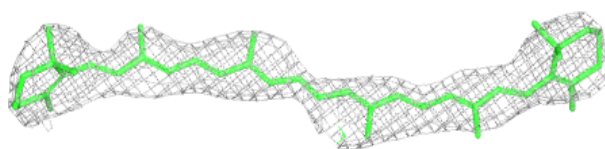


Electron density around CLA BB 5620:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

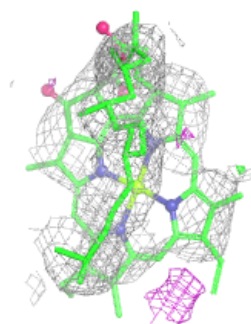
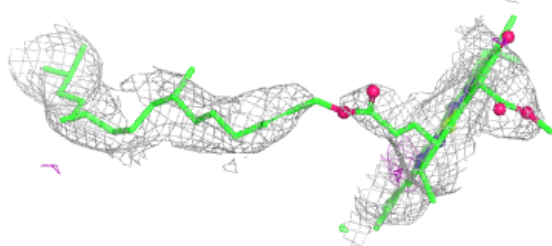
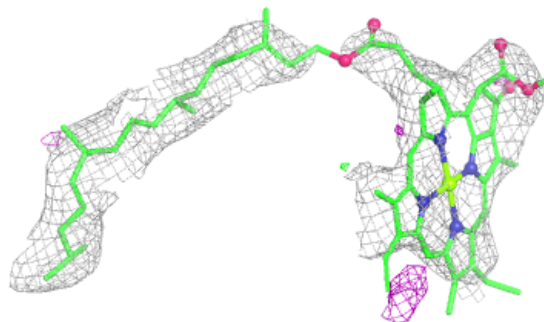
**Electron density around BCR AB 619:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

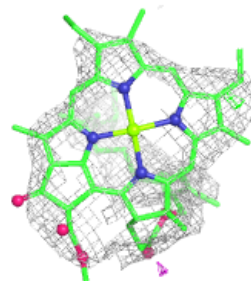
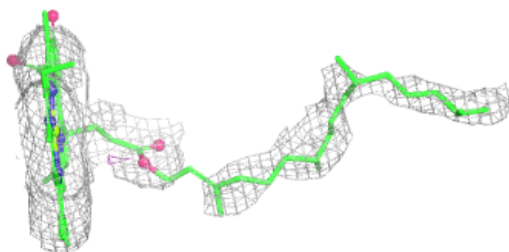
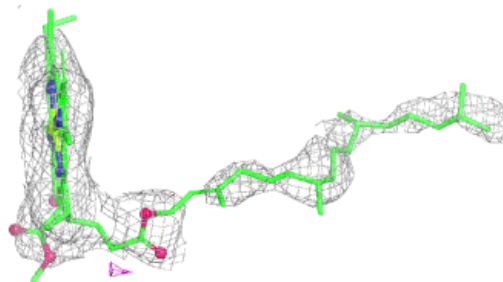


Electron density around CLA AB 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

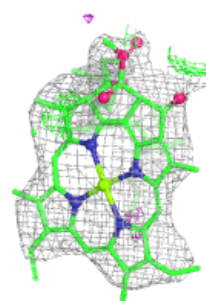
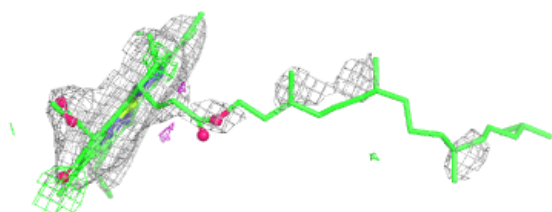
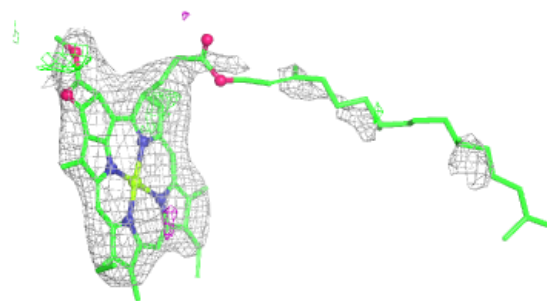
**Electron density around CLA BB 5610:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

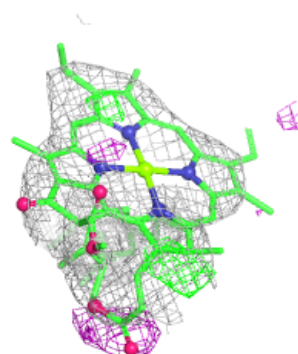
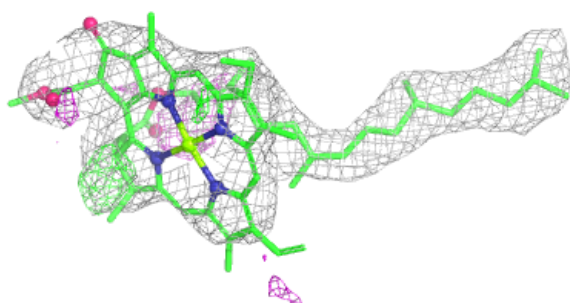
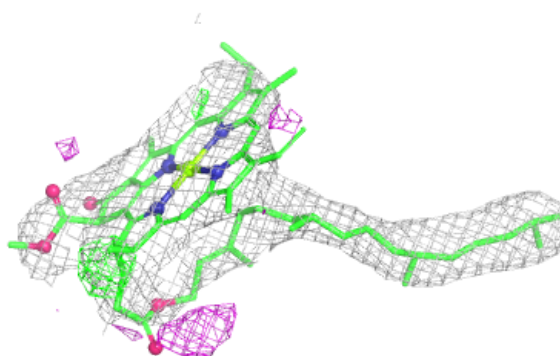


Electron density around CLA AA 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

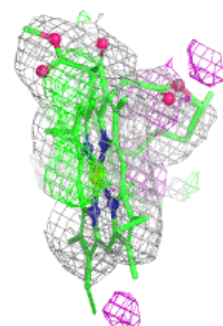
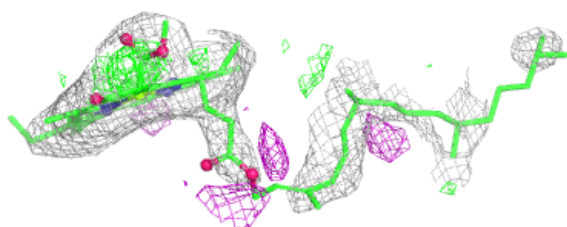
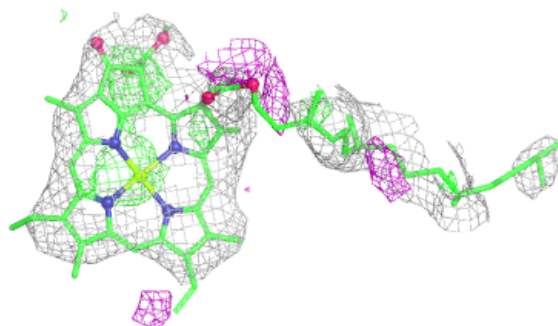
**Electron density around CLA AC 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

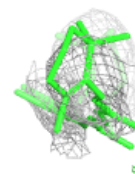
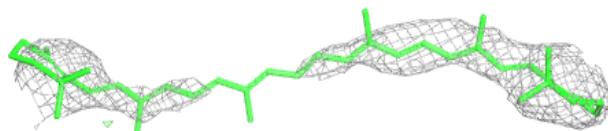
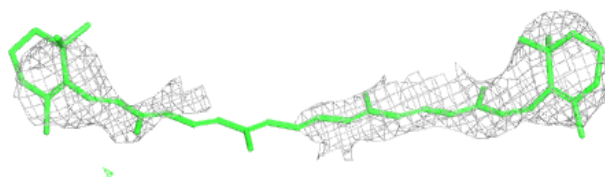


Electron density around CLA AA 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

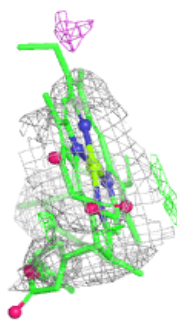
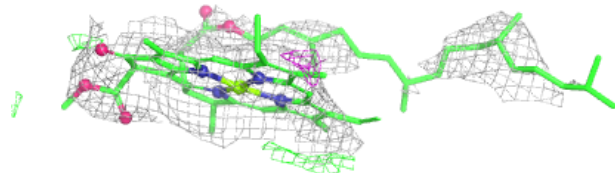
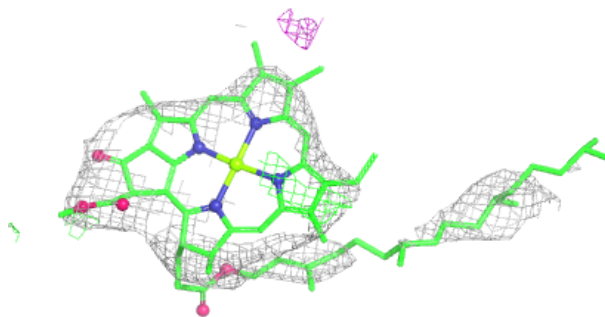
**Electron density around BCR BC 5514:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

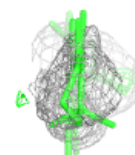
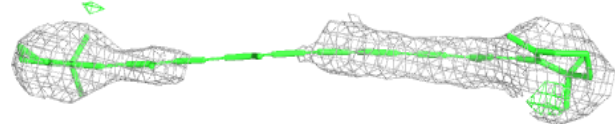
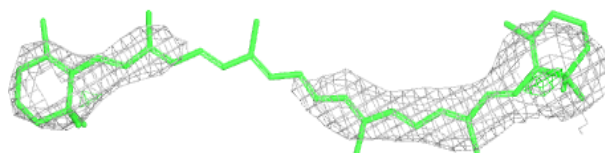


Electron density around CLA BC 5501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

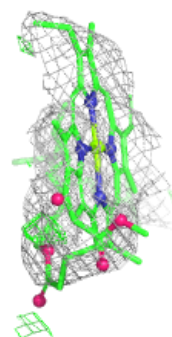
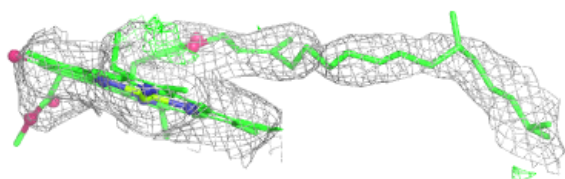
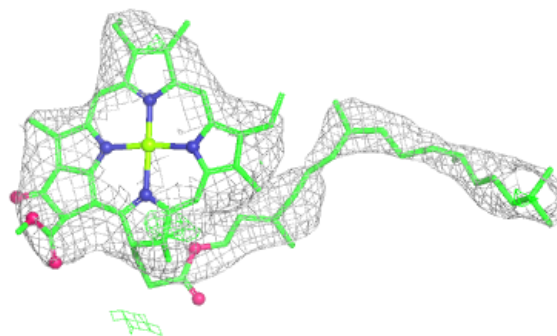
**Electron density around BCR AK 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

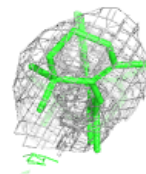
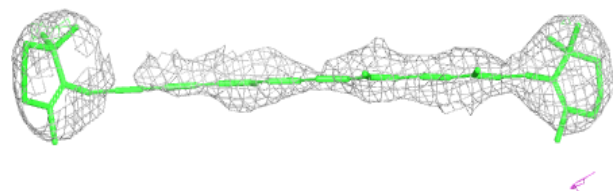
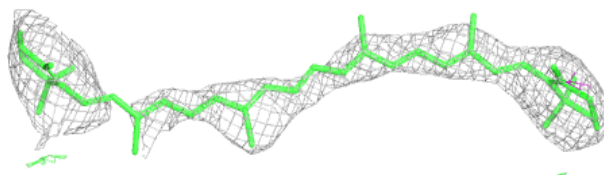


Electron density around CLA BB 5607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

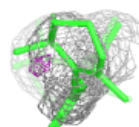
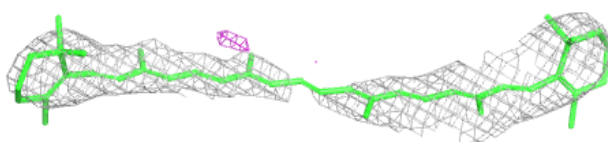
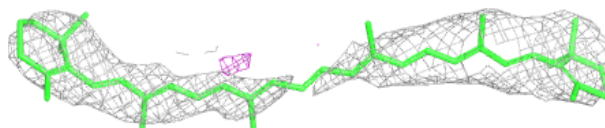
**Electron density around BCR BA 5411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

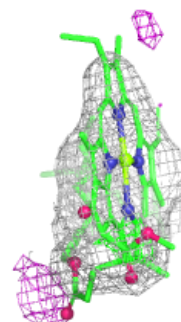
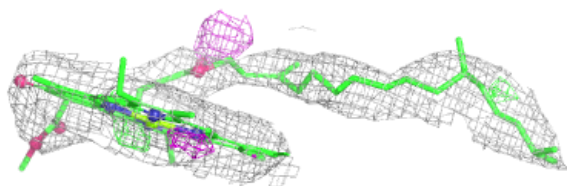
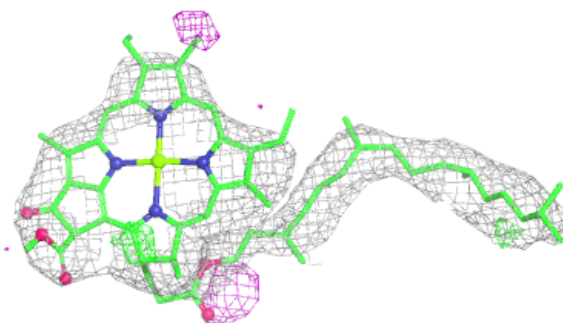


Electron density around BCR BB 5623:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

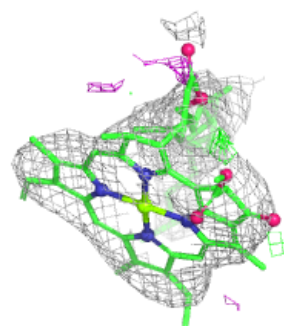
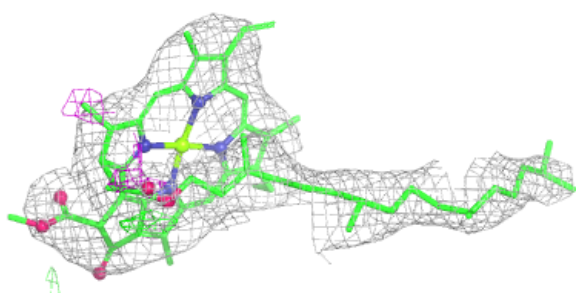
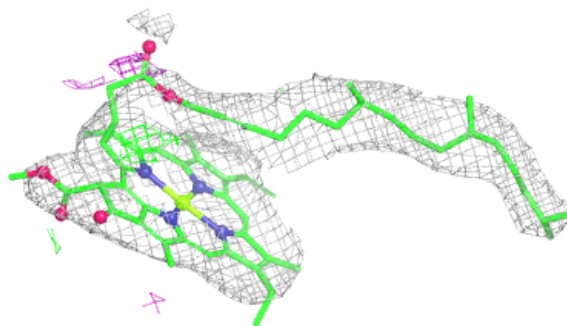
**Electron density around CLA AB 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

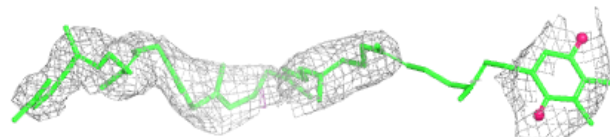
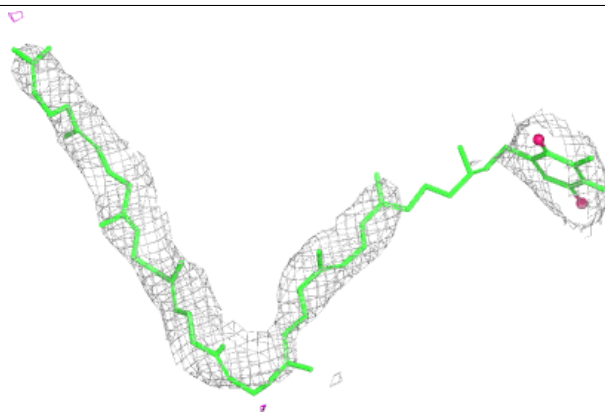


Electron density around CLA BB 5612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

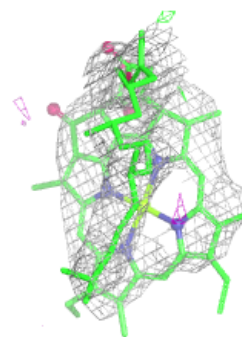
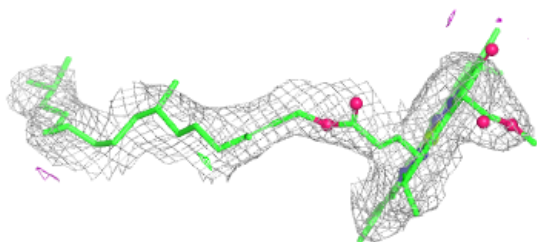
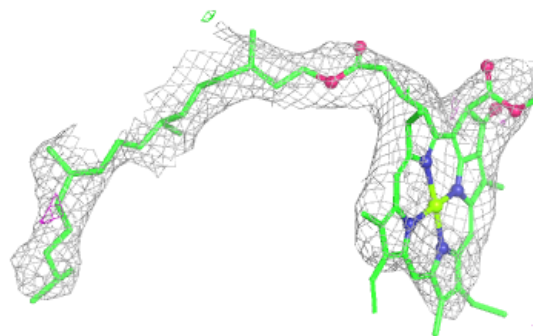
**Electron density around PL9 BD 5406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

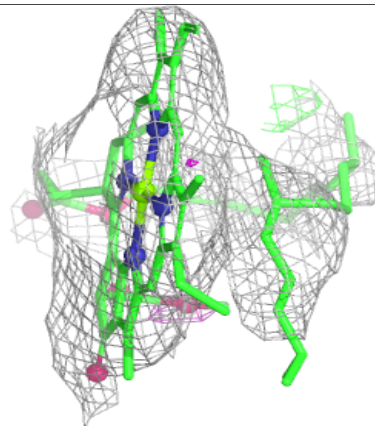
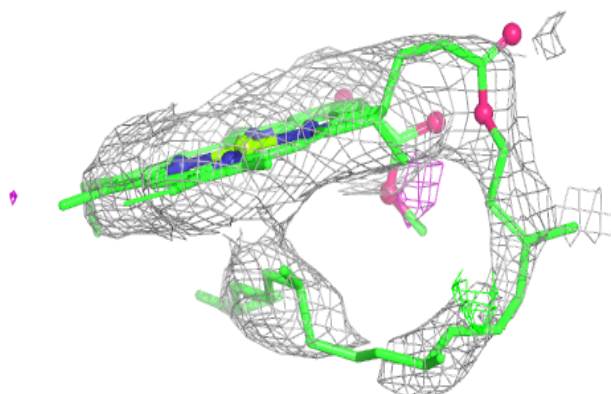
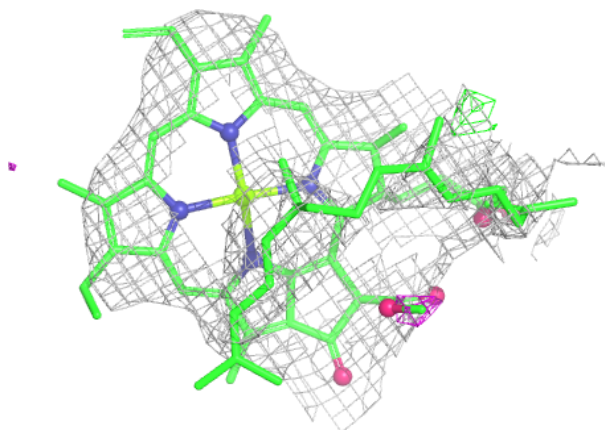


Electron density around CLA BB 5613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

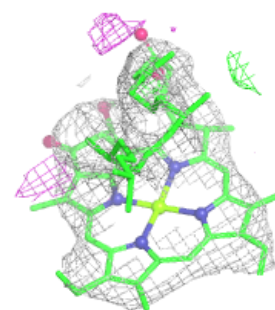
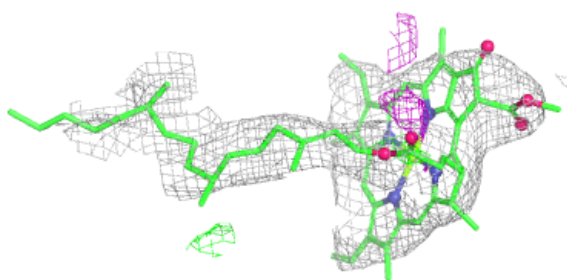
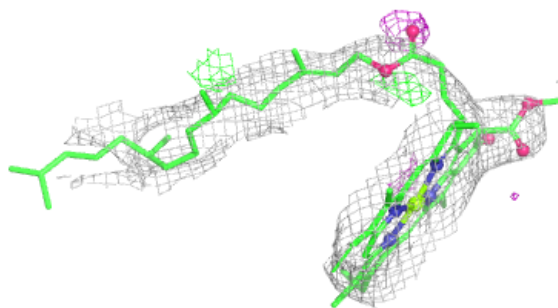
**Electron density around CLA BC 5510:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

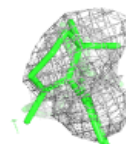
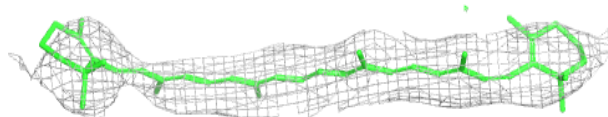
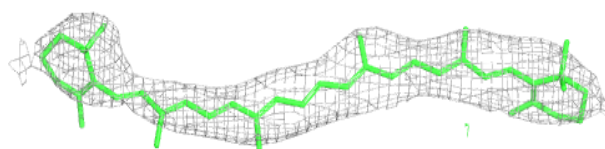


Electron density around CLA AC 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

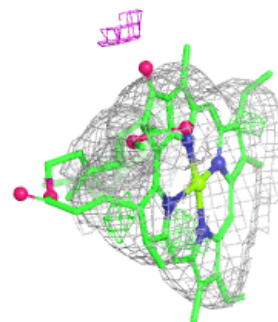
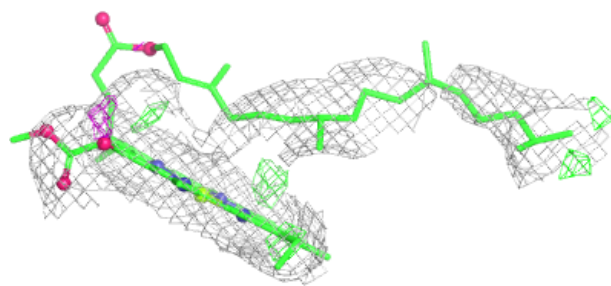
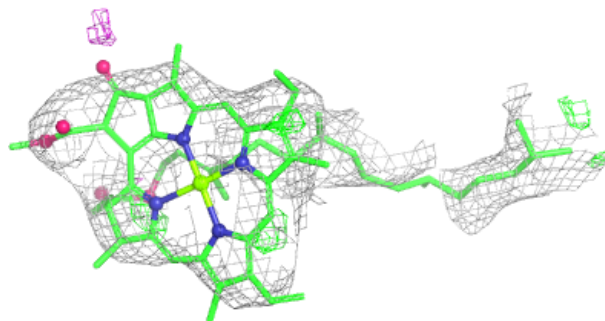
**Electron density around BCR AC 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



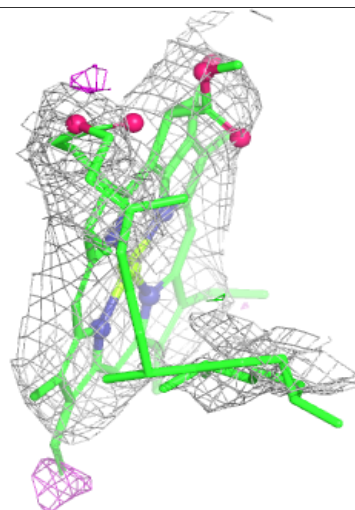
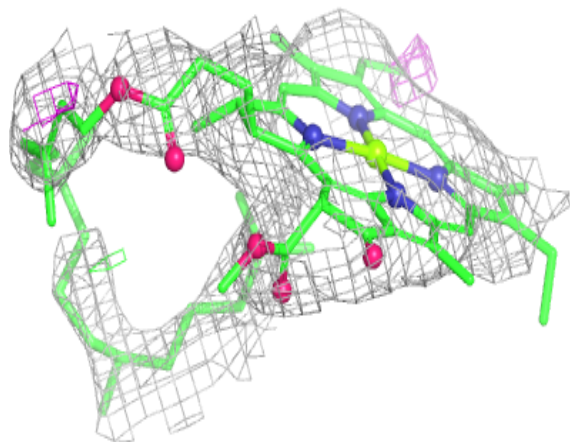
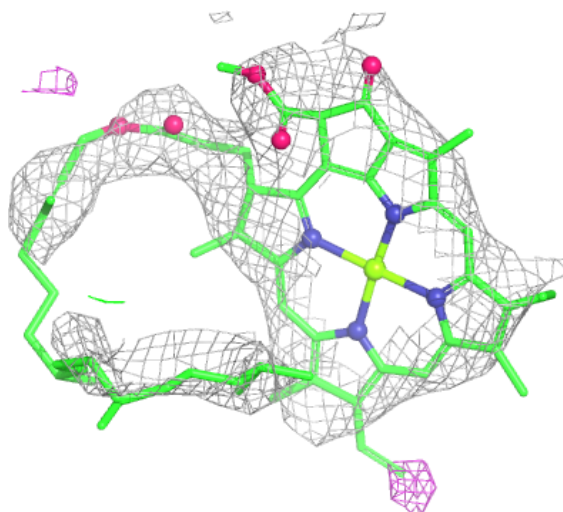
Electron density around CLA AB 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



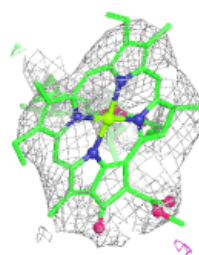
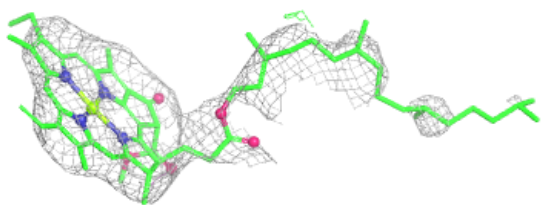
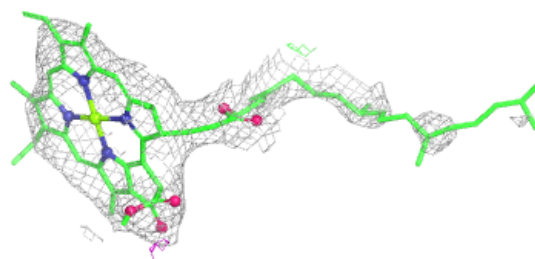
Electron density around CLA AB 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

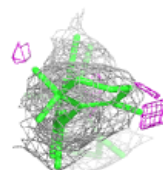
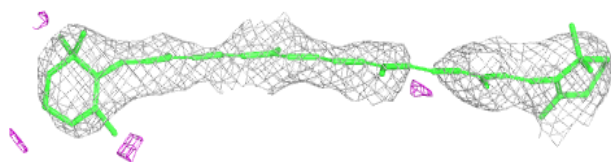
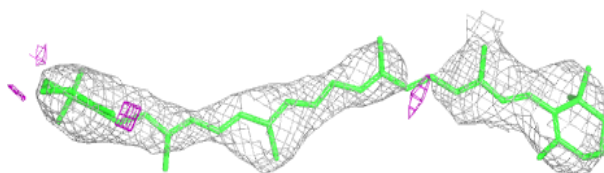


Electron density around CLA BC 5502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

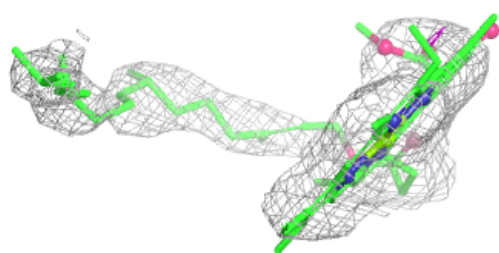
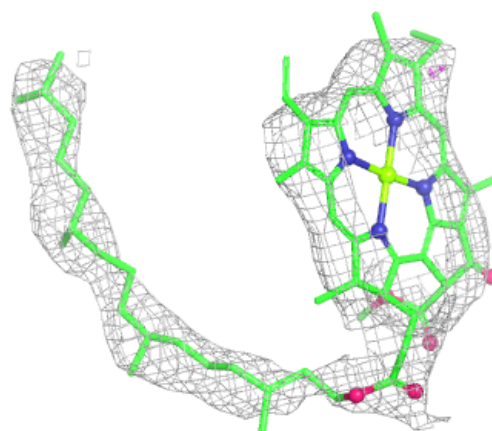
**Electron density around BCR BB 5621:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

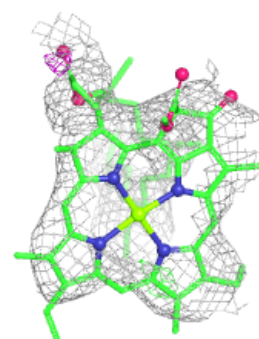
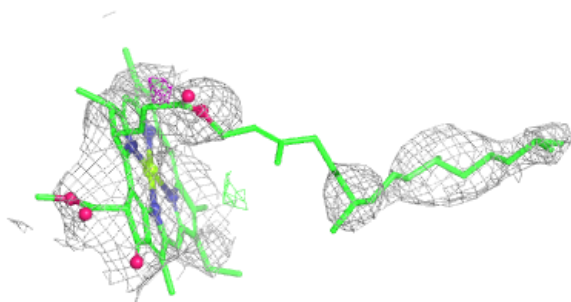
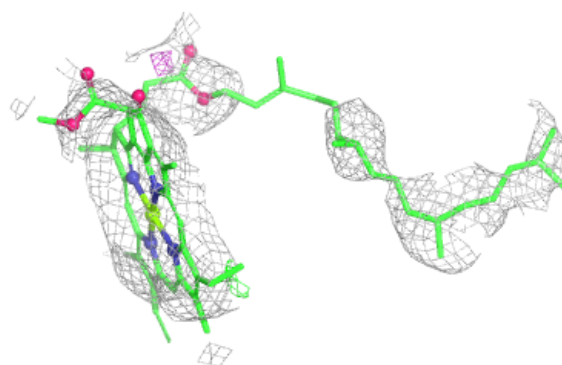


Electron density around CLA BC 5507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

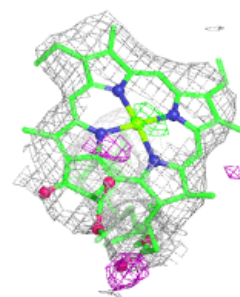
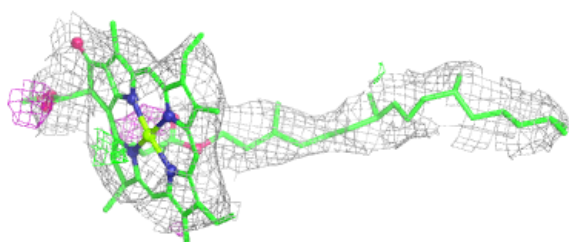
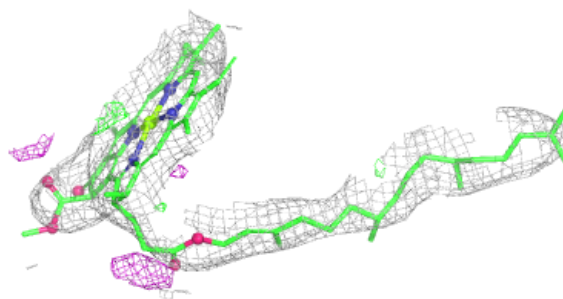
**Electron density around CLA BC 5508:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



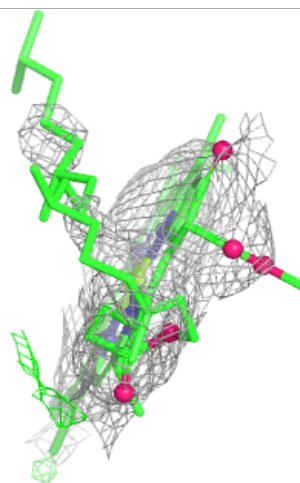
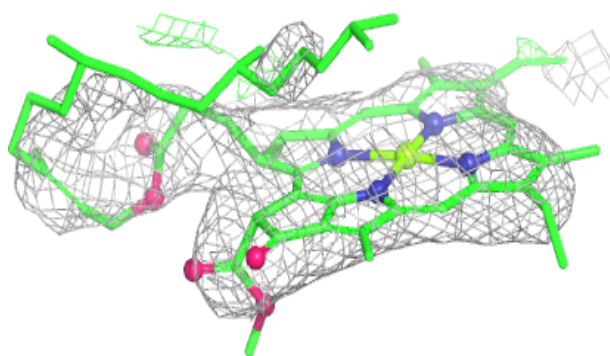
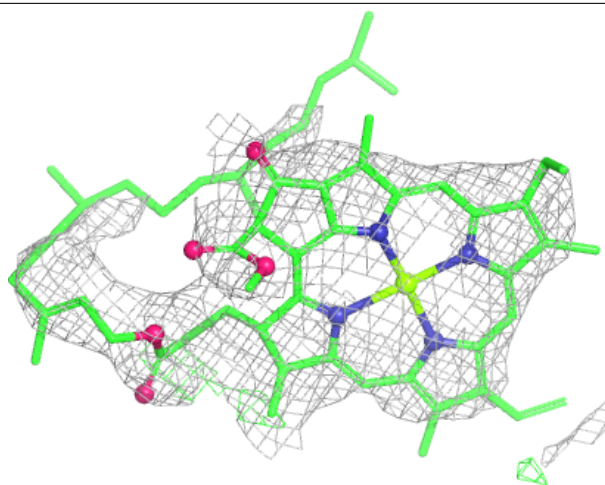
Electron density around CLA BB 5611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



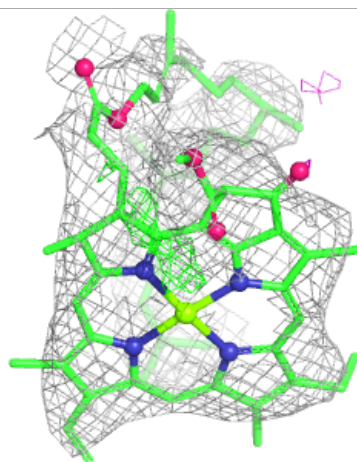
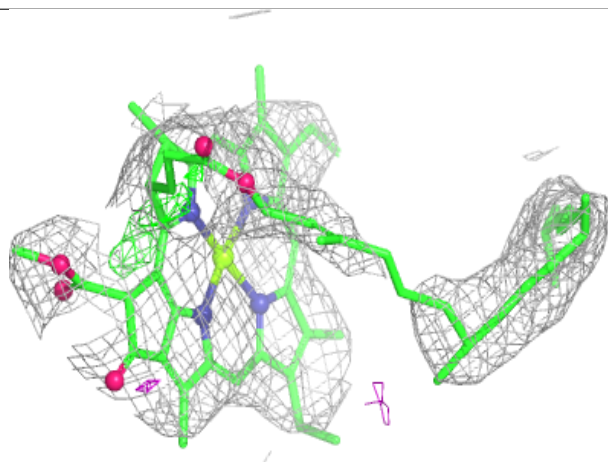
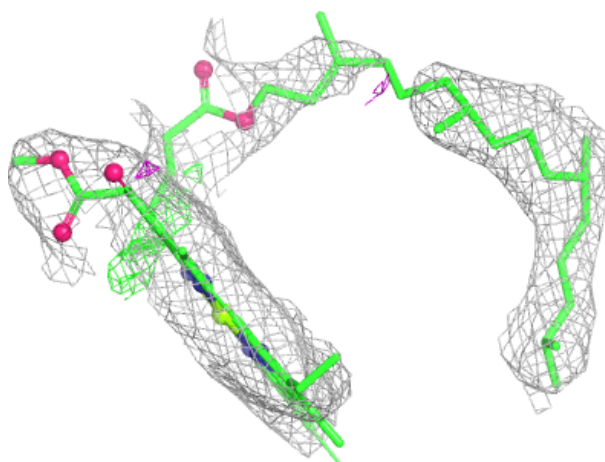
Electron density around CLA BC 5509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



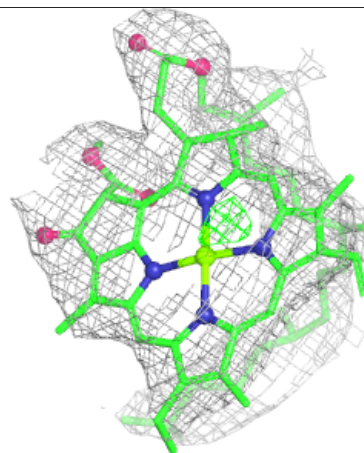
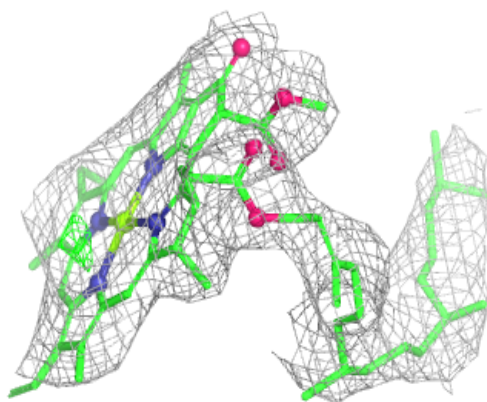
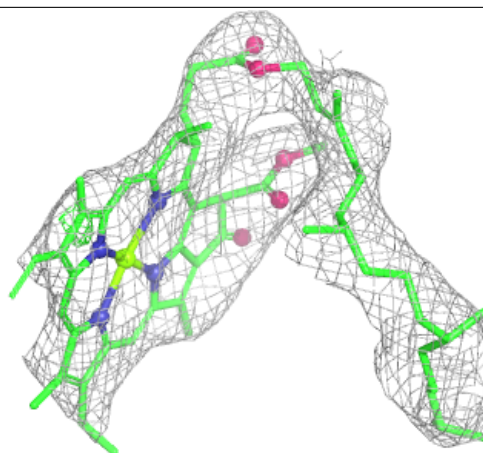
Electron density around CLA AB 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



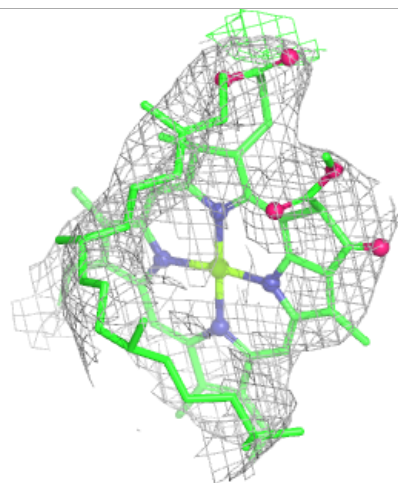
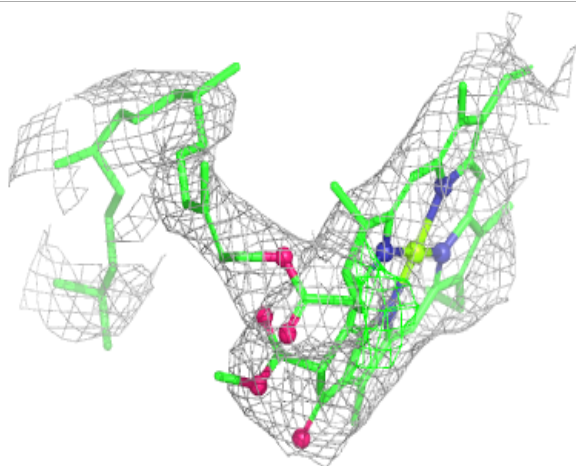
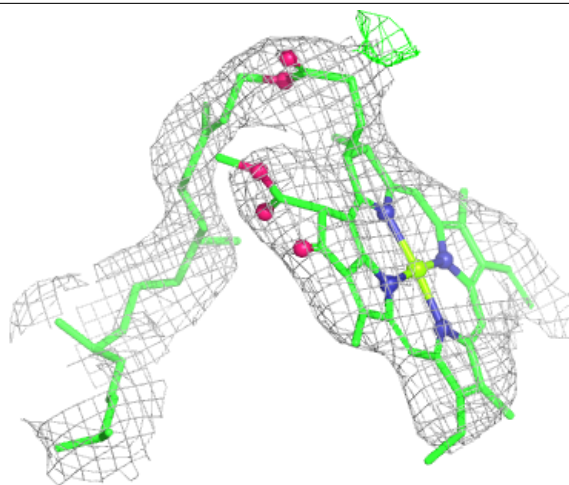
Electron density around CLA AB 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



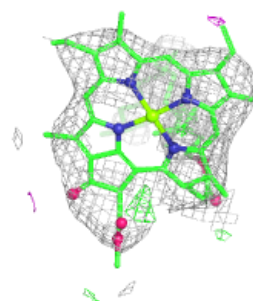
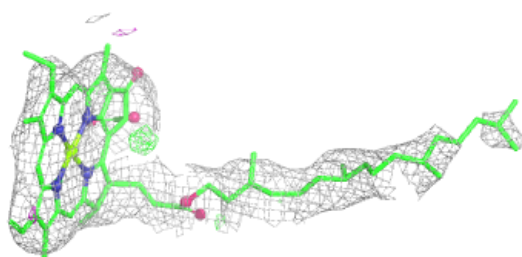
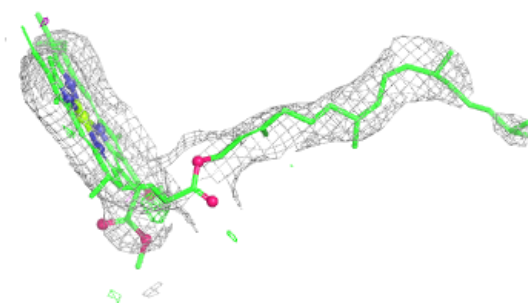
Electron density around CLA BB 5617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

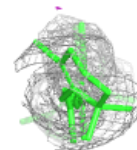
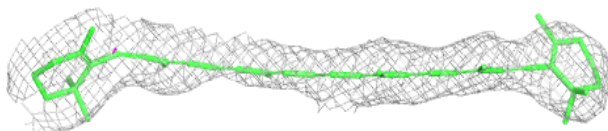
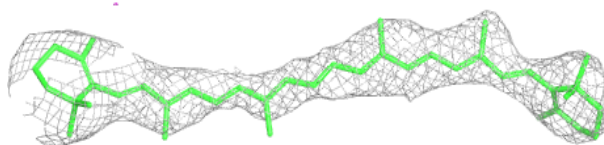


Electron density around CLA AB 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

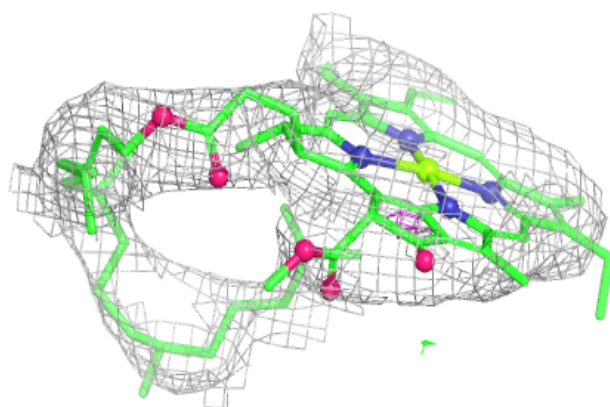
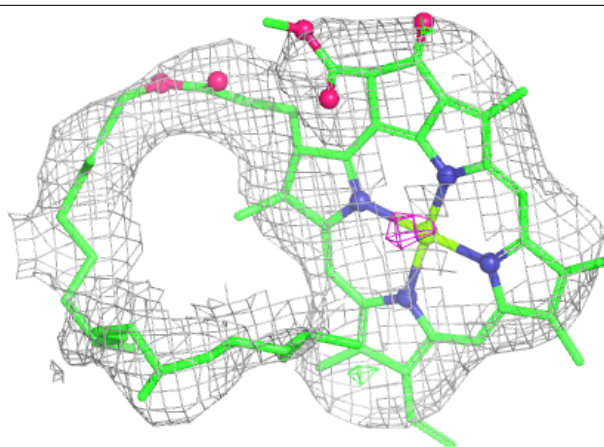
**Electron density around BCR BB 5622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



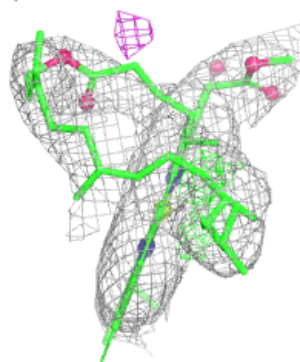
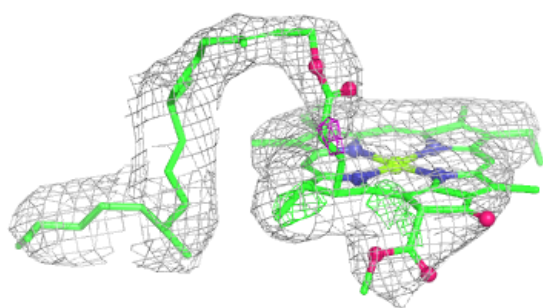
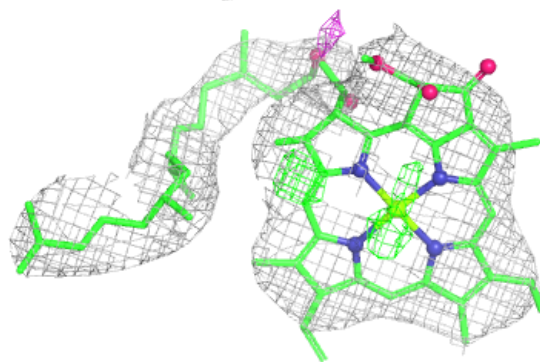
Electron density around CLA BB 5619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

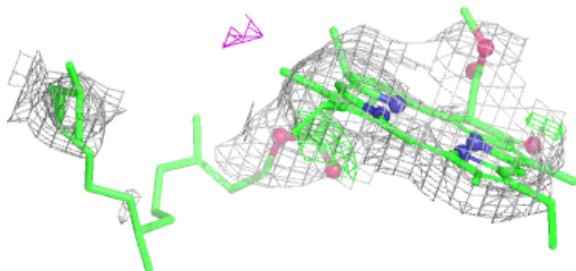
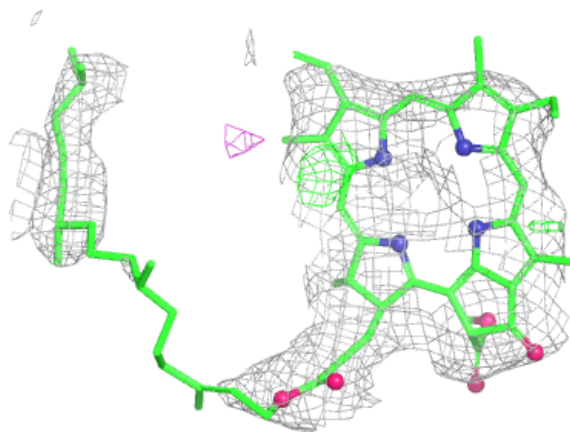


Electron density around CLA BA 5406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

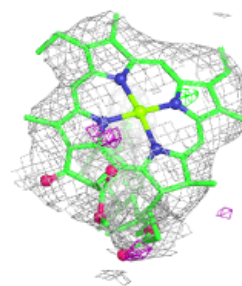
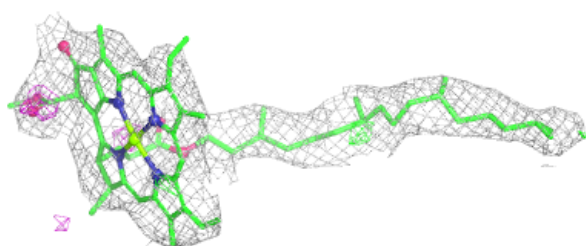
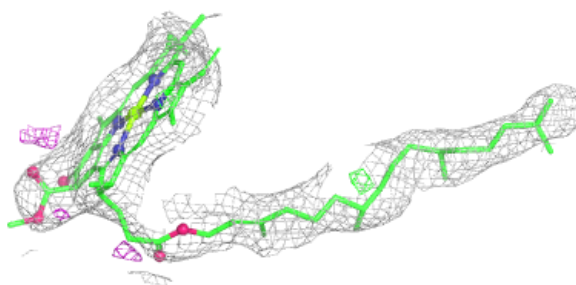
**Electron density around PHO BD 5404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

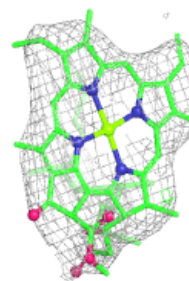
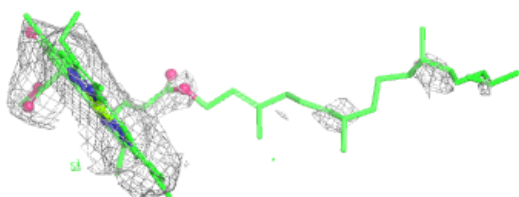
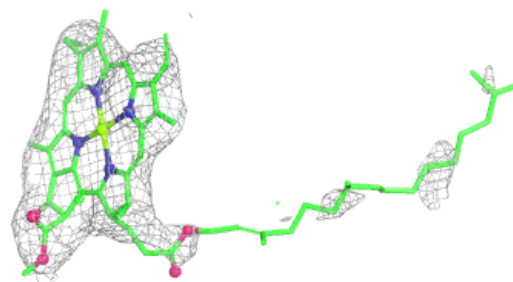


Electron density around CLA AB 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

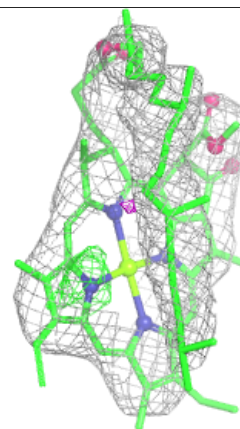
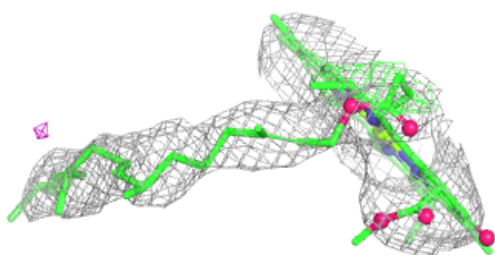
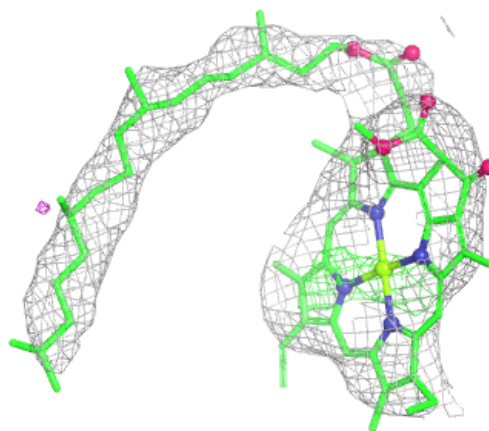
**Electron density around CLA BA 5408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

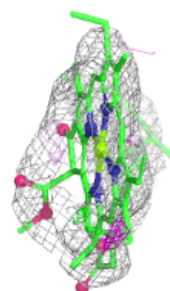
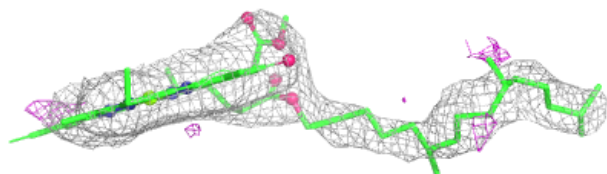
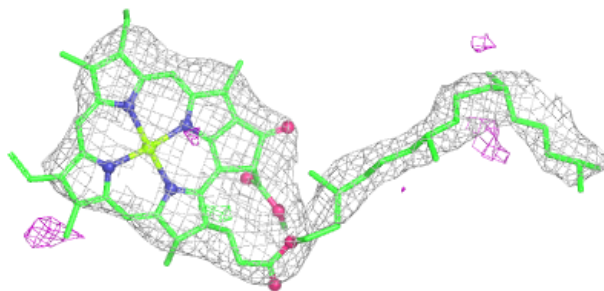


Electron density around CLA AC 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

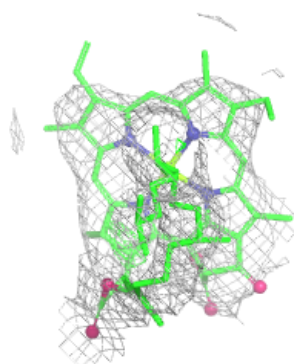
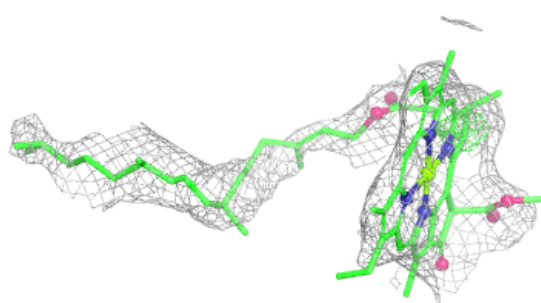
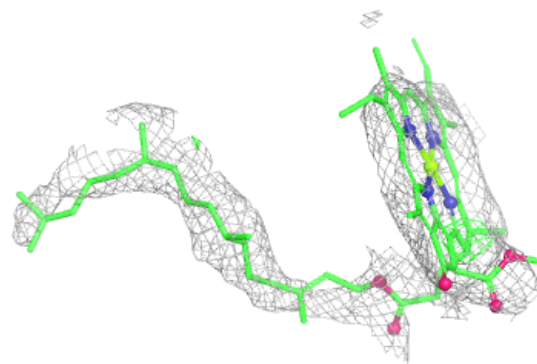
**Electron density around CLA BB 5606:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

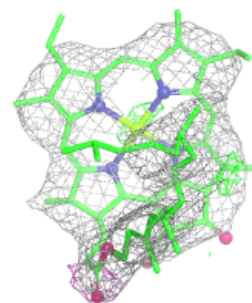
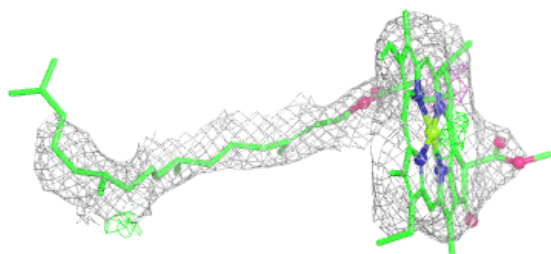
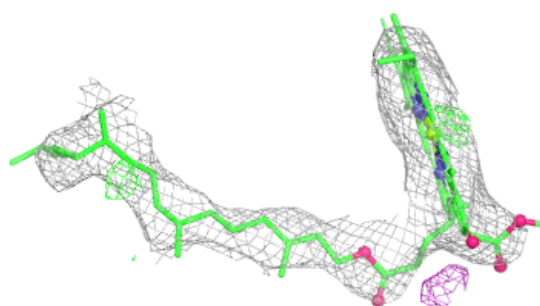


Electron density around CLA AC 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

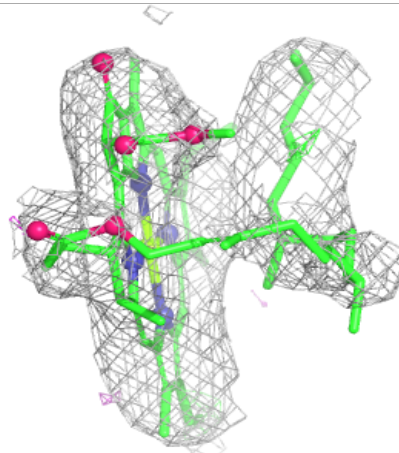
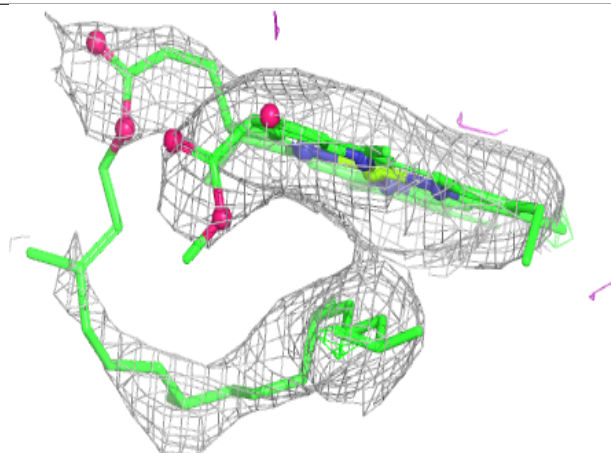
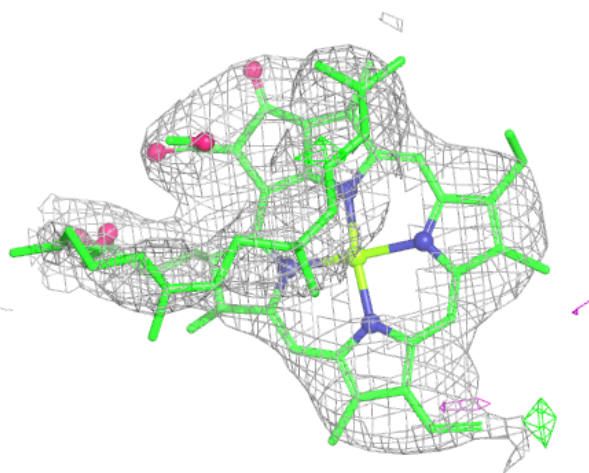
**Electron density around CLA BB 5609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



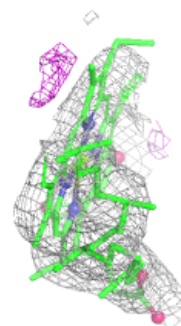
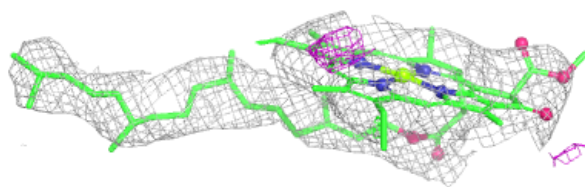
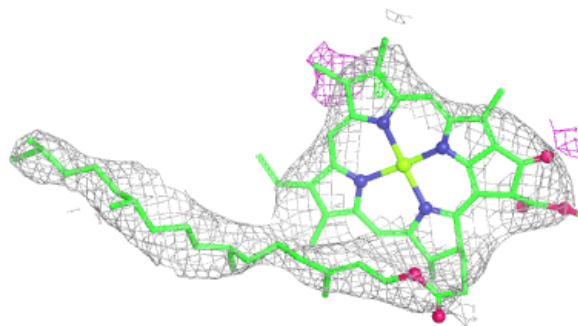
Electron density around CLA AC 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



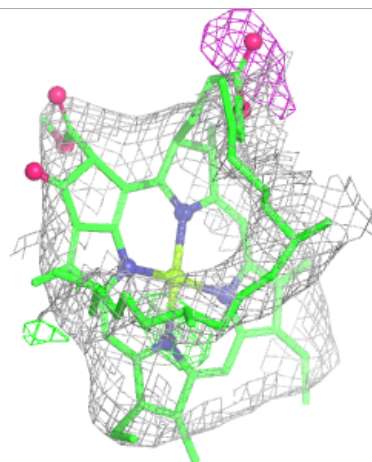
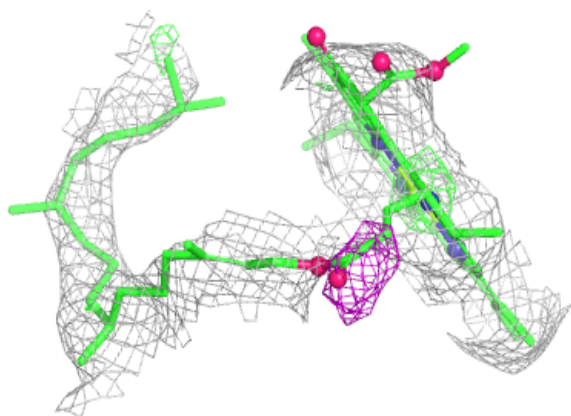
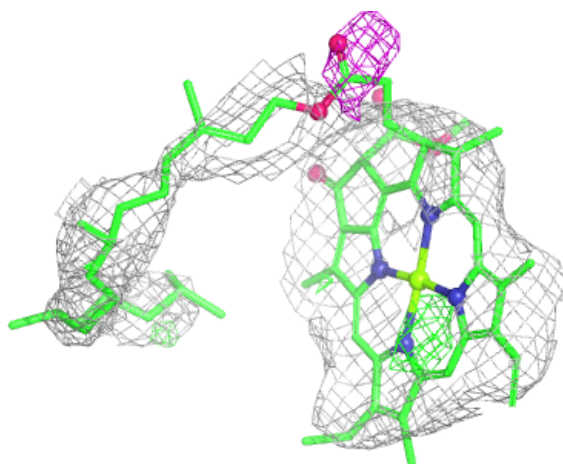
Electron density around CLA AC 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



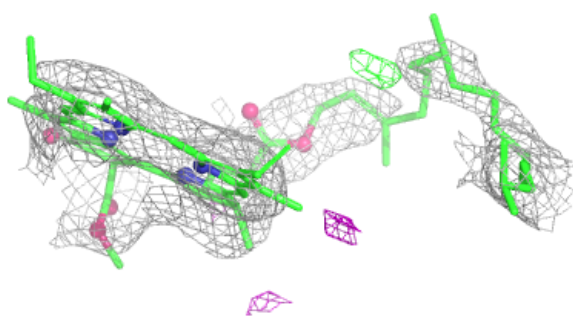
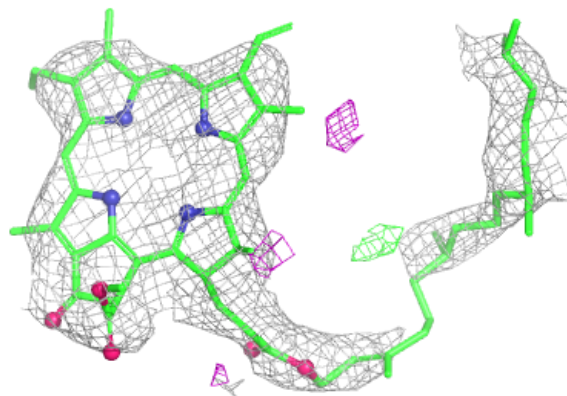
Electron density around CLA AC 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



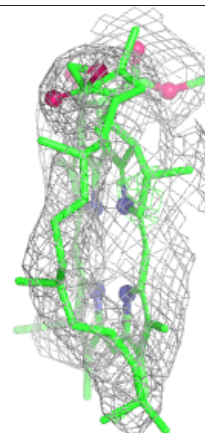
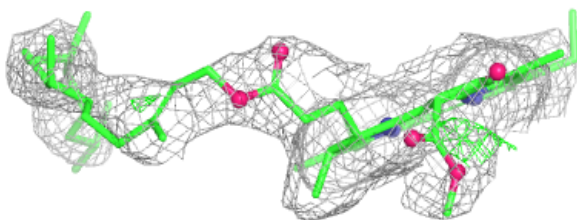
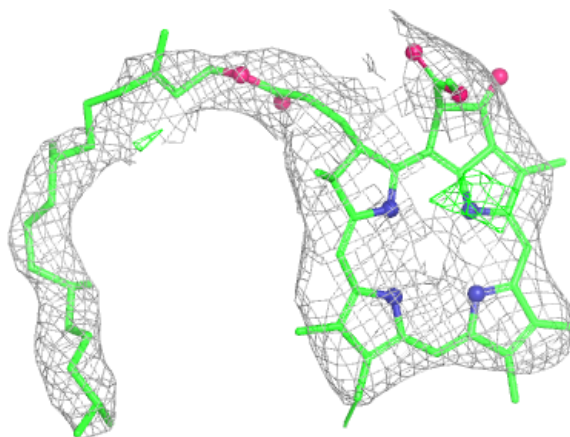
Electron density around PHO AD 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



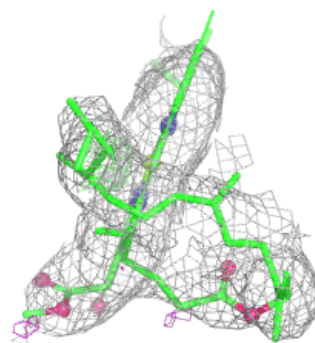
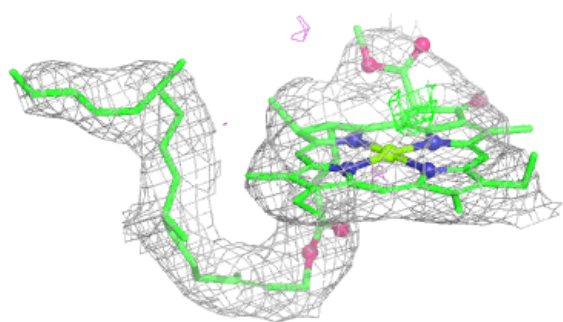
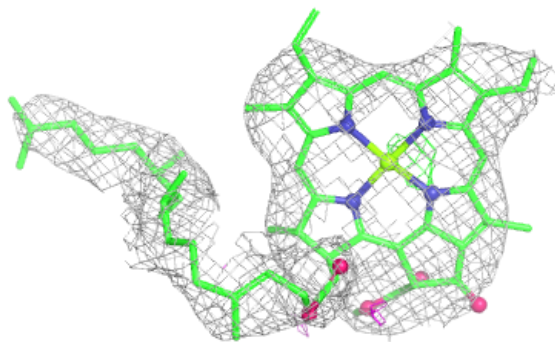
Electron density around PHO BD 5403:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

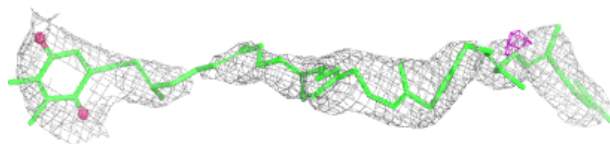
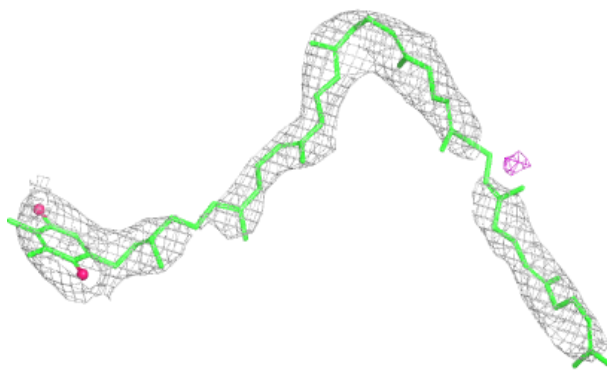


Electron density around CLA AA 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

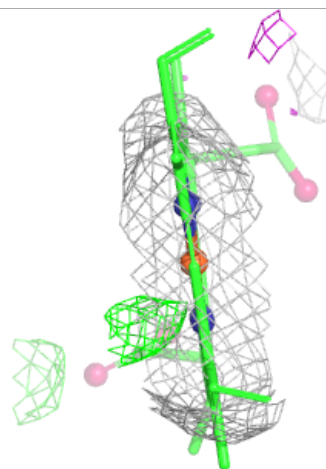
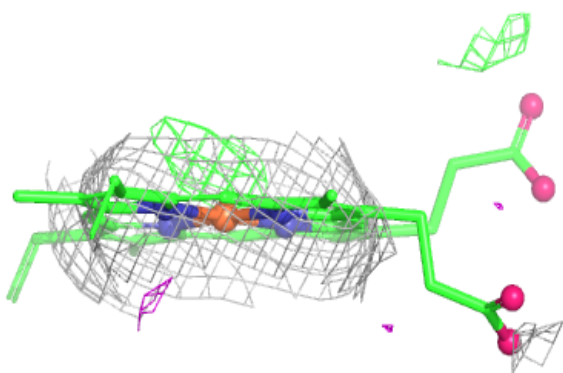
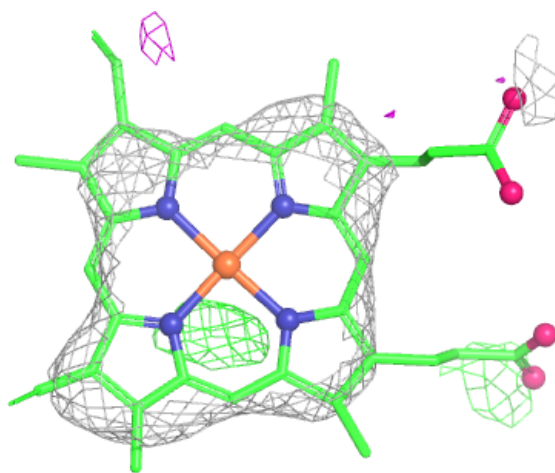
**Electron density around PL9 AD 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



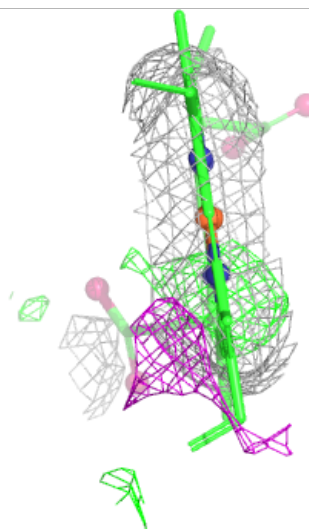
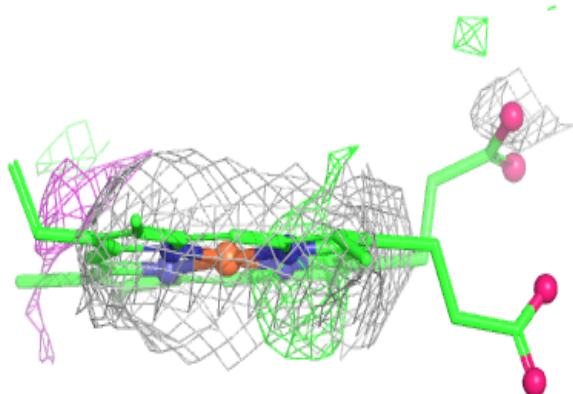
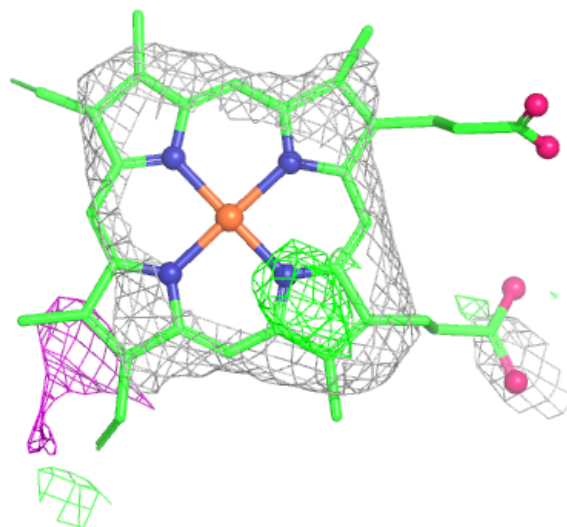
Electron density around HEM AF 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



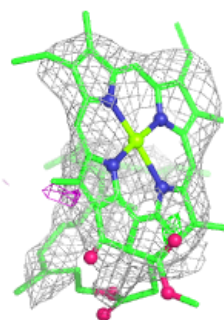
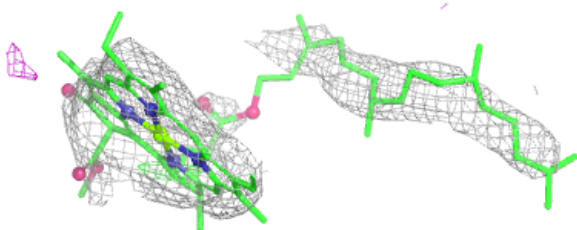
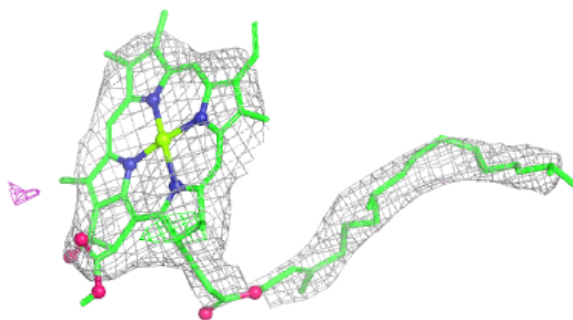
Electron density around HEM BF 5101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

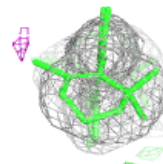
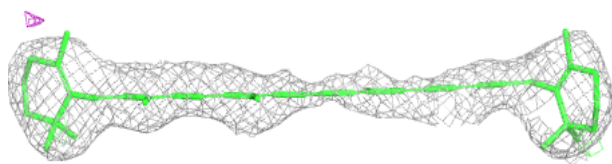
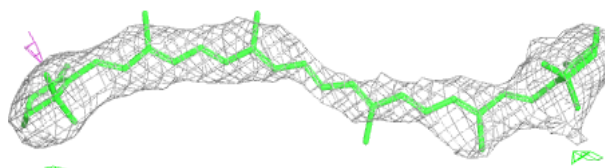


Electron density around CLA AC 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

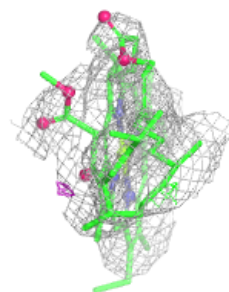
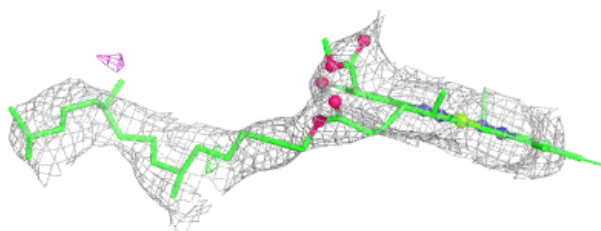
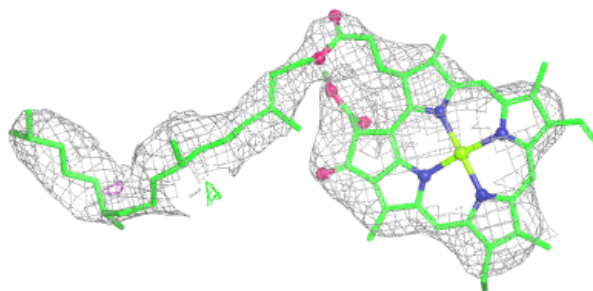
**Electron density around BCR AA 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

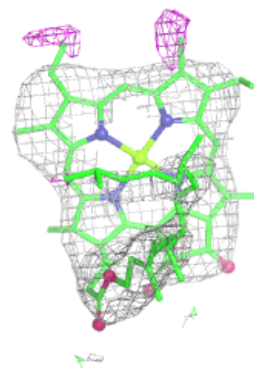
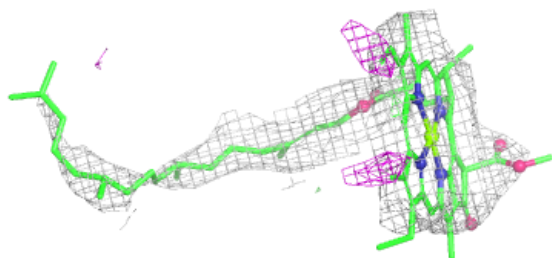
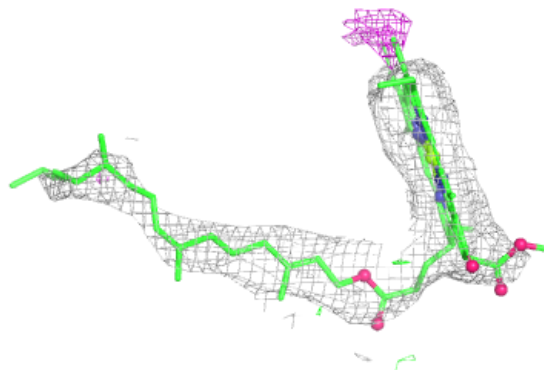


Electron density around CLA AB 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

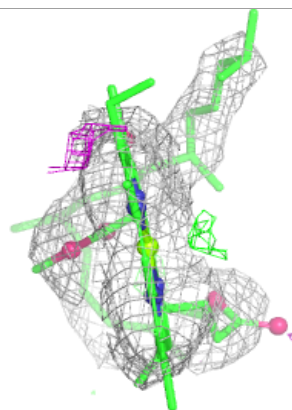
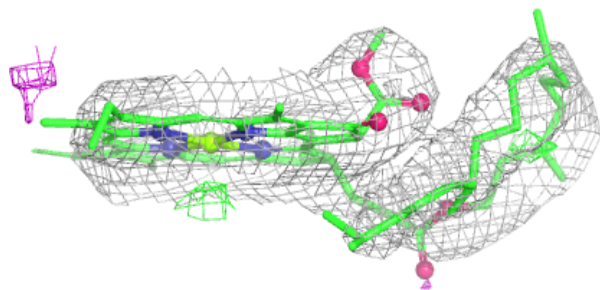
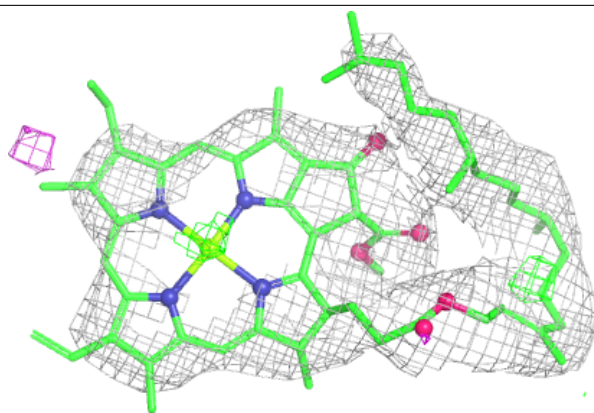
**Electron density around CLA AB 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



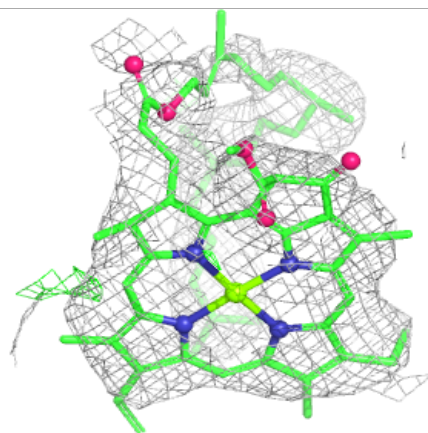
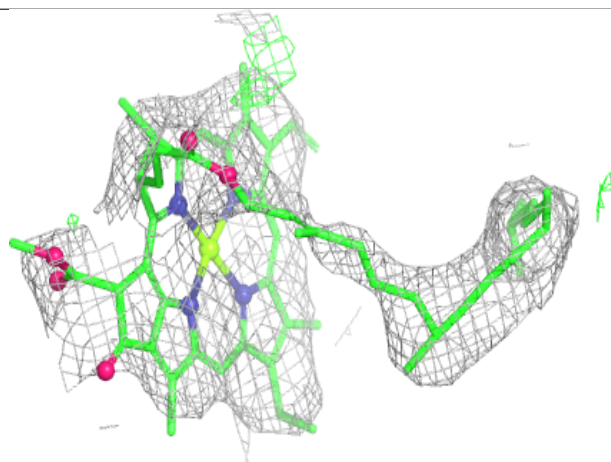
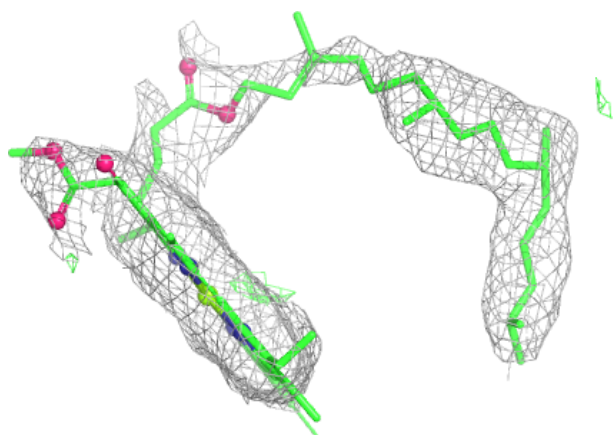
Electron density around CLA BB 5614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



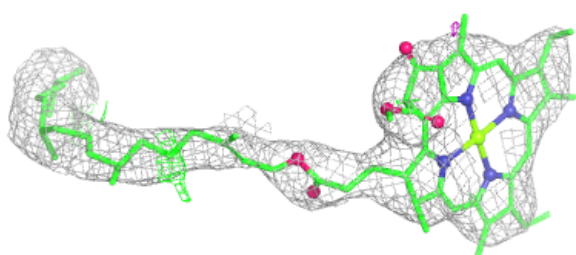
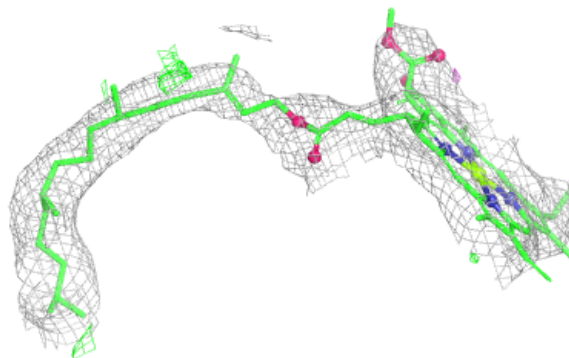
Electron density around CLA BB 5615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

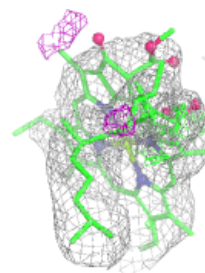
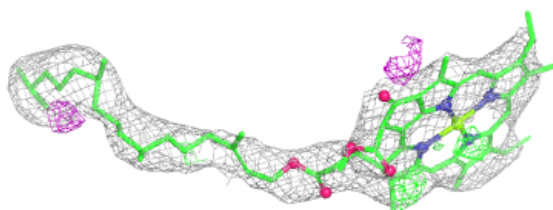
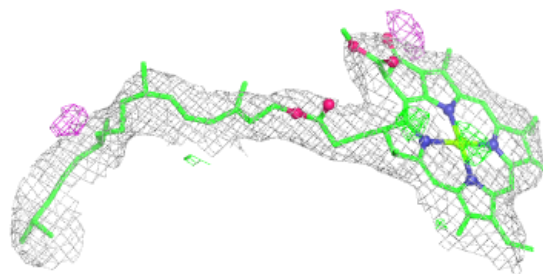


Electron density around CLA AD 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

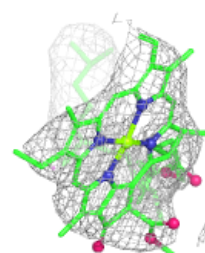
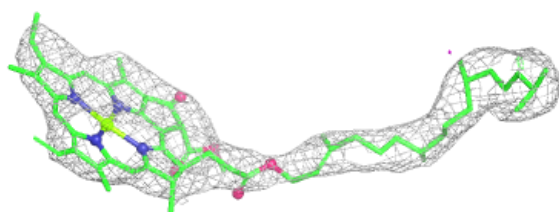
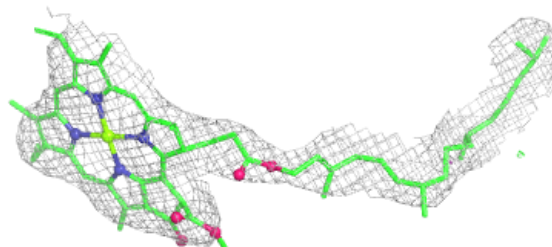
**Electron density around CLA AA 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

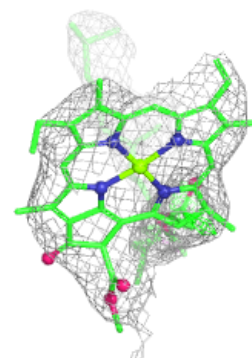
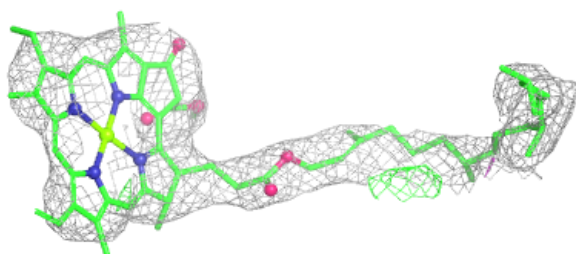
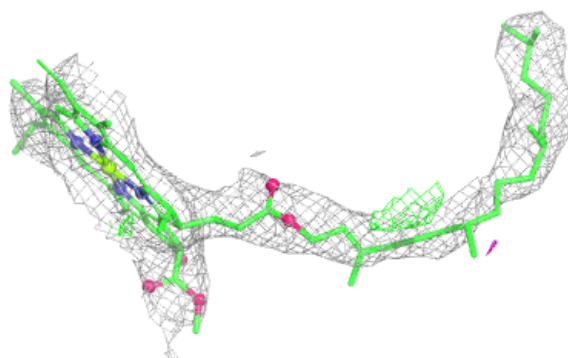


Electron density around CLA BA 5405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

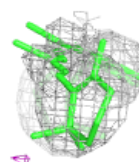
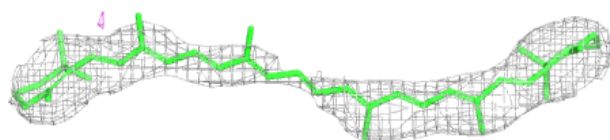
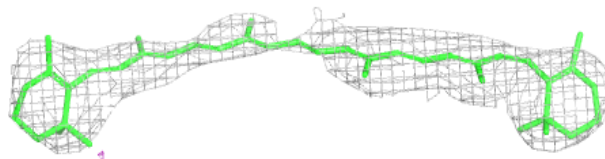
**Electron density around CLA BD 5402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



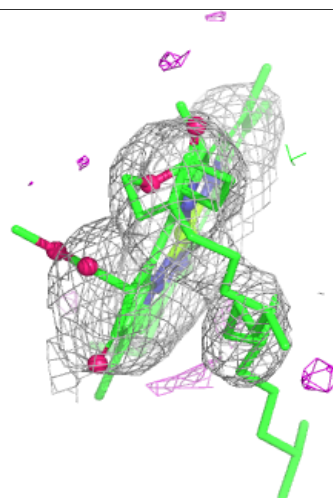
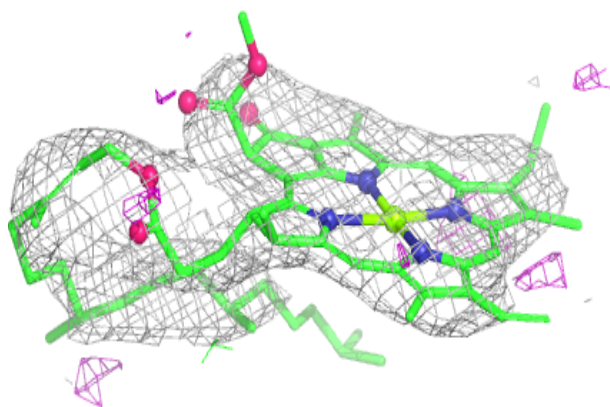
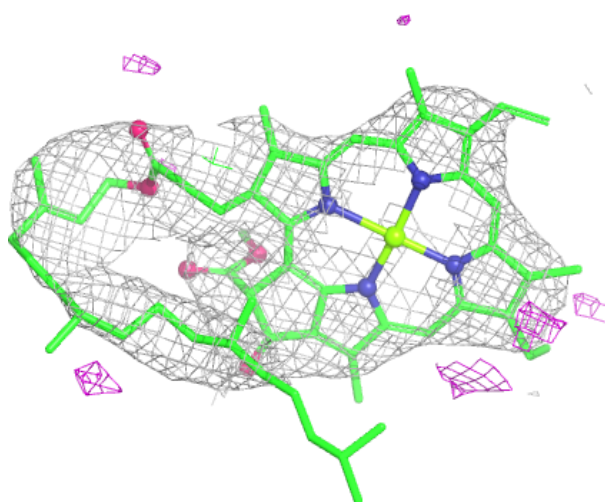
Electron density around BCR AC 514:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



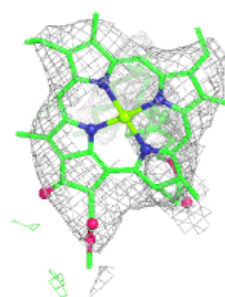
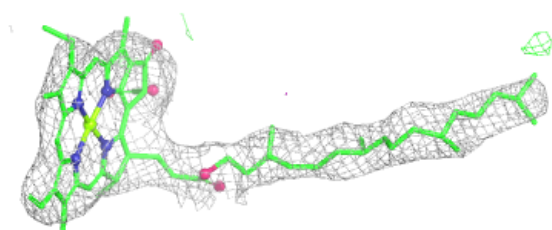
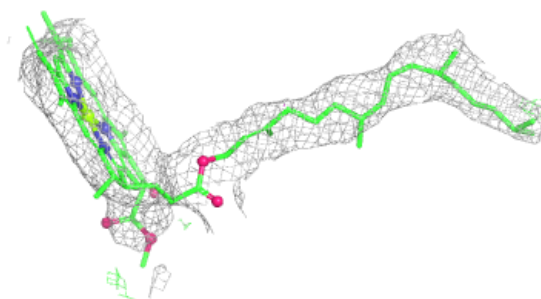
Electron density around CLA AC 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

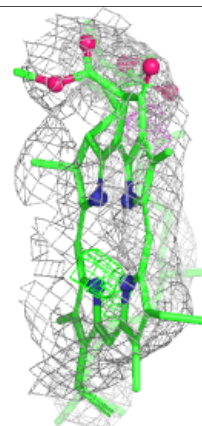
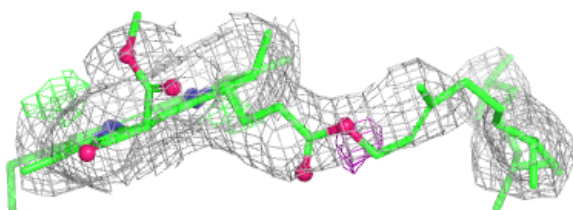
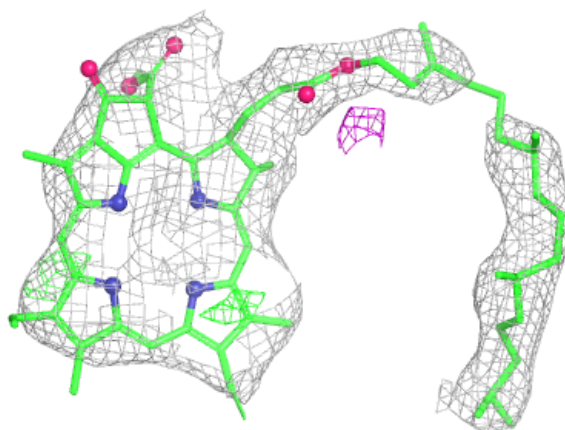


Electron density around CLA BB 5608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

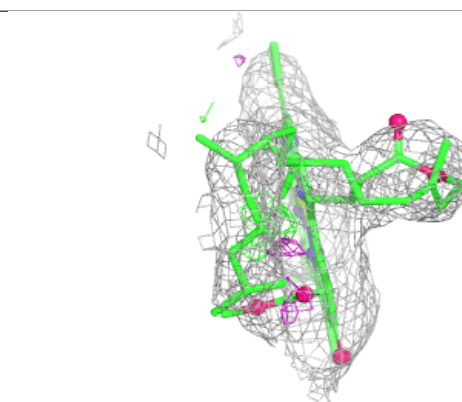
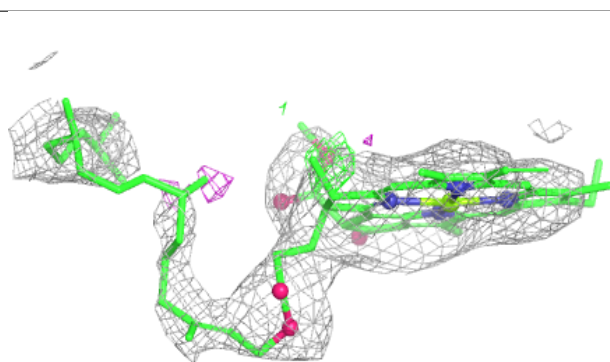
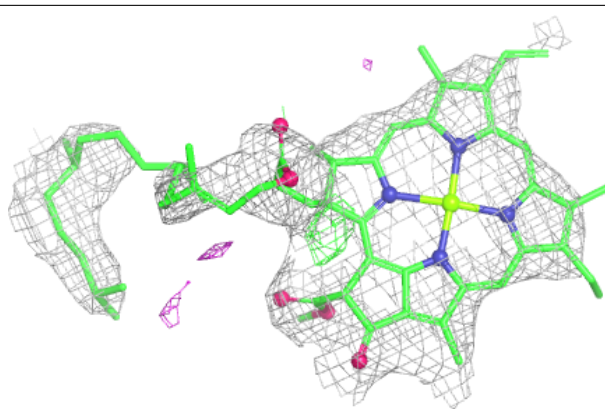
**Electron density around PHO AD 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

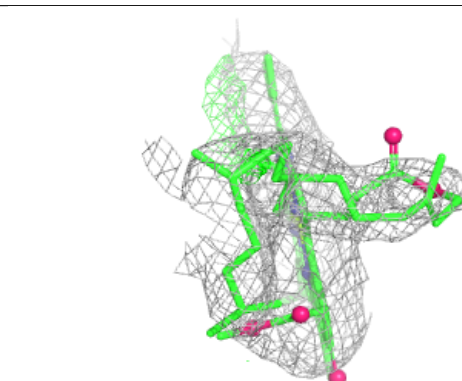
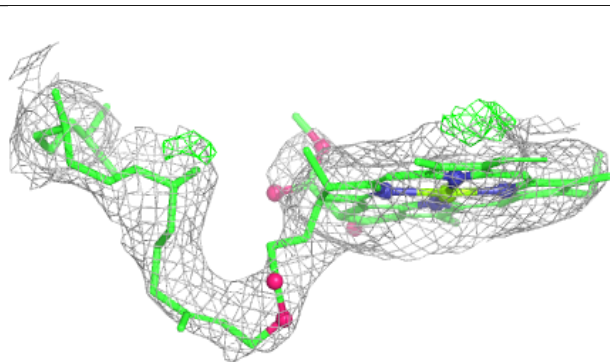
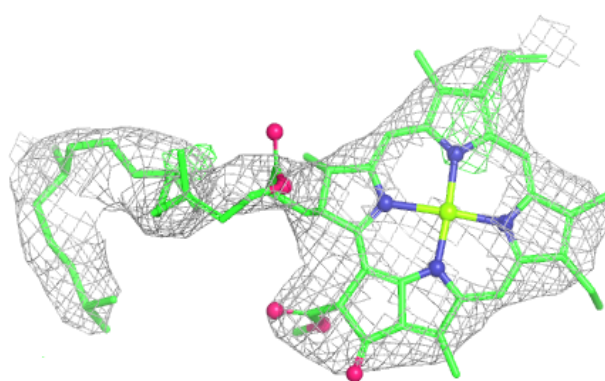


Electron density around CLA AB 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

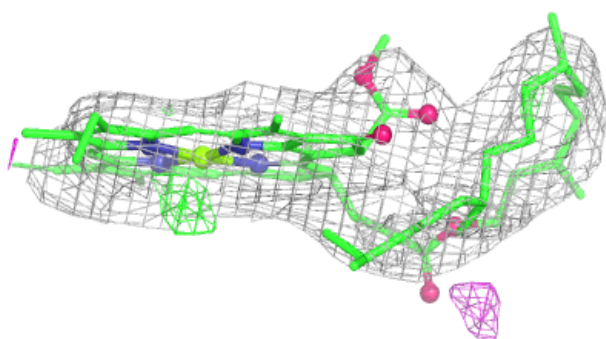
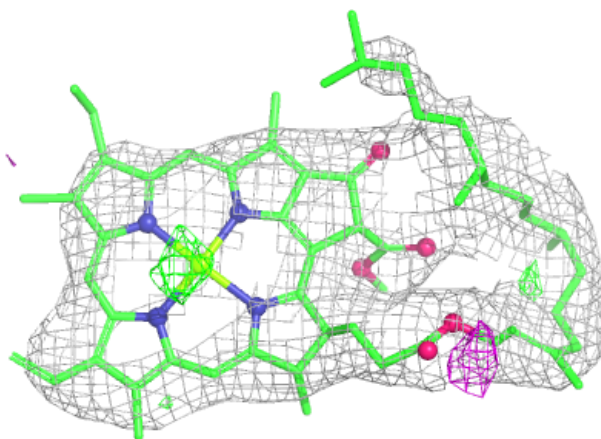
**Electron density around CLA BB 5616:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



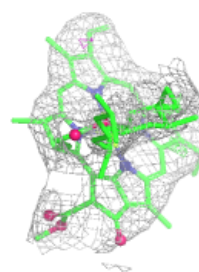
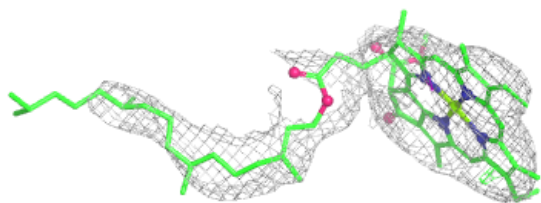
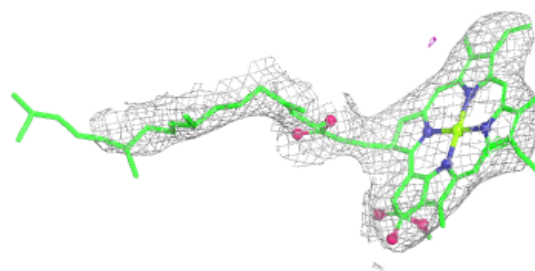
Electron density around CLA AB 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



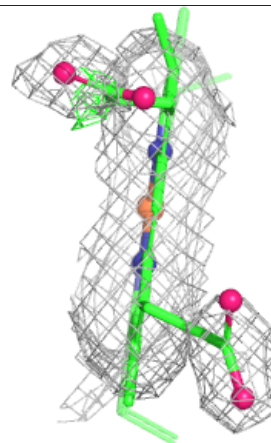
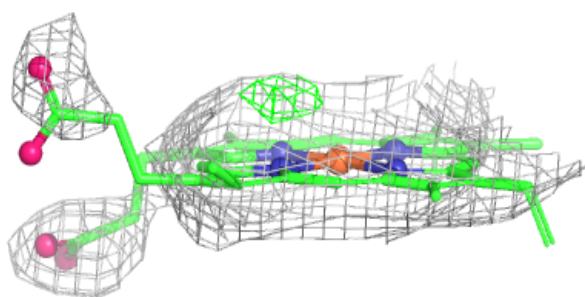
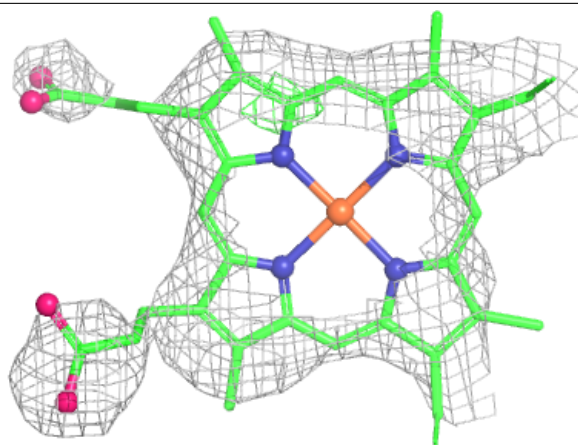
Electron density around CLA AC 502:

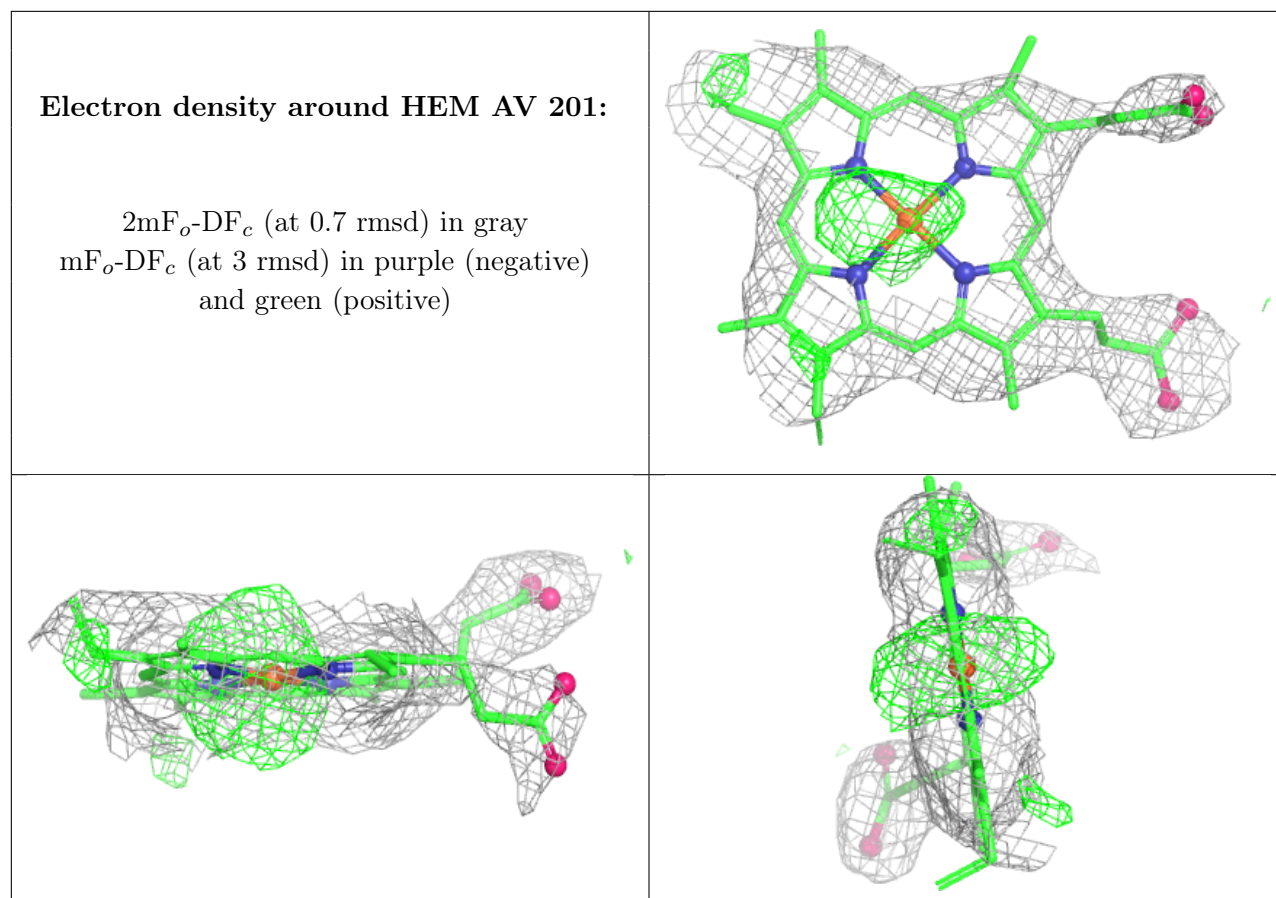
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM BV 5201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.