



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:16 AM EDT

PDB ID : 3AG3 / pdb_00003ag3
Title : Bovine Heart Cytochrome c Oxidase in the Nitric Oxide-bound Fully Reduced State at 100 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

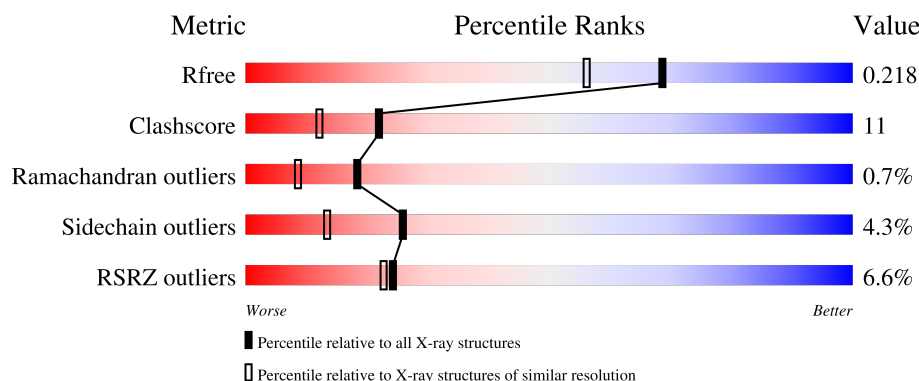
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



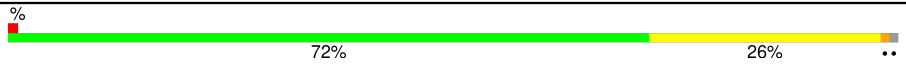
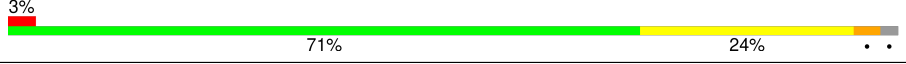
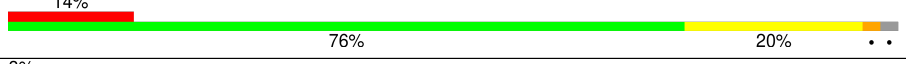
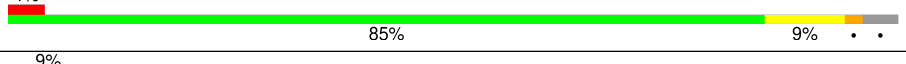
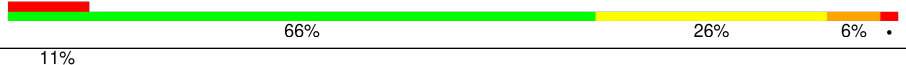
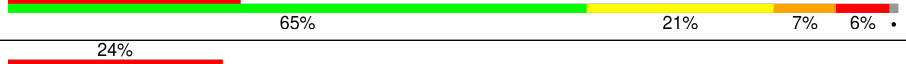
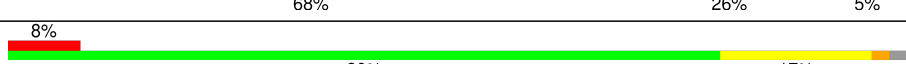
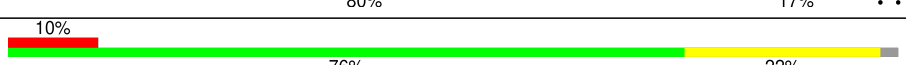
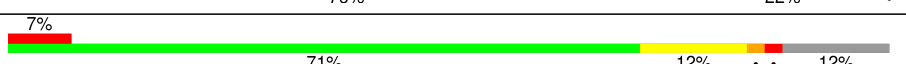
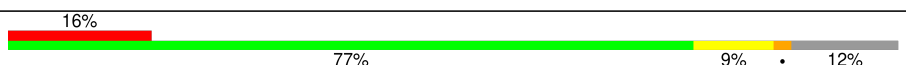
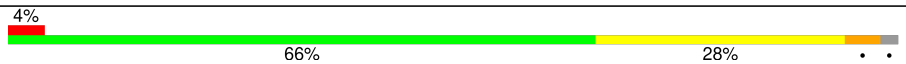
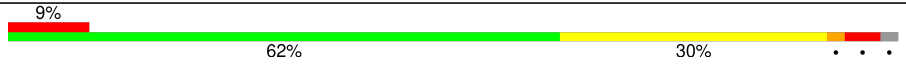
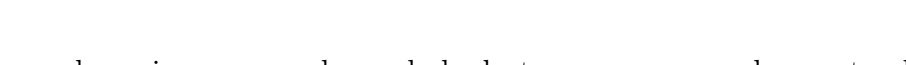
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	514	0% 70% 25% ..
1	N	514	2% 68% 28% ..
2	B	227	6% 67% 24% 7% .
2	O	227	7% 69% 28% ..

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Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
1	FME	N	1	-	X	-	-
2	FME	B	1	-	X	-	-
22	PSC	B	229	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1059	X	-	-	-
24	UNX	C	262	-	-	-	X
24	UNX	P	262	-	-	-	X
25	PEK	G	1263	-	-	X	-
25	PEK	T	263	-	-	X	-
26	CDL	C	270	-	-	X	-
26	CDL	G	269	-	-	X	-
26	CDL	P	1270	-	-	X	-
26	CDL	T	1269	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			
1	N	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

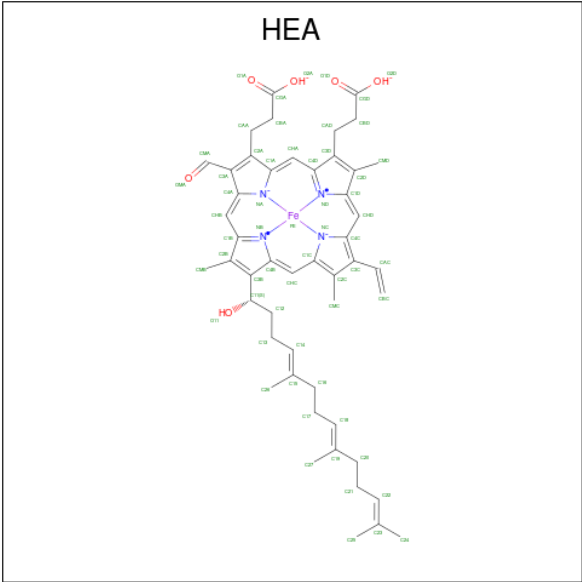
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

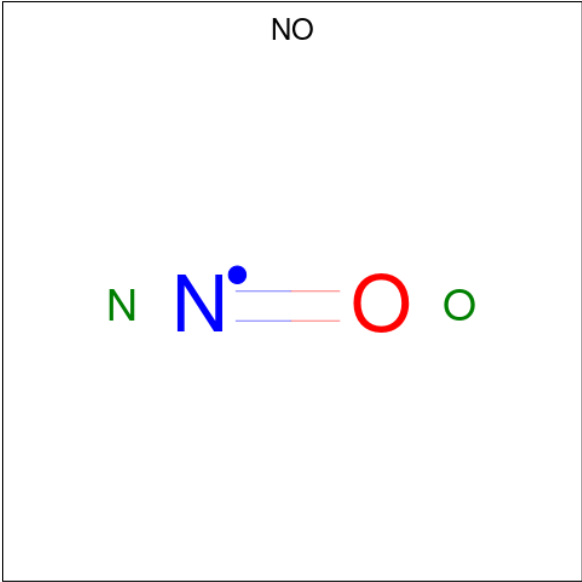
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total N O 2 1 1	0	0
15	N	1	Total N O 2 1 1	0	0

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Cu 1 1	0	0
16	N	1	Total Cu 1 1	0	0

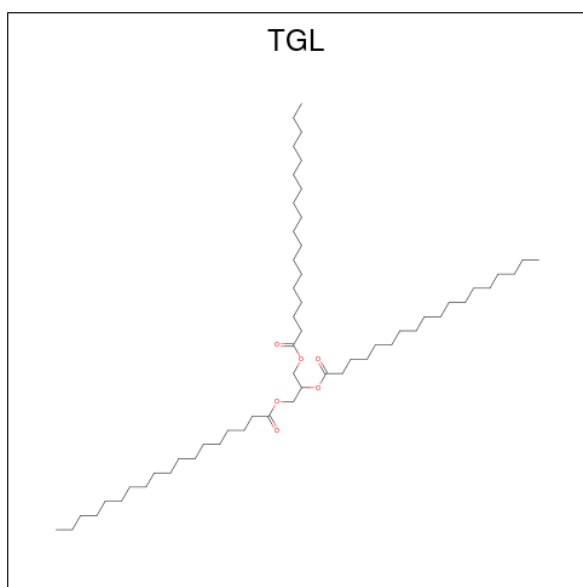
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Mg 1 1	0	0
17	N	1	Total Mg 1 1	0	0

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

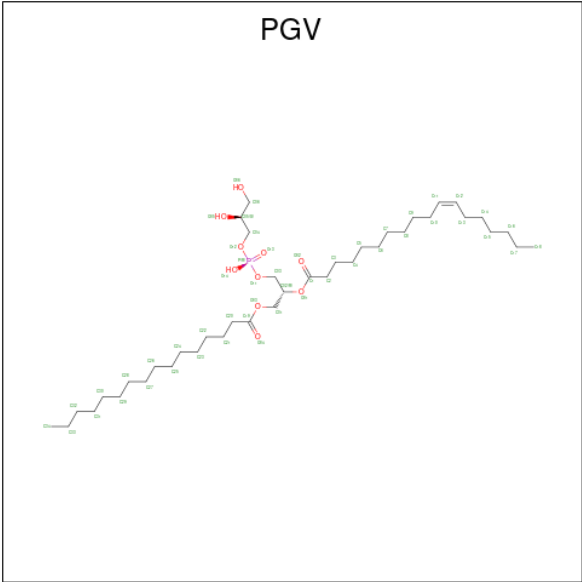
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



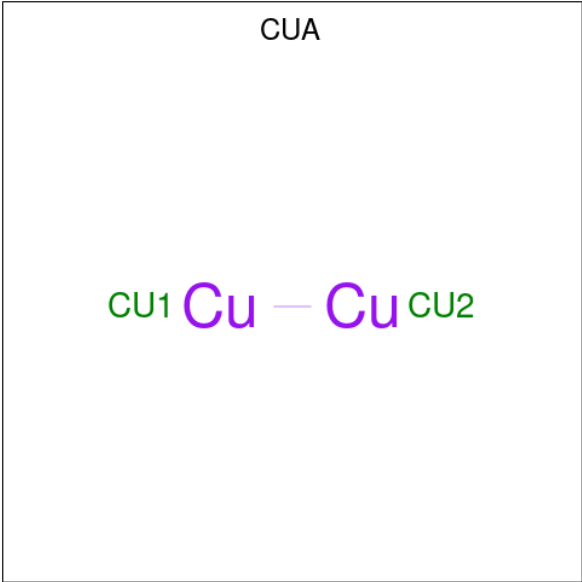
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



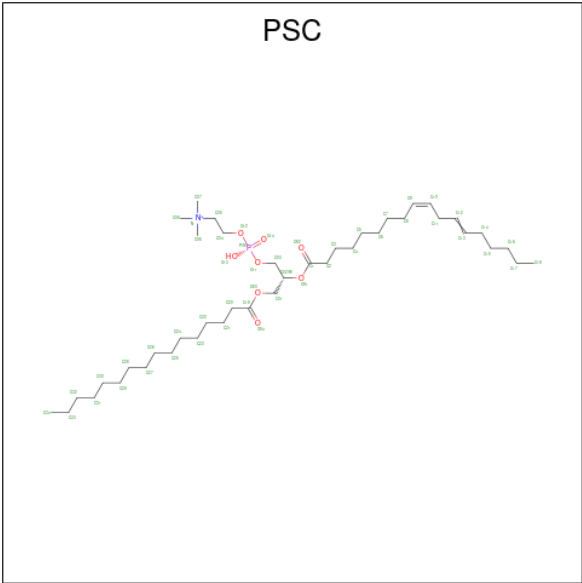
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	M	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



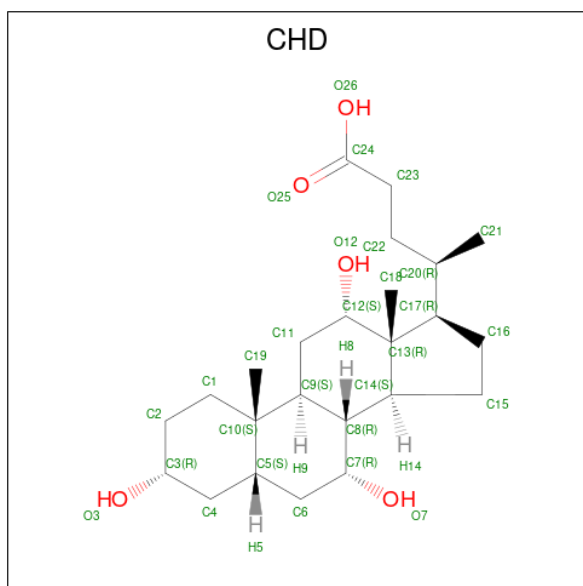
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	R	1	Total	C	N	O	P	
			52	42	1	8	1	
							0	0

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).

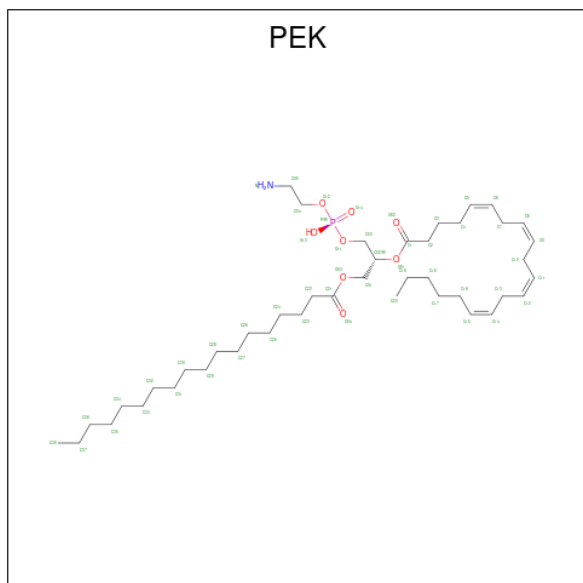


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O		
			29	24	5	0	0
23	C	1	Total	C	O		
			29	24	5	0	0
23	C	1	Total	C	O		
			29	24	5	0	0
23	J	1	Total	C	O		
			29	24	5	0	0
23	O	1	Total	C	O		
			29	24	5	0	0
23	P	1	Total	C	O		
			29	24	5	0	0
23	P	1	Total	C	O		
			29	24	5	0	0
23	W	1	Total	C	O		
			29	24	5	0	0

- Molecule 24 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

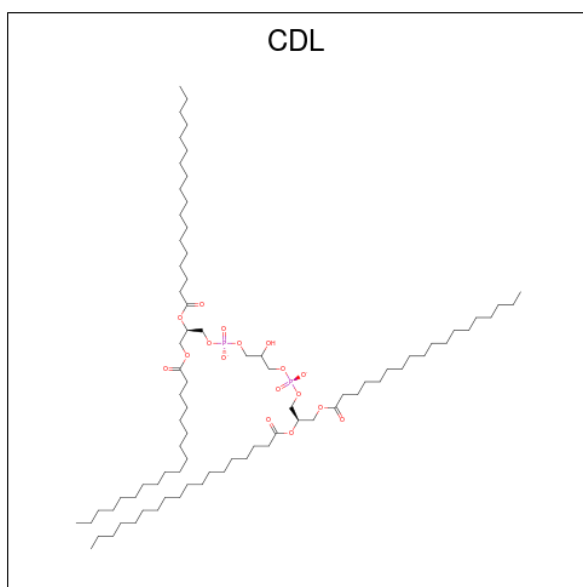
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total X 1 1	0	0
24	P	1	Total X 1 1	0	0

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C N O P 53 43 1 8 1	0	0
25	G	1	Total C N O P 53 43 1 8 1	0	0
25	G	1	Total C N O P 53 43 1 8 1	0	0
25	P	1	Total C N O P 53 43 1 8 1	0	0
25	P	1	Total C N O P 53 43 1 8 1	0	0
25	T	1	Total C N O P 53 43 1 8 1	0	0

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

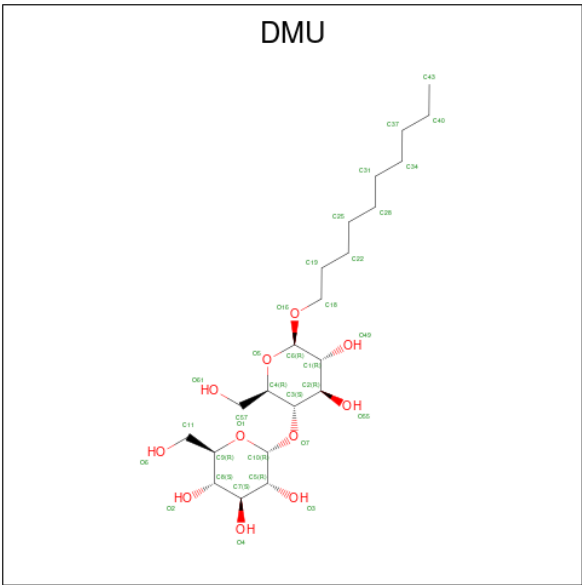


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	F	1	Total	Zn	0	0
			1	1		
27	S	1	Total	Zn	0	0
			1	1		

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	G	1	Total	C	O	0	0
			33	22	11		
28	M	1	Total	C	O	0	0
			33	22	11		
28	P	1	Total	C	O	0	0
			33	22	11		
28	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	218	Total	O	0	0
			218	218		
29	B	143	Total	O	0	0
			143	143		
29	C	116	Total	O	0	0
			116	116		
29	D	80	Total	O	0	0
			80	80		
29	E	49	Total	O	0	0
			49	49		
29	F	61	Total	O	0	0
			61	61		
29	G	45	Total	O	0	0
			45	45		
29	H	51	Total	O	0	0
			51	51		

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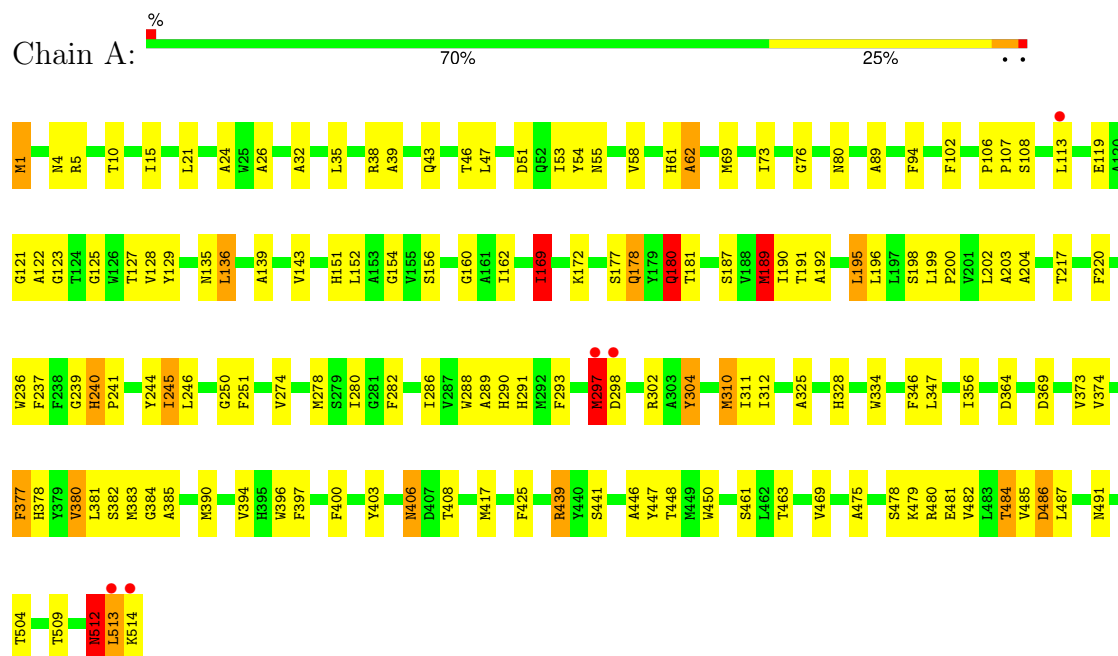
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	I	37	Total 37	O 37	0	0
29	J	24	Total 24	O 24	0	0
29	K	29	Total 29	O 29	0	0
29	L	23	Total 23	O 23	0	0
29	M	31	Total 31	O 31	0	0
29	N	222	Total 222	O 222	0	0
29	O	137	Total 137	O 137	0	0
29	P	102	Total 102	O 102	0	0
29	Q	65	Total 65	O 65	0	0
29	R	47	Total 47	O 47	0	0
29	S	64	Total 64	O 64	0	0
29	T	47	Total 47	O 47	0	0
29	U	49	Total 49	O 49	0	0
29	V	27	Total 27	O 27	0	0
29	W	19	Total 19	O 19	0	0
29	X	22	Total 22	O 22	0	0
29	Y	21	Total 21	O 21	0	0
29	Z	14	Total 14	O 14	0	0

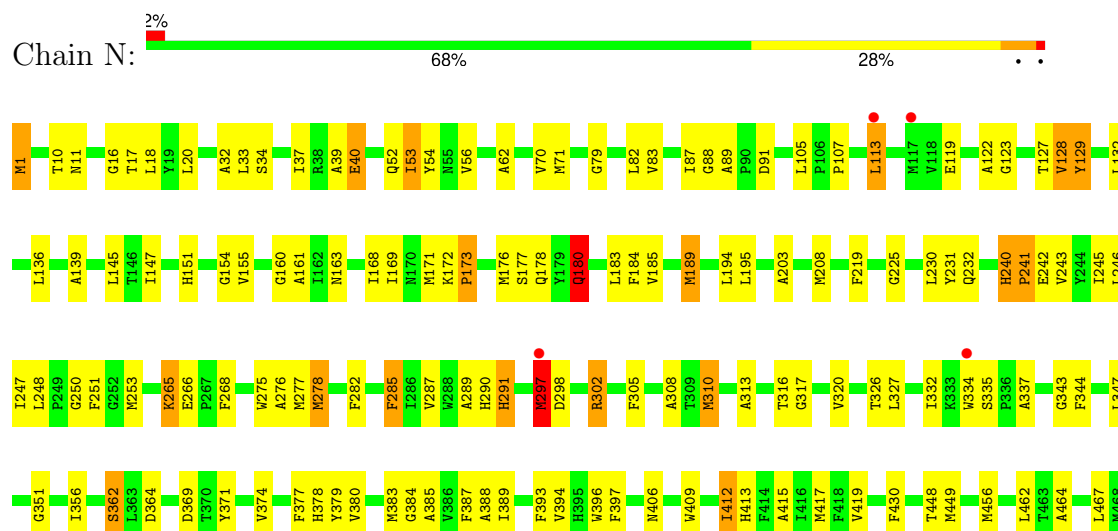
3 Residue-property plots

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

• Molecule 1: Cytochrome c oxidase subunit 1

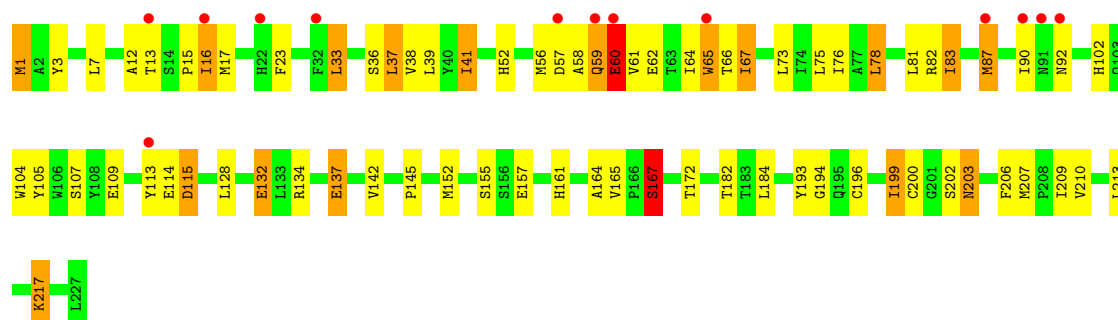


• Molecule 1: Cytochrome c oxidase subunit 1

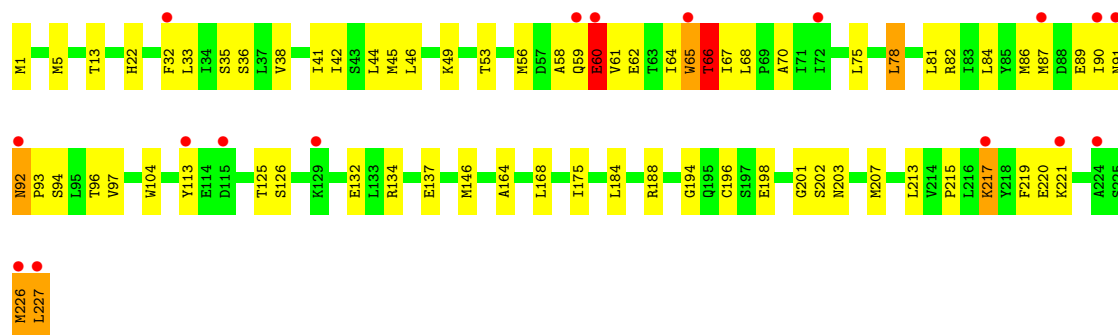




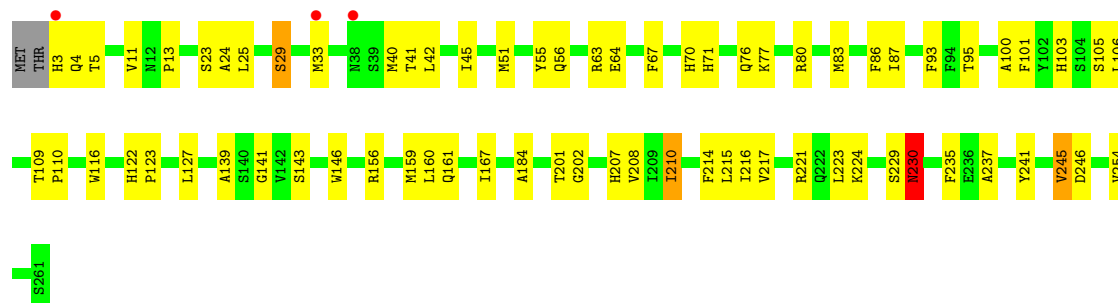
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

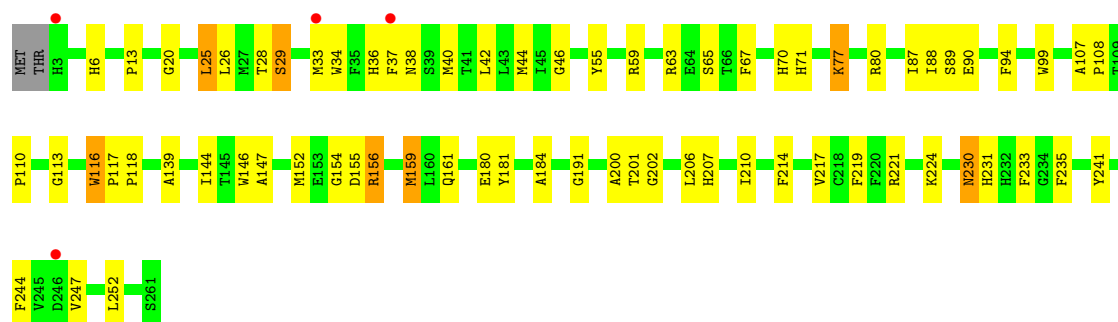


• Molecule 3: Cytochrome c oxidase subunit 3

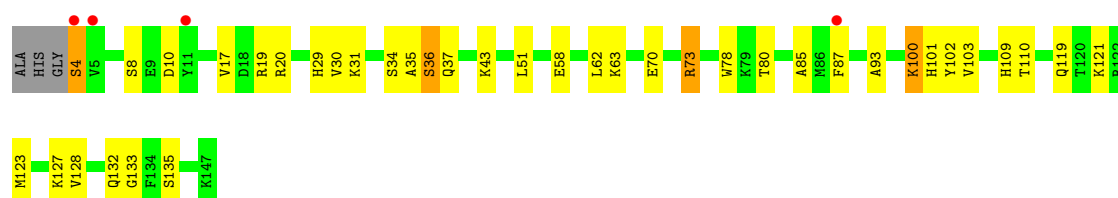


• Molecule 3: Cytochrome c oxidase subunit 3

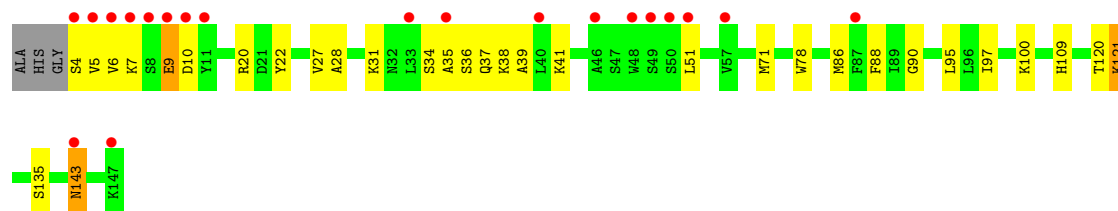
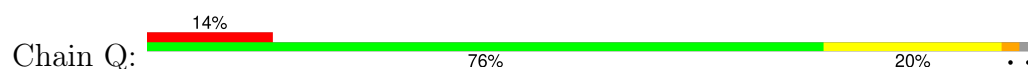




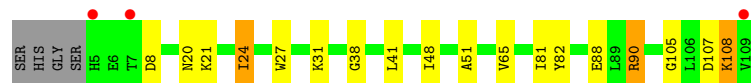
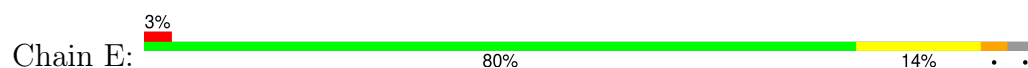
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



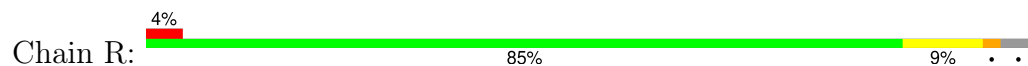
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 5: Cytochrome c oxidase subunit 5A

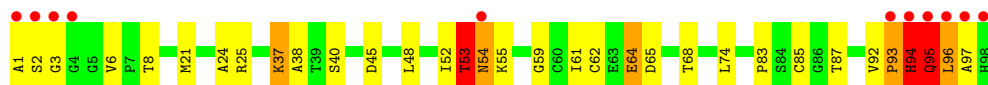


- Molecule 6: Cytochrome c oxidase subunit 5B

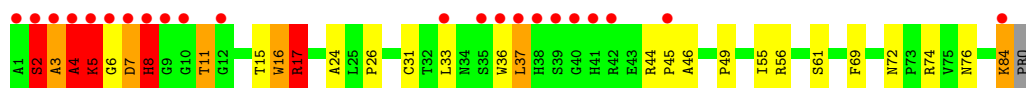




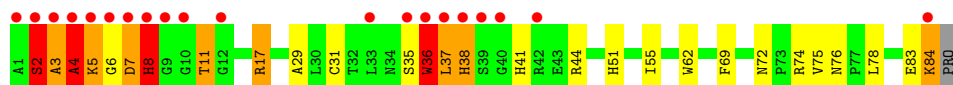
- Molecule 6: Cytochrome c oxidase subunit 5B



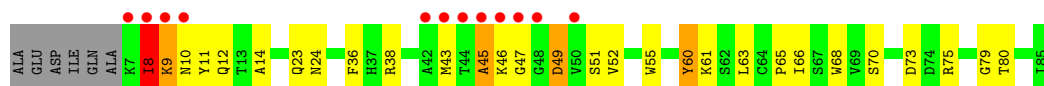
- Molecule 7: Cytochrome c oxidase subunit 6A2



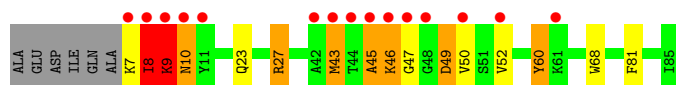
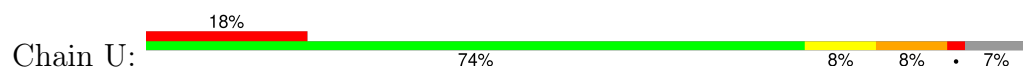
- Molecule 7: Cytochrome c oxidase subunit 6A2



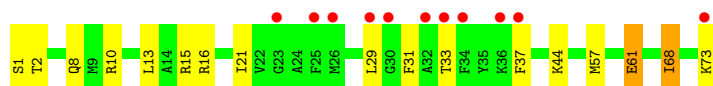
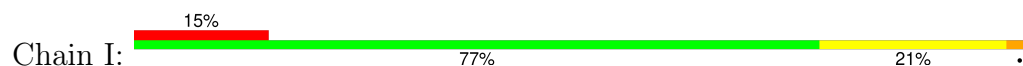
- Molecule 8: Cytochrome c oxidase subunit 6B1



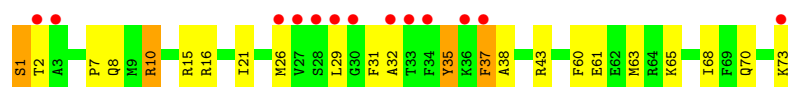
- Molecule 8: Cytochrome c oxidase subunit 6B1



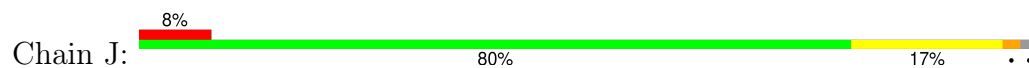
- Molecule 9: Cytochrome c oxidase subunit 6C



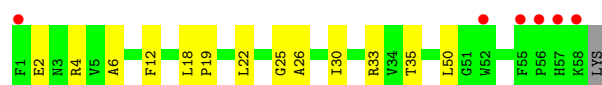
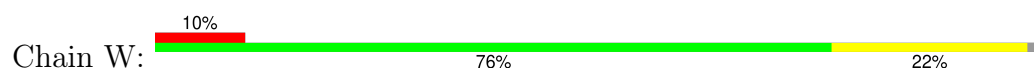
- Molecule 9: Cytochrome c oxidase subunit 6C



• Molecule 10: Cytochrome c oxidase polypeptide 7A1



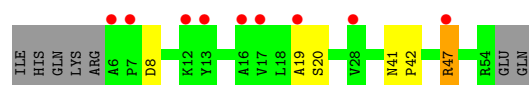
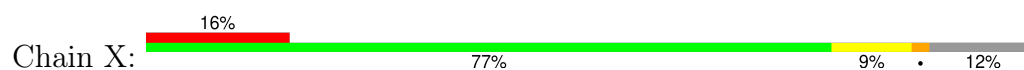
• Molecule 10: Cytochrome c oxidase polypeptide 7A1



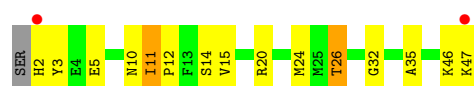
• Molecule 11: Cytochrome c oxidase subunit 7B



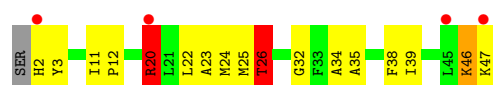
• Molecule 11: Cytochrome c oxidase subunit 7B



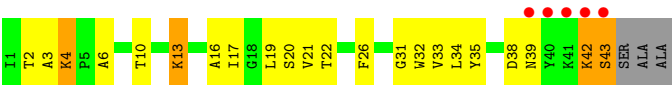
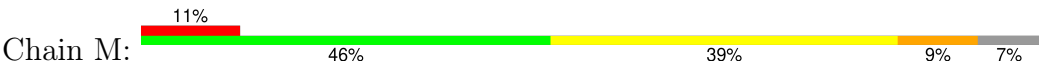
• Molecule 12: Cytochrome c oxidase subunit 7C



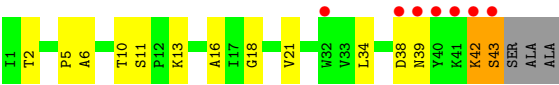
• Molecule 12: Cytochrome c oxidase subunit 7C



● Molecule 13: Cytochrome c oxidase subunit 8B



● Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.29Å 208.36Å 177.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 99.6 (40.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.175 , 0.203 0.192 , 0.218	Depositor DCC
R_{free} test set	30652 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32545	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HEA, TGL, CUA, DMU, PSC, CHD, NA, PGV, PEK, FME, NO, UNX, ZN, SAC, TPO, CDL, CU

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	2.11	101/4189 (2.4%)	1.68	50/5722 (0.9%)
1	N	2.11	94/4189 (2.2%)	1.64	55/5722 (1.0%)
2	B	2.10	46/1860 (2.5%)	1.70	20/2534 (0.8%)
2	O	1.85	24/1860 (1.3%)	1.57	16/2534 (0.6%)
3	C	1.88	36/2197 (1.6%)	1.55	20/3005 (0.7%)
3	P	1.93	38/2197 (1.7%)	1.54	21/3005 (0.7%)
4	D	1.90	19/1229 (1.5%)	1.52	22/1658 (1.3%)
4	Q	1.67	9/1229 (0.7%)	1.42	14/1658 (0.8%)
5	E	1.80	8/871 (0.9%)	1.48	6/1182 (0.5%)
5	R	1.59	5/871 (0.6%)	1.37	3/1182 (0.3%)
6	F	2.12	20/765 (2.6%)	1.67	10/1038 (1.0%)
6	S	1.97	15/765 (2.0%)	1.76	18/1038 (1.7%)
7	G	1.99	15/690 (2.2%)	1.67	10/937 (1.1%)
7	T	1.86	12/690 (1.7%)	1.64	12/937 (1.3%)
8	H	1.90	16/682 (2.3%)	1.48	4/921 (0.4%)
8	U	1.54	5/682 (0.7%)	1.44	5/921 (0.5%)
9	I	1.69	5/605 (0.8%)	1.38	2/802 (0.2%)
9	V	1.68	3/605 (0.5%)	1.45	4/802 (0.5%)
10	J	1.61	2/471 (0.4%)	1.48	3/636 (0.5%)
10	W	1.81	8/471 (1.7%)	1.46	2/636 (0.3%)
11	K	1.78	4/398 (1.0%)	1.59	7/546 (1.3%)
11	X	1.49	2/398 (0.5%)	1.39	2/546 (0.4%)
12	L	1.87	5/393 (1.3%)	1.56	4/526 (0.8%)
12	Y	1.92	8/393 (2.0%)	1.51	1/526 (0.2%)
13	M	2.02	10/345 (2.9%)	1.54	2/470 (0.4%)
13	Z	1.72	6/345 (1.7%)	1.48	1/470 (0.2%)
All	All	1.93	516/29390 (1.8%)	1.58	314/39954 (0.8%)

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	1
2	B	1	0
6	F	0	1
6	S	0	1
All	All	1	3

All (516) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	512	ASN	CA-CB	11.95	1.72	1.53
1	N	310	MET	SD-CE	-10.19	1.54	1.79
1	A	482	VAL	CA-CB	10.15	1.64	1.54
1	N	189	MET	CB-CG	10.09	1.82	1.52
6	S	54	ASN	CB-CG	-10.08	1.26	1.52
7	T	17	ARG	CD-NE	-9.90	1.32	1.46
7	G	17	ARG	CD-NE	-9.72	1.32	1.46
1	A	310	MET	SD-CE	-9.66	1.55	1.79
3	P	20	GLY	N-CA	9.58	1.57	1.45
2	O	175	ILE	CA-CB	9.51	1.61	1.54
3	P	46	GLY	N-CA	9.38	1.57	1.45
1	N	122	ALA	CA-CB	9.21	1.64	1.53
1	A	189	MET	CG-SD	-9.16	1.57	1.80
1	N	419	VAL	CA-CB	9.15	1.66	1.54
1	N	83	VAL	CA-CB	8.99	1.59	1.54
6	F	92	VAL	CA-CB	8.89	1.65	1.54
1	A	122	ALA	CA-CB	8.81	1.66	1.53
2	B	87	MET	CG-SD	8.70	2.02	1.80
3	C	29	SER	CA-CB	8.60	1.67	1.53
1	A	512	ASN	CB-CG	-8.46	1.30	1.52
1	A	297	MET	CG-SD	8.41	2.01	1.80
4	Q	6	VAL	CA-CB	8.40	1.62	1.54
4	Q	121	LYS	CE-NZ	8.33	1.74	1.49
1	A	203	ALA	N-CA	8.32	1.56	1.46
12	L	35	ALA	CA-CB	8.31	1.63	1.53
1	A	240	HIS	N-CA	8.29	1.53	1.46
1	A	298	ASP	N-CA	8.27	1.56	1.46
1	N	483	LEU	C-O	8.26	1.30	1.23
1	A	113	LEU	CB-CG	8.16	1.69	1.53
13	Z	16	ALA	CA-CB	8.16	1.66	1.53
2	B	142	VAL	CA-CB	8.12	1.62	1.53
6	S	54	ASN	CA-C	-8.05	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	231	HIS	CA-C	-8.04	1.43	1.52
1	A	154	GLY	N-CA	8.00	1.55	1.45
1	N	11	ASN	C-O	8.00	1.33	1.24
1	N	415	ALA	CA-CB	7.99	1.65	1.53
7	T	3	ALA	CA-C	7.97	1.63	1.52
1	A	302	ARG	CZ-NH1	7.96	1.43	1.32
1	A	54	TYR	CA-C	7.93	1.63	1.52
3	P	77	LYS	CA-CB	-7.93	1.40	1.53
2	B	113	TYR	N-CA	7.91	1.56	1.46
11	X	41	ASN	C-O	7.87	1.27	1.23
2	B	167	SER	CB-OG	-7.85	1.26	1.42
1	A	298	ASP	CG-OD2	7.81	1.40	1.25
1	N	163	ASN	N-CA	7.78	1.55	1.46
1	N	113	LEU	CB-CG	7.78	1.69	1.53
6	S	3	GLY	N-CA	7.77	1.52	1.45
1	N	155	VAL	CA-CB	7.73	1.63	1.54
1	N	397	PHE	CA-C	7.64	1.62	1.52
1	A	55	ASN	N-CA	7.62	1.55	1.46
13	M	17	ILE	CA-C	7.60	1.62	1.52
6	F	29	ASP	N-CA	7.56	1.54	1.46
13	Z	11	SER	C-O	7.52	1.33	1.23
8	H	8	ILE	CA-CB	7.52	1.64	1.54
1	A	397	PHE	CA-C	7.50	1.62	1.52
1	N	484	THR	CB-CG2	7.48	1.77	1.52
1	A	89	ALA	CA-CB	7.48	1.66	1.53
1	N	79	GLY	N-CA	7.47	1.55	1.45
3	P	230	ASN	CB-CG	-7.43	1.33	1.52
3	C	217	VAL	CA-CB	7.43	1.63	1.54
10	W	26	ALA	CA-CB	7.40	1.65	1.53
2	B	59	GLN	CG-CD	7.39	1.70	1.52
7	T	2	SER	CA-C	7.38	1.62	1.52
7	G	2	SER	CA-C	7.38	1.62	1.52
7	G	55	ILE	CA-CB	7.38	1.62	1.54
6	F	92	VAL	C-O	-7.37	1.15	1.24
1	N	297	MET	CG-SD	7.35	1.99	1.80
1	N	326	THR	CA-C	7.33	1.62	1.52
1	N	203	ALA	N-CA	7.32	1.55	1.46
3	P	200	ALA	N-CA	7.31	1.55	1.46
1	A	24	ALA	CA-CB	7.31	1.64	1.53
1	A	439	ARG	CD-NE	7.31	1.56	1.46
7	T	55	ILE	C-O	7.22	1.31	1.24
6	F	3	GLY	N-CA	7.20	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	73	ASP	N-CA	7.20	1.55	1.46
1	A	190	ILE	CA-CB	7.19	1.63	1.54
3	C	223	LEU	N-CA	7.18	1.55	1.46
6	F	70	ILE	CA-CB	7.17	1.62	1.54
3	P	107	ALA	CA-CB	7.16	1.62	1.53
4	D	103	VAL	CA-CB	7.14	1.62	1.55
6	F	56	ARG	CZ-NH1	7.13	1.42	1.32
1	A	397	PHE	N-CA	7.11	1.53	1.46
1	N	337	ALA	N-CA	7.11	1.54	1.46
6	F	69	VAL	C-O	7.09	1.32	1.24
1	A	240	HIS	CA-C	7.05	1.60	1.52
1	N	277	MET	N-CA	7.05	1.55	1.46
1	A	143	VAL	N-CA	7.04	1.55	1.46
5	R	75	ALA	CA-CB	7.04	1.65	1.53
4	D	36	SER	N-CA	7.03	1.55	1.46
2	B	182	THR	C-O	-6.99	1.15	1.23
5	E	20	ASN	N-CA	6.98	1.55	1.46
6	S	2	SER	N-CA	6.98	1.54	1.46
4	D	100	LYS	CE-NZ	6.97	1.70	1.49
7	G	4	ALA	CA-CB	-6.97	1.41	1.53
1	N	119	GLU	CA-C	-6.91	1.47	1.53
1	A	403	TYR	N-CA	6.90	1.54	1.45
1	A	123	GLY	C-O	6.89	1.33	1.23
1	A	374	VAL	CA-CB	6.88	1.63	1.54
1	A	154	GLY	C-O	-6.87	1.15	1.23
1	N	268	PHE	C-O	6.86	1.32	1.23
6	F	2	SER	N-CA	6.85	1.54	1.46
1	A	46	THR	C-O	6.84	1.32	1.24
2	B	61	VAL	N-CA	-6.82	1.37	1.46
1	N	248	LEU	CA-CB	6.75	1.62	1.53
5	E	81	ILE	C-O	6.74	1.31	1.24
1	N	195	LEU	CB-CG	6.72	1.66	1.53
5	R	56	ARG	N-CA	6.69	1.54	1.46
8	H	12	GLN	CA-C	6.63	1.58	1.52
1	N	378	HIS	N-CA	6.63	1.55	1.46
7	T	36	TRP	CB-CG	6.63	1.70	1.50
1	A	390	MET	N-CA	6.59	1.54	1.46
3	C	139	ALA	N-CA	6.58	1.54	1.46
6	F	59	GLY	CA-C	-6.57	1.47	1.52
1	A	245	ILE	C-O	6.56	1.31	1.24
1	A	26	ALA	CA-C	-6.55	1.44	1.52
5	E	82	TYR	CA-C	6.55	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	57	ILE	CA-CB	6.53	1.61	1.54
1	A	128	VAL	N-CA	6.52	1.54	1.46
1	N	456	MET	C-O	6.52	1.31	1.24
4	D	110	THR	CA-CB	6.50	1.65	1.53
3	C	11	VAL	CA-CB	6.50	1.62	1.54
2	O	90	ILE	CA-CB	6.50	1.63	1.54
4	D	128	VAL	N-CA	6.49	1.54	1.46
3	C	5	THR	N-CA	-6.49	1.38	1.46
3	C	93	PHE	N-CA	6.49	1.54	1.46
1	A	450	TRP	N-CA	6.48	1.54	1.46
3	P	252	LEU	N-CA	6.48	1.54	1.46
1	A	220	PHE	N-CA	6.47	1.53	1.46
1	N	91	ASP	CA-CB	6.47	1.62	1.53
1	N	183	LEU	C-O	6.46	1.31	1.24
10	W	30	ILE	CA-C	6.46	1.60	1.52
7	G	36	TRP	CB-CG	6.46	1.70	1.50
12	Y	32	GLY	N-CA	6.45	1.53	1.45
1	N	185	VAL	C-O	-6.44	1.16	1.24
3	P	29	SER	CB-OG	-6.43	1.29	1.42
6	F	74	LEU	N-CA	6.42	1.54	1.46
1	A	302	ARG	N-CA	6.42	1.54	1.46
2	O	59	GLN	CG-CD	6.41	1.68	1.52
13	M	10	THR	CA-CB	6.41	1.62	1.53
1	A	251	PHE	N-CA	6.38	1.54	1.46
2	B	23	PHE	C-O	6.37	1.31	1.24
7	T	5	LYS	CB-CG	6.36	1.71	1.52
1	N	33	LEU	CA-CB	6.35	1.63	1.53
1	N	388	ALA	CA-CB	6.34	1.63	1.53
1	N	173	PRO	CA-CB	6.33	1.59	1.53
7	G	3	ALA	CA-C	6.32	1.61	1.52
6	F	61	ILE	CA-CB	6.32	1.60	1.53
1	A	408	THR	CA-CB	6.31	1.63	1.53
1	N	317	GLY	N-CA	6.31	1.53	1.45
1	N	371	TYR	CA-C	6.30	1.61	1.52
8	H	8	ILE	CA-C	6.28	1.60	1.52
6	F	3	GLY	C-O	6.28	1.29	1.23
6	F	37	LYS	C-O	-6.27	1.16	1.23
4	D	29	HIS	CA-C	6.26	1.60	1.52
2	B	3	TYR	CA-CB	6.26	1.61	1.54
13	M	4	LYS	CD-CE	-6.26	1.33	1.52
1	A	236	TRP	C-O	6.25	1.31	1.24
3	P	147	ALA	N-CA	6.25	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	LYS	CB-CG	6.24	1.71	1.52
1	N	113	LEU	CG-CD1	6.22	1.73	1.52
1	A	43	GLN	CA-CB	6.22	1.62	1.53
4	D	20	ARG	CD-NE	-6.22	1.37	1.46
13	M	22	THR	N-CA	6.21	1.53	1.46
1	A	106	PRO	CA-C	6.21	1.57	1.52
1	A	113	LEU	CG-CD1	6.20	1.73	1.52
6	S	83	PRO	N-CA	6.20	1.54	1.47
1	A	119	GLU	CA-C	-6.17	1.47	1.53
1	N	362	SER	N-CA	6.13	1.53	1.46
1	N	511	VAL	CA-CB	6.13	1.62	1.54
7	T	55	ILE	CA-CB	6.13	1.61	1.54
1	A	196	LEU	N-CA	6.12	1.53	1.46
2	B	145	PRO	C-O	6.12	1.30	1.23
1	N	297	MET	CA-CB	6.12	1.63	1.53
3	C	83	MET	N-CA	6.11	1.53	1.46
4	D	35	ALA	CA-CB	6.11	1.62	1.53
7	G	16	TRP	CA-C	6.10	1.60	1.52
3	P	139	ALA	CA-CB	6.10	1.62	1.53
7	T	3	ALA	N-CA	6.10	1.54	1.46
6	S	52	ILE	N-CA	-6.09	1.40	1.46
6	S	61	ILE	CA-CB	6.09	1.60	1.53
1	N	147	ILE	CA-CB	6.09	1.61	1.54
1	N	169	ILE	CA-CB	6.09	1.62	1.54
1	A	38	ARG	CZ-NH2	6.08	1.41	1.33
2	B	38	VAL	CA-CB	6.08	1.62	1.54
8	U	8	ILE	CA-CB	6.08	1.62	1.54
2	O	38	VAL	CA-CB	6.06	1.62	1.54
2	O	198	GLU	C-O	6.05	1.30	1.23
1	A	169	ILE	CG1-CD1	-6.02	1.28	1.51
3	P	90	GLU	N-CA	6.02	1.53	1.46
1	N	464	ALA	N-CA	6.01	1.53	1.46
7	G	7	ASP	N-CA	6.00	1.53	1.46
12	Y	20	ARG	CD-NE	6.00	1.54	1.46
4	D	63	LYS	N-CA	6.00	1.53	1.46
5	E	51	ALA	N-CA	5.99	1.53	1.46
11	X	19	ALA	CA-CB	5.99	1.62	1.53
5	R	40	ASP	CA-CB	5.99	1.60	1.52
1	A	385	ALA	CA-CB	5.97	1.62	1.53
12	L	12	PRO	C-O	5.97	1.29	1.23
3	C	123	PRO	C-O	5.96	1.30	1.23
9	I	57	MET	N-CA	5.96	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	109	GLU	N-CA	5.96	1.53	1.46
4	D	132	GLN	C-O	-5.96	1.16	1.24
7	G	15	THR	CA-CB	5.96	1.62	1.53
6	F	1	ALA	C-O	5.96	1.35	1.23
1	A	139	ALA	CA-CB	5.95	1.63	1.53
4	Q	120	THR	N-CA	5.95	1.53	1.46
4	D	30	VAL	CA-C	-5.95	1.45	1.52
12	Y	23	ALA	CA-CB	5.95	1.62	1.53
12	L	15	VAL	CA-C	5.93	1.60	1.52
2	B	206	PHE	N-CA	5.93	1.54	1.46
13	M	21	VAL	CA-C	5.93	1.60	1.52
7	T	75	VAL	N-CA	5.93	1.51	1.46
1	N	302	ARG	CZ-NH1	5.92	1.41	1.32
3	P	13	PRO	CA-CB	5.92	1.61	1.53
1	A	289	ALA	CA-CB	5.92	1.63	1.53
3	C	33	MET	CG-SD	5.91	1.95	1.80
2	B	83	ILE	CA-C	-5.90	1.45	1.52
2	B	36	SER	CA-C	5.88	1.60	1.52
8	H	63	LEU	N-CA	5.87	1.53	1.46
10	W	22	LEU	N-CA	5.87	1.54	1.45
1	N	396	TRP	N-CA	5.86	1.53	1.46
1	N	462	LEU	CA-C	5.86	1.60	1.52
7	G	5	LYS	CA-C	5.86	1.60	1.52
13	M	20	SER	CA-C	-5.86	1.45	1.52
1	A	328	HIS	N-CA	5.85	1.53	1.46
2	B	152	MET	CB-CG	-5.85	1.34	1.52
6	S	2	SER	CA-C	5.85	1.59	1.52
5	E	27	TRP	N-CA	5.84	1.53	1.46
2	O	96	THR	C-O	5.84	1.31	1.24
1	N	246	LEU	N-CA	5.83	1.53	1.46
8	H	55	TRP	N-CA	-5.83	1.39	1.46
6	S	45	ASP	CA-C	5.83	1.60	1.52
1	A	198	SER	N-CA	5.82	1.53	1.46
1	N	467	LEU	C-O	5.82	1.31	1.24
1	A	286	ILE	CA-CB	5.82	1.60	1.54
1	N	40	GLU	C-O	5.81	1.30	1.24
3	P	33	MET	CG-SD	5.80	1.95	1.80
7	G	46	ALA	CA-C	5.80	1.59	1.52
1	N	297	MET	CB-CG	5.80	1.69	1.52
13	M	31	GLY	N-CA	5.79	1.53	1.45
13	M	33	VAL	CA-CB	5.79	1.61	1.54
4	D	4	SER	N-CA	5.79	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	37	ILE	CA-CB	5.79	1.61	1.54
3	C	216	ILE	N-CA	5.79	1.53	1.46
3	P	118	PRO	C-O	5.79	1.30	1.23
1	A	191	THR	N-CA	5.79	1.53	1.46
2	B	105	TYR	C-O	5.79	1.30	1.23
1	N	470	PHE	N-CA	5.78	1.53	1.46
2	B	137	GLU	N-CA	5.77	1.53	1.45
8	H	14	ALA	C-N	5.77	1.40	1.33
1	A	5	ARG	CD-NE	5.76	1.54	1.46
2	O	134	ARG	CD-NE	5.76	1.54	1.46
3	P	159	MET	N-CA	5.76	1.53	1.46
2	O	56	MET	SD-CE	5.75	1.94	1.79
2	B	199	ILE	C-O	5.74	1.30	1.24
2	B	132	GLU	CD-OE2	5.72	1.36	1.25
8	H	61	LYS	CE-NZ	5.71	1.66	1.49
1	N	247	ILE	C-O	5.71	1.30	1.24
4	Q	135	SER	N-CA	5.71	1.53	1.46
1	A	192	ALA	CA-CB	5.71	1.62	1.53
3	P	155	ASP	CA-CB	5.70	1.60	1.53
1	N	16	GLY	N-CA	5.70	1.53	1.45
7	T	4	ALA	CA-CB	-5.70	1.43	1.53
2	B	115	ASP	CB-CG	5.69	1.66	1.52
3	C	237	ALA	CA-CB	5.69	1.62	1.53
6	S	94	HIS	CA-C	-5.68	1.45	1.52
3	P	184	ALA	CA-CB	5.68	1.62	1.53
3	C	184	ALA	CA-CB	5.68	1.62	1.53
2	B	200	CYS	N-CA	5.67	1.52	1.46
6	F	73	TRP	C-O	5.66	1.30	1.23
1	N	230	LEU	N-CA	5.66	1.53	1.46
1	N	163	ASN	CA-CB	5.66	1.62	1.53
1	A	513	LEU	CA-C	-5.65	1.46	1.53
1	N	139	ALA	CA-CB	5.65	1.62	1.53
1	N	448	THR	CA-CB	5.64	1.62	1.53
6	F	82	CYS	N-CA	5.64	1.52	1.45
2	B	161	HIS	CA-CB	5.63	1.61	1.53
1	N	287	VAL	CA-CB	5.63	1.60	1.54
2	O	219	PHE	CA-CB	5.63	1.62	1.53
12	L	10	ASN	C-N	5.62	1.38	1.33
2	B	90	ILE	C-O	5.62	1.30	1.24
1	N	32	ALA	N-CA	5.62	1.53	1.46
12	Y	46	LYS	CD-CE	-5.62	1.35	1.52
12	Y	20	ARG	NE-CZ	5.62	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	92	ASN	CB-CG	5.61	1.66	1.52
1	A	406	ASN	CA-CB	5.61	1.60	1.53
5	R	71	VAL	C-O	5.61	1.30	1.24
8	H	68	TRP	N-CA	5.60	1.53	1.46
2	B	107	SER	C-O	5.59	1.31	1.23
1	A	189	MET	SD-CE	-5.58	1.65	1.79
1	A	53	ILE	CG1-CD1	5.58	1.73	1.51
1	A	491	ASN	CA-CB	5.58	1.58	1.53
1	A	32	ALA	CA-CB	5.57	1.62	1.53
2	O	44	LEU	N-CA	5.57	1.53	1.46
7	T	29	ALA	N-CA	5.57	1.53	1.46
5	R	40	ASP	CA-C	-5.57	1.47	1.53
3	C	201	THR	CA-CB	5.56	1.62	1.53
3	C	210	ILE	CA-CB	5.56	1.61	1.54
3	P	244	PHE	CA-CB	5.56	1.62	1.53
1	N	413	HIS	CA-C	5.55	1.59	1.52
3	C	160	LEU	CA-CB	5.55	1.61	1.53
1	N	154	GLY	N-CA	5.55	1.52	1.45
10	J	14	GLU	CA-C	5.54	1.59	1.52
1	A	58	VAL	CA-CB	5.54	1.61	1.54
3	C	167	ILE	C-O	5.54	1.30	1.24
1	N	70	VAL	C-O	5.54	1.30	1.24
1	N	243	VAL	C-O	5.54	1.30	1.24
13	Z	10	THR	CA-CB	5.53	1.62	1.53
1	A	217	THR	C-O	5.53	1.31	1.23
1	N	132	LEU	N-CA	5.52	1.53	1.46
1	N	88	GLY	N-CA	5.52	1.53	1.45
2	B	155	SER	CA-CB	5.51	1.61	1.53
3	P	38	ASN	N-CA	-5.51	1.39	1.46
1	N	245	ILE	CA-CB	5.50	1.62	1.54
3	P	201	THR	CA-CB	5.50	1.62	1.53
1	A	199	LEU	N-CA	5.49	1.52	1.46
2	B	202	SER	N-CA	5.49	1.53	1.46
2	O	97	VAL	N-CA	5.49	1.52	1.46
3	P	87	ILE	CA-C	5.49	1.59	1.52
6	S	68	THR	CA-CB	5.48	1.60	1.53
2	B	165	VAL	CA-CB	5.48	1.61	1.54
3	C	141	GLY	N-CA	5.48	1.52	1.45
2	O	202	SER	CA-CB	5.48	1.62	1.53
5	E	38	GLY	N-CA	5.47	1.53	1.45
4	Q	97	ILE	CA-CB	5.47	1.60	1.54
3	C	13	PRO	CA-C	-5.47	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	55	TYR	CA-CB	5.47	1.61	1.53
2	B	17	MET	CG-SD	5.47	1.94	1.80
13	Z	5	PRO	C-O	5.47	1.30	1.23
1	A	189	MET	N-CA	5.47	1.52	1.46
3	C	33	MET	N-CA	5.47	1.52	1.46
1	A	204	ALA	C-O	5.46	1.30	1.24
2	B	92	ASN	CG-OD1	5.46	1.33	1.23
3	C	86	PHE	CA-CB	5.46	1.61	1.53
1	N	123	GLY	CA-C	5.46	1.59	1.51
3	P	231	HIS	C-O	5.45	1.30	1.24
13	Z	6	ALA	C-O	5.45	1.30	1.23
1	N	364	ASP	CA-C	5.45	1.60	1.52
1	A	62	ALA	N-CA	5.44	1.53	1.46
1	A	162	ILE	CA-CB	5.44	1.60	1.54
3	P	28	THR	C-O	5.44	1.30	1.24
2	B	15	PRO	CA-C	5.43	1.60	1.52
1	A	346	PHE	CD1-CE1	5.42	1.54	1.38
9	I	61	GLU	CG-CD	-5.41	1.38	1.52
3	C	4	GLN	CA-C	-5.41	1.45	1.52
1	N	53	ILE	CG1-CD1	5.41	1.72	1.51
1	N	483	LEU	CA-C	5.41	1.58	1.53
1	A	127	THR	CA-CB	5.41	1.62	1.53
6	S	24	ALA	C-O	-5.40	1.17	1.24
10	W	19	PRO	N-CA	5.40	1.52	1.46
3	C	24	ALA	CA-CB	5.40	1.61	1.53
1	N	195	LEU	N-CA	5.40	1.52	1.46
12	L	26	THR	CA-CB	5.40	1.61	1.53
1	A	394	VAL	N-CA	5.40	1.52	1.46
1	A	417	MET	N-CA	5.39	1.52	1.46
4	Q	28	ALA	CA-CB	-5.39	1.44	1.53
2	B	213	LEU	CA-C	5.38	1.59	1.52
6	S	25	ARG	CA-C	5.38	1.60	1.52
1	N	20	LEU	N-CA	5.38	1.52	1.46
2	B	39	LEU	CA-C	5.38	1.59	1.52
2	B	199	ILE	CA-CB	5.38	1.60	1.54
2	O	221	LYS	N-CA	5.38	1.52	1.46
1	A	61	HIS	N-CA	5.36	1.52	1.46
3	C	76	GLN	CD-OE1	5.36	1.33	1.23
4	D	43	LYS	CA-C	5.36	1.59	1.52
2	O	184	LEU	CA-C	5.36	1.59	1.52
1	A	509	THR	CA-CB	5.36	1.62	1.53
3	P	217	VAL	CA-CB	5.35	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ILE	CA-CB	5.35	1.61	1.54
1	A	475	ALA	C-O	5.35	1.30	1.24
1	A	192	ALA	N-CA	5.35	1.52	1.46
8	U	27	ARG	CA-C	5.35	1.59	1.52
1	N	320	VAL	N-CA	5.34	1.52	1.46
1	N	240	HIS	CA-C	5.34	1.59	1.52
1	A	447	TYR	N-CA	5.34	1.53	1.46
3	C	245	VAL	CA-CB	5.33	1.61	1.54
11	K	39	GLU	CA-CB	5.33	1.60	1.53
1	N	184	PHE	N-CA	5.33	1.53	1.46
4	Q	20	ARG	N-CA	5.33	1.52	1.46
13	M	3	ALA	CA-CB	5.32	1.63	1.53
1	N	298	ASP	CG-OD2	5.32	1.35	1.25
7	G	56	ARG	CZ-NH1	5.31	1.40	1.32
8	H	9	LYS	N-CA	5.30	1.53	1.46
3	P	214	PHE	N-CA	-5.30	1.40	1.46
1	A	244	TYR	N-CA	5.30	1.52	1.46
1	A	297	MET	CA-CB	5.30	1.62	1.53
3	C	235	PHE	CA-CB	5.29	1.61	1.53
9	V	7	PRO	C-O	5.29	1.30	1.23
1	A	39	ALA	CA-C	5.29	1.59	1.52
1	N	129	TYR	C-O	5.29	1.31	1.24
1	N	389	ILE	CA-CB	-5.28	1.47	1.54
3	C	214	PHE	CA-C	5.28	1.59	1.52
3	C	230	ASN	CB-CG	-5.28	1.38	1.52
6	F	65	ASP	N-CA	5.27	1.52	1.46
3	P	116	TRP	CA-C	5.26	1.57	1.52
11	K	29	TRP	CE3-CZ3	5.26	1.54	1.38
4	D	93	ALA	CA-CB	-5.25	1.44	1.53
7	T	51	HIS	CA-C	5.25	1.59	1.52
1	N	161	ALA	CA-C	5.24	1.59	1.52
10	W	12	PHE	N-CA	-5.24	1.39	1.46
1	A	480	ARG	CZ-NH2	5.24	1.40	1.33
9	V	21	ILE	CG1-CD1	5.23	1.72	1.51
10	J	30	ILE	CA-CB	-5.23	1.47	1.54
2	B	172	THR	CA-CB	5.23	1.62	1.53
9	I	13	LEU	C-O	5.23	1.30	1.24
13	Z	18	GLY	N-CA	5.22	1.52	1.45
6	F	20	VAL	CA-CB	5.22	1.60	1.54
1	N	285	PHE	CD1-CE1	5.22	1.54	1.38
2	O	64	ILE	CA-CB	5.22	1.60	1.54
3	P	94	PHE	CA-C	-5.21	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	27	VAL	C-O	5.21	1.29	1.23
1	A	246	LEU	N-CA	5.20	1.52	1.46
12	Y	20	ARG	CG-CD	5.19	1.68	1.52
1	A	38	ARG	CD-NE	5.19	1.53	1.46
1	N	275	TRP	CA-CB	5.19	1.61	1.53
9	I	16	ARG	NE-CZ	5.19	1.38	1.33
1	N	242	GLU	N-CA	5.18	1.52	1.46
3	C	70	HIS	N-CA	5.18	1.52	1.46
1	N	113	LEU	CG-CD2	5.18	1.69	1.52
12	Y	26	THR	CA-CB	5.18	1.61	1.53
2	O	125	THR	CA-C	5.17	1.59	1.52
9	V	65	LYS	N-CA	5.17	1.52	1.46
1	A	162	ILE	N-CA	5.17	1.52	1.46
1	N	247	ILE	CA-CB	5.17	1.61	1.54
2	O	137	GLU	N-CA	5.16	1.52	1.45
1	N	10	THR	C-O	-5.16	1.17	1.24
1	A	156	SER	C-O	5.16	1.30	1.24
2	B	41	ILE	CA-CB	-5.16	1.48	1.54
4	D	85	ALA	CA-C	5.16	1.59	1.52
3	P	89	SER	C-O	5.16	1.30	1.24
4	Q	5	VAL	CA-C	5.16	1.59	1.52
10	W	25	GLY	N-CA	5.16	1.52	1.44
8	H	70	SER	C-O	5.15	1.30	1.24
8	H	79	GLY	CA-C	5.14	1.58	1.51
6	S	92	VAL	C-N	5.14	1.39	1.33
3	C	100	ALA	CA-CB	5.14	1.61	1.53
1	A	94	PHE	CA-C	5.14	1.58	1.52
2	B	209	ILE	C-O	-5.14	1.18	1.24
2	O	35	SER	CA-C	5.14	1.59	1.52
3	P	219	PHE	N-CA	5.14	1.52	1.46
1	A	487	LEU	CA-CB	5.14	1.61	1.53
2	B	38	VAL	N-CA	-5.14	1.40	1.46
4	D	20	ARG	N-CA	5.14	1.52	1.46
1	N	232	GLN	C-O	5.14	1.30	1.24
3	P	26	LEU	N-CA	5.14	1.52	1.46
3	C	33	MET	SD-CE	5.13	1.92	1.79
6	F	18	ARG	N-CA	5.13	1.52	1.46
1	N	231	TYR	N-CA	5.13	1.52	1.46
13	M	35	TYR	CA-C	5.13	1.59	1.52
1	A	448	THR	CA-CB	5.12	1.61	1.53
2	B	73	LEU	CA-CB	5.12	1.61	1.53
1	A	293	PHE	CB-CG	5.12	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	146	TRP	N-CA	5.11	1.52	1.46
10	W	35	THR	C-O	5.11	1.29	1.24
1	N	176	MET	CA-C	5.11	1.59	1.52
1	A	297	MET	SD-CE	-5.10	1.66	1.79
5	E	65	VAL	N-CA	-5.10	1.40	1.46
7	G	7	ASP	CA-C	5.10	1.59	1.52
11	K	28	VAL	CA-C	5.10	1.61	1.52
3	P	37	PHE	CA-C	-5.09	1.46	1.53
10	W	6	ALA	N-CA	5.09	1.52	1.46
8	U	49	ASP	CA-C	5.09	1.58	1.52
9	I	21	ILE	CG1-CD1	5.09	1.71	1.51
1	A	446	ALA	CA-CB	5.09	1.61	1.53
8	H	80	THR	N-CA	5.09	1.52	1.46
8	H	49	ASP	CA-C	5.08	1.58	1.52
3	P	108	PRO	N-CA	-5.08	1.41	1.47
12	Y	39	ILE	CA-CB	5.08	1.60	1.54
2	B	65	TRP	CB-CG	-5.08	1.34	1.50
1	N	39	ALA	CA-CB	-5.08	1.45	1.53
3	P	59	ARG	C-O	5.08	1.30	1.24
8	U	68	TRP	N-CA	5.08	1.52	1.46
2	O	59	GLN	CB-CG	5.08	1.67	1.52
3	P	144	ILE	CA-CB	5.07	1.61	1.54
2	B	12	ALA	CA-C	5.07	1.59	1.52
2	O	113	TYR	C-O	-5.07	1.17	1.24
1	N	71	MET	SD-CE	-5.06	1.66	1.79
1	A	69	MET	CA-C	5.06	1.57	1.52
1	A	191	THR	CA-C	-5.06	1.46	1.52
1	A	298	ASP	CB-CG	5.06	1.64	1.52
8	H	66	ILE	CA-CB	5.06	1.60	1.54
4	D	80	THR	CA-C	5.06	1.59	1.52
1	A	121	GLY	N-CA	5.05	1.50	1.45
1	N	385	ALA	CA-CB	5.05	1.61	1.53
2	O	201	GLY	CA-C	5.05	1.57	1.52
2	B	59	GLN	CB-CG	5.05	1.67	1.52
4	D	19	ARG	CZ-NH2	5.05	1.40	1.33
6	S	21	MET	CA-C	5.04	1.59	1.52
8	H	24	ASN	CA-CB	5.04	1.59	1.53
1	N	316	THR	CA-C	5.04	1.59	1.52
1	A	135	ASN	C-O	5.04	1.30	1.24
1	N	471	ILE	C-O	5.04	1.30	1.24
3	C	127	LEU	CG-CD2	-5.04	1.35	1.52
3	C	71	HIS	N-CA	5.03	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	25	LEU	N-CA	5.03	1.52	1.46
4	D	73	ARG	C-O	-5.03	1.17	1.23
8	U	9	LYS	N-CA	5.03	1.51	1.46
1	A	240	HIS	CE1-NE2	5.03	1.37	1.32
7	G	49	PRO	N-CD	5.03	1.54	1.47
3	C	254	VAL	CA-CB	5.02	1.60	1.54
1	N	128	VAL	CA-C	5.02	1.59	1.52
5	E	24	ILE	C-O	5.02	1.29	1.24
11	K	54	ARG	CZ-NH1	5.02	1.39	1.32
3	P	155	ASP	N-CA	5.02	1.53	1.46
1	A	129	TYR	C-O	5.02	1.30	1.24
3	C	146	TRP	C-N	5.01	1.40	1.33
2	O	53	THR	C-O	5.01	1.30	1.24
1	A	469	VAL	CA-C	5.01	1.59	1.52
1	A	288	TRP	CA-C	-5.01	1.45	1.52
2	B	90	ILE	N-CA	5.01	1.52	1.46
2	O	188	ARG	CA-C	5.01	1.57	1.52
1	A	479	LYS	C-O	5.01	1.30	1.23
2	B	16	ILE	CG1-CD1	5.01	1.71	1.51
1	N	168	ILE	C-O	5.00	1.30	1.24
2	B	203	ASN	CG-OD1	-5.00	1.14	1.23
2	O	90	ILE	N-CA	5.00	1.52	1.46

All (314) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	54	ASN	CB-CA-C	-11.26	88.11	109.72
7	G	17	ARG	NE-CZ-NH2	-11.19	109.13	119.20
7	T	17	ARG	NE-CZ-NH2	-10.77	109.50	119.20
4	D	20	ARG	NE-CZ-NH2	-10.56	109.69	119.20
1	N	250	GLY	N-CA-C	-10.31	99.57	112.77
7	T	17	ARG	NE-CZ-NH1	10.31	131.81	121.50
7	G	17	ARG	NE-CZ-NH1	9.96	131.46	121.50
1	N	240	HIS	CA-CB-CG	-9.46	104.34	113.80
1	N	278	MET	CG-SD-CE	-9.46	80.08	100.90
2	O	175	ILE	N-CA-CB	-9.29	102.53	112.37
2	B	65	TRP	CB-CA-C	9.18	127.33	110.36
1	A	240	HIS	CA-CB-CG	-9.14	104.66	113.80
1	A	108	SER	N-CA-C	-8.98	101.57	111.36
2	B	60	GLU	N-CA-C	-8.95	91.74	110.80
4	Q	20	ARG	NE-CZ-NH2	-8.90	111.19	119.20
3	C	29	SER	CA-CB-OG	-8.76	93.58	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	ALA	N-CA-C	-8.76	101.81	111.36
4	Q	9	GLU	N-CA-C	-8.57	99.79	111.87
7	G	17	ARG	CB-CG-CD	-8.47	91.81	111.30
1	N	89	ALA	CA-C-N	-8.44	111.44	120.47
1	N	89	ALA	C-N-CA	-8.44	111.44	120.47
10	W	18	LEU	CA-C-N	-8.35	112.12	120.31
10	W	18	LEU	C-N-CA	-8.35	112.12	120.31
2	B	82	ARG	CG-CD-NE	-8.30	93.73	112.00
8	H	38	ARG	N-CA-C	-8.29	102.19	111.14
11	K	41	ASN	CA-C-N	-8.18	112.23	120.98
11	K	41	ASN	C-N-CA	-8.18	112.23	120.98
1	N	310	MET	CG-SD-CE	-7.98	83.34	100.90
2	B	66	THR	OG1-CB-CG2	7.90	125.11	109.30
7	T	17	ARG	CB-CG-CD	-7.85	93.25	111.30
1	A	250	GLY	N-CA-C	-7.81	102.77	112.77
2	O	66	THR	OG1-CB-CG2	7.80	124.91	109.30
4	D	20	ARG	NE-CZ-NH1	7.70	129.20	121.50
1	N	513	LEU	CA-C-N	-7.62	107.98	121.70
1	N	513	LEU	C-N-CA	-7.62	107.98	121.70
1	N	316	THR	N-CA-C	-7.60	103.07	111.36
1	A	189	MET	CG-SD-CE	-7.58	84.23	100.90
3	P	80	ARG	CG-CD-NE	-7.57	95.35	112.00
9	V	21	ILE	N-CA-C	-7.42	102.91	111.00
1	A	280	ILE	N-CA-C	-7.38	103.27	110.72
12	Y	38	PHE	N-CA-C	7.36	120.36	111.82
1	N	485	VAL	N-CA-CB	-7.35	99.39	111.44
3	C	41	THR	N-CA-C	7.34	118.97	110.97
7	G	8	HIS	N-CA-C	7.27	126.28	110.80
3	P	161	GLN	CB-CG-CD	-7.26	100.26	112.60
1	N	145	LEU	N-CA-C	-7.25	103.46	111.36
3	C	215	LEU	N-CA-C	-7.22	103.44	111.82
1	A	297	MET	CG-SD-CE	-7.21	85.03	100.90
3	C	87	ILE	CA-C-O	-7.19	113.47	120.95
1	N	469	VAL	N-CA-C	-7.15	103.50	110.72
6	S	64	GLU	CA-C-N	-7.14	113.81	126.45
6	S	64	GLU	C-N-CA	-7.14	113.81	126.45
3	P	200	ALA	N-CA-C	-7.13	102.70	111.40
7	T	44	ARG	N-CA-C	7.13	117.80	109.60
6	S	53	THR	CB-CA-C	-7.02	98.25	114.41
1	N	276	ALA	N-CA-C	-6.90	103.68	111.14
1	A	202	LEU	N-CA-C	-6.87	103.87	111.36
1	N	343	GLY	N-CA-C	-6.87	104.54	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	20	ARG	NE-CZ-NH1	6.85	128.35	121.50
4	D	19	ARG	NE-CZ-NH1	-6.85	114.65	121.50
1	A	373	VAL	N-CA-C	-6.83	103.83	110.72
1	A	513	LEU	CA-C-N	-6.82	109.42	121.70
1	A	513	LEU	C-N-CA	-6.82	109.42	121.70
3	P	37	PHE	N-CA-C	-6.80	102.27	112.54
4	D	36	SER	N-CA-CB	6.79	120.21	110.16
4	Q	135	SER	CA-CB-OG	-6.77	97.55	111.10
12	L	5	GLU	CA-C-N	-6.77	111.24	121.87
12	L	5	GLU	C-N-CA	-6.77	111.24	121.87
4	D	20	ARG	CA-CB-CG	6.72	127.54	114.10
1	A	136	LEU	CB-CG-CD2	-6.69	90.63	110.70
8	U	9	LYS	N-CA-C	6.67	118.78	109.31
1	N	512	ASN	CB-CA-C	-6.63	97.25	109.46
4	D	31	LYS	CB-CG-CD	-6.63	96.06	111.30
4	D	10	ASP	N-CA-C	6.62	121.02	113.15
5	E	108	LYS	CB-CA-C	6.60	120.56	109.48
3	P	6	HIS	N-CA-C	-6.56	99.78	109.81
4	Q	20	ARG	CD-NE-CZ	6.55	133.57	124.40
8	U	43	MET	N-CA-C	6.53	119.22	111.71
3	P	113	GLY	N-CA-C	-6.52	105.51	114.64
2	O	65	TRP	CB-CA-C	6.52	122.49	110.11
1	A	189	MET	CA-CB-CG	-6.51	101.08	114.10
7	G	7	ASP	N-CA-C	6.50	124.64	110.80
7	T	44	ARG	CA-C-N	-6.49	113.95	120.31
7	T	44	ARG	C-N-CA	-6.49	113.95	120.31
4	D	62	LEU	N-CA-C	-6.46	104.09	112.23
1	A	62	ALA	CA-C-N	-6.46	111.12	120.29
1	A	62	ALA	C-N-CA	-6.46	111.12	120.29
7	T	8	HIS	N-CA-C	6.45	124.55	110.80
1	A	169	ILE	CB-CA-C	-6.45	103.60	112.24
1	A	180	GLN	CA-CB-CG	-6.44	101.21	114.10
1	A	160	GLY	N-CA-C	-6.41	105.04	112.73
1	A	512	ASN	CB-CA-C	-6.40	97.02	109.76
11	K	47	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	N	251	PHE	CB-CA-C	-6.40	100.17	110.79
11	K	20	SER	CB-CA-C	-6.38	100.01	110.85
1	N	10	THR	N-CA-C	-6.37	103.17	111.71
3	P	181	TYR	N-CA-C	-6.35	104.44	111.36
6	S	59	GLY	N-CA-C	-6.33	101.02	110.71
2	B	157	GLU	CA-CB-CG	-6.33	101.45	114.10
1	N	510	TYR	CA-C-N	-6.32	114.01	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	510	TYR	C-N-CA	-6.32	114.01	122.98
2	O	36	SER	CB-CA-C	6.31	122.79	110.67
6	F	93	PRO	CA-C-N	6.30	133.58	121.54
6	F	93	PRO	C-N-CA	6.30	133.58	121.54
1	N	160	GLY	N-CA-C	-6.29	104.72	112.77
2	B	87	MET	CA-CB-CG	6.29	126.67	114.10
11	K	21	GLY	N-CA-C	-6.26	105.24	112.50
6	S	93	PRO	CA-C-N	6.24	133.46	121.54
6	S	93	PRO	C-N-CA	6.24	133.46	121.54
3	C	106	LEU	CA-C-N	-6.22	116.00	122.85
3	C	106	LEU	C-N-CA	-6.22	116.00	122.85
8	H	8	ILE	CB-CA-C	6.22	121.49	111.29
7	T	41	HIS	N-CA-C	6.22	118.73	109.59
1	N	52	GLN	N-CA-C	-6.21	104.43	111.07
1	A	244	TYR	CA-CB-CG	-6.21	102.73	113.90
2	O	202	SER	CA-CB-OG	-6.20	98.71	111.10
3	C	229	SER	N-CA-C	-6.19	104.98	112.54
1	A	312	ILE	CA-CB-CG1	-6.17	99.91	110.40
3	C	143	SER	N-CA-C	6.16	118.79	111.71
1	N	105	LEU	CA-C-N	-6.16	114.04	120.38
1	N	105	LEU	C-N-CA	-6.16	114.04	120.38
1	N	278	MET	CA-CB-CG	-6.16	101.79	114.10
4	D	4	SER	N-CA-CB	6.15	120.96	110.50
1	N	53	ILE	CB-CG1-CD1	-6.15	100.88	113.80
1	A	191	THR	N-CA-C	-6.14	104.59	111.28
1	A	311	ILE	CA-CB-CG1	-6.09	100.05	110.40
2	B	64	ILE	CB-CA-C	-6.06	103.86	112.22
6	S	53	THR	OG1-CB-CG2	6.06	121.41	109.30
1	N	230	LEU	N-CA-C	-6.04	104.69	111.28
4	Q	9	GLU	CA-C-N	6.04	131.22	121.98
4	Q	9	GLU	C-N-CA	6.04	131.22	121.98
1	A	102	PHE	CA-CB-CG	-6.01	107.79	113.80
6	F	92	VAL	CA-C-N	-6.01	113.78	119.85
6	F	92	VAL	C-N-CA	-6.01	113.78	119.85
1	A	187	SER	N-CA-C	-5.98	104.88	111.82
1	A	304	TYR	N-CA-C	-5.97	104.69	111.14
7	G	44	ARG	N-CA-C	5.96	117.22	109.64
13	Z	21	VAL	N-CA-C	-5.96	104.70	110.72
3	P	152	MET	CA-CB-CG	-5.95	102.20	114.10
3	P	88	ILE	N-CA-C	-5.95	104.71	110.42
5	E	88	GLU	N-CA-C	5.94	117.76	111.28
5	R	29	LEU	N-CA-C	-5.94	104.72	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	36	PHE	N-CA-C	5.93	117.42	111.07
1	A	125	GLY	CA-C-O	-5.93	117.08	122.24
2	B	67	ILE	CB-CA-C	-5.92	104.04	112.22
6	F	64	GLU	CA-C-N	-5.91	116.00	126.45
6	F	64	GLU	C-N-CA	-5.91	116.00	126.45
2	O	60	GLU	N-CA-C	-5.88	98.28	110.80
3	P	156	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	A	237	PHE	N-CA-C	-5.84	104.91	111.28
5	E	90	ARG	CG-CD-NE	-5.82	99.19	112.00
3	P	29	SER	CB-CA-C	-5.82	100.78	110.68
10	J	57	HIS	CB-CA-C	5.82	120.55	110.72
1	A	53	ILE	CB-CG1-CD1	-5.81	101.61	113.80
3	C	80	ARG	CG-CD-NE	-5.80	99.23	112.00
1	A	396	TRP	N-CA-C	-5.80	105.53	113.30
2	B	37	LEU	CB-CG-CD1	-5.79	93.32	110.70
2	B	114	GLU	CA-C-N	-5.78	113.09	122.34
2	B	114	GLU	C-N-CA	-5.78	113.09	122.34
1	A	35	LEU	N-CA-C	-5.74	104.63	111.69
1	N	335	SER	CA-C-N	-5.74	113.11	119.19
1	N	335	SER	C-N-CA	-5.74	113.11	119.19
3	C	64	GLU	N-CA-C	5.72	118.29	111.71
3	C	56	GLN	CA-CB-CG	-5.72	102.66	114.10
7	G	33	LEU	CA-CB-CG	5.71	136.30	116.30
3	P	99	TRP	N-CA-C	-5.71	105.14	111.36
7	G	24	ALA	N-CA-C	-5.70	104.70	111.03
4	D	8	SER	N-CA-C	-5.70	105.15	111.71
1	A	417	MET	CG-SD-CE	-5.70	88.36	100.90
1	N	393	PHE	N-CA-C	-5.65	104.74	111.69
3	C	230	ASN	N-CA-C	5.64	121.05	113.72
1	N	253	MET	CA-CB-CG	-5.64	102.82	114.10
3	C	123	PRO	CB-CA-C	-5.63	103.85	111.12
1	A	377	PHE	CA-CB-CG	5.62	119.42	113.80
1	N	308	ALA	N-CA-C	-5.61	105.25	111.36
11	X	41	ASN	CB-CA-C	-5.60	106.13	111.00
2	B	59	GLN	CB-CG-CD	5.59	122.11	112.60
9	V	35	TYR	N-CA-C	-5.59	105.19	112.23
5	E	107	ASP	CA-C-N	-5.58	114.33	122.65
5	E	107	ASP	C-N-CA	-5.58	114.33	122.65
2	B	36	SER	CB-CA-C	5.58	121.76	110.38
6	S	54	ASN	N-CA-C	5.58	120.09	113.28
7	G	61	SER	CA-CB-OG	-5.58	99.95	111.10
4	Q	71	MET	N-CA-C	-5.58	105.35	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	N-CA-CB	5.57	116.99	110.42
1	A	10	THR	N-CA-C	-5.56	104.25	111.71
4	D	121	LYS	N-CA-C	5.56	117.34	111.28
2	B	66	THR	N-CA-C	-5.56	106.43	113.43
9	I	68	ILE	CG1-CB-CG2	5.56	127.37	110.70
1	N	189	MET	CA-CB-CG	-5.56	102.98	114.10
12	L	32	GLY	N-CA-C	-5.55	106.06	112.50
4	D	20	ARG	CD-NE-CZ	5.55	132.17	124.40
6	F	87	THR	N-CA-CB	5.55	118.13	109.97
6	S	64	GLU	CA-CB-CG	-5.55	103.00	114.10
7	T	78	LEU	N-CA-C	-5.54	103.76	110.13
13	M	22	THR	N-CA-C	-5.53	105.15	111.07
1	N	169	ILE	CB-CA-C	-5.52	103.16	112.16
6	F	95	GLN	N-CA-C	5.52	122.56	110.80
4	Q	90	GLY	N-CA-C	-5.52	105.71	112.77
6	F	70	ILE	N-CA-CB	-5.48	104.79	111.21
3	C	40	MET	CA-CB-CG	-5.48	103.14	114.10
1	N	326	THR	N-CA-C	-5.47	105.40	111.36
10	J	51	GLY	N-CA-C	-5.46	106.17	112.50
2	O	202	SER	CB-CA-C	-5.46	99.56	110.42
9	V	8	GLN	CB-CG-CD	-5.45	103.34	112.60
2	B	16	ILE	CA-CB-CG1	-5.43	101.16	110.40
1	N	82	LEU	CA-C-N	-5.43	115.98	120.33
1	N	82	LEU	C-N-CA	-5.43	115.98	120.33
6	S	45	ASP	CA-C-N	-5.43	114.98	120.31
6	S	45	ASP	C-N-CA	-5.43	114.98	120.31
4	Q	88	PHE	N-CA-C	5.43	117.20	111.28
10	J	28	ASP	N-CA-C	-5.43	105.44	111.36
6	S	40	SER	N-CA-C	-5.41	106.63	113.18
13	M	26	PHE	CB-CA-C	-5.41	99.89	110.11
3	P	36	HIS	N-CA-C	5.41	121.63	114.12
1	N	327	LEU	N-CA-C	-5.40	105.39	111.28
1	N	412	ILE	CB-CA-C	-5.39	104.78	112.22
5	E	90	ARG	NE-CZ-NH2	-5.39	114.35	119.20
2	O	35	SER	CA-CB-OG	-5.38	100.33	111.10
3	C	23	SER	CA-CB-OG	-5.37	100.36	111.10
4	Q	143	ASN	N-CA-C	5.37	118.60	111.30
1	N	56	VAL	N-CA-C	5.36	116.09	110.62
1	A	202	LEU	CA-C-O	-5.36	114.74	120.42
9	I	68	ILE	N-CA-C	5.35	119.94	112.50
1	N	313	ALA	N-CA-C	-5.35	105.62	111.82
2	O	66	THR	CB-CA-C	5.34	118.47	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	483	LEU	CA-C-N	5.33	130.94	122.94
1	N	483	LEU	C-N-CA	5.33	130.94	122.94
1	A	425	PHE	CA-C-N	-5.33	113.43	120.09
1	A	425	PHE	C-N-CA	-5.33	113.43	120.09
6	F	63	GLU	CA-CB-CG	-5.32	103.46	114.10
4	D	133	GLY	N-CA-C	5.32	121.83	113.86
5	R	71	VAL	N-CA-C	5.32	115.94	110.36
2	O	66	THR	N-CA-CB	-5.31	101.10	110.34
2	O	92	ASN	N-CA-C	5.31	121.53	109.81
1	A	15	ILE	N-CA-C	-5.30	105.21	110.62
2	B	66	THR	CA-CB-OG1	5.30	117.55	109.60
2	O	226	MET	N-CA-C	-5.30	106.66	113.02
12	L	11	ILE	N-CA-C	-5.30	104.85	109.19
1	N	17	THR	CA-CB-OG1	-5.29	101.67	109.60
1	N	39	ALA	N-CA-C	-5.29	105.57	112.23
3	C	221	ARG	NE-CZ-NH1	-5.28	116.22	121.50
3	P	221	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	310	MET	N-CA-C	5.28	117.03	111.28
1	N	203	ALA	N-CA-C	-5.28	105.53	111.28
2	O	60	GLU	N-CA-CB	5.28	119.41	110.49
2	O	66	THR	CA-CB-CG2	5.28	119.47	110.50
11	K	54	ARG	CA-C-O	5.27	129.76	120.80
4	D	20	ARG	CB-CA-C	-5.27	102.05	110.79
4	Q	5	VAL	CA-C-N	5.26	127.55	120.50
4	Q	5	VAL	C-N-CA	5.26	127.55	120.50
1	N	266	GLU	N-CA-CB	-5.25	105.59	111.10
7	T	3	ALA	N-CA-C	5.24	121.97	110.80
4	D	31	LYS	N-CA-C	5.24	119.80	113.41
1	A	485	VAL	CA-C-O	-5.23	115.00	120.76
4	Q	22	TYR	N-CA-C	-5.23	101.23	108.76
1	A	475	ALA	N-CA-C	-5.23	105.49	111.14
1	A	486	ASP	CB-CA-C	-5.23	99.57	110.40
1	A	239	GLY	CA-C-N	-5.22	113.31	119.78
1	A	239	GLY	C-N-CA	-5.22	113.31	119.78
1	A	463	THR	N-CA-C	-5.22	105.59	111.28
1	N	291	HIS	CA-CB-CG	-5.22	108.58	113.80
3	P	70	HIS	CA-C-N	-5.22	114.33	122.16
3	P	70	HIS	C-N-CA	-5.22	114.33	122.16
6	S	97	ALA	N-CA-C	5.21	117.85	110.50
2	B	184	LEU	N-CA-CB	-5.20	101.81	111.13
4	D	17	VAL	CB-CA-C	-5.20	101.71	110.71
3	C	45	ILE	CB-CA-C	-5.19	105.05	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ILE	N-CA-C	-5.18	105.66	110.53
1	N	484	THR	CB-CA-C	-5.18	99.47	109.37
3	P	206	LEU	N-CA-C	-5.18	105.71	111.36
6	S	93	PRO	O-C-N	5.17	128.95	123.01
4	D	135	SER	CA-CB-OG	-5.16	100.78	111.10
6	S	8	THR	N-CA-C	-5.16	102.55	110.14
2	B	7	LEU	N-CA-C	-5.15	107.55	113.88
2	B	60	GLU	N-CA-CB	5.14	119.17	110.49
1	N	225	GLY	N-CA-C	-5.14	108.14	115.64
11	K	29	TRP	N-CA-C	-5.13	105.77	111.36
1	N	171	MET	CA-C-N	-5.13	114.17	122.48
1	N	171	MET	C-N-CA	-5.13	114.17	122.48
1	A	461	SER	CA-CB-OG	-5.13	100.84	111.10
1	N	180	GLN	CA-CB-CG	-5.13	103.85	114.10
1	N	332	ILE	CB-CA-C	-5.12	104.49	111.15
3	C	101	PHE	N-CA-C	5.12	117.25	111.11
1	A	47	LEU	N-CA-C	-5.11	106.13	112.93
4	D	119	GLN	CB-CG-CD	-5.11	103.91	112.60
2	O	67	ILE	CB-CA-C	-5.11	105.17	112.22
9	V	8	GLN	CA-CB-CG	-5.11	103.89	114.10
8	U	81	PHE	CA-C-N	-5.10	115.01	120.47
8	U	81	PHE	C-N-CA	-5.10	115.01	120.47
5	R	47	ILE	N-CA-C	-5.09	105.88	110.82
4	D	20	ARG	N-CA-C	-5.09	105.73	111.28
7	T	2	SER	CA-C-N	5.08	131.23	121.54
7	T	2	SER	C-N-CA	5.08	131.23	121.54
3	P	233	PHE	CA-C-N	-5.07	113.80	120.14
3	P	233	PHE	C-N-CA	-5.07	113.80	120.14
8	H	75	ARG	CA-CB-CG	-5.06	103.98	114.10
8	U	8	ILE	CB-CA-C	5.06	119.59	111.29
1	A	244	TYR	N-CA-C	-5.06	105.85	111.36
3	C	230	ASN	N-CA-CB	-5.05	103.23	110.65
2	O	132	GLU	CG-CD-OE1	-5.05	106.79	118.40
1	A	195	LEU	N-CA-C	-5.04	105.67	111.07
11	X	19	ALA	N-CA-C	5.04	116.47	111.07
7	G	16	TRP	CA-CB-CG	-5.04	104.03	113.60
6	S	2	SER	N-CA-C	5.04	115.95	108.60
3	C	161	GLN	N-CA-CB	-5.03	102.71	110.16
4	D	123	MET	CA-CB-CG	-5.03	104.04	114.10
3	P	217	VAL	N-CA-C	-5.02	105.60	110.42
3	P	235	PHE	N-CA-C	-5.02	105.89	111.36
4	D	19	ARG	NE-CZ-NH2	5.01	123.71	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	5.01	121.48	110.80
1	N	113	LEU	CB-CA-C	5.01	119.11	110.79
2	B	184	LEU	N-CA-C	-5.01	100.54	109.06
1	N	145	LEU	CA-CB-CG	-5.00	98.79	116.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	66	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	TYR	Sidechain
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4060	0	4037	59	0
1	N	4060	0	4037	71	0
2	B	1824	0	1833	30	0
2	O	1824	0	1833	37	1
3	C	2110	0	2027	30	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	11	0
5	E	852	0	845	8	0
5	R	852	0	845	8	1
6	F	748	0	728	17	0
6	S	748	0	728	19	1
7	G	675	0	643	43	0
7	T	675	0	643	51	0
8	H	662	0	623	13	0
8	U	662	0	623	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	601	0	613	6	1
9	V	601	0	613	16	0
10	J	460	0	459	4	0
10	W	460	0	459	6	0
11	K	384	0	366	1	0
11	X	384	0	366	4	0
12	L	380	0	380	10	0
12	Y	380	0	380	11	0
13	M	335	0	352	10	0
13	Z	335	0	352	3	0
14	A	120	0	107	6	0
14	N	120	0	108	3	0
15	A	2	0	0	0	0
15	N	2	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	8	0
19	D	63	0	110	8	0
19	L	63	0	110	15	0
19	N	63	0	110	15	0
19	O	63	0	110	10	0
19	Q	63	0	110	12	0
20	A	51	0	76	0	0
20	C	102	0	152	8	0
20	M	51	0	76	15	0
20	N	102	0	152	9	0
20	P	102	0	152	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	26	0
22	R	52	0	80	15	0
23	B	29	0	36	2	0
23	C	58	0	73	4	0
23	J	29	0	36	1	0
23	O	29	0	39	3	0
23	P	58	0	73	6	0
23	W	29	0	36	1	0
24	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	P	1	0	0	0	0
25	C	53	0	77	8	0
25	G	106	0	154	43	0
25	P	106	0	154	24	0
25	T	53	0	77	21	0
26	C	100	0	156	25	0
26	G	100	0	156	30	0
26	P	100	0	156	25	0
26	T	100	0	156	27	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	37	4	0
28	M	33	0	37	0	0
28	P	33	0	39	6	0
28	Z	33	0	38	2	0
29	A	218	0	0	6	0
29	B	143	0	0	7	0
29	C	116	0	0	3	0
29	D	80	0	0	3	0
29	E	49	0	0	0	0
29	F	61	0	0	2	0
29	G	45	0	0	2	0
29	H	51	0	0	1	0
29	I	37	0	0	2	0
29	J	24	0	0	0	0
29	K	29	0	0	0	0
29	L	23	0	0	1	0
29	M	31	0	0	2	0
29	N	222	0	0	7	0
29	O	137	0	0	5	0
29	P	102	0	0	0	0
29	Q	65	0	0	3	0
29	R	47	0	0	0	0
29	S	64	0	0	0	0
29	T	47	0	0	2	0
29	U	49	0	0	2	0
29	V	27	0	0	2	0
29	W	19	0	0	0	0
29	X	22	0	0	3	0
29	Y	21	0	0	1	0
29	Z	14	0	0	1	0
All	All	32545	0	31351	662	2

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 (662) 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)
25:P:1265:PEK:H383	26:T:1269:CDL:C27	1.21	1.67
1:N:484:THR:CB	1:N:484:THR:CG2	1.77	1.60
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.70	1.55
1:N:189:MET:CG	1:N:189:MET:CB	1.82	1.52
4:Q:121:LYS:NZ	4:Q:121:LYS:CE	1.74	1.50
2:B:87:MET:CG	2:B:87:MET:SD	2.02	1.47
1:A:297:MET:CG	1:A:297:MET:SD	2.01	1.47
25:P:1265:PEK:C38	26:T:1269:CDL:C27	2.06	1.32
22:B:229:PSC:H343	22:B:229:PSC:H142	1.23	1.18
1:N:513:LEU:O	1:N:514:LYS:HB2	1.41	1.16
7:T:84:LYS:HD2	7:T:84:LYS:H	1.09	1.16
25:P:1265:PEK:C38	26:T:1269:CDL:H273	1.69	1.15
1:A:513:LEU:O	1:A:514:LYS:HB2	1.37	1.15
22:B:229:PSC:H343	22:B:229:PSC:C14	1.78	1.14
22:R:1229:PSC:H142	22:R:1229:PSC:C34	1.79	1.13
20:M:524:PGV:H22	20:M:524:PGV:H011	1.12	1.11
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.16	1.10
7:T:2:SER:O	25:T:263:PEK:H331	1.52	1.08
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.31	1.07
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.70	1.06
20:C:267:PGV:H172	26:C:270:CDL:H662	1.33	1.05
6:F:85:CYS:SG	6:F:87:THR:HG23	1.96	1.05
7:G:84:LYS:HD2	7:G:84:LYS:N	1.69	1.04
22:B:229:PSC:H072	9:I:10:ARG:HH21	1.20	1.04
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.41	1.02
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.42	1.01
25:P:1265:PEK:C38	26:T:1269:CDL:H272	1.81	1.00
2:O:227:LEU:HD21	29:O:4852:HOH:O	1.60	0.99
7:G:84:LYS:HD2	7:G:84:LYS:H	0.83	0.99
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.43	0.99
7:G:84:LYS:H	7:G:84:LYS:CD	1.76	0.98
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.44	0.98
25:P:1264:PEK:H12	25:P:1264:PEK:H242	1.46	0.98
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.29	0.97
25:P:1265:PEK:H383	26:T:1269:CDL:H272	0.98	0.97
6:F:97:ALA:HB2	29:F:4812:HOH:O	1.61	0.97
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.06	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:229:PSC:H142	22:B:229:PSC:C34	1.96	0.96
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.26	0.94
13:M:39:ASN:O	13:M:43:SER:OG	1.86	0.94
20:M:524:PGV:H011	20:M:524:PGV:C2	1.97	0.94
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.48	0.94
22:R:1229:PSC:H142	22:R:1229:PSC:H343	1.48	0.93
25:C:264:PEK:H101	25:C:264:PEK:H161	1.52	0.92
8:H:9:LYS:O	8:H:10:ASN:HB2	1.69	0.92
1:A:513:LEU:O	1:A:514:LYS:CB	2.09	0.91
20:M:524:PGV:H22	20:M:524:PGV:C01	2.01	0.91
6:S:85:CYS:SG	6:S:87:THR:HG23	2.11	0.91
1:A:406:ASN:HD21	20:M:524:PGV:H21	1.36	0.90
1:A:297:MET:CG	1:A:297:MET:CE	2.50	0.90
19:A:521:TGL:H111	19:A:521:TGL:H283	1.52	0.89
25:P:1265:PEK:H381	26:T:1269:CDL:H273	1.49	0.89
7:T:5:LYS:CD	25:T:263:PEK:H371	2.03	0.88
25:P:1264:PEK:H71	25:P:1264:PEK:H32	1.56	0.88
1:N:417:MET:CE	29:N:3166:HOH:O	2.22	0.88
7:G:3:ALA:CB	25:G:1263:PEK:H382	2.03	0.87
8:H:9:LYS:HG3	8:H:10:ASN:H	1.38	0.87
25:G:265:PEK:H371	26:G:269:CDL:C27	2.05	0.86
7:T:5:LYS:HD2	25:T:263:PEK:C37	2.05	0.86
7:G:2:SER:OG	25:G:1263:PEK:C29	2.23	0.86
20:N:1524:PGV:H22	20:N:1524:PGV:H011	1.57	0.86
3:P:224:LYS:HE3	26:P:1270:CDL:HB31	1.58	0.86
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.38	0.85
10:W:2:GLU:HB2	10:W:4:ARG:NH1	1.90	0.85
1:A:297:MET:HE2	1:A:297:MET:CB	2.07	0.85
13:M:19:LEU:HD23	20:M:524:PGV:H311	1.57	0.84
3:P:34:TRP:HE1	28:P:1272:DMU:H29	1.40	0.84
1:N:513:LEU:O	1:N:514:LYS:CB	2.14	0.84
7:G:72:ASN:H	7:G:76:ASN:HD22	1.23	0.84
8:H:9:LYS:HG3	8:H:10:ASN:N	1.92	0.83
26:T:1269:CDL:HA21	26:T:1269:CDL:H111	1.60	0.83
19:L:522:TGL:H231	19:L:522:TGL:CA9	2.03	0.83
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.61	0.83
7:T:84:LYS:H	7:T:84:LYS:CD	1.89	0.83
3:P:224:LYS:CD	26:P:1270:CDL:HB32	2.09	0.82
22:R:1229:PSC:H343	22:R:1229:PSC:C14	2.09	0.82
7:T:84:LYS:HD2	7:T:84:LYS:N	1.93	0.82
29:A:4501:HOH:O	25:C:264:PEK:H381	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:1:SAC:OAC	9:V:1:SAC:HB3	1.79	0.81
1:A:1:FME:CE	1:A:4:ASN:HD22	1.94	0.81
1:N:417:MET:HE1	29:N:3166:HOH:O	1.78	0.81
1:A:297:MET:CE	1:A:297:MET:CB	2.59	0.81
26:C:270:CDL:H522	26:C:270:CDL:OB9	1.80	0.81
22:B:229:PSC:O02	22:B:229:PSC:H032	1.80	0.80
19:A:521:TGL:H241	19:A:521:TGL:H201	1.64	0.79
8:U:27:ARG:HG2	29:U:4871:HOH:O	1.79	0.79
20:C:267:PGV:C17	26:C:270:CDL:H662	2.12	0.79
25:P:1265:PEK:H383	26:T:1269:CDL:H271	1.58	0.79
26:G:269:CDL:H511	26:G:269:CDL:H201	1.65	0.78
26:P:1270:CDL:PA1	26:P:1270:CDL:HB22	2.15	0.78
29:A:4740:HOH:O	3:C:77:LYS:HE2	1.84	0.78
19:N:1522:TGL:H231	19:N:1522:TGL:HA92	1.65	0.78
25:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.28	0.77
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.66	0.77
25:C:264:PEK:HN2	7:G:76:ASN:HD21	1.32	0.77
7:G:2:SER:OG	25:G:1263:PEK:H291	1.84	0.77
26:P:1270:CDL:H192	26:P:1270:CDL:H231	1.65	0.76
7:T:5:LYS:HD2	25:T:263:PEK:C38	2.15	0.76
7:T:72:ASN:H	7:T:76:ASN:HD22	1.34	0.76
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.66	0.75
19:O:1521:TGL:H241	19:O:1521:TGL:H201	1.67	0.75
26:C:270:CDL:H672	26:C:270:CDL:H252	1.68	0.75
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.67	0.75
19:A:521:TGL:HA92	19:A:521:TGL:H252	1.70	0.74
26:G:269:CDL:H352	2:O:78:LEU:HD12	1.70	0.74
22:B:229:PSC:C14	22:B:229:PSC:C34	2.59	0.73
26:P:1270:CDL:H242	26:P:1270:CDL:H661	1.70	0.73
25:G:265:PEK:H371	26:G:269:CDL:H272	1.68	0.73
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.53	0.73
25:C:264:PEK:H32	25:C:264:PEK:H71	1.69	0.73
25:G:265:PEK:C38	26:G:269:CDL:C27	2.66	0.73
1:N:189:MET:CG	1:N:189:MET:CA	2.65	0.73
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.71	0.73
28:G:272:DMU:O1	28:G:272:DMU:H29	1.89	0.73
25:G:265:PEK:C37	26:G:269:CDL:C27	2.67	0.73
1:N:383[B]:MET:O	1:N:387:PHE:HB2	1.89	0.73
25:G:265:PEK:H371	26:G:269:CDL:H273	1.69	0.73
6:F:1:ALA:H1	25:G:265:PEK:H042	1.53	0.72
7:G:69:PHE:HZ	28:G:272:DMU:H1	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:269:CDL:H782	26:G:269:CDL:H562	1.70	0.72
1:N:351:GLY:HA3	1:N:380[A]:VAL:HG13	1.70	0.72
3:P:224:LYS:HE3	26:P:1270:CDL:CB3	2.19	0.72
4:Q:100:LYS:HE2	29:Q:4794:HOH:O	1.88	0.72
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.71	0.71
22:R:1229:PSC:C07	9:V:10:ARG:HH21	2.03	0.71
22:B:229:PSC:H072	9:I:10:ARG:NH2	2.02	0.71
19:O:1521:TGL:H101	19:O:1521:TGL:C28	2.20	0.71
22:B:229:PSC:C07	9:I:10:ARG:HH21	2.00	0.71
25:G:265:PEK:C37	26:G:269:CDL:H272	2.21	0.71
19:N:1522:TGL:H362	29:Y:4638:HOH:O	1.91	0.71
26:T:1269:CDL:H762	26:T:1269:CDL:H561	1.73	0.71
22:R:1229:PSC:C34	22:R:1229:PSC:C14	2.64	0.70
8:U:23:GLN:HG3	29:U:4345:HOH:O	1.91	0.70
7:G:5:LYS:CD	25:G:1263:PEK:H371	2.21	0.70
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.71	0.70
3:C:246:ASP:HB2	29:C:4099:HOH:O	1.91	0.70
2:B:81:LEU:HD12	26:T:1269:CDL:H351	1.73	0.70
8:H:45:ALA:O	8:H:47:GLY:N	2.24	0.70
6:F:1:ALA:HB3	6:S:65:ASP:OD1	1.93	0.69
19:L:522:TGL:HC62	19:L:522:TGL:CC2	2.19	0.69
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.73	0.69
1:N:189:MET:CB	1:N:189:MET:SD	2.79	0.69
3:P:34:TRP:NE1	28:P:1272:DMU:H29	2.09	0.68
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.75	0.68
9:I:44:LYS:HE2	29:I:4840:HOH:O	1.94	0.68
22:B:229:PSC:H343	22:B:229:PSC:H141	1.70	0.68
29:N:4526:HOH:O	2:O:87:MET:SD	2.52	0.68
20:N:1524:PGV:H22	20:N:1524:PGV:C01	2.23	0.68
7:G:11:TPO:CG2	7:G:11:TPO:O	2.42	0.67
1:N:177:SER:H	1:N:180:GLN:HE21	1.43	0.67
25:P:1265:PEK:H042	6:S:1:ALA:N	2.08	0.67
1:N:189:MET:CB	1:N:189:MET:HE2	2.24	0.67
8:U:45:ALA:O	8:U:47:GLY:N	2.28	0.66
10:W:2:GLU:CB	10:W:4:ARG:NH1	2.57	0.66
25:C:264:PEK:H161	25:C:264:PEK:C10	2.25	0.66
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.59	0.66
3:P:63:ARG:HE	26:P:1270:CDL:CA2	2.08	0.66
1:A:484:THR:HB	13:M:2:THR:OG1	1.95	0.66
12:L:46:LYS:O	12:L:47:LYS:HB2	1.96	0.66
23:O:229:CHD:H12	23:O:229:CHD:H212	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:73:LYS:CA	9:V:73:LYS:HE3	2.25	0.66
6:S:53:THR:HG22	6:S:54:ASN:H	1.61	0.66
23:P:1271:CHD:H162	23:P:1271:CHD:H232	1.77	0.65
8:U:9:LYS:O	8:U:10:ASN:HB2	1.95	0.65
9:V:73:LYS:HE3	9:V:73:LYS:HA	1.77	0.65
12:Y:22:LEU:O	12:Y:26:THR:HB	1.95	0.65
25:G:265:PEK:H383	26:G:269:CDL:C27	2.25	0.65
1:A:282:PHE:HA	7:T:4:ALA:CB	2.26	0.65
29:A:4197:HOH:O	22:B:229:PSC:H21	1.97	0.65
1:A:484:THR:HG22	29:A:4618:HOH:O	1.96	0.65
1:A:297:MET:HE2	1:A:297:MET:HB2	1.79	0.64
20:P:1267:PGV:H172	26:P:1270:CDL:H652	1.80	0.64
26:T:1269:CDL:OA8	26:T:1269:CDL:H331	1.97	0.64
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.07	0.64
4:Q:7:LYS:O	4:Q:10:ASP:HB2	1.98	0.64
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.28	0.64
7:T:5:LYS:HB2	25:T:263:PEK:C36	2.24	0.64
6:S:94:HIS:O	6:S:95:GLN:HB2	1.96	0.64
7:G:3:ALA:HB1	25:G:1263:PEK:C38	2.28	0.64
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.62	0.64
2:O:49:LYS:HD2	29:Q:3076:HOH:O	1.98	0.63
8:H:52:VAL:HG12	8:U:46:LYS:HB2	1.79	0.63
6:S:64:GLU:O	6:S:65:ASP:HB2	1.98	0.63
19:N:1522:TGL:HA92	19:N:1522:TGL:C23	2.28	0.63
19:O:1521:TGL:H101	19:O:1521:TGL:H281	1.79	0.63
8:H:9:LYS:HA	29:H:4747:HOH:O	1.97	0.63
22:R:1229:PSC:H071	9:V:10:ARG:HH21	1.64	0.63
25:P:1265:PEK:H042	6:S:1:ALA:H1	1.64	0.63
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.63	0.63
1:A:1:FME:HE2	1:A:4:ASN:HD22	1.61	0.63
2:O:226:MET:O	2:O:227:LEU:C	2.41	0.63
3:P:224:LYS:CE	26:P:1270:CDL:HB31	2.28	0.63
6:F:1:ALA:N	25:G:265:PEK:H042	2.13	0.62
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG12	1.82	0.62
2:B:13:THR:OG1	2:B:167:SER:HB2	2.00	0.62
28:G:272:DMU:H29	28:G:272:DMU:C10	2.29	0.62
3:P:224:LYS:HD2	26:P:1270:CDL:HB32	1.80	0.62
8:H:9:LYS:CG	8:H:10:ASN:H	2.08	0.62
19:O:1521:TGL:H201	19:O:1521:TGL:C24	2.30	0.62
7:T:2:SER:OG	25:T:263:PEK:C29	2.48	0.62
7:G:17:ARG:HD2	29:O:2446:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1265:PEK:C04	6:S:1:ALA:N	2.62	0.61
19:Q:1523:TGL:HG32	19:Q:1523:TGL:OB1	2.00	0.61
26:T:1269:CDL:H511	26:T:1269:CDL:H201	1.82	0.61
6:F:1:ALA:N	25:G:265:PEK:C04	2.64	0.61
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.82	0.61
8:U:9:LYS:HG3	8:U:10:ASN:H	1.65	0.61
2:O:42:ILE:HG21	19:Q:1523:TGL:H231	1.81	0.61
1:A:51:ASP:OD1	1:A:441:SER:OG	2.15	0.61
20:C:267:PGV:H172	26:C:270:CDL:C66	2.22	0.61
26:C:270:CDL:HB21	26:C:270:CDL:PA1	2.40	0.61
7:G:3:ALA:CB	25:G:1263:PEK:C38	2.77	0.61
10:W:2:GLU:CB	10:W:4:ARG:HH11	2.14	0.61
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.30	0.61
4:Q:86:MET:HE1	29:X:4865:HOH:O	2.01	0.60
22:B:229:PSC:O02	22:B:229:PSC:C03	2.50	0.60
3:C:210:ILE:HD13	20:C:267:PGV:H301	1.82	0.60
7:G:69:PHE:CZ	28:G:272:DMU:H1	2.36	0.60
1:N:177:SER:H	1:N:180:GLN:NE2	1.98	0.60
1:A:514:LYS:NZ	29:A:2645:HOH:O	2.33	0.60
7:G:2:SER:O	25:G:1263:PEK:H331	2.01	0.60
10:W:2:GLU:HB2	10:W:4:ARG:HH12	1.66	0.60
2:B:78:LEU:HD12	26:T:1269:CDL:H352	1.84	0.60
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.65	0.60
7:G:5:LYS:HD2	25:G:1263:PEK:C37	2.31	0.60
7:G:5:LYS:CB	25:G:1263:PEK:H362	2.19	0.60
10:J:52:TRP:O	10:J:57:HIS:HE1	1.85	0.60
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.85	0.59
2:B:78:LEU:CD1	26:T:1269:CDL:H352	2.33	0.59
3:C:63:ARG:NE	26:C:270:CDL:HA22	2.14	0.59
3:C:224:LYS:CD	26:C:270:CDL:HB32	2.33	0.59
20:C:268:PGV:H031	29:C:4819:HOH:O	2.02	0.59
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.85	0.59
7:G:5:LYS:HB3	1:N:278:MET:SD	2.43	0.59
1:A:297:MET:CE	1:A:297:MET:HB3	2.32	0.59
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.37	0.58
1:N:449:MET:SD	2:O:5:MET:HG2	2.43	0.58
29:B:3446:HOH:O	7:T:17:ARG:CD	2.51	0.58
1:N:189:MET:CB	1:N:189:MET:CE	2.80	0.58
7:G:37:LEU:HD11	26:G:269:CDL:H361	1.84	0.58
2:O:89:GLU:O	2:O:91:ASN:ND2	2.36	0.58
4:Q:95:LEU:HD22	28:Z:1526:DMU:H13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:84:LEU:HA	2:O:87:MET:HE2	1.84	0.58
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.86	0.58
3:C:210:ILE:HG12	20:C:267:PGV:H132	1.86	0.58
7:T:11:TPO:HG22	7:T:11:TPO:O	2.04	0.58
19:N:1522:TGL:H231	19:N:1522:TGL:CA9	2.32	0.57
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.68	0.57
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.40	0.57
7:T:36:TRP:HB3	29:T:4707:HOH:O	2.03	0.57
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	2.03	0.57
20:M:524:PGV:C30	20:M:524:PGV:H141	2.35	0.57
7:T:2:SER:OG	25:T:263:PEK:H291	2.04	0.57
22:B:229:PSC:H071	5:E:8:ASP:HA	1.85	0.57
22:R:1229:PSC:H212	22:R:1229:PSC:O01	2.05	0.57
7:T:8:HIS:CD2	25:T:263:PEK:H232	2.39	0.57
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.02	0.57
19:L:522:TGL:HA92	19:L:522:TGL:C23	2.20	0.57
12:Y:20:ARG:HH11	12:Y:20:ARG:HB3	1.68	0.57
7:G:2:SER:OG	25:G:1263:PEK:H301	2.05	0.57
7:T:3:ALA:CB	25:T:263:PEK:H382	2.34	0.57
25:G:1263:PEK:H132	3:P:247:VAL:HG12	1.86	0.57
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.39	0.57
3:P:34:TRP:CZ2	28:P:1272:DMU:O5	2.58	0.57
25:P:1265:PEK:C37	26:T:1269:CDL:H272	2.34	0.57
1:N:351:GLY:CA	1:N:380[A]:VAL:HG13	2.34	0.56
28:P:1272:DMU:H30	7:T:62:TRP:HB3	1.87	0.56
8:U:49:ASP:O	8:U:52:VAL:HG22	2.06	0.56
29:B:3446:HOH:O	7:T:17:ARG:HD3	2.04	0.56
4:D:34:SER:H	4:D:37:GLN:NE2	2.03	0.56
26:G:269:CDL:H241	26:G:269:CDL:H531	1.87	0.56
1:N:484:THR:CG2	1:N:484:THR:C	2.79	0.56
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.22	0.56
3:C:95:THR:HG21	20:C:268:PGV:H282	1.85	0.56
8:H:45:ALA:C	8:H:47:GLY:H	2.13	0.56
25:P:1265:PEK:H8	29:T:4897:HOH:O	2.05	0.56
19:Q:1523:TGL:H242	19:Q:1523:TGL:HA91	1.86	0.56
3:P:224:LYS:CE	26:P:1270:CDL:CB3	2.84	0.56
25:P:1265:PEK:H041	7:T:17:ARG:HH22	1.69	0.56
7:T:5:LYS:CB	25:T:263:PEK:H362	2.26	0.56
6:F:64:GLU:O	6:F:65:ASP:HB2	2.06	0.56
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.41	0.55
26:C:270:CDL:HA4	26:C:270:CDL:H122	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:269:CDL:H201	26:G:269:CDL:C51	2.36	0.55
19:N:1522:TGL:HC51	19:N:1522:TGL:OC1	2.06	0.55
19:Q:1523:TGL:HC21	19:Q:1523:TGL:CG1	2.37	0.55
4:D:34:SER:H	4:D:37:GLN:HE21	1.55	0.55
7:G:2:SER:O	25:G:1263:PEK:H322	2.07	0.55
7:G:3:ALA:O	7:G:4:ALA:HB2	2.05	0.55
7:G:17:ARG:CD	29:O:2446:HOH:O	2.54	0.55
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.88	0.55
26:C:270:CDL:HB21	26:C:270:CDL:OA5	2.06	0.55
26:G:269:CDL:H352	2:O:78:LEU:CD1	2.35	0.55
1:N:297:MET:CE	1:N:302:ARG:HG2	2.37	0.55
3:P:224:LYS:CD	26:P:1270:CDL:CB3	2.84	0.55
1:A:177:SER:H	1:A:180:GLN:HE21	1.55	0.55
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.88	0.55
8:U:43:MET:HE3	8:U:49:ASP:N	2.21	0.55
26:G:269:CDL:H451	2:O:70:ALA:HB1	1.89	0.55
1:N:409:TRP:HA	1:N:412:ILE:HD12	1.89	0.55
2:O:32:PHE:CE2	19:O:1521:TGL:HA51	2.41	0.55
20:P:1267:PGV:C18	26:P:1270:CDL:H662	2.36	0.55
19:A:521:TGL:H363	19:A:521:TGL:H221	1.89	0.54
3:C:224:LYS:HE3	26:C:270:CDL:HB32	1.88	0.54
22:B:229:PSC:H071	5:E:8:ASP:OD1	2.07	0.54
29:N:3132:HOH:O	3:P:191:GLY:HA3	2.07	0.54
1:A:377:PHE:HA	1:A:380[B]:VAL:HG22	1.90	0.54
13:M:19:LEU:HD23	20:M:524:PGV:C31	2.32	0.54
1:A:334:TRP:CE3	19:D:523:TGL:HA31	2.43	0.54
1:A:478:SER:O	13:M:6:ALA:HB1	2.08	0.54
19:A:521:TGL:H283	19:A:521:TGL:C11	2.32	0.54
7:G:3:ALA:O	7:G:4:ALA:CB	2.55	0.54
12:L:11:ILE:CG2	19:L:522:TGL:H272	2.38	0.54
20:M:524:PGV:H062	29:M:2126:HOH:O	2.07	0.54
26:G:269:CDL:H561	26:G:269:CDL:H762	1.89	0.54
7:G:11:TPO:O	7:G:11:TPO:HG22	2.08	0.53
19:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.90	0.53
25:P:1265:PEK:C04	6:S:1:ALA:H2	2.21	0.53
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.53
26:G:269:CDL:H351	2:O:81:LEU:HD12	1.89	0.53
22:R:1229:PSC:O01	22:R:1229:PSC:C21	2.57	0.53
7:G:2:SER:OG	25:G:1263:PEK:C30	2.56	0.53
1:N:1:FME:HE2	12:Y:3:TYR:CE1	2.43	0.53
7:T:83:GLU:HA	7:T:84:LYS:NZ	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:LEU:HD12	19:N:1522:TGL:H141	1.89	0.53
7:T:37:LEU:HD21	26:T:1269:CDL:H361	1.90	0.53
2:O:226:MET:O	2:O:227:LEU:OXT	2.27	0.53
1:A:21:LEU:HD23	19:L:522:TGL:H211	1.90	0.53
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.91	0.53
19:Q:1523:TGL:OB1	19:Q:1523:TGL:CG3	2.57	0.53
2:B:56:MET:HB3	22:B:229:PSC:H211	1.91	0.53
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.23	0.53
5:R:108:LYS:O	5:R:108:LYS:HG2	2.09	0.52
20:N:1524:PGV:H011	20:N:1524:PGV:H221	1.91	0.52
2:O:66:THR:HG21	23:O:229:CHD:H3	1.91	0.52
26:P:1270:CDL:H661	26:P:1270:CDL:C24	2.38	0.52
2:B:1:FME:HCN	2:B:193:TYR:HB2	1.92	0.52
1:N:136:LEU:HD12	29:N:4821:HOH:O	2.08	0.52
2:O:13:THR:HB	2:O:168:LEU:HD23	1.91	0.52
5:E:31:LYS:HE2	6:F:83:PRO:O	2.09	0.52
7:T:11:TPO:O	7:T:11:TPO:CG2	2.57	0.52
26:T:1269:CDL:H331	26:T:1269:CDL:OA7	2.08	0.52
25:G:265:PEK:C37	26:G:269:CDL:H273	2.37	0.52
25:G:265:PEK:H292	29:O:4943:HOH:O	2.09	0.52
2:O:227:LEU:CD2	29:O:4852:HOH:O	2.34	0.52
23:P:1271:CHD:H232	23:P:1271:CHD:C16	2.38	0.52
7:T:37:LEU:CD2	26:T:1269:CDL:H361	2.40	0.52
7:T:38:HIS:CE1	26:T:1269:CDL:H122	2.45	0.52
2:B:1:FME:CN	2:B:193:TYR:H	2.23	0.52
7:G:72:ASN:H	7:G:76:ASN:ND2	1.99	0.52
1:N:53:ILE:HG12	29:N:3704:HOH:O	2.08	0.52
3:P:34:TRP:HE1	28:P:1272:DMU:C57	2.18	0.52
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.44	0.52
13:M:13:LYS:HE3	29:M:4807:HOH:O	2.09	0.51
1:A:297:MET:HE2	1:A:297:MET:HB3	1.90	0.51
12:L:14:SER:H	19:L:522:TGL:HC31	1.75	0.51
7:G:5:LYS:HD2	25:G:1263:PEK:C38	2.40	0.51
26:G:269:CDL:H112	26:G:269:CDL:HA21	1.93	0.51
2:B:41:ILE:HD13	22:B:229:PSC:H342	1.93	0.51
20:M:524:PGV:H141	20:M:524:PGV:H302	1.91	0.51
20:P:1267:PGV:H172	26:P:1270:CDL:C65	2.40	0.51
7:T:38:HIS:HE2	26:T:1269:CDL:H122	1.75	0.51
26:G:269:CDL:HA21	26:G:269:CDL:C11	2.41	0.51
20:N:1524:PGV:C01	20:N:1524:PGV:H221	2.40	0.51
1:N:351:GLY:C	1:N:380[A]:VAL:HG13	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:1266:PGV:H183	25:P:1264:PEK:H332	1.93	0.51
26:C:270:CDL:H651	26:C:270:CDL:H772	1.92	0.51
19:O:1521:TGL:H241	19:O:1521:TGL:C20	2.38	0.51
20:M:524:PGV:O01	20:M:524:PGV:O13	2.29	0.51
10:W:2:GLU:HB3	10:W:4:ARG:HH11	1.75	0.51
7:T:84:LYS:CD	7:T:84:LYS:N	2.64	0.50
3:C:67:PHE:CE1	26:C:270:CDL:H1	2.39	0.50
23:O:229:CHD:H212	23:O:229:CHD:C12	2.41	0.50
3:P:40:MET:O	3:P:44:MET:HG2	2.11	0.50
11:X:8:ASP:HB2	29:X:4890:HOH:O	2.11	0.50
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.77	0.50
3:P:224:LYS:HD3	26:P:1270:CDL:HB32	1.91	0.50
5:R:107:ASP:OD2	5:R:107:ASP:N	2.45	0.50
7:T:2:SER:O	25:T:263:PEK:C33	2.43	0.50
26:G:269:CDL:H771	29:G:4678:HOH:O	2.12	0.50
19:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.94	0.50
2:O:58:ALA:O	2:O:62:GLU:HG3	2.12	0.50
4:Q:78:TRP:HA	19:Q:1523:TGL:HB22	1.94	0.50
3:C:224:LYS:CE	26:C:270:CDL:HB32	2.42	0.50
8:H:43:MET:CE	8:H:49:ASP:H	2.23	0.50
12:L:24:MET:SD	19:L:522:TGL:H161	2.51	0.50
25:T:263:PEK:O04	25:T:263:PEK:H242	2.11	0.50
2:B:58:ALA:O	2:B:62:GLU:HG3	2.12	0.50
22:B:229:PSC:H222	22:B:229:PSC:O04	2.11	0.50
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.42	0.50
5:E:21:LYS:HE2	5:E:24:ILE:HA	1.93	0.50
25:G:265:PEK:H383	26:G:269:CDL:H271	1.93	0.50
1:N:113:LEU:HD12	19:N:1522:TGL:C14	2.42	0.50
4:Q:78:TRP:CA	19:Q:1523:TGL:HB22	2.41	0.50
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.00	0.49
8:H:43:MET:HE3	8:H:49:ASP:N	2.27	0.49
7:T:38:HIS:NE2	26:T:1269:CDL:H122	2.27	0.49
1:A:278:MET:SD	7:T:5:LYS:HB3	2.53	0.49
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.93	0.49
12:L:2:HIS:CG	12:L:3:TYR:H	2.30	0.49
20:P:1267:PGV:H182	26:P:1270:CDL:H662	1.94	0.49
7:T:3:ALA:O	7:T:4:ALA:HB2	2.12	0.49
25:P:1265:PEK:C04	6:S:1:ALA:H1	2.25	0.49
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.48	0.49
1:N:484:THR:HB	13:Z:2:THR:OG1	2.12	0.49
7:T:7:ASP:OD1	7:T:8:HIS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MET:O	1:A:189:MET:HG3	2.12	0.49
5:R:80:GLU:H	5:R:80:GLU:CD	2.20	0.49
6:S:55:LYS:HA	6:S:74:LEU:O	2.12	0.49
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.95	0.49
1:A:240:HIS:C	1:A:240:HIS:CD2	2.90	0.49
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.94	0.49
1:A:347:LEU:HD13	1:A:383[B]:MET:HB3	1.95	0.49
1:N:34:SER:HB2	14:N:515:HEA:C2B	2.43	0.49
1:N:113:LEU:HD12	19:N:1522:TGL:C13	2.43	0.48
19:N:1522:TGL:CC3	12:Y:20:ARG:HH21	2.25	0.48
2:B:57:ASP:H	22:B:229:PSC:H201	1.77	0.48
7:G:17:ARG:HH22	25:G:265:PEK:H041	1.79	0.48
2:O:82:ARG:NH1	2:O:86:MET:HE1	2.28	0.48
8:U:9:LYS:O	8:U:10:ASN:CB	2.61	0.48
1:A:325:ALA:HA	22:B:229:PSC:H291	1.96	0.48
3:C:103:HIS:HA	20:C:268:PGV:H012	1.95	0.48
2:O:84:LEU:HA	2:O:87:MET:CE	2.43	0.48
8:U:9:LYS:HG3	8:U:10:ASN:N	2.28	0.48
11:X:8:ASP:HB3	29:X:4788:HOH:O	2.13	0.48
26:G:269:CDL:H782	26:G:269:CDL:C56	2.40	0.48
19:A:521:TGL:H111	19:A:521:TGL:C28	2.34	0.48
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.95	0.48
1:N:334:TRP:CZ3	19:Q:1523:TGL:HA51	2.48	0.48
3:P:63:ARG:HE	26:P:1270:CDL:HA21	1.78	0.48
7:T:2:SER:OG	25:T:263:PEK:H292	2.14	0.47
1:A:377:PHE:CD1	14:A:516:HEA:HAD1	2.49	0.47
3:C:122:HIS:HD2	29:C:4553:HOH:O	1.95	0.47
26:C:270:CDL:HB22	10:J:8:LYS:NZ	2.29	0.47
1:N:351:GLY:C	1:N:380[A]:VAL:CG1	2.87	0.47
22:R:1229:PSC:H142	22:R:1229:PSC:H341	1.82	0.47
3:C:207:HIS:HD2	3:C:241:TYR:OH	1.97	0.47
25:G:265:PEK:C38	26:G:269:CDL:H273	2.44	0.47
25:G:1263:PEK:H132	3:P:247:VAL:CG1	2.44	0.47
9:V:35:TYR:C	9:V:37:PHE:H	2.21	0.47
1:A:334:TRP:CZ3	19:D:523:TGL:HA52	2.49	0.47
7:G:8:HIS:HE1	25:G:1263:PEK:H321	1.80	0.47
1:N:189:MET:HE2	1:N:189:MET:HB3	1.94	0.47
7:T:35:SER:C	7:T:37:LEU:H	2.23	0.47
2:B:1:FME:HCN	2:B:193:TYR:H	1.80	0.47
6:F:1:ALA:N	25:G:265:PEK:H041	2.30	0.47
1:N:18:LEU:CD2	19:N:1522:TGL:HB21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.47
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.95	0.47
5:R:41:LEU:CD2	22:R:1229:PSC:H041	2.45	0.47
7:T:7:ASP:CG	7:T:8:HIS:N	2.71	0.47
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.13	0.47
7:G:5:LYS:HG3	25:G:1263:PEK:C38	2.32	0.47
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.50	0.47
22:B:229:PSC:C28	22:B:229:PSC:H322	2.45	0.47
3:C:3:HIS:HE1	6:F:96:LEU:CD2	2.28	0.47
23:C:271:CHD:H232	23:C:271:CHD:H162	1.97	0.47
8:U:60:TYR:CD1	8:U:60:TYR:C	2.92	0.47
6:F:1:ALA:H2	25:G:265:PEK:C04	2.28	0.46
19:L:522:TGL:H182	19:L:522:TGL:OA1	2.15	0.46
1:N:240:HIS:CD2	1:N:240:HIS:C	2.93	0.46
19:A:521:TGL:HC22	29:D:2606:HOH:O	2.16	0.46
22:B:229:PSC:C07	5:E:8:ASP:HA	2.46	0.46
25:P:1264:PEK:H32	25:P:1264:PEK:C7	2.35	0.46
29:B:3446:HOH:O	7:T:17:ARG:HD2	2.14	0.46
23:C:271:CHD:H112	23:C:271:CHD:H12A	1.45	0.46
2:O:217:LYS:HE2	2:O:220:GLU:OE2	2.16	0.46
26:P:1270:CDL:HB22	26:P:1270:CDL:OA5	2.15	0.46
7:T:38:HIS:ND1	7:T:38:HIS:N	2.63	0.46
26:G:269:CDL:H562	26:G:269:CDL:C78	2.41	0.46
9:V:15:ARG:HD2	29:V:4529:HOH:O	2.16	0.46
8:H:60:TYR:CD1	8:H:60:TYR:C	2.93	0.46
1:A:334:TRP:CD1	19:D:523:TGL:HC41	2.51	0.46
12:L:20:ARG:HH22	19:L:522:TGL:HC61	1.80	0.46
1:N:488:THR:HB	1:N:495:LEU:HD13	1.97	0.46
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.50	0.46
3:P:210:ILE:HG12	20:P:1267:PGV:H132	1.98	0.46
1:A:400:PHE:HB3	19:L:522:TGL:H283	1.98	0.45
19:Q:1523:TGL:H351	9:V:16:ARG:HH21	1.81	0.45
2:B:56:MET:HA	22:B:229:PSC:H202	1.97	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.45
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.98	0.45
23:B:1085:CHD:H112	23:B:1085:CHD:H12A	1.82	0.45
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.77	0.45
11:X:42:PRO:HG2	11:X:47:ARG:NE	2.31	0.45
10:J:4:ARG:HD3	10:J:7:GLU:OE2	2.17	0.45
23:P:1271:CHD:C16	23:P:1271:CHD:C23	2.95	0.45
6:S:53:THR:CG2	6:S:54:ASN:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:GLY:HA3	25:C:264:PEK:H21	1.98	0.45
1:N:18:LEU:HD22	19:N:1522:TGL:HB21	1.98	0.45
25:P:1265:PEK:H041	6:S:1:ALA:N	2.31	0.45
5:R:11:PHE:HB3	22:R:1229:PSC:H073	1.99	0.45
1:A:364:ASP:OD2	14:A:516:HEA:O1A	2.35	0.45
26:G:269:CDL:H762	26:G:269:CDL:C56	2.47	0.45
26:G:269:CDL:H182	26:G:269:CDL:H152	1.60	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.45
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.68	0.45
1:A:274:VAL:HG12	1:A:278:MET:HE2	1.98	0.45
2:O:22:HIS:CE1	9:V:43:ARG:HG2	2.52	0.45
3:P:202:GLY:HA3	25:P:1264:PEK:H21	1.99	0.45
1:N:380[B]:VAL:O	1:N:384[B]:GLY:HA3	2.17	0.45
3:P:116:TRP:HA	3:P:117:PRO:C	2.42	0.45
3:P:156:ARG:HE	23:P:1271:CHD:C24	2.29	0.44
1:A:382[B]:SER:OG	14:A:515:HEA:H121	2.18	0.44
29:L:4824:HOH:O	13:M:32:TRP:HH2	1.99	0.44
23:B:1085:CHD:H12	23:B:1085:CHD:H212	1.99	0.44
4:D:109:HIS:HB3	29:D:4632:HOH:O	2.18	0.44
26:G:269:CDL:H561	26:G:269:CDL:H592	1.29	0.44
19:O:1521:TGL:H282	19:O:1521:TGL:H252	1.73	0.44
28:Z:1526:DMU:H9	28:Z:1526:DMU:H15	1.33	0.44
8:H:9:LYS:HD2	8:H:11:TYR:HB2	1.97	0.44
26:C:270:CDL:OB7	26:C:270:CDL:OA3	2.36	0.44
10:J:33:ARG:HG2	23:J:60:CHD:C15	2.48	0.44
3:C:67:PHE:HE1	26:C:270:CDL:C1	2.27	0.44
1:N:347:LEU:HD13	1:N:383[B]:MET:SD	2.58	0.44
2:B:59:GLN:O	2:B:60:GLU:HG3	2.17	0.44
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.44
1:N:87:ILE:O	1:N:173:PRO:HD3	2.18	0.44
1:N:344:PHE:CD1	1:N:344:PHE:C	2.95	0.44
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.60	0.44
22:B:229:PSC:C07	9:I:10:ARG:NH2	2.72	0.43
1:N:362:SER:OG	2:O:87:MET:HE2	2.18	0.43
22:R:1229:PSC:H221	22:R:1229:PSC:H251	1.67	0.43
11:X:42:PRO:HG2	11:X:47:ARG:HE	1.83	0.43
1:A:195:LEU:CD2	1:A:245:ILE:HD13	2.47	0.43
4:D:101:HIS:HD2	4:D:102:TYR:CZ	2.36	0.43
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.99	0.43
4:D:70:GLU:O	4:D:73:ARG:NH1	2.52	0.43
20:M:524:PGV:P	20:M:524:PGV:H061	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379:TYR:O	1:N:383[A]:MET:HB2	2.18	0.43
20:M:524:PGV:C2	20:M:524:PGV:C01	2.75	0.43
1:N:472:ILE:HG21	19:N:1522:TGL:HA91	2.01	0.43
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.16	0.43
1:A:377:PHE:O	1:A:381[A]:LEU:HB3	2.19	0.43
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.32	0.43
19:O:1521:TGL:H101	19:O:1521:TGL:H283	1.98	0.43
6:S:94:HIS:CD2	6:S:95:GLN:H	2.37	0.43
8:H:43:MET:HE3	8:H:49:ASP:H	1.83	0.43
20:M:524:PGV:H302	20:M:524:PGV:C14	2.48	0.43
1:N:240:HIS:O	1:N:241:PRO:C	2.59	0.43
28:P:1272:DMU:H1	7:T:69:PHE:HZ	1.84	0.43
19:Q:1523:TGL:HA91	19:Q:1523:TGL:C24	2.48	0.43
6:F:1:ALA:H1	25:G:265:PEK:C04	2.21	0.43
2:B:16:ILE:HG13	29:B:4955:HOH:O	2.19	0.43
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.00	0.43
4:D:78:TRP:CA	19:D:523:TGL:HB22	2.49	0.43
25:G:1263:PEK:H331	25:G:1263:PEK:H361	1.86	0.43
1:N:53:ILE:HD13	1:N:53:ILE:HG21	1.74	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.19	0.43
5:E:105:GLY:O	5:E:108:LYS:HE2	2.18	0.42
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.93	0.42
2:O:146:MET:HA	2:O:213:LEU:HD12	2.01	0.42
26:P:1270:CDL:H652	26:P:1270:CDL:H622	1.33	0.42
22:R:1229:PSC:H072	9:V:10:ARG:HH21	1.83	0.42
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.42
1:N:1:FME:HE2	12:Y:3:TYR:HE1	1.84	0.42
1:N:417:MET:HE2	29:N:3166:HOH:O	2.03	0.42
1:A:1:FME:HE2	1:A:4:ASN:ND2	2.30	0.42
1:A:136:LEU:HD12	29:A:4591:HOH:O	2.18	0.42
14:A:515:HEA:HBC1	14:A:515:HEA:HMC3	2.01	0.42
3:C:224:LYS:HE3	26:C:270:CDL:CB3	2.49	0.42
26:T:1269:CDL:C56	26:T:1269:CDL:H782	2.48	0.42
4:D:87:PHE:CZ	20:M:524:PGV:H152	2.54	0.42
22:B:229:PSC:C34	22:B:229:PSC:H141	2.37	0.42
22:B:229:PSC:H041	5:E:41:LEU:HD23	2.02	0.42
26:C:270:CDL:H672	26:C:270:CDL:C25	2.45	0.42
7:G:2:SER:OG	25:G:1263:PEK:H292	2.15	0.42
20:N:1524:PGV:H062	29:Z:4423:HOH:O	2.19	0.42
19:A:521:TGL:H201	19:A:521:TGL:C24	2.43	0.42
26:C:270:CDL:H642	26:C:270:CDL:H192	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:310:MET:HE3	1:N:356:ILE:HG23	2.00	0.42
6:S:95:GLN:NE2	6:S:95:GLN:HA	2.32	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.20	0.42
3:C:230:ASN:HB2	29:F:2400:HOH:O	2.19	0.42
4:D:109:HIS:HD2	29:D:2122:HOH:O	2.03	0.42
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.86	0.42
10:W:33:ARG:HG2	23:W:1059:CHD:C15	2.50	0.42
1:A:512:ASN:HD22	1:A:512:ASN:HA	1.51	0.42
3:C:51:MET:HB3	26:C:270:CDL:H381	2.02	0.42
3:C:156:ARG:HE	23:C:271:CHD:C24	2.33	0.42
26:T:1269:CDL:H542	26:T:1269:CDL:H241	2.01	0.42
1:A:380[B]:VAL:O	1:A:384[B]:GLY:HA3	2.20	0.42
2:B:87:MET:HE2	29:B:4235:HOH:O	2.19	0.42
1:N:208:MET:HG2	1:N:219:PHE:CE1	2.54	0.42
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.84	0.42
1:N:430:PHE:HE1	19:O:1521:TGL:HB21	1.85	0.42
4:D:127:LYS:HD2	29:I:2618:HOH:O	2.20	0.42
20:N:1524:PGV:H321	20:N:1524:PGV:C15	2.49	0.42
2:O:32:PHE:HE2	19:O:1521:TGL:HA51	1.84	0.42
5:R:23:ASP:OD2	5:R:23:ASP:N	2.49	0.42
2:B:102:HIS:O	2:B:104:TRP:HA	2.20	0.41
23:C:271:CHD:H212	23:C:271:CHD:H12	2.01	0.41
26:G:269:CDL:H542	26:G:269:CDL:C24	2.50	0.41
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.20	0.41
7:T:5:LYS:CD	25:T:263:PEK:C38	2.94	0.41
9:V:31:PHE:O	9:V:32:ALA:C	2.61	0.41
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.44	0.41
29:B:2562:HOH:O	19:D:523:TGL:HC72	2.19	0.41
3:C:109:THR:HB	3:C:110:PRO:HD2	2.02	0.41
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.03	0.41
3:C:3:HIS:CE1	6:F:96:LEU:CD2	3.04	0.41
3:C:207:HIS:CD2	3:C:241:TYR:OH	2.73	0.41
19:D:523:TGL:H231	19:D:523:TGL:H201	1.34	0.41
26:C:270:CDL:H252	26:C:270:CDL:C67	2.45	0.41
13:M:42:LYS:HA	13:M:42:LYS:HD2	1.60	0.41
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.18	0.41
1:A:378:HIS:HA	1:A:382[A]:SER:OG	2.20	0.41
2:B:128:LEU:HD11	2:B:134:ARG:HA	2.02	0.41
7:G:5:LYS:CG	25:G:1263:PEK:H383	2.35	0.41
7:G:31:CYS:SG	26:G:269:CDL:H532	2.61	0.41
13:M:16:ALA:HA	20:M:524:PGV:H312	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.55	0.41
9:V:15:ARG:HB2	29:V:4529:HOH:O	2.19	0.41
13:Z:39:ASN:O	13:Z:43:SER:OG	2.28	0.41
2:B:217:LYS:CE	29:B:4805:HOH:O	2.68	0.41
12:L:47:LYS:HB2	12:L:47:LYS:HE2	1.86	0.41
1:N:127:THR:HB	1:N:129:TYR:CE2	2.55	0.41
4:Q:41:LYS:HB3	4:Q:41:LYS:HE3	1.82	0.41
12:Y:34:ALA:O	12:Y:35:ALA:C	2.64	0.41
1:A:169:ILE:N	1:A:169:ILE:HD13	2.34	0.41
1:A:310:MET:HE1	2:B:76:ILE:HG21	2.03	0.41
1:A:439:ARG:HD3	2:B:199:ILE:HB	2.03	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.77	0.41
2:B:56:MET:HA	22:B:229:PSC:C20	2.51	0.41
3:C:105:SER:HA	3:C:116:TRP:CE3	2.56	0.41
7:G:45:PRO:HD2	29:G:2099:HOH:O	2.21	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.72	0.41
26:P:1270:CDL:PA1	26:P:1270:CDL:CB2	2.97	0.41
19:Q:1523:TGL:HB92	19:Q:1523:TGL:H122	1.79	0.41
6:S:37:LYS:HD2	6:S:37:LYS:HA	1.91	0.41
1:A:107:PRO:HB3	3:C:25:LEU:HB2	2.03	0.41
2:B:52:HIS:HE1	22:B:229:PSC:H212	1.85	0.41
5:E:48:ILE:HD13	5:E:48:ILE:HA	1.91	0.41
1:N:512:ASN:HD22	1:N:512:ASN:HA	1.63	0.41
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.56	0.41
20:P:1268:PGV:H51	20:P:1268:PGV:H21	1.82	0.41
7:T:5:LYS:HD2	25:T:263:PEK:H381	2.00	0.41
13:Z:42:LYS:HD2	13:Z:42:LYS:HA	1.96	0.41
25:C:264:PEK:H32	25:C:264:PEK:C7	2.40	0.40
6:F:1:ALA:H2	25:G:265:PEK:H041	1.85	0.40
5:R:11:PHE:CB	22:R:1229:PSC:H073	2.50	0.40
8:U:50:VAL:C	8:U:52:VAL:N	2.79	0.40
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.03	0.40
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.57	0.40
19:N:1522:TGL:HC32	12:Y:20:ARG:HH21	1.86	0.40
2:O:227:LEU:HD23	2:O:227:LEU:HA	1.34	0.40
9:V:37:PHE:CD1	9:V:37:PHE:C	2.99	0.40
1:A:310:MET:CE	1:A:356:ILE:HG23	2.51	0.40
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.04	0.40
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.03	0.40
14:A:515:HEA:HAC	14:A:515:HEA:HH2	1.93	0.40
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:62:GLU:O	2:O:66:THR:HB	2.21	0.40
5:R:41:LEU:HD23	22:R:1229:PSC:H041	2.02	0.40
7:T:3:ALA:HB3	25:T:263:PEK:H361	2.02	0.40
1:A:76:GLY:O	1:A:80:ASN:HB2	2.22	0.40
2:B:83:ILE:O	2:B:87:MET:HG3	2.22	0.40
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.70	0.40
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.04	0.40
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.57	0.40
7:T:3:ALA:HB3	25:T:263:PEK:H382	2.03	0.40
9:V:37:PHE:CD1	9:V:38:ALA:N	2.90	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:OG1	5:R:80:GLU:OE1[3_647]	1.64	0.56
2:O:126:SER:O	6:S:94:HIS:CB[2_684]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/514 (101%)	504 (98%)	13 (2%)	0	100	100
1	N	517/514 (101%)	501 (97%)	16 (3%)	0	100	100
2	B	225/227 (99%)	220 (98%)	4 (2%)	1 (0%)	30	19
2	O	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	30	19
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	18	8
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
7	G	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	1	0
7	T	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	1	0
8	H	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	1	0
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	1	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3514/3614 (97%)	3380 (96%)	108 (3%)	26 (1%)	18	8

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
8	H	45	ALA
8	H	46	LYS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS

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Mol	Chain	Res	Type
8	U	45	ALA
8	U	46	LYS
2	B	60	GLU
8	H	8	ILE
2	O	60	GLU
6	S	94	HIS
8	U	8	ILE
8	U	10	ASN
6	F	96	LEU
7	G	6	GLY
8	H	51	SER
4	Q	35	ALA
7	G	37	LEU
6	S	96	LEU
7	T	6	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/426 (101%)	415 (96%)	15 (4%)	32	19
1	N	430/426 (101%)	420 (98%)	10 (2%)	44	33
2	B	210/210 (100%)	200 (95%)	10 (5%)	23	11
2	O	210/210 (100%)	199 (95%)	11 (5%)	21	9
3	C	224/226 (99%)	222 (99%)	2 (1%)	70	67
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	34
4	D	128/129 (99%)	124 (97%)	4 (3%)	35	23
4	Q	128/129 (99%)	122 (95%)	6 (5%)	23	11
5	E	92/95 (97%)	91 (99%)	1 (1%)	65	60
5	R	92/95 (97%)	90 (98%)	2 (2%)	45	34
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	18
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	2
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	2
8	H	71/75 (95%)	67 (94%)	4 (6%)	19	8
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	8
9	I	57/57 (100%)	49 (86%)	8 (14%)	3	1
9	V	57/57 (100%)	50 (88%)	7 (12%)	4	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	38
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	38
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	9
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	9
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	28
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7	2
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	1
All	All	3048/3082 (99%)	2917 (96%)	131 (4%)	26	13

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	LEU
1	A	169	ILE
1	A	178	GLN
1	A	180	GLN
1	A	189	MET
1	A	200	PRO
1	A	241	PRO
1	A	297	MET
1	A	369	ASP
1	A	380[A]	VAL
1	A	380[B]	VAL
1	A	484	THR
1	A	486	ASP
1	A	504	THR
1	A	512	ASN
2	B	33	LEU
2	B	37	LEU
2	B	60	GLU

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Mol	Chain	Res	Type
2	B	65	TRP
2	B	67	ILE
2	B	75	LEU
2	B	78	LEU
2	B	115	ASP
2	B	167	SER
2	B	217	LYS
3	C	159	MET
3	C	230	ASN
4	D	4	SER
4	D	36	SER
4	D	51	LEU
4	D	58	GLU
5	E	90	ARG
6	F	48	LEU
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	5	LYS
7	G	17	ARG
7	G	26	PRO
7	G	74	ARG
7	G	84	LYS
8	H	8	ILE
8	H	23	GLN
8	H	60	TYR
8	H	65	PRO
9	I	8	GLN
9	I	15	ARG
9	I	29	LEU
9	I	33	THR
9	I	37	PHE
9	I	61	GLU
9	I	68	ILE
9	I	73	LYS
10	J	50	LEU
11	K	47	ARG
11	K	54	ARG
12	L	26	THR
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP

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Mol	Chain	Res	Type
13	M	42	LYS
13	M	43	SER
1	N	128	VAL
1	N	180	GLN
1	N	241	PRO
1	N	265	LYS
1	N	297	MET
1	N	369	ASP
1	N	394	VAL
1	N	484	THR
1	N	504	THR
1	N	512	ASN
2	O	33	LEU
2	O	60	GLU
2	O	61	VAL
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	217	LYS
2	O	227	LEU
3	P	77	LYS
3	P	110	PRO
3	P	159	MET
3	P	180	GLU
3	P	230	ASN
4	Q	4	SER
4	Q	9	GLU
4	Q	31	LYS
4	Q	38	LYS
4	Q	51	LEU
4	Q	143	ASN
5	R	80	GLU
5	R	108	LYS
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU

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Mol	Chain	Res	Type
7	T	2	SER
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	74	ARG
7	T	84	LYS
8	U	7	LYS
8	U	8	ILE
8	U	9	LYS
8	U	60	TYR
9	V	2	THR
9	V	10	ARG
9	V	26	MET
9	V	29	LEU
9	V	37	PHE
9	V	61	GLU
9	V	70	GLN
10	W	50	LEU
11	X	20	SER
11	X	47	ARG
12	Y	2	HIS
12	Y	11	ILE
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	10	GLN
2	B	181	GLN
3	C	3	HIS
3	C	68	GLN

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Mol	Chain	Res	Type
3	C	161	GLN
3	C	230	ASN
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
4	D	119	GLN
5	E	94	ASN
7	G	8	HIS
7	G	34	ASN
7	G	76	ASN
8	H	31	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	43	GLN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	422	ASN
1	N	512	ASN
2	O	91	ASN
2	O	181	GLN
2	O	203	ASN
3	P	3	HIS
3	P	68	GLN
3	P	76	GLN
3	P	207	HIS
3	P	230	ASN
4	Q	37	GLN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	94	HIS
6	S	95	GLN
7	T	34	ASN
7	T	41	HIS
7	T	76	ASN
8	U	28	ASN
8	U	31	GLN
8	U	32	ASN

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Mol	Chain	Res	Type
10	W	57	HIS
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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
9	SAC	I	1	9	7,8,9	2.78	2 (28%)	7,9,11	2.02	3 (42%)
7	TPO	G	11	7	8,10,11	3.05	6 (75%)	10,14,16	1.74	3 (30%)
1	FME	A	1	1	8,9,10	2.15	2 (25%)	8,9,11	8.37	5 (62%)
2	FME	O	1	2	8,9,10	1.79	3 (37%)	8,9,11	6.12	3 (37%)
2	FME	B	1	2	8,9,10	3.71	6 (75%)	8,9,11	7.39	6 (75%)
1	FME	N	1	1	8,9,10	1.15	1 (12%)	8,9,11	7.49	5 (62%)
9	SAC	V	1	9	7,8,9	3.10	2 (28%)	7,9,11	3.06	2 (28%)
7	TPO	T	11	7	8,10,11	3.30	5 (62%)	10,14,16	2.22	5 (50%)

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
9	SAC	I	1	9	-	4/7/8/10	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	1/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	5/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-
7	TPO	T	11	7	-	3/9/11/13	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	7.13	1.72	1.59
2	B	1	FME	CN-N	6.83	1.55	1.33
9	V	1	SAC	CA-N	5.92	1.55	1.46
7	G	11	TPO	P-OG1	5.87	1.69	1.59
1	A	1	FME	CA-N	5.34	1.54	1.46
9	I	1	SAC	OAC-C1A	5.19	1.34	1.23
9	V	1	SAC	OAC-C1A	5.15	1.34	1.23
2	B	1	FME	O1-CN	-4.59	1.03	1.22
2	B	1	FME	CA-N	4.47	1.53	1.46
7	G	11	TPO	P-O1P	4.45	1.64	1.50
9	I	1	SAC	CA-N	4.14	1.52	1.46
7	T	11	TPO	P-O1P	3.80	1.62	1.50
2	O	1	FME	O1-CN	-3.44	1.08	1.22
2	B	1	FME	CG-SD	-3.25	1.64	1.81
7	T	11	TPO	P-O3P	2.63	1.64	1.54
2	B	1	FME	CB-CA	2.56	1.58	1.53
7	G	11	TPO	P-O2P	2.50	1.64	1.54
2	O	1	FME	CG-SD	-2.46	1.68	1.81
1	A	1	FME	O1-CN	-2.33	1.13	1.22
2	O	1	FME	CB-CG	2.29	1.60	1.51
1	N	1	FME	CA-N	2.24	1.49	1.46
7	G	11	TPO	CG2-CB	2.22	1.56	1.51
7	G	11	TPO	P-O3P	2.15	1.62	1.54
7	T	11	TPO	O-C	2.13	1.28	1.20
7	T	11	TPO	P-O2P	2.12	1.62	1.54
2	B	1	FME	CB-CG	2.08	1.59	1.51
7	G	11	TPO	O-C	2.03	1.27	1.20

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CA-N-CN	-22.50	88.22	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CA-N-CN	-19.41	92.96	122.82
2	O	1	FME	CA-N-CN	-16.83	96.94	122.82
2	B	1	FME	CA-N-CN	-13.91	101.44	122.82
2	B	1	FME	O1-CN-N	-13.08	91.52	125.32
9	V	1	SAC	C-CA-N	7.24	123.47	109.50
2	B	1	FME	C-CA-N	7.24	123.47	109.50
1	N	1	FME	O1-CN-N	6.64	142.48	125.32
1	A	1	FME	O1-CN-N	4.72	137.52	125.32
7	T	11	TPO	O3P-P-OG1	3.89	120.99	105.85
1	N	1	FME	CB-CA-N	3.76	117.37	110.52
9	I	1	SAC	C-CA-N	3.75	116.73	109.50
1	A	1	FME	CE-SD-CG	3.58	118.87	100.32
7	G	11	TPO	O2P-P-OG1	3.38	119.01	105.85
2	B	1	FME	CG-CB-CA	-3.19	103.10	112.87
7	T	11	TPO	P-OG1-CB	3.11	131.78	123.33
1	A	1	FME	CB-CA-N	2.84	115.68	110.52
7	T	11	TPO	OG1-P-O1P	-2.72	99.65	109.33
7	G	11	TPO	O-C-CA	-2.69	117.85	124.77
7	T	11	TPO	O-C-CA	-2.59	118.11	124.77
7	G	11	TPO	CG2-CB-CA	2.54	118.22	113.26
7	T	11	TPO	O2P-P-OG1	2.46	115.42	105.85
9	I	1	SAC	C2A-C1A-N	-2.45	112.05	116.12
1	A	1	FME	C-CA-N	2.34	114.02	109.50
2	O	1	FME	CG-CB-CA	-2.34	105.72	112.87
9	I	1	SAC	CB-CA-C	-2.33	106.22	111.35
9	V	1	SAC	O-C-CA	-2.33	118.79	124.77
1	N	1	FME	C-CA-N	2.27	113.88	109.50
2	B	1	FME	CB-CA-N	2.15	114.44	110.52
2	O	1	FME	O-C-CA	-2.14	119.27	124.77
1	N	1	FME	CE-SD-CG	2.12	111.27	100.32
2	B	1	FME	O-C-CA	-2.01	119.59	124.77

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
9	I	1	SAC	N-CA-CB-OG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	O-C-CA-CB
9	V	1	SAC	C-CA-CB-OG
9	V	1	SAC	N-CA-CB-OG
1	N	1	FME	CA-CB-CG-SD
9	I	1	SAC	C-CA-N-C1A
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
9	I	1	SAC	CB-CA-N-C1A
7	G	11	TPO	CB-OG1-P-O1P

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	3	0
1	A	1	FME	3	0
2	B	1	FME	3	0
1	N	1	FME	2	0
9	V	1	SAC	1	0
7	T	11	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 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$
21	CUA	B	228	2	0,1,1	-	-	-		
23	CHD	C	525	-	32,32,32	1.79	8 (25%)	51,51,51	5.08	35 (68%)
21	CUA	O	228	2	0,1,1	-	-	-		
23	CHD	O	229	-	32,32,32	2.00	12 (37%)	51,51,51	5.52	32 (62%)
25	PEK	T	263	-	52,52,52	1.28	4 (7%)	55,57,57	1.41	7 (12%)
28	DMU	P	1272	-	34,34,34	1.71	6 (17%)	45,45,45	3.48	27 (60%)
15	NO	A	520	16,14	0,1,1	-	-	-		
23	CHD	C	271	-	32,32,32	1.10	2 (6%)	51,51,51	5.03	32 (62%)
20	PGV	N	1524	-	50,50,50	1.32	3 (6%)	53,56,56	1.38	8 (15%)
20	PGV	C	268	-	50,50,50	1.38	4 (8%)	53,56,56	1.70	6 (11%)
20	PGV	N	1266	-	50,50,50	1.25	5 (10%)	53,56,56	1.57	9 (16%)
23	CHD	W	1059	-	32,32,32	1.02	1 (3%)	51,51,51	5.12	36 (70%)
26	CDL	G	269	-	99,99,99	1.56	13 (13%)	105,111,111	1.60	22 (20%)
26	CDL	P	1270	-	99,99,99	1.59	15 (15%)	105,111,111	1.89	23 (21%)
23	CHD	B	1085	-	32,32,32	2.19	11 (34%)	51,51,51	5.33	35 (68%)
14	HEA	A	515	1	67,67,67	2.14	19 (28%)	81,103,103	2.21	26 (32%)
25	PEK	G	1263	-	52,52,52	1.46	4 (7%)	55,57,57	1.45	7 (12%)
19	TGL	N	1522	-	62,62,62	1.72	10 (16%)	65,65,65	1.97	17 (26%)
25	PEK	P	1264	-	52,52,52	0.97	2 (3%)	55,57,57	2.26	12 (21%)
23	CHD	J	60	-	32,32,32	1.18	2 (6%)	51,51,51	5.09	33 (64%)
20	PGV	P	1268	-	50,50,50	1.49	3 (6%)	53,56,56	1.74	9 (16%)
19	TGL	O	1521	-	62,62,62	1.48	6 (9%)	65,65,65	1.77	12 (18%)
14	HEA	A	516	1,15	67,67,67	1.74	14 (20%)	81,103,103	2.69	33 (40%)
26	CDL	C	270	-	99,99,99	1.58	15 (15%)	105,111,111	1.84	19 (18%)
28	DMU	G	272	-	34,34,34	1.47	6 (17%)	45,45,45	3.58	24 (53%)
19	TGL	L	522	-	62,62,62	1.77	7 (11%)	65,65,65	2.17	16 (24%)
20	PGV	M	524	-	50,50,50	1.23	2 (4%)	53,56,56	1.50	9 (16%)
20	PGV	A	522	-	50,50,50	1.20	4 (8%)	53,56,56	1.53	9 (16%)
23	CHD	P	1271	-	32,32,32	0.99	1 (3%)	51,51,51	5.17	35 (68%)
28	DMU	Z	1526	-	34,34,34	1.15	4 (11%)	45,45,45	3.44	25 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	C	264	-	52,52,52	1.16	5 (9%)	55,57,57	2.19	12 (21%)
26	CDL	T	1269	-	99,99,99	1.47	12 (12%)	105,111,111	1.71	21 (20%)
14	HEA	N	515	1	67,67,67	1.81	18 (26%)	81,103,103	2.10	32 (39%)
22	PSC	B	229	-	51,51,51	1.28	3 (5%)	57,59,59	1.25	8 (14%)
22	PSC	R	1229	-	51,51,51	1.43	3 (5%)	57,59,59	1.31	6 (10%)
19	TGL	D	523	-	62,62,62	1.64	7 (11%)	65,65,65	1.76	15 (23%)
19	TGL	Q	1523	-	62,62,62	1.58	7 (11%)	65,65,65	1.49	8 (12%)
23	CHD	P	1525	-	32,32,32	2.00	13 (40%)	51,51,51	5.47	37 (72%)
14	HEA	N	516	1,15	67,67,67	1.72	20 (29%)	81,103,103	2.30	37 (45%)
20	PGV	P	1267	-	50,50,50	1.04	2 (4%)	53,56,56	1.67	11 (20%)
25	PEK	G	265	-	52,52,52	1.51	4 (7%)	55,57,57	1.66	9 (16%)
28	DMU	M	526	-	34,34,34	1.23	4 (11%)	45,45,45	3.60	27 (60%)
15	NO	N	520	16,14	0,1,1	-	-	-	-	-
19	TGL	A	521	-	62,62,62	1.42	6 (9%)	65,65,65	1.80	13 (20%)
20	PGV	C	267	-	50,50,50	0.92	1 (2%)	53,56,56	1.40	11 (20%)
25	PEK	P	1265	-	52,52,52	1.49	6 (11%)	55,57,57	1.54	8 (14%)

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
23	CHD	C	525	-	-	1/9/74/74	0/4/4/4
23	CHD	O	229	-	-	3/9/74/74	0/4/4/4
25	PEK	T	263	-	-	31/56/56/56	-
28	DMU	P	1272	-	6/6/10/10	13/19/59/59	0/2/2/2
23	CHD	C	271	-	1/1/12/12	5/9/74/74	0/4/4/4
20	PGV	N	1524	-	-	25/55/55/55	-
20	PGV	C	268	-	-	35/55/55/55	-
20	PGV	N	1266	-	-	17/55/55/55	-
23	CHD	W	1059	-	1/1/12/12	6/9/74/74	0/4/4/4
26	CDL	G	269	-	-	58/110/110/110	-
26	CDL	P	1270	-	-	68/110/110/110	-
23	CHD	B	1085	-	-	2/9/74/74	0/4/4/4
14	HEA	A	515	1	-	5/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	G	1263	-	-	30/56/56/56	-
19	TGL	N	1522	-	-	42/65/65/65	-
25	PEK	P	1264	-	-	22/56/56/56	-
23	CHD	J	60	-	2/2/12/12	6/9/74/74	0/4/4/4
20	PGV	P	1268	-	-	26/55/55/55	-
19	TGL	O	1521	-	-	30/65/65/65	-
14	HEA	A	516	1,15	-	5/36/76/76	-
26	CDL	C	270	-	-	69/110/110/110	-
28	DMU	G	272	-	6/6/10/10	11/19/59/59	0/2/2/2
19	TGL	L	522	-	-	36/65/65/65	-
20	PGV	M	524	-	-	34/55/55/55	-
20	PGV	A	522	-	-	8/55/55/55	-
23	CHD	P	1271	-	1/1/12/12	3/9/74/74	0/4/4/4
28	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
25	PEK	C	264	-	-	21/56/56/56	-
26	CDL	T	1269	-	-	59/110/110/110	-
14	HEA	N	515	1	-	5/36/76/76	-
22	PSC	B	229	-	-	39/55/55/55	-
22	PSC	R	1229	-	-	30/55/55/55	-
19	TGL	D	523	-	-	40/65/65/65	-
19	TGL	Q	1523	-	-	37/65/65/65	-
23	CHD	P	1525	-	-	4/9/74/74	0/4/4/4
14	HEA	N	516	1,15	-	6/36/76/76	-
20	PGV	P	1267	-	-	13/55/55/55	-
25	PEK	G	265	-	-	28/56/56/56	-
28	DMU	M	526	-	4/4/10/10	7/19/59/59	0/2/2/2
19	TGL	A	521	-	-	39/65/65/65	-
20	PGV	C	267	-	-	11/55/55/55	-
25	PEK	P	1265	-	-	30/56/56/56	-

All (294) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515	HEA	C11-C3B	9.21	1.62	1.51
20	P	1268	PGV	O01-C1	7.63	1.55	1.34
19	L	522	TGL	OG2-CB1	7.53	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1522	TGL	OG2-CB1	7.31	1.54	1.34
20	C	268	PGV	O01-C1	6.46	1.52	1.34
28	P	1272	DMU	O16-C6	6.33	1.50	1.40
25	G	1263	PEK	O03-C21	6.06	1.51	1.33
25	T	263	PEK	O03-C21	6.05	1.51	1.33
25	P	1265	PEK	O03-C21	5.98	1.50	1.33
25	G	265	PEK	O01-C1	5.98	1.51	1.34
25	G	1263	PEK	O01-C1	5.80	1.50	1.34
28	G	272	DMU	O16-C6	5.79	1.49	1.40
25	G	265	PEK	O03-C21	5.72	1.50	1.33
19	D	523	TGL	OB1-CB1	5.70	1.39	1.22
23	O	229	CHD	C18-C13	5.70	1.63	1.54
23	B	1085	CHD	C18-C13	5.67	1.63	1.54
26	G	269	CDL	OB6-CB5	5.66	1.50	1.34
26	G	269	CDL	OA6-CA5	5.59	1.50	1.34
23	B	1085	CHD	C10-C5	-5.48	1.46	1.55
20	M	524	PGV	O03-C19	5.46	1.49	1.33
26	C	270	CDL	OA8-CA7	5.44	1.49	1.33
20	N	1524	PGV	O03-C19	5.43	1.49	1.33
26	C	270	CDL	OB8-CB7	5.34	1.48	1.33
25	P	1265	PEK	O01-C1	5.32	1.49	1.34
19	O	1521	TGL	OG2-CB1	5.31	1.49	1.34
19	Q	1523	TGL	OG1-CA1	5.30	1.48	1.33
26	T	1269	CDL	OA6-CA5	5.29	1.49	1.34
19	Q	1523	TGL	OG2-CB1	5.29	1.49	1.34
22	R	1229	PSC	O01-C1	5.28	1.49	1.34
26	P	1270	CDL	OA8-CA7	5.28	1.48	1.33
19	L	522	TGL	OG1-CA1	5.22	1.48	1.33
19	D	523	TGL	OG2-CB1	5.20	1.49	1.34
14	A	516	HEA	C11-C3B	5.02	1.57	1.51
26	G	269	CDL	OB8-CB7	4.89	1.47	1.33
19	A	521	TGL	OG1-CA1	4.88	1.47	1.33
19	O	1521	TGL	OG1-CA1	4.88	1.47	1.33
26	P	1270	CDL	OA6-CA5	4.80	1.47	1.34
26	T	1269	CDL	OB6-CB5	4.80	1.47	1.34
26	P	1270	CDL	OB8-CB7	4.75	1.47	1.33
22	B	229	PSC	O01-C1	4.74	1.47	1.34
19	O	1521	TGL	OG3-CC1	4.70	1.47	1.33
22	R	1229	PSC	O03-C19	4.69	1.47	1.33
19	D	523	TGL	OG1-CA1	4.68	1.47	1.33
14	A	515	HEA	CHA-C1A	4.67	1.47	1.38
14	N	516	HEA	CHC-C4B	4.66	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	521	TGL	OG3-CC1	4.66	1.46	1.33
23	P	1525	CHD	C6-C5	-4.63	1.46	1.53
14	N	516	HEA	CHD-C1D	4.59	1.47	1.38
19	N	1522	TGL	OG3-CC1	4.55	1.46	1.33
19	N	1522	TGL	OG1-CA1	4.55	1.46	1.33
14	A	515	HEA	C1A-C2A	-4.54	1.37	1.45
22	B	229	PSC	O03-C19	4.50	1.46	1.33
19	Q	1523	TGL	OB1-CB1	4.42	1.35	1.22
19	A	521	TGL	OG2-CB1	4.42	1.46	1.34
14	N	515	HEA	CHA-C1A	4.42	1.47	1.38
19	Q	1523	TGL	OG3-CC1	4.40	1.46	1.33
19	L	522	TGL	OG3-CC1	4.39	1.46	1.33
26	T	1269	CDL	OA8-CA7	4.37	1.46	1.33
22	R	1229	PSC	C13-C12	4.33	1.56	1.31
19	L	522	TGL	C20-CA9	-4.31	1.30	1.51
26	T	1269	CDL	OB8-CB7	4.28	1.45	1.33
26	G	269	CDL	OA8-CA7	4.22	1.45	1.33
19	D	523	TGL	OG3-CC1	4.13	1.45	1.33
26	C	270	CDL	OA6-CA5	4.11	1.45	1.34
26	P	1270	CDL	C59-C58	-4.11	1.31	1.51
23	C	525	CHD	C11-C12	-4.10	1.46	1.53
14	A	515	HEA	C4C-NC	-4.09	1.31	1.39
20	N	1266	PGV	O03-C19	4.02	1.45	1.33
25	T	263	PEK	O01-C1	4.00	1.45	1.34
26	C	270	CDL	C59-C58	-3.98	1.32	1.51
23	P	1525	CHD	C10-C5	-3.97	1.49	1.55
20	N	1266	PGV	O01-C1	3.95	1.45	1.34
14	N	515	HEA	C1B-C2B	-3.95	1.36	1.44
14	A	516	HEA	C4A-NA	-3.90	1.32	1.39
26	C	270	CDL	OB6-CB5	3.88	1.45	1.34
26	C	270	CDL	C79-C78	-3.86	1.32	1.51
19	N	1522	TGL	C20-CA9	-3.80	1.32	1.51
26	G	269	CDL	C42-C41	-3.79	1.33	1.51
25	P	1265	PEK	P-O12	3.74	1.74	1.59
20	N	1524	PGV	O01-C1	3.72	1.44	1.34
14	A	516	HEA	CHB-C4A	3.69	1.45	1.38
20	P	1268	PGV	O03-C19	3.66	1.44	1.33
19	L	522	TGL	C10-CB9	-3.66	1.33	1.51
20	C	268	PGV	O03-C19	3.65	1.44	1.33
26	P	1270	CDL	PB2-OB3	3.65	1.63	1.50
26	P	1270	CDL	C62-C61	-3.65	1.33	1.51
23	C	525	CHD	C23-C24	3.62	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515	HEA	FE-NC	3.61	2.07	1.95
20	M	524	PGV	O01-C1	3.61	1.44	1.34
14	N	515	HEA	CHC-C4B	3.61	1.45	1.38
14	N	515	HEA	C1A-C2A	-3.60	1.38	1.45
19	O	1521	TGL	C10-CB9	-3.57	1.34	1.51
26	T	1269	CDL	C59-C58	-3.57	1.34	1.51
23	C	525	CHD	C11-C9	3.57	1.59	1.53
22	B	229	PSC	C13-C12	3.57	1.52	1.31
19	N	1522	TGL	C10-CB9	-3.54	1.34	1.51
25	G	265	PEK	P-O12	3.52	1.73	1.59
20	A	522	PGV	C01-C02	3.52	1.61	1.50
26	P	1270	CDL	C79-C78	-3.50	1.34	1.51
26	P	1270	CDL	C82-C81	-3.49	1.34	1.51
19	O	1521	TGL	C20-CA9	-3.48	1.34	1.51
14	A	515	HEA	FE-NB	3.47	2.05	1.94
26	G	269	CDL	C59-C58	-3.47	1.34	1.51
26	P	1270	CDL	C19-C18	-3.47	1.34	1.51
19	D	523	TGL	C20-CA9	-3.47	1.34	1.51
19	A	521	TGL	C10-CB9	-3.46	1.34	1.51
14	N	515	HEA	FE-ND	3.45	2.05	1.94
19	A	521	TGL	C20-CA9	-3.43	1.34	1.51
26	C	270	CDL	C62-C61	-3.43	1.34	1.51
26	T	1269	CDL	C79-C78	-3.40	1.34	1.51
26	C	270	CDL	C82-C81	-3.38	1.35	1.51
14	A	516	HEA	C1D-ND	-3.37	1.34	1.40
19	L	522	TGL	CC2-CC1	3.35	1.60	1.50
26	C	270	CDL	C19-C18	-3.32	1.35	1.51
26	T	1269	CDL	C42-C41	-3.32	1.35	1.51
23	B	1085	CHD	C8-C7	-3.32	1.47	1.53
14	A	516	HEA	CHD-C1D	3.31	1.45	1.38
23	P	1271	CHD	C20-C17	3.31	1.60	1.54
26	T	1269	CDL	C19-C18	-3.31	1.35	1.51
19	Q	1523	TGL	C10-CB9	-3.30	1.35	1.51
23	P	1525	CHD	O12-C12	3.30	1.49	1.43
26	P	1270	CDL	C22-C21	-3.28	1.35	1.51
23	C	525	CHD	C15-C14	-3.28	1.47	1.54
23	P	1525	CHD	C1-C10	-3.26	1.48	1.54
28	M	526	DMU	C3-C4	-3.26	1.44	1.52
26	G	269	CDL	C19-C18	-3.24	1.35	1.51
26	G	269	CDL	C62-C61	-3.23	1.35	1.51
19	Q	1523	TGL	C15-CC9	-3.23	1.35	1.51
14	N	516	HEA	C16-C15	3.22	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	C79-C78	-3.22	1.35	1.51
14	A	516	HEA	O11-C11	3.22	1.50	1.42
19	D	523	TGL	C15-CC9	-3.21	1.35	1.51
28	Z	1526	DMU	C3-C4	-3.20	1.44	1.52
23	O	229	CHD	C22-C20	3.16	1.62	1.54
26	C	270	CDL	C22-C21	-3.16	1.36	1.51
26	G	269	CDL	C39-C38	-3.15	1.36	1.51
26	G	269	CDL	C22-C21	-3.14	1.36	1.51
23	C	525	CHD	C10-C5	-3.13	1.50	1.55
26	T	1269	CDL	C22-C21	-3.13	1.36	1.51
23	O	229	CHD	C6-C7	-3.10	1.46	1.52
14	A	516	HEA	CHA-C4D	3.10	1.46	1.39
26	P	1270	CDL	C39-C38	-3.09	1.36	1.51
25	C	264	PEK	C2-C1	3.08	1.59	1.50
19	Q	1523	TGL	C20-CA9	-3.08	1.36	1.51
19	N	1522	TGL	CG3-CG2	3.07	1.60	1.50
26	P	1270	CDL	OB6-CB5	3.07	1.42	1.34
26	G	269	CDL	C82-C81	-3.04	1.36	1.51
14	N	516	HEA	FE-NB	3.02	2.04	1.94
23	B	1085	CHD	O12-C12	3.01	1.48	1.43
23	B	1085	CHD	C13-C14	-2.99	1.50	1.55
26	T	1269	CDL	C62-C61	-2.99	1.36	1.51
14	A	515	HEA	C12-C13	2.98	1.63	1.53
20	C	268	PGV	P-O11	2.98	1.71	1.59
26	C	270	CDL	C39-C38	-2.97	1.37	1.51
14	A	515	HEA	C22-C23	2.97	1.41	1.32
14	N	515	HEA	C1C-NC	-2.97	1.34	1.39
20	P	1267	PGV	C01-C02	2.96	1.60	1.50
26	C	270	CDL	PB2-OB3	2.96	1.61	1.50
23	O	229	CHD	O12-C12	2.93	1.48	1.43
26	T	1269	CDL	C39-C38	-2.93	1.37	1.51
23	P	1525	CHD	C10-C9	2.92	1.61	1.56
19	O	1521	TGL	C15-CC9	-2.89	1.37	1.51
28	P	1272	DMU	O1-C10	2.89	1.49	1.41
23	C	525	CHD	C18-C13	2.86	1.58	1.54
25	G	265	PEK	P-O11	2.85	1.70	1.59
26	T	1269	CDL	C82-C81	-2.85	1.37	1.51
26	C	270	CDL	PA1-OA5	2.83	1.70	1.59
14	A	515	HEA	C1D-ND	-2.83	1.35	1.40
14	N	515	HEA	C3B-C2B	2.82	1.41	1.34
23	P	1525	CHD	C11-C9	2.81	1.58	1.53
14	N	516	HEA	C4C-NC	-2.81	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	516	HEA	CHD-C4C	2.80	1.45	1.39
20	A	522	PGV	O01-C1	2.80	1.42	1.34
19	L	522	TGL	C15-CC9	-2.78	1.37	1.51
25	C	264	PEK	O01-C1	2.77	1.42	1.34
26	C	270	CDL	C42-C41	-2.77	1.38	1.51
28	P	1272	DMU	O5-C4	2.77	1.51	1.44
19	N	1522	TGL	C15-CC9	-2.76	1.38	1.51
28	M	526	DMU	C6-C1	-2.74	1.44	1.52
23	P	1525	CHD	C6-C7	-2.73	1.47	1.52
20	A	522	PGV	O01-C02	-2.72	1.40	1.46
14	A	516	HEA	CHA-C1A	2.71	1.43	1.38
25	P	1265	PEK	P-O11	2.70	1.70	1.59
25	G	1263	PEK	C03-C02	2.68	1.59	1.50
23	O	229	CHD	C13-C12	-2.67	1.50	1.54
23	P	1525	CHD	C19-C10	2.67	1.58	1.54
14	N	516	HEA	CHB-C4A	2.66	1.43	1.38
14	A	515	HEA	C12-C11	-2.65	1.48	1.53
28	P	1272	DMU	C2-C1	2.64	1.59	1.52
14	N	516	HEA	CHB-C1B	2.64	1.45	1.39
20	P	1268	PGV	P-O11	2.64	1.69	1.59
25	C	264	PEK	O03-C01	-2.63	1.39	1.45
14	A	515	HEA	C4A-NA	-2.63	1.34	1.39
23	B	1085	CHD	C4-C5	2.62	1.58	1.53
14	A	516	HEA	C3B-C2B	2.61	1.40	1.34
26	C	270	CDL	PB2-OB2	2.61	1.69	1.59
25	P	1264	PEK	C2-C1	2.60	1.58	1.50
20	A	522	PGV	O03-C19	2.58	1.40	1.33
14	N	516	HEA	CHC-C1C	2.58	1.45	1.39
19	A	521	TGL	C15-CC9	-2.58	1.38	1.51
23	O	229	CHD	O7-C7	2.58	1.48	1.43
23	B	1085	CHD	C23-C24	2.57	1.56	1.50
23	O	229	CHD	C13-C14	-2.57	1.51	1.55
28	P	1272	DMU	O5-C6	2.56	1.48	1.41
14	A	515	HEA	O11-C11	2.56	1.48	1.42
23	W	1059	CHD	C20-C17	2.55	1.58	1.54
20	N	1266	PGV	O01-C02	-2.54	1.40	1.46
19	D	523	TGL	C10-CB9	-2.54	1.39	1.51
14	N	516	HEA	C4B-C3B	-2.53	1.40	1.44
23	O	229	CHD	C19-C10	2.52	1.58	1.54
23	B	1085	CHD	C13-C12	-2.51	1.50	1.54
14	N	515	HEA	CHD-C1D	2.51	1.43	1.38
14	N	516	HEA	C1A-NA	-2.50	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	M	526	DMU	O16-C6	2.49	1.44	1.40
23	C	271	CHD	O26-C24	-2.49	1.22	1.30
14	N	516	HEA	CHA-C1A	2.49	1.43	1.38
25	G	1263	PEK	P-O11	2.48	1.69	1.59
23	C	525	CHD	O25-C24	2.47	1.30	1.22
28	Z	1526	DMU	O16-C6	2.46	1.44	1.40
26	P	1270	CDL	C42-C41	-2.45	1.39	1.51
14	N	516	HEA	CMB-C2B	2.45	1.55	1.50
19	N	1522	TGL	OG2-CG2	2.43	1.52	1.46
23	C	271	CHD	C10-C9	-2.41	1.51	1.56
26	G	269	CDL	C17-C16	2.41	1.63	1.51
23	J	60	CHD	C20-C17	2.41	1.58	1.54
28	G	272	DMU	O5-C6	2.41	1.48	1.41
19	N	1522	TGL	OB1-CB1	2.41	1.29	1.22
14	A	516	HEA	C1A-C2A	-2.40	1.41	1.45
14	N	516	HEA	C4D-C3D	-2.39	1.41	1.45
14	N	515	HEA	CHA-C4D	2.38	1.44	1.39
14	A	515	HEA	C21-C22	2.36	1.57	1.50
14	A	515	HEA	C4B-NB	-2.35	1.36	1.40
26	P	1270	CDL	PB2-OB2	2.35	1.68	1.59
14	N	515	HEA	CHD-C4C	2.34	1.44	1.39
14	A	515	HEA	CBD-CGD	2.34	1.56	1.50
25	C	264	PEK	C23-C22	-2.33	1.43	1.52
14	N	515	HEA	C12-C13	2.33	1.60	1.53
14	N	516	HEA	C3B-C2B	2.31	1.40	1.34
14	A	516	HEA	CMB-C2B	2.30	1.55	1.50
14	A	516	HEA	CMA-C3A	2.28	1.50	1.45
23	C	525	CHD	C22-C20	2.27	1.60	1.54
20	N	1524	PGV	C21-C20	2.27	1.60	1.52
28	Z	1526	DMU	O16-C18	2.27	1.49	1.43
23	P	1525	CHD	C13-C12	-2.25	1.51	1.54
14	N	515	HEA	CHC-C1C	2.24	1.44	1.39
23	O	229	CHD	C10-C5	-2.24	1.51	1.55
23	P	1525	CHD	C13-C17	2.23	1.59	1.55
23	O	229	CHD	C4-C5	2.23	1.57	1.53
14	A	515	HEA	CHD-C1D	2.23	1.43	1.38
14	N	515	HEA	C4B-C3B	-2.23	1.40	1.44
20	C	268	PGV	O04-C19	-2.22	1.15	1.22
23	J	60	CHD	C11-C9	2.22	1.57	1.53
25	P	1265	PEK	C22-C21	2.21	1.57	1.50
26	P	1270	CDL	PA1-OA5	2.20	1.68	1.59
23	B	1085	CHD	C21-C20	2.20	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	1266	PGV	C04-C05	2.19	1.58	1.51
23	P	1525	CHD	O7-C7	2.18	1.47	1.43
28	P	1272	DMU	O7-C10	2.18	1.47	1.41
23	B	1085	CHD	C4-C3	2.18	1.55	1.52
14	N	516	HEA	O11-C11	2.17	1.47	1.42
25	P	1264	PEK	O03-C21	2.17	1.39	1.33
20	N	1266	PGV	C01-C02	2.17	1.57	1.50
14	A	515	HEA	CHC-C1C	2.17	1.44	1.39
14	A	516	HEA	CBD-CGD	2.16	1.55	1.50
28	G	272	DMU	O1-C10	2.16	1.47	1.41
28	G	272	DMU	C3-C4	-2.16	1.47	1.52
28	Z	1526	DMU	C2-C1	2.16	1.57	1.52
14	N	515	HEA	C4D-ND	-2.15	1.34	1.38
23	O	229	CHD	C1-C2	-2.15	1.49	1.53
20	P	1267	PGV	O05-C05	2.14	1.49	1.43
23	P	1525	CHD	C16-C17	2.14	1.58	1.54
23	P	1525	CHD	C21-C20	2.14	1.58	1.53
14	N	515	HEA	CMA-C3A	2.13	1.50	1.45
28	G	272	DMU	O7-C10	2.13	1.47	1.41
14	N	515	HEA	O11-C11	2.12	1.47	1.42
14	N	515	HEA	FE-NC	2.11	2.02	1.95
14	N	516	HEA	O2D-CGD	-2.11	1.23	1.30
14	A	516	HEA	C14-C15	2.09	1.37	1.33
14	N	516	HEA	FE-NA	2.09	2.02	1.95
20	C	267	PGV	O01-C02	-2.09	1.41	1.46
14	A	515	HEA	CHA-C4D	2.07	1.43	1.39
14	N	516	HEA	CHA-C4D	2.07	1.43	1.39
28	G	272	DMU	C2-C1	2.06	1.57	1.52
19	N	1522	TGL	CG1-CG2	2.06	1.57	1.50
14	N	515	HEA	CMB-C2B	2.05	1.55	1.50
28	M	526	DMU	C8-C9	-2.03	1.48	1.53
14	A	515	HEA	CAA-C2A	2.02	1.56	1.51
14	N	516	HEA	C3A-C4A	-2.02	1.42	1.46
25	T	263	PEK	C03-C02	2.02	1.57	1.50
25	P	1265	PEK	C03-C02	2.01	1.57	1.50
25	C	264	PEK	P-O14	2.01	1.57	1.50
25	T	263	PEK	C01-C02	2.01	1.57	1.50
23	O	229	CHD	C8-C9	2.00	1.57	1.53
23	B	1085	CHD	C16-C17	2.00	1.58	1.54

All (813) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C6-C5-C10	15.58	129.24	112.66
23	O	229	CHD	C6-C5-C10	15.40	129.05	112.66
23	O	229	CHD	C14-C13-C12	13.96	120.18	107.42
23	B	1085	CHD	C1-C10-C5	13.82	127.58	107.75
23	C	271	CHD	C10-C9-C8	13.42	126.80	111.84
23	P	1525	CHD	C14-C13-C12	12.98	119.28	107.42
23	O	229	CHD	C1-C10-C5	12.85	126.19	107.75
23	P	1525	CHD	C6-C5-C10	12.77	126.25	112.66
23	P	1271	CHD	C10-C9-C8	12.74	126.04	111.84
23	C	525	CHD	C6-C5-C10	12.00	125.43	112.66
25	P	1264	PEK	C2-C3-C4	11.93	139.41	113.35
23	P	1525	CHD	C1-C10-C5	11.87	124.78	107.75
23	B	1085	CHD	C14-C13-C12	11.32	117.76	107.42
23	O	229	CHD	C19-C10-C9	-11.25	96.05	111.18
23	P	1525	CHD	C19-C10-C9	-11.11	96.25	111.18
23	C	525	CHD	C14-C13-C12	11.10	117.56	107.42
23	J	60	CHD	C10-C9-C8	10.85	123.93	111.84
23	O	229	CHD	C18-C13-C12	-10.79	98.26	109.06
23	C	525	CHD	C19-C10-C9	-10.78	96.68	111.18
23	P	1271	CHD	C6-C5-C10	10.67	124.01	112.66
23	W	1059	CHD	C10-C9-C8	10.53	123.57	111.84
23	C	525	CHD	C1-C10-C5	10.33	122.58	107.75
23	P	1271	CHD	C18-C13-C12	-10.03	99.01	109.06
23	P	1525	CHD	C17-C13-C12	9.98	126.64	117.67
23	J	60	CHD	C13-C17-C20	9.87	131.44	119.48
25	C	264	PEK	C2-C3-C4	9.70	134.54	113.35
23	J	60	CHD	C18-C13-C12	-9.51	99.54	109.06
23	B	1085	CHD	C19-C10-C9	-9.35	98.61	111.18
23	C	525	CHD	C4-C3-C2	9.30	121.96	110.62
23	C	271	CHD	C18-C13-C12	-9.27	99.77	109.06
23	B	1085	CHD	C6-C5-C4	-9.24	100.67	111.23
23	B	1085	CHD	C18-C13-C12	-9.11	99.94	109.06
23	W	1059	CHD	C13-C17-C20	9.07	130.48	119.48
23	B	1085	CHD	C18-C13-C17	-9.03	97.06	111.20
14	A	516	HEA	C3C-C4C-NC	9.02	117.39	109.80
23	C	271	CHD	C6-C5-C10	9.02	122.25	112.66
23	W	1059	CHD	C14-C8-C7	9.01	123.81	111.85
23	P	1525	CHD	C15-C14-C13	9.01	112.28	103.54
23	W	1059	CHD	C18-C13-C12	-8.80	100.24	109.06
23	C	271	CHD	C14-C13-C12	8.80	115.46	107.42
28	G	272	DMU	O16-C6-C1	8.79	121.63	108.27
28	M	526	DMU	O1-C10-C5	8.69	128.23	110.37
23	O	229	CHD	C4-C3-C2	8.69	121.22	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C1-C10-C5	8.66	120.18	107.75
23	C	271	CHD	C1-C10-C5	8.65	120.17	107.75
23	P	1525	CHD	C18-C13-C12	-8.60	100.44	109.06
23	P	1271	CHD	C6-C7-C8	8.53	120.82	111.50
19	L	522	TGL	OG3-CC1-OC1	-8.44	102.51	123.63
23	C	271	CHD	C6-C7-C8	8.44	120.71	111.50
23	W	1059	CHD	C14-C13-C12	8.26	114.96	107.42
23	C	271	CHD	O7-C7-C6	-8.19	89.49	109.86
23	J	60	CHD	C14-C13-C12	8.15	114.87	107.42
23	P	1271	CHD	C1-C2-C3	8.07	121.18	110.48
23	J	60	CHD	C14-C8-C7	7.90	122.33	111.85
23	B	1085	CHD	C10-C9-C8	7.74	120.47	111.84
23	J	60	CHD	C6-C7-C8	7.71	119.92	111.50
28	G	272	DMU	O1-C9-C8	7.70	123.57	109.70
28	Z	1526	DMU	O1-C9-C8	7.69	123.56	109.70
23	C	271	CHD	C11-C9-C8	7.69	122.27	110.89
23	P	1525	CHD	C4-C3-C2	7.67	119.98	110.62
23	C	271	CHD	C4-C3-C2	7.63	119.93	110.62
23	W	1059	CHD	C1-C2-C3	7.63	120.59	110.48
23	P	1271	CHD	C16-C17-C20	7.63	123.72	112.18
23	O	229	CHD	C6-C5-C4	-7.61	102.53	111.23
23	C	525	CHD	C18-C13-C17	-7.59	99.31	111.20
23	W	1059	CHD	C6-C7-C8	7.58	119.78	111.50
23	C	271	CHD	C15-C14-C8	7.53	128.69	118.36
23	B	1085	CHD	C17-C13-C12	7.46	124.38	117.67
23	W	1059	CHD	C15-C14-C13	7.38	110.70	103.54
23	J	60	CHD	C17-C13-C12	7.37	124.30	117.67
23	J	60	CHD	C1-C10-C5	7.35	118.30	107.75
23	W	1059	CHD	C1-C10-C5	7.31	118.25	107.75
23	C	525	CHD	O12-C12-C13	-7.31	98.67	111.02
28	Z	1526	DMU	O1-C10-C5	7.29	125.36	110.37
20	C	268	PGV	O03-C19-C20	7.29	134.07	111.83
23	O	229	CHD	C9-C8-C7	7.24	120.97	111.86
23	W	1059	CHD	C4-C5-C10	7.23	120.35	112.66
23	C	525	CHD	C18-C13-C14	-7.17	99.97	111.20
23	W	1059	CHD	C17-C13-C12	7.16	124.11	117.67
23	P	1271	CHD	C15-C14-C8	7.10	128.10	118.36
23	O	229	CHD	C10-C9-C8	7.08	119.73	111.84
23	J	60	CHD	C1-C2-C3	7.05	119.82	110.48
23	P	1525	CHD	C18-C13-C14	-7.04	100.17	111.20
23	J	60	CHD	C9-C11-C12	6.98	123.43	114.29
28	Z	1526	DMU	O16-C6-C1	6.97	118.85	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	O7-C7-C6	-6.96	92.55	109.86
23	J	60	CHD	C6-C5-C10	6.94	120.05	112.66
28	G	272	DMU	C18-O16-C6	6.93	125.52	113.68
14	A	515	HEA	O11-C11-C12	6.91	127.47	109.14
26	C	270	CDL	CB4-OB6-CB5	-6.89	101.30	117.80
28	Z	1526	DMU	O5-C6-C1	6.89	124.53	110.37
23	C	525	CHD	C17-C13-C12	6.89	123.87	117.67
23	C	271	CHD	C19-C10-C9	-6.89	101.92	111.18
26	P	1270	CDL	CB4-OB6-CB5	-6.88	101.32	117.80
28	G	272	DMU	O5-C4-C57	6.86	123.45	106.44
23	C	271	CHD	C16-C17-C20	6.83	122.51	112.18
23	C	271	CHD	C15-C14-C13	6.79	110.13	103.54
23	W	1059	CHD	C16-C17-C13	6.76	110.10	103.54
23	W	1059	CHD	C4-C3-C2	6.72	118.82	110.62
23	J	60	CHD	C4-C3-C2	6.68	118.77	110.62
23	P	1271	CHD	C23-C22-C20	-6.63	102.07	114.46
23	J	60	CHD	C16-C17-C13	6.61	109.95	103.54
28	M	526	DMU	O1-C9-C8	6.58	121.55	109.70
23	P	1271	CHD	C5-C4-C3	6.57	122.62	112.71
23	W	1059	CHD	C9-C10-C5	6.54	117.60	108.51
23	P	1525	CHD	C23-C22-C20	-6.52	102.27	114.46
23	P	1271	CHD	C17-C13-C12	6.51	123.52	117.67
26	P	1270	CDL	OA6-CA5-C11	6.51	125.56	111.48
23	B	1085	CHD	C4-C3-C2	6.50	118.55	110.62
23	C	525	CHD	C15-C14-C13	6.49	109.83	103.54
23	J	60	CHD	C15-C14-C13	6.47	109.82	103.54
26	T	1269	CDL	OB6-CB5-C51	6.47	125.48	111.48
28	G	272	DMU	O1-C10-C5	6.44	123.59	110.37
19	D	523	TGL	OG2-CB1-CB2	-6.38	97.67	111.48
23	J	60	CHD	C5-C4-C3	6.38	122.33	112.71
23	B	1085	CHD	C17-C13-C14	6.34	106.48	100.11
23	P	1271	CHD	C14-C13-C12	6.31	113.19	107.42
14	A	516	HEA	CHA-C4D-C3D	-6.28	115.61	124.77
28	M	526	DMU	O5-C4-C57	6.28	122.01	106.44
23	P	1271	CHD	C11-C9-C8	6.28	120.18	110.89
26	C	270	CDL	OA6-CA5-C11	6.26	125.02	111.48
28	M	526	DMU	O16-C6-C1	6.24	117.75	108.27
19	O	1521	TGL	OG2-CB1-CB2	6.23	124.97	111.48
23	C	271	CHD	C16-C17-C13	6.22	109.58	103.54
23	W	1059	CHD	C5-C6-C7	6.22	121.80	114.40
28	P	1272	DMU	O1-C9-C8	6.21	120.88	109.70
23	J	60	CHD	C5-C6-C7	6.19	121.76	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C23-C22-C20	-6.18	102.91	114.46
14	A	515	HEA	O11-C11-C3B	-6.17	99.95	111.26
25	G	265	PEK	O03-C21-C22	6.16	130.62	111.83
26	G	269	CDL	OA6-CA5-C11	6.16	124.80	111.48
23	C	525	CHD	C22-C20-C17	-6.13	97.61	110.33
23	C	271	CHD	C1-C2-C3	6.12	118.59	110.48
23	W	1059	CHD	C6-C5-C10	6.12	119.17	112.66
23	O	229	CHD	C15-C14-C13	6.09	109.44	103.54
28	P	1272	DMU	O1-C9-C11	6.09	121.52	106.44
28	M	526	DMU	C6-O5-C4	6.08	125.60	113.72
28	P	1272	DMU	C8-C7-C5	6.08	121.51	110.83
19	A	521	TGL	CG2-OG2-CB1	6.06	132.31	117.80
28	P	1272	DMU	O1-C10-C5	6.05	122.81	110.37
28	P	1272	DMU	O5-C4-C3	6.05	122.22	109.72
23	B	1085	CHD	O12-C12-C13	-6.05	100.81	111.02
23	P	1271	CHD	C11-C12-C13	6.03	117.40	111.26
23	P	1525	CHD	C11-C9-C10	6.03	119.82	113.70
23	W	1059	CHD	C11-C12-C13	6.01	117.38	111.26
19	N	1522	TGL	CG2-OG2-CB1	6.01	132.17	117.80
23	C	525	CHD	C10-C9-C8	6.00	118.53	111.84
23	O	229	CHD	C18-C13-C14	-5.94	101.89	111.20
19	O	1521	TGL	CG2-OG2-CB1	5.93	132.00	117.80
23	W	1059	CHD	C15-C14-C8	5.90	126.45	118.36
23	O	229	CHD	C21-C20-C17	-5.90	104.03	112.88
28	Z	1526	DMU	C8-C7-C5	5.89	121.17	110.83
28	P	1272	DMU	O5-C6-O16	5.87	123.92	110.04
23	W	1059	CHD	C9-C11-C12	5.85	121.95	114.29
14	A	515	HEA	C13-C12-C11	-5.85	105.05	114.39
23	C	525	CHD	C11-C9-C10	5.84	119.63	113.70
23	P	1525	CHD	C5-C4-C3	5.84	121.51	112.71
14	A	516	HEA	C4C-C3C-C2C	-5.82	100.06	107.30
23	J	60	CHD	C11-C12-C13	5.82	117.19	111.26
23	P	1271	CHD	C15-C14-C13	5.82	109.18	103.54
23	O	229	CHD	C1-C2-C3	5.79	118.16	110.48
26	C	270	CDL	OB8-CB7-C71	5.76	129.38	111.83
26	T	1269	CDL	OA6-CA5-C11	5.68	123.77	111.48
23	P	1525	CHD	C18-C13-C17	-5.68	102.31	111.20
23	O	229	CHD	O12-C12-C13	-5.65	101.48	111.02
23	P	1525	CHD	C22-C20-C17	-5.65	98.62	110.33
23	J	60	CHD	C15-C14-C8	5.64	126.10	118.36
23	J	60	CHD	C4-C5-C10	5.64	118.66	112.66
20	P	1268	PGV	O03-C19-C20	5.60	128.90	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Z	1526	DMU	O1-C9-C11	5.58	120.28	106.44
23	P	1271	CHD	C19-C10-C1	-5.57	99.45	108.31
26	P	1270	CDL	OB8-CB7-C71	5.56	128.78	111.83
23	J	60	CHD	C2-C1-C10	5.55	122.11	112.74
14	N	516	HEA	C4C-CHD-C1D	-5.51	113.30	126.25
23	P	1271	CHD	C4-C3-C2	5.50	117.33	110.62
28	M	526	DMU	C8-C7-C5	5.50	120.48	110.83
28	M	526	DMU	C2-C3-C4	5.49	123.11	110.93
19	L	522	TGL	CC3-CC2-CC1	5.49	133.81	113.69
19	L	522	TGL	CG2-OG2-CB1	5.45	130.84	117.80
28	P	1272	DMU	O16-C6-C1	5.45	116.55	108.27
23	P	1525	CHD	O12-C12-C13	-5.44	101.83	111.02
28	P	1272	DMU	O5-C4-C57	5.40	119.83	106.44
23	O	229	CHD	C11-C9-C10	5.40	119.18	113.70
23	C	271	CHD	C5-C4-C3	5.39	120.83	112.71
25	P	1264	PEK	O01-C1-O02	-5.38	111.13	123.70
28	Z	1526	DMU	C2-C3-C4	5.38	122.86	110.93
23	J	60	CHD	C19-C10-C5	-5.38	101.45	110.44
28	G	272	DMU	C2-C3-C4	5.37	122.83	110.93
23	J	60	CHD	C9-C10-C5	5.36	115.96	108.51
23	O	229	CHD	C9-C11-C12	5.35	121.30	114.29
23	C	525	CHD	C17-C13-C14	5.35	105.48	100.11
28	G	272	DMU	C6-O5-C4	5.34	124.14	113.72
23	W	1059	CHD	C5-C4-C3	5.32	120.74	112.71
23	P	1271	CHD	C16-C17-C13	5.32	108.70	103.54
23	W	1059	CHD	C11-C9-C8	5.31	118.75	110.89
23	P	1525	CHD	O3-C3-C4	5.30	120.39	109.84
20	P	1268	PGV	O01-C1-C2	5.29	122.92	111.48
23	P	1271	CHD	O12-C12-C11	-5.28	98.39	109.12
23	O	229	CHD	C17-C13-C14	5.27	105.40	100.11
28	G	272	DMU	C8-C7-C5	5.25	120.05	110.83
23	P	1525	CHD	C10-C9-C8	5.22	117.66	111.84
19	N	1522	TGL	OG3-CC1-OC1	-5.21	110.60	123.63
23	C	271	CHD	C5-C6-C7	5.19	120.57	114.40
28	M	526	DMU	O7-C10-C5	-5.17	95.36	108.09
25	C	264	PEK	O01-C1-O02	-5.15	111.67	123.70
23	P	1271	CHD	C18-C13-C17	-5.13	103.16	111.20
23	O	229	CHD	C17-C13-C12	5.07	122.23	117.67
23	P	1525	CHD	C4-C5-C10	-5.07	107.27	112.66
28	P	1272	DMU	C6-C1-C2	5.06	120.66	110.01
19	L	522	TGL	OG3-CC1-CC2	5.06	127.25	111.83
14	A	516	HEA	C2B-C1B-NB	5.01	115.70	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C5-C4-C3	5.00	120.25	112.71
26	P	1270	CDL	C52-C51-CB5	-5.00	95.38	113.69
14	N	515	HEA	O2A-CGA-CBA	4.99	129.77	114.00
23	W	1059	CHD	C19-C10-C5	-4.99	102.10	110.44
26	T	1269	CDL	OA8-CA7-C31	4.99	127.04	111.83
14	A	516	HEA	C2D-C1D-ND	4.98	115.57	109.84
23	C	525	CHD	C11-C12-C13	4.98	116.33	111.26
28	P	1272	DMU	C18-O16-C6	4.97	122.17	113.68
23	P	1525	CHD	C13-C17-C20	4.96	125.50	119.48
19	Q	1523	TGL	OG1-CG1-CG2	4.96	122.68	108.40
23	W	1059	CHD	C2-C1-C10	4.95	121.10	112.74
14	N	515	HEA	C13-C12-C11	-4.95	106.48	114.39
28	M	526	DMU	O5-C6-C1	4.94	120.53	110.37
28	P	1272	DMU	C6-O5-C4	4.94	123.36	113.72
20	N	1524	PGV	C4-C3-C2	-4.92	95.03	113.13
19	A	521	TGL	OG2-CB1-CB2	4.90	122.08	111.48
20	N	1266	PGV	O01-C1-O02	-4.89	112.27	123.70
14	A	516	HEA	C3D-C4D-ND	4.89	115.08	110.35
25	G	1263	PEK	O01-C1-C2	4.87	122.02	111.48
14	A	516	HEA	C16-C15-C14	-4.87	110.25	121.17
23	C	271	CHD	C17-C13-C12	4.86	122.04	117.67
26	C	270	CDL	C52-C51-CB5	-4.84	95.95	113.69
23	P	1525	CHD	C9-C8-C7	4.84	117.95	111.86
25	P	1265	PEK	O01-C1-C2	4.82	121.92	111.48
23	C	271	CHD	C2-C1-C10	4.82	120.87	112.74
23	P	1271	CHD	C14-C8-C7	4.80	118.22	111.85
28	Z	1526	DMU	O7-C10-C5	-4.78	96.33	108.09
28	Z	1526	DMU	C18-O16-C6	4.75	121.79	113.68
23	C	525	CHD	C9-C8-C7	4.75	117.83	111.86
23	J	60	CHD	C6-C5-C4	-4.73	105.82	111.23
28	P	1272	DMU	O61-C57-C4	4.72	127.39	111.33
25	G	265	PEK	O03-C21-O04	-4.71	111.86	123.63
23	C	271	CHD	C4-C5-C10	4.70	117.67	112.66
23	B	1085	CHD	C4-C5-C10	-4.67	107.69	112.66
28	M	526	DMU	C7-C8-C9	4.65	118.67	110.23
23	C	525	CHD	O3-C3-C4	4.65	119.10	109.84
28	M	526	DMU	O55-C2-C3	4.64	121.83	109.94
23	P	1271	CHD	C17-C13-C14	4.62	104.75	100.11
23	O	229	CHD	C11-C9-C8	4.61	117.71	110.89
28	P	1272	DMU	C1-C2-C3	4.58	120.08	109.68
14	N	516	HEA	C13-C12-C11	-4.58	107.08	114.39
25	P	1265	PEK	O03-C21-C22	4.57	125.78	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C11-C9-C8	4.56	117.64	110.89
28	Z	1526	DMU	O5-C4-C3	4.56	119.15	109.72
19	N	1522	TGL	CB4-CB3-CB2	-4.56	96.37	113.13
23	W	1059	CHD	C16-C17-C20	4.55	119.06	112.18
20	C	268	PGV	O01-C1-C2	4.55	121.32	111.48
23	O	229	CHD	O7-C7-C6	-4.52	98.62	109.86
23	C	525	CHD	C11-C9-C8	4.52	117.58	110.89
23	W	1059	CHD	C22-C20-C17	4.52	119.69	110.33
28	M	526	DMU	O3-C5-C7	4.51	121.01	110.38
25	T	263	PEK	O03-C21-C22	4.49	125.52	111.83
23	C	525	CHD	C9-C11-C12	4.49	120.16	114.29
25	G	1263	PEK	C02-O01-C1	4.48	128.53	117.80
23	J	60	CHD	C13-C14-C8	4.48	120.39	114.72
23	P	1271	CHD	C9-C11-C12	4.46	120.13	114.29
20	A	522	PGV	O01-C1-O02	-4.46	113.28	123.70
14	A	516	HEA	C1D-ND-C4D	-4.45	99.94	105.21
23	P	1525	CHD	C5-C6-C7	4.45	119.69	114.40
14	N	515	HEA	CAA-CBA-CGA	-4.45	101.87	113.67
28	G	272	DMU	O1-C9-C11	4.43	117.43	106.44
23	P	1525	CHD	C6-C5-C4	-4.43	106.17	111.23
14	A	516	HEA	OMA-CMA-C3A	-4.42	115.63	125.62
28	M	526	DMU	O1-C9-C11	4.42	117.39	106.44
23	B	1085	CHD	C9-C8-C7	4.40	117.40	111.86
28	G	272	DMU	O61-C57-C4	4.39	126.28	111.33
23	B	1085	CHD	C11-C9-C10	4.37	118.14	113.70
28	Z	1526	DMU	C6-O5-C4	4.33	122.17	113.72
23	P	1271	CHD	C2-C1-C10	4.32	120.04	112.74
19	D	523	TGL	OG2-CB1-OB1	4.31	133.78	123.70
23	P	1525	CHD	O12-C12-C11	-4.30	100.38	109.12
28	G	272	DMU	O5-C4-C3	4.29	118.58	109.72
14	N	516	HEA	C1C-CHC-C4B	-4.27	116.20	126.25
19	Q	1523	TGL	CG3-CG2-CG1	-4.26	101.85	111.78
19	N	1522	TGL	OG3-CC1-CC2	4.25	124.80	111.83
14	A	515	HEA	CAD-C3D-C4D	4.24	132.09	124.70
23	W	1059	CHD	C6-C5-C4	-4.23	106.39	111.23
23	J	60	CHD	C11-C9-C10	4.23	118.00	113.70
23	C	525	CHD	C13-C17-C20	4.23	124.61	119.48
23	P	1525	CHD	C14-C8-C9	4.23	115.65	109.75
14	A	516	HEA	CHA-C1A-NA	4.22	129.05	124.45
23	J	60	CHD	C22-C20-C17	4.22	119.08	110.33
26	G	269	CDL	OB6-CB5-C51	4.20	120.57	111.48
28	M	526	DMU	C1-C2-C3	4.19	119.19	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C1-C2-C3	4.18	116.02	110.48
23	O	229	CHD	C15-C14-C8	4.17	124.08	118.36
20	P	1268	PGV	C03-C02-C01	-4.17	102.07	111.78
14	A	516	HEA	CHA-C4D-ND	4.16	128.90	124.42
14	N	516	HEA	C3A-C2A-C1A	-4.15	103.12	107.05
14	N	516	HEA	CMC-C2C-C1C	4.15	131.73	125.42
23	W	1059	CHD	C1-C10-C9	-4.14	104.90	111.34
14	N	516	HEA	CHC-C4B-NB	4.14	129.49	124.37
28	G	272	DMU	O7-C3-C2	4.13	117.73	107.23
25	G	265	PEK	O01-C1-C2	4.11	120.38	111.48
28	G	272	DMU	C6-C1-C2	4.11	118.65	110.01
28	P	1272	DMU	C10-O1-C9	4.10	121.72	113.72
14	A	516	HEA	C1A-CHA-C4D	-4.10	117.31	126.02
25	C	264	PEK	C24-C23-C22	-4.10	98.08	113.13
28	Z	1526	DMU	O5-C4-C57	4.09	116.58	106.44
19	L	522	TGL	CA4-CA3-CA2	-4.09	98.09	113.13
14	A	515	HEA	C17-C18-C19	-4.09	118.26	127.62
20	P	1267	PGV	O01-C1-O02	-4.09	114.14	123.70
23	C	525	CHD	C5-C4-C3	4.08	118.86	112.71
23	C	525	CHD	C6-C7-C8	4.08	115.96	111.50
14	A	516	HEA	C17-C18-C19	4.08	136.96	127.62
23	O	229	CHD	C14-C8-C9	4.08	115.44	109.75
23	P	1271	CHD	C4-C5-C10	4.07	116.99	112.66
19	D	523	TGL	OG1-CA1-CA2	4.05	124.19	111.83
28	G	272	DMU	O5-C6-C1	4.04	118.68	110.37
14	A	515	HEA	C2A-C1A-NA	4.03	114.21	110.32
28	G	272	DMU	C7-C8-C9	4.02	117.52	110.23
28	Z	1526	DMU	O3-C5-C7	4.02	119.85	110.38
23	O	229	CHD	C5-C6-C7	4.01	119.17	114.40
14	A	515	HEA	CHD-C1D-ND	-4.01	119.40	124.37
14	A	516	HEA	C4C-NC-C1C	-4.00	99.30	105.82
23	P	1525	CHD	C11-C12-C13	3.99	115.32	111.26
23	C	271	CHD	C17-C13-C14	3.98	104.11	100.11
20	C	267	PGV	C22-C21-C20	-3.97	98.55	113.13
20	N	1524	PGV	O03-C19-C20	3.96	123.90	111.83
23	J	60	CHD	C11-C9-C8	3.96	116.75	110.89
28	M	526	DMU	O49-C1-C2	3.94	119.67	110.38
23	B	1085	CHD	C14-C8-C9	3.94	115.25	109.75
23	B	1085	CHD	C19-C10-C5	-3.94	103.85	110.44
23	C	271	CHD	C11-C12-C13	3.93	115.26	111.26
26	P	1270	CDL	CA4-OA6-CA5	3.92	127.17	117.80
23	J	60	CHD	C16-C17-C20	3.91	118.10	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	C13-C14-C15	-3.90	118.69	127.62
25	C	264	PEK	O03-C01-C02	-3.90	97.17	108.40
23	P	1525	CHD	C9-C11-C12	3.89	119.38	114.29
23	P	1271	CHD	C19-C10-C9	-3.88	105.96	111.18
14	A	516	HEA	O11-C11-C3B	-3.88	104.15	111.26
28	P	1272	DMU	O7-C10-O1	3.88	120.90	110.69
14	N	516	HEA	CHC-C1C-NC	3.87	130.88	123.86
23	C	525	CHD	O7-C7-C8	-3.86	100.67	109.52
14	A	515	HEA	CHA-C4D-C3D	-3.86	119.14	124.77
14	A	516	HEA	CHA-C1A-C2A	-3.86	118.78	124.86
23	C	525	CHD	C6-C5-C4	-3.85	106.82	111.23
23	O	229	CHD	C9-C10-C5	-3.85	103.16	108.51
28	Z	1526	DMU	C57-C4-C3	3.85	124.20	113.38
23	J	60	CHD	C1-C10-C9	-3.83	105.39	111.34
23	B	1085	CHD	C9-C11-C12	3.83	119.31	114.29
25	T	263	PEK	O01-C1-C2	3.83	119.77	111.48
26	G	269	CDL	CB6-CB4-CB3	-3.83	102.86	111.78
23	J	60	CHD	C18-C13-C14	-3.80	105.25	111.20
28	P	1272	DMU	C7-C8-C9	3.79	117.11	110.23
19	L	522	TGL	C26-C25-C24	-3.78	95.24	114.37
23	P	1525	CHD	C2-C1-C10	3.77	119.11	112.74
23	C	525	CHD	O7-C7-C6	-3.77	100.47	109.86
14	A	516	HEA	CHB-C1B-C2B	-3.74	119.12	125.03
26	T	1269	CDL	OA8-CA7-OA9	-3.74	114.28	123.63
20	M	524	PGV	C02-O01-C1	3.74	126.74	117.80
19	N	1522	TGL	OG1-CA1-CA2	3.72	123.19	111.83
14	A	515	HEA	C3D-C4D-ND	3.72	113.95	110.35
25	T	263	PEK	O03-C01-C02	3.72	119.12	108.40
20	C	268	PGV	O04-C19-C20	-3.71	109.26	123.78
14	A	516	HEA	C3B-C4B-NB	3.71	114.10	109.84
20	P	1267	PGV	C27-C26-C25	-3.71	95.63	114.37
22	B	229	PSC	C29-C28-C27	-3.69	95.70	114.37
23	O	229	CHD	C18-C13-C17	-3.69	105.42	111.20
26	G	269	CDL	CB6-OB8-CB7	3.69	130.59	117.12
26	P	1270	CDL	C42-C41-C40	3.67	132.94	114.37
19	O	1521	TGL	CG3-OG3-CC1	3.67	130.53	117.12
19	A	521	TGL	OG2-CG2-CG3	3.63	121.37	108.34
19	Q	1523	TGL	OG3-CC1-CC2	3.60	122.83	111.83
14	N	516	HEA	C3C-C4C-NC	3.60	112.83	109.80
23	P	1525	CHD	O7-C7-C6	-3.60	100.91	109.86
23	C	525	CHD	O26-C24-O25	-3.59	114.09	123.33
25	G	1263	PEK	C2-C3-C4	3.59	121.20	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	522	PGV	O03-C19-O04	-3.58	114.68	123.63
23	B	1085	CHD	C11-C9-C8	3.57	116.17	110.89
23	B	1085	CHD	O26-C24-C23	3.56	125.26	114.00
23	C	271	CHD	O12-C12-C11	-3.56	101.87	109.12
14	A	515	HEA	C2D-C1D-ND	3.55	113.92	109.84
23	B	1085	CHD	O25-C24-C23	-3.55	111.82	123.09
23	W	1059	CHD	C18-C13-C14	-3.55	105.64	111.20
14	N	515	HEA	O2D-CGD-CBD	3.53	125.15	114.00
20	A	522	PGV	C23-C22-C21	-3.53	96.53	114.37
25	T	263	PEK	O01-C1-O02	-3.53	115.46	123.70
28	M	526	DMU	O7-C3-C2	3.52	116.18	107.23
23	W	1059	CHD	C13-C14-C8	3.52	119.18	114.72
26	C	270	CDL	OA6-CA5-OA7	-3.52	115.48	123.70
23	P	1271	CHD	C21-C20-C17	3.52	118.16	112.88
20	N	1266	PGV	O01-C02-C01	-3.51	95.74	108.34
19	A	521	TGL	CG3-OG3-CC1	3.51	129.94	117.12
26	C	270	CDL	C39-C38-C37	3.50	132.08	114.37
14	A	515	HEA	O1A-CGA-CBA	-3.50	111.99	123.09
23	C	525	CHD	C15-C16-C17	3.49	111.98	105.14
26	T	1269	CDL	OA6-CA5-OA7	-3.49	115.55	123.70
19	O	1521	TGL	OG1-CA1-CA2	3.49	122.47	111.83
23	B	1085	CHD	C15-C14-C13	3.49	106.92	103.54
19	O	1521	TGL	OG3-CC1-CC2	3.49	122.46	111.83
28	M	526	DMU	C57-C4-C3	3.48	123.17	113.38
23	W	1059	CHD	O7-C7-C6	-3.48	101.20	109.86
25	C	264	PEK	C03-C02-C01	-3.47	103.69	111.78
23	B	1085	CHD	C6-C7-C8	3.47	115.29	111.50
22	R	1229	PSC	C02-O01-C1	3.47	126.10	117.80
25	P	1265	PEK	O03-C21-O04	-3.46	114.96	123.63
28	G	272	DMU	O7-C10-C5	3.46	116.61	108.09
23	W	1059	CHD	O12-C12-C11	-3.46	102.09	109.12
14	A	516	HEA	C4B-NB-C1B	-3.45	101.12	105.21
14	N	516	HEA	CHC-C4B-C3B	-3.45	117.10	125.80
19	D	523	TGL	CB3-CB2-CB1	3.43	126.27	113.69
25	C	264	PEK	C25-C24-C23	-3.43	97.03	114.37
20	P	1267	PGV	O14-P-O13	3.43	128.38	112.44
28	Z	1526	DMU	C1-C2-C3	3.42	117.45	109.68
25	C	264	PEK	O02-C1-C2	3.42	137.17	123.78
14	N	515	HEA	CHA-C4D-C3D	-3.42	119.79	124.77
14	N	515	HEA	CAD-C3D-C2D	3.41	134.26	127.87
14	N	515	HEA	CHA-C4D-ND	3.41	128.10	124.42
25	P	1264	PEK	O03-C21-C22	-3.40	101.47	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	C25-C23-C24	-3.38	106.80	114.59
14	A	516	HEA	CAD-C3D-C4D	3.38	130.59	124.70
23	C	525	CHD	C19-C10-C5	-3.38	104.80	110.44
14	N	516	HEA	CAA-C2A-C1A	3.37	131.70	124.85
26	G	269	CDL	OB8-CB6-CB4	3.37	118.11	108.40
19	A	521	TGL	OG1-CA1-CA2	3.37	122.10	111.83
22	B	229	PSC	O01-C1-C2	3.36	118.75	111.48
28	Z	1526	DMU	C7-C8-C9	3.35	116.31	110.23
28	G	272	DMU	O7-C3-C4	3.34	118.24	109.48
26	T	1269	CDL	CB6-CB4-CB3	-3.33	104.03	111.78
20	P	1268	PGV	O01-C02-C03	3.32	120.26	108.34
14	N	516	HEA	CAD-C3D-C4D	3.32	130.48	124.70
28	P	1272	DMU	O7-C10-C5	3.32	116.25	108.09
23	C	271	CHD	C23-C22-C20	-3.30	108.30	114.46
26	T	1269	CDL	C83-C82-C81	3.30	131.04	114.37
14	N	516	HEA	CHC-C1C-C2C	-3.29	117.87	127.43
20	M	524	PGV	C8-C9-C10	-3.26	98.17	113.86
28	G	272	DMU	C1-C2-C3	3.26	117.08	109.68
20	N	1524	PGV	O03-C19-O04	-3.25	115.51	123.63
19	N	1522	TGL	CC3-CC2-CC1	3.24	125.58	113.69
14	N	516	HEA	CHA-C4D-C3D	-3.24	120.04	124.77
25	P	1264	PEK	O11-P-O14	-3.24	96.09	108.94
14	N	515	HEA	O2A-CGA-O1A	-3.24	115.01	123.33
23	B	1085	CHD	C15-C14-C8	3.23	122.79	118.36
23	P	1271	CHD	C5-C6-C7	3.23	118.24	114.40
23	C	271	CHD	C11-C9-C10	-3.22	110.43	113.70
20	P	1268	PGV	C02-O01-C1	3.22	125.50	117.80
28	M	526	DMU	C11-C9-C8	3.22	120.92	113.02
19	L	522	TGL	OG1-CA1-CA2	3.21	121.64	111.83
20	M	524	PGV	O01-C1-O02	-3.20	116.23	123.70
23	C	271	CHD	C9-C11-C12	3.20	118.48	114.29
23	B	1085	CHD	C16-C17-C13	3.19	106.64	103.54
20	A	522	PGV	C8-C7-C6	3.18	130.44	114.37
23	O	229	CHD	O12-C12-C11	-3.18	102.65	109.12
19	A	521	TGL	OG3-CC1-CC2	3.18	121.52	111.83
28	M	526	DMU	O7-C10-O1	-3.18	102.34	110.69
14	N	516	HEA	O1A-CGA-CBA	-3.17	113.03	123.09
23	W	1059	CHD	C9-C8-C7	3.15	115.83	111.86
26	P	1270	CDL	OA6-CA5-OA7	-3.15	116.35	123.70
20	A	522	PGV	O03-C19-C20	3.14	121.42	111.83
20	P	1268	PGV	O02-C1-C2	-3.14	111.49	123.78
23	P	1271	CHD	O12-C12-C13	-3.14	105.71	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C14-C8-C9	3.13	114.12	109.75
20	N	1266	PGV	O03-C19-C20	3.13	121.37	111.83
14	A	515	HEA	C4A-C3A-C2A	-3.12	104.11	106.81
19	D	523	TGL	OG1-CA1-OA1	-3.12	115.83	123.63
19	A	521	TGL	C15-CC9-CC8	3.12	130.12	114.37
14	A	515	HEA	C1D-ND-C4D	-3.11	101.52	105.21
26	T	1269	CDL	C80-C79-C78	3.11	130.09	114.37
19	L	522	TGL	C15-CC9-CC8	3.11	130.08	114.37
19	O	1521	TGL	C15-CC9-CC8	3.11	130.07	114.37
14	N	516	HEA	CHD-C4C-NC	3.10	129.49	123.86
14	N	516	HEA	C3B-C4B-NB	3.10	113.40	109.84
20	P	1267	PGV	O03-C19-O04	-3.10	115.87	123.63
26	C	270	CDL	CA6-OA8-CA7	3.09	128.41	117.12
22	R	1229	PSC	O03-C19-C20	3.08	121.23	111.83
26	P	1270	CDL	C39-C38-C37	3.07	129.88	114.37
22	R	1229	PSC	O01-C1-C2	3.07	118.12	111.48
28	G	272	DMU	O4-C7-C5	3.06	117.59	110.38
23	J	60	CHD	C9-C8-C7	3.06	115.71	111.86
19	N	1522	TGL	OG3-CG3-CG2	3.06	117.21	108.40
23	B	1085	CHD	C16-C17-C20	3.06	116.80	112.18
23	P	1525	CHD	C17-C13-C14	3.05	103.17	100.11
28	P	1272	DMU	O4-C7-C5	3.05	117.56	110.38
26	C	270	CDL	O1-C1-CB2	3.04	120.22	109.70
23	P	1525	CHD	C1-C10-C9	-3.04	106.62	111.34
14	N	515	HEA	C13-C14-C15	-3.03	120.69	127.62
14	N	516	HEA	CHB-C4A-NA	3.03	127.75	124.45
25	P	1264	PEK	C25-C24-C23	-3.01	99.13	114.37
20	P	1267	PGV	O03-C01-C02	-3.01	99.72	108.40
25	P	1265	PEK	C35-C34-C33	-3.00	99.19	114.37
14	A	515	HEA	CAD-CBD-CGD	-3.00	105.71	113.67
14	N	515	HEA	C1C-CHC-C4B	-3.00	119.20	126.25
25	G	265	PEK	C24-C23-C22	2.99	124.12	113.13
28	Z	1526	DMU	O61-C57-C4	2.99	121.52	111.33
14	A	516	HEA	C2C-C1C-NC	2.99	114.93	110.14
23	C	525	CHD	C22-C23-C24	-2.99	104.53	112.49
23	C	271	CHD	C18-C13-C17	-2.98	106.53	111.20
25	G	265	PEK	O03-C01-C02	2.97	116.95	108.40
19	D	523	TGL	C21-C20-CA9	2.97	129.36	114.37
28	P	1272	DMU	C2-C3-C4	2.96	117.49	110.93
20	P	1268	PGV	O12-P-O13	-2.96	97.21	108.94
23	O	229	CHD	O3-C3-C4	2.96	115.73	109.84
19	D	523	TGL	C10-CB9-CB8	2.95	129.30	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	516	HEA	CHD-C1D-ND	2.94	128.01	124.37
19	L	522	TGL	OG2-CG2-CG3	2.94	118.89	108.34
19	A	521	TGL	OG3-CC1-OC1	-2.94	116.28	123.63
20	P	1268	PGV	O03-C19-O04	-2.92	116.32	123.63
25	P	1264	PEK	C02-O01-C1	2.91	124.77	117.80
20	M	524	PGV	O01-C02-C01	2.91	118.79	108.34
23	P	1525	CHD	C19-C10-C5	-2.91	105.57	110.44
28	G	272	DMU	C10-O1-C9	2.91	119.40	113.72
25	P	1264	PEK	O02-C1-C2	2.91	135.15	123.78
14	N	515	HEA	O2D-CGD-O1D	-2.90	115.87	123.33
23	P	1525	CHD	C19-C10-C1	2.90	112.91	108.31
23	C	271	CHD	C19-C10-C5	-2.89	105.60	110.44
25	P	1264	PEK	O04-C21-C22	2.89	135.08	123.78
20	N	1266	PGV	O03-C19-O04	-2.89	116.40	123.63
19	D	523	TGL	OG3-CC1-OC1	-2.88	116.42	123.63
23	C	525	CHD	C15-C14-C8	2.88	122.31	118.36
26	P	1270	CDL	OA8-CA7-C31	2.88	120.61	111.83
19	Q	1523	TGL	OG1-CA1-CA2	2.88	120.60	111.83
25	G	1263	PEK	C01-O03-C21	2.87	127.61	117.12
26	C	270	CDL	OB8-CB7-OB9	-2.87	116.45	123.63
14	N	516	HEA	CAD-C3D-C2D	-2.87	122.49	127.87
28	P	1272	DMU	O16-C18-C19	2.86	119.08	109.37
28	M	526	DMU	C6-C1-C2	2.86	116.03	110.01
19	N	1522	TGL	OG2-CG2-CG3	2.86	118.61	108.34
19	Q	1523	TGL	OG3-CC1-OC1	-2.86	116.47	123.63
28	P	1272	DMU	O49-C1-C2	2.86	117.11	110.38
25	P	1265	PEK	O03-C01-C02	2.86	116.63	108.40
19	N	1522	TGL	C26-C25-C24	-2.86	99.93	114.37
14	N	515	HEA	CHC-C1C-C2C	-2.84	119.17	127.43
25	G	1263	PEK	O03-C21-C22	2.84	120.49	111.83
14	N	516	HEA	C1A-CHA-C4D	-2.83	120.00	126.02
26	T	1269	CDL	OB8-CB7-OB9	-2.82	116.57	123.63
26	P	1270	CDL	C55-C54-C53	-2.82	100.10	114.37
14	N	516	HEA	CHA-C1A-C2A	-2.81	120.42	124.86
28	P	1272	DMU	O5-C6-C1	2.81	116.14	110.37
19	O	1521	TGL	OG2-CG2-CG1	2.81	118.42	108.34
26	C	270	CDL	OA6-CA4-CA3	2.80	118.39	108.34
23	B	1085	CHD	C13-C17-C20	2.80	122.87	119.48
14	A	516	HEA	C4A-CHB-C1B	-2.80	120.08	126.02
19	O	1521	TGL	OG2-CG2-CG3	2.79	118.33	108.34
26	P	1270	CDL	OA8-CA7-OA9	-2.78	116.66	123.63
28	Z	1526	DMU	O49-C1-C2	2.78	116.94	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	OA6-CA4-CA6	2.78	118.33	108.34
20	C	268	PGV	O03-C19-O04	-2.78	116.67	123.63
26	C	270	CDL	CB6-OB8-CB7	2.78	127.28	117.12
25	G	265	PEK	O11-P-O14	-2.78	97.92	108.94
23	C	271	CHD	C14-C8-C7	2.78	115.54	111.85
25	P	1264	PEK	O03-C01-C02	-2.77	100.41	108.40
20	M	524	PGV	C4-C3-C2	-2.77	102.95	113.13
14	N	515	HEA	C26-C15-C16	2.76	120.03	115.23
23	P	1271	CHD	O26-C24-O25	2.76	130.43	123.33
14	N	515	HEA	CMB-C2B-C1B	-2.75	120.74	125.03
23	P	1271	CHD	C13-C14-C8	2.74	118.19	114.72
26	C	270	CDL	PA1-OA5-CA3	2.74	137.07	121.35
14	N	515	HEA	C3C-C4C-NC	2.74	112.11	109.80
23	P	1525	CHD	C15-C14-C8	2.74	122.11	118.36
26	C	270	CDL	C40-C39-C38	2.74	128.20	114.37
19	A	521	TGL	OG1-CA1-OA1	-2.73	116.79	123.63
26	G	269	CDL	C83-C82-C81	2.73	128.17	114.37
23	O	229	CHD	C4-C5-C10	-2.73	109.76	112.66
26	C	270	CDL	CA4-OA6-CA5	2.72	124.31	117.80
19	D	523	TGL	CG3-OG3-CC1	2.72	127.05	117.12
26	P	1270	CDL	CB2-C1-CA2	-2.71	104.85	112.65
20	N	1266	PGV	O01-C1-C2	2.70	117.32	111.48
26	T	1269	CDL	C39-C38-C37	2.70	128.00	114.37
23	B	1085	CHD	C16-C15-C14	2.69	110.41	105.14
23	C	525	CHD	O25-C24-C23	2.69	131.63	123.09
26	P	1270	CDL	OB9-CB7-C71	-2.69	113.26	123.78
14	A	516	HEA	C26-C15-C16	2.69	119.89	115.23
26	C	270	CDL	OA8-CA7-C31	2.69	120.03	111.83
14	N	516	HEA	C2A-C1A-NA	2.68	112.91	110.32
20	M	524	PGV	C01-O03-C19	2.68	126.91	117.12
28	G	272	DMU	C10-C5-C7	2.68	115.64	110.01
14	N	516	HEA	CMD-C2D-C1D	2.68	129.22	125.03
26	G	269	CDL	CB4-OB6-CB5	2.67	124.19	117.80
26	C	270	CDL	O1-C1-CA2	-2.67	100.47	109.70
14	A	516	HEA	C4D-C3D-C2D	-2.67	103.01	106.89
23	C	525	CHD	C18-C13-C12	-2.66	106.39	109.06
20	C	267	PGV	C21-C20-C19	-2.66	103.95	113.69
14	N	515	HEA	C1A-CHA-C4D	-2.65	120.38	126.02
23	O	229	CHD	C5-C4-C3	2.65	116.71	112.71
14	N	516	HEA	CHD-C1D-C2D	-2.65	119.42	126.95
14	N	515	HEA	CAD-CBD-CGD	-2.65	106.64	113.67
23	O	229	CHD	C22-C20-C17	-2.64	104.86	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	521	TGL	CB7-CB6-CB5	-2.63	101.05	114.37
19	O	1521	TGL	OB1-CB1-CB2	-2.63	113.48	123.78
26	C	270	CDL	C42-C41-C40	2.63	127.67	114.37
23	P	1525	CHD	C22-C23-C24	-2.63	105.48	112.49
20	P	1267	PGV	C04-C05-C06	-2.62	102.93	111.77
20	C	268	PGV	P-O11-C03	2.62	136.38	121.35
28	Z	1526	DMU	O7-C3-C2	2.62	113.90	107.23
23	B	1085	CHD	C9-C10-C5	-2.62	104.88	108.51
14	N	515	HEA	O11-C11-C3B	-2.62	106.46	111.26
28	M	526	DMU	C31-C28-C25	-2.61	101.15	114.37
23	J	60	CHD	O7-C7-C6	-2.61	103.35	109.86
19	N	1522	TGL	CG3-OG3-CC1	2.61	126.66	117.12
14	N	516	HEA	C13-C14-C15	2.61	133.60	127.62
23	P	1271	CHD	C6-C5-C4	-2.61	108.24	111.23
19	D	523	TGL	OG3-CC1-CC2	2.61	119.79	111.83
26	P	1270	CDL	OA8-CA6-CA4	2.60	115.89	108.40
14	N	515	HEA	O1A-CGA-CBA	-2.60	114.85	123.09
19	Q	1523	TGL	OG2-CG2-CG1	2.59	117.63	108.34
25	G	265	PEK	O13-P-O11	2.58	119.24	107.57
14	N	515	HEA	CHB-C4A-NA	2.57	127.25	124.45
28	P	1272	DMU	O49-C1-C6	-2.57	103.96	110.08
14	N	516	HEA	CBD-CAD-C3D	2.57	119.63	112.53
28	Z	1526	DMU	O7-C10-O1	-2.56	103.95	110.69
28	Z	1526	DMU	O5-C6-O16	2.56	116.10	110.04
20	A	522	PGV	O05-C05-C04	-2.56	100.85	109.70
19	L	522	TGL	CG3-CG2-CG1	-2.55	105.84	111.78
20	C	267	PGV	O01-C1-C2	2.55	116.99	111.48
28	M	526	DMU	O55-C2-C1	2.54	116.36	110.38
14	A	515	HEA	CAA-CBA-CGA	-2.53	106.94	113.67
23	B	1085	CHD	C1-C10-C9	-2.53	107.40	111.34
19	L	522	TGL	CB7-CB6-CB5	-2.53	101.57	114.37
19	N	1522	TGL	OG2-CB1-OB1	2.53	129.61	123.70
23	O	229	CHD	C11-C12-C13	2.52	113.83	111.26
25	C	264	PEK	C27-C26-C25	-2.52	101.62	114.37
20	C	267	PGV	O14-P-O12	2.52	118.98	107.57
26	T	1269	CDL	C82-C81-C80	2.51	127.07	114.37
28	P	1272	DMU	C10-C5-C7	2.50	115.26	110.01
14	N	516	HEA	CHA-C4D-ND	2.49	127.11	124.42
25	P	1265	PEK	C24-C23-C22	2.49	122.28	113.13
23	B	1085	CHD	O12-C12-C11	-2.48	104.07	109.12
28	Z	1526	DMU	C10-C5-C7	2.48	115.22	110.01
20	M	524	PGV	C28-C27-C26	-2.48	101.85	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	1272	DMU	O7-C3-C4	2.47	115.96	109.48
22	R	1229	PSC	C27-C26-C25	-2.47	101.87	114.37
26	P	1270	CDL	C58-C57-C56	-2.47	101.90	114.37
26	C	270	CDL	OB9-CB7-C71	-2.46	114.16	123.78
26	T	1269	CDL	CB6-OB8-CB7	2.46	126.10	117.12
26	G	269	CDL	CB2-C1-CA2	-2.45	105.58	112.65
26	T	1269	CDL	OA6-CA4-CA6	2.45	117.14	108.34
14	N	516	HEA	C4A-C3A-C2A	2.45	108.94	106.81
20	N	1266	PGV	C03-C02-C01	-2.45	106.08	111.78
14	A	515	HEA	C12-C13-C14	2.45	118.59	112.16
23	P	1525	CHD	C15-C16-C17	2.44	109.92	105.14
26	P	1270	CDL	CA6-CA4-CA3	-2.44	106.09	111.78
28	G	272	DMU	O5-C6-O16	2.44	115.81	110.04
14	A	516	HEA	CMB-C2B-C1B	2.44	128.84	125.03
28	G	272	DMU	C11-C9-C8	2.44	119.00	113.02
19	N	1522	TGL	CB3-CB2-CB1	2.43	122.61	113.69
22	R	1229	PSC	C21-C20-C19	-2.43	104.78	113.69
26	G	269	CDL	C23-C22-C21	2.43	126.66	114.37
25	P	1265	PEK	P-O12-C04	2.43	132.82	121.26
28	M	526	DMU	C34-C31-C28	-2.43	102.11	114.37
19	O	1521	TGL	CG1-OG1-CA1	2.43	125.98	117.12
23	B	1085	CHD	C18-C13-C14	-2.42	107.41	111.20
23	P	1271	CHD	C13-C17-C20	2.42	122.41	119.48
19	D	523	TGL	C25-C24-C23	2.41	126.57	114.37
22	R	1229	PSC	C3-C2-C1	2.41	122.53	113.69
26	P	1270	CDL	C80-C79-C78	2.41	126.54	114.37
20	C	267	PGV	O01-C1-O02	-2.41	118.08	123.70
20	N	1266	PGV	C9-C10-C11	2.40	126.05	112.60
14	N	515	HEA	C3B-C4B-NB	2.40	112.60	109.84
19	N	1522	TGL	C15-CC9-CC8	2.40	126.49	114.37
14	N	515	HEA	C4B-C3B-C2B	-2.40	103.41	107.44
14	A	516	HEA	CHD-C1D-ND	-2.40	121.40	124.37
23	C	525	CHD	C2-C1-C10	2.39	116.77	112.74
25	T	263	PEK	C18-C17-C16	-2.39	102.37	113.86
22	B	229	PSC	C3-C2-C1	2.39	122.44	113.69
14	N	515	HEA	CHD-C4C-NC	2.39	128.19	123.86
25	C	264	PEK	C32-C31-C30	-2.38	102.33	114.37
25	P	1265	PEK	C36-C35-C34	2.38	126.38	114.37
19	L	522	TGL	C25-C24-C23	-2.37	102.38	114.37
20	M	524	PGV	O03-C19-C20	2.37	119.05	111.83
28	M	526	DMU	C22-C19-C18	-2.36	103.19	113.47
14	N	516	HEA	C2D-C1D-ND	2.36	112.55	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	1522	TGL	OG1-CG1-CG2	2.35	115.18	108.40
14	N	516	HEA	C1D-ND-C4D	-2.35	102.42	105.21
14	A	515	HEA	OMA-CMA-C3A	-2.34	120.35	125.62
26	G	269	CDL	C80-C79-C78	2.34	126.18	114.37
14	N	516	HEA	C12-C11-C3B	-2.33	108.47	112.12
26	G	269	CDL	CA4-OA6-CA5	2.33	123.37	117.80
20	P	1267	PGV	C22-C21-C20	-2.33	104.58	113.13
23	W	1059	CHD	C19-C10-C9	-2.33	108.05	111.18
14	N	516	HEA	CMC-C2C-C3C	-2.32	121.09	126.55
26	G	269	CDL	OB7-CB5-C51	-2.32	114.71	123.78
25	G	1263	PEK	O03-C01-C02	2.32	115.08	108.40
28	M	526	DMU	O5-C4-C3	2.32	114.52	109.72
14	N	515	HEA	CHC-C4B-NB	2.32	127.23	124.37
19	A	521	TGL	CC3-CC2-CC1	2.32	122.18	113.69
20	N	1524	PGV	O01-C02-C03	2.32	116.65	108.34
26	G	269	CDL	CA6-CA4-CA3	-2.31	106.39	111.78
26	G	269	CDL	OA6-CA5-OA7	-2.31	118.30	123.70
25	C	264	PEK	C01-O03-C21	2.31	125.57	117.12
20	P	1268	PGV	O04-C19-C20	-2.31	114.74	123.78
20	C	267	PGV	O03-C19-O04	-2.31	117.85	123.63
23	J	60	CHD	C19-C10-C1	-2.31	104.64	108.31
26	T	1269	CDL	C40-C39-C38	2.31	126.04	114.37
14	A	516	HEA	CHC-C4B-C3B	-2.31	119.98	125.80
26	C	270	CDL	CB6-CB4-CB3	2.30	117.16	111.78
23	W	1059	CHD	C21-C20-C17	2.30	116.34	112.88
23	C	271	CHD	O12-C12-C13	-2.30	107.13	111.02
19	D	523	TGL	CG2-OG2-CB1	2.30	123.30	117.80
28	P	1272	DMU	O55-C2-C1	2.29	115.78	110.38
25	P	1264	PEK	C24-C23-C22	-2.29	104.70	113.13
19	D	523	TGL	CG3-CG2-CG1	-2.29	106.44	111.78
19	N	1522	TGL	C24-C23-C22	-2.29	102.78	114.37
19	L	522	TGL	C24-C23-C22	-2.29	102.78	114.37
25	P	1264	PEK	C32-C31-C30	-2.29	102.78	114.37
28	M	526	DMU	O4-C7-C5	-2.29	104.98	110.38
25	G	265	PEK	P-O11-C03	2.29	134.46	121.35
14	N	516	HEA	O2D-CGD-CBD	2.29	121.22	114.00
26	T	1269	CDL	C22-C21-C20	2.28	125.92	114.37
14	N	515	HEA	C4C-CHD-C1D	-2.28	120.88	126.25
14	A	515	HEA	C16-C15-C14	-2.28	116.05	121.17
19	N	1522	TGL	CA8-CA7-CA6	-2.28	102.85	114.37
23	C	271	CHD	C21-C20-C22	2.28	113.86	110.34
19	L	522	TGL	CA8-CA7-CA6	-2.28	102.85	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	1270	CDL	OB8-CB7-OB9	-2.27	117.94	123.63
14	N	516	HEA	C21-C20-C19	2.27	120.71	113.19
20	C	267	PGV	C27-C26-C25	-2.27	102.89	114.37
14	N	515	HEA	C24-C23-C22	2.27	129.47	122.66
26	T	1269	CDL	OB6-CB5-OB7	-2.27	118.40	123.70
14	N	515	HEA	CHC-C4B-C3B	-2.27	120.08	125.80
23	P	1271	CHD	C19-C10-C5	-2.26	106.66	110.44
25	C	264	PEK	O13-P-O14	2.26	122.94	112.44
20	P	1267	PGV	C9-C10-C11	-2.25	99.98	112.60
26	T	1269	CDL	C23-C22-C21	2.25	125.74	114.37
20	C	267	PGV	O03-C01-C02	-2.25	101.91	108.40
19	Q	1523	TGL	C24-C23-C22	2.25	125.73	114.37
20	A	522	PGV	C7-C6-C5	-2.25	103.02	114.37
25	T	263	PEK	O04-C21-C22	-2.24	115.00	123.78
20	C	268	PGV	O12-P-O13	-2.24	100.04	108.94
14	N	516	HEA	CAD-CBD-CGD	-2.24	107.72	113.67
26	P	1270	CDL	OA6-CA4-CA3	2.24	116.38	108.34
14	N	516	HEA	CHD-C4C-C3C	-2.24	117.66	127.37
28	Z	1526	DMU	C10-O1-C9	2.24	118.09	113.72
26	G	269	CDL	C42-C41-C40	2.24	125.68	114.37
19	O	1521	TGL	C33-C19-C18	2.24	125.67	114.37
20	N	1524	PGV	O01-C02-C01	2.23	116.36	108.34
20	N	1524	PGV	C5-C4-C3	-2.23	103.11	114.37
26	G	269	CDL	C62-C61-C60	2.23	125.62	114.37
14	A	516	HEA	C26-C15-C14	2.22	129.33	123.63
14	A	515	HEA	O2A-CGA-CBA	2.22	121.00	114.00
26	T	1269	CDL	PA1-OA5-CA3	2.21	134.02	121.35
26	G	269	CDL	OB6-CB4-CB6	2.21	116.27	108.34
14	A	516	HEA	CAA-C2A-C1A	2.21	129.34	124.85
22	B	229	PSC	C32-C31-C30	-2.21	103.21	114.37
20	C	267	PGV	C02-O01-C1	2.21	123.08	117.80
19	L	522	TGL	OA1-CA1-CA2	-2.20	115.16	123.78
19	O	1521	TGL	OG3-CC1-OC1	-2.19	118.14	123.63
19	L	522	TGL	CC4-CC3-CC2	-2.18	105.11	113.13
20	N	1266	PGV	C5-C4-C3	-2.18	103.36	114.37
23	W	1059	CHD	C19-C10-C1	-2.17	104.85	108.31
26	P	1270	CDL	C32-C31-CA7	2.16	121.63	113.69
22	B	229	PSC	C21-C20-C19	-2.16	105.79	113.69
14	N	516	HEA	C26-C15-C16	2.15	118.97	115.23
14	A	515	HEA	CMC-C2C-C1C	2.15	128.70	125.42
26	G	269	CDL	C39-C38-C37	2.14	125.20	114.37
26	G	269	CDL	O1-C1-CB2	2.14	117.09	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	521	TGL	CA3-CA2-CA1	-2.14	105.86	113.69
25	G	1263	PEK	P-O11-C03	2.13	133.58	121.35
20	M	524	PGV	C7-C6-C5	2.13	125.14	114.37
14	A	516	HEA	O2D-CGD-O1D	2.13	128.81	123.33
23	B	1085	CHD	O7-C7-C6	-2.13	104.57	109.86
22	B	229	PSC	C11-C12-C13	-2.12	105.65	123.57
20	C	267	PGV	C31-C30-C29	2.12	125.09	114.37
20	A	522	PGV	O01-C1-C2	2.12	116.07	111.48
19	D	523	TGL	C16-C15-CC9	2.12	125.08	114.37
26	P	1270	CDL	C82-C81-C80	2.12	125.06	114.37
28	Z	1526	DMU	O4-C7-C8	-2.11	105.39	110.38
25	P	1264	PEK	C30-C29-C28	-2.11	103.70	114.37
19	N	1522	TGL	CA5-CA4-CA3	-2.11	103.70	114.37
23	W	1059	CHD	C11-C9-C10	2.11	115.84	113.70
25	C	264	PEK	O04-C21-C22	2.11	132.02	123.78
23	C	271	CHD	C18-C13-C14	-2.11	107.90	111.20
23	O	229	CHD	C15-C16-C17	2.10	109.26	105.14
14	A	515	HEA	CAD-C3D-C2D	-2.10	123.94	127.87
14	A	515	HEA	C4D-C3D-C2D	-2.10	103.84	106.89
22	B	229	PSC	C27-C26-C25	-2.09	103.82	114.37
20	P	1267	PGV	C31-C30-C29	2.08	124.89	114.37
26	T	1269	CDL	C62-C61-C60	2.08	124.89	114.37
20	N	1524	PGV	C26-C25-C24	2.08	124.88	114.37
19	D	523	TGL	CC4-CC3-CC2	-2.08	105.49	113.13
14	A	515	HEA	CHA-C1A-C2A	-2.07	121.59	124.86
20	P	1267	PGV	C02-O01-C1	2.07	122.75	117.80
14	A	516	HEA	C3A-C2A-C1A	-2.07	105.09	107.05
26	P	1270	CDL	CB6-OB8-CB7	2.06	124.67	117.12
28	G	272	DMU	O55-C2-C3	2.06	115.22	109.94
14	N	515	HEA	CAA-C2A-C1A	2.06	129.04	124.85
26	P	1270	CDL	C20-C19-C18	2.06	124.78	114.37
26	T	1269	CDL	C13-C12-C11	2.06	120.69	113.13
20	N	1524	PGV	C01-O03-C19	2.06	124.64	117.12
19	A	521	TGL	OG1-CG1-CG2	-2.06	102.46	108.40
20	A	522	PGV	C8-C9-C10	-2.05	103.98	113.86
28	M	526	DMU	O16-C18-C19	2.05	116.33	109.37
26	G	269	CDL	OA8-CA7-OA9	-2.05	118.51	123.63
20	N	1266	PGV	C30-C29-C28	2.05	124.71	114.37
20	C	267	PGV	C4-C3-C2	-2.05	105.61	113.13
28	Z	1526	DMU	O7-C3-C4	2.04	114.84	109.48
20	P	1267	PGV	C21-C20-C19	-2.04	106.22	113.69
14	A	516	HEA	O1D-CGD-CBD	-2.04	116.62	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	CHC-C1C-NC	2.04	127.56	123.86
25	T	263	PEK	P-O11-C03	2.04	133.02	121.35
22	B	229	PSC	O01-C1-O02	-2.03	118.95	123.70
14	A	516	HEA	C1B-C2B-C3B	-2.03	104.44	106.80
19	Q	1523	TGL	C10-CB9-CB8	2.02	124.58	114.37
26	G	269	CDL	C22-C21-C20	2.02	124.57	114.37
14	A	515	HEA	CBD-CAD-C3D	-2.02	106.95	112.53
14	N	515	HEA	CHC-C1C-NC	2.01	127.51	123.86
25	G	265	PEK	P-O12-C04	2.01	130.85	121.26
23	P	1525	CHD	C21-C20-C17	-2.01	109.86	112.88
28	P	1272	DMU	O3-C5-C10	-2.01	105.28	110.08
14	N	515	HEA	C17-C18-C19	-2.01	123.03	127.62
26	T	1269	CDL	OB5-PB2-OB3	-2.01	100.98	108.94
14	N	515	HEA	CHD-C1D-C2D	-2.00	121.26	126.95

All (26) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	271	CHD	C9
23	J	60	CHD	C9
23	J	60	CHD	C17
23	P	1271	CHD	C9
23	W	1059	CHD	C17
28	G	272	DMU	C5
28	G	272	DMU	C9
28	G	272	DMU	C2
28	G	272	DMU	C4
28	G	272	DMU	C3
28	G	272	DMU	C6
28	M	526	DMU	C9
28	M	526	DMU	C2
28	M	526	DMU	C4
28	M	526	DMU	C5
28	P	1272	DMU	C5
28	P	1272	DMU	C9
28	P	1272	DMU	C2
28	P	1272	DMU	C4
28	P	1272	DMU	C6
28	P	1272	DMU	C10
28	Z	1526	DMU	C6
28	Z	1526	DMU	C5
28	Z	1526	DMU	C9

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Mol	Chain	Res	Type	Atom
28	Z	1526	DMU	C2
28	Z	1526	DMU	C4

All (970) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	C	267	PGV	C10-C11-C12-C13
20	C	268	PGV	O03-C01-C02-O01
20	C	268	PGV	C04-C05-C06-O06
20	C	268	PGV	O02-C1-O01-C02
20	M	524	PGV	C03-O11-P-O12
20	M	524	PGV	C03-O11-P-O14
20	M	524	PGV	C04-O12-P-O11
20	M	524	PGV	C04-O12-P-O13
20	M	524	PGV	C04-O12-P-O14
20	M	524	PGV	C02-C03-O11-P
20	M	524	PGV	O12-C04-C05-C06
20	M	524	PGV	O02-C1-O01-C02
20	M	524	PGV	C2-C1-O01-C02
20	N	1524	PGV	C04-O12-P-O11
20	N	1524	PGV	C04-O12-P-O13
20	N	1524	PGV	C04-O12-P-O14
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
20	P	1268	PGV	C03-O11-P-O13
20	P	1268	PGV	C02-C03-O11-P
20	P	1268	PGV	O12-C04-C05-C06
20	P	1268	PGV	C2-C1-O01-C02
22	B	229	PSC	C03-O11-P-O12
22	B	229	PSC	C03-O11-P-O13
22	B	229	PSC	C04-O12-P-O11
22	B	229	PSC	C04-O12-P-O14
22	B	229	PSC	C03-C02-O01-C1
22	B	229	PSC	C10-C11-C12-C13
22	R	1229	PSC	C03-O11-P-O12
22	R	1229	PSC	C03-O11-P-O13
22	R	1229	PSC	C04-O12-P-O11
22	R	1229	PSC	C04-O12-P-O13
22	R	1229	PSC	C03-C02-O01-C1
22	R	1229	PSC	O12-C04-C05-N
22	R	1229	PSC	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
23	J	60	CHD	C16-C17-C20-C21
23	W	1059	CHD	C16-C17-C20-C21
23	W	1059	CHD	C16-C17-C20-C22
25	C	264	PEK	C6-C7-C8-C9
25	C	264	PEK	C12-C13-C14-C15
25	G	265	PEK	C04-O12-P-O11
25	G	265	PEK	C04-O12-P-O13
25	G	1263	PEK	C03-O11-P-O12
25	G	1263	PEK	C03-O11-P-O13
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O03-C01-C02-O01
25	P	1265	PEK	C04-O12-P-O11
25	T	263	PEK	C03-O11-P-O12
25	T	263	PEK	C03-O11-P-O13
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O03-C01-C02-O01
25	T	263	PEK	O12-C04-C05-N
25	T	263	PEK	C11-C10-C9-C8
26	C	270	CDL	CB2-C1-CA2-OA2
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CA3-OA5-PA1-OA2
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	OA7-CA5-OA6-CA4
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB3-OB5-PB2-OB2
26	C	270	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
26	P	1270	CDL	CB2-C1-CA2-OA2
26	P	1270	CDL	CA2-C1-CB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CA3-OA5-PA1-OA2
26	P	1270	CDL	CA3-OA5-PA1-OA3
26	P	1270	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	T	1269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA3-OA5-PA1-OA2
26	T	1269	CDL	CA3-OA5-PA1-OA3
26	T	1269	CDL	CA3-OA5-PA1-OA4
26	T	1269	CDL	C11-CA5-OA6-CA4
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	T	1269	CDL	OB6-CB4-CB6-OB8
28	G	272	DMU	O5-C6-O16-C18
28	Z	1526	DMU	O5-C6-O16-C18
19	D	523	TGL	OC1-CC1-OG3-CG3
19	Q	1523	TGL	OC1-CC1-OG3-CG3
19	Q	1523	TGL	CC2-CC1-OG3-CG3
20	M	524	PGV	O04-C19-O03-C01
23	J	60	CHD	C16-C17-C20-C22
19	A	521	TGL	OB1-CB1-OG2-CG2
20	P	1268	PGV	O02-C1-O01-C02
26	T	1269	CDL	OA7-CA5-OA6-CA4
20	M	524	PGV	C20-C19-O03-C01
20	N	1524	PGV	C20-C19-O03-C01
28	Z	1526	DMU	O6-C11-C9-O1
20	C	268	PGV	C2-C1-O01-C02
26	P	1270	CDL	C51-CB5-OB6-CB4
19	L	522	TGL	OA1-CA1-OG1-CG1
19	N	1522	TGL	OA1-CA1-OG1-CG1
19	D	523	TGL	CC2-CC1-OG3-CG3
19	L	522	TGL	CA2-CA1-OG1-CG1
19	N	1522	TGL	CA2-CA1-OG1-CG1
20	C	268	PGV	C10-C11-C12-C13
20	P	1267	PGV	C10-C11-C12-C13
22	B	229	PSC	C11-C10-C9-C8
25	C	264	PEK	C7-C8-C9-C10
25	G	1263	PEK	C4-C5-C6-C7
25	G	1263	PEK	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	P	1265	PEK	C7-C8-C9-C10
20	N	1524	PGV	O04-C19-O03-C01
19	Q	1523	TGL	CB9-C10-C11-C12
28	Z	1526	DMU	O5-C4-C57-O61
20	P	1268	PGV	O12-C04-C05-O05
22	R	1229	PSC	C20-C19-O03-C01
28	M	526	DMU	O5-C4-C57-O61
19	A	521	TGL	CB2-CB1-OG2-CG2
26	G	269	CDL	C15-C16-C17-C18
20	N	1524	PGV	C19-C20-C21-C22
26	G	269	CDL	C79-C80-C81-C82
19	D	523	TGL	C17-C18-C19-C33
28	M	526	DMU	O6-C11-C9-C8
22	R	1229	PSC	O04-C19-O03-C01
19	Q	1523	TGL	C21-C22-C23-C24
26	T	1269	CDL	C79-C80-C81-C82
28	Z	1526	DMU	C19-C22-C25-C28
26	P	1270	CDL	C62-C63-C64-C65
20	P	1268	PGV	C10-C11-C12-C13
25	C	264	PEK	C10-C11-C12-C13
25	G	265	PEK	C7-C8-C9-C10
25	G	265	PEK	C10-C11-C12-C13
25	G	265	PEK	C13-C14-C15-C16
25	P	1264	PEK	C10-C11-C12-C13
25	P	1264	PEK	C13-C14-C15-C16
25	T	263	PEK	C10-C11-C12-C13
22	R	1229	PSC	C22-C23-C24-C25
26	P	1270	CDL	C82-C83-C84-C85
26	T	1269	CDL	CA7-C31-C32-C33
23	C	271	CHD	C21-C20-C22-C23
28	P	1272	DMU	C28-C31-C34-C37
19	O	1521	TGL	OB1-CB1-OG2-CG2
26	G	269	CDL	CA2-C1-CB2-OB2
22	B	229	PSC	C20-C19-O03-C01
25	T	263	PEK	C22-C21-O03-C01
26	G	269	CDL	C31-CA7-OA8-CA6
19	D	523	TGL	C13-C14-C29-C30
20	M	524	PGV	C4-C5-C6-C7
26	P	1270	CDL	C20-C21-C22-C23
26	P	1270	CDL	C38-C39-C40-C41
26	T	1269	CDL	C22-C23-C24-C25
22	B	229	PSC	C04-C05-N-C06

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C60-C61-C62-C63
28	P	1272	DMU	O6-C11-C9-O1
23	C	271	CHD	C17-C20-C22-C23
28	G	272	DMU	O6-C11-C9-C8
19	D	523	TGL	C20-C21-C22-C23
26	T	1269	CDL	C15-C16-C17-C18
28	P	1272	DMU	C1-C6-O16-C18
19	N	1522	TGL	C17-C18-C19-C33
26	G	269	CDL	C56-C57-C58-C59
22	R	1229	PSC	C1-C2-C3-C4
20	M	524	PGV	O12-C04-C05-O05
26	P	1270	CDL	O1-C1-CB2-OB2
26	G	269	CDL	OA9-CA7-OA8-CA6
28	G	272	DMU	O5-C4-C57-O61
26	G	269	CDL	CA5-C11-C12-C13
26	P	1270	CDL	OB7-CB5-OB6-CB4
26	C	270	CDL	OB5-CB3-CB4-OB6
28	P	1272	DMU	O5-C4-C57-O61
19	N	1522	TGL	CC1-CC2-CC3-CC4
19	L	522	TGL	CC3-CC4-CC5-CC6
19	L	522	TGL	CC1-CC2-CC3-CC4
25	P	1265	PEK	C1-C2-C3-C4
26	G	269	CDL	CA7-C31-C32-C33
19	A	521	TGL	C16-C15-CC9-CC8
19	D	523	TGL	CB9-C10-C11-C12
22	R	1229	PSC	C19-C20-C21-C22
26	C	270	CDL	CB7-C71-C72-C73
26	G	269	CDL	CB5-C51-C52-C53
26	G	269	CDL	CB7-C71-C72-C73
26	T	1269	CDL	CB7-C71-C72-C73
25	G	1263	PEK	C33-C34-C35-C36
22	R	1229	PSC	C04-C05-N-C06
20	P	1268	PGV	C1-C2-C3-C4
22	B	229	PSC	C1-C2-C3-C4
25	G	265	PEK	C1-C2-C3-C4
26	C	270	CDL	C51-CB5-OB6-CB4
19	A	521	TGL	CA1-CA2-CA3-CA4
19	O	1521	TGL	CA1-CA2-CA3-CA4
26	C	270	CDL	CA7-C31-C32-C33
22	B	229	PSC	O04-C19-O03-C01
20	C	268	PGV	C2-C3-C4-C5
26	C	270	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	O1-C1-CB2-OB2
26	P	1270	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CB2-OB2
19	D	523	TGL	CB1-CB2-CB3-CB4
19	Q	1523	TGL	CB1-CB2-CB3-CB4
25	C	264	PEK	C1-C2-C3-C4
26	P	1270	CDL	CB7-C71-C72-C73
25	T	263	PEK	C29-C30-C31-C32
22	R	1229	PSC	C11-C12-C13-C14
25	P	1265	PEK	C4-C5-C6-C7
25	T	263	PEK	O04-C21-O03-C01
25	G	1263	PEK	C22-C21-O03-C01
23	W	1059	CHD	C13-C17-C20-C22
19	N	1522	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	C38-C39-C40-C41
19	Q	1523	TGL	C13-C14-C29-C30
22	B	229	PSC	C04-C05-N-C07
19	N	1522	TGL	CB2-CB1-OG2-CG2
19	O	1521	TGL	CB2-CB1-OG2-CG2
26	C	270	CDL	OB7-CB5-OB6-CB4
20	M	524	PGV	C04-C05-C06-O06
19	D	523	TGL	CG3-CG2-OG2-CB1
19	Q	1523	TGL	CG3-CG2-OG2-CB1
25	G	1263	PEK	O04-C21-O03-C01
26	T	1269	CDL	C37-C38-C39-C40
26	P	1270	CDL	OB5-CB3-CB4-OB6
20	P	1268	PGV	C20-C19-O03-C01
23	J	60	CHD	C13-C17-C20-C21
22	B	229	PSC	C04-C05-N-C08
20	M	524	PGV	C19-C20-C21-C22
23	P	1271	CHD	C21-C20-C22-C23
19	N	1522	TGL	C22-C23-C24-C25
19	Q	1523	TGL	C16-C17-C18-C19
20	C	267	PGV	C7-C8-C9-C10
20	M	524	PGV	C2-C3-C4-C5
26	T	1269	CDL	C61-C62-C63-C64
19	L	522	TGL	C22-C23-C24-C25
19	L	522	TGL	C23-C24-C25-C26
25	G	1263	PEK	C25-C26-C27-C28
25	P	1265	PEK	C29-C30-C31-C32
26	G	269	CDL	C59-C60-C61-C62
28	M	526	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
20	M	524	PGV	C10-C11-C12-C13
25	P	1265	PEK	C10-C11-C12-C13
25	T	263	PEK	C4-C5-C6-C7
22	B	229	PSC	C2-C3-C4-C5
26	P	1270	CDL	C37-C38-C39-C40
26	P	1270	CDL	C77-C78-C79-C80
26	T	1269	CDL	C17-C18-C19-C20
26	C	270	CDL	C31-CA7-OA8-CA6
19	N	1522	TGL	CB5-CB6-CB7-CB8
19	Q	1523	TGL	C12-C13-C14-C29
19	Q	1523	TGL	C17-C18-C19-C33
20	A	522	PGV	C25-C26-C27-C28
20	C	267	PGV	C13-C14-C15-C16
25	P	1264	PEK	C16-C17-C18-C19
26	P	1270	CDL	C35-C36-C37-C38
26	P	1270	CDL	C83-C84-C85-C86
28	Z	1526	DMU	C25-C28-C31-C34
20	C	268	PGV	O05-C05-C06-O06
20	N	1266	PGV	C26-C27-C28-C29
25	T	263	PEK	C31-C32-C33-C34
26	C	270	CDL	C76-C77-C78-C79
26	G	269	CDL	C37-C38-C39-C40
25	G	1263	PEK	C2-C3-C4-C5
23	J	60	CHD	C13-C17-C20-C22
20	C	268	PGV	C22-C23-C24-C25
26	P	1270	CDL	C80-C81-C82-C83
26	G	269	CDL	C51-CB5-OB6-CB4
26	T	1269	CDL	C51-CB5-OB6-CB4
20	P	1267	PGV	C14-C15-C16-C17
25	G	1263	PEK	C16-C17-C18-C19
25	G	1263	PEK	C31-C32-C33-C34
26	C	270	CDL	C43-C44-C45-C46
22	R	1229	PSC	C5-C6-C7-C8
26	C	270	CDL	C53-C54-C55-C56
19	L	522	TGL	CB5-CB6-CB7-CB8
22	B	229	PSC	C24-C25-C26-C27
26	C	270	CDL	C51-C52-C53-C54
26	P	1270	CDL	C16-C17-C18-C19
26	T	1269	CDL	C40-C41-C42-C43
19	O	1521	TGL	CA9-C20-C21-C22
26	G	269	CDL	C19-C20-C21-C22
22	B	229	PSC	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
19	O	1521	TGL	C13-C14-C29-C30
22	R	1229	PSC	C24-C25-C26-C27
26	G	269	CDL	OB7-CB5-OB6-CB4
20	N	1266	PGV	C23-C24-C25-C26
20	P	1267	PGV	C7-C8-C9-C10
19	D	523	TGL	CA5-CA6-CA7-CA8
19	O	1521	TGL	CA2-CA3-CA4-CA5
20	N	1266	PGV	C6-C7-C8-C9
26	C	270	CDL	C11-C12-C13-C14
26	C	270	CDL	C14-C15-C16-C17
26	G	269	CDL	C43-C44-C45-C46
26	G	269	CDL	C52-C53-C54-C55
26	P	1270	CDL	C15-C16-C17-C18
22	R	1229	PSC	C29-C30-C31-C32
19	L	522	TGL	CA3-CA4-CA5-CA6
19	Q	1523	TGL	C15-C16-C17-C18
26	G	269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C73-C74-C75-C76
19	N	1522	TGL	CA5-CA6-CA7-CA8
19	Q	1523	TGL	CC2-CC3-CC4-CC5
22	R	1229	PSC	C2-C3-C4-C5
26	C	270	CDL	C64-C65-C66-C67
19	A	521	TGL	CB7-CB8-CB9-C10
20	C	268	PGV	C3-C4-C5-C6
20	P	1268	PGV	C2-C3-C4-C5
25	C	264	PEK	C2-C3-C4-C5
25	G	1263	PEK	C15-C16-C17-C18
25	P	1265	PEK	C13-C14-C15-C16
19	A	521	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C73-C74-C75-C76
26	P	1270	CDL	C36-C37-C38-C39
23	P	1271	CHD	C20-C22-C23-C24
20	P	1268	PGV	C22-C23-C24-C25
26	G	269	CDL	C35-C36-C37-C38
26	P	1270	CDL	C74-C75-C76-C77
19	D	523	TGL	CB2-CB3-CB4-CB5
19	Q	1523	TGL	C21-C20-CA9-CA8
20	A	522	PGV	C29-C30-C31-C32
20	C	268	PGV	C23-C24-C25-C26
25	C	264	PEK	C26-C27-C28-C29
26	G	269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
19	N	1522	TGL	C15-C16-C17-C18
19	O	1521	TGL	C11-C10-CB9-CB8
20	N	1524	PGV	C22-C23-C24-C25
25	T	263	PEK	C25-C26-C27-C28
19	A	521	TGL	CB3-CB4-CB5-CB6
19	A	521	TGL	CB4-CB5-CB6-CB7
19	D	523	TGL	C21-C20-CA9-CA8
19	L	522	TGL	C21-C20-CA9-CA8
20	C	268	PGV	C28-C29-C30-C31
25	C	264	PEK	C23-C24-C25-C26
25	C	264	PEK	C28-C29-C30-C31
25	T	263	PEK	C30-C31-C32-C33
19	Q	1523	TGL	C23-C24-C25-C26
20	P	1268	PGV	C3-C4-C5-C6
26	P	1270	CDL	C73-C74-C75-C76
19	D	523	TGL	C23-C24-C25-C26
26	C	270	CDL	C81-C82-C83-C84
26	T	1269	CDL	C36-C37-C38-C39
19	D	523	TGL	C16-C15-CC9-CC8
22	B	229	PSC	C2-C1-O01-C02
25	G	265	PEK	C2-C1-O01-C02
25	P	1265	PEK	C2-C1-O01-C02
26	G	269	CDL	C11-CA5-OA6-CA4
19	D	523	TGL	C33-C34-C35-C36
25	P	1264	PEK	C15-C16-C17-C18
19	N	1522	TGL	C25-C26-C27-C28
19	N	1522	TGL	CB3-CB4-CB5-CB6
26	G	269	CDL	C58-C59-C60-C61
26	T	1269	CDL	C57-C58-C59-C60
20	P	1267	PGV	C13-C14-C15-C16
20	P	1268	PGV	C23-C24-C25-C26
20	N	1524	PGV	C23-C24-C25-C26
26	P	1270	CDL	C63-C64-C65-C66
22	R	1229	PSC	C11-C10-C9-C8
25	T	263	PEK	C13-C14-C15-C16
19	L	522	TGL	C18-C19-C33-C34
19	N	1522	TGL	C19-C33-C34-C35
25	G	265	PEK	C25-C26-C27-C28
20	C	268	PGV	C6-C7-C8-C9
20	N	1266	PGV	C5-C6-C7-C8
26	P	1270	CDL	C75-C76-C77-C78
28	G	272	DMU	C28-C31-C34-C37

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Mol	Chain	Res	Type	Atoms
20	P	1268	PGV	O04-C19-O03-C01
26	C	270	CDL	OA9-CA7-OA8-CA6
19	O	1521	TGL	C21-C20-CA9-CA8
19	O	1521	TGL	C12-C13-C14-C29
20	M	524	PGV	C24-C25-C26-C27
19	L	522	TGL	CB2-CB3-CB4-CB5
25	G	265	PEK	O02-C1-O01-C02
20	C	268	PGV	O01-C02-C03-O11
20	P	1268	PGV	O01-C02-C03-O11
26	P	1270	CDL	C78-C79-C80-C81
20	C	267	PGV	C30-C31-C32-C33
26	T	1269	CDL	C58-C59-C60-C61
23	W	1059	CHD	C13-C17-C20-C21
19	D	523	TGL	OG1-CG1-CG2-OG2
25	P	1265	PEK	C15-C16-C17-C18
26	C	270	CDL	C41-C42-C43-C44
25	P	1264	PEK	C25-C26-C27-C28
26	C	270	CDL	C59-C60-C61-C62
26	G	269	CDL	C61-C62-C63-C64
26	T	1269	CDL	C62-C63-C64-C65
20	N	1524	PGV	C5-C6-C7-C8
20	N	1266	PGV	C30-C31-C32-C33
19	N	1522	TGL	CC6-CC7-CC8-CC9
19	O	1521	TGL	CC2-CC3-CC4-CC5
19	Q	1523	TGL	C10-C11-C12-C13
26	C	270	CDL	C36-C37-C38-C39
26	C	270	CDL	C72-C73-C74-C75
26	G	269	CDL	C57-C58-C59-C60
20	C	268	PGV	C30-C31-C32-C33
25	P	1264	PEK	C28-C29-C30-C31
25	P	1265	PEK	O02-C1-O01-C02
25	C	264	PEK	C27-C28-C29-C30
20	C	268	PGV	C20-C19-O03-C01
26	G	269	CDL	C11-C12-C13-C14
26	P	1270	CDL	C58-C59-C60-C61
19	O	1521	TGL	CA5-CA6-CA7-CA8
25	P	1265	PEK	C26-C27-C28-C29
19	D	523	TGL	CC6-CC7-CC8-CC9
25	G	1263	PEK	C30-C31-C32-C33
26	P	1270	CDL	C71-C72-C73-C74
26	T	1269	CDL	C80-C81-C82-C83
19	A	521	TGL	CA5-CA6-CA7-CA8

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C60-C61-C62-C63
19	D	523	TGL	CA3-CA4-CA5-CA6
19	L	522	TGL	C16-C15-CC9-CC8
22	B	229	PSC	C13-C14-C15-C16
19	A	521	TGL	OC1-CC1-OG3-CG3
19	D	523	TGL	CA6-CA7-CA8-CA9
19	Q	1523	TGL	C18-C19-C33-C34
22	B	229	PSC	C26-C27-C28-C29
25	P	1264	PEK	C27-C28-C29-C30
25	G	265	PEK	C01-C02-C03-O11
25	P	1265	PEK	C01-C02-C03-O11
25	T	263	PEK	C01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-CB6
26	P	1270	CDL	OA5-CA3-CA4-CA6
22	B	229	PSC	O02-C1-O01-C02
19	N	1522	TGL	C18-C19-C33-C34
26	C	270	CDL	C21-C22-C23-C24
19	L	522	TGL	C12-C13-C14-C29
19	O	1521	TGL	CB4-CB5-CB6-CB7
19	Q	1523	TGL	CA2-CA1-OG1-CG1
19	A	521	TGL	CB1-CB2-CB3-CB4
19	D	523	TGL	C16-C17-C18-C19
19	D	523	TGL	CC2-CC3-CC4-CC5
26	G	269	CDL	C73-C74-C75-C76
23	C	271	CHD	C20-C22-C23-C24
19	A	521	TGL	C13-C14-C29-C30
19	L	522	TGL	C11-C12-C13-C14
20	M	524	PGV	C3-C4-C5-C6
20	N	1524	PGV	C21-C22-C23-C24
26	T	1269	CDL	C43-C44-C45-C46
19	O	1521	TGL	CC7-CC8-CC9-C15
25	G	265	PEK	C28-C29-C30-C31
25	P	1265	PEK	C22-C21-O03-C01
20	P	1267	PGV	C30-C31-C32-C33
26	T	1269	CDL	C39-C40-C41-C42
19	L	522	TGL	C25-C26-C27-C28
28	G	272	DMU	C1-C6-O16-C18
28	P	1272	DMU	C5-C10-O7-C3
20	A	522	PGV	C10-C11-C12-C13
25	C	264	PEK	C4-C5-C6-C7
25	C	264	PEK	C13-C14-C15-C16
25	P	1264	PEK	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
19	N	1522	TGL	CC3-CC4-CC5-CC6
20	C	268	PGV	O03-C01-C02-C03
20	M	524	PGV	O03-C01-C02-C03
20	N	1524	PGV	O03-C01-C02-C03
25	G	1263	PEK	O03-C01-C02-C03
25	T	263	PEK	O03-C01-C02-C03
26	C	270	CDL	CA3-CA4-CA6-OA8
26	G	269	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CB3-CB4-CB6-OB8
19	O	1521	TGL	C15-C16-C17-C18
20	N	1524	PGV	C7-C8-C9-C10
25	P	1264	PEK	C2-C3-C4-C5
25	T	263	PEK	C2-C3-C4-C5
25	T	263	PEK	C15-C16-C17-C18
19	N	1522	TGL	CC7-CC8-CC9-C15
26	C	270	CDL	C15-C16-C17-C18
26	T	1269	CDL	C32-C33-C34-C35
26	T	1269	CDL	C33-C34-C35-C36
19	L	522	TGL	C11-C10-CB9-CB8
19	O	1521	TGL	CA3-CA4-CA5-CA6
19	O	1521	TGL	CC4-CC5-CC6-CC7
25	G	265	PEK	C29-C30-C31-C32
20	M	524	PGV	C26-C27-C28-C29
26	C	270	CDL	CA5-C11-C12-C13
28	G	272	DMU	C4-C3-O7-C10
26	P	1270	CDL	C53-C54-C55-C56
19	A	521	TGL	CC5-CC6-CC7-CC8
19	Q	1523	TGL	CA6-CA7-CA8-CA9
26	C	270	CDL	C19-C20-C21-C22
19	O	1521	TGL	OC1-CC1-OG3-CG3
19	A	521	TGL	CB6-CB7-CB8-CB9
26	C	270	CDL	C20-C21-C22-C23
25	T	263	PEK	C16-C17-C18-C19
22	B	229	PSC	C5-C6-C7-C8
26	P	1270	CDL	C43-C44-C45-C46
19	A	521	TGL	CG1-CG2-OG2-CB1
20	M	524	PGV	C01-C02-O01-C1
26	G	269	CDL	C41-C42-C43-C44
25	G	265	PEK	C2-C3-C4-C5
19	L	522	TGL	CC4-CC5-CC6-CC7
25	C	264	PEK	C25-C26-C27-C28
14	N	515	HEA	C2A-C3A-CMA-OMA

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C10-C11-C12-C13
25	G	1263	PEK	C13-C14-C15-C16
19	A	521	TGL	CC2-CC1-OG3-CG3
19	O	1521	TGL	CC2-CC1-OG3-CG3
20	P	1268	PGV	C14-C15-C16-C17
19	N	1522	TGL	C20-C21-C22-C23
25	P	1265	PEK	C28-C29-C30-C31
20	P	1267	PGV	C15-C16-C17-C18
19	O	1521	TGL	C11-C12-C13-C14
25	T	263	PEK	C34-C35-C36-C37
26	G	269	CDL	C62-C63-C64-C65
25	P	1264	PEK	C23-C24-C25-C26
26	T	1269	CDL	C72-C73-C74-C75
19	N	1522	TGL	C29-C30-C31-C32
20	C	268	PGV	C15-C16-C17-C18
19	A	521	TGL	C11-C10-CB9-CB8
19	D	523	TGL	CA2-CA3-CA4-CA5
26	C	270	CDL	C74-C75-C76-C77
19	Q	1523	TGL	OG1-CG1-CG2-OG2
20	M	524	PGV	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
20	C	268	PGV	C31-C32-C33-C34
19	A	521	TGL	C16-C17-C18-C19
19	L	522	TGL	CA2-CA3-CA4-CA5
22	R	1229	PSC	C04-C05-N-C08
26	C	270	CDL	C58-C59-C60-C61
26	G	269	CDL	C64-C65-C66-C67
20	C	268	PGV	C11-C10-C9-C8
25	G	265	PEK	C15-C16-C17-C18
20	A	522	PGV	C31-C32-C33-C34
20	C	267	PGV	C31-C32-C33-C34
19	Q	1523	TGL	OA1-CA1-OG1-CG1
25	P	1265	PEK	O04-C21-O03-C01
19	D	523	TGL	CC3-CC4-CC5-CC6
19	L	522	TGL	C21-C22-C23-C24
20	P	1267	PGV	C31-C32-C33-C34
22	B	229	PSC	C31-C32-C33-C34
22	B	229	PSC	C14-C15-C16-C17
26	C	270	CDL	C13-C14-C15-C16
19	N	1522	TGL	CC5-CC6-CC7-CC8
19	Q	1523	TGL	CC3-CC4-CC5-CC6
20	N	1524	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
22	B	229	PSC	C23-C24-C25-C26
26	C	270	CDL	C31-C32-C33-C34
19	D	523	TGL	CA9-C20-C21-C22
25	G	1263	PEK	C34-C35-C36-C37
26	T	1269	CDL	C59-C60-C61-C62
22	B	229	PSC	C21-C22-C23-C24
25	G	265	PEK	C4-C5-C6-C7
25	P	1264	PEK	C4-C5-C6-C7
20	C	268	PGV	C24-C25-C26-C27
19	L	522	TGL	OB1-CB1-OG2-CG2
28	Z	1526	DMU	C19-C18-O16-C6
22	B	229	PSC	C4-C5-C6-C7
26	P	1270	CDL	C79-C80-C81-C82
20	M	524	PGV	C05-C04-O12-P
20	C	268	PGV	O04-C19-O03-C01
26	G	269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C81-C82-C83-C84
19	N	1522	TGL	C12-C13-C14-C29
28	Z	1526	DMU	C34-C37-C40-C43
19	A	521	TGL	C23-C24-C25-C26
20	P	1268	PGV	C13-C14-C15-C16
20	N	1524	PGV	C24-C25-C26-C27
26	C	270	CDL	C22-C23-C24-C25
26	T	1269	CDL	C63-C64-C65-C66
20	C	268	PGV	C01-C02-C03-O11
20	N	1524	PGV	C01-C02-C03-O11
20	P	1268	PGV	C01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-CA6
26	P	1270	CDL	OB5-CB3-CB4-CB6
28	M	526	DMU	C25-C28-C31-C34
26	G	269	CDL	C60-C61-C62-C63
28	G	272	DMU	C34-C37-C40-C43
26	T	1269	CDL	C31-CA7-OA8-CA6
19	Q	1523	TGL	C11-C10-CB9-CB8
28	P	1272	DMU	C22-C25-C28-C31
20	M	524	PGV	C31-C32-C33-C34
28	M	526	DMU	C34-C37-C40-C43
19	N	1522	TGL	OG2-CB1-CB2-CB3
25	G	265	PEK	C24-C25-C26-C27
20	N	1266	PGV	C11-C10-C9-C8
25	P	1265	PEK	C16-C17-C18-C19
19	L	522	TGL	C17-C18-C19-C33

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Mol	Chain	Res	Type	Atoms
19	N	1522	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	OG1-CG1-CG2-CG3
20	C	267	PGV	C15-C16-C17-C18
19	A	521	TGL	CC6-CC7-CC8-CC9
26	P	1270	CDL	C13-C14-C15-C16
26	G	269	CDL	C44-C45-C46-C47
19	Q	1523	TGL	CB5-CB6-CB7-CB8
20	C	268	PGV	C14-C15-C16-C17
26	C	270	CDL	C63-C64-C65-C66
26	G	269	CDL	C71-C72-C73-C74
19	N	1522	TGL	C10-C11-C12-C13
28	P	1272	DMU	C3-C4-C57-O61
20	P	1268	PGV	C15-C16-C17-C18
19	A	521	TGL	CA3-CA4-CA5-CA6
26	P	1270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	CA4-CA3-OA5-PA1
25	G	1263	PEK	C21-C22-C23-C24
20	N	1524	PGV	C28-C29-C30-C31
26	G	269	CDL	C81-C82-C83-C84
25	T	263	PEK	C27-C28-C29-C30
19	L	522	TGL	CC7-CC8-CC9-C15
20	N	1266	PGV	C25-C26-C27-C28
25	P	1265	PEK	C24-C25-C26-C27
25	P	1265	PEK	C33-C34-C35-C36
19	A	521	TGL	CA6-CA7-CA8-CA9
25	P	1264	PEK	C30-C31-C32-C33
20	N	1524	PGV	O03-C01-C02-O01
22	B	229	PSC	C9-C10-C11-C12
22	R	1229	PSC	C9-C10-C11-C12
22	R	1229	PSC	C10-C11-C12-C13
25	C	264	PEK	C11-C10-C9-C8
25	C	264	PEK	C9-C10-C11-C12
25	G	265	PEK	C5-C6-C7-C8
25	G	265	PEK	C11-C10-C9-C8
25	P	1264	PEK	C5-C6-C7-C8
25	P	1264	PEK	C9-C10-C11-C12
25	P	1264	PEK	C12-C13-C14-C15
25	P	1265	PEK	C5-C6-C7-C8
25	T	263	PEK	C5-C6-C7-C8
25	T	263	PEK	C9-C10-C11-C12
25	T	263	PEK	C12-C13-C14-C15
19	L	522	TGL	CC2-CC3-CC4-CC5

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Mol	Chain	Res	Type	Atoms
25	P	1264	PEK	C1-C2-C3-C4
26	P	1270	CDL	C40-C41-C42-C43
20	P	1268	PGV	C4-C5-C6-C7
26	G	269	CDL	C55-C56-C57-C58
19	O	1521	TGL	C14-C29-C30-C31
26	G	269	CDL	C14-C15-C16-C17
19	N	1522	TGL	CB1-CB2-CB3-CB4
28	M	526	DMU	O5-C6-O16-C18
22	B	229	PSC	C27-C28-C29-C30
20	P	1268	PGV	C30-C31-C32-C33
22	R	1229	PSC	C04-C05-N-C07
20	M	524	PGV	C29-C30-C31-C32
28	P	1272	DMU	O6-C11-C9-C8
26	T	1269	CDL	C82-C83-C84-C85
28	M	526	DMU	C22-C25-C28-C31
25	T	263	PEK	C28-C29-C30-C31
19	A	521	TGL	CA2-CA3-CA4-CA5
26	P	1270	CDL	C22-C23-C24-C25
19	N	1522	TGL	C33-C34-C35-C36
19	A	521	TGL	CA4-CA5-CA6-CA7
26	G	269	CDL	C31-C32-C33-C34
20	M	524	PGV	C01-C02-C03-O11
25	G	1263	PEK	C01-C02-C03-O11
20	C	267	PGV	C29-C30-C31-C32
26	C	270	CDL	C1-CA2-OA2-PA1
22	R	1229	PSC	C02-C01-O03-C19
19	D	523	TGL	CB6-CB7-CB8-CB9
19	O	1521	TGL	CA6-CA7-CA8-CA9
19	O	1521	TGL	C16-C17-C18-C19
20	P	1268	PGV	C28-C29-C30-C31
19	A	521	TGL	C18-C19-C33-C34
22	R	1229	PSC	C26-C27-C28-C29
20	P	1267	PGV	C1-C2-C3-C4
19	D	523	TGL	C22-C23-C24-C25
19	L	522	TGL	CB2-CB1-OG2-CG2
25	G	265	PEK	C26-C27-C28-C29
19	N	1522	TGL	OG1-CA1-CA2-CA3
20	N	1266	PGV	C12-C13-C14-C15
26	C	270	CDL	C62-C63-C64-C65
26	T	1269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	C53-C54-C55-C56
25	G	265	PEK	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	OA5-CA3-CA4-OA6
28	Z	1526	DMU	C28-C31-C34-C37
19	D	523	TGL	OG1-CG1-CG2-CG3
26	G	269	CDL	CA3-CA4-CA6-OA8
20	M	524	PGV	C14-C15-C16-C17
28	G	272	DMU	C3-C4-C57-O61
20	C	268	PGV	C9-C10-C11-C12
26	T	1269	CDL	C32-C31-CA7-OA8
22	R	1229	PSC	C27-C28-C29-C30
19	N	1522	TGL	C11-C12-C13-C14
19	N	1522	TGL	OG2-CG2-CG3-OG3
19	Q	1523	TGL	OG2-CG2-CG3-OG3
19	L	522	TGL	CA6-CA7-CA8-CA9
25	P	1265	PEK	C22-C23-C24-C25
20	M	524	PGV	C13-C14-C15-C16
26	P	1270	CDL	C11-C12-C13-C14
22	B	229	PSC	O12-C04-C05-N
19	O	1521	TGL	CC5-CC6-CC7-CC8
25	P	1264	PEK	C24-C25-C26-C27
19	A	521	TGL	CC4-CC5-CC6-CC7
19	D	523	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	CC6-CC7-CC8-CC9
25	C	264	PEK	C33-C34-C35-C36
20	M	524	PGV	O05-C05-C06-O06
19	L	522	TGL	C13-C14-C29-C30
20	A	522	PGV	C5-C6-C7-C8
26	T	1269	CDL	C75-C76-C77-C78
26	T	1269	CDL	C52-C53-C54-C55
26	G	269	CDL	OA5-CA3-CA4-CA6
19	D	523	TGL	CA7-CA8-CA9-C20
26	C	270	CDL	C40-C41-C42-C43
19	N	1522	TGL	CB4-CB5-CB6-CB7
20	A	522	PGV	C7-C8-C9-C10
26	P	1270	CDL	C31-C32-C33-C34
19	O	1521	TGL	C29-C30-C31-C32
20	P	1267	PGV	C02-C03-O11-P
26	P	1270	CDL	C1-CA2-OA2-PA1
26	C	270	CDL	C34-C35-C36-C37
25	G	1263	PEK	O01-C02-C03-O11
25	P	1265	PEK	O01-C02-C03-O11
25	T	263	PEK	O01-C02-C03-O11
26	T	1269	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
14	N	515	HEA	C4A-C3A-CMA-OMA
19	O	1521	TGL	C17-C18-C19-C33
19	D	523	TGL	OG2-CG2-CG3-OG3
26	C	270	CDL	OA6-CA4-CA6-OA8
26	T	1269	CDL	C77-C78-C79-C80
19	N	1522	TGL	CG1-CG2-CG3-OG3
22	B	229	PSC	O03-C01-C02-C03
25	C	264	PEK	C17-C18-C19-C20
26	P	1270	CDL	OB9-CB7-OB8-CB6
26	T	1269	CDL	C24-C25-C26-C27
19	N	1522	TGL	C16-C15-CC9-CC8
19	N	1522	TGL	C21-C20-CA9-CA8
28	G	272	DMU	C19-C22-C25-C28
20	C	268	PGV	C03-O11-P-O13
22	B	229	PSC	C04-O12-P-O13
25	C	264	PEK	O12-C04-C05-N
25	G	265	PEK	C04-O12-P-O14
25	P	1265	PEK	C04-O12-P-O14
26	C	270	CDL	CA3-OA5-PA1-OA3
26	C	270	CDL	CB2-OB2-PB2-OB5
26	G	269	CDL	CA2-OA2-PA1-OA4
26	G	269	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	C24-C25-C26-C27
23	P	1271	CHD	C16-C17-C20-C22
20	C	267	PGV	C02-C03-O11-P
20	C	268	PGV	C02-C03-O11-P
20	C	268	PGV	C05-C04-O12-P
20	N	1524	PGV	C05-C04-O12-P
25	T	263	PEK	C02-C03-O11-P
26	G	269	CDL	CA4-CA3-OA5-PA1
22	B	229	PSC	C15-C16-C17-C18
25	T	263	PEK	C26-C27-C28-C29
19	O	1521	TGL	CB1-CB2-CB3-CB4
19	O	1521	TGL	CG1-CG2-OG2-CB1
19	L	522	TGL	C19-C33-C34-C35
26	C	270	CDL	C71-C72-C73-C74
23	P	1525	CHD	C13-C17-C20-C22
25	G	265	PEK	C22-C23-C24-C25
28	Z	1526	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
25	C	264	PEK	C35-C36-C37-C38
22	R	1229	PSC	C28-C29-C30-C31
26	C	270	CDL	C42-C43-C44-C45
19	L	522	TGL	CA9-C20-C21-C22
20	N	1524	PGV	C9-C10-C11-C12
20	N	1524	PGV	C26-C27-C28-C29
25	T	263	PEK	C32-C33-C34-C35
20	P	1268	PGV	C24-C25-C26-C27
19	L	522	TGL	OG1-CA1-CA2-CA3
19	A	521	TGL	C29-C30-C31-C32
19	D	523	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	C76-C77-C78-C79
26	G	269	CDL	OB9-CB7-OB8-CB6
22	B	229	PSC	C28-C29-C30-C31
14	A	515	HEA	C26-C15-C16-C17
19	N	1522	TGL	C14-C29-C30-C31
14	A	515	HEA	C14-C15-C16-C17
22	R	1229	PSC	C23-C24-C25-C26
20	C	267	PGV	C9-C10-C11-C12
25	G	1263	PEK	C3-C4-C5-C6
28	G	272	DMU	C5-C10-O7-C3
20	N	1266	PGV	C10-C11-C12-C13
20	N	1266	PGV	O03-C19-C20-C21
26	T	1269	CDL	CB5-C51-C52-C53
19	Q	1523	TGL	C29-C30-C31-C32
26	P	1270	CDL	C71-CB7-OB8-CB6
20	P	1268	PGV	C05-C04-O12-P
20	C	268	PGV	C7-C8-C9-C10
26	P	1270	CDL	C72-C73-C74-C75
26	C	270	CDL	C78-C79-C80-C81
20	C	268	PGV	C13-C14-C15-C16
19	D	523	TGL	C12-C13-C14-C29
19	Q	1523	TGL	CA3-CA4-CA5-CA6
22	B	229	PSC	C02-C01-O03-C19
25	P	1264	PEK	C33-C34-C35-C36
26	G	269	CDL	C80-C81-C82-C83
26	P	1270	CDL	C41-C42-C43-C44
28	P	1272	DMU	C31-C34-C37-C40
20	N	1266	PGV	C4-C5-C6-C7
20	C	268	PGV	C25-C26-C27-C28
20	P	1268	PGV	C6-C7-C8-C9
25	G	265	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
28	G	272	DMU	O16-C18-C19-C22
14	A	516	HEA	CAD-CBD-CGD-O1D
26	C	270	CDL	C1-CB2-OB2-PB2
26	P	1270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C51-C52-C53-C54
22	B	229	PSC	C7-C8-C9-C10
25	P	1264	PEK	C3-C4-C5-C6
19	A	521	TGL	C19-C33-C34-C35
20	N	1266	PGV	C31-C32-C33-C34
26	P	1270	CDL	C32-C33-C34-C35
19	Q	1523	TGL	CA9-C20-C21-C22
25	G	1263	PEK	C26-C27-C28-C29
20	P	1267	PGV	C29-C30-C31-C32
20	N	1524	PGV	C03-C02-O01-C1
26	G	269	CDL	CA3-CA4-OA6-CA5
26	G	269	CDL	CA6-CA4-OA6-CA5
20	C	268	PGV	C12-C13-C14-C15
20	N	1266	PGV	C24-C25-C26-C27
23	B	1085	CHD	C22-C23-C24-O25
23	W	1059	CHD	C22-C23-C24-O25
19	A	521	TGL	C15-C16-C17-C18
14	A	516	HEA	CAA-CBA-CGA-O1A
20	P	1267	PGV	C19-C20-C21-C22
19	A	521	TGL	C17-C18-C19-C33
19	D	523	TGL	CA2-CA1-OG1-CG1
25	G	1263	PEK	C02-C03-O11-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
23	O	229	CHD	C22-C23-C24-O26
14	N	516	HEA	C26-C15-C16-C17
28	P	1272	DMU	O16-C18-C19-C22
14	A	515	HEA	CAD-CBD-CGD-O1D
23	O	229	CHD	C22-C23-C24-O25
19	L	522	TGL	C24-C25-C26-C27
20	P	1267	PGV	C9-C10-C11-C12
14	N	516	HEA	CAA-CBA-CGA-O1A
26	C	270	CDL	C39-C40-C41-C42
25	G	1263	PEK	C5-C6-C7-C8
25	G	1263	PEK	C9-C10-C11-C12
25	P	1265	PEK	C6-C7-C8-C9
19	A	521	TGL	C10-C11-C12-C13
20	P	1268	PGV	C11-C10-C9-C8
26	P	1270	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	O	1521	TGL	OG1-CA1-CA2-CA3
22	B	229	PSC	C29-C30-C31-C32
19	N	1522	TGL	CC4-CC5-CC6-CC7
19	N	1522	TGL	CC2-CC3-CC4-CC5
14	A	516	HEA	CAD-CBD-CGD-O2D
23	J	60	CHD	C22-C23-C24-O26
23	W	1059	CHD	C22-C23-C24-O26
20	N	1266	PGV	C29-C30-C31-C32
19	Q	1523	TGL	CA5-CA6-CA7-CA8
19	O	1521	TGL	C10-C11-C12-C13
20	C	268	PGV	C26-C27-C28-C29
25	P	1265	PEK	C2-C3-C4-C5
19	N	1522	TGL	CA9-C20-C21-C22
14	A	516	HEA	C26-C15-C16-C17
23	J	60	CHD	C22-C23-C24-O25
20	P	1267	PGV	C05-C04-O12-P
25	G	265	PEK	C02-C03-O11-P
26	C	270	CDL	C32-C33-C34-C35
26	G	269	CDL	C75-C76-C77-C78
19	D	523	TGL	OA1-CA1-OG1-CG1
19	N	1522	TGL	C21-C22-C23-C24
19	N	1522	TGL	CA4-CA5-CA6-CA7
26	P	1270	CDL	CA3-CA4-CA6-OA8
26	C	270	CDL	C23-C24-C25-C26
26	G	269	CDL	C71-CB7-OB8-CB6
23	O	229	CHD	C21-C20-C22-C23
23	B	1085	CHD	C22-C23-C24-O26
14	A	515	HEA	CAD-CBD-CGD-O2D
14	A	516	HEA	CAA-CBA-CGA-O2A
14	N	516	HEA	CAA-CBA-CGA-O2A
25	T	263	PEK	C3-C4-C5-C6
25	P	1265	PEK	C17-C18-C19-C20
19	D	523	TGL	OG1-CA1-CA2-CA3
20	M	524	PGV	C25-C26-C27-C28
14	N	515	HEA	CAD-CBD-CGD-O1D
14	N	516	HEA	CAD-CBD-CGD-O1D
26	P	1270	CDL	CA5-C11-C12-C13
19	L	522	TGL	OG2-CB1-CB2-CB3
26	G	269	CDL	CB4-CB3-OB5-PB2
26	C	270	CDL	CB4-CB6-OB8-CB7
19	L	522	TGL	C10-C11-C12-C13
14	N	516	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	R	1229	PSC	C12-C13-C14-C15
19	Q	1523	TGL	OG2-CB1-CB2-CB3
20	M	524	PGV	C21-C22-C23-C24
25	P	1265	PEK	C25-C26-C27-C28
22	B	229	PSC	C12-C13-C14-C15
25	P	1264	PEK	C14-C15-C16-C17
25	G	265	PEK	C17-C18-C19-C20
19	A	521	TGL	CB2-CB3-CB4-CB5
25	G	265	PEK	C33-C34-C35-C36
14	N	516	HEA	C2A-C3A-CMA-OMA
28	P	1272	DMU	C34-C37-C40-C43
28	Z	1526	DMU	C18-C19-C22-C25
20	N	1266	PGV	C11-C12-C13-C14
19	Q	1523	TGL	CG1-CG2-CG3-OG3
26	C	270	CDL	CB3-CB4-CB6-OB8
23	P	1525	CHD	C22-C23-C24-O25
19	O	1521	TGL	C19-C33-C34-C35
25	C	264	PEK	O01-C1-C2-C3
19	N	1522	TGL	OA1-CA1-CA2-CA3
20	M	524	PGV	C9-C10-C11-C12
20	N	1266	PGV	C7-C8-C9-C10
26	T	1269	CDL	OB9-CB7-OB8-CB6
26	C	270	CDL	C32-C31-CA7-OA8
25	P	1265	PEK	C3-C4-C5-C6
20	C	267	PGV	C05-C04-O12-P
19	L	522	TGL	CB4-CB5-CB6-CB7
26	C	270	CDL	C12-C11-CA5-OA6
14	N	515	HEA	CAD-CBD-CGD-O2D
20	N	1266	PGV	C9-C10-C11-C12
25	G	1263	PEK	C14-C15-C16-C17
19	D	523	TGL	CB5-CB6-CB7-CB8
19	Q	1523	TGL	C33-C34-C35-C36
26	P	1270	CDL	C23-C24-C25-C26
26	P	1270	CDL	C19-C20-C21-C22
19	D	523	TGL	OG3-CC1-CC2-CC3
19	L	522	TGL	OG3-CC1-CC2-CC3
22	R	1229	PSC	O03-C19-C20-C21
25	P	1264	PEK	O01-C1-C2-C3
19	D	523	TGL	C15-C16-C17-C18
22	B	229	PSC	O03-C19-C20-C21
26	G	269	CDL	O1-C1-CA2-OA2
19	L	522	TGL	CG1-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	CB3-CB4-CB6-OB8
28	P	1272	DMU	O5-C6-O16-C18
19	A	521	TGL	OG1-CA1-CA2-CA3
19	A	521	TGL	OG3-CC1-CC2-CC3
19	Q	1523	TGL	OG3-CC1-CC2-CC3
26	T	1269	CDL	C55-C56-C57-C58
19	A	521	TGL	C24-C25-C26-C27
20	C	268	PGV	C5-C6-C7-C8
26	C	270	CDL	C57-C58-C59-C60
25	G	265	PEK	O04-C21-O03-C01
28	P	1272	DMU	C19-C22-C25-C28
19	D	523	TGL	C21-C22-C23-C24
23	P	1525	CHD	C22-C23-C24-O26
19	Q	1523	TGL	C20-C21-C22-C23
20	A	522	PGV	C26-C27-C28-C29
20	A	522	PGV	O03-C19-C20-C21
26	C	270	CDL	C32-C31-CA7-OA9
25	G	1263	PEK	C22-C23-C24-C25
25	P	1265	PEK	C02-C03-O11-P
23	C	271	CHD	C22-C23-C24-O26
26	P	1270	CDL	C44-C45-C46-C47
26	T	1269	CDL	C32-C31-CA7-OA9
19	A	521	TGL	OC1-CC1-CC2-CC3
19	N	1522	TGL	OB1-CB1-CB2-CB3
25	C	264	PEK	O02-C1-C2-C3
23	C	525	CHD	C22-C23-C24-O25
19	A	521	TGL	OA1-CA1-CA2-CA3
25	P	1264	PEK	O02-C1-C2-C3
20	C	268	PGV	O12-C04-C05-O05
20	C	268	PGV	C4-C5-C6-C7
25	G	1263	PEK	C27-C28-C29-C30
25	G	1263	PEK	C28-C29-C30-C31
26	T	1269	CDL	C71-CB7-OB8-CB6
19	N	1522	TGL	C23-C24-C25-C26
19	A	521	TGL	CC3-CC4-CC5-CC6
26	P	1270	CDL	OB6-CB4-CB6-OB8
23	C	271	CHD	C16-C17-C20-C22
19	L	522	TGL	OC1-CC1-CC2-CC3
19	D	523	TGL	CG1-CG2-CG3-OG3
14	N	515	HEA	CAA-CBA-CGA-O1A
25	P	1265	PEK	O01-C1-C2-C3
19	Q	1523	TGL	OC1-CC1-CC2-CC3

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Mol	Chain	Res	Type	Atoms
19	A	521	TGL	C25-C26-C27-C28
23	P	1525	CHD	C13-C17-C20-C21
19	D	523	TGL	OC1-CC1-CC2-CC3
22	B	229	PSC	O04-C19-C20-C21
20	C	267	PGV	C1-C2-C3-C4
19	Q	1523	TGL	OG1-CA1-CA2-CA3
20	M	524	PGV	O03-C19-C20-C21
14	A	515	HEA	CAA-CBA-CGA-O2A
25	P	1265	PEK	O02-C1-C2-C3
25	G	265	PEK	O01-C1-C2-C3

There are no ring outliers.

38 monomers are involved in 361 short contacts:

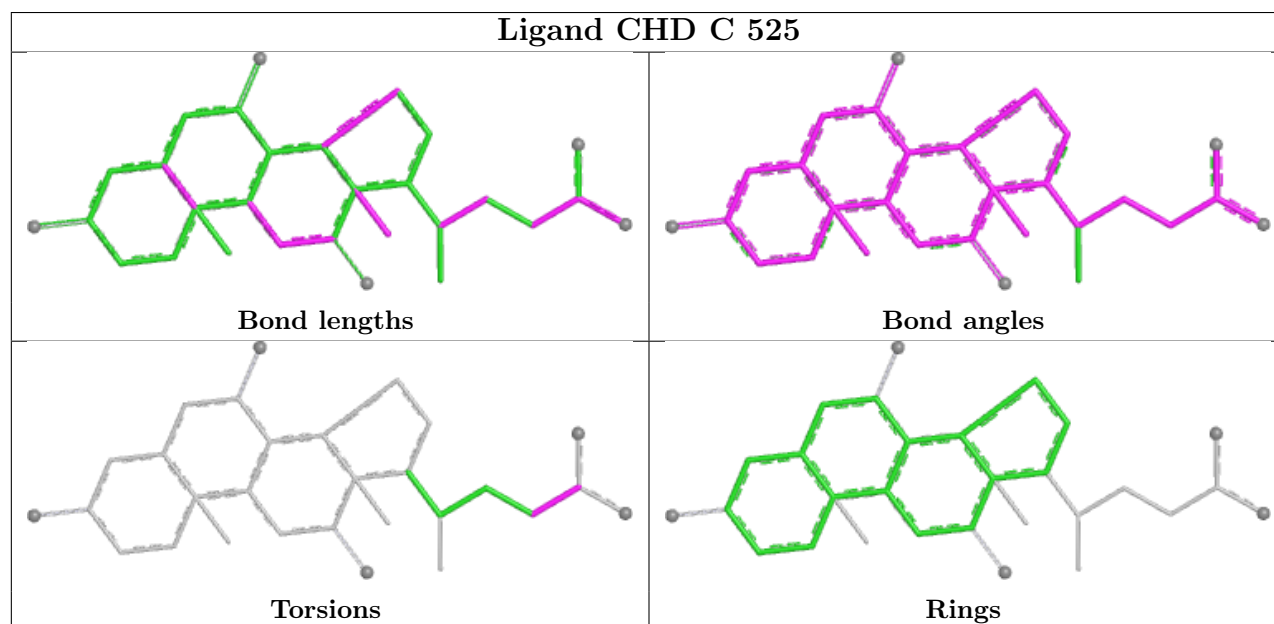
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	O	229	CHD	3	0
25	T	263	PEK	21	0
28	P	1272	DMU	6	0
23	C	271	CHD	4	0
20	N	1524	PGV	8	0
20	C	268	PGV	3	0
20	N	1266	PGV	1	0
23	W	1059	CHD	1	0
26	G	269	CDL	30	0
26	P	1270	CDL	25	0
23	B	1085	CHD	2	0
14	A	515	HEA	4	0
25	G	1263	PEK	24	0
19	N	1522	TGL	15	0
25	P	1264	PEK	7	0
23	J	60	CHD	1	0
20	P	1268	PGV	1	0
19	O	1521	TGL	10	0
14	A	516	HEA	2	0
26	C	270	CDL	25	0
28	G	272	DMU	4	0
19	L	522	TGL	15	0
20	M	524	PGV	15	0
23	P	1271	CHD	5	0
28	Z	1526	DMU	2	0
25	C	264	PEK	8	0
26	T	1269	CDL	27	0

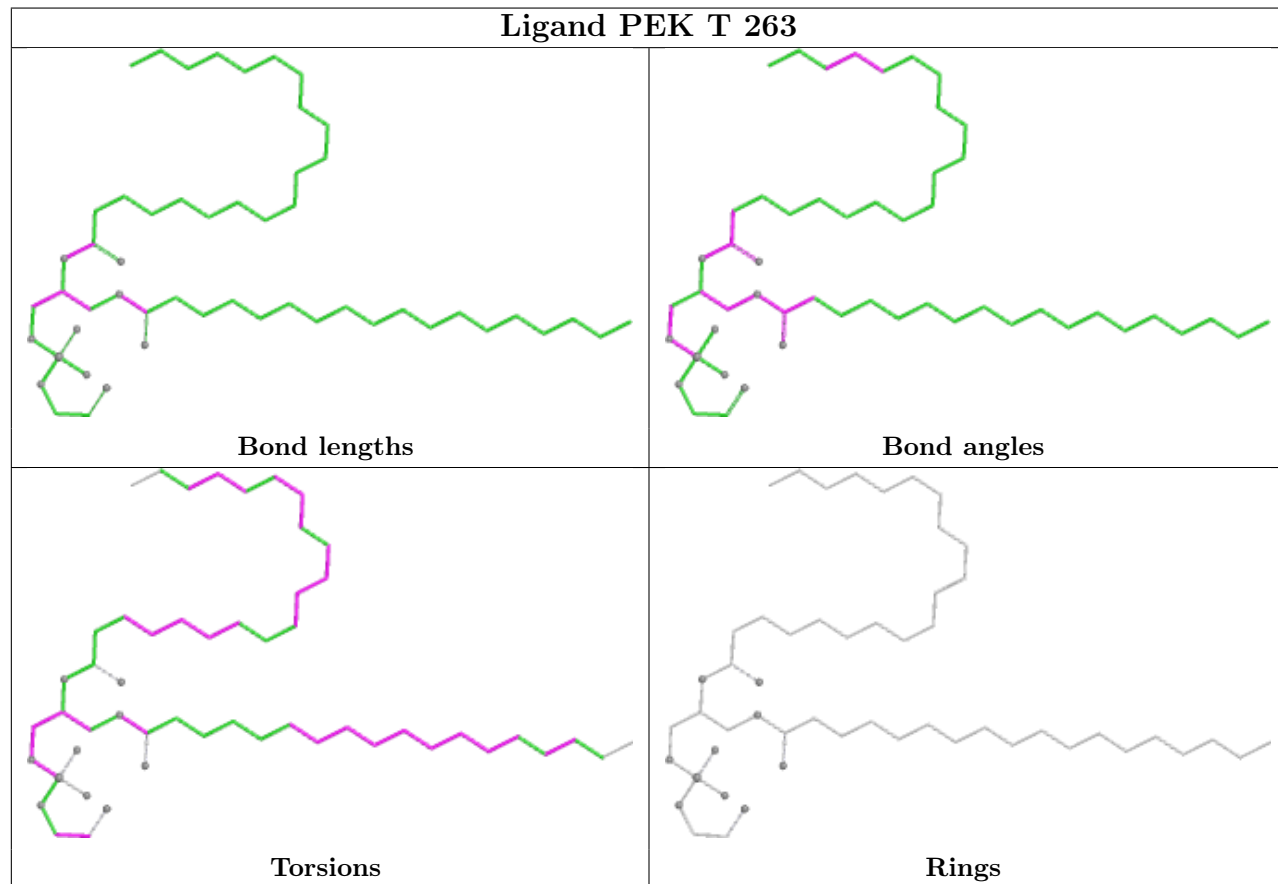
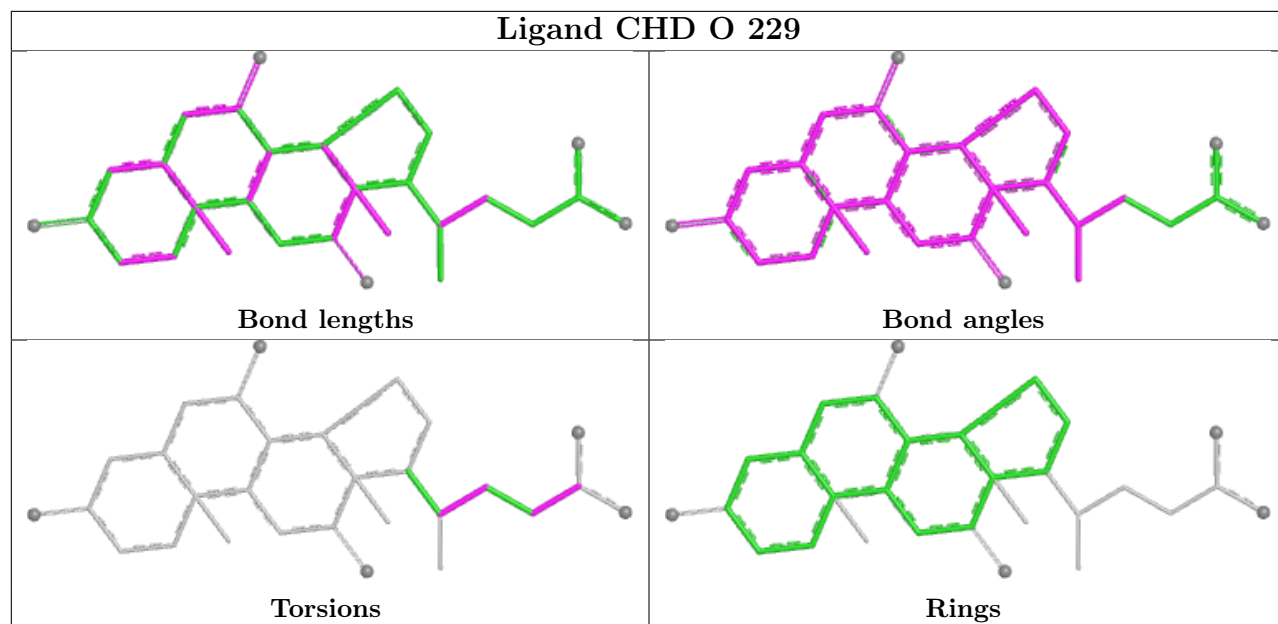
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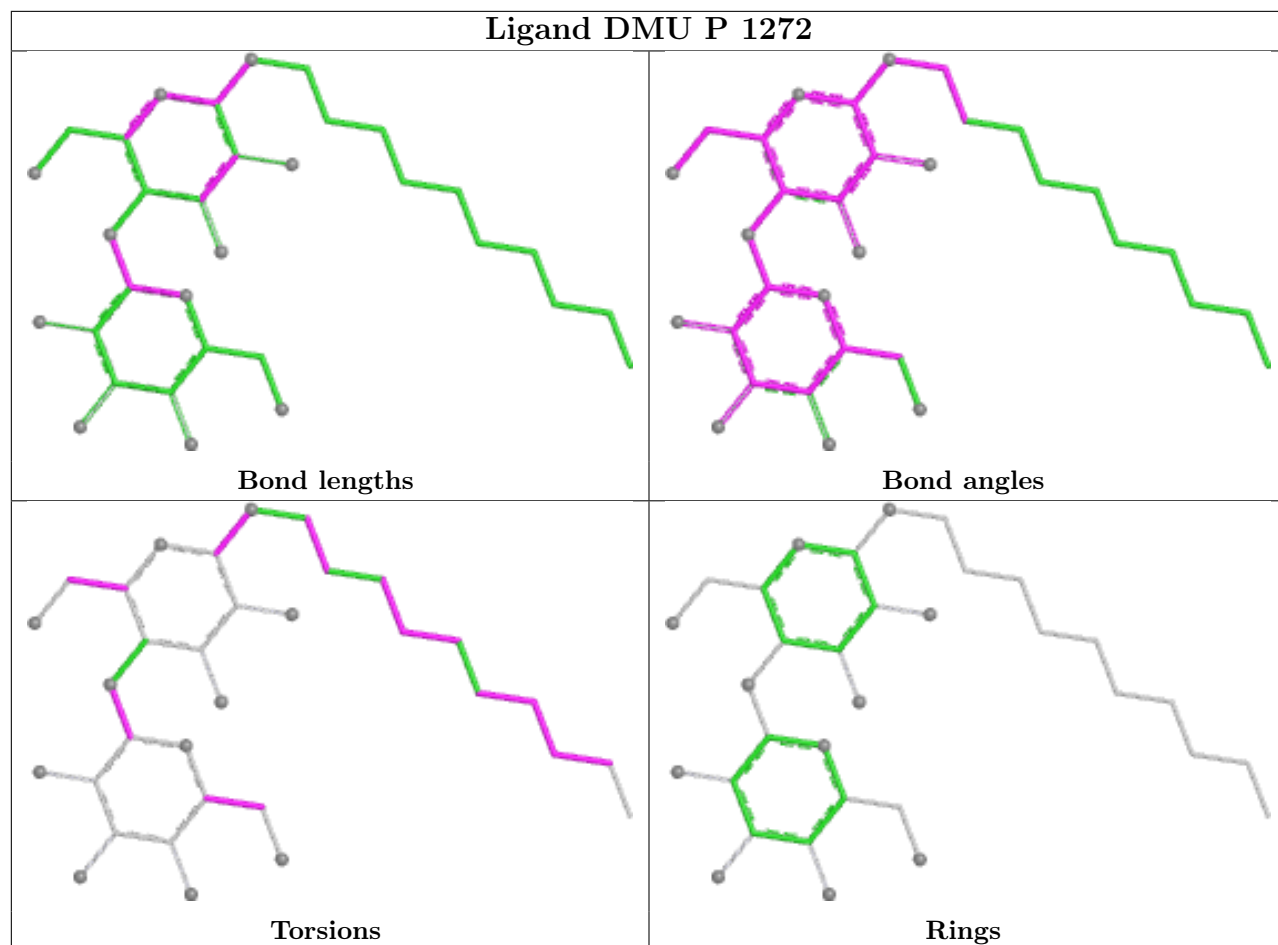
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	515	HEA	3	0
22	B	229	PSC	26	0
22	R	1229	PSC	15	0
19	D	523	TGL	8	0
19	Q	1523	TGL	12	0
23	P	1525	CHD	1	0
20	P	1267	PGV	5	0
25	G	265	PEK	19	0
19	A	521	TGL	8	0
20	C	267	PGV	5	0
25	P	1265	PEK	17	0

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.

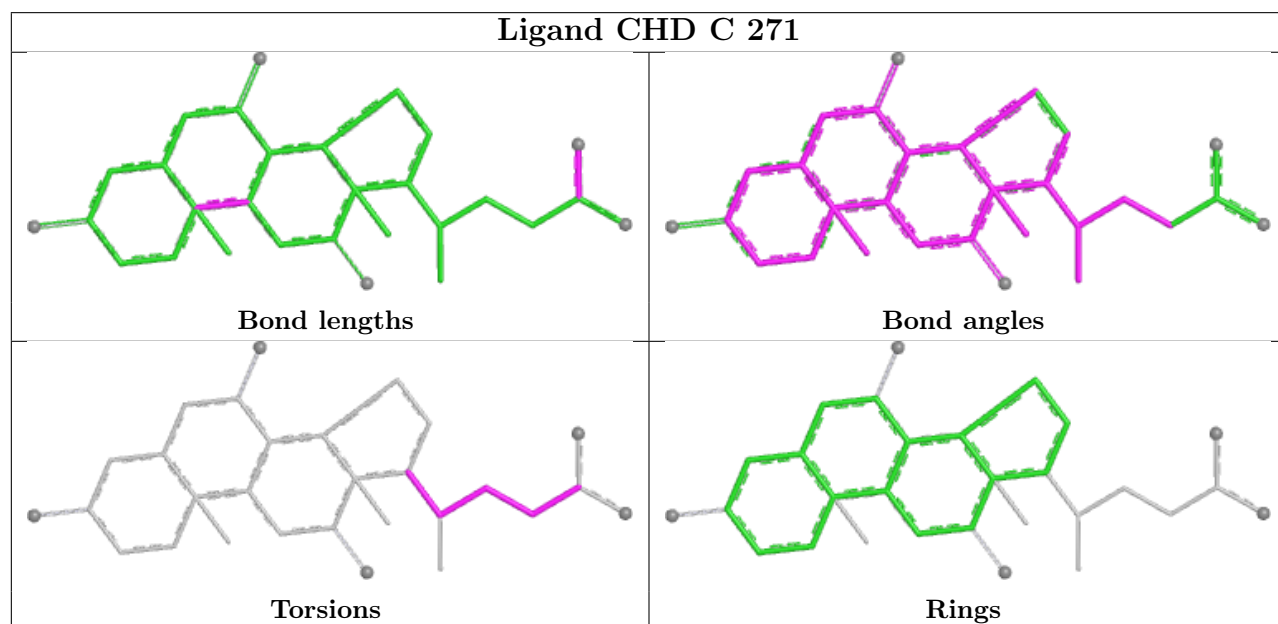


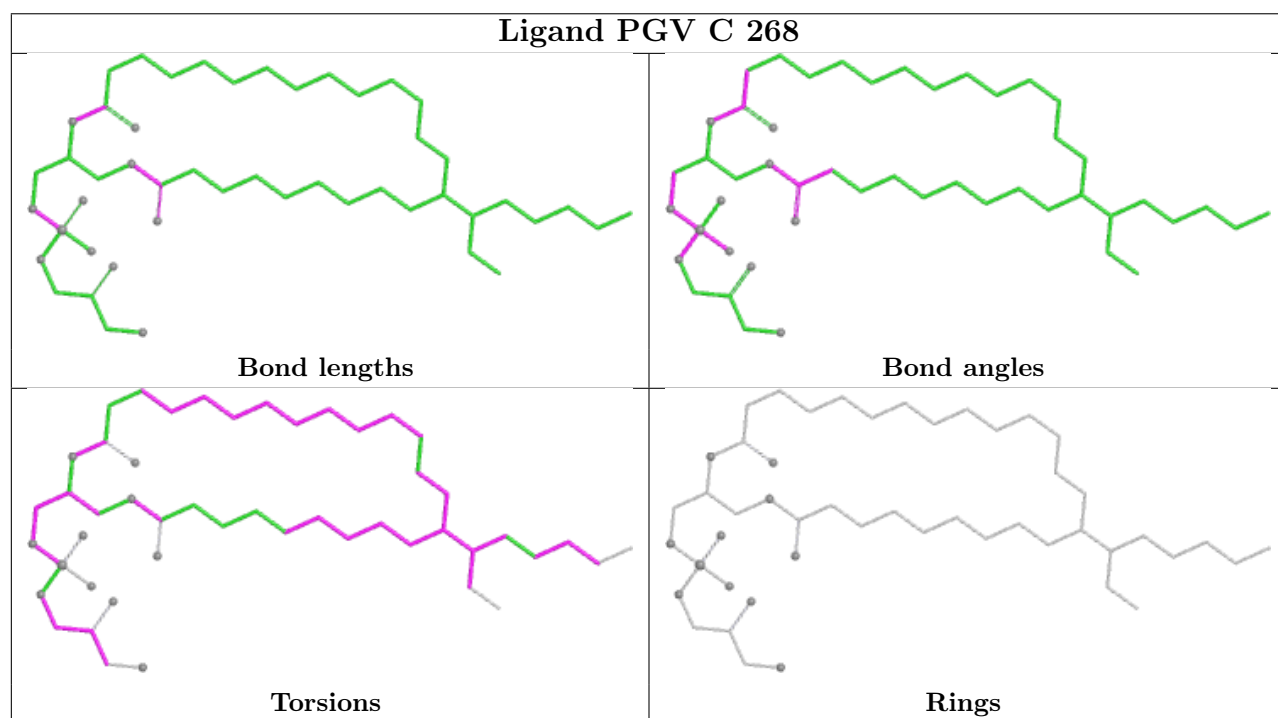
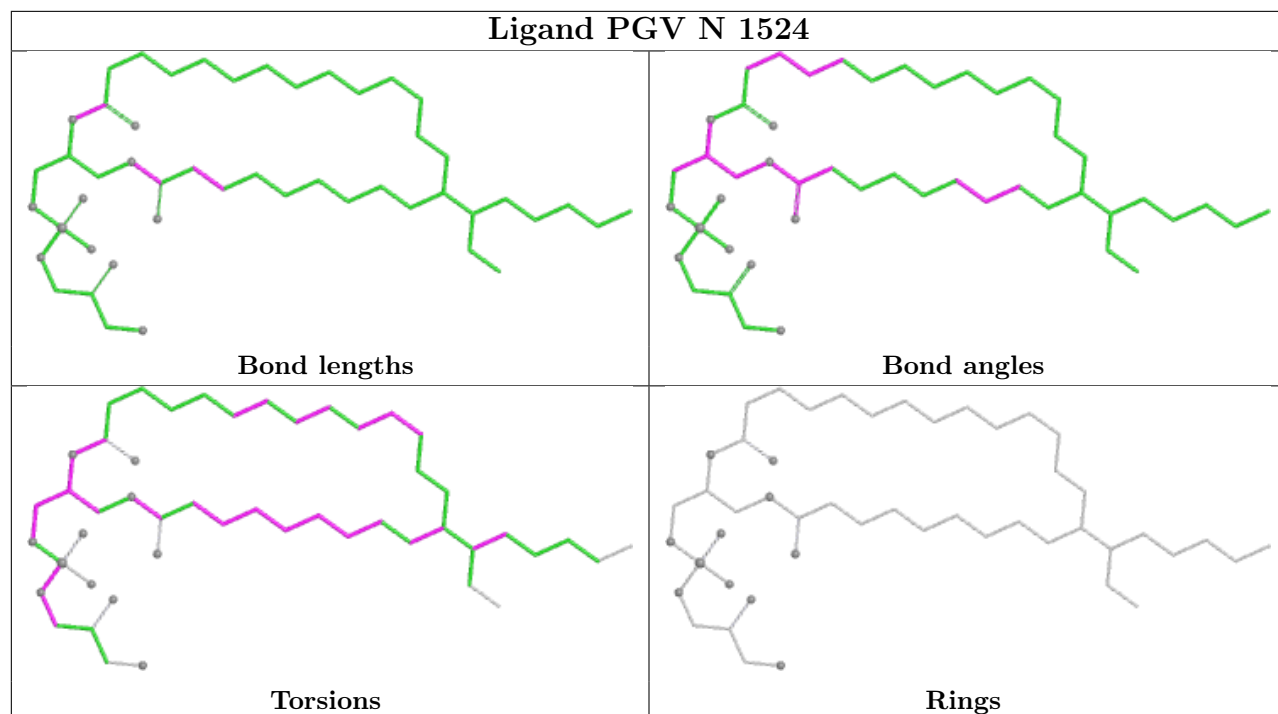


Ligand DMU P 1272

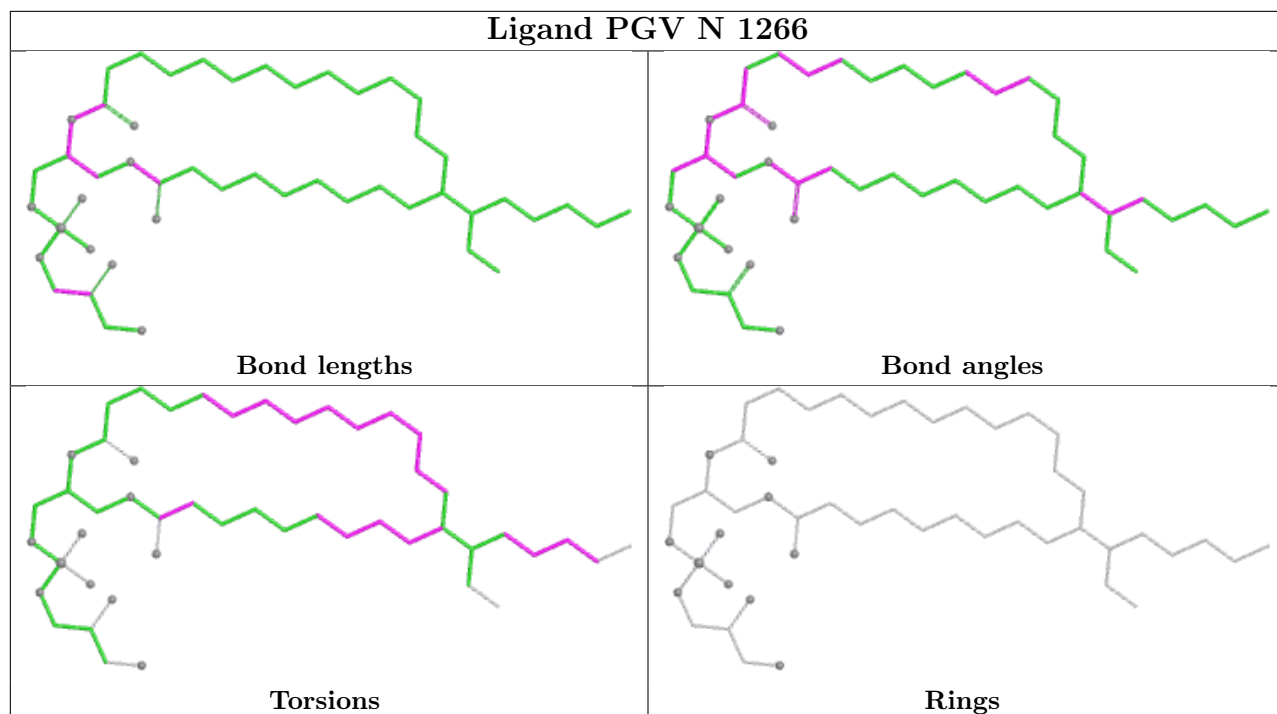


Ligand CHD C 271

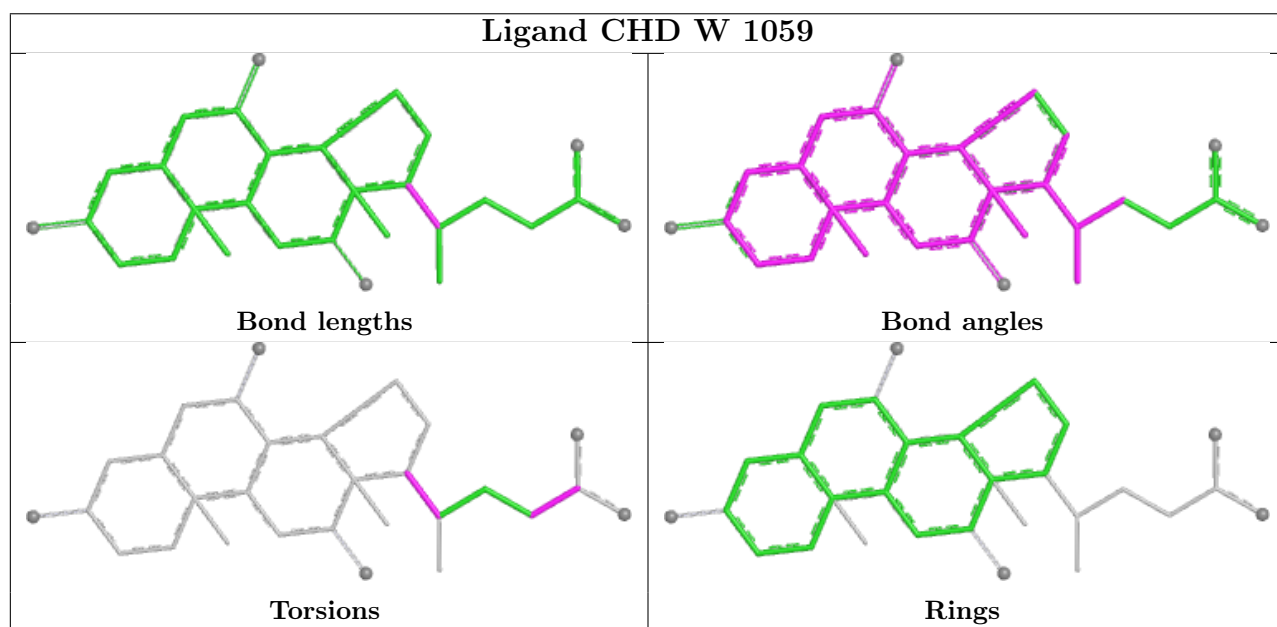


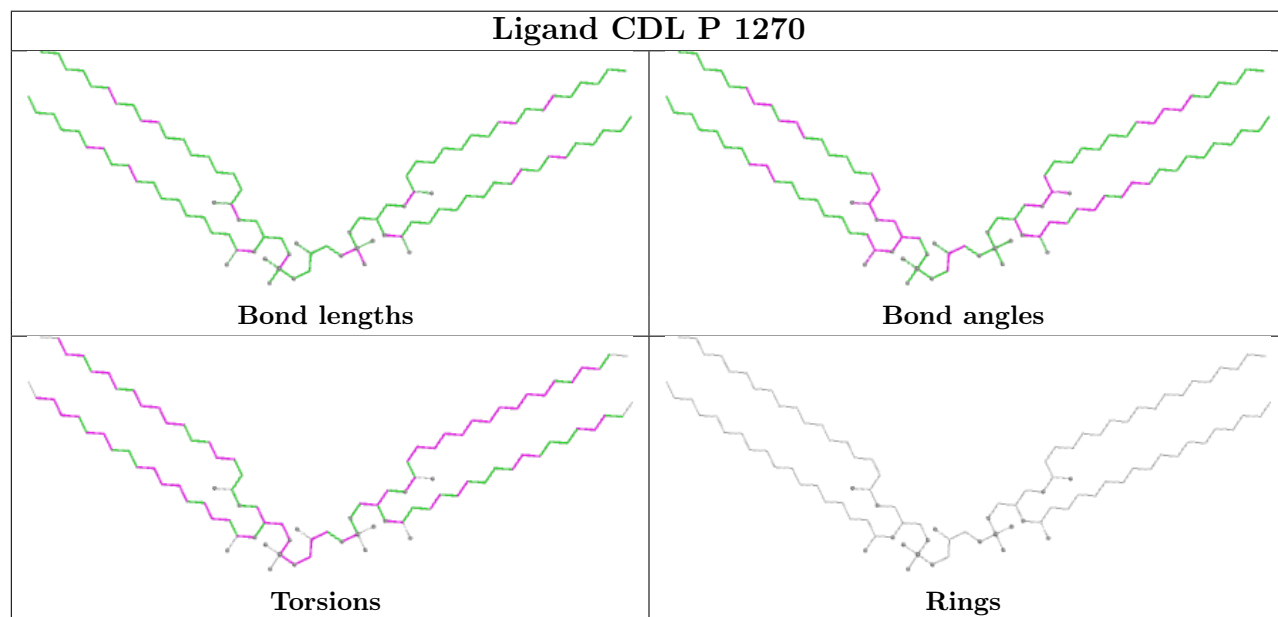
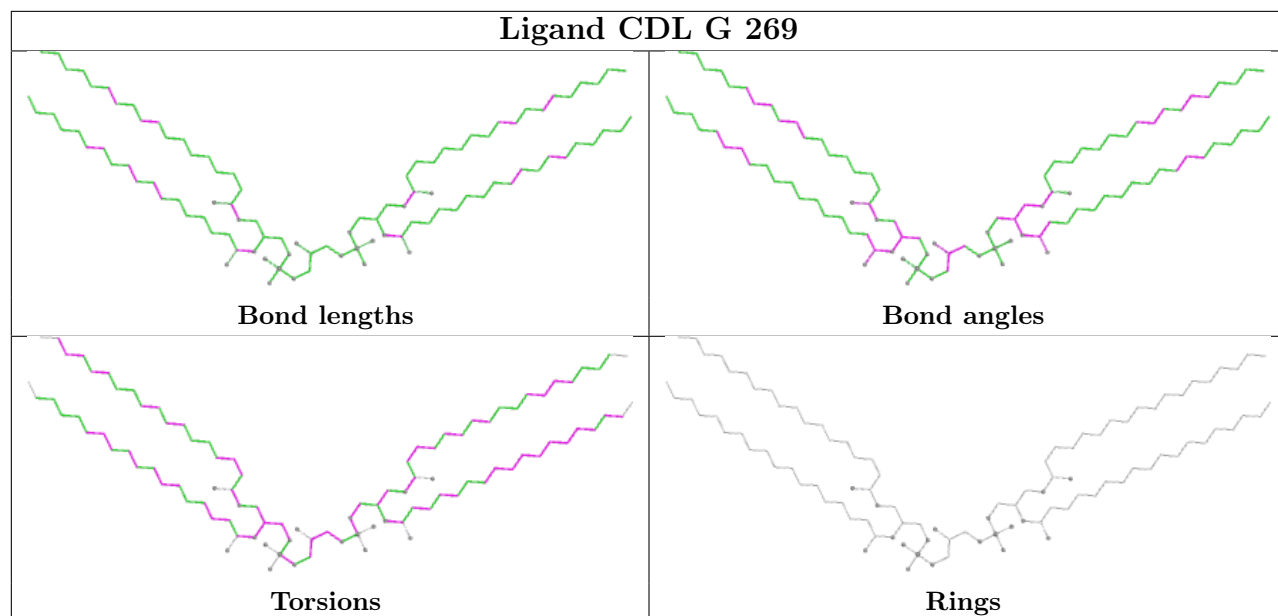


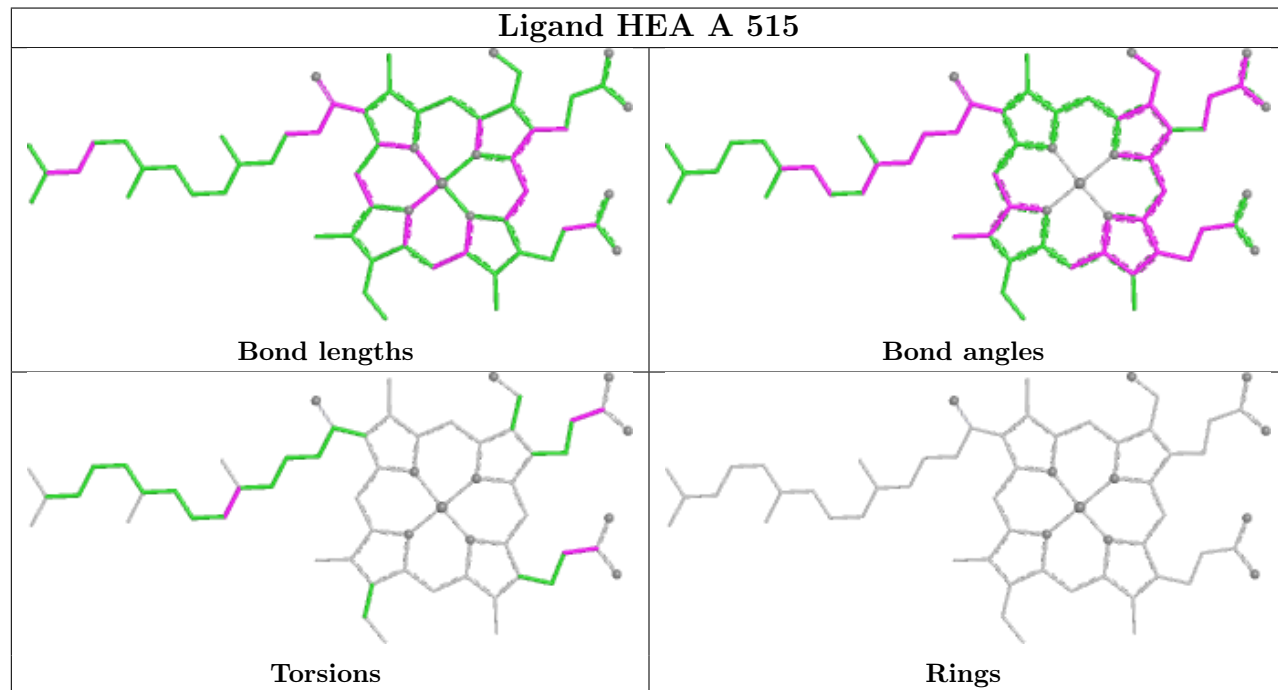
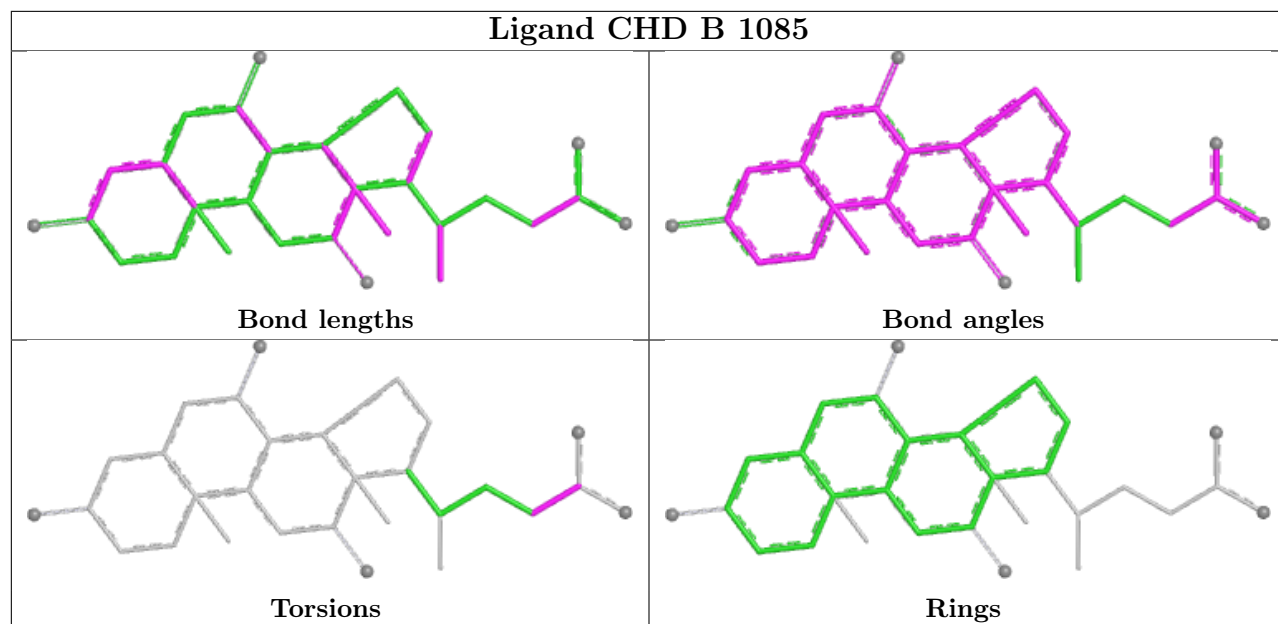
Ligand PGV N 1266

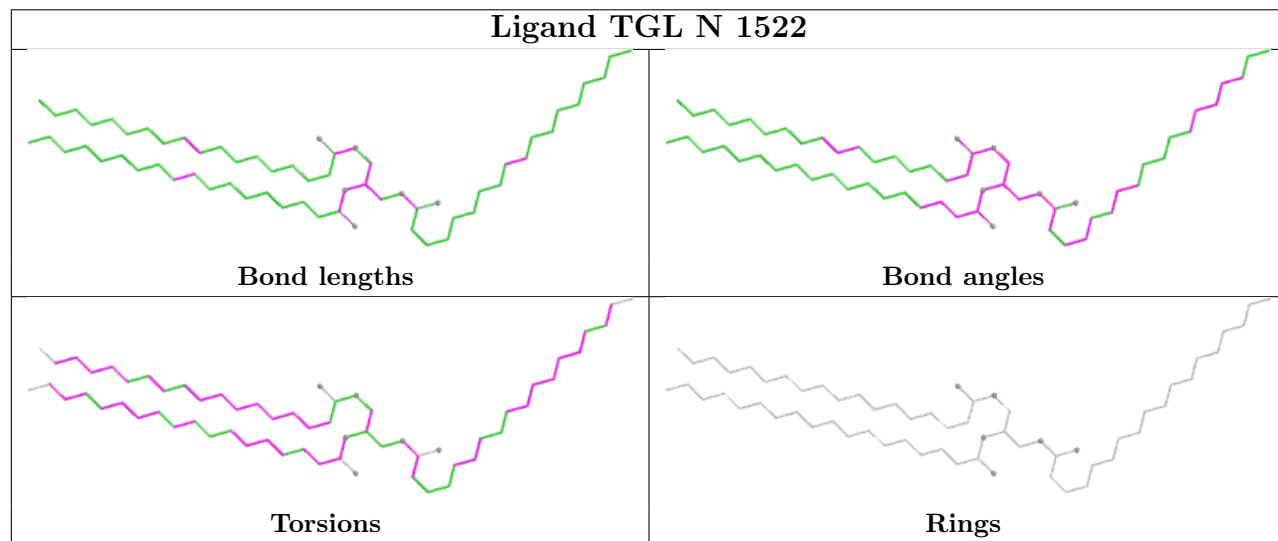
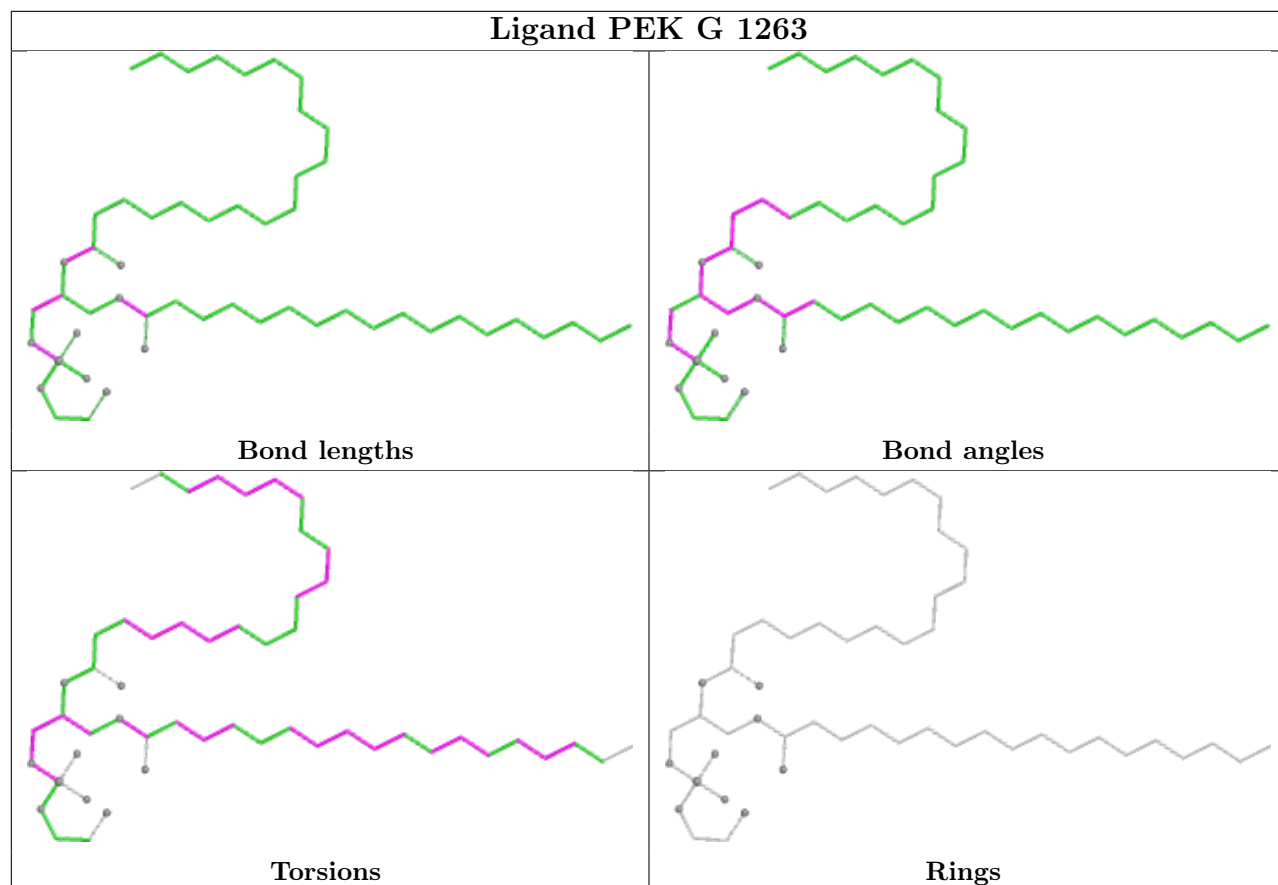


Ligand CHD W 1059

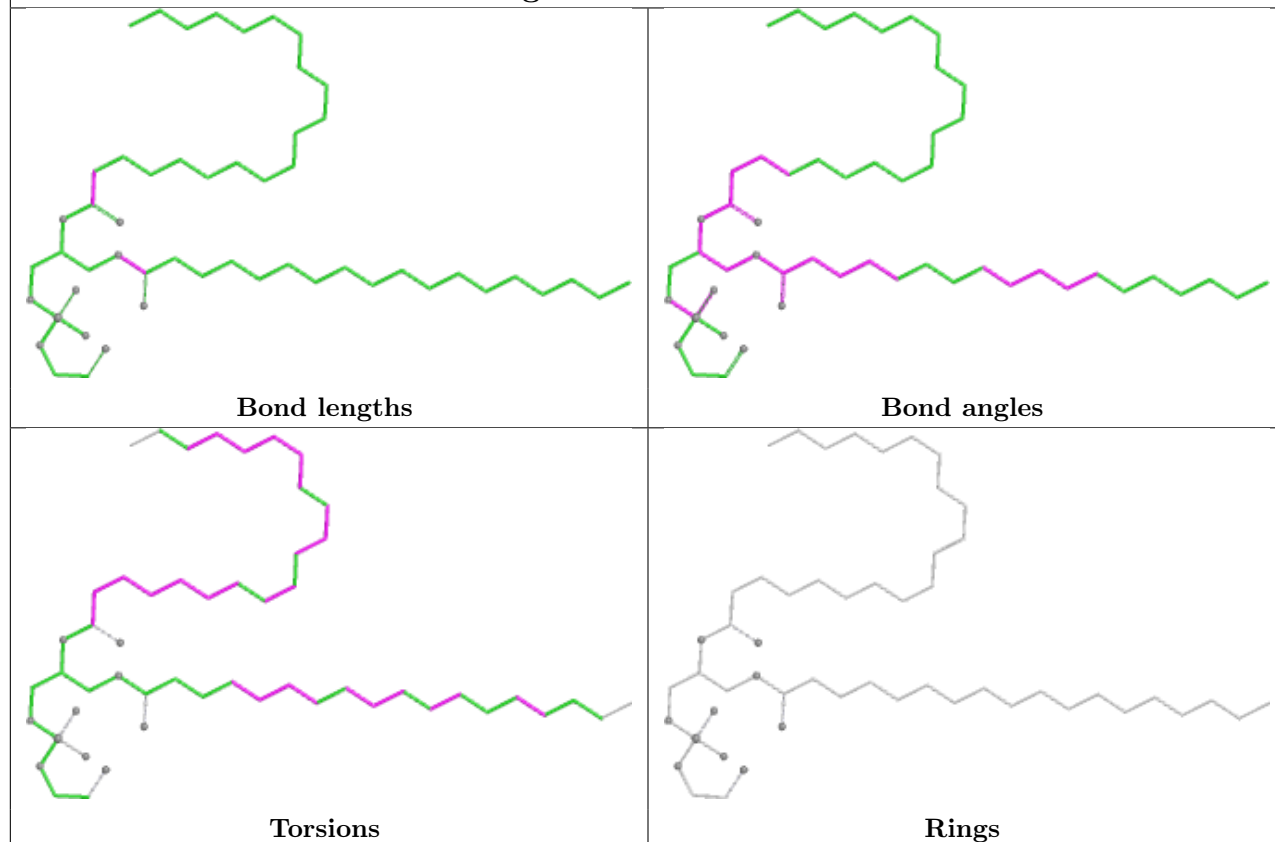




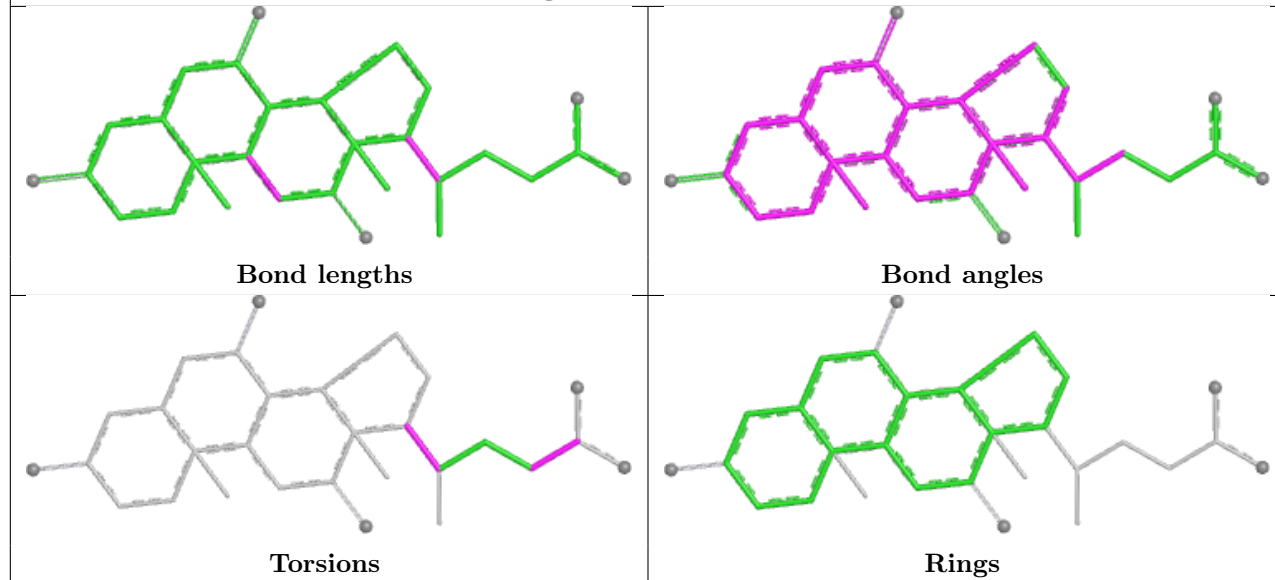


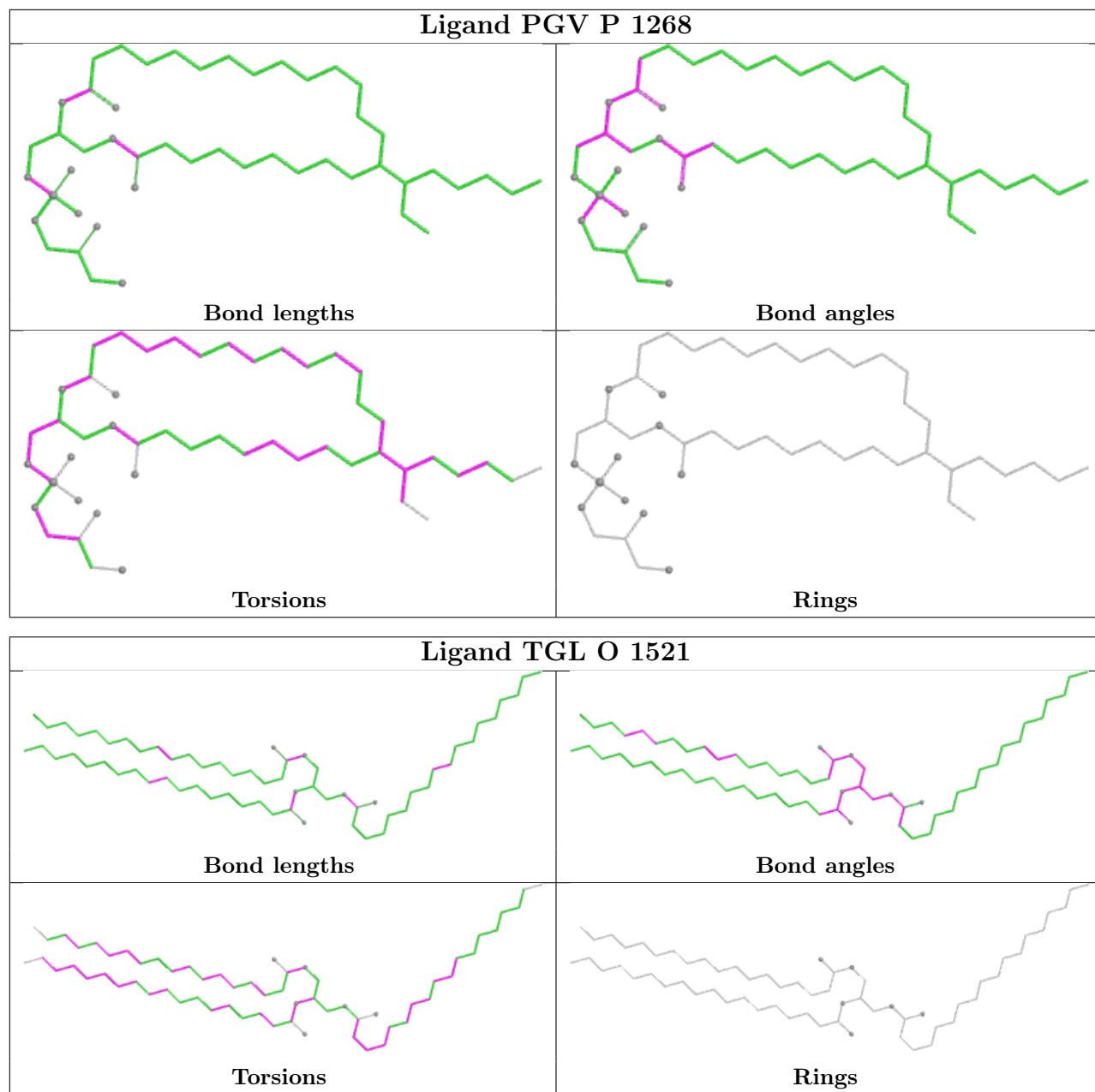


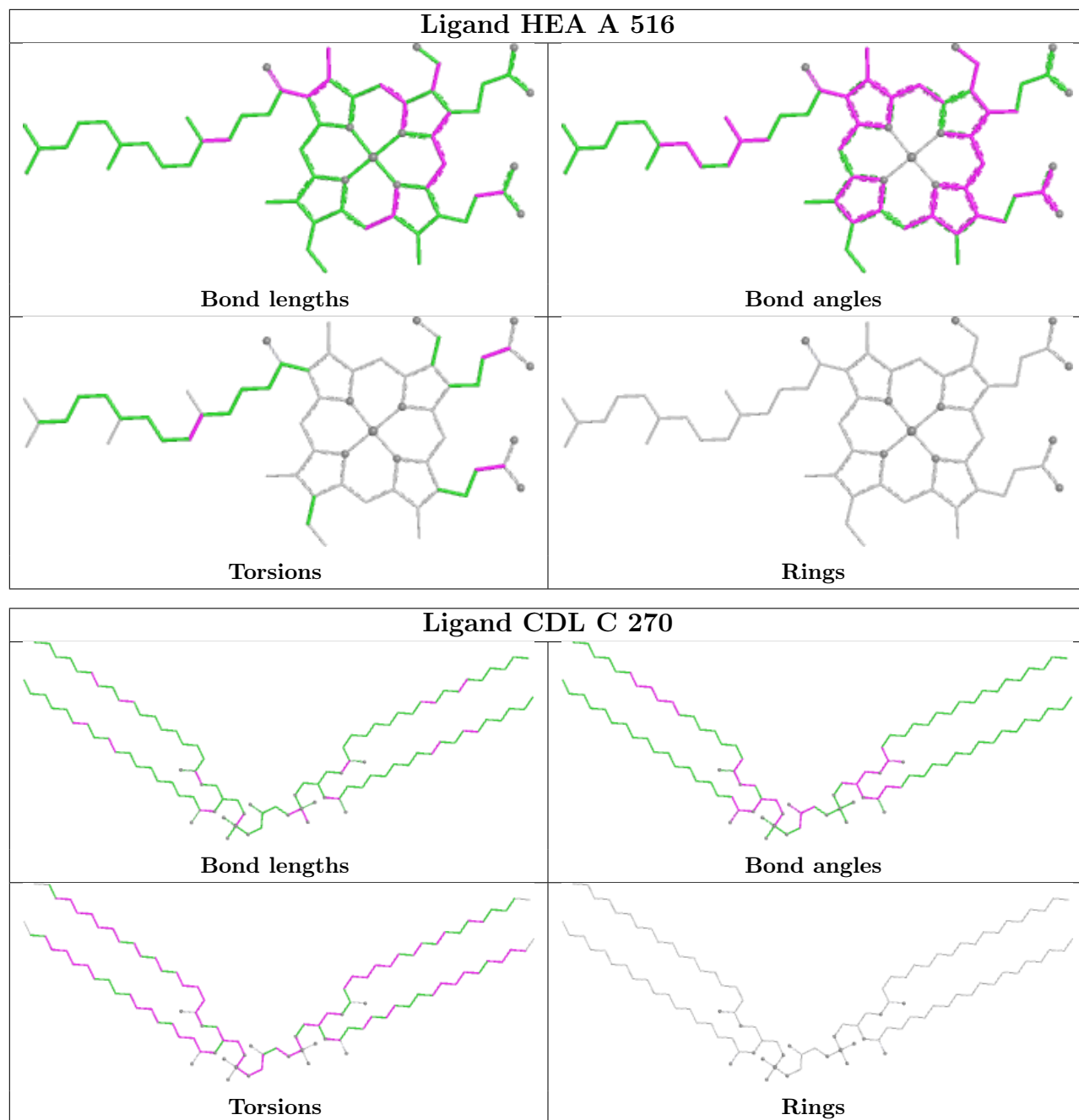
Ligand PEK P 1264

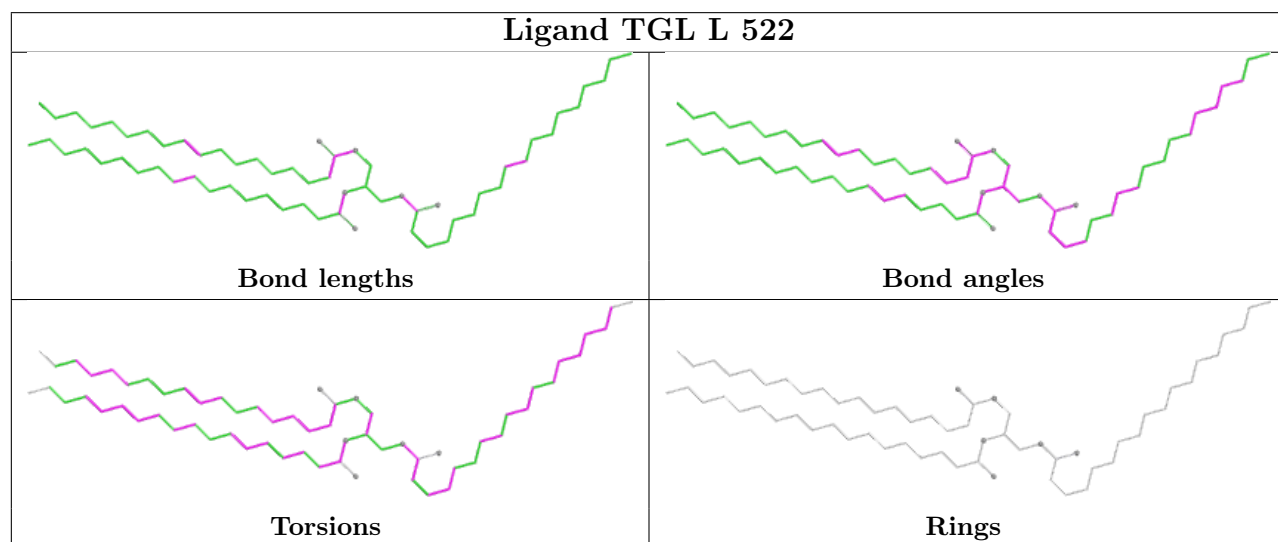
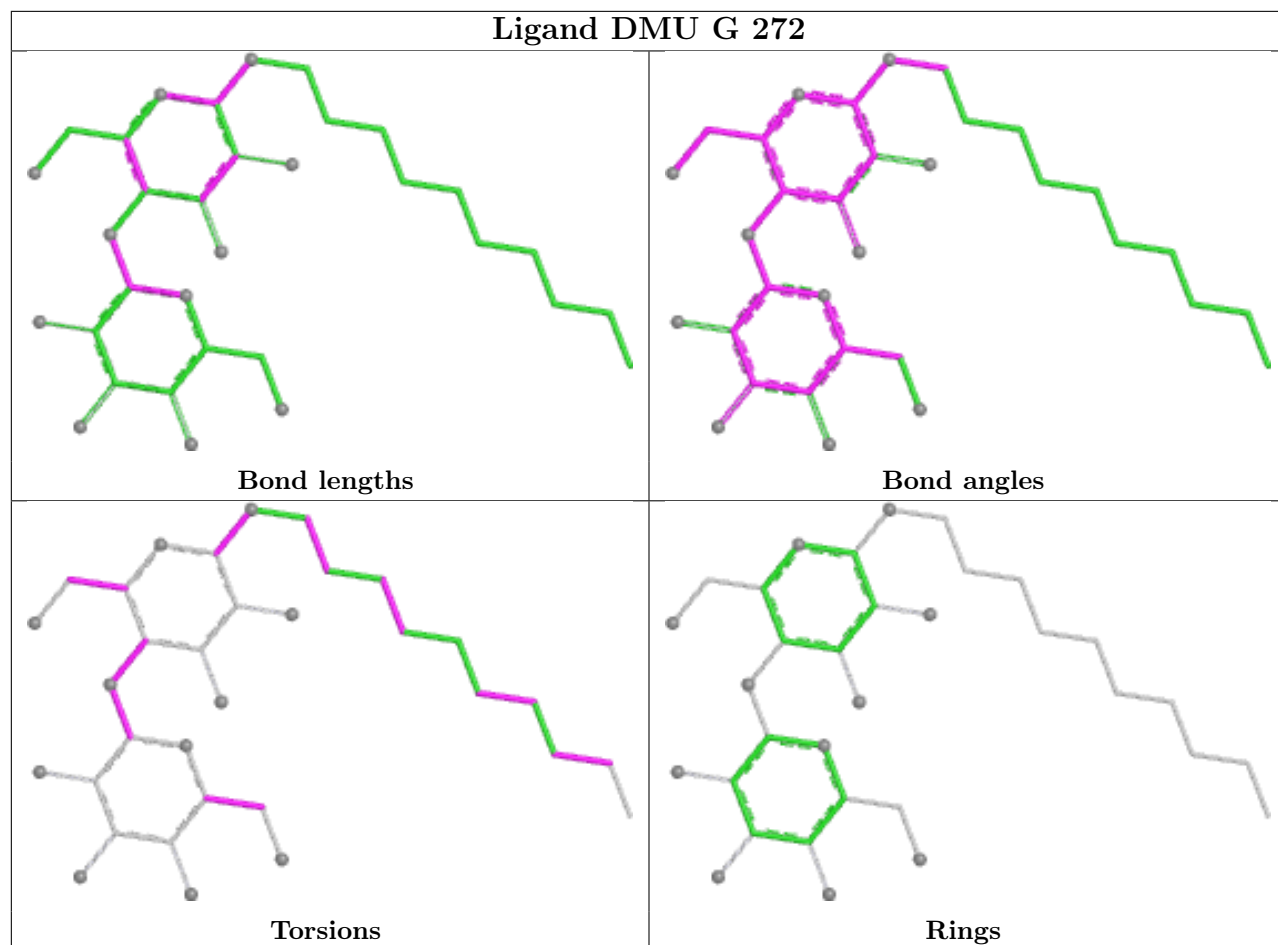


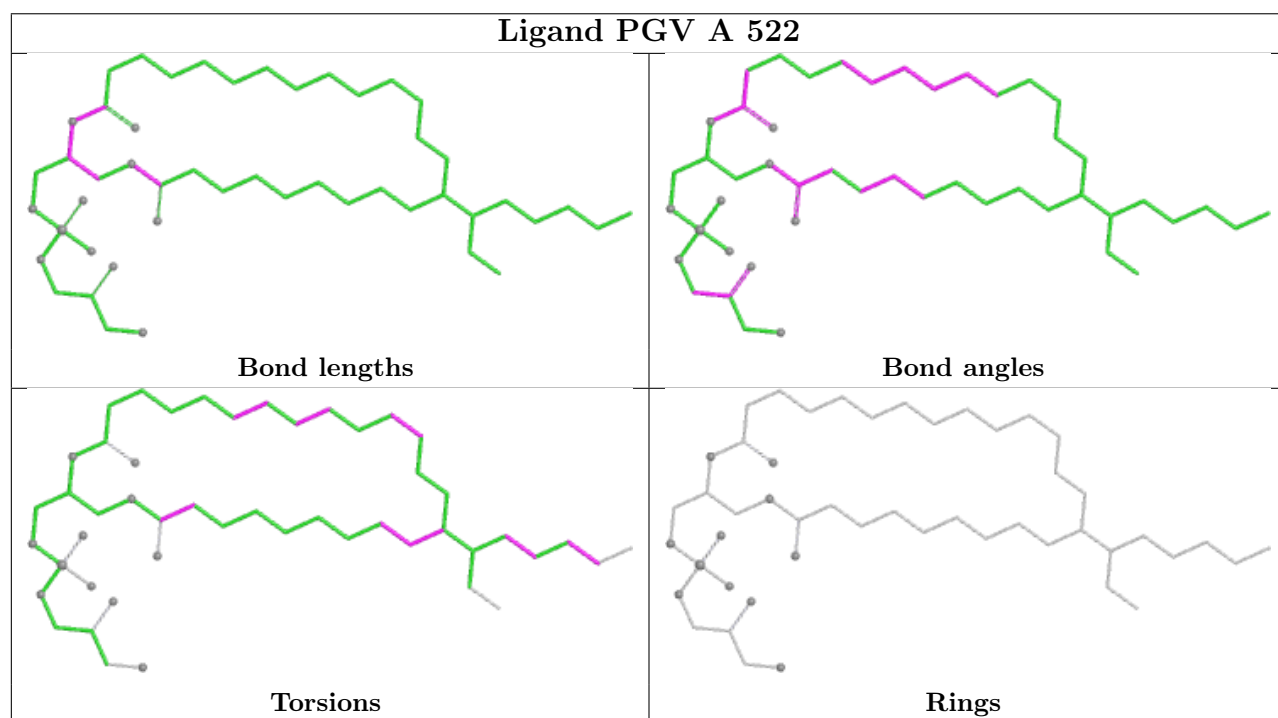
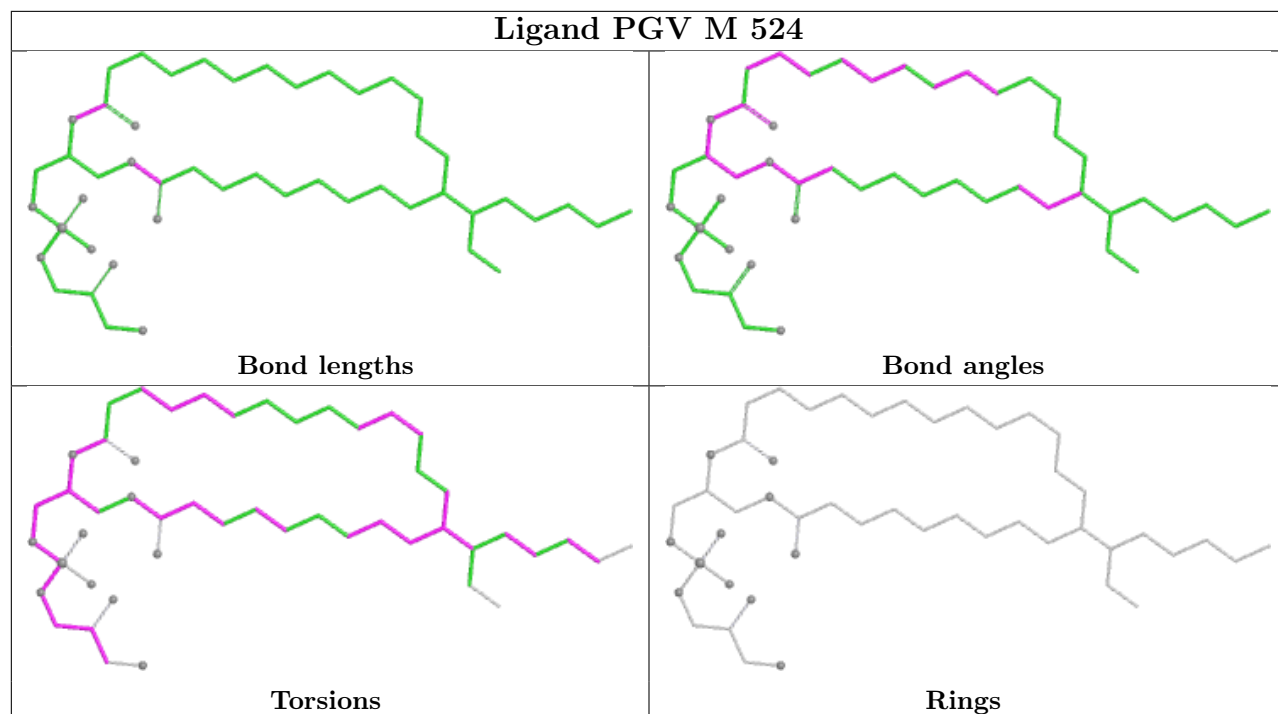
Ligand CHD J 60



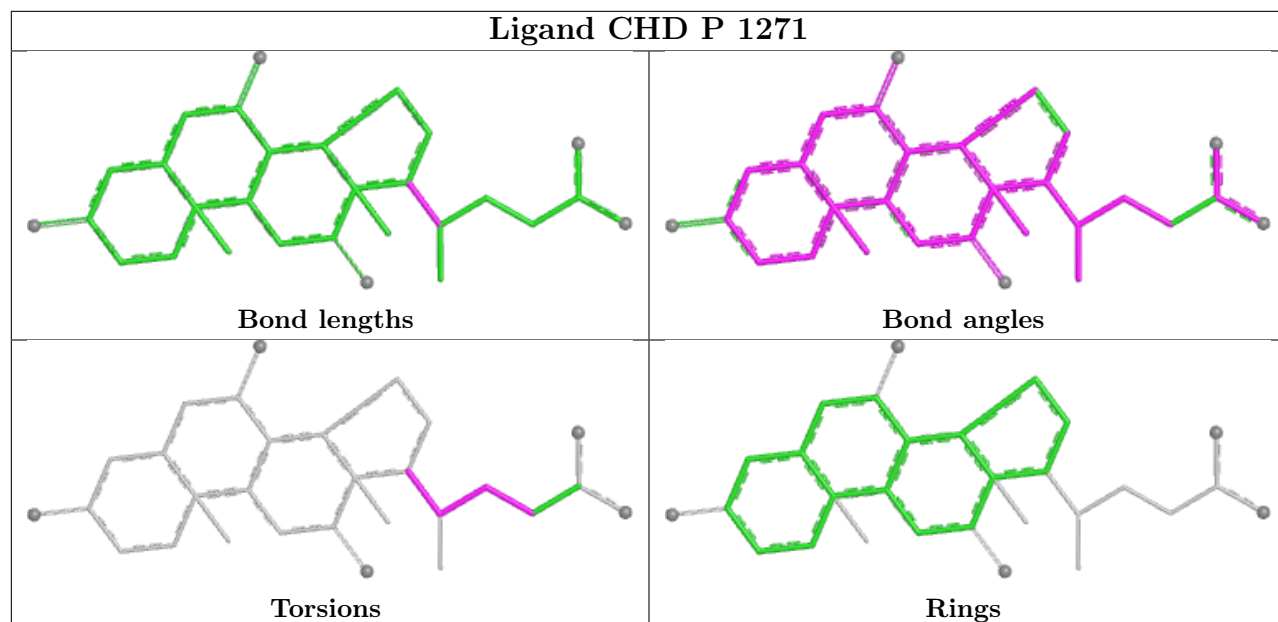




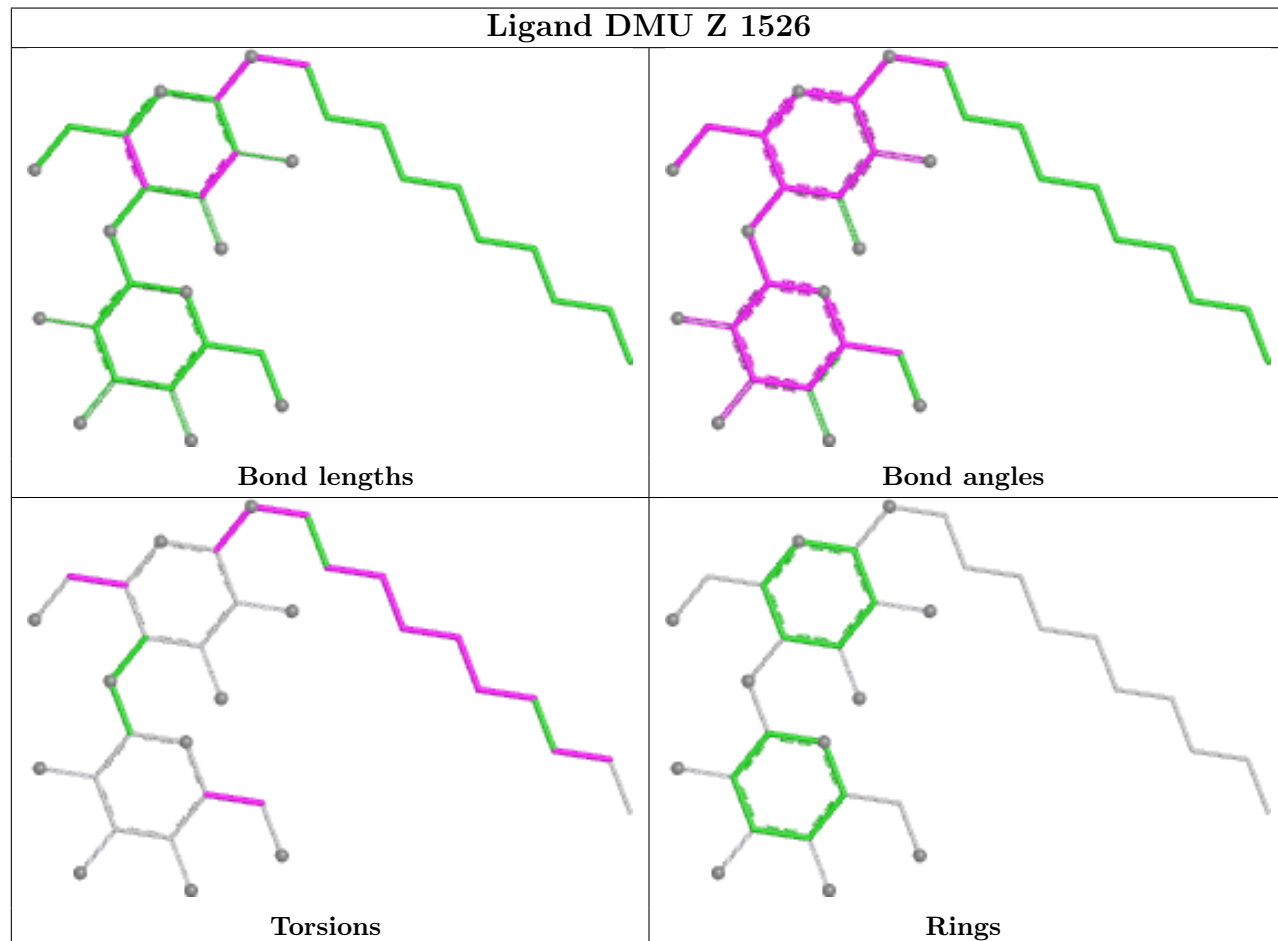


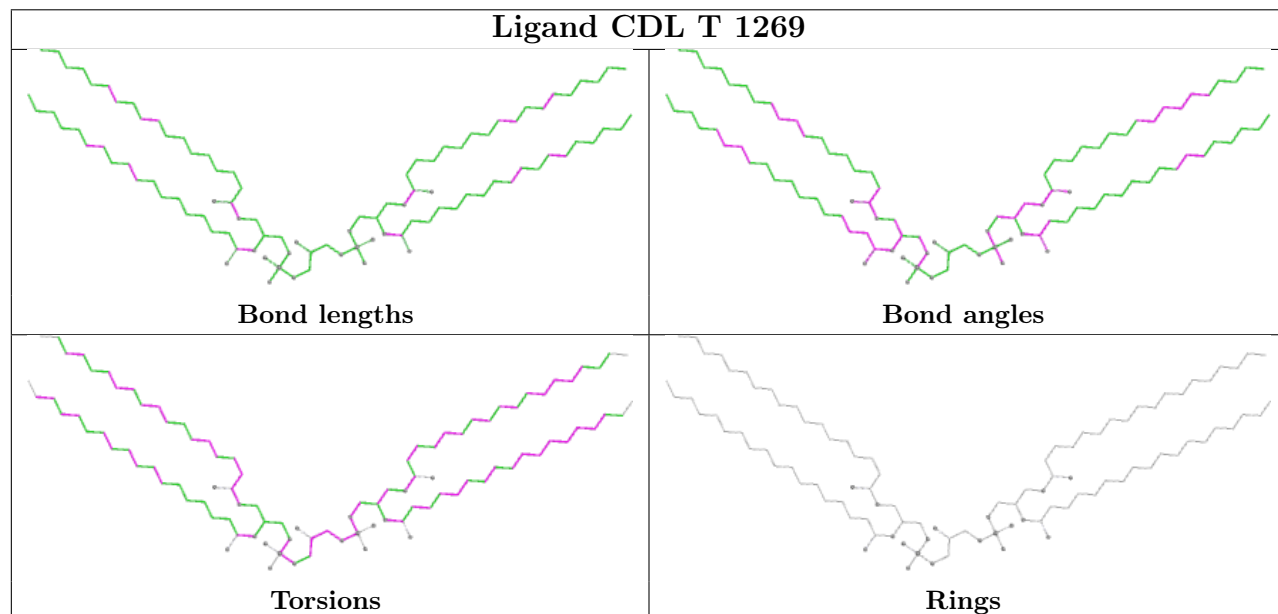
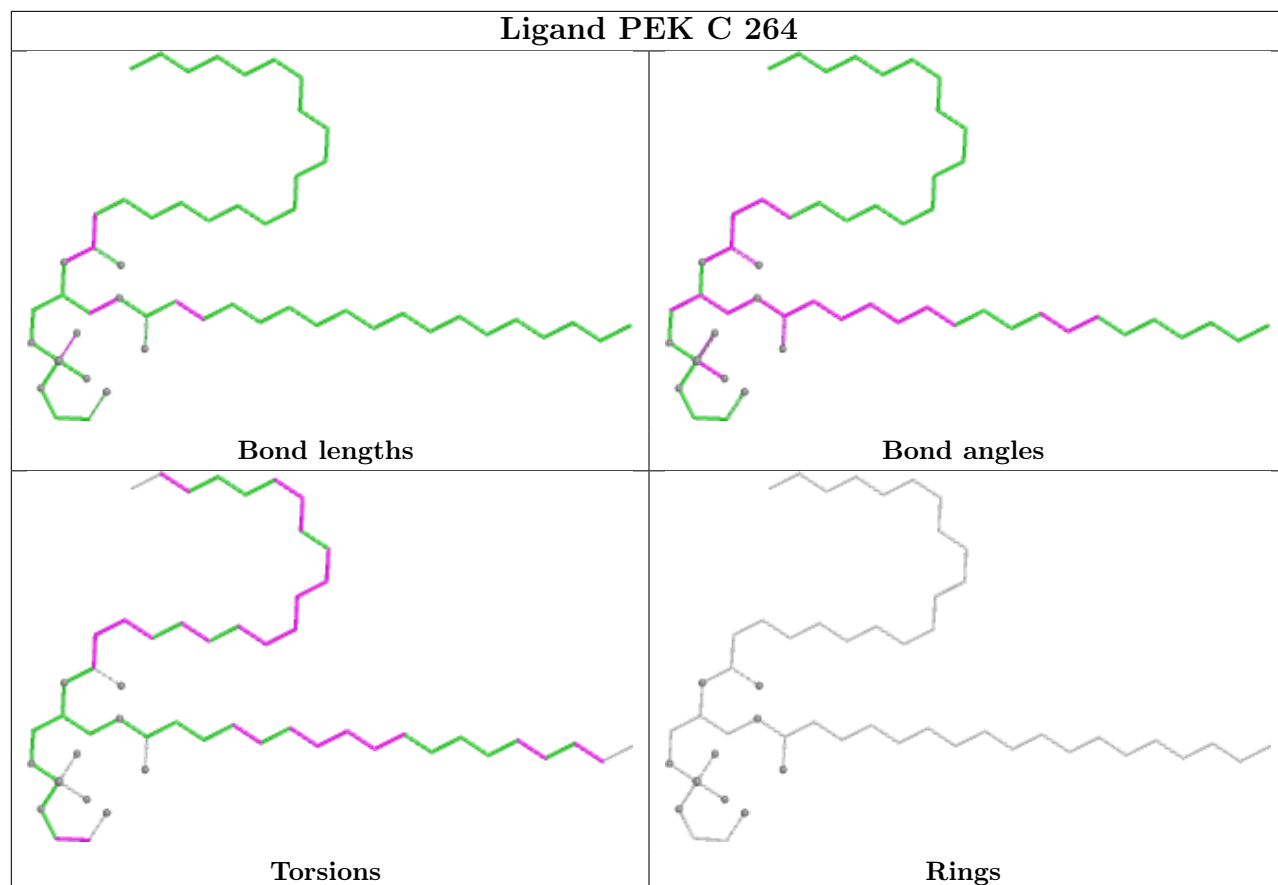


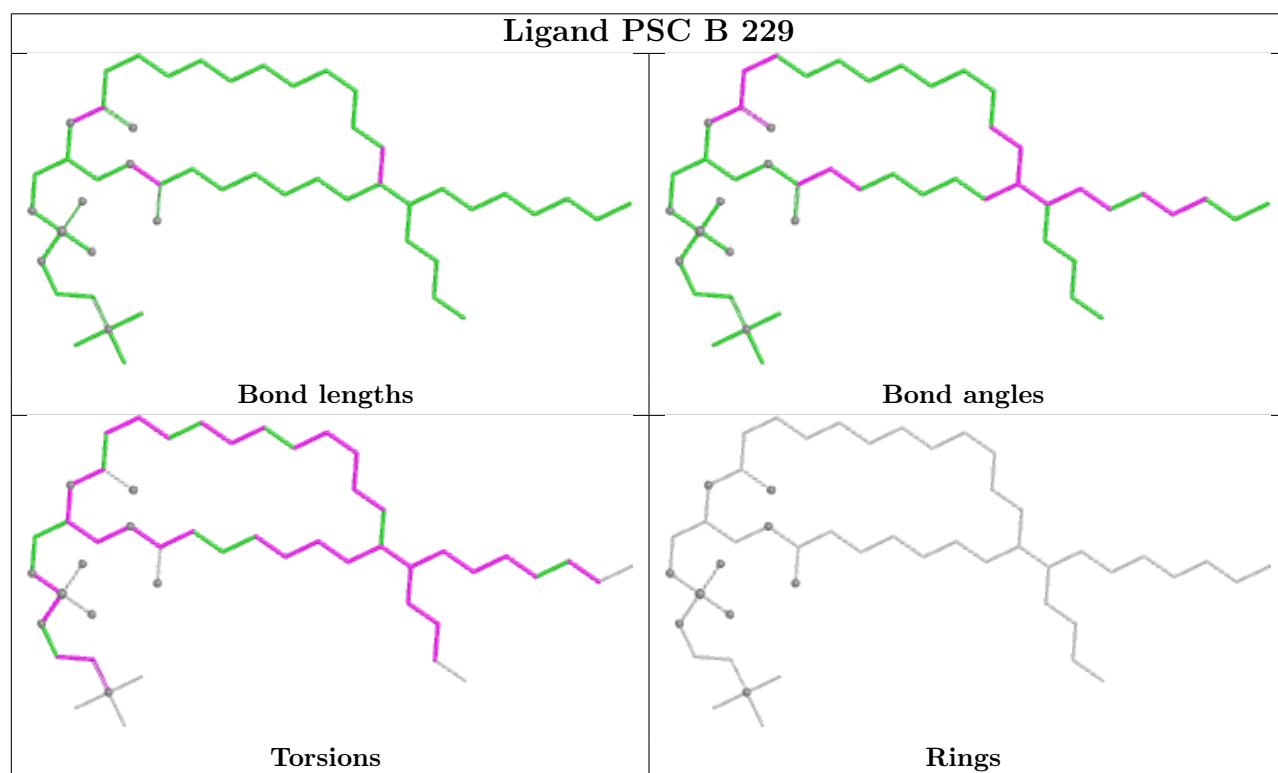
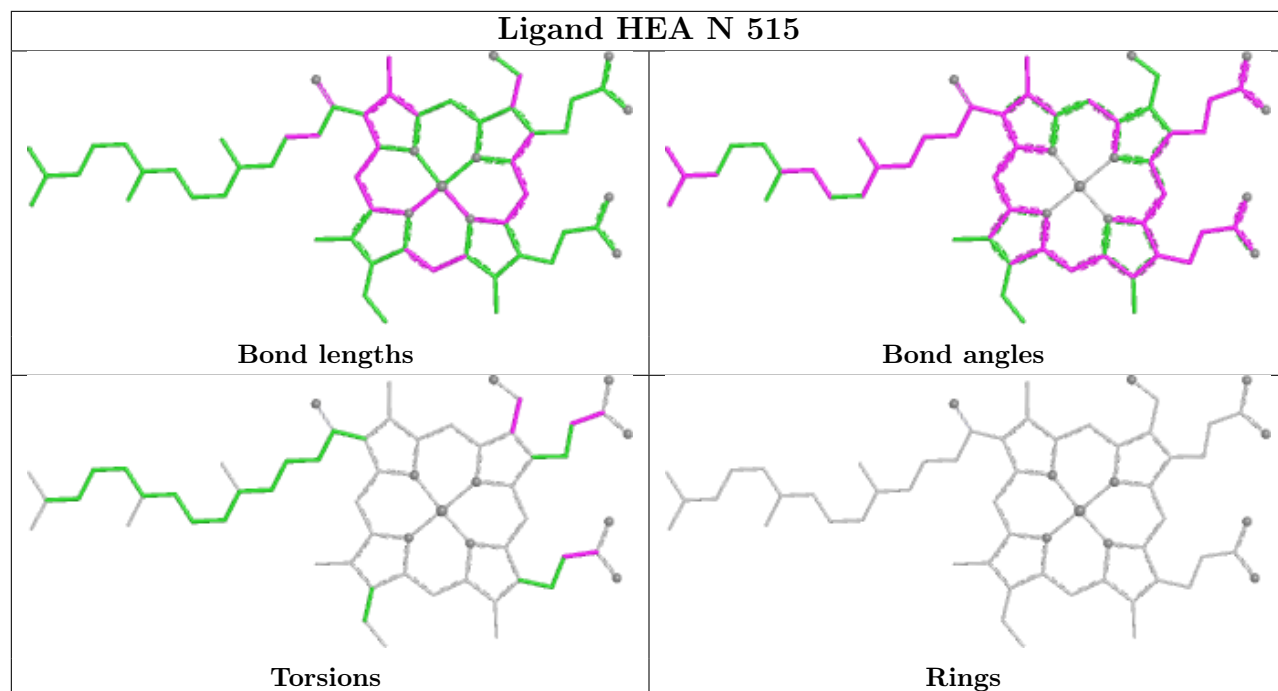
Ligand CHD P 1271

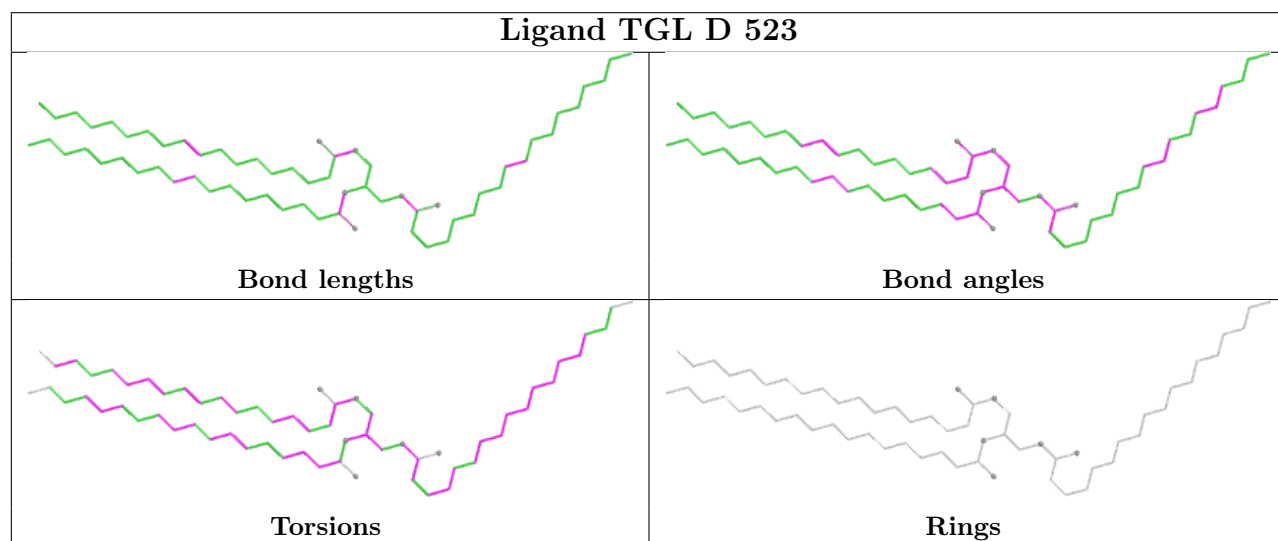
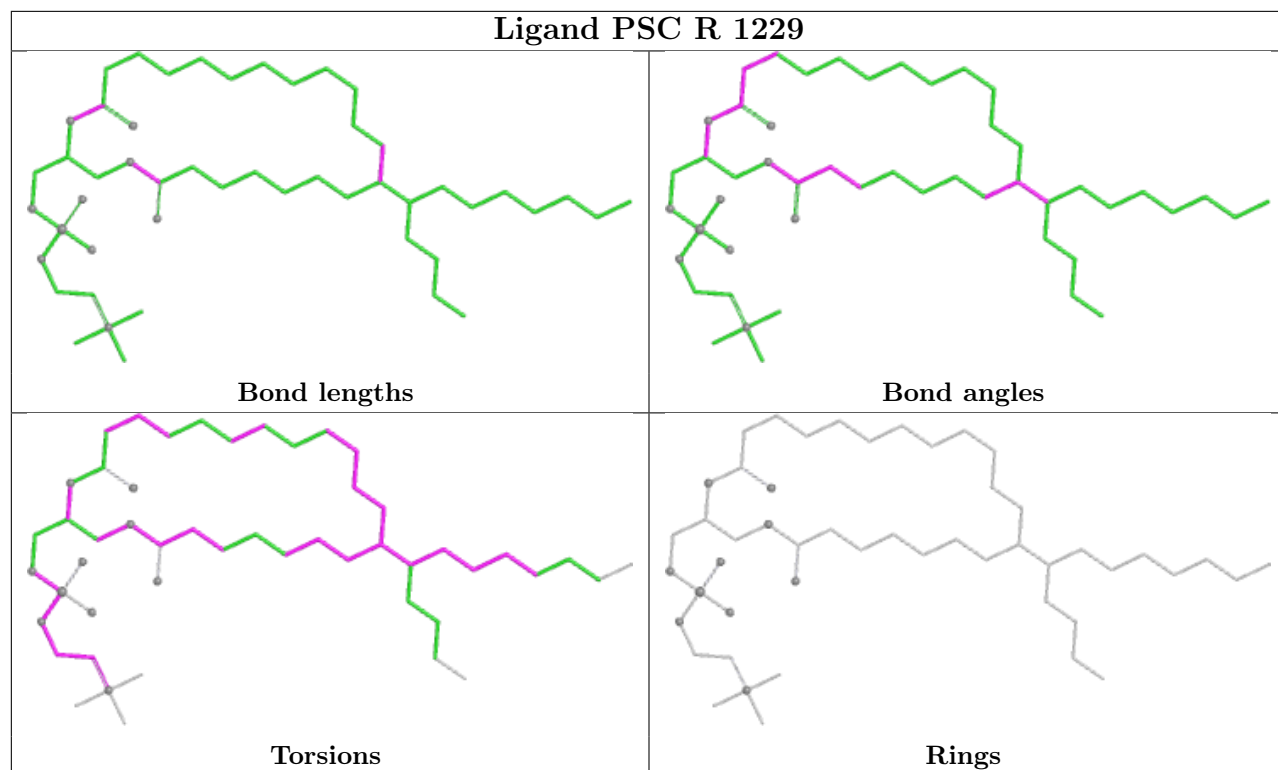


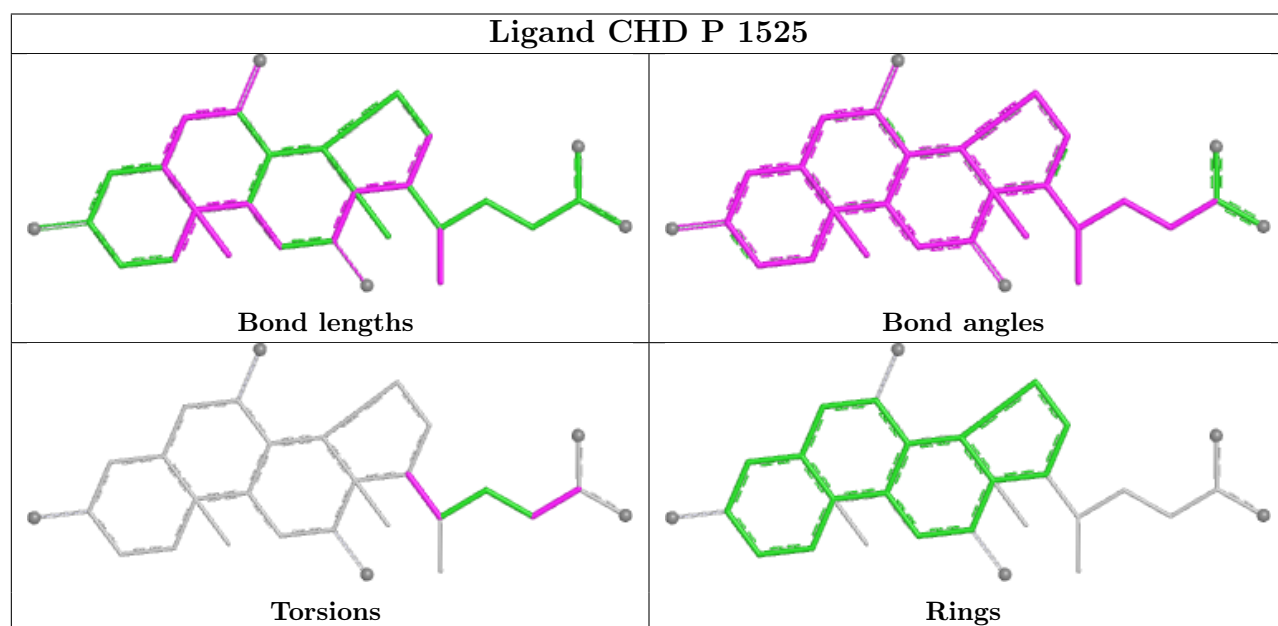
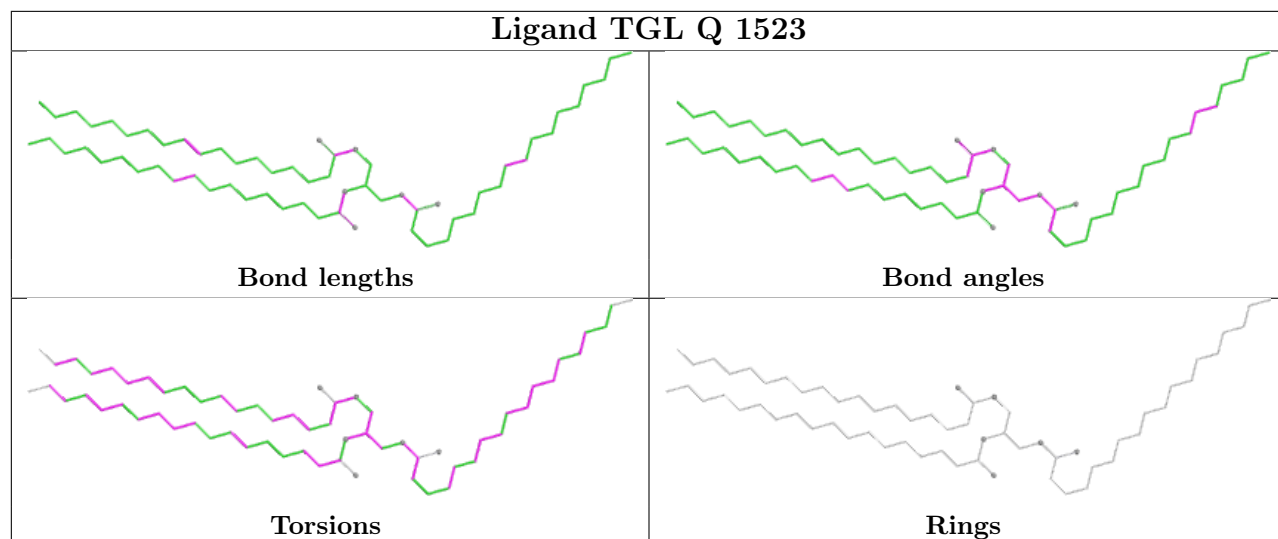
Ligand DMU Z 1526

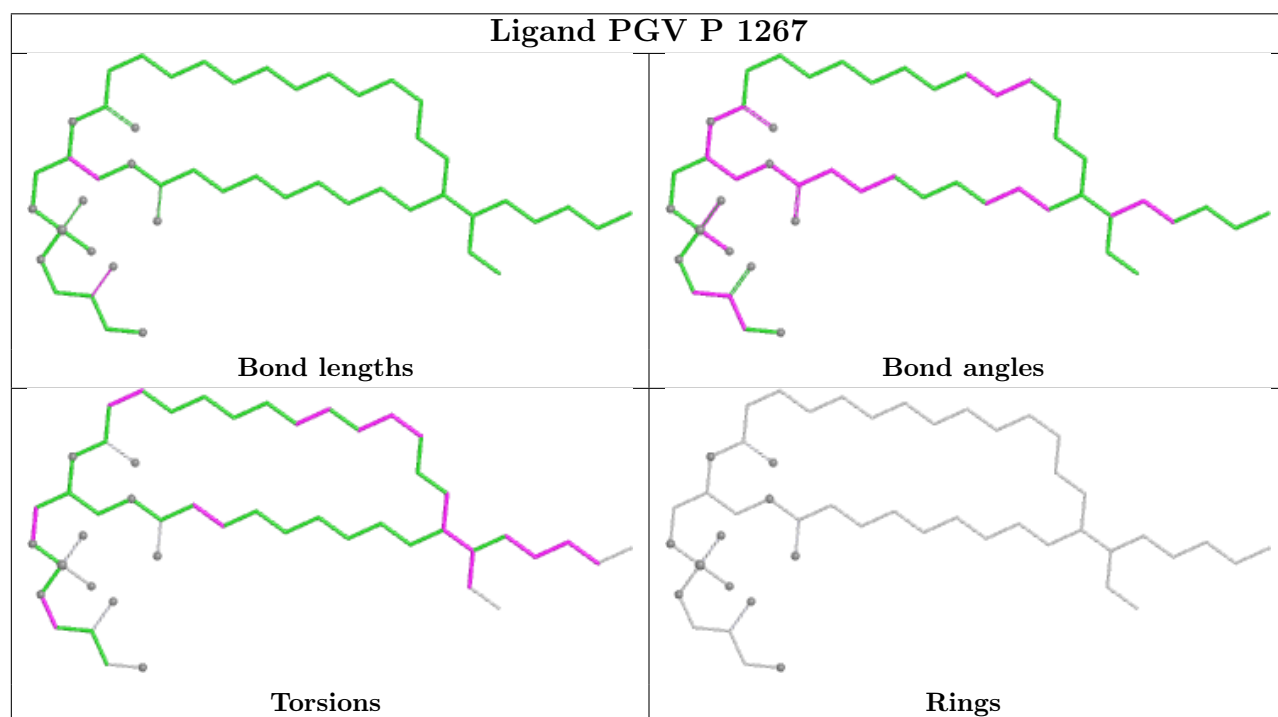
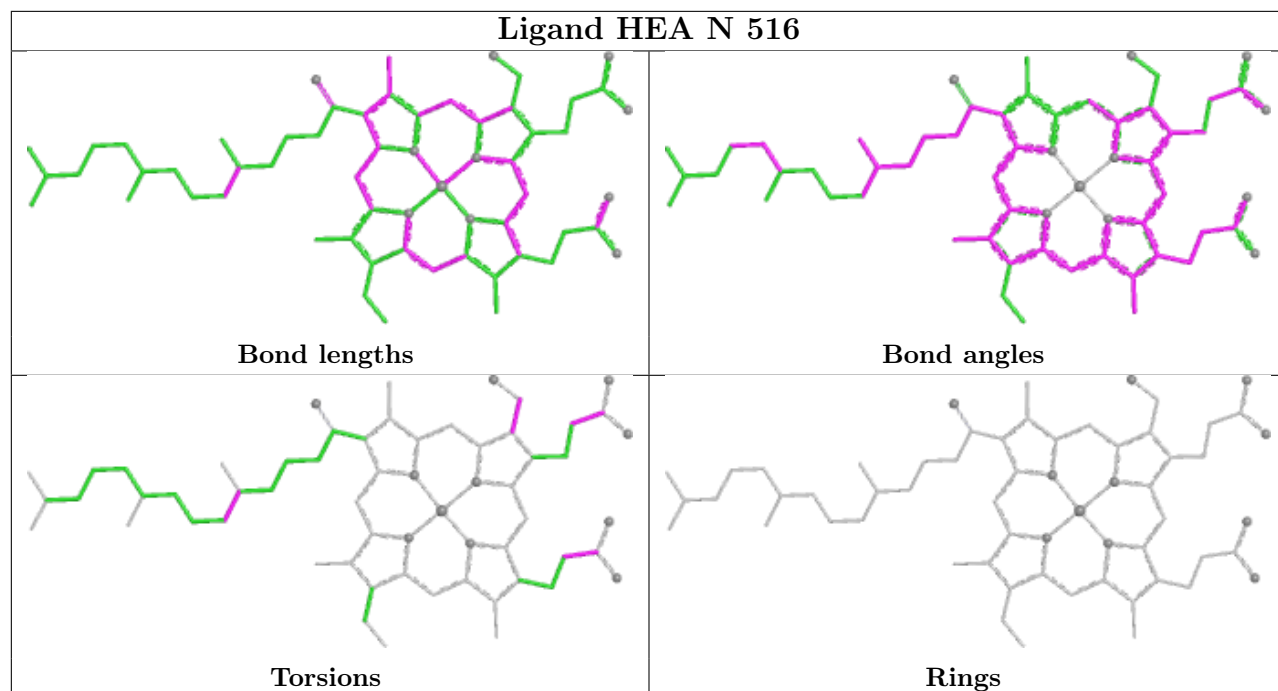


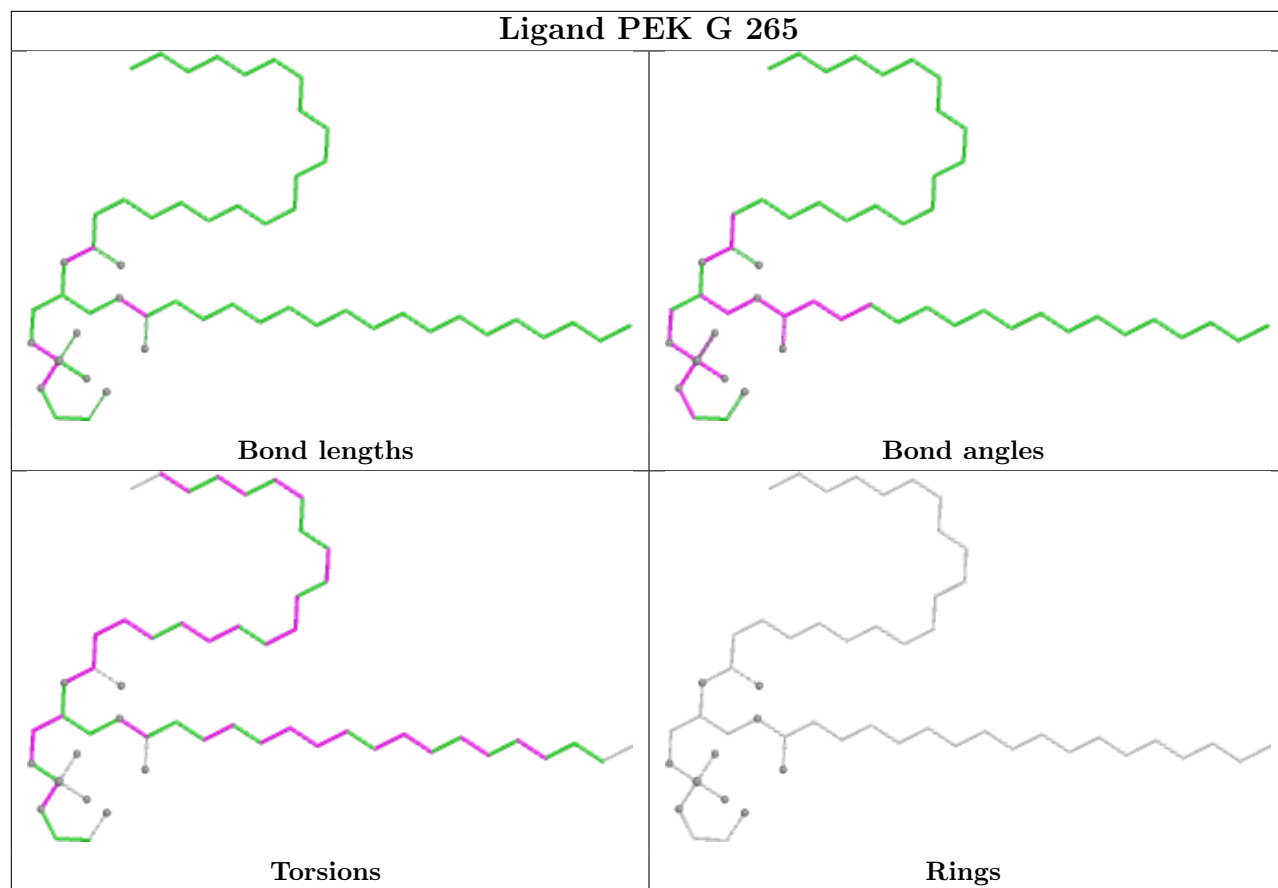




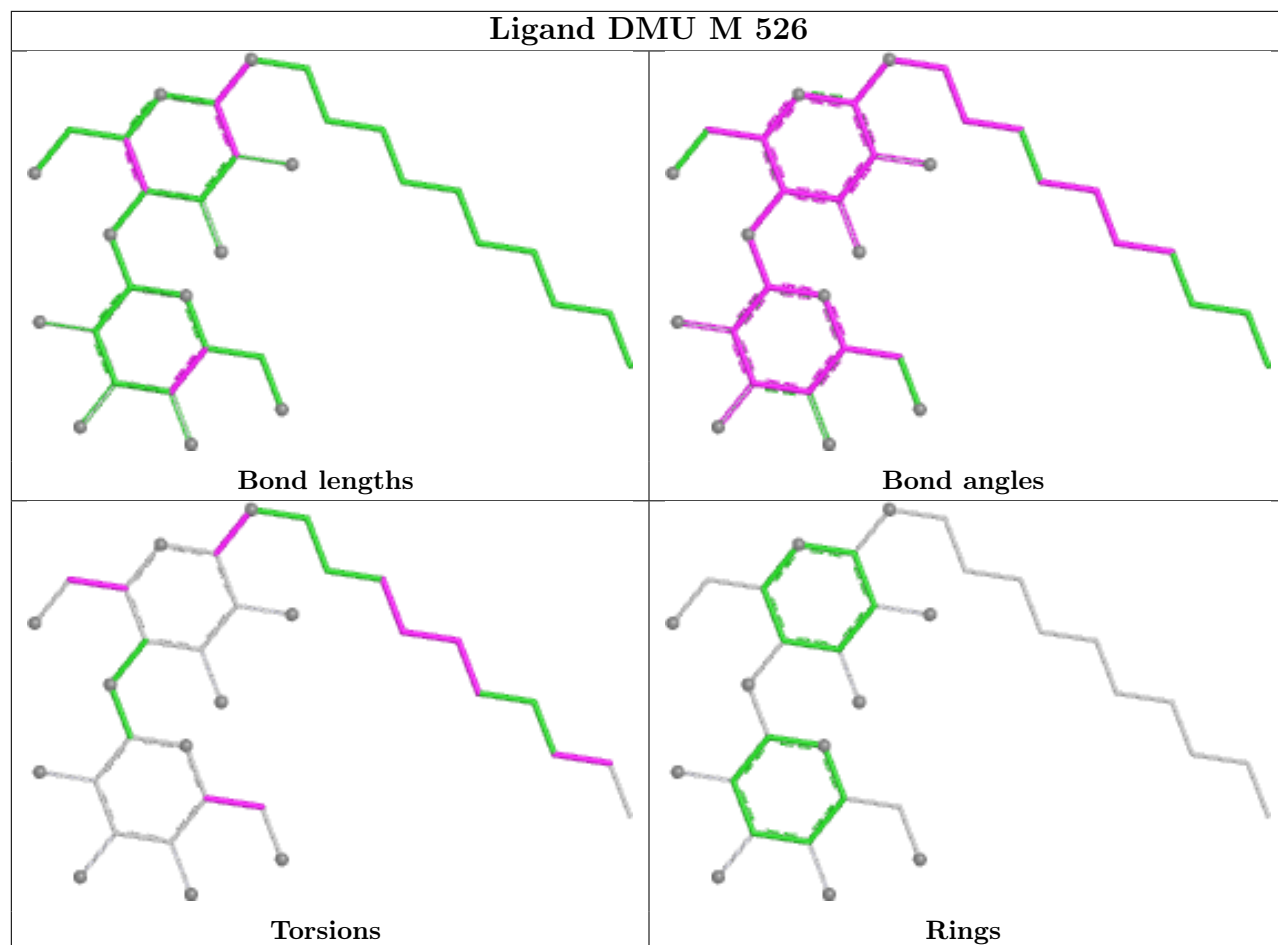




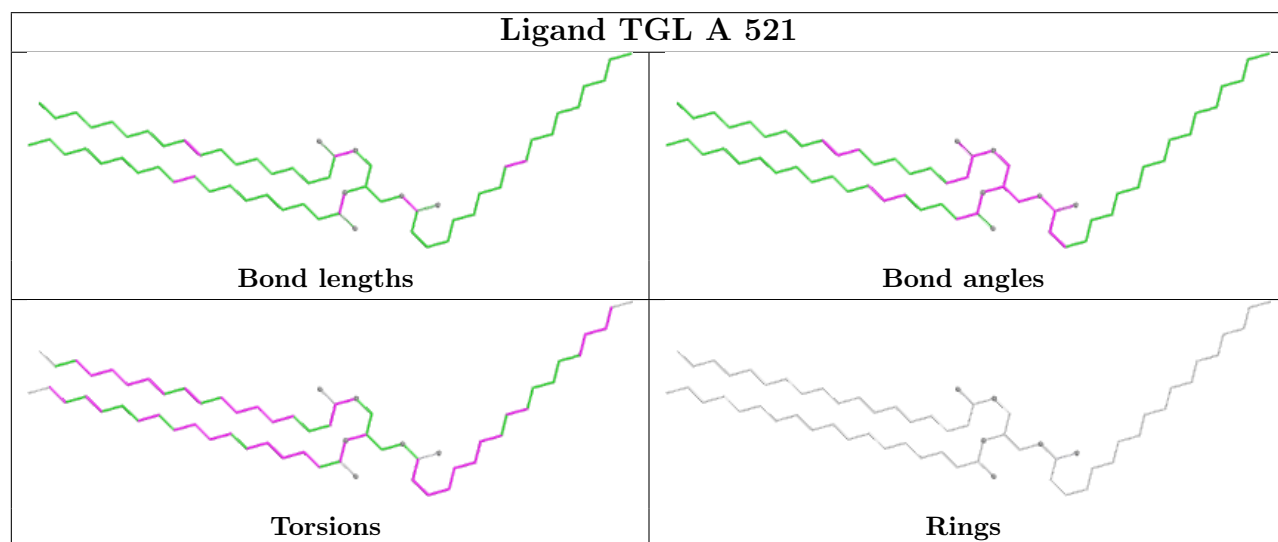


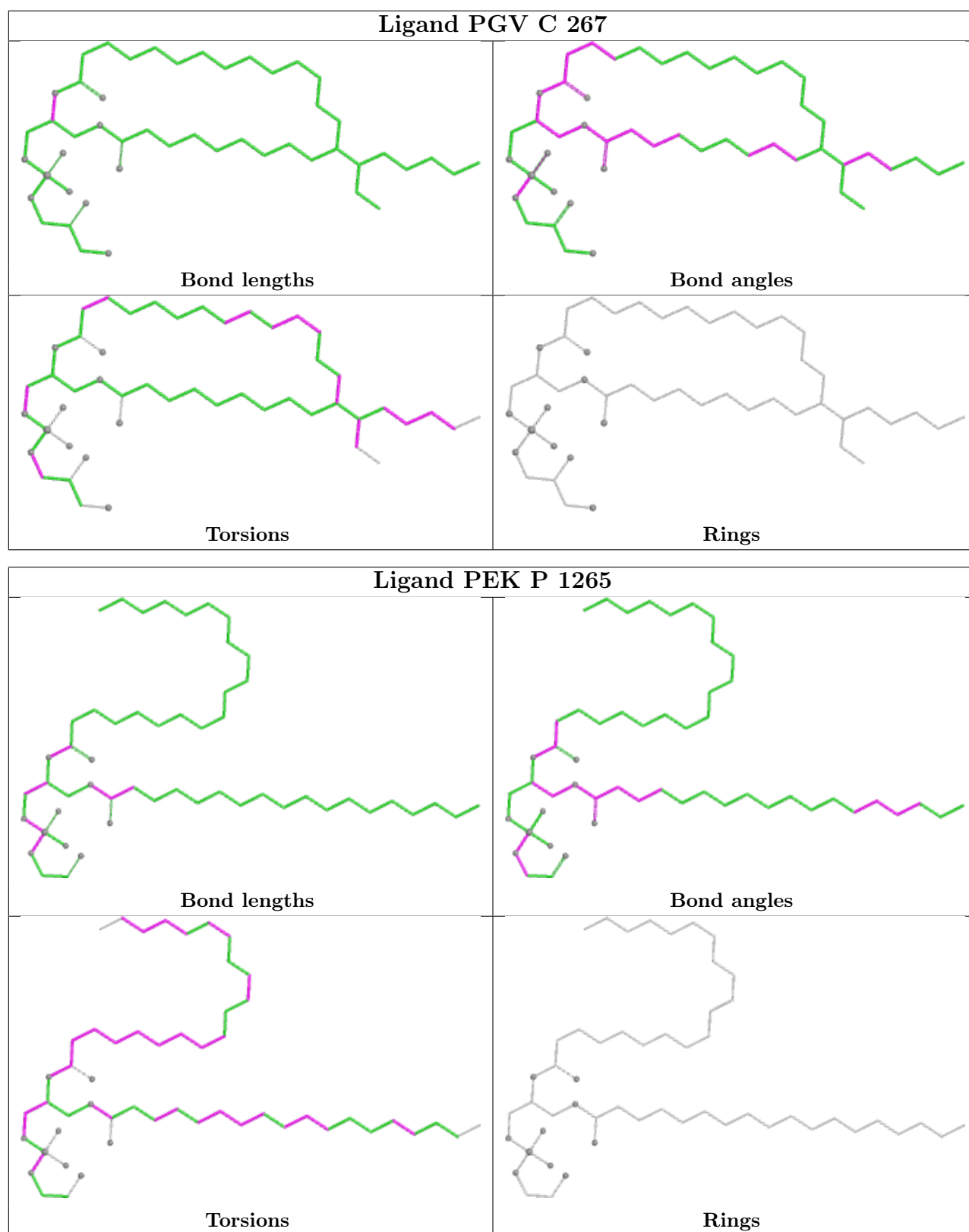


Ligand DMU M 526



Ligand TGL A 521





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.43	5 (0%) 79 80	12, 25, 33, 64	5 (0%)
1	N	513/514 (99%)	-0.08	8 (1%) 70 71	14, 28, 36, 63	5 (0%)
2	B	226/227 (99%)	0.13	13 (5%) 29 27	20, 30, 48, 68	0
2	O	226/227 (99%)	0.53	17 (7%) 20 18	25, 34, 58, 80	0
3	C	259/261 (99%)	-0.22	3 (1%) 76 77	23, 27, 39, 61	0
3	P	259/261 (99%)	0.10	4 (1%) 72 72	25, 30, 41, 58	0
4	D	144/147 (97%)	0.33	4 (2%) 55 55	27, 34, 48, 64	0
4	Q	144/147 (97%)	1.16	20 (13%) 6 5	31, 40, 65, 115	0
5	E	105/109 (96%)	0.35	3 (2%) 53 53	28, 33, 58, 98	0
5	R	105/109 (96%)	0.76	4 (3%) 44 44	29, 37, 58, 101	0
6	F	98/98 (100%)	0.72	9 (9%) 14 12	26, 35, 79, 127	0
6	S	98/98 (100%)	1.00	11 (11%) 10 8	27, 37, 85, 121	0
7	G	83/85 (97%)	1.20	22 (26%) 1 1	25, 33, 90, 108	0
7	T	83/85 (97%)	1.35	20 (24%) 2 1	26, 34, 91, 107	0
8	H	79/85 (92%)	0.91	12 (15%) 5 4	27, 37, 83, 109	0
8	U	79/85 (92%)	1.10	15 (18%) 3 2	30, 41, 88, 109	0
9	I	72/73 (98%)	0.80	11 (15%) 5 4	28, 40, 57, 66	0
9	V	72/73 (98%)	1.19	13 (18%) 3 3	30, 44, 61, 77	0
10	J	58/59 (98%)	0.58	5 (8%) 16 14	27, 35, 56, 97	0
10	W	58/59 (98%)	0.99	6 (10%) 12 10	29, 37, 57, 102	0
11	K	49/56 (87%)	0.84	4 (8%) 17 15	30, 37, 52, 66	0
11	X	49/56 (87%)	1.27	9 (18%) 3 2	34, 42, 56, 72	0
12	L	46/47 (97%)	0.17	2 (4%) 40 39	25, 31, 48, 73	0
12	Y	46/47 (97%)	0.76	4 (8%) 16 14	29, 34, 51, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.68	5 (11%) 9 8	27, 31, 69, 98	0
13	Z	43/46 (93%)	1.17	7 (16%) 4 3	32, 37, 79, 106	0
All	All	3550/3614 (98%)	0.33	236 (6%) 24 23	12, 31, 58, 127	10 (0%)

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	19.4
6	F	1	ALA	14.0
4	Q	6	VAL	13.1
6	S	97	ALA	11.0
8	U	8	ILE	9.5
6	F	96	LEU	9.1
8	H	8	ILE	8.8
7	T	3	ALA	8.2
8	H	47	GLY	8.1
4	Q	5	VAL	8.0
6	S	94	HIS	8.0
7	G	36	TRP	7.6
2	O	227	LEU	7.5
6	S	98	HIS	7.5
6	S	96	LEU	7.3
7	T	4	ALA	6.6
7	G	7	ASP	6.6
7	T	36	TRP	6.5
7	G	1	ALA	6.3
7	G	9	GLY	6.3
6	F	97	ALA	6.1
5	R	109	VAL	5.9
7	G	2	SER	5.9
4	Q	4	SER	5.8
2	B	59	GLN	5.8
7	G	37	LEU	5.7
7	T	9	GLY	5.6
7	T	5	LYS	5.5
9	V	3	ALA	5.5
6	S	95	GLN	5.5
7	G	10	GLY	5.4
9	I	37	PHE	5.4
7	G	5	LYS	5.3
2	O	59	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
12	L	47	LYS	5.3
9	V	2	THR	5.3
7	G	3	ALA	5.2
7	G	4	ALA	5.2
7	G	8	HIS	5.2
6	S	3	GLY	5.2
7	T	2	SER	5.2
6	S	2	SER	5.0
2	O	90	ILE	5.0
4	Q	7	LYS	5.0
7	T	37	LEU	4.9
2	O	226	MET	4.9
8	U	44	THR	4.9
8	H	7	LYS	4.9
2	O	113	TYR	4.8
13	M	40	TYR	4.8
8	H	48	GLY	4.8
7	T	8	HIS	4.8
2	B	92	ASN	4.7
11	K	6	ALA	4.7
7	G	6	GLY	4.7
7	T	1	ALA	4.6
2	B	90	ILE	4.6
7	T	10	GLY	4.6
4	Q	8	SER	4.5
6	F	94	HIS	4.5
11	X	7	PRO	4.5
7	T	7	ASP	4.5
12	L	2	HIS	4.5
8	U	47	GLY	4.5
10	W	58	LYS	4.5
7	T	84	LYS	4.4
10	J	58	LYS	4.4
11	X	6	ALA	4.4
13	M	43	SER	4.4
5	R	5	HIS	4.4
13	Z	40	TYR	4.4
8	U	45	ALA	4.3
13	Z	42	LYS	4.3
6	F	3	GLY	4.2
9	V	37	PHE	4.2
2	B	113	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
3	P	33	MET	4.1
6	F	98	HIS	4.0
8	H	9	LYS	4.0
6	F	2	SER	4.0
4	Q	51	LEU	4.0
5	E	5	HIS	3.9
3	P	37	PHE	3.9
9	V	36	LYS	3.9
6	F	95	GLN	3.8
7	T	6	GLY	3.8
1	N	484	THR	3.7
3	C	3	HIS	3.7
4	D	4	SER	3.7
4	Q	9	GLU	3.7
8	U	9	LYS	3.7
10	J	1	PHE	3.6
7	G	41	HIS	3.6
9	V	27	VAL	3.6
7	T	38	HIS	3.6
2	B	87	MET	3.6
12	Y	47	LYS	3.6
4	Q	48	TRP	3.5
13	Z	43	SER	3.5
8	U	42	ALA	3.5
8	U	48	GLY	3.5
13	Z	41	LYS	3.5
7	G	12	GLY	3.5
8	U	7	LYS	3.5
7	T	12	GLY	3.4
13	M	42	LYS	3.4
7	G	38	HIS	3.4
13	M	41	LYS	3.4
10	W	52	TRP	3.4
2	O	224	ALA	3.4
10	W	57	HIS	3.3
7	G	40	GLY	3.3
8	H	50	VAL	3.3
3	C	33	MET	3.3
10	W	55	PHE	3.3
7	G	84	LYS	3.3
1	A	514	LYS	3.3
6	S	93	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	O	32	PHE	3.3
2	B	65	TRP	3.3
11	K	47	ARG	3.2
8	H	10	ASN	3.2
12	Y	2	HIS	3.2
8	H	45	ALA	3.2
5	E	109	VAL	3.2
2	O	87	MET	3.2
7	G	39	SER	3.2
2	O	65	TRP	3.1
2	B	91	ASN	3.1
8	U	43	MET	3.1
8	H	44	THR	3.1
4	Q	35	ALA	3.1
9	V	30	GLY	3.1
11	X	47	ARG	3.1
11	X	16	ALA	3.1
11	X	19	ALA	3.1
4	Q	33	LEU	3.0
12	Y	45	LEU	3.0
8	U	50	VAL	3.0
7	T	39	SER	3.0
4	Q	46	ALA	3.0
8	H	46	LYS	3.0
11	K	7	PRO	3.0
13	Z	38	ASP	2.9
2	O	60	GLU	2.9
3	C	38	ASN	2.9
2	B	16	ILE	2.9
1	A	298	ASP	2.9
13	Z	39	ASN	2.9
7	T	42	ARG	2.9
4	D	11	TYR	2.8
8	H	43	MET	2.8
10	W	1	PHE	2.8
8	U	10	ASN	2.8
1	N	514	LYS	2.8
1	N	113	LEU	2.8
4	Q	40	LEU	2.7
8	U	61	LYS	2.7
1	N	297	MET	2.7
9	V	33	THR	2.7

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Mol	Chain	Res	Type	RSRZ
10	J	56	PRO	2.7
9	V	73	LYS	2.7
8	H	42	ALA	2.7
9	I	29	LEU	2.7
4	Q	10	ASP	2.6
11	X	12	LYS	2.6
6	S	4	GLY	2.6
12	Y	20	ARG	2.6
8	U	46	LYS	2.6
9	I	36	LYS	2.6
2	B	32	PHE	2.6
10	W	56	PRO	2.6
1	A	113	LEU	2.6
9	I	32	ALA	2.6
2	O	129	LYS	2.6
2	O	217	LYS	2.6
4	Q	50	SER	2.6
3	P	3	HIS	2.5
4	Q	11	TYR	2.5
11	K	54	ARG	2.5
7	T	33	LEU	2.5
13	Z	32	TRP	2.5
7	G	33	LEU	2.5
7	G	42	ARG	2.5
2	O	92	ASN	2.4
1	A	297	MET	2.4
6	F	93	PRO	2.4
2	B	60	GLU	2.4
11	X	17	VAL	2.4
9	I	30	GLY	2.4
4	Q	49	SER	2.4
1	N	513	LEU	2.4
7	G	45	PRO	2.4
9	V	28	SER	2.4
4	Q	147	LYS	2.4
9	I	33	THR	2.3
4	D	5	VAL	2.3
11	X	28	VAL	2.3
1	N	512	ASN	2.3
2	O	91	ASN	2.3
9	I	23	GLY	2.3
7	T	35	SER	2.3

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Mol	Chain	Res	Type	RSRZ
13	M	39	ASN	2.3
9	V	26	MET	2.3
1	N	334	TRP	2.2
2	B	57	ASP	2.2
5	R	94	ASN	2.2
3	P	246	ASP	2.2
7	G	35	SER	2.2
8	U	11	TYR	2.2
1	A	513	LEU	2.2
10	J	55	PHE	2.2
9	I	73	LYS	2.2
5	E	7	THR	2.2
5	R	93	LEU	2.2
10	J	57	HIS	2.1
4	Q	87	PHE	2.1
4	Q	143	ASN	2.1
7	T	40	GLY	2.1
9	V	34	PHE	2.1
2	B	13	THR	2.1
4	Q	57	VAL	2.1
2	O	221	LYS	2.1
2	B	22	HIS	2.1
9	V	29	LEU	2.1
9	I	34	PHE	2.1
11	X	13	TYR	2.1
6	S	54	ASN	2.1
9	V	32	ALA	2.1
1	N	117	MET	2.0
9	I	26	MET	2.0
2	O	115	ASP	2.0
2	O	72	ILE	2.0
4	D	87	PHE	2.0
9	I	25	PHE	2.0
8	U	52	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	TPO	T	11	11/12	0.57	0.28	71,80,101,104	0
7	TPO	G	11	11/12	0.58	0.32	66,75,101,101	0
9	SAC	V	1	9/10	0.66	0.20	83,86,88,88	0
9	SAC	I	1	9/10	0.72	0.20	63,66,69,73	0
1	FME	N	1	10/11	0.86	0.17	42,48,77,80	0
1	FME	A	1	10/11	0.91	0.14	38,41,68,76	0
2	FME	B	1	10/11	0.95	0.09	20,30,40,52	0
2	FME	O	1	10/11	0.96	0.10	33,34,40,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	UNX	C	262	1/1	0.61	0.55	81,81,81,81	0
23	CHD	J	60	29/29	0.71	0.27	99,104,108,108	0
24	UNX	P	262	1/1	0.71	0.43	82,82,82,82	0
20	PGV	P	1268	51/51	0.73	0.26	57,77,111,112	0
28	DMU	P	1272	33/33	0.73	0.23	72,106,119,121	0
20	PGV	N	1524	51/51	0.74	0.26	41,76,121,123	0
23	CHD	W	1059	29/29	0.75	0.24	101,108,110,112	0
25	PEK	G	265	53/53	0.75	0.25	47,79,103,105	0
25	PEK	G	1263	53/53	0.75	0.28	51,96,123,124	0
25	PEK	P	1265	53/53	0.75	0.25	46,76,107,110	0
25	PEK	T	263	53/53	0.75	0.26	48,94,121,122	0
28	DMU	G	272	33/33	0.75	0.22	72,100,115,116	0
19	TGL	Q	1523	63/63	0.75	0.27	56,74,100,102	0
26	CDL	T	1269	100/100	0.77	0.24	59,86,115,118	0
19	TGL	N	1522	63/63	0.77	0.25	49,64,84,89	0
26	CDL	P	1270	100/100	0.77	0.26	36,86,117,120	0
20	PGV	C	268	51/51	0.78	0.26	51,79,108,111	0
26	CDL	G	269	100/100	0.78	0.23	58,86,116,120	0
19	TGL	D	523	63/63	0.78	0.25	53,67,97,99	0
20	PGV	M	524	51/51	0.79	0.24	40,70,127,129	0
19	TGL	A	521	63/63	0.79	0.24	53,72,88,92	0

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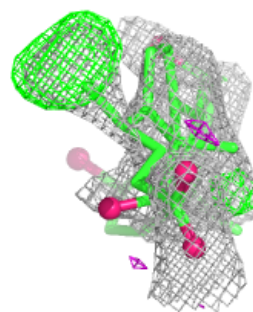
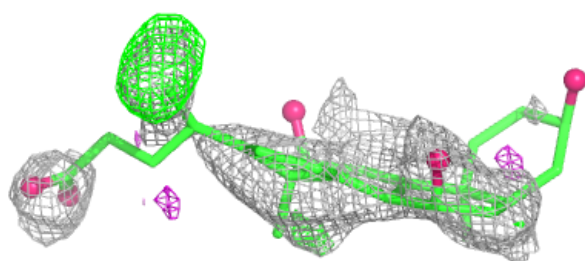
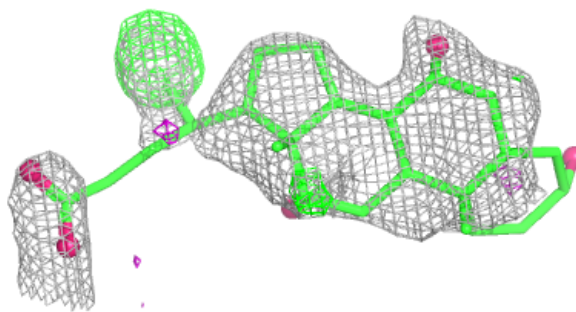
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CDL	C	270	100/100	0.80	0.23	42,84,109,110	0
19	TGL	L	522	63/63	0.80	0.23	36,62,78,81	0
22	PSC	R	1229	52/52	0.80	0.27	49,95,129,135	0
19	TGL	O	1521	63/63	0.81	0.21	53,75,88,92	0
22	PSC	B	229	52/52	0.82	0.25	45,95,136,139	0
23	CHD	C	271	29/29	0.87	0.13	54,61,65,73	0
28	DMU	Z	1526	33/33	0.87	0.14	40,50,71,75	0
23	CHD	P	1271	29/29	0.90	0.12	51,63,68,69	0
28	DMU	M	526	33/33	0.92	0.10	35,44,61,65	0
25	PEK	P	1264	53/53	0.94	0.14	25,49,81,82	0
20	PGV	N	1266	51/51	0.95	0.11	23,36,59,64	0
25	PEK	C	264	53/53	0.95	0.12	24,45,77,80	0
20	PGV	P	1267	51/51	0.95	0.12	23,37,80,82	0
23	CHD	O	229	29/29	0.96	0.07	21,25,31,33	0
23	CHD	P	1525	29/29	0.96	0.07	27,31,35,37	0
18	NA	N	519	1/1	0.96	0.09	31,31,31,31	0
23	CHD	C	525	29/29	0.96	0.07	21,30,35,38	0
20	PGV	C	267	51/51	0.97	0.10	22,33,73,74	0
23	CHD	B	1085	29/29	0.97	0.06	23,26,31,37	0
18	NA	A	519	1/1	0.97	0.09	28,28,28,28	0
17	MG	N	518	1/1	0.97	0.05	29,29,29,29	0
20	PGV	A	522	51/51	0.97	0.10	20,33,67,71	0
15	NO	A	520	2/2	0.98	0.06	24,24,24,25	0
17	MG	A	518	1/1	0.98	0.04	24,24,24,24	0
14	HEA	A	515	60/60	0.98	0.06	19,23,38,41	0
21	CUA	O	228	2/2	0.98	0.03	27,27,27,27	0
14	HEA	N	515	60/60	0.98	0.06	21,26,40,44	0
27	ZN	F	99	1/1	0.99	0.03	31,31,31,31	0
27	ZN	S	99	1/1	0.99	0.03	33,33,33,33	0
21	CUA	B	228	2/2	0.99	0.03	23,23,23,23	0
14	HEA	N	516	60/60	0.99	0.06	22,26,31,36	0
14	HEA	A	516	60/60	0.99	0.05	19,22,30,34	0
15	NO	N	520	2/2	0.99	0.05	26,26,26,31	0
16	CU	A	517	1/1	1.00	0.03	24,24,24,24	0
16	CU	N	517	1/1	1.00	0.04	26,26,26,26	0

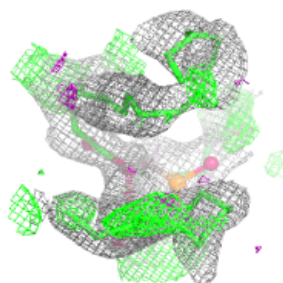
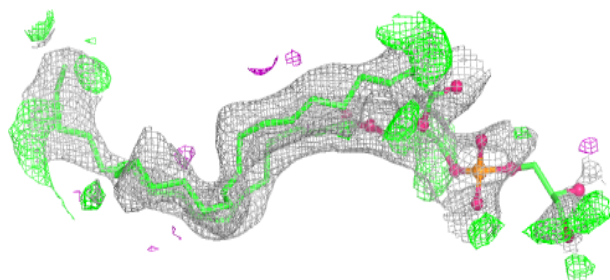
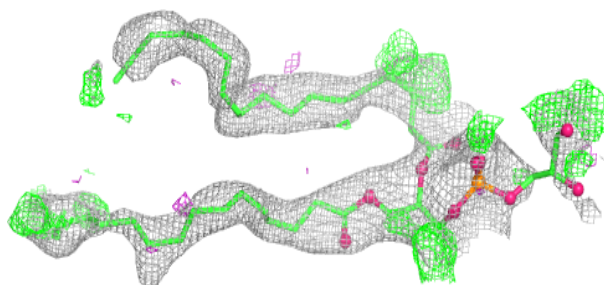
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD J 60:

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

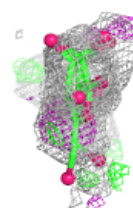
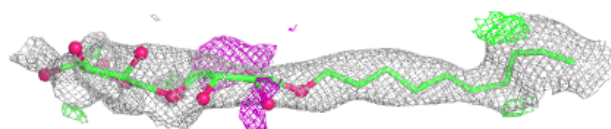
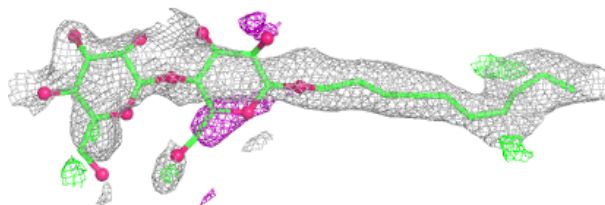
**Electron density around PGV P 1268:**

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

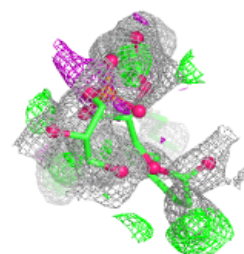
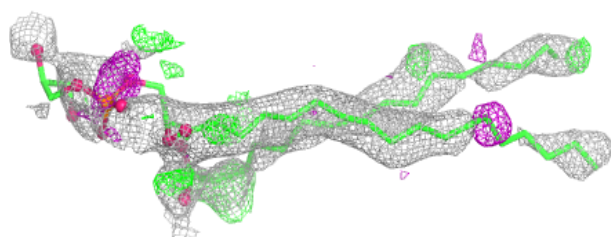
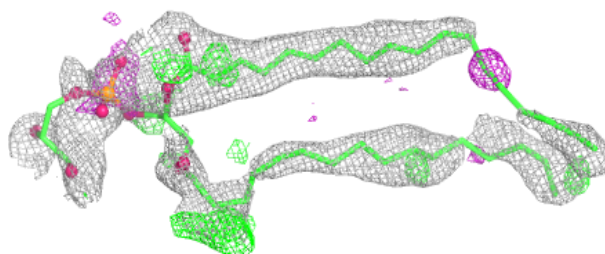


Electron density around DMU P 1272:

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

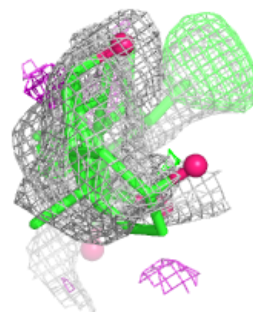
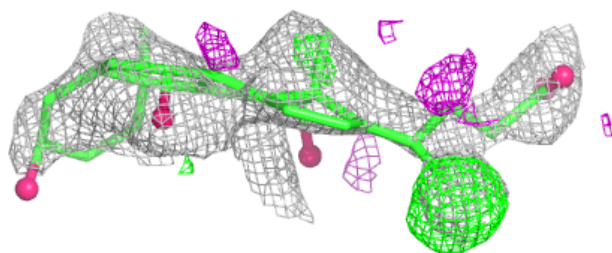
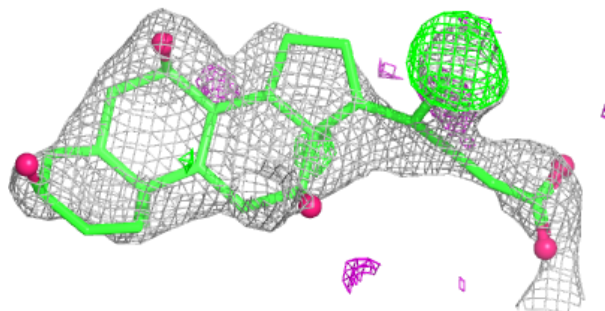
**Electron density around PGV N 1524:**

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



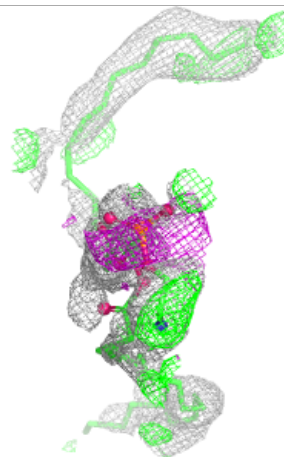
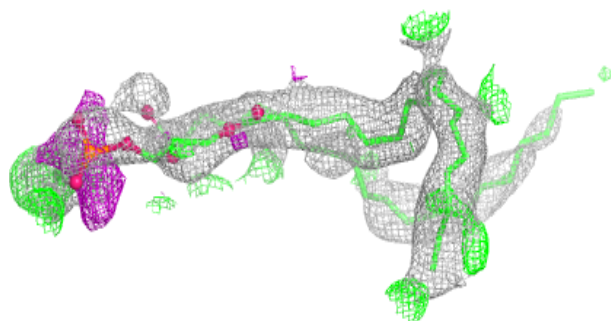
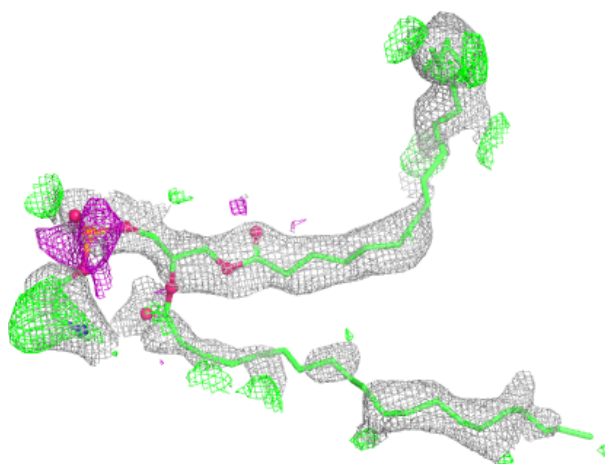
Electron density around CHD W 1059:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



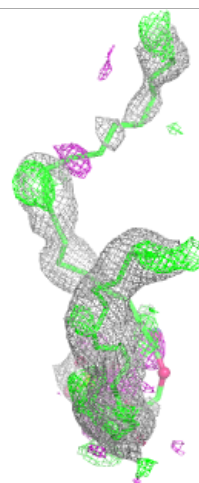
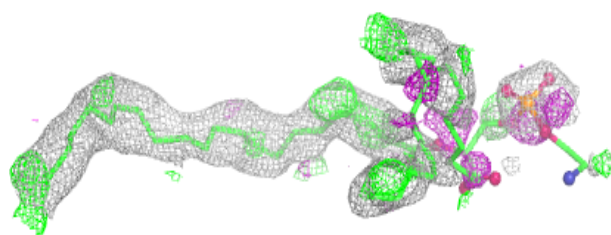
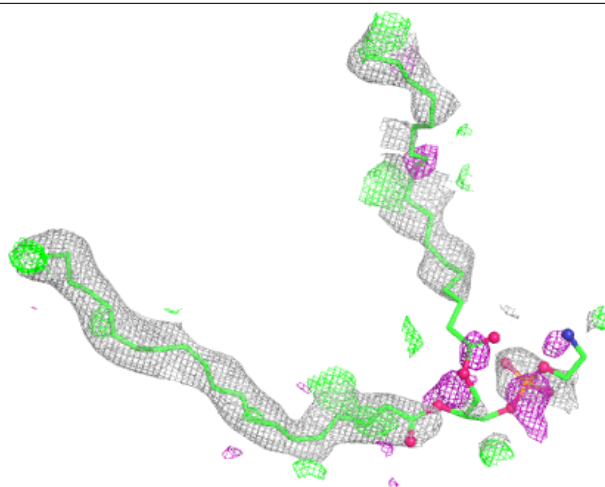
Electron density around PEK G 265:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



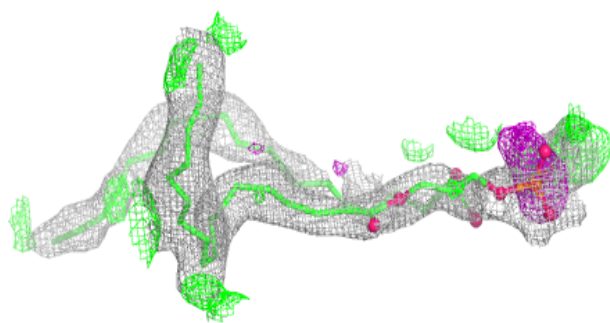
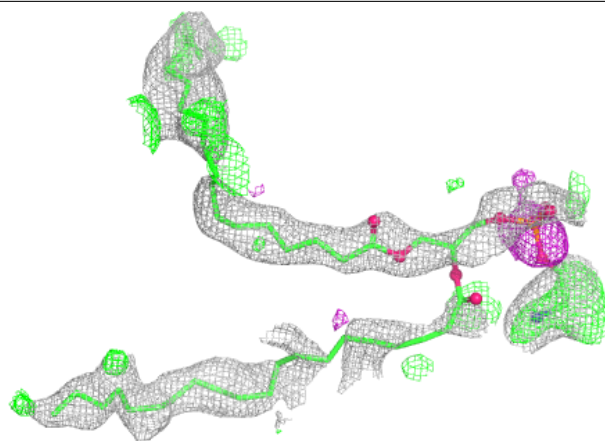
Electron density around PEK G 1263:

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



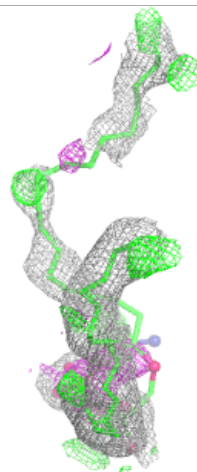
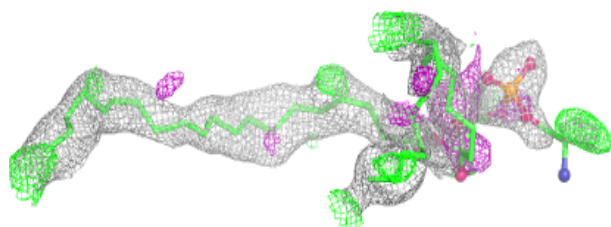
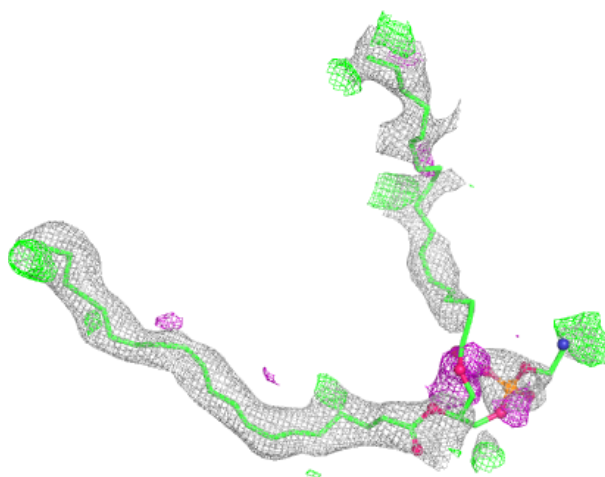
Electron density around PEK P 1265:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



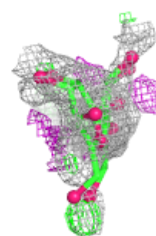
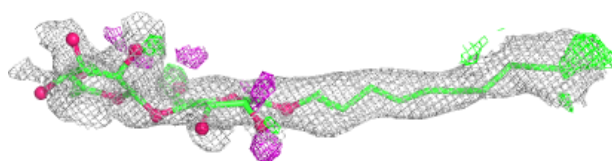
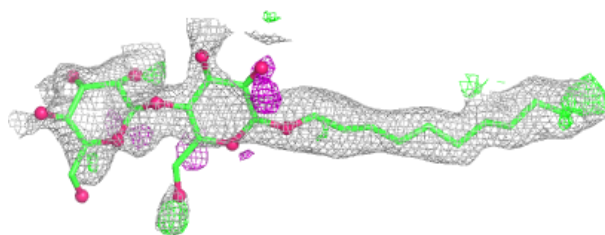
Electron density around PEK T 263:

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

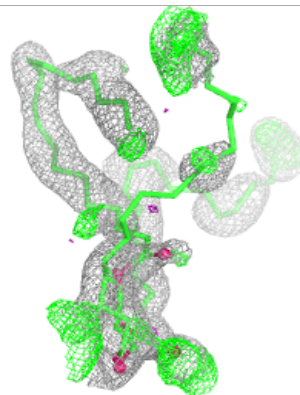
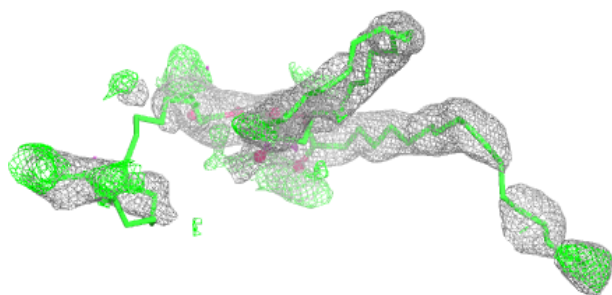
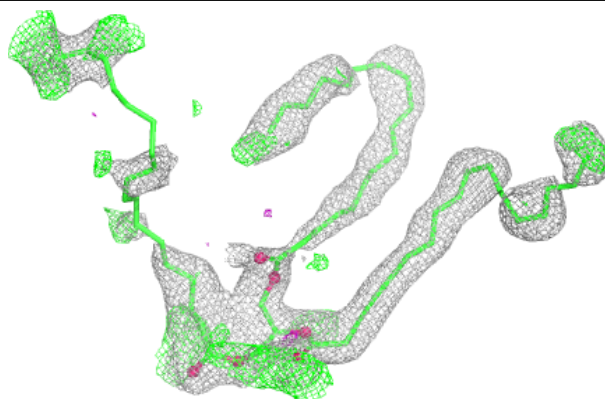


Electron density around DMU G 272:

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

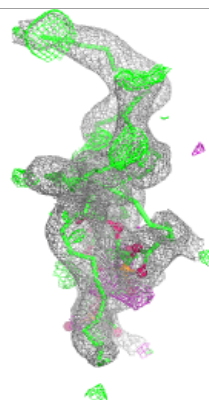
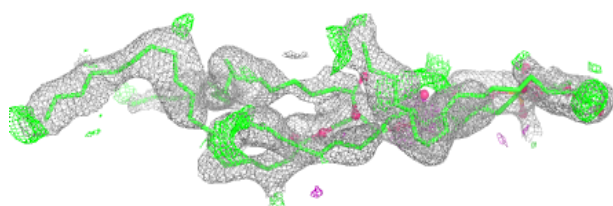
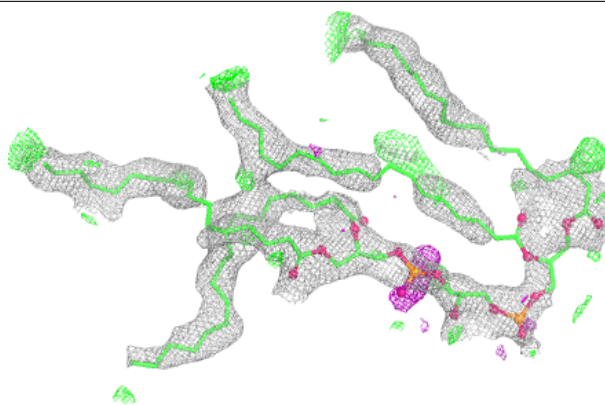
**Electron density around TGL Q 1523:**

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and green (positive)

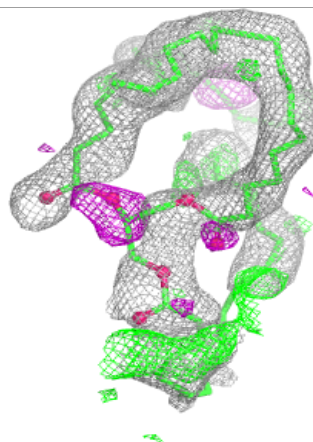
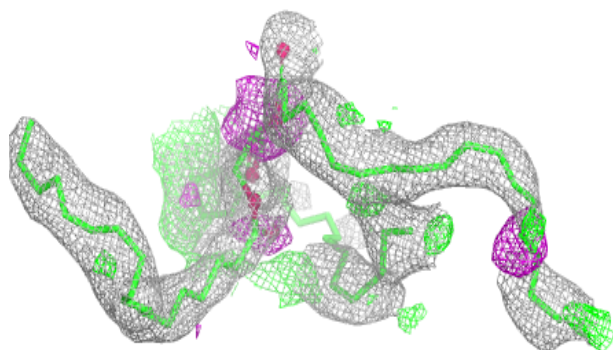
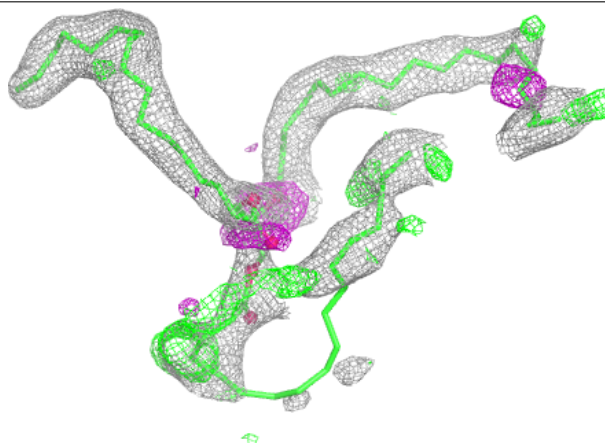


Electron density around CDL T 1269:

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

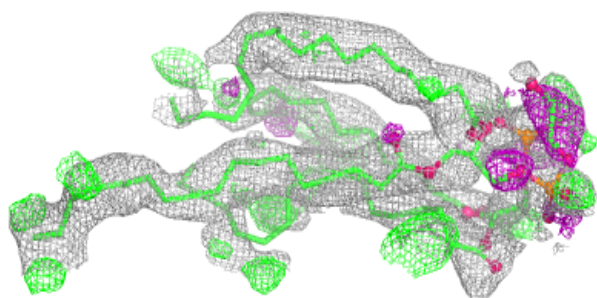
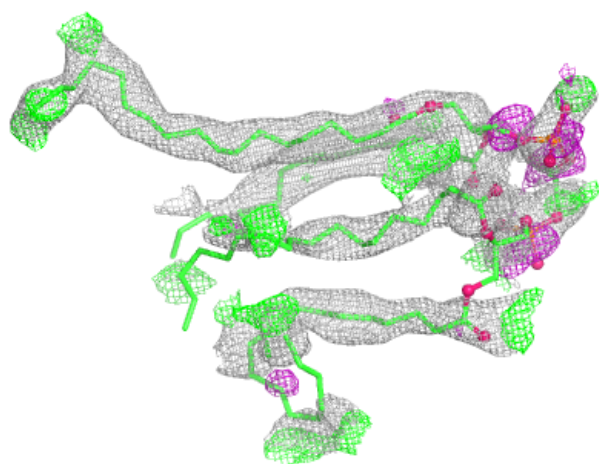
**Electron density around TGL N 1522:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



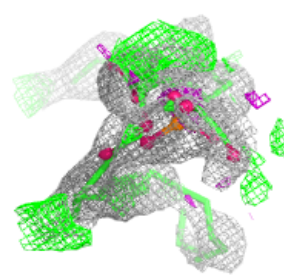
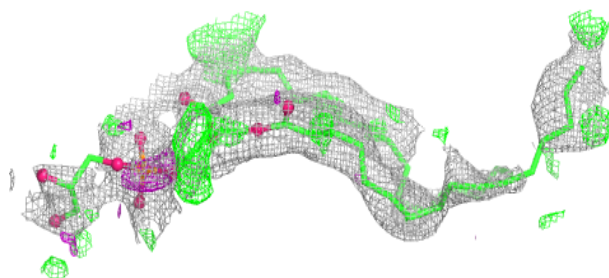
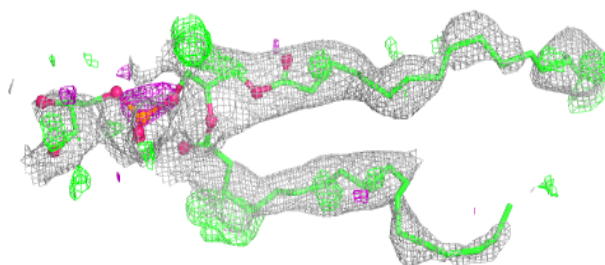
Electron density around CDL P 1270:

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and green (positive)

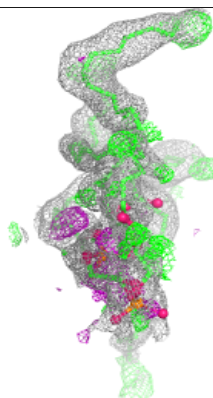
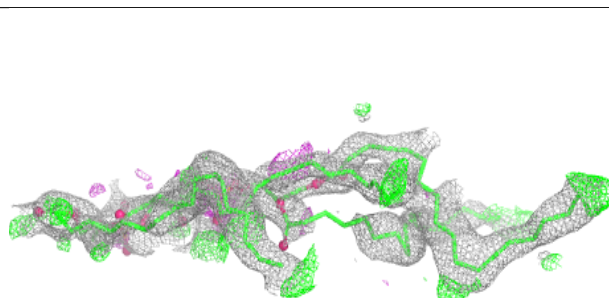
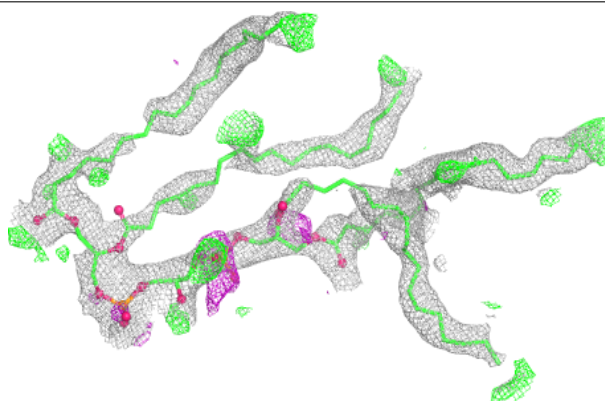


Electron density around PGV C 268:

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

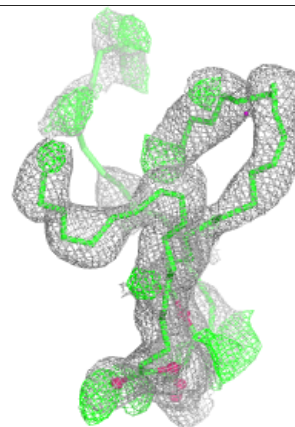
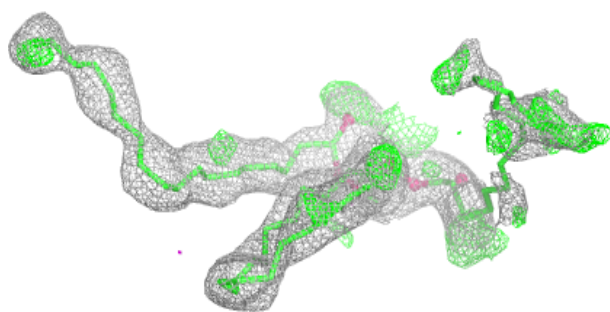
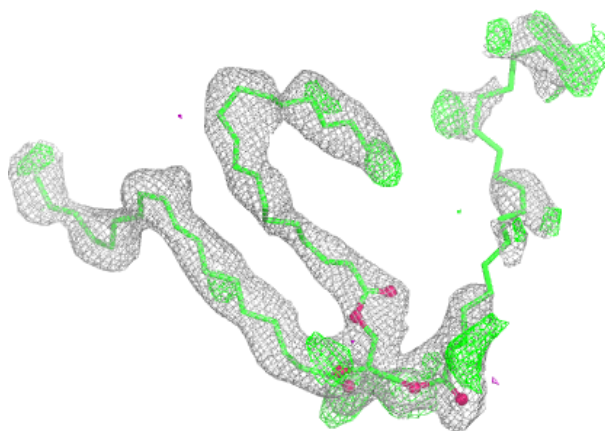
**Electron density around CDL G 269:**

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and green (positive)

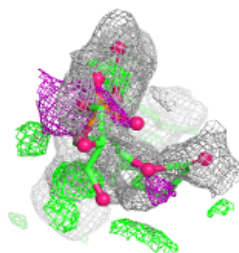
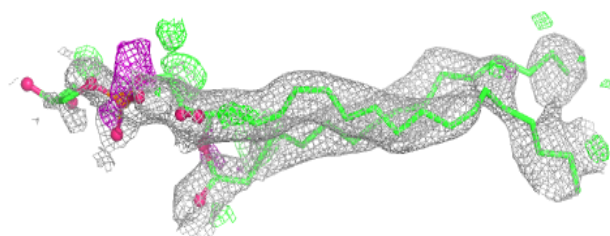
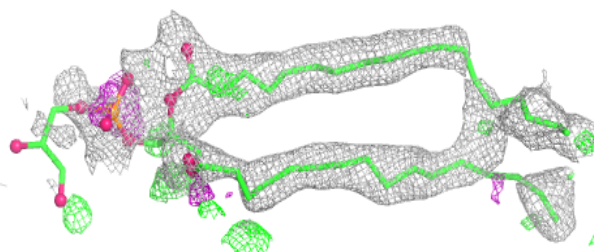


Electron density around TGL D 523:

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

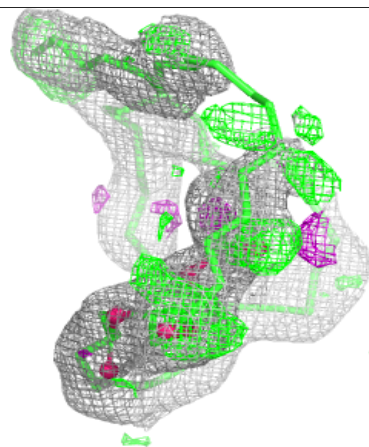
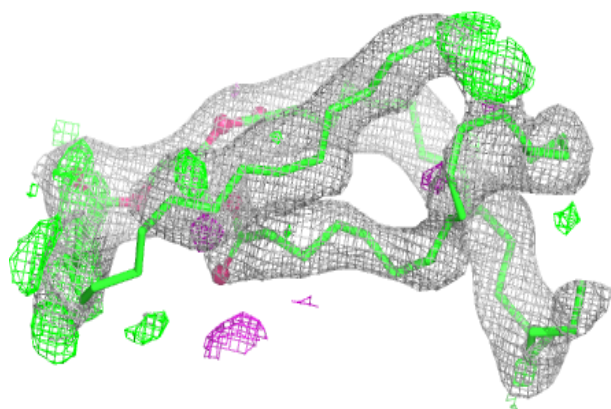
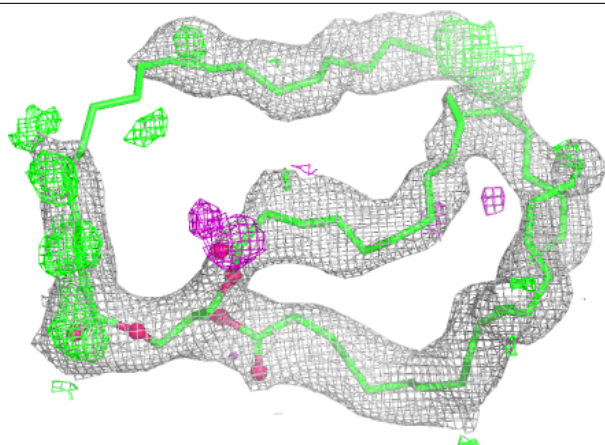
**Electron density around PGV M 524:**

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



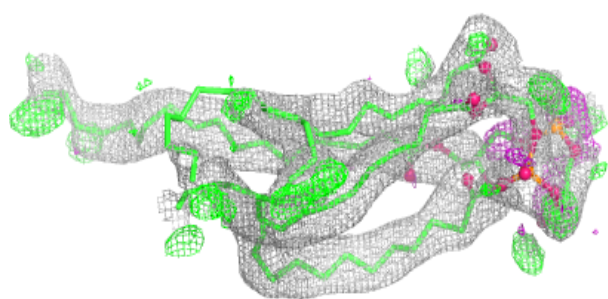
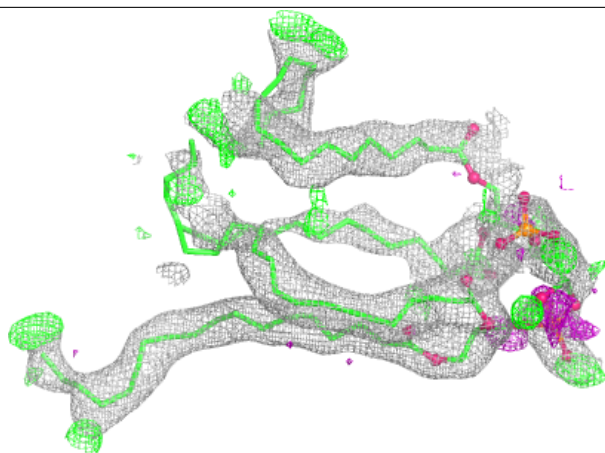
Electron density around TGL A 521:

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



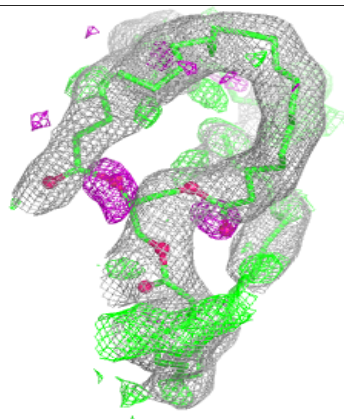
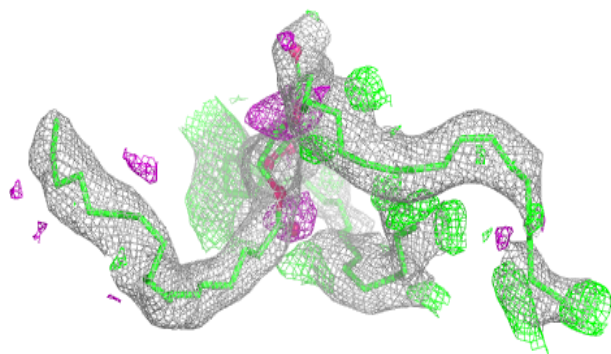
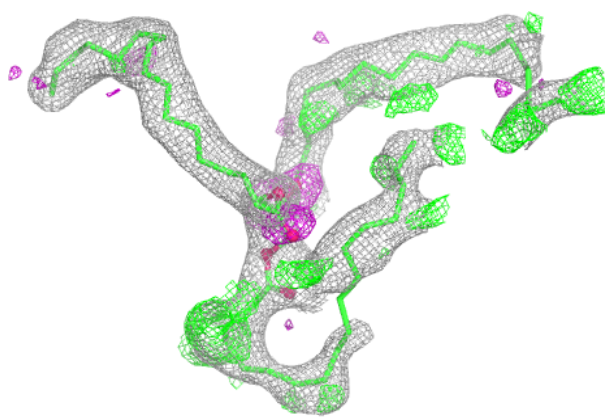
Electron density around CDL C 270:

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

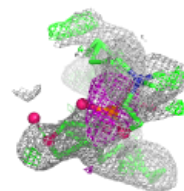
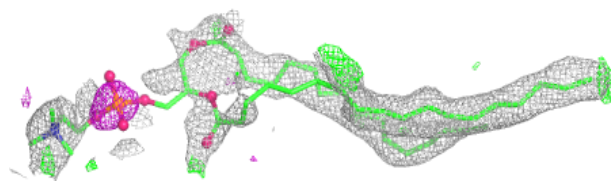
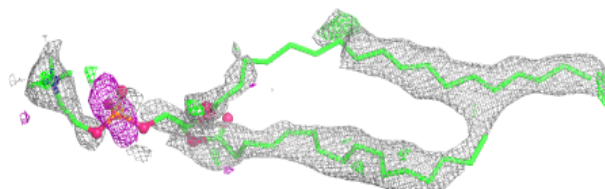


Electron density around TGL L 522:

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

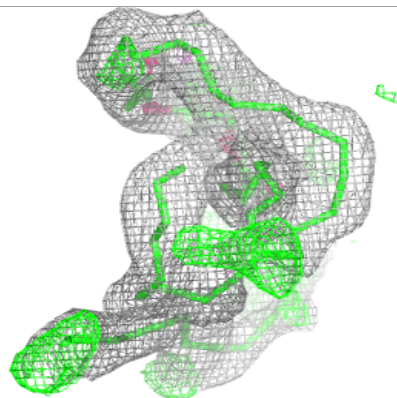
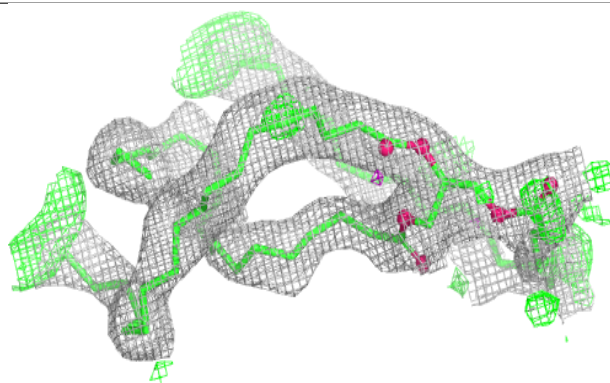
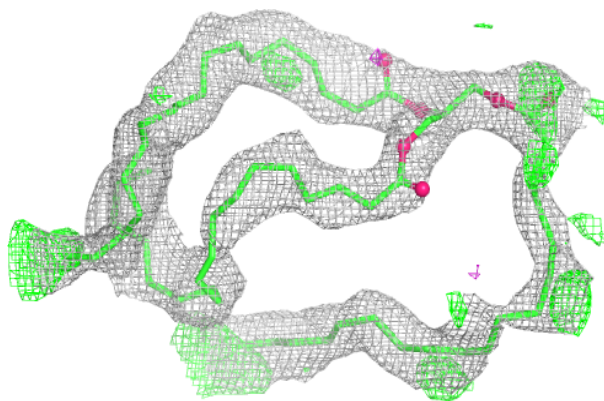
**Electron density around PSC R 1229:**

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

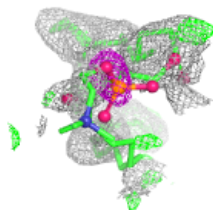
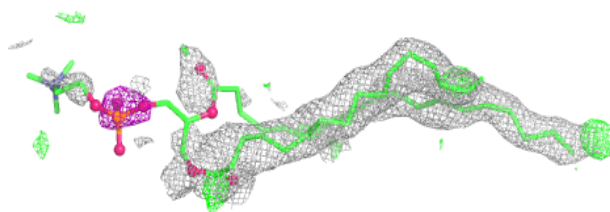
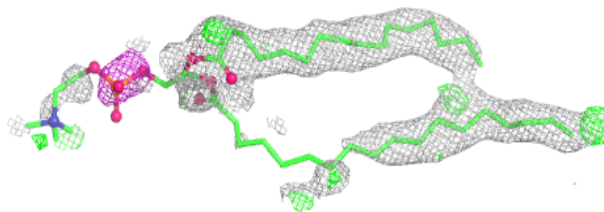


Electron density around TGL O 1521:

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

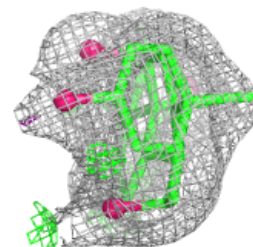
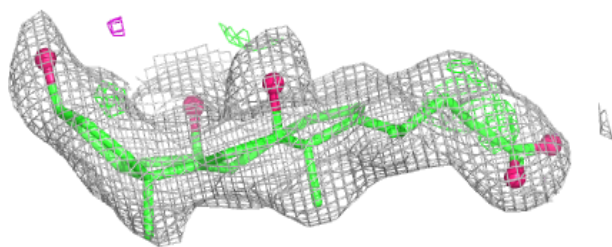
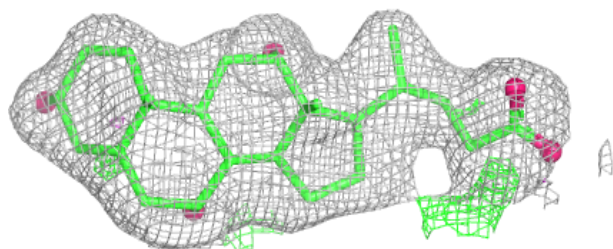
**Electron density around PSC B 229:**

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

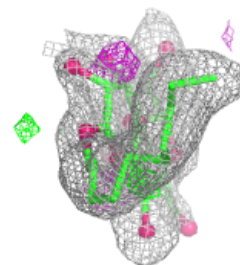
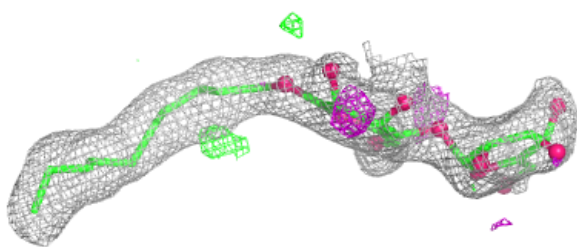
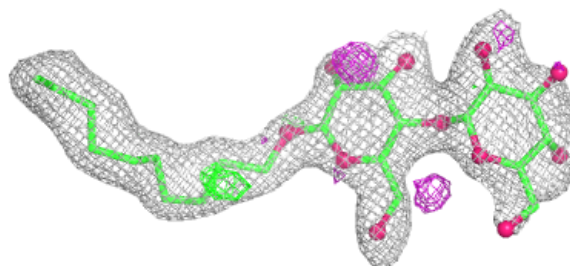


Electron density around CHD C 271:

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

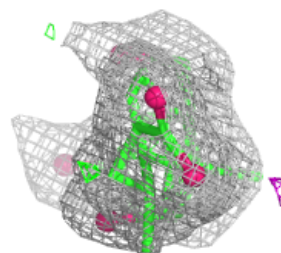
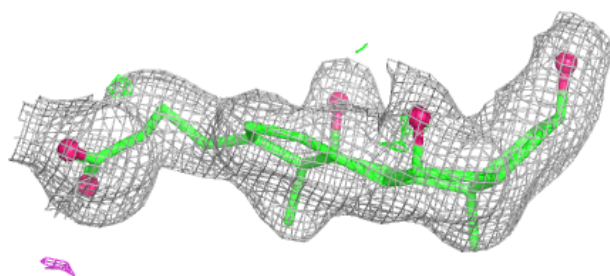
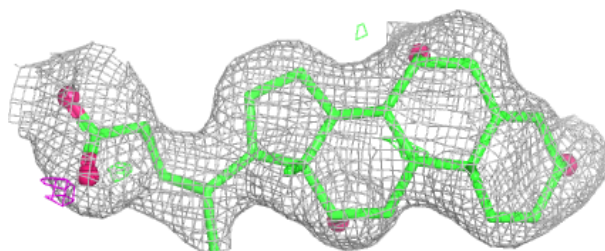
**Electron density around DMU Z 1526:**

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

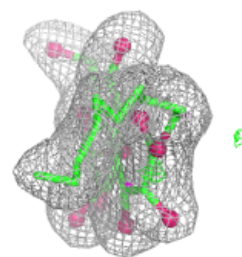
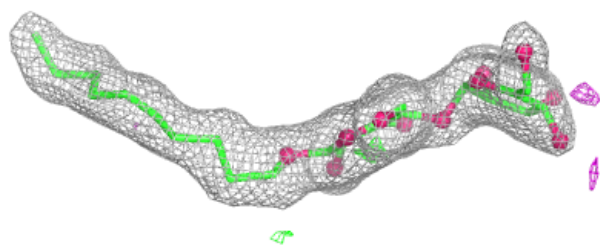


Electron density around CHD P 1271:

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

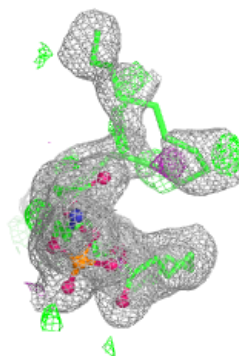
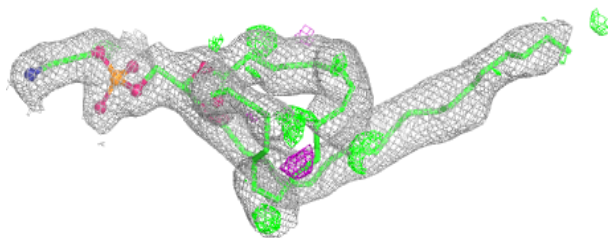
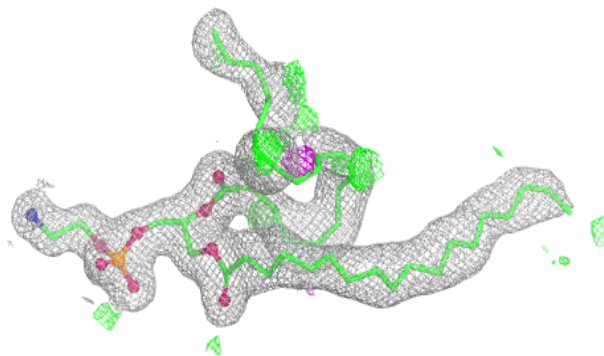
**Electron density around DMU M 526:**

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

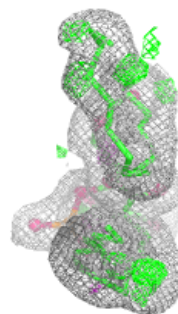
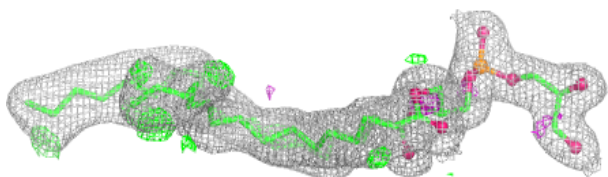
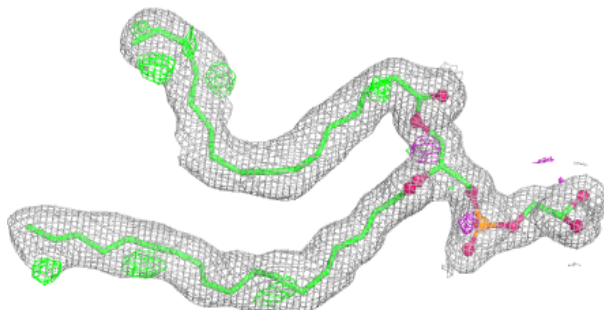


Electron density around PEK P 1264:

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

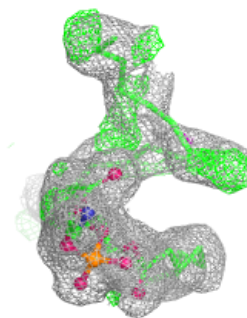
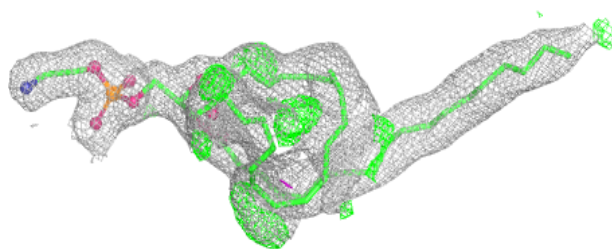
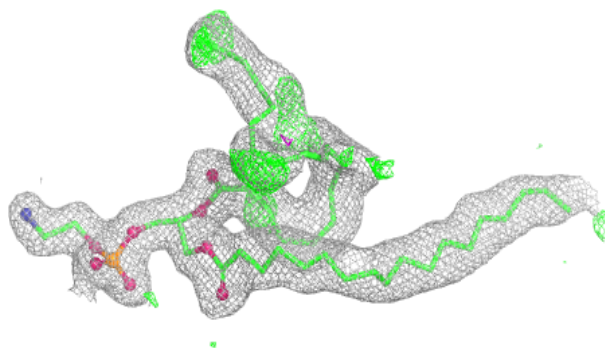
**Electron density around PGV N 1266:**

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

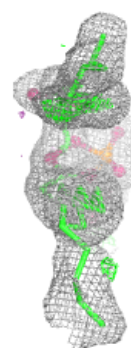
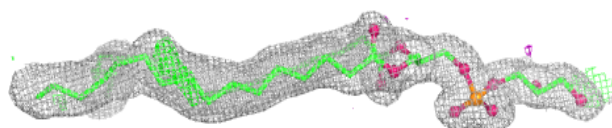
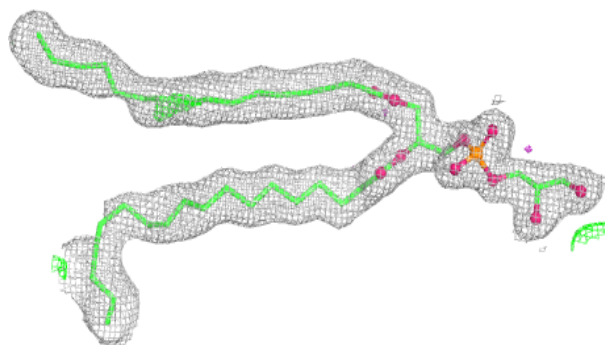


Electron density around PEK C 264:

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

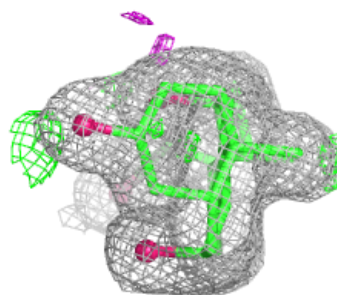
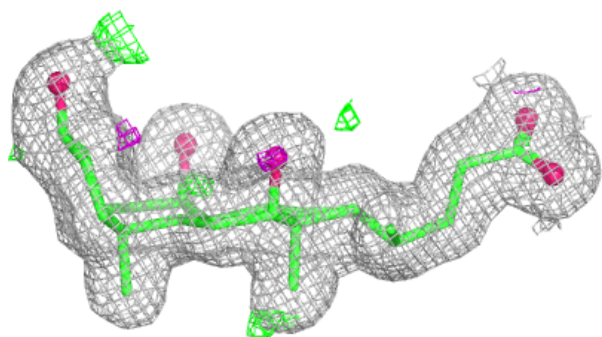
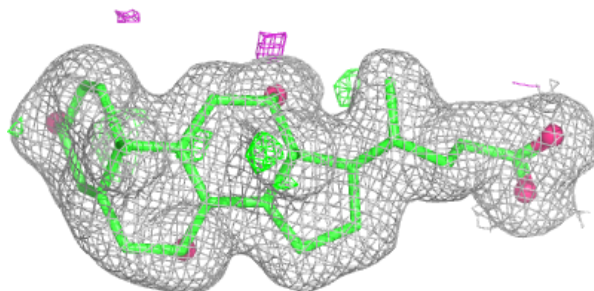
**Electron density around PGV P 1267:**

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

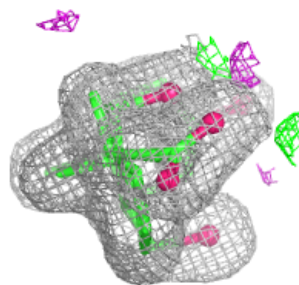
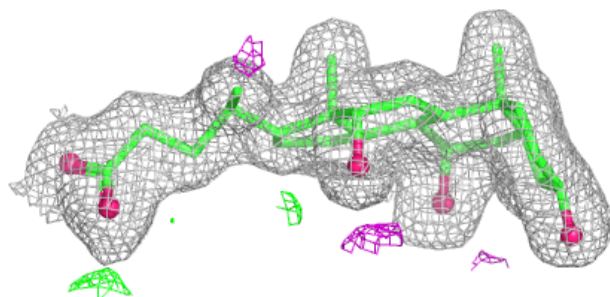
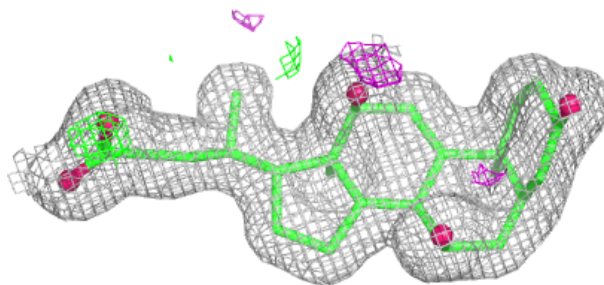


Electron density around CHD O 229:

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

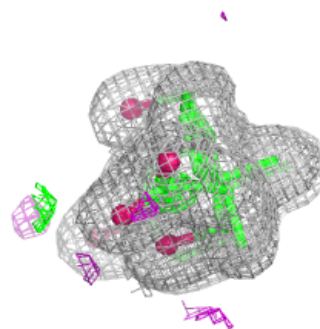
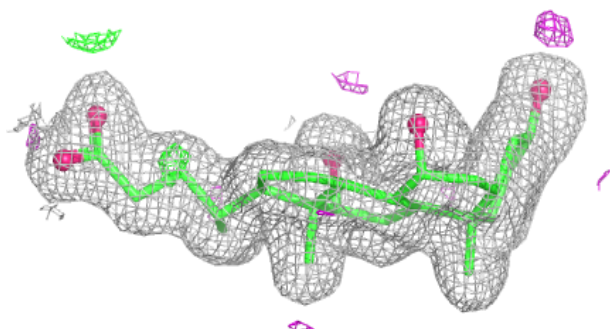
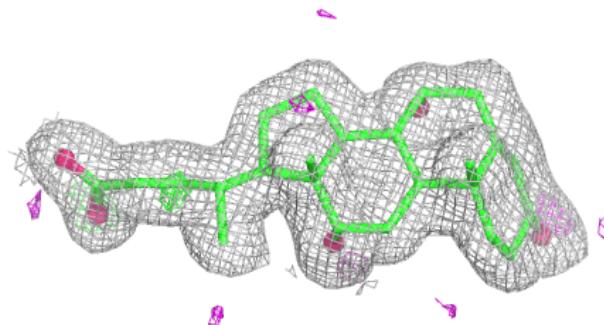
**Electron density around CHD P 1525:**

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

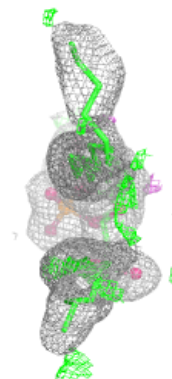
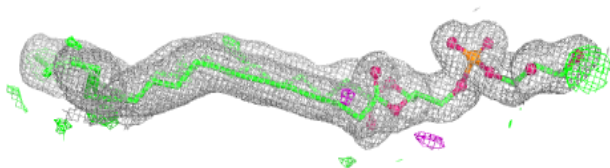
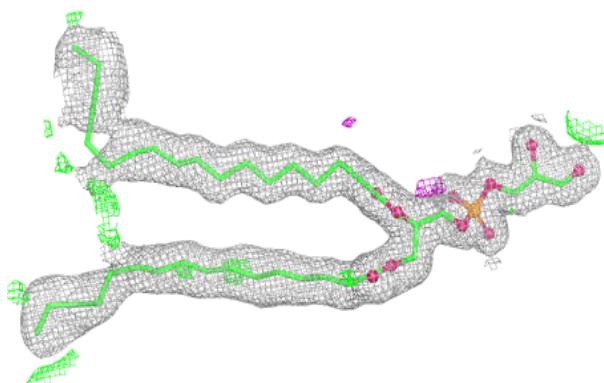


Electron density around CHD C 525:

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

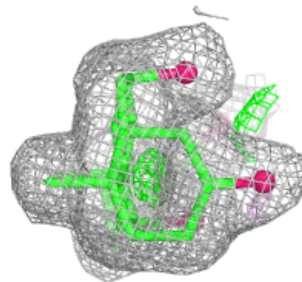
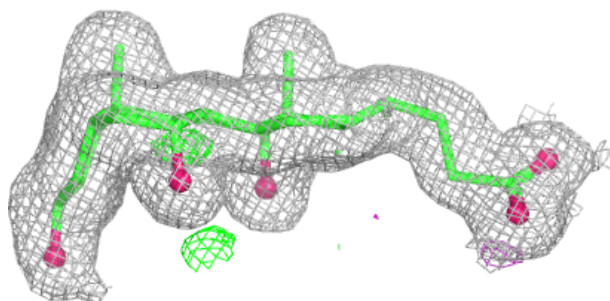
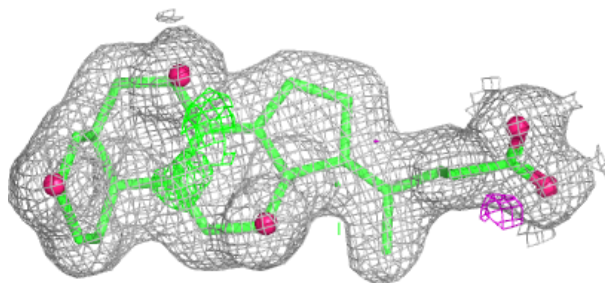
**Electron density around PGV C 267:**

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

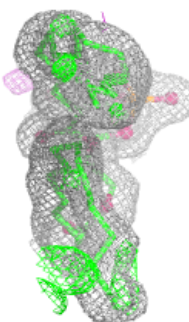
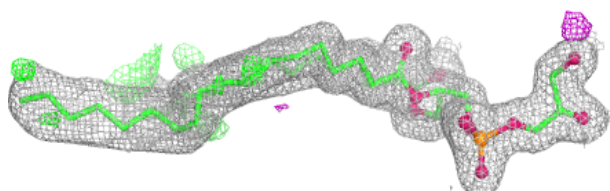
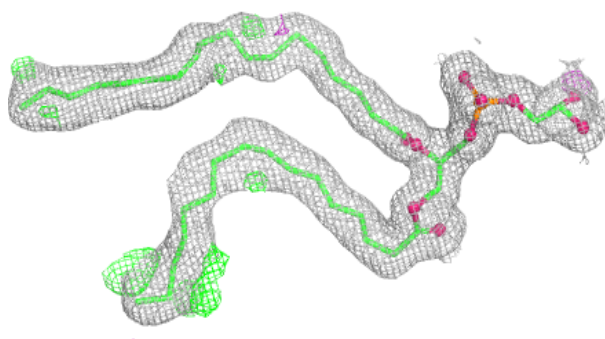


Electron density around CHD B 1085:

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

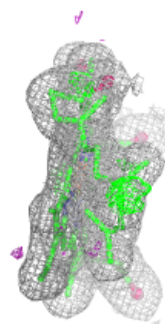
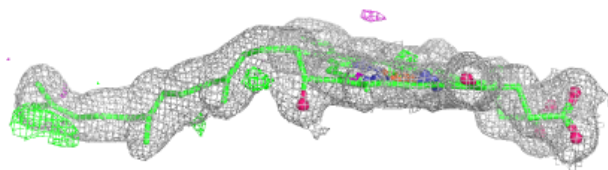
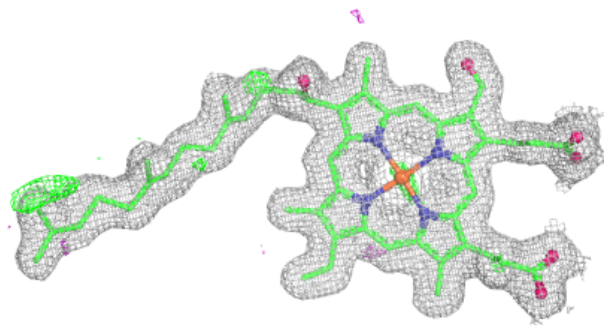
**Electron density around PGV A 522:**

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

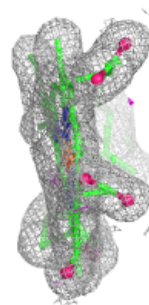
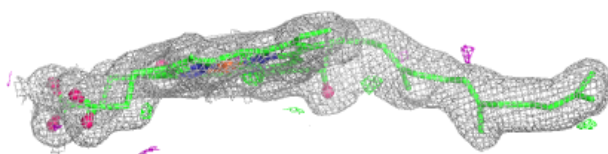
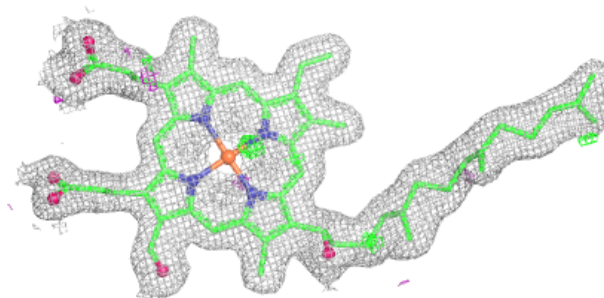


Electron density around HEA A 515:

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

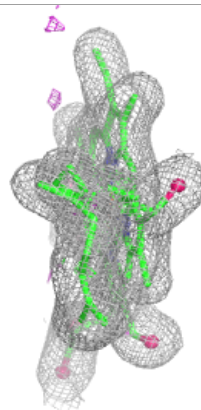
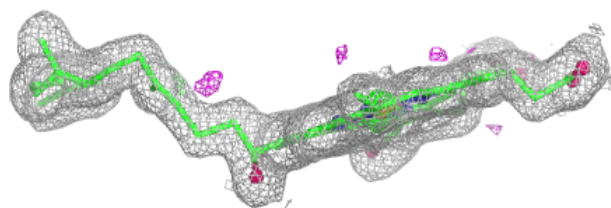
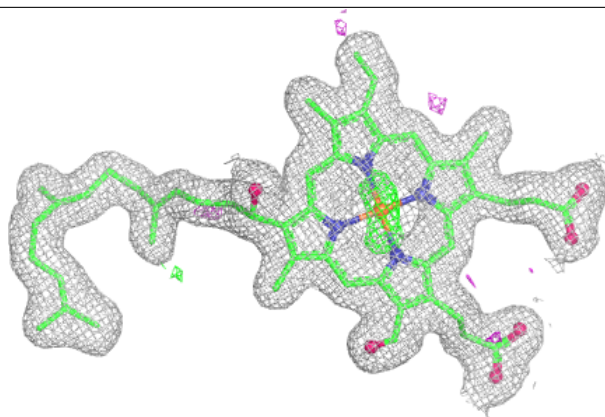
**Electron density around HEA N 515:**

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

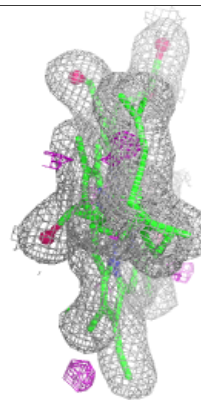
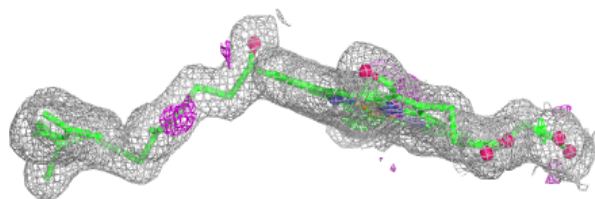
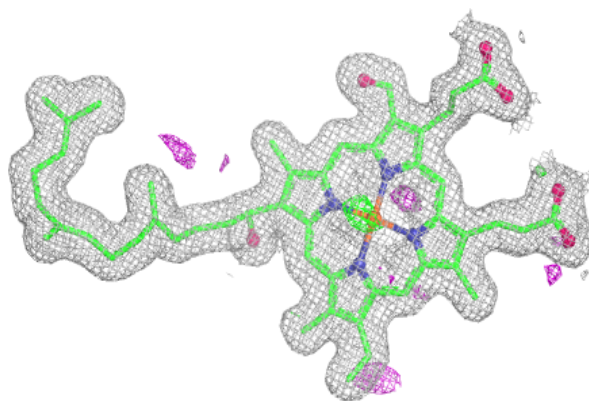


Electron density around HEA N 516:

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

**Electron density around HEA A 516:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.