



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:04 AM UTC

PDB ID : 2ZXW / pdb_00002zxw
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (1-s X-ray exposure dataset)
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Hirata, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.
Deposited on : 2009-01-08
Resolution : 2.50 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

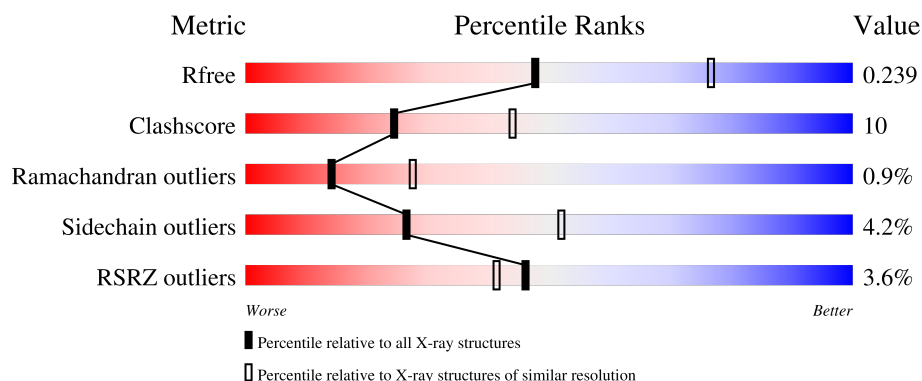
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

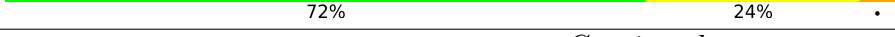
The reported resolution of this entry is 2.50 Å.

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.



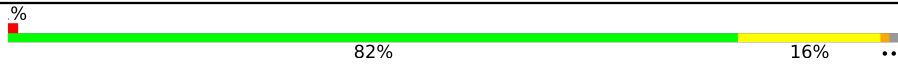
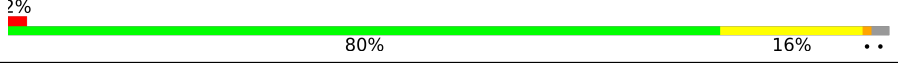
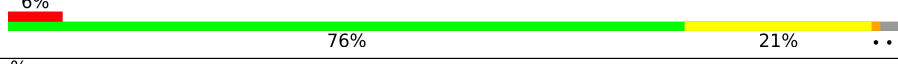
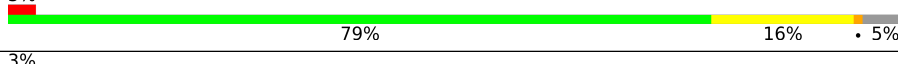
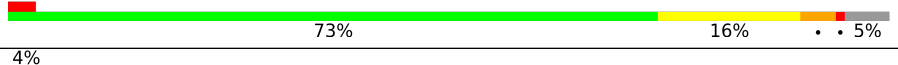
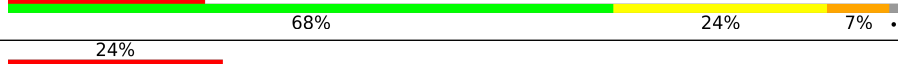
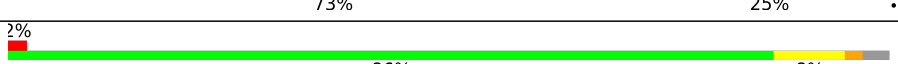
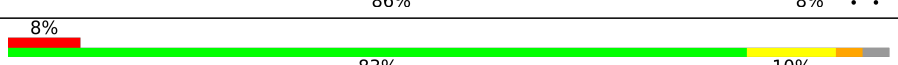
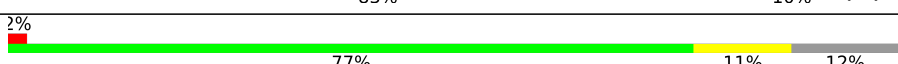
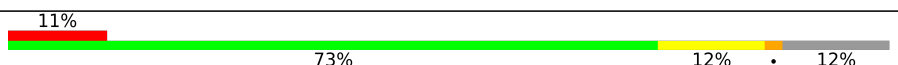
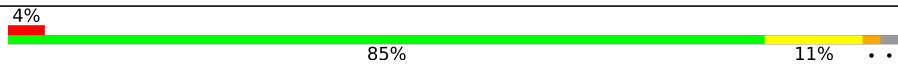
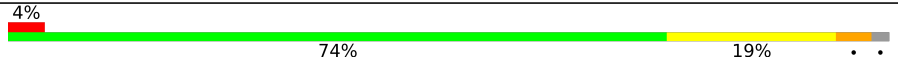
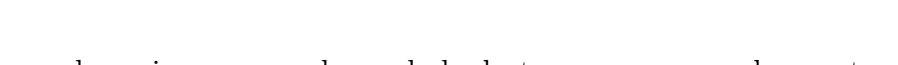
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	 78%21%.
1	N	514	 79%20%.
2	B	227	 2%75%22%.
2	O	227	 4%72%24%.

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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
23	CHD	B	1086	X	-	-	-
23	CHD	C	271	X	-	-	-
23	CHD	C	525	X	-	-	-
23	CHD	G	86	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 31827 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

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

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 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			

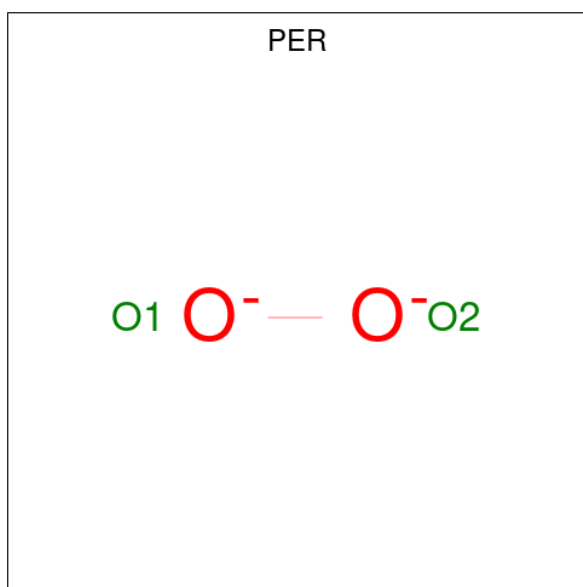
- Molecule 13 is a protein called Cytochrome c oxidase polypeptide 8H.

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 COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 15 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



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

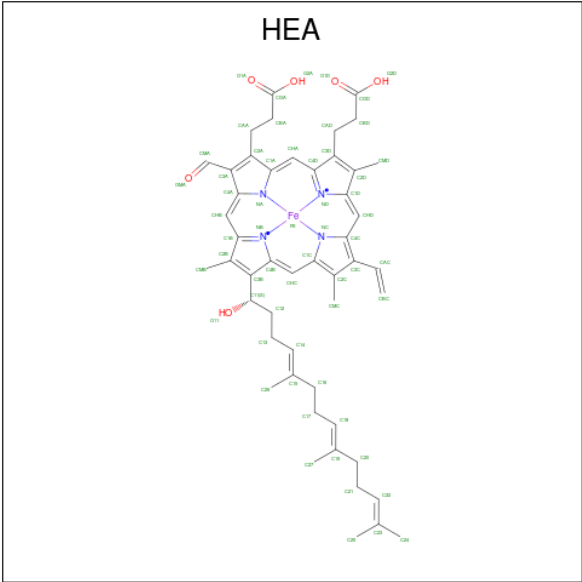
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

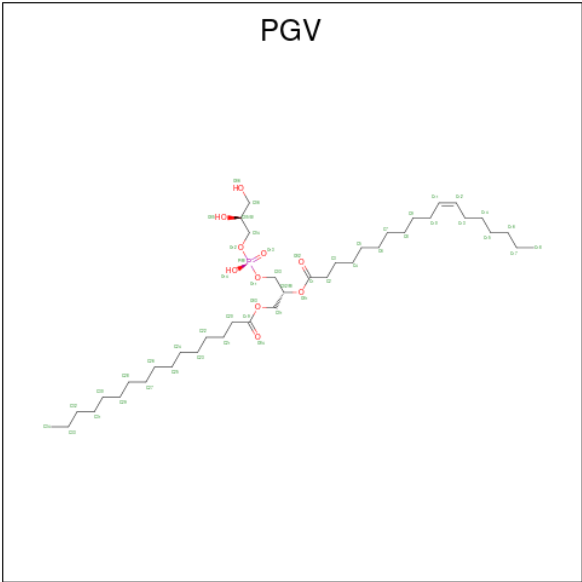
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



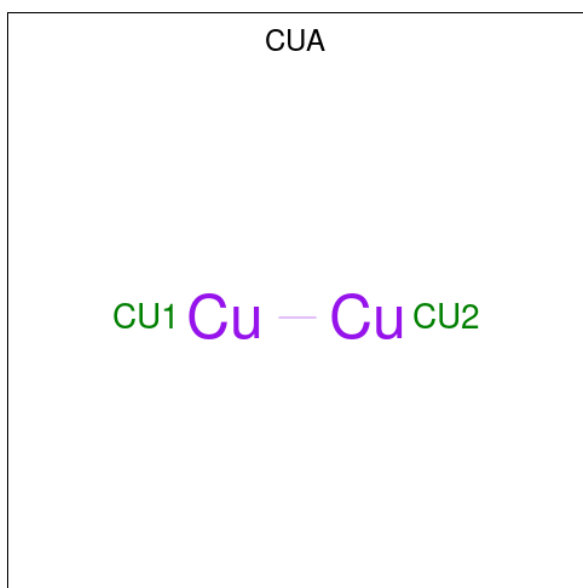
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY} (HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



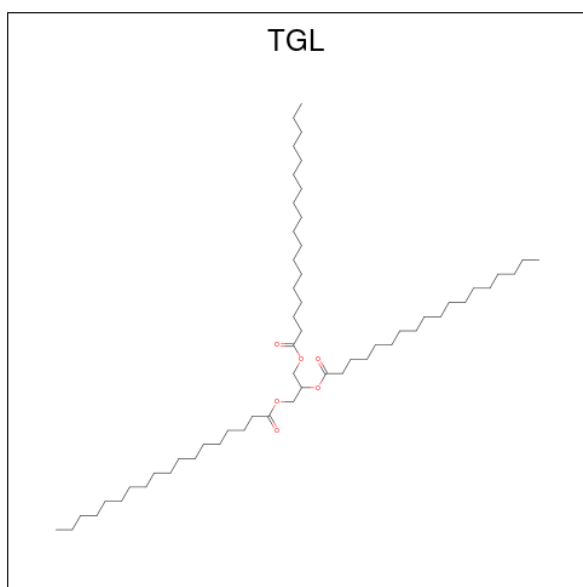
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O P 51 40 10 1	0	0
19	A	1	Total C O P 51 40 10 1	0	0
19	C	1	Total C O P 51 40 10 1	0	0
19	C	1	Total C O P 51 40 10 1	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	P	1	Total C O P 51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

- Molecule 20 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



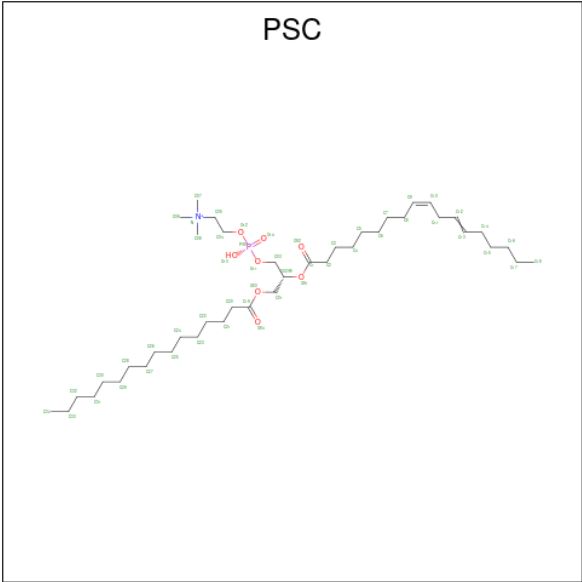
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total Cu 2 2	0	0
20	O	1	Total Cu 2 2	0	0

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



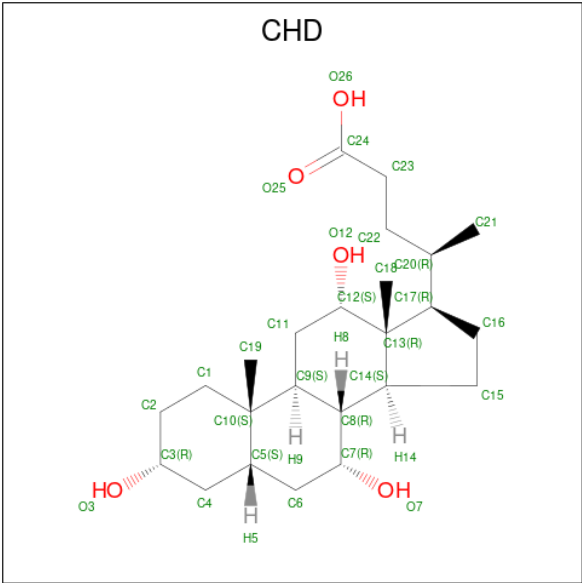
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)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		
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



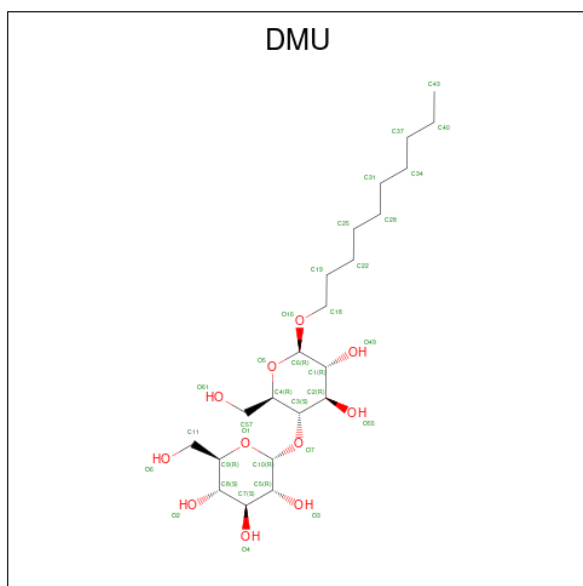
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).

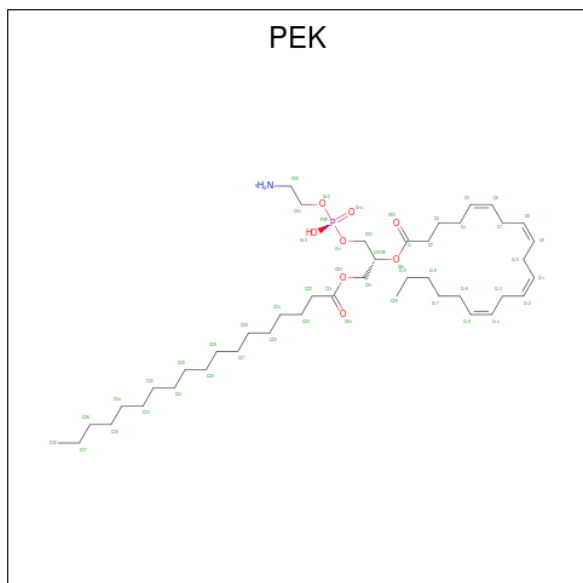


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

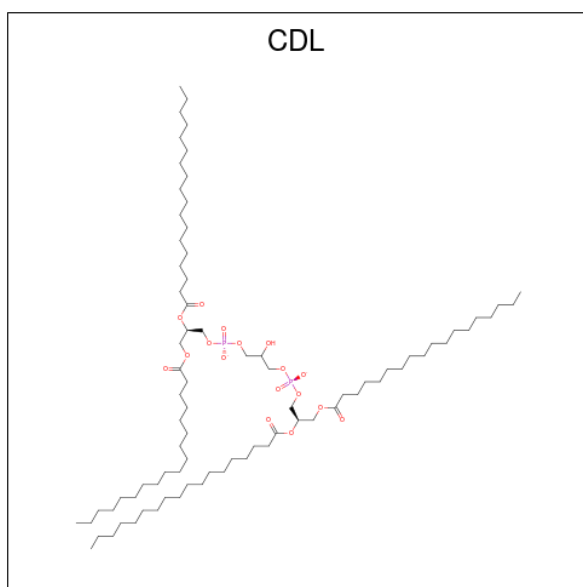
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total X 1 1	0	0
25	P	1	Total X 1 1	0	0

- Molecule 26 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
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 27 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	186	Total	O	0	0
			186	186		
29	B	97	Total	O	0	0
			97	97		
29	C	86	Total	O	0	0
			86	86		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	66	Total O 66 66	0	0
29	E	43	Total O 43 43	0	0
29	F	61	Total O 61 61	0	0
29	G	42	Total O 42 42	0	0
29	H	27	Total O 27 27	0	0
29	I	23	Total O 23 23	0	0
29	J	12	Total O 12 12	0	0
29	K	14	Total O 14 14	0	0
29	L	17	Total O 17 17	0	0
29	M	13	Total O 13 13	0	0
29	N	171	Total O 171 171	0	0
29	O	90	Total O 90 90	0	0
29	P	80	Total O 80 80	0	0
29	Q	43	Total O 43 43	0	0
29	R	37	Total O 37 37	0	0
29	S	50	Total O 50 50	0	0
29	T	37	Total O 37 37	0	0
29	U	31	Total O 31 31	0	0
29	V	20	Total O 20 20	0	0
29	W	9	Total O 9 9	0	0
29	X	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Y	17	Total 17	O 17	0	0
29	Z	8	Total 8	O 8	0	0

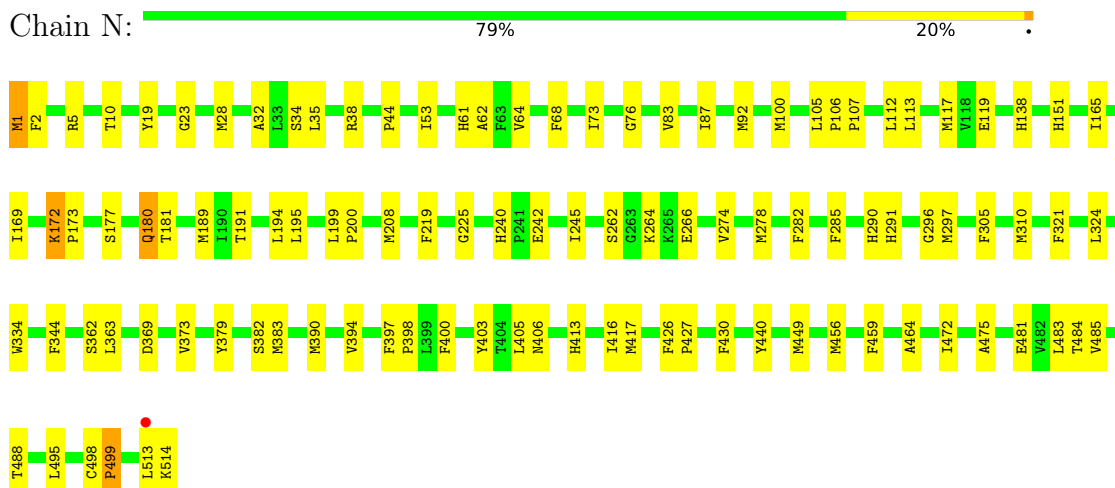
3 Residue-property plots

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.

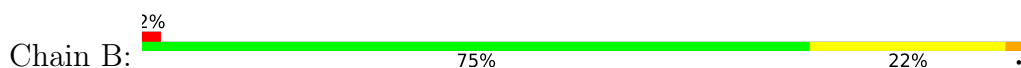
• Molecule 1: Cytochrome c oxidase subunit 1

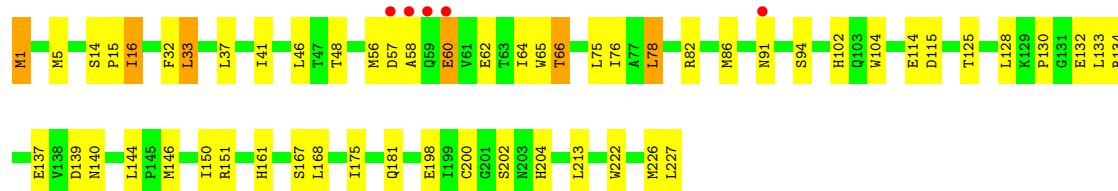


• Molecule 1: Cytochrome c oxidase subunit 1

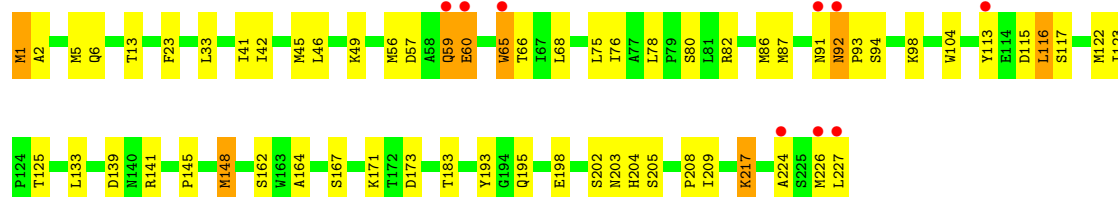


• Molecule 2: Cytochrome c oxidase subunit 2

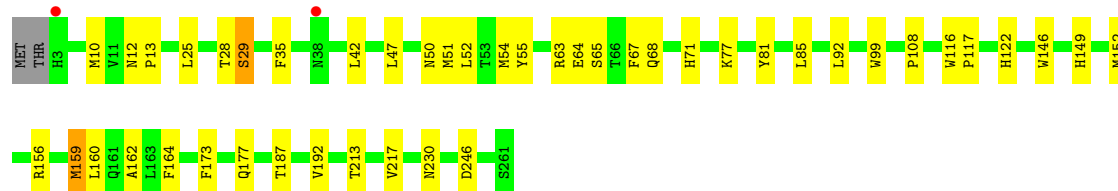
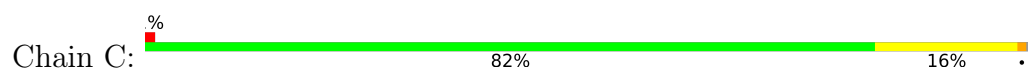




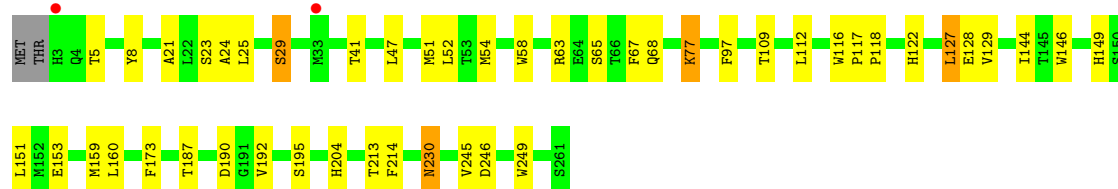
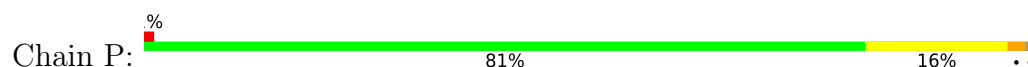
• Molecule 2: Cytochrome c oxidase subunit 2



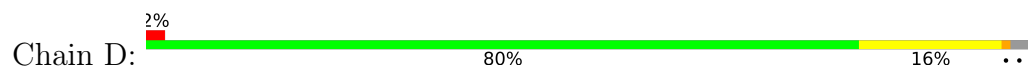
• Molecule 3: Cytochrome c oxidase subunit 3



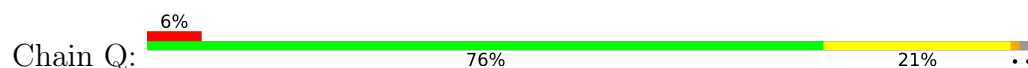
• Molecule 3: Cytochrome c oxidase subunit 3

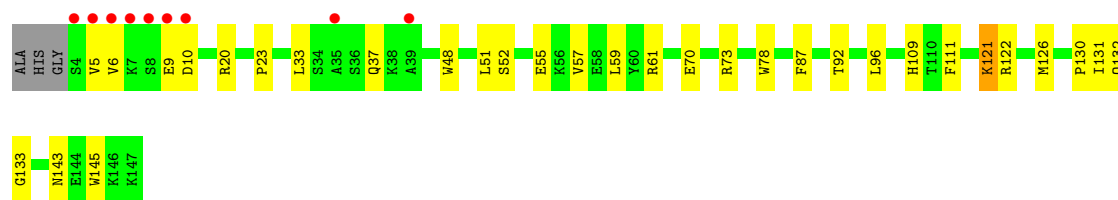


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

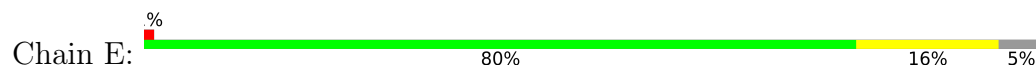


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

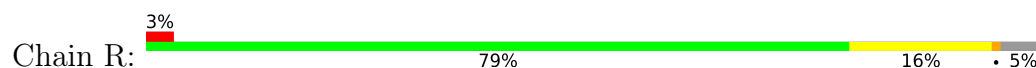




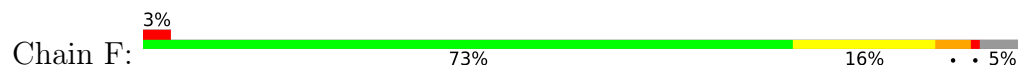
• Molecule 5: Cytochrome c oxidase subunit 5A



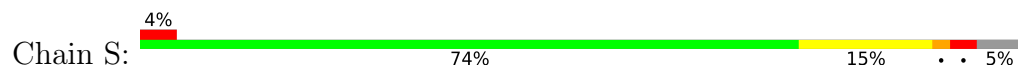
• Molecule 5: Cytochrome c oxidase subunit 5A



• Molecule 6: Cytochrome c oxidase subunit 5B



• Molecule 6: Cytochrome c oxidase subunit 5B



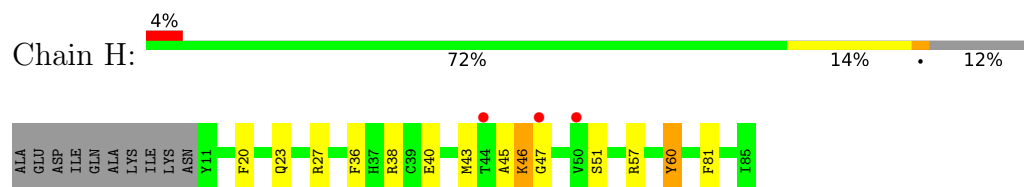
• Molecule 7: Cytochrome c oxidase polypeptide 6A2



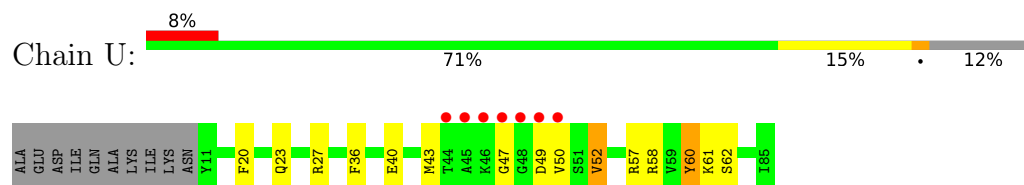
• Molecule 7: Cytochrome c oxidase polypeptide 6A2



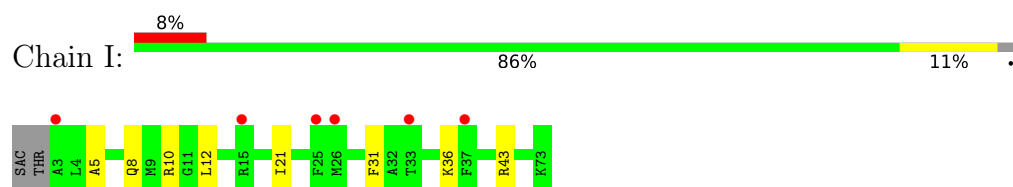
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



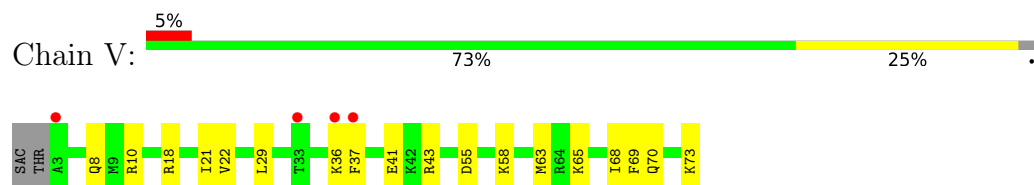
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



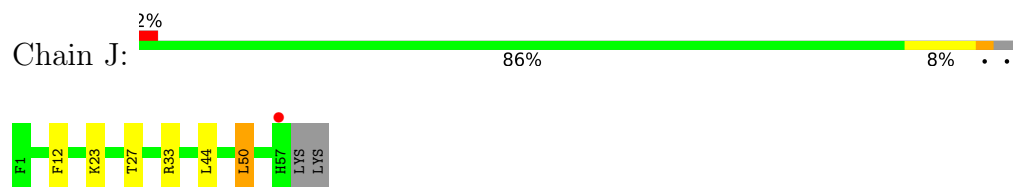
- Molecule 9: Cytochrome c oxidase polypeptide VIc



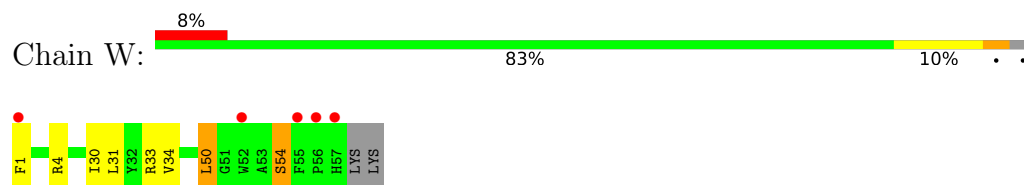
- Molecule 9: Cytochrome c oxidase polypeptide VIc



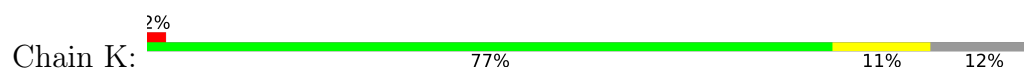
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1

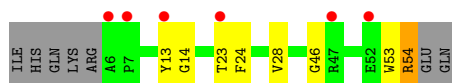
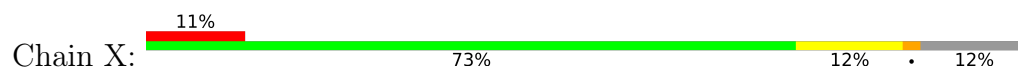


- Molecule 11: Cytochrome c oxidase polypeptide 7B

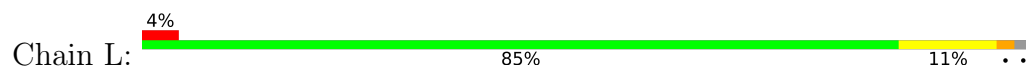




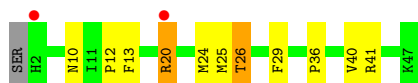
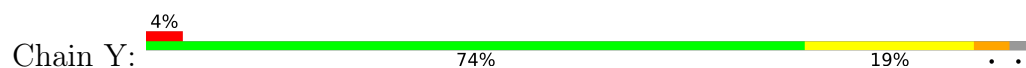
- Molecule 11: Cytochrome c oxidase polypeptide 7B



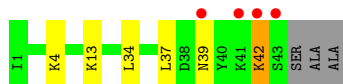
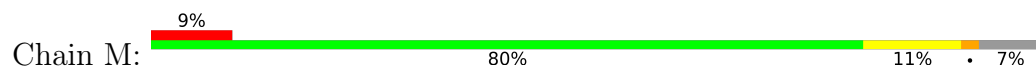
- Molecule 12: Cytochrome c oxidase subunit 7C



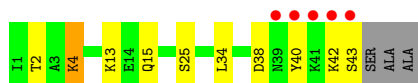
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase polypeptide 8H



- Molecule 13: Cytochrome c oxidase polypeptide 8H



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.16Å 207.62Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.50) 91.4 (40.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.185 , 0.233 0.192 , 0.239	Depositor DCC
R_{free} test set	10030 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31827	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: CDL, TGL, PEK, DMU, ZN, UNX, PER, FME, CU, CHD, TPO, PGV, HEA, MG, CUA, NA, PSC

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	1.23	7/4156 (0.2%)	1.15	12/5678 (0.2%)
1	N	1.14	2/4156 (0.0%)	1.14	18/5678 (0.3%)
2	B	1.21	2/1860 (0.1%)	1.17	3/2534 (0.1%)
2	O	1.13	1/1860 (0.1%)	1.17	3/2534 (0.1%)
3	C	1.12	0/2197	1.08	1/3005 (0.0%)
3	P	1.08	2/2197 (0.1%)	1.10	7/3005 (0.2%)
4	D	1.09	0/1229	1.12	4/1658 (0.2%)
4	Q	1.02	2/1229 (0.2%)	1.08	3/1658 (0.2%)
5	E	1.11	0/860	1.08	0/1167
5	R	1.00	0/860	1.10	2/1167 (0.2%)
6	F	1.12	2/733 (0.3%)	1.26	4/996 (0.4%)
6	S	1.04	0/733	1.24	7/996 (0.7%)
7	G	1.16	0/690	1.18	3/937 (0.3%)
7	T	1.11	0/690	1.23	7/937 (0.7%)
8	H	1.05	0/648	1.13	3/877 (0.3%)
8	U	0.98	0/648	1.03	0/877
9	I	1.10	0/598	1.12	0/792
9	V	1.03	0/598	1.13	1/792 (0.1%)
10	J	1.03	0/462	1.06	1/625 (0.2%)
10	W	0.96	0/462	1.08	0/625
11	K	1.15	0/398	1.15	1/546 (0.2%)
11	X	1.00	0/398	1.07	0/546
12	L	1.08	0/393	1.15	1/526 (0.2%)
12	Y	0.93	0/393	1.12	1/526 (0.2%)
13	M	1.14	0/345	1.17	0/470
13	Z	0.95	0/345	1.21	2/470 (0.4%)
All	All	1.12	18/29138 (0.1%)	1.14	84/39622 (0.2%)

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
6	S	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	10.15	1.36	1.24
2	O	198	GLU	C-O	9.59	1.35	1.23
1	A	240	HIS	N-CA	-9.12	1.40	1.46
4	Q	5	VAL	CA-C	7.39	1.60	1.53
4	Q	5	VAL	CA-CB	7.32	1.63	1.53
2	B	175	ILE	CA-C	7.18	1.57	1.52
1	A	299	VAL	CA-CB	6.84	1.63	1.54
1	A	141	ALA	CA-CB	-6.72	1.42	1.53
1	A	83	VAL	CA-CB	6.36	1.57	1.54
3	P	245	VAL	CA-C	5.72	1.59	1.52
6	F	6	VAL	CA-CB	5.67	1.61	1.54
1	A	295	VAL	CA-CB	5.45	1.61	1.54
3	P	23	SER	CA-C	5.44	1.60	1.52
1	N	373	VAL	CA-CB	5.38	1.61	1.54
1	N	83	VAL	CA-CB	5.37	1.57	1.54
1	A	258	VAL	CA-CB	5.34	1.60	1.54
6	F	92	VAL	CA-CB	5.23	1.60	1.54
1	A	511	VAL	CA-CB	5.07	1.60	1.54

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	N-CA-CB	9.32	119.25	110.39
1	N	172	LYS	CA-C-N	-9.14	112.99	119.66
1	N	172	LYS	C-N-CA	-9.14	112.99	119.66
6	S	94	HIS	N-CA-C	7.90	127.62	110.80
1	A	240	HIS	N-CA-CB	7.89	117.89	110.39
13	Z	4	LYS	CA-C-N	-7.38	112.72	120.03
13	Z	4	LYS	C-N-CA	-7.38	112.72	120.03
4	Q	10	ASP	N-CA-C	-7.34	103.40	112.88
4	Q	133	GLY	N-CA-C	6.93	120.87	112.49
11	K	21	GLY	N-CA-C	-6.87	104.18	112.49
1	N	266	GLU	CA-C-N	6.81	126.72	119.85
1	N	266	GLU	C-N-CA	6.81	126.72	119.85
2	O	65	TRP	N-CA-C	6.75	120.49	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	122	HIS	CA-C-N	6.73	126.71	119.78
3	P	122	HIS	C-N-CA	6.73	126.71	119.78
2	O	92	ASN	CA-C-N	6.66	126.64	119.78
2	O	92	ASN	C-N-CA	6.66	126.64	119.78
5	R	47	ILE	N-CA-C	-6.49	104.53	110.82
1	N	10	THR	N-CA-C	-6.33	103.74	112.03
3	P	8	TYR	N-CA-C	6.28	119.03	110.55
1	N	83	VAL	N-CA-CB	6.27	115.34	110.45
3	P	128	GLU	CA-C-N	-6.14	116.37	120.24
3	P	128	GLU	C-N-CA	-6.14	116.37	120.24
12	Y	20	ARG	N-CA-C	-6.12	104.68	111.36
3	C	99	TRP	N-CA-C	-6.03	104.62	111.07
4	D	5	VAL	N-CA-C	6.01	116.47	107.51
6	F	93	PRO	N-CA-C	6.01	120.67	111.11
1	N	64	VAL	N-CA-C	-6.00	104.89	110.53
1	N	499	PRO	CA-C-N	-5.99	114.21	120.38
1	N	499	PRO	C-N-CA	-5.99	114.21	120.38
10	J	44	LEU	N-CA-C	-5.96	104.86	111.36
12	L	20	ARG	N-CA-C	-5.96	104.79	111.28
1	N	92	MET	N-CA-C	-5.94	101.72	110.52
6	S	53	THR	CA-C-N	5.91	129.30	120.31
6	S	53	THR	C-N-CA	5.91	129.30	120.31
1	A	237	PHE	N-CA-C	-5.88	104.95	111.71
1	A	49	GLY	N-CA-C	-5.84	102.93	110.69
1	N	119	GLU	CB-CA-C	-5.82	109.85	116.54
7	T	58	LYS	CA-C-N	-5.81	113.80	119.78
7	T	58	LYS	C-N-CA	-5.81	113.80	119.78
5	R	44	GLU	N-CA-C	5.79	116.26	109.60
4	D	24	LEU	CA-C-N	5.79	126.59	120.11
4	D	24	LEU	C-N-CA	5.79	126.59	120.11
1	A	7	LEU	N-CA-C	-5.76	106.59	113.97
4	D	133	GLY	N-CA-C	5.76	119.46	112.49
1	A	280	ILE	N-CA-C	-5.75	104.91	110.72
4	Q	5	VAL	N-CA-C	5.72	115.53	106.32
6	F	95	GLN	N-CA-C	5.68	122.90	110.80
1	A	105	LEU	CA-C-N	-5.65	114.56	120.38
1	A	105	LEU	C-N-CA	-5.65	114.56	120.38
2	B	48	THR	N-CA-C	5.60	118.59	109.24
6	S	29	ASP	CA-C-N	5.58	125.25	119.56
6	S	29	ASP	C-N-CA	5.58	125.25	119.56
6	S	52	ILE	N-CA-C	-5.58	106.87	112.17
1	A	472	ILE	N-CA-C	-5.51	105.15	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	72	ASN	CA-C-N	5.49	125.14	119.05
7	T	72	ASN	C-N-CA	5.49	125.14	119.05
2	B	64	ILE	N-CA-C	-5.48	105.16	110.42
8	H	38	ARG	N-CA-C	-5.45	105.26	111.14
9	V	69	PHE	N-CA-C	5.43	118.52	110.48
7	T	6	GLY	N-CA-C	5.35	125.85	113.18
6	S	20	VAL	N-CA-C	-5.33	105.18	110.62
1	N	105	LEU	CA-C-N	-5.30	114.92	120.38
1	N	105	LEU	C-N-CA	-5.30	114.92	120.38
3	P	245	VAL	N-CA-C	5.23	115.85	110.36
7	T	8	HIS	N-CA-C	5.22	121.93	110.80
1	N	262	SER	N-CA-C	-5.17	106.97	113.28
1	A	262	SER	N-CA-C	-5.16	106.77	113.16
3	P	129	VAL	N-CA-CB	5.13	113.73	110.50
2	B	161	HIS	N-CA-C	-5.13	101.63	108.86
1	A	129	TYR	CA-C-N	-5.12	115.11	120.38
1	A	129	TYR	C-N-CA	-5.12	115.11	120.38
1	N	274	VAL	N-CA-C	-5.10	105.74	110.53
1	N	305	PHE	N-CA-C	5.08	118.26	111.75
7	G	57	THR	N-CA-C	-5.08	107.12	113.72
8	H	81	PHE	CA-C-N	-5.06	114.53	119.64
8	H	81	PHE	C-N-CA	-5.06	114.53	119.64
1	N	240	HIS	CA-CB-CG	-5.06	108.74	113.80
6	F	82	CYS	CA-C-N	5.03	124.69	119.56
6	F	82	CYS	C-N-CA	5.03	124.69	119.56
7	G	58	LYS	CA-C-N	-5.02	115.06	120.03
7	G	58	LYS	C-N-CA	-5.02	115.06	120.03
7	T	21	PHE	N-CA-C	5.01	118.55	112.23
1	A	208	MET	CG-SD-CE	5.01	111.93	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	78	0
1	N	4027	0	4001	84	0
2	B	1824	0	1833	39	0
2	O	1824	0	1833	45	0
3	C	2110	0	2027	36	0
3	P	2110	0	2027	34	0
4	D	1195	0	1183	23	0
4	Q	1195	0	1183	24	0
5	E	842	0	838	9	0
5	R	842	0	838	10	0
6	F	717	0	700	11	0
6	S	717	0	700	13	0
7	G	675	0	644	24	0
7	T	675	0	644	38	0
8	H	628	0	580	10	0
8	U	628	0	580	15	0
9	I	585	0	597	9	0
9	V	585	0	597	9	0
10	J	451	0	446	3	0
10	W	451	0	446	6	0
11	K	384	0	366	5	0
11	X	384	0	366	9	0
12	L	380	0	380	11	0
12	Y	380	0	380	10	0
13	M	335	0	352	3	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	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	120	0	108	12	0
18	N	120	0	108	7	0
19	A	102	0	152	5	0
19	C	102	0	152	5	0
19	N	153	0	228	13	0
19	P	51	0	76	5	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	63	0	110	10	0
21	D	63	0	110	5	0
21	L	63	0	110	13	0
21	N	126	0	220	26	0
21	O	63	0	110	6	0
22	B	52	0	80	13	0
22	O	52	0	80	12	0
23	B	29	0	37	0	0
23	C	58	0	73	5	0
23	G	29	0	36	2	0
23	J	29	0	35	2	0
23	P	58	0	73	5	0
23	W	29	0	35	1	0
24	C	33	0	37	2	0
24	M	33	0	38	0	0
24	P	33	0	37	3	0
24	Z	33	0	38	2	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	53	0	77	4	0
26	G	106	0	154	16	0
26	P	106	0	154	13	0
26	T	53	0	77	14	0
27	C	100	0	156	13	0
27	G	100	0	156	17	0
27	P	100	0	156	9	0
27	T	100	0	156	18	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	186	0	0	2	0
29	B	97	0	0	2	0
29	C	86	0	0	5	0
29	D	66	0	0	0	0
29	E	43	0	0	1	0
29	F	61	0	0	2	0
29	G	42	0	0	4	0
29	H	27	0	0	1	0
29	I	23	0	0	6	0
29	J	12	0	0	0	0
29	K	14	0	0	0	0
29	L	17	0	0	2	0
29	M	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	N	171	0	0	2	0
29	O	90	0	0	2	0
29	P	80	0	0	2	0
29	Q	43	0	0	1	0
29	R	37	0	0	0	0
29	S	50	0	0	4	0
29	T	37	0	0	2	0
29	U	31	0	0	0	0
29	V	20	0	0	0	0
29	W	9	0	0	0	0
29	X	11	0	0	0	0
29	Y	17	0	0	0	0
29	Z	8	0	0	1	0
All	All	31827	0	31063	612	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (612) 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)
26:P:1265:PEK:C7	26:P:1265:PEK:C6	1.88	1.48
15:A:520:PER:O2	15:A:520:PER:O1	1.70	1.08
26:P:1265:PEK:H383	27:T:1269:CDL:H272	1.33	1.08
15:N:520:PER:O1	15:N:520:PER:O2	1.70	1.08
6:S:52:ILE:O	6:S:94:HIS:CE1	2.09	1.05
3:C:63:ARG:HE	27:C:270:CDL:HA22	1.23	1.03
21:O:1523:TGL:HC21	21:O:1523:TGL:HG11	1.42	1.01
21:N:1522:TGL:HC62	21:N:1522:TGL:HC22	1.45	0.99
21:D:523:TGL:HC21	21:D:523:TGL:HG11	1.44	0.98
21:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.44	0.98
3:P:63:ARG:HE	27:P:1270:CDL:HA22	1.27	0.97
21:N:1521:TGL:H101	21:N:1521:TGL:H281	1.44	0.96
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.47	0.96
7:G:72:ASN:H	7:G:76:ASN:HD22	1.04	0.92
7:G:5:LYS:HG3	26:G:1263:PEK:H383	1.52	0.92
7:T:5:LYS:HG3	26:T:263:PEK:H383	1.54	0.90
24:C:272:DMU:H30	24:C:272:DMU:O1	1.72	0.89
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.55	0.89
27:T:1269:CDL:H571	27:T:1269:CDL:H782	1.54	0.89
19:C:267:PGV:H182	27:C:270:CDL:H671	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:264:PEK:H102	26:G:264:PEK:H161	1.56	0.87
2:O:56:MET:HA	22:O:1230:PSC:H202	1.54	0.87
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.38	0.86
1:A:468:MET:HE1	18:A:515:HEA:H212	1.58	0.86
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.57	0.85
1:A:514:LYS:HE2	29:F:2322:HOH:O	1.74	0.85
3:C:50:ASN:ND2	3:C:54:MET:HE2	1.91	0.85
26:P:1265:PEK:C7	26:P:1265:PEK:C5	2.56	0.84
2:B:56:MET:HG2	22:B:230:PSC:H211	1.59	0.84
2:O:224:ALA:O	2:O:227:LEU:HG	1.78	0.84
4:D:34:SER:H	4:D:37:GLN:HE21	1.23	0.84
12:L:13:PHE:HA	21:L:522:TGL:HC31	1.61	0.83
7:T:72:ASN:H	7:T:76:ASN:HD22	1.23	0.82
1:A:400:PHE:HB3	21:L:522:TGL:H283	1.62	0.81
7:T:2:SER:OG	26:T:263:PEK:H301	1.81	0.81
7:G:45:PRO:HD2	29:G:2141:HOH:O	1.79	0.81
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.64	0.80
27:G:269:CDL:H541	27:G:269:CDL:H231	1.64	0.80
19:P:1267:PGV:H182	27:P:1270:CDL:C67	2.12	0.80
8:U:40:GLU:HG3	8:U:50:VAL:HG13	1.63	0.80
3:P:25:LEU:O	3:P:29:SER:HB2	1.82	0.80
19:P:1267:PGV:H182	27:P:1270:CDL:H671	1.63	0.79
7:T:45:PRO:HD2	29:T:3141:HOH:O	1.83	0.79
26:P:1265:PEK:H383	27:T:1269:CDL:C27	2.14	0.78
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.66	0.78
3:C:25:LEU:O	3:C:29:SER:HB2	1.83	0.78
27:G:269:CDL:H522	27:G:269:CDL:H202	1.65	0.77
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.66	0.76
7:G:5:LYS:HB3	1:N:278:MET:SD	2.26	0.76
7:G:84:LYS:H	7:G:84:LYS:HD2	1.52	0.75
1:N:112:LEU:HG	29:N:3070:HOH:O	1.87	0.74
1:A:278:MET:SD	7:T:5:LYS:HB3	2.27	0.74
3:C:50:ASN:HD21	3:C:54:MET:HE2	1.53	0.74
9:I:5:ALA:CB	29:I:4239:HOH:O	2.35	0.74
1:N:177:SER:H	1:N:180:GLN:NE2	1.86	0.73
26:C:265:PEK:H383	27:G:269:CDL:H272	1.70	0.72
7:T:5:LYS:CG	26:T:263:PEK:H383	2.18	0.72
8:U:40:GLU:HG3	8:U:50:VAL:CG1	2.19	0.72
19:C:267:PGV:H12	19:C:267:PGV:H161	1.70	0.72
3:P:214:PHE:CD1	19:P:1267:PGV:H62	2.25	0.71
7:G:76:ASN:HD21	26:G:264:PEK:HN2	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:HB2	26:T:263:PEK:H362	1.71	0.71
1:N:400:PHE:HB3	21:N:1522:TGL:C28	2.21	0.71
3:C:160:LEU:HD13	23:C:271:CHD:C18	2.20	0.71
7:T:31:CYS:SG	27:T:1269:CDL:H532	2.31	0.71
1:N:400:PHE:HB3	21:N:1522:TGL:H283	1.73	0.71
7:T:3:ALA:HB1	26:T:263:PEK:H382	1.73	0.70
21:N:1522:TGL:HC22	21:N:1522:TGL:CC6	2.19	0.70
26:P:1265:PEK:C6	26:P:1265:PEK:C8	2.70	0.70
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.72	0.70
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.21	0.70
7:T:8:HIS:CD2	26:T:263:PEK:H232	2.27	0.70
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.57	0.69
21:B:521:TGL:HC22	29:I:2365:HOH:O	1.92	0.69
2:O:41:ILE:CD1	22:O:1230:PSC:H342	2.22	0.69
7:G:72:ASN:H	7:G:76:ASN:ND2	1.84	0.69
3:C:246:ASP:HB2	29:C:4041:HOH:O	1.92	0.69
7:T:2:SER:O	26:T:263:PEK:H322	1.92	0.69
7:T:5:LYS:HD2	26:T:263:PEK:C38	2.23	0.69
8:U:43:MET:HE2	8:U:52:VAL:HG21	1.74	0.68
7:G:2:SER:OG	26:G:1263:PEK:H301	1.94	0.68
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.27	0.67
27:G:269:CDL:H782	27:G:269:CDL:H571	1.76	0.67
19:A:524:PGV:H062	29:M:2148:HOH:O	1.94	0.67
9:I:5:ALA:HB2	29:I:4239:HOH:O	1.92	0.67
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.07	0.67
19:N:1524:PGV:H012	29:N:4082:HOH:O	1.95	0.67
12:L:5:GLU:HB2	29:L:4231:HOH:O	1.94	0.67
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.77	0.67
12:L:20:ARG:HH22	21:L:522:TGL:HC62	1.58	0.66
19:C:268:PGV:H062	29:C:4330:HOH:O	1.95	0.66
1:N:310:MET:HE1	2:O:76:ILE:HG21	1.78	0.66
21:N:1521:TGL:H281	21:N:1521:TGL:C10	2.21	0.66
21:N:1522:TGL:H361	21:N:1522:TGL:HB91	1.77	0.66
21:B:521:TGL:H222	21:B:521:TGL:HA82	1.76	0.66
27:C:270:CDL:HB22	27:C:270:CDL:OA5	1.96	0.66
3:P:160:LEU:HD13	23:P:1271:CHD:C18	2.25	0.65
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.77	0.65
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.78	0.65
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.77	0.65
19:C:267:PGV:H182	27:C:270:CDL:C67	2.26	0.65
27:T:1269:CDL:H782	27:T:1269:CDL:C57	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HG21	21:L:522:TGL:HA91	1.79	0.65
4:D:130:PRO:HG2	4:D:131:ILE:HD12	1.79	0.65
2:O:116:LEU:HD12	2:O:117:SER:N	2.12	0.65
21:O:1523:TGL:HG11	21:O:1523:TGL:CC2	2.22	0.65
19:N:1524:PGV:H062	29:Z:3148:HOH:O	1.97	0.64
2:B:56:MET:HA	22:B:230:PSC:H202	1.79	0.64
26:C:265:PEK:H383	27:G:269:CDL:C27	2.28	0.64
21:N:1522:TGL:H242	21:N:1522:TGL:H202	1.80	0.64
24:C:272:DMU:H30	24:C:272:DMU:C10	2.27	0.64
11:K:24:PHE:O	11:K:28:VAL:HG12	1.98	0.64
21:N:1521:TGL:H101	21:N:1521:TGL:C28	2.22	0.64
1:N:362:SER:HA	2:O:87:MET:HE1	1.81	0.63
12:L:20:ARG:NH2	21:L:522:TGL:HC32	2.14	0.62
1:A:87:ILE:O	1:A:173:PRO:HD3	1.99	0.62
1:N:514:LYS:HE2	29:S:3322:HOH:O	1.97	0.62
21:B:521:TGL:C28	21:B:521:TGL:H101	2.29	0.62
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.81	0.62
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.35	0.62
22:B:230:PSC:H322	22:B:230:PSC:H281	1.82	0.61
3:P:246:ASP:HB2	29:P:4136:HOH:O	1.98	0.61
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.00	0.61
3:P:67:PHE:HE1	27:P:1270:CDL:H1	1.64	0.61
4:D:78:TRP:HA	21:D:523:TGL:HB22	1.83	0.61
7:G:31:CYS:SG	27:G:269:CDL:H532	2.40	0.60
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.82	0.60
3:P:213:THR:HG23	27:P:1270:CDL:H762	1.82	0.60
1:N:100:MET:HE1	19:N:1266:PGV:H81	1.84	0.60
6:F:64:GLU:O	6:F:65:ASP:HB2	2.01	0.60
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.82	0.60
4:D:131:ILE:HD12	4:D:131:ILE:N	2.17	0.60
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.34	0.60
1:A:52:GLN:O	1:A:56:VAL:HG23	2.02	0.59
5:E:78:HIS:HD2	9:I:12:LEU:HD13	1.68	0.59
1:A:233:HIS:CE1	1:A:292:MET:HE1	2.38	0.59
21:N:1522:TGL:H202	21:N:1522:TGL:C24	2.32	0.59
24:P:1272:DMU:H30	24:P:1272:DMU:O1	2.01	0.59
26:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.48	0.59
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.83	0.59
9:I:5:ALA:N	29:I:4239:HOH:O	2.30	0.59
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.38	0.58
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:LYS:HG3	26:G:1263:PEK:C38	2.28	0.58
21:O:1523:TGL:HB22	4:Q:78:TRP:HA	1.84	0.58
27:G:269:CDL:H541	27:G:269:CDL:C23	2.33	0.58
8:H:60:TYR:CD1	8:H:60:TYR:C	2.81	0.58
11:X:24:PHE:O	11:X:28:VAL:HG12	2.03	0.58
2:B:37:LEU:HB2	29:I:4437:HOH:O	2.02	0.58
12:L:20:ARG:HH22	21:L:522:TGL:CC6	2.16	0.58
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.68	0.58
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.04	0.58
1:N:87:ILE:O	1:N:173:PRO:HD3	2.03	0.57
27:T:1269:CDL:H541	27:T:1269:CDL:H232	1.85	0.57
7:T:72:ASN:H	7:T:76:ASN:ND2	1.99	0.57
1:A:28:MET:CE	18:A:515:HEA:H271	2.33	0.57
1:N:488:THR:HB	1:N:495:LEU:HD13	1.84	0.57
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.40	0.57
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.38	0.57
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.86	0.57
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.87	0.57
26:P:1265:PEK:C38	27:T:1269:CDL:H272	2.22	0.57
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.86	0.57
12:L:20:ARG:HH22	21:L:522:TGL:HC32	1.69	0.56
1:N:28:MET:CE	18:N:515:HEA:H271	2.35	0.56
2:B:56:MET:HA	22:B:230:PSC:C20	2.34	0.56
21:D:523:TGL:HC21	21:D:523:TGL:CG1	2.27	0.56
7:G:84:LYS:H	7:G:84:LYS:CD	2.18	0.56
1:A:240:HIS:O	1:A:243:VAL:HG22	2.06	0.56
22:B:230:PSC:H343	22:B:230:PSC:H142	1.87	0.56
8:H:43:MET:HE1	8:U:43:MET:HE1	1.87	0.56
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.86	0.56
1:A:38:ARG:HD2	18:A:515:HEA:OMA	2.05	0.56
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.86	0.56
19:N:1524:PGV:H22	19:N:1524:PGV:H011	1.88	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.70	0.56
6:S:52:ILE:C	6:S:94:HIS:CE1	2.84	0.56
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.87	0.55
7:T:84:LYS:HD2	7:T:84:LYS:H	1.71	0.55
27:T:1269:CDL:OB4	27:T:1269:CDL:H1	2.06	0.55
26:G:1263:PEK:H042	3:P:77:LYS:NZ	2.22	0.55
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.88	0.55
21:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.41	0.55
2:B:82:ARG:HH11	2:B:86:MET:HE1	1.70	0.55
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.41	0.55
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.89	0.55
10:J:50:LEU:HD22	10:J:50:LEU:O	2.06	0.55
1:A:1:FME:HCN	1:A:4:ASN:H	1.71	0.55
18:A:516:HEA:OMA	18:A:516:HEA:HHB	2.05	0.55
3:P:47:LEU:O	3:P:51:MET:HG2	2.06	0.55
4:D:9:GLU:OE2	4:D:9:GLU:N	2.35	0.55
27:G:269:CDL:H111	27:G:269:CDL:HA21	1.89	0.55
3:P:230:ASN:HB2	29:P:3271:HOH:O	2.06	0.55
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.41	0.54
8:H:46:LYS:HB2	8:U:52:VAL:HG12	1.89	0.54
1:A:112:LEU:HD12	29:A:2070:HOH:O	2.06	0.54
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.53	0.54
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.89	0.54
3:P:149:HIS:O	3:P:153:GLU:HG3	2.08	0.54
1:N:35:LEU:HB3	24:Z:1526:DMU:H24	1.90	0.54
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.23	0.54
1:A:379:TYR:O	1:A:383:MET:HB2	2.08	0.54
5:E:78:HIS:CD2	9:I:12:LEU:HD13	2.42	0.54
26:G:1263:PEK:H12	29:G:4260:HOH:O	2.08	0.54
1:N:151:HIS:CD2	26:P:1264:PEK:H382	2.43	0.54
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.43	0.54
1:A:1:FME:HE2	1:A:1:FME:HA	1.89	0.53
5:E:105:GLY:O	5:E:108:LYS:HG2	2.07	0.53
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.16	0.53
2:B:58:ALA:O	2:B:62:GLU:HG3	2.08	0.53
4:D:34:SER:H	4:D:37:GLN:NE2	1.99	0.53
27:G:269:CDL:H761	1:N:282:PHE:HZ	1.73	0.53
4:Q:122:ARG:O	4:Q:126:MET:HG2	2.09	0.53
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.90	0.53
3:P:127:LEU:HG	27:T:1269:CDL:OB3	2.09	0.53
3:P:187:THR:HG22	26:P:1264:PEK:H052	1.89	0.53
19:C:268:PGV:H101	29:C:4467:HOH:O	2.08	0.53
21:L:522:TGL:HC62	21:L:522:TGL:HC22	1.90	0.53
22:O:1230:PSC:H21	22:O:1230:PSC:H222	1.90	0.53
26:G:1263:PEK:H042	3:P:77:LYS:HZ1	1.73	0.53
26:P:1265:PEK:H6	26:P:1265:PEK:H221	1.89	0.53
9:V:65:LYS:O	11:X:54:ARG:NH1	2.34	0.53
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:70:ILE:HG13	6:S:84:SER:HB3	1.91	0.53
7:G:4:ALA:CB	1:N:282:PHE:HA	2.39	0.52
21:N:1521:TGL:HA92	21:N:1521:TGL:H301	1.91	0.52
6:F:22:LEU:HD12	29:F:4476:HOH:O	2.09	0.52
4:Q:33:LEU:HA	4:Q:37:GLN:HE21	1.74	0.52
9:V:55:ASP:OD2	9:V:58:LYS:HB2	2.09	0.52
21:B:521:TGL:H101	21:B:521:TGL:H281	1.91	0.52
21:B:521:TGL:H281	21:B:521:TGL:C10	2.38	0.52
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.45	0.52
7:G:3:ALA:HB1	26:G:1263:PEK:H382	1.90	0.52
3:P:52:LEU:HD21	27:P:1270:CDL:H412	1.91	0.52
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.09	0.52
1:N:177:SER:H	1:N:180:GLN:HE21	1.54	0.52
3:C:67:PHE:HE1	27:C:270:CDL:H1	1.73	0.52
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.45	0.52
27:P:1270:CDL:H642	27:P:1270:CDL:H231	1.92	0.52
7:T:3:ALA:CB	26:T:263:PEK:H382	2.39	0.52
7:G:2:SER:O	26:G:1263:PEK:H322	2.10	0.51
6:S:25:ARG:HD3	29:S:4299:HOH:O	2.09	0.51
6:S:95:GLN:HG2	29:S:4510:HOH:O	2.10	0.51
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.74	0.51
21:N:1522:TGL:HC62	21:N:1522:TGL:CC2	2.18	0.51
1:A:28:MET:HE2	18:A:515:HEA:H271	1.91	0.51
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.44	0.51
3:P:190:ASP:HB3	7:T:53:LEU:HD22	1.92	0.51
26:C:265:PEK:C38	27:G:269:CDL:H273	2.40	0.51
1:N:472:ILE:HG21	21:N:1522:TGL:CA9	2.41	0.51
7:G:72:ASN:N	7:G:76:ASN:HD22	1.89	0.51
21:N:1521:TGL:H241	21:N:1521:TGL:H201	1.93	0.51
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.45	0.51
1:A:35:LEU:HD11	1:A:462:LEU:HD22	1.93	0.51
7:G:3:ALA:O	7:G:4:ALA:HB2	2.10	0.51
7:G:5:LYS:HD2	26:G:1263:PEK:H371	1.91	0.51
18:N:515:HEA:HBC1	18:N:515:HEA:CMC	2.38	0.51
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.41	0.51
26:C:265:PEK:C38	27:G:269:CDL:C27	2.89	0.50
27:C:270:CDL:H661	27:C:270:CDL:H242	1.93	0.50
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.76	0.50
1:N:113:LEU:HD13	21:N:1522:TGL:H292	1.93	0.50
1:N:117:MET:HB3	10:W:54:SER:OG	2.11	0.50
1:A:160:GLY:HA3	29:A:2061:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PRO:HD2	29:B:2132:HOH:O	2.12	0.50
19:N:1524:PGV:H061	19:N:1524:PGV:O11	2.11	0.50
24:P:1272:DMU:H30	24:P:1272:DMU:C10	2.41	0.50
7:T:5:LYS:HD2	26:T:263:PEK:H371	1.93	0.50
1:N:400:PHE:HB3	21:N:1522:TGL:H282	1.94	0.50
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.29	0.50
19:A:524:PGV:P	19:A:524:PGV:H061	2.51	0.50
19:A:524:PGV:H152	19:A:524:PGV:H321	1.92	0.50
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.47	0.50
2:O:125:THR:N	29:O:3143:HOH:O	2.45	0.50
2:O:65:TRP:CZ3	22:O:1230:PSC:H331	2.47	0.50
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.93	0.50
7:T:23:LEU:HD12	27:T:1269:CDL:H273	1.93	0.50
27:G:269:CDL:H541	27:G:269:CDL:H241	1.92	0.50
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.75	0.50
1:A:449:MET:SD	2:B:5:MET:HG2	2.51	0.50
4:D:93:ALA:HB3	11:K:28:VAL:HG22	1.94	0.50
1:A:390:MET:HE2	1:A:413:HIS:CE1	2.47	0.49
1:A:488:THR:HB	1:A:495:LEU:HD13	1.93	0.49
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.47	0.49
1:N:426:PHE:HB3	1:N:427:PRO:HD3	1.94	0.49
1:A:377:PHE:CE2	1:A:378:HIS:CE1	3.01	0.49
4:Q:109:HIS:HD2	29:Q:3147:HOH:O	1.95	0.49
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.94	0.49
1:N:398:PRO:HA	1:N:403:TYR:O	2.12	0.49
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.95	0.49
27:P:1270:CDL:H352	27:P:1270:CDL:H162	1.94	0.49
2:B:1:FME:SD	2:B:133:LEU:CD1	3.00	0.49
3:C:55:TYR:CD1	27:C:270:CDL:H532	2.48	0.49
1:A:21:LEU:HD23	21:L:522:TGL:H212	1.95	0.49
27:G:269:CDL:H473	29:G:4294:HOH:O	2.13	0.49
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.94	0.49
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.27	0.49
21:B:521:TGL:H222	21:B:521:TGL:CA8	2.41	0.49
3:C:63:ARG:NE	27:C:270:CDL:HA22	2.07	0.49
21:D:523:TGL:HB62	21:D:523:TGL:HA52	1.95	0.48
2:O:1:FME:SD	2:O:133:LEU:HD13	2.53	0.48
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.27	0.48
3:C:116:TRP:HA	3:C:117:PRO:C	2.38	0.48
1:A:169:ILE:HG23	7:T:9:GLY:HA2	1.95	0.48
1:N:1:FME:CN	1:N:2:PHE:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PHE:HZ	21:B:521:TGL:HA31	1.78	0.48
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.96	0.48
2:B:102:HIS:O	2:B:104:TRP:HA	2.14	0.48
6:S:53:THR:HB	6:S:54:ASN:H	1.33	0.48
7:T:84:LYS:H	7:T:84:LYS:CD	2.25	0.48
3:C:213:THR:O	3:C:217:VAL:HG23	2.13	0.48
7:G:3:ALA:O	29:G:4448:HOH:O	2.20	0.48
7:T:38:HIS:HE2	27:T:1269:CDL:H111	1.79	0.48
27:C:270:CDL:H522	27:C:270:CDL:OB9	2.13	0.48
18:N:515:HEA:C16	18:N:515:HEA:H273	2.43	0.48
2:B:57:ASP:H	22:B:230:PSC:H201	1.78	0.47
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.27	0.47
23:C:271:CHD:H112	23:C:271:CHD:H12A	1.63	0.47
7:G:1:ALA:HB2	19:N:1268:PGV:H312	1.97	0.47
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.95	0.47
12:L:20:ARG:HD2	29:L:4423:HOH:O	2.13	0.47
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.79	0.47
19:A:524:PGV:H321	19:A:524:PGV:C15	2.45	0.47
2:O:226:MET:HG3	2:O:226:MET:O	2.14	0.47
3:C:156:ARG:HE	23:C:271:CHD:C24	2.27	0.47
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.15	0.47
26:G:1263:PEK:H312	26:G:1263:PEK:H282	1.67	0.47
2:O:1:FME:HCN	2:O:193:TYR:HB2	1.96	0.47
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.79	0.47
1:A:172:LYS:HZ2	1:A:178:GLN:NE2	2.13	0.47
1:A:278:MET:HB3	7:T:5:LYS:HG2	1.97	0.47
1:A:115:SER:HB2	1:A:142:SER:O	2.15	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.47
1:A:430:PHE:HE1	21:B:521:TGL:HB21	1.79	0.47
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.30	0.47
18:N:515:HEA:C16	18:N:515:HEA:C27	2.92	0.47
9:V:37:PHE:HA	9:V:41:GLU:HB2	1.97	0.47
1:A:37:ILE:HG21	18:A:515:HEA:CMA	2.45	0.47
2:B:62:GLU:O	2:B:66:THR:HB	2.15	0.47
2:O:162:SER:HA	2:O:173:ASP:HA	1.97	0.47
7:T:17:ARG:HD2	29:T:3293:HOH:O	2.14	0.47
1:A:32:ALA:CB	12:L:36:PRO:HG2	2.42	0.46
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.50	0.46
1:N:199:LEU:N	1:N:200:PRO:CD	2.79	0.46
19:N:1266:PGV:H181	26:P:1264:PEK:H321	1.97	0.46
3:P:204:HIS:CE1	3:P:249:TRP:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:MET:HB3	7:T:5:LYS:CG	2.45	0.46
26:G:264:PEK:H71	26:G:264:PEK:H32	1.98	0.46
3:C:108:PRO:HA	29:C:2192:HOH:O	2.15	0.46
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.97	0.46
1:A:172:LYS:NZ	1:A:178:GLN:NE2	2.64	0.46
3:C:149:HIS:HA	3:C:152:MET:HE2	1.97	0.46
5:E:63:SER:O	5:E:67:ILE:HG13	2.16	0.46
2:O:57:ASP:H	22:O:1230:PSC:C20	2.28	0.46
10:W:30:ILE:O	10:W:34:VAL:HG23	2.15	0.46
6:F:85:CYS:SG	6:F:87:THR:HG23	2.55	0.46
23:G:86:CHD:H212	23:G:86:CHD:H12	1.96	0.46
23:P:1525:CHD:H12	23:P:1525:CHD:H212	1.97	0.46
2:O:59:GLN:O	2:O:59:GLN:HG3	2.15	0.46
22:O:1230:PSC:H212	22:O:1230:PSC:C02	2.46	0.46
3:P:54:MET:HB3	3:P:58:TRP:CZ3	2.50	0.46
1:A:24:ALA:HA	18:A:515:HEA:H22	1.97	0.46
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.51	0.46
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.97	0.46
5:R:89:LEU:O	5:R:93:LEU:HG	2.16	0.46
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.46	0.46
3:C:159:MET:SD	3:C:159:MET:C	2.99	0.46
21:N:1522:TGL:HA82	12:Y:29:PHE:HZ	1.80	0.46
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.66	0.46
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.51	0.46
22:O:1230:PSC:H212	22:O:1230:PSC:O01	2.15	0.46
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.85	0.46
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.80	0.46
4:D:78:TRP:CA	21:D:523:TGL:HB22	2.46	0.46
27:G:269:CDL:H152	27:G:269:CDL:H182	1.70	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.46
2:O:141:ARG:HG3	9:V:70:GLN:HE22	1.81	0.46
2:B:1:FME:SD	2:B:133:LEU:HD11	2.56	0.45
4:D:9:GLU:H	4:D:9:GLU:CD	2.22	0.45
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.16	0.45
3:P:63:ARG:NE	27:P:1270:CDL:HA22	2.11	0.45
1:A:209:LEU:O	1:A:213:ARG:HG3	2.16	0.45
18:A:516:HEA:HHC	18:A:516:HEA:O11	2.16	0.45
2:O:82:ARG:HG2	2:O:86:MET:CE	2.47	0.45
27:G:269:CDL:H222	27:G:269:CDL:H252	1.73	0.45
1:N:472:ILE:HG21	21:N:1522:TGL:HA91	1.97	0.45
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:65:SER:HB2	19:P:1267:PGV:H041	1.98	0.45
7:T:5:LYS:CD	26:T:263:PEK:H383	2.46	0.45
21:L:522:TGL:H251	21:L:522:TGL:H282	1.64	0.45
1:N:169:ILE:HD11	1:N:189:MET:SD	2.57	0.45
3:C:51:MET:HB3	27:C:270:CDL:H622	1.99	0.45
21:O:1523:TGL:HC21	21:O:1523:TGL:CG1	2.30	0.45
26:P:1265:PEK:C38	27:T:1269:CDL:C27	2.87	0.45
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.99	0.45
2:O:98:LYS:HE2	8:U:62:SER:O	2.17	0.45
7:T:5:LYS:CD	26:T:263:PEK:C38	2.95	0.45
2:B:139:ASP:OD2	2:B:140:ASN:N	2.49	0.45
4:D:132:GLN:OE1	9:I:43:ARG:HD3	2.16	0.45
13:Z:42:LYS:HA	13:Z:42:LYS:HD2	1.82	0.45
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.82	0.45
27:C:270:CDL:H642	27:C:270:CDL:H192	1.97	0.45
4:D:78:TRP:O	4:D:82:VAL:HG23	2.16	0.45
18:N:515:HEA:C27	18:N:515:HEA:H161	2.47	0.45
1:A:1:FME:HA	1:A:1:FME:CE	2.47	0.45
1:A:127:THR:HG22	1:A:235:PHE:CE2	2.52	0.45
21:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.99	0.45
7:T:5:LYS:HD2	26:T:263:PEK:C37	2.47	0.45
1:A:377:PHE:HE2	1:A:378:HIS:CE1	2.35	0.44
3:C:52:LEU:HD23	27:C:270:CDL:H362	1.99	0.44
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.99	0.44
4:Q:70:GLU:O	4:Q:73:ARG:HG2	2.18	0.44
1:A:11:ASN:HB2	1:A:502:TYR:CZ	2.51	0.44
1:A:407:ASP:O	1:A:411:LYS:HG3	2.18	0.44
3:C:187:THR:HG22	26:G:264:PEK:H052	2.00	0.44
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.51	0.44
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.54	0.44
8:U:58:ARG:HD2	8:U:58:ARG:HA	1.84	0.44
1:A:148:PHE:HB3	3:C:28:THR:HB	2.00	0.44
4:D:109:HIS:HE1	4:D:115:TRP:CZ3	2.35	0.44
1:N:191:THR:HG23	1:N:245:ILE:HG23	2.00	0.44
3:C:47:LEU:O	3:C:51:MET:HG2	2.18	0.44
2:B:146:MET:HA	2:B:213:LEU:HD12	2.00	0.44
5:E:81:ILE:O	5:E:85:VAL:HG23	2.17	0.44
3:P:116:TRP:HA	3:P:117:PRO:C	2.42	0.44
1:A:314:ILE:HB	1:A:315:PRO:CD	2.47	0.44
1:A:350:VAL:HG13	21:B:521:TGL:HB81	2.00	0.44
2:B:82:ARG:HG2	2:B:86:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:1263:PEK:H331	26:G:1263:PEK:H362	1.70	0.44
2:O:1:FME:SD	2:O:133:LEU:CD1	3.06	0.44
6:S:51:SER:O	6:S:94:HIS:N	2.37	0.44
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.99	0.43
27:T:1269:CDL:H111	27:T:1269:CDL:HA21	2.00	0.43
2:B:144:LEU:HD22	2:B:150:ILE:HD13	2.00	0.43
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.82	0.43
21:N:1521:TGL:H282	21:N:1521:TGL:H252	1.80	0.43
2:O:217:LYS:HA	2:O:217:LYS:HE2	2.00	0.43
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.53	0.43
7:T:77:PRO:HD3	7:T:82:TYR:CE1	2.52	0.43
2:O:13:THR:HG22	2:O:13:THR:O	2.18	0.43
2:O:86:MET:HE3	2:O:86:MET:HB2	1.88	0.43
4:Q:132:GLN:OE1	9:V:43:ARG:HD3	2.18	0.43
1:N:379:TYR:O	1:N:383:MET:HB2	2.17	0.43
7:T:3:ALA:O	7:T:4:ALA:CB	2.66	0.43
22:O:1230:PSC:H343	22:O:1230:PSC:C14	2.48	0.43
24:P:1272:DMU:H25	26:P:1264:PEK:H341	2.00	0.43
6:S:87:THR:HG22	29:S:3333:HOH:O	2.18	0.43
27:T:1269:CDL:H541	27:T:1269:CDL:C23	2.48	0.43
8:H:27:ARG:NH1	29:H:2287:HOH:O	2.52	0.43
10:J:12:PHE:O	10:J:23:LYS:HE2	2.19	0.43
6:S:18:ARG:HA	6:S:21:MET:HE2	2.00	0.43
24:Z:1526:DMU:H9	24:Z:1526:DMU:H15	1.79	0.43
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.07	0.43
2:B:65:TRP:HZ3	22:B:230:PSC:H331	1.84	0.43
5:E:31:LYS:HE3	6:F:83:PRO:O	2.18	0.43
2:O:141:ARG:HG3	9:V:70:GLN:NE2	2.34	0.43
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.62	0.43
11:X:13:TYR:O	11:X:14:GLY:C	2.62	0.43
18:A:515:HEA:HBC1	18:A:515:HEA:HMC1	2.00	0.43
22:B:230:PSC:C07	9:I:10:ARG:HE	2.32	0.43
7:G:8:HIS:ND1	26:G:1263:PEK:H312	2.34	0.43
1:N:417:MET:HE2	1:N:464:ALA:HB1	2.00	0.43
19:N:1524:PGV:H222	13:Z:15:GLN:HE22	1.83	0.43
2:O:59:GLN:O	2:O:59:GLN:CG	2.67	0.43
3:P:214:PHE:CE1	19:P:1267:PGV:H62	2.54	0.43
1:A:90:PRO:HB2	3:C:10:MET:CE	2.48	0.43
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.53	0.43
3:C:173:PHE:CD2	3:C:173:PHE:C	2.96	0.43
21:L:522:TGL:CC6	21:L:522:TGL:HC22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.19	0.43
1:N:397:PHE:N	1:N:398:PRO:CD	2.81	0.42
6:S:94:HIS:O	6:S:95:GLN:HB2	2.19	0.42
7:T:38:HIS:NE2	27:T:1269:CDL:H111	2.34	0.42
1:A:378:HIS:CG	1:A:425:PHE:CE2	3.07	0.42
1:A:397:PHE:HB3	1:A:398:PRO:HD3	2.01	0.42
1:N:34:SER:HB3	1:N:61:HIS:CE1	2.54	0.42
2:O:49:LYS:NZ	21:O:1523:TGL:HC71	2.34	0.42
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.18	0.42
10:W:1:PHE:HD1	10:W:1:PHE:H1	1.65	0.42
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.54	0.42
2:B:222:TRP:O	2:B:226:MET:HB2	2.19	0.42
22:B:230:PSC:H142	22:B:230:PSC:C34	2.49	0.42
1:N:5:ARG:NH2	12:Y:10:ASN:HA	2.34	0.42
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.54	0.42
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.19	0.42
1:N:449:MET:SD	2:O:5:MET:CG	3.07	0.42
1:N:459:PHE:HB3	4:Q:92:THR:HG23	2.01	0.42
19:N:1524:PGV:H151	4:Q:87:PHE:CZ	2.54	0.42
1:A:269:GLY:O	1:A:273:MET:HG2	2.20	0.42
1:N:400:PHE:O	21:N:1522:TGL:H283	2.19	0.42
4:Q:33:LEU:HB3	4:Q:37:GLN:HB3	2.01	0.42
18:A:516:HEA:HHD	18:A:516:HEA:HAC	1.72	0.42
2:B:1:FME:SD	2:B:133:LEU:HD13	2.59	0.42
6:F:47:ASN:HB2	6:F:89:TYR:CD1	2.54	0.42
27:G:269:CDL:H541	27:G:269:CDL:C24	2.49	0.42
2:O:1:FME:HE1	2:O:133:LEU:HD22	2.00	0.42
27:T:1269:CDL:H552	27:T:1269:CDL:H521	1.75	0.42
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.84	0.42
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.82	0.42
1:A:66:ILE:HG23	1:A:246:LEU:HD21	2.02	0.42
22:B:230:PSC:H212	22:B:230:PSC:C02	2.50	0.42
21:N:1522:TGL:H282	21:N:1522:TGL:H251	1.71	0.42
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.20	0.42
4:Q:145:TRP:CD1	11:X:46:GLY:H	2.37	0.42
7:T:47:PHE:CE2	7:T:77:PRO:HB2	2.54	0.42
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.82	0.42
1:N:405:LEU:HD23	1:N:475:ALA:HB2	2.00	0.42
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.19	0.42
1:A:310:MET:HE2	1:A:356:ILE:HG23	2.02	0.42
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:1523:TGL:HB81	21:O:1523:TGL:H122	2.02	0.42
27:T:1269:CDL:H592	27:T:1269:CDL:H561	1.85	0.42
12:Y:24:MET:HA	12:Y:24:MET:HE2	2.02	0.42
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.54	0.42
4:D:107:ILE:HB	4:D:108:PRO:HD2	2.02	0.42
4:D:131:ILE:HD12	4:D:131:ILE:H	1.83	0.42
3:P:192:VAL:HA	3:P:195:SER:HB2	2.02	0.42
4:Q:48:TRP:CD1	5:R:56:ARG:HH12	2.38	0.42
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.84	0.41
1:A:254:ILE:HD13	1:A:254:ILE:HA	1.95	0.41
3:C:164:PHE:CD1	23:C:271:CHD:H193	2.55	0.41
1:N:169:ILE:N	1:N:169:ILE:HD13	2.34	0.41
1:N:344:PHE:CD1	1:N:344:PHE:C	2.97	0.41
3:P:63:ARG:O	3:P:68:GLN:HG3	2.20	0.41
1:A:28:MET:HE2	18:A:515:HEA:C27	2.50	0.41
7:G:78:LEU:HB3	7:G:79:PRO:HD2	2.02	0.41
1:N:165:ILE:O	1:N:169:ILE:HG12	2.20	0.41
4:Q:48:TRP:CE2	5:R:56:ARG:NH1	2.88	0.41
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.03	0.41
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.55	0.41
27:C:270:CDL:H621	27:C:270:CDL:H652	1.79	0.41
1:N:225:GLY:HA2	3:P:109:THR:OG1	2.19	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.41
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.01	0.41
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.74	0.41
21:B:521:TGL:H241	21:B:521:TGL:H201	2.03	0.41
27:G:269:CDL:H761	1:N:282:PHE:CZ	2.55	0.41
19:N:1268:PGV:H21	19:N:1268:PGV:H51	1.84	0.41
4:Q:51:LEU:HD21	4:Q:59:LEU:CD1	2.51	0.41
4:Q:121:LYS:HG2	11:X:53:TRP:HD1	1.86	0.41
8:U:49:ASP:O	8:U:52:VAL:HG22	2.20	0.41
1:A:344:PHE:CD1	1:A:344:PHE:C	2.98	0.41
1:A:486:ASP:OD2	4:D:19:ARG:HD3	2.20	0.41
1:N:191:THR:CG2	1:N:245:ILE:HG23	2.50	0.41
22:O:1230:PSC:H281	22:O:1230:PSC:H322	2.01	0.41
26:T:263:PEK:H282	26:T:263:PEK:H312	1.82	0.41
2:B:128:LEU:HD11	2:B:134:ARG:HA	2.02	0.41
4:D:8:SER:OG	13:M:4:LYS:NZ	2.53	0.41
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.02	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.84	0.41
1:N:35:LEU:HD23	1:N:35:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.17	0.41
3:C:29:SER:HB3	3:C:42:LEU:HD13	2.03	0.41
1:N:113:LEU:O	1:N:117:MET:HG2	2.20	0.41
1:N:208:MET:HB3	1:N:219:PHE:CD1	2.56	0.41
1:N:472:ILE:HG21	21:N:1522:TGL:HA92	2.03	0.41
10:W:50:LEU:O	10:W:50:LEU:HD22	2.21	0.41
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.56	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.41
2:B:200:CYS:SG	2:B:204:HIS:HA	2.60	0.41
3:C:12:ASN:O	3:C:13:PRO:C	2.64	0.41
3:C:35:PHE:HA	7:G:61:SER:OG	2.21	0.41
4:D:121:LYS:HG2	11:K:53:TRP:HD1	1.86	0.41
5:E:46:LYS:HG2	29:E:4386:HOH:O	2.20	0.41
6:F:6:VAL:HA	6:F:7:PRO:HD2	1.92	0.41
12:L:20:ARG:HH12	21:L:522:TGL:HC61	1.86	0.41
2:O:123:ILE:HD11	2:O:139:ASP:HA	2.03	0.41
2:O:209:ILE:HA	29:O:3146:HOH:O	2.19	0.41
3:P:21:ALA:O	3:P:24:ALA:HB3	2.20	0.41
3:P:173:PHE:CD2	3:P:173:PHE:C	2.98	0.41
8:U:40:GLU:HG3	8:U:50:VAL:HG11	2.00	0.41
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.88	0.41
2:B:37:LEU:HD13	29:I:4437:HOH:O	2.20	0.41
23:J:60:CHD:H183	23:J:60:CHD:H222	2.03	0.41
1:N:430:PHE:HE1	21:N:1521:TGL:HB21	1.86	0.41
2:O:122:MET:HB2	2:O:208:PRO:HD2	2.03	0.41
5:R:72:LYS:HB2	5:R:82:TYR:CD2	2.56	0.41
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.21	0.40
4:D:121:LYS:HG2	11:K:53:TRP:CD1	2.56	0.40
12:L:27:LEU:HD23	12:L:27:LEU:HA	1.92	0.40
1:N:195:LEU:HD23	1:N:245:ILE:HD13	2.02	0.40
1:N:498:CYS:HA	1:N:499:PRO:HA	1.77	0.40
1:A:472:ILE:HG21	21:L:522:TGL:CA9	2.48	0.40
3:C:122:HIS:HB3	29:C:4383:HOH:O	2.20	0.40
8:H:20:PHE:HE2	8:H:27:ARG:HG2	1.86	0.40
8:H:43:MET:HE1	8:U:43:MET:CE	2.50	0.40
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.57	0.40
1:N:180:GLN:HE21	1:N:180:GLN:HB2	1.63	0.40
5:R:44:GLU:O	5:R:45:PRO:C	2.62	0.40
7:T:31:CYS:SG	27:T:1269:CDL:H551	2.61	0.40
3:C:81:TYR:O	3:C:85:LEU:HG	2.20	0.40
4:D:24:LEU:HD12	5:E:30:ARG:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:164:ALA:HB2	2:O:171:LYS:HG3	2.04	0.40
5:R:48:ILE:O	5:R:52:LEU:HG	2.21	0.40
1:A:169:ILE:HD12	7:T:7:ASP:O	2.22	0.40
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.40
1:N:28:MET:HE2	1:N:28:MET:N	2.36	0.40
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.85	0.40
2:O:45:MET:HA	2:O:45:MET:HE2	2.02	0.40
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.22	0.40
1:A:92:MET:HE3	1:A:92:MET:HB3	2.00	0.40
1:A:204:ALA:O	1:A:208:MET:HG3	2.22	0.40
1:A:383:MET:HA	1:A:387:PHE:CD2	2.56	0.40
2:B:125:THR:N	29:B:2143:HOH:O	2.54	0.40
6:F:82:CYS:HA	6:F:83:PRO:HD3	1.97	0.40
23:G:86:CHD:H12A	23:G:86:CHD:H112	1.56	0.40
8:H:43:MET:CE	8:U:43:MET:HE1	2.51	0.40
1:N:416:ILE:HG22	1:N:464:ALA:HB2	2.04	0.40
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.56	0.40
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	494 (96%)	18 (4%)	0	100	100
1	N	512/514 (100%)	492 (96%)	20 (4%)	0	100	100
2	B	225/227 (99%)	209 (93%)	13 (6%)	3 (1%)	9	18
2	O	225/227 (99%)	210 (93%)	12 (5%)	3 (1%)	9	18
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
5	E	102/109 (94%)	100 (98%)	1 (1%)	1 (1%)	12	24
5	R	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	11	22
6	S	91/98 (93%)	84 (92%)	5 (6%)	2 (2%)	5	9
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	0	0
7	T	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	0	0
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	2	3
8	U	73/85 (86%)	68 (93%)	4 (6%)	1 (1%)	9	17
9	I	69/73 (94%)	64 (93%)	4 (6%)	1 (1%)	9	17
9	V	69/73 (94%)	66 (96%)	2 (3%)	1 (1%)	9	17
10	J	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
10	W	55/59 (93%)	55 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	44 (100%)	0	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	3478/3614 (96%)	3315 (95%)	132 (4%)	31 (1%)	14	27

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	39	SER
6	S	95	GLN
7	T	4	ALA
7	T	8	HIS
2	B	60	GLU
2	B	202	SER
7	G	6	GLY

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Mol	Chain	Res	Type
7	G	8	HIS
7	G	37	LEU
7	G	40	GLY
2	O	59	GLN
2	O	202	SER
7	T	3	ALA
7	T	7	ASP
7	T	39	SER
7	T	40	GLY
8	U	47	GLY
7	G	3	ALA
8	H	46	LYS
2	O	60	GLU
7	T	6	GLY
5	E	79	LYS
9	I	36	LYS
9	V	36	LYS
8	H	45	ALA
8	H	47	GLY
6	S	94	HIS
2	B	130	PRO

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	426/426 (100%)	415 (97%)	11 (3%)	40	68
1	N	426/426 (100%)	414 (97%)	12 (3%)	38	66
2	B	210/210 (100%)	200 (95%)	10 (5%)	23	46
2	O	210/210 (100%)	193 (92%)	17 (8%)	11	23
3	C	224/226 (99%)	218 (97%)	6 (3%)	39	67
3	P	224/226 (99%)	218 (97%)	6 (3%)	39	67
4	D	128/129 (99%)	124 (97%)	4 (3%)	35	62
4	Q	128/129 (99%)	124 (97%)	4 (3%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	91/95 (96%)	87 (96%)	4 (4%)	25	50
5	R	91/95 (96%)	89 (98%)	2 (2%)	45	73
6	F	79/81 (98%)	74 (94%)	5 (6%)	16	34
6	S	79/81 (98%)	74 (94%)	5 (6%)	16	34
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	19
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	36
8	H	67/75 (89%)	64 (96%)	3 (4%)	24	49
8	U	67/75 (89%)	64 (96%)	3 (4%)	24	49
9	I	56/57 (98%)	54 (96%)	2 (4%)	31	58
9	V	56/57 (98%)	51 (91%)	5 (9%)	9	20
10	J	48/50 (96%)	46 (96%)	2 (4%)	26	52
10	W	48/50 (96%)	45 (94%)	3 (6%)	16	34
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	68
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	43
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	68
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	43
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	13
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	13
All	All	3022/3082 (98%)	2894 (96%)	128 (4%)	26	52

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	128	VAL
1	A	138	HIS
1	A	152	LEU
1	A	180	GLN
1	A	297	MET
1	A	306	THR
1	A	369	ASP
1	A	382	SER
1	A	507	GLU
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU

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Mol	Chain	Res	Type
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	115	ASP
2	B	167	SER
3	C	29	SER
3	C	77	LYS
3	C	92	LEU
3	C	159	MET
3	C	192	VAL
3	C	230	ASN
4	D	15	SER
4	D	45	LYS
4	D	51	LEU
4	D	131	ILE
5	E	7	THR
5	E	70	VAL
5	E	90	ARG
5	E	109	VAL
6	F	48	LEU
6	F	53	THR
6	F	87	THR
6	F	92	VAL
6	F	95	GLN
7	G	17	ARG
7	G	33	LEU
7	G	37	LEU
7	G	43	GLU
7	G	74	ARG
7	G	84	LYS
8	H	40	GLU
8	H	51	SER
8	H	60	TYR
9	I	8	GLN
9	I	21	ILE
10	J	27	THR
10	J	50	LEU
11	K	47	ARG
12	L	26	THR

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Mol	Chain	Res	Type
13	M	13	LYS
13	M	34	LEU
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	138	HIS
1	N	180	GLN
1	N	264	LYS
1	N	297	MET
1	N	363	LEU
1	N	369	ASP
1	N	382	SER
1	N	394	VAL
1	N	484	THR
1	N	485	VAL
1	N	513	LEU
2	O	33	LEU
2	O	42	ILE
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	113	TYR
2	O	115	ASP
2	O	116	LEU
2	O	148	MET
2	O	167	SER
2	O	183	THR
2	O	205	SER
2	O	217	LYS
3	P	29	SER
3	P	41	THR
3	P	77	LYS
3	P	127	LEU
3	P	144	ILE
3	P	230	ASN
4	Q	6	VAL
4	Q	9	GLU
4	Q	121	LYS

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Mol	Chain	Res	Type
4	Q	143	ASN
5	R	70	VAL
5	R	90	ARG
6	S	48	LEU
6	S	53	THR
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	17	ARG
7	T	33	LEU
7	T	37	LEU
7	T	84	LYS
8	U	52	VAL
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	10	ARG
9	V	21	ILE
9	V	22	VAL
9	V	29	LEU
10	W	4	ARG
10	W	50	LEU
10	W	54	SER
11	X	23	THR
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	43	GLN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	10	GLN

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Mol	Chain	Res	Type
2	B	52	HIS
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	161	GLN
3	C	222	GLN
4	D	32	ASN
4	D	37	GLN
4	D	109	HIS
5	E	78	HIS
5	E	94	ASN
7	G	76	ASN
8	H	22	ASN
8	H	31	GLN
10	J	57	HIS
11	K	35	GLN
12	L	42	HIS
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	503	HIS
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	92	ASN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	70	HIS
3	P	76	GLN
4	Q	29	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	119	GLN
4	Q	143	ASN
5	R	78	HIS
5	R	94	ASN
6	S	94	HIS
7	T	41	HIS

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Mol	Chain	Res	Type
7	T	71	HIS
7	T	76	ASN
8	U	28	ASN
8	U	31	GLN
8	U	32	ASN
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 ⓘ

6 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
7	TPO	G	11	7	8,10,11	2.09	3 (37%)	10,14,16	1.49	3 (30%)
7	TPO	T	11	7	8,10,11	1.88	2 (25%)	10,14,16	1.72	3 (30%)
2	FME	O	1	2	8,9,10	0.64	0	8,9,11	2.59	2 (25%)
1	FME	A	1	1	8,9,10	0.68	0	8,9,11	2.12	3 (37%)
2	FME	B	1	2	8,9,10	0.76	0	8,9,11	3.12	2 (25%)
1	FME	N	1	1	8,9,10	0.53	0	8,9,11	3.17	4 (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
7	TPO	G	11	7	-	4/9/11/13	-

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.54	1.65	1.59
7	T	11	TPO	P-O1P	3.37	1.61	1.50
7	G	11	TPO	P-O1P	2.96	1.59	1.50
7	T	11	TPO	P-OG1	2.64	1.64	1.59
7	G	11	TPO	P-O2P	2.01	1.62	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-7.29	111.62	122.82
1	N	1	FME	CA-N-CN	-7.22	111.72	122.82
2	O	1	FME	CA-N-CN	-5.38	114.54	122.82
1	A	1	FME	CA-N-CN	-4.21	116.34	122.82
7	T	11	TPO	CG2-CB-CA	4.08	121.20	113.26
2	O	1	FME	C-CA-N	4.02	117.26	109.50
2	B	1	FME	C-CA-N	3.74	116.71	109.50
1	N	1	FME	CB-CA-N	3.70	117.27	110.52
7	G	11	TPO	O2P-P-OG1	2.87	117.03	105.85
1	N	1	FME	CE-SD-CG	2.66	114.07	100.32
1	A	1	FME	CE-SD-CG	2.65	114.05	100.32
1	A	1	FME	O1-CN-N	-2.58	118.66	125.32
1	N	1	FME	O-C-CA	-2.39	118.63	124.77
7	T	11	TPO	O2P-P-OG1	2.26	114.66	105.85
7	T	11	TPO	O-C-CA	-2.12	119.31	124.77
7	G	11	TPO	O-C-CA	-2.10	119.36	124.77
7	G	11	TPO	CG2-CB-CA	2.01	117.17	113.26

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
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
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	O-C-CA-CB
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
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	N	1	FME	CB-CG-SD-CE
7	G	11	TPO	O-C-CA-CB
7	T	11	TPO	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
2	O	1	FME	4	0
1	A	1	FME	3	0
2	B	1	FME	3	0
1	N	1	FME	1	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
19	PGV	P	1267	-	50,50,50	0.89	2 (4%)	53,56,56	1.03	3 (5%)
15	PER	A	520	14,18	1,1,1	1.98	0	-		
26	PEK	G	264	-	52,52,52	0.99	3 (5%)	55,57,57	1.25	5 (9%)
26	PEK	P	1265	-	52,52,52	1.54	4 (7%)	55,57,57	1.26	5 (9%)
18	HEA	N	515	1	67,67,67	1.88	20 (29%)	81,103,103	1.89	18 (22%)
21	TGL	O	1523	-	62,62,62	1.47	6 (9%)	65,65,65	1.23	9 (13%)
26	PEK	G	1263	-	52,52,52	1.31	2 (3%)	55,57,57	1.24	5 (9%)
21	TGL	N	1521	-	62,62,62	1.55	7 (11%)	65,65,65	1.63	13 (20%)
26	PEK	T	263	-	52,52,52	1.45	6 (11%)	55,57,57	1.37	7 (12%)
23	CHD	C	271	-	32,32,32	0.87	0	51,51,51	4.72	33 (64%)
23	CHD	J	60	-	32,32,32	1.00	2 (6%)	51,51,51	4.87	33 (64%)
23	CHD	P	1271	-	32,32,32	0.86	0	51,51,51	4.86	30 (58%)
20	CUA	B	228	2	0,1,1	-	-	-		
21	TGL	B	521	-	62,62,62	1.35	6 (9%)	65,65,65	1.70	11 (16%)
23	CHD	W	1060	-	32,32,32	1.16	4 (12%)	51,51,51	5.07	33 (64%)
18	HEA	A	515	1	67,67,67	1.98	21 (31%)	81,103,103	1.95	21 (25%)
23	CHD	B	1086	-	32,32,32	1.25	4 (12%)	51,51,51	5.30	34 (66%)
24	DMU	C	272	-	34,34,34	1.19	2 (5%)	45,45,45	3.32	24 (53%)
19	PGV	N	1524	-	50,50,50	1.13	2 (4%)	53,56,56	1.22	5 (9%)
19	PGV	N	1268	-	50,50,50	1.21	2 (4%)	53,56,56	1.38	5 (9%)
27	CDL	C	270	-	99,99,99	1.44	13 (13%)	105,111,111	1.34	11 (10%)
19	PGV	N	1266	-	50,50,50	0.95	2 (4%)	53,56,56	1.39	6 (11%)
21	TGL	D	523	-	62,62,62	1.52	6 (9%)	65,65,65	1.49	13 (20%)
27	CDL	T	1269	-	99,99,99	1.40	11 (11%)	105,111,111	1.43	12 (11%)
23	CHD	C	525	-	32,32,32	1.24	2 (6%)	51,51,51	4.89	36 (70%)
24	DMU	Z	1526	-	34,34,34	0.95	2 (5%)	45,45,45	3.17	19 (42%)
19	PGV	A	524	-	50,50,50	1.20	2 (4%)	53,56,56	1.20	5 (9%)
24	DMU	P	1272	-	34,34,34	1.21	2 (5%)	45,45,45	3.24	24 (53%)
27	CDL	G	269	-	99,99,99	1.47	12 (12%)	105,111,111	1.26	10 (9%)
19	PGV	A	521	-	50,50,50	1.09	2 (4%)	53,56,56	1.28	5 (9%)
18	HEA	A	516	15,1	67,67,67	3.05	28 (41%)	81,103,103	4.02	44 (54%)
18	HEA	N	516	15,1	67,67,67	2.24	26 (38%)	81,103,103	1.64	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGV	C	267	-	50,50,50	0.87	2 (4%)	53,56,56	1.19	5 (9%)
20	CUA	O	228	2	0,1,1	-	-	-	-	-
21	TGL	L	522	-	62,62,62	1.42	5 (8%)	65,65,65	1.50	8 (12%)
21	TGL	N	1522	-	62,62,62	1.57	6 (9%)	65,65,65	1.38	10 (15%)
23	CHD	G	86	-	32,32,32	1.12	2 (6%)	51,51,51	5.02	33 (64%)
27	CDL	P	1270	-	99,99,99	1.42	11 (11%)	105,111,111	1.30	12 (11%)
24	DMU	M	526	-	34,34,34	0.80	2 (5%)	45,45,45	3.13	23 (51%)
19	PGV	C	268	-	50,50,50	1.20	2 (4%)	53,56,56	1.33	4 (7%)
26	PEK	P	1264	-	52,52,52	0.99	4 (7%)	55,57,57	1.48	8 (14%)
22	PSC	B	230	-	51,51,51	1.30	3 (5%)	57,59,59	1.22	6 (10%)
15	PER	N	520	14,18	1,1,1	1.98	0	-	-	-
26	PEK	C	265	-	52,52,52	1.38	4 (7%)	55,57,57	1.26	4 (7%)
23	CHD	P	1525	-	32,32,32	0.97	2 (6%)	51,51,51	5.12	37 (72%)
22	PSC	O	1230	-	51,51,51	1.23	3 (5%)	57,59,59	1.09	3 (5%)

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
19	PGV	P	1267	-	-	13/55/55/55	-
26	PEK	G	264	-	-	24/56/56/56	-
26	PEK	P	1265	-	-	27/56/56/56	-
18	HEA	N	515	1	-	8/36/76/76	-
21	TGL	O	1523	-	-	32/65/65/65	-
26	PEK	G	1263	-	-	33/56/56/56	-
21	TGL	N	1521	-	-	28/65/65/65	-
26	PEK	T	263	-	-	30/56/56/56	-
23	CHD	C	271	-	2/2/12/12	8/9/74/74	0/4/4/4
23	CHD	J	60	-	1/1/12/12	7/9/74/74	0/4/4/4
23	CHD	P	1271	-	2/2/12/12	8/9/74/74	0/4/4/4
21	TGL	B	521	-	-	33/65/65/65	-
23	CHD	W	1060	-	1/1/12/12	7/9/74/74	0/4/4/4
23	CHD	B	1086	-	1/1/12/12	3/9/74/74	0/4/4/4
18	HEA	A	515	1	-	9/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DMU	C	272	-	5/5/10/10	11/19/59/59	0/2/2/2
19	PGV	N	1524	-	-	35/55/55/55	-
19	PGV	N	1268	-	-	27/55/55/55	-
27	CDL	C	270	-	-	68/110/110/110	-
19	PGV	N	1266	-	-	14/55/55/55	-
21	TGL	D	523	-	-	38/65/65/65	-
27	CDL	T	1269	-	-	62/110/110/110	-
23	CHD	C	525	-	1/1/12/12	2/9/74/74	0/4/4/4
24	DMU	Z	1526	-	5/5/10/10	11/19/59/59	0/2/2/2
19	PGV	A	524	-	-	31/55/55/55	-
24	DMU	P	1272	-	5/5/10/10	11/19/59/59	0/2/2/2
27	CDL	G	269	-	-	61/110/110/110	-
19	PGV	A	521	-	-	14/55/55/55	-
18	HEA	A	516	15,1	-	9/36/76/76	-
18	HEA	N	516	15,1	-	8/36/76/76	-
23	CHD	G	86	-	1/1/12/12	3/9/74/74	0/4/4/4
19	PGV	C	267	-	-	17/55/55/55	-
21	TGL	L	522	-	-	34/65/65/65	-
21	TGL	N	1522	-	-	34/65/65/65	-
27	CDL	P	1270	-	-	58/110/110/110	-
24	DMU	M	526	-	5/5/10/10	10/19/59/59	0/2/2/2
19	PGV	C	268	-	-	34/55/55/55	-
26	PEK	P	1264	-	-	26/56/56/56	-
22	PSC	B	230	-	-	28/55/55/55	-
26	PEK	C	265	-	-	27/56/56/56	-
23	CHD	P	1525	-	1/1/12/12	2/9/74/74	0/4/4/4
22	PSC	O	1230	-	-	35/55/55/55	-

All (247) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	FE-ND	9.06	2.22	1.94
18	A	516	HEA	C3A-C4A	-7.66	1.32	1.46
18	N	516	HEA	FE-NC	7.55	2.20	1.95
18	A	516	HEA	FE-NC	6.84	2.17	1.95
18	A	516	HEA	C4D-C3D	-6.78	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	515	HEA	FE-NC	6.31	2.16	1.95
18	N	516	HEA	FE-NA	6.30	2.15	1.95
18	A	515	HEA	FE-NA	6.17	2.15	1.95
26	T	263	PEK	O03-C21	6.03	1.50	1.33
19	A	524	PGV	O03-C19	5.76	1.50	1.33
18	A	516	HEA	CHB-C1B	5.74	1.52	1.39
18	A	516	HEA	CHA-C1A	5.69	1.49	1.38
21	N	1522	TGL	OG2-CB1	5.69	1.50	1.34
21	N	1522	TGL	OG1-CA1	5.68	1.49	1.33
21	D	523	TGL	OG3-CC1	5.58	1.49	1.33
19	N	1268	PGV	O01-C1	5.50	1.49	1.34
26	G	1263	PEK	O03-C21	5.50	1.49	1.33
18	A	516	HEA	C4B-NB	-5.50	1.30	1.40
21	L	522	TGL	OG1-CA1	5.45	1.49	1.33
27	P	1270	CDL	OA8-CA7	5.39	1.49	1.33
19	C	268	PGV	O01-C1	5.34	1.49	1.34
21	L	522	TGL	OG2-CB1	5.27	1.49	1.34
19	N	1524	PGV	O03-C19	5.26	1.48	1.33
26	T	263	PEK	O01-C1	5.25	1.49	1.34
26	C	265	PEK	O03-C21	5.24	1.48	1.33
21	O	1523	TGL	OG2-CB1	5.24	1.49	1.34
26	P	1265	PEK	C7-C6	5.24	1.88	1.51
21	D	523	TGL	OG2-CB1	5.23	1.49	1.34
22	B	230	PSC	O01-C1	5.19	1.49	1.34
26	P	1265	PEK	O03-C21	5.18	1.48	1.33
18	A	516	HEA	CHD-C1D	5.16	1.48	1.38
27	G	269	CDL	OA6-CA5	5.16	1.48	1.34
21	N	1521	TGL	OG1-CA1	5.15	1.48	1.33
27	C	270	CDL	OA8-CA7	5.13	1.48	1.33
27	T	1269	CDL	OB6-CB5	5.12	1.48	1.34
26	P	1265	PEK	O01-C1	5.04	1.48	1.34
27	G	269	CDL	OB8-CB7	5.03	1.48	1.33
21	D	523	TGL	OG1-CA1	4.98	1.47	1.33
27	T	1269	CDL	OB8-CB7	4.96	1.47	1.33
26	G	1263	PEK	O01-C1	4.94	1.48	1.34
27	G	269	CDL	OB6-CB5	4.92	1.48	1.34
27	P	1270	CDL	OA6-CA5	4.85	1.48	1.34
27	C	270	CDL	OA6-CA5	4.84	1.48	1.34
21	O	1523	TGL	OG1-CA1	4.83	1.47	1.33
18	A	516	HEA	C4C-NC	-4.82	1.30	1.39
21	N	1521	TGL	OG2-CB1	4.80	1.47	1.34
26	C	265	PEK	O01-C1	4.76	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	1272	DMU	O16-C6	4.75	1.48	1.40
27	P	1270	CDL	OB8-CB7	4.73	1.47	1.33
21	B	521	TGL	OG1-CA1	4.70	1.47	1.33
21	O	1523	TGL	OG3-CC1	4.70	1.47	1.33
19	A	521	PGV	O03-C19	4.66	1.46	1.33
18	A	516	HEA	C4A-NA	-4.64	1.30	1.39
18	A	516	HEA	C4D-ND	-4.60	1.29	1.38
27	T	1269	CDL	OA6-CA5	4.60	1.47	1.34
19	A	521	PGV	O01-C1	4.59	1.47	1.34
22	B	230	PSC	O03-C19	4.59	1.46	1.33
21	B	521	TGL	OG2-CB1	4.56	1.47	1.34
18	A	516	HEA	C4B-C3B	-4.55	1.36	1.44
18	A	516	HEA	CHB-C4A	4.46	1.47	1.38
27	C	270	CDL	OB8-CB7	4.45	1.46	1.33
24	C	272	DMU	O16-C6	4.40	1.47	1.40
21	N	1521	TGL	OG3-CC1	4.38	1.46	1.33
21	N	1522	TGL	OG3-CC1	4.37	1.46	1.33
19	C	268	PGV	O03-C19	4.37	1.46	1.33
19	N	1266	PGV	O03-C19	4.35	1.46	1.33
27	G	269	CDL	OA8-CA7	4.35	1.46	1.33
27	P	1270	CDL	OB6-CB5	4.34	1.46	1.34
19	N	1268	PGV	O03-C19	4.33	1.46	1.33
18	A	515	HEA	FE-NB	4.31	2.08	1.94
18	N	516	HEA	FE-NB	4.31	2.08	1.94
22	O	1230	PSC	C13-C12	4.28	1.56	1.31
21	N	1521	TGL	CA6-CA5	4.26	1.73	1.51
22	O	1230	PSC	O01-C1	4.24	1.46	1.34
27	T	1269	CDL	OA8-CA7	4.23	1.45	1.33
18	A	516	HEA	CHC-C1C	4.22	1.48	1.39
19	N	1524	PGV	O01-C1	4.14	1.46	1.34
22	B	230	PSC	C13-C12	4.06	1.54	1.31
19	P	1267	PGV	O03-C19	4.04	1.45	1.33
27	C	270	CDL	OB6-CB5	4.00	1.45	1.34
26	G	264	PEK	O01-C1	3.95	1.45	1.34
19	A	524	PGV	O01-C1	3.93	1.45	1.34
22	O	1230	PSC	O03-C19	3.92	1.44	1.33
18	A	516	HEA	FE-NA	3.84	2.07	1.95
18	N	516	HEA	CHD-C1D	3.84	1.46	1.38
19	C	267	PGV	O03-C19	3.80	1.44	1.33
18	A	515	HEA	C4A-NA	-3.79	1.32	1.39
18	N	516	HEA	C1C-NC	-3.76	1.32	1.39
21	L	522	TGL	OG3-CC1	3.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	C3A-C4A	-3.71	1.39	1.46
18	A	515	HEA	C1C-NC	-3.71	1.32	1.39
18	N	515	HEA	FE-ND	3.68	2.06	1.94
26	P	1264	PEK	O01-C1	3.68	1.44	1.34
27	C	270	CDL	C59-C58	-3.67	1.33	1.51
21	L	522	TGL	C20-CA9	-3.66	1.33	1.51
21	N	1521	TGL	C10-CB9	-3.64	1.33	1.51
21	L	522	TGL	C10-CB9	-3.59	1.33	1.51
21	B	521	TGL	OG3-CC1	3.59	1.43	1.33
18	N	516	HEA	C4C-NC	-3.57	1.32	1.39
21	N	1522	TGL	C20-CA9	-3.53	1.34	1.51
27	P	1270	CDL	C59-C58	-3.49	1.34	1.51
18	A	516	HEA	OMA-CMA	3.46	1.29	1.22
27	P	1270	CDL	C62-C61	-3.46	1.34	1.51
27	G	269	CDL	C42-C41	-3.45	1.34	1.51
21	N	1522	TGL	C10-CB9	-3.42	1.34	1.51
18	A	516	HEA	CAA-C2A	3.41	1.60	1.51
18	A	515	HEA	C1D-ND	-3.40	1.34	1.40
27	G	269	CDL	C39-C38	-3.40	1.34	1.51
21	D	523	TGL	C15-CC9	-3.39	1.34	1.51
27	G	269	CDL	C59-C58	-3.39	1.34	1.51
27	C	270	CDL	C79-C78	-3.38	1.34	1.51
23	B	1086	CHD	C13-C14	-3.37	1.49	1.55
21	B	521	TGL	C10-CB9	-3.35	1.35	1.51
21	O	1523	TGL	C15-CC9	-3.34	1.35	1.51
18	A	515	HEA	C1A-C2A	-3.34	1.39	1.45
18	A	515	HEA	CHA-C1A	3.33	1.44	1.38
18	N	515	HEA	FE-NA	3.33	2.06	1.95
23	C	525	CHD	C18-C13	3.31	1.59	1.54
27	P	1270	CDL	C22-C21	-3.30	1.35	1.51
27	P	1270	CDL	C19-C18	-3.28	1.35	1.51
27	T	1269	CDL	C62-C61	-3.27	1.35	1.51
27	G	269	CDL	C19-C18	-3.26	1.35	1.51
18	N	516	HEA	CHA-C1A	3.26	1.44	1.38
21	N	1521	TGL	C20-CA9	-3.25	1.35	1.51
18	N	515	HEA	C1A-C2A	-3.25	1.39	1.45
21	O	1523	TGL	C10-CB9	-3.23	1.35	1.51
27	T	1269	CDL	C19-C18	-3.23	1.35	1.51
18	A	516	HEA	CMA-C3A	3.22	1.52	1.45
27	C	270	CDL	C62-C61	-3.22	1.35	1.51
18	N	515	HEA	C3A-C4A	-3.22	1.40	1.46
18	N	515	HEA	C4D-C3D	-3.21	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	516	HEA	O11-C11	3.21	1.50	1.42
27	G	269	CDL	C62-C61	-3.21	1.35	1.51
18	A	516	HEA	CHC-C4B	3.20	1.44	1.38
18	N	516	HEA	CHD-C4C	3.20	1.46	1.39
27	C	270	CDL	C22-C21	-3.20	1.35	1.51
21	B	521	TGL	C20-CA9	-3.19	1.35	1.51
19	C	267	PGV	O01-C1	3.19	1.43	1.34
18	N	516	HEA	CHB-C4A	3.18	1.44	1.38
27	T	1269	CDL	C42-C41	-3.18	1.36	1.51
26	P	1264	PEK	O03-C01	-3.16	1.38	1.45
27	C	270	CDL	C39-C38	-3.11	1.36	1.51
21	D	523	TGL	C20-CA9	-3.11	1.36	1.51
18	N	515	HEA	CHA-C1A	3.09	1.44	1.38
27	T	1269	CDL	C39-C38	-3.08	1.36	1.51
21	D	523	TGL	C10-CB9	-3.07	1.36	1.51
24	Z	1526	DMU	C3-C4	-3.05	1.44	1.52
23	W	1060	CHD	C11-C9	3.05	1.58	1.53
21	N	1522	TGL	C15-CC9	-3.04	1.36	1.51
27	T	1269	CDL	C59-C58	-3.03	1.36	1.51
18	A	516	HEA	CHD-C4C	3.02	1.46	1.39
27	C	270	CDL	C42-C41	-3.02	1.36	1.51
18	N	515	HEA	CHB-C4A	2.99	1.44	1.38
18	A	516	HEA	C11-C3B	2.96	1.55	1.51
27	C	270	CDL	C19-C18	-2.95	1.37	1.51
27	C	270	CDL	C82-C81	-2.95	1.37	1.51
18	N	516	HEA	CHA-C4D	2.92	1.45	1.39
21	N	1521	TGL	C15-CC9	-2.92	1.37	1.51
21	O	1523	TGL	C20-CA9	-2.92	1.37	1.51
18	N	515	HEA	CHC-C4B	2.92	1.44	1.38
26	G	264	PEK	O03-C21	2.91	1.41	1.33
18	N	515	HEA	C1D-ND	-2.91	1.35	1.40
18	A	515	HEA	C1A-NA	-2.86	1.34	1.39
26	P	1265	PEK	C6-C5	2.85	1.47	1.31
23	B	1086	CHD	C10-C5	-2.84	1.51	1.55
27	G	269	CDL	C82-C81	-2.83	1.37	1.51
27	T	1269	CDL	C22-C21	-2.83	1.37	1.51
21	B	521	TGL	C15-CC9	-2.82	1.37	1.51
27	P	1270	CDL	C39-C38	-2.79	1.37	1.51
19	N	1266	PGV	O01-C1	2.77	1.42	1.34
18	A	515	HEA	C1B-NB	-2.76	1.33	1.38
27	T	1269	CDL	C82-C81	-2.76	1.38	1.51
18	N	516	HEA	C4B-NB	-2.74	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	1267	PGV	O01-C1	2.71	1.41	1.34
18	N	516	HEA	CHC-C4B	2.70	1.43	1.38
23	C	525	CHD	C13-C14	-2.69	1.51	1.55
24	M	526	DMU	C3-C4	-2.68	1.45	1.52
18	N	515	HEA	C4B-NB	-2.68	1.35	1.40
18	N	516	HEA	C1D-ND	-2.66	1.35	1.40
18	N	516	HEA	CHB-C1B	2.65	1.45	1.39
26	G	264	PEK	O03-C01	-2.64	1.39	1.45
18	A	516	HEA	C1A-NA	2.59	1.44	1.39
18	A	515	HEA	FE-NC	2.57	2.03	1.95
23	W	1060	CHD	C20-C17	2.57	1.58	1.54
24	Z	1526	DMU	O16-C6	2.55	1.44	1.40
26	P	1264	PEK	O03-C21	2.53	1.40	1.33
26	C	265	PEK	C05-C04	2.53	1.60	1.49
18	N	515	HEA	CHC-C1C	2.51	1.45	1.39
18	A	515	HEA	CHC-C4B	2.51	1.43	1.38
18	A	515	HEA	CHD-C1D	2.51	1.43	1.38
18	N	515	HEA	CHD-C1D	2.50	1.43	1.38
18	N	516	HEA	C4A-NA	-2.50	1.34	1.39
18	N	516	HEA	C1A-C2A	-2.48	1.40	1.45
18	A	516	HEA	C20-C19	2.48	1.56	1.51
23	P	1525	CHD	C13-C14	-2.47	1.51	1.55
18	N	515	HEA	CHB-C1B	2.45	1.44	1.39
27	P	1270	CDL	C42-C41	-2.45	1.39	1.51
27	G	269	CDL	C22-C21	-2.43	1.39	1.51
18	N	516	HEA	C1B-NB	-2.42	1.34	1.38
18	A	515	HEA	CHD-C4C	2.41	1.44	1.39
18	N	515	HEA	C4A-NA	-2.41	1.35	1.39
18	N	515	HEA	FE-NB	2.40	2.02	1.94
18	A	515	HEA	CHA-C4D	2.39	1.44	1.39
24	C	272	DMU	O1-C10	2.39	1.48	1.41
18	A	515	HEA	C4D-C3D	-2.39	1.41	1.45
18	N	516	HEA	C3D-C2D	2.38	1.41	1.36
26	C	265	PEK	P-O12	2.37	1.68	1.59
23	G	86	CHD	C11-C9	2.35	1.57	1.53
18	N	516	HEA	C4B-C3B	-2.34	1.40	1.44
27	P	1270	CDL	C82-C81	-2.33	1.40	1.51
18	N	516	HEA	C18-C19	2.31	1.38	1.33
18	N	515	HEA	C4C-NC	-2.31	1.35	1.39
18	N	516	HEA	FE-ND	2.29	2.01	1.94
27	C	270	CDL	OB6-CB4	-2.28	1.41	1.46
23	G	86	CHD	C10-C5	-2.28	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	515	HEA	CHD-C4C	2.27	1.44	1.39
23	B	1086	CHD	C13-C12	-2.27	1.51	1.54
18	A	516	HEA	CAD-C3D	2.26	1.57	1.51
18	A	515	HEA	C4B-NB	-2.26	1.36	1.40
26	P	1264	PEK	O01-C02	-2.25	1.41	1.46
18	A	515	HEA	C4C-NC	-2.23	1.35	1.39
18	A	515	HEA	O11-C11	2.22	1.47	1.42
18	A	515	HEA	C1D-C2D	-2.21	1.40	1.44
24	P	1272	DMU	O1-C10	2.18	1.47	1.41
18	N	516	HEA	C22-C23	2.17	1.39	1.32
18	N	515	HEA	C3B-C2B	2.16	1.39	1.34
24	M	526	DMU	O16-C6	2.16	1.43	1.40
26	T	263	PEK	P-O11	2.15	1.67	1.59
23	J	60	CHD	C11-C9	2.13	1.57	1.53
18	N	516	HEA	C3B-C2B	2.11	1.39	1.34
27	G	269	CDL	C79-C78	-2.10	1.41	1.51
23	W	1060	CHD	O12-C12	2.10	1.47	1.43
18	N	516	HEA	CHC-C1C	2.10	1.44	1.39
18	A	516	HEA	C14-C15	2.09	1.37	1.33
18	A	515	HEA	CHB-C4A	2.09	1.42	1.38
18	A	516	HEA	CHA-C4D	2.09	1.44	1.39
23	J	60	CHD	O12-C12	2.08	1.47	1.43
26	T	263	PEK	C9-C8	2.08	1.43	1.31
18	N	516	HEA	C1A-NA	-2.07	1.35	1.39
23	B	1086	CHD	C1-C10	-2.04	1.50	1.54
26	T	263	PEK	C03-C02	2.04	1.57	1.50
23	W	1060	CHD	C11-C12	2.03	1.56	1.53
18	N	515	HEA	CHA-C4D	2.03	1.43	1.39
26	T	263	PEK	C01-C02	2.02	1.57	1.50
18	A	516	HEA	CAC-C3C	2.02	1.52	1.47
18	A	516	HEA	C18-C19	2.02	1.37	1.33
23	P	1525	CHD	C8-C9	2.01	1.57	1.53

All (649) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1086	CHD	C18-C13-C12	-14.15	94.89	109.06
23	C	271	CHD	C10-C9-C8	13.32	126.68	111.84
23	P	1271	CHD	C10-C9-C8	13.28	126.64	111.84
23	C	525	CHD	C6-C5-C10	13.23	126.73	112.66
23	P	1525	CHD	C6-C5-C10	12.41	125.86	112.66
23	C	525	CHD	C10-C9-C8	11.50	124.66	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	86	CHD	C6-C5-C10	11.42	124.82	112.66
18	A	516	HEA	CMB-C2B-C1B	11.40	142.85	125.03
23	P	1525	CHD	C1-C10-C5	11.28	123.94	107.75
23	B	1086	CHD	C1-C10-C5	11.17	123.78	107.75
18	A	516	HEA	CHA-C4D-C3D	-10.82	108.99	124.77
23	B	1086	CHD	C10-C9-C8	10.74	123.81	111.84
23	P	1271	CHD	C15-C14-C8	10.68	133.00	118.36
23	P	1525	CHD	C14-C13-C12	10.43	116.95	107.42
23	B	1086	CHD	C14-C13-C12	10.42	116.94	107.42
23	C	525	CHD	C1-C10-C5	10.27	122.48	107.75
23	W	1060	CHD	C13-C17-C20	10.17	131.81	119.48
23	B	1086	CHD	C17-C13-C12	10.16	126.81	117.67
18	A	516	HEA	CMB-C2B-C3B	-10.15	110.64	130.28
18	A	516	HEA	CMD-C2D-C1D	10.14	140.88	125.03
23	G	86	CHD	C1-C10-C5	9.89	121.94	107.75
23	J	60	CHD	C10-C9-C8	9.79	122.76	111.84
23	G	86	CHD	C18-C13-C12	-9.78	99.27	109.06
23	J	60	CHD	C15-C14-C13	9.74	112.99	103.54
23	G	86	CHD	C17-C13-C12	9.58	126.28	117.67
23	G	86	CHD	C10-C9-C8	9.55	122.48	111.84
23	P	1525	CHD	C10-C9-C8	9.32	122.22	111.84
23	W	1060	CHD	C10-C9-C8	9.31	122.22	111.84
23	C	271	CHD	C15-C14-C8	9.31	131.13	118.36
23	J	60	CHD	C16-C17-C13	9.26	112.52	103.54
23	G	86	CHD	C14-C13-C12	9.23	115.85	107.42
18	A	516	HEA	C3D-C4D-ND	9.12	119.17	110.35
23	B	1086	CHD	C6-C5-C10	9.07	122.31	112.66
23	B	1086	CHD	C19-C10-C9	-8.93	99.18	111.18
23	B	1086	CHD	C1-C2-C3	8.80	122.14	110.48
24	C	272	DMU	O16-C6-C1	8.70	121.49	108.27
23	G	86	CHD	C19-C10-C9	-8.60	99.62	111.18
23	W	1060	CHD	C14-C8-C7	8.60	123.26	111.85
23	C	525	CHD	C17-C13-C12	8.52	125.33	117.67
24	M	526	DMU	O1-C9-C8	8.50	125.01	109.70
23	P	1525	CHD	C17-C13-C12	8.46	125.28	117.67
23	W	1060	CHD	C6-C5-C4	-8.45	101.57	111.23
23	C	271	CHD	C11-C12-C13	8.44	119.85	111.26
23	J	60	CHD	C13-C17-C20	8.43	129.69	119.48
23	P	1525	CHD	C4-C3-C2	8.40	120.87	110.62
18	A	516	HEA	CAD-C3D-C2D	8.39	143.58	127.87
18	A	516	HEA	CAA-C2A-C1A	8.38	141.88	124.85
24	P	1272	DMU	O16-C6-C1	8.19	120.71	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C15-C14-C13	8.18	111.48	103.54
23	P	1525	CHD	C19-C10-C9	-8.17	100.20	111.18
23	P	1525	CHD	C15-C14-C13	8.16	111.46	103.54
23	C	525	CHD	C14-C13-C12	8.05	114.77	107.42
23	C	525	CHD	C4-C3-C2	8.05	120.44	110.62
23	W	1060	CHD	C15-C14-C13	7.96	111.26	103.54
23	G	86	CHD	C5-C4-C3	7.94	124.68	112.71
23	P	1271	CHD	C4-C3-C2	7.93	120.29	110.62
23	W	1060	CHD	C4-C5-C10	7.93	121.10	112.66
23	B	1086	CHD	C6-C7-C8	7.90	120.13	111.50
23	P	1271	CHD	C1-C10-C5	7.62	118.68	107.75
23	C	271	CHD	C6-C7-C8	7.57	119.77	111.50
23	W	1060	CHD	C6-C7-C8	7.57	119.77	111.50
23	J	60	CHD	C14-C8-C7	7.52	121.83	111.85
23	C	271	CHD	C15-C14-C13	7.52	110.83	103.54
23	W	1060	CHD	C1-C2-C3	7.45	120.34	110.48
23	J	60	CHD	C1-C2-C3	7.44	120.34	110.48
23	P	1271	CHD	C6-C7-C8	7.42	119.60	111.50
23	P	1271	CHD	C11-C12-C13	7.41	118.81	111.26
23	C	271	CHD	C5-C6-C7	7.39	123.19	114.40
23	W	1060	CHD	C16-C17-C13	7.30	110.62	103.54
23	C	525	CHD	C18-C13-C12	-7.29	101.76	109.06
23	W	1060	CHD	C11-C9-C10	7.29	121.10	113.70
18	A	516	HEA	CAD-C3D-C4D	-7.28	112.02	124.70
23	J	60	CHD	C4-C5-C10	7.17	120.28	112.66
23	B	1086	CHD	C5-C4-C3	7.16	123.51	112.71
18	A	515	HEA	C26-C15-C16	7.15	127.63	115.23
23	C	271	CHD	C4-C5-C10	7.08	120.20	112.66
23	P	1271	CHD	C5-C6-C7	7.07	122.81	114.40
23	B	1086	CHD	C18-C13-C17	-6.92	100.37	111.20
23	B	1086	CHD	C17-C13-C14	6.89	107.03	100.11
24	Z	1526	DMU	O1-C9-C8	6.86	122.06	109.70
23	G	86	CHD	C18-C13-C17	-6.83	100.50	111.20
23	P	1271	CHD	C14-C8-C7	6.81	120.89	111.85
23	C	271	CHD	C1-C2-C3	6.81	119.50	110.48
23	P	1271	CHD	C16-C17-C13	6.79	110.13	103.54
23	C	525	CHD	C19-C10-C9	-6.78	102.06	111.18
23	P	1271	CHD	C17-C13-C12	-6.77	111.57	117.67
18	A	516	HEA	CHA-C4D-ND	6.77	131.71	124.42
24	M	526	DMU	O5-C6-C1	6.77	124.28	110.37
23	J	60	CHD	C5-C6-C7	6.76	122.44	114.40
23	W	1060	CHD	C5-C6-C7	6.74	122.42	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	86	CHD	C15-C14-C13	6.70	110.04	103.54
23	C	271	CHD	C16-C17-C13	6.70	110.03	103.54
23	W	1060	CHD	C9-C11-C12	6.68	123.04	114.29
18	A	516	HEA	C2A-C1A-NA	-6.67	103.89	110.32
23	P	1271	CHD	C6-C5-C10	6.62	119.71	112.66
23	C	271	CHD	C1-C10-C5	6.62	117.25	107.75
23	C	525	CHD	C15-C14-C13	6.60	109.94	103.54
23	G	86	CHD	C1-C2-C3	6.59	119.21	110.48
23	J	60	CHD	C6-C7-C8	6.59	118.69	111.50
24	C	272	DMU	O1-C10-C5	6.57	123.88	110.37
23	J	60	CHD	C14-C13-C12	6.57	113.42	107.42
23	C	271	CHD	C6-C5-C10	6.56	119.64	112.66
24	Z	1526	DMU	O5-C6-C1	6.56	123.84	110.37
23	J	60	CHD	C6-C5-C10	6.53	119.61	112.66
24	Z	1526	DMU	O1-C10-C5	6.47	123.66	110.37
23	C	271	CHD	C4-C3-C2	6.45	118.49	110.62
23	P	1525	CHD	C18-C13-C12	-6.44	102.61	109.06
24	P	1272	DMU	O1-C9-C8	6.44	121.30	109.70
23	P	1525	CHD	C18-C13-C14	-6.43	101.13	111.20
23	W	1060	CHD	C6-C5-C10	6.41	119.48	112.66
23	W	1060	CHD	C11-C12-C13	6.39	117.76	111.26
24	M	526	DMU	O1-C10-C5	6.37	123.46	110.37
24	P	1272	DMU	O1-C10-C5	6.35	123.41	110.37
23	W	1060	CHD	C9-C10-C5	6.31	117.28	108.51
23	W	1060	CHD	C15-C14-C8	6.27	126.96	118.36
23	P	1525	CHD	C6-C5-C4	-6.26	104.08	111.23
23	C	525	CHD	C5-C4-C3	6.25	122.13	112.71
23	P	1271	CHD	C11-C9-C8	6.24	120.13	110.89
23	J	60	CHD	C9-C11-C12	6.23	122.45	114.29
18	N	515	HEA	C12-C11-C3B	6.23	121.86	112.12
24	C	272	DMU	O1-C9-C8	6.22	120.90	109.70
23	J	60	CHD	C5-C4-C3	6.20	122.06	112.71
23	W	1060	CHD	C4-C3-C2	6.19	118.17	110.62
24	Z	1526	DMU	O1-C9-C11	6.17	121.74	106.44
23	G	86	CHD	C6-C7-C8	6.16	118.22	111.50
23	J	60	CHD	C6-C5-C4	-6.12	104.23	111.23
23	C	271	CHD	C13-C17-C20	6.11	126.88	119.48
23	J	60	CHD	C1-C10-C5	6.11	116.51	107.75
24	P	1272	DMU	O5-C4-C3	6.10	122.34	109.72
23	C	271	CHD	C2-C1-C10	6.10	123.03	112.74
24	C	272	DMU	C8-C7-C5	6.08	121.51	110.83
18	N	515	HEA	C27-C19-C20	6.08	125.77	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1086	CHD	C9-C11-C12	6.02	122.17	114.29
23	J	60	CHD	C2-C1-C10	6.00	122.86	112.74
23	C	271	CHD	C14-C8-C7	5.98	119.79	111.85
23	P	1525	CHD	C1-C2-C3	5.98	118.40	110.48
23	J	60	CHD	C4-C3-C2	5.96	117.89	110.62
23	W	1060	CHD	C2-C1-C10	5.96	122.80	112.74
19	N	1268	PGV	O01-C1-C2	5.95	124.36	111.48
24	Z	1526	DMU	O5-C4-C3	5.95	122.02	109.72
23	C	525	CHD	C11-C12-C13	5.93	117.30	111.26
24	C	272	DMU	O5-C4-C3	5.91	121.95	109.72
23	P	1271	CHD	C5-C4-C3	5.87	121.57	112.71
23	G	86	CHD	C16-C17-C20	5.83	121.00	112.18
23	W	1060	CHD	C5-C4-C3	5.81	121.47	112.71
23	P	1525	CHD	C5-C4-C3	5.81	121.47	112.71
23	W	1060	CHD	C1-C10-C5	5.79	116.06	107.75
23	J	60	CHD	C11-C9-C10	5.79	119.58	113.70
21	B	521	TGL	CG2-OG2-CB1	5.78	131.62	117.80
23	C	271	CHD	C5-C4-C3	5.74	121.37	112.71
23	P	1271	CHD	C2-C1-C10	5.74	122.43	112.74
23	P	1271	CHD	C4-C5-C10	5.74	118.77	112.66
23	G	86	CHD	C4-C3-C2	5.74	117.62	110.62
23	J	60	CHD	C9-C10-C5	5.73	116.47	108.51
23	P	1271	CHD	C1-C2-C3	5.72	118.06	110.48
23	G	86	CHD	C17-C13-C14	5.71	105.84	100.11
24	C	272	DMU	O5-C6-C1	5.70	122.08	110.37
24	M	526	DMU	O16-C6-C1	5.70	116.92	108.27
18	N	515	HEA	C26-C15-C16	5.66	125.06	115.23
23	C	525	CHD	C6-C7-C8	5.66	117.68	111.50
24	P	1272	DMU	C8-C7-C5	5.61	120.68	110.83
19	C	268	PGV	O01-C1-C2	5.61	123.61	111.48
23	C	525	CHD	C2-C1-C10	5.60	122.19	112.74
23	G	86	CHD	C11-C9-C8	5.60	119.18	110.89
24	M	526	DMU	C2-C3-C4	5.57	123.28	110.93
18	A	516	HEA	CMC-C2C-C1C	5.52	133.82	125.42
23	P	1525	CHD	C18-C13-C17	-5.51	102.57	111.20
22	B	230	PSC	O01-C1-C2	5.50	123.38	111.48
23	J	60	CHD	C11-C12-C13	5.49	116.84	111.26
23	J	60	CHD	C15-C14-C8	5.48	125.87	118.36
23	P	1525	CHD	C11-C9-C8	5.48	119.00	110.89
27	T	1269	CDL	OA6-CA5-C11	5.47	123.32	111.48
23	W	1060	CHD	C14-C13-C12	5.46	112.41	107.42
24	P	1272	DMU	O5-C6-C1	5.45	121.57	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	CAA-CBA-CGA	-5.44	99.23	113.67
23	W	1060	CHD	C22-C20-C17	5.43	121.58	110.33
23	C	525	CHD	C6-C5-C4	-5.40	105.06	111.23
23	P	1525	CHD	C6-C7-C8	5.38	117.37	111.50
27	C	270	CDL	OA6-CA5-C11	5.33	123.02	111.48
24	Z	1526	DMU	O5-C4-C57	5.33	119.65	106.44
26	T	263	PEK	O01-C1-C2	5.31	122.98	111.48
24	M	526	DMU	O5-C4-C3	5.24	120.55	109.72
23	P	1525	CHD	C11-C12-C13	5.24	116.59	111.26
23	C	525	CHD	C18-C13-C17	-5.23	103.00	111.20
23	C	271	CHD	C11-C9-C8	5.22	118.62	110.89
24	P	1272	DMU	O1-C9-C11	5.22	119.37	106.44
27	T	1269	CDL	OB6-CB5-C51	5.22	122.77	111.48
18	A	516	HEA	CHB-C1B-C2B	5.20	133.23	125.03
21	L	522	TGL	OG3-CC1-OC1	-5.19	110.66	123.63
18	A	516	HEA	OMA-CMA-C3A	5.18	137.32	125.62
27	G	269	CDL	OA6-CA5-C11	5.15	122.62	111.48
23	G	86	CHD	O12-C12-C13	-5.12	102.37	111.02
23	G	86	CHD	C11-C12-C13	5.12	116.47	111.26
23	W	1060	CHD	C19-C10-C5	-5.11	101.89	110.44
19	N	1266	PGV	O03-C19-C20	5.11	127.42	111.83
23	J	60	CHD	C9-C8-C7	5.11	118.29	111.86
26	G	1263	PEK	O01-C1-C2	5.07	122.45	111.48
18	N	516	HEA	C27-C19-C20	5.07	124.02	115.23
23	J	60	CHD	C18-C13-C12	-5.06	103.99	109.06
24	Z	1526	DMU	O16-C6-C1	5.03	115.91	108.27
23	B	1086	CHD	C15-C14-C13	5.02	108.41	103.54
19	N	1268	PGV	O03-C19-C20	4.94	126.90	111.83
27	P	1270	CDL	OA6-CA5-C11	4.93	122.14	111.48
23	P	1271	CHD	C13-C17-C20	4.93	125.45	119.48
23	C	271	CHD	C16-C17-C20	4.93	119.63	112.18
24	C	272	DMU	O1-C9-C11	4.91	118.61	106.44
23	B	1086	CHD	O7-C7-C6	-4.90	97.68	109.86
23	C	525	CHD	O12-C12-C13	-4.89	102.76	111.02
23	C	525	CHD	C17-C13-C14	4.85	104.98	100.11
23	P	1271	CHD	C18-C13-C12	-4.82	104.23	109.06
18	A	516	HEA	CHB-C1B-NB	-4.82	119.24	124.42
24	Z	1526	DMU	C2-C3-C4	4.82	121.61	110.93
23	G	86	CHD	C2-C1-C10	4.81	120.86	112.74
23	G	86	CHD	C6-C5-C4	-4.80	105.74	111.23
18	A	516	HEA	CHB-C4A-C3A	-4.79	117.14	125.21
23	B	1086	CHD	C4-C3-C2	4.73	116.39	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	O7-C3-C2	4.72	119.23	107.23
27	G	269	CDL	OB6-CB5-C51	4.72	121.69	111.48
23	C	271	CHD	C9-C11-C12	4.70	120.45	114.29
18	A	516	HEA	CHB-C4A-NA	4.70	129.57	124.45
23	W	1060	CHD	C18-C13-C12	-4.69	104.36	109.06
18	A	516	HEA	CHD-C1D-ND	-4.68	118.58	124.37
21	N	1521	TGL	CG2-OG2-CB1	4.67	128.98	117.80
24	Z	1526	DMU	C7-C8-C9	4.65	118.66	110.23
23	P	1525	CHD	O7-C7-C6	-4.64	98.31	109.86
18	N	516	HEA	OMA-CMA-C3A	-4.62	115.19	125.62
19	C	268	PGV	O03-C19-C20	4.60	125.87	111.83
23	W	1060	CHD	C1-C10-C9	-4.60	104.20	111.34
23	P	1271	CHD	C16-C17-C20	4.57	119.09	112.18
18	A	516	HEA	CHA-C1A-C2A	4.57	132.07	124.86
23	C	525	CHD	C11-C9-C8	4.56	117.64	110.89
18	A	516	HEA	C12-C11-C3B	4.55	119.23	112.12
26	C	265	PEK	O03-C21-C22	4.53	125.66	111.83
21	B	521	TGL	OG2-CG2-CG3	4.52	124.56	108.34
22	O	1230	PSC	O01-C1-C2	4.52	121.25	111.48
19	A	521	PGV	O03-C19-C20	4.51	125.58	111.83
19	A	521	PGV	O03-C19-O04	-4.47	112.44	123.63
19	N	1266	PGV	O03-C19-O04	-4.46	112.48	123.63
24	Z	1526	DMU	C8-C7-C5	4.45	118.65	110.83
23	P	1525	CHD	C17-C13-C14	4.43	104.56	100.11
18	A	515	HEA	C12-C11-C3B	4.43	119.05	112.12
23	P	1525	CHD	C9-C8-C7	4.42	117.42	111.86
23	B	1086	CHD	C6-C5-C4	-4.42	106.18	111.23
26	P	1264	PEK	O03-C01-C02	-4.37	95.79	108.40
23	P	1525	CHD	O12-C12-C11	-4.36	100.25	109.12
23	C	525	CHD	C18-C13-C14	-4.36	104.38	111.20
23	W	1060	CHD	C9-C8-C7	4.36	117.34	111.86
23	B	1086	CHD	C11-C9-C10	4.35	118.12	113.70
21	D	523	TGL	OG3-CC1-CC2	4.32	125.01	111.83
24	C	272	DMU	O5-C4-C57	4.32	117.14	106.44
18	A	516	HEA	O11-C11-C3B	4.32	119.18	111.26
24	P	1272	DMU	C7-C8-C9	4.31	118.04	110.23
23	B	1086	CHD	C14-C8-C9	4.30	115.76	109.75
18	A	516	HEA	CMD-C2D-C3D	-4.30	114.53	126.15
23	P	1271	CHD	C14-C13-C12	4.28	111.33	107.42
24	M	526	DMU	O5-C4-C57	4.28	117.05	106.44
23	C	271	CHD	C19-C10-C1	-4.24	101.57	108.31
18	A	516	HEA	C3B-C4B-NB	4.23	114.70	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	C2-C3-C4	4.23	120.31	110.93
18	A	516	HEA	O11-C11-C12	-4.23	97.92	109.14
26	P	1265	PEK	O01-C1-C2	4.21	120.58	111.48
24	M	526	DMU	O1-C9-C11	4.20	116.86	106.44
23	P	1525	CHD	C13-C17-C20	4.18	124.55	119.48
23	W	1060	CHD	C17-C13-C12	4.14	121.39	117.67
23	J	60	CHD	C19-C10-C5	-4.11	103.57	110.44
23	C	525	CHD	C16-C17-C13	4.09	107.50	103.54
24	C	272	DMU	O7-C3-C4	4.08	120.19	109.48
23	C	525	CHD	C9-C11-C12	4.08	119.63	114.29
23	P	1271	CHD	C9-C11-C12	4.07	119.61	114.29
24	P	1272	DMU	O5-C4-C57	4.06	116.50	106.44
26	P	1264	PEK	O01-C1-O02	-4.05	114.23	123.70
19	A	524	PGV	O03-C19-C20	4.04	124.15	111.83
23	B	1086	CHD	C11-C9-C8	4.02	116.85	110.89
24	M	526	DMU	C8-C7-C5	4.02	117.89	110.83
23	C	525	CHD	C16-C17-C20	4.02	118.26	112.18
23	C	271	CHD	C6-C5-C4	-4.02	106.63	111.23
26	P	1265	PEK	O03-C21-C22	4.02	124.09	111.83
23	W	1060	CHD	O7-C7-C6	-4.01	99.87	109.86
23	C	525	CHD	C1-C2-C3	4.01	115.80	110.48
23	P	1271	CHD	C19-C10-C5	-4.00	103.76	110.44
26	G	264	PEK	O01-C1-O02	-4.00	114.36	123.70
23	P	1525	CHD	C11-C9-C10	4.00	117.76	113.70
19	N	1524	PGV	O01-C1-C2	3.99	120.12	111.48
24	M	526	DMU	C10-C5-C7	3.99	118.41	110.01
23	P	1271	CHD	C9-C10-C5	3.99	114.05	108.51
23	B	1086	CHD	C19-C10-C5	-3.98	103.78	110.44
24	P	1272	DMU	O7-C10-C5	3.98	117.88	108.09
26	C	265	PEK	O01-C1-C2	3.98	120.09	111.48
24	C	272	DMU	C7-C8-C9	3.98	117.45	110.23
27	P	1270	CDL	OB8-CB7-C71	3.96	123.90	111.83
24	P	1272	DMU	C1-C2-C3	3.93	118.60	109.68
24	M	526	DMU	C7-C8-C9	3.91	117.32	110.23
24	P	1272	DMU	C2-C3-C4	3.91	119.59	110.93
26	P	1264	PEK	C24-C23-C22	-3.90	98.80	113.13
21	L	522	TGL	OG3-CC1-CC2	3.90	123.72	111.83
23	P	1525	CHD	C1-C10-C9	-3.89	105.30	111.34
19	N	1524	PGV	O03-C19-C20	3.89	123.69	111.83
23	J	60	CHD	C22-C20-C17	3.83	118.27	110.33
21	D	523	TGL	OG2-CB1-CB2	3.81	119.72	111.48
27	T	1269	CDL	OB8-CB6-CB4	3.80	119.34	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	521	TGL	OG2-CB1-CB2	3.77	119.64	111.48
24	P	1272	DMU	O7-C3-C4	3.77	119.36	109.48
24	C	272	DMU	O7-C10-C5	3.77	117.36	108.09
24	C	272	DMU	C10-O1-C9	3.76	121.06	113.72
23	P	1525	CHD	C22-C20-C17	-3.76	102.54	110.33
18	A	515	HEA	O11-C11-C3B	-3.75	104.38	111.26
24	P	1272	DMU	C6-C1-C2	3.74	117.88	110.01
18	N	515	HEA	C16-C17-C18	3.73	130.49	112.02
26	C	265	PEK	O03-C21-O04	-3.72	114.33	123.63
18	A	516	HEA	C3C-C4C-NC	3.71	112.93	109.80
23	P	1525	CHD	C16-C17-C13	3.71	107.14	103.54
21	N	1521	TGL	OG1-CA1-CA2	3.71	123.14	111.83
23	G	86	CHD	C9-C8-C7	3.70	116.52	111.86
21	N	1521	TGL	OG1-CG1-CG2	3.70	119.07	108.40
18	A	515	HEA	C3A-C2A-C1A	-3.70	103.55	107.05
26	T	263	PEK	O03-C01-C02	3.69	119.04	108.40
21	O	1523	TGL	OG3-CC1-CC2	3.66	123.00	111.83
24	P	1272	DMU	C10-O1-C9	3.66	120.87	113.72
18	N	516	HEA	C3A-C2A-C1A	-3.66	103.59	107.05
26	G	264	PEK	O01-C1-C2	3.65	119.38	111.48
18	N	515	HEA	C12-C13-C14	-3.65	102.58	112.16
18	A	515	HEA	C2D-C1D-ND	3.64	114.03	109.84
23	P	1525	CHD	C9-C11-C12	3.64	119.06	114.29
23	C	271	CHD	C9-C10-C5	3.64	113.56	108.51
24	Z	1526	DMU	C6-C1-C2	3.63	117.65	110.01
23	C	525	CHD	C14-C8-C9	3.63	114.82	109.75
23	B	1086	CHD	C1-C10-C9	-3.62	105.72	111.34
23	G	86	CHD	C15-C14-C8	3.62	123.32	118.36
26	G	1263	PEK	O03-C21-C22	3.62	122.86	111.83
21	D	523	TGL	OG1-CG1-CG2	3.60	118.77	108.40
23	G	86	CHD	C11-C9-C10	3.60	117.35	113.70
24	C	272	DMU	C6-C1-C2	3.59	117.56	110.01
21	L	522	TGL	OG1-CA1-CA2	3.59	122.77	111.83
23	G	86	CHD	C9-C11-C12	3.58	118.98	114.29
21	N	1522	TGL	OG2-CB1-CB2	3.58	119.22	111.48
24	Z	1526	DMU	C10-C5-C7	3.58	117.53	110.01
24	C	272	DMU	C1-C2-C3	3.57	117.78	109.68
23	B	1086	CHD	C5-C6-C7	3.57	118.64	114.40
23	P	1271	CHD	C19-C10-C9	-3.55	106.41	111.18
27	C	270	CDL	OA8-CA7-C31	3.54	122.64	111.83
21	N	1521	TGL	OG2-CB1-CB2	3.54	119.14	111.48
21	B	521	TGL	OG1-CA1-CA2	3.53	122.61	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	86	CHD	C18-C13-C14	-3.53	105.68	111.20
19	C	267	PGV	O01-C1-C2	3.52	119.10	111.48
21	N	1521	TGL	CG3-OG3-CC1	3.48	129.84	117.12
27	T	1269	CDL	OA6-CA5-OA7	-3.48	115.57	123.70
23	G	86	CHD	C14-C8-C9	3.48	114.61	109.75
27	T	1269	CDL	C83-C82-C81	3.46	131.88	114.37
24	M	526	DMU	O7-C10-C5	-3.46	99.56	108.09
18	N	516	HEA	CAD-CBD-CGD	-3.46	104.48	113.67
23	J	60	CHD	C1-C10-C9	-3.46	105.96	111.34
23	G	86	CHD	C1-C10-C9	-3.43	106.01	111.34
26	T	263	PEK	O03-C21-C22	3.43	122.30	111.83
21	N	1521	TGL	CA6-CA5-CA4	-3.43	97.02	114.37
23	C	525	CHD	C15-C14-C8	3.42	123.05	118.36
23	J	60	CHD	C11-C9-C8	3.41	115.94	110.89
22	O	1230	PSC	O01-C1-O02	-3.41	115.73	123.70
21	N	1522	TGL	OG1-CA1-CA2	3.40	122.21	111.83
23	P	1525	CHD	C14-C8-C9	3.40	114.50	109.75
26	P	1264	PEK	C2-C3-C4	3.39	120.77	113.35
18	A	515	HEA	C16-C17-C18	3.39	128.79	112.02
21	N	1521	TGL	OG2-CG2-CG3	3.37	120.45	108.34
18	A	515	HEA	C12-C13-C14	-3.37	103.32	112.16
23	C	271	CHD	C17-C13-C14	3.36	103.48	100.11
24	P	1272	DMU	O16-C18-C19	3.34	120.69	109.37
23	C	525	CHD	C13-C17-C20	3.34	123.53	119.48
18	A	516	HEA	CBA-CAA-C2A	-3.33	103.33	112.53
24	C	272	DMU	O4-C7-C5	3.31	118.17	110.38
24	C	272	DMU	C6-O5-C4	3.30	120.16	113.72
18	N	516	HEA	C3C-C4C-NC	3.29	112.57	109.80
27	P	1270	CDL	OA8-CA7-C31	3.29	121.87	111.83
21	L	522	TGL	CC3-CC2-CC1	3.29	125.74	113.69
21	B	521	TGL	CG3-OG3-CC1	3.28	129.12	117.12
23	J	60	CHD	C21-C20-C22	3.28	115.42	110.34
23	C	525	CHD	C11-C9-C10	3.28	117.03	113.70
18	N	515	HEA	C21-C20-C19	-3.28	102.33	113.19
23	P	1525	CHD	C2-C1-C10	3.28	118.27	112.74
23	P	1525	CHD	C23-C22-C20	-3.27	108.35	114.46
23	P	1271	CHD	C17-C13-C14	3.26	103.39	100.11
23	C	271	CHD	C18-C13-C12	-3.26	105.79	109.06
23	G	86	CHD	O12-C12-C11	-3.24	102.52	109.12
18	A	515	HEA	C3B-C4B-NB	3.24	113.56	109.84
27	C	270	CDL	OB8-CB7-C71	3.23	121.69	111.83
18	A	515	HEA	C2B-C1B-NB	3.23	113.64	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	O7-C3-C2	3.23	115.43	107.23
26	P	1264	PEK	O01-C1-C2	3.23	118.46	111.48
18	A	515	HEA	C26-C15-C14	-3.22	115.36	123.63
23	B	1086	CHD	C18-C13-C14	-3.21	106.18	111.20
18	A	516	HEA	CHC-C4B-C3B	-3.21	117.71	125.80
24	M	526	DMU	C57-C4-C3	3.20	122.39	113.38
24	P	1272	DMU	C6-O5-C4	3.20	119.97	113.72
19	N	1268	PGV	O03-C19-O04	-3.20	115.62	123.63
23	P	1525	CHD	O12-C12-C13	-3.18	105.65	111.02
24	Z	1526	DMU	O55-C2-C3	3.18	118.09	109.94
27	P	1270	CDL	OB8-CB7-OB9	-3.17	115.69	123.63
19	N	1266	PGV	O01-C1-O02	-3.17	116.30	123.70
24	M	526	DMU	C6-C1-C2	3.15	116.65	110.01
27	C	270	CDL	OB8-CB7-OB9	-3.15	115.75	123.63
18	N	515	HEA	C27-C19-C18	-3.15	115.55	123.63
21	N	1522	TGL	OG3-CC1-OC1	-3.14	115.78	123.63
24	Z	1526	DMU	O5-C6-O16	3.12	117.41	110.04
23	C	271	CHD	C14-C13-C12	3.11	110.26	107.42
21	O	1523	TGL	OG2-CB1-CB2	3.10	118.20	111.48
26	G	1263	PEK	O03-C01-C02	3.10	117.34	108.40
26	G	264	PEK	O03-C01-C02	-3.10	99.47	108.40
21	D	523	TGL	C21-C20-CA9	3.10	130.02	114.37
18	N	516	HEA	C4C-C3C-C2C	-3.08	103.47	107.30
24	C	272	DMU	C18-O16-C6	3.07	118.92	113.68
23	J	60	CHD	C16-C17-C20	3.06	116.81	112.18
23	G	86	CHD	O7-C7-C6	-3.06	102.26	109.86
23	C	525	CHD	C9-C8-C7	3.04	115.69	111.86
24	C	272	DMU	C11-C9-C8	3.04	120.49	113.02
18	N	515	HEA	O2D-CGD-O1D	-3.04	115.52	123.33
21	D	523	TGL	CG3-OG3-CC1	3.03	128.18	117.12
23	P	1525	CHD	C16-C17-C20	3.02	116.75	112.18
21	B	521	TGL	OG3-CC1-OC1	-3.02	116.08	123.63
27	T	1269	CDL	OA8-CA7-C31	3.02	121.03	111.83
23	P	1525	CHD	C15-C14-C8	3.01	122.49	118.36
18	A	515	HEA	C1D-C2D-C3D	-3.00	103.83	106.98
23	B	1086	CHD	C16-C17-C20	3.00	116.71	112.18
19	C	268	PGV	O03-C19-O04	-2.97	116.19	123.63
26	P	1265	PEK	C7-C6-C5	-2.97	98.48	123.57
23	B	1086	CHD	C11-C12-C13	2.97	114.28	111.26
23	B	1086	CHD	C16-C17-C13	2.97	106.42	103.54
21	N	1522	TGL	OG3-CC1-CC2	2.96	120.86	111.83
23	P	1525	CHD	C19-C10-C5	-2.96	105.49	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	1521	TGL	CG1-OG1-CA1	-2.95	106.33	117.12
23	B	1086	CHD	O12-C12-C13	-2.93	106.07	111.02
23	C	271	CHD	O7-C7-C6	-2.92	102.59	109.86
19	A	524	PGV	C01-O03-C19	2.91	127.75	117.12
26	T	263	PEK	C02-O01-C1	2.91	124.75	117.80
18	A	516	HEA	C13-C14-C15	-2.89	121.00	127.62
19	A	521	PGV	O01-C1-C2	2.89	117.73	111.48
23	C	271	CHD	C22-C23-C24	-2.89	104.78	112.49
23	B	1086	CHD	C15-C14-C8	2.88	122.31	118.36
23	G	86	CHD	C16-C17-C13	2.88	106.33	103.54
24	Z	1526	DMU	C1-C2-C3	2.87	116.20	109.68
19	A	524	PGV	O01-C1-C2	2.87	117.69	111.48
23	W	1060	CHD	C16-C17-C20	2.87	116.52	112.18
23	P	1271	CHD	C22-C23-C24	-2.86	104.87	112.49
26	P	1265	PEK	O03-C21-O04	-2.85	116.50	123.63
24	Z	1526	DMU	C10-O1-C9	2.85	119.28	113.72
26	G	264	PEK	C24-C23-C22	-2.84	102.68	113.13
24	M	526	DMU	C10-O7-C3	2.84	124.71	117.98
19	N	1524	PGV	C01-O03-C19	2.82	127.42	117.12
24	M	526	DMU	C6-O5-C4	2.82	119.22	113.72
18	A	516	HEA	O2A-CGA-CBA	2.82	122.90	114.00
27	G	269	CDL	OA6-CA5-OA7	-2.81	117.12	123.70
27	T	1269	CDL	OA8-CA7-OA9	-2.81	116.61	123.63
18	A	516	HEA	O2D-CGD-CBD	2.80	122.86	114.00
23	W	1060	CHD	C18-C13-C14	-2.80	106.82	111.20
19	N	1266	PGV	O03-C01-C02	2.78	116.40	108.40
24	M	526	DMU	O7-C3-C2	2.78	114.28	107.23
24	M	526	DMU	C1-C2-C3	2.77	115.97	109.68
24	P	1272	DMU	C57-C4-C3	2.76	121.14	113.38
23	W	1060	CHD	C13-C14-C8	2.76	118.21	114.72
21	L	522	TGL	OG1-CG1-CG2	2.76	116.34	108.40
18	N	516	HEA	C20-C19-C18	-2.75	115.00	121.17
21	O	1523	TGL	OG1-CA1-CA2	2.75	120.20	111.83
19	N	1268	PGV	C03-C02-C01	-2.72	105.43	111.78
18	N	515	HEA	O1A-CGA-CBA	-2.72	114.47	123.09
23	P	1525	CHD	C5-C6-C7	2.71	117.62	114.40
24	P	1272	DMU	O5-C6-O16	2.70	116.42	110.04
24	Z	1526	DMU	O7-C10-C5	-2.68	101.49	108.09
24	C	272	DMU	C57-C4-C3	2.67	120.89	113.38
18	N	516	HEA	CHB-C1B-NB	2.67	127.29	124.42
26	P	1264	PEK	C3-C2-C1	-2.66	103.93	113.69
21	N	1522	TGL	OG1-CG1-CG2	2.66	116.06	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	C10-C5-C7	2.65	115.58	110.01
18	A	516	HEA	CMC-C2C-C3C	-2.63	120.36	126.55
23	C	525	CHD	O7-C7-C6	-2.63	103.32	109.86
18	N	515	HEA	C1D-C2D-C3D	-2.63	104.22	106.98
19	C	267	PGV	O03-C19-O04	-2.62	117.08	123.63
23	P	1271	CHD	C6-C5-C4	-2.62	108.23	111.23
23	W	1060	CHD	C11-C9-C8	2.62	114.77	110.89
23	P	1271	CHD	C19-C10-C1	-2.61	104.15	108.31
23	P	1271	CHD	O7-C7-C6	-2.61	103.37	109.86
21	O	1523	TGL	OG1-CA1-OA1	-2.61	117.11	123.63
27	T	1269	CDL	C82-C81-C80	2.59	127.47	114.37
18	N	516	HEA	C2D-C1D-ND	2.58	112.80	109.84
18	A	516	HEA	CHD-C4C-NC	2.56	128.51	123.86
27	G	269	CDL	OA8-CA7-C31	2.56	119.65	111.83
21	N	1522	TGL	CG1-OG1-CA1	2.56	126.48	117.12
24	P	1272	DMU	C11-C9-C8	2.56	119.31	113.02
18	A	515	HEA	OMA-CMA-C3A	-2.56	119.84	125.62
22	B	230	PSC	O01-C1-O02	-2.55	117.74	123.70
21	B	521	TGL	OG3-CC1-CC2	2.55	119.60	111.83
21	D	523	TGL	OG1-CA1-CA2	2.54	119.59	111.83
23	C	271	CHD	C19-C10-C5	-2.54	106.19	110.44
21	O	1523	TGL	C21-C20-CA9	2.54	127.19	114.37
21	N	1521	TGL	CA7-CA6-CA5	-2.53	101.58	114.37
19	P	1267	PGV	O03-C19-O04	-2.52	117.33	123.63
23	G	86	CHD	C19-C10-C5	-2.52	106.23	110.44
19	N	1524	PGV	C02-O01-C1	2.51	123.80	117.80
23	P	1525	CHD	O3-C3-C4	2.51	114.83	109.84
21	D	523	TGL	CG2-OG2-CB1	2.50	123.78	117.80
18	N	516	HEA	C1D-C2D-C3D	-2.49	104.36	106.98
19	A	521	PGV	O12-P-O13	2.49	118.80	108.94
24	Z	1526	DMU	C6-O5-C4	2.48	118.57	113.72
21	N	1521	TGL	OG3-CC1-CC2	2.48	119.39	111.83
27	G	269	CDL	OB8-CB7-OB9	-2.48	117.43	123.63
27	P	1270	CDL	OA8-CA6-CA4	2.47	115.53	108.40
23	J	60	CHD	C17-C13-C12	2.47	119.89	117.67
21	N	1521	TGL	CB7-CB6-CB5	-2.47	101.90	114.37
18	A	516	HEA	C16-C15-C14	2.46	126.70	121.17
27	C	270	CDL	OA8-CA6-CA4	2.44	115.44	108.40
23	J	60	CHD	C13-C14-C8	2.44	117.81	114.72
18	N	515	HEA	CHB-C1B-C2B	-2.44	121.18	125.03
27	G	269	CDL	CA6-OA8-CA7	2.44	126.02	117.12
23	C	525	CHD	C5-C6-C7	2.43	117.29	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	524	PGV	C02-O01-C1	2.43	123.62	117.80
18	A	515	HEA	C25-C23-C22	-2.43	115.36	122.66
23	B	1086	CHD	C2-C1-C10	2.43	116.84	112.74
27	G	269	CDL	OB8-CB7-C71	2.43	119.24	111.83
24	M	526	DMU	O7-C3-C4	2.43	115.84	109.48
18	A	515	HEA	CHC-C4B-NB	-2.42	121.37	124.37
27	C	270	CDL	C52-C51-CB5	-2.42	104.82	113.69
27	T	1269	CDL	C43-C42-C41	2.42	126.61	114.37
21	B	521	TGL	OG1-CG1-CG2	2.42	115.36	108.40
26	T	263	PEK	C01-O03-C21	2.42	125.95	117.12
24	M	526	DMU	O7-C10-O1	-2.41	104.34	110.69
27	C	270	CDL	C39-C38-C37	2.41	126.57	114.37
21	O	1523	TGL	OG2-CG2-CG3	2.41	116.99	108.34
19	N	1524	PGV	O03-C19-O04	-2.40	117.62	123.63
18	A	515	HEA	C3C-C4C-NC	2.40	111.82	109.80
21	D	523	TGL	C11-C10-CB9	2.39	126.45	114.37
18	A	516	HEA	CHC-C4B-NB	2.39	127.32	124.37
21	N	1522	TGL	C15-CC9-CC8	2.38	126.40	114.37
18	N	516	HEA	CHA-C4D-C3D	-2.37	121.32	124.77
23	G	86	CHD	C5-C6-C7	2.37	117.21	114.40
18	N	515	HEA	CMC-C2C-C1C	2.37	129.02	125.42
27	C	270	CDL	OA8-CA7-OA9	-2.37	117.71	123.63
18	N	516	HEA	C2A-C1A-NA	2.36	112.60	110.32
18	N	516	HEA	CHB-C4A-C3A	2.35	129.18	125.21
21	D	523	TGL	C10-CB9-CB8	2.35	126.24	114.37
27	P	1270	CDL	C78-C77-C76	-2.35	102.51	114.37
21	N	1522	TGL	C24-C23-C22	-2.35	102.51	114.37
18	A	516	HEA	C1D-ND-C4D	-2.34	102.43	105.21
23	W	1060	CHD	C19-C10-C1	-2.34	104.58	108.31
23	C	271	CHD	O12-C12-C11	-2.34	104.37	109.12
27	P	1270	CDL	OB6-CB5-C51	2.33	116.53	111.48
21	B	521	TGL	CG1-OG1-CA1	-2.33	108.59	117.12
19	P	1267	PGV	O03-C19-C20	2.33	118.94	111.83
27	P	1270	CDL	OA8-CA7-OA9	-2.33	117.81	123.63
27	P	1270	CDL	OA6-CA5-OA7	-2.32	118.28	123.70
23	C	271	CHD	C13-C14-C8	2.32	117.65	114.72
18	A	516	HEA	O1A-CGA-CBA	-2.31	115.75	123.09
18	N	515	HEA	C2B-C1B-NB	2.31	112.57	109.90
24	C	272	DMU	O5-C6-O16	2.31	115.49	110.04
26	T	263	PEK	O01-C1-O02	-2.30	118.33	123.70
18	N	516	HEA	CHA-C4D-ND	2.30	126.89	124.42
18	A	516	HEA	C1A-CHA-C4D	-2.29	121.14	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	C17-C16-C15	2.29	120.79	113.19
23	J	60	CHD	O7-C7-C6	-2.29	104.15	109.86
18	A	516	HEA	O1D-CGD-CBD	-2.29	115.82	123.09
27	C	270	CDL	OA6-CA5-OA7	-2.29	118.34	123.70
18	N	515	HEA	C2D-C1D-ND	2.29	112.47	109.84
21	D	523	TGL	C20-CA9-CA8	2.28	125.91	114.37
21	N	1522	TGL	CB9-CB8-CB7	-2.28	102.84	114.37
21	N	1521	TGL	OG1-CA1-OA1	-2.27	117.94	123.63
18	A	516	HEA	C1D-C2D-C3D	-2.27	104.59	106.98
27	C	270	CDL	CA6-CA4-CA3	-2.27	106.49	111.78
21	O	1523	TGL	CG3-OG3-CC1	2.27	125.41	117.12
21	L	522	TGL	OG2-CB1-CB2	2.26	116.38	111.48
19	N	1268	PGV	O02-C1-C2	-2.26	114.94	123.78
23	C	525	CHD	O3-C3-C4	2.25	114.33	109.84
18	A	515	HEA	C4C-C3C-C2C	-2.25	104.50	107.30
23	C	525	CHD	C22-C23-C24	-2.24	106.51	112.49
18	A	516	HEA	CHC-C1C-NC	-2.24	119.80	123.86
21	D	523	TGL	CG3-CG2-CG1	-2.23	106.58	111.78
23	C	525	CHD	C19-C10-C5	-2.22	106.72	110.44
21	B	521	TGL	CB7-CB6-CB5	-2.22	103.14	114.37
21	O	1523	TGL	OG3-CC1-OC1	-2.22	118.08	123.63
27	G	269	CDL	OA8-CA7-OA9	-2.20	118.12	123.63
26	G	1263	PEK	O01-C1-O02	-2.20	118.57	123.70
27	T	1269	CDL	CA4-OA6-CA5	-2.19	112.55	117.80
27	P	1270	CDL	C39-C38-C37	2.18	125.41	114.37
23	C	271	CHD	C19-C10-C9	-2.18	108.24	111.18
27	G	269	CDL	CB6-OB8-CB7	2.18	125.08	117.12
18	N	515	HEA	C3C-C2C-C1C	-2.17	104.61	107.17
23	P	1525	CHD	O7-C7-C8	-2.17	104.54	109.52
26	P	1264	PEK	O01-C02-C01	-2.17	100.55	108.34
23	C	525	CHD	C1-C10-C9	-2.17	107.97	111.34
24	M	526	DMU	O5-C6-O16	2.17	115.17	110.04
18	N	515	HEA	C26-C15-C14	-2.16	118.08	123.63
23	C	271	CHD	C18-C13-C17	-2.16	107.83	111.20
27	P	1270	CDL	C20-C19-C18	2.15	125.24	114.37
22	B	230	PSC	O03-C19-C20	2.15	118.39	111.83
21	O	1523	TGL	C11-C10-CB9	2.15	125.22	114.37
19	A	524	PGV	O01-C02-C01	2.15	116.05	108.34
18	A	515	HEA	CHC-C1C-C2C	-2.14	121.21	127.43
21	L	522	TGL	CG2-OG2-CB1	2.14	122.91	117.80
18	N	516	HEA	O11-C11-C3B	-2.13	107.35	111.26
27	P	1270	CDL	O1-C1-CA2	-2.13	102.33	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	1521	TGL	C15-CC9-CC8	2.12	125.09	114.37
23	B	1086	CHD	O7-C7-C8	-2.12	104.67	109.52
23	B	1086	CHD	O25-C24-C23	-2.12	116.38	123.09
27	G	269	CDL	C83-C82-C81	2.11	125.05	114.37
21	D	523	TGL	CC3-CC2-CC1	-2.11	105.96	113.69
24	C	272	DMU	C10-C5-C7	2.11	114.45	110.01
19	P	1267	PGV	C27-C26-C25	-2.11	103.71	114.37
26	G	264	PEK	C3-C2-C1	-2.11	105.97	113.69
26	G	1263	PEK	C01-O03-C21	2.11	124.81	117.12
19	N	1266	PGV	C15-C14-C13	-2.10	103.75	113.86
19	C	267	PGV	O03-C19-C20	2.10	118.24	111.83
19	N	1266	PGV	C01-O03-C19	-2.09	109.48	117.12
18	A	515	HEA	C4B-C3B-C2B	-2.09	103.93	107.44
23	C	525	CHD	C22-C20-C17	-2.08	106.02	110.33
24	M	526	DMU	C11-C9-C8	2.07	118.11	113.02
23	G	86	CHD	C13-C14-C8	2.07	117.34	114.72
26	C	265	PEK	C01-O03-C21	2.07	124.69	117.12
19	C	268	PGV	O03-C01-C02	2.07	114.36	108.40
23	J	60	CHD	C19-C10-C1	-2.07	105.02	108.31
18	A	515	HEA	O2D-CGD-O1D	-2.06	118.03	123.33
23	B	1086	CHD	C14-C8-C7	2.06	114.58	111.85
18	A	516	HEA	C2B-C1B-NB	-2.05	107.53	109.90
21	D	523	TGL	OC1-CC1-CC2	-2.05	115.77	123.78
22	B	230	PSC	C3-C2-C1	2.05	121.20	113.69
24	P	1272	DMU	O7-C3-C2	2.05	112.43	107.23
18	N	516	HEA	CHB-C4A-NA	-2.04	122.23	124.45
22	O	1230	PSC	O03-C19-C20	2.04	118.05	111.83
26	T	263	PEK	O04-C21-C22	-2.04	115.81	123.78
18	A	515	HEA	CHA-C1A-NA	2.04	126.67	124.45
19	C	267	PGV	C9-C10-C11	-2.04	101.20	112.60
19	C	267	PGV	C27-C26-C25	-2.04	104.08	114.37
18	N	515	HEA	C3D-C4D-ND	2.03	112.32	110.35
18	A	516	HEA	CHD-C4C-C3C	-2.03	118.55	127.37
22	B	230	PSC	C32-C31-C30	-2.03	104.10	114.37
18	A	515	HEA	C21-C20-C19	-2.03	106.45	113.19
21	N	1522	TGL	CG2-OG2-CB1	2.03	122.66	117.80
18	N	516	HEA	CHA-C1A-NA	-2.03	122.24	124.45
24	P	1272	DMU	O4-C7-C5	2.03	115.16	110.38
22	B	230	PSC	C29-C28-C27	-2.03	104.11	114.37
27	C	270	CDL	C57-C56-C55	-2.03	104.11	114.37
24	C	272	DMU	O16-C18-C19	2.02	116.24	109.37
19	A	521	PGV	C26-C25-C24	-2.02	104.15	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	526	DMU	O55-C2-C1	2.02	115.14	110.38
18	N	515	HEA	CHD-C1D-C2D	-2.02	121.21	126.95
27	T	1269	CDL	C23-C22-C21	2.02	124.56	114.37
24	P	1272	DMU	O7-C10-O1	2.02	116.00	110.69
26	P	1264	PEK	O13-P-O14	2.01	121.81	112.44
23	B	1086	CHD	O12-C12-C11	-2.01	105.03	109.12
23	C	525	CHD	O26-C24-C23	2.01	120.35	114.00
21	L	522	TGL	CG1-OG1-CA1	2.01	124.46	117.12
18	A	516	HEA	C4A-C3A-C2A	2.01	108.55	106.81
26	P	1265	PEK	O03-C01-C02	2.01	114.18	108.40
21	B	521	TGL	OG1-CA1-OA1	-2.01	118.61	123.63
23	C	271	CHD	C23-C22-C20	-2.00	110.72	114.46
27	T	1269	CDL	OB8-CB7-C71	2.00	117.94	111.83

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	1086	CHD	C9
23	C	525	CHD	C9
23	C	271	CHD	C14
23	C	271	CHD	C9
23	G	86	CHD	C9
23	J	60	CHD	C17
23	P	1525	CHD	C9
23	P	1271	CHD	C14
23	P	1271	CHD	C9
23	W	1060	CHD	C17
24	C	272	DMU	C2
24	C	272	DMU	C4
24	C	272	DMU	C6
24	C	272	DMU	C5
24	C	272	DMU	C9
24	M	526	DMU	C6
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C5
24	M	526	DMU	C9
24	P	1272	DMU	C2
24	P	1272	DMU	C4
24	P	1272	DMU	C6
24	P	1272	DMU	C5
24	P	1272	DMU	C9

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Mol	Chain	Res	Type	Atom
24	Z	1526	DMU	C6
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C5
24	Z	1526	DMU	C9

All (980) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	515	HEA	C2A-C3A-CMA-OMA
18	A	515	HEA	C16-C17-C18-C19
18	A	516	HEA	C2A-C3A-CMA-OMA
18	N	515	HEA	C16-C17-C18-C19
19	A	524	PGV	C03-O11-P-O14
19	A	524	PGV	C04-O12-P-O11
19	A	524	PGV	C04-O12-P-O13
19	A	524	PGV	C04-O12-P-O14
19	A	524	PGV	C02-C03-O11-P
19	A	524	PGV	O02-C1-O01-C02
19	A	524	PGV	O04-C19-O03-C01
19	A	524	PGV	C20-C19-O03-C01
19	C	268	PGV	C04-O12-P-O11
19	C	268	PGV	C04-O12-P-O14
19	C	268	PGV	C04-C05-C06-O06
19	N	1524	PGV	C04-O12-P-O11
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
21	N	1522	TGL	CB2-CB1-OG2-CG2
22	B	230	PSC	C03-O11-P-O14
22	B	230	PSC	C2-C1-O01-C02
22	O	1230	PSC	C03-O11-P-O12
22	O	1230	PSC	C03-O11-P-O14
22	O	1230	PSC	C04-O12-P-O11
22	O	1230	PSC	C04-O12-P-O14
23	C	271	CHD	C16-C17-C20-C22
23	J	60	CHD	C13-C17-C20-C22
23	J	60	CHD	C16-C17-C20-C21
23	J	60	CHD	C16-C17-C20-C22
23	P	1271	CHD	C16-C17-C20-C22
23	W	1060	CHD	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22
26	C	265	PEK	C03-O11-P-O12
26	C	265	PEK	C03-O11-P-O13
26	C	265	PEK	O12-C04-C05-N
26	G	264	PEK	O12-C04-C05-N
26	G	1263	PEK	C03-O11-P-O12
26	G	1263	PEK	C03-O11-P-O13
26	G	1263	PEK	C03-O11-P-O14
26	G	1263	PEK	O03-C01-C02-O01
26	G	1263	PEK	O12-C04-C05-N
26	P	1264	PEK	O12-C04-C05-N
26	P	1265	PEK	C04-O12-P-O14
26	P	1265	PEK	O12-C04-C05-N
26	T	263	PEK	C03-O11-P-O12
26	T	263	PEK	C03-O11-P-O13
26	T	263	PEK	O03-C01-C02-O01
26	T	263	PEK	O12-C04-C05-N
27	C	270	CDL	CA2-OA2-PA1-OA3
27	C	270	CDL	CA3-OA5-PA1-OA2
27	C	270	CDL	CA3-OA5-PA1-OA3
27	C	270	CDL	C11-CA5-OA6-CA4
27	C	270	CDL	CB2-OB2-PB2-OB3
27	C	270	CDL	CB2-OB2-PB2-OB4
27	G	269	CDL	C1-CB2-OB2-PB2
27	G	269	CDL	CB3-OB5-PB2-OB2
27	G	269	CDL	CB3-OB5-PB2-OB3
27	P	1270	CDL	CA2-C1-CB2-OB2
27	P	1270	CDL	CA2-OA2-PA1-OA3
27	P	1270	CDL	CA2-OA2-PA1-OA5
27	P	1270	CDL	CA3-OA5-PA1-OA2
27	P	1270	CDL	C11-CA5-OA6-CA4
27	P	1270	CDL	CB2-OB2-PB2-OB5
27	T	1269	CDL	O1-C1-CA2-OA2
27	T	1269	CDL	C1-CB2-OB2-PB2
27	T	1269	CDL	CB3-OB5-PB2-OB2
27	T	1269	CDL	CB3-OB5-PB2-OB3
21	D	523	TGL	OC1-CC1-OG3-CG3
21	N	1521	TGL	CG2-CG3-OG3-CC1
21	D	523	TGL	CC2-CC1-OG3-CG3
19	N	1524	PGV	O04-C19-O03-C01
21	O	1523	TGL	OC1-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
23	C	271	CHD	C16-C17-C20-C21
23	P	1271	CHD	C16-C17-C20-C21
21	N	1522	TGL	OB1-CB1-OG2-CG2
22	B	230	PSC	O02-C1-O01-C02
22	O	1230	PSC	O02-C1-O01-C02
27	P	1270	CDL	OA7-CA5-OA6-CA4
19	N	1524	PGV	C20-C19-O03-C01
21	O	1523	TGL	CC2-CC1-OG3-CG3
19	A	524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
22	O	1230	PSC	C2-C1-O01-C02
23	P	1271	CHD	C13-C17-C20-C22
18	A	515	HEA	C26-C15-C16-C17
18	N	515	HEA	C26-C15-C16-C17
18	A	515	HEA	C14-C15-C16-C17
18	N	515	HEA	C14-C15-C16-C17
21	L	522	TGL	OA1-CA1-OG1-CG1
21	N	1522	TGL	OA1-CA1-OG1-CG1
21	O	1523	TGL	CA2-CA1-OG1-CG1
22	B	230	PSC	C20-C19-O03-C01
22	O	1230	PSC	C20-C19-O03-C01
27	T	1269	CDL	C31-CA7-OA8-CA6
19	C	267	PGV	C10-C11-C12-C13
26	C	265	PEK	C4-C5-C6-C7
26	C	265	PEK	C13-C14-C15-C16
26	G	1263	PEK	C4-C5-C6-C7
26	P	1265	PEK	C4-C5-C6-C7
26	P	1265	PEK	C13-C14-C15-C16
26	T	263	PEK	C4-C5-C6-C7
27	C	270	CDL	OA7-CA5-OA6-CA4
21	D	523	TGL	C21-C20-CA9-CA8
27	C	270	CDL	O1-C1-CB2-OB2
27	P	1270	CDL	O1-C1-CB2-OB2
24	Z	1526	DMU	O6-C11-C9-O1
19	C	268	PGV	C2-C1-O01-C02
21	L	522	TGL	CB2-CB1-OG2-CG2
27	G	269	CDL	C11-CA5-OA6-CA4
27	T	1269	CDL	C11-CA5-OA6-CA4
21	N	1522	TGL	CC3-CC4-CC5-CC6
21	L	522	TGL	CA2-CA1-OG1-CG1
21	N	1522	TGL	CA2-CA1-OG1-CG1
21	O	1523	TGL	OA1-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	O04-C19-O03-C01
22	O	1230	PSC	O04-C19-O03-C01
27	T	1269	CDL	OA9-CA7-OA8-CA6
27	G	269	CDL	OA7-CA5-OA6-CA4
21	N	1522	TGL	C21-C20-CA9-CA8
24	C	272	DMU	O5-C6-O16-C18
24	M	526	DMU	O5-C6-O16-C18
24	Z	1526	DMU	O5-C6-O16-C18
27	P	1270	CDL	C20-C21-C22-C23
21	B	521	TGL	CA2-CA1-OG1-CG1
19	P	1267	PGV	C10-C11-C12-C13
22	B	230	PSC	C11-C10-C9-C8
26	G	264	PEK	C13-C14-C15-C16
26	G	1263	PEK	C10-C11-C12-C13
26	P	1264	PEK	C13-C14-C15-C16
26	P	1265	PEK	C10-C11-C12-C13
26	T	263	PEK	C7-C8-C9-C10
26	T	263	PEK	C13-C14-C15-C16
27	G	269	CDL	C15-C16-C17-C18
27	T	1269	CDL	C80-C81-C82-C83
27	G	269	CDL	C22-C23-C24-C25
19	C	268	PGV	O02-C1-O01-C02
21	L	522	TGL	OB1-CB1-OG2-CG2
19	A	524	PGV	O12-C04-C05-C06
27	C	270	CDL	CA2-C1-CB2-OB2
27	G	269	CDL	CA2-C1-CB2-OB2
21	N	1521	TGL	CC2-CC1-OG3-CG3
27	G	269	CDL	C31-CA7-OA8-CA6
24	C	272	DMU	O6-C11-C9-C8
21	D	523	TGL	C11-C10-CB9-CB8
21	O	1523	TGL	C11-C10-CB9-CB8
24	M	526	DMU	C19-C22-C25-C28
24	Z	1526	DMU	O5-C4-C57-O61
23	P	1271	CHD	C17-C20-C22-C23
27	C	270	CDL	C20-C21-C22-C23
27	T	1269	CDL	C73-C74-C75-C76
26	G	1263	PEK	C28-C29-C30-C31
23	P	1271	CHD	C21-C20-C22-C23
21	N	1521	TGL	CA2-CA1-OG1-CG1
24	M	526	DMU	O5-C4-C57-O61
22	B	230	PSC	C20-C21-C22-C23
21	B	521	TGL	OA1-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
27	G	269	CDL	OA9-CA7-OA8-CA6
24	P	1272	DMU	C3-C4-C57-O61
24	P	1272	DMU	O6-C11-C9-C8
24	Z	1526	DMU	C19-C22-C25-C28
22	O	1230	PSC	C11-C10-C9-C8
26	C	265	PEK	C7-C8-C9-C10
26	C	265	PEK	C10-C11-C12-C13
21	N	1521	TGL	OC1-CC1-OG3-CG3
27	T	1269	CDL	C15-C16-C17-C18
23	C	271	CHD	C17-C20-C22-C23
21	B	521	TGL	CC2-CC1-OG3-CG3
21	B	521	TGL	C21-C20-CA9-CA8
27	C	270	CDL	C83-C84-C85-C86
26	T	263	PEK	C28-C29-C30-C31
27	T	1269	CDL	OA7-CA5-OA6-CA4
24	C	272	DMU	C3-C4-C57-O61
24	C	272	DMU	O16-C18-C19-C22
21	N	1521	TGL	CA1-CA2-CA3-CA4
26	G	264	PEK	C1-C2-C3-C4
27	T	1269	CDL	CA5-C11-C12-C13
19	N	1268	PGV	C2-C1-O01-C02
27	P	1270	CDL	C51-CB5-OB6-CB4
19	A	524	PGV	C19-C20-C21-C22
27	G	269	CDL	CA5-C11-C12-C13
27	G	269	CDL	CA7-C31-C32-C33
24	P	1272	DMU	O5-C6-O16-C18
21	L	522	TGL	CC3-CC4-CC5-CC6
19	A	524	PGV	O12-C04-C05-O05
19	C	268	PGV	O12-C04-C05-O05
19	N	1268	PGV	O12-C04-C05-O05
27	G	269	CDL	O1-C1-CB2-OB2
27	T	1269	CDL	O1-C1-CB2-OB2
21	N	1522	TGL	CB1-CB2-CB3-CB4
27	P	1270	CDL	CB7-C71-C72-C73
21	N	1521	TGL	OB1-CB1-OG2-CG2
24	M	526	DMU	O6-C11-C9-O1
23	C	271	CHD	C21-C20-C22-C23
21	B	521	TGL	OC1-CC1-OG3-CG3
21	B	521	TGL	CG2-CG3-OG3-CC1
24	M	526	DMU	O6-C11-C9-C8
27	G	269	CDL	C40-C41-C42-C43
26	P	1264	PEK	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
27	C	270	CDL	CB7-C71-C72-C73
24	C	272	DMU	C4-C3-O7-C10
21	B	521	TGL	CA9-C20-C21-C22
27	T	1269	CDL	C40-C41-C42-C43
19	N	1268	PGV	O02-C1-O01-C02
27	P	1270	CDL	OB7-CB5-OB6-CB4
19	C	268	PGV	O12-C04-C05-C06
19	N	1268	PGV	O12-C04-C05-C06
27	T	1269	CDL	CA2-C1-CB2-OB2
23	P	1271	CHD	C13-C17-C20-C21
24	P	1272	DMU	O16-C18-C19-C22
21	D	523	TGL	C16-C15-CC9-CC8
21	N	1521	TGL	CB2-CB1-OG2-CG2
22	O	1230	PSC	C11-C12-C13-C14
26	G	1263	PEK	C7-C8-C9-C10
26	G	1263	PEK	C13-C14-C15-C16
21	L	522	TGL	CB1-CB2-CB3-CB4
22	O	1230	PSC	C20-C21-C22-C23
19	A	524	PGV	C04-C05-C06-O06
22	O	1230	PSC	C1-C2-C3-C4
27	C	270	CDL	C60-C61-C62-C63
21	N	1521	TGL	OA1-CA1-OG1-CG1
27	G	269	CDL	C59-C60-C61-C62
21	B	521	TGL	C14-C29-C30-C31
21	O	1523	TGL	CB5-CB6-CB7-CB8
26	G	264	PEK	C25-C26-C27-C28
27	C	270	CDL	C76-C77-C78-C79
27	C	270	CDL	C82-C83-C84-C85
19	N	1266	PGV	C23-C24-C25-C26
21	D	523	TGL	C19-C33-C34-C35
21	L	522	TGL	CA7-CA8-CA9-C20
21	N	1521	TGL	CA5-CA6-CA7-CA8
26	G	1263	PEK	C31-C32-C33-C34
27	C	270	CDL	C73-C74-C75-C76
27	P	1270	CDL	C58-C59-C60-C61
19	A	524	PGV	C24-C25-C26-C27
21	D	523	TGL	CB3-CB4-CB5-CB6
21	D	523	TGL	CB5-CB6-CB7-CB8
27	C	270	CDL	C72-C73-C74-C75
27	P	1270	CDL	C72-C73-C74-C75
27	P	1270	CDL	C73-C74-C75-C76
21	B	521	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	O05-C05-C06-O06
19	N	1524	PGV	O05-C05-C06-O06
19	C	268	PGV	C24-C25-C26-C27
19	N	1524	PGV	C4-C5-C6-C7
19	N	1268	PGV	C13-C14-C15-C16
21	L	522	TGL	CB9-C10-C11-C12
21	O	1523	TGL	CC4-CC5-CC6-CC7
19	C	267	PGV	C1-C2-C3-C4
21	D	523	TGL	CB1-CB2-CB3-CB4
19	A	521	PGV	C6-C7-C8-C9
19	C	268	PGV	C30-C31-C32-C33
19	N	1268	PGV	C26-C27-C28-C29
21	L	522	TGL	C21-C22-C23-C24
19	P	1267	PGV	C13-C14-C15-C16
21	N	1522	TGL	CA7-CA8-CA9-C20
19	N	1266	PGV	C5-C6-C7-C8
19	N	1266	PGV	C6-C7-C8-C9
21	N	1522	TGL	C24-C25-C26-C27
19	C	268	PGV	C20-C21-C22-C23
21	N	1522	TGL	CA5-CA6-CA7-CA8
21	N	1522	TGL	CB4-CB5-CB6-CB7
22	B	230	PSC	C24-C25-C26-C27
19	N	1268	PGV	C27-C28-C29-C30
26	G	264	PEK	C31-C32-C33-C34
26	T	263	PEK	C25-C26-C27-C28
27	C	270	CDL	C36-C37-C38-C39
27	C	270	CDL	C42-C43-C44-C45
27	T	1269	CDL	C60-C61-C62-C63
27	P	1270	CDL	C79-C80-C81-C82
24	P	1272	DMU	C19-C22-C25-C28
27	P	1270	CDL	C11-C12-C13-C14
24	Z	1526	DMU	C28-C31-C34-C37
26	G	1263	PEK	C25-C26-C27-C28
21	L	522	TGL	CB6-CB7-CB8-CB9
21	N	1521	TGL	CA6-CA7-CA8-CA9
21	O	1523	TGL	C17-C18-C19-C33
22	B	230	PSC	C26-C27-C28-C29
26	C	265	PEK	C25-C26-C27-C28
26	P	1265	PEK	C25-C26-C27-C28
27	P	1270	CDL	C15-C16-C17-C18
21	B	521	TGL	CB1-CB2-CB3-CB4
21	O	1523	TGL	CB1-CB2-CB3-CB4

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C1-C2-C3-C4
19	A	524	PGV	C20-C21-C22-C23
19	N	1524	PGV	C22-C23-C24-C25
19	N	1266	PGV	C7-C8-C9-C10
21	N	1522	TGL	C12-C13-C14-C29
24	P	1272	DMU	C28-C31-C34-C37
26	C	265	PEK	C16-C17-C18-C19
26	T	263	PEK	C31-C32-C33-C34
27	C	270	CDL	C57-C58-C59-C60
27	C	270	CDL	C59-C60-C61-C62
27	G	269	CDL	C13-C14-C15-C16
24	Z	1526	DMU	C25-C28-C31-C34
26	G	1263	PEK	C33-C34-C35-C36
26	G	1263	PEK	C29-C30-C31-C32
19	A	521	PGV	C5-C6-C7-C8
21	L	522	TGL	C24-C25-C26-C27
27	P	1270	CDL	C36-C37-C38-C39
21	N	1521	TGL	CB1-CB2-CB3-CB4
26	P	1265	PEK	C1-C2-C3-C4
21	N	1522	TGL	CC9-C15-C16-C17
19	C	268	PGV	C12-C13-C14-C15
19	N	1268	PGV	C20-C19-O03-C01
26	C	265	PEK	C22-C21-O03-C01
22	B	230	PSC	C11-C12-C13-C14
21	N	1522	TGL	C10-C11-C12-C13
27	C	270	CDL	C41-C42-C43-C44
21	N	1521	TGL	C13-C14-C29-C30
21	N	1522	TGL	CC6-CC7-CC8-CC9
21	O	1523	TGL	C15-C16-C17-C18
19	N	1268	PGV	C25-C26-C27-C28
21	N	1522	TGL	CC4-CC5-CC6-CC7
27	C	270	CDL	C38-C39-C40-C41
27	G	269	CDL	C81-C82-C83-C84
26	G	264	PEK	C29-C30-C31-C32
26	T	263	PEK	C29-C30-C31-C32
27	G	269	CDL	C62-C63-C64-C65
19	N	1268	PGV	C14-C15-C16-C17
27	P	1270	CDL	C13-C14-C15-C16
23	J	60	CHD	C13-C17-C20-C21
19	N	1268	PGV	C24-C25-C26-C27
27	C	270	CDL	C11-C12-C13-C14
27	C	270	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
27	G	269	CDL	C61-C62-C63-C64
27	G	269	CDL	C73-C74-C75-C76
27	P	1270	CDL	CA5-C11-C12-C13
27	T	1269	CDL	C71-CB7-OB8-CB6
19	N	1268	PGV	C30-C31-C32-C33
21	O	1523	TGL	CB2-CB3-CB4-CB5
26	G	264	PEK	C27-C28-C29-C30
27	G	269	CDL	C56-C57-C58-C59
21	D	523	TGL	C10-C11-C12-C13
24	M	526	DMU	C25-C28-C31-C34
26	G	1263	PEK	C27-C28-C29-C30
24	P	1272	DMU	C1-C6-O16-C18
19	C	268	PGV	C13-C14-C15-C16
27	G	269	CDL	C82-C83-C84-C85
22	B	230	PSC	C23-C24-C25-C26
26	G	1263	PEK	C16-C17-C18-C19
26	P	1264	PEK	C16-C17-C18-C19
27	G	269	CDL	C54-C55-C56-C57
21	N	1521	TGL	C15-C16-C17-C18
22	O	1230	PSC	C5-C6-C7-C8
23	W	1060	CHD	C13-C17-C20-C21
21	B	521	TGL	CB2-CB1-OG2-CG2
27	C	270	CDL	C51-CB5-OB6-CB4
21	L	522	TGL	C25-C26-C27-C28
19	A	521	PGV	C4-C5-C6-C7
22	O	1230	PSC	C29-C30-C31-C32
19	C	268	PGV	C11-C10-C9-C8
19	N	1268	PGV	C11-C10-C9-C8
21	L	522	TGL	CC2-CC3-CC4-CC5
22	B	230	PSC	C29-C30-C31-C32
21	L	522	TGL	C17-C18-C19-C33
21	D	523	TGL	CC6-CC7-CC8-CC9
21	N	1522	TGL	C16-C17-C18-C19
21	O	1523	TGL	C18-C19-C33-C34
26	C	265	PEK	C32-C33-C34-C35
22	O	1230	PSC	C04-C05-N-C08
21	L	522	TGL	C10-C11-C12-C13
21	L	522	TGL	CC9-C15-C16-C17
21	N	1521	TGL	C16-C17-C18-C19
26	T	263	PEK	C27-C28-C29-C30
27	G	269	CDL	C79-C80-C81-C82
27	P	1270	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
27	P	1270	CDL	C51-C52-C53-C54
27	P	1270	CDL	C59-C60-C61-C62
19	C	268	PGV	C26-C27-C28-C29
21	L	522	TGL	CC6-CC7-CC8-CC9
24	P	1272	DMU	C4-C3-O7-C10
26	T	263	PEK	C30-C31-C32-C33
26	C	265	PEK	O04-C21-O03-C01
19	N	1524	PGV	C14-C15-C16-C17
27	C	270	CDL	C74-C75-C76-C77
19	P	1267	PGV	C1-C2-C3-C4
27	C	270	CDL	C78-C79-C80-C81
19	A	521	PGV	C7-C8-C9-C10
21	N	1521	TGL	CA3-CA4-CA5-CA6
21	O	1523	TGL	CC6-CC7-CC8-CC9
21	L	522	TGL	CA3-CA4-CA5-CA6
27	C	270	CDL	C40-C41-C42-C43
27	G	269	CDL	CB7-C71-C72-C73
19	C	268	PGV	C14-C15-C16-C17
19	A	524	PGV	C11-C10-C9-C8
19	N	1524	PGV	C11-C10-C9-C8
19	N	1268	PGV	C12-C13-C14-C15
26	C	265	PEK	C15-C16-C17-C18
21	N	1521	TGL	C14-C29-C30-C31
19	A	524	PGV	C22-C23-C24-C25
21	D	523	TGL	CB2-CB3-CB4-CB5
21	N	1521	TGL	CA4-CA5-CA6-CA7
26	P	1264	PEK	C26-C27-C28-C29
27	C	270	CDL	C61-C62-C63-C64
27	P	1270	CDL	C74-C75-C76-C77
27	T	1269	CDL	C72-C73-C74-C75
19	N	1266	PGV	C29-C30-C31-C32
27	T	1269	CDL	C77-C78-C79-C80
21	N	1522	TGL	CA2-CA3-CA4-CA5
24	C	272	DMU	C19-C22-C25-C28
26	P	1265	PEK	C29-C30-C31-C32
27	T	1269	CDL	C36-C37-C38-C39
21	B	521	TGL	CA5-CA6-CA7-CA8
27	C	270	CDL	C51-C52-C53-C54
27	G	269	CDL	C72-C73-C74-C75
27	T	1269	CDL	C62-C63-C64-C65
19	A	521	PGV	C30-C31-C32-C33
27	C	270	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	C	270	CDL	C75-C76-C77-C78
27	P	1270	CDL	C60-C61-C62-C63
19	N	1266	PGV	C4-C5-C6-C7
27	T	1269	CDL	C23-C24-C25-C26
19	N	1268	PGV	O04-C19-O03-C01
21	D	523	TGL	CA9-C20-C21-C22
26	P	1264	PEK	C7-C8-C9-C10
26	C	265	PEK	C34-C35-C36-C37
24	P	1272	DMU	C22-C25-C28-C31
26	P	1264	PEK	C25-C26-C27-C28
26	G	1263	PEK	C26-C27-C28-C29
26	P	1264	PEK	C15-C16-C17-C18
26	P	1265	PEK	C15-C16-C17-C18
19	N	1524	PGV	C24-C25-C26-C27
27	G	269	CDL	C35-C36-C37-C38
27	G	269	CDL	C36-C37-C38-C39
27	C	270	CDL	OA5-CA3-CA4-CA6
27	C	270	CDL	OB5-CB3-CB4-CB6
21	L	522	TGL	C20-C21-C22-C23
21	O	1523	TGL	CB3-CB4-CB5-CB6
21	N	1521	TGL	CB9-C10-C11-C12
19	N	1524	PGV	C19-C20-C21-C22
22	O	1230	PSC	C23-C24-C25-C26
19	N	1268	PGV	C22-C23-C24-C25
21	B	521	TGL	C15-C16-C17-C18
27	T	1269	CDL	C55-C56-C57-C58
19	N	1266	PGV	C19-C20-C21-C22
21	O	1523	TGL	CA9-C20-C21-C22
26	P	1265	PEK	C24-C25-C26-C27
27	C	270	CDL	C32-C33-C34-C35
19	C	268	PGV	C10-C11-C12-C13
19	A	524	PGV	O03-C01-C02-C03
21	N	1521	TGL	OG1-CG1-CG2-CG3
26	G	1263	PEK	O03-C01-C02-C03
26	P	1264	PEK	O03-C01-C02-C03
26	T	263	PEK	O03-C01-C02-C03
27	C	270	CDL	CA3-CA4-CA6-OA8
27	P	1270	CDL	CA3-CA4-CA6-OA8
27	T	1269	CDL	CA3-CA4-CA6-OA8
24	C	272	DMU	C22-C25-C28-C31
26	P	1264	PEK	C24-C25-C26-C27
19	A	521	PGV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C27-C28-C29-C30
21	B	521	TGL	C16-C17-C18-C19
26	P	1264	PEK	C31-C32-C33-C34
27	C	270	CDL	C19-C20-C21-C22
27	G	269	CDL	C37-C38-C39-C40
19	N	1524	PGV	C2-C3-C4-C5
27	T	1269	CDL	OB9-CB7-OB8-CB6
24	M	526	DMU	C3-C4-C57-O61
19	C	267	PGV	C30-C31-C32-C33
27	G	269	CDL	C78-C79-C80-C81
22	O	1230	PSC	C04-C05-N-C07
21	D	523	TGL	C17-C18-C19-C33
22	O	1230	PSC	C26-C27-C28-C29
24	C	272	DMU	O5-C4-C57-O61
21	B	521	TGL	CA4-CA5-CA6-CA7
26	T	263	PEK	C16-C17-C18-C19
27	C	270	CDL	C16-C17-C18-C19
27	C	270	CDL	C43-C44-C45-C46
27	P	1270	CDL	C35-C36-C37-C38
27	T	1269	CDL	C71-C72-C73-C74
27	C	270	CDL	C71-C72-C73-C74
26	G	264	PEK	C16-C17-C18-C19
19	C	268	PGV	C29-C30-C31-C32
21	N	1521	TGL	CA9-C20-C21-C22
27	T	1269	CDL	C11-C12-C13-C14
26	G	264	PEK	C24-C25-C26-C27
27	G	269	CDL	C55-C56-C57-C58
27	T	1269	CDL	C31-C32-C33-C34
19	N	1524	PGV	C12-C13-C14-C15
21	N	1522	TGL	CB6-CB7-CB8-CB9
27	P	1270	CDL	C71-C72-C73-C74
18	N	516	HEA	C2A-C3A-CMA-OMA
21	L	522	TGL	CC4-CC5-CC6-CC7
27	P	1270	CDL	CA7-C31-C32-C33
19	N	1268	PGV	C10-C11-C12-C13
26	G	264	PEK	C10-C11-C12-C13
19	C	268	PGV	O01-C02-C03-O11
19	C	267	PGV	C24-C25-C26-C27
27	P	1270	CDL	C41-C42-C43-C44
26	P	1265	PEK	C22-C21-O03-C01
27	P	1270	CDL	C31-CA7-OA8-CA6
21	N	1521	TGL	CB3-CB4-CB5-CB6

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Mol	Chain	Res	Type	Atoms
26	C	265	PEK	C29-C30-C31-C32
27	G	269	CDL	C44-C45-C46-C47
19	C	267	PGV	C7-C8-C9-C10
19	P	1267	PGV	C22-C23-C24-C25
21	N	1522	TGL	C16-C15-CC9-CC8
22	O	1230	PSC	C27-C28-C29-C30
21	N	1522	TGL	C11-C12-C13-C14
26	G	1263	PEK	C30-C31-C32-C33
22	O	1230	PSC	O03-C01-C02-O01
27	T	1269	CDL	C64-C65-C66-C67
24	Z	1526	DMU	C22-C25-C28-C31
27	G	269	CDL	C33-C34-C35-C36
26	C	265	PEK	C22-C23-C24-C25
21	L	522	TGL	C21-C20-CA9-CA8
21	B	521	TGL	C25-C26-C27-C28
21	D	523	TGL	C33-C34-C35-C36
24	P	1272	DMU	C34-C37-C40-C43
18	A	516	HEA	C3B-C11-C12-C13
18	N	516	HEA	C3B-C11-C12-C13
21	L	522	TGL	CA2-CA3-CA4-CA5
27	P	1270	CDL	C55-C56-C57-C58
19	C	268	PGV	C31-C32-C33-C34
26	P	1264	PEK	C27-C28-C29-C30
21	N	1522	TGL	C29-C30-C31-C32
19	P	1267	PGV	C23-C24-C25-C26
26	T	263	PEK	C26-C27-C28-C29
19	P	1267	PGV	C25-C26-C27-C28
19	P	1267	PGV	C31-C32-C33-C34
19	A	521	PGV	C19-C20-C21-C22
27	G	269	CDL	CB5-C51-C52-C53
19	N	1524	PGV	C10-C11-C12-C13
26	P	1264	PEK	C10-C11-C12-C13
26	T	263	PEK	C10-C11-C12-C13
19	P	1267	PGV	C15-C16-C17-C18
21	N	1522	TGL	CB5-CB6-CB7-CB8
21	D	523	TGL	C15-C16-C17-C18
27	T	1269	CDL	C54-C55-C56-C57
27	C	270	CDL	OB7-CB5-OB6-CB4
19	A	524	PGV	O05-C05-C06-O06
19	A	524	PGV	C05-C04-O12-P
27	C	270	CDL	CA4-CA3-OA5-PA1
26	G	264	PEK	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
21	D	523	TGL	C13-C14-C29-C30
26	G	264	PEK	C32-C33-C34-C35
27	G	269	CDL	C75-C76-C77-C78
19	C	267	PGV	C25-C26-C27-C28
19	C	268	PGV	C25-C26-C27-C28
21	N	1522	TGL	C22-C23-C24-C25
19	A	524	PGV	C01-C02-C03-O11
19	C	268	PGV	C01-C02-C03-O11
19	N	1524	PGV	C01-C02-C03-O11
26	P	1265	PEK	C01-C02-C03-O11
27	P	1270	CDL	OB5-CB3-CB4-CB6
27	T	1269	CDL	OA5-CA3-CA4-CA6
24	M	526	DMU	C28-C31-C34-C37
26	G	264	PEK	C26-C27-C28-C29
27	G	269	CDL	C64-C65-C66-C67
27	P	1270	CDL	C44-C45-C46-C47
21	B	521	TGL	CB9-C10-C11-C12
27	T	1269	CDL	C44-C45-C46-C47
26	C	265	PEK	C31-C32-C33-C34
19	C	267	PGV	C31-C32-C33-C34
24	M	526	DMU	C34-C37-C40-C43
27	P	1270	CDL	C61-C62-C63-C64
21	O	1523	TGL	C19-C33-C34-C35
19	N	1524	PGV	C28-C29-C30-C31
19	C	267	PGV	C13-C14-C15-C16
19	P	1267	PGV	C7-C8-C9-C10
26	G	264	PEK	C34-C35-C36-C37
21	B	521	TGL	C13-C14-C29-C30
27	P	1270	CDL	C57-C58-C59-C60
27	C	270	CDL	C77-C78-C79-C80
27	T	1269	CDL	CB2-C1-CA2-OA2
21	D	523	TGL	CA2-CA1-OG1-CG1
19	N	1524	PGV	O03-C01-C02-C03
22	B	230	PSC	O03-C01-C02-C03
27	C	270	CDL	CB3-CB4-CB6-OB8
27	P	1270	CDL	CB3-CB4-CB6-OB8
22	O	1230	PSC	C21-C22-C23-C24
19	A	521	PGV	C31-C32-C33-C34
21	D	523	TGL	C16-C17-C18-C19
24	P	1272	DMU	C25-C28-C31-C34
27	T	1269	CDL	C21-C22-C23-C24
19	C	267	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	N	1522	TGL	C21-C22-C23-C24
27	T	1269	CDL	CA7-C31-C32-C33
27	T	1269	CDL	C13-C14-C15-C16
19	C	267	PGV	C22-C23-C24-C25
21	O	1523	TGL	C16-C15-CC9-CC8
19	N	1268	PGV	O01-C02-C03-O11
26	G	1263	PEK	O01-C02-C03-O11
27	C	270	CDL	OB5-CB3-CB4-OB6
21	B	521	TGL	C20-C21-C22-C23
26	P	1265	PEK	C22-C23-C24-C25
27	G	269	CDL	C80-C81-C82-C83
26	P	1265	PEK	O04-C21-O03-C01
27	T	1269	CDL	C61-C62-C63-C64
21	B	521	TGL	CA6-CA7-CA8-CA9
27	G	269	CDL	C42-C43-C44-C45
19	C	268	PGV	O03-C01-C02-O01
21	N	1521	TGL	OG1-CG1-CG2-OG2
22	B	230	PSC	O03-C01-C02-O01
27	P	1270	CDL	OA6-CA4-CA6-OA8
22	B	230	PSC	C9-C10-C11-C12
22	O	1230	PSC	C9-C10-C11-C12
22	O	1230	PSC	C10-C11-C12-C13
26	C	265	PEK	C5-C6-C7-C8
26	G	264	PEK	C9-C10-C11-C12
26	G	1263	PEK	C11-C10-C9-C8
26	P	1264	PEK	C9-C10-C11-C12
26	P	1265	PEK	C5-C6-C7-C8
26	P	1265	PEK	C6-C7-C8-C9
26	T	263	PEK	C11-C10-C9-C8
21	D	523	TGL	CB6-CB7-CB8-CB9
27	G	269	CDL	C31-C32-C33-C34
27	C	270	CDL	C55-C56-C57-C58
21	B	521	TGL	C16-C15-CC9-CC8
27	C	270	CDL	C58-C59-C60-C61
26	P	1264	PEK	C2-C3-C4-C5
22	O	1230	PSC	C31-C32-C33-C34
19	C	268	PGV	C23-C24-C25-C26
24	C	272	DMU	C1-C6-O16-C18
19	A	521	PGV	C29-C30-C31-C32
21	O	1523	TGL	C12-C13-C14-C29
27	C	270	CDL	C84-C85-C86-C87
27	P	1270	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
27	T	1269	CDL	C82-C83-C84-C85
19	N	1268	PGV	C15-C16-C17-C18
26	T	263	PEK	C01-C02-C03-O11
27	P	1270	CDL	OA5-CA3-CA4-CA6
21	L	522	TGL	C29-C30-C31-C32
21	O	1523	TGL	C33-C34-C35-C36
27	G	269	CDL	C71-CB7-OB8-CB6
21	D	523	TGL	CB9-C10-C11-C12
19	A	524	PGV	C10-C11-C12-C13
21	L	522	TGL	CC5-CC6-CC7-CC8
26	G	1263	PEK	C32-C33-C34-C35
21	L	522	TGL	OG1-CA1-CA2-CA3
27	C	270	CDL	C80-C81-C82-C83
27	G	269	CDL	C39-C40-C41-C42
19	A	524	PGV	C25-C26-C27-C28
19	A	524	PGV	C03-C02-O01-C1
19	N	1524	PGV	C03-C02-O01-C1
21	D	523	TGL	CG3-CG2-OG2-CB1
21	D	523	TGL	OA1-CA1-OG1-CG1
22	B	230	PSC	C31-C32-C33-C34
19	N	1524	PGV	O12-C04-C05-O05
26	G	1263	PEK	C21-C22-C23-C24
27	P	1270	CDL	OA5-CA3-CA4-OA6
27	T	1269	CDL	OA5-CA3-CA4-OA6
22	O	1230	PSC	O03-C01-C02-C03
21	B	521	TGL	C22-C23-C24-C25
27	P	1270	CDL	OA9-CA7-OA8-CA6
19	N	1266	PGV	C31-C32-C33-C34
21	B	521	TGL	CA3-CA4-CA5-CA6
21	L	522	TGL	CB7-CB8-CB9-C10
27	G	269	CDL	C14-C15-C16-C17
26	P	1264	PEK	C32-C33-C34-C35
27	P	1270	CDL	C43-C44-C45-C46
27	C	270	CDL	OA6-CA4-CA6-OA8
27	C	270	CDL	OB6-CB4-CB6-OB8
21	N	1521	TGL	CB4-CB5-CB6-CB7
19	C	268	PGV	C20-C19-O03-C01
27	T	1269	CDL	C33-C34-C35-C36
22	O	1230	PSC	C04-C05-N-C06
19	N	1524	PGV	C6-C7-C8-C9
19	N	1524	PGV	C21-C22-C23-C24
26	P	1264	PEK	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	O04-C19-O03-C01
19	C	267	PGV	C28-C29-C30-C31
19	A	524	PGV	C26-C27-C28-C29
19	A	524	PGV	C28-C29-C30-C31
19	N	1524	PGV	C26-C27-C28-C29
27	T	1269	CDL	C19-C20-C21-C22
26	P	1264	PEK	C29-C30-C31-C32
26	P	1264	PEK	C17-C18-C19-C20
26	C	265	PEK	C1-C2-C3-C4
23	C	271	CHD	C13-C17-C20-C21
27	T	1269	CDL	C79-C80-C81-C82
21	N	1521	TGL	C18-C19-C33-C34
21	O	1523	TGL	CA5-CA6-CA7-CA8
27	C	270	CDL	C35-C36-C37-C38
24	Z	1526	DMU	C3-C4-C57-O61
21	O	1523	TGL	CA6-CA7-CA8-CA9
26	P	1265	PEK	O01-C02-C03-O11
27	C	270	CDL	OA5-CA3-CA4-OA6
27	P	1270	CDL	OB5-CB3-CB4-OB6
27	C	270	CDL	CA5-C11-C12-C13
26	G	264	PEK	C2-C1-O01-C02
22	B	230	PSC	C3-C4-C5-C6
27	G	269	CDL	C24-C25-C26-C27
18	A	515	HEA	C4A-C3A-CMA-OMA
18	A	516	HEA	C4A-C3A-CMA-OMA
18	N	516	HEA	C4A-C3A-CMA-OMA
19	A	521	PGV	C9-C10-C11-C12
21	N	1522	TGL	C17-C18-C19-C33
27	G	269	CDL	OB9-CB7-OB8-CB6
19	N	1524	PGV	O03-C01-C02-O01
26	P	1264	PEK	O03-C01-C02-O01
26	P	1265	PEK	O03-C01-C02-O01
27	P	1270	CDL	OB6-CB4-CB6-OB8
27	T	1269	CDL	OA6-CA4-CA6-OA8
26	G	264	PEK	C4-C5-C6-C7
21	N	1522	TGL	CB2-CB3-CB4-CB5
27	G	269	CDL	CA3-CA4-CA6-OA8
26	G	1263	PEK	C17-C18-C19-C20
19	C	268	PGV	C27-C28-C29-C30
27	G	269	CDL	C34-C35-C36-C37
27	P	1270	CDL	C19-C20-C21-C22
26	G	264	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
27	T	1269	CDL	C16-C17-C18-C19
21	B	521	TGL	CC5-CC6-CC7-CC8
18	N	515	HEA	O11-C11-C3B-C2B
19	N	1524	PGV	C04-O12-P-O13
19	N	1266	PGV	C04-O12-P-O13
22	B	230	PSC	C03-O11-P-O12
22	O	1230	PSC	C03-O11-P-O13
22	O	1230	PSC	C04-O12-P-O13
26	C	265	PEK	C03-O11-P-O14
26	C	265	PEK	C04-O12-P-O11
27	C	270	CDL	CA2-OA2-PA1-OA5
27	C	270	CDL	CB2-OB2-PB2-OB5
27	G	269	CDL	CA2-OA2-PA1-OA3
27	G	269	CDL	CB3-OB5-PB2-OB4
27	P	1270	CDL	CA2-OA2-PA1-OA4
27	P	1270	CDL	CA3-OA5-PA1-OA3
27	T	1269	CDL	CB3-OB5-PB2-OB4
26	C	265	PEK	C30-C31-C32-C33
22	O	1230	PSC	C22-C23-C24-C25
21	O	1523	TGL	CB6-CB7-CB8-CB9
27	C	270	CDL	C34-C35-C36-C37
19	C	267	PGV	C02-C03-O11-P
19	N	1524	PGV	C05-C04-O12-P
19	N	1268	PGV	C02-C03-O11-P
19	N	1268	PGV	C05-C04-O12-P
19	P	1267	PGV	C02-C03-O11-P
23	C	271	CHD	C13-C17-C20-C22
27	G	269	CDL	CB4-CB3-OB5-PB2
27	T	1269	CDL	C39-C40-C41-C42
19	C	268	PGV	C15-C16-C17-C18
27	P	1270	CDL	C84-C85-C86-C87
19	N	1268	PGV	C4-C5-C6-C7
26	T	263	PEK	C21-C22-C23-C24
19	N	1266	PGV	C9-C10-C11-C12
19	N	1266	PGV	C30-C31-C32-C33
21	D	523	TGL	C24-C25-C26-C27
22	O	1230	PSC	C03-C02-O01-C1
21	D	523	TGL	CA7-CA8-CA9-C20
26	P	1265	PEK	C23-C24-C25-C26
19	N	1268	PGV	C01-C02-C03-O11
22	B	230	PSC	C01-C02-C03-O11
26	G	1263	PEK	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
19	P	1267	PGV	C9-C10-C11-C12
26	T	263	PEK	O01-C02-C03-O11
19	P	1267	PGV	C24-C25-C26-C27
21	N	1522	TGL	CB3-CB4-CB5-CB6
26	C	265	PEK	C23-C24-C25-C26
27	T	1269	CDL	C24-C25-C26-C27
19	A	521	PGV	O03-C19-C20-C21
23	G	86	CHD	C17-C20-C22-C23
21	D	523	TGL	OG2-CG2-CG3-OG3
21	B	521	TGL	CB3-CB4-CB5-CB6
19	C	268	PGV	C3-C4-C5-C6
27	P	1270	CDL	C81-C82-C83-C84
21	L	522	TGL	OG2-CB1-CB2-CB3
27	G	269	CDL	C20-C21-C22-C23
19	P	1267	PGV	C30-C31-C32-C33
19	N	1524	PGV	O03-C19-C20-C21
19	N	1266	PGV	O03-C19-C20-C21
21	O	1523	TGL	C13-C14-C29-C30
19	N	1524	PGV	C9-C10-C11-C12
22	O	1230	PSC	C7-C8-C9-C10
19	A	524	PGV	C7-C8-C9-C10
21	N	1521	TGL	C20-C21-C22-C23
24	M	526	DMU	C19-C18-O16-C6
24	Z	1526	DMU	C19-C18-O16-C6
27	T	1269	CDL	C75-C76-C77-C78
27	T	1269	CDL	CB4-CB3-OB5-PB2
19	N	1268	PGV	C23-C24-C25-C26
21	N	1521	TGL	C11-C10-CB9-CB8
27	C	270	CDL	C81-C82-C83-C84
26	P	1265	PEK	C33-C34-C35-C36
27	P	1270	CDL	C34-C35-C36-C37
27	G	269	CDL	O1-C1-CA2-OA2
27	T	1269	CDL	C58-C59-C60-C61
27	G	269	CDL	OB6-CB4-CB6-OB8
24	C	272	DMU	C25-C28-C31-C34
26	P	1265	PEK	C7-C8-C9-C10
26	P	1264	PEK	C34-C35-C36-C37
19	A	524	PGV	C21-C22-C23-C24
23	W	1060	CHD	C17-C20-C22-C23
19	C	268	PGV	C7-C8-C9-C10
26	T	263	PEK	C33-C34-C35-C36
23	P	1271	CHD	C22-C23-C24-O26

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	O12-C04-C05-C06
27	T	1269	CDL	C53-C54-C55-C56
23	P	1271	CHD	C22-C23-C24-O25
23	B	1086	CHD	C17-C20-C22-C23
23	C	271	CHD	C22-C23-C24-O25
19	N	1524	PGV	C20-C21-C22-C23
23	G	86	CHD	C22-C23-C24-O25
21	B	521	TGL	CG3-CG2-OG2-CB1
21	D	523	TGL	CC3-CC4-CC5-CC6
27	P	1270	CDL	C16-C17-C18-C19
27	C	270	CDL	C31-CA7-OA8-CA6
21	N	1521	TGL	CC5-CC6-CC7-CC8
21	O	1523	TGL	CC2-CC3-CC4-CC5
26	G	264	PEK	C23-C24-C25-C26
18	N	516	HEA	CAD-CBD-CGD-O1D
23	B	1086	CHD	C22-C23-C24-O26
19	C	267	PGV	C12-C13-C14-C15
21	O	1523	TGL	CB7-CB8-CB9-C10
19	C	268	PGV	C02-C03-O11-P
19	C	268	PGV	C05-C04-O12-P
26	G	1263	PEK	C02-C03-O11-P
27	C	270	CDL	C1-CA2-OA2-PA1
27	P	1270	CDL	CA4-CA3-OA5-PA1
27	T	1269	CDL	OB5-CB3-CB4-CB6
19	A	521	PGV	C28-C29-C30-C31
21	O	1523	TGL	C14-C29-C30-C31
19	N	1268	PGV	C7-C8-C9-C10
19	A	521	PGV	C11-C12-C13-C14
18	A	516	HEA	CAA-CBA-CGA-O1A
18	N	516	HEA	CAA-CBA-CGA-O1A
26	T	263	PEK	C22-C23-C24-C25
22	B	230	PSC	C10-C11-C12-C13
26	C	265	PEK	C6-C7-C8-C9
26	C	265	PEK	C9-C10-C11-C12
26	C	265	PEK	C11-C12-C13-C14
26	G	264	PEK	C11-C10-C9-C8
26	G	1263	PEK	C6-C7-C8-C9
26	G	1263	PEK	C9-C10-C11-C12
26	G	1263	PEK	C12-C13-C14-C15
26	P	1265	PEK	C11-C10-C9-C8
23	J	60	CHD	C22-C23-C24-O25
23	W	1060	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
23	J	60	CHD	C17-C20-C22-C23
19	A	521	PGV	C23-C24-C25-C26
23	C	271	CHD	C22-C23-C24-O26
18	N	516	HEA	CAD-CBD-CGD-O2D
19	C	267	PGV	C29-C30-C31-C32
22	O	1230	PSC	C25-C26-C27-C28
23	B	1086	CHD	C22-C23-C24-O25
19	A	524	PGV	C31-C32-C33-C34
26	T	263	PEK	C34-C35-C36-C37
27	C	270	CDL	C52-C53-C54-C55
23	W	1060	CHD	C22-C23-C24-O26
21	B	521	TGL	CB4-CB5-CB6-CB7
18	A	516	HEA	C2A-CAA-CBA-CGA
21	B	521	TGL	OG1-CG1-CG2-CG3
21	O	1523	TGL	OG1-CG1-CG2-CG3
18	N	516	HEA	CAA-CBA-CGA-O2A
27	G	269	CDL	C23-C24-C25-C26
27	C	270	CDL	C24-C25-C26-C27
21	L	522	TGL	CA5-CA6-CA7-CA8
21	D	523	TGL	CA5-CA6-CA7-CA8
23	C	525	CHD	C22-C23-C24-O26
23	J	60	CHD	C22-C23-C24-O26
18	A	516	HEA	CAD-CBD-CGD-O2D
21	N	1522	TGL	OG2-CB1-CB2-CB3
18	A	516	HEA	CAA-CBA-CGA-O2A
27	P	1270	CDL	C18-C19-C20-C21
27	G	269	CDL	OA5-CA3-CA4-CA6
21	O	1523	TGL	OG2-CG2-CG3-OG3
27	T	1269	CDL	OB6-CB4-CB6-OB8
19	N	1266	PGV	C20-C21-C22-C23
19	C	267	PGV	C9-C10-C11-C12
26	G	1263	PEK	C3-C4-C5-C6
21	L	522	TGL	C16-C17-C18-C19
26	P	1265	PEK	C32-C33-C34-C35
27	C	270	CDL	C62-C63-C64-C65
23	P	1525	CHD	C22-C23-C24-O26
18	A	516	HEA	CAD-CBD-CGD-O1D
23	G	86	CHD	C22-C23-C24-O26
26	G	1263	PEK	C15-C16-C17-C18
27	T	1269	CDL	C35-C36-C37-C38
21	O	1523	TGL	CB9-C10-C11-C12
23	P	1525	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
27	G	269	CDL	C71-C72-C73-C74
21	O	1523	TGL	CG1-CG2-OG2-CB1
22	B	230	PSC	C03-C02-O01-C1
19	N	1266	PGV	C11-C12-C13-C14
26	G	264	PEK	C3-C4-C5-C6
19	C	268	PGV	C19-C20-C21-C22
21	N	1521	TGL	C29-C30-C31-C32
23	C	525	CHD	C22-C23-C24-O25
27	T	1269	CDL	C56-C57-C58-C59
22	B	230	PSC	C04-C05-N-C08
21	B	521	TGL	C12-C13-C14-C29
27	P	1270	CDL	C75-C76-C77-C78
18	A	515	HEA	CAD-CBD-CGD-O1D
18	A	516	HEA	O11-C11-C12-C13
18	N	516	HEA	O11-C11-C12-C13
27	C	270	CDL	C53-C54-C55-C56
19	C	268	PGV	C21-C22-C23-C24
21	B	521	TGL	CB6-CB7-CB8-CB9
26	P	1264	PEK	C28-C29-C30-C31
26	C	265	PEK	C35-C36-C37-C38
21	B	521	TGL	OG1-CA1-CA2-CA3
21	D	523	TGL	OG1-CA1-CA2-CA3
27	T	1269	CDL	C37-C38-C39-C40
19	N	1268	PGV	C6-C7-C8-C9
21	D	523	TGL	OG1-CG1-CG2-OG2
21	N	1522	TGL	OG3-CC1-CC2-CC3
22	O	1230	PSC	O01-C1-C2-C3
26	T	263	PEK	C23-C24-C25-C26
22	B	230	PSC	O01-C1-C2-C3
26	P	1264	PEK	C14-C15-C16-C17
26	T	263	PEK	C3-C4-C5-C6
19	C	267	PGV	C05-C04-O12-P
21	D	523	TGL	C18-C19-C33-C34
21	N	1522	TGL	CA6-CA7-CA8-CA9
21	O	1523	TGL	CA4-CA5-CA6-CA7
21	D	523	TGL	CA1-CA2-CA3-CA4
21	N	1522	TGL	OG1-CA1-CA2-CA3
19	C	267	PGV	O04-C19-O03-C01
26	P	1264	PEK	O01-C1-C2-C3
27	T	1269	CDL	C20-C21-C22-C23
19	N	1268	PGV	C31-C32-C33-C34
21	N	1522	TGL	C11-C10-CB9-CB8

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Mol	Chain	Res	Type	Atoms
27	G	269	CDL	C63-C64-C65-C66
21	D	523	TGL	C21-C22-C23-C24
18	A	515	HEA	CAA-CBA-CGA-O1A
26	T	263	PEK	C2-C1-O01-C02
24	C	272	DMU	C5-C10-O7-C3
21	D	523	TGL	CC4-CC5-CC6-CC7
18	A	515	HEA	CAD-CBD-CGD-O2D
18	N	515	HEA	CAA-CBA-CGA-O1A
18	N	515	HEA	CAD-CBD-CGD-O1D
24	Z	1526	DMU	C18-C19-C22-C25
27	G	269	CDL	C18-C19-C20-C21
26	T	263	PEK	O02-C1-O01-C02
21	D	523	TGL	C12-C13-C14-C29
26	P	1265	PEK	C34-C35-C36-C37
18	A	515	HEA	CAA-CBA-CGA-O2A
21	D	523	TGL	C29-C30-C31-C32
26	G	1263	PEK	O01-C1-C2-C3
27	C	270	CDL	OA9-CA7-OA8-CA6
21	L	522	TGL	CG1-CG2-CG3-OG3
27	T	1269	CDL	CB3-CB4-CB6-OB8
21	L	522	TGL	CB4-CB5-CB6-CB7
21	O	1523	TGL	OG3-CC1-CC2-CC3
27	T	1269	CDL	C63-C64-C65-C66
18	N	515	HEA	CAA-CBA-CGA-O2A
18	N	515	HEA	CAD-CBD-CGD-O2D
26	P	1265	PEK	C26-C27-C28-C29
27	P	1270	CDL	C32-C31-CA7-OA8
21	L	522	TGL	OG3-CC1-CC2-CC3
26	G	264	PEK	C15-C16-C17-C18
19	A	524	PGV	C14-C15-C16-C17
26	G	264	PEK	O01-C1-C2-C3
26	P	1264	PEK	C3-C4-C5-C6
22	B	230	PSC	C04-C05-N-C07
26	T	263	PEK	O01-C1-C2-C3
27	C	270	CDL	C37-C38-C39-C40
27	G	269	CDL	C58-C59-C60-C61
27	P	1270	CDL	C83-C84-C85-C86
21	N	1522	TGL	OC1-CC1-CC2-CC3
26	P	1264	PEK	O02-C1-C2-C3
26	G	1263	PEK	O02-C1-C2-C3
21	L	522	TGL	C15-C16-C17-C18
24	Z	1526	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
21	L	522	TGL	C19-C33-C34-C35
27	G	269	CDL	C32-C33-C34-C35
22	B	230	PSC	O02-C1-C2-C3
27	T	1269	CDL	OB7-CB5-OB6-CB4
21	D	523	TGL	CG1-CG2-CG3-OG3
27	G	269	CDL	CB3-CB4-CB6-OB8
21	B	521	TGL	OA1-CA1-CA2-CA3
27	C	270	CDL	C64-C65-C66-C67
27	T	1269	CDL	CB7-C71-C72-C73
26	P	1265	PEK	C31-C32-C33-C34
19	N	1524	PGV	O01-C1-C2-C3
19	N	1524	PGV	C25-C26-C27-C28
22	O	1230	PSC	C24-C25-C26-C27
21	D	523	TGL	OG2-CB1-CB2-CB3
27	G	269	CDL	C52-C51-CB5-OB6
27	T	1269	CDL	C51-CB5-OB6-CB4
22	O	1230	PSC	O02-C1-C2-C3
26	G	264	PEK	O02-C1-C2-C3
26	T	263	PEK	O02-C1-C2-C3
22	B	230	PSC	C7-C8-C9-C10
26	P	1265	PEK	C14-C15-C16-C17
19	A	524	PGV	O01-C1-C2-C3
21	B	521	TGL	CC6-CC7-CC8-CC9

There are no ring outliers.

39 monomers are involved in 246 short contacts:

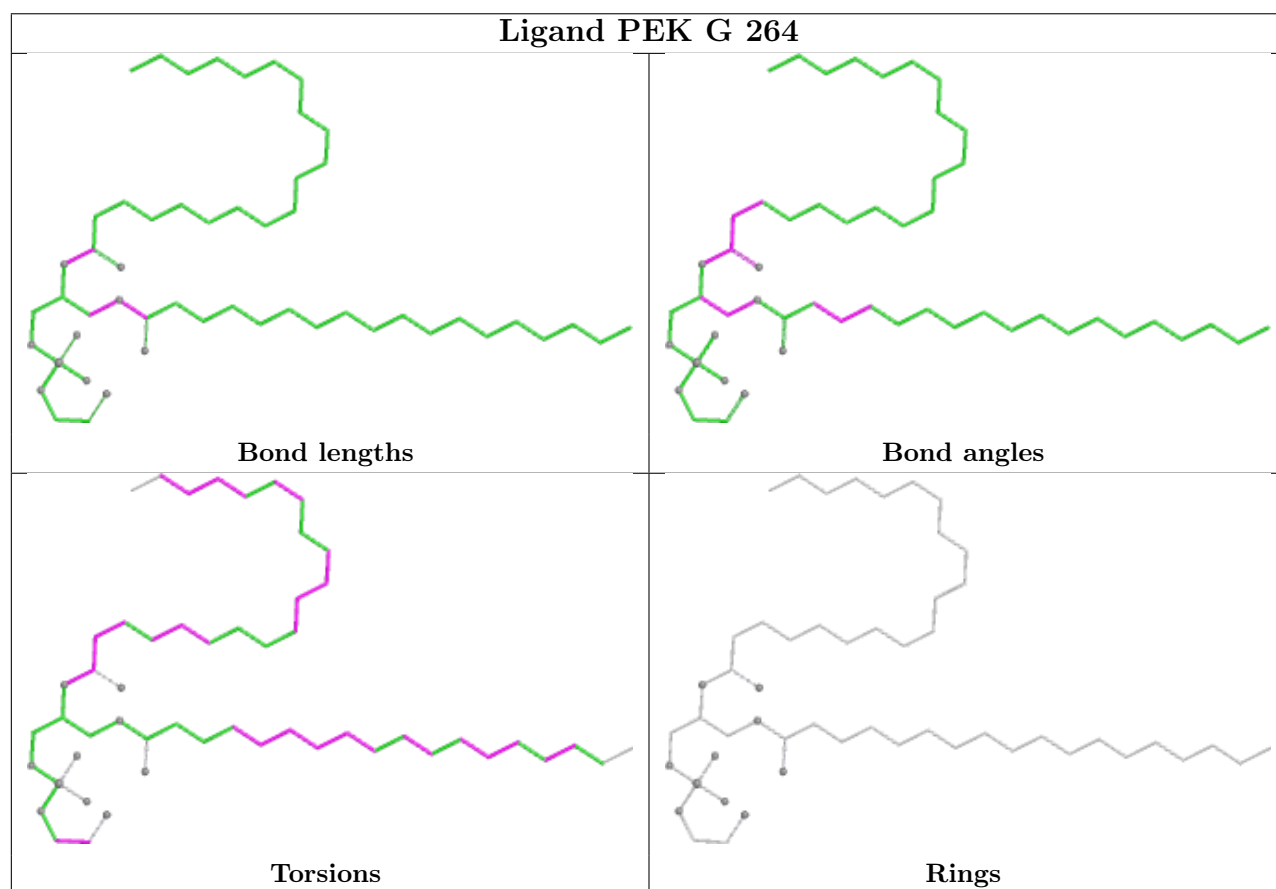
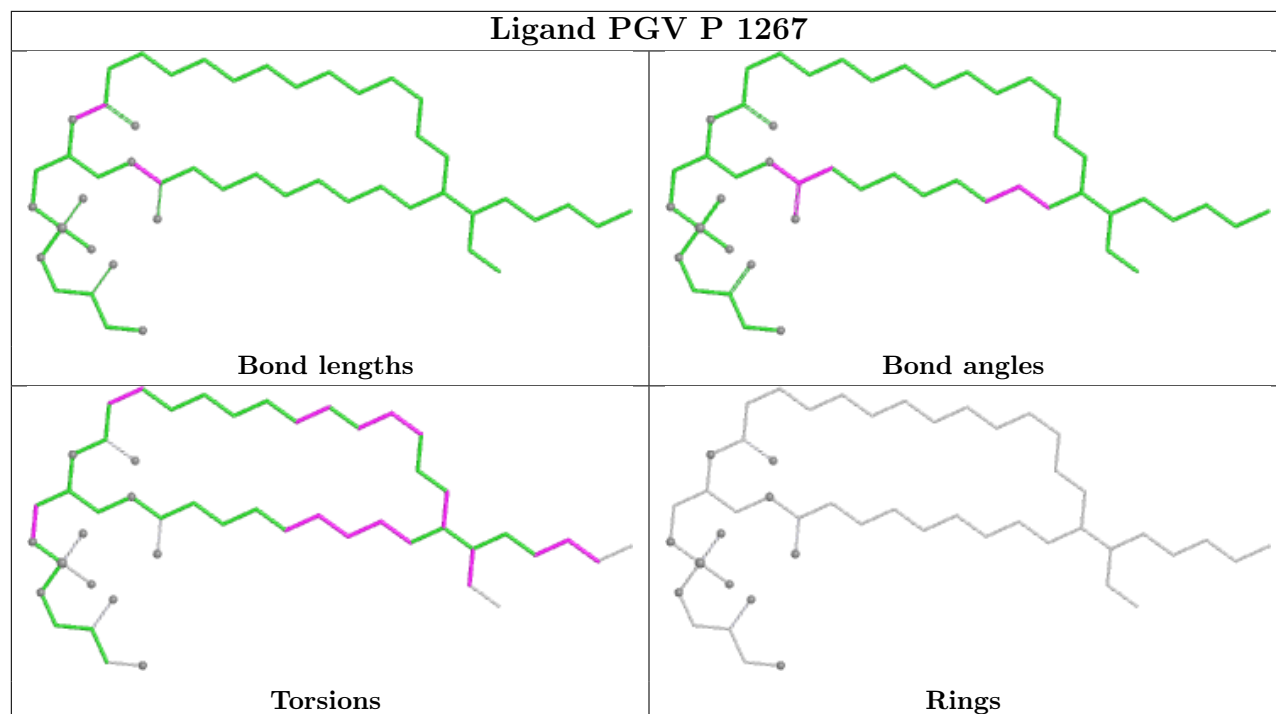
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	1267	PGV	5	0
15	A	520	PER	1	0
26	G	264	PEK	4	0
26	P	1265	PEK	8	0
18	N	515	HEA	7	0
21	O	1523	TGL	6	0
26	G	1263	PEK	12	0
21	N	1521	TGL	7	0
26	T	263	PEK	14	0
23	C	271	CHD	5	0
23	J	60	CHD	2	0
23	P	1271	CHD	3	0
21	B	521	TGL	10	0
23	W	1060	CHD	1	0

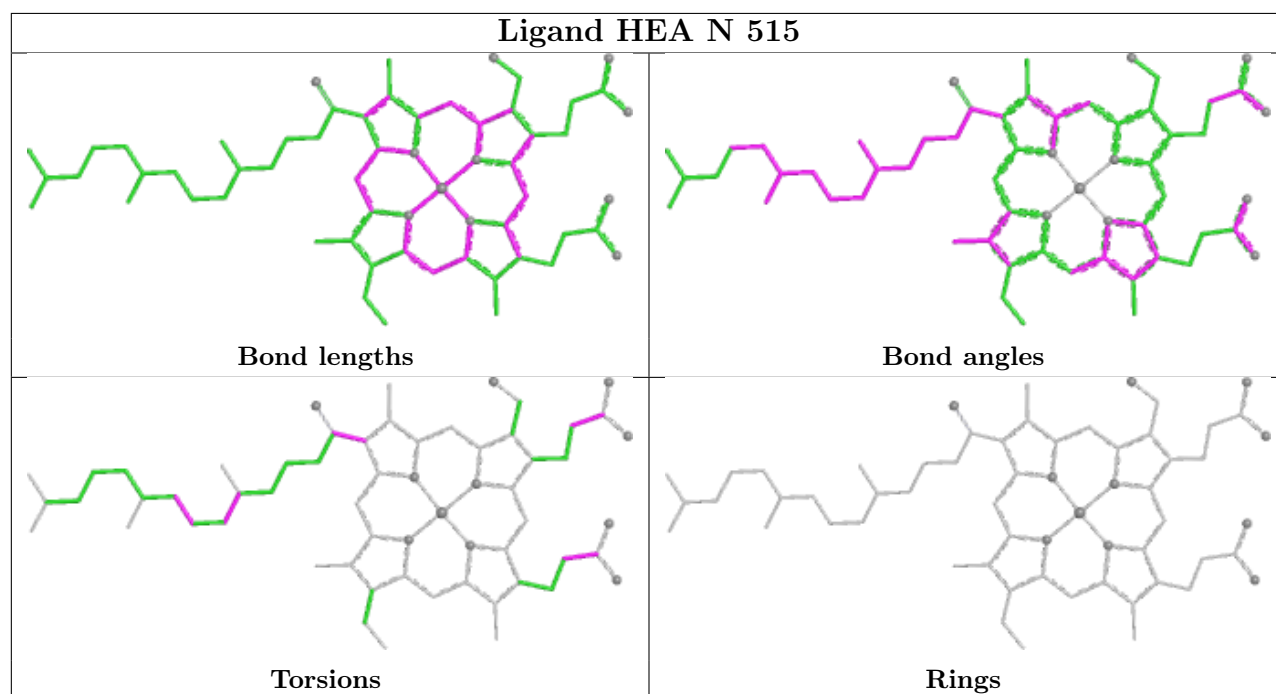
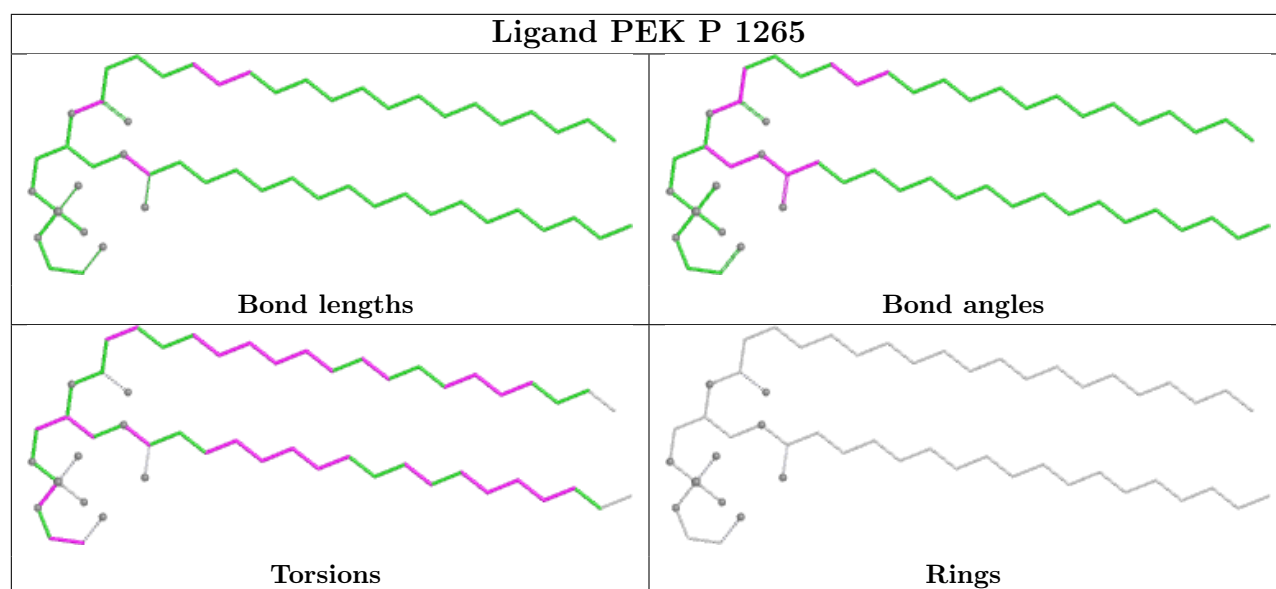
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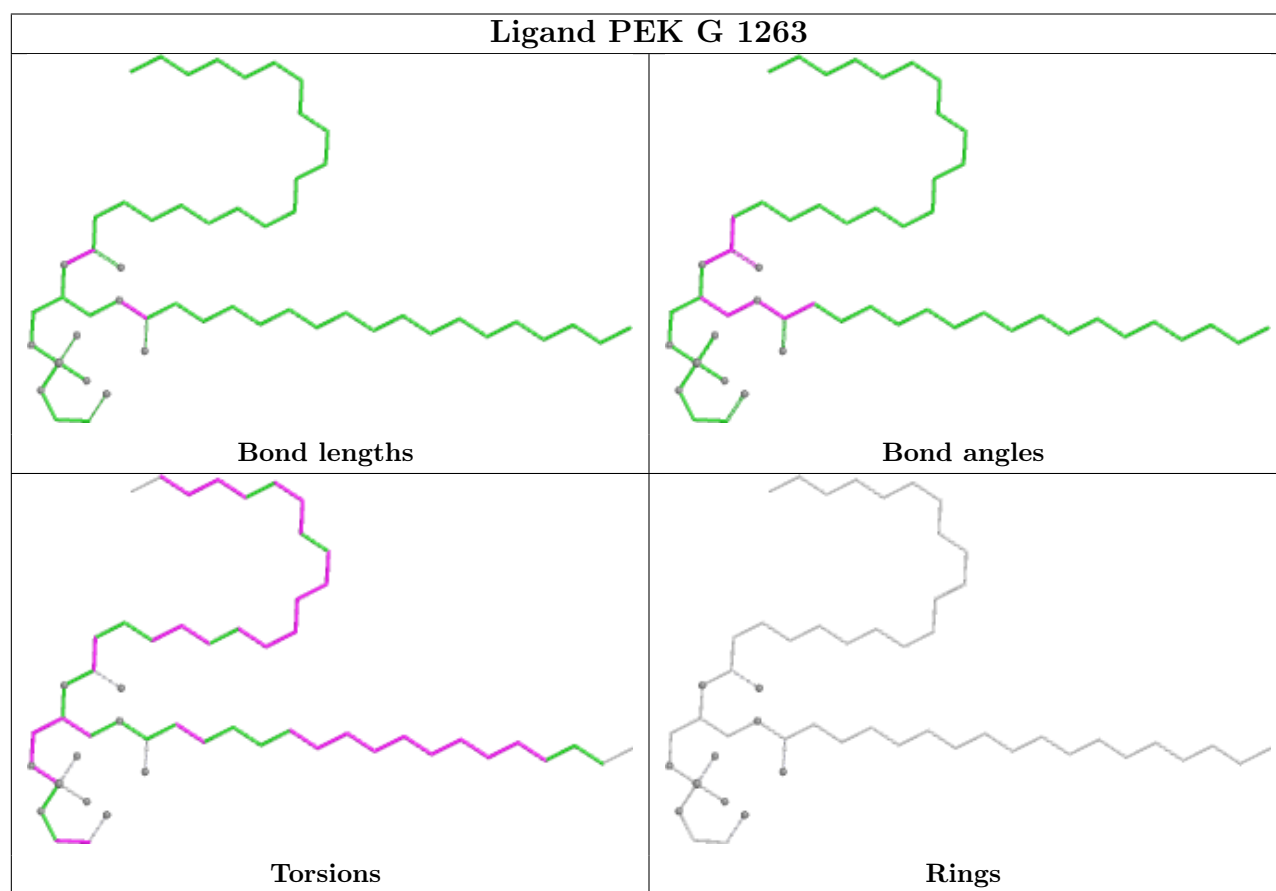
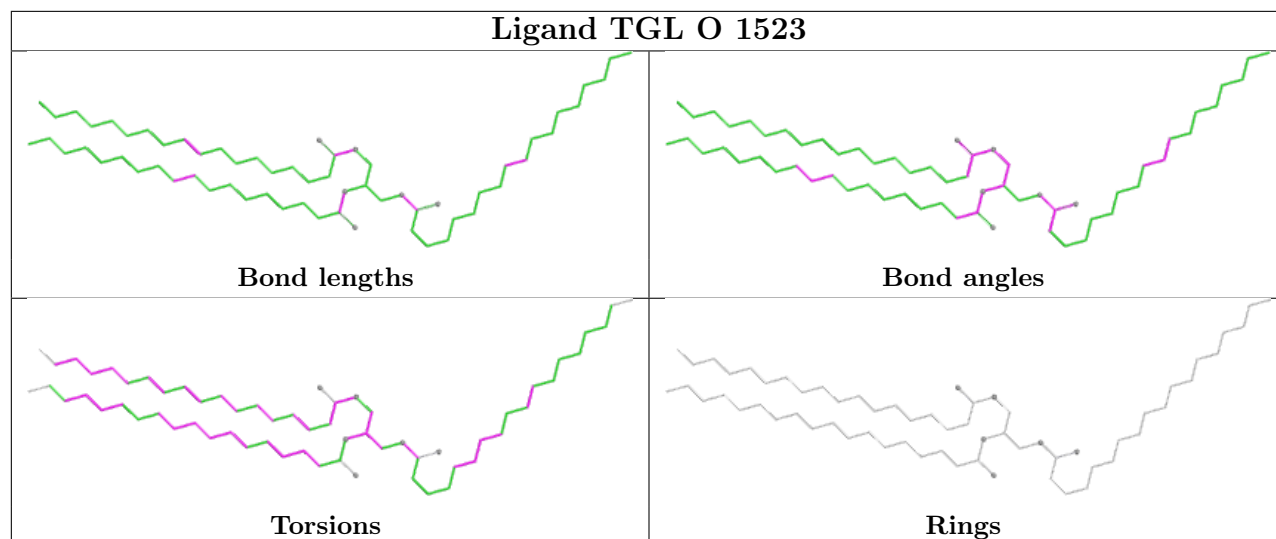
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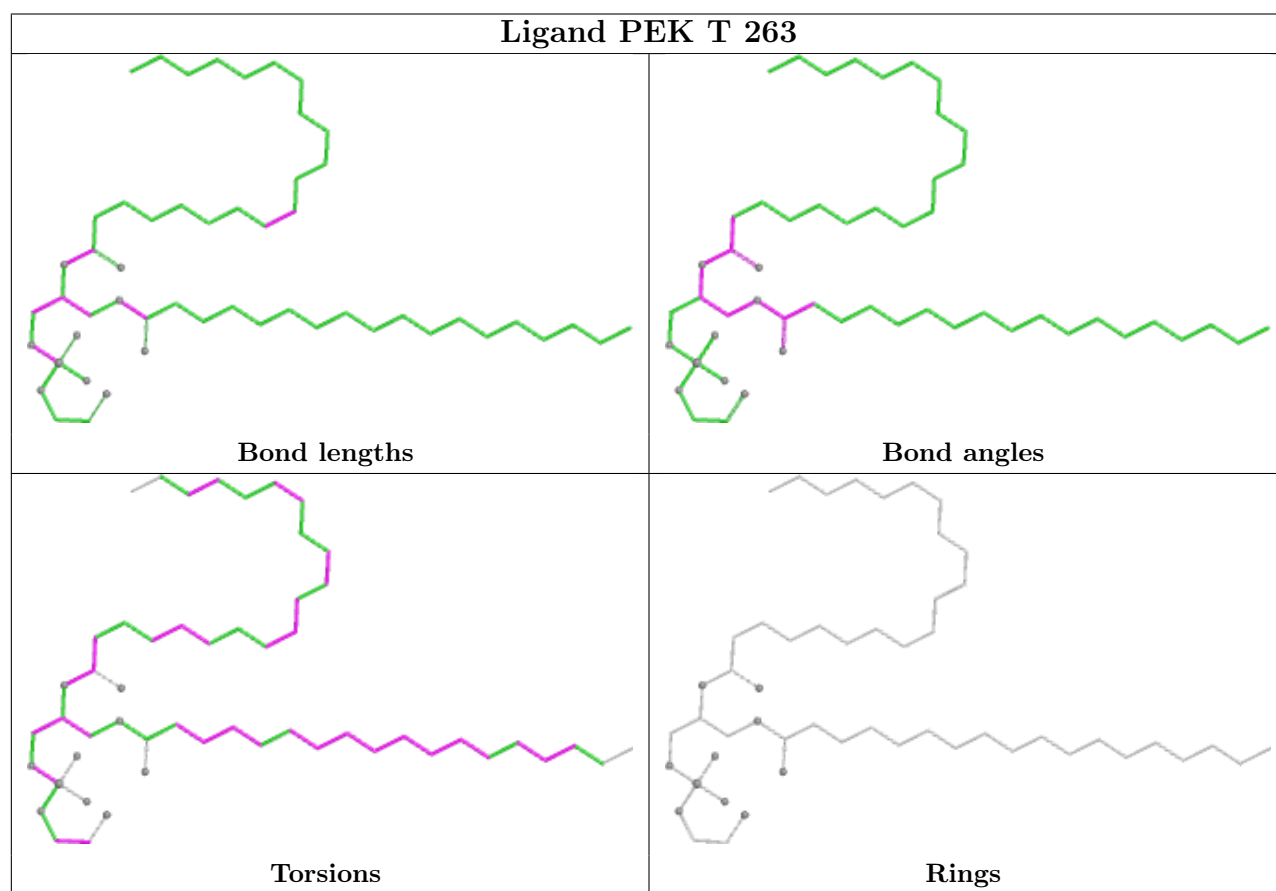
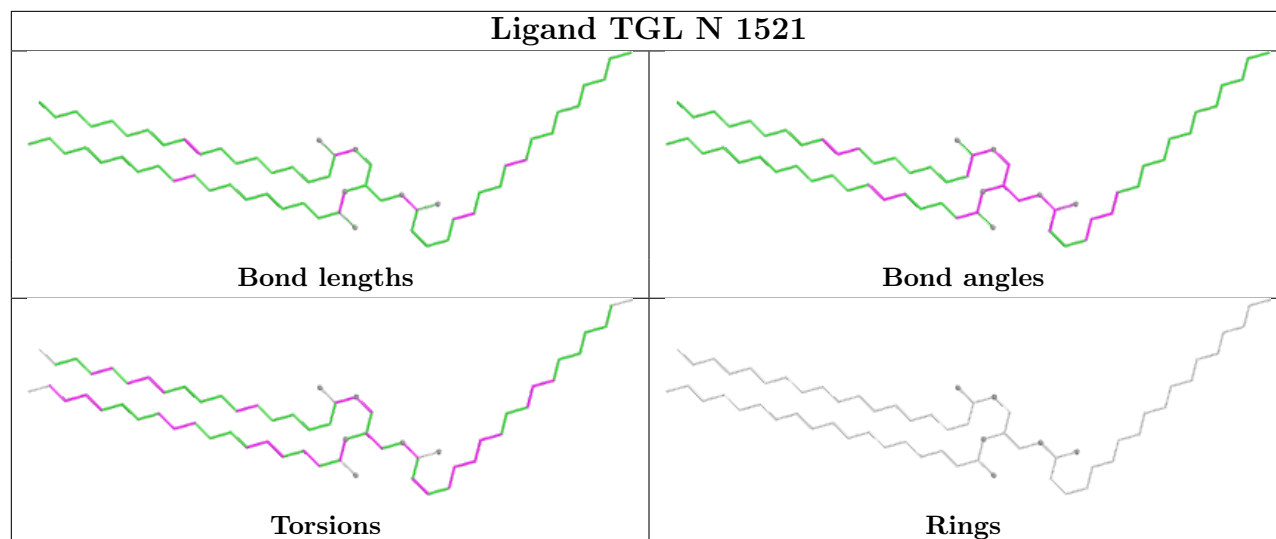
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	8	0
24	C	272	DMU	2	0
19	N	1524	PGV	9	0
19	N	1268	PGV	2	0
27	C	270	CDL	13	0
19	N	1266	PGV	2	0
21	D	523	TGL	5	0
27	T	1269	CDL	18	0
24	Z	1526	DMU	2	0
19	A	524	PGV	5	0
24	P	1272	DMU	3	0
27	G	269	CDL	17	0
18	A	516	HEA	4	0
19	C	267	PGV	3	0
21	L	522	TGL	13	0
21	N	1522	TGL	19	0
23	G	86	CHD	2	0
27	P	1270	CDL	9	0
19	C	268	PGV	2	0
26	P	1264	PEK	5	0
22	B	230	PSC	13	0
15	N	520	PER	1	0
26	C	265	PEK	4	0
23	P	1525	CHD	2	0
22	O	1230	PSC	12	0

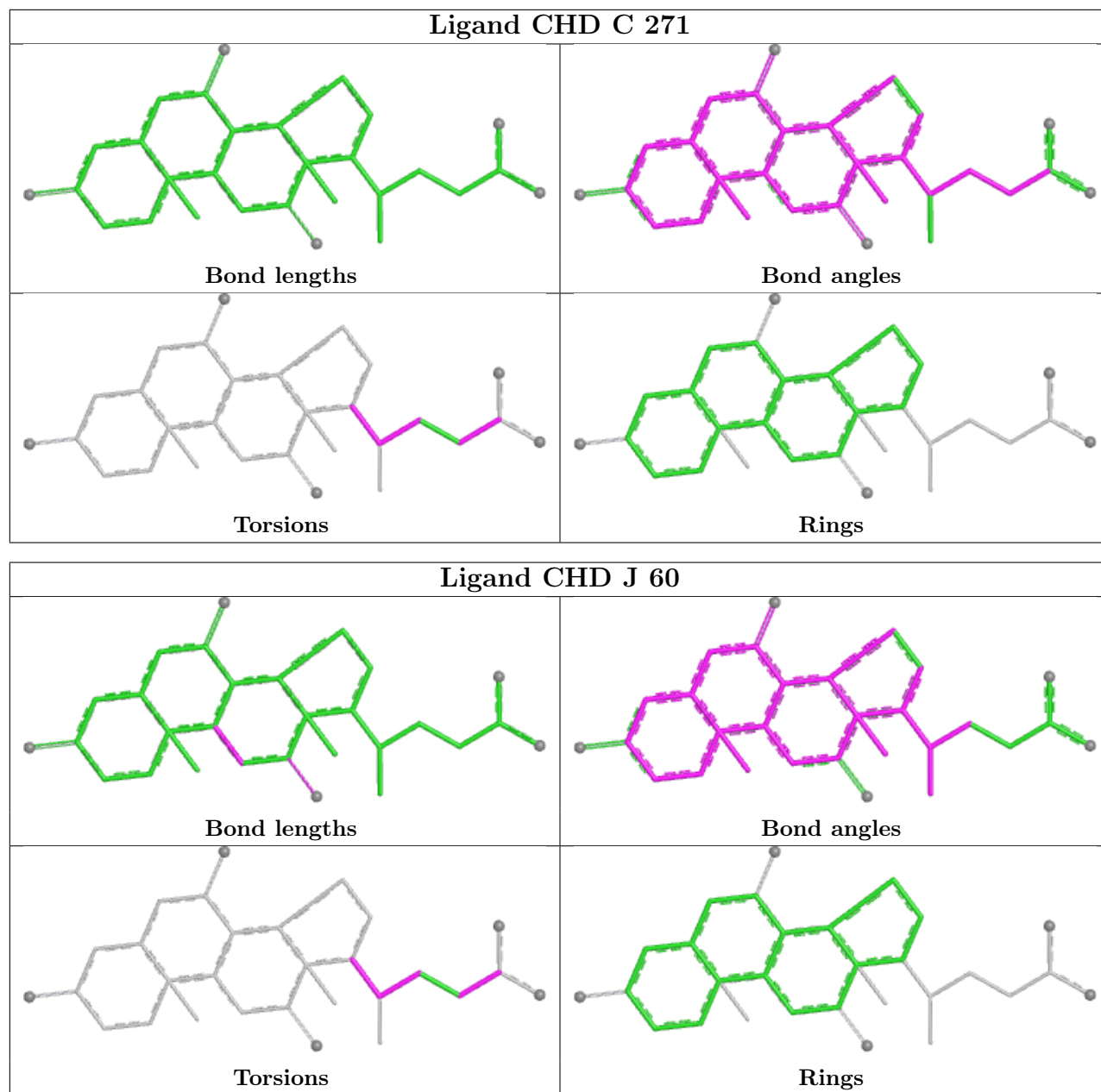
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



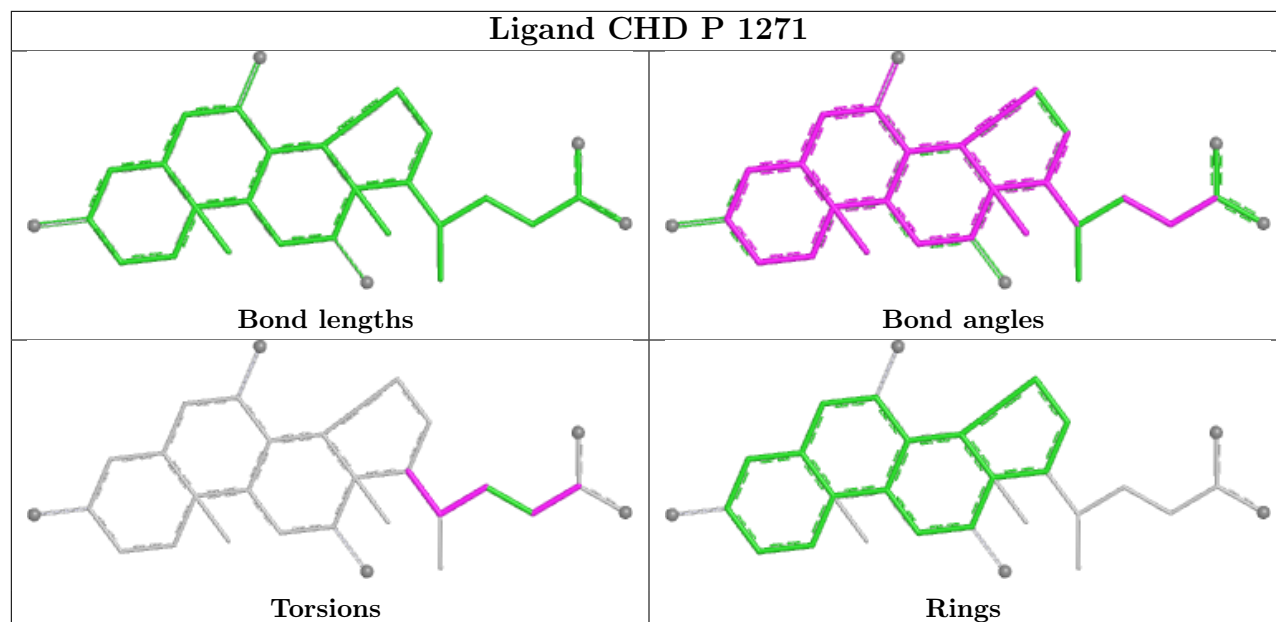




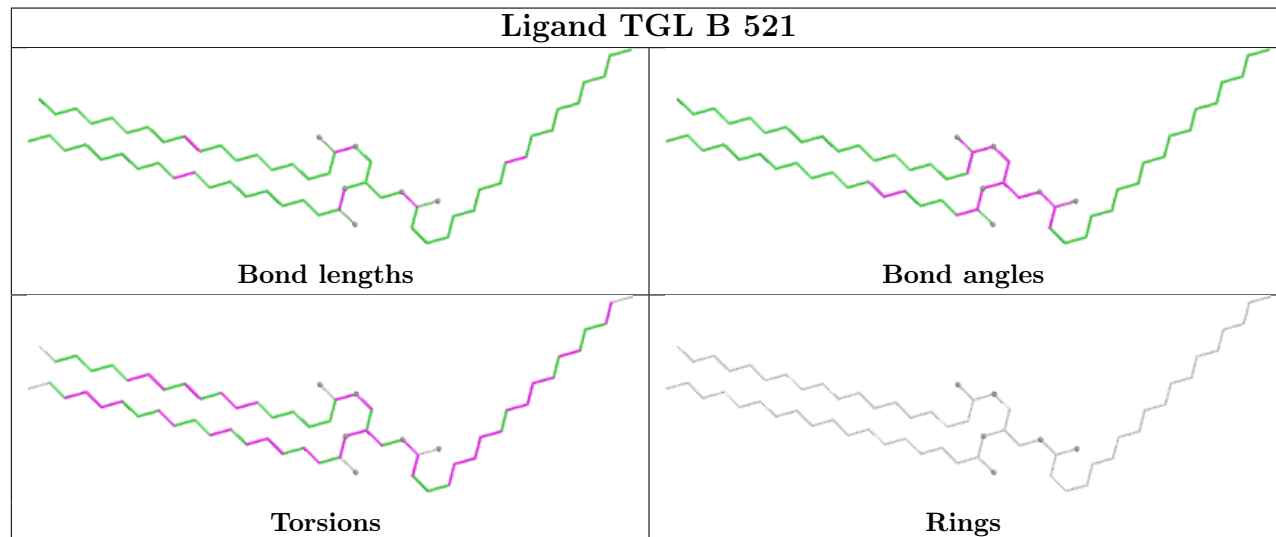




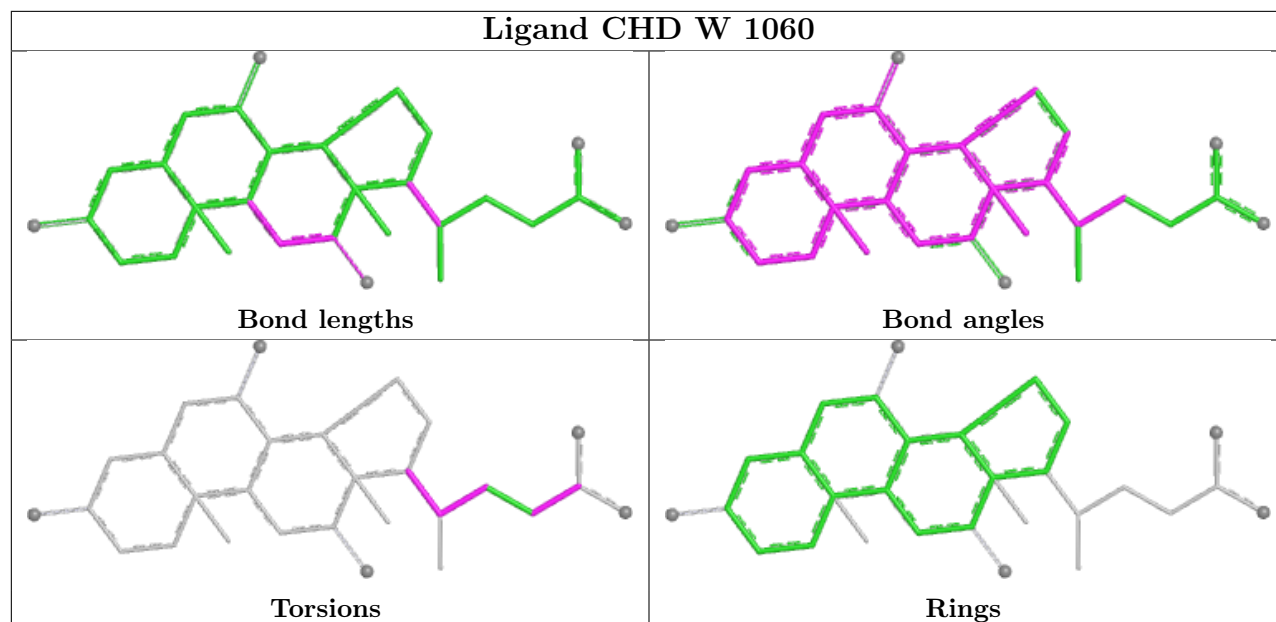
Ligand CHD P 1271



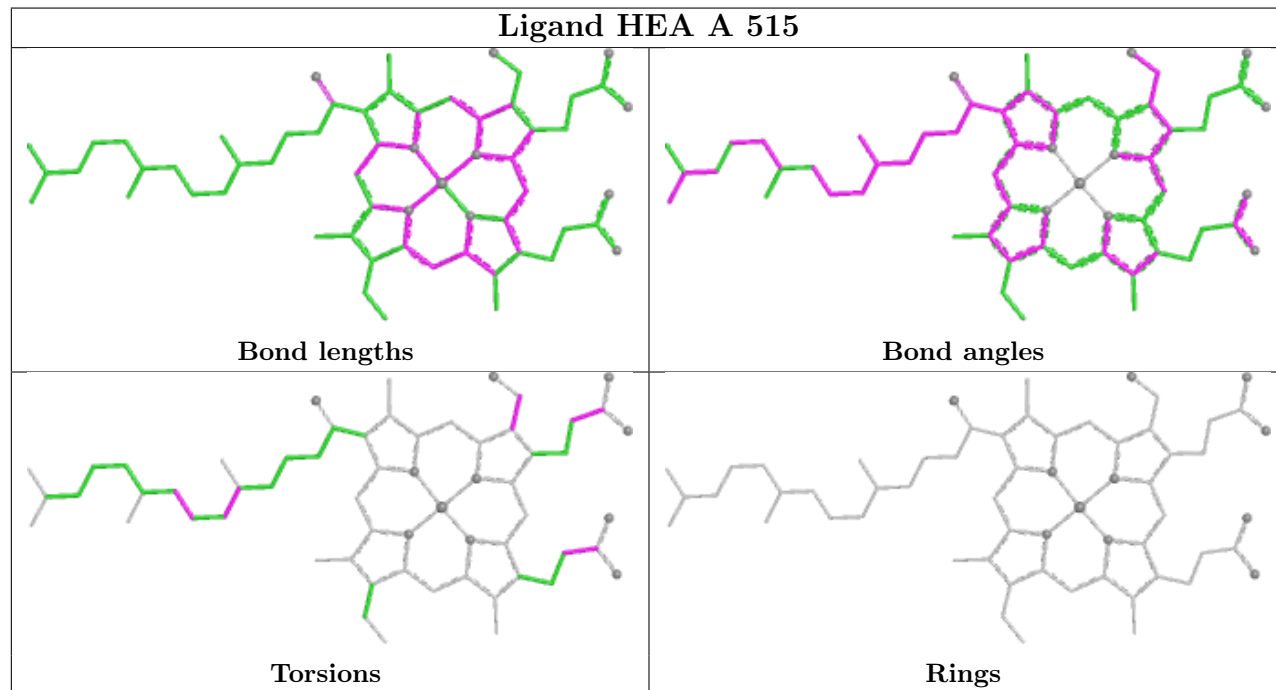
Ligand TGL B 521



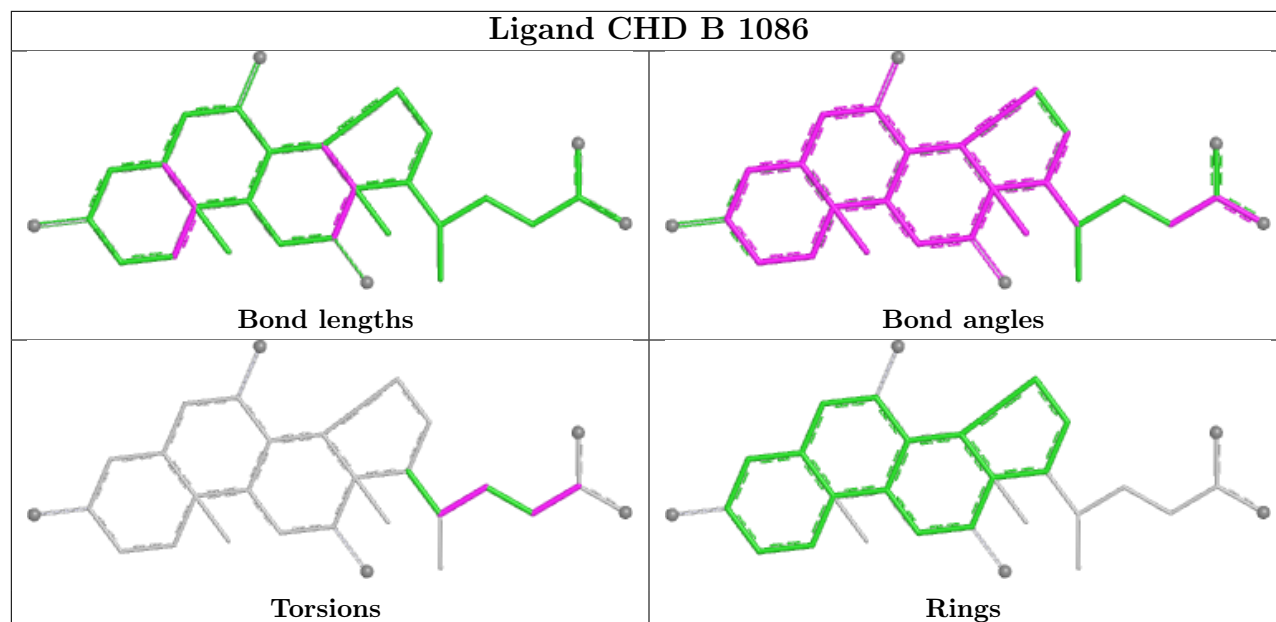
Ligand CHD W 1060



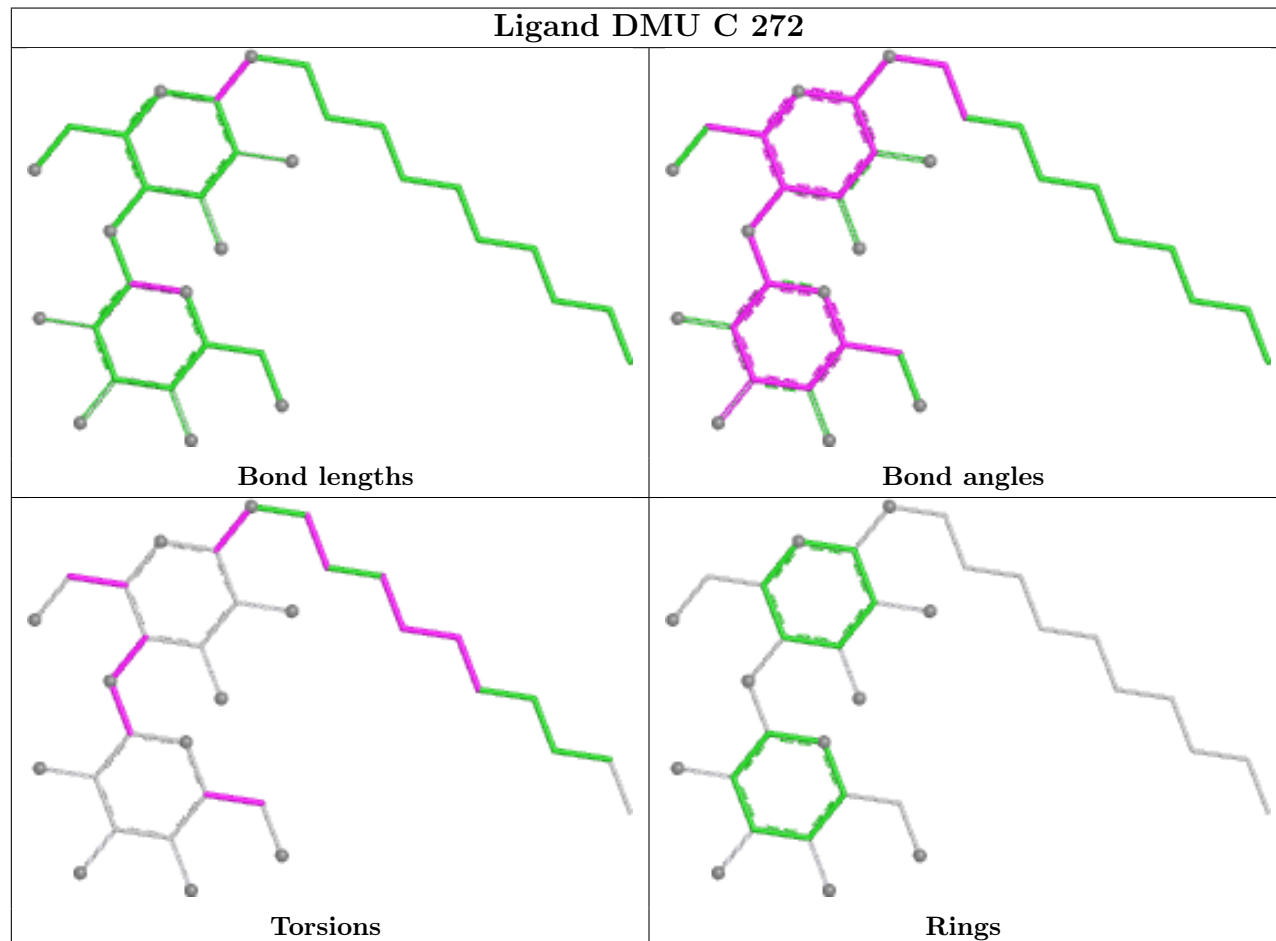
Ligand HEA A 515



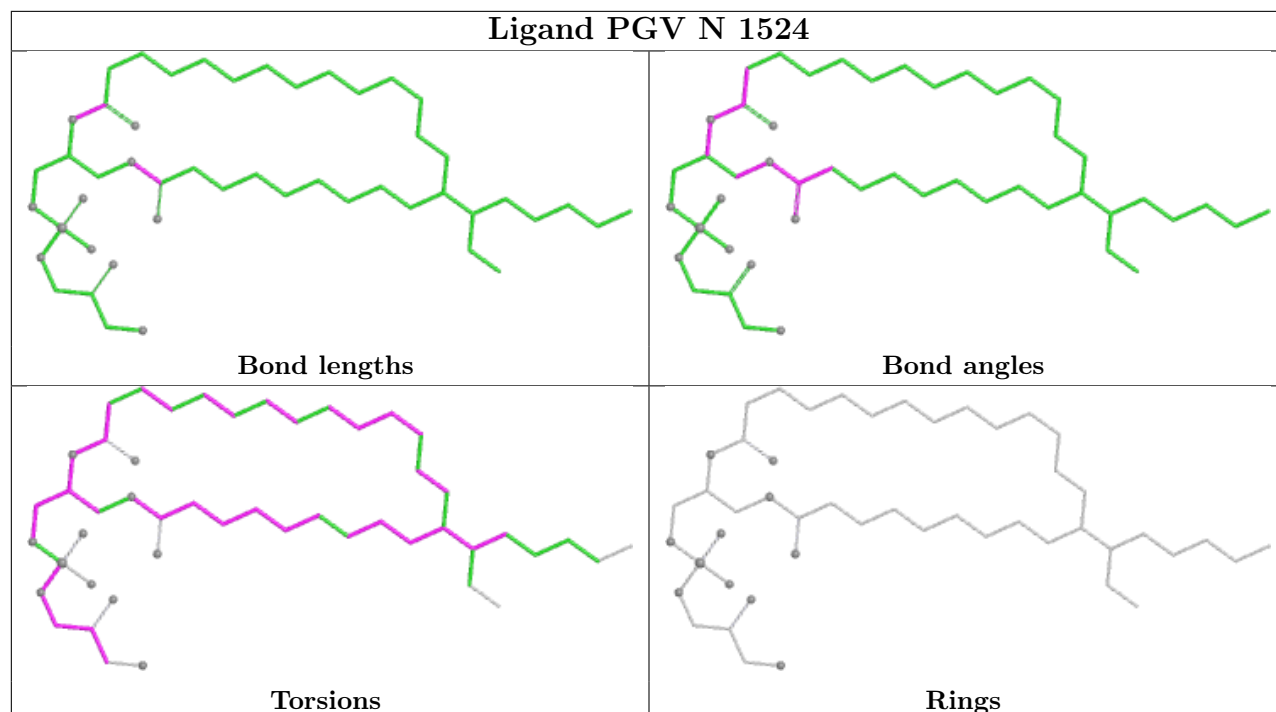
Ligand CHD B 1086



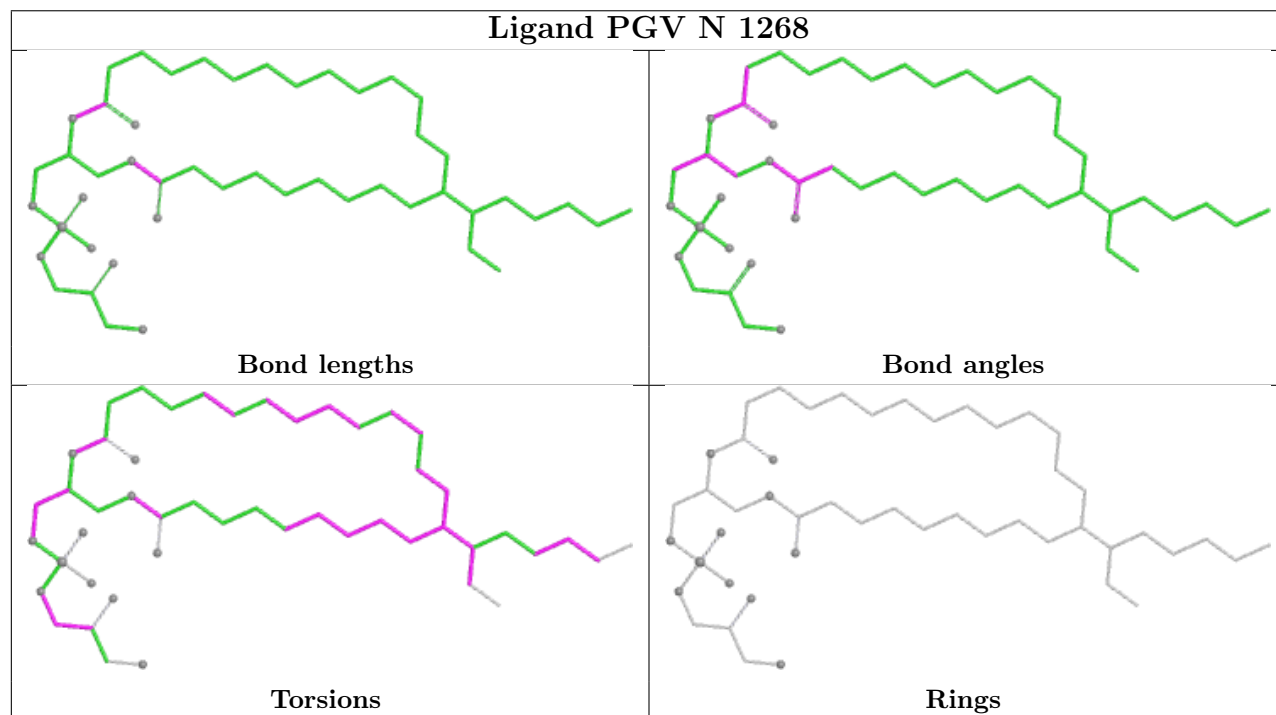
Ligand DMU C 272

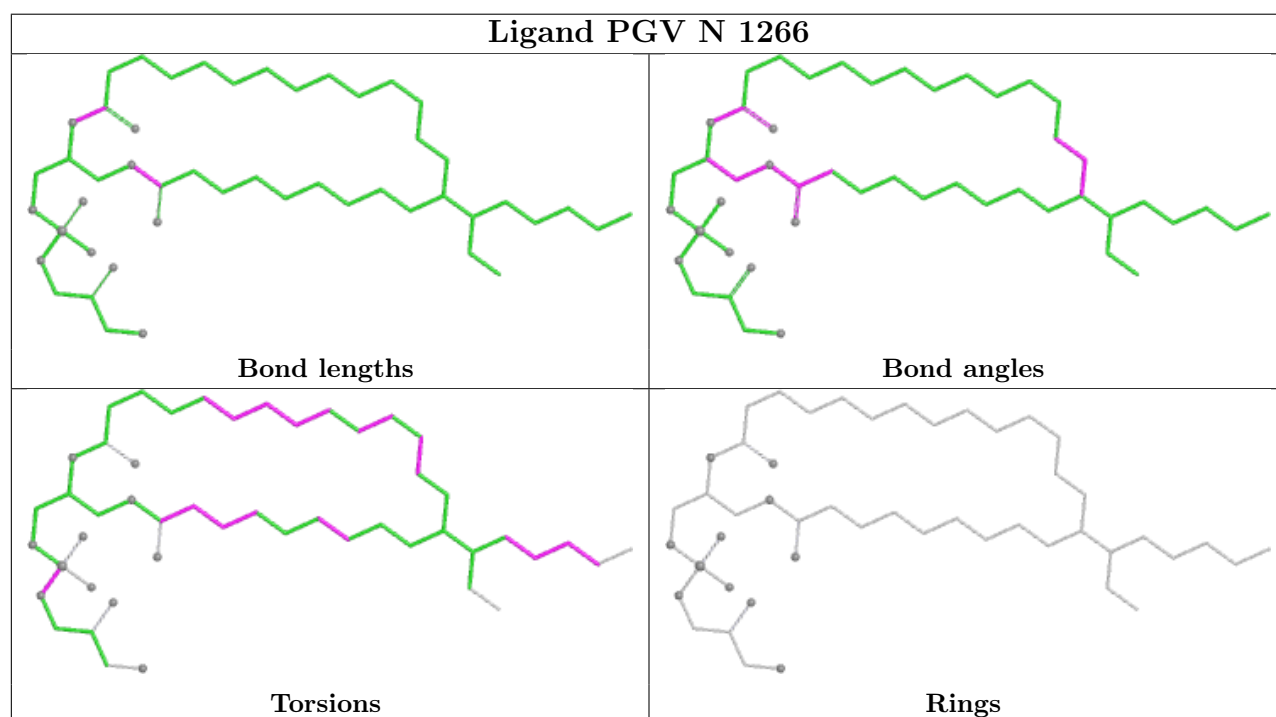
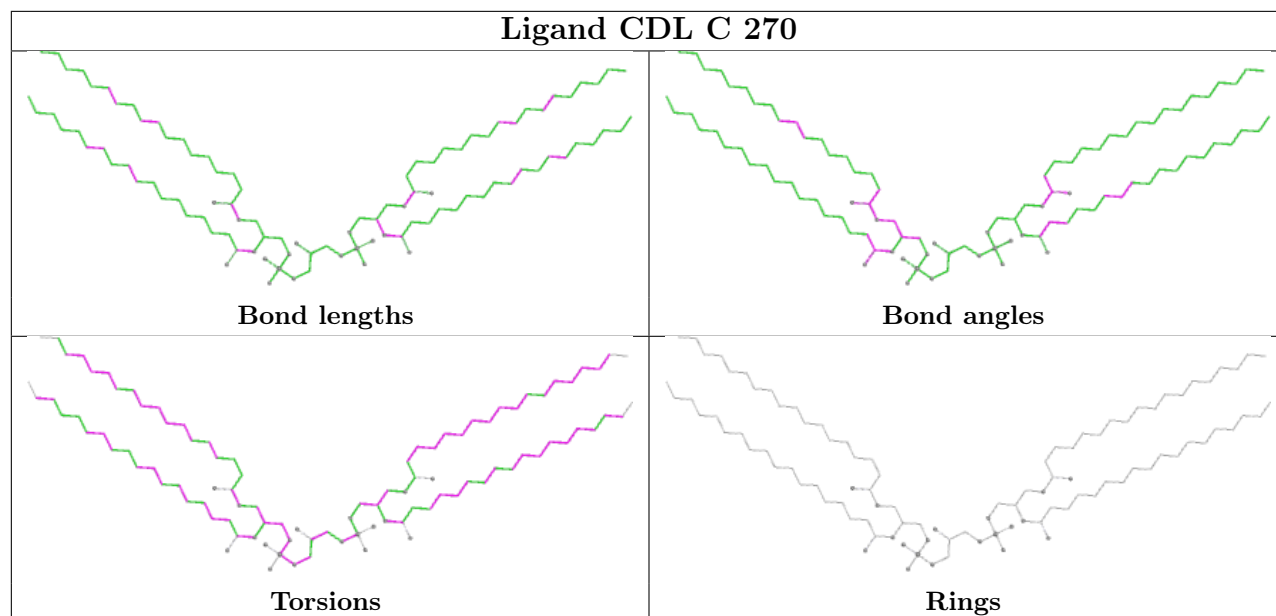


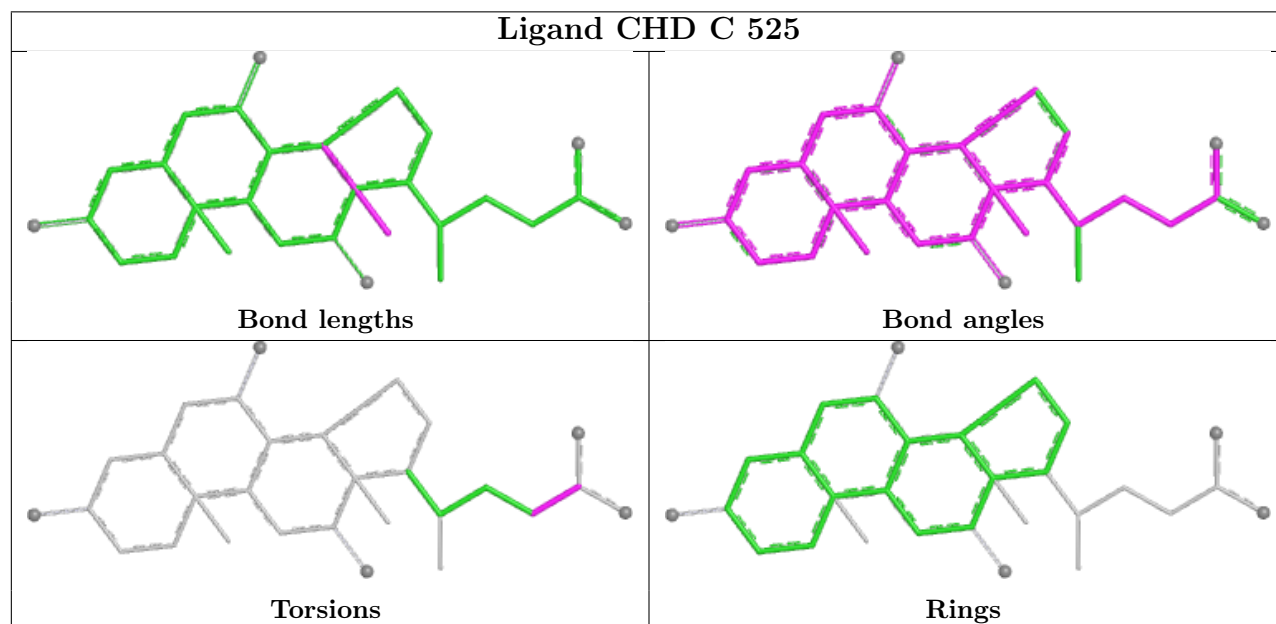
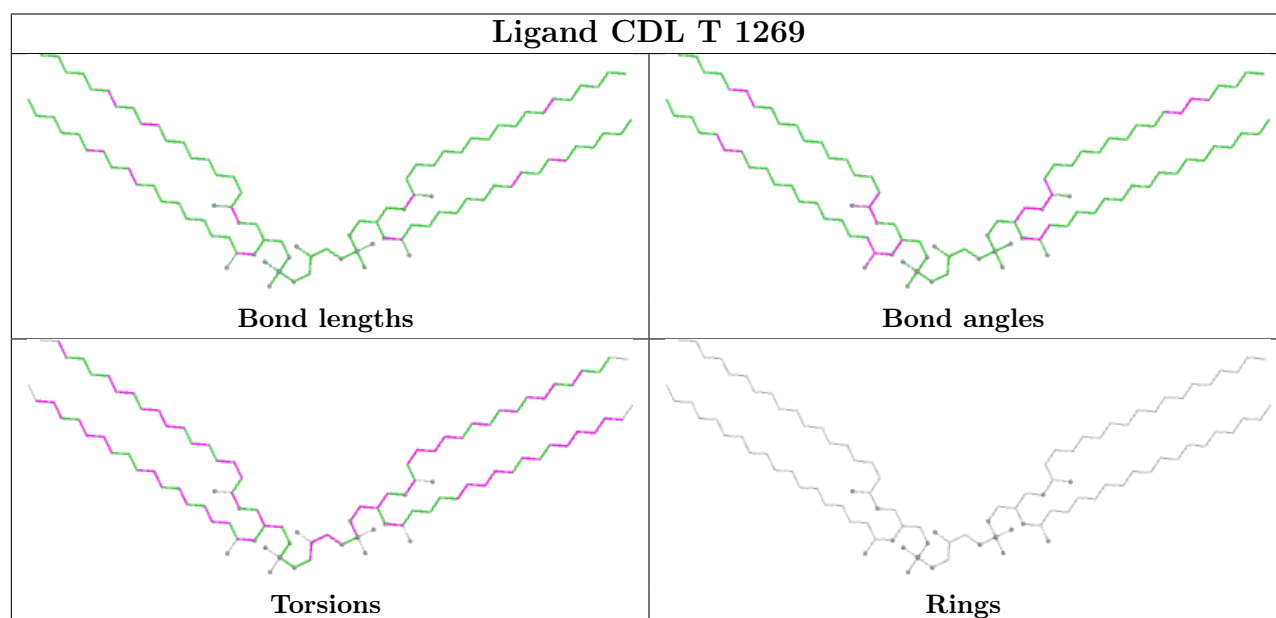
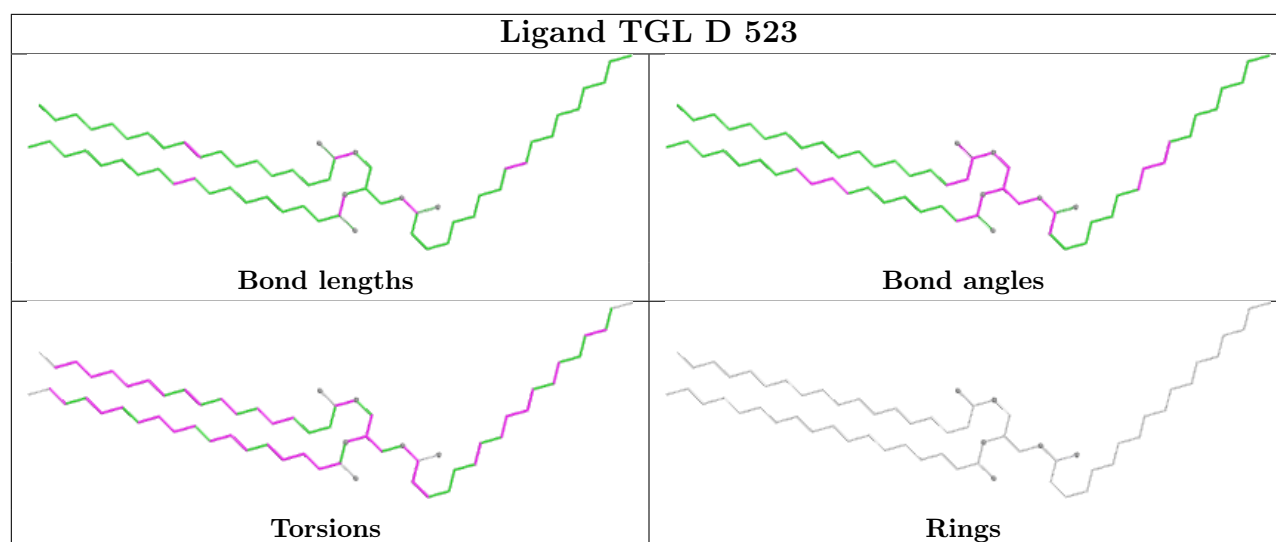
Ligand PGV N 1524



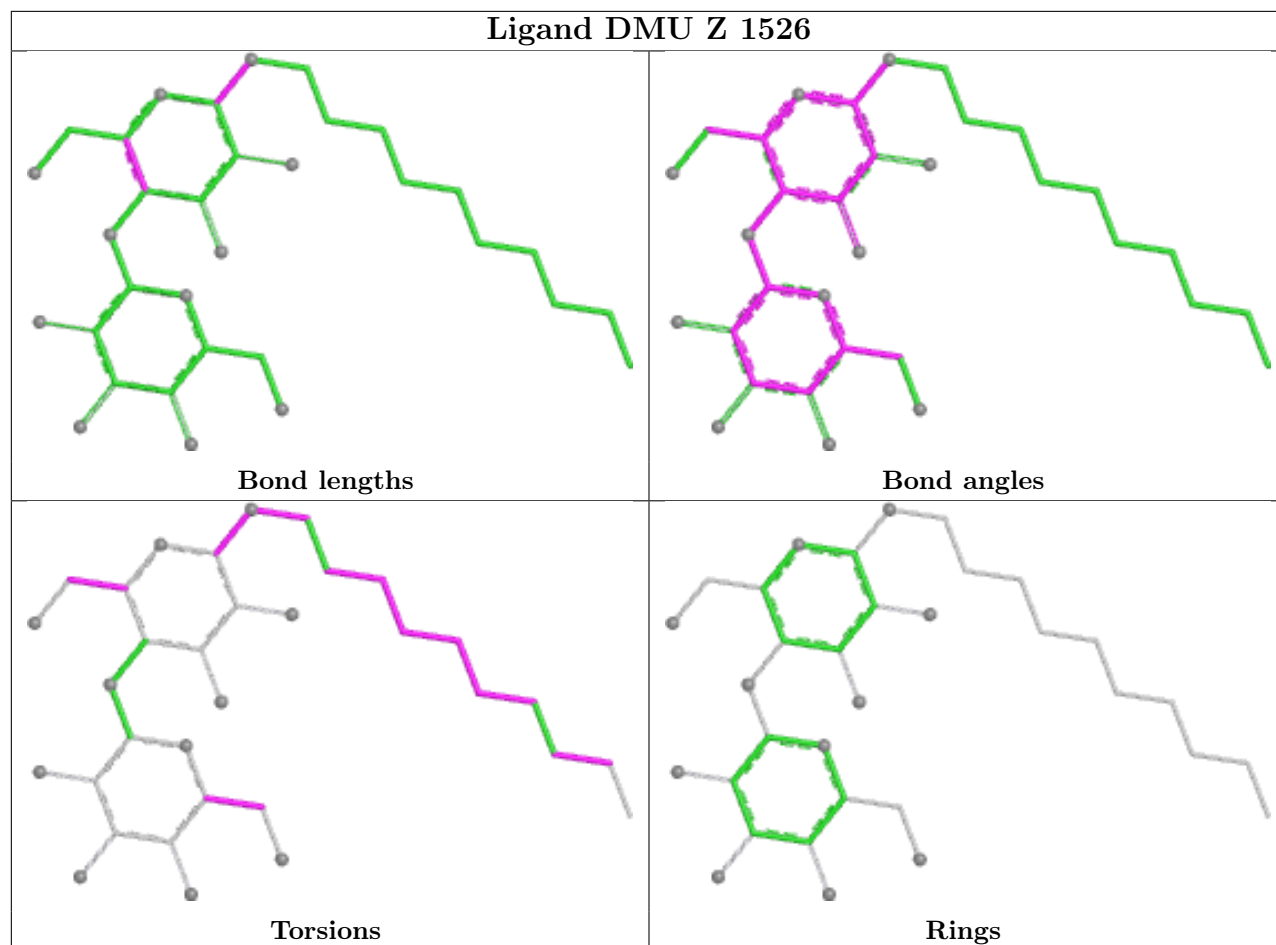
Ligand PGV N 1268



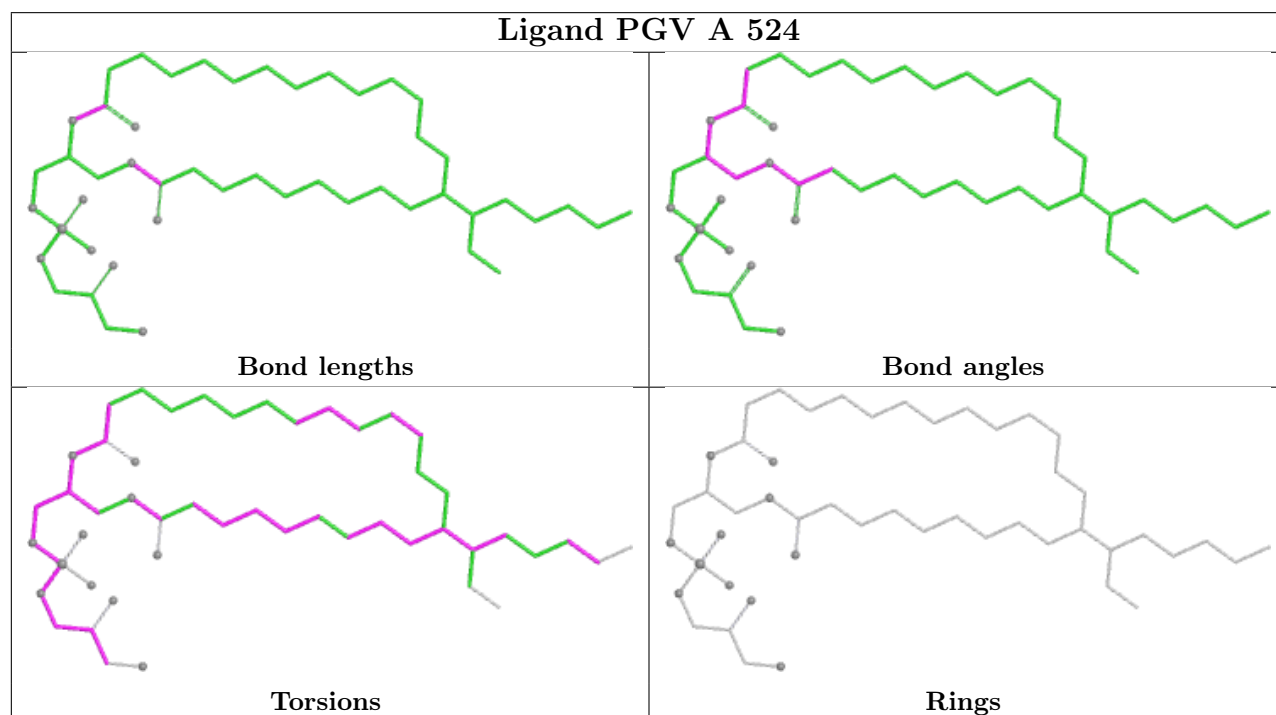




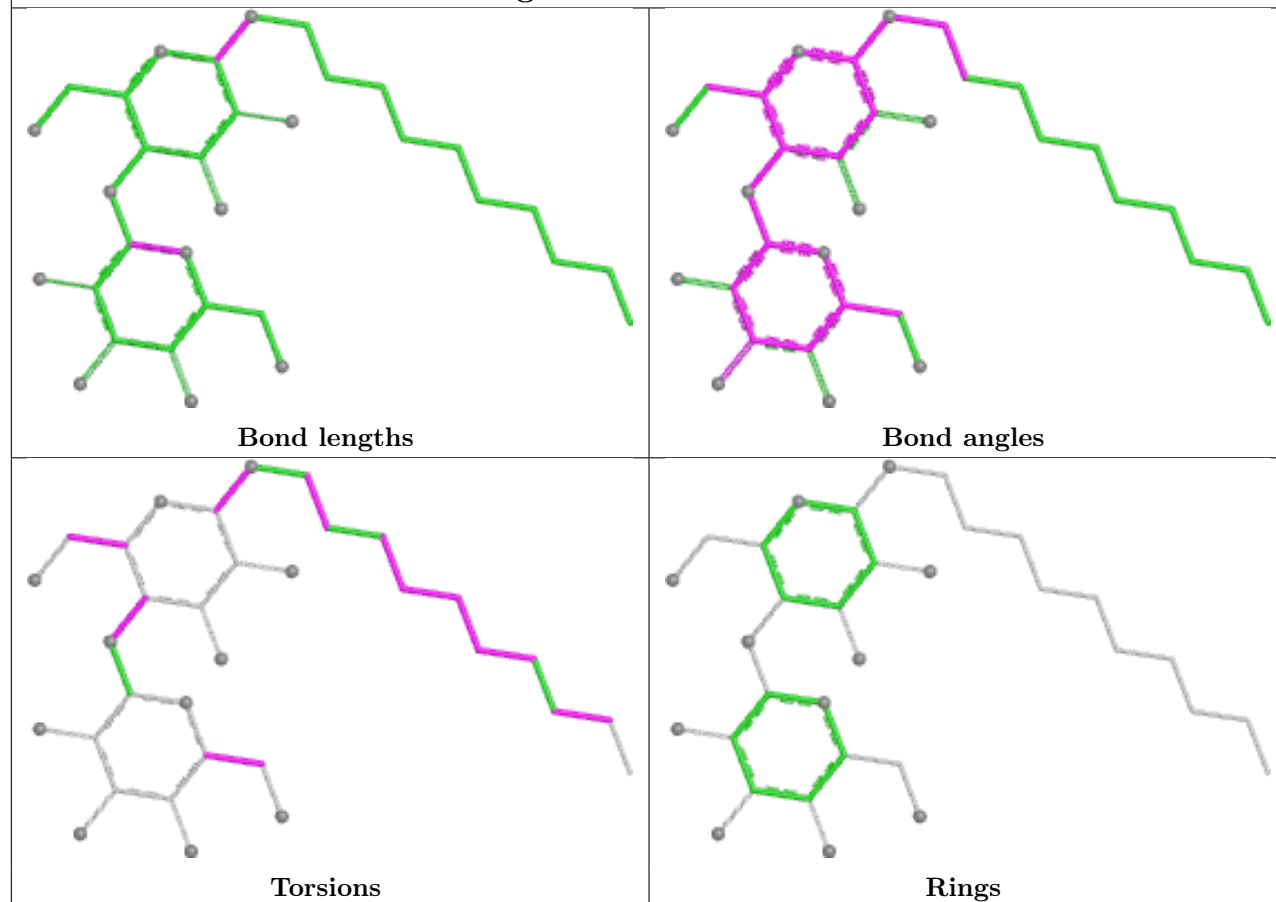
Ligand DMU Z 1526



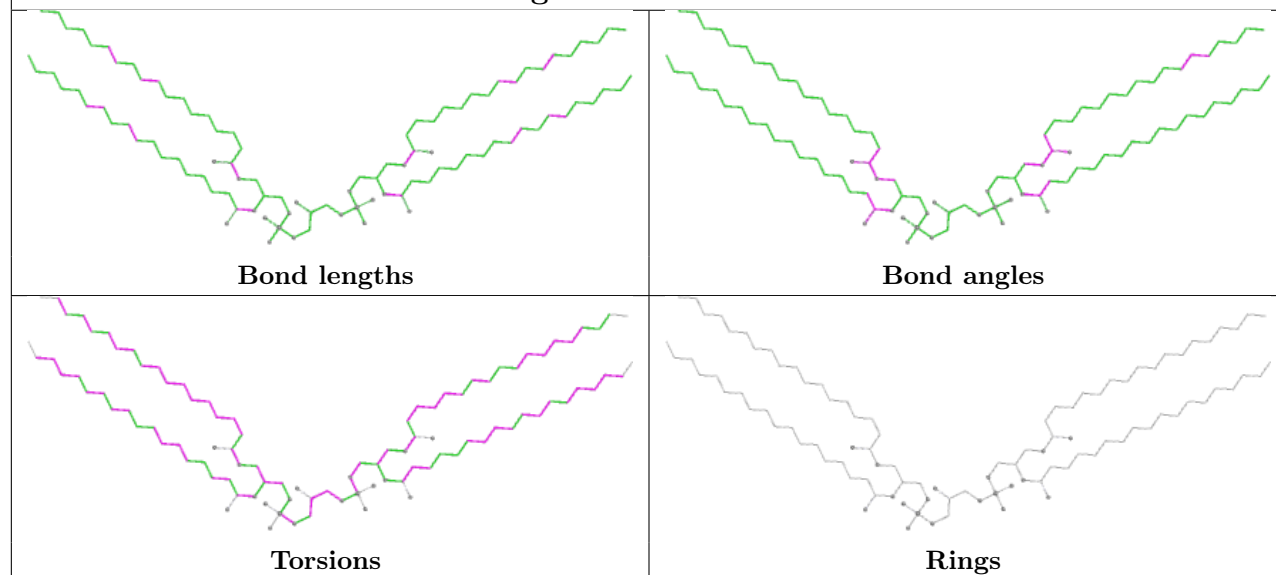
Ligand PGV A 524

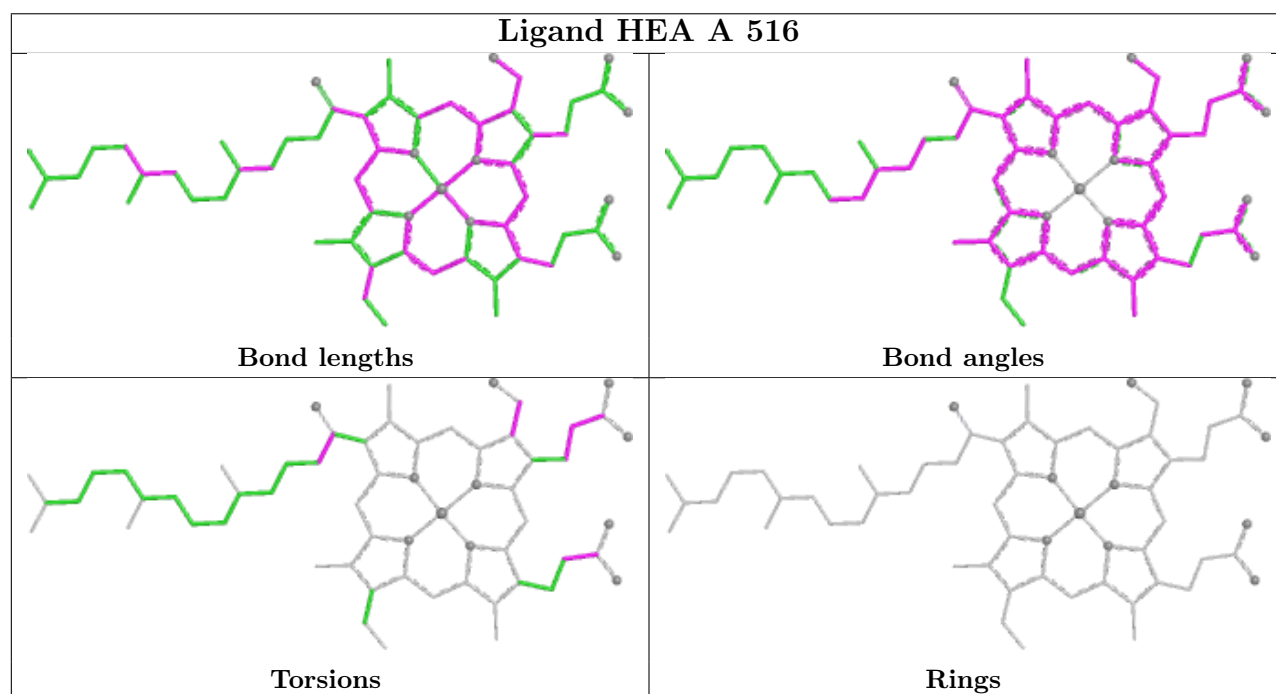
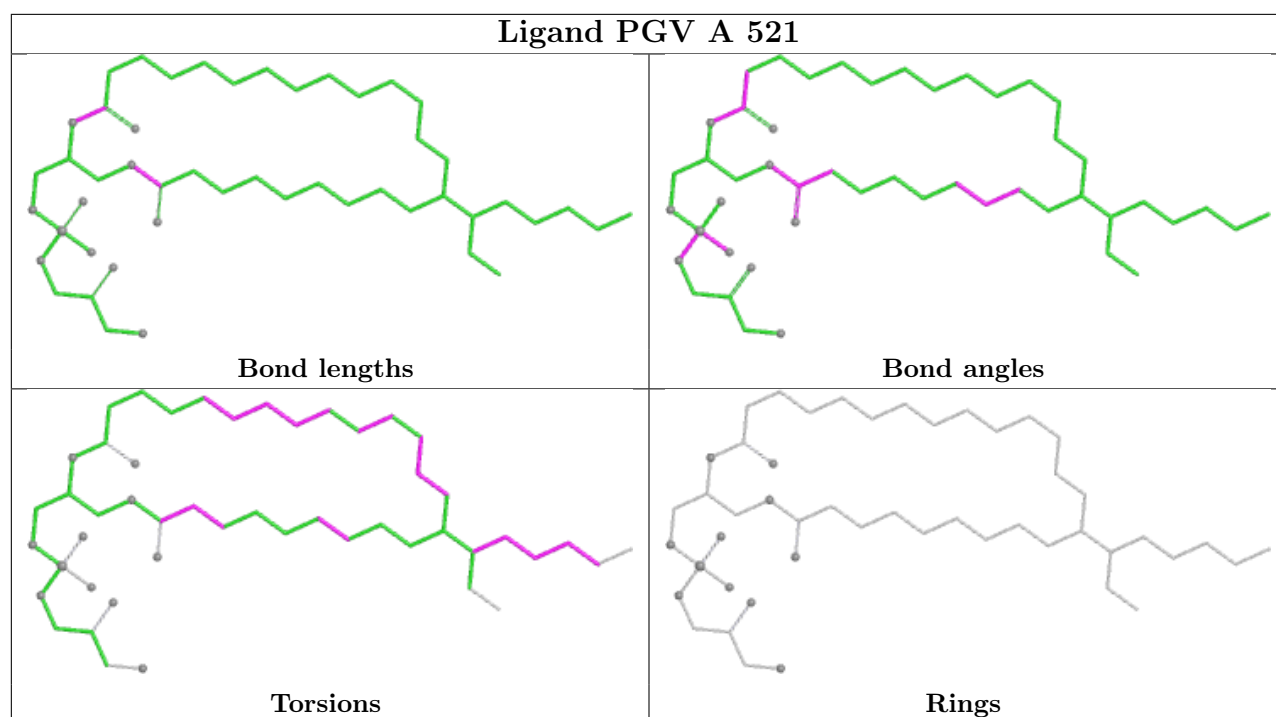


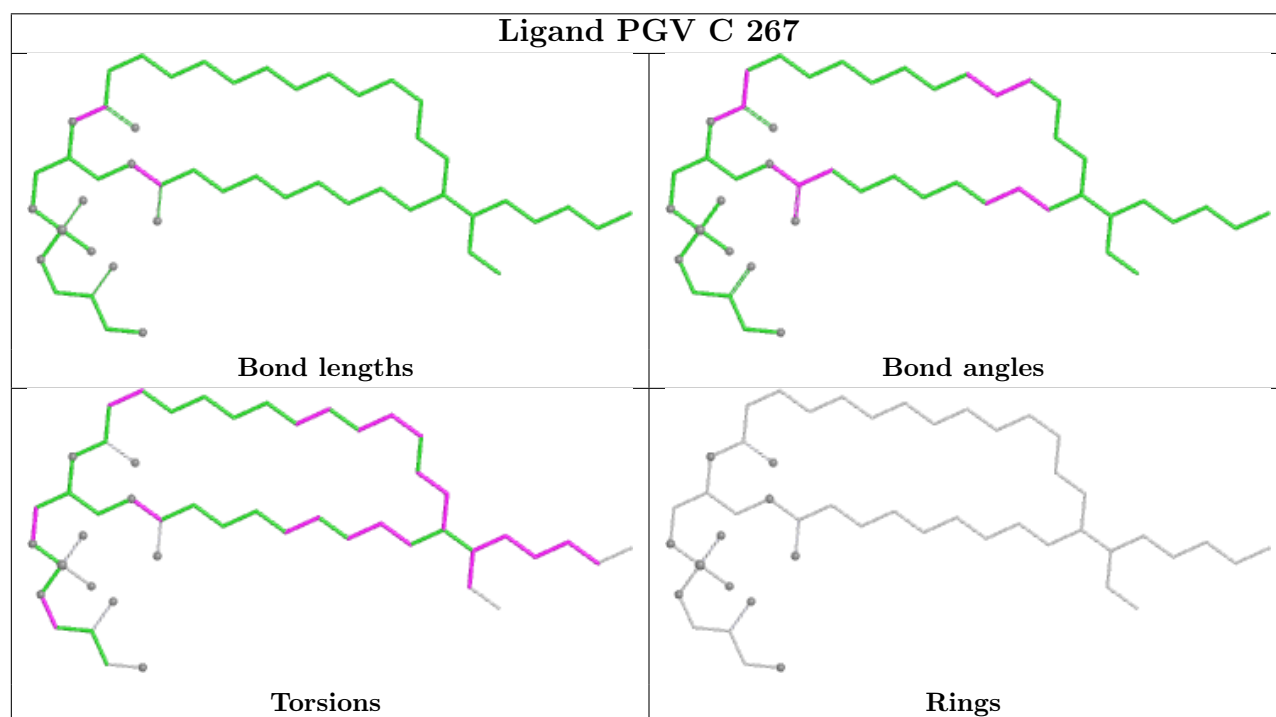
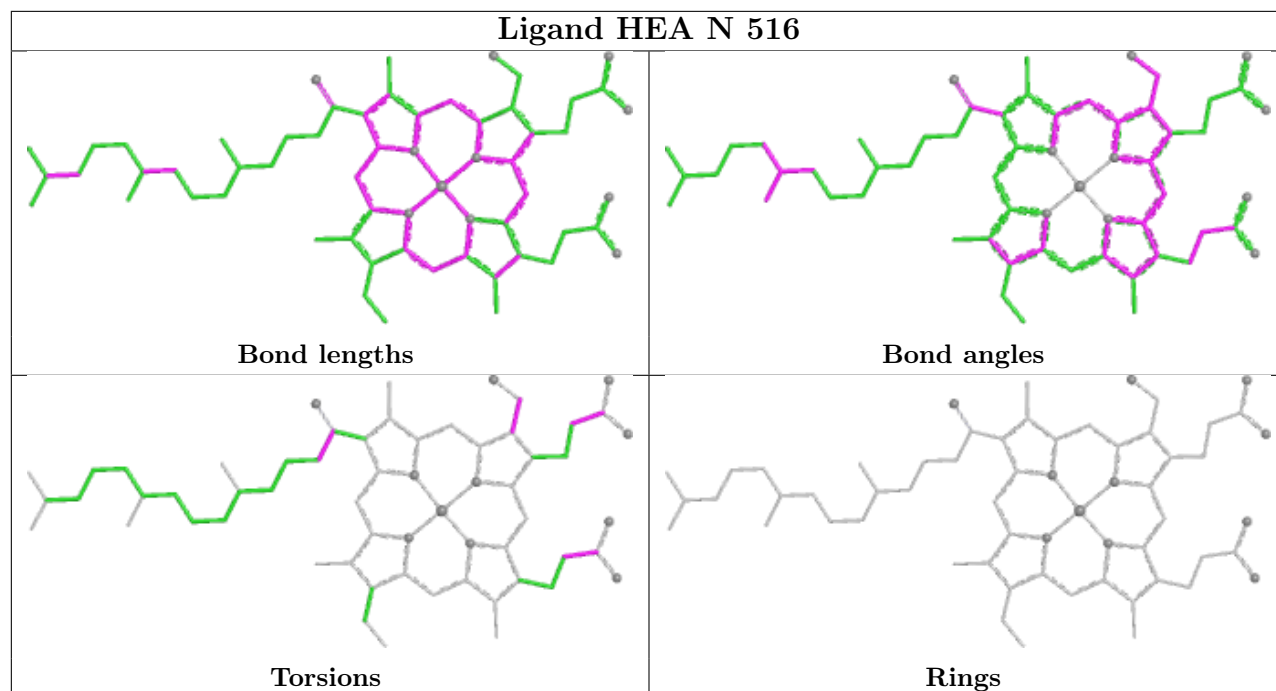
Ligand DMU P 1272

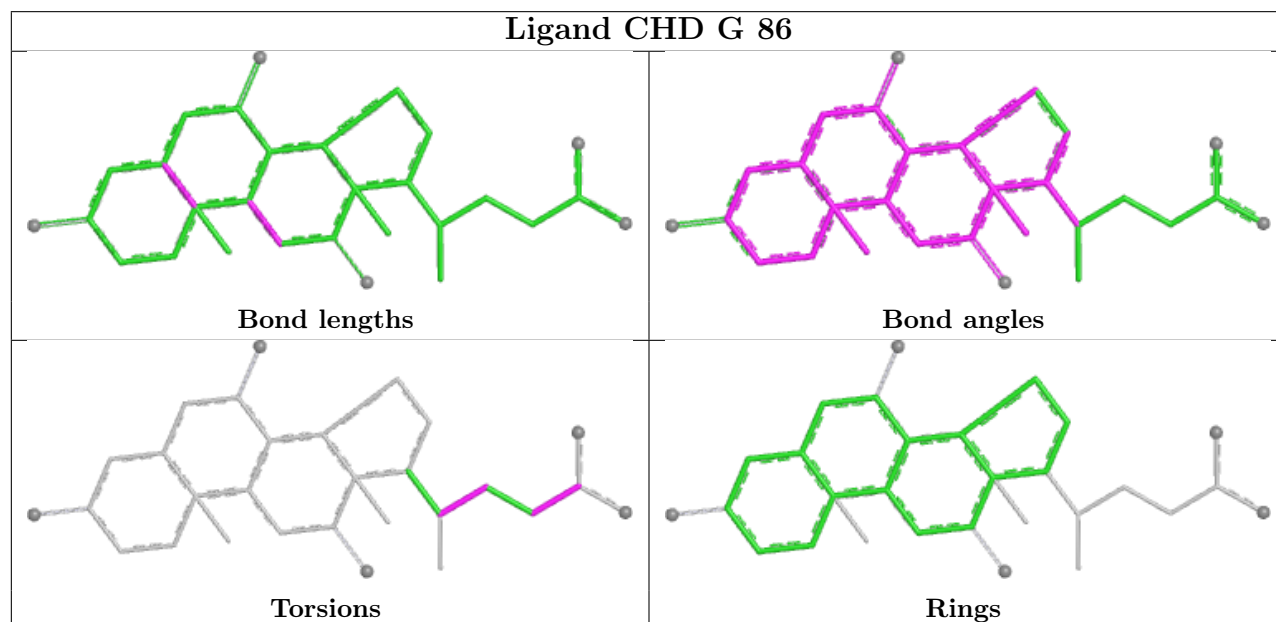
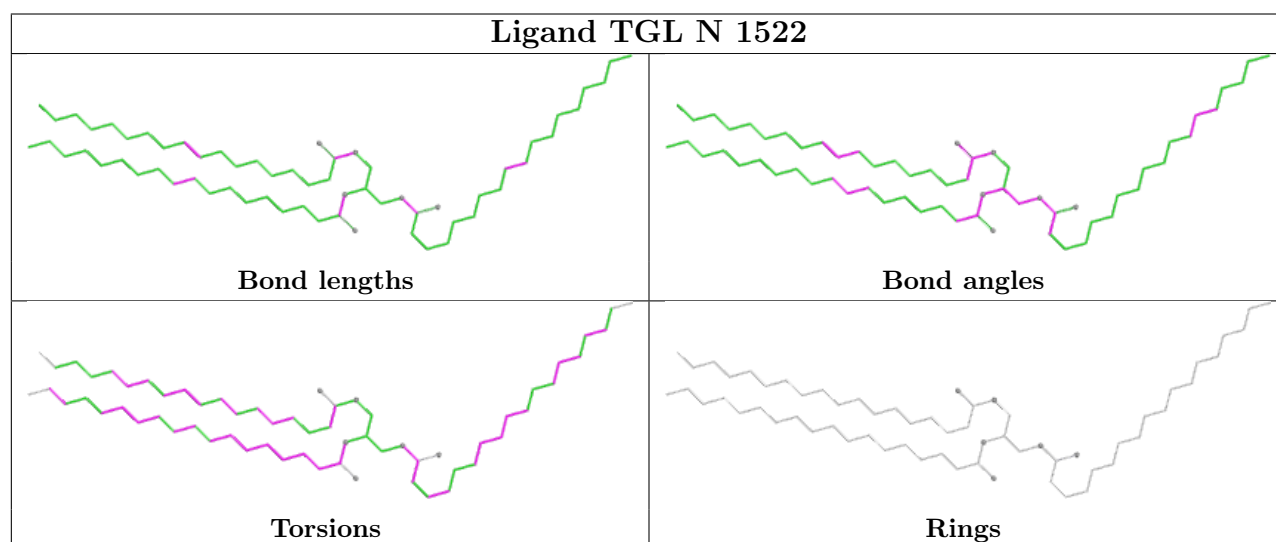
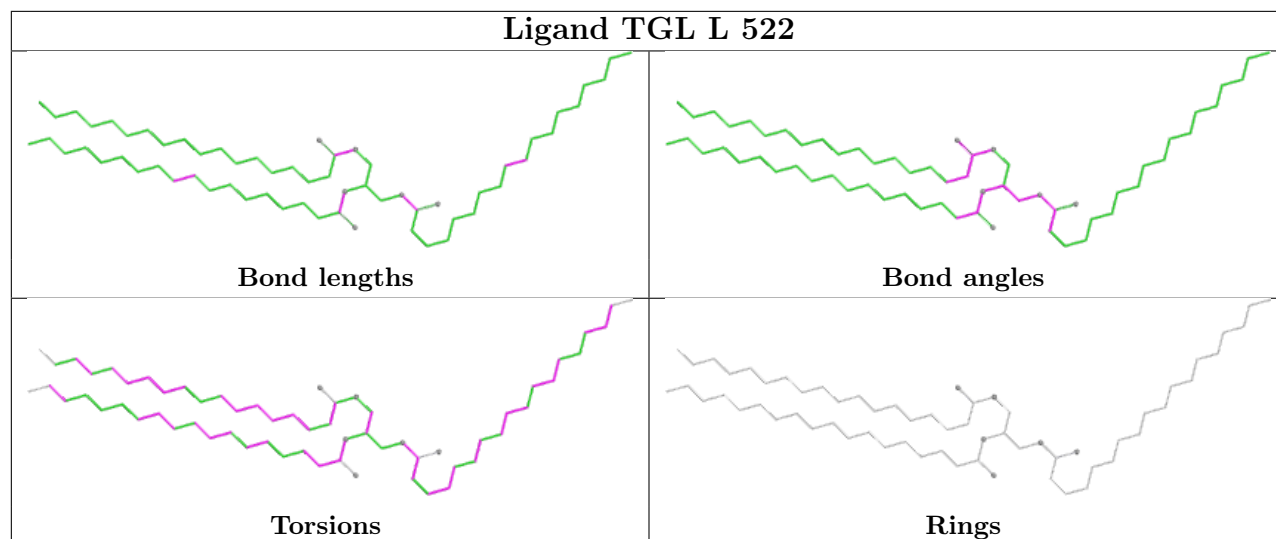


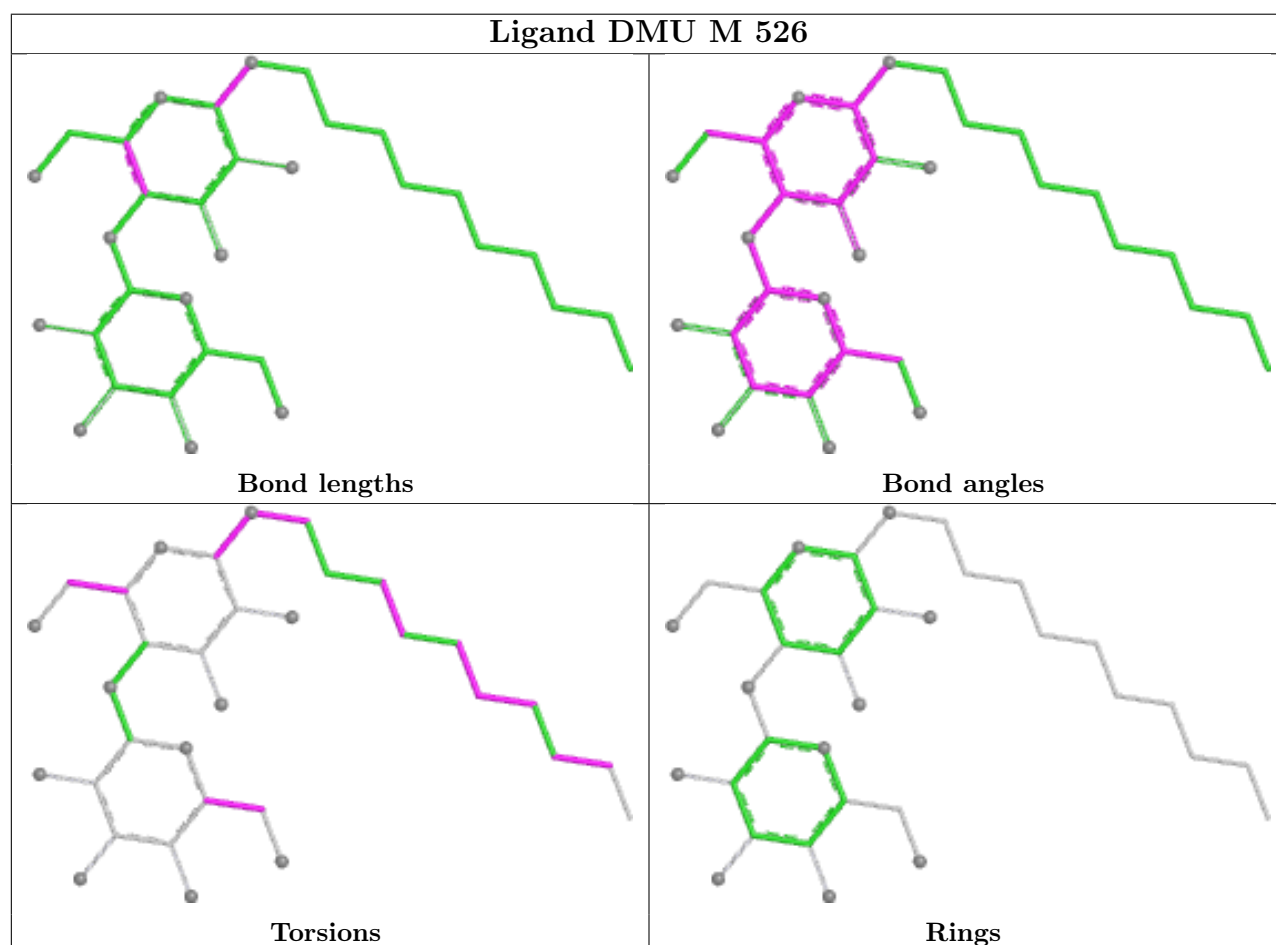
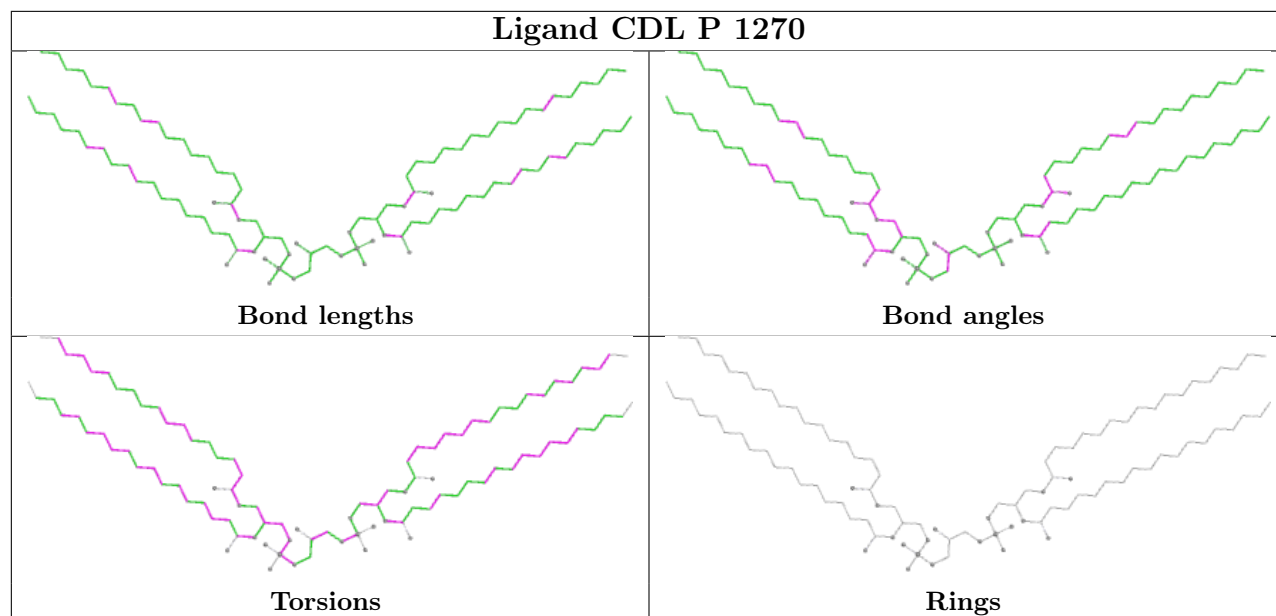
Ligand CDL G 269

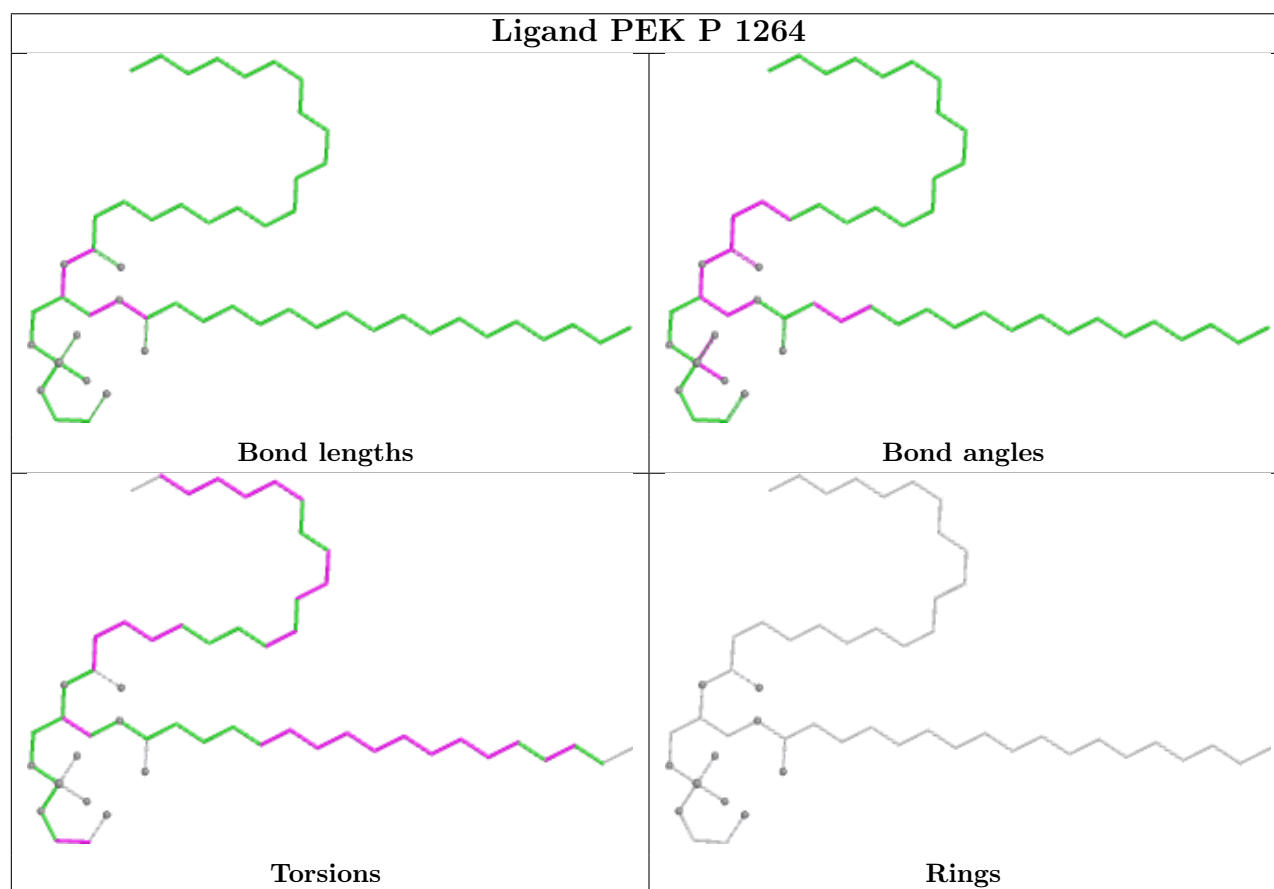
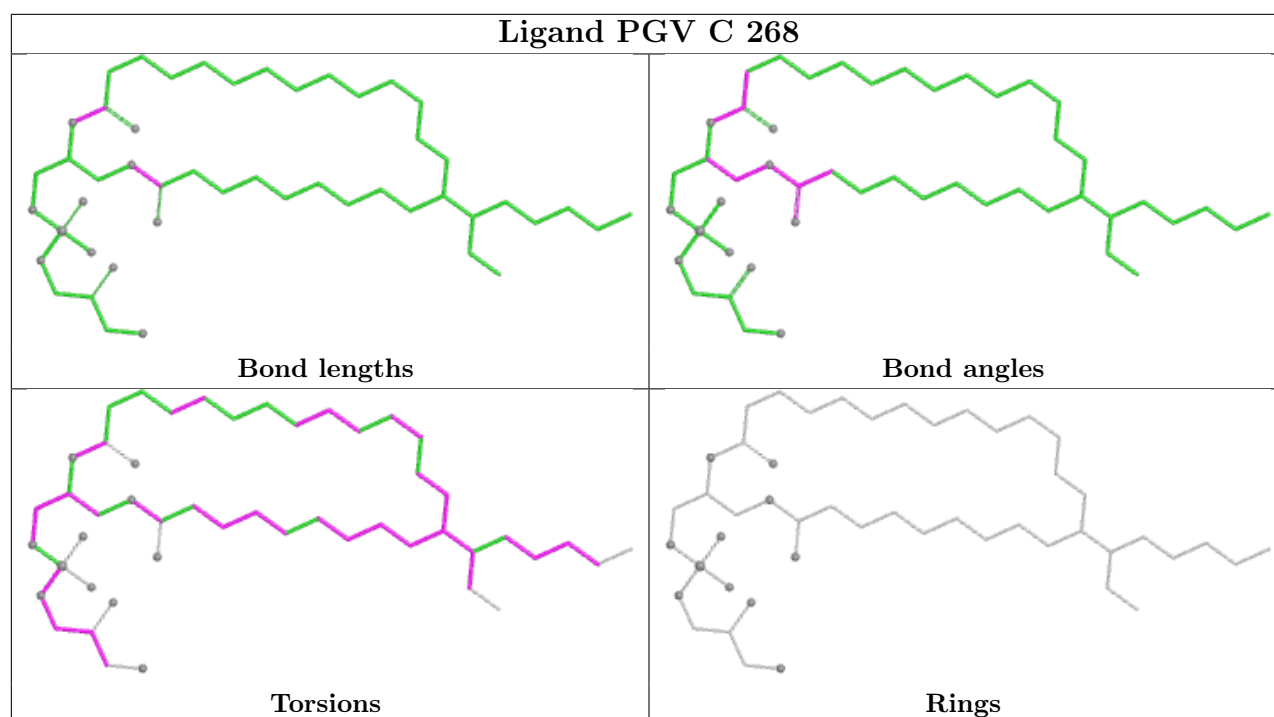




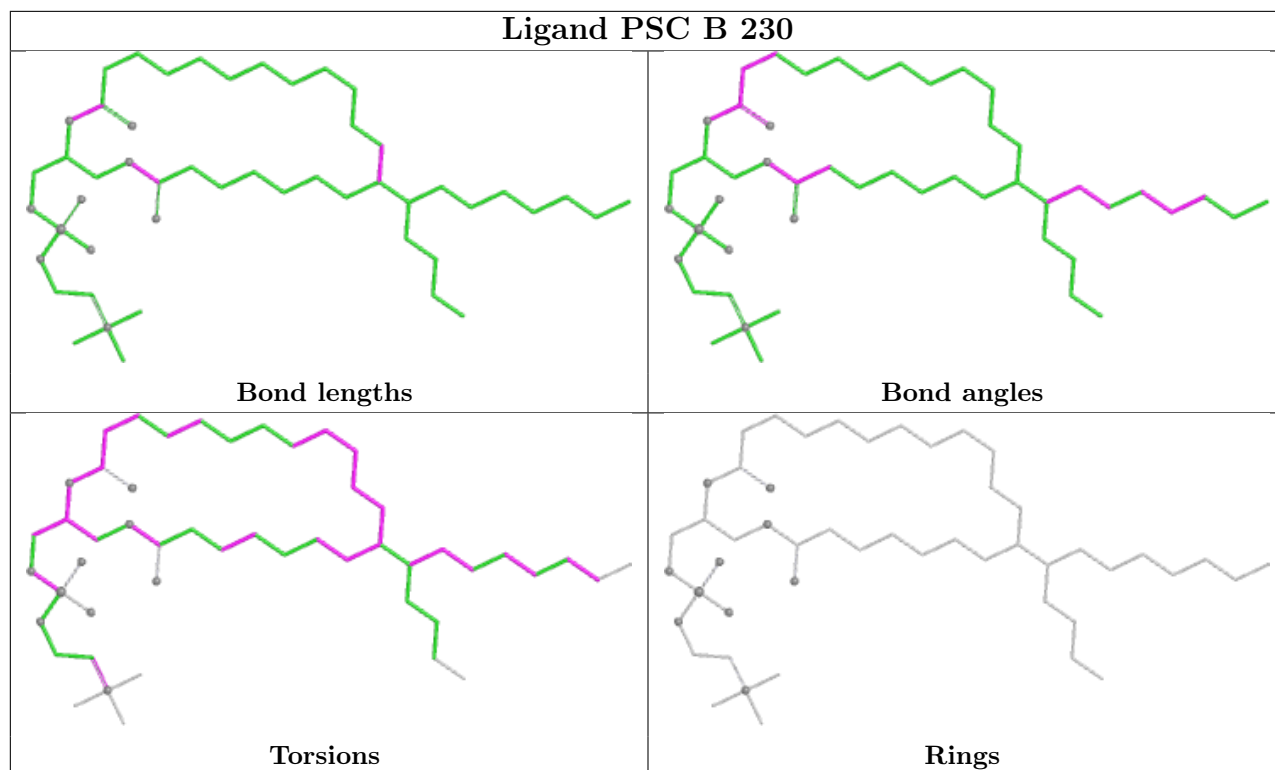




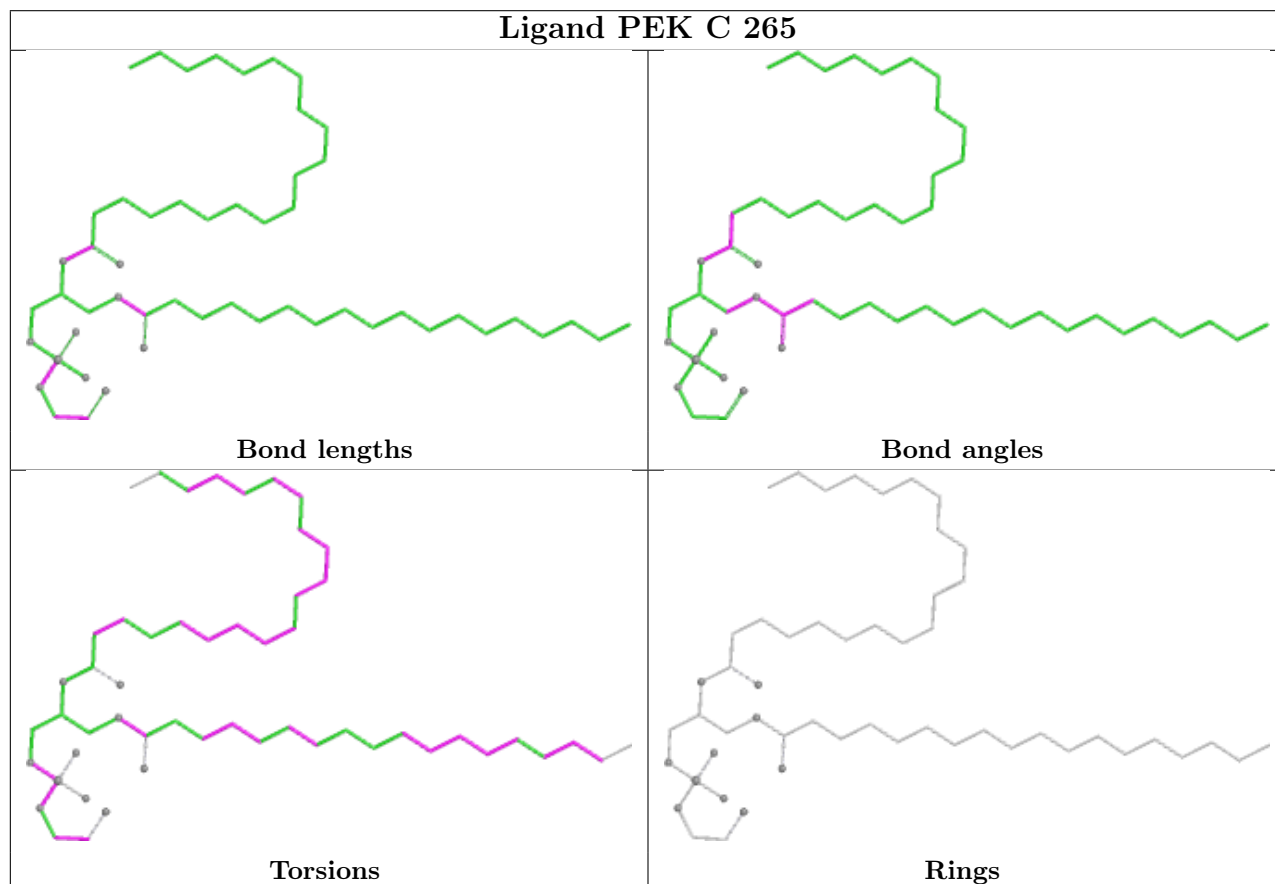


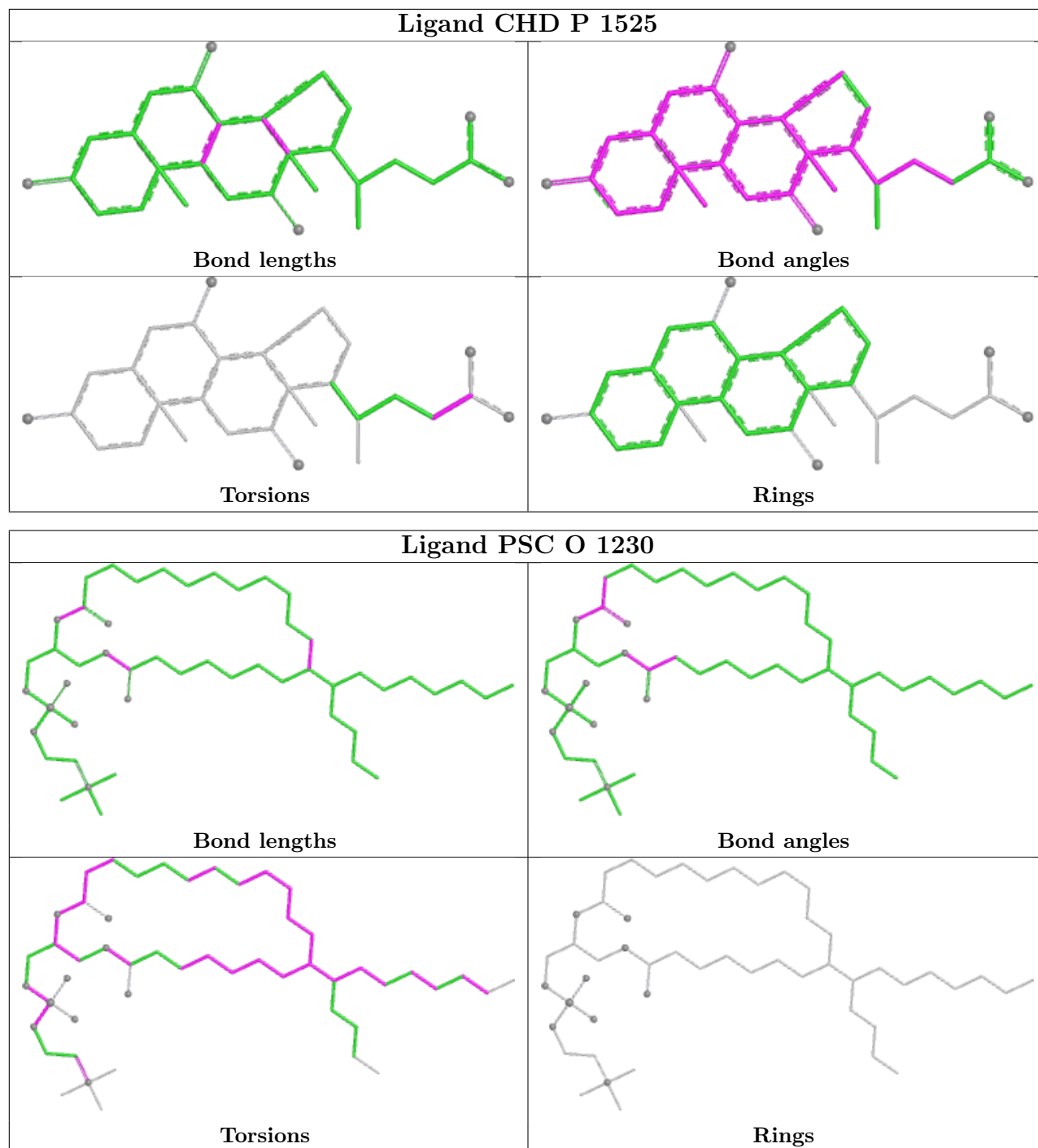


Ligand PSC B 230



Ligand PEK C 265





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.86	0 100 100	11, 17, 25, 51	0
1	N	513/514 (99%)	-0.55	1 (0%) 91 89	15, 23, 33, 56	0
2	B	226/227 (99%)	-0.50	5 (2%) 62 58	12, 22, 49, 86	0
2	O	226/227 (99%)	-0.07	9 (3%) 42 38	20, 30, 60, 84	0
3	C	259/261 (99%)	-0.66	2 (0%) 82 80	13, 21, 34, 58	0
3	P	259/261 (99%)	-0.48	2 (0%) 82 80	16, 24, 40, 64	0
4	D	144/147 (97%)	-0.41	3 (2%) 63 59	14, 26, 48, 70	0
4	Q	144/147 (97%)	0.62	9 (6%) 26 23	27, 41, 63, 105	0
5	E	104/109 (95%)	-0.46	1 (0%) 79 76	18, 27, 54, 75	0
5	R	104/109 (95%)	0.09	3 (2%) 53 49	23, 35, 57, 77	0
6	F	93/98 (94%)	-0.23	3 (3%) 50 46	15, 27, 49, 94	0
6	S	93/98 (94%)	0.13	4 (4%) 40 35	20, 33, 55, 102	0
7	G	83/85 (97%)	0.67	19 (22%) 2 1	15, 28, 99, 105	0
7	T	83/85 (97%)	0.82	20 (24%) 2 1	17, 33, 98, 102	0
8	H	75/85 (88%)	-0.19	3 (4%) 42 38	18, 29, 70, 78	0
8	U	75/85 (88%)	0.18	7 (9%) 14 12	24, 34, 72, 79	0
9	I	71/73 (97%)	0.15	6 (8%) 16 14	21, 34, 60, 65	0
9	V	71/73 (97%)	0.55	4 (5%) 30 26	23, 45, 60, 70	0
10	J	57/59 (96%)	-0.15	1 (1%) 67 64	19, 32, 59, 82	0
10	W	57/59 (96%)	0.39	5 (8%) 15 14	25, 37, 68, 92	0
11	K	49/56 (87%)	-0.13	1 (2%) 65 61	19, 31, 43, 50	0
11	X	49/56 (87%)	0.65	6 (12%) 8 7	33, 42, 59, 71	0
12	L	46/47 (97%)	-0.39	2 (4%) 40 35	17, 26, 48, 74	0
12	Y	46/47 (97%)	0.34	2 (4%) 40 35	26, 35, 60, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.07	4 (9%) 14 12	15, 24, 72, 97	0
13	Z	43/46 (93%)	0.52	5 (11%) 9 8	28, 36, 89, 106	0
All	All	3526/3614 (97%)	-0.27	127 (3%) 46 41	11, 26, 57, 106	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	11.3
4	Q	5	VAL	8.9
4	Q	8	SER	7.9
6	S	96	LEU	7.9
7	T	3	ALA	7.9
4	Q	4	SER	7.8
6	S	95	GLN	7.0
7	G	5	LYS	6.6
6	S	94	HIS	6.4
7	G	4	ALA	6.2
7	T	2	SER	5.7
7	T	5	LYS	5.6
7	G	7	ASP	5.5
2	B	59	GLN	5.3
2	O	227	LEU	5.3
4	Q	7	LYS	5.2
7	G	36	TRP	5.1
7	G	9	GLY	5.1
7	T	1	ALA	5.1
6	F	96	LEU	5.0
7	G	3	ALA	4.9
7	T	4	ALA	4.9
13	Z	43	SER	4.9
7	T	36	TRP	4.8
2	O	226	MET	4.8
7	G	8	HIS	4.7
7	T	10	GLY	4.6
7	T	9	GLY	4.5
9	V	3	ALA	4.5
7	G	1	ALA	4.4
2	B	60	GLU	4.3
4	D	4	SER	4.2
7	G	12	GLY	4.2
11	X	6	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	O	59	GLN	4.1
6	S	93	PRO	4.1
13	M	43	SER	4.1
4	Q	9	GLU	4.1
7	G	37	LEU	4.1
1	N	513	LEU	4.0
7	T	8	HIS	4.0
13	M	39	ASN	3.9
7	T	38	HIS	3.9
6	F	94	HIS	3.9
12	Y	20	ARG	3.8
7	T	37	LEU	3.8
7	T	39	SER	3.7
4	Q	35	ALA	3.7
7	G	2	SER	3.6
9	V	37	PHE	3.6
13	Z	41	LYS	3.6
8	U	45	ALA	3.6
12	L	2	HIS	3.5
7	G	38	HIS	3.5
10	W	52	TRP	3.5
10	W	57	HIS	3.5
7	T	84	LYS	3.4
11	X	7	PRO	3.4
7	G	40	GLY	3.3
7	T	12	GLY	3.3
13	Z	40	TYR	3.3
7	T	42	ARG	3.3
7	G	10	GLY	3.3
2	O	113	TYR	3.2
6	F	95	GLN	3.2
8	U	48	GLY	3.2
7	G	39	SER	3.1
8	U	46	LYS	3.1
13	M	42	LYS	3.1
3	P	3	HIS	3.1
9	I	37	PHE	3.0
5	R	79	LYS	3.0
9	I	3	ALA	3.0
2	O	224	ALA	2.9
7	T	7	ASP	2.9
8	H	47	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	5	VAL	2.9
10	W	56	PRO	2.9
5	E	6	GLU	2.8
7	G	41	HIS	2.8
7	G	42	ARG	2.7
2	O	60	GLU	2.7
4	D	6	VAL	2.7
10	J	57	HIS	2.6
2	O	65	TRP	2.6
8	U	44	THR	2.6
8	U	47	GLY	2.6
2	B	91	ASN	2.6
10	W	1	PHE	2.5
11	X	47	ARG	2.5
7	G	6	GLY	2.5
7	T	40	GLY	2.5
2	O	92	ASN	2.5
9	V	33	THR	2.5
8	H	50	VAL	2.4
13	Z	39	ASN	2.4
7	G	43	GLU	2.4
7	T	6	GLY	2.4
2	O	91	ASN	2.4
3	P	33	MET	2.3
2	B	57	ASP	2.3
13	M	41	LYS	2.3
13	Z	42	LYS	2.3
4	Q	39	ALA	2.3
3	C	38	ASN	2.3
7	T	43	GLU	2.2
5	R	109	VAL	2.2
9	I	15	ARG	2.2
3	C	3	HIS	2.2
8	U	50	VAL	2.2
2	B	58	ALA	2.2
9	V	36	LYS	2.2
10	W	55	PHE	2.2
11	X	52	GLU	2.1
7	T	41	HIS	2.1
11	X	23	THR	2.1
12	L	47	LYS	2.1
5	R	108	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
9	I	26	MET	2.1
8	H	44	THR	2.1
11	X	13	TYR	2.1
9	I	25	PHE	2.0
11	K	6	ALA	2.0
4	Q	10	ASP	2.0
8	U	49	ASP	2.0
12	Y	2	HIS	2.0
9	I	33	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
7	TPO	T	11	11/12	0.52	0.28	74,80,100,101	0
7	TPO	G	11	11/12	0.53	0.29	74,81,102,102	0
1	FME	N	1	10/11	0.81	0.18	48,50,63,64	0
1	FME	A	1	10/11	0.84	0.15	44,46,62,65	0
2	FME	O	1	10/11	0.95	0.11	30,31,37,38	0
2	FME	B	1	10/11	0.97	0.08	19,21,26,33	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(Å ²)	Q<0.9
24	DMU	P	1272	33/33	0.66	0.25	74,102,105,106	0
23	CHD	W	1060	29/29	0.70	0.30	97,100,102,103	0
24	DMU	C	272	33/33	0.72	0.24	64,101,103,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	PEK	C	265	53/53	0.72	0.27	39,87,101,104	0
25	UNX	P	1262	1/1	0.74	0.35	29,29,29,29	0
26	PEK	G	1263	53/53	0.74	0.27	46,88,115,116	0
26	PEK	T	263	53/53	0.74	0.25	35,81,112,112	0
21	TGL	N	1522	63/63	0.75	0.25	25,66,80,81	0
19	PGV	N	1268	51/51	0.75	0.24	62,89,99,101	0
23	CHD	J	60	29/29	0.77	0.26	95,98,101,103	0
27	CDL	T	1269	100/100	0.77	0.22	43,76,109,113	0
19	PGV	A	524	51/51	0.78	0.24	30,65,100,103	0
21	TGL	O	1523	63/63	0.78	0.25	34,64,86,90	0
27	CDL	G	269	100/100	0.78	0.23	42,77,109,113	0
27	CDL	P	1270	100/100	0.78	0.26	44,89,104,105	0
22	PSC	O	1230	52/52	0.78	0.24	38,82,113,115	0
19	PGV	C	268	51/51	0.79	0.24	53,87,97,98	0
19	PGV	N	1524	51/51	0.79	0.21	36,68,102,102	0
27	CDL	C	270	100/100	0.79	0.23	40,86,103,105	0
26	PEK	P	1265	53/53	0.80	0.25	32,83,103,103	0
21	TGL	B	521	63/63	0.80	0.22	31,58,87,89	0
21	TGL	D	523	63/63	0.80	0.22	38,57,83,86	0
25	UNX	C	262	1/1	0.81	0.30	26,26,26,26	0
21	TGL	L	522	63/63	0.83	0.21	25,61,74,78	0
21	TGL	N	1521	63/63	0.83	0.20	43,63,85,90	0
23	CHD	P	1271	29/29	0.83	0.19	74,82,84,84	0
22	PSC	B	230	52/52	0.83	0.21	31,86,112,114	0
23	CHD	C	271	29/29	0.85	0.19	71,83,86,86	0
24	DMU	Z	1526	33/33	0.88	0.13	32,50,66,68	0
16	MG	N	1518	1/1	0.90	0.08	26,26,26,26	0
23	CHD	P	1525	29/29	0.93	0.08	17,27,31,35	0
23	CHD	C	525	29/29	0.94	0.07	14,24,31,33	0
24	DMU	M	526	33/33	0.94	0.09	15,38,57,59	0
26	PEK	P	1264	53/53	0.94	0.12	20,37,65,65	0
26	PEK	G	264	53/53	0.95	0.10	15,31,57,58	0
23	CHD	B	1086	29/29	0.96	0.07	11,20,27,33	0
23	CHD	G	86	29/29	0.96	0.06	17,21,25,26	0
19	PGV	N	1266	51/51	0.97	0.07	15,28,50,52	0
17	NA	A	519	1/1	0.97	0.03	16,16,16,16	0
19	PGV	P	1267	51/51	0.97	0.08	16,28,59,60	0
19	PGV	A	521	51/51	0.97	0.07	12,24,48,57	0
19	PGV	C	267	51/51	0.97	0.08	13,24,55,58	0
17	NA	N	1519	1/1	0.97	0.06	24,24,24,24	0
18	HEA	N	515	60/60	0.97	0.07	14,25,37,39	0
16	MG	A	518	1/1	0.98	0.03	21,21,21,21	0

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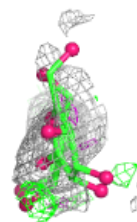
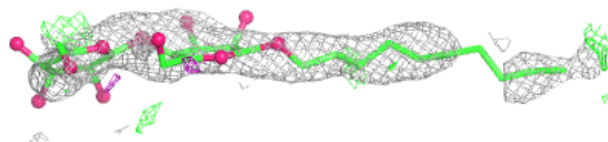
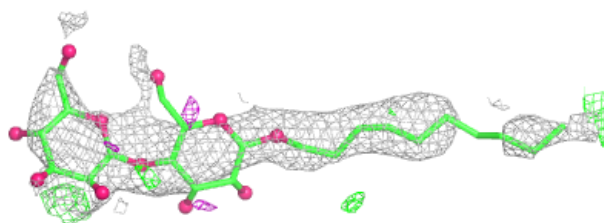
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	HEA	N	516	60/60	0.98	0.07	9,20,26,28	0
18	HEA	A	515	60/60	0.98	0.06	8,17,40,45	0
15	PER	N	520	2/2	0.99	0.06	13,13,13,13	0
14	CU	N	517	1/1	0.99	0.02	18,18,18,18	0
20	CUA	B	228	2/2	0.99	0.03	17,17,17,18	0
20	CUA	O	228	2/2	0.99	0.03	25,25,25,26	0
15	PER	A	520	2/2	0.99	0.08	8,8,8,10	0
18	HEA	A	516	60/60	0.99	0.05	9,16,24,27	0
14	CU	A	517	1/1	1.00	0.01	17,17,17,17	0
28	ZN	F	99	1/1	1.00	0.02	26,26,26,26	0
28	ZN	S	99	1/1	1.00	0.01	28,28,28,28	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.

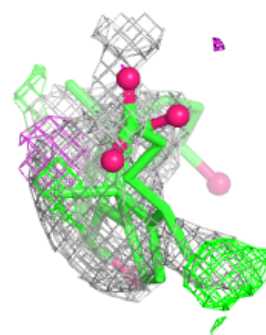
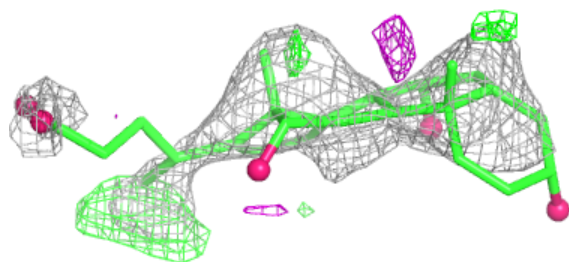
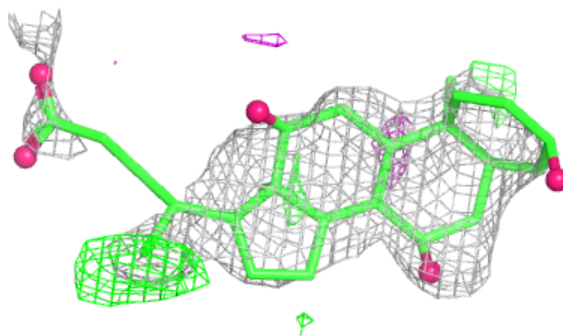
Electron density around DMU P 1272:

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

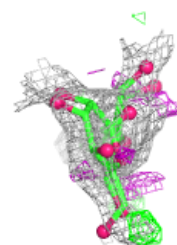
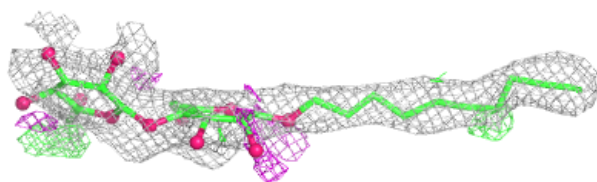
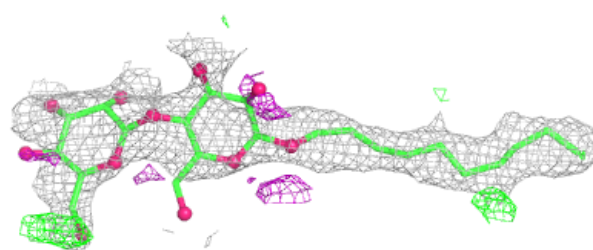


Electron density around CHD W 1060:

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

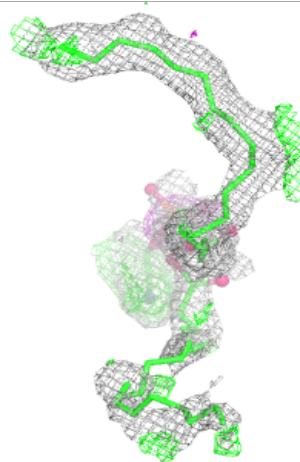
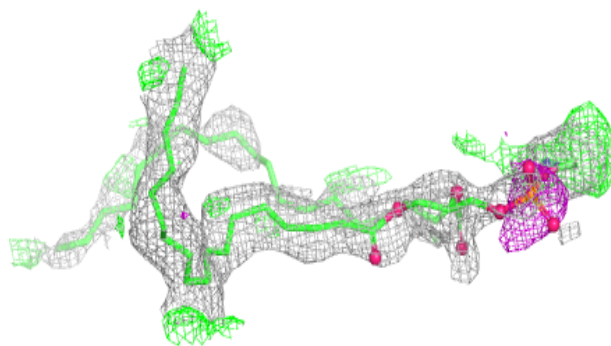
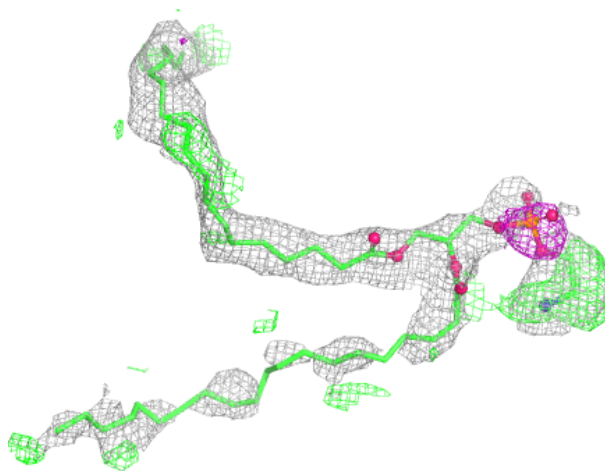
**Electron density around DMU C 272:**

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



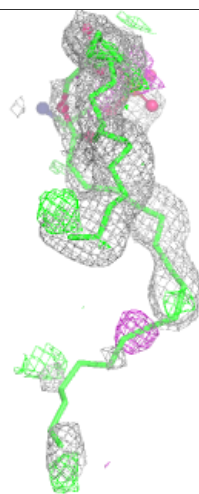
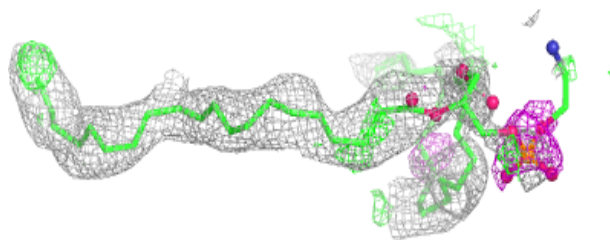
Electron density around PEK C 265:

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



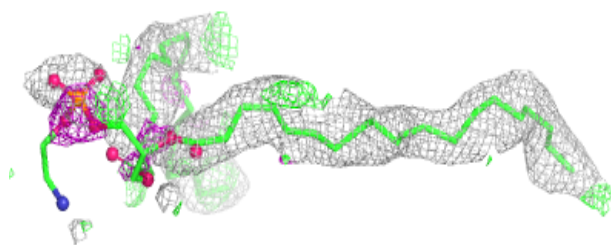
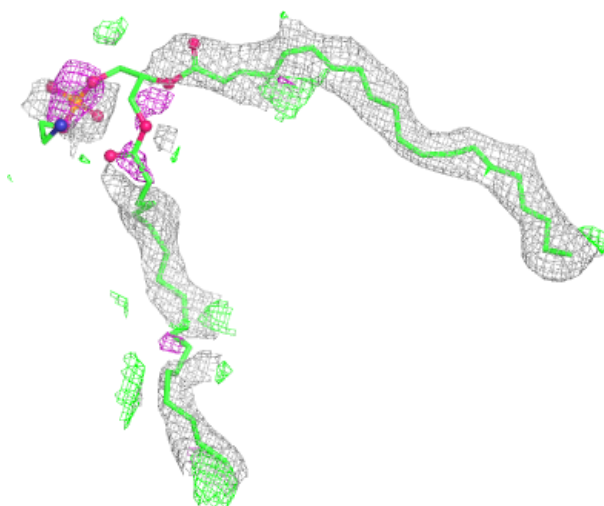
Electron density around PEK G 1263:

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



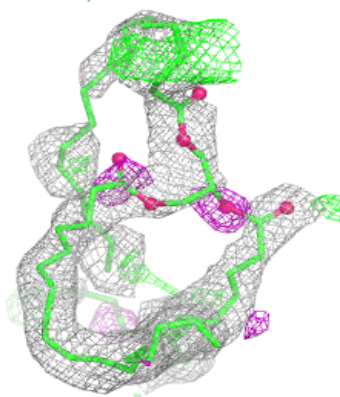
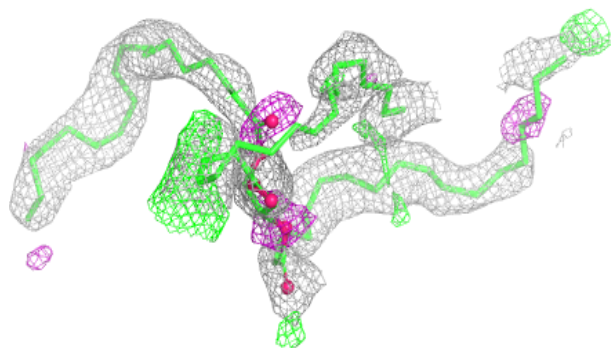
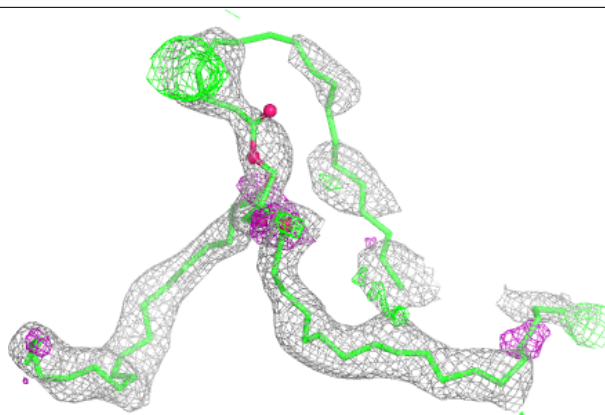
Electron density around PEK T 263:

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

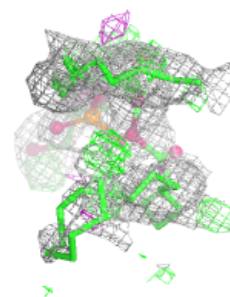
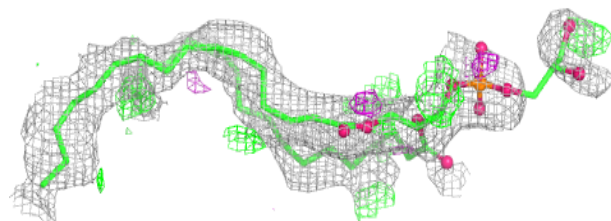
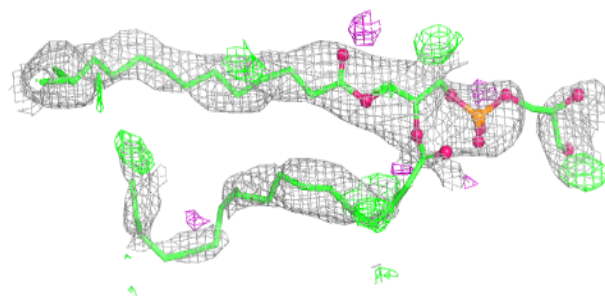


Electron density around TGL N 1522:

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

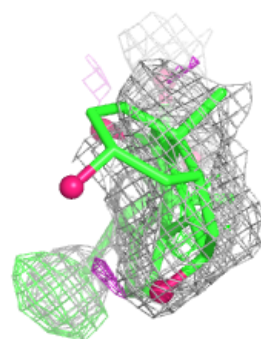
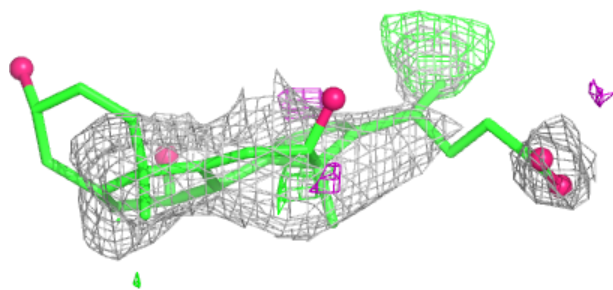
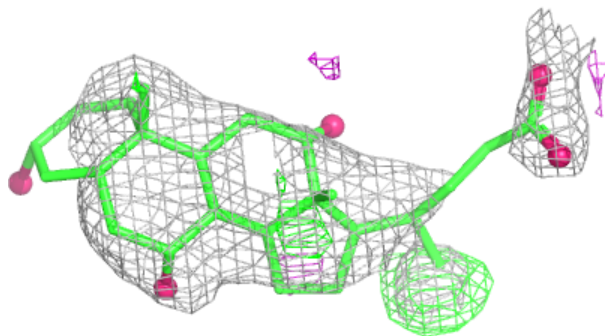
**Electron density around PGV N 1268:**

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

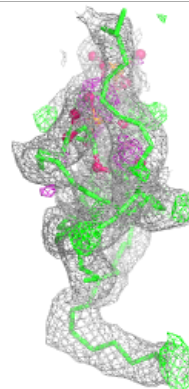
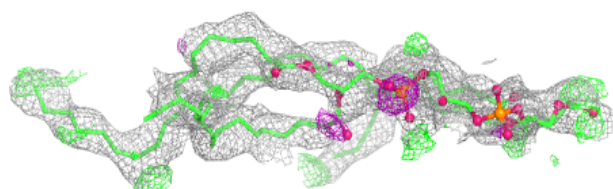
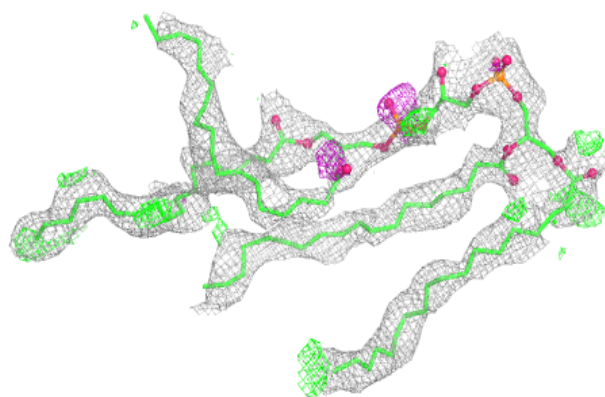


Electron density around CHD J 60:

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

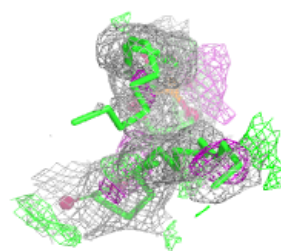
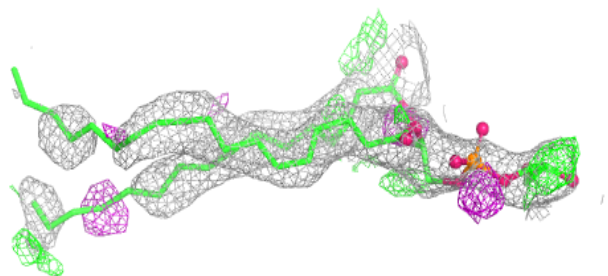
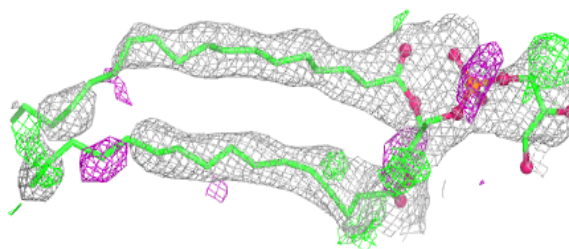
**Electron density around CDL T 1269:**

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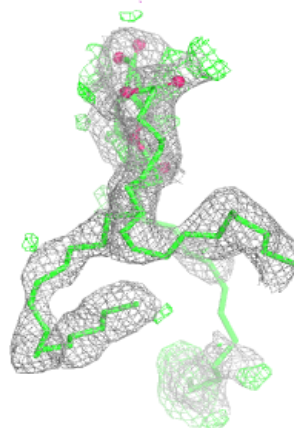
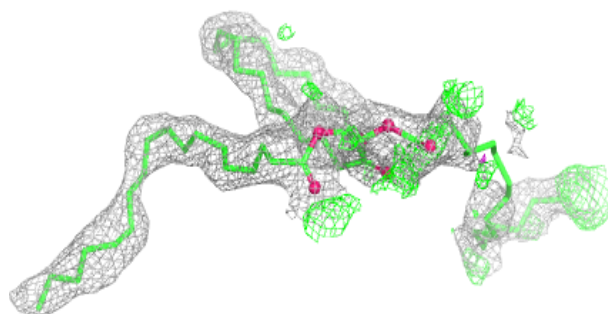
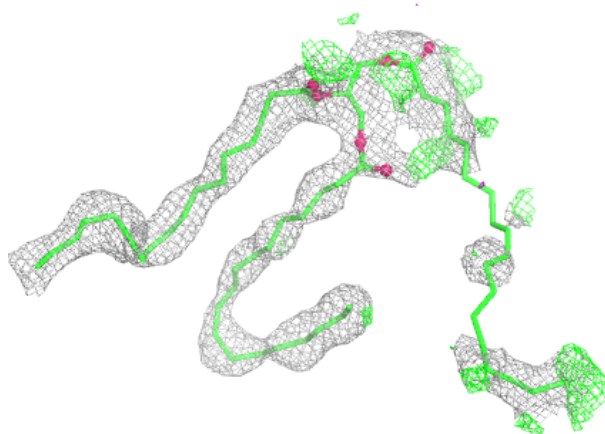


Electron density around PGV A 524:

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

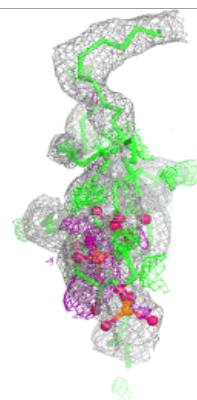
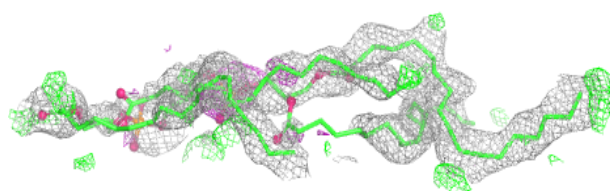
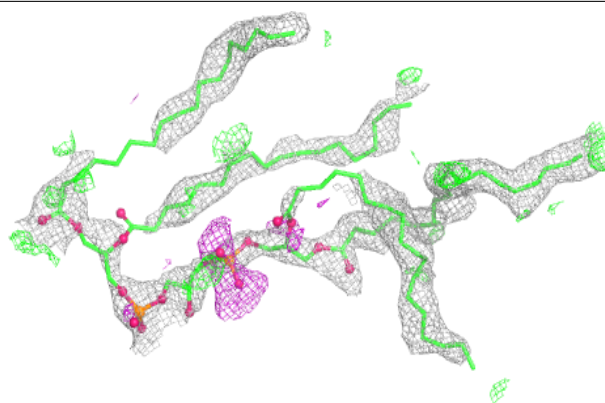
**Electron density around TGL O 1523:**

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

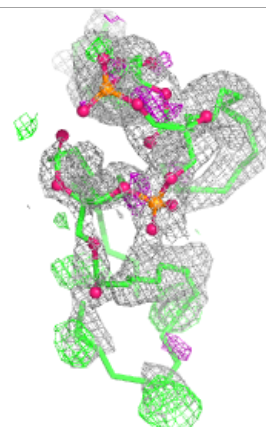
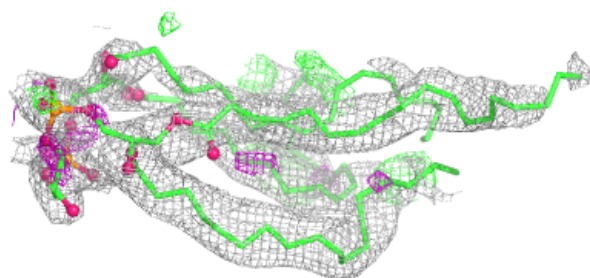
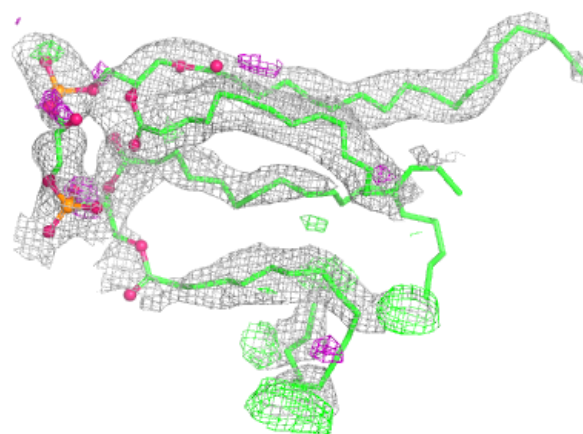


Electron density around CDL G 269:

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and green (positive)

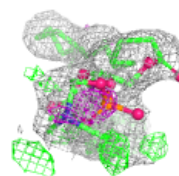
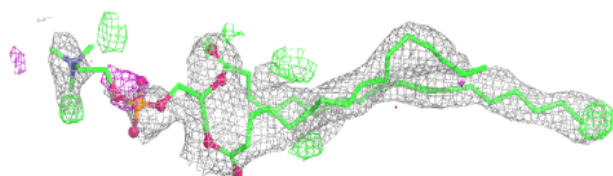
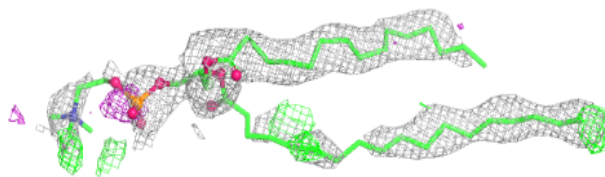
**Electron density around CDL P 1270:**

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

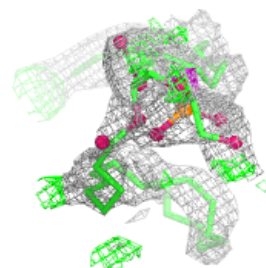
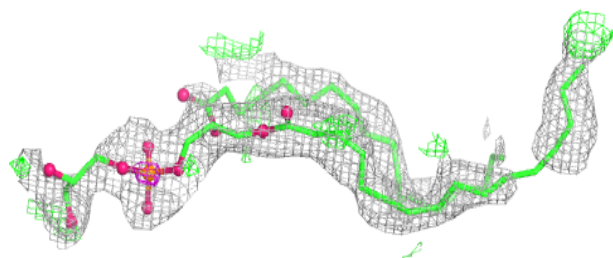
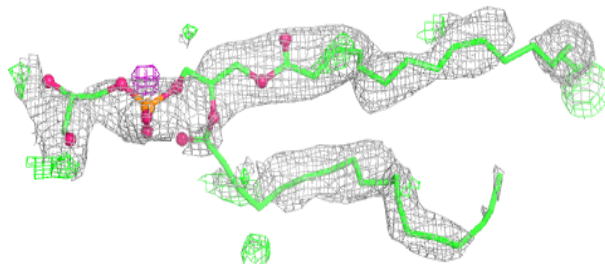


Electron density around PSC O 1230:

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

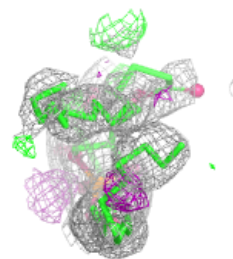
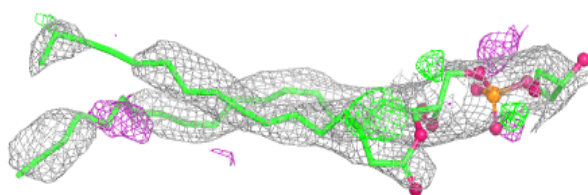
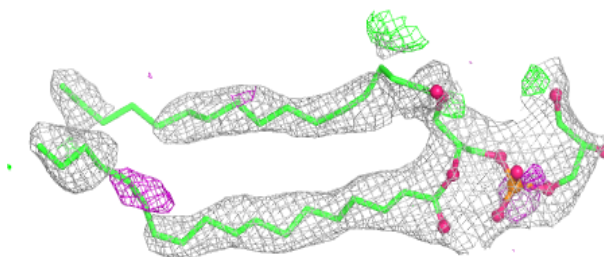
**Electron density around PGV C 268:**

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



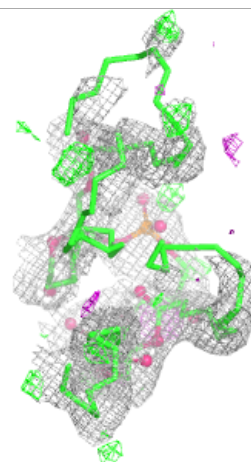
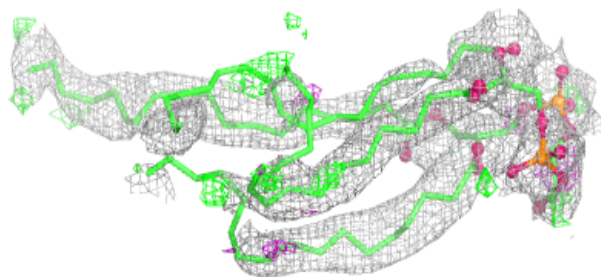
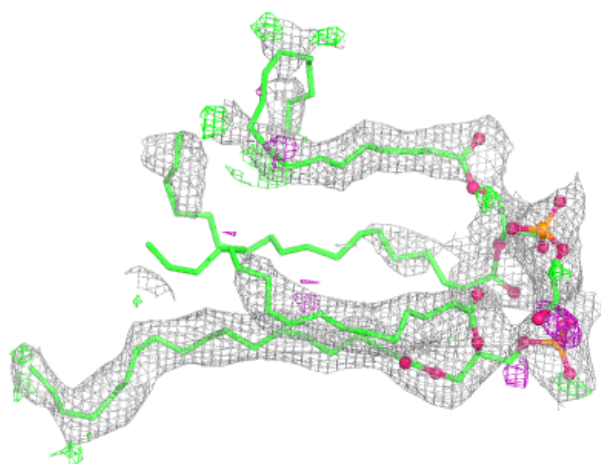
Electron density around PGV N 1524:

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



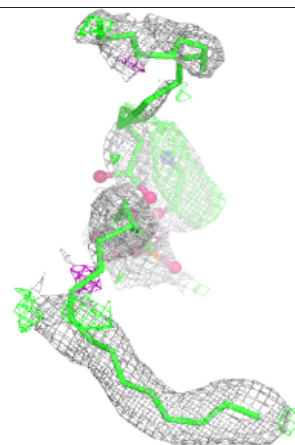
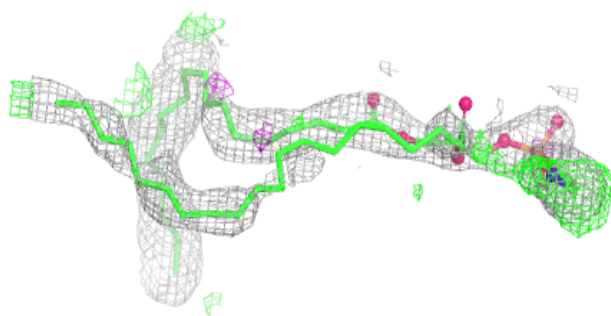
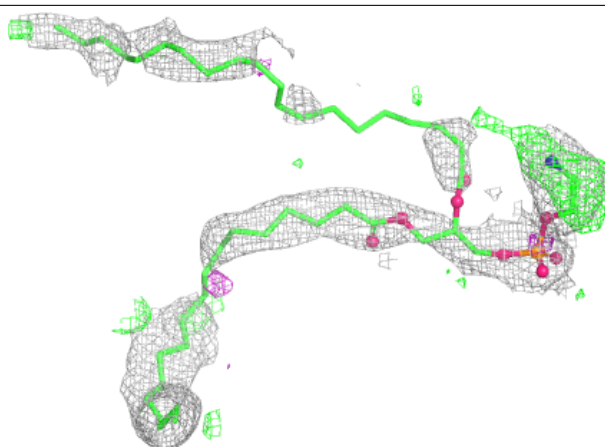
Electron density around CDL C 270:

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

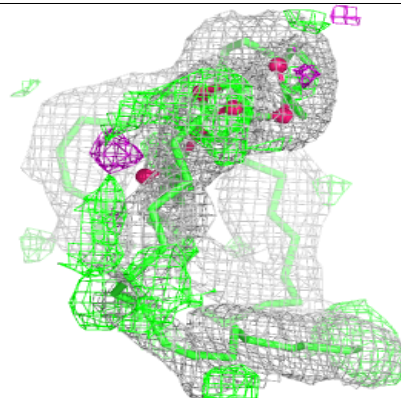
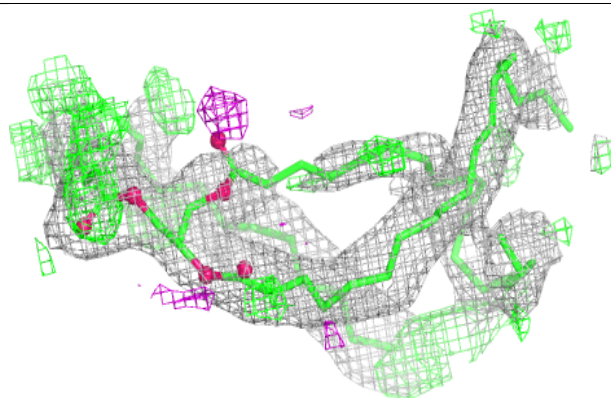
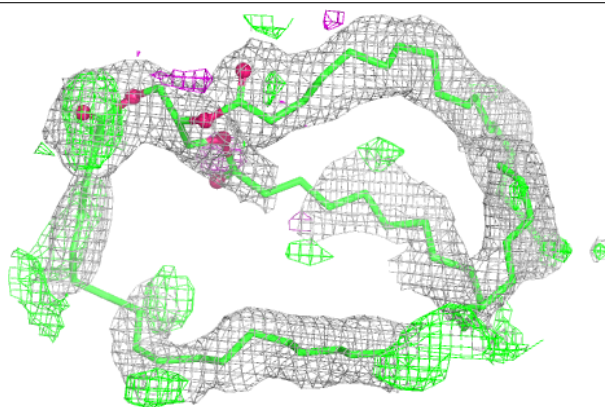


Electron density around PEK P 1265:

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

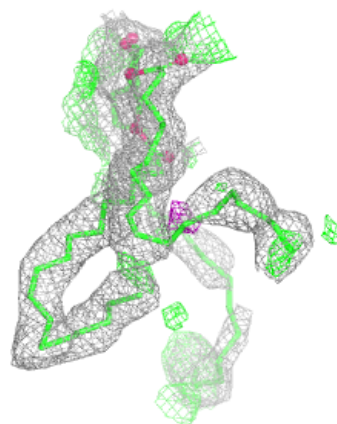
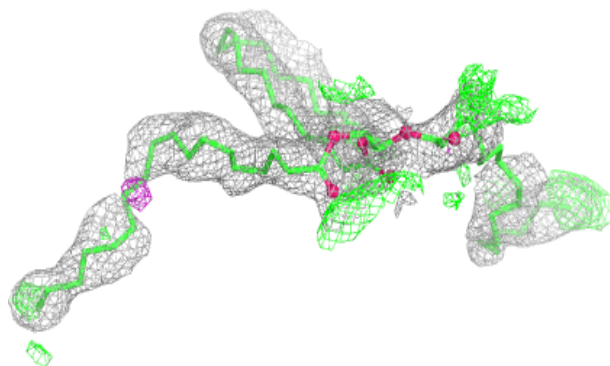
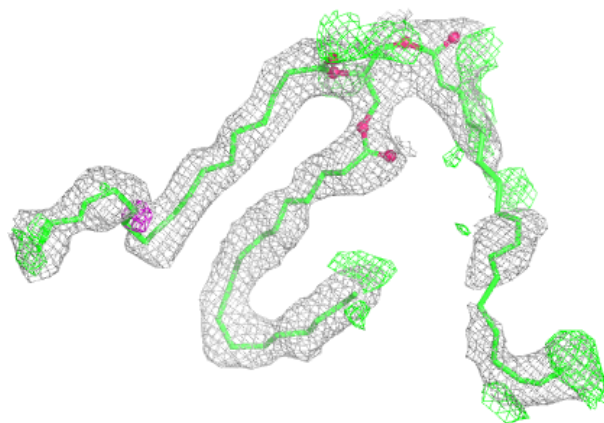
**Electron density around TGL B 521:**

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



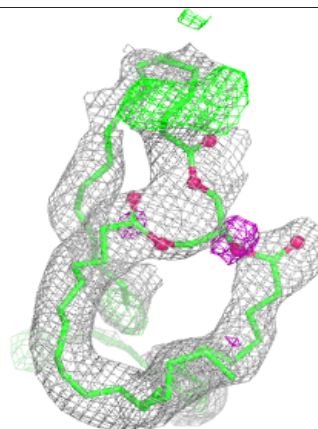
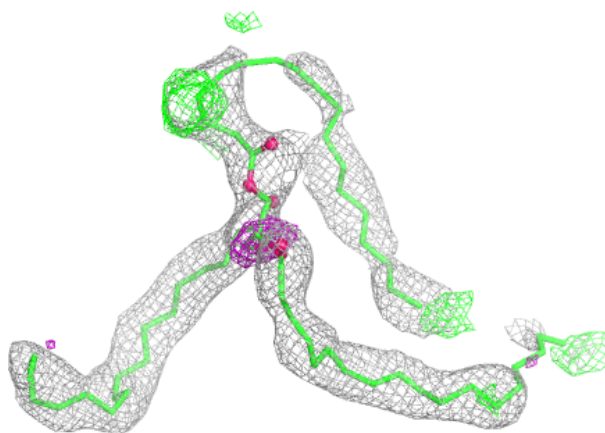
Electron density around TGL D 523:

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



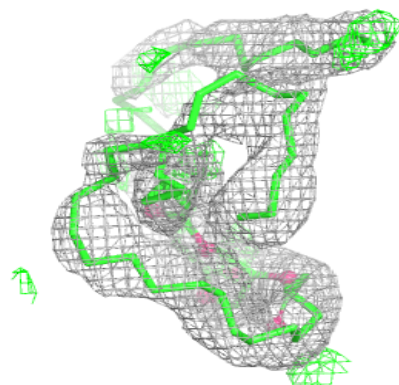
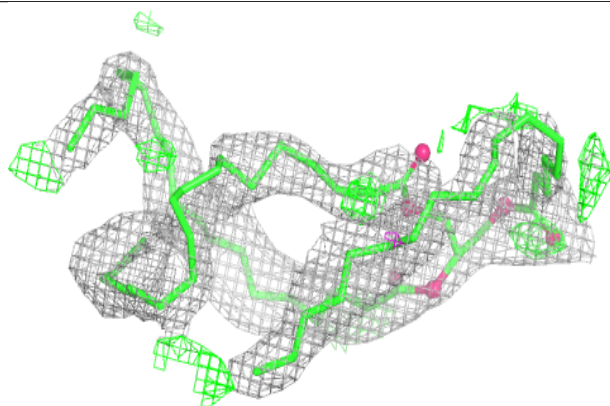
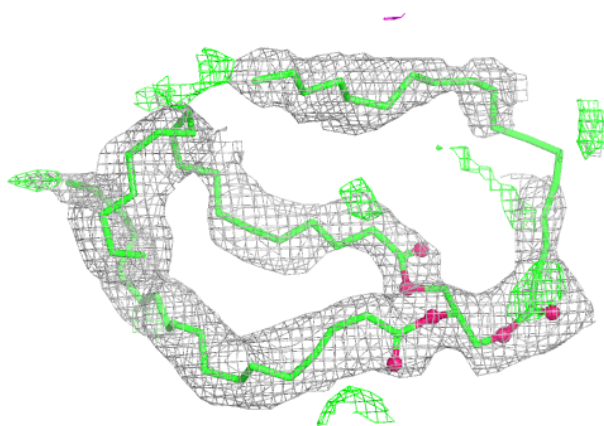
Electron density around TGL L 522:

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

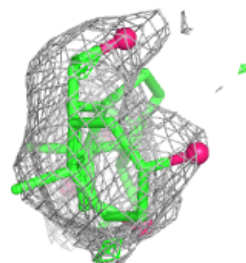
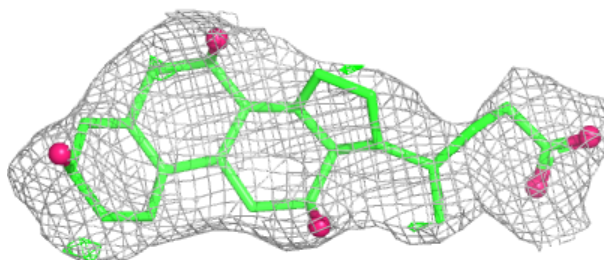


Electron density around TGL N 1521:

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

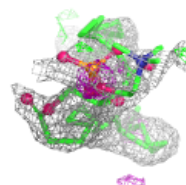
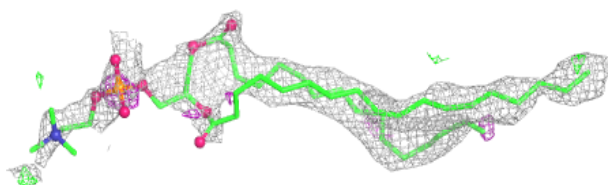
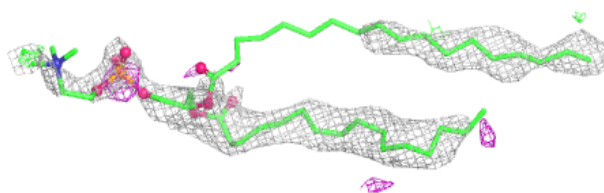
**Electron density around CHD P 1271:**

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

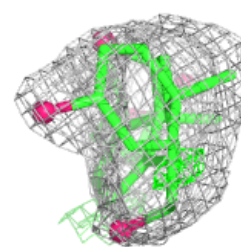
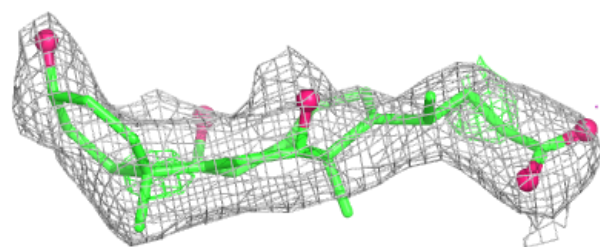
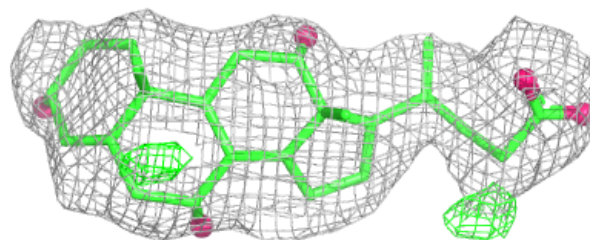


Electron density around PSC B 230:

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

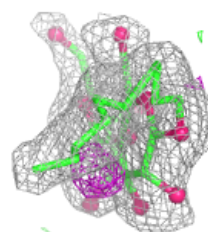
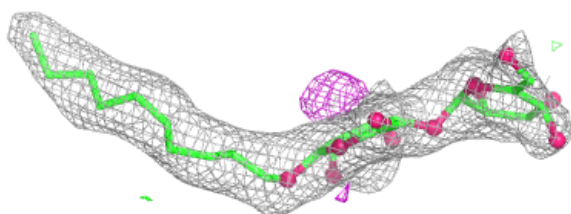
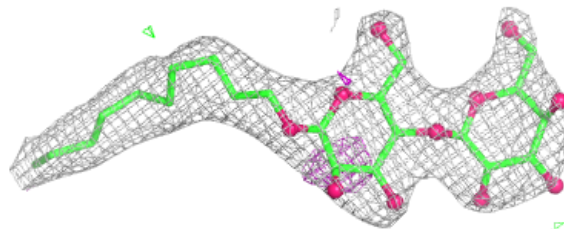
**Electron density around CHD C 271:**

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

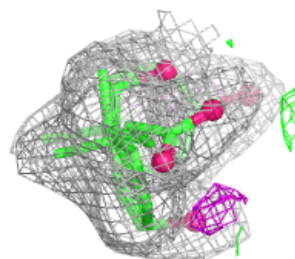
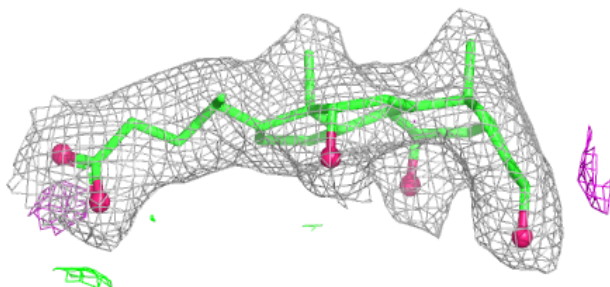
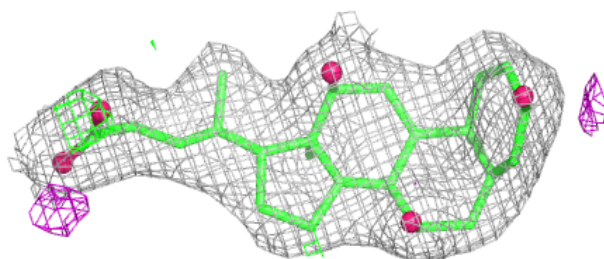


Electron density around DMU Z 1526:

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

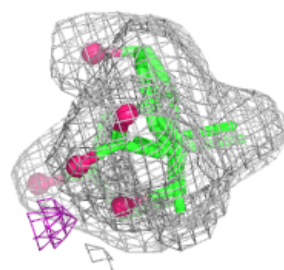
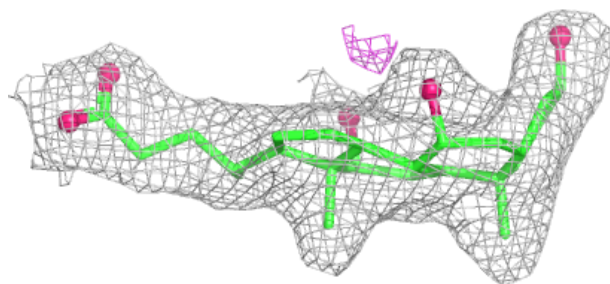
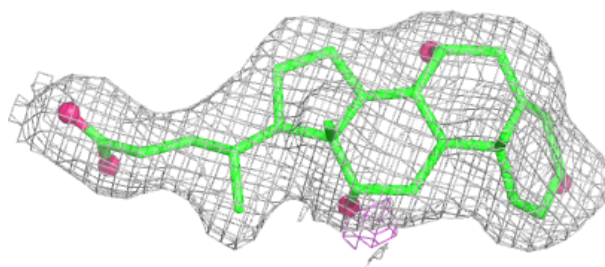
**Electron density around CHD P 1525:**

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

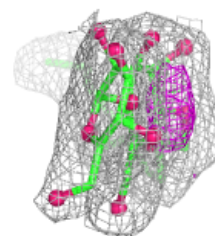
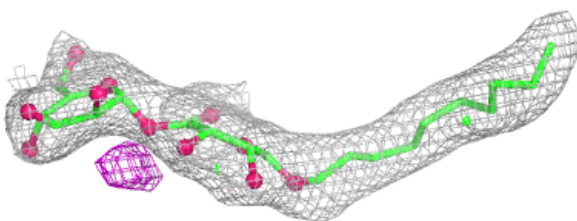
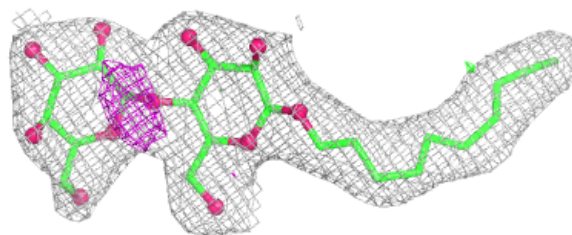


Electron density around CHD C 525:

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

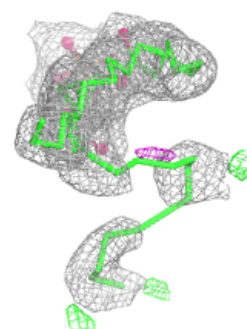
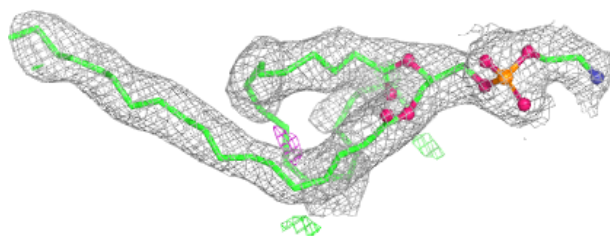
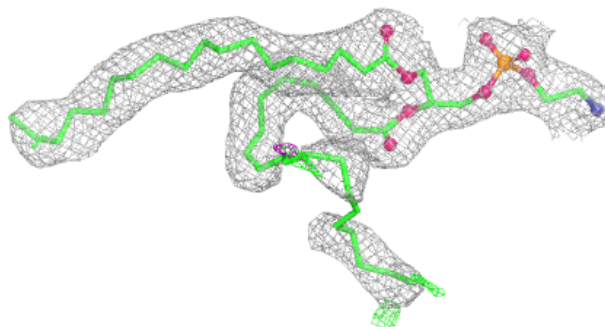
**Electron density around DMU M 526:**

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

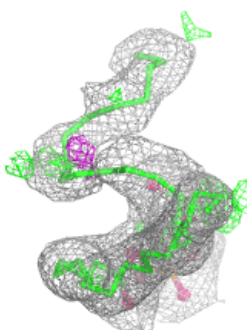
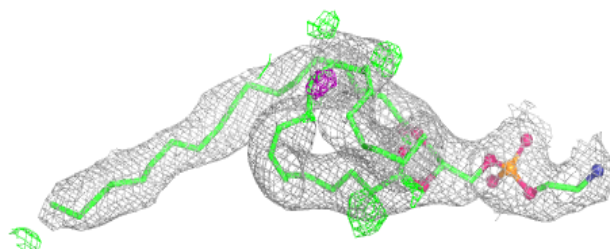
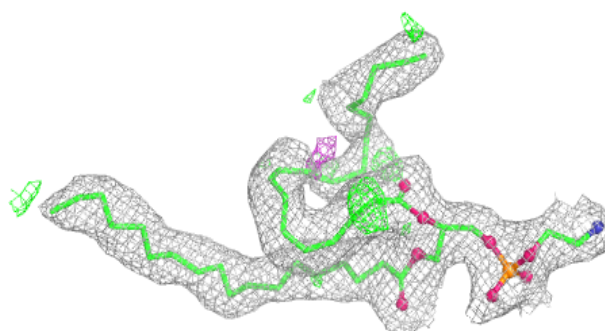


Electron density around PEK P 1264:

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

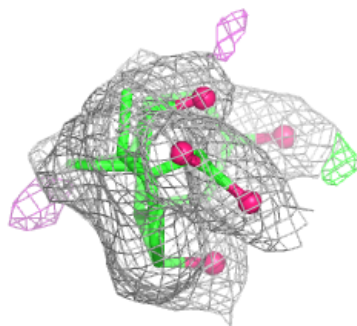
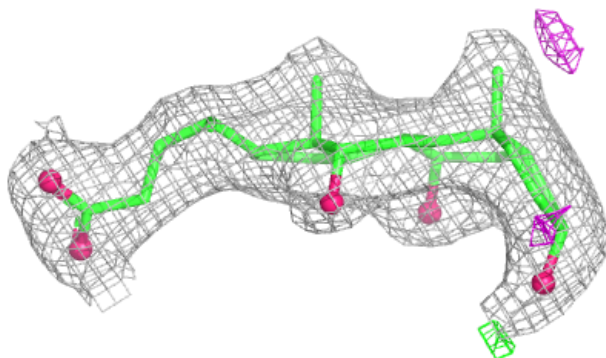
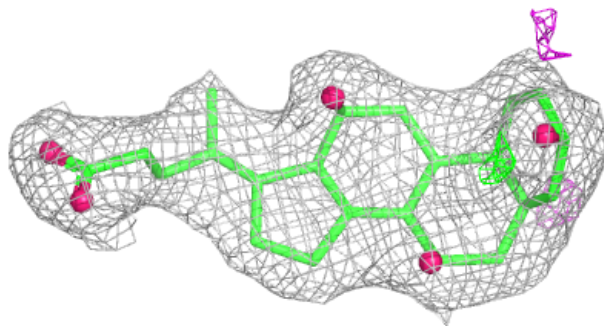
**Electron density around PEK G 264:**

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

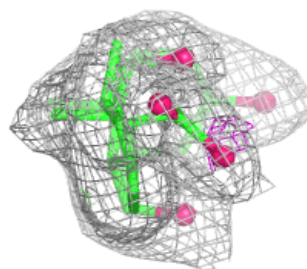
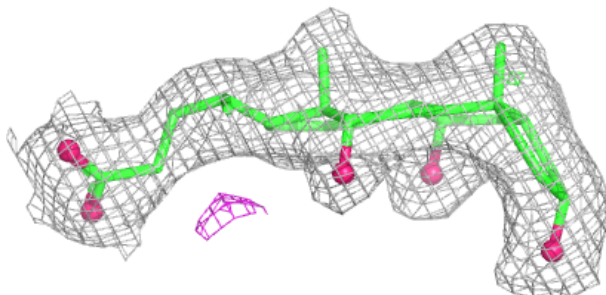
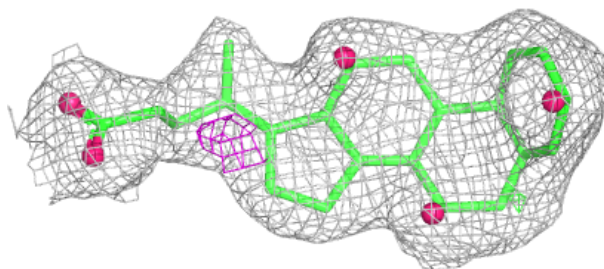


Electron density around CHD B 1086:

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

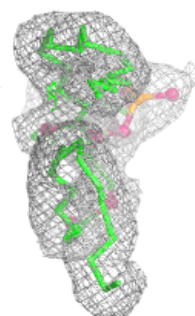
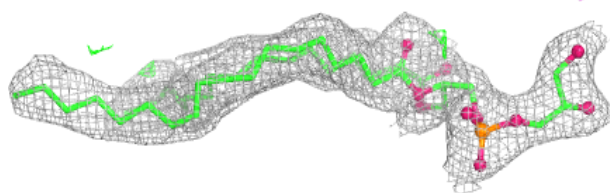
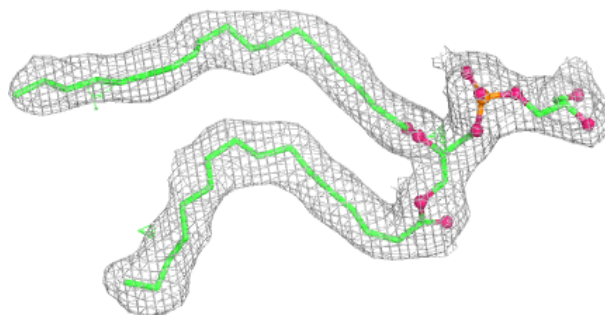
**Electron density around CHD G 86:**

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

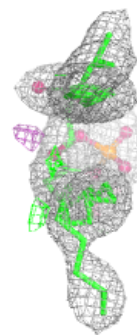
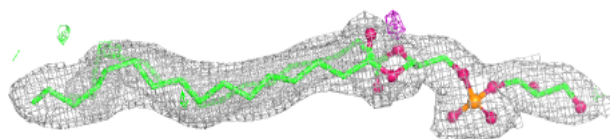
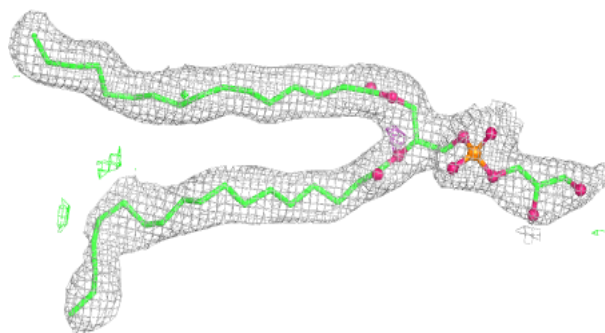


Electron density around PGV N 1266:

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

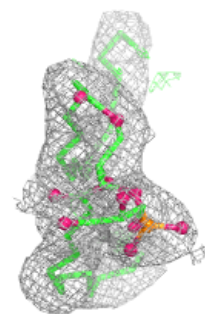
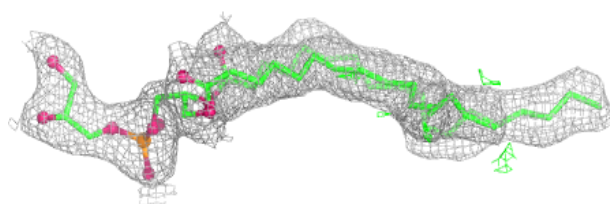
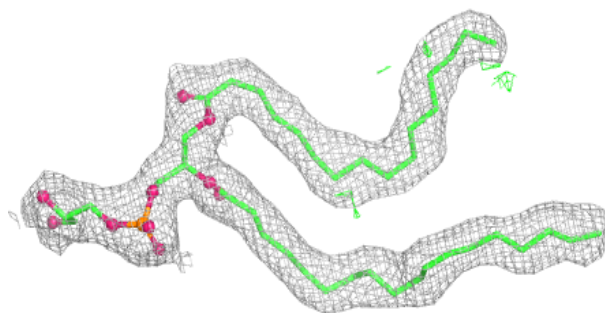
**Electron density around PGV P 1267:**

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

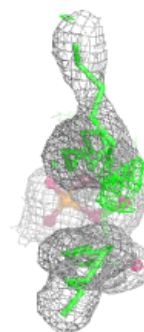
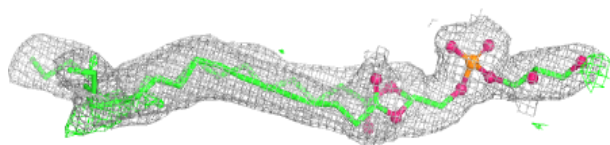
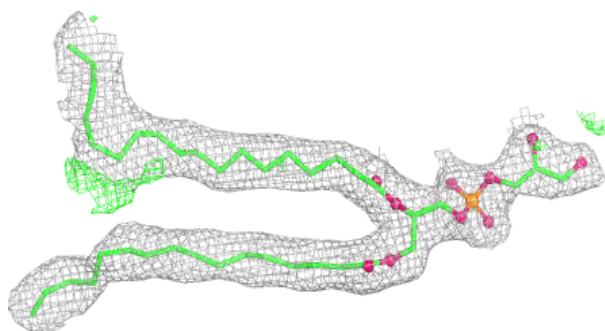


Electron density around PGV A 521:

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

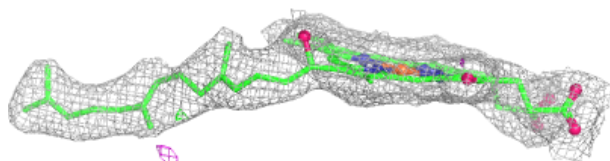
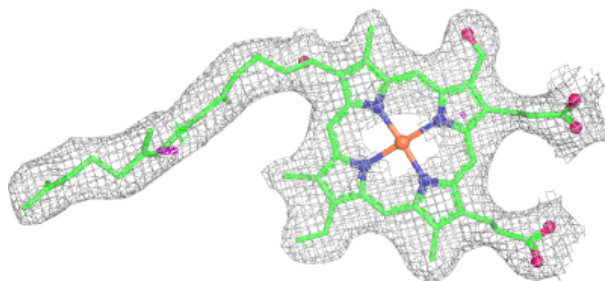
**Electron density around PGV C 267:**

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

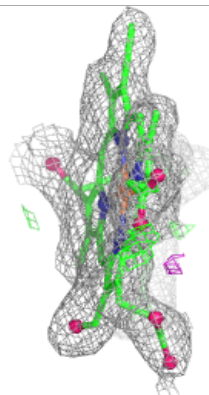
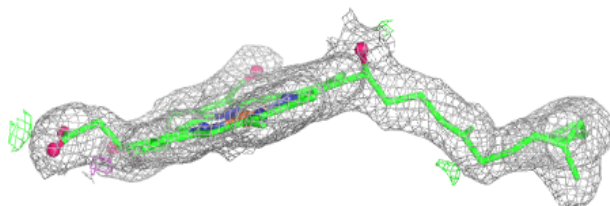
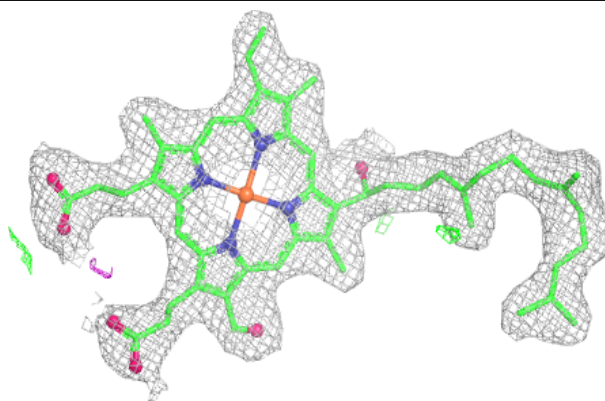


Electron density around HEA N 515:

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

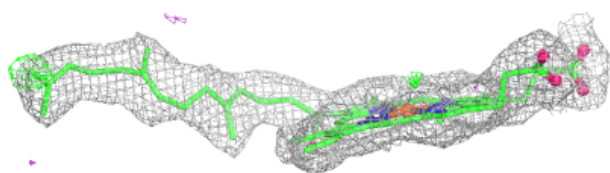
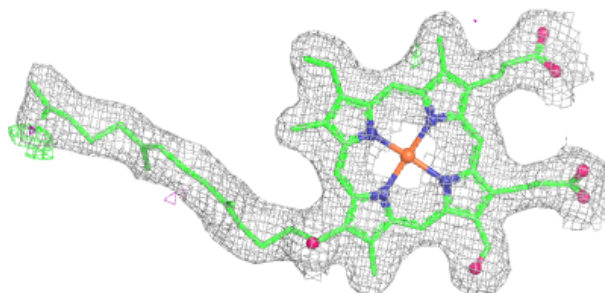
**Electron density around HEA N 516:**

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

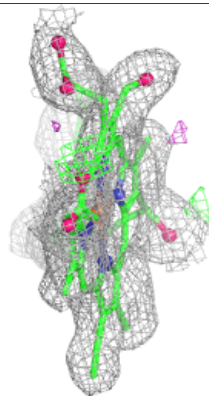
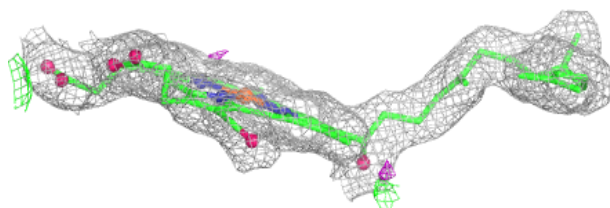
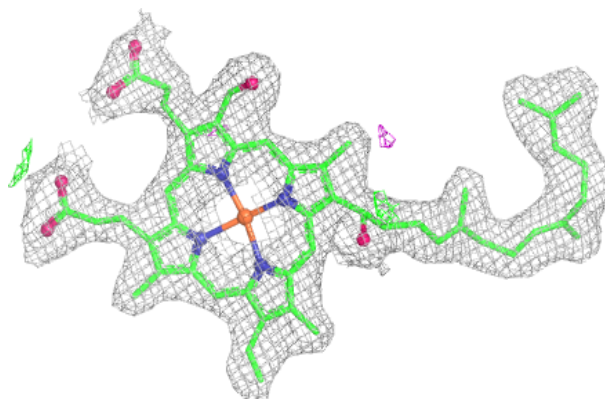


Electron density around HEA A 515:

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

**Electron density around HEA 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.