



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 10:47 PM EDT

PDB ID : 7SA3 / pdb_00007sa3
EMDB ID : EMD-24943
Title : Structure of a monomeric photosystem II core complex from a cyanobacterium acclimated to far-red light
Authors : Gisriel, C.J.; Bryant, D.A.; Brudvig, G.W.
Deposited on : 2021-09-22
Resolution : 2.25 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

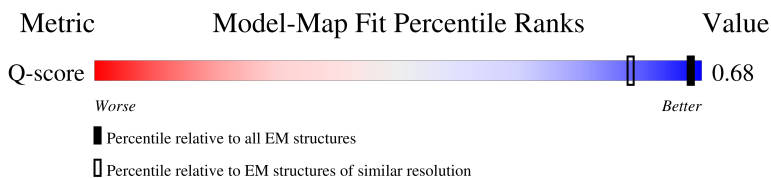
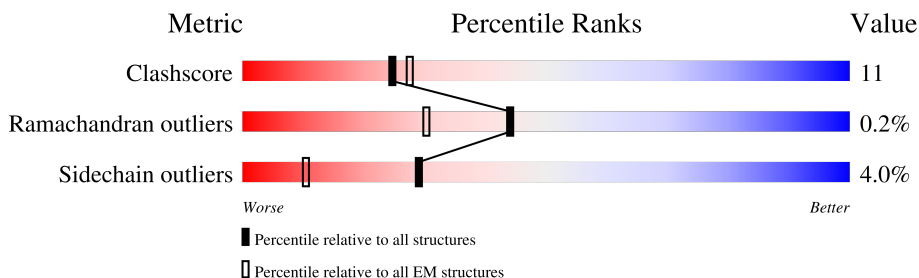
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.25 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.



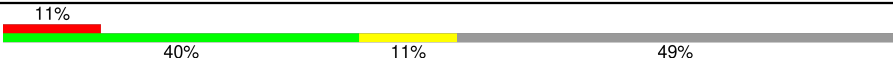
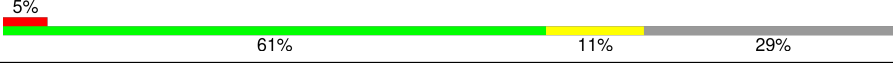
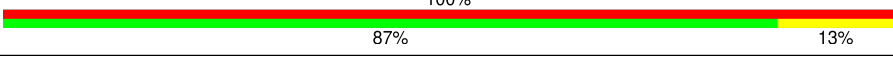
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3458 (1.75 - 2.75)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	
2	B	509	
3	C	482	
4	D	352	

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Mol	Chain	Length	Quality of chain
5	E	80	
6	F	44	
7	I	38	
8	K	45	
9	N	23	

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
13	CL7	A	404	X	-	-	-
17	F6C	B	603	X	-	-	-
17	F6C	B	606	X	-	-	-
17	F6C	B	612	X	-	-	-
17	F6C	C	507	X	-	-	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 15960 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	303	Total	C	N	O	S	0	0
			2382	1572	392	403	15		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	conflict	UNP B4WKH9
A	2	THR	-	conflict	UNP B4WKH9
A	3	THR	-	conflict	UNP B4WKH9
A	4	ILE	-	conflict	UNP B4WKH9
A	5	SER	-	conflict	UNP B4WKH9
A	6	THR	-	conflict	UNP B4WKH9
A	7	ARG	-	conflict	UNP B4WKH9
A	8	PRO	-	conflict	UNP B4WKH9
A	9	THR	-	conflict	UNP B4WKH9
A	10	SER	-	conflict	UNP B4WKH9
A	11	ARG	-	conflict	UNP B4WKH9
A	12	PHE	-	conflict	UNP B4WKH9
A	13	PRO	-	conflict	UNP B4WKH9
A	14	THR	-	conflict	UNP B4WKH9
A	15	TRP	-	conflict	UNP B4WKH9
A	16	ASP	-	conflict	UNP B4WKH9
A	17	ARG	-	conflict	UNP B4WKH9
A	18	PHE	-	conflict	UNP B4WKH9
A	19	CYS	-	conflict	UNP B4WKH9
A	20	ASN	-	conflict	UNP B4WKH9
A	21	TRP	-	conflict	UNP B4WKH9
A	22	VAL	-	conflict	UNP B4WKH9
A	23	THR	-	conflict	UNP B4WKH9
A	24	SER	-	conflict	UNP B4WKH9
A	25	THR	-	conflict	UNP B4WKH9
A	26	GLU	-	conflict	UNP B4WKH9
A	27	ASN	-	conflict	UNP B4WKH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ARG	-	conflict	UNP B4WKH9
A	29	LEU	-	conflict	UNP B4WKH9
A	30	TYR	-	conflict	UNP B4WKH9
A	31	ILE	-	conflict	UNP B4WKH9
A	32	GLY	-	conflict	UNP B4WKH9
A	33	TRP	-	conflict	UNP B4WKH9
A	34	PHE	-	conflict	UNP B4WKH9
A	35	GLY	-	conflict	UNP B4WKH9
A	36	VAL	-	conflict	UNP B4WKH9
A	37	LEU	-	conflict	UNP B4WKH9

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	450	Total	C	N	O	S	0	0
			3528	2316	593	607	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	420	Total	C	N	O	S	0	0
			3272	2154	553	554	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	336	Total	C	N	O	S	0	0
			2671	1770	435	452	14		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	41	Total	C	N	O	0	0
			330	225	49	56		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			243	165	41	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	27	Total	C	N	O	S	0	0
			213	150	28	34	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	37	Total	C	N	O	0	0
			294	206	45	43		

- Molecule 9 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Ca	0
			1	1	

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Cl	0
			1	1	

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).

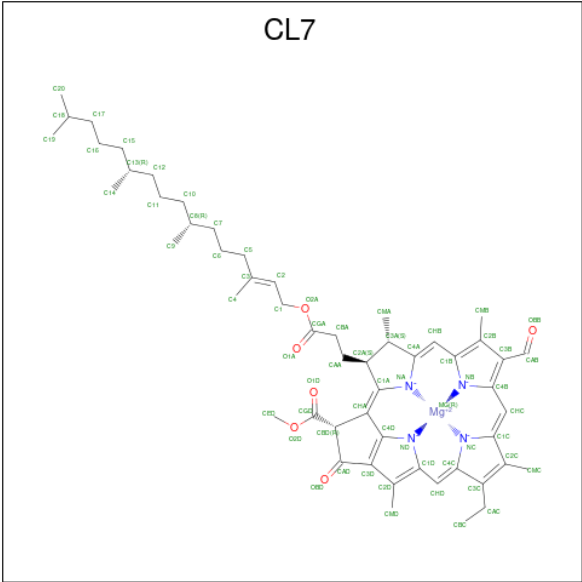


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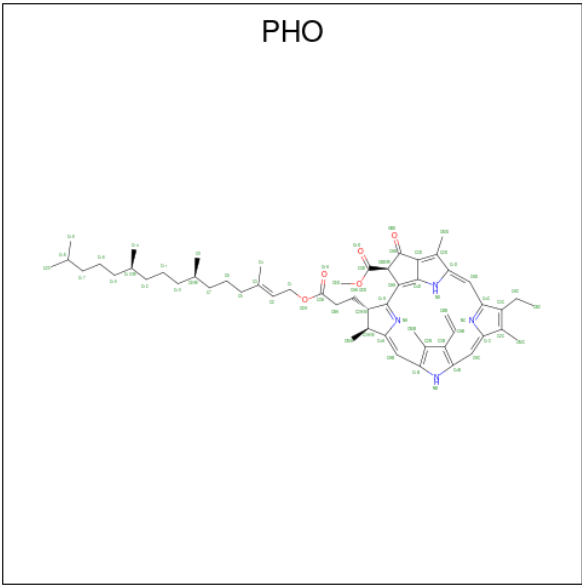
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 13 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



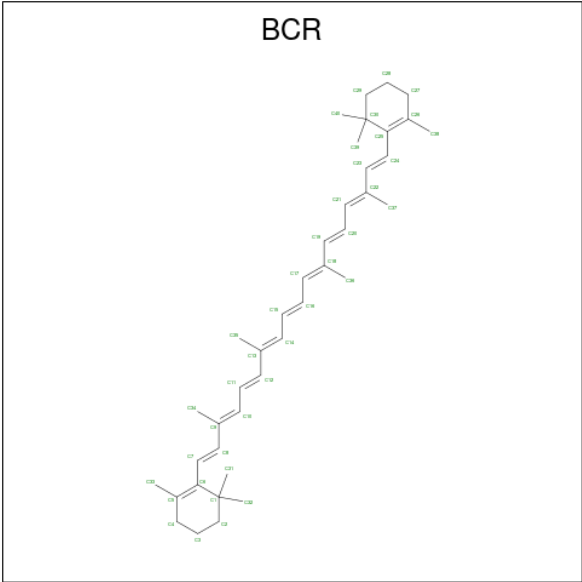
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 14 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



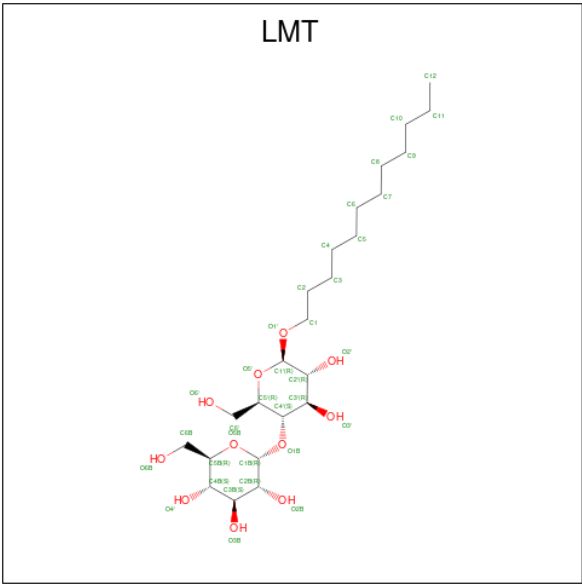
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	N	O	0
			64	55	4	5	
14	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



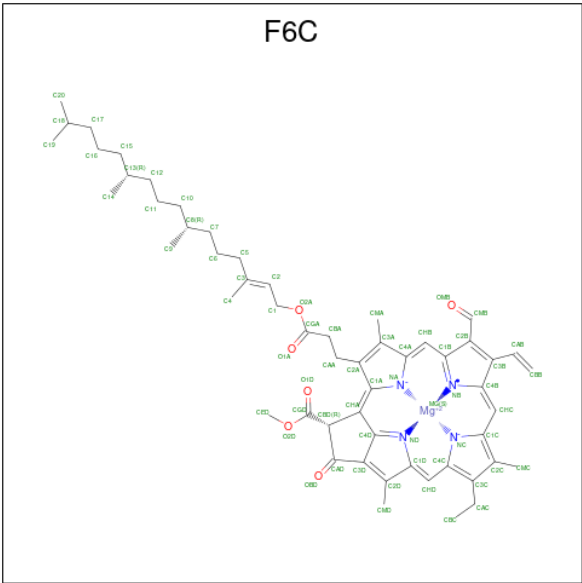
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	C	1	Total	C	0
			40	40	
15	C	1	Total	C	0
			40	40	
15	D	1	Total	C	0
			26	26	

- Molecule 16 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



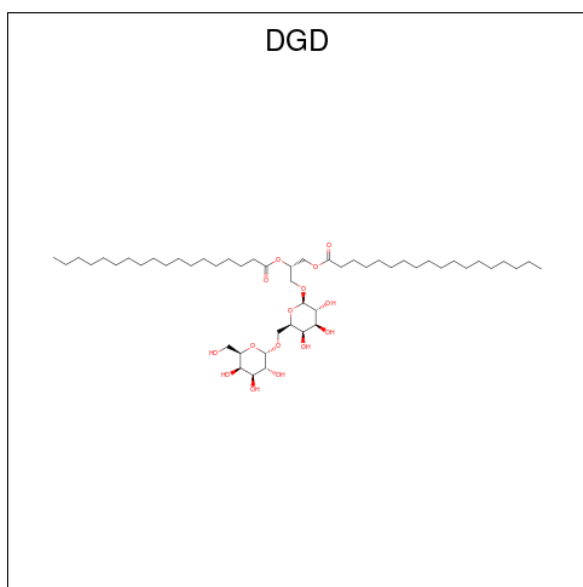
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			35	24	11	
16	A	1	Total	C	O	0
			31	20	11	
16	B	1	Total	C	O	0
			35	24	11	
16	B	1	Total	C	O	0
			30	19	11	
16	C	1	Total	C	O	0
			34	23	11	
16	D	1	Total	C	O	0
			20	15	5	

- Molecule 17 is Chlorophyll F (CCD ID: F6C) (formula: C₅₅H₆₈MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



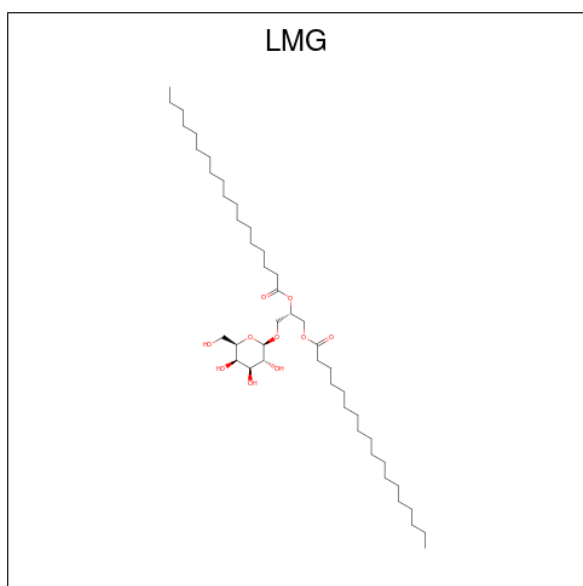
Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	B	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
17	B	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
17	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 18 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			47	38	9	
18	C	1	Total	C	O	0
			47	32	15	

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			40	30	10	

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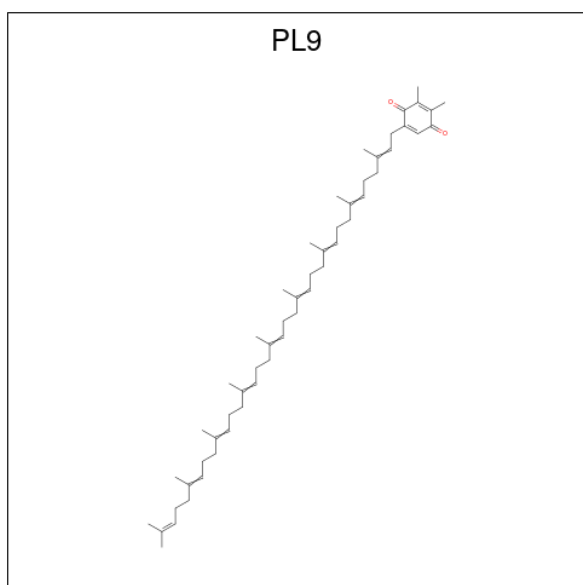
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Mol	Chain	Residues	Atoms			AltConf
19	D	1	Total	C	O	0
			33	23	10	

- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

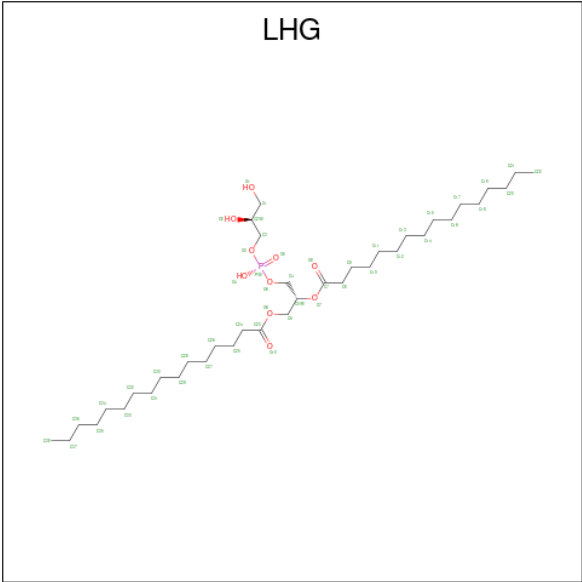
Mol	Chain	Residues	Atoms			AltConf
20	D	1	Total	Fe		0
			1	1		

- Molecule 21 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).



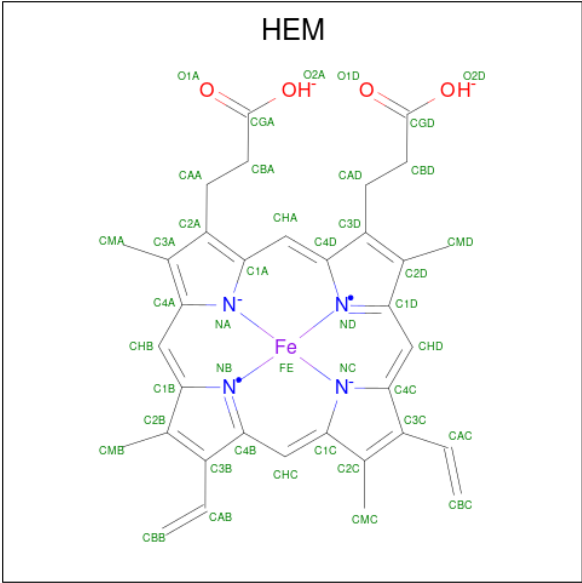
Mol	Chain	Residues	Atoms			AltConf
21	D	1	Total	C	O	0
			45	43	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
22	D	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 23 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

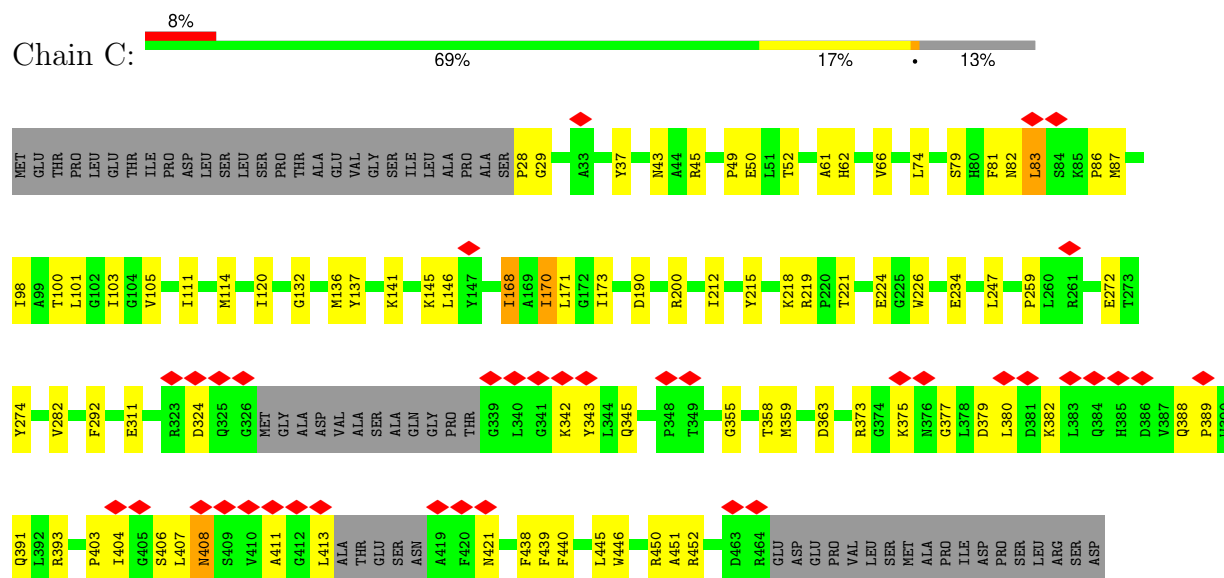


Mol	Chain	Residues	Atoms					AltConf
23	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

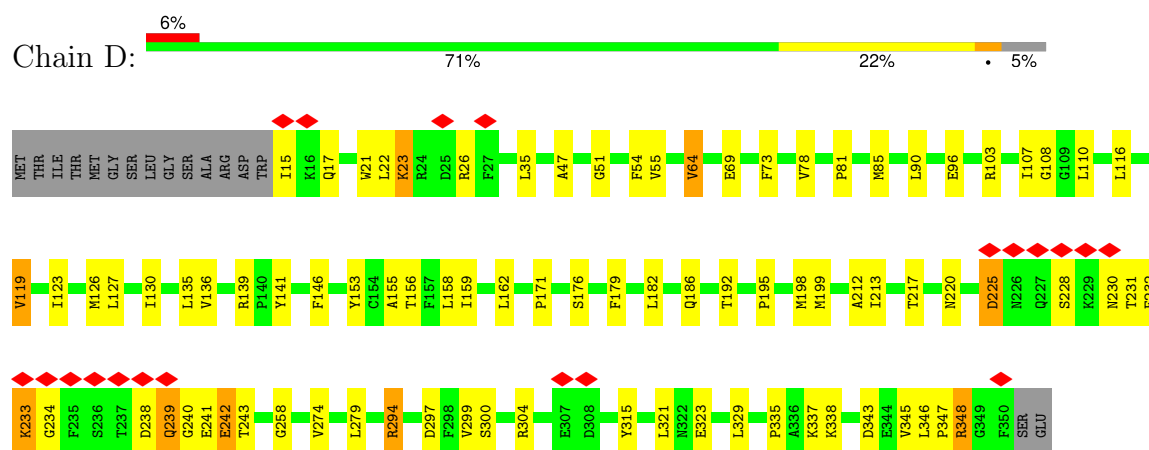
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	A	61	Total 61	O 61	0
24	B	59	Total 59	O 59	0
24	C	44	Total 44	O 44	0
24	D	65	Total 65	O 65	0
24	I	1	Total 1	O 1	0

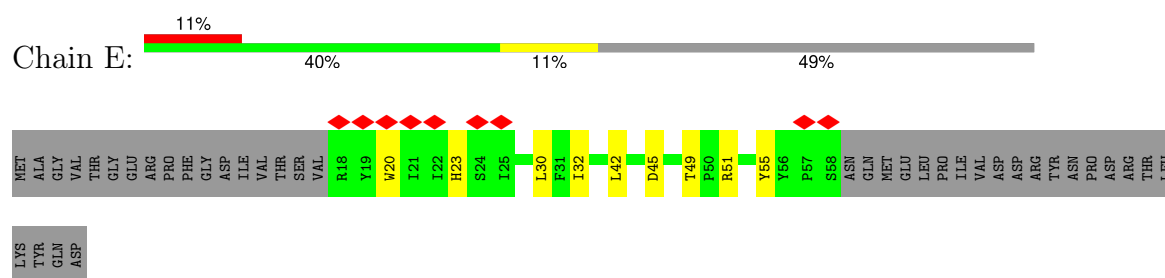
- Molecule 3: Photosystem II CP43 reaction center protein



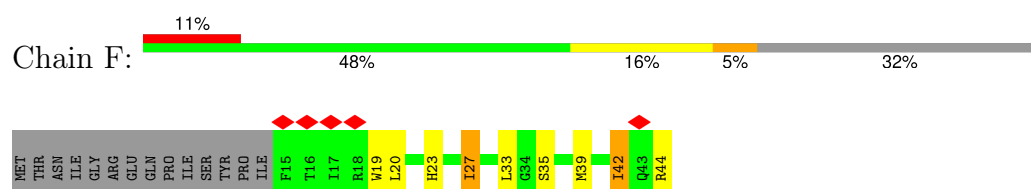
- Molecule 4: Photosystem II D2 protein



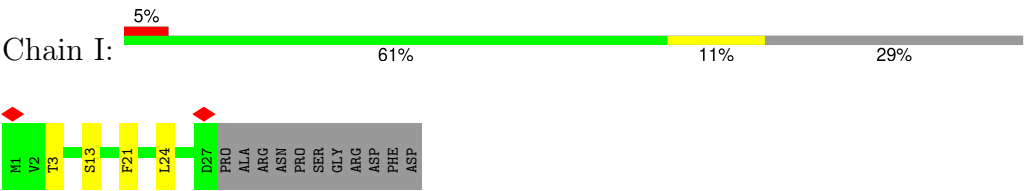
- Molecule 5: Cytochrome b559 subunit alpha



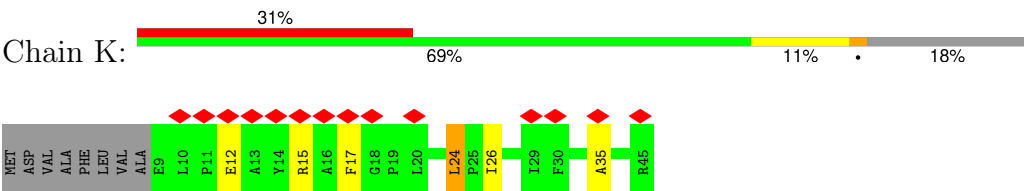
- Molecule 6: Cytochrome b559 subunit beta



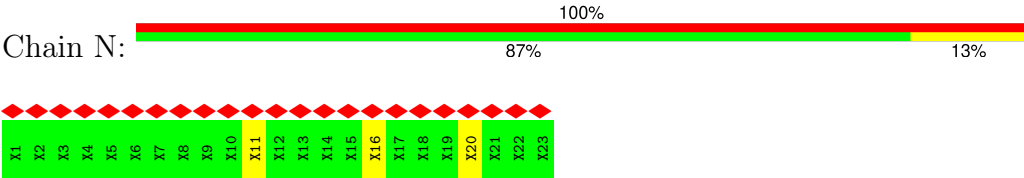
● Molecule 7: Photosystem II reaction center protein I



● Molecule 8: Photosystem II reaction center protein K



● Molecule 9: Unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	315307	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, LMG, CA, DGD, CLA, HEM, F6C, LMT, CL7, LHG, FE2, CL, PL9, BCR

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	A	0.39	0/2462	0.56	0/3362
2	B	0.38	0/3651	0.57	1/4966 (0.0%)
3	C	0.36	0/3384	0.59	1/4608 (0.0%)
4	D	0.40	0/2760	0.56	0/3751
5	E	0.28	0/345	0.51	0/476
6	F	0.29	0/250	0.71	0/337
7	I	0.21	0/218	0.49	0/294
8	K	0.30	0/305	0.77	0/417
All	All	0.37	0/13375	0.58	2/18211 (0.0%)

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	A	0	2
2	B	0	6
8	K	0	1
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	LEU	N-CA-C	-6.11	106.37	113.88
3	C	226	TRP	N-CA-CB	-5.21	101.69	110.49

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	ARG	Peptide
1	A	340	PHE	Peptide
2	B	135	LEU	Peptide
2	B	384	ARG	Peptide
2	B	385	GLN	Peptide
2	B	386	ALA	Peptide
2	B	387	GLU	Peptide
2	B	388	SER	Peptide
8	K	17	PHE	Peptide

5.2 Too-close contacts [i](#)

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	A	2382	0	2311	75	0
2	B	3528	0	3377	49	0
3	C	3272	0	3190	66	0
4	D	2671	0	2592	83	0
5	E	330	0	310	6	0
6	F	243	0	252	6	0
7	I	213	0	226	3	0
8	K	294	0	301	4	0
9	N	115	0	25	2	0
10	A	1	0	0	0	0
11	A	1	0	0	0	0
12	A	175	0	170	12	0
12	B	610	0	562	38	0
12	C	695	0	688	40	0
12	D	105	0	92	3	0
13	A	65	0	70	3	0
14	A	64	0	74	5	0
14	D	64	0	74	2	0
15	A	40	0	49	5	0
15	B	40	0	49	2	0
15	C	80	0	98	6	0
15	D	26	0	29	1	0
16	A	66	0	78	3	0
16	B	65	0	78	1	0
16	C	34	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	D	20	0	24	0	0
17	B	168	0	0	8	0
17	C	61	0	0	2	0
18	B	47	0	66	1	0
18	C	47	0	52	2	0
19	B	40	0	50	1	0
19	D	33	0	36	2	0
20	D	1	0	0	0	0
21	D	45	0	61	4	0
22	D	46	0	65	7	0
23	F	43	0	30	4	0
24	A	61	0	0	6	0
24	B	59	0	0	1	0
24	C	44	0	0	6	0
24	D	65	0	0	2	0
24	I	1	0	0	0	0
All	All	15960	0	15119	327	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 11.

All (327) 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:A:330:GLU:OE1	3:C:408:ASN:ND2	1.64	1.30
1:A:190:GLU:O	3:C:407:LEU:HG	1.30	1.29
24:A:556:HOH:O	3:C:407:LEU:HD23	1.55	1.05
1:A:335:ARG:NH2	24:A:501:HOH:O	1.89	1.03
2:B:388:SER:OG	2:B:394:GLN:NE2	2.01	0.93
3:C:411:ALA:HB2	24:C:612:HOH:O	1.69	0.91
3:C:440:PHE:HA	12:C:508:CLA:HMC2	1.49	0.91
4:D:225:ASP:CG	4:D:234:GLY:O	2.17	0.87
3:C:411:ALA:CB	24:C:612:HOH:O	2.20	0.87
4:D:225:ASP:OD2	4:D:234:GLY:O	1.98	0.81
12:B:604:CLA:HBB1	12:B:604:CLA:HMB1	1.63	0.81
1:A:190:GLU:O	3:C:407:LEU:CG	2.23	0.76
12:C:508:CLA:HMB3	12:C:508:CLA:HBB1	1.67	0.75
17:C:507:F6C:CED	12:C:509:CLA:H92	2.18	0.74
3:C:403:PRO:O	24:C:601:HOH:O	2.07	0.72
1:A:249:ILE:CD1	4:D:238:ASP:O	2.37	0.71
1:A:339:ASN:HD21	3:C:406:SER:HB2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASN:HD22	3:C:421:ASN:HD21	1.37	0.70
4:D:241:GLU:C	4:D:243:THR:H	2.01	0.68
4:D:192:THR:HG23	12:D:403:CLA:HBC2	1.75	0.68
4:D:119:VAL:HG11	4:D:158:LEU:HD11	1.77	0.67
1:A:122:PRO:HG3	18:C:515:DGD:HAT1	1.77	0.65
2:B:255:THR:HG21	12:B:601:CLA:HED1	1.78	0.65
12:B:604:CLA:HMA2	12:B:605:CLA:HMA2	1.78	0.65
1:A:249:ILE:HD13	4:D:239:GLN:O	1.96	0.65
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.78	0.65
5:E:30:LEU:HD21	6:F:27:ILE:HG23	1.79	0.64
2:B:385:GLN:O	2:B:385:GLN:NE2	2.30	0.64
2:B:357:ARG:NH2	4:D:337:LYS:O	2.30	0.64
1:A:193:ILE:HG13	1:A:294:MET:HE1	1.80	0.63
1:A:94:PHE:HZ	12:A:407:CLA:HAA1	1.63	0.63
2:B:341:LEU:HD21	2:B:431:GLU:HG2	1.79	0.63
4:D:239:GLN:HA	4:D:239:GLN:OE1	2.00	0.61
1:A:199:HIS:HA	1:A:287:VAL:HG23	1.81	0.61
1:A:249:ILE:CD1	4:D:239:GLN:O	2.47	0.61
2:B:103:PHE:CZ	12:B:604:CLA:HMC1	2.36	0.61
3:C:87:MET:HE2	3:C:111:ILE:HD11	1.80	0.61
1:A:186:VAL:O	1:A:190:GLU:HG2	2.00	0.61
1:A:128:LEU:HD13	1:A:145:CYS:HB2	1.83	0.61
6:F:23:HIS:NE2	23:F:101:HEM:NA	2.48	0.60
2:B:182:ALA:HB2	16:B:619:LMT:H6D	1.83	0.60
4:D:241:GLU:O	4:D:243:THR:N	2.34	0.60
3:C:170:ILE:HG22	3:C:171:LEU:HD22	1.83	0.60
3:C:200:ARG:NH2	3:C:234:GLU:OE2	2.32	0.59
4:D:241:GLU:C	4:D:243:THR:N	2.60	0.59
12:A:407:CLA:H102	7:I:13:SER:HA	1.85	0.59
4:D:85:MET:HB3	4:D:90:LEU:HD21	1.84	0.59
1:A:249:ILE:HD12	4:D:238:ASP:O	2.03	0.59
4:D:225:ASP:OD1	4:D:225:ASP:N	2.34	0.59
3:C:219:ARG:NH2	3:C:224:GLU:OE1	2.36	0.58
3:C:389:PRO:HB2	3:C:393:ARG:HH21	1.69	0.58
12:C:508:CLA:HBB1	12:C:508:CLA:CMB	2.34	0.57
4:D:279:LEU:HD22	14:D:402:PHO:HBC3	1.86	0.57
12:B:604:CLA:H8	12:B:605:CLA:HBB1	1.85	0.57
2:B:348:ASP:HB3	2:B:354:LEU:HD11	1.85	0.57
3:C:440:PHE:HA	12:C:508:CLA:CMC	2.29	0.57
4:D:156:THR:HG22	4:D:171:PRO:HG3	1.86	0.57
1:A:28:ARG:NH2	4:D:258:GLY:O	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:119:VAL:HG12	4:D:153:TYR:HE2	1.68	0.57
3:C:215:TYR:HA	3:C:218:LYS:HD3	1.87	0.57
3:C:66:VAL:HG12	12:C:503:CLA:HHD	1.87	0.57
5:E:45:ASP:OD1	5:E:51:ARG:NH1	2.38	0.57
12:B:611:CLA:H12	12:B:613:CLA:HBA2	1.86	0.57
4:D:199:MET:HG2	21:D:406:PL9:H322	1.86	0.57
1:A:93:HIS:NE2	3:C:363:ASP:OD2	2.35	0.56
3:C:37:TYR:CE2	12:C:508:CLA:HED1	2.40	0.56
3:C:274:TYR:O	24:C:602:HOH:O	2.18	0.56
12:B:607:CLA:HMB2	4:D:126:MET:HE2	1.86	0.56
3:C:345:GLN:HE21	3:C:355:GLY:HA2	1.70	0.56
4:D:69:GLU:OE1	5:E:55:TYR:OH	2.23	0.56
1:A:163:PRO:HB3	1:A:169:PHE:HA	1.86	0.56
22:D:407:LHG:O3	22:D:407:LHG:O1	2.21	0.56
17:B:603:F6C:O1A	12:B:604:CLA:O1A	2.23	0.56
12:B:607:CLA:H193	4:D:35:LEU:HB3	1.88	0.55
1:A:249:ILE:HD11	4:D:238:ASP:O	2.06	0.55
1:A:325:ALA:HB2	4:D:329:LEU:HD13	1.88	0.55
15:C:517:BCR:H391	8:K:35:ALA:HB2	1.89	0.55
12:B:604:CLA:HMA2	12:B:605:CLA:CMA	2.37	0.55
1:A:269:SER:OG	4:D:240:GLY:O	2.15	0.55
17:B:603:F6C:CBA	17:B:603:F6C:CBD	2.85	0.55
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.89	0.54
1:A:44:VAL:HG13	15:A:408:BCR:H362	1.89	0.54
1:A:330:GLU:CD	3:C:408:ASN:HD21	2.13	0.54
3:C:190:ASP:OD2	3:C:200:ARG:NH1	2.37	0.54
3:C:74:LEU:HD22	12:C:503:CLA:HED3	1.90	0.54
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.89	0.54
2:B:365:ASN:HD21	4:D:323:GLU:HG3	1.73	0.54
2:B:388:SER:HB2	2:B:391:GLY:N	2.22	0.54
4:D:73:PHE:HE2	19:D:408:LMG:H322	1.73	0.54
18:B:616:DGD:HAF2	4:D:162:LEU:HD13	1.88	0.54
1:A:125:LEU:HD22	12:C:505:CLA:HBB2	1.90	0.53
3:C:100:THR:HG22	12:C:501:CLA:HED1	1.89	0.53
3:C:411:ALA:HB1	24:C:612:HOH:O	1.95	0.53
4:D:228:SER:OG	4:D:230:ASN:O	2.26	0.53
3:C:324:ASP:OD2	3:C:342:LYS:NZ	2.34	0.53
2:B:475:PHE:HB3	2:B:478:VAL:HG22	1.90	0.53
3:C:137:TYR:HD1	3:C:141:LYS:HE2	1.73	0.53
4:D:126:MET:HB2	4:D:146:PHE:HD2	1.74	0.53
4:D:15:ILE:N	4:D:17:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PRO:HA	1:A:113:TYR:CG	2.44	0.53
1:A:141:ARG:HH22	22:D:407:LHG:HC41	1.74	0.53
3:C:439:PHE:O	12:C:508:CLA:HAC1	2.09	0.53
1:A:128:LEU:HD11	3:C:445:LEU:HD13	1.91	0.52
1:A:132:TRP:HZ2	3:C:452:ARG:HG3	1.74	0.52
1:A:335:ARG:HB2	1:A:335:ARG:CZ	2.39	0.52
3:C:343:TYR:O	3:C:355:GLY:N	2.41	0.52
12:B:604:CLA:CHC	12:B:604:CLA:H72	2.40	0.52
4:D:21:TRP:O	4:D:26:ARG:NH2	2.27	0.52
1:A:41:LEU:HD13	1:A:122:PRO:HB2	1.90	0.52
2:B:329:ARG:HH12	19:B:617:LMG:HC61	1.74	0.52
1:A:83:VAL:HB	1:A:175:MET:HB2	1.92	0.52
3:C:168:ILE:CG2	3:C:247:LEU:O	2.58	0.52
4:D:213:ILE:HG21	21:D:406:PL9:HC71	1.92	0.51
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.93	0.51
4:D:231:THR:C	4:D:233:LYS:H	2.18	0.51
1:A:162:TYR:HA	1:A:295:ALA:HB2	1.91	0.51
2:B:75:TRP:HA	2:B:88:PRO:HG3	1.93	0.51
2:B:471:LEU:HD21	4:D:130:ILE:HG12	1.92	0.51
4:D:225:ASP:CB	4:D:234:GLY:O	2.58	0.51
5:E:23:HIS:NE2	23:F:101:HEM:ND	2.59	0.51
12:B:613:CLA:H12	12:B:614:CLA:HBB2	1.92	0.50
3:C:98:ILE:HG22	3:C:103:ILE:HB	1.94	0.50
1:A:307:VAL:HG11	4:D:64:VAL:HG11	1.94	0.50
1:A:332:MET:HB2	4:D:321:LEU:HD23	1.94	0.50
1:A:333:HIS:O	24:A:501:HOH:O	2.20	0.50
2:B:258:TYR:OH	4:D:162:LEU:O	2.25	0.50
4:D:51:GLY:HA2	4:D:55:VAL:HB	1.93	0.50
22:D:407:LHG:H222	9:N:11:UNK:HA	1.94	0.50
1:A:249:ILE:HA	1:A:252:ALA:HB3	1.93	0.50
1:A:302:ASN:HD22	3:C:421:ASN:ND2	2.08	0.50
2:B:60:CYS:HB3	2:B:63:MET:HB2	1.94	0.50
2:B:330:MET:HA	2:B:444:ARG:HB2	1.92	0.50
6:F:39:MET:HA	6:F:42:ILE:HG13	1.93	0.50
2:B:137:LYS:HD2	2:B:217:ILE:HG23	1.93	0.50
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.47	0.49
3:C:379:ASP:HB3	3:C:382:LYS:HG3	1.93	0.49
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.94	0.49
2:B:142:HIS:ND1	12:B:609:CLA:OBD	2.41	0.49
2:B:311:PHE:O	2:B:317:ASN:ND2	2.45	0.49
3:C:43:ASN:N	12:C:508:CLA:O1A	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HA	1:A:287:VAL:HG12	1.95	0.49
1:A:309:ASP:OD1	1:A:313:ARG:N	2.43	0.49
17:B:603:F6C:CBA	17:B:603:F6C:CHA	2.90	0.49
1:A:197:PRO:HA	1:A:200:MET:HB2	1.94	0.49
2:B:69:LEU:HD11	12:B:602:CLA:HMD1	1.94	0.49
3:C:388:GLN:HG2	3:C:391:GLN:HE21	1.78	0.49
3:C:98:ILE:HD12	3:C:120:ILE:HG21	1.94	0.48
4:D:90:LEU:HD22	4:D:107:ILE:HD12	1.94	0.48
1:A:88:ASN:HD22	3:C:359:MET:HE3	1.78	0.48
15:D:405:BCR:H351	15:D:405:BCR:H15C	1.68	0.48
2:B:103:PHE:CE2	12:B:604:CLA:HMC1	2.48	0.48
3:C:446:TRP:HH2	22:D:407:LHG:HC61	1.78	0.48
2:B:315:ILE:HG22	2:B:426:LEU:HB3	1.96	0.48
14:A:406:PHO:H13	14:A:406:PHO:H102	1.68	0.48
24:A:556:HOH:O	3:C:411:ALA:CB	2.62	0.48
12:B:610:CLA:C3B	17:B:612:F6C:CMA	2.92	0.48
12:C:509:CLA:H102	12:C:509:CLA:HAA2	1.95	0.48
1:A:36:VAL:HA	15:A:408:BCR:H322	1.96	0.48
1:A:101:ALA:N	1:A:105:GLU:OE2	2.43	0.48
12:B:607:CLA:H2	4:D:127:LEU:HD22	1.95	0.48
5:E:30:LEU:HD22	23:F:101:HEM:HBB1	1.96	0.48
17:B:603:F6C:C5	12:B:611:CLA:H191	2.44	0.47
4:D:242:GLU:CD	4:D:242:GLU:H	2.22	0.47
1:A:133:GLU:OE1	1:A:137:ARG:NH1	2.41	0.47
12:B:602:CLA:H72	12:B:602:CLA:HBB1	1.96	0.47
2:B:81:THR:OG1	2:B:82:GLY:N	2.47	0.47
3:C:168:ILE:HG22	3:C:247:LEU:O	2.15	0.47
4:D:294:ARG:NH1	24:D:502:HOH:O	2.28	0.47
1:A:308:LEU:HD23	1:A:312:GLY:HA2	1.97	0.47
24:A:556:HOH:O	3:C:411:ALA:HB3	2.14	0.47
15:C:517:BCR:H24C	15:C:517:BCR:H371	1.54	0.47
6:F:35:SER:O	6:F:39:MET:HG3	2.15	0.47
1:A:309:ASP:HB3	1:A:315:LEU:HD21	1.96	0.47
2:B:244:VAL:HG13	12:B:602:CLA:H93	1.97	0.47
1:A:143:TRP:HZ2	3:C:450:ARG:HB2	1.80	0.46
4:D:343:ASP:O	4:D:348:ARG:NH1	2.48	0.46
1:A:222:SER:HB2	4:D:139:ARG:O	2.15	0.46
13:A:404:CL7:HBA1	13:A:404:CL7:H3A	1.63	0.46
12:B:604:CLA:HHD	12:B:604:CLA:HBC2	1.98	0.46
12:C:503:CLA:H8	12:C:503:CLA:H51	1.62	0.46
23:F:101:HEM:HBC2	23:F:101:HEM:HMC2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HE	1:A:65:ARG:HB3	1.51	0.46
1:A:282:VAL:HG11	22:D:407:LHG:H191	1.97	0.46
3:C:81:PHE:CE1	3:C:111:ILE:HD13	2.50	0.46
12:C:503:CLA:H72	12:C:503:CLA:H112	1.70	0.46
4:D:54:PHE:O	5:E:49:THR:OG1	2.28	0.46
2:B:25:MET:HE1	2:B:108:PHE:HE1	1.81	0.46
2:B:357:ARG:NH1	24:B:710:HOH:O	2.42	0.46
3:C:259:PRO:HA	12:C:506:CLA:HED3	1.98	0.46
7:I:21:PHE:HA	7:I:24:LEU:HB2	1.96	0.46
1:A:46:ILE:HG12	14:A:406:PHO:H71	1.98	0.46
12:A:405:CLA:H3A	12:A:405:CLA:HBA2	1.72	0.45
16:A:410:LMT:O6B	16:C:516:LMT:O2'	2.23	0.45
15:C:514:BCR:H15C	15:C:514:BCR:H351	1.79	0.45
1:A:177:ILE:HD11	21:D:406:PL9:H401	1.97	0.45
14:D:402:PHO:H112	14:D:402:PHO:H72	1.79	0.45
3:C:83:LEU:HD22	3:C:83:LEU:HA	1.85	0.45
4:D:274:VAL:HG22	21:D:406:PL9:H222	1.98	0.45
9:N:16:UNK:O	9:N:20:UNK:N	2.49	0.45
2:B:323:GLY:HA3	2:B:326:ARG:HG3	1.98	0.45
12:B:611:CLA:H102	12:B:611:CLA:H61	1.68	0.45
22:D:407:LHG:H251	22:D:407:LHG:H281	1.61	0.45
2:B:442:LEU:HD11	4:D:299:VAL:HG21	1.97	0.45
12:B:604:CLA:C7	12:B:604:CLA:C4B	2.95	0.45
12:C:502:CLA:HMB1	12:C:502:CLA:HBB1	1.99	0.45
6:F:19:TRP:HE3	6:F:20:LEU:HD22	1.82	0.45
1:A:94:PHE:HB2	3:C:221:THR:HG21	1.99	0.45
1:A:299:ASN:HD22	3:C:407:LEU:HD21	1.82	0.45
13:A:404:CL7:H71C	14:A:406:PHO:HMB2	1.99	0.45
16:A:409:LMT:O3B	4:D:304:ARG:NH2	2.50	0.45
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.52	0.45
2:B:291:SER:HB2	2:B:296:LYS:NZ	2.32	0.45
12:B:607:CLA:H162	4:D:35:LEU:HB3	1.99	0.45
3:C:137:TYR:OH	12:C:513:CLA:O1D	2.25	0.44
2:B:385:GLN:NE2	2:B:385:GLN:C	2.75	0.44
12:C:505:CLA:H62	12:C:505:CLA:H2	1.74	0.44
4:D:335:PRO:O	4:D:338:LYS:NZ	2.50	0.44
1:A:51:THR:HG22	15:A:408:BCR:H271	1.99	0.44
2:B:239:ALA:O	2:B:466:HIS:ND1	2.42	0.44
1:A:277:ALA:HA	4:D:212:ALA:HA	2.00	0.44
1:A:184:MET:HA	12:A:403:CLA:HMD1	2.00	0.44
3:C:272:GLU:HG2	3:C:451:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:508:CLA:H202	12:C:508:CLA:H161	1.61	0.44
12:A:405:CLA:HMD3	4:D:182:LEU:HD11	1.99	0.44
12:C:508:CLA:HBC2	22:D:407:LHG:H342	2.00	0.44
12:A:403:CLA:H122	14:A:406:PHO:H3A	1.99	0.44
12:B:604:CLA:HAA1	12:B:604:CLA:HBD	1.99	0.44
3:C:28:PRO:HB2	3:C:29:GLY:H	1.65	0.44
4:D:294:ARG:NH2	24:D:501:HOH:O	2.28	0.44
12:C:510:CLA:HBA1	12:C:510:CLA:H3A	1.80	0.44
4:D:186:GLN:HB2	12:D:403:CLA:HBC1	2.00	0.44
2:B:242:LEU:HD21	12:B:610:CLA:CAB	2.48	0.43
3:C:45:ARG:NH1	12:C:511:CLA:OBD	2.49	0.43
16:C:516:LMT:H5B	16:C:516:LMT:H6D	2.00	0.43
1:A:269:SER:CB	4:D:240:GLY:O	2.66	0.43
12:C:502:CLA:H102	12:C:502:CLA:H62	1.68	0.43
12:B:611:CLA:H162	12:B:611:CLA:H193	1.77	0.43
3:C:132:GLY:O	3:C:136:MET:HG3	2.17	0.43
1:A:340:PHE:HA	1:A:341:PRO:HD2	1.65	0.43
12:B:604:CLA:H42	12:B:604:CLA:CHD	2.49	0.43
12:C:506:CLA:H71	15:C:514:BCR:H331	2.00	0.43
4:D:139:ARG:HD3	4:D:141:TYR:CE1	2.54	0.43
4:D:47:ALA:HB1	4:D:110:LEU:HD22	2.00	0.43
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.43
12:A:407:CLA:H71	7:I:13:SER:HA	2.01	0.43
15:A:408:BCR:H24C	15:A:408:BCR:H371	1.74	0.43
4:D:297:ASP:O	4:D:315:TYR:OH	2.26	0.43
1:A:270:ARG:HD2	4:D:231:THR:O	2.18	0.43
2:B:149:LEU:HB3	12:B:602:CLA:HAC1	2.00	0.43
12:B:610:CLA:H8	12:B:610:CLA:H51	1.76	0.43
4:D:23:LYS:HG3	4:D:135:LEU:HD11	2.01	0.43
12:B:604:CLA:C4B	12:B:604:CLA:H71	2.49	0.42
4:D:22:LEU:HD11	4:D:35:LEU:HD11	2.01	0.42
1:A:132:TRP:CH2	12:C:505:CLA:HAA2	2.54	0.42
12:C:509:CLA:H141	12:C:509:CLA:H161	1.84	0.42
12:A:407:CLA:H92	12:A:407:CLA:H61	1.80	0.42
12:B:607:CLA:CBB	4:D:123:ILE:HG12	2.50	0.42
12:C:502:CLA:H2	12:C:503:CLA:C1D	2.49	0.42
18:C:515:DGD:HA21	18:C:515:DGD:HA52	1.82	0.42
14:A:406:PHO:H41	14:A:406:PHO:H61	1.63	0.42
4:D:119:VAL:HG12	4:D:153:TYR:CE2	2.52	0.42
1:A:268:ASN:CG	1:A:271:GLN:HG3	2.44	0.42
1:A:332:MET:SD	4:D:347:PRO:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:GLY:O	2:B:439:SER:HB3	2.19	0.42
12:B:613:CLA:H93	12:B:613:CLA:H111	1.85	0.42
16:A:409:LMT:H31	16:A:409:LMT:H61	1.81	0.42
3:C:101:LEU:HD11	12:C:503:CLA:HBA1	2.01	0.42
19:D:408:LMG:O5	6:F:44:ARG:NH2	2.49	0.42
1:A:190:GLU:HB2	1:A:191:HIS:CD2	2.55	0.42
4:D:96:GLU:O	4:D:103:ARG:NH1	2.53	0.42
1:A:249:ILE:HD11	4:D:239:GLN:O	2.19	0.42
12:B:610:CLA:CAB	17:B:612:F6C:CMA	2.97	0.42
8:K:24:LEU:HD23	8:K:24:LEU:HA	1.87	0.42
8:K:26:ILE:H	8:K:26:ILE:HG13	1.74	0.42
1:A:94:PHE:CZ	12:A:407:CLA:HAA1	2.49	0.41
12:C:501:CLA:H92	12:C:501:CLA:H62	1.89	0.41
2:B:53:ASN:HD22	2:B:53:ASN:HA	1.68	0.41
2:B:27:ASN:HD21	12:B:611:CLA:H11	1.85	0.41
3:C:62:HIS:CE1	12:C:509:CLA:HMA2	2.55	0.41
4:D:195:PRO:O	4:D:199:MET:HG3	2.20	0.41
4:D:346:LEU:O	4:D:348:ARG:NH1	2.53	0.41
2:B:29:LEU:HD13	17:B:612:F6C:CMD	2.50	0.41
15:B:615:BCR:H24C	15:B:615:BCR:H371	1.80	0.41
3:C:49:PRO:HA	3:C:52:THR:HG23	2.02	0.41
1:A:339:ASN:ND2	3:C:406:SER:HB2	2.29	0.41
2:B:336:LEU:HD12	2:B:337:PRO:HD2	2.02	0.41
3:C:87:MET:HE3	3:C:87:MET:HB2	1.95	0.41
4:D:81:PRO:HB3	4:D:90:LEU:HD11	2.02	0.41
2:B:52:LEU:HD23	2:B:52:LEU:HA	1.92	0.41
12:C:505:CLA:HHD	24:C:618:HOH:O	2.20	0.41
15:A:408:BCR:H351	15:A:408:BCR:H15C	1.72	0.41
3:C:61:ALA:HB1	15:C:517:BCR:H373	2.02	0.41
3:C:114:MET:HB3	3:C:114:MET:HE3	1.74	0.41
12:C:501:CLA:C1D	12:C:503:CLA:H2	2.50	0.41
12:C:505:CLA:HMD3	17:C:507:F6C:CAB	2.50	0.41
12:C:511:CLA:HBA1	15:C:517:BCR:H271	2.02	0.41
4:D:139:ARG:HD3	4:D:141:TYR:HE1	1.85	0.41
4:D:155:ALA:HA	4:D:159:ILE:HB	2.03	0.41
12:D:404:CLA:HHC	12:D:404:CLA:HBB1	2.03	0.41
8:K:12:GLU:HA	8:K:15:ARG:HD3	2.03	0.41
2:B:149:LEU:HD12	2:B:149:LEU:HA	1.91	0.41
12:B:604:CLA:H72	12:B:604:CLA:C4B	2.51	0.41
15:B:615:BCR:H15C	15:B:615:BCR:H351	1.78	0.41
12:C:501:CLA:H71	12:C:501:CLA:HBB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:503:CLA:H203	12:C:510:CLA:HAB	2.01	0.41
4:D:81:PRO:HA	4:D:108:GLY:HA3	2.03	0.41
1:A:37:LEU:HD21	12:C:505:CLA:H143	2.02	0.41
1:A:285:TRP:CD1	3:C:438:PHE:HZ	2.39	0.41
1:A:181:PHE:HB3	1:A:185:PHE:CZ	2.56	0.40
12:A:403:CLA:H142	12:A:403:CLA:H112	1.86	0.40
12:A:403:CLA:HBA1	12:A:403:CLA:H3A	1.78	0.40
12:B:602:CLA:H61	12:B:602:CLA:H41	1.48	0.40
4:D:116:LEU:O	4:D:119:VAL:HG22	2.20	0.40
4:D:225:ASP:HB2	4:D:234:GLY:O	2.21	0.40
1:A:194:LEU:HD21	12:A:403:CLA:C2C	2.51	0.40
3:C:373:ARG:NH2	3:C:377:GLY:HA2	2.36	0.40
12:C:502:CLA:H202	12:C:502:CLA:H161	1.77	0.40
12:C:503:CLA:H193	12:C:503:CLA:H161	1.89	0.40
12:B:601:CLA:HED3	12:B:602:CLA:HMA2	2.02	0.40
1:A:170:SER:O	24:A:502:HOH:O	2.22	0.40
2:B:185:TRP:HZ3	2:B:204:ALA:HB2	1.87	0.40
3:C:50:GLU:O	3:C:145:LYS:HB3	2.21	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.86	0.40
1:A:141:ARG:HB2	4:D:220:ASN:HA	2.03	0.40
1:A:144:ILE:HD11	4:D:217:THR:HA	2.03	0.40
13:A:404:CL7:HED2	4:D:198:MET:SD	2.62	0.40
2:B:33:PHE:CE2	17:B:603:F6C:OMB	2.75	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 PDB entries followed by that with respect to all EM entries.

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	A	297/361 (82%)	290 (98%)	7 (2%)	0	100	100
2	B	444/509 (87%)	427 (96%)	16 (4%)	1 (0%)	43	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	414/482 (86%)	391 (94%)	22 (5%)	1 (0%)	43	50
4	D	334/352 (95%)	324 (97%)	8 (2%)	2 (1%)	21	21
5	E	39/80 (49%)	37 (95%)	2 (5%)	0	100	100
6	F	28/44 (64%)	25 (89%)	3 (11%)	0	100	100
7	I	25/38 (66%)	25 (100%)	0	0	100	100
8	K	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
All	All	1616/1911 (85%)	1552 (96%)	60 (4%)	4 (0%)	44	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	384	ARG
3	C	86	PRO
4	D	242	GLU
4	D	232	PHE

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 PDB entries followed by that with respect to all EM entries.

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	A	249/299 (83%)	243 (98%)	6 (2%)	43	54
2	B	358/410 (87%)	349 (98%)	9 (2%)	42	52
3	C	321/372 (86%)	303 (94%)	18 (6%)	19	20
4	D	273/290 (94%)	261 (96%)	12 (4%)	25	29
5	E	33/69 (48%)	30 (91%)	3 (9%)	9	7
6	F	24/37 (65%)	21 (88%)	3 (12%)	4	3
7	I	24/33 (73%)	23 (96%)	1 (4%)	26	31
8	K	29/37 (78%)	28 (97%)	1 (3%)	32	40
All	All	1311/1547 (85%)	1258 (96%)	53 (4%)	29	34

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	61	ILE
1	A	128	LEU
1	A	221	THR
1	A	250	LEU
1	A	340	PHE
2	B	22	VAL
2	B	84	THR
2	B	149	LEU
2	B	331	VAL
2	B	385	GLN
2	B	389	LYS
2	B	394	GLN
2	B	461	LEU
2	B	474	LEU
3	C	79	SER
3	C	82	ASN
3	C	83	LEU
3	C	105	VAL
3	C	146	LEU
3	C	168	ILE
3	C	170	ILE
3	C	173	ILE
3	C	212	ILE
3	C	282	VAL
3	C	292	PHE
3	C	311	GLU
3	C	358	THR
3	C	375	LYS
3	C	380	LEU
3	C	404	ILE
3	C	408	ASN
3	C	413	LEU
4	D	23	LYS
4	D	64	VAL
4	D	119	VAL
4	D	136	VAL
4	D	176	SER
4	D	225	ASP
4	D	233	LYS
4	D	239	GLN
4	D	294	ARG
4	D	300	SER

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Mol	Chain	Res	Type
4	D	345	VAL
4	D	348	ARG
5	E	20	TRP
5	E	32	ILE
5	E	42	LEU
6	F	27	ILE
6	F	33	LEU
6	F	42	ILE
7	I	3	THR
8	K	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	182	ASN
1	A	271	GLN
1	A	339	ASN
2	B	26	HIS
2	B	53	ASN
2	B	87	ASN
2	B	193	HIS
2	B	202	HIS
2	B	365	ASN
2	B	385	GLN
2	B	394	GLN
2	B	425	GLN
2	B	455	HIS
3	C	62	HIS
3	C	80	HIS
3	C	82	ASN
3	C	285	GLN
3	C	314	GLN
3	C	345	GLN
3	C	391	GLN
3	C	408	ASN
3	C	421	ASN
4	D	61	HIS
4	D	219	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 56 ligands modelled in this entry, 3 are monoatomic - leaving 53 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	$\# Z > 2$
12	CLA	C	501	3	69,73,73	2.20	21 (30%)	82,113,113	2.52	27 (32%)
15	BCR	A	408	-	41,41,41	2.74	6 (14%)	56,56,56	6.60	24 (42%)
12	CLA	D	404	4	49,53,73	2.51	22 (44%)	58,89,113	2.83	24 (41%)
12	CLA	C	503	3	69,73,73	2.19	21 (30%)	82,113,113	2.46	26 (31%)
15	BCR	C	517	-	41,41,41	2.64	6 (14%)	56,56,56	6.57	21 (37%)
12	CLA	B	604	2	59,63,73	2.43	22 (37%)	70,101,113	2.64	26 (37%)
14	PHO	A	406	-	58,69,69	2.09	9 (15%)	55,99,99	1.54	6 (10%)
12	CLA	C	502	3	69,73,73	2.21	21 (30%)	82,113,113	2.49	25 (30%)
12	CLA	C	513	-	49,53,73	2.54	21 (42%)	58,89,113	2.71	21 (36%)
18	DGD	C	515	-	48,48,67	1.16	4 (8%)	62,62,81	1.35	5 (8%)
15	BCR	C	514	-	41,41,41	2.68	6 (14%)	56,56,56	6.55	18 (32%)
17	F6C	B	603	2	57,59,74	3.08	30 (52%)	65,96,114	3.49	34 (52%)
12	CLA	A	405	24	54,58,73	2.52	22 (40%)	64,95,113	2.79	27 (42%)
12	CLA	B	602	2	59,63,73	2.41	20 (33%)	70,101,113	2.66	29 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CL7	A	404	24	69,73,73	2.27	22 (31%)	80,113,113	2.36	25 (31%)
16	LMT	D	409	-	20,20,36	1.42	4 (20%)	23,24,47	1.73	4 (17%)
17	F6C	B	612	2	62,64,74	2.93	30 (48%)	71,102,114	3.38	32 (45%)
12	CLA	C	506	3	59,63,73	2.44	22 (37%)	70,101,113	2.54	27 (38%)
19	LMG	B	617	-	40,40,55	1.20	4 (10%)	48,48,63	1.26	5 (10%)
12	CLA	B	607	2	69,73,73	2.25	21 (30%)	82,113,113	2.39	30 (36%)
12	CLA	B	608	2	49,53,73	2.53	23 (46%)	58,89,113	2.84	21 (36%)
17	F6C	C	507	24	67,69,74	2.83	30 (44%)	77,108,114	3.25	32 (41%)
21	PL9	D	406	-	45,45,55	1.54	5 (11%)	56,57,69	1.50	10 (17%)
17	F6C	B	606	24	67,69,74	2.84	27 (40%)	77,108,114	3.57	34 (44%)
23	HEM	F	101	5,6	50,50,50	1.41	9 (18%)	67,82,82	1.06	3 (4%)
12	CLA	B	605	2	59,63,73	2.41	20 (33%)	70,101,113	2.63	27 (38%)
19	LMG	D	408	-	33,33,55	1.15	2 (6%)	41,41,63	1.10	3 (7%)
16	LMT	A	409	-	36,36,36	1.17	6 (16%)	47,47,47	1.14	3 (6%)
12	CLA	C	511	3	49,53,73	2.50	21 (42%)	58,89,113	2.82	23 (39%)
12	CLA	C	512	3	49,53,73	2.50	19 (38%)	58,89,113	2.80	22 (37%)
12	CLA	B	609	-	49,53,73	2.51	21 (42%)	58,89,113	2.86	23 (39%)
12	CLA	C	505	3	69,73,73	2.23	20 (28%)	82,113,113	2.39	24 (29%)
12	CLA	B	610	2	59,63,73	2.39	19 (32%)	70,101,113	2.58	28 (40%)
12	CLA	A	407	1	64,68,73	2.30	20 (31%)	76,107,113	2.53	24 (31%)
22	LHG	D	407	-	45,45,48	0.92	2 (4%)	48,51,54	1.13	5 (10%)
12	CLA	C	508	3	69,73,73	2.24	23 (33%)	82,113,113	2.48	26 (31%)
12	CLA	D	403	4	64,68,73	2.27	20 (31%)	76,107,113	2.74	25 (32%)
16	LMT	C	516	-	35,35,36	1.18	6 (17%)	46,46,47	0.96	0
12	CLA	B	611	2	69,73,73	2.20	20 (28%)	82,113,113	2.48	24 (29%)
12	CLA	C	504	24	54,58,73	2.49	21 (38%)	64,95,113	2.76	25 (39%)
12	CLA	B	614	2	54,58,73	2.49	23 (42%)	64,95,113	2.80	27 (42%)
12	CLA	A	403	1	69,73,73	2.19	20 (28%)	82,113,113	2.53	27 (32%)
16	LMT	A	410	-	32,32,36	1.29	5 (15%)	43,43,47	1.25	5 (11%)
14	PHO	D	402	-	58,69,69	2.15	9 (15%)	55,99,99	1.70	10 (18%)
12	CLA	C	510	3	69,73,73	2.21	21 (30%)	82,113,113	2.56	27 (32%)
15	BCR	B	615	-	41,41,41	2.76	6 (14%)	56,56,56	6.52	22 (39%)
16	LMT	B	618	-	36,36,36	1.13	4 (11%)	47,47,47	1.11	3 (6%)
15	BCR	D	405	-	25,26,41	3.08	5 (20%)	32,34,56	7.21	14 (43%)
18	DGD	B	616	-	47,47,67	0.96	4 (8%)	55,55,81	1.40	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	LMT	B	619	-	31,31,36	1.36	7 (22%)	42,42,47	1.27	4 (9%)
12	CLA	C	509	3	69,73,73	2.25	22 (31%)	82,113,113	2.48	28 (34%)
12	CLA	B	613	-	69,73,73	2.22	20 (28%)	82,113,113	2.52	27 (32%)
12	CLA	B	601	2	59,63,73	2.40	21 (35%)	70,101,113	2.64	24 (34%)

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
12	CLA	C	501	3	-	11/39/115/115	-
15	BCR	A	408	-	-	10/29/63/63	0/2/2/2
12	CLA	D	404	4	-	4/15/91/115	-
12	CLA	C	503	3	-	12/39/115/115	-
15	BCR	C	517	-	-	11/29/63/63	0/2/2/2
12	CLA	B	604	2	-	13/27/103/115	-
14	PHO	A	406	-	-	9/37/103/103	0/5/6/6
12	CLA	C	502	3	-	17/39/115/115	-
12	CLA	C	513	-	-	3/15/91/115	-
18	DGD	C	515	-	-	15/36/76/95	0/2/2/2
15	BCR	C	514	-	-	5/29/63/63	0/2/2/2
17	F6C	B	603	2	1/1/7/16	9/23/79/97	-
12	CLA	A	405	24	-	7/21/97/115	-
12	CLA	B	602	2	-	10/27/103/115	-
13	CL7	A	404	24	2/2/15/20	21/39/115/115	-
16	LMT	D	409	-	-	9/12/28/61	0/1/1/2
17	F6C	B	612	2	1/1/8/16	13/29/85/97	-
12	CLA	C	506	3	-	8/27/103/115	-
19	LMG	B	617	-	-	9/35/55/70	0/1/1/1
17	F6C	C	507	24	1/1/9/16	17/35/91/97	-
12	CLA	B	607	2	-	13/39/115/115	-
12	CLA	B	608	2	-	11/15/91/115	-
21	PL9	D	406	-	-	14/41/61/73	0/1/1/1
17	F6C	B	606	24	1/1/9/16	17/35/91/97	-
23	HEM	F	101	5,6	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	605	2	-	9/27/103/115	-
19	LMG	D	408	-	-	5/28/48/70	0/1/1/1
16	LMT	A	409	-	-	8/21/61/61	0/2/2/2
12	CLA	C	511	3	-	3/15/91/115	-
12	CLA	C	512	3	-	8/15/91/115	-
12	CLA	B	609	-	-	7/15/91/115	-
12	CLA	C	505	3	-	19/39/115/115	-
12	CLA	B	610	2	-	11/27/103/115	-
12	CLA	A	407	1	-	12/33/109/115	-
22	LHG	D	407	-	-	21/50/50/53	-
12	CLA	C	508	3	-	18/39/115/115	-
12	CLA	D	403	4	-	6/33/109/115	-
16	LMT	C	516	-	-	12/20/60/61	0/2/2/2
12	CLA	B	611	2	-	15/39/115/115	-
12	CLA	C	504	24	-	6/21/97/115	-
12	CLA	B	614	2	-	2/21/97/115	-
12	CLA	A	403	1	-	8/39/115/115	-
16	LMT	A	410	-	-	7/17/57/61	0/2/2/2
14	PHO	D	402	-	-	6/37/103/103	0/5/6/6
12	CLA	C	510	3	-	20/39/115/115	-
15	BCR	B	615	-	-	9/29/63/63	0/2/2/2
16	LMT	B	618	-	-	11/21/61/61	0/2/2/2
15	BCR	D	405	-	-	10/20/37/63	0/1/1/2
18	DGD	B	616	-	-	19/41/61/95	0/1/1/2
16	LMT	B	619	-	-	6/16/56/61	0/2/2/2
12	CLA	C	509	3	-	10/39/115/115	-
12	CLA	B	613	-	-	17/39/115/115	-
12	CLA	B	601	2	-	9/27/103/115	-

All (835) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	606	F6C	C1A-CHA	10.21	1.51	1.35
14	D	402	PHO	C3B-C4B	9.60	1.51	1.41
14	A	406	PHO	C1B-C2B	9.53	1.50	1.39
17	B	603	F6C	MG-NA	9.33	2.24	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	507	F6C	MG-NA	9.24	2.24	2.05
17	B	603	F6C	C1A-CHA	9.21	1.50	1.35
17	B	612	F6C	MG-NA	9.08	2.23	2.05
17	B	606	F6C	MG-NA	8.91	2.23	2.05
17	B	612	F6C	C1A-CHA	8.86	1.49	1.35
17	C	507	F6C	C1A-CHA	8.79	1.49	1.35
15	B	615	BCR	C8-C9	-8.72	1.27	1.46
13	A	404	CL7	MG-NA	8.66	2.23	2.05
14	D	402	PHO	C1B-C2B	8.65	1.49	1.39
15	A	408	BCR	C8-C9	-8.50	1.27	1.46
15	D	405	BCR	C8-C9	-8.41	1.28	1.46
15	C	514	BCR	C8-C9	-8.34	1.28	1.46
15	D	405	BCR	C11-C10	-8.27	1.17	1.43
15	B	615	BCR	C11-C10	-8.27	1.17	1.43
15	C	517	BCR	C8-C9	-8.26	1.28	1.46
15	A	408	BCR	C11-C10	-8.19	1.17	1.43
14	A	406	PHO	C3B-C4B	8.12	1.49	1.41
15	C	514	BCR	C11-C10	-8.07	1.18	1.43
15	C	517	BCR	C11-C10	-8.04	1.18	1.43
15	B	615	BCR	C16-C17	-7.74	1.19	1.43
17	B	603	F6C	C2A-C3A	7.69	1.53	1.36
15	A	408	BCR	C20-C21	-7.65	1.19	1.43
15	B	615	BCR	C20-C21	-7.59	1.19	1.43
12	B	608	CLA	MG-NA	7.58	2.24	2.06
12	C	503	CLA	MG-NA	7.58	2.24	2.06
17	C	507	F6C	C2A-C3A	7.54	1.53	1.36
15	A	408	BCR	C16-C17	-7.54	1.19	1.43
17	B	612	F6C	C2A-C3A	7.47	1.52	1.36
12	B	607	CLA	MG-NA	7.47	2.24	2.06
12	B	604	CLA	MG-NA	7.47	2.24	2.06
15	C	514	BCR	C20-C21	-7.46	1.20	1.43
12	C	504	CLA	MG-NA	7.44	2.24	2.06
12	B	602	CLA	MG-NA	7.43	2.23	2.06
12	B	609	CLA	MG-NA	7.40	2.23	2.06
12	C	508	CLA	MG-NA	7.40	2.23	2.06
12	B	614	CLA	MG-NA	7.40	2.23	2.06
15	D	405	BCR	C16-C17	-7.36	1.20	1.43
12	C	512	CLA	MG-NA	7.36	2.23	2.06
12	C	502	CLA	MG-NA	7.35	2.23	2.06
12	B	613	CLA	MG-NA	7.34	2.23	2.06
15	C	517	BCR	C16-C17	-7.33	1.20	1.43
15	C	514	BCR	C16-C17	-7.32	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	601	CLA	MG-NA	7.29	2.23	2.06
15	C	517	BCR	C20-C21	-7.29	1.20	1.43
12	C	511	CLA	MG-NA	7.27	2.23	2.06
12	D	404	CLA	MG-NA	7.25	2.23	2.06
12	C	505	CLA	MG-NA	7.24	2.23	2.06
12	C	513	CLA	MG-NA	7.21	2.23	2.06
12	C	506	CLA	MG-NA	7.21	2.23	2.06
12	B	605	CLA	MG-NA	7.19	2.23	2.06
12	B	610	CLA	MG-NA	7.18	2.23	2.06
12	C	501	CLA	MG-NA	7.17	2.23	2.06
12	A	405	CLA	MG-NA	7.14	2.23	2.06
12	C	509	CLA	MG-NA	7.09	2.23	2.06
12	A	403	CLA	MG-NA	7.09	2.23	2.06
12	B	611	CLA	MG-NA	7.07	2.23	2.06
12	A	407	CLA	MG-NA	7.04	2.23	2.06
12	C	510	CLA	MG-NA	6.92	2.22	2.06
17	B	606	F6C	C2A-C3A	6.92	1.51	1.36
12	D	403	CLA	MG-NA	6.90	2.22	2.06
21	D	406	PL9	C3-C4	-5.96	1.40	1.49
13	A	404	CL7	O2A-C1	5.58	1.61	1.46
12	B	607	CLA	O2A-C1	5.43	1.60	1.46
12	B	610	CLA	O2A-C1	5.42	1.60	1.46
12	A	405	CLA	O2A-C1	5.36	1.60	1.46
17	B	603	F6C	O2A-C1	5.35	1.60	1.46
12	B	602	CLA	O2A-C1	5.35	1.60	1.46
12	B	614	CLA	O2A-C1	5.34	1.60	1.46
12	C	509	CLA	O2A-C1	5.33	1.60	1.46
17	C	507	F6C	O2A-C1	5.31	1.60	1.46
12	C	508	CLA	O2A-C1	5.29	1.60	1.46
17	B	612	F6C	O2A-C1	5.29	1.60	1.46
12	C	506	CLA	O2A-C1	5.28	1.60	1.46
12	B	605	CLA	O2A-C1	5.28	1.60	1.46
12	B	604	CLA	O2A-C1	5.24	1.60	1.46
17	B	606	F6C	O2A-C1	5.20	1.60	1.46
12	A	407	CLA	O2A-C1	5.20	1.60	1.46
12	B	601	CLA	O2A-C1	5.16	1.60	1.46
12	B	613	CLA	O2A-C1	5.16	1.60	1.46
12	C	504	CLA	O2A-C1	5.15	1.60	1.46
12	B	609	CLA	O2D-CGD	5.15	1.45	1.33
12	D	403	CLA	O2A-C1	5.14	1.60	1.46
12	C	502	CLA	O2A-C1	5.11	1.59	1.46
12	B	608	CLA	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	510	CLA	O2A-C1	5.08	1.59	1.46
12	C	508	CLA	O2D-CGD	5.08	1.45	1.33
17	C	507	F6C	O2D-CGD	5.07	1.45	1.33
12	C	505	CLA	O2A-C1	5.05	1.59	1.46
12	C	501	CLA	O2A-C1	5.04	1.59	1.46
12	B	604	CLA	O2D-CGD	5.04	1.45	1.33
17	B	612	F6C	O2D-CGD	5.03	1.45	1.33
12	A	407	CLA	O2D-CGD	5.01	1.45	1.33
17	B	603	F6C	O2D-CGD	5.00	1.45	1.33
12	C	510	CLA	O2D-CGD	4.98	1.45	1.33
12	B	604	CLA	CHC-C1C	4.97	1.48	1.38
12	C	513	CLA	O2D-CGD	4.97	1.45	1.33
12	B	611	CLA	O2A-C1	4.96	1.59	1.46
12	A	403	CLA	O2A-C1	4.95	1.59	1.46
12	C	505	CLA	O2D-CGD	4.93	1.45	1.33
12	C	503	CLA	O2A-C1	4.93	1.59	1.46
12	C	502	CLA	O2D-CGD	4.93	1.45	1.33
12	C	506	CLA	O2D-CGD	4.93	1.45	1.33
12	C	509	CLA	O2D-CGD	4.90	1.45	1.33
12	C	504	CLA	O2D-CGD	4.88	1.45	1.33
12	B	605	CLA	O2D-CGD	4.87	1.45	1.33
12	B	602	CLA	C3D-C4D	-4.86	1.33	1.44
12	B	613	CLA	O2D-CGD	4.84	1.45	1.33
12	C	506	CLA	CHD-C1D	4.83	1.47	1.38
17	C	507	F6C	CHC-C4B	4.83	1.48	1.38
12	B	601	CLA	O2D-CGD	4.82	1.45	1.33
12	C	508	CLA	CHC-C1C	4.81	1.48	1.38
12	A	405	CLA	O2D-CGD	4.81	1.45	1.33
12	B	614	CLA	O2D-CGD	4.81	1.45	1.33
12	B	607	CLA	C3D-C4D	-4.80	1.33	1.44
12	B	611	CLA	O2D-CGD	4.80	1.45	1.33
12	C	503	CLA	O2D-CGD	4.79	1.45	1.33
17	B	612	F6C	CHC-C4B	4.77	1.48	1.38
12	A	403	CLA	C3D-C4D	-4.77	1.33	1.44
12	B	610	CLA	O2D-CGD	4.76	1.44	1.33
17	B	606	F6C	O2D-CGD	4.75	1.44	1.33
12	B	608	CLA	CHC-C1C	4.74	1.48	1.38
12	D	403	CLA	O2D-CGD	4.74	1.44	1.33
12	B	607	CLA	O2D-CGD	4.73	1.44	1.33
12	C	510	CLA	C3D-C4D	-4.72	1.33	1.44
12	D	404	CLA	O2D-CGD	4.71	1.44	1.33
12	C	513	CLA	CHC-C1C	4.70	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	602	CLA	O2D-CGD	4.70	1.44	1.33
12	C	512	CLA	O2D-CGD	4.69	1.44	1.33
12	B	610	CLA	C3D-C4D	-4.67	1.33	1.44
12	D	403	CLA	C3D-C4D	-4.64	1.33	1.44
12	C	509	CLA	CHC-C1C	4.64	1.47	1.38
15	B	615	BCR	C10-C9	-4.64	1.25	1.35
17	B	603	F6C	CHC-C4B	4.64	1.47	1.38
12	C	501	CLA	O2D-CGD	4.62	1.44	1.33
12	B	613	CLA	CHC-C1C	4.59	1.47	1.38
12	A	407	CLA	C3D-C4D	-4.56	1.33	1.44
12	B	601	CLA	C3D-C4D	-4.56	1.33	1.44
12	C	509	CLA	C3D-C4D	-4.55	1.33	1.44
12	B	611	CLA	CHC-C1C	4.55	1.47	1.38
12	B	613	CLA	C3D-C4D	-4.55	1.34	1.44
15	A	408	BCR	C10-C9	-4.54	1.25	1.35
12	B	611	CLA	C3D-C4D	-4.54	1.34	1.44
12	A	405	CLA	C3C-C2C	4.53	1.46	1.36
12	C	505	CLA	CHC-C1C	4.53	1.47	1.38
12	C	503	CLA	C3D-C4D	-4.52	1.34	1.44
12	C	508	CLA	CHD-C1D	4.52	1.47	1.38
15	C	514	BCR	C10-C9	-4.52	1.25	1.35
12	C	506	CLA	C3C-C2C	4.51	1.46	1.36
12	A	405	CLA	C3D-C4D	-4.51	1.34	1.44
12	C	501	CLA	C3D-C4D	-4.51	1.34	1.44
12	A	407	CLA	C3C-C2C	4.51	1.46	1.36
12	D	403	CLA	CHC-C1C	4.51	1.47	1.38
15	D	405	BCR	C10-C9	-4.51	1.25	1.35
12	B	609	CLA	C3C-C2C	4.50	1.46	1.36
12	C	508	CLA	C3C-C2C	4.49	1.46	1.36
12	C	512	CLA	C3D-C4D	-4.48	1.34	1.44
12	B	604	CLA	CHD-C1D	4.48	1.47	1.38
12	C	510	CLA	C3C-C2C	4.47	1.46	1.36
12	A	405	CLA	CHC-C1C	4.47	1.47	1.38
12	C	511	CLA	O2D-CGD	4.47	1.44	1.33
12	B	601	CLA	CHC-C1C	4.46	1.47	1.38
12	C	505	CLA	C3D-C4D	-4.46	1.34	1.44
12	A	403	CLA	O2D-CGD	4.45	1.44	1.33
12	B	605	CLA	CHC-C1C	4.44	1.47	1.38
12	B	604	CLA	C3C-C2C	4.44	1.46	1.36
12	C	513	CLA	C3C-C2C	4.44	1.46	1.36
12	B	605	CLA	C3D-C4D	-4.43	1.34	1.44
12	C	502	CLA	C3D-C4D	-4.43	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	405	CLA	CHD-C1D	4.43	1.47	1.38
12	C	512	CLA	CHC-C1C	4.42	1.47	1.38
19	B	617	LMG	O8-C28	4.42	1.46	1.33
12	A	403	CLA	CHC-C1C	4.42	1.47	1.38
12	B	604	CLA	C3D-C4D	-4.42	1.34	1.44
12	B	614	CLA	C3C-C2C	4.41	1.46	1.36
12	C	513	CLA	C3D-C4D	-4.41	1.34	1.44
12	C	505	CLA	C3C-C2C	4.41	1.46	1.36
12	C	501	CLA	CHC-C1C	4.41	1.47	1.38
13	A	404	CL7	O2D-CGD	4.41	1.44	1.33
12	C	511	CLA	C3C-C2C	4.40	1.46	1.36
12	D	404	CLA	C3D-C4D	-4.40	1.34	1.44
12	C	511	CLA	C3D-C4D	-4.40	1.34	1.44
15	C	517	BCR	C10-C9	-4.39	1.25	1.35
17	B	612	F6C	CHD-C1D	4.39	1.47	1.38
12	C	508	CLA	C3D-C4D	-4.39	1.34	1.44
12	D	404	CLA	CHC-C1C	4.38	1.47	1.38
17	C	507	F6C	CHD-C1D	4.38	1.47	1.38
12	B	609	CLA	CHC-C1C	4.37	1.47	1.38
17	B	606	F6C	CHC-C4B	4.37	1.47	1.38
12	C	511	CLA	CHC-C1C	4.36	1.47	1.38
12	C	504	CLA	CHC-C1C	4.36	1.47	1.38
12	C	510	CLA	CHC-C1C	4.36	1.47	1.38
12	B	602	CLA	CHD-C1D	4.34	1.46	1.38
12	A	403	CLA	C3C-C2C	4.33	1.46	1.36
12	C	503	CLA	CHC-C1C	4.33	1.47	1.38
12	B	605	CLA	C3C-C2C	4.33	1.46	1.36
12	B	602	CLA	CHC-C1C	4.33	1.47	1.38
17	B	606	F6C	C4A-NA	-4.32	1.32	1.37
12	B	608	CLA	C3C-C2C	4.31	1.46	1.36
12	C	506	CLA	C3D-C4D	-4.31	1.34	1.44
12	C	509	CLA	C3C-C2C	4.31	1.46	1.36
12	C	513	CLA	CHD-C1D	4.31	1.46	1.38
12	B	609	CLA	CHD-C1D	4.31	1.46	1.38
12	B	614	CLA	CHD-C1D	4.31	1.46	1.38
12	C	503	CLA	CHD-C1D	4.31	1.46	1.38
13	A	404	CL7	C3C-C2C	4.30	1.46	1.36
12	B	601	CLA	C3C-C2C	4.30	1.46	1.36
12	B	607	CLA	C3C-C2C	4.30	1.46	1.36
12	C	509	CLA	CHD-C1D	4.29	1.46	1.38
12	C	511	CLA	CHD-C1D	4.29	1.46	1.38
12	B	611	CLA	C3C-C2C	4.29	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	407	CLA	CHC-C1C	4.29	1.47	1.38
12	D	404	CLA	C3C-C2C	4.28	1.46	1.36
12	B	607	CLA	CHC-C1C	4.27	1.47	1.38
12	C	504	CLA	C3D-C4D	-4.27	1.34	1.44
12	A	407	CLA	CHD-C1D	4.27	1.46	1.38
12	D	403	CLA	C3C-C2C	4.26	1.46	1.36
12	B	613	CLA	CHD-C1D	4.26	1.46	1.38
12	C	504	CLA	CHD-C1D	4.25	1.46	1.38
12	C	510	CLA	CHD-C1D	4.25	1.46	1.38
12	B	614	CLA	CHC-C1C	4.24	1.47	1.38
19	D	408	LMG	O7-C10	4.24	1.46	1.34
12	C	504	CLA	C3C-C2C	4.24	1.45	1.36
12	B	610	CLA	C1D-ND	-4.24	1.32	1.37
12	C	501	CLA	C3C-C2C	4.24	1.45	1.36
17	B	603	F6C	CHD-C1D	4.23	1.47	1.38
12	B	608	CLA	C3D-C4D	-4.23	1.34	1.44
12	C	502	CLA	C3C-C2C	4.22	1.45	1.36
12	B	605	CLA	CHD-C1D	4.22	1.46	1.38
13	A	404	CL7	CHD-C4C	4.22	1.46	1.38
12	B	613	CLA	C3C-C2C	4.22	1.45	1.36
12	D	403	CLA	C1D-ND	-4.22	1.32	1.37
12	B	601	CLA	CHD-C1D	4.21	1.46	1.38
12	B	602	CLA	C3C-C2C	4.19	1.45	1.36
12	B	608	CLA	CHD-C1D	4.19	1.46	1.38
12	C	506	CLA	CHC-C1C	4.19	1.46	1.38
12	C	505	CLA	C1D-ND	-4.19	1.32	1.37
12	C	506	CLA	CHD-C4C	4.18	1.48	1.39
19	D	408	LMG	O8-C28	4.17	1.45	1.33
12	C	503	CLA	C3C-C2C	4.16	1.45	1.36
12	B	614	CLA	C3D-C4D	-4.16	1.34	1.44
12	B	610	CLA	C1B-NB	-4.16	1.32	1.37
12	B	610	CLA	C1C-NC	-4.16	1.31	1.37
12	B	607	CLA	C1B-NB	-4.15	1.32	1.37
12	C	512	CLA	C3C-C2C	4.15	1.45	1.36
12	C	502	CLA	CHD-C1D	4.15	1.46	1.38
12	B	609	CLA	C3D-C4D	-4.15	1.34	1.44
17	B	603	F6C	C4A-NA	-4.13	1.32	1.37
13	A	404	CL7	CHC-C1C	4.11	1.46	1.38
12	D	404	CLA	CHD-C1D	4.11	1.46	1.38
13	A	404	CL7	C1C-NC	-4.10	1.32	1.37
17	B	612	F6C	C4A-NA	-4.10	1.32	1.37
12	B	607	CLA	CHD-C1D	4.08	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	CLA	CHC-C1C	4.04	1.46	1.38
12	C	501	CLA	CHD-C1D	4.03	1.46	1.38
12	C	512	CLA	CHD-C1D	4.02	1.46	1.38
22	D	407	LHG	O7-C7	4.00	1.45	1.34
17	C	507	F6C	C4A-NA	-4.00	1.32	1.37
12	B	607	CLA	C1D-ND	-3.99	1.32	1.37
17	B	612	F6C	MG-NC	3.95	2.13	2.05
17	B	612	F6C	CHB-C1B	3.95	1.48	1.39
17	C	507	F6C	CHC-C1C	3.94	1.48	1.39
12	A	405	CLA	CHD-C4C	3.94	1.48	1.39
12	C	505	CLA	CHD-C1D	3.94	1.46	1.38
17	B	612	F6C	CHD-C4C	3.94	1.48	1.39
23	F	101	HEM	FE-NA	3.93	2.08	1.95
12	A	407	CLA	CHD-C4C	3.93	1.48	1.39
12	A	403	CLA	CHD-C1D	3.92	1.46	1.38
12	B	604	CLA	CHC-C4B	3.91	1.48	1.39
12	C	510	CLA	CHD-C4C	3.91	1.48	1.39
17	C	507	F6C	CHD-C4C	3.91	1.48	1.39
12	C	508	CLA	CHC-C4B	3.90	1.48	1.39
17	B	603	F6C	MG-NC	3.90	2.13	2.05
12	B	610	CLA	CHC-C1C	3.90	1.46	1.38
17	C	507	F6C	MG-NC	3.89	2.13	2.05
17	C	507	F6C	CHB-C1B	3.89	1.48	1.39
14	D	402	PHO	C1D-C2D	3.89	1.43	1.39
12	C	504	CLA	CHD-C4C	3.89	1.48	1.39
12	C	508	CLA	CHD-C4C	3.89	1.48	1.39
12	C	509	CLA	CHD-C4C	3.89	1.48	1.39
12	C	513	CLA	CHD-C4C	3.87	1.48	1.39
17	B	603	F6C	CHB-C1B	3.87	1.48	1.39
12	C	508	CLA	CHB-C1B	3.86	1.48	1.39
12	B	601	CLA	CHD-C4C	3.85	1.48	1.39
12	D	403	CLA	CHB-C1B	3.85	1.48	1.39
12	C	511	CLA	CHD-C4C	3.85	1.48	1.39
12	B	611	CLA	CHD-C1D	3.83	1.45	1.38
17	B	606	F6C	CHC-C1C	3.83	1.48	1.39
17	B	612	F6C	CHC-C1C	3.83	1.48	1.39
19	B	617	LMG	O7-C10	3.82	1.45	1.34
12	A	407	CLA	C1D-ND	-3.81	1.32	1.37
12	A	403	CLA	CHD-C4C	3.81	1.47	1.39
12	D	404	CLA	CHD-C4C	3.81	1.47	1.39
14	A	406	PHO	C1D-C2D	3.81	1.43	1.39
12	D	404	CLA	CHC-C4B	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	501	CLA	CHB-C1B	3.80	1.47	1.39
12	C	512	CLA	CHD-C4C	3.80	1.47	1.39
12	B	604	CLA	CHD-C4C	3.80	1.47	1.39
22	D	407	LHG	O8-C23	3.80	1.44	1.33
12	B	605	CLA	CHD-C4C	3.79	1.47	1.39
17	B	606	F6C	CHD-C1D	3.79	1.46	1.38
12	C	510	CLA	CHB-C1B	3.78	1.47	1.39
15	B	615	BCR	C11-C12	-3.78	1.24	1.34
12	C	506	CLA	C1B-NB	-3.78	1.32	1.37
12	B	607	CLA	CHD-C4C	3.78	1.47	1.39
12	B	605	CLA	C1D-ND	-3.78	1.32	1.37
12	B	608	CLA	CHD-C4C	3.77	1.47	1.39
17	B	603	F6C	CHC-C1C	3.76	1.47	1.39
12	B	604	CLA	CHB-C1B	3.76	1.47	1.39
12	C	501	CLA	CHD-C4C	3.76	1.47	1.39
12	B	614	CLA	OBD-CAD	3.76	1.29	1.22
17	B	606	F6C	MG-NC	3.76	2.13	2.05
12	C	503	CLA	CHD-C4C	3.76	1.47	1.39
12	A	403	CLA	C1D-ND	-3.75	1.32	1.37
12	B	611	CLA	C1D-ND	-3.75	1.32	1.37
12	C	513	CLA	OBD-CAD	3.75	1.28	1.22
13	A	404	CL7	C4C-NC	-3.75	1.32	1.37
12	C	513	CLA	CHC-C4B	3.74	1.47	1.39
12	B	614	CLA	CHB-C1B	3.73	1.47	1.39
17	B	606	F6C	C3D-C4D	-3.72	1.34	1.44
12	C	509	CLA	CHC-C4B	3.71	1.47	1.39
17	B	612	F6C	OBD-CAD	3.71	1.28	1.22
12	C	502	CLA	C1C-NC	-3.70	1.32	1.37
12	B	610	CLA	CHD-C1D	3.70	1.45	1.38
12	B	608	CLA	CHC-C4B	3.70	1.47	1.39
17	B	606	F6C	CHD-C4C	3.70	1.47	1.39
12	B	613	CLA	CHC-C4B	3.70	1.47	1.39
12	B	602	CLA	CHD-C4C	3.69	1.47	1.39
15	D	405	BCR	C11-C12	-3.69	1.25	1.34
12	C	501	CLA	CHC-C4B	3.69	1.47	1.39
17	C	507	F6C	C3D-C4D	-3.68	1.34	1.44
12	B	602	CLA	C1D-ND	-3.68	1.33	1.37
12	B	611	CLA	CHC-C4B	3.68	1.47	1.39
17	B	612	F6C	C3D-C4D	-3.67	1.34	1.44
12	C	502	CLA	CHB-C1B	3.67	1.47	1.39
12	C	503	CLA	CHC-C4B	3.66	1.47	1.39
12	C	501	CLA	C1D-ND	-3.66	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	507	F6C	OBD-CAD	3.66	1.28	1.22
21	D	406	PL9	C7-C3	-3.66	1.46	1.51
12	C	508	CLA	OBD-CAD	3.66	1.28	1.22
12	B	601	CLA	CHC-C4B	3.65	1.47	1.39
12	B	613	CLA	CHD-C4C	3.65	1.47	1.39
12	A	405	CLA	C1D-ND	-3.65	1.33	1.37
12	B	609	CLA	CHD-C4C	3.65	1.47	1.39
12	C	509	CLA	C1D-ND	-3.64	1.33	1.37
12	B	610	CLA	C3C-C2C	3.64	1.44	1.36
12	B	609	CLA	OBD-CAD	3.63	1.28	1.22
17	B	603	F6C	C3D-C4D	-3.63	1.34	1.44
12	C	512	CLA	CHC-C4B	3.63	1.47	1.39
12	B	608	CLA	CHB-C1B	3.63	1.47	1.39
12	B	609	CLA	CHB-C1B	3.62	1.47	1.39
16	D	409	LMT	O3'-C3'	-3.62	1.35	1.43
12	B	614	CLA	CHD-C4C	3.62	1.47	1.39
17	B	603	F6C	CHD-C4C	3.62	1.47	1.39
12	B	608	CLA	OBD-CAD	3.61	1.28	1.22
12	D	404	CLA	C1D-ND	-3.61	1.33	1.37
13	A	404	CL7	CHC-C4B	3.61	1.47	1.39
12	B	614	CLA	CHC-C4B	3.59	1.47	1.39
12	B	610	CLA	MG-ND	-3.59	1.98	2.05
12	C	503	CLA	CHB-C1B	3.59	1.47	1.39
17	B	606	F6C	C1C-NC	-3.58	1.33	1.37
12	C	510	CLA	C1B-NB	-3.58	1.33	1.37
12	B	604	CLA	OBD-CAD	3.57	1.28	1.22
13	A	404	CL7	C1D-ND	-3.57	1.33	1.37
12	C	509	CLA	CHB-C1B	3.57	1.47	1.39
12	B	601	CLA	C1D-ND	-3.57	1.33	1.37
12	C	512	CLA	CHB-C1B	3.57	1.47	1.39
15	A	408	BCR	C11-C12	-3.57	1.25	1.34
12	C	511	CLA	CHB-C1B	3.56	1.47	1.39
17	B	606	F6C	OBD-CAD	3.55	1.28	1.22
12	B	602	CLA	MG-ND	-3.54	1.98	2.05
12	B	610	CLA	OBD-CAD	3.54	1.28	1.22
12	C	504	CLA	CHB-C1B	3.54	1.47	1.39
17	B	606	F6C	CHB-C1B	3.54	1.47	1.39
12	A	403	CLA	CHC-C4B	3.54	1.47	1.39
12	C	513	CLA	CHB-C1B	3.53	1.47	1.39
12	B	610	CLA	CHB-C1B	3.53	1.47	1.39
12	C	511	CLA	CHC-C4B	3.52	1.47	1.39
13	A	404	CL7	CHB-C1B	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	609	CLA	CHC-C4B	3.52	1.47	1.39
12	C	506	CLA	C1D-ND	-3.52	1.33	1.37
12	B	605	CLA	OBD-CAD	3.51	1.28	1.22
12	C	505	CLA	CHC-C4B	3.50	1.47	1.39
12	C	511	CLA	OBD-CAD	3.49	1.28	1.22
12	B	611	CLA	CHD-C4C	3.49	1.47	1.39
12	B	613	CLA	CHB-C1B	3.49	1.47	1.39
12	C	502	CLA	CHD-C4C	3.49	1.47	1.39
12	C	505	CLA	CHB-C1B	3.49	1.47	1.39
12	C	505	CLA	CHD-C4C	3.49	1.47	1.39
12	D	403	CLA	CHC-C4B	3.48	1.47	1.39
12	B	607	CLA	OBD-CAD	3.48	1.28	1.22
15	C	514	BCR	C11-C12	-3.48	1.25	1.34
12	B	602	CLA	CHC-C4B	3.48	1.47	1.39
17	B	606	F6C	C3B-C2B	3.47	1.47	1.39
12	B	601	CLA	CHB-C1B	3.47	1.47	1.39
12	C	504	CLA	CHC-C4B	3.47	1.47	1.39
12	B	605	CLA	CHC-C4B	3.47	1.47	1.39
13	A	404	CL7	C1B-NB	-3.46	1.33	1.37
17	B	603	F6C	OBD-CAD	3.46	1.28	1.22
12	A	403	CLA	CHB-C1B	3.44	1.47	1.39
12	C	501	CLA	OBD-CAD	3.44	1.28	1.22
12	D	403	CLA	CHD-C4C	3.44	1.47	1.39
12	B	607	CLA	MG-ND	-3.44	1.99	2.05
12	D	404	CLA	CHB-C1B	3.44	1.47	1.39
12	B	607	CLA	CHC-C4B	3.44	1.47	1.39
15	C	517	BCR	C11-C12	-3.43	1.25	1.34
12	A	407	CLA	CHC-C4B	3.43	1.47	1.39
12	C	505	CLA	OBD-CAD	3.43	1.28	1.22
12	B	611	CLA	CHB-C1B	3.42	1.47	1.39
12	C	512	CLA	C1B-NB	-3.42	1.33	1.37
12	C	510	CLA	CHC-C4B	3.40	1.47	1.39
12	A	407	CLA	CHB-C1B	3.40	1.47	1.39
12	C	506	CLA	C3D-C2D	3.40	1.48	1.39
12	C	513	CLA	C1D-ND	-3.40	1.33	1.37
12	C	511	CLA	C1D-ND	-3.39	1.33	1.37
12	B	605	CLA	C1B-NB	-3.39	1.33	1.37
12	B	602	CLA	OBD-CAD	3.39	1.28	1.22
12	B	602	CLA	CHB-C1B	3.38	1.47	1.39
12	B	605	CLA	CHB-C1B	3.37	1.47	1.39
12	C	510	CLA	OBD-CAD	3.35	1.28	1.22
12	C	510	CLA	C1D-ND	-3.34	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	403	CLA	CHD-C1D	3.34	1.44	1.38
12	B	605	CLA	MG-ND	-3.33	1.99	2.05
14	D	402	PHO	C4D-CHA	3.31	1.44	1.39
12	D	403	CLA	C1B-NB	-3.30	1.33	1.37
12	C	504	CLA	OBD-CAD	3.30	1.28	1.22
12	A	405	CLA	CHC-C4B	3.30	1.46	1.39
12	B	601	CLA	OBD-CAD	3.30	1.28	1.22
23	F	101	HEM	CAC-C3C	3.29	1.56	1.47
12	A	405	CLA	C4B-NB	-3.28	1.33	1.37
12	C	503	CLA	C1D-ND	-3.27	1.33	1.37
23	F	101	HEM	FE-ND	3.27	2.05	1.94
12	C	502	CLA	C1D-ND	-3.27	1.33	1.37
12	B	611	CLA	OBD-CAD	3.27	1.28	1.22
12	C	505	CLA	C1B-NB	-3.27	1.33	1.37
12	C	506	CLA	OBD-CAD	3.27	1.28	1.22
12	A	405	CLA	C1B-NB	-3.26	1.33	1.37
12	B	607	CLA	CHB-C1B	3.26	1.46	1.39
12	C	509	CLA	OBD-CAD	3.26	1.28	1.22
12	B	613	CLA	OBD-CAD	3.25	1.28	1.22
12	C	502	CLA	C4B-NB	-3.25	1.33	1.37
12	C	502	CLA	OBD-CAD	3.25	1.28	1.22
12	A	405	CLA	OBD-CAD	3.25	1.28	1.22
12	B	613	CLA	C1B-NB	-3.24	1.33	1.37
12	C	512	CLA	OBD-CAD	3.23	1.28	1.22
12	C	506	CLA	CHB-C1B	3.22	1.46	1.39
12	C	502	CLA	CHC-C4B	3.22	1.46	1.39
12	B	613	CLA	C1D-ND	-3.21	1.33	1.37
17	C	507	F6C	C3B-C2B	3.20	1.46	1.39
12	C	504	CLA	C1B-NB	-3.19	1.33	1.37
12	A	403	CLA	C1B-NB	-3.19	1.33	1.37
12	B	601	CLA	C1B-NB	-3.19	1.33	1.37
12	A	405	CLA	C1C-NC	-3.18	1.32	1.37
12	B	605	CLA	C1C-NC	-3.18	1.32	1.37
12	C	503	CLA	OBD-CAD	3.18	1.28	1.22
12	C	505	CLA	MG-ND	-3.17	1.99	2.05
12	A	407	CLA	OBD-CAD	3.17	1.27	1.22
12	C	512	CLA	C1D-ND	-3.17	1.33	1.37
12	A	405	CLA	CHB-C1B	3.16	1.46	1.39
12	C	504	CLA	C1D-ND	-3.16	1.33	1.37
12	A	407	CLA	C1B-NB	-3.15	1.33	1.37
12	C	511	CLA	C1B-NB	-3.15	1.33	1.37
12	C	506	CLA	C1C-NC	-3.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	608	CLA	C1D-ND	-3.15	1.33	1.37
12	B	602	CLA	C1B-NB	-3.14	1.33	1.37
17	B	612	F6C	C3B-C2B	3.11	1.46	1.39
13	A	404	CL7	C1A-CHA	3.11	1.51	1.38
12	D	404	CLA	OBD-CAD	3.10	1.27	1.22
12	B	604	CLA	MG-NC	3.10	2.13	2.06
12	C	502	CLA	C3D-C2D	3.10	1.47	1.39
12	D	404	CLA	C1C-NC	-3.09	1.33	1.37
12	B	609	CLA	C3D-C2D	3.09	1.47	1.39
12	B	610	CLA	CHD-C4C	3.08	1.46	1.39
14	A	406	PHO	C4D-ND	-3.08	1.33	1.38
12	B	601	CLA	C3D-C2D	3.08	1.47	1.39
13	A	404	CL7	MG-NC	3.08	2.11	2.05
12	D	404	CLA	C1B-NB	-3.07	1.33	1.37
13	A	404	CL7	OBD-CAD	3.07	1.27	1.22
12	A	405	CLA	C3D-C2D	3.07	1.47	1.39
12	B	604	CLA	C3D-C2D	3.06	1.47	1.39
23	F	101	HEM	CAB-C3B	3.06	1.55	1.47
17	B	603	F6C	C3B-C2B	3.06	1.46	1.39
12	B	611	CLA	C1B-NB	-3.06	1.33	1.37
12	C	509	CLA	C3D-C2D	3.06	1.47	1.39
12	A	407	CLA	C4B-NB	-3.06	1.33	1.37
12	C	508	CLA	MG-NC	3.05	2.13	2.06
12	A	403	CLA	OBD-CAD	3.05	1.27	1.22
12	C	505	CLA	C4B-NB	-3.05	1.33	1.37
17	B	603	F6C	C3D-C2D	3.05	1.47	1.39
14	A	406	PHO	CMD-C2D	-3.04	1.45	1.51
12	B	614	CLA	C1D-ND	-3.04	1.33	1.37
17	B	612	F6C	C3D-C2D	3.04	1.47	1.39
12	C	502	CLA	C1B-NB	-3.03	1.33	1.37
17	C	507	F6C	C3D-C2D	3.02	1.47	1.39
12	C	506	CLA	MG-ND	-3.02	1.99	2.05
12	A	407	CLA	C3D-C2D	3.02	1.47	1.39
12	C	509	CLA	MG-ND	-3.02	1.99	2.05
12	D	403	CLA	OBD-CAD	3.01	1.27	1.22
12	C	503	CLA	MG-NC	3.00	2.13	2.06
12	B	611	CLA	MG-ND	-2.99	1.99	2.05
12	B	610	CLA	C3D-C2D	2.99	1.47	1.39
12	C	508	CLA	C3D-C2D	2.99	1.47	1.39
12	C	511	CLA	C3D-C2D	2.98	1.47	1.39
12	B	614	CLA	C1B-C2B	2.98	1.50	1.43
12	B	614	CLA	C3D-C2D	2.98	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	603	F6C	C1C-NC	-2.97	1.34	1.37
12	C	501	CLA	C1C-NC	-2.97	1.33	1.37
12	C	501	CLA	C3D-C2D	2.97	1.47	1.39
12	B	610	CLA	CHC-C4B	2.97	1.46	1.39
12	B	609	CLA	C1D-ND	-2.96	1.34	1.37
12	A	403	CLA	MG-ND	-2.95	1.99	2.05
12	D	403	CLA	C4B-NB	-2.95	1.34	1.37
12	C	505	CLA	MG-NC	2.95	2.13	2.06
12	C	509	CLA	MG-NC	2.95	2.13	2.06
12	B	605	CLA	C3D-C2D	2.95	1.47	1.39
12	C	513	CLA	C3D-C2D	2.95	1.47	1.39
12	B	608	CLA	C4D-CHA	2.94	1.48	1.38
12	A	403	CLA	C4B-NB	-2.94	1.34	1.37
12	B	609	CLA	C4D-CHA	2.94	1.48	1.38
12	C	512	CLA	C3D-C2D	2.94	1.47	1.39
18	B	616	DGD	C4D-C5D	2.94	1.59	1.52
12	A	403	CLA	C1C-NC	-2.94	1.33	1.37
12	C	504	CLA	C1C-NC	-2.93	1.33	1.37
12	C	503	CLA	MG-ND	-2.93	2.00	2.05
12	B	613	CLA	MG-NC	2.93	2.13	2.06
12	B	601	CLA	MG-NC	2.92	2.13	2.06
12	B	608	CLA	MG-NC	2.92	2.13	2.06
17	B	606	F6C	C4C-NC	-2.92	1.34	1.37
14	D	402	PHO	CMC-C2C	-2.92	1.46	1.50
19	B	617	LMG	C37-C36	-2.92	1.33	1.51
12	B	608	CLA	C1B-NB	-2.91	1.34	1.37
12	C	506	CLA	CHC-C4B	2.91	1.46	1.39
12	B	613	CLA	C3D-C2D	2.91	1.46	1.39
12	B	614	CLA	MG-NC	2.90	2.13	2.06
12	C	502	CLA	C4D-CHA	2.90	1.48	1.38
12	D	404	CLA	C3D-C2D	2.90	1.46	1.39
17	C	507	F6C	C3C-C2C	2.90	1.46	1.38
12	B	609	CLA	C1B-C2B	2.89	1.49	1.43
17	B	612	F6C	C3C-C2C	2.89	1.46	1.38
12	B	614	CLA	C4D-CHA	2.89	1.48	1.38
12	D	403	CLA	C1C-NC	-2.89	1.33	1.37
12	A	405	CLA	MG-NC	2.89	2.13	2.06
12	C	502	CLA	MG-ND	-2.89	2.00	2.05
12	B	609	CLA	C1B-NB	-2.89	1.34	1.37
12	B	611	CLA	C3D-C2D	2.88	1.46	1.39
17	C	507	F6C	C1D-C2D	2.88	1.50	1.44
12	C	504	CLA	MG-NC	2.88	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	605	CLA	MG-NC	2.88	2.13	2.06
12	B	601	CLA	C4D-CHA	2.88	1.48	1.38
12	D	404	CLA	MG-NC	2.88	2.13	2.06
12	C	504	CLA	C3D-C2D	2.87	1.46	1.39
17	B	612	F6C	C1D-C2D	2.87	1.50	1.44
12	D	404	CLA	MG-ND	-2.87	2.00	2.05
12	B	609	CLA	MG-NC	2.87	2.13	2.06
14	D	402	PHO	CMD-C2D	-2.87	1.45	1.51
12	D	403	CLA	MG-ND	-2.86	2.00	2.05
12	B	611	CLA	C1C-NC	-2.86	1.33	1.37
12	C	512	CLA	C4D-CHA	2.85	1.48	1.38
12	C	506	CLA	C4D-CHA	2.85	1.48	1.38
12	C	505	CLA	C4D-CHA	2.85	1.48	1.38
12	B	613	CLA	C4D-CHA	2.85	1.48	1.38
12	C	503	CLA	C1C-NC	-2.85	1.33	1.37
12	B	608	CLA	C3D-C2D	2.84	1.46	1.39
17	B	606	F6C	C1D-ND	-2.84	1.33	1.37
12	C	513	CLA	C1B-NB	-2.83	1.34	1.37
12	C	503	CLA	C3D-C2D	2.83	1.46	1.39
21	D	406	PL9	C52-C5	-2.83	1.45	1.50
12	C	508	CLA	C1B-C2B	2.83	1.49	1.43
14	D	402	PHO	C4D-ND	-2.83	1.34	1.38
12	C	511	CLA	MG-ND	-2.82	2.00	2.05
12	B	602	CLA	MG-NC	2.82	2.13	2.06
12	C	501	CLA	C4B-NB	-2.82	1.34	1.37
12	B	601	CLA	MG-ND	-2.82	2.00	2.05
12	B	605	CLA	C4B-NB	-2.82	1.34	1.37
12	C	501	CLA	C1B-NB	-2.82	1.34	1.37
12	B	614	CLA	C1C-NC	-2.81	1.33	1.37
12	D	403	CLA	C1B-C2B	2.81	1.49	1.43
12	C	504	CLA	C4D-CHA	2.81	1.48	1.38
21	D	406	PL9	C6-C1	-2.81	1.43	1.48
12	B	602	CLA	C1C-NC	-2.81	1.33	1.37
12	C	501	CLA	MG-ND	-2.80	2.00	2.05
18	B	616	DGD	C4D-C3D	2.80	1.59	1.52
14	A	406	PHO	CAC-C3C	-2.80	1.46	1.51
12	C	512	CLA	C4B-NB	-2.79	1.34	1.37
12	B	613	CLA	MG-ND	-2.79	2.00	2.05
12	B	604	CLA	C1D-ND	-2.79	1.34	1.37
12	C	501	CLA	C1B-C2B	2.79	1.49	1.43
12	B	607	CLA	C4D-CHA	2.78	1.47	1.38
12	C	511	CLA	MG-NC	2.78	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	510	CLA	C1B-C2B	2.78	1.49	1.43
12	D	403	CLA	MG-NC	2.78	2.12	2.06
12	C	509	CLA	C4D-CHA	2.78	1.47	1.38
12	B	607	CLA	C1C-NC	-2.77	1.33	1.37
13	A	404	CL7	MG-ND	-2.77	2.00	2.05
12	C	505	CLA	C3D-C2D	2.77	1.46	1.39
17	B	603	F6C	C3C-C2C	2.77	1.46	1.38
12	B	609	CLA	MG-ND	-2.77	2.00	2.05
13	A	404	CL7	C4B-NB	-2.77	1.34	1.37
12	B	614	CLA	C1B-NB	-2.77	1.34	1.37
17	B	606	F6C	C3C-C2C	2.76	1.46	1.38
12	B	610	CLA	C4D-CHA	2.75	1.47	1.38
12	C	512	CLA	MG-NC	2.75	2.12	2.06
12	C	508	CLA	C4D-CHA	2.74	1.47	1.38
12	C	513	CLA	C4D-CHA	2.74	1.47	1.38
12	C	511	CLA	C1C-NC	-2.74	1.33	1.37
12	C	503	CLA	C4D-CHA	2.73	1.47	1.38
12	A	407	CLA	MG-ND	-2.73	2.00	2.05
14	A	406	PHO	C4D-CHA	2.73	1.43	1.39
12	B	611	CLA	C1B-C2B	2.73	1.49	1.43
12	B	611	CLA	C4D-CHA	2.73	1.47	1.38
12	C	509	CLA	C1B-C2B	2.73	1.49	1.43
12	A	403	CLA	C4D-CHA	2.72	1.47	1.38
12	C	512	CLA	MG-ND	-2.72	2.00	2.05
12	C	513	CLA	MG-ND	-2.72	2.00	2.05
12	B	611	CLA	C4B-NB	-2.72	1.34	1.37
12	C	504	CLA	MG-ND	-2.72	2.00	2.05
12	C	505	CLA	C1C-NC	-2.71	1.33	1.37
17	B	603	F6C	C1A-C2A	2.71	1.51	1.45
12	B	604	CLA	C4D-CHA	2.71	1.47	1.38
12	B	610	CLA	C4B-NB	-2.71	1.34	1.37
18	C	515	DGD	O2G-C2G	-2.70	1.40	1.46
14	A	406	PHO	CMC-C2C	-2.70	1.46	1.50
12	B	611	CLA	MG-NC	2.70	2.12	2.06
12	C	510	CLA	C4D-CHA	2.70	1.47	1.38
12	C	510	CLA	MG-ND	-2.70	2.00	2.05
17	B	606	F6C	C3D-C2D	2.70	1.46	1.39
12	C	506	CLA	C4C-C3C	2.69	1.49	1.45
12	A	407	CLA	C1C-NC	-2.69	1.33	1.37
12	B	601	CLA	C4B-NB	-2.69	1.34	1.37
12	C	513	CLA	C4B-NB	-2.69	1.34	1.37
12	B	608	CLA	MG-ND	-2.69	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	618	LMT	O3'-C3'	-2.68	1.36	1.43
12	B	613	CLA	C1C-NC	-2.68	1.33	1.37
12	C	513	CLA	MG-NC	2.68	2.12	2.06
13	A	404	CL7	CHD-C1D	2.68	1.45	1.39
12	B	607	CLA	MG-NC	2.68	2.12	2.06
12	B	602	CLA	C4B-NB	-2.68	1.34	1.37
12	B	602	CLA	C4D-CHA	2.68	1.47	1.38
12	C	511	CLA	C4D-CHA	2.68	1.47	1.38
12	A	405	CLA	C4D-CHA	2.68	1.47	1.38
12	B	613	CLA	C4B-NB	-2.67	1.34	1.37
12	C	502	CLA	C1B-C2B	2.67	1.49	1.43
12	D	404	CLA	C4D-CHA	2.67	1.47	1.38
12	A	403	CLA	MG-NC	2.67	2.12	2.06
12	C	503	CLA	C1B-NB	-2.67	1.34	1.37
12	C	501	CLA	MG-NC	2.67	2.12	2.06
12	C	506	CLA	C4B-NB	-2.66	1.34	1.37
12	A	403	CLA	C1B-C2B	2.66	1.49	1.43
12	C	510	CLA	C3D-C2D	2.66	1.46	1.39
12	C	509	CLA	C4B-NB	-2.65	1.34	1.37
12	C	505	CLA	C1B-C2B	2.65	1.49	1.43
12	C	510	CLA	C1C-NC	-2.65	1.33	1.37
18	B	616	DGD	O2G-C2G	-2.65	1.40	1.46
12	B	604	CLA	C1B-NB	-2.64	1.34	1.37
17	B	606	F6C	CMB-C2B	2.64	1.51	1.45
12	C	506	CLA	MG-NC	2.64	2.12	2.06
16	A	410	LMT	O3'-C3'	-2.64	1.36	1.43
17	C	507	F6C	C1C-NC	-2.64	1.34	1.37
12	C	510	CLA	MG-NC	2.63	2.12	2.06
21	D	406	PL9	C53-C6	-2.63	1.45	1.50
12	C	512	CLA	C1B-C2B	2.63	1.49	1.43
12	C	508	CLA	C1D-ND	-2.63	1.34	1.37
17	B	606	F6C	C1A-C2A	2.62	1.51	1.45
12	B	604	CLA	C1B-C2B	2.62	1.49	1.43
12	C	501	CLA	C4D-CHA	2.62	1.47	1.38
12	B	604	CLA	C4B-NB	-2.62	1.34	1.37
12	B	608	CLA	C1C-NC	-2.61	1.33	1.37
12	B	607	CLA	C3D-C2D	2.61	1.46	1.39
12	B	605	CLA	C4D-CHA	2.61	1.47	1.38
12	C	502	CLA	MG-NC	2.60	2.12	2.06
12	B	613	CLA	C1B-C2B	2.60	1.49	1.43
12	C	510	CLA	C4B-NB	-2.59	1.34	1.37
12	C	509	CLA	C1C-NC	-2.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	509	CLA	C1B-NB	-2.59	1.34	1.37
12	C	511	CLA	C1B-C2B	2.59	1.49	1.43
17	B	612	F6C	C1C-NC	-2.58	1.34	1.37
12	B	609	CLA	C1C-NC	-2.58	1.33	1.37
17	B	603	F6C	C1D-C2D	2.58	1.49	1.44
12	C	508	CLA	C1B-NB	-2.58	1.34	1.37
12	B	601	CLA	C1B-C2B	2.57	1.49	1.43
12	B	601	CLA	C1C-NC	-2.57	1.33	1.37
12	A	407	CLA	C4D-CHA	2.57	1.47	1.38
12	A	407	CLA	MG-NC	2.56	2.12	2.06
16	C	516	LMT	O2'-C2'	-2.56	1.36	1.43
12	D	403	CLA	C4D-CHA	2.55	1.47	1.38
16	D	409	LMT	C3'-C2'	2.55	1.56	1.52
17	B	612	F6C	C2B-C1B	2.54	1.49	1.44
12	C	503	CLA	C1B-C2B	2.54	1.49	1.43
12	D	403	CLA	C3D-C2D	2.54	1.45	1.39
12	C	513	CLA	C1C-NC	-2.53	1.33	1.37
12	C	508	CLA	C1D-C2D	2.53	1.50	1.45
17	B	606	F6C	C2B-C1B	2.52	1.49	1.44
17	C	507	F6C	C2B-C1B	2.52	1.49	1.44
12	C	504	CLA	C4B-NB	-2.51	1.34	1.37
12	A	407	CLA	C1B-C2B	2.51	1.49	1.43
17	B	606	F6C	C4B-NB	-2.51	1.34	1.37
16	A	409	LMT	O2'-C2'	-2.51	1.36	1.43
12	C	512	CLA	C1C-NC	-2.50	1.34	1.37
17	C	507	F6C	C4A-C3A	2.50	1.50	1.45
12	B	607	CLA	C4B-NB	-2.49	1.34	1.37
13	A	404	CL7	C1B-C2B	2.49	1.49	1.43
17	C	507	F6C	CMB-C2B	2.48	1.50	1.45
12	C	508	CLA	C4B-NB	-2.48	1.34	1.37
12	B	608	CLA	C1B-C2B	2.48	1.48	1.43
16	B	618	LMT	O2'-C2'	-2.47	1.36	1.43
12	A	405	CLA	MG-ND	-2.46	2.00	2.05
12	A	403	CLA	C3D-C2D	2.46	1.45	1.39
12	B	604	CLA	C1D-C2D	2.46	1.50	1.45
12	B	602	CLA	C3D-C2D	2.45	1.45	1.39
17	B	612	F6C	C4A-C3A	2.45	1.50	1.45
19	B	617	LMG	C19-C18	-2.45	1.32	1.50
12	C	506	CLA	C1D-C2D	2.45	1.50	1.45
14	A	406	PHO	CMB-C2B	-2.44	1.46	1.51
12	D	404	CLA	C1B-C2B	2.44	1.48	1.43
12	B	604	CLA	C1C-NC	-2.43	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	602	CLA	C1B-C2B	2.43	1.48	1.43
17	B	603	F6C	C2B-C1B	2.43	1.49	1.44
17	B	612	F6C	CMB-C2B	2.42	1.50	1.45
12	C	513	CLA	C1B-C2B	2.42	1.48	1.43
12	B	614	CLA	MG-ND	-2.42	2.01	2.05
17	B	603	F6C	C1D-ND	-2.42	1.34	1.37
18	C	515	DGD	O5D-C6D	-2.42	1.39	1.43
12	C	504	CLA	C1B-C2B	2.41	1.48	1.43
23	F	101	HEM	FE-NC	2.41	2.03	1.95
12	C	511	CLA	C4B-NB	-2.41	1.34	1.37
17	B	603	F6C	C4C-NC	-2.40	1.34	1.37
16	A	409	LMT	O2B-C2B	-2.40	1.37	1.43
17	B	603	F6C	C4A-C3A	2.40	1.50	1.45
16	A	409	LMT	O4'-C4B	-2.39	1.37	1.43
18	C	515	DGD	O1G-C1G	-2.38	1.39	1.45
16	A	410	LMT	O2'-C2'	-2.38	1.37	1.43
16	B	618	LMT	O2B-C2B	-2.38	1.37	1.43
13	A	404	CL7	C1D-C2D	2.37	1.48	1.43
17	B	606	F6C	MG-ND	-2.37	2.00	2.06
12	C	503	CLA	C4B-NB	-2.37	1.34	1.37
16	A	409	LMT	O3'-C3'	-2.36	1.37	1.43
16	C	516	LMT	O3'-C3'	-2.36	1.37	1.43
12	B	608	CLA	C4B-NB	-2.35	1.34	1.37
12	C	513	CLA	C1D-C2D	2.34	1.50	1.45
16	B	619	LMT	O3'-C3'	-2.34	1.37	1.43
12	B	604	CLA	MG-ND	-2.33	2.01	2.05
16	C	516	LMT	O3B-C3B	-2.33	1.37	1.43
16	D	409	LMT	O1'-C1'	-2.33	1.36	1.40
17	B	612	F6C	C1D-ND	-2.32	1.34	1.37
17	B	612	F6C	C4C-NC	-2.31	1.34	1.37
16	B	619	LMT	O3B-C3B	-2.31	1.37	1.43
17	C	507	F6C	C1A-C2A	2.31	1.50	1.45
12	B	609	CLA	C4B-NB	-2.30	1.34	1.37
12	C	508	CLA	MG-ND	-2.29	2.01	2.05
17	B	603	F6C	CMB-C2B	2.29	1.50	1.45
12	B	608	CLA	C1D-C2D	2.28	1.49	1.45
16	B	619	LMT	O2'-C2'	-2.28	1.37	1.43
17	C	507	F6C	C1C-C2C	2.28	1.48	1.43
12	D	404	CLA	C3B-C4B	2.27	1.49	1.42
12	C	508	CLA	C1C-NC	-2.27	1.34	1.37
16	D	409	LMT	O2'-C2'	-2.27	1.37	1.43
14	D	402	PHO	CMB-C2B	-2.27	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	405	CLA	C1B-C2B	2.27	1.48	1.43
14	D	402	PHO	CAC-C3C	-2.27	1.47	1.51
12	D	404	CLA	C4B-NB	-2.26	1.34	1.37
17	B	603	F6C	MG-ND	-2.26	2.00	2.06
17	B	603	F6C	C4B-NB	-2.25	1.34	1.37
12	B	614	CLA	C1D-C2D	2.25	1.49	1.45
12	B	604	CLA	C4C-C3C	2.24	1.48	1.45
16	A	409	LMT	O3B-C3B	-2.24	1.37	1.43
16	A	410	LMT	O2B-C2B	-2.24	1.37	1.43
12	A	405	CLA	C4C-C3C	2.24	1.48	1.45
16	B	619	LMT	O2B-C2B	-2.23	1.37	1.43
17	B	612	F6C	C1C-C2C	2.22	1.48	1.43
12	C	510	CLA	C1D-C2D	2.21	1.49	1.45
16	A	410	LMT	O3B-C3B	-2.20	1.37	1.43
17	B	612	F6C	C1A-C2A	2.20	1.50	1.45
16	A	409	LMT	O1'-C1'	-2.19	1.36	1.40
12	B	607	CLA	C4C-C3C	2.19	1.48	1.45
12	C	508	CLA	C4C-C3C	2.19	1.48	1.45
17	C	507	F6C	C4C-NC	-2.19	1.35	1.37
12	C	501	CLA	C1D-C2D	2.19	1.49	1.45
17	C	507	F6C	C1D-ND	-2.18	1.34	1.37
12	B	614	CLA	C3B-C4B	2.18	1.49	1.42
16	B	619	LMT	O4'-C4B	-2.17	1.37	1.43
17	B	612	F6C	C4C-C3C	2.16	1.48	1.44
12	C	511	CLA	C1D-C2D	2.15	1.49	1.45
17	B	606	F6C	CHB-C4A	-2.15	1.34	1.38
12	C	509	CLA	C4C-C3C	2.14	1.48	1.45
17	C	507	F6C	C4C-C3C	2.14	1.48	1.44
12	B	610	CLA	MG-NC	2.14	2.11	2.06
17	B	603	F6C	C4D-CHA	2.14	1.48	1.42
13	A	404	CL7	C3D-C4D	-2.13	1.34	1.40
17	C	507	F6C	MG-ND	-2.13	2.01	2.06
16	B	619	LMT	O5B-C5B	-2.13	1.39	1.44
17	B	603	F6C	C1C-C2C	2.13	1.48	1.43
16	C	516	LMT	O1'-C1'	-2.12	1.36	1.40
17	B	606	F6C	C1D-C2D	2.12	1.48	1.44
12	C	502	CLA	C4C-C3C	2.12	1.48	1.45
23	F	101	HEM	CMB-C2B	2.11	1.55	1.50
12	D	404	CLA	C1D-C2D	2.11	1.49	1.45
12	C	509	CLA	C1D-C2D	2.11	1.49	1.45
12	C	513	CLA	C3B-C4B	2.11	1.48	1.42
17	B	603	F6C	C4C-C3C	2.10	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	612	F6C	MG-ND	-2.10	2.01	2.06
12	A	405	CLA	C1D-C2D	2.09	1.49	1.45
12	C	506	CLA	C1B-C2B	2.09	1.48	1.43
12	B	609	CLA	C1D-C2D	2.09	1.49	1.45
13	A	404	CL7	C3B-C4B	2.09	1.48	1.42
23	F	101	HEM	CMC-C2C	2.09	1.55	1.50
12	B	608	CLA	C1A-CHA	2.08	1.51	1.43
12	C	504	CLA	C1D-C2D	2.08	1.49	1.45
16	B	618	LMT	O3B-C3B	-2.08	1.37	1.43
17	C	507	F6C	C4B-NB	-2.08	1.34	1.37
17	B	612	F6C	C4B-NB	-2.06	1.34	1.37
12	B	614	CLA	C1A-CHA	2.06	1.51	1.43
23	F	101	HEM	CMA-C3A	2.06	1.55	1.50
12	C	503	CLA	C3B-C4B	2.06	1.48	1.42
12	B	601	CLA	C1D-C2D	2.06	1.49	1.45
12	B	608	CLA	C3B-C4B	2.06	1.48	1.42
12	B	605	CLA	C1B-C2B	2.05	1.47	1.43
12	B	608	CLA	C1C-C2C	2.05	1.48	1.44
18	C	515	DGD	O3G-C3G	-2.05	1.40	1.43
23	F	101	HEM	CMD-C2D	2.05	1.55	1.50
12	B	614	CLA	C4C-C3C	2.05	1.48	1.45
16	A	410	LMT	O4'-C4B	-2.04	1.37	1.43
12	D	404	CLA	C4C-C3C	2.04	1.48	1.45
16	C	516	LMT	O2B-C2B	-2.03	1.37	1.43
16	B	619	LMT	O5'-C5'	-2.03	1.39	1.44
17	B	612	F6C	C4D-CHA	2.03	1.47	1.42
17	C	507	F6C	C4D-CHA	2.02	1.47	1.42
12	B	609	CLA	C1A-CHA	2.02	1.51	1.43
16	C	516	LMT	O4'-C4B	-2.02	1.38	1.43
18	B	616	DGD	O1G-C1G	-2.01	1.40	1.45
12	C	508	CLA	C3B-C4B	2.01	1.48	1.42
12	C	511	CLA	C3B-C4B	2.01	1.48	1.42
12	B	607	CLA	C3B-C4B	2.00	1.48	1.42

All (1042) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	517	BCR	C20-C21-C22	21.29	157.14	127.28
15	B	615	BCR	C20-C21-C22	20.90	156.59	127.28
15	B	615	BCR	C15-C16-C17	20.83	166.15	123.52
15	A	408	BCR	C15-C16-C17	20.68	165.83	123.52
15	A	408	BCR	C20-C21-C22	20.67	156.27	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	517	BCR	C15-C16-C17	20.65	165.77	123.52
15	C	514	BCR	C20-C21-C22	20.58	156.14	127.28
15	C	514	BCR	C15-C16-C17	20.36	165.18	123.52
15	C	514	BCR	C16-C17-C18	20.36	155.83	127.28
15	D	405	BCR	C15-C16-C17	19.96	164.37	123.52
15	D	405	BCR	C16-C17-C18	19.93	155.23	127.28
15	B	615	BCR	C16-C17-C18	19.58	154.74	127.28
15	A	408	BCR	C16-C17-C18	19.42	154.51	127.28
15	D	405	BCR	C10-C11-C12	19.19	178.79	123.20
15	C	517	BCR	C10-C11-C12	18.78	177.61	123.20
15	B	615	BCR	C10-C11-C12	18.64	177.21	123.20
15	A	408	BCR	C10-C11-C12	18.43	176.59	123.20
15	C	517	BCR	C16-C17-C18	18.18	152.78	127.28
15	C	514	BCR	C10-C11-C12	18.00	175.35	123.20
15	A	408	BCR	C21-C20-C19	14.48	165.14	123.20
15	C	517	BCR	C21-C20-C19	14.15	164.21	123.20
17	B	606	F6C	CAA-C2A-C3A	-14.13	101.40	127.87
15	B	615	BCR	C21-C20-C19	13.52	162.36	123.20
15	C	514	BCR	C11-C10-C9	13.50	146.21	127.28
15	C	514	BCR	C21-C20-C19	13.14	161.29	123.20
15	C	517	BCR	C16-C15-C14	12.73	149.56	123.52
15	A	408	BCR	C11-C10-C9	12.70	145.09	127.28
15	D	405	BCR	C11-C10-C9	12.48	144.78	127.28
15	D	405	BCR	C16-C15-C14	12.23	148.54	123.52
15	C	514	BCR	C11-C12-C13	12.15	159.67	126.36
15	C	514	BCR	C16-C15-C14	11.95	147.97	123.52
15	C	517	BCR	C11-C10-C9	11.89	143.96	127.28
15	B	615	BCR	C11-C10-C9	11.71	143.70	127.28
15	A	408	BCR	C11-C12-C13	11.70	158.44	126.36
17	B	606	F6C	C3B-C2B-C1B	-11.69	100.43	106.46
15	A	408	BCR	C16-C15-C14	11.56	147.18	123.52
15	B	615	BCR	C16-C15-C14	11.47	146.99	123.52
15	D	405	BCR	C11-C12-C13	10.97	156.44	126.36
15	B	615	BCR	C11-C12-C13	10.66	155.59	126.36
15	C	517	BCR	C11-C12-C13	10.41	154.91	126.36
17	C	507	F6C	C3B-C2B-C1B	-10.41	101.09	106.46
17	B	612	F6C	C3B-C2B-C1B	-10.06	101.27	106.46
17	B	603	F6C	C3B-C2B-C1B	-9.96	101.32	106.46
17	B	603	F6C	CAA-C2A-C3A	-9.79	109.54	127.87
17	B	612	F6C	CAA-C2A-C3A	-9.36	110.34	127.87
17	B	612	F6C	C1D-ND-C4D	-9.20	102.48	106.68
17	C	507	F6C	CAA-C2A-C3A	-9.19	110.66	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	507	F6C	C1D-ND-C4D	-9.18	102.49	106.68
17	B	606	F6C	C1D-ND-C4D	-9.08	102.54	106.68
12	C	510	CLA	CMD-C2D-C1D	9.03	140.64	124.73
12	A	403	CLA	CMD-C2D-C1D	8.94	140.47	124.73
17	C	507	F6C	CMD-C2D-C1D	8.92	138.97	125.03
17	B	612	F6C	CMD-C2D-C1D	8.83	138.84	125.03
17	B	606	F6C	CMD-C2D-C1D	8.63	138.52	125.03
17	B	603	F6C	C1D-ND-C4D	-8.52	102.79	106.68
17	B	603	F6C	CMD-C2D-C1D	8.50	138.32	125.03
12	D	403	CLA	CMD-C2D-C1D	8.37	139.47	124.73
12	B	608	CLA	CMD-C2D-C1D	8.31	139.36	124.73
12	B	607	CLA	CMD-C2D-C1D	8.23	139.22	124.73
12	C	508	CLA	CMD-C2D-C1D	8.11	139.00	124.73
12	C	513	CLA	CMD-C2D-C1D	8.05	138.91	124.73
12	C	503	CLA	CMD-C2D-C1D	8.04	138.88	124.73
12	B	614	CLA	CMD-C2D-C1D	8.00	138.81	124.73
12	B	602	CLA	CMD-C2D-C1D	7.95	138.72	124.73
12	D	404	CLA	CMD-C2D-C1D	7.93	138.69	124.73
12	B	604	CLA	CMD-C2D-C1D	7.90	138.63	124.73
12	C	504	CLA	CMD-C2D-C1D	7.89	138.62	124.73
12	B	605	CLA	CMD-C2D-C1D	7.84	138.54	124.73
12	C	501	CLA	CMD-C2D-C1D	7.83	138.51	124.73
15	C	514	BCR	C20-C19-C18	7.76	147.63	126.36
12	C	509	CLA	CMD-C2D-C1D	7.64	138.19	124.73
13	A	404	CL7	CMD-C2D-C1D	7.62	137.02	125.42
12	A	405	CLA	CMD-C2D-C1D	7.62	138.14	124.73
15	B	615	BCR	C20-C19-C18	7.61	147.23	126.36
12	B	611	CLA	CMD-C2D-C1D	7.58	138.07	124.73
12	B	613	CLA	CMD-C2D-C1D	7.57	138.06	124.73
12	C	511	CLA	CMD-C2D-C1D	7.54	138.00	124.73
12	B	609	CLA	CMD-C2D-C1D	7.50	137.94	124.73
12	C	506	CLA	CMD-C2D-C1D	7.45	137.85	124.73
12	B	610	CLA	CMD-C2D-C1D	7.39	137.75	124.73
12	C	512	CLA	CMD-C2D-C1D	7.39	137.74	124.73
12	B	601	CLA	CMD-C2D-C1D	7.38	137.72	124.73
14	D	402	PHO	C4D-CHA-CBD	-7.37	104.92	108.45
12	D	403	CLA	C4A-NA-C1A	7.22	109.97	106.68
12	C	502	CLA	CMD-C2D-C1D	7.22	137.43	124.73
12	A	407	CLA	CMD-C2D-C1D	7.04	137.13	124.73
17	B	612	F6C	CAA-C2A-C1A	-6.85	108.86	128.01
14	A	406	PHO	C4D-CHA-CBD	-6.69	105.25	108.45
17	C	507	F6C	CAA-C2A-C1A	-6.62	109.52	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	403	CLA	C2D-C1D-ND	6.60	116.66	110.13
15	C	517	BCR	C24-C23-C22	-6.59	116.49	126.23
12	C	509	CLA	O2D-CGD-CBD	6.56	122.70	111.23
12	B	602	CLA	O2D-CGD-CBD	6.55	122.68	111.23
12	C	506	CLA	C2C-C1C-NC	6.53	116.84	109.98
12	B	610	CLA	C4A-NA-C1A	6.44	109.61	106.68
12	C	502	CLA	O2D-CGD-CBD	6.42	122.46	111.23
12	C	511	CLA	C4A-NA-C1A	6.42	109.61	106.68
12	B	614	CLA	C2C-C1C-NC	6.39	116.70	109.98
13	A	404	CL7	C2C-C1C-NC	6.36	116.42	110.13
12	B	609	CLA	O2D-CGD-CBD	6.35	122.33	111.23
12	C	502	CLA	C2C-C1C-NC	6.33	116.63	109.98
15	A	408	BCR	C20-C19-C18	6.29	143.62	126.36
12	C	505	CLA	CMD-C2D-C1D	6.26	135.75	124.73
12	A	405	CLA	C2C-C1C-NC	6.25	116.55	109.98
15	C	517	BCR	C20-C19-C18	6.24	143.46	126.36
12	B	609	CLA	C2C-C1C-NC	6.21	116.51	109.98
12	B	611	CLA	C4A-NA-C1A	6.20	109.51	106.68
12	B	602	CLA	C2C-C1C-NC	6.19	116.49	109.98
12	C	503	CLA	C2C-C1C-NC	6.17	116.46	109.98
12	D	403	CLA	C3D-C2D-C1D	-6.16	97.42	105.83
12	C	510	CLA	C1C-C2C-C3C	-6.14	100.52	106.98
12	C	512	CLA	C2C-C1C-NC	6.13	116.42	109.98
12	B	605	CLA	O2D-CGD-CBD	6.13	121.95	111.23
12	D	403	CLA	C1D-ND-C4D	-6.09	102.04	106.31
12	B	601	CLA	C2C-C1C-NC	6.05	116.33	109.98
12	D	404	CLA	C2C-C1C-NC	6.04	116.33	109.98
12	C	502	CLA	C4A-NA-C1A	6.04	109.43	106.68
12	C	512	CLA	C1C-C2C-C3C	-6.03	100.64	106.98
12	A	407	CLA	O2D-CGD-CBD	5.98	121.68	111.23
12	C	505	CLA	C2C-C1C-NC	5.97	116.25	109.98
12	B	611	CLA	O2D-CGD-CBD	5.91	121.56	111.23
12	C	510	CLA	C2C-C1C-NC	5.90	116.18	109.98
12	B	605	CLA	C2C-C1C-NC	5.88	116.16	109.98
12	A	405	CLA	C1C-C2C-C3C	-5.87	100.81	106.98
12	B	601	CLA	O2A-CGA-O1A	-5.85	108.98	123.63
12	C	501	CLA	C2C-C1C-NC	5.85	116.13	109.98
12	B	613	CLA	C2C-C1C-NC	5.84	116.12	109.98
12	B	602	CLA	C1C-C2C-C3C	-5.83	100.85	106.98
12	B	610	CLA	C3D-C2D-C1D	-5.83	97.88	105.83
12	C	505	CLA	C4A-NA-C1A	5.82	109.33	106.68
12	C	510	CLA	C4A-NA-C1A	5.81	109.33	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	603	F6C	O2D-CGD-CBD	5.81	121.38	111.23
12	B	614	CLA	C4A-NA-C1A	5.77	109.31	106.68
12	C	503	CLA	C1C-C2C-C3C	-5.77	100.91	106.98
12	C	505	CLA	O2D-CGD-CBD	5.76	121.29	111.23
12	B	609	CLA	C4A-NA-C1A	5.74	109.30	106.68
12	C	509	CLA	C2C-C1C-NC	5.74	116.01	109.98
17	B	603	F6C	C1A-C2A-C3A	-5.72	100.94	106.97
12	B	609	CLA	C1C-C2C-C3C	-5.71	100.97	106.98
12	C	511	CLA	C2C-C1C-NC	5.70	115.97	109.98
17	B	603	F6C	C2C-C1C-NC	5.69	116.23	110.33
12	C	504	CLA	C2C-C1C-NC	5.68	115.95	109.98
12	A	407	CLA	C2C-C1C-NC	5.68	115.95	109.98
12	B	613	CLA	C4A-NA-C1A	5.67	109.27	106.68
12	C	508	CLA	C2C-C1C-NC	5.67	115.94	109.98
12	A	405	CLA	C3B-C2B-C1B	-5.66	100.49	107.17
12	C	509	CLA	C3B-C2B-C1B	-5.66	100.49	107.17
12	B	611	CLA	C3B-C2B-C1B	-5.65	100.51	107.17
12	A	407	CLA	C1C-C2C-C3C	-5.65	101.04	106.98
12	B	601	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
12	B	611	CLA	C2C-C1C-NC	5.64	115.91	109.98
12	D	403	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
12	C	508	CLA	C1D-ND-C4D	-5.63	102.36	106.31
12	B	604	CLA	C2C-C1C-NC	5.63	115.90	109.98
13	A	404	CL7	C2D-C1D-ND	5.63	116.16	110.33
12	C	501	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
12	A	403	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
12	C	502	CLA	C3D-C2D-C1D	-5.60	98.18	105.83
12	B	604	CLA	O2D-CGD-CBD	5.60	121.01	111.23
12	A	403	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
12	B	607	CLA	C2C-C1C-NC	5.59	115.85	109.98
17	B	606	F6C	C2C-C1C-NC	5.59	116.12	110.33
12	C	509	CLA	O2A-CGA-O1A	-5.58	109.67	123.63
12	D	404	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
12	B	611	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
12	A	407	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
12	C	504	CLA	O2D-CGD-CBD	5.57	120.96	111.23
17	B	612	F6C	C2C-C1C-NC	5.56	116.09	110.33
12	B	610	CLA	C2D-C1D-ND	5.56	115.63	110.13
17	B	606	F6C	O2D-CGD-CBD	5.54	120.91	111.23
17	B	606	F6C	CAA-C2A-C1A	-5.53	112.55	128.01
12	D	404	CLA	O2D-CGD-CBD	5.53	120.89	111.23
12	C	501	CLA	O2D-CGD-CBD	5.51	120.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	613	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
12	C	501	CLA	C4A-NA-C1A	5.50	109.19	106.68
17	C	507	F6C	C1A-C2A-C3A	-5.50	101.18	106.97
12	A	405	CLA	C4A-NA-C1A	5.48	109.18	106.68
17	B	612	F6C	C1A-C2A-C3A	-5.48	101.20	106.97
12	C	512	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
12	D	403	CLA	C2C-C1C-NC	5.46	115.72	109.98
17	C	507	F6C	C2C-C1C-NC	5.45	115.98	110.33
12	B	608	CLA	C3D-C2D-C1D	-5.44	98.40	105.83
15	A	408	BCR	C38-C26-C25	-5.43	118.56	124.48
12	A	403	CLA	C2C-C1C-NC	5.43	115.69	109.98
12	B	601	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
12	C	510	CLA	O2D-CGD-CBD	5.43	120.72	111.23
17	B	606	F6C	C2D-C1D-ND	5.43	115.68	109.98
12	C	512	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
12	B	607	CLA	O2D-CGD-CBD	5.41	120.69	111.23
12	C	503	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
12	B	613	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
12	C	501	CLA	C2D-C1D-ND	5.39	115.46	110.13
12	C	511	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
12	D	404	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
12	B	613	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
12	C	513	CLA	O2D-CGD-CBD	5.36	120.61	111.23
12	B	608	CLA	O2D-CGD-CBD	5.36	120.60	111.23
12	B	613	CLA	C2D-C1D-ND	5.35	115.42	110.13
12	B	614	CLA	O2D-CGD-CBD	5.35	120.59	111.23
12	C	512	CLA	O2D-CGD-CBD	5.35	120.58	111.23
12	A	403	CLA	C4A-NA-C1A	5.34	109.12	106.68
12	B	604	CLA	C1D-ND-C4D	-5.33	102.57	106.31
12	B	608	CLA	C4A-NA-C1A	5.33	109.11	106.68
12	B	614	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
12	B	608	CLA	C2C-C1C-NC	5.32	115.57	109.98
12	B	610	CLA	O2D-CGD-CBD	5.32	120.53	111.23
12	C	501	CLA	C3D-C2D-C1D	-5.32	98.58	105.83
12	B	614	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
17	B	606	F6C	O2A-CGA-O1A	-5.31	110.34	123.63
12	C	501	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
12	B	601	CLA	O2D-CGD-CBD	5.31	120.51	111.23
12	C	508	CLA	O2D-CGD-CBD	5.31	120.51	111.23
12	C	504	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
12	C	505	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	C	502	CLA	C2D-C1D-ND	5.29	115.37	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	609	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
12	C	504	CLA	C4A-NA-C1A	5.28	109.09	106.68
12	B	609	CLA	C2D-C1D-ND	5.27	115.34	110.13
17	B	603	F6C	O2A-CGA-O1A	-5.26	110.46	123.63
12	A	403	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
12	B	605	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
12	C	513	CLA	C2C-C1C-NC	5.26	115.50	109.98
12	C	508	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
12	C	505	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
12	B	608	CLA	C2D-C1D-ND	5.26	115.33	110.13
12	D	403	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
12	D	404	CLA	C2D-C1D-ND	5.25	115.32	110.13
12	B	614	CLA	C2D-C1D-ND	5.25	115.32	110.13
12	B	608	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
12	B	602	CLA	O2A-CGA-O1A	-5.24	110.52	123.63
12	C	504	CLA	O2A-CGA-O1A	-5.23	110.54	123.63
12	B	604	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
17	B	612	F6C	O2D-CGD-CBD	5.22	120.36	111.23
12	C	512	CLA	C2D-C1D-ND	5.22	115.30	110.13
12	B	610	CLA	O2A-CGA-O1A	-5.22	110.57	123.63
12	B	609	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
12	D	404	CLA	C4A-NA-C1A	5.21	109.06	106.68
12	C	513	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
12	B	608	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
12	C	504	CLA	C1C-C2C-C3C	-5.20	101.52	106.98
12	B	601	CLA	C4A-NA-C1A	5.19	109.05	106.68
12	A	407	CLA	C2D-C1D-ND	5.19	115.27	110.13
12	B	601	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
12	B	605	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
12	C	503	CLA	O2D-CGD-CBD	5.18	120.28	111.23
12	C	506	CLA	O2A-CGA-O1A	-5.17	110.69	123.63
12	B	604	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
12	B	607	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
12	B	611	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
12	C	509	CLA	C4A-NA-C1A	5.16	109.03	106.68
12	C	501	CLA	C1D-ND-C4D	-5.15	102.70	106.31
12	C	509	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
12	C	508	CLA	C2D-C1D-ND	5.12	115.19	110.13
12	C	508	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
12	C	513	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
12	C	508	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
15	A	408	BCR	C24-C23-C22	-5.11	118.68	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	407	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
12	C	511	CLA	C3B-C2B-C1B	-5.10	101.15	107.17
12	B	605	CLA	C4A-NA-C1A	5.10	109.01	106.68
12	C	504	CLA	C2D-C1D-ND	5.09	115.16	110.13
12	B	611	CLA	C2D-C1D-ND	5.09	115.16	110.13
12	C	512	CLA	C4A-NA-C1A	5.09	109.00	106.68
12	C	512	CLA	O2A-CGA-O1A	-5.08	110.27	123.33
17	B	603	F6C	C2D-C1D-ND	5.07	115.31	109.98
12	C	505	CLA	C2D-C1D-ND	5.07	115.14	110.13
12	C	513	CLA	C1C-C2C-C3C	-5.06	101.65	106.98
12	B	613	CLA	O2D-CGD-CBD	5.05	120.07	111.23
17	B	612	F6C	O2A-CGA-O1A	-5.04	111.02	123.63
12	B	604	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
12	C	506	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
12	A	405	CLA	O2A-CGA-O1A	-5.03	111.05	123.63
12	C	506	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
12	C	510	CLA	O2A-CGA-O1A	-5.02	111.07	123.63
17	B	606	F6C	C3D-C2D-C1D	-5.02	98.56	105.83
12	B	605	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
12	C	508	CLA	O2A-CGA-O1A	-5.01	111.09	123.63
12	A	405	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
17	C	507	F6C	O2A-CGA-O1A	-5.00	111.13	123.63
17	C	507	F6C	O2D-CGD-CBD	4.99	119.94	111.23
12	B	604	CLA	C2D-C1D-ND	4.98	115.05	110.13
12	C	511	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
12	C	503	CLA	C2D-C1D-ND	4.97	115.05	110.13
12	C	506	CLA	O2D-CGD-CBD	4.97	119.92	111.23
17	B	603	F6C	CAA-C2A-C1A	-4.97	114.13	128.01
12	A	405	CLA	C2D-C1D-ND	4.97	115.04	110.13
12	C	503	CLA	C4A-NA-C1A	4.96	108.94	106.68
13	A	404	CL7	C3B-C2B-C1B	-4.96	101.33	107.17
12	C	501	CLA	O2A-CGA-O1A	-4.96	111.23	123.63
17	B	612	F6C	C2D-C1D-ND	4.96	115.19	109.98
12	C	511	CLA	O2D-CGD-CBD	4.95	119.88	111.23
12	B	604	CLA	O2A-CGA-O1A	-4.95	111.25	123.63
12	C	504	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
12	C	509	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
12	B	602	CLA	C4A-NA-C1A	4.94	108.93	106.68
12	B	601	CLA	C2D-C1D-ND	4.93	115.01	110.13
12	C	505	CLA	O2A-CGA-O1A	-4.93	111.29	123.63
17	B	603	F6C	C3D-C2D-C1D	-4.93	98.69	105.83
12	C	503	CLA	C3B-C2B-C1B	-4.93	101.36	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	506	CLA	C4A-NA-C1A	4.93	108.93	106.68
12	B	610	CLA	C2C-C1C-NC	4.91	115.14	109.98
13	A	404	CL7	C1D-ND-C4D	-4.91	102.87	106.31
15	C	517	BCR	C19-C18-C17	4.90	126.72	119.01
12	C	513	CLA	C2D-C1D-ND	4.90	114.97	110.13
12	B	605	CLA	O2A-CGA-O1A	-4.88	111.43	123.63
12	B	607	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
15	B	615	BCR	C7-C8-C9	-4.87	119.03	126.23
12	B	608	CLA	O2A-CGA-O1A	-4.86	110.83	123.33
17	C	507	F6C	C2D-C1D-ND	4.86	115.08	109.98
12	C	510	CLA	C1D-ND-C4D	-4.86	102.91	106.31
17	B	606	F6C	C4A-NA-C1A	4.85	109.72	106.31
12	B	602	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
17	B	612	F6C	C1C-C2C-C3C	-4.84	101.27	106.82
12	C	510	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
12	B	613	CLA	C1D-ND-C4D	-4.84	102.92	106.31
12	A	407	CLA	C1D-ND-C4D	-4.83	102.92	106.31
12	C	511	CLA	C2D-C1D-ND	4.83	114.90	110.13
12	B	601	CLA	O2A-CGA-CBA	4.82	126.54	111.83
13	A	404	CL7	O2A-CGA-O1A	-4.81	111.59	123.63
12	A	403	CLA	O2A-CGA-O1A	-4.80	111.61	123.63
17	B	612	F6C	C3D-C2D-C1D	-4.80	98.88	105.83
12	C	503	CLA	O2A-CGA-O1A	-4.79	111.64	123.63
12	B	611	CLA	O2A-CGA-O1A	-4.78	111.67	123.63
12	D	404	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
12	A	407	CLA	C4A-NA-C1A	4.77	108.85	106.68
17	C	507	F6C	C3D-C2D-C1D	-4.76	98.93	105.83
12	B	602	CLA	O2A-CGA-CBA	4.76	126.36	111.83
17	B	606	F6C	C1C-C2C-C3C	-4.73	101.40	106.82
12	C	510	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
15	B	615	BCR	C24-C23-C22	-4.72	119.25	126.23
12	D	404	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
17	C	507	F6C	C1C-C2C-C3C	-4.70	101.43	106.82
17	B	603	F6C	C1C-C2C-C3C	-4.70	101.43	106.82
12	C	505	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
13	A	404	CL7	O2D-CGD-CBD	4.69	119.42	111.23
12	A	403	CLA	O2D-CGD-CBD	4.68	119.42	111.23
12	B	613	CLA	O2A-CGA-O1A	-4.68	111.93	123.63
12	A	405	CLA	O2D-CGD-CBD	4.67	119.40	111.23
12	B	614	CLA	C1D-ND-C4D	-4.66	103.04	106.31
12	C	502	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
12	A	405	CLA	C1D-ND-C4D	-4.64	103.06	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	403	CLA	C2D-C1D-ND	4.63	114.71	110.13
12	A	405	CLA	O2A-CGA-CBA	4.62	125.91	111.83
12	C	502	CLA	O2A-CGA-O1A	-4.61	112.10	123.63
12	D	404	CLA	C1D-ND-C4D	-4.60	103.08	106.31
12	B	605	CLA	C2D-C1D-ND	4.60	114.68	110.13
12	C	509	CLA	C2D-C1D-ND	4.59	114.66	110.13
12	B	609	CLA	C1D-ND-C4D	-4.57	103.11	106.31
12	C	513	CLA	C4A-NA-C1A	4.57	108.76	106.68
12	C	513	CLA	O2A-CGA-O1A	-4.55	111.63	123.33
12	C	511	CLA	O2A-CGA-O1A	-4.55	111.64	123.33
12	C	513	CLA	C1D-ND-C4D	-4.55	103.12	106.31
12	C	511	CLA	C1D-ND-C4D	-4.54	103.13	106.31
12	C	510	CLA	C2D-C1D-ND	4.53	114.61	110.13
12	B	608	CLA	C1D-ND-C4D	-4.52	103.14	106.31
12	B	614	CLA	O2A-CGA-O1A	-4.50	112.37	123.63
12	C	508	CLA	C4A-NA-C1A	4.50	108.73	106.68
12	C	512	CLA	C1D-ND-C4D	-4.49	103.16	106.31
12	B	609	CLA	O2A-CGA-O1A	-4.48	111.82	123.33
12	C	502	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
12	D	403	CLA	O2A-CGA-O1A	-4.47	112.44	123.63
12	C	504	CLA	C1D-ND-C4D	-4.43	103.20	106.31
15	A	408	BCR	C7-C8-C9	-4.40	119.72	126.23
12	C	506	CLA	O2A-CGA-CBA	4.38	125.19	111.83
12	B	607	CLA	O2A-CGA-O1A	-4.36	112.72	123.63
12	B	611	CLA	C1D-ND-C4D	-4.36	103.25	106.31
15	A	408	BCR	C33-C5-C6	-4.35	119.74	124.48
13	A	404	CL7	C1C-C2C-C3C	-4.35	100.52	106.97
17	B	606	F6C	O2A-CGA-CBA	4.33	125.05	111.83
12	B	614	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
12	D	403	CLA	CHD-C1D-ND	-4.33	118.71	124.80
12	B	607	CLA	C4A-NA-C1A	4.31	108.65	106.68
12	B	607	CLA	C2D-C1D-ND	4.31	114.39	110.13
12	B	610	CLA	O2A-CGA-CBA	4.30	124.95	111.83
17	B	606	F6C	C4A-C3A-C2A	-4.30	100.60	106.97
12	C	506	CLA	C2D-C1D-ND	4.26	114.34	110.13
12	B	611	CLA	C2B-C1B-NB	4.24	114.73	110.33
12	B	605	CLA	C2B-C1B-NB	4.23	114.72	110.33
17	B	606	F6C	O2A-C1-C2	4.23	124.39	108.11
12	A	405	CLA	C2B-C1B-NB	4.23	114.71	110.33
12	A	407	CLA	O2A-CGA-O1A	-4.22	113.07	123.63
18	C	515	DGD	O3G-C3G-C2G	-4.22	100.56	110.82
15	C	517	BCR	C33-C5-C6	-4.21	119.89	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	505	CLA	C1D-ND-C4D	-4.21	103.36	106.31
12	B	601	CLA	C1D-ND-C4D	-4.21	103.36	106.31
12	B	607	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
17	B	603	F6C	O2A-CGA-CBA	4.20	124.64	111.83
12	C	502	CLA	C1D-ND-C4D	-4.17	103.39	106.31
12	C	503	CLA	C1D-ND-C4D	-4.17	103.39	106.31
17	B	606	F6C	C1-C2-C3	-4.16	119.39	126.20
13	A	404	CL7	O2A-C1-C2	4.15	124.06	108.11
12	A	403	CLA	C2B-C1B-NB	4.14	114.61	110.33
12	C	511	CLA	C2B-C1B-NB	4.13	114.61	110.33
12	B	602	CLA	O2A-C1-C2	4.11	123.93	108.11
12	C	510	CLA	O2A-CGA-CBA	4.11	124.36	111.83
12	C	509	CLA	O2A-CGA-CBA	4.10	124.33	111.83
12	A	403	CLA	O2A-CGA-CBA	4.10	124.32	111.83
15	C	517	BCR	C7-C8-C9	-4.10	120.18	126.23
12	C	509	CLA	C2B-C1B-NB	4.09	114.57	110.33
17	B	612	F6C	O2A-CGA-CBA	4.08	124.26	111.83
17	C	507	F6C	O2A-CGA-CBA	4.07	124.26	111.83
16	D	409	LMT	C1'-O5'-C5'	4.07	117.64	113.13
22	D	407	LHG	O7-C7-C8	4.06	120.27	111.48
12	D	403	CLA	O2D-CGD-CBD	4.06	118.33	111.23
12	B	602	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
12	C	511	CLA	CMA-C3A-C4A	4.06	122.68	111.77
12	C	512	CLA	C2B-C1B-NB	4.05	114.53	110.33
12	C	509	CLA	C1D-ND-C4D	-4.05	103.47	106.31
15	C	517	BCR	C36-C18-C17	-4.04	116.28	122.82
17	B	606	F6C	C3A-C4A-NA	4.03	114.12	110.13
13	A	404	CL7	O2A-CGA-CBA	4.03	124.13	111.83
12	D	403	CLA	O2A-C1-C2	4.03	123.63	108.11
12	A	407	CLA	CHD-C1D-ND	-4.03	119.14	124.80
12	B	605	CLA	CHD-C1D-ND	-4.02	119.14	124.80
12	B	614	CLA	C1-C2-C3	-4.01	120.28	126.76
12	C	508	CLA	O2A-CGA-CBA	4.00	124.03	111.83
12	C	501	CLA	CHD-C1D-ND	-4.00	119.18	124.80
12	C	504	CLA	C1-C2-C3	-3.98	120.32	126.76
12	C	505	CLA	O2A-CGA-CBA	3.97	123.95	111.83
16	D	409	LMT	C3'-C4'-C5'	-3.97	104.48	111.19
12	A	403	CLA	CHD-C1D-ND	-3.97	119.22	124.80
12	C	511	CLA	CHD-C1D-ND	-3.96	119.23	124.80
12	B	608	CLA	C2B-C1B-NB	3.96	114.43	110.33
12	B	607	CLA	O2A-CGA-CBA	3.95	123.89	111.83
12	B	604	CLA	O2A-CGA-CBA	3.95	123.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	610	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
12	B	605	CLA	O2D-CGD-O1D	-3.94	116.18	123.85
14	D	402	PHO	CMB-C2B-C3B	3.94	132.55	124.68
19	D	408	LMG	O7-C10-C11	3.94	120.00	111.48
12	C	513	CLA	C2B-C1B-NB	3.92	114.39	110.33
12	A	403	CLA	C1D-ND-C4D	-3.92	103.56	106.31
12	C	513	CLA	CHD-C1D-ND	-3.92	119.29	124.80
12	A	403	CLA	O2A-C1-C2	3.91	123.15	108.11
17	B	606	F6C	C1A-C2A-C3A	-3.90	102.86	106.97
12	C	502	CLA	C1-C2-C3	-3.89	119.82	126.20
17	B	603	F6C	C1-C2-C3	-3.88	120.49	126.76
12	B	613	CLA	O2A-CGA-CBA	3.88	123.66	111.83
17	C	507	F6C	C4A-C3A-C2A	-3.87	101.23	106.97
12	A	407	CLA	C2B-C1B-NB	3.86	114.33	110.33
12	C	501	CLA	O2A-CGA-CBA	3.85	123.58	111.83
13	A	404	CL7	C1-O2A-CGA	3.84	125.96	116.65
19	B	617	LMG	O7-C10-C11	3.84	119.80	111.48
12	C	510	CLA	CHD-C1D-ND	-3.84	119.40	124.80
17	B	612	F6C	C4A-C3A-C2A	-3.83	101.29	106.97
18	B	616	DGD	O3G-C3G-C2G	-3.83	101.51	110.82
12	B	611	CLA	CHD-C1D-ND	-3.83	119.42	124.80
12	B	614	CLA	O2A-CGA-CBA	3.82	123.49	111.83
12	B	601	CLA	C2B-C1B-NB	3.82	114.29	110.33
17	B	603	F6C	C4A-NA-C1A	3.81	108.98	106.31
12	B	604	CLA	C1-C2-C3	-3.81	119.96	126.20
12	C	502	CLA	O2A-CGA-CBA	3.80	123.41	111.83
12	B	607	CLA	C1-C2-C3	-3.79	119.99	126.20
12	C	506	CLA	CHD-C1D-ND	-3.78	119.48	124.80
12	D	404	CLA	C2B-C1B-NB	3.78	114.25	110.33
12	C	504	CLA	O2A-CGA-CBA	3.77	123.32	111.83
12	C	506	CLA	C3B-C2B-C1B	-3.77	102.73	107.17
12	B	607	CLA	C2B-C1B-NB	3.76	114.23	110.33
12	C	502	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
12	A	405	CLA	CHD-C1D-ND	-3.76	119.52	124.80
12	A	405	CLA	O2A-C1-C2	3.75	122.52	108.11
12	B	611	CLA	O2A-CGA-CBA	3.74	123.23	111.83
12	C	504	CLA	C2B-C1B-NB	3.74	114.20	110.33
12	B	613	CLA	C2B-C1B-NB	3.73	114.20	110.33
15	C	514	BCR	C24-C23-C22	-3.72	120.73	126.23
12	D	404	CLA	CHD-C1D-ND	-3.70	119.59	124.80
12	B	610	CLA	C1D-ND-C4D	-3.70	103.72	106.31
12	C	504	CLA	CHD-C1D-ND	-3.68	119.62	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	407	CLA	CAA-C2A-C3A	-3.67	103.08	113.00
12	B	605	CLA	O2A-CGA-CBA	3.66	123.00	111.83
17	C	507	F6C	C3A-C4A-NA	3.66	113.75	110.13
13	A	404	CL7	C2B-C1B-NB	3.66	114.12	110.33
15	C	517	BCR	C38-C26-C25	-3.65	120.50	124.48
17	B	603	F6C	C4A-C3A-C2A	-3.65	101.56	106.97
12	B	604	CLA	C4A-NA-C1A	3.64	108.34	106.68
12	C	504	CLA	O2A-C1-C2	3.64	122.11	108.11
12	D	403	CLA	C2B-C1B-NB	3.63	114.09	110.33
12	B	614	CLA	CMB-C2B-C1B	3.63	130.94	125.42
12	C	503	CLA	O2A-CGA-CBA	3.62	122.89	111.83
12	C	503	CLA	CHD-C1D-ND	-3.62	119.70	124.80
12	D	404	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
17	B	603	F6C	C3A-C4A-NA	3.60	113.69	110.13
12	D	403	CLA	O2A-CGA-CBA	3.60	122.81	111.83
12	B	609	CLA	C2B-C1B-NB	3.58	114.04	110.33
17	B	612	F6C	C1-C2-C3	-3.58	120.33	126.20
12	B	614	CLA	O2A-C1-C2	3.57	121.86	108.11
21	D	406	PL9	C7-C8-C9	-3.57	120.69	126.83
12	B	608	CLA	CMC-C2C-C1C	3.56	130.60	125.03
12	B	608	CLA	CHD-C1D-ND	-3.56	119.79	124.80
17	B	612	F6C	C3A-C4A-NA	3.56	113.65	110.13
12	C	508	CLA	CHD-C1D-ND	-3.55	119.80	124.80
12	B	604	CLA	CHD-C1D-ND	-3.55	119.81	124.80
12	B	607	CLA	C1D-ND-C4D	-3.54	103.83	106.31
17	C	507	F6C	C1-C2-C3	-3.53	120.41	126.20
16	D	409	LMT	O5'-C1'-C2'	3.52	117.61	110.37
12	C	505	CLA	C2B-C1B-NB	3.52	113.97	110.33
12	B	607	CLA	CHD-C1D-ND	-3.51	119.86	124.80
12	B	610	CLA	O2A-C1-C2	3.50	121.58	108.11
12	C	508	CLA	C1-C2-C3	-3.50	120.46	126.20
12	C	512	CLA	CHD-C1D-ND	-3.50	119.88	124.80
12	B	609	CLA	CHD-C1D-ND	-3.50	119.88	124.80
12	B	602	CLA	C2D-C1D-ND	3.49	113.58	110.13
12	C	505	CLA	C1-C2-C3	-3.49	120.49	126.20
18	B	616	DGD	C1D-C2D-C3D	-3.48	102.69	110.01
12	B	605	CLA	C1D-ND-C4D	-3.48	103.87	106.31
12	B	610	CLA	CHD-C1D-ND	-3.48	119.91	124.80
12	A	403	CLA	CAA-C2A-C3A	-3.47	103.62	113.00
12	C	506	CLA	C2B-C1B-NB	3.47	113.92	110.33
12	C	503	CLA	C2B-C1B-NB	3.46	113.92	110.33
12	C	510	CLA	C2B-C1B-NB	3.46	113.92	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	514	BCR	C38-C26-C25	-3.46	120.71	124.48
18	C	515	DGD	O6D-C1D-O3G	-3.45	101.90	110.04
12	D	403	CLA	CMC-C2C-C1C	3.44	130.41	125.03
14	A	406	PHO	C2B-C1B-NB	-3.44	106.94	109.43
12	C	506	CLA	O2A-C1-C2	3.44	121.33	108.11
12	A	407	CLA	O2A-CGA-CBA	3.43	122.30	111.83
12	C	512	CLA	O2A-CGA-CBA	3.43	124.83	114.00
12	C	508	CLA	O2A-C1-C2	3.42	121.29	108.11
12	B	601	CLA	CHD-C1D-ND	-3.42	119.99	124.80
12	C	510	CLA	C1-C2-C3	-3.42	120.59	126.20
12	C	504	CLA	CMA-C3A-C4A	3.41	120.95	111.77
12	C	509	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
12	C	509	CLA	CHD-C1D-ND	-3.41	120.00	124.80
17	B	612	F6C	C4A-NA-C1A	3.40	108.69	106.31
12	B	602	CLA	C4D-C3D-CAD	3.39	111.79	108.11
12	B	610	CLA	C3B-C2B-C1B	-3.38	103.18	107.17
12	B	613	CLA	CAA-C2A-C3A	-3.37	103.91	113.00
17	C	507	F6C	O2A-C1-C2	3.36	121.05	108.11
12	C	511	CLA	O2A-CGA-CBA	3.36	124.62	114.00
13	A	404	CL7	C3C-C4C-NC	3.34	113.68	110.20
12	C	505	CLA	O2A-C1-C2	3.33	120.92	108.11
12	C	510	CLA	C4D-C3D-CAD	3.31	111.70	108.11
12	C	510	CLA	O2A-C1-C2	3.31	120.84	108.11
15	C	514	BCR	C3-C4-C5	-3.30	108.18	114.06
17	C	507	F6C	C4A-NA-C1A	3.29	108.62	106.31
12	C	510	CLA	CMD-C2D-C3D	-3.29	120.14	127.69
12	C	502	CLA	O2A-C1-C2	3.29	120.76	108.11
12	B	601	CLA	C4-C3-C5	3.29	120.93	115.23
12	D	404	CLA	O2A-CGA-CBA	3.29	124.38	114.00
12	C	501	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
12	B	602	CLA	C2B-C1B-NB	3.28	113.73	110.33
12	B	602	CLA	C1D-ND-C4D	-3.28	104.01	106.31
12	C	501	CLA	C1-C2-C3	-3.27	120.83	126.20
21	D	406	PL9	O1-C4-C3	-3.27	117.28	120.73
12	B	604	CLA	C3D-C4D-ND	3.25	115.27	109.99
17	B	612	F6C	O2A-C1-C2	3.24	120.59	108.11
12	C	508	CLA	C3D-C4D-ND	3.24	115.25	109.99
12	C	503	CLA	C1-C2-C3	-3.24	120.89	126.20
12	B	613	CLA	CHD-C1D-ND	-3.23	120.25	124.80
15	A	408	BCR	C35-C13-C12	3.23	123.02	118.09
13	A	404	CL7	C3A-C4A-CHB	-3.22	118.92	123.66
12	B	604	CLA	O2A-C1-C2	3.22	120.50	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	605	CLA	CMB-C2B-C3B	3.19	134.06	126.55
14	D	402	PHO	O2D-CGD-O1D	-3.19	117.64	123.85
12	B	614	CLA	CHD-C1D-ND	-3.18	120.32	124.80
12	B	608	CLA	O2A-CGA-CBA	3.18	124.03	114.00
17	B	606	F6C	CMA-C3A-C4A	-3.17	119.14	124.73
12	B	613	CLA	O2A-C1-C2	3.17	120.32	108.11
12	B	611	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
14	A	406	PHO	CMB-C2B-C3B	3.17	131.02	124.68
17	B	612	F6C	CHA-C1A-C2A	-3.17	121.88	130.41
17	B	612	F6C	C3D-C4D-ND	3.17	115.15	109.93
17	C	507	F6C	C3D-C4D-ND	3.17	115.15	109.93
17	B	603	F6C	CHA-C4D-ND	3.15	136.07	133.05
12	C	501	CLA	C2B-C1B-NB	3.15	113.60	110.33
12	B	601	CLA	O2A-C1-C2	3.15	120.24	108.11
17	C	507	F6C	CHA-C1A-C2A	-3.15	121.95	130.41
12	C	513	CLA	O2A-CGA-CBA	3.14	123.92	114.00
12	A	407	CLA	C1-C2-C3	-3.13	121.08	126.20
17	B	603	F6C	O2A-C1-C2	3.12	120.13	108.11
12	C	503	CLA	CMC-C2C-C1C	3.12	129.91	125.03
15	B	615	BCR	C33-C5-C4	3.12	120.25	113.60
12	A	407	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
12	C	501	CLA	CMB-C2B-C1B	3.12	130.16	125.42
12	C	502	CLA	CHD-C1D-ND	-3.11	120.42	124.80
12	B	613	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	B	615	BCR	C33-C5-C6	-3.10	121.10	124.48
12	B	604	CLA	C2B-C1B-NB	3.10	113.54	110.33
12	B	609	CLA	CMA-C3A-C4A	3.10	120.10	111.77
12	C	501	CLA	C3D-C4D-ND	3.09	115.01	109.99
12	B	611	CLA	O2A-C1-C2	3.09	119.99	108.11
16	B	619	LMT	C3'-C4'-C5'	-3.09	104.09	110.93
12	B	604	CLA	CMA-C3A-C4A	3.08	120.04	111.77
12	C	506	CLA	C1-C2-C3	-3.07	121.16	126.20
21	D	406	PL9	C7-C3-C4	3.07	119.44	116.91
12	C	510	CLA	C3D-C4D-ND	3.06	114.97	109.99
17	B	612	F6C	CHA-C4D-ND	3.06	135.98	133.05
12	C	502	CLA	C3C-C4C-NC	3.06	114.35	110.43
12	C	512	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
12	B	607	CLA	CMB-C2B-C3B	3.05	133.73	126.55
15	C	517	BCR	C39-C30-C25	-3.05	105.46	110.24
12	C	508	CLA	CMA-C3A-C4A	3.05	119.97	111.77
12	A	405	CLA	C3D-C4D-ND	3.05	114.94	109.99
12	B	613	CLA	CMC-C2C-C1C	3.04	129.79	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	508	CLA	C2B-C1B-NB	3.04	113.48	110.33
17	B	603	F6C	C3C-C4C-NC	3.04	113.65	110.32
16	B	619	LMT	C1'-O5'-C5'	-3.03	107.80	113.72
16	A	409	LMT	C3B-C4B-C5B	-3.03	104.74	110.23
15	C	514	BCR	C34-C9-C8	3.03	122.72	118.09
12	D	403	CLA	C3D-C4D-ND	3.03	114.91	109.99
12	B	610	CLA	C1-C2-C3	-3.02	121.24	126.20
12	C	506	CLA	CAC-C3C-C4C	3.02	128.72	124.79
12	C	506	CLA	C1D-ND-C4D	-3.01	104.20	106.31
17	C	507	F6C	CHA-C4D-ND	3.01	135.93	133.05
12	A	407	CLA	C3D-C4D-ND	3.01	114.89	109.99
12	B	614	CLA	C2B-C1B-NB	3.01	113.44	110.33
12	C	512	CLA	CMC-C2C-C1C	3.01	129.73	125.03
17	B	606	F6C	C3C-C4C-NC	3.01	113.61	110.32
17	B	606	F6C	CHB-C4A-C3A	-3.00	119.24	125.49
15	B	615	BCR	C4-C5-C6	-3.00	118.65	122.70
12	B	601	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
12	B	610	CLA	C2B-C1B-NB	2.99	113.43	110.33
12	A	403	CLA	CMC-C2C-C1C	2.98	129.70	125.03
16	A	410	LMT	C3'-C4'-C5'	-2.98	104.32	110.93
12	C	503	CLA	C4-C3-C5	2.98	120.40	115.23
12	C	503	CLA	O2A-C1-C2	2.98	119.57	108.11
17	B	612	F6C	CMA-C3A-C4A	-2.98	119.49	124.73
12	C	511	CLA	C3D-C4D-ND	2.97	114.82	109.99
12	B	607	CLA	O2A-C1-C2	2.97	119.55	108.11
12	D	404	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
12	A	403	CLA	CMD-C2D-C3D	-2.97	120.88	127.69
12	C	503	CLA	CMA-C3A-C4A	2.96	119.73	111.77
17	B	606	F6C	CHD-C1D-ND	-2.96	119.85	124.31
12	B	602	CLA	C1-C2-C3	-2.96	121.35	126.20
12	C	509	CLA	C1-C2-C3	-2.96	121.35	126.20
12	D	403	CLA	CAA-C2A-C3A	-2.95	105.02	113.00
12	B	613	CLA	C4-C3-C5	2.95	120.35	115.23
12	D	403	CLA	CAA-CBA-CGA	-2.95	104.84	113.21
12	B	605	CLA	C1-O2A-CGA	2.95	123.79	116.65
12	D	403	CLA	C4-C3-C5	2.95	120.34	115.23
12	C	502	CLA	C2B-C1B-NB	2.95	113.38	110.33
12	C	513	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
17	B	606	F6C	CMA-C3A-C2A	-2.94	118.20	126.15
12	D	404	CLA	CMB-C2B-C1B	2.94	129.89	125.42
12	C	505	CLA	C3C-C4C-NC	2.94	114.19	110.43
12	A	407	CLA	O2A-C1-C2	2.93	119.39	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	602	CLA	CMD-C2D-C3D	-2.92	120.98	127.69
17	C	507	F6C	CHD-C1D-ND	-2.92	119.91	124.31
16	B	618	LMT	C3'-C4'-C5'	-2.92	104.45	110.93
12	B	602	CLA	C4-C3-C5	2.91	120.28	115.23
12	D	404	CLA	CMC-C2C-C1C	2.91	129.58	125.03
17	B	612	F6C	CHD-C1D-ND	-2.91	119.93	124.31
12	C	509	CLA	C3D-C4D-ND	2.91	114.71	109.99
16	A	410	LMT	C3B-C4B-C5B	-2.91	104.96	110.23
12	B	608	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	D	402	PHO	O2D-CGD-CBD	2.90	114.13	110.95
12	B	609	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
12	C	509	CLA	O2A-C1-C2	2.89	119.23	108.11
17	C	507	F6C	C3C-C4C-NC	2.87	113.46	110.32
12	B	601	CLA	CMC-C2C-C1C	2.87	129.52	125.03
12	A	405	CLA	C1-C2-C3	-2.87	122.12	126.76
12	B	609	CLA	O2A-CGA-CBA	2.86	123.04	114.00
16	A	410	LMT	O5B-C5B-C6B	2.86	113.53	106.44
12	C	501	CLA	O2A-C1-C2	2.86	119.12	108.11
21	D	406	PL9	C7-C3-C2	-2.86	120.02	123.39
12	B	613	CLA	C1-C2-C3	-2.86	121.52	126.20
12	B	609	CLA	CAA-C2A-C3A	-2.85	105.28	113.00
17	B	603	F6C	OMB-CMB-C2B	-2.85	119.19	125.62
13	A	404	CL7	C3D-C4D-ND	2.84	114.17	110.20
12	B	602	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
12	C	502	CLA	C4C-C3C-C2C	-2.84	102.75	106.89
17	B	603	F6C	C3D-C4D-ND	2.83	114.59	109.93
17	B	606	F6C	C3D-C4D-ND	2.83	114.59	109.93
12	B	602	CLA	C1-O2A-CGA	2.83	123.49	116.65
12	C	513	CLA	C3D-C4D-ND	2.82	114.58	109.99
12	B	604	CLA	C4-C3-C5	2.82	120.13	115.23
17	C	507	F6C	CMA-C3A-C4A	-2.82	119.77	124.73
19	B	617	LMG	C8-O7-C10	-2.81	111.06	117.80
17	B	603	F6C	CHA-C1A-C2A	-2.81	122.86	130.41
12	B	602	CLA	O1D-CGD-CBD	-2.80	118.99	124.52
12	C	509	CLA	C4-C3-C5	2.79	120.08	115.23
12	B	610	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
12	C	506	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
15	D	405	BCR	C34-C9-C8	2.79	122.35	118.09
15	D	405	BCR	C36-C18-C17	-2.78	118.30	122.82
12	C	502	CLA	C4-C3-C5	2.78	120.06	115.23
17	B	612	F6C	C3C-C4C-NC	2.78	113.37	110.32
22	D	407	LHG	O8-C23-C24	2.78	120.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	515	DGD	C1D-C2D-C3D	-2.78	104.17	110.01
18	B	616	DGD	C3G-C2G-C1G	-2.76	105.34	111.78
12	C	501	CLA	C6-C5-C3	-2.76	106.74	113.47
17	B	606	F6C	O1D-CGD-CBD	-2.76	119.07	124.52
12	D	404	CLA	C3D-C4D-ND	2.76	114.47	109.99
12	C	505	CLA	CHD-C1D-ND	-2.75	120.93	124.80
12	B	614	CLA	CMA-C3A-C4A	2.75	119.16	111.77
12	C	501	CLA	CAA-C2A-C3A	-2.75	105.58	113.00
12	B	614	CLA	C3C-C4C-NC	2.74	113.95	110.43
21	D	406	PL9	C36-C34-C33	-2.74	115.01	121.17
17	B	606	F6C	C4-C3-C5	2.74	119.99	115.23
17	B	603	F6C	O2D-CGD-O1D	-2.74	118.51	123.85
12	B	607	CLA	C4D-C3D-CAD	2.74	111.08	108.11
12	C	511	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
15	B	615	BCR	C8-C7-C6	-2.74	119.68	127.00
13	A	404	CL7	C3D-C2D-C1D	-2.74	97.66	106.40
12	C	513	CLA	C4D-C3D-CAD	2.73	111.08	108.11
17	B	612	F6C	C4-C3-C5	2.73	119.97	115.23
15	C	514	BCR	C23-C24-C25	-2.73	119.70	127.00
12	B	614	CLA	C1-O2A-CGA	2.73	123.26	116.65
17	C	507	F6C	C4-C3-C5	2.73	119.97	115.23
17	B	603	F6C	CHB-C4A-C3A	-2.72	119.82	125.49
17	B	606	F6C	CHA-C4D-ND	2.72	135.65	133.05
12	B	611	CLA	C1-C2-C3	-2.71	121.76	126.20
12	B	604	CLA	CMC-C2C-C1C	2.71	129.27	125.03
12	B	610	CLA	C3C-C4C-NC	2.71	113.90	110.43
12	C	504	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
12	D	403	CLA	C4D-C3D-CAD	2.70	111.04	108.11
15	B	615	BCR	C3-C4-C5	-2.70	109.24	114.06
12	C	508	CLA	C4-C3-C5	2.70	119.91	115.23
12	B	611	CLA	CMC-C2C-C1C	2.69	129.24	125.03
12	A	405	CLA	CMA-C3A-C4A	2.69	118.99	111.77
12	C	512	CLA	CMA-C3A-C4A	2.68	118.98	111.77
12	B	605	CLA	C4-C3-C5	2.68	119.88	115.23
12	C	511	CLA	CMC-C2C-C1C	2.67	129.21	125.03
12	C	505	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
12	B	610	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
12	B	610	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
12	B	613	CLA	OBD-CAD-C3D	-2.67	122.18	128.42
12	B	608	CLA	C4D-C3D-CAD	2.67	111.00	108.11
12	B	608	CLA	C3C-C4C-NC	2.67	113.85	110.43
14	A	406	PHO	O2D-CGD-O1D	-2.67	118.66	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	512	CLA	CMB-C2B-C3B	2.66	132.82	126.55
17	C	507	F6C	O2D-CGD-O1D	-2.66	118.66	123.85
12	B	601	CLA	C3D-C4D-ND	2.66	114.32	109.99
12	B	607	CLA	CMD-C2D-C3D	-2.66	121.60	127.69
12	B	608	CLA	CMA-C3A-C4A	2.65	118.91	111.77
12	B	611	CLA	C3D-C4D-ND	2.65	114.30	109.99
12	C	508	CLA	CMC-C2C-C1C	2.65	129.17	125.03
12	B	607	CLA	C4-C3-C5	2.65	119.82	115.23
12	C	506	CLA	C3D-C4D-ND	2.64	114.28	109.99
12	B	605	CLA	C4D-C3D-CAD	2.64	110.97	108.11
13	A	404	CL7	CHD-C1D-ND	-2.63	120.10	124.05
13	A	404	CL7	O2D-CGD-O1D	-2.62	118.75	123.85
12	B	601	CLA	C1-C2-C3	-2.62	121.91	126.20
12	B	614	CLA	C4D-C3D-CAD	2.62	110.95	108.11
12	B	614	CLA	C3D-C4D-ND	2.62	114.24	109.99
12	B	613	CLA	C4D-C3D-CAD	2.62	110.95	108.11
21	D	406	PL9	C41-C39-C40	2.61	120.61	114.59
12	A	403	CLA	C4-C3-C5	2.61	119.76	115.23
15	C	517	BCR	C15-C14-C13	-2.61	123.62	127.28
12	B	605	CLA	CAC-C3C-C4C	2.61	128.18	124.79
12	B	605	CLA	CAA-C2A-C3A	-2.61	105.96	113.00
12	B	602	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
17	B	603	F6C	CHD-C1D-ND	-2.60	120.39	124.31
12	B	613	CLA	C3D-C4D-ND	2.60	114.21	109.99
12	C	504	CLA	C3D-C4D-ND	2.60	114.21	109.99
12	B	602	CLA	CMC-C2C-C1C	2.59	129.09	125.03
17	B	603	F6C	CMA-C3A-C4A	-2.59	120.16	124.73
17	B	603	F6C	CMC-C2C-C1C	2.59	129.36	125.42
12	C	513	CLA	CMC-C2C-C1C	2.58	129.07	125.03
17	C	507	F6C	CHB-C4A-C3A	-2.58	120.12	125.49
12	B	609	CLA	C3D-C4D-ND	2.58	114.18	109.99
12	C	508	CLA	CMB-C2B-C1B	2.57	129.33	125.42
12	B	602	CLA	CHD-C1D-ND	-2.57	121.19	124.80
12	B	609	CLA	O1D-CGD-CBD	-2.56	119.46	124.52
12	B	604	CLA	CMB-C2B-C1B	2.56	129.32	125.42
12	B	607	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
12	A	407	CLA	CMC-C2C-C1C	2.56	129.04	125.03
12	C	505	CLA	CMC-C2C-C1C	2.56	129.03	125.03
12	B	609	CLA	C3C-C4C-NC	2.56	113.71	110.43
21	D	406	PL9	C22-C23-C24	-2.56	121.77	127.62
12	C	508	CLA	C4D-C3D-CAD	2.55	110.88	108.11
15	B	615	BCR	C35-C13-C12	2.54	121.97	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	D	402	PHO	C1-C2-C3	-2.54	122.04	126.20
12	C	506	CLA	C4-C3-C5	2.54	119.63	115.23
12	C	506	CLA	C4B-C3B-C2B	-2.53	104.15	107.30
12	A	405	CLA	C1-O2A-CGA	2.53	122.78	116.65
12	C	503	CLA	C6-C5-C3	-2.53	107.30	113.47
12	A	403	CLA	C6-C5-C3	-2.53	107.30	113.47
12	B	610	CLA	CMB-C2B-C3B	2.53	132.50	126.55
15	C	517	BCR	C28-C27-C26	-2.53	109.55	114.06
12	B	611	CLA	C4-C3-C5	2.53	119.61	115.23
17	B	612	F6C	CHB-C4A-C3A	-2.52	120.24	125.49
12	C	503	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
12	C	502	CLA	CMA-C3A-C4A	2.52	118.54	111.77
12	A	403	CLA	O1D-CGD-CBD	-2.52	119.56	124.52
12	B	611	CLA	C3C-C4C-NC	2.51	113.65	110.43
12	C	508	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
12	C	502	CLA	CMC-C2C-C3C	2.51	132.95	126.15
17	B	612	F6C	OMB-CMB-C2B	-2.51	119.96	125.62
12	A	403	CLA	C4D-C3D-CAD	2.51	110.83	108.11
12	C	505	CLA	C4D-C3D-CAD	2.51	110.83	108.11
15	A	408	BCR	C19-C18-C17	2.50	122.94	119.01
15	C	514	BCR	C35-C13-C12	2.50	121.90	118.09
17	B	612	F6C	CMC-C2C-C1C	2.50	129.22	125.42
17	B	612	F6C	O2D-CGD-O1D	-2.50	118.99	123.85
12	B	613	CLA	C3C-C4C-NC	2.49	113.62	110.43
17	C	507	F6C	CMC-C2C-C1C	2.49	129.22	125.42
12	C	501	CLA	CMC-C2C-C1C	2.49	128.93	125.03
17	C	507	F6C	OMB-CMB-C2B	-2.49	120.00	125.62
12	C	505	CLA	C3D-C4D-ND	2.49	114.04	109.99
17	B	606	F6C	CED-O2D-CGD	2.49	121.56	115.92
12	B	602	CLA	C3D-C4D-ND	2.49	114.03	109.99
21	D	406	PL9	O2-C1-C6	2.49	124.44	120.48
12	B	604	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
15	A	408	BCR	C38-C26-C27	2.49	118.90	113.60
14	D	402	PHO	C2D-C1D-ND	-2.49	107.63	109.43
15	D	405	BCR	C7-C8-C9	-2.48	122.56	126.23
12	C	509	CLA	C3C-C4C-NC	2.48	113.61	110.43
12	B	602	CLA	CMA-C3A-C4A	2.48	118.43	111.77
12	C	512	CLA	C3D-C4D-ND	2.47	114.00	109.99
12	C	510	CLA	CAA-C2A-C3A	-2.47	106.34	113.00
12	C	503	CLA	C3D-C4D-ND	2.46	113.99	109.99
15	D	405	BCR	C35-C13-C12	2.46	121.84	118.09
17	B	612	F6C	CMA-C3A-C2A	-2.46	119.50	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	502	CLA	C3D-C4D-ND	2.45	113.98	109.99
12	B	609	CLA	CMC-C2C-C1C	2.45	128.86	125.03
12	D	403	CLA	C3C-C4C-NC	2.45	113.56	110.43
12	C	501	CLA	C4D-C3D-CAD	2.44	110.76	108.11
12	B	613	CLA	C1-O2A-CGA	2.44	122.56	116.65
15	B	615	BCR	C1-C6-C5	-2.44	119.30	122.64
12	B	611	CLA	C4D-C3D-CAD	2.44	110.75	108.11
17	C	507	F6C	CMD-C2D-C3D	-2.44	122.10	127.69
19	B	617	LMG	O8-C28-C29	2.43	119.23	111.83
12	A	405	CLA	CMB-C2B-C1B	2.43	129.11	125.42
14	D	402	PHO	C2B-C1B-NB	-2.42	107.68	109.43
12	C	506	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
12	C	508	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
15	C	517	BCR	C34-C9-C10	-2.42	118.89	122.82
12	A	405	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
12	C	506	CLA	CMC-C2C-C3C	2.42	132.70	126.15
15	D	405	BCR	C3-C4-C5	-2.42	109.74	114.06
21	D	406	PL9	C27-C28-C29	-2.42	122.09	127.62
12	D	403	CLA	CED-O2D-CGD	2.42	121.40	115.92
17	B	606	F6C	OMB-CMB-C2B	-2.42	120.17	125.62
12	D	404	CLA	CAC-C3C-C4C	2.41	127.93	124.79
12	B	605	CLA	C3D-C4D-ND	2.41	113.91	109.99
12	D	403	CLA	C1-C2-C3	-2.41	122.25	126.20
12	C	512	CLA	C4D-C3D-CAD	2.41	110.72	108.11
12	C	503	CLA	C3C-C4C-NC	2.41	113.51	110.43
15	C	517	BCR	C31-C1-C6	-2.40	106.47	110.24
12	B	608	CLA	C3D-C4D-ND	2.40	113.89	109.99
12	C	504	CLA	CMC-C2C-C1C	2.40	128.79	125.03
15	B	615	BCR	C36-C18-C17	-2.40	118.92	122.82
12	C	509	CLA	CMC-C2C-C1C	2.40	128.79	125.03
12	C	512	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
15	A	408	BCR	C36-C18-C17	-2.40	118.93	122.82
12	C	511	CLA	C4D-C3D-CAD	2.39	110.71	108.11
12	A	403	CLA	C3D-C4D-ND	2.39	113.88	109.99
17	B	603	F6C	C5-C3-C4	2.39	120.09	114.59
18	B	616	DGD	O6D-C1D-O3G	-2.39	104.40	110.04
14	A	406	PHO	O1D-CGD-CBD	2.39	128.34	124.72
12	C	509	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
12	C	513	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
18	C	515	DGD	O5D-C6D-C5D	-2.38	104.06	109.42
12	B	608	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
15	D	405	BCR	C15-C14-C13	-2.38	123.94	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	607	CLA	CAA-C2A-C3A	-2.38	106.58	113.00
12	B	607	CLA	C3D-C4D-ND	2.37	113.84	109.99
12	C	510	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
12	C	506	CLA	C3B-C4B-NB	2.37	112.64	110.53
15	A	408	BCR	C33-C5-C4	2.37	118.64	113.60
17	B	606	F6C	C4A-CHB-C1B	2.37	131.05	126.02
12	B	601	CLA	C4D-C3D-CAD	2.36	110.67	108.11
12	B	614	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
22	D	407	LHG	O8-C23-O10	-2.36	117.73	123.63
12	C	502	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
16	B	618	LMT	C1'-O5'-C5'	-2.36	109.12	113.72
12	A	405	CLA	CED-O2D-CGD	2.36	121.26	115.92
12	D	404	CLA	C4D-C3D-CAD	2.36	110.67	108.11
17	B	612	F6C	CMD-C2D-C3D	-2.36	122.28	127.69
12	C	503	CLA	CMB-C2B-C1B	2.36	129.01	125.42
12	C	501	CLA	CMA-C3A-C4A	2.35	118.10	111.77
12	C	509	CLA	CMB-C2B-C3B	2.35	132.07	126.55
12	D	404	CLA	C3C-C4C-NC	2.35	113.44	110.43
12	A	403	CLA	C3C-C4C-NC	2.34	113.43	110.43
12	C	510	CLA	C4-C3-C5	2.34	119.29	115.23
15	B	615	BCR	C29-C28-C27	2.34	116.42	111.28
12	B	605	CLA	C6-C5-C3	-2.34	107.77	113.47
12	A	407	CLA	C1-O2A-CGA	2.34	122.31	116.65
12	C	513	CLA	CAA-C2A-C3A	-2.34	106.69	113.00
12	B	604	CLA	C4D-C3D-CAD	2.32	110.63	108.11
13	A	404	CL7	CMB-C2B-C1B	2.32	128.96	125.42
15	C	514	BCR	C36-C18-C17	-2.32	119.05	122.82
12	B	605	CLA	CHB-C1B-C2B	-2.32	120.70	127.43
15	A	408	BCR	C15-C14-C13	-2.32	124.03	127.28
12	C	508	CLA	C3C-C4C-NC	2.31	113.39	110.43
12	B	604	CLA	CAC-C3C-C4C	2.31	127.80	124.79
14	D	402	PHO	O1D-CGD-CBD	2.31	128.22	124.72
12	B	604	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
12	B	604	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
12	D	404	CLA	C4B-CHC-C1C	2.30	131.65	126.25
12	B	607	CLA	CMC-C2C-C1C	2.30	128.62	125.03
13	A	404	CL7	C4-C3-C2	-2.30	117.73	123.63
12	B	609	CLA	C4D-C3D-CAD	2.30	110.60	108.11
15	A	408	BCR	C37-C22-C21	-2.30	119.09	122.82
16	A	409	LMT	C1'-O5'-C5'	-2.29	109.25	113.72
12	A	407	CLA	CMA-C3A-C4A	2.28	117.91	111.77
12	B	607	CLA	CHB-C1B-C2B	-2.28	120.80	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	511	CLA	C3C-C4C-NC	2.28	113.35	110.43
18	B	616	DGD	C5B-C4B-C3B	-2.28	102.84	114.37
12	B	608	CLA	CED-O2D-CGD	2.28	121.09	115.92
12	B	613	CLA	CMB-C2B-C1B	2.28	128.89	125.42
12	C	513	CLA	CMB-C2B-C3B	2.28	131.91	126.55
12	B	604	CLA	C3C-C4C-NC	2.28	113.35	110.43
15	B	615	BCR	C15-C14-C13	-2.28	124.09	127.28
19	B	617	LMG	C7-O1-C1	-2.27	108.92	113.80
12	B	605	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
12	C	510	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
12	B	601	CLA	CMB-C2B-C1B	2.27	128.88	125.42
12	A	405	CLA	CAC-C3C-C4C	2.27	127.74	124.79
12	C	503	CLA	CAC-C3C-C4C	2.27	127.74	124.79
12	C	504	CLA	C4D-C3D-CAD	2.27	110.57	108.11
12	A	407	CLA	C4-C3-C5	2.27	119.16	115.23
12	A	403	CLA	CMB-C2B-C3B	2.26	131.88	126.55
12	C	505	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
22	D	407	LHG	C6-C5-C4	-2.26	106.51	111.78
15	C	514	BCR	C33-C5-C6	-2.26	122.02	124.48
12	C	513	CLA	C3C-C4C-NC	2.25	113.32	110.43
23	F	101	HEM	C1B-NB-C4B	2.25	107.87	105.21
12	C	509	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
12	B	611	CLA	CMB-C2B-C3B	2.24	131.83	126.55
16	B	619	LMT	O1'-C1'-C2'	2.24	111.67	108.27
17	B	603	F6C	O1D-CGD-CBD	-2.24	120.10	124.52
12	B	605	CLA	CMA-C3A-C4A	2.23	117.77	111.77
12	B	605	CLA	C3C-C4C-NC	2.23	113.29	110.43
12	B	601	CLA	C3C-C4C-NC	2.23	113.28	110.43
12	B	614	CLA	C5-C3-C4	2.22	119.70	114.59
14	A	406	PHO	C2D-C1D-ND	-2.22	107.83	109.43
12	A	405	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
12	A	405	CLA	C4D-C3D-CAD	2.22	110.52	108.11
12	A	407	CLA	CMB-C2B-C3B	2.22	131.77	126.55
12	B	614	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
17	C	507	F6C	CMA-C3A-C2A	-2.22	120.16	126.15
12	B	610	CLA	CAC-C3C-C4C	2.21	127.67	124.79
12	A	403	CLA	CAA-C2A-C1A	-2.21	104.73	111.97
12	B	614	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
15	D	405	BCR	C17-C18-C19	2.21	122.48	116.80
12	A	403	CLA	CAA-CBA-CGA	-2.21	106.94	113.21
12	B	602	CLA	C3C-C4C-NC	2.20	113.25	110.43
12	C	510	CLA	CAA-CBA-CGA	-2.20	106.96	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	406	PL9	C8-C7-C3	2.20	117.71	112.03
12	C	503	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
12	C	509	CLA	C11-C10-C8	-2.19	108.67	115.97
12	C	503	CLA	C4D-C3D-CAD	2.19	110.49	108.11
12	C	504	CLA	C3C-C4C-NC	2.19	113.24	110.43
12	B	611	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	C	510	CLA	CMC-C2C-C1C	2.18	128.45	125.03
12	B	607	CLA	CAC-C3C-C4C	2.18	127.63	124.79
12	C	505	CLA	C4-C3-C5	2.18	119.02	115.23
13	A	404	CL7	CHC-C1C-NC	-2.18	121.73	124.80
12	C	510	CLA	CAA-C2A-C1A	-2.18	104.83	111.97
15	B	615	BCR	C12-C13-C14	-2.18	115.58	119.01
12	C	501	CLA	C3C-C4C-NC	2.17	113.21	110.43
18	B	616	DGD	C1D-O6D-C5D	-2.17	109.93	113.63
12	B	607	CLA	C3C-C4C-NC	2.17	113.21	110.43
12	D	403	CLA	CMB-C2B-C1B	2.17	128.72	125.42
12	B	610	CLA	C4-C3-C5	2.17	118.99	115.23
12	C	509	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
12	C	501	CLA	C4-C3-C5	2.16	118.98	115.23
17	B	606	F6C	CHA-C1A-C2A	-2.16	124.61	130.41
13	A	404	CL7	CHD-C4C-C3C	-2.15	121.46	124.86
12	C	509	CLA	CAC-C3C-C4C	2.14	127.58	124.79
12	C	504	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
12	B	613	CLA	CAC-C3C-C4C	2.14	127.57	124.79
14	D	402	PHO	CBA-CAA-C2A	-2.14	107.49	113.78
12	C	511	CLA	CMB-C2B-C3B	2.14	131.57	126.55
15	C	517	BCR	C34-C9-C8	2.14	121.35	118.09
17	B	612	F6C	CHC-C1C-C2C	-2.13	121.23	127.43
12	A	405	CLA	C5-C3-C4	2.13	119.49	114.59
12	D	404	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
16	B	619	LMT	C6'-C5'-C4'	2.13	119.37	113.38
12	C	509	CLA	CHB-C4A-NA	2.13	127.47	124.40
22	D	407	LHG	C5-O7-C7	-2.13	112.70	117.80
17	B	603	F6C	CAC-C3C-C4C	2.13	127.84	124.91
12	B	610	CLA	C3D-C4D-ND	2.13	113.44	109.99
12	B	605	CLA	O2A-C1-C2	2.13	116.29	108.11
12	C	508	CLA	CAC-C3C-C4C	2.12	127.55	124.79
16	D	409	LMT	O6'-C6'-C5'	-2.12	106.32	111.77
13	A	404	CL7	C4B-CHC-C1C	2.12	131.20	124.66
17	B	603	F6C	CHC-C1C-C2C	-2.11	121.30	127.43
12	B	614	CLA	CHC-C1C-C2C	-2.11	120.96	126.95
12	B	602	CLA	CMB-C2B-C1B	2.11	128.63	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	502	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
12	A	405	CLA	CMD-C2D-C3D	-2.10	122.86	127.69
16	A	409	LMT	C4B-C3B-C2B	-2.10	107.14	110.83
17	B	606	F6C	CMC-C2C-C1C	2.10	128.62	125.42
12	C	505	CLA	CAA-CBA-CGA	-2.10	107.24	113.21
12	A	405	CLA	CMC-C2C-C1C	2.10	128.31	125.03
15	A	408	BCR	C12-C13-C14	-2.10	115.71	119.01
23	F	101	HEM	C4D-ND-C1D	2.09	107.69	105.21
12	B	610	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
15	C	514	BCR	C37-C22-C21	-2.09	119.42	122.82
12	B	610	CLA	CMA-C3A-C4A	2.09	117.40	111.77
12	B	607	CLA	CHA-C4D-ND	2.09	136.86	132.55
15	A	408	BCR	C34-C9-C8	2.09	121.28	118.09
12	C	501	CLA	C1-O2A-CGA	2.09	121.71	116.65
12	B	610	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
12	B	611	CLA	C6-C5-C3	-2.09	108.38	113.47
16	A	410	LMT	C1B-C2B-C3B	2.09	114.40	110.01
12	C	501	CLA	CMD-C2D-C3D	-2.09	122.91	127.69
12	C	510	CLA	CED-O2D-CGD	2.08	120.64	115.92
12	C	502	CLA	C11-C12-C13	-2.08	109.04	115.97
12	D	404	CLA	CMA-C3A-C4A	2.08	117.36	111.77
17	B	606	F6C	CMD-C2D-C3D	-2.08	122.92	127.69
23	F	101	HEM	CMB-C2B-C1B	-2.08	121.79	125.03
19	D	408	LMG	O8-C28-C29	2.08	118.16	111.83
12	C	506	CLA	C4C-C3C-C2C	-2.08	103.87	106.89
12	B	607	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
15	D	405	BCR	C34-C9-C10	-2.07	119.46	122.82
15	A	408	BCR	C34-C9-C10	-2.07	119.47	122.82
12	C	511	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
12	B	602	CLA	C4-C3-C2	-2.06	118.32	123.63
12	C	506	CLA	CHB-C1B-C2B	-2.06	121.43	127.43
12	B	607	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
12	C	504	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
15	A	408	BCR	C23-C24-C25	-2.06	121.48	127.00
12	C	509	CLA	C4D-C3D-CAD	2.06	110.35	108.11
12	B	610	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
12	A	403	CLA	CMA-C3A-C4A	2.06	117.31	111.77
12	B	609	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
16	A	410	LMT	C1'-O5'-C5'	-2.06	109.70	113.72
14	D	402	PHO	CAA-CBA-CGA	-2.06	107.36	113.21
13	A	404	CL7	C4-C3-C5	2.05	118.79	115.23
17	B	603	F6C	C4A-CHB-C1B	2.05	130.38	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	512	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
12	C	511	CLA	CAA-CBA-CGA	-2.05	107.02	112.49
12	B	609	CLA	CMB-C2B-C3B	2.05	131.37	126.55
12	B	613	CLA	CHB-C4A-NA	2.05	127.36	124.40
17	B	603	F6C	CMD-C2D-C3D	-2.05	122.99	127.69
12	B	610	CLA	CHC-C1C-C2C	-2.04	121.14	126.95
17	B	606	F6C	CMC-C2C-C3C	2.04	129.95	125.62
12	C	510	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
17	C	507	F6C	CHC-C1C-C2C	-2.04	121.52	127.43
12	C	511	CLA	CAA-C2A-C3A	-2.04	107.50	113.00
12	D	403	CLA	O1D-CGD-CBD	-2.03	120.50	124.52
12	B	614	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
12	B	607	CLA	C7-C6-C5	-2.03	107.84	113.26
19	D	408	LMG	O7-C10-O9	-2.03	118.96	123.70
16	B	618	LMT	C3B-C4B-C5B	-2.03	106.56	110.23
13	A	404	CL7	CAC-C3C-C2C	2.02	131.27	127.56
12	C	508	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
12	B	602	CLA	CHA-C4D-ND	2.02	136.72	132.55
12	C	505	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
12	B	601	CLA	CAC-C3C-C4C	2.02	127.41	124.79
12	A	407	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
12	B	601	CLA	CHB-C4A-NA	2.02	127.31	124.40
19	B	617	LMG	O6-C1-C2	-2.01	106.23	110.37
12	C	506	CLA	CED-O2D-CGD	2.01	120.48	115.92
18	C	515	DGD	C3G-C2G-C1G	-2.01	107.10	111.78
12	C	506	CLA	CMB-C2B-C3B	2.01	131.28	126.55
12	C	504	CLA	CAC-C3C-C4C	2.01	127.40	124.79
12	C	504	CLA	CED-O2D-CGD	2.01	120.47	115.92
12	C	512	CLA	C3C-C4C-NC	2.00	113.00	110.43

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	404	CL7	NA
13	A	404	CL7	NC
17	B	603	F6C	NA
17	B	606	F6C	NA
17	B	612	F6C	NA
17	C	507	F6C	NA

All (565) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	403	CLA	CBD-CGD-O2D-CED
12	B	607	CLA	C2-C1-O2A-CGA
12	B	607	CLA	CBD-CGD-O2D-CED
12	B	608	CLA	C3A-C2A-CAA-CBA
12	B	608	CLA	C2B-C3B-CAB-CBB
12	B	608	CLA	C4B-C3B-CAB-CBB
12	B	608	CLA	CAD-CBD-CGD-O1D
12	B	608	CLA	CAD-CBD-CGD-O2D
12	B	608	CLA	CBD-CGD-O2D-CED
12	B	609	CLA	CBD-CGD-O2D-CED
12	B	611	CLA	C2-C1-O2A-CGA
12	B	611	CLA	CAD-CBD-CGD-O2D
12	B	613	CLA	C1A-C2A-CAA-CBA
12	C	501	CLA	CBD-CGD-O2D-CED
12	C	503	CLA	CBD-CGD-O2D-CED
12	C	509	CLA	C2-C1-O2A-CGA
12	C	510	CLA	CBD-CGD-O2D-CED
12	C	511	CLA	CBD-CGD-O2D-CED
12	C	512	CLA	CAD-CBD-CGD-O2D
12	C	513	CLA	CBD-CGD-O2D-CED
13	A	404	CL7	C2-C1-O2A-CGA
13	A	404	CL7	C1A-C2A-CAA-CBA
13	A	404	CL7	C3A-C2A-CAA-CBA
14	A	406	PHO	C4-C3-C5-C6
14	D	402	PHO	CHA-CBD-CGD-O2D
15	A	408	BCR	C7-C8-C9-C10
15	C	517	BCR	C11-C10-C9-C8
15	C	517	BCR	C11-C10-C9-C34
15	C	517	BCR	C10-C11-C12-C13
15	D	405	BCR	C7-C8-C9-C10
15	D	405	BCR	C11-C10-C9-C8
15	D	405	BCR	C11-C10-C9-C34
16	A	409	LMT	C2-C1-O1'-C1'
16	B	618	LMT	C2'-C1'-O1'-C1
16	B	618	LMT	O5'-C1'-O1'-C1
16	D	409	LMT	O5'-C1'-O1'-C1
16	D	409	LMT	C4'-C5'-C6'-O6'
16	D	409	LMT	O5'-C5'-C6'-O6'
17	B	603	F6C	C1A-C2A-CAA-CBA
17	B	603	F6C	C1B-C2B-CMB-OMB
17	B	603	F6C	C3B-C2B-CMB-OMB
17	B	606	F6C	C1A-C2A-CAA-CBA
17	B	606	F6C	C3B-C2B-CMB-OMB

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Mol	Chain	Res	Type	Atoms
17	B	612	F6C	C2-C1-O2A-CGA
17	C	507	F6C	C2B-C3B-CAB-CBB
17	C	507	F6C	C1B-C2B-CMB-OMB
17	C	507	F6C	C3B-C2B-CMB-OMB
17	C	507	F6C	C6-C7-C8-C9
18	B	616	DGD	C2B-C1B-O2G-C2G
18	B	616	DGD	O1B-C1B-O2G-C2G
21	D	406	PL9	C7-C8-C9-C11
21	D	406	PL9	C22-C23-C24-C26
21	D	406	PL9	C27-C28-C29-C31
21	D	406	PL9	C32-C33-C34-C35
21	D	406	PL9	C37-C38-C39-C40
22	D	407	LHG	O6-C4-C5-O7
12	C	510	CLA	O1D-CGD-O2D-CED
12	B	604	CLA	CBD-CGD-O2D-CED
12	B	610	CLA	CBD-CGD-O2D-CED
12	B	614	CLA	CBD-CGD-O2D-CED
12	C	502	CLA	CBD-CGD-O2D-CED
12	D	403	CLA	CBD-CGD-O2D-CED
12	B	602	CLA	O1A-CGA-O2A-C1
21	D	406	PL9	C37-C38-C39-C41
12	B	602	CLA	CBA-CGA-O2A-C1
12	A	405	CLA	O1A-CGA-O2A-C1
12	B	604	CLA	O1A-CGA-O2A-C1
13	A	404	CL7	O1A-CGA-O2A-C1
18	B	616	DGD	O1A-C1A-O1G-C1G
12	C	501	CLA	O1D-CGD-O2D-CED
12	C	511	CLA	O1D-CGD-O2D-CED
12	C	506	CLA	CBD-CGD-O2D-CED
12	B	609	CLA	O1D-CGD-O2D-CED
12	B	602	CLA	C3-C5-C6-C7
12	C	502	CLA	C3-C5-C6-C7
12	C	510	CLA	C3-C5-C6-C7
13	A	404	CL7	C3-C5-C6-C7
17	B	606	F6C	C3-C5-C6-C7
17	B	612	F6C	C3-C5-C6-C7
12	A	405	CLA	CBA-CGA-O2A-C1
12	B	604	CLA	CBA-CGA-O2A-C1
12	D	404	CLA	CBD-CGD-O2D-CED
17	B	606	F6C	CBD-CGD-O2D-CED
12	A	403	CLA	O1D-CGD-O2D-CED
12	B	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	B	608	CLA	O1D-CGD-O2D-CED
12	B	614	CLA	O1D-CGD-O2D-CED
12	C	503	CLA	O1D-CGD-O2D-CED
12	C	513	CLA	O1D-CGD-O2D-CED
12	B	604	CLA	O1D-CGD-O2D-CED
12	B	610	CLA	O1D-CGD-O2D-CED
12	C	502	CLA	C4-C3-C5-C6
17	B	606	F6C	C4-C3-C5-C6
12	C	502	CLA	C2-C3-C5-C6
14	A	406	PHO	C2-C3-C5-C6
17	B	606	F6C	C2-C3-C5-C6
16	B	619	LMT	O5B-C5B-C6B-O6B
12	A	403	CLA	C3-C5-C6-C7
12	C	508	CLA	C3-C5-C6-C7
12	B	601	CLA	CBA-CGA-O2A-C1
12	B	613	CLA	CBA-CGA-O2A-C1
12	C	509	CLA	CBA-CGA-O2A-C1
13	A	404	CL7	CBA-CGA-O2A-C1
17	C	507	F6C	CBA-CGA-O2A-C1
18	B	616	DGD	C2A-C1A-O1G-C1G
21	D	406	PL9	C7-C8-C9-C10
21	D	406	PL9	C32-C33-C34-C36
12	C	505	CLA	O1A-CGA-O2A-C1
12	C	508	CLA	O1A-CGA-O2A-C1
12	C	509	CLA	O1A-CGA-O2A-C1
17	C	507	F6C	O1A-CGA-O2A-C1
12	B	605	CLA	CBD-CGD-O2D-CED
12	B	607	CLA	CBA-CGA-O2A-C1
17	B	603	F6C	CBA-CGA-O2A-C1
16	A	409	LMT	O5'-C5'-C6'-O6'
12	B	601	CLA	O1A-CGA-O2A-C1
16	B	619	LMT	C4B-C5B-C6B-O6B
16	A	410	LMT	O5B-C5B-C6B-O6B
16	C	516	LMT	O5'-C5'-C6'-O6'
12	D	403	CLA	O1D-CGD-O2D-CED
16	B	618	LMT	O5B-C5B-C6B-O6B
12	C	505	CLA	CBA-CGA-O2A-C1
12	C	508	CLA	CBA-CGA-O2A-C1
12	B	607	CLA	O1A-CGA-O2A-C1
12	B	613	CLA	O1A-CGA-O2A-C1
17	B	603	F6C	O1A-CGA-O2A-C1
16	B	619	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
17	B	606	F6C	C2A-CAA-CBA-CGA
16	A	409	LMT	C4'-C5'-C6'-O6'
12	B	604	CLA	C2A-CAA-CBA-CGA
16	A	410	LMT	O5'-C1'-O1'-C1
18	B	616	DGD	O6D-C1D-O3G-C3G
12	C	502	CLA	O1D-CGD-O2D-CED
12	B	611	CLA	CBD-CGD-O2D-CED
19	B	617	LMG	O6-C5-C6-O5
16	A	410	LMT	C4B-C5B-C6B-O6B
16	B	618	LMT	O5'-C5'-C6'-O6'
12	B	611	CLA	CBA-CGA-O2A-C1
12	C	504	CLA	CBA-CGA-O2A-C1
17	B	606	F6C	CBA-CGA-O2A-C1
12	A	407	CLA	CBD-CGD-O2D-CED
12	C	506	CLA	O1D-CGD-O2D-CED
16	B	618	LMT	C4B-C5B-C6B-O6B
16	B	619	LMT	C4'-C5'-C6'-O6'
12	B	602	CLA	C4-C3-C5-C6
12	B	602	CLA	C2-C3-C5-C6
12	B	604	CLA	C3-C5-C6-C7
12	A	407	CLA	C6-C7-C8-C9
12	C	509	CLA	C6-C7-C8-C9
13	A	404	CL7	C6-C7-C8-C9
14	A	406	PHO	C11-C10-C8-C9
16	C	516	LMT	C4'-C5'-C6'-O6'
16	A	410	LMT	C2'-C1'-O1'-C1
18	B	616	DGD	C2D-C1D-O3G-C3G
12	D	404	CLA	O1D-CGD-O2D-CED
17	B	606	F6C	O1D-CGD-O2D-CED
15	A	408	BCR	C7-C8-C9-C34
15	A	408	BCR	C11-C12-C13-C35
15	A	408	BCR	C36-C18-C19-C20
15	B	615	BCR	C7-C8-C9-C34
15	D	405	BCR	C7-C8-C9-C34
15	B	615	BCR	C7-C8-C9-C10
12	C	502	CLA	C2C-C3C-CAC-CBC
16	B	618	LMT	C4'-C5'-C6'-O6'
19	B	617	LMG	C4-C5-C6-O5
12	C	504	CLA	O1A-CGA-O2A-C1
12	C	508	CLA	C15-C16-C17-C18
12	C	503	CLA	C15-C16-C17-C18
21	D	406	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	D	406	PL9	C29-C31-C32-C33
12	B	611	CLA	O1A-CGA-O2A-C1
12	A	403	CLA	C15-C16-C17-C18
12	C	510	CLA	C15-C16-C17-C18
14	A	406	PHO	C5-C6-C7-C8
12	B	601	CLA	C2A-CAA-CBA-CGA
12	B	602	CLA	C2A-CAA-CBA-CGA
12	B	605	CLA	C2A-CAA-CBA-CGA
12	C	512	CLA	C2A-CAA-CBA-CGA
15	B	615	BCR	C10-C11-C12-C13
12	B	605	CLA	C5-C6-C7-C8
12	B	613	CLA	C15-C16-C17-C18
12	C	502	CLA	C8-C10-C11-C12
13	A	404	CL7	C5-C6-C7-C8
18	B	616	DGD	C1A-C2A-C3A-C4A
18	B	616	DGD	C1B-C2B-C3B-C4B
16	B	619	LMT	O5'-C1'-O1'-C1
16	C	516	LMT	O5'-C1'-O1'-C1
12	B	601	CLA	C5-C6-C7-C8
12	C	502	CLA	C5-C6-C7-C8
17	C	507	F6C	C8-C10-C11-C12
12	B	613	CLA	C5-C6-C7-C8
12	B	605	CLA	O1D-CGD-O2D-CED
19	B	617	LMG	C10-C11-C12-C13
12	A	407	CLA	C5-C6-C7-C8
12	B	607	CLA	C15-C16-C17-C18
12	C	503	CLA	C8-C10-C11-C12
12	C	510	CLA	CBA-CGA-O2A-C1
16	C	516	LMT	C2'-C1'-O1'-C1
12	B	613	CLA	C16-C17-C18-C19
15	A	408	BCR	C11-C10-C9-C34
15	C	517	BCR	C11-C12-C13-C35
15	A	408	BCR	C17-C18-C19-C20
12	B	609	CLA	C2A-CAA-CBA-CGA
12	C	502	CLA	C15-C16-C17-C18
17	C	507	F6C	C11-C12-C13-C15
22	D	407	LHG	C25-C26-C27-C28
17	B	606	F6C	O1A-CGA-O2A-C1
15	A	408	BCR	C11-C10-C9-C8
17	B	612	F6C	CBA-CGA-O2A-C1
14	D	402	PHO	CBD-CGD-O2D-CED
12	B	613	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
12	B	610	CLA	C6-C7-C8-C9
12	B	613	CLA	C16-C17-C18-C20
16	D	409	LMT	C2-C3-C4-C5
12	B	611	CLA	C8-C10-C11-C12
12	A	405	CLA	C4B-C3B-CAB-CBB
18	C	515	DGD	C1B-C2B-C3B-C4B
12	B	610	CLA	C6-C7-C8-C10
12	C	509	CLA	C16-C17-C18-C19
12	C	510	CLA	C16-C17-C18-C19
17	B	612	F6C	C6-C7-C8-C9
17	B	612	F6C	C6-C7-C8-C10
17	C	507	F6C	C11-C12-C13-C14
18	B	616	DGD	CDA-CEA-CFA-CGA
16	D	409	LMT	O1'-C1-C2-C3
12	B	609	CLA	C3A-C2A-CAA-CBA
12	B	613	CLA	C3A-C2A-CAA-CBA
12	C	506	CLA	C3A-C2A-CAA-CBA
18	C	515	DGD	C8A-C9A-CAA-CBA
12	C	503	CLA	C5-C6-C7-C8
22	D	407	LHG	C28-C29-C30-C31
18	C	515	DGD	C7A-C8A-C9A-CAA
19	B	617	LMG	C29-C30-C31-C32
22	D	407	LHG	C11-C12-C13-C14
15	A	408	BCR	C23-C24-C25-C26
15	A	408	BCR	C23-C24-C25-C30
15	C	514	BCR	C1-C6-C7-C8
15	C	514	BCR	C5-C6-C7-C8
12	B	611	CLA	O1D-CGD-O2D-CED
16	B	618	LMT	O1'-C1-C2-C3
12	A	405	CLA	C2A-CAA-CBA-CGA
12	C	510	CLA	O1A-CGA-O2A-C1
17	B	612	F6C	O1A-CGA-O2A-C1
15	D	405	BCR	C10-C11-C12-C13
13	A	404	CL7	C10-C11-C12-C13
22	D	407	LHG	C13-C14-C15-C16
16	A	409	LMT	C11-C10-C9-C8
18	B	616	DGD	CCA-CDA-CEA-CFA
16	D	409	LMT	C2'-C1'-O1'-C1
16	C	516	LMT	C1-C2-C3-C4
12	C	502	CLA	C4C-C3C-CAC-CBC
18	C	515	DGD	C5A-C6A-C7A-C8A
16	A	409	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
15	B	615	BCR	C11-C12-C13-C35
12	A	407	CLA	C11-C12-C13-C14
12	A	407	CLA	C11-C12-C13-C15
12	C	505	CLA	C16-C17-C18-C20
12	C	509	CLA	C16-C17-C18-C20
12	C	504	CLA	CBD-CGD-O2D-CED
17	B	612	F6C	C4-C3-C5-C6
16	C	516	LMT	C4-C5-C6-C7
12	C	508	CLA	C8-C10-C11-C12
17	C	507	F6C	C4B-C3B-CAB-CBB
22	D	407	LHG	C31-C32-C33-C34
12	C	510	CLA	C16-C17-C18-C20
22	D	407	LHG	C9-C10-C11-C12
22	D	407	LHG	C30-C31-C32-C33
12	C	501	CLA	C2A-CAA-CBA-CGA
12	C	505	CLA	C2A-CAA-CBA-CGA
13	A	404	CL7	C2A-CAA-CBA-CGA
18	C	515	DGD	C6A-C7A-C8A-C9A
12	B	607	CLA	C10-C11-C12-C13
12	A	407	CLA	O1D-CGD-O2D-CED
12	A	405	CLA	C1A-C2A-CAA-CBA
12	A	407	CLA	C1A-C2A-CAA-CBA
12	B	604	CLA	C1A-C2A-CAA-CBA
12	B	605	CLA	C1A-C2A-CAA-CBA
12	B	607	CLA	C1A-C2A-CAA-CBA
12	B	608	CLA	C1A-C2A-CAA-CBA
12	B	609	CLA	C1A-C2A-CAA-CBA
12	B	610	CLA	C1A-C2A-CAA-CBA
12	C	501	CLA	C1A-C2A-CAA-CBA
12	C	506	CLA	C1A-C2A-CAA-CBA
12	C	508	CLA	C1A-C2A-CAA-CBA
12	C	511	CLA	C1A-C2A-CAA-CBA
18	B	616	DGD	C3A-C4A-C5A-C6A
12	B	611	CLA	C15-C16-C17-C18
14	A	406	PHO	C8-C10-C11-C12
22	D	407	LHG	O6-C4-C5-C6
14	D	402	PHO	C3-C5-C6-C7
13	A	404	CL7	C11-C10-C8-C7
17	B	606	F6C	C11-C10-C8-C7
12	B	611	CLA	C10-C11-C12-C13
12	A	407	CLA	C4-C3-C5-C6
12	C	510	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	A	410	LMT	C3-C4-C5-C6
12	C	505	CLA	C5-C6-C7-C8
12	C	510	CLA	C10-C11-C12-C13
12	B	608	CLA	C2A-CAA-CBA-CGA
12	B	613	CLA	C11-C12-C13-C14
13	A	404	CL7	C14-C13-C15-C16
14	A	406	PHO	C6-C7-C8-C9
12	D	403	CLA	C11-C12-C13-C15
12	C	501	CLA	CBA-CGA-O2A-C1
21	D	406	PL9	C22-C23-C24-C25
18	C	515	DGD	O6E-C5E-C6E-O5E
19	D	408	LMG	O6-C5-C6-O5
12	B	602	CLA	C6-C7-C8-C9
12	C	502	CLA	C16-C17-C18-C19
12	C	501	CLA	O1A-CGA-O2A-C1
14	D	402	PHO	CHA-CBD-CGD-O1D
12	C	510	CLA	C2-C3-C5-C6
12	C	508	CLA	C10-C11-C12-C13
16	A	410	LMT	O5'-C5'-C6'-O6'
17	B	603	F6C	C2C-C3C-CAC-CBC
17	C	507	F6C	C1A-C2A-CAA-CBA
15	B	615	BCR	C11-C10-C9-C8
12	B	604	CLA	C2C-C3C-CAC-CBC
21	D	406	PL9	C15-C14-C16-C17
12	A	407	CLA	C2-C3-C5-C6
18	B	616	DGD	C5B-C6B-C7B-C8B
22	D	407	LHG	C29-C30-C31-C32
18	C	515	DGD	C3A-C4A-C5A-C6A
18	B	616	DGD	C4A-C5A-C6A-C7A
16	A	410	LMT	O1'-C1-C2-C3
12	C	503	CLA	C2A-CAA-CBA-CGA
16	B	619	LMT	O1'-C1-C2-C3
18	C	515	DGD	O6D-C5D-C6D-O5D
18	B	616	DGD	C4B-C5B-C6B-C7B
12	A	403	CLA	CBA-CGA-O2A-C1
12	B	610	CLA	CBA-CGA-O2A-C1
12	B	613	CLA	C11-C10-C8-C9
12	C	505	CLA	C6-C7-C8-C9
12	C	505	CLA	C11-C12-C13-C14
12	C	508	CLA	C6-C7-C8-C9
12	C	508	CLA	C11-C10-C8-C9
12	C	508	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	A	404	CL7	C11-C10-C8-C9
17	B	606	F6C	C11-C10-C8-C9
12	C	501	CLA	C4B-C3B-CAB-CBB
16	C	516	LMT	C2-C3-C4-C5
17	B	612	F6C	C3A-C2A-CAA-CBA
12	C	505	CLA	C13-C15-C16-C17
12	D	403	CLA	C11-C12-C13-C14
18	B	616	DGD	CBA-CCA-CDA-CEA
16	C	516	LMT	C3-C4-C5-C6
12	B	607	CLA	C11-C10-C8-C7
12	B	611	CLA	C12-C13-C15-C16
12	C	505	CLA	C6-C7-C8-C10
12	C	505	CLA	C11-C12-C13-C15
12	C	508	CLA	C6-C7-C8-C10
12	C	508	CLA	C11-C10-C8-C7
12	C	508	CLA	C11-C12-C13-C15
14	A	406	PHO	C6-C7-C8-C10
14	A	406	PHO	C11-C10-C8-C7
19	D	408	LMG	C28-C29-C30-C31
22	D	407	LHG	C19-C20-C21-C22
12	A	405	CLA	C3A-C2A-CAA-CBA
12	B	604	CLA	C3A-C2A-CAA-CBA
12	C	512	CLA	C3A-C2A-CAA-CBA
12	C	502	CLA	CBA-CGA-O2A-C1
18	B	616	DGD	C7A-C8A-C9A-CAA
22	D	407	LHG	C4-C5-C6-O8
13	A	404	CL7	C8-C10-C11-C12
16	D	409	LMT	C1-C2-C3-C4
15	C	514	BCR	C23-C24-C25-C30
15	C	517	BCR	C1-C6-C7-C8
15	D	405	BCR	C1-C6-C7-C8
18	C	515	DGD	C4D-C5D-C6D-O5D
12	C	502	CLA	C16-C17-C18-C20
18	B	616	DGD	CFA-CGA-CHA-CIA
14	D	402	PHO	O1D-CGD-O2D-CED
12	C	506	CLA	C5-C6-C7-C8
13	A	404	CL7	C2C-C3C-CAC-CBC
12	C	506	CLA	CBA-CGA-O2A-C1
12	B	605	CLA	C6-C7-C8-C10
16	A	409	LMT	C9-C10-C11-C12
13	A	404	CL7	C15-C16-C17-C18
15	B	615	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
12	C	503	CLA	C16-C17-C18-C19
12	C	505	CLA	C16-C17-C18-C19
12	A	407	CLA	C8-C10-C11-C12
12	C	509	CLA	C6-C7-C8-C10
15	A	408	BCR	C11-C12-C13-C14
15	B	615	BCR	C11-C12-C13-C14
15	C	517	BCR	C11-C12-C13-C14
12	A	403	CLA	O1A-CGA-O2A-C1
13	A	404	CL7	C4-C3-C5-C6
12	C	502	CLA	O1A-CGA-O2A-C1
12	C	506	CLA	O1A-CGA-O2A-C1
14	A	406	PHO	C10-C11-C12-C13
15	C	514	BCR	C19-C20-C21-C22
12	B	601	CLA	C6-C7-C8-C9
12	B	602	CLA	C6-C7-C8-C10
12	B	610	CLA	O1A-CGA-O2A-C1
22	D	407	LHG	C14-C15-C16-C17
18	C	515	DGD	C2B-C3B-C4B-C5B
12	C	505	CLA	C15-C16-C17-C18
17	B	612	F6C	C2-C3-C5-C6
16	C	516	LMT	C7-C8-C9-C10
12	B	613	CLA	C6-C7-C8-C9
18	B	616	DGD	C6B-C7B-C8B-C9B
12	C	504	CLA	O1D-CGD-O2D-CED
17	C	507	F6C	C3A-C2A-CAA-CBA
12	B	604	CLA	C4-C3-C5-C6
12	C	503	CLA	C4B-C3B-CAB-CBB
17	B	603	F6C	C4C-C3C-CAC-CBC
12	C	510	CLA	C12-C13-C15-C16
12	B	604	CLA	C6-C7-C8-C10
19	B	617	LMG	O9-C10-O7-C8
19	B	617	LMG	C11-C10-O7-C8
12	B	607	CLA	C11-C10-C8-C9
12	B	602	CLA	C5-C6-C7-C8
12	B	601	CLA	C6-C7-C8-C10
17	B	606	F6C	C1B-C2B-CMB-OMB
22	D	407	LHG	O7-C5-C6-O8
16	D	409	LMT	C3-C4-C5-C6
12	B	607	CLA	C4-C3-C5-C6
12	C	502	CLA	CAD-CBD-CGD-O2D
12	C	504	CLA	CAD-CBD-CGD-O2D
12	C	505	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	B	606	F6C	CAD-CBD-CGD-O2D
19	B	617	LMG	C11-C12-C13-C14
16	C	516	LMT	C11-C10-C9-C8
12	B	611	CLA	CAD-CBD-CGD-O1D
12	C	502	CLA	CAD-CBD-CGD-O1D
12	C	504	CLA	CAD-CBD-CGD-O1D
12	C	505	CLA	CAD-CBD-CGD-O1D
12	C	512	CLA	CAD-CBD-CGD-O1D
15	D	405	BCR	C9-C10-C11-C12
17	B	606	F6C	CAD-CBD-CGD-O1D
17	B	612	F6C	CHA-CBD-CGD-O1D
17	B	612	F6C	CHA-CBD-CGD-O2D
22	D	407	LHG	C4-O6-P-O5
12	A	405	CLA	C2B-C3B-CAB-CBB
21	D	406	PL9	C13-C14-C16-C17
12	C	508	CLA	C16-C17-C18-C20
12	B	605	CLA	C6-C7-C8-C9
12	B	605	CLA	C4-C3-C5-C6
12	B	613	CLA	C10-C11-C12-C13
12	B	611	CLA	C14-C13-C15-C16
12	B	613	CLA	C6-C7-C8-C10
17	B	603	F6C	C3A-C2A-CAA-CBA
17	B	612	F6C	C1A-C2A-CAA-CBA
17	C	507	F6C	CBD-CGD-O2D-CED
17	B	612	F6C	C5-C6-C7-C8
19	D	408	LMG	O1-C7-C8-O7
12	D	403	CLA	O1A-CGA-O2A-C1
22	D	407	LHG	C10-C11-C12-C13
16	B	618	LMT	C6-C7-C8-C9
12	B	601	CLA	CAA-CBA-CGA-O2A
12	C	510	CLA	C14-C13-C15-C16
16	B	618	LMT	C3-C4-C5-C6
12	B	601	CLA	C4B-C3B-CAB-CBB
23	F	101	HEM	C3D-CAD-CBD-CGD
12	C	503	CLA	C16-C17-C18-C20
12	B	605	CLA	C2-C3-C5-C6
19	D	408	LMG	C29-C30-C31-C32
22	D	407	LHG	C24-C25-C26-C27
12	B	610	CLA	C3-C5-C6-C7
18	C	515	DGD	O2G-C2G-C3G-O3G
12	C	505	CLA	C4-C3-C5-C6
15	C	517	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	C	512	CLA	O1D-CGD-O2D-CED
12	B	610	CLA	C4-C3-C5-C6
12	B	607	CLA	C2-C3-C5-C6
12	C	508	CLA	C2A-CAA-CBA-CGA
18	C	515	DGD	C1G-C2G-C3G-O3G
12	C	508	CLA	C14-C13-C15-C16
17	C	507	F6C	O1D-CGD-O2D-CED
12	C	512	CLA	C1A-C2A-CAA-CBA
12	B	611	CLA	C16-C17-C18-C19
22	D	407	LHG	C27-C28-C29-C30
12	B	601	CLA	C2B-C3B-CAB-CBB
12	B	613	CLA	C2B-C3B-CAB-CBB
12	C	503	CLA	C2B-C3B-CAB-CBB
15	C	514	BCR	C23-C24-C25-C26
15	C	517	BCR	C5-C6-C7-C8
15	C	517	BCR	C23-C24-C25-C26
15	C	517	BCR	C23-C24-C25-C30
15	D	405	BCR	C5-C6-C7-C8
13	A	404	CL7	C13-C15-C16-C17
12	C	503	CLA	C4-C3-C5-C6
16	D	409	LMT	C4-C5-C6-C7
17	B	603	F6C	C2A-CAA-CBA-CGA
12	C	502	CLA	C6-C7-C8-C10
12	C	508	CLA	C12-C13-C15-C16
12	C	510	CLA	C11-C10-C8-C7
12	B	609	CLA	CAA-CBA-CGA-O2A
12	D	403	CLA	CBA-CGA-O2A-C1
12	B	609	CLA	CAA-CBA-CGA-O1A
15	D	405	BCR	C17-C18-C19-C20
21	D	406	PL9	C30-C29-C31-C32
12	B	604	CLA	C2-C3-C5-C6
12	B	610	CLA	C2-C3-C5-C6
12	C	512	CLA	CBD-CGD-O2D-CED
12	C	505	CLA	C8-C10-C11-C12
17	B	606	F6C	C10-C11-C12-C13
12	C	505	CLA	C2-C3-C5-C6
13	A	404	CL7	C4C-C3C-CAC-CBC
12	B	602	CLA	C4B-C3B-CAB-CBB
12	B	613	CLA	C4B-C3B-CAB-CBB
12	C	509	CLA	C8-C10-C11-C12
12	B	613	CLA	C4-C3-C5-C6
12	C	505	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	D	407	LHG	C2-C3-O3-P
22	D	407	LHG	C11-C10-C9-C8
12	C	501	CLA	C13-C15-C16-C17
18	B	616	DGD	C5A-C6A-C7A-C8A
12	C	503	CLA	C3A-C2A-CAA-CBA
16	C	516	LMT	O1'-C1-C2-C3
12	C	501	CLA	C8-C10-C11-C12
12	C	509	CLA	C13-C15-C16-C17
12	A	407	CLA	C3-C5-C6-C7
12	C	501	CLA	C3-C5-C6-C7
12	B	608	CLA	CAA-CBA-CGA-O1A
12	B	608	CLA	CAA-CBA-CGA-O2A
12	A	403	CLA	C6-C7-C8-C10
12	A	407	CLA	C6-C7-C8-C10
12	C	505	CLA	C12-C13-C15-C16
13	A	404	CL7	C6-C7-C8-C10
12	C	501	CLA	C2B-C3B-CAB-CBB
12	C	508	CLA	C2B-C3B-CAB-CBB
15	B	615	BCR	C23-C24-C25-C26
15	B	615	BCR	C23-C24-C25-C30
12	D	404	CLA	CAA-CBA-CGA-O1A
16	B	618	LMT	C5-C6-C7-C8
12	B	604	CLA	C4C-C3C-CAC-CBC
13	A	404	CL7	C2-C3-C5-C6
12	B	611	CLA	CAA-CBA-CGA-O2A
12	B	610	CLA	C5-C6-C7-C8
12	D	404	CLA	CAA-CBA-CGA-O2A
12	C	510	CLA	CAA-CBA-CGA-O2A
12	C	510	CLA	C11-C10-C8-C9
16	A	409	LMT	C4-C5-C6-C7
17	B	606	F6C	CAA-CBA-CGA-O2A
15	C	517	BCR	C19-C20-C21-C22
19	B	617	LMG	O10-C28-O8-C9
16	B	618	LMT	C4-C5-C6-C7
15	D	405	BCR	C36-C18-C19-C20
12	C	510	CLA	C2-C1-O2A-CGA
12	C	509	CLA	C11-C12-C13-C15
12	C	510	CLA	C6-C7-C8-C10
17	C	507	F6C	C6-C7-C8-C10
16	C	516	LMT	C5'-C4'-O1B-C1B
12	B	611	CLA	CAA-CBA-CGA-O1A
19	B	617	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
12	A	403	CLA	C6-C7-C8-C9
12	B	607	CLA	C13-C15-C16-C17
12	C	510	CLA	CAA-CBA-CGA-O1A
18	C	515	DGD	C5D-C6D-O5D-C1E
19	D	408	LMG	C8-C7-O1-C1
12	C	512	CLA	CAA-CBA-CGA-O2A
12	C	513	CLA	CAA-CBA-CGA-O2A
23	F	101	HEM	CAA-CBA-CGA-O2A
12	C	510	CLA	CAD-CBD-CGD-O2D
17	C	507	F6C	CAD-CBD-CGD-O2D
23	F	101	HEM	CAA-CBA-CGA-O1A
17	C	507	F6C	C5-C6-C7-C8
18	C	515	DGD	O6E-C1E-O5D-C6D
14	D	402	PHO	C8-C10-C11-C12
16	A	409	LMT	C7-C8-C9-C10
12	C	506	CLA	CAA-CBA-CGA-O2A
18	C	515	DGD	C2A-C3A-C4A-C5A
22	D	407	LHG	C26-C27-C28-C29

There are no ring outliers.

47 monomers are involved in 142 short contacts:

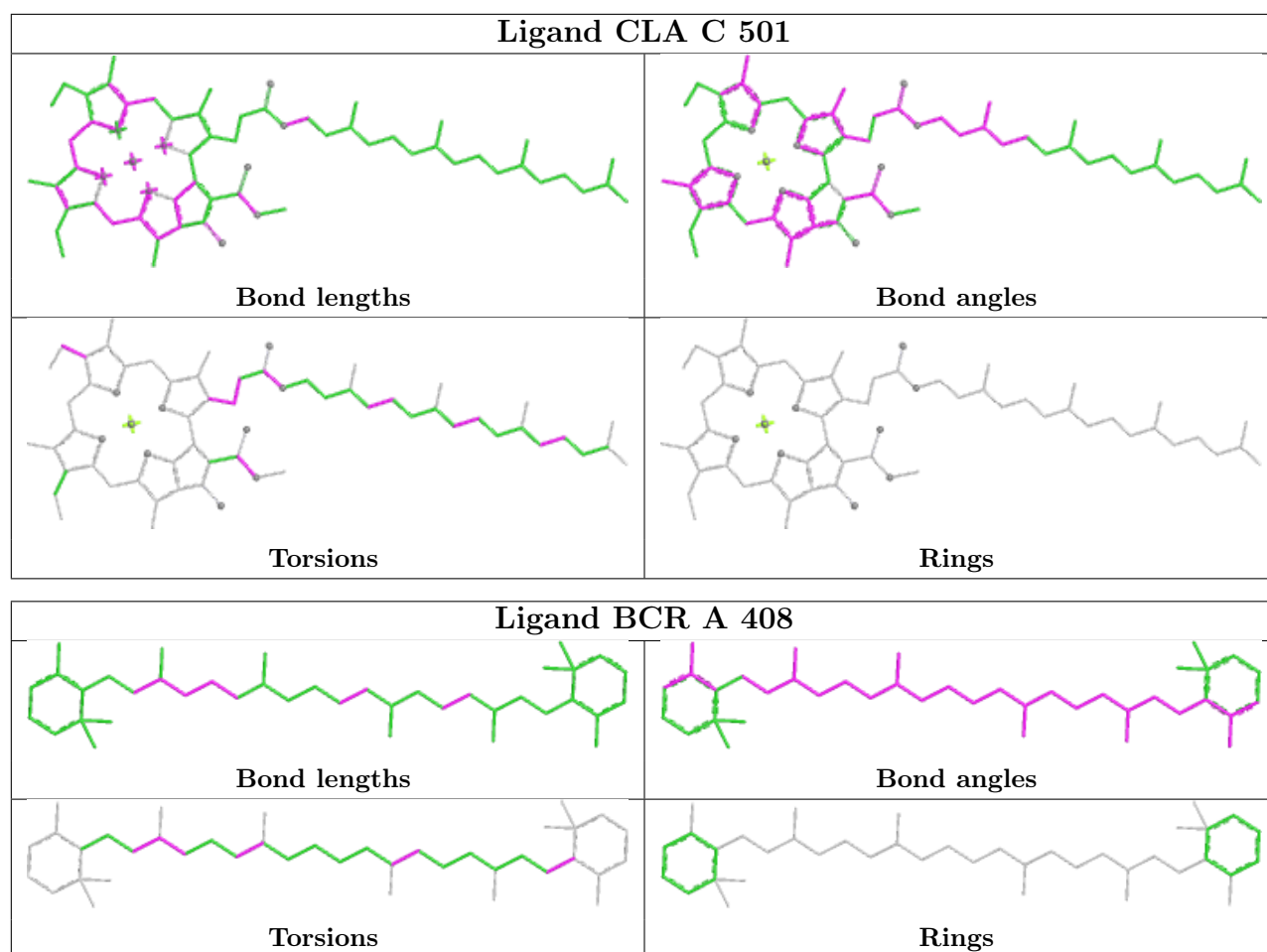
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	501	CLA	4	0
15	A	408	BCR	5	0
12	D	404	CLA	1	0
12	C	503	CLA	9	0
15	C	517	BCR	4	0
12	B	604	CLA	14	0
14	A	406	PHO	5	0
12	C	502	CLA	4	0
12	C	513	CLA	1	0
18	C	515	DGD	2	0
15	C	514	BCR	2	0
17	B	603	F6C	5	0
12	A	405	CLA	2	0
12	B	602	CLA	6	0
13	A	404	CL7	3	0
17	B	612	F6C	3	0
12	C	506	CLA	2	0
19	B	617	LMG	1	0
12	B	607	CLA	5	0

Continued on next page...

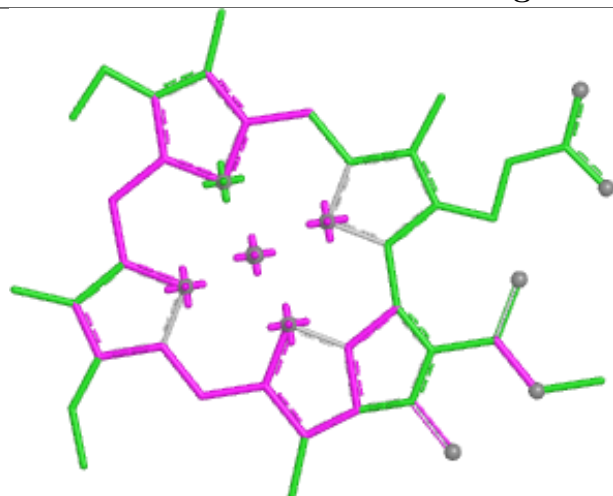
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	507	F6C	2	0
21	D	406	PL9	4	0
23	F	101	HEM	4	0
12	B	605	CLA	3	0
19	D	408	LMG	2	0
16	A	409	LMT	2	0
12	C	511	CLA	2	0
12	B	609	CLA	1	0
12	C	505	CLA	6	0
12	B	610	CLA	4	0
12	A	407	CLA	5	0
22	D	407	LHG	7	0
12	C	508	CLA	9	0
12	D	403	CLA	2	0
16	C	516	LMT	2	0
12	B	611	CLA	5	0
12	B	614	CLA	1	0
12	A	403	CLA	5	0
16	A	410	LMT	1	0
14	D	402	PHO	2	0
12	C	510	CLA	2	0
15	B	615	BCR	2	0
15	D	405	BCR	1	0
18	B	616	DGD	1	0
16	B	619	LMT	1	0
12	C	509	CLA	4	0
12	B	613	CLA	3	0
12	B	601	CLA	2	0

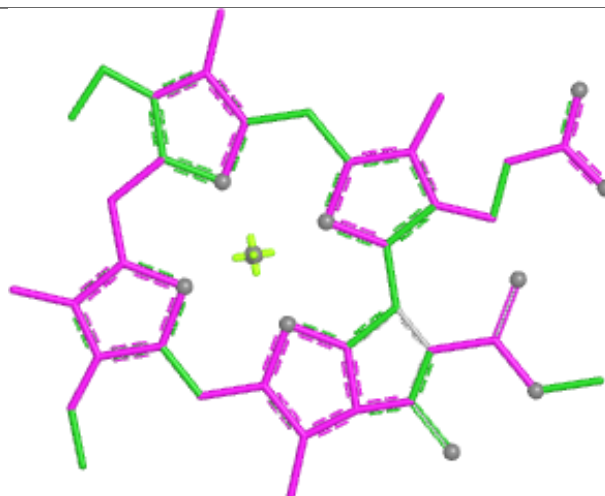
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



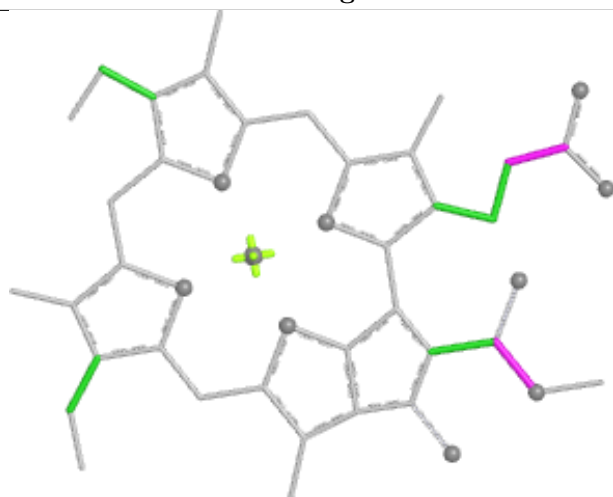
Ligand CLA D 404



Bond lengths



Bond angles

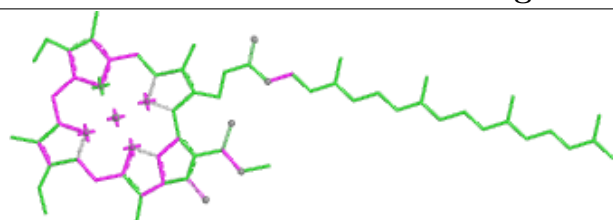


Torsions

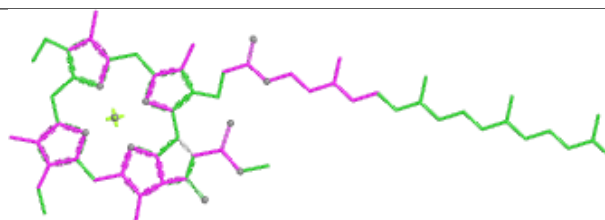


Rings

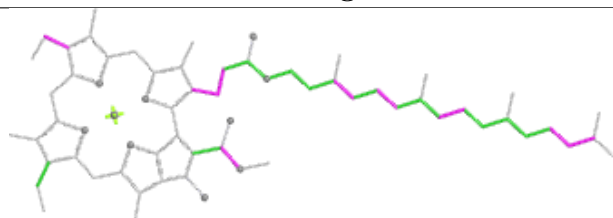
Ligand CLA C 503



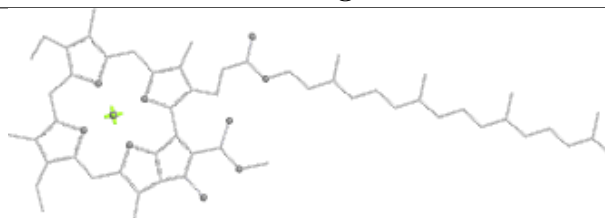
Bond lengths



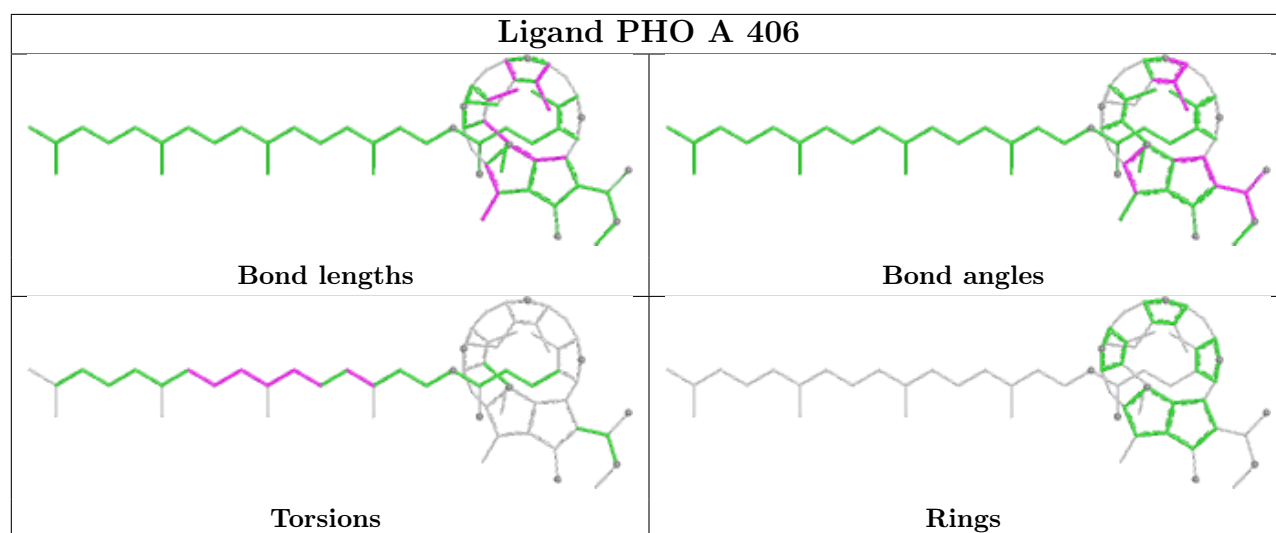
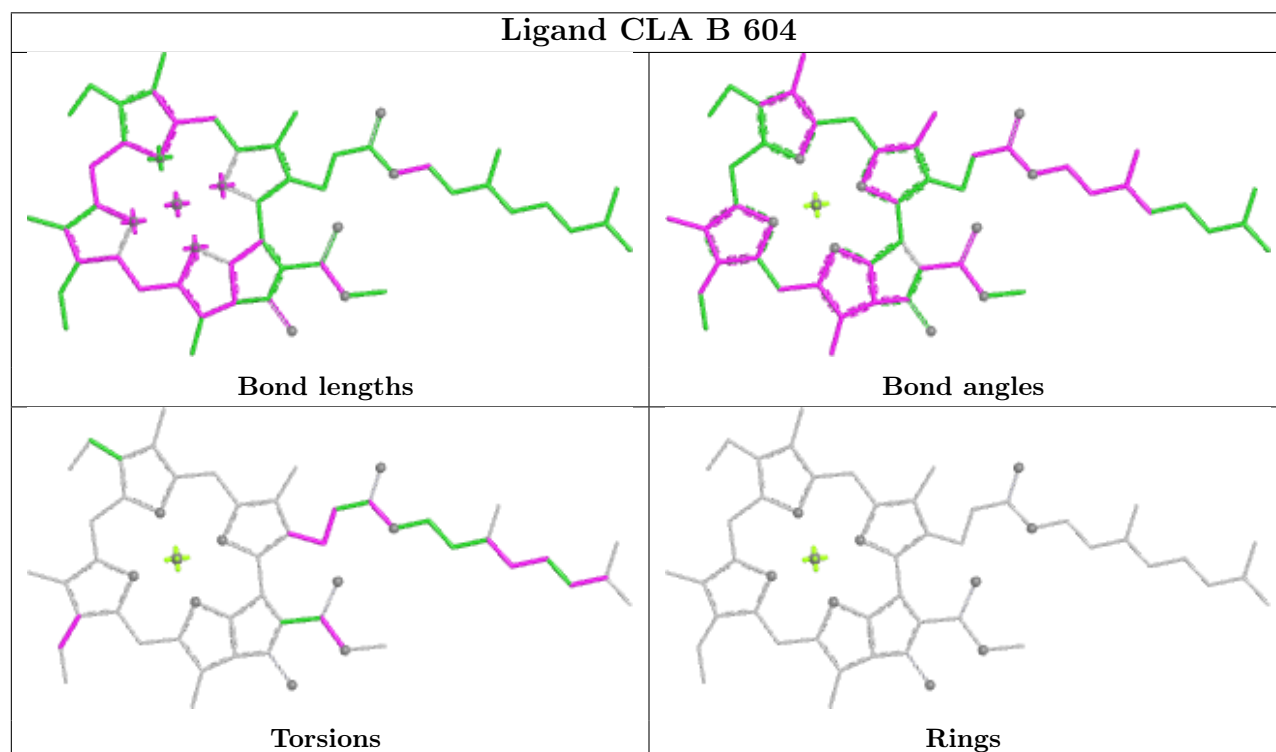
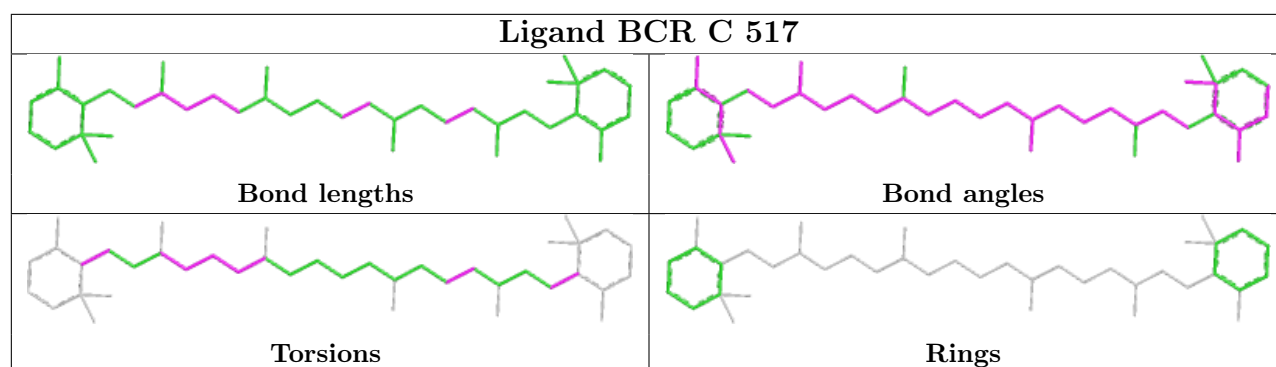
Bond angles

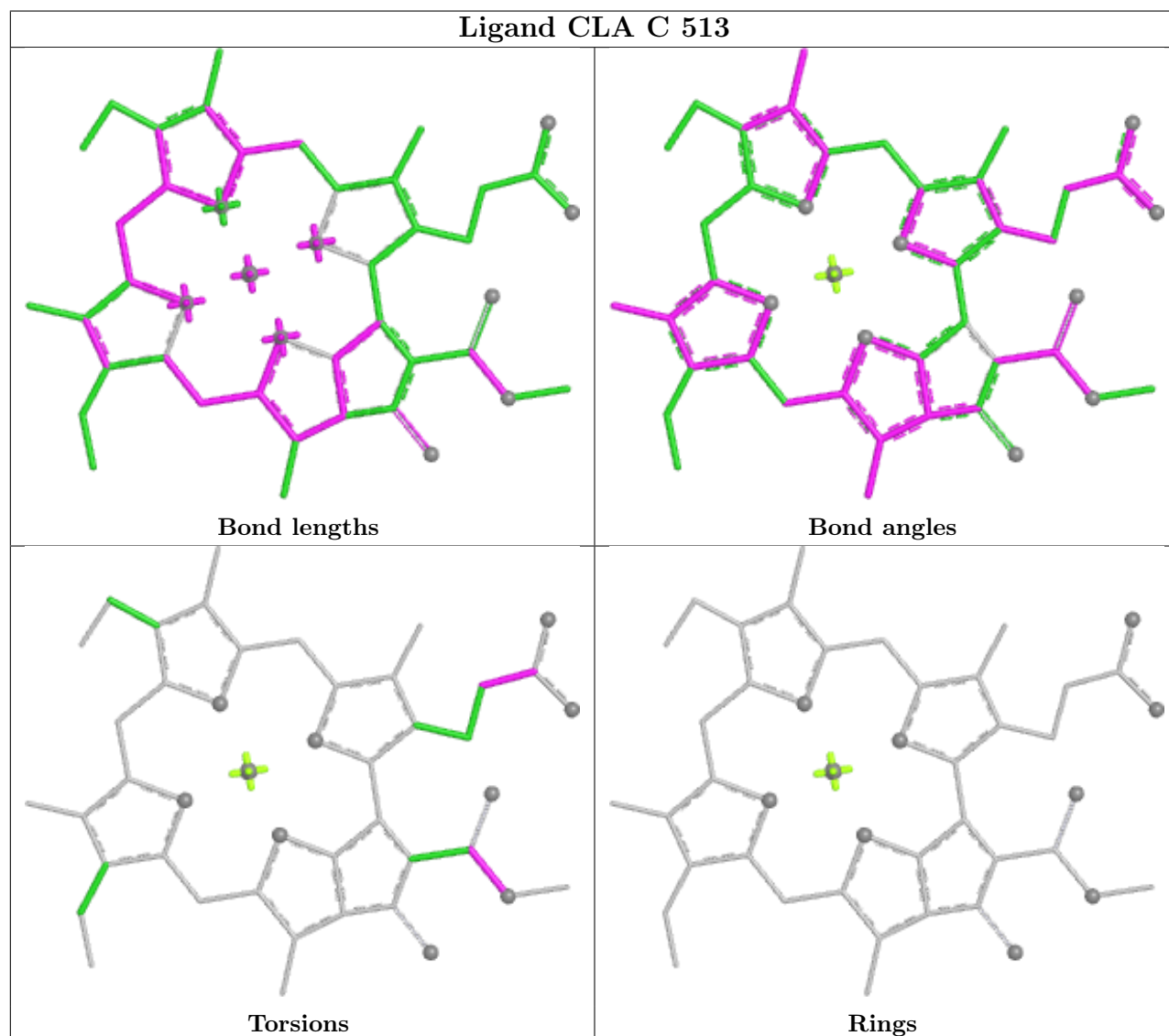
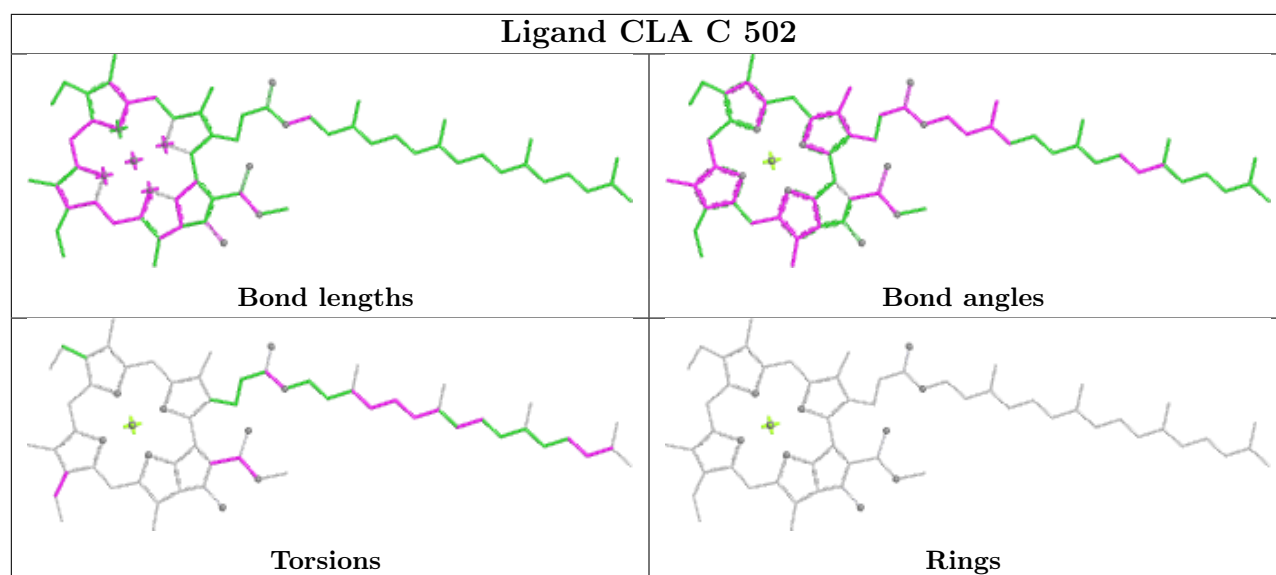


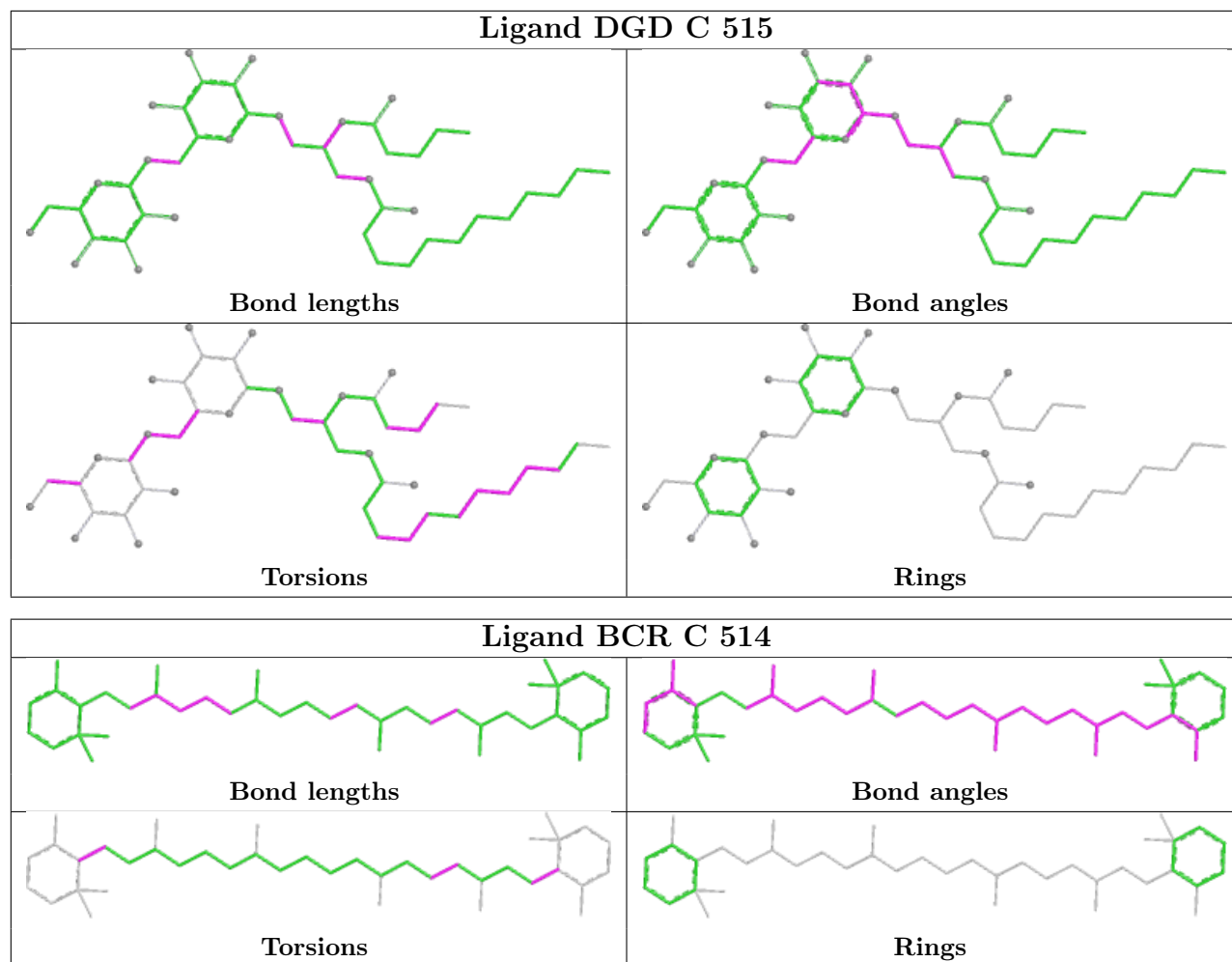
Torsions

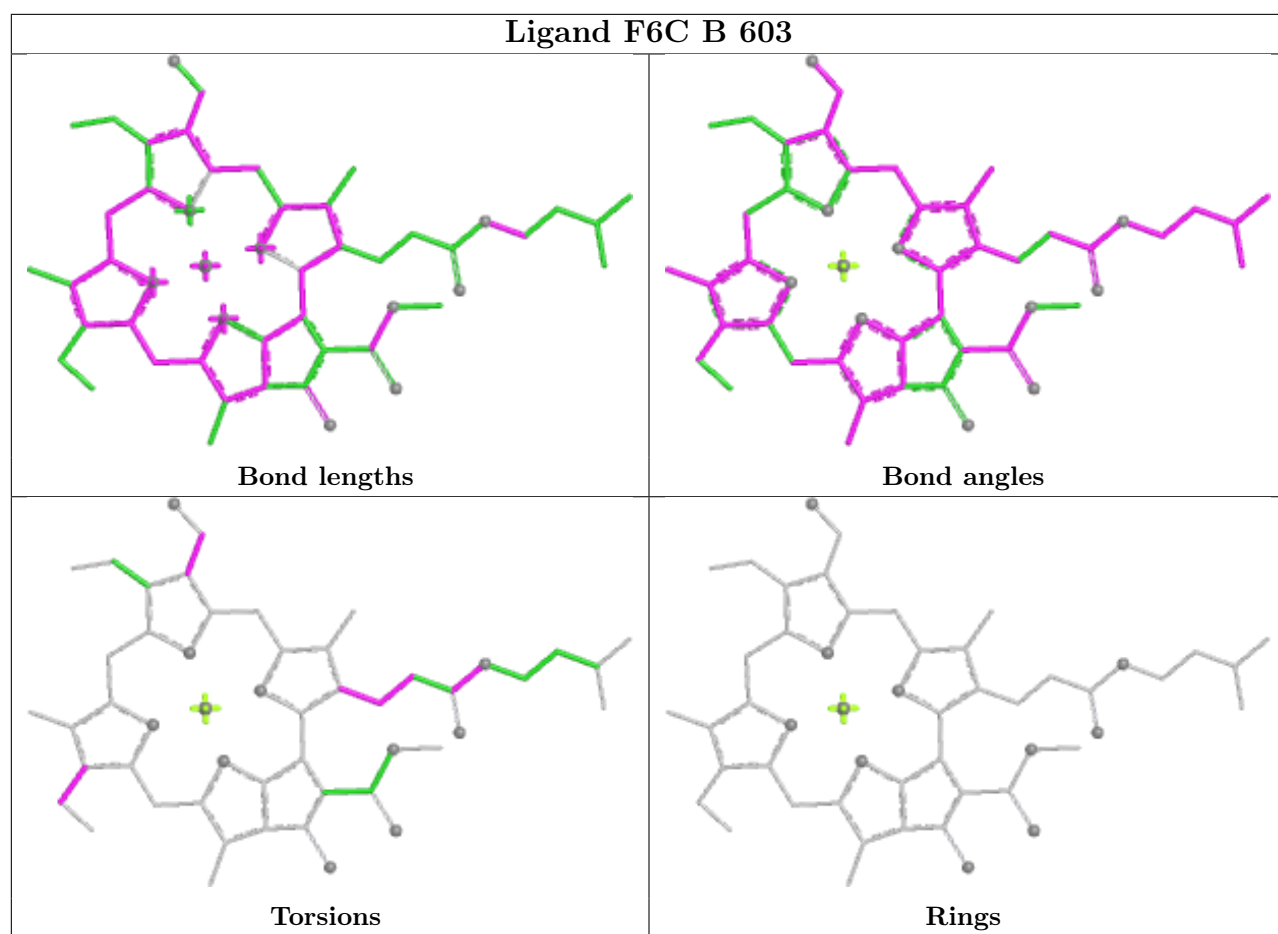


Rings

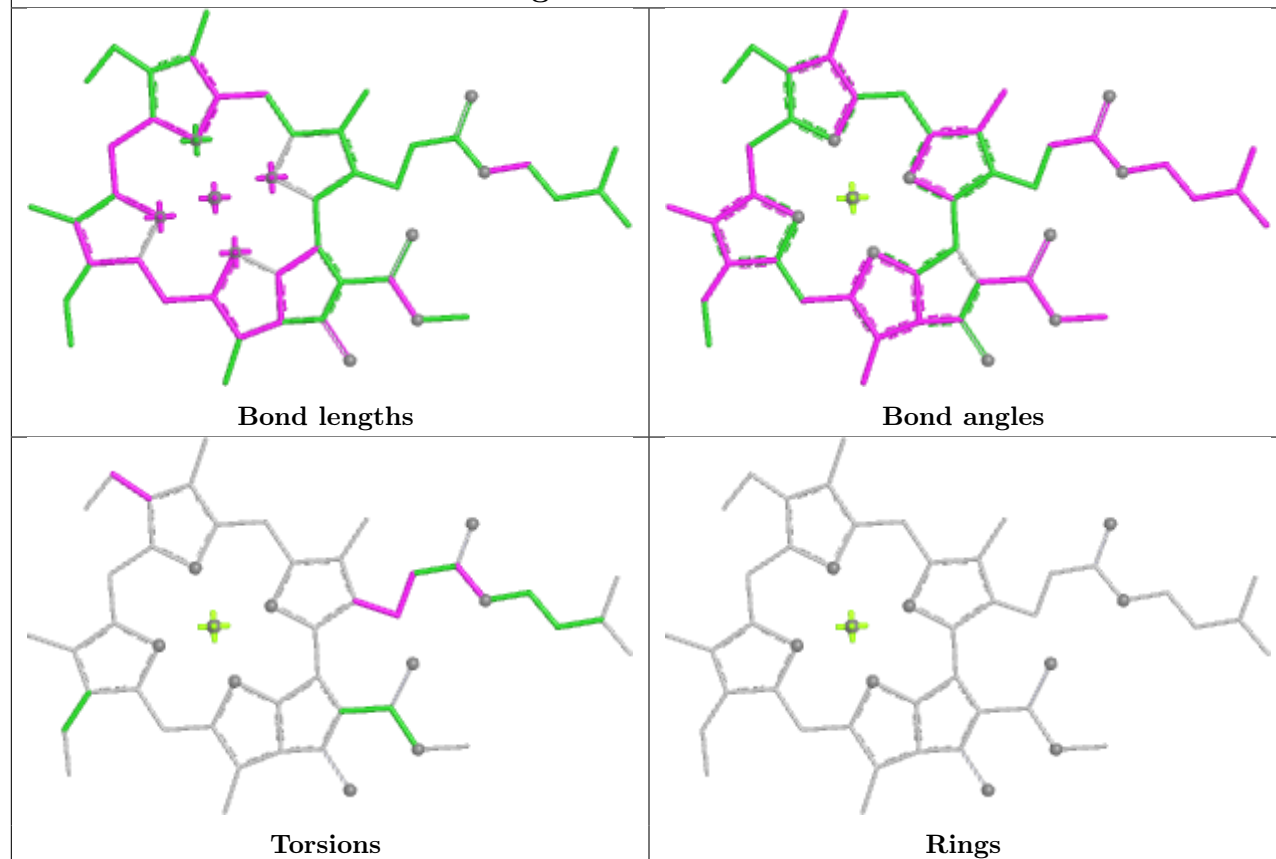




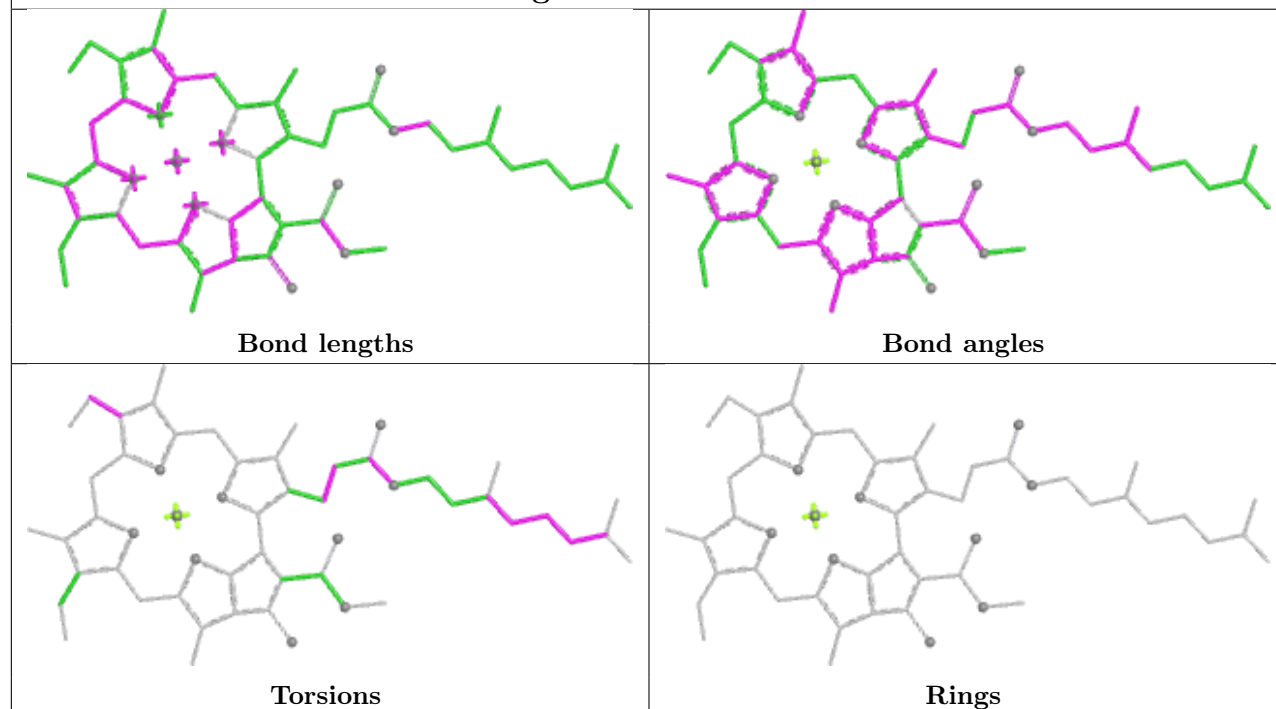


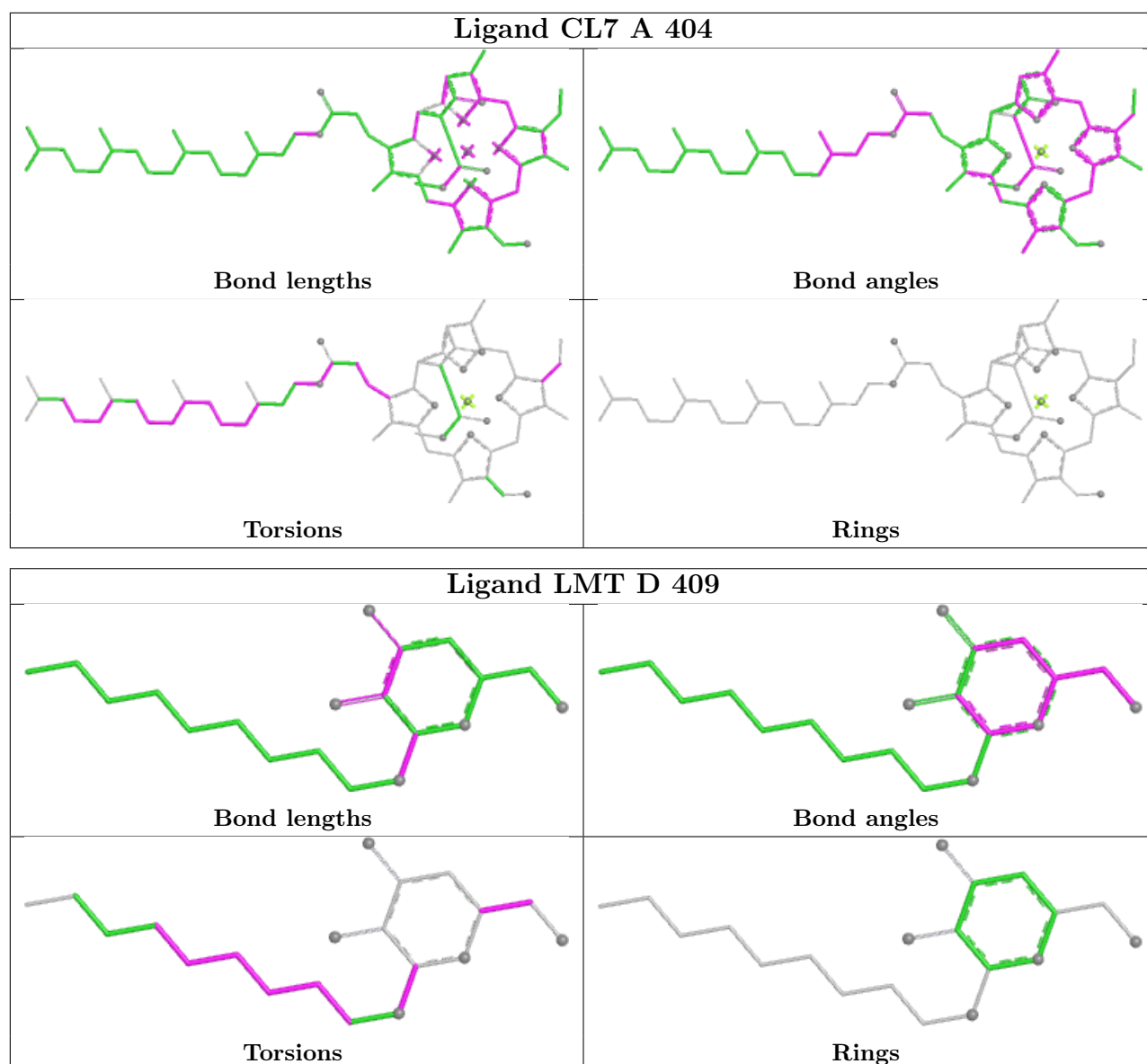


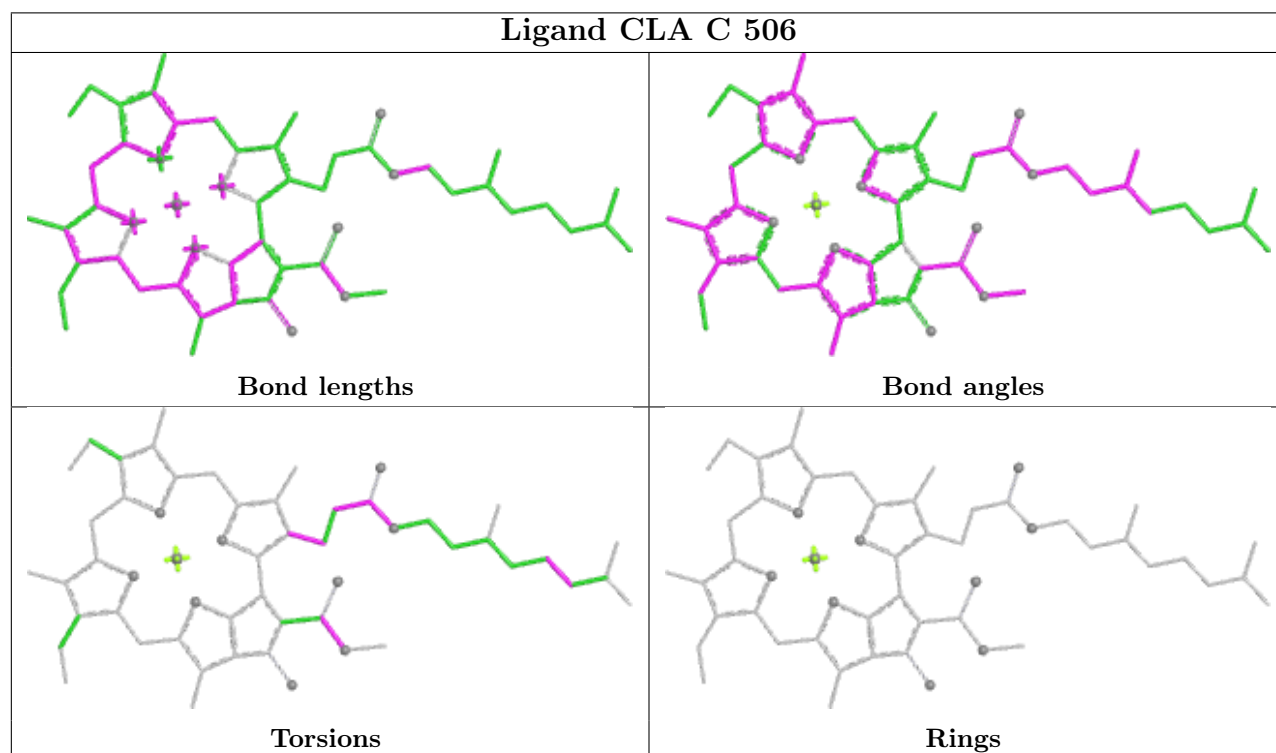
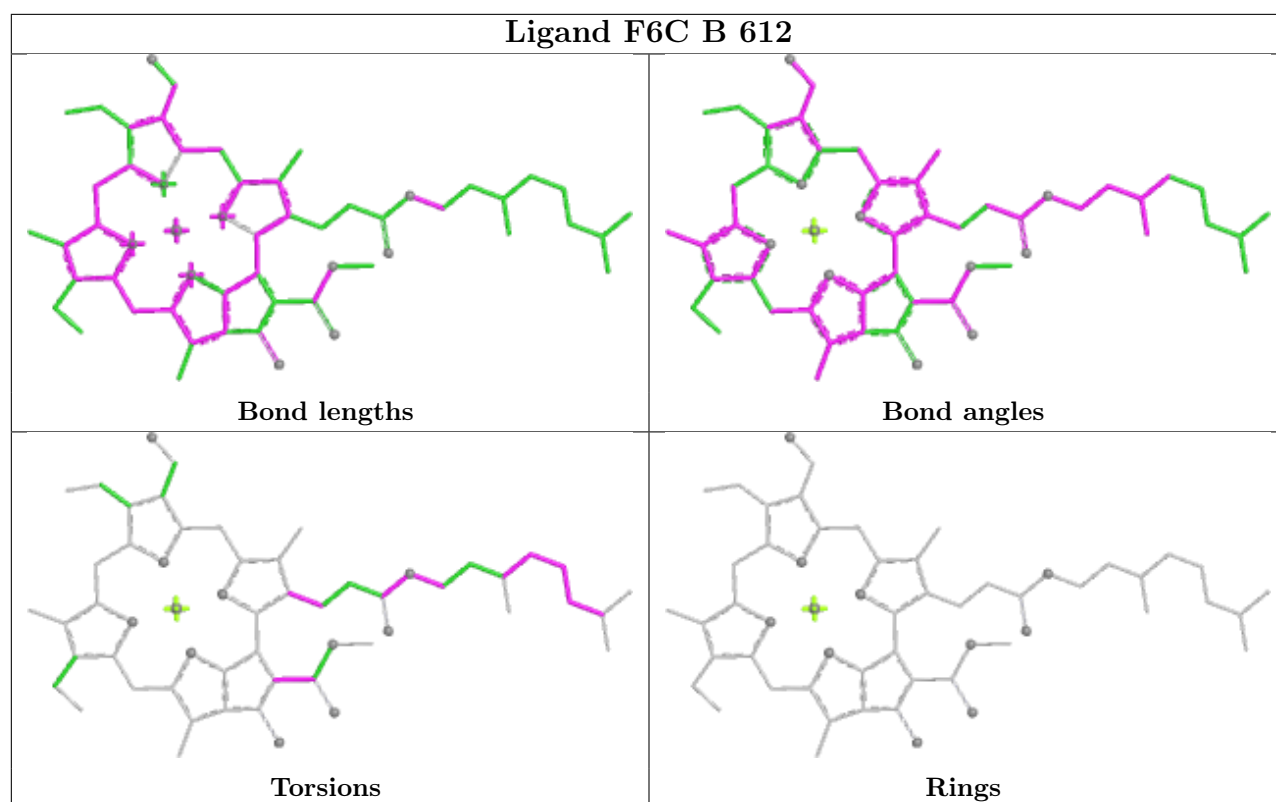
Ligand CLA A 405

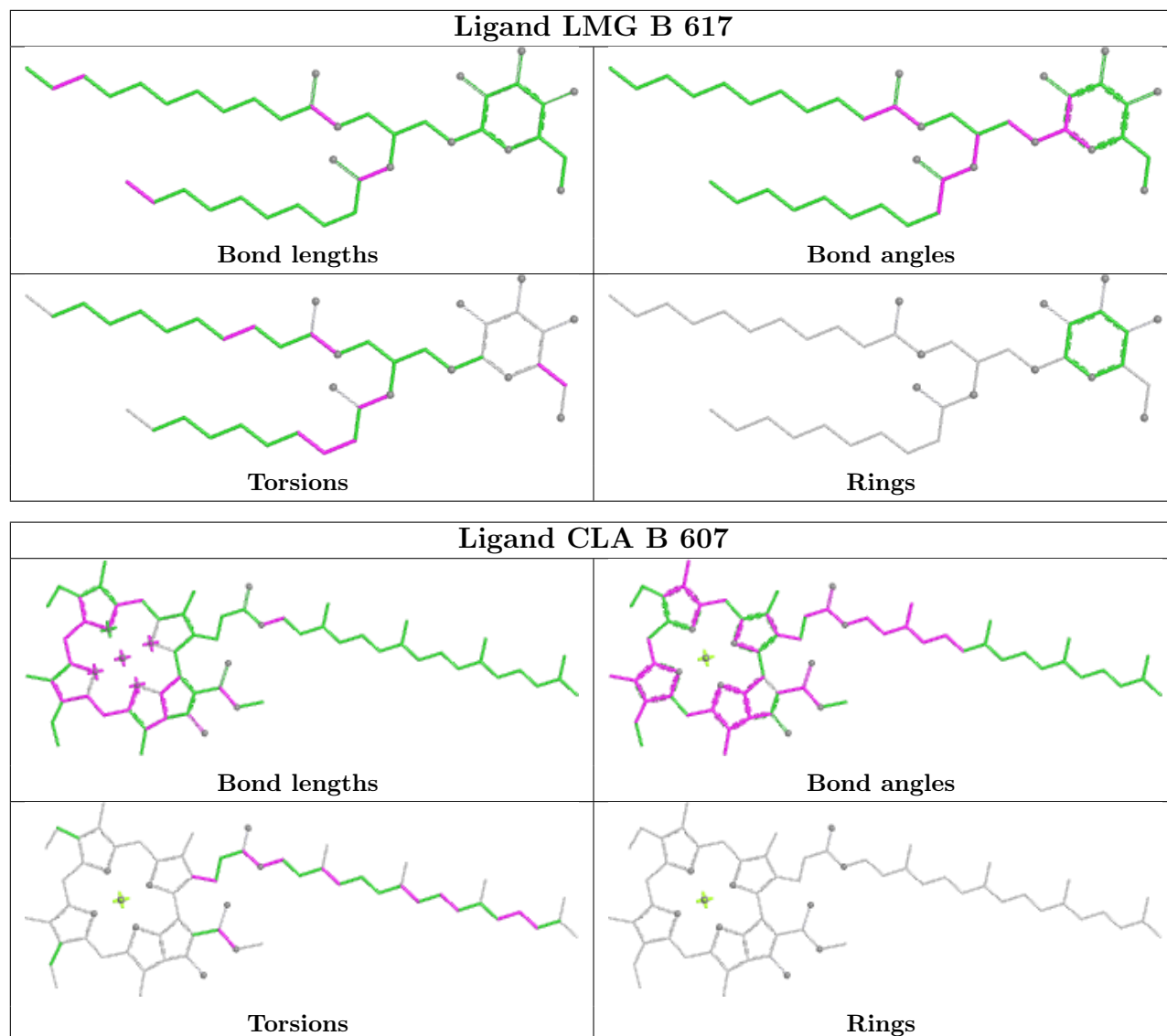


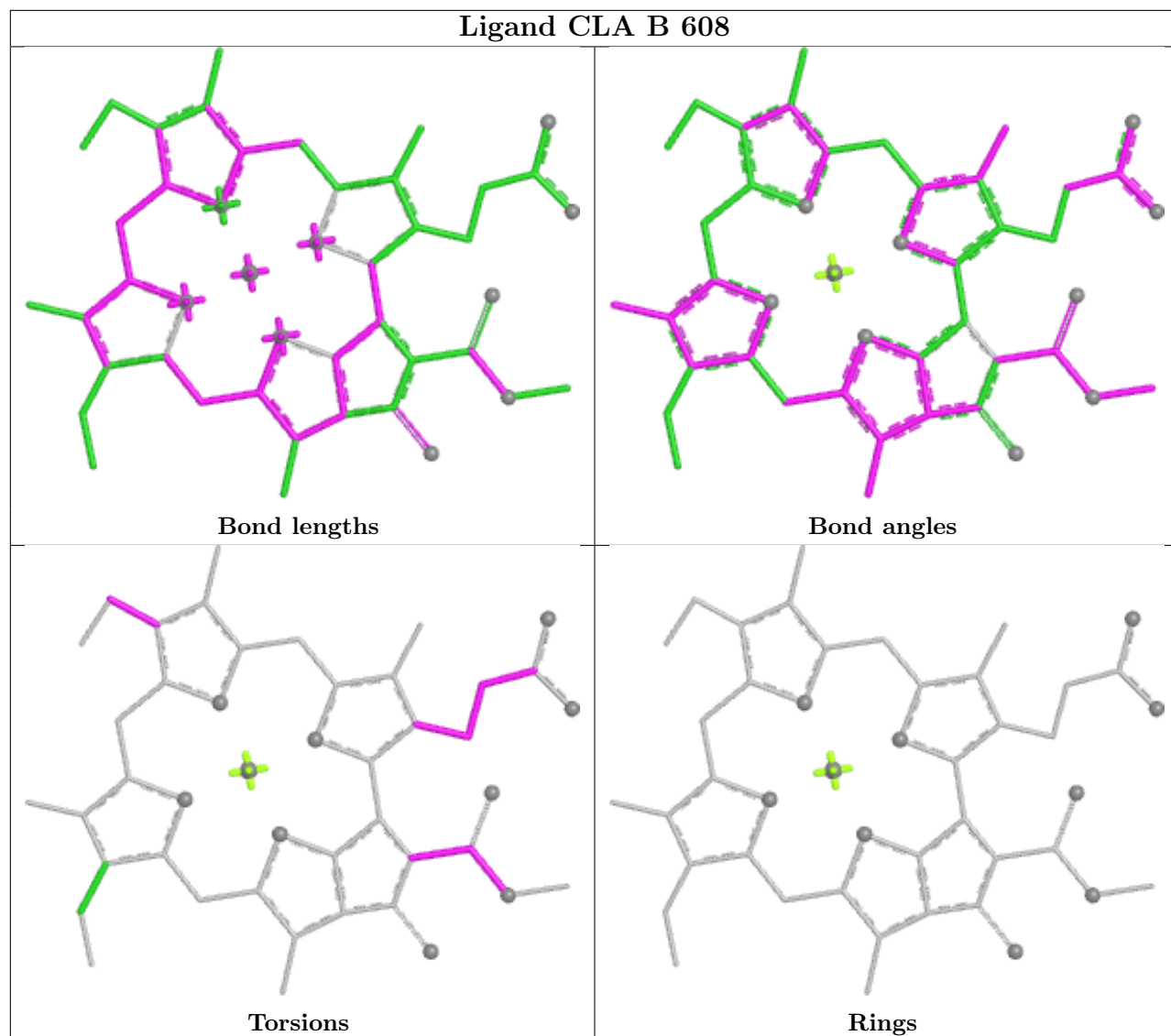
Ligand CLA B 602

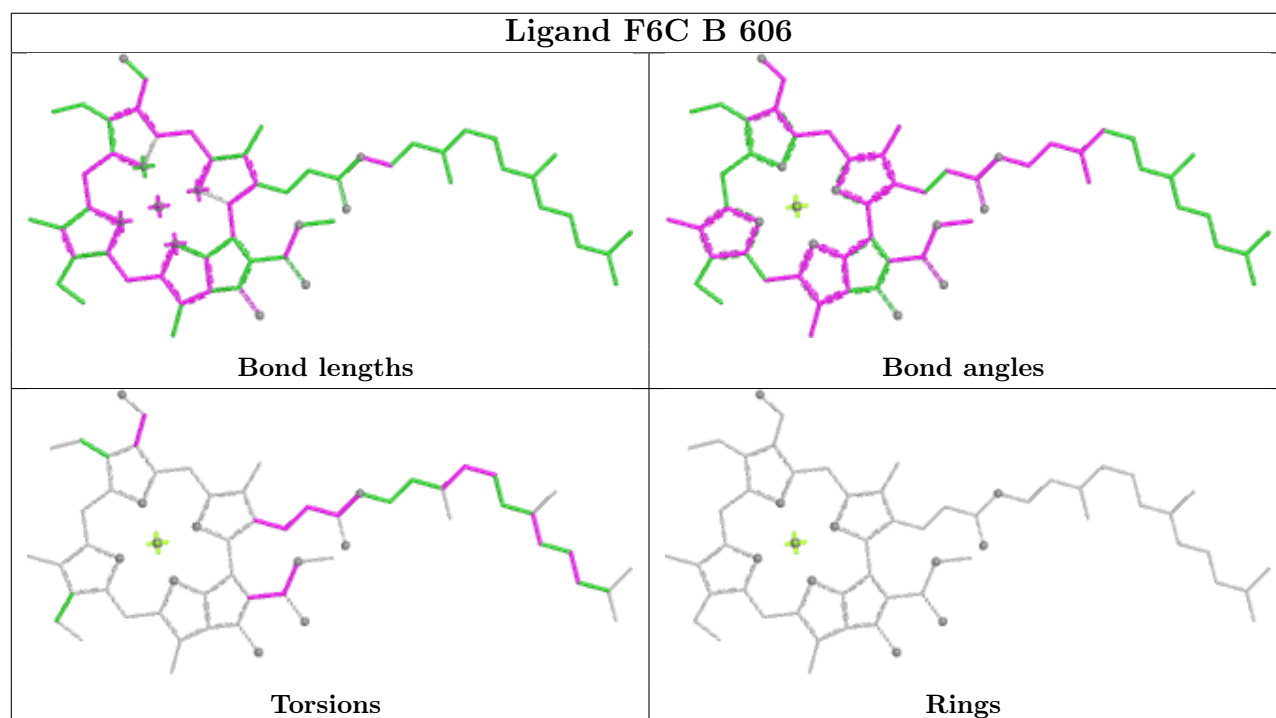
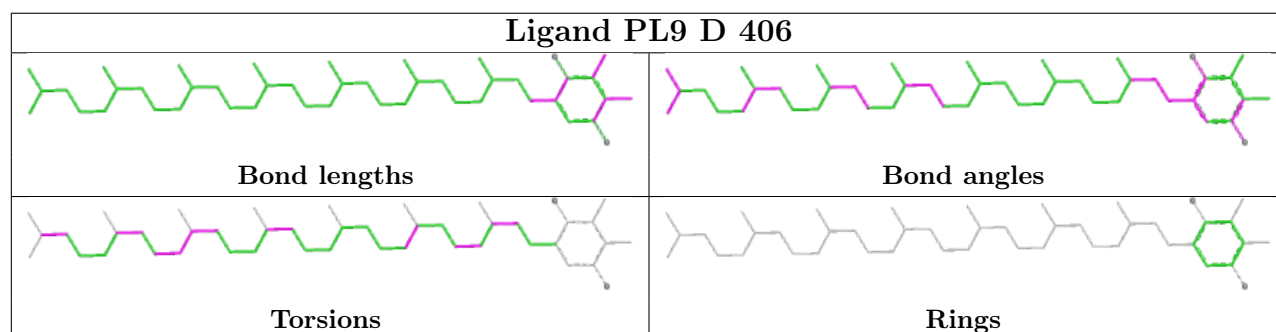
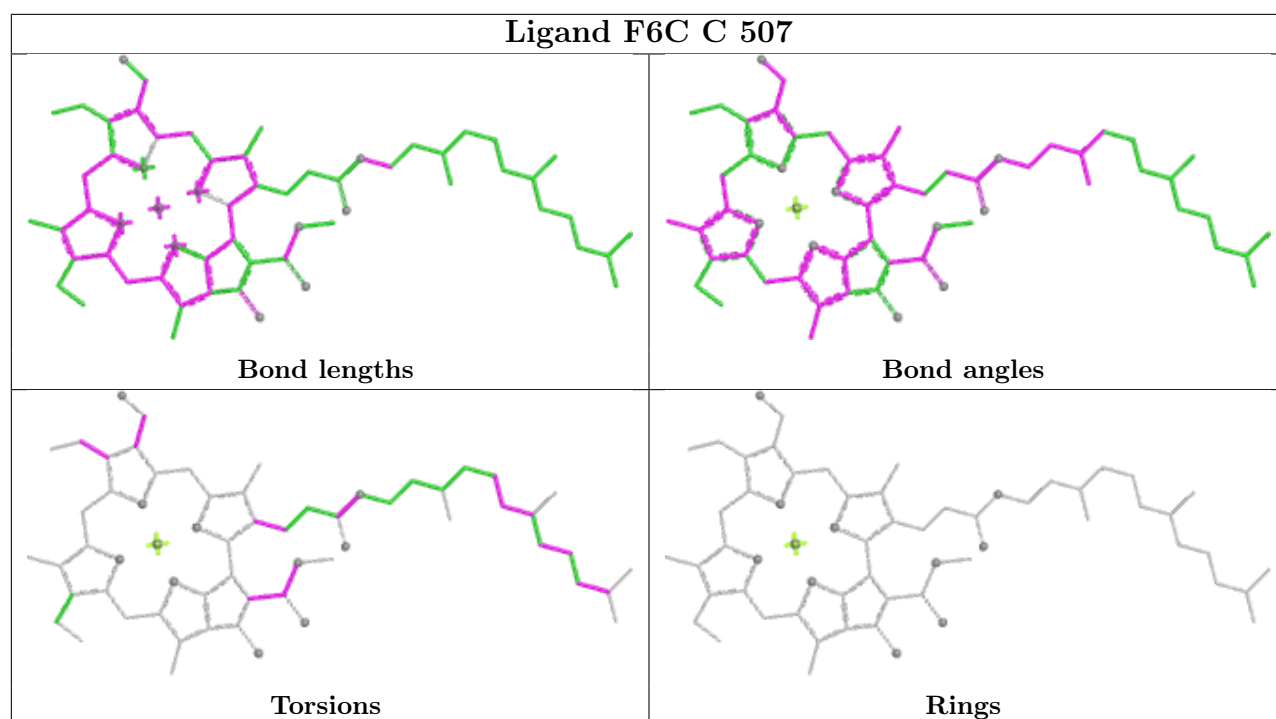


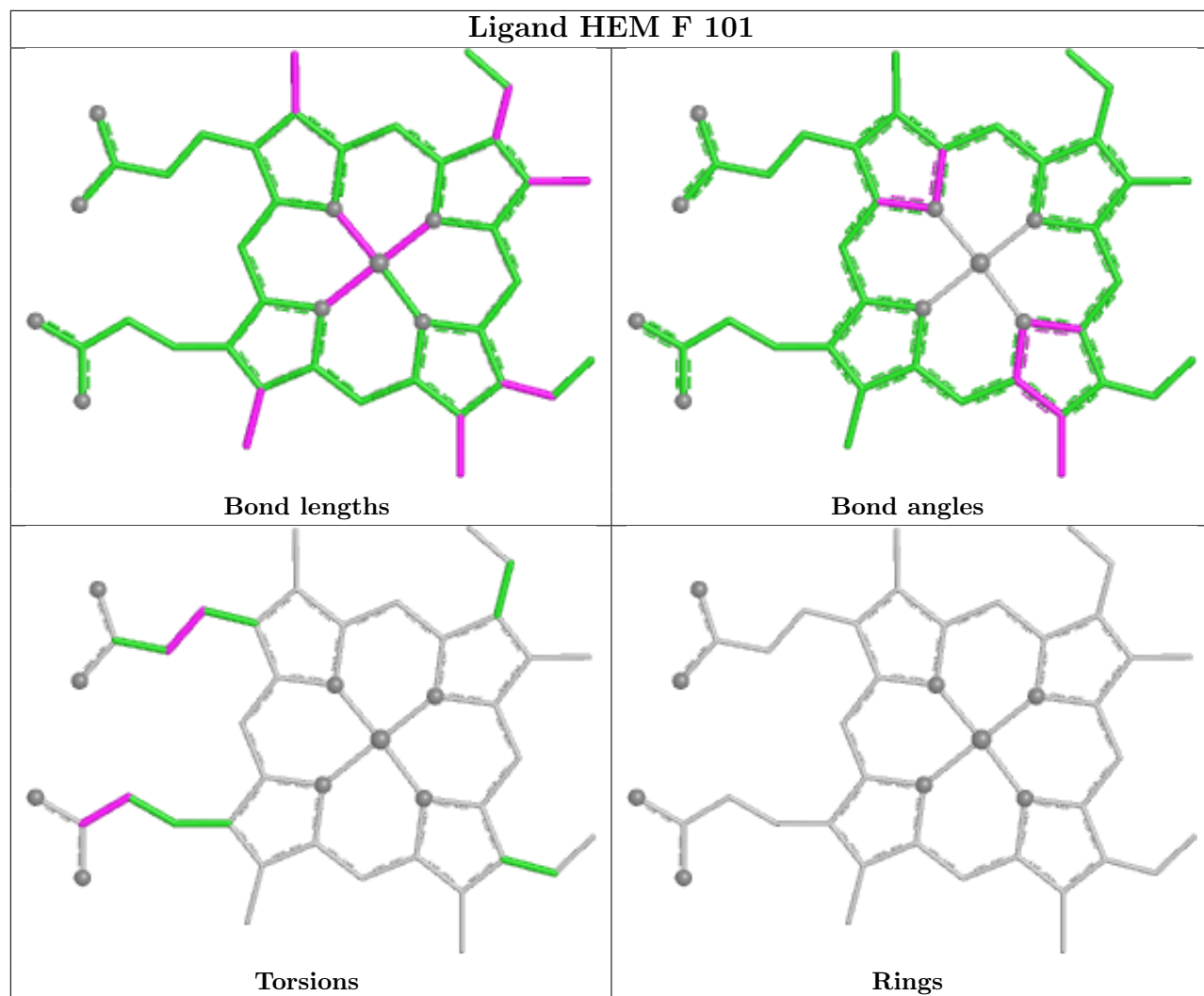


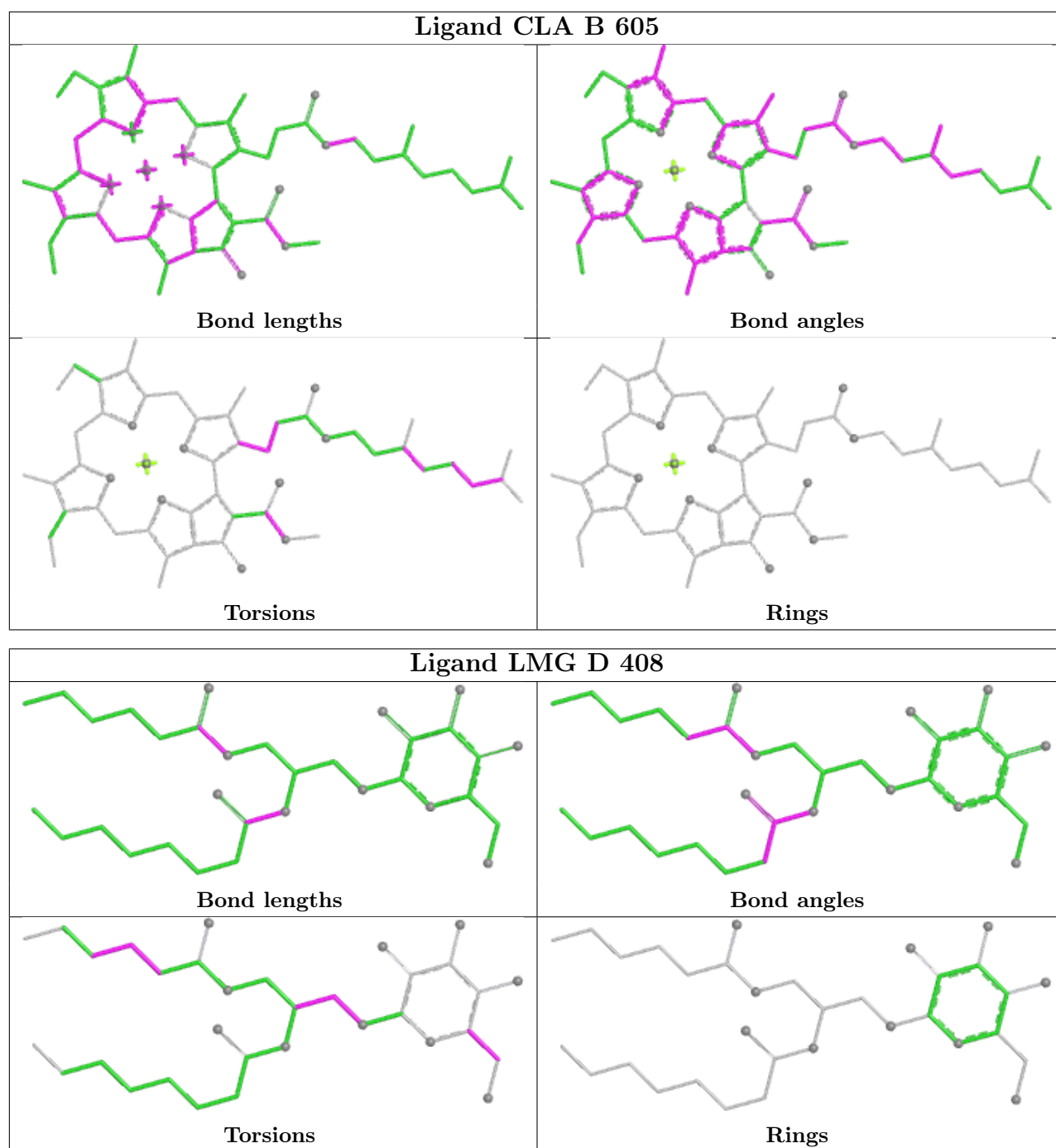


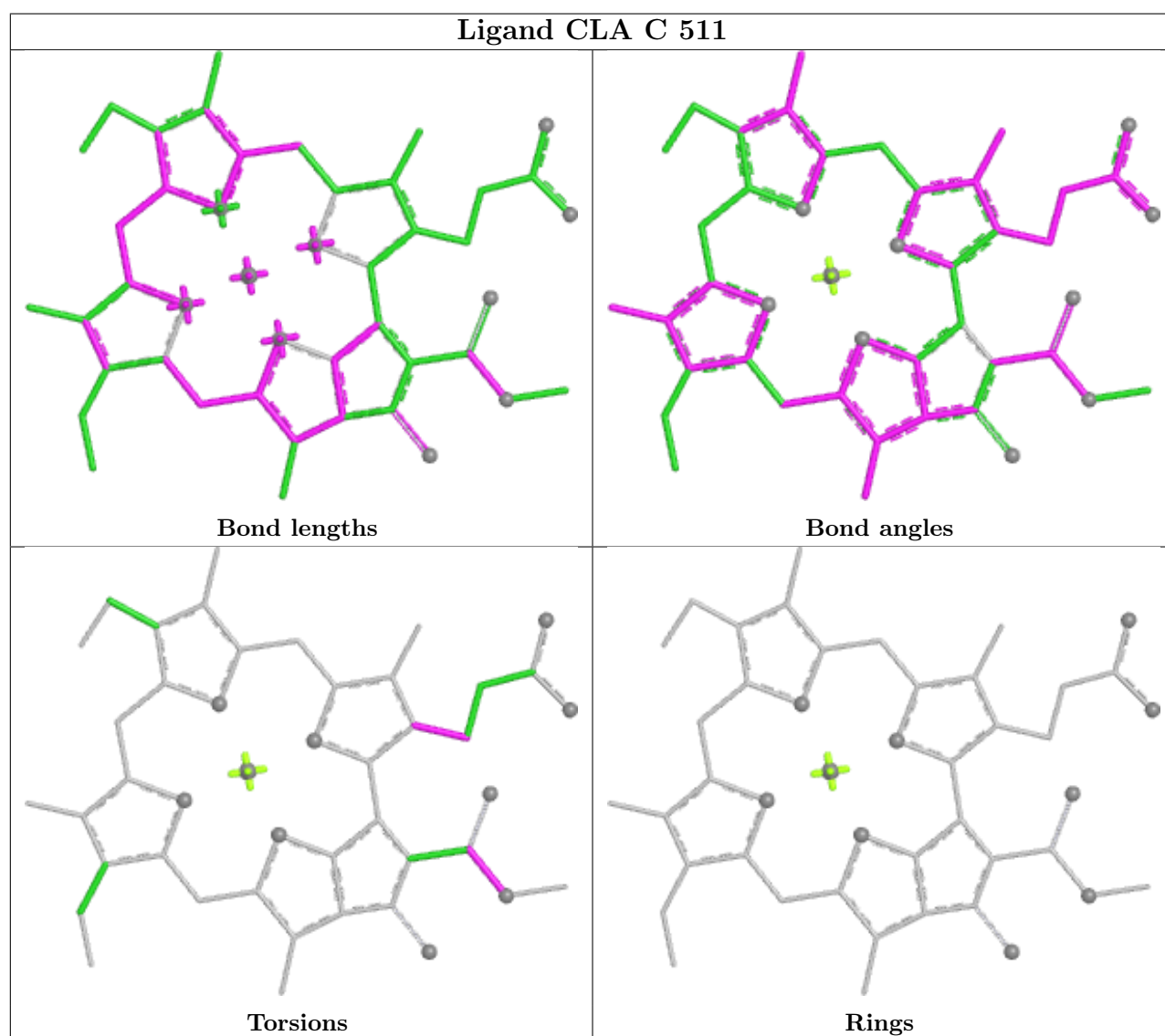
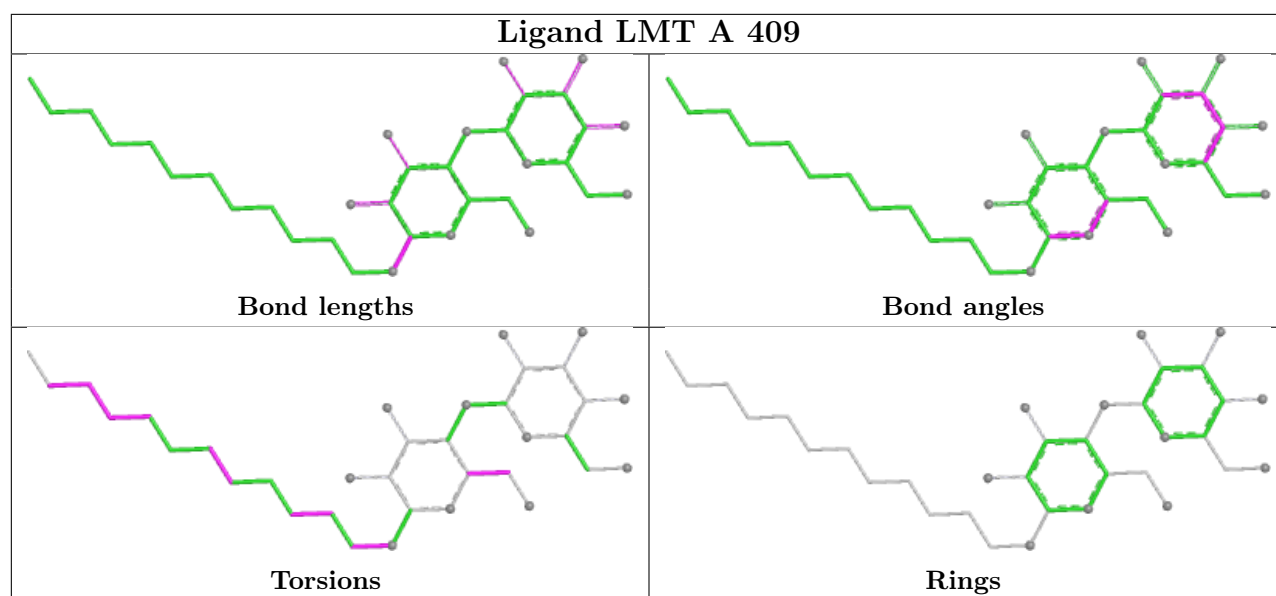


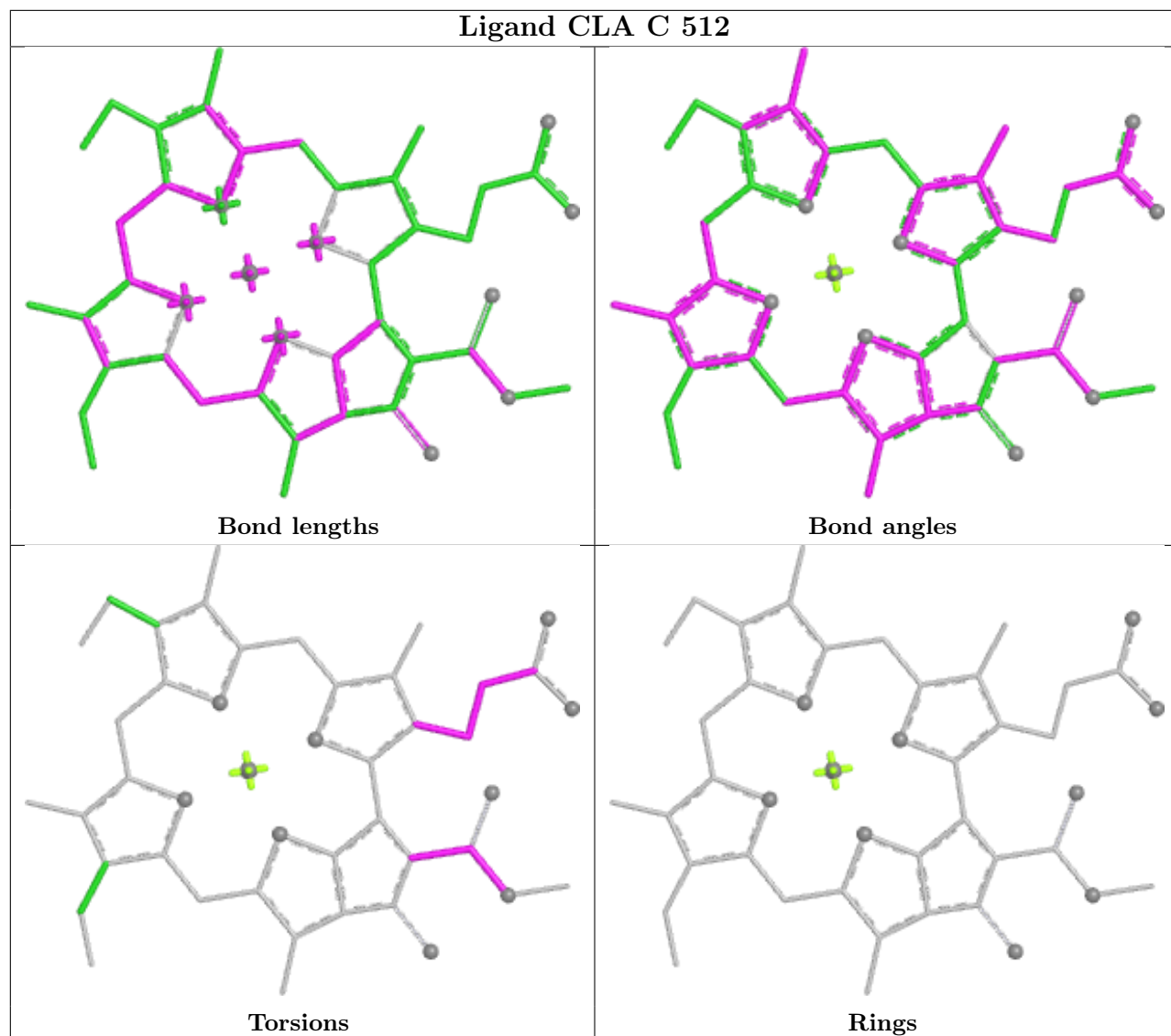




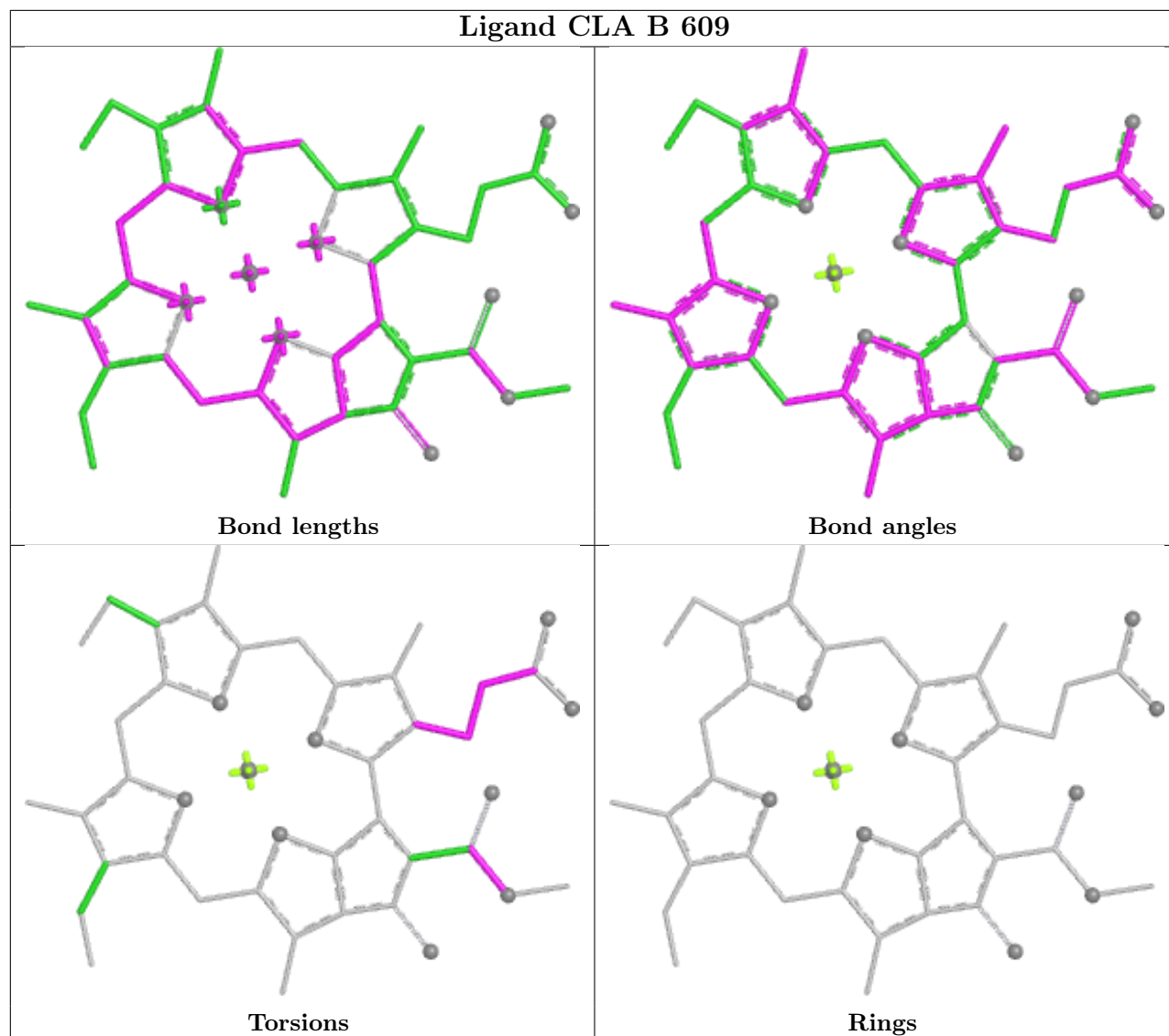




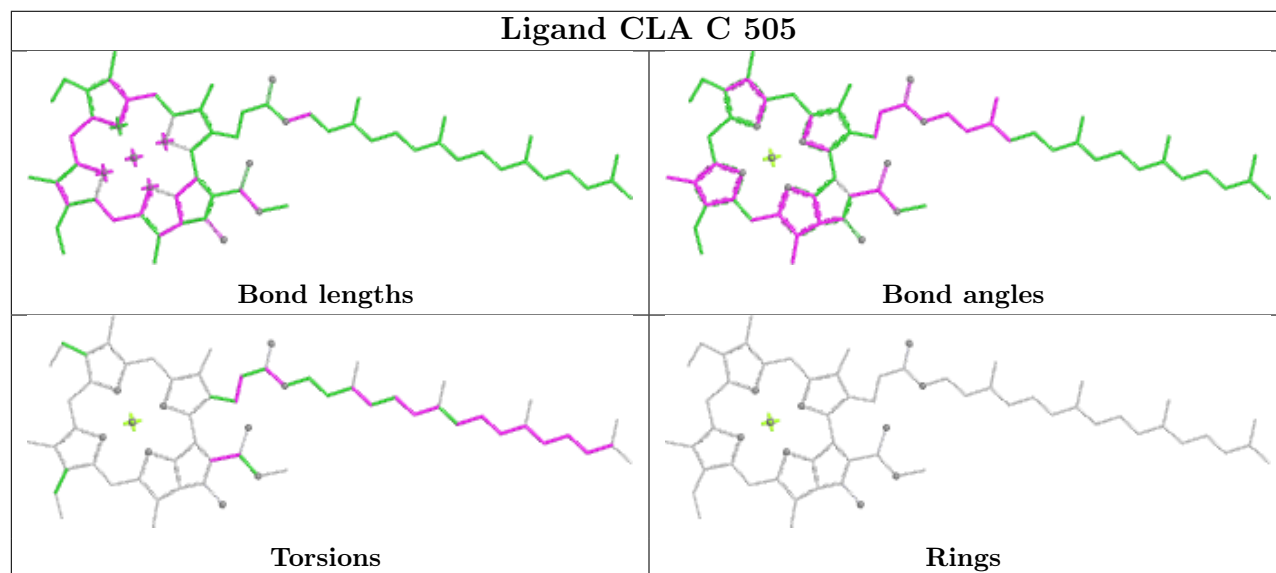




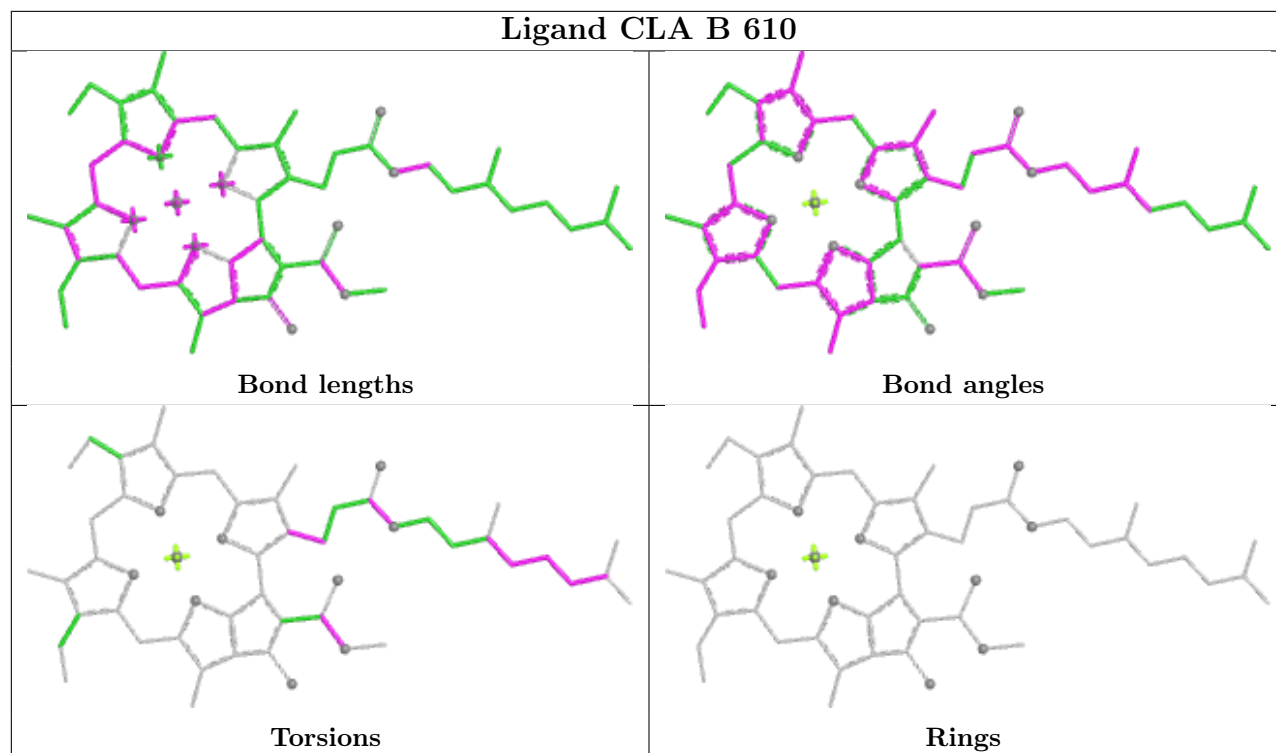
Ligand CLA B 609



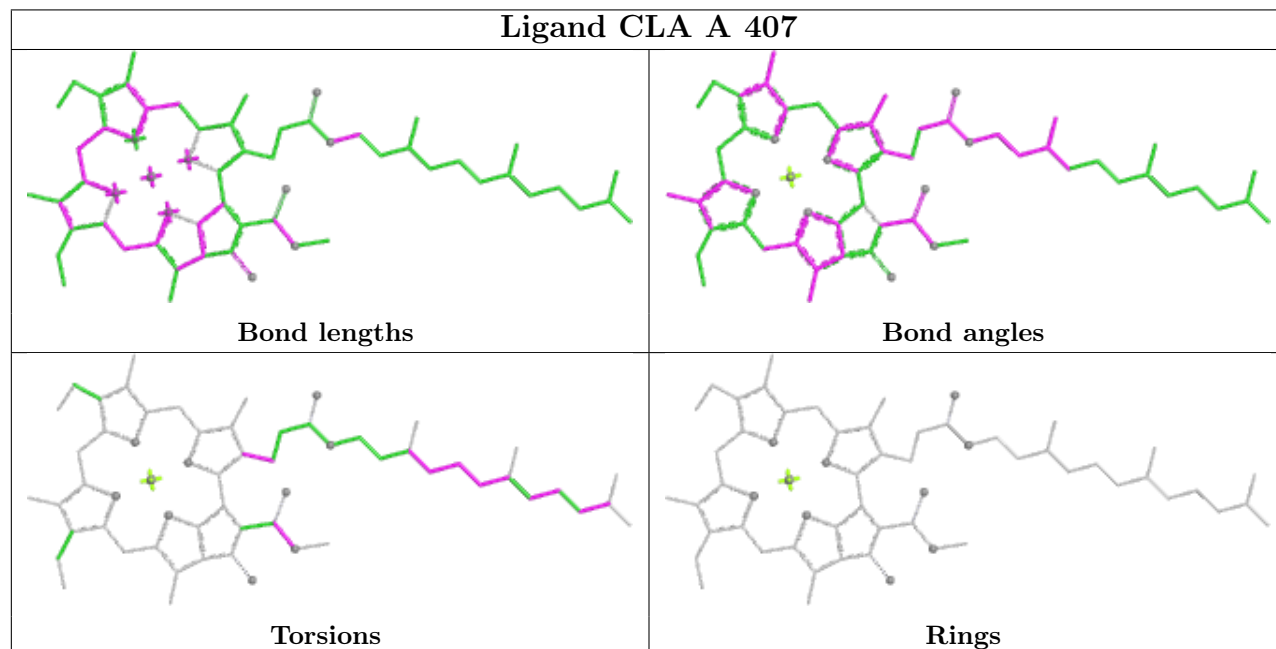
Ligand CLA C 505

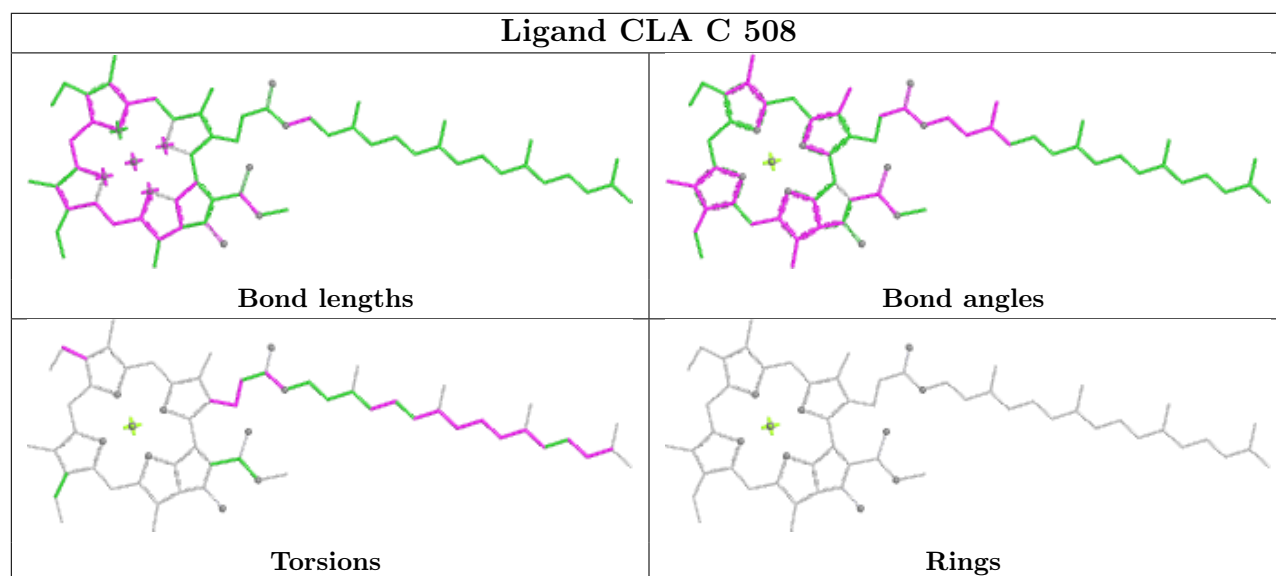
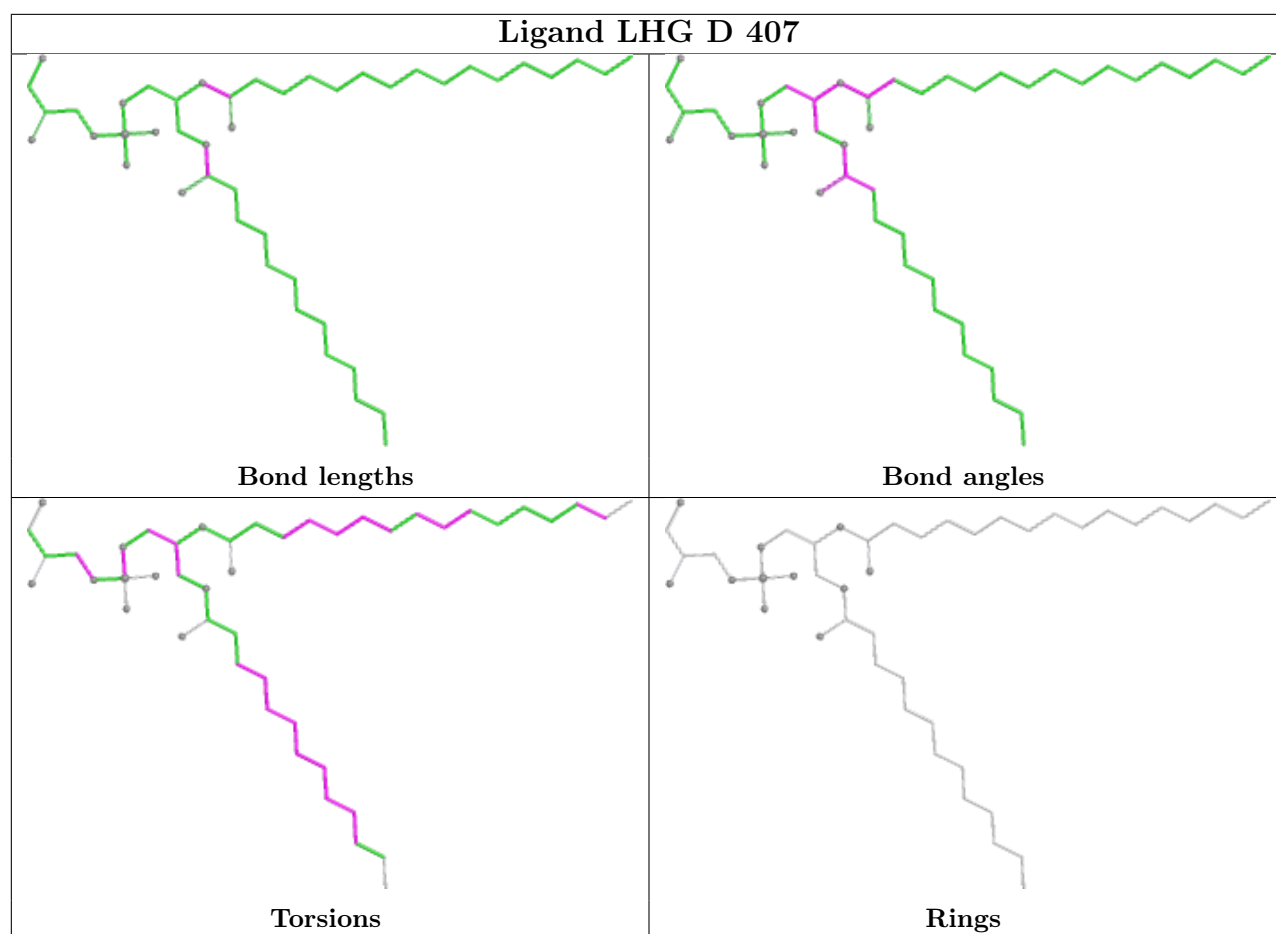


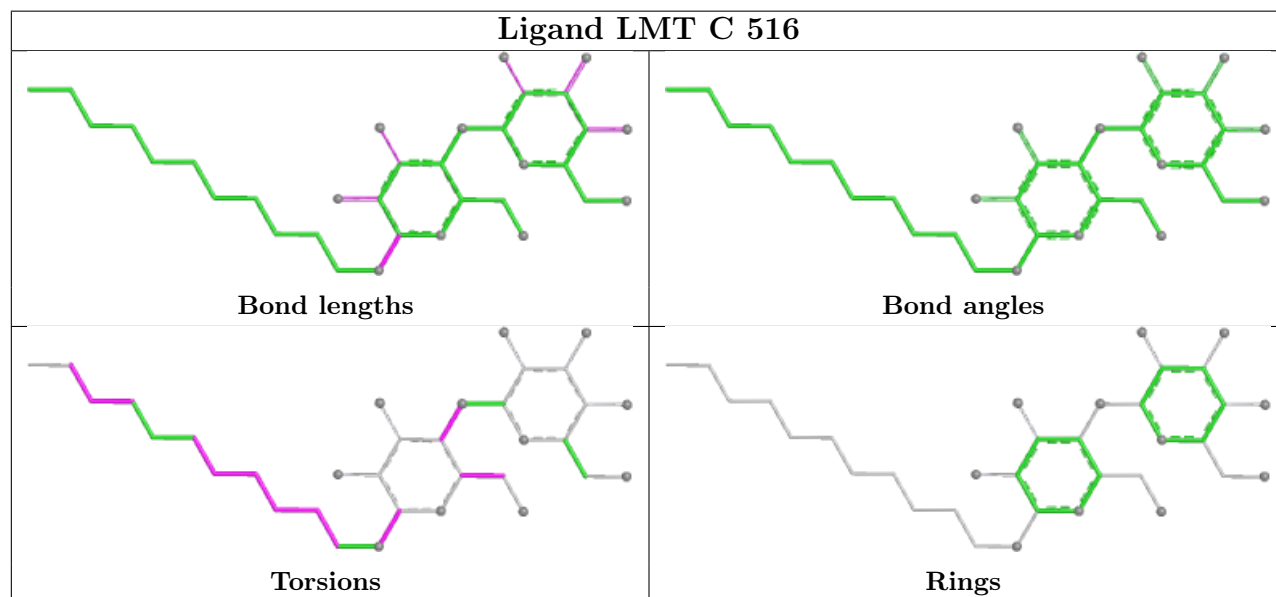
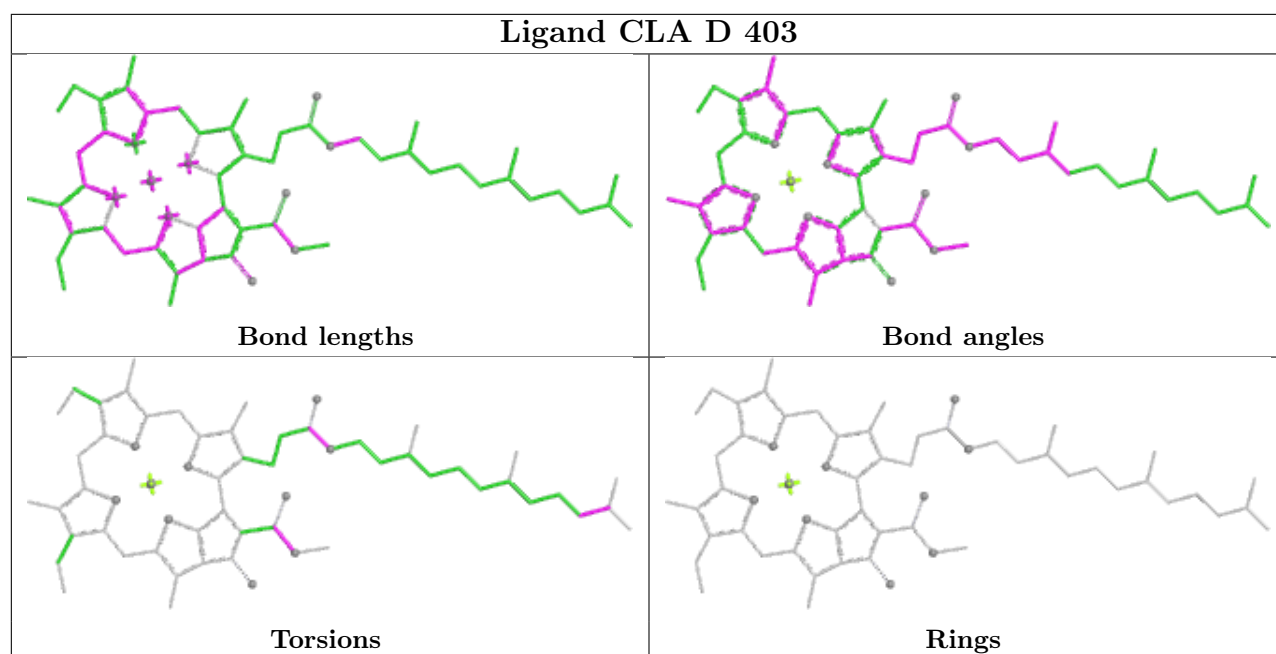
Ligand CLA B 610



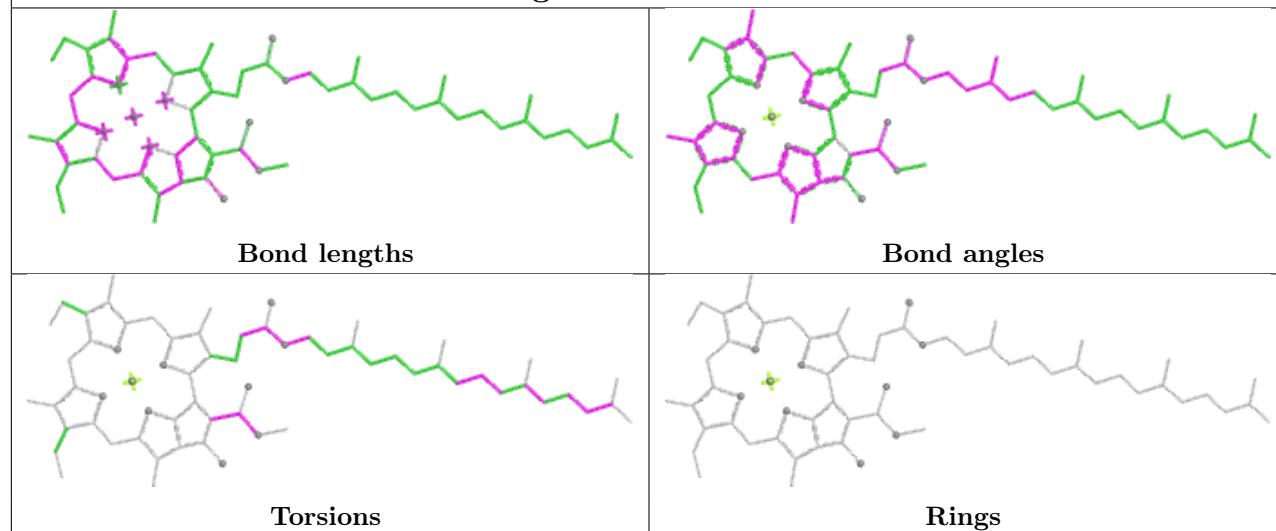
Ligand CLA A 407



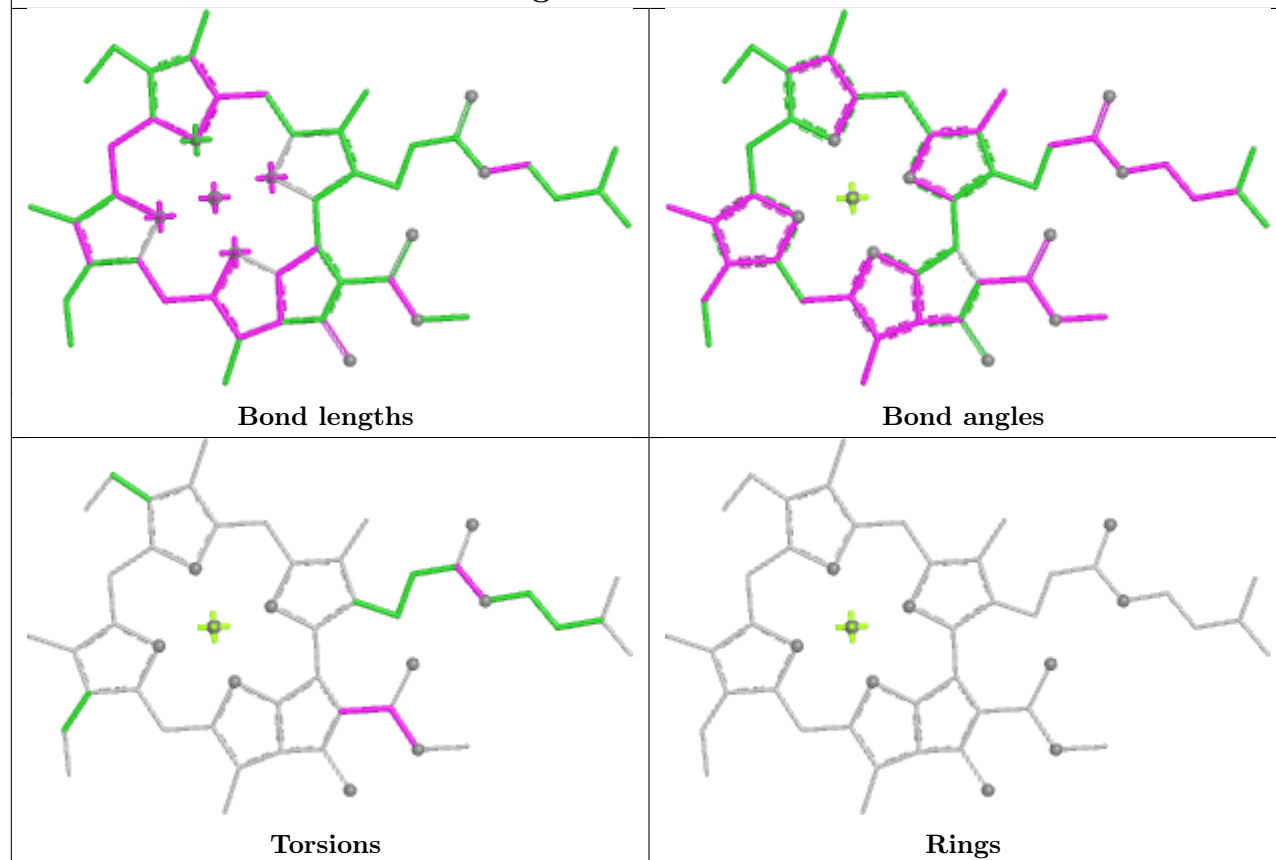




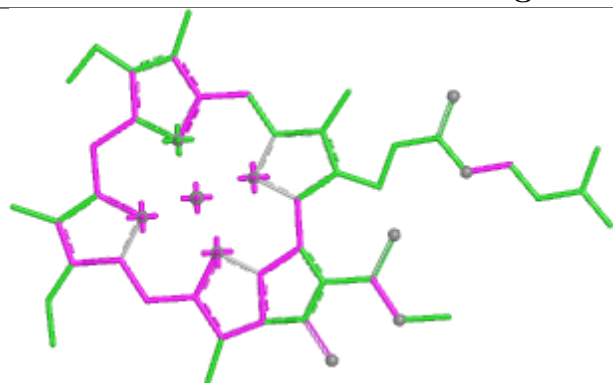
Ligand CLA B 611



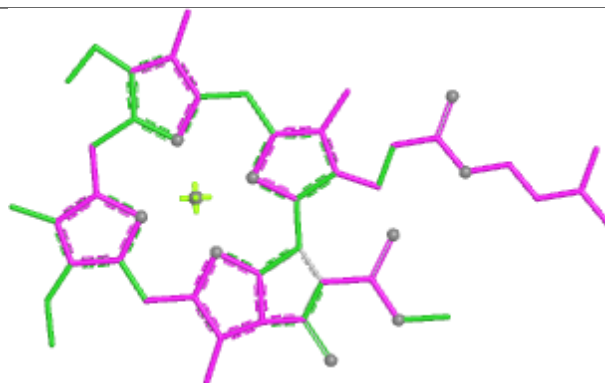
Ligand CLA C 504



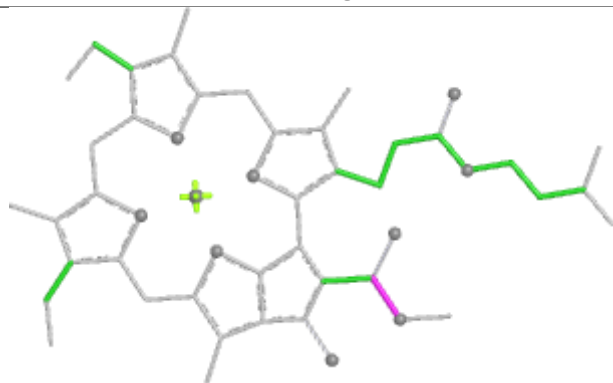
Ligand CLA B 614



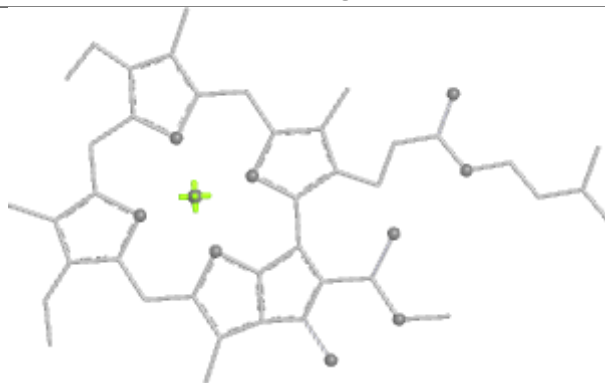
Bond lengths



Bond angles

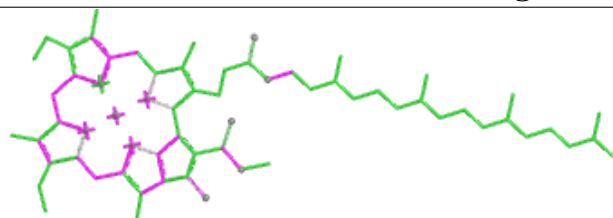


Torsions

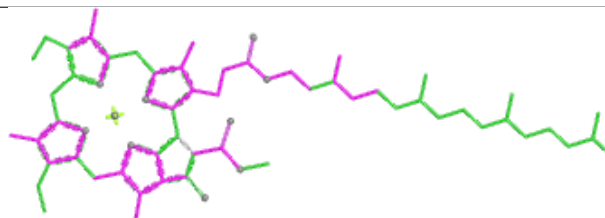


Rings

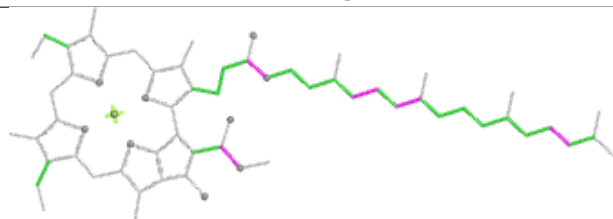
Ligand CLA A 403



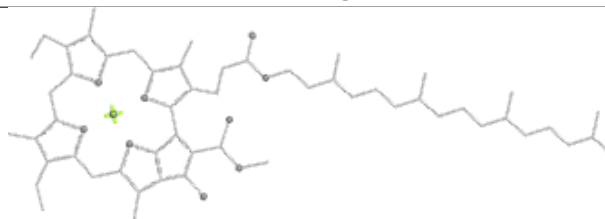
Bond lengths



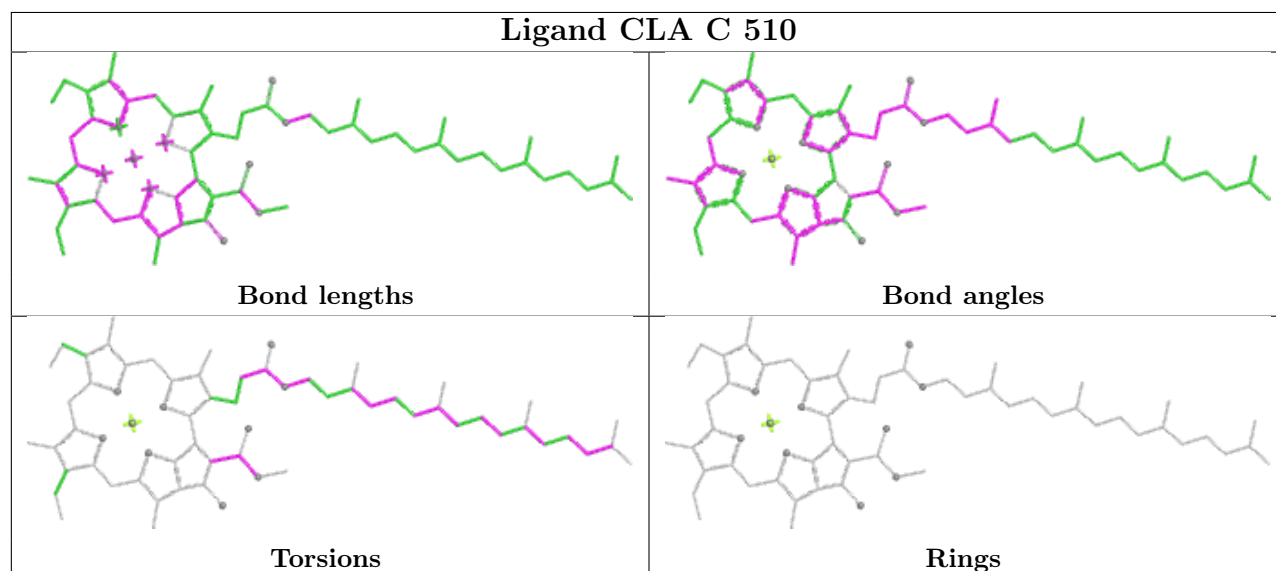
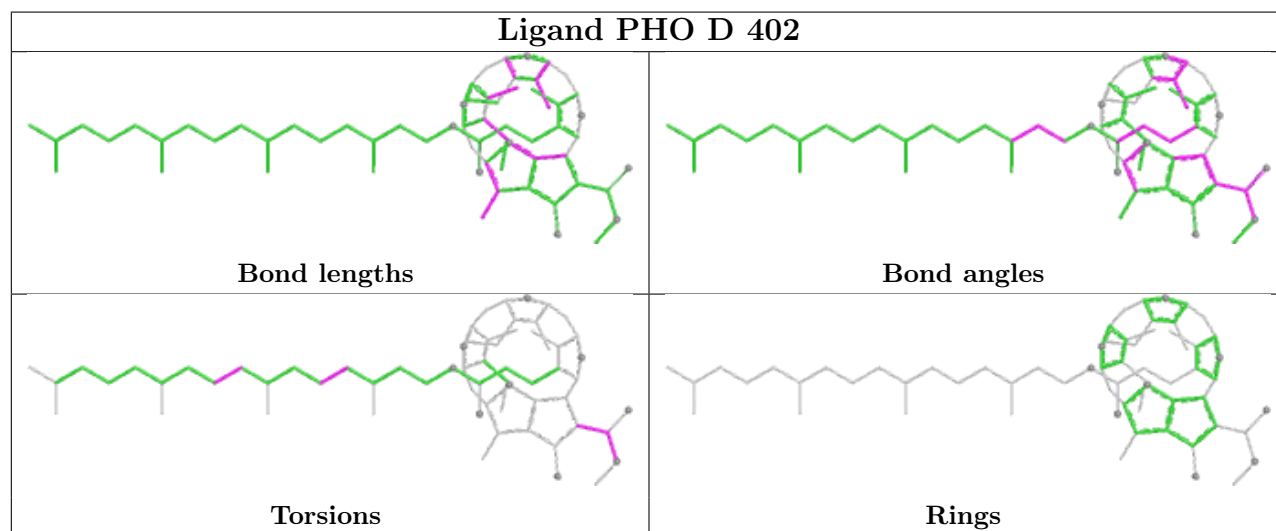
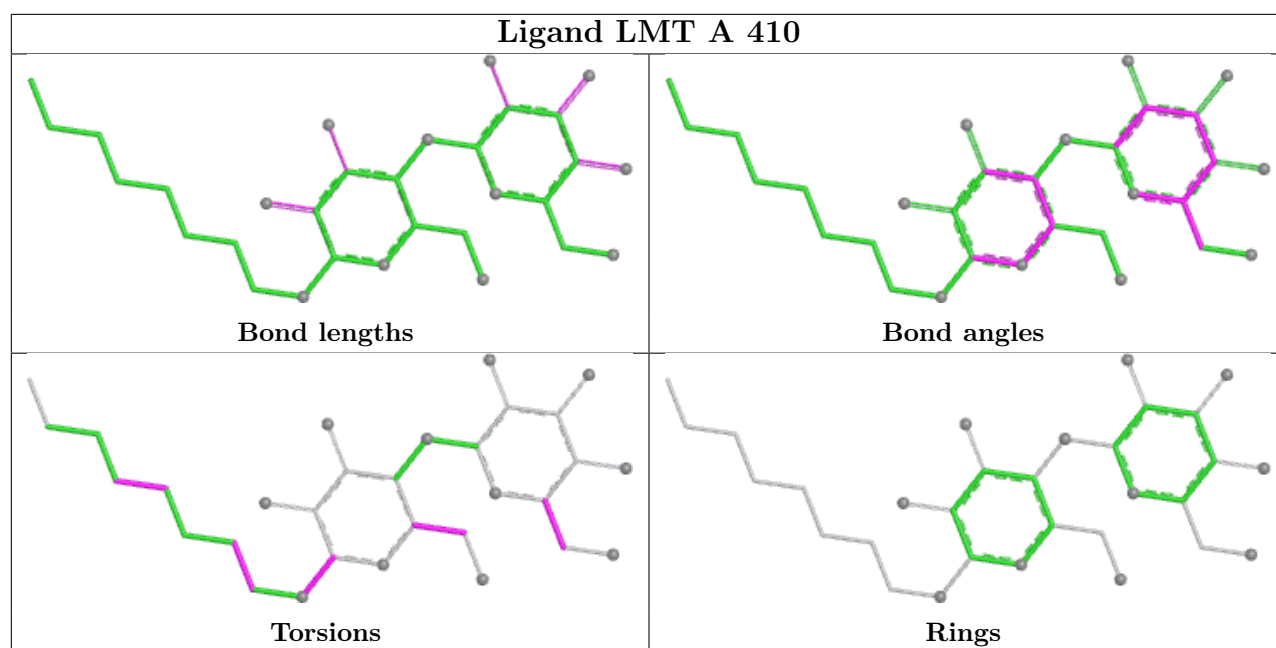
Bond angles

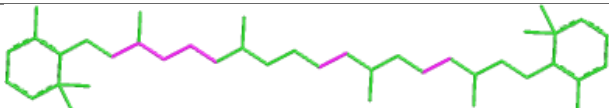
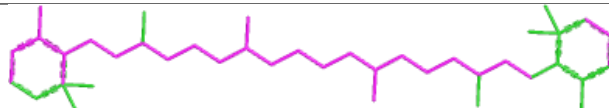
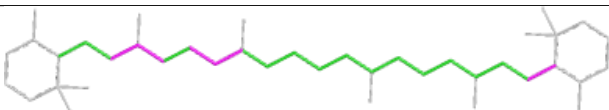
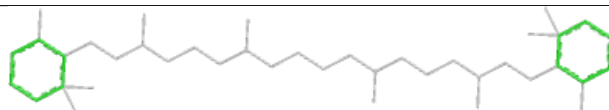


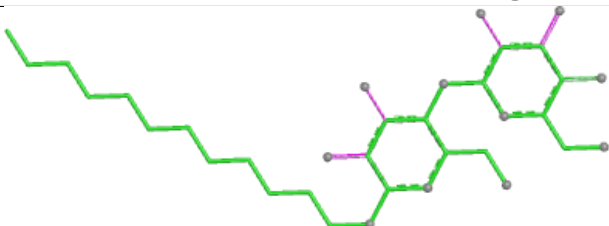
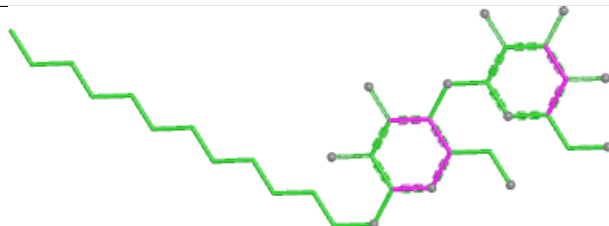
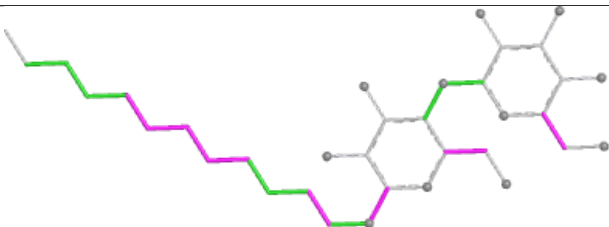
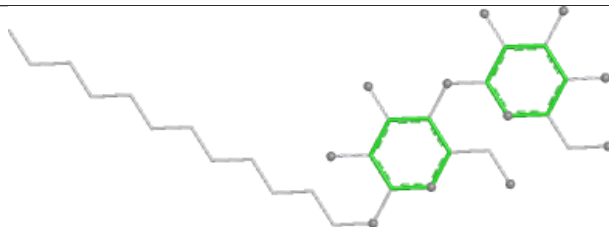
Torsions

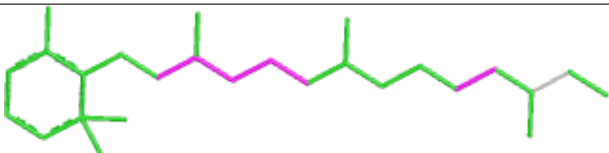
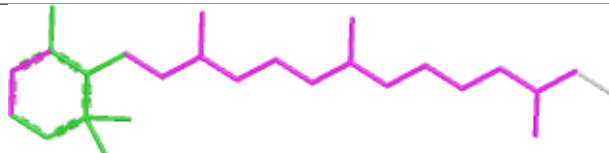
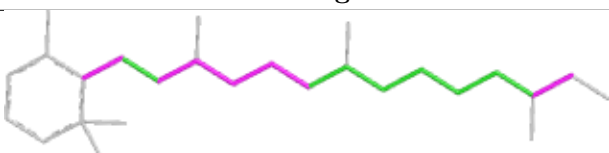
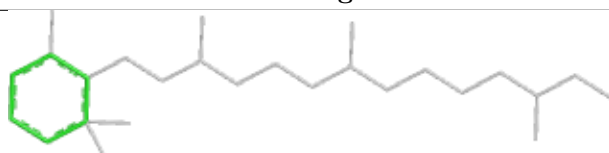


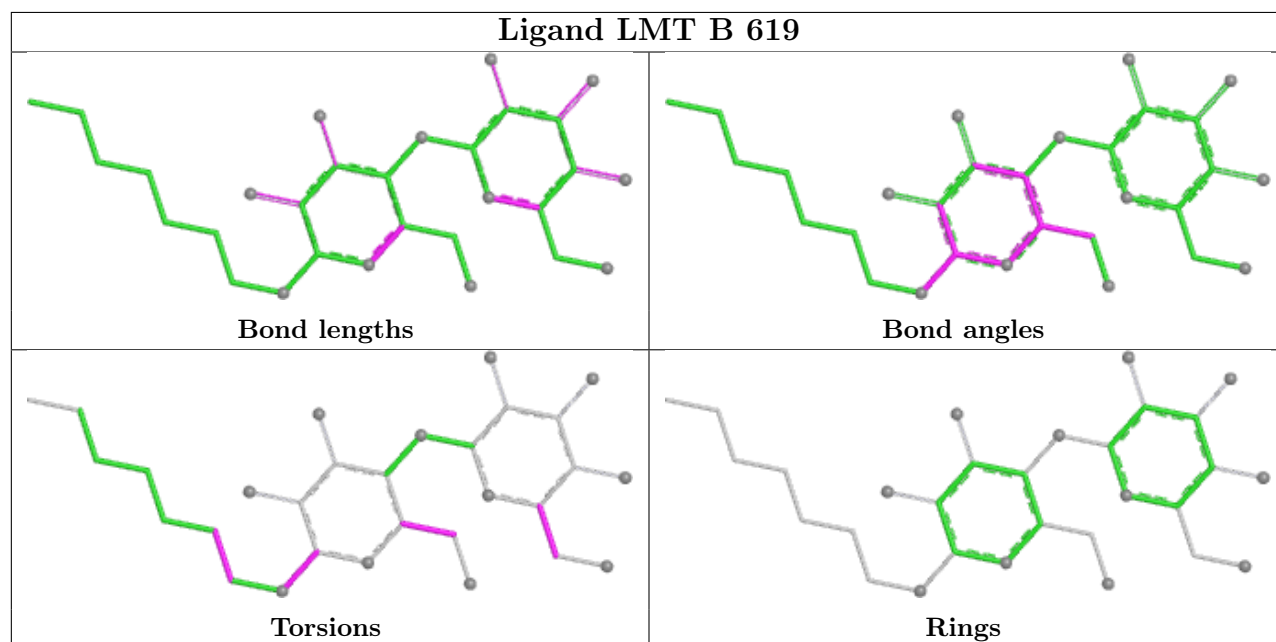
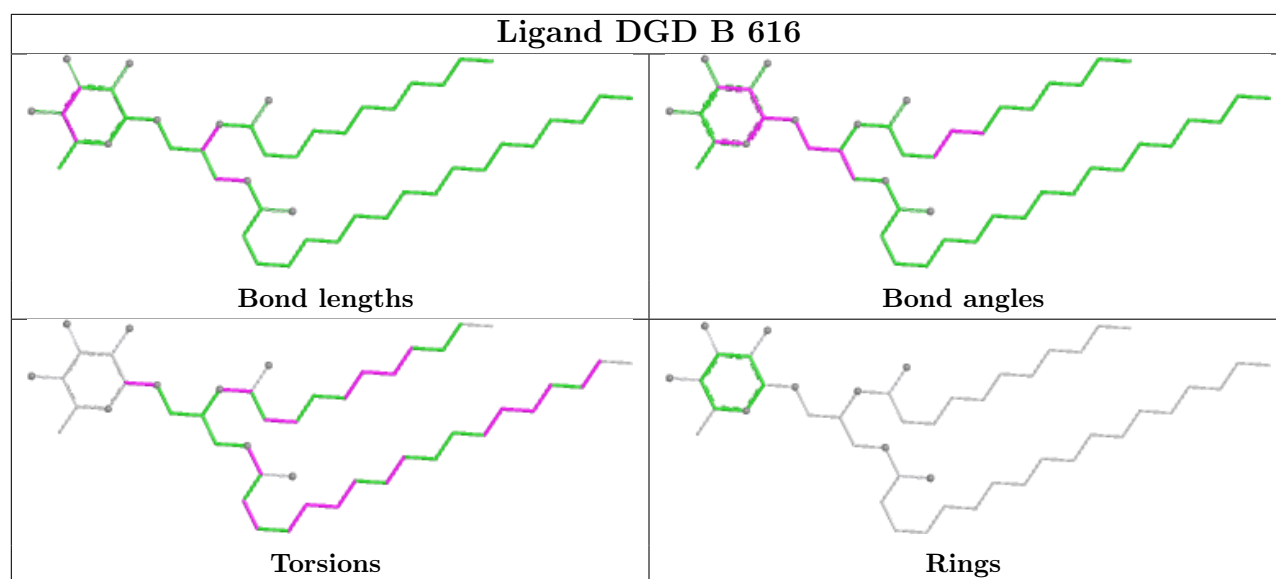
Rings

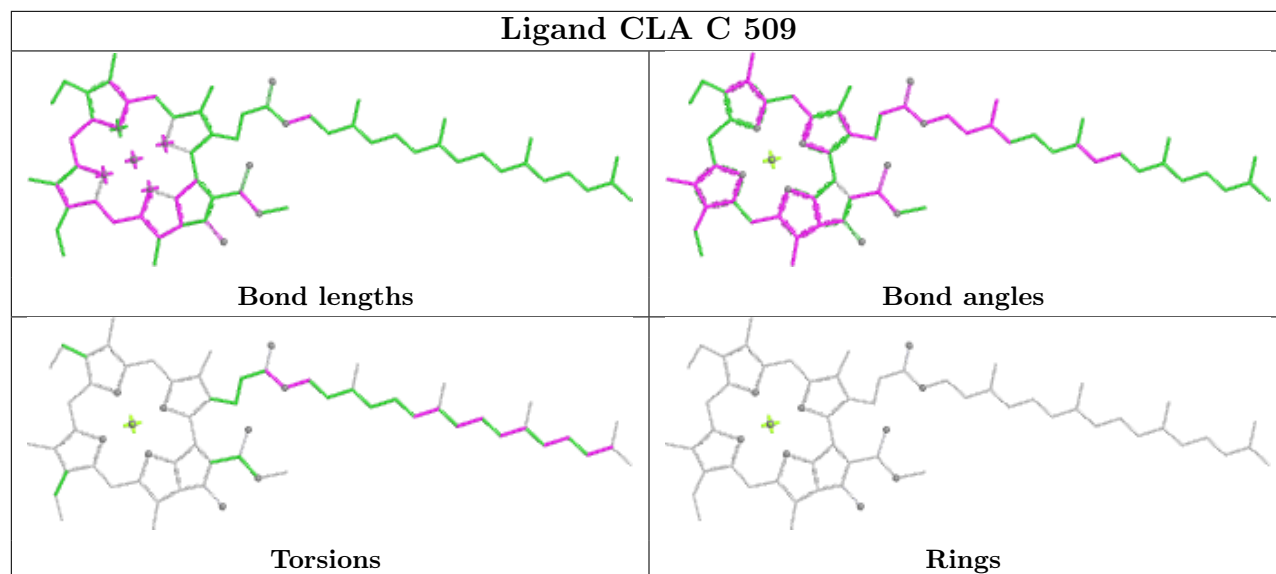
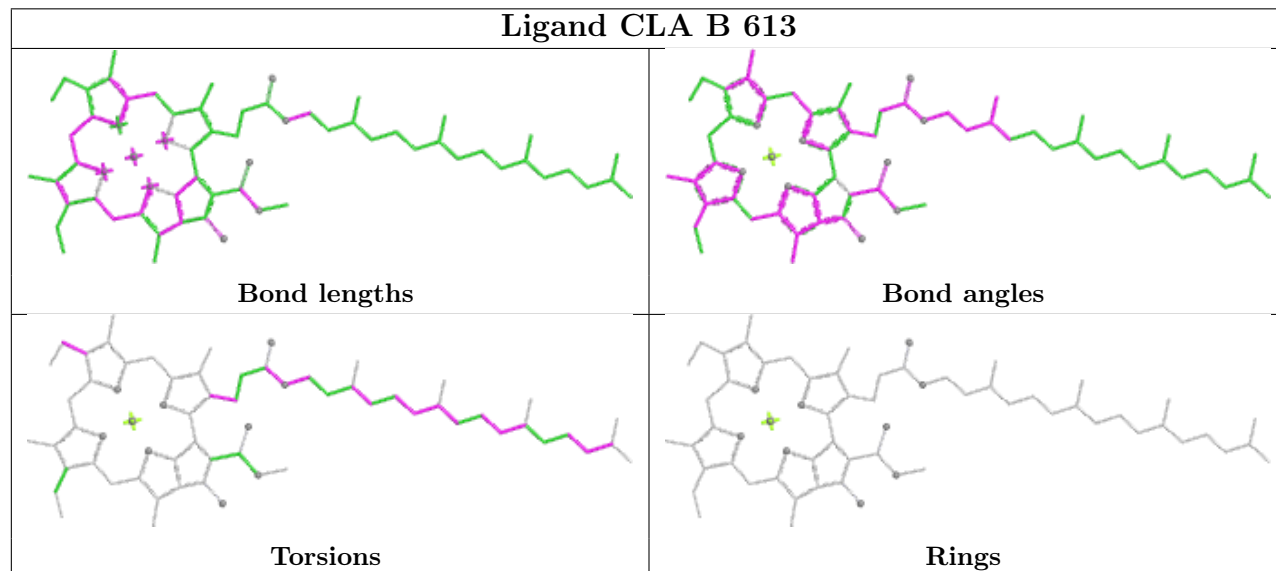


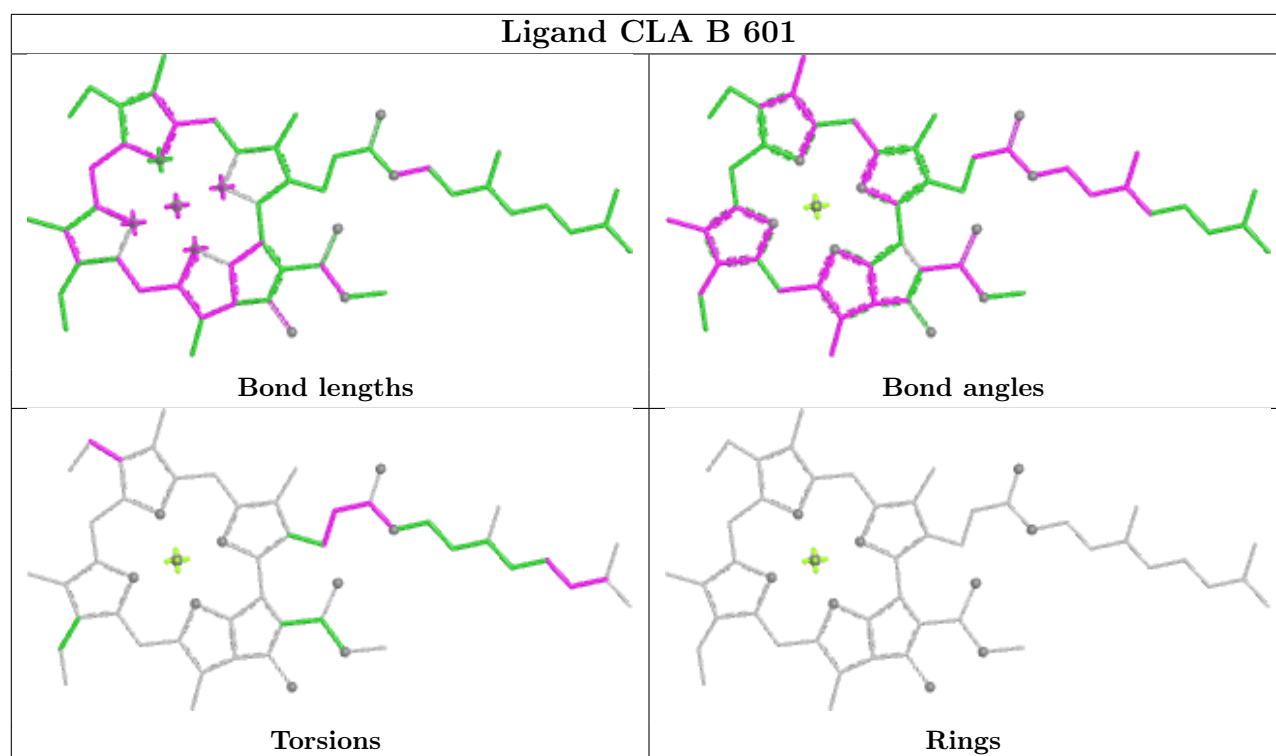
Ligand BCR B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings



Ligand CLA C 509**Ligand CLA B 613**



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.

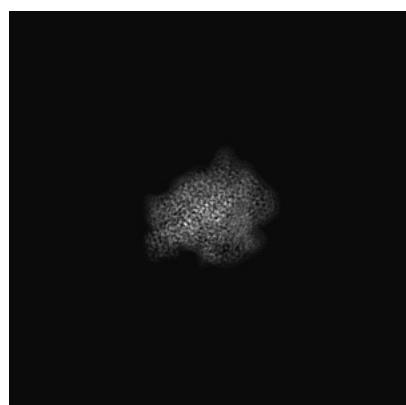
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24943. These allow visual inspection of the internal detail of the map and identification of artifacts.

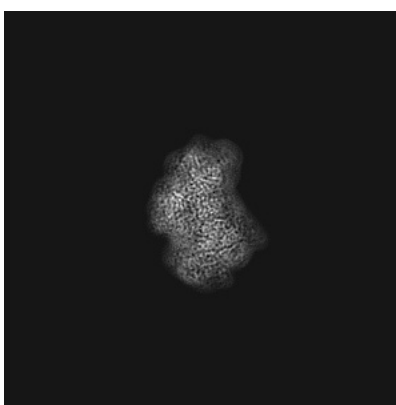
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

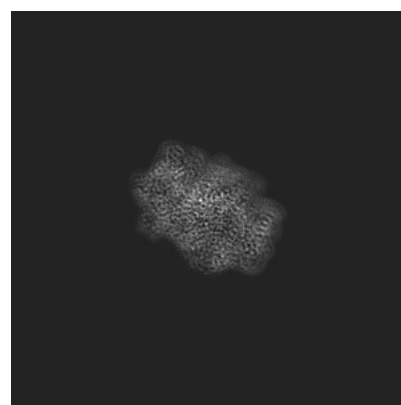
6.1.1 Primary map



X



Y

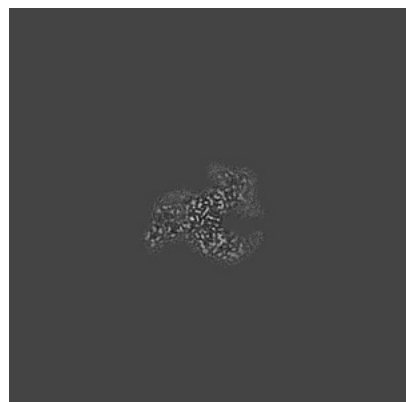


Z

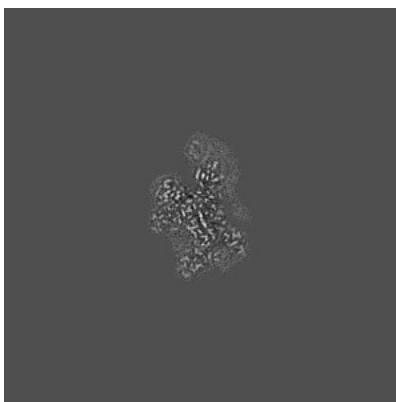
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

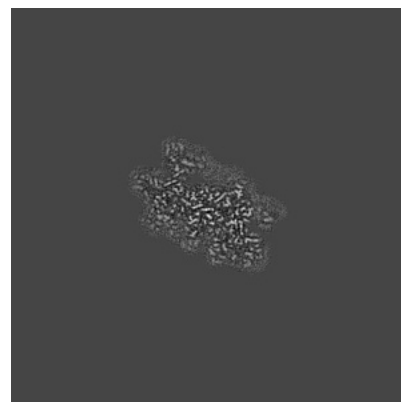
6.2.1 Primary map



X Index: 192



Y Index: 192

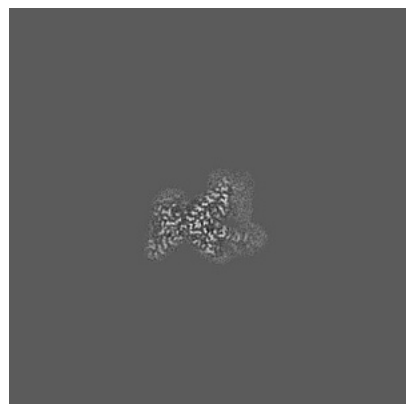


Z Index: 192

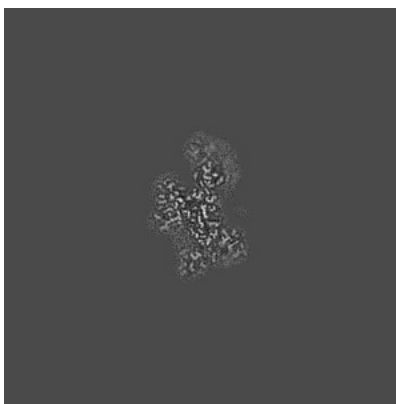
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

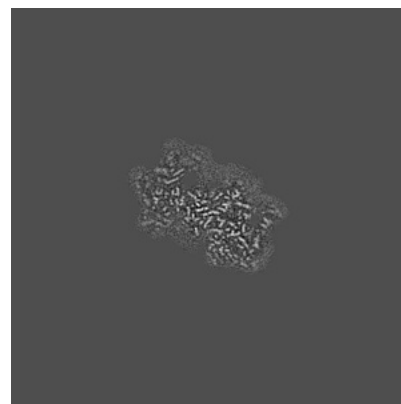
6.3.1 Primary map



X Index: 202



Y Index: 190

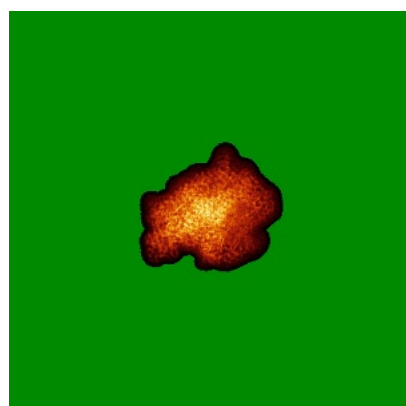


Z Index: 187

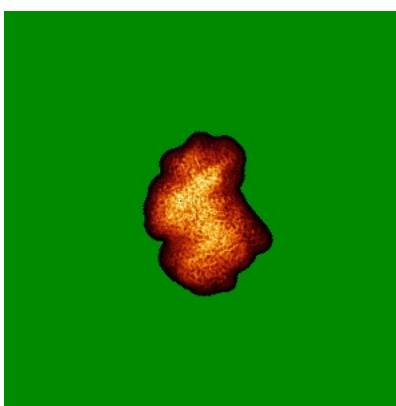
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

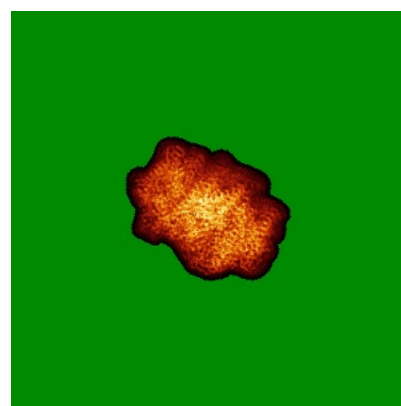
6.4.1 Primary map



X



Y

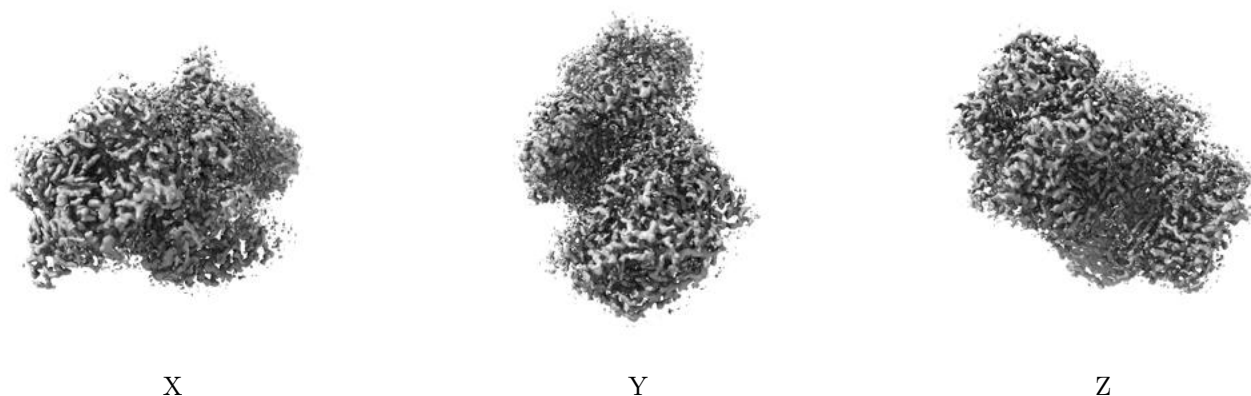


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

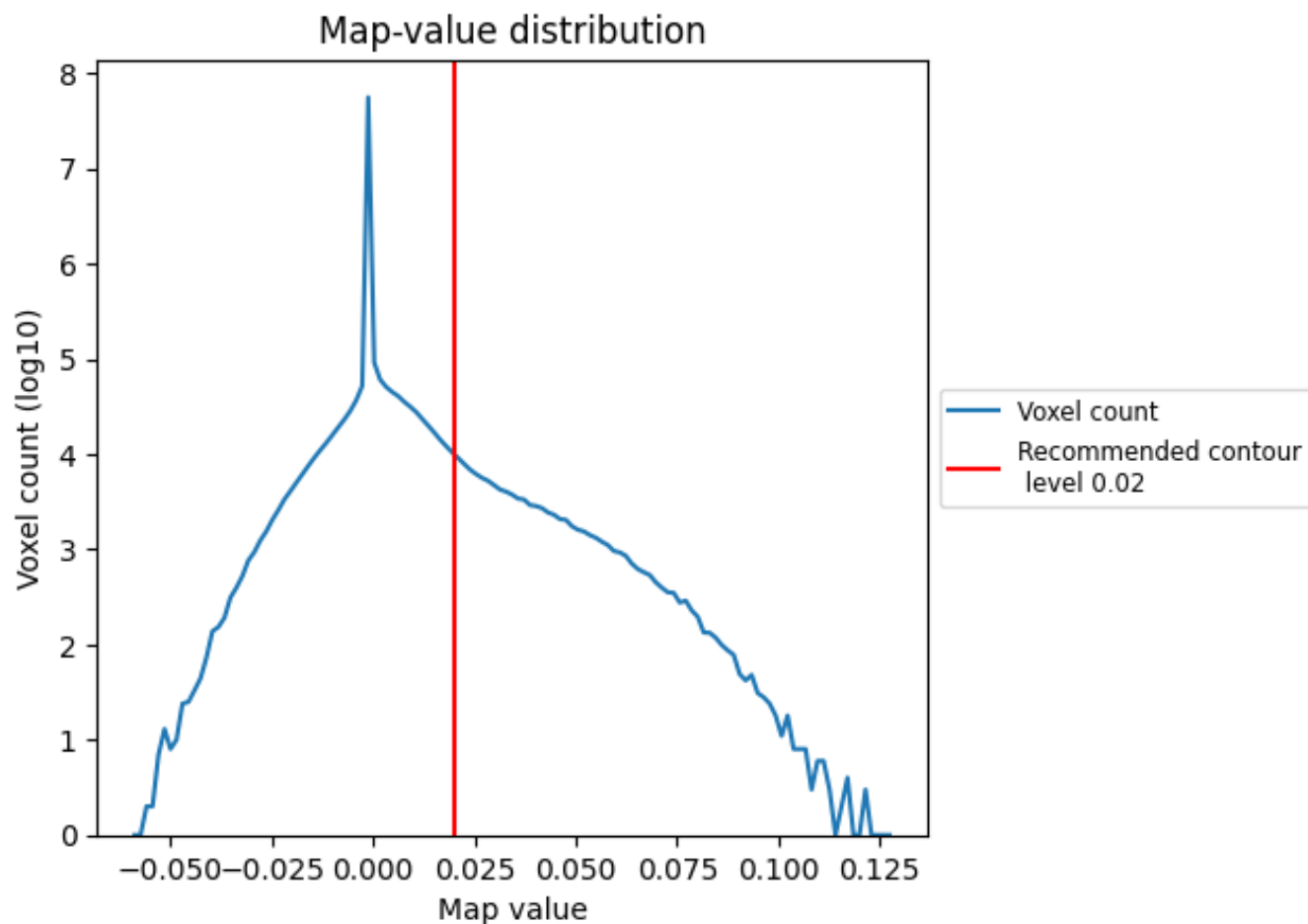
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

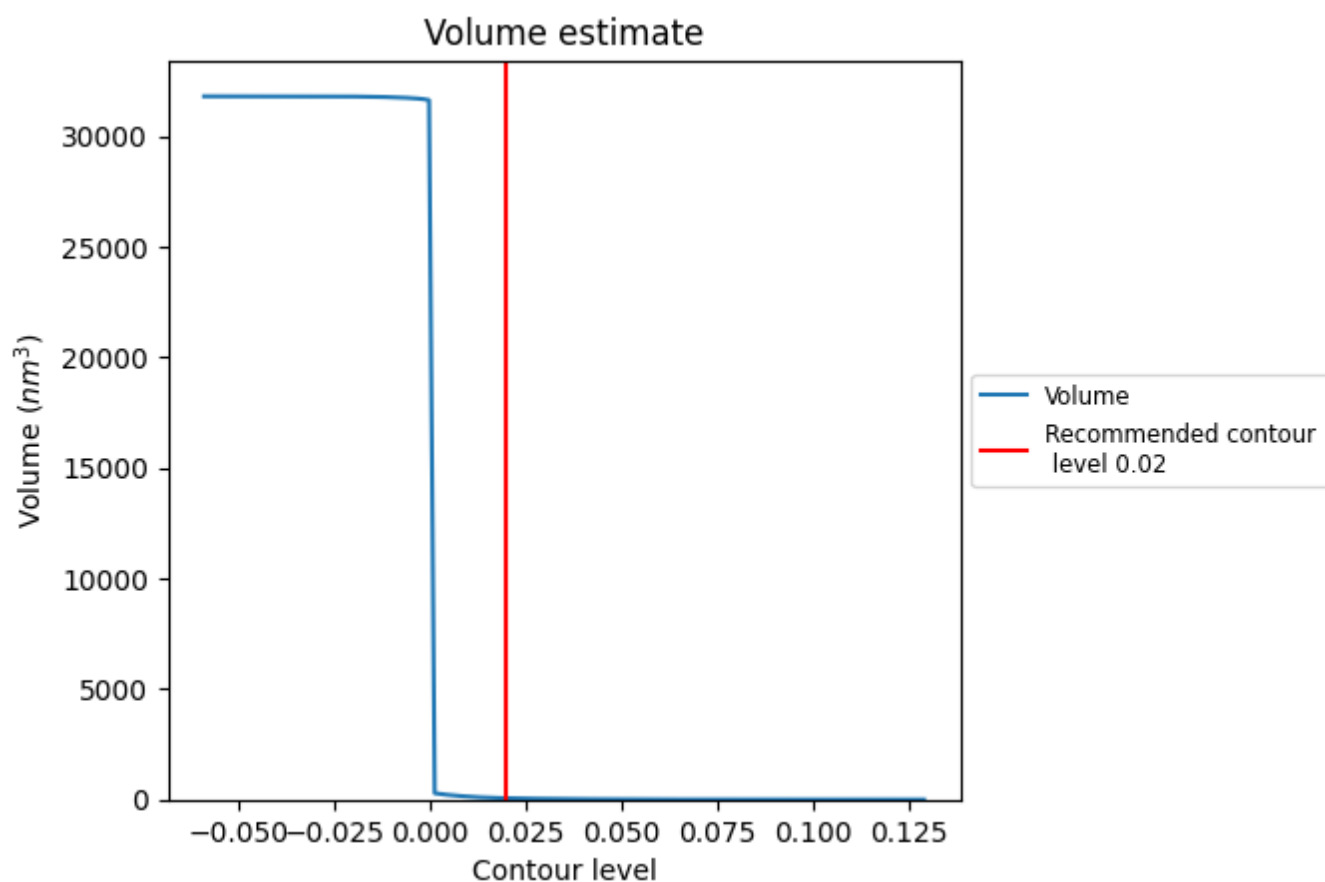
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

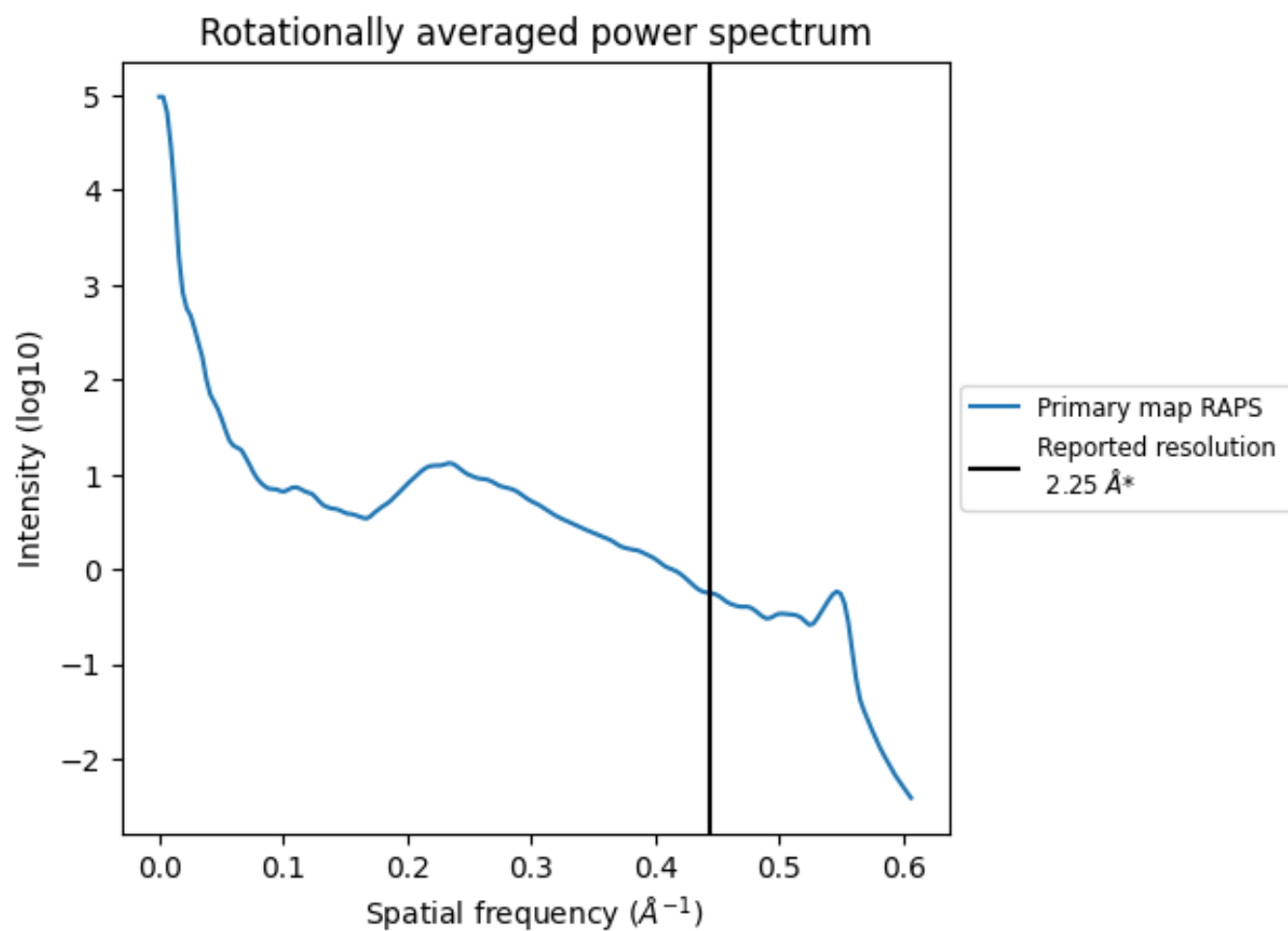
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm^3 ; this corresponds to an approximate mass of 54 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

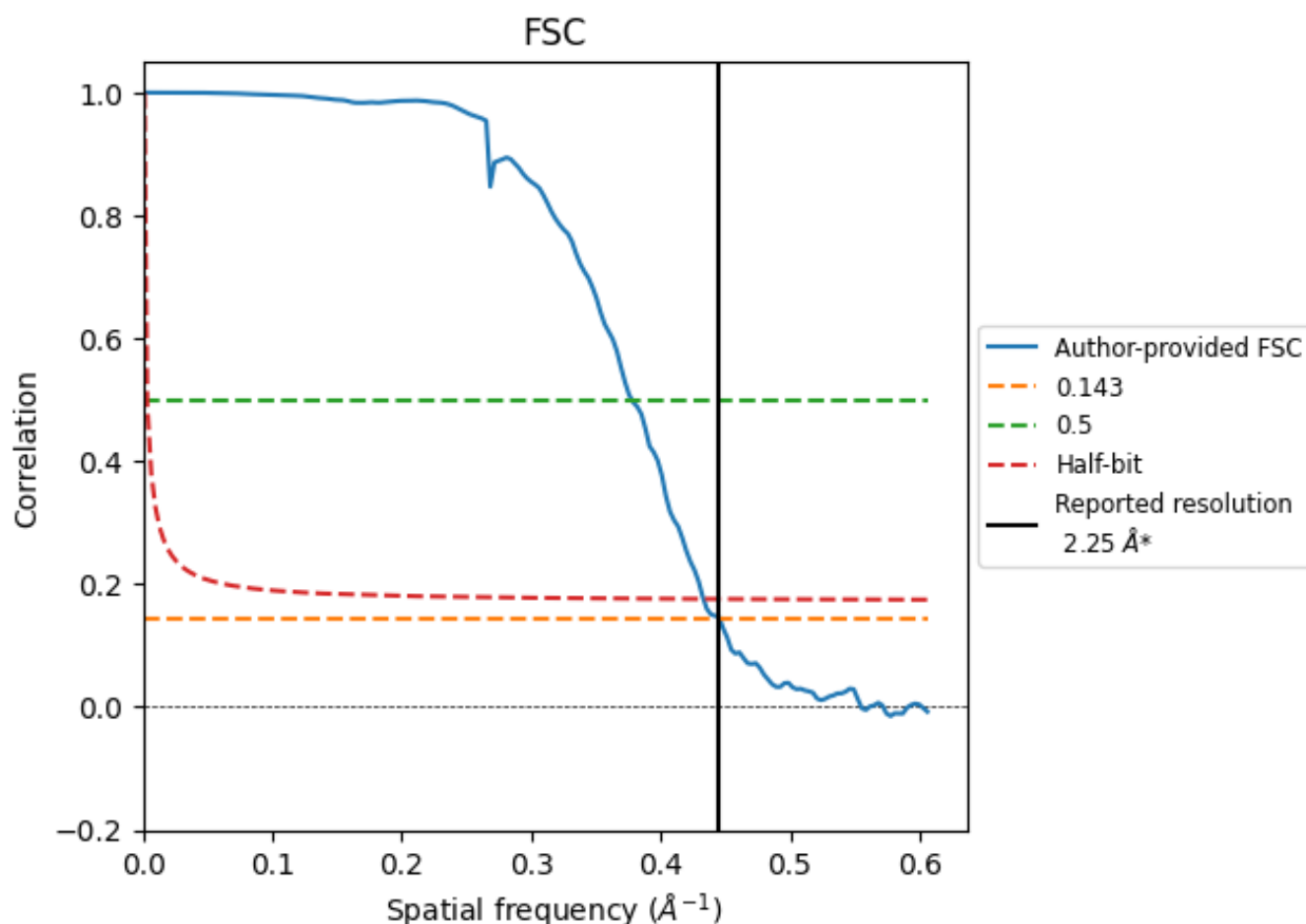


*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

8.2 Resolution estimates [i](#)

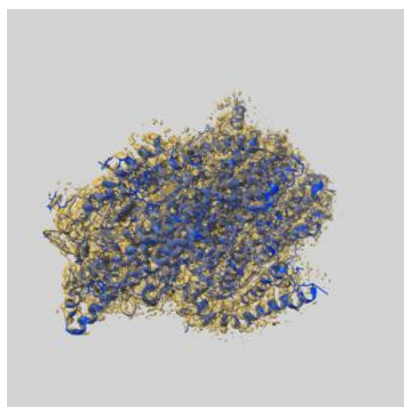
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.24	2.65	2.31
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

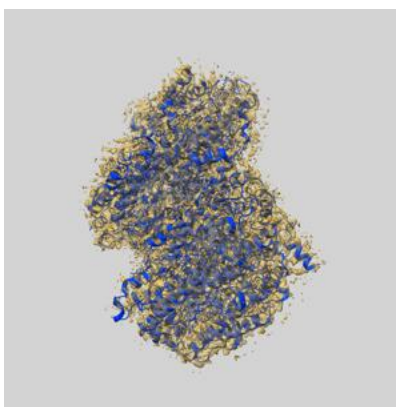
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24943 and PDB model 7SA3. Per-residue inclusion information can be found in section [3](#) on page [16](#).

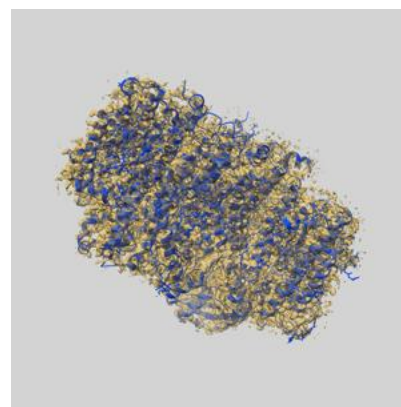
9.1 Map-model overlay [i](#)



X



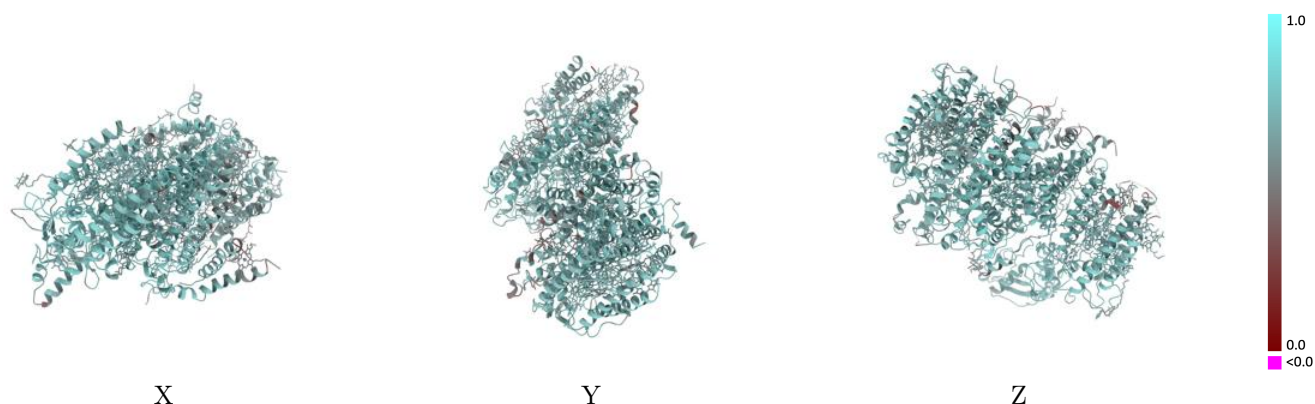
Y



Z

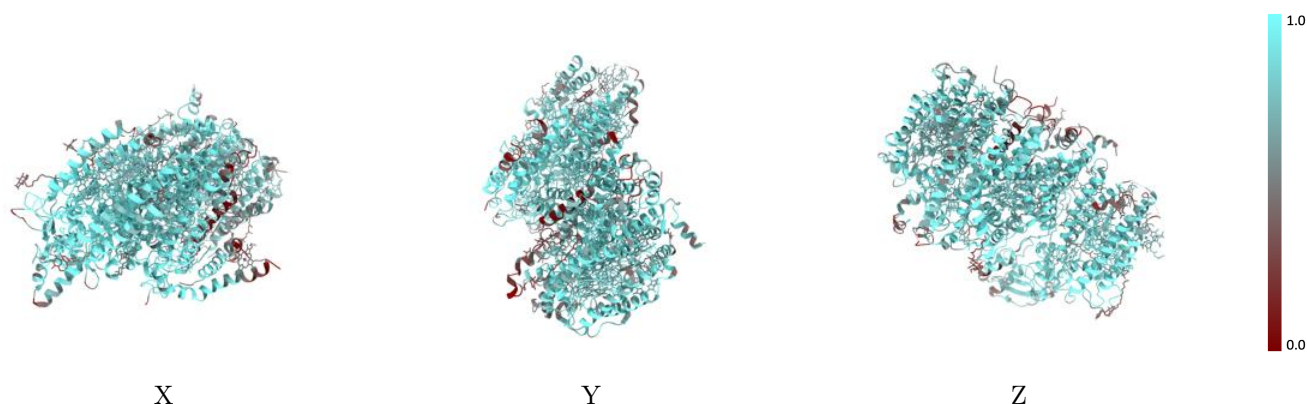
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



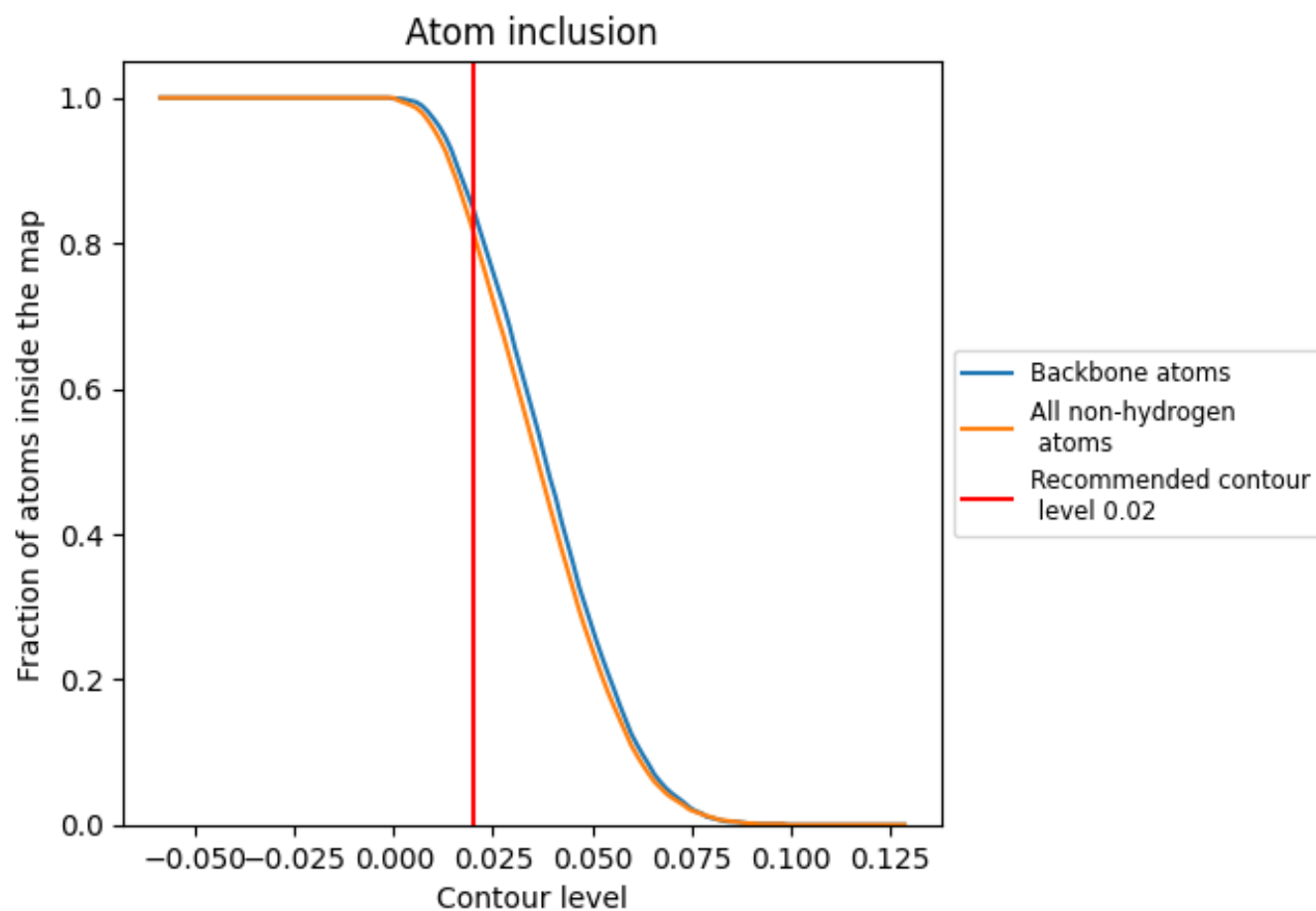
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.6800
A	0.8630	0.7030
B	0.8470	0.6850
C	0.7830	0.6650
D	0.8710	0.7060
E	0.7170	0.6340
F	0.6390	0.5940
I	0.7500	0.6480
K	0.4760	0.5710
N	0.1300	0.4730

1.0

0.0

<0.0