Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 08:41 AM EDT

PDB ID	:	2ZXW
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 (i) 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 (i)) were used in the production of this report:

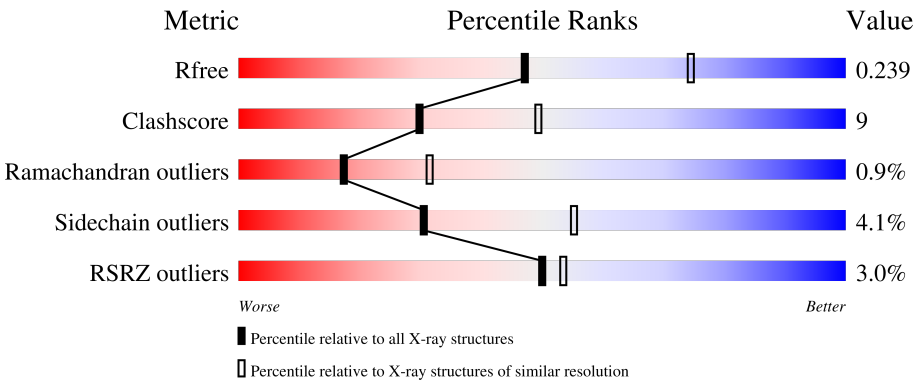
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	82% 16% •
1	N	514	82% 17%
2	B	227	78% 19% •
2	O	227	2% 73% 24% •

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Mol	Chain	Length	Quality of chain
3	C	261	84% 15%
3	P	261	85% 13%
4	D	147	82% 15%
4	Q	147	8% 80% 18%
5	E	109	3% 81% 15% 5%
5	R	109	% 82% 14% 5%
6	F	98	3% 76% 17% 5%
6	S	98	4% 78% 13% 5%
7	G	85	15% 68% 24% 7%
7	T	85	18% 67% 20% 12%
8	H	85	4% 73% 12% 12%
8	U	85	4% 69% 15% 12%
9	I	73	8% 84% 14%
9	V	73	5% 75% 22%
10	J	59	8% 88% 7%
10	W	59	14% 85% 8%
11	K	56	79% 9% 12%
11	X	56	11% 79% 7% 12%
12	L	47	2% 83% 15%
12	Y	47	4% 77% 21%
13	M	46	11% 80% 11% 7%
13	Z	46	11% 74% 20% 7%

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	-	-	X
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	X	-	-	-
23	CHD	W	1060	X	-	-	X
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	514	4027	2691	623	678	35	0	0	0
1	N	514	4027	2691	623	678	35	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	104	842	538	141	161	2	0	0	0
5	R	104	842	538	141	161	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

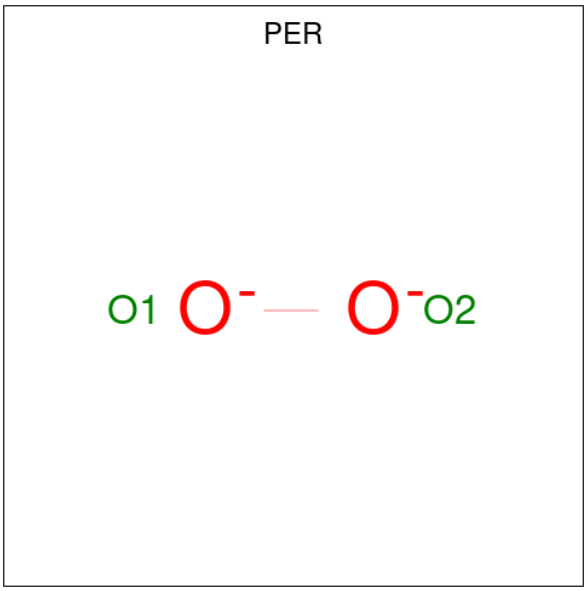
- Molecule 13 is a protein called Cytochrome c oxidase polypeptide 8H.

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

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 15 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



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 (three-letter code: MG) (formula: Mg).

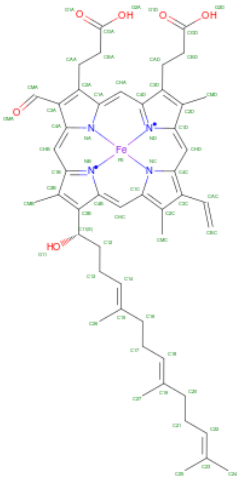
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0

- Molecule 17 is SODIUM ION (three-letter code: 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 (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

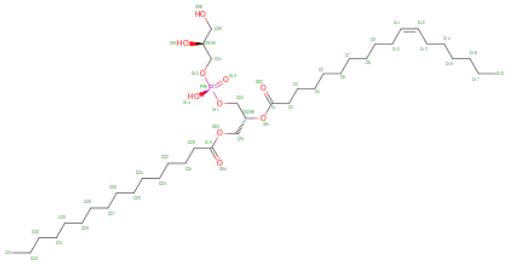
HEA



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

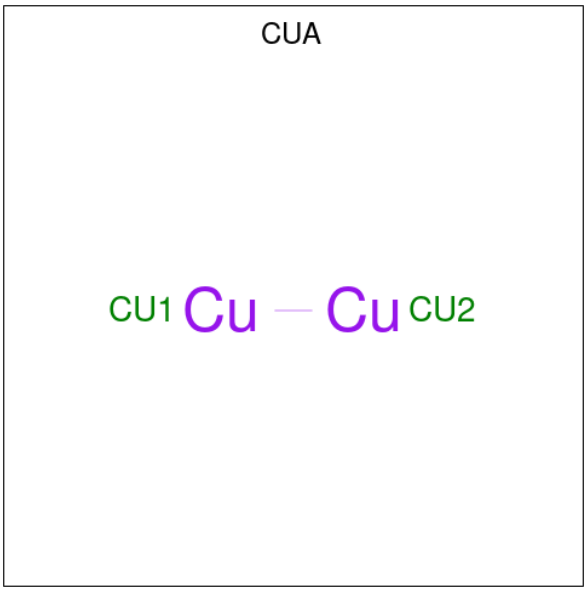
- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).

PGV



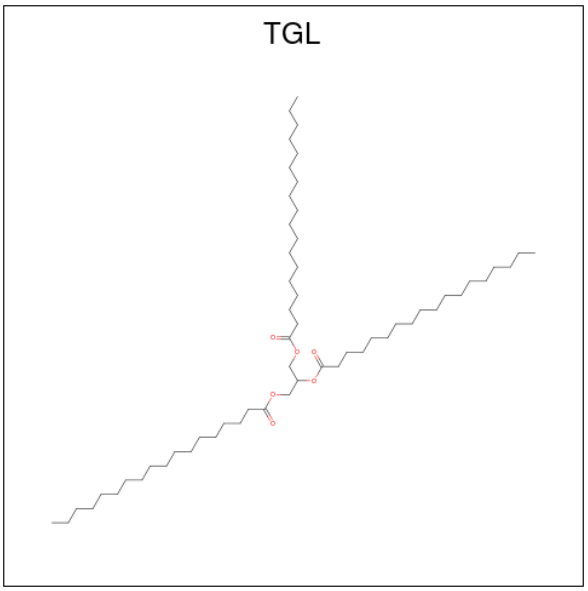
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
19	A	1	51	40	10	1	0	0
			Total	C	O	P		
19	A	1	51	40	10	1	0	0
			Total	C	O	P		
19	C	1	51	40	10	1	0	0
			Total	C	O	P		
19	C	1	51	40	10	1	0	0
			Total	C	O	P		
19	N	1	51	40	10	1	0	0
			Total	C	O	P		
19	N	1	51	40	10	1	0	0
			Total	C	O	P		
19	N	1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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



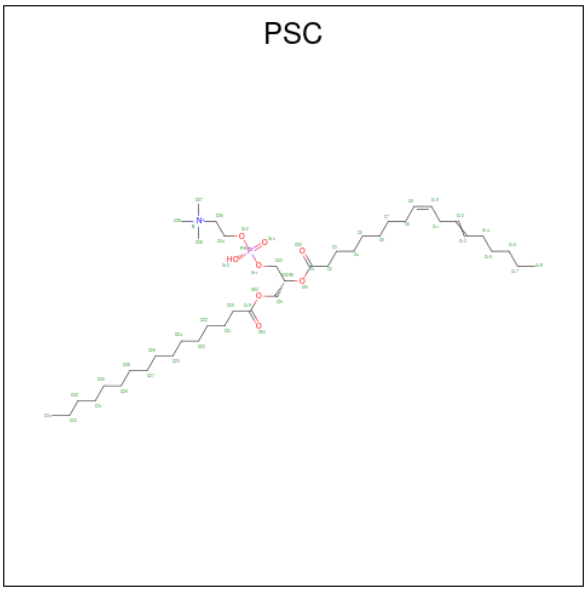
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
20	B	1	2	2	0	0
			Total	Cu		
20	O	1	2	2	0	0

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



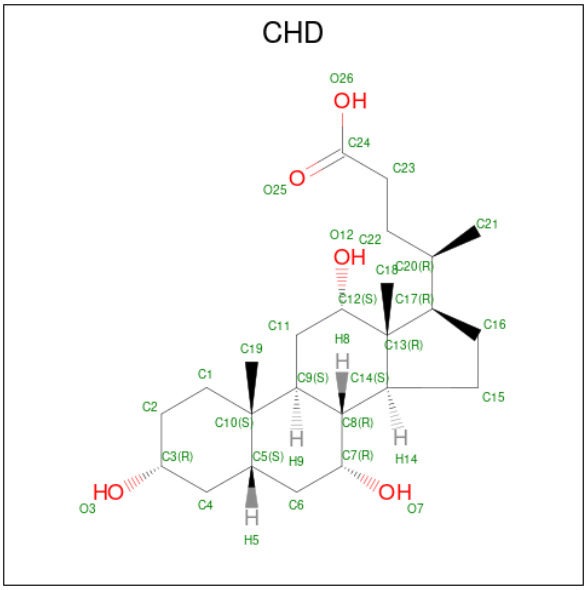
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	B	1	63	57	6	0	0
21	D	1	63	57	6	0	0
21	L	1	63	57	6	0	0
21	N	1	63	57	6	0	0
21	N	1	63	57	6	0	0
21	O	1	63	57	6	0	0

- 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 (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

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



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

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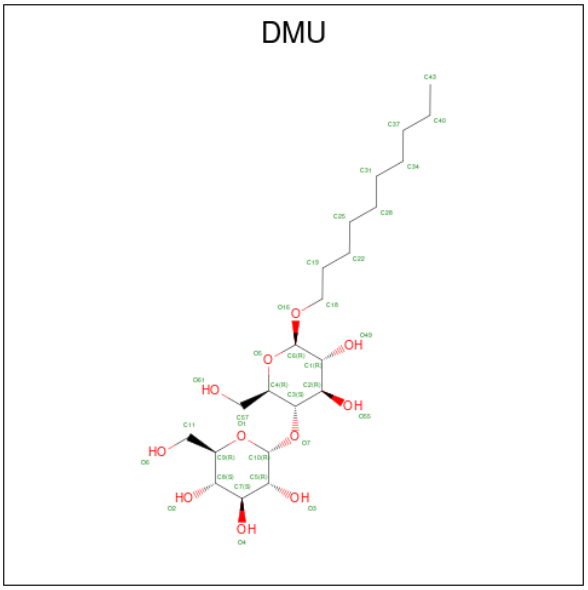
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
23	C	1	29	24	5	0	0
23	G	1	29	24	5	0	0
23	J	1	29	24	5	0	0
23	P	1	29	24	5	0	0
23	P	1	29	24	5	0	0
23	W	1	29	24	5	0	0

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

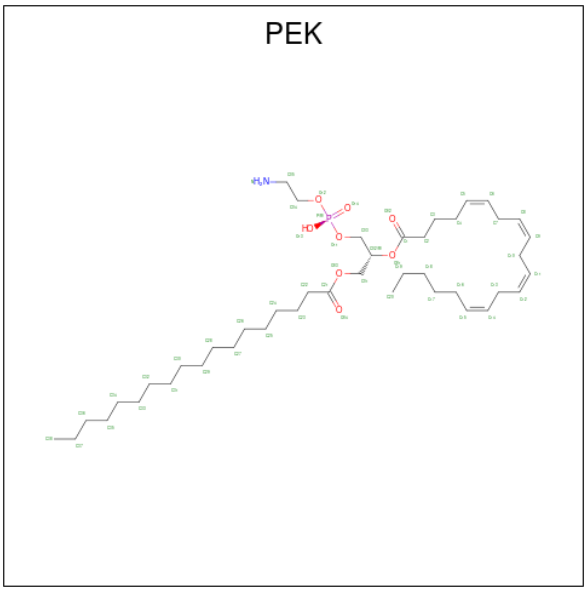


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
24	C	1	33	22	11	0	0
24	M	1	33	22	11	0	0
24	P	1	33	22	11	0	0
24	Z	1	33	22	11	0	0

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

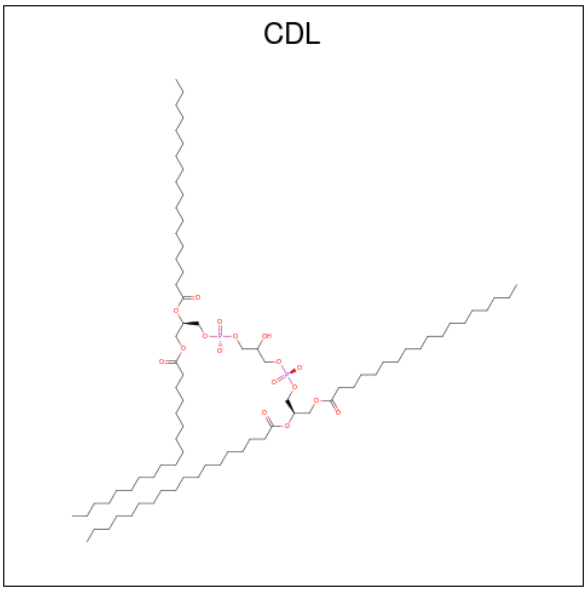
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
25	C	1	1	1	0	0
			Total	X		
25	P	1	1	1	0	0

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

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

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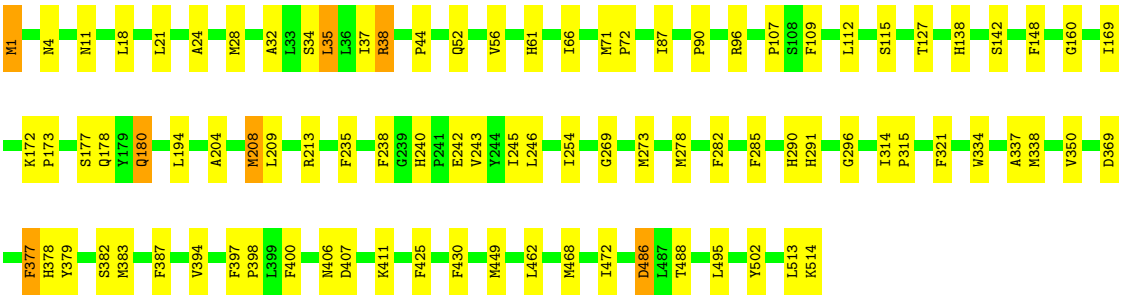
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Y	17	Total O 17 17	0	0
29	Z	8	Total O 8 8	0	0

3 Residue-property plots (i)

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.

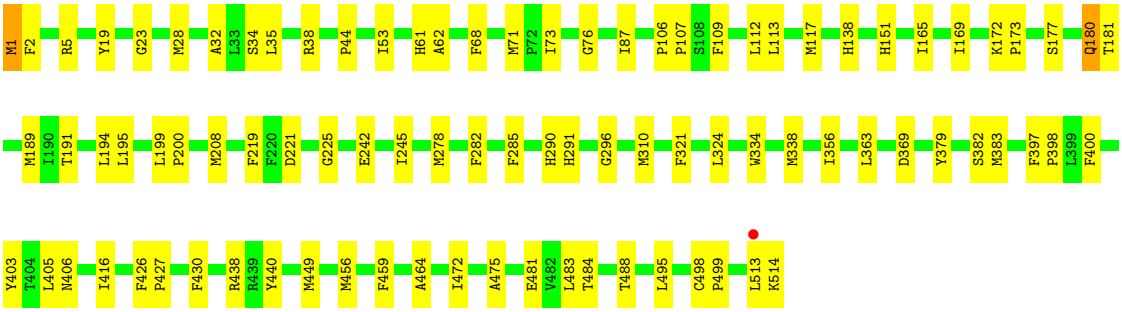
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



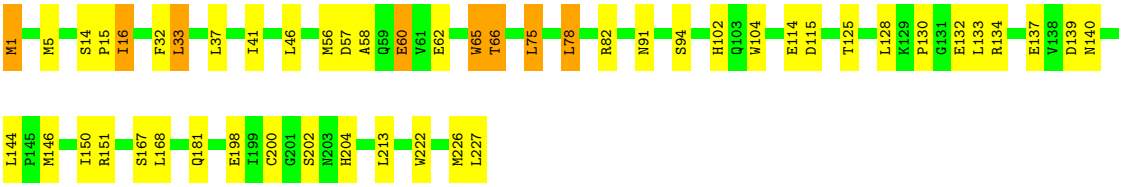
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



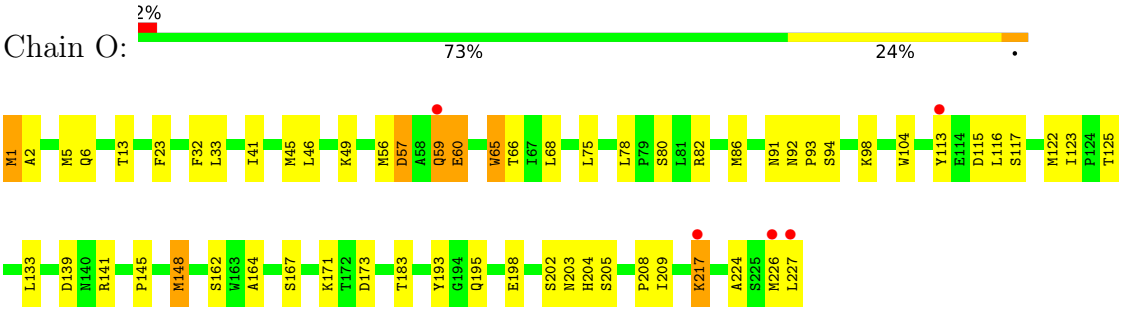
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



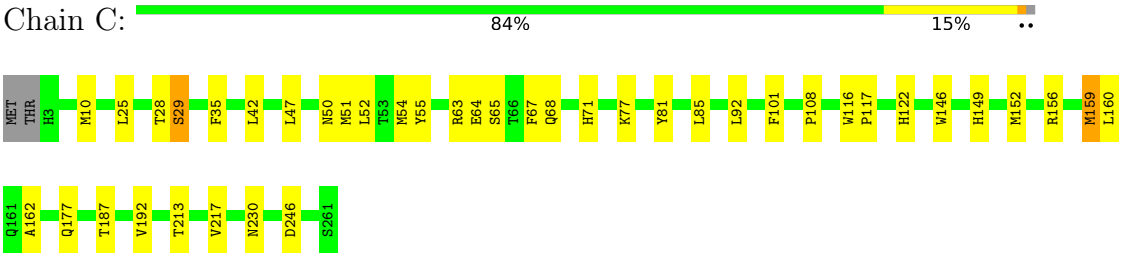
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



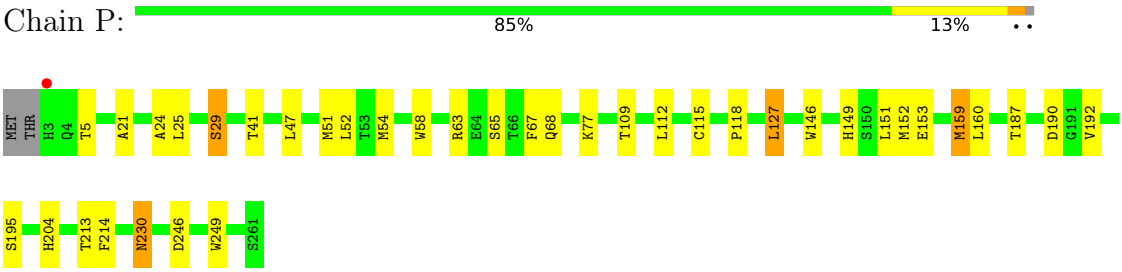
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



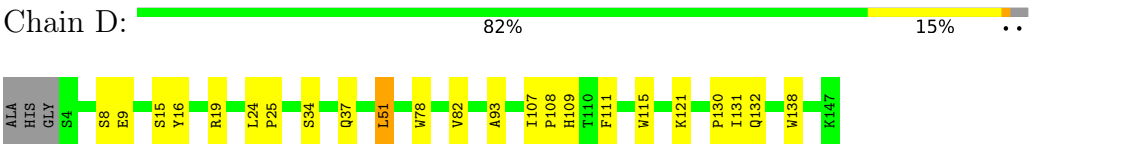
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



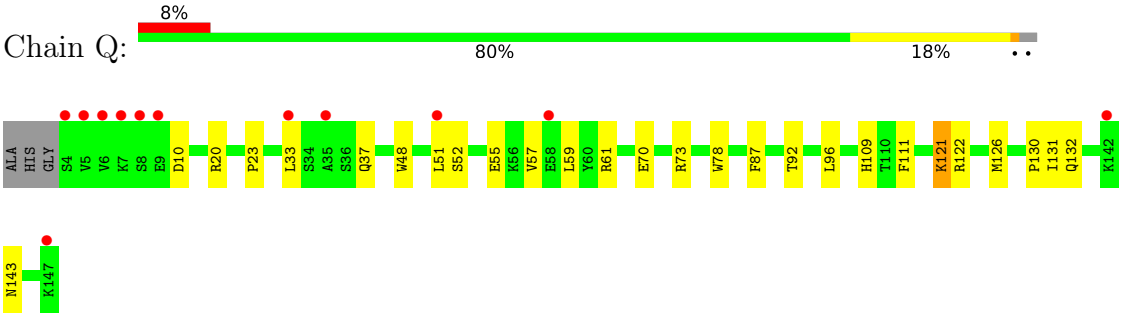
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



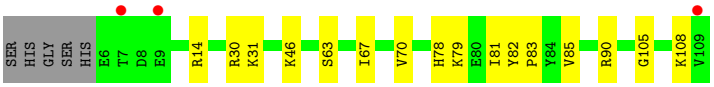
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



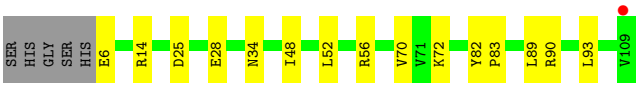
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:



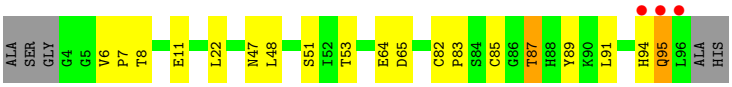
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:



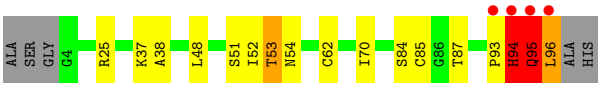
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain F:



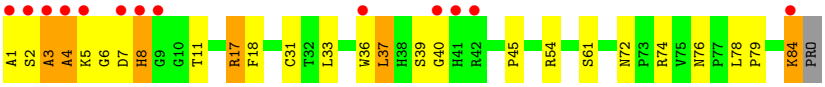
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain S:



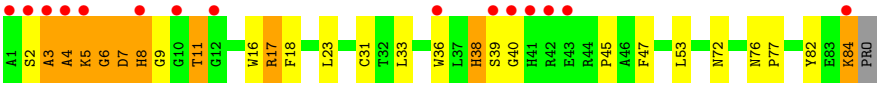
• Molecule 7: Cytochrome c oxidase polypeptide 6A2

Chain G:



• Molecule 7: Cytochrome c oxidase polypeptide 6A2

Chain T:

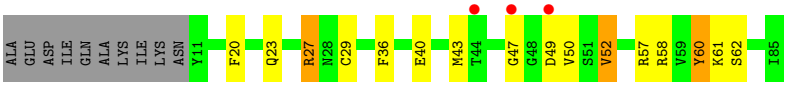


• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:

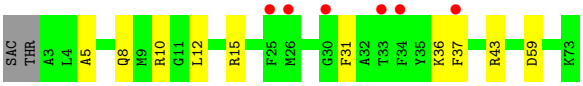
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:



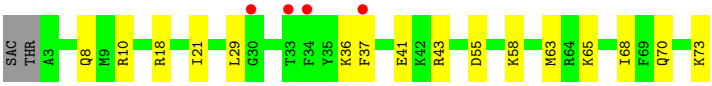
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



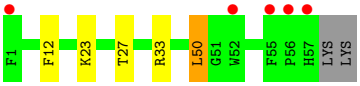
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



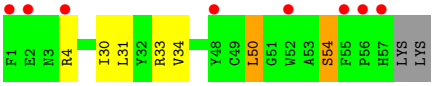
• Molecule 10: Cytochrome c oxidase polypeptide 7A1

Chain J:



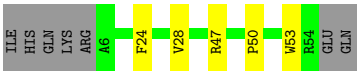
• Molecule 10: Cytochrome c oxidase polypeptide 7A1

Chain W:



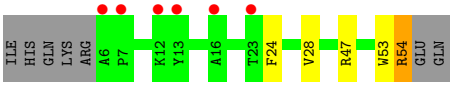
• Molecule 11: Cytochrome c oxidase polypeptide 7B

Chain K:



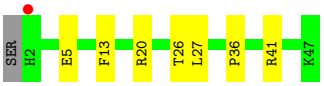
• Molecule 11: Cytochrome c oxidase polypeptide 7B

Chain X:



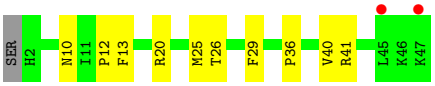
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:



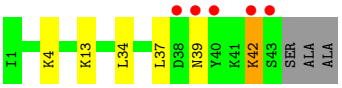
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:



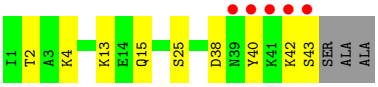
• Molecule 13: Cytochrome c oxidase polypeptide 8H

Chain M:



• Molecule 13: Cytochrome c oxidase polypeptide 8H

Chain Z:



4 Data and refinement statistics (i)

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 38.33 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.50) 91.1 (38.33-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CUA, MG, PGV, PER, DMU, FME, UNX, NA, CHD, HEA, CU, CDL, PEK, TPO, TGL, 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	1.01	0/4156	0.85	5/5678 (0.1%)
1	N	0.96	0/4156	0.81	3/5678 (0.1%)
2	B	0.97	1/1860 (0.1%)	0.91	2/2534 (0.1%)
2	O	0.91	1/1860 (0.1%)	0.90	0/2534
3	C	0.98	1/2197 (0.0%)	0.77	0/3005
3	P	0.93	1/2197 (0.0%)	0.81	1/3005 (0.0%)
4	D	0.99	0/1229	0.82	1/1658 (0.1%)
4	Q	0.84	0/1229	0.76	0/1658
5	E	0.94	0/860	0.87	1/1167 (0.1%)
5	R	0.85	0/860	0.78	0/1167
6	F	0.89	0/733	0.94	0/996
6	S	0.83	0/733	0.93	1/996 (0.1%)
7	G	0.98	1/690 (0.1%)	0.88	0/937
7	T	0.94	2/690 (0.3%)	0.88	2/937 (0.2%)
8	H	0.96	0/648	0.82	1/877 (0.1%)
8	U	0.82	0/648	0.73	0/877
9	I	1.00	0/598	0.89	1/792 (0.1%)
9	V	0.93	0/598	0.79	0/792
10	J	0.87	0/462	0.76	0/625
10	W	0.80	0/462	0.82	0/625
11	K	0.97	0/398	0.85	0/546
11	X	0.81	0/398	0.76	0/546
12	L	0.96	0/393	0.85	1/526 (0.2%)
12	Y	0.81	0/393	0.78	0/526
13	M	0.96	0/345	0.80	0/470
13	Z	0.75	0/345	0.69	0/470
All	All	0.94	7/29138 (0.0%)	0.83	19/39622 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	7.94	1.64	1.50
2	B	198	GLU	C-O	6.96	1.36	1.23
7	T	36	TRP	CB-CG	6.95	1.62	1.50
2	O	198	GLU	C-O	6.42	1.35	1.23
7	T	5	LYS	CB-CG	5.51	1.67	1.52
3	P	115	CYS	CB-SG	5.49	1.91	1.82
3	C	101	PHE	CE1-CZ	5.24	1.47	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	MET	CG-SD-CE	7.33	111.93	100.20
1	A	35	LEU	CB-CG-CD1	-6.52	99.91	111.00
3	P	152	MET	CG-SD-CE	6.22	110.15	100.20
6	S	94	HIS	N-CA-C	6.16	127.62	111.00
1	A	96	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	96	ARG	NE-CZ-NH1	6.13	123.37	120.30
9	I	59	ASP	CB-CG-OD1	-5.34	113.49	118.30
7	T	33	LEU	CA-CB-CG	5.33	127.55	115.30
1	N	221	ASP	CB-CG-OD1	5.31	123.08	118.30
1	N	221	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	B	75	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	486	ASP	CB-CG-OD1	5.22	123.00	118.30
8	H	27	ARG	NE-CZ-NH1	5.17	122.88	120.30
4	D	51	LEU	CA-CB-CG	5.16	127.17	115.30
1	N	438	ARG	NE-CZ-NH2	-5.16	117.72	120.30
12	L	41	ARG	NE-CZ-NH1	5.10	122.85	120.30
7	T	6	GLY	N-CA-C	5.10	125.85	113.10
2	B	82	ARG	NE-CZ-NH2	-5.04	117.78	120.30
5	E	14	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	69	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	35	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	34	0
3	P	2110	0	2027	31	0
4	D	1195	0	1183	23	0
4	Q	1195	0	1183	22	0
5	E	842	0	838	9	0
5	R	842	0	838	8	0
6	F	717	0	700	11	0
6	S	717	0	700	12	0
7	G	675	0	644	24	0
7	T	675	0	644	37	0
8	H	628	0	580	7	0
8	U	628	0	580	12	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	5	0
11	K	384	0	366	5	0
11	X	384	0	366	7	0
12	L	380	0	380	11	0
12	Y	380	0	380	9	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	N	1	0	0	0	0
18	A	120	0	108	12	0
18	N	120	0	108	8	0
19	A	102	0	152	5	0
19	C	102	0	152	5	0
19	N	153	0	228	12	0
19	P	51	0	76	5	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
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	4	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	17	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	578	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 9.

All (578) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.50	0.94
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
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
18:A:515:HEA:HBC1	18:A:515:HEA:HMC1	1.78	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
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
18:N:516:HEA:HMC1	18:N:516:HEA:HBC1	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
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
8:U:43:MET:HE2	8:U:52:VAL:HG21	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:O:82:ARG:HG2	2:O:86:MET:HE3	1.86	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.88	0.55
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.41	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
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
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
5:E:105:GLY:O	5:E:108:LYS:HG2	2.07	0.53
8:H:60:TYR:CD1	8:H:60:TYR:C	2.81	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: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
3:C:149:HIS:HA	3:C:152:MET:HE2	1.90	0.53
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.90	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
21:N:1522:TGL:HC62	21:N:1522:TGL:CC2	2.18	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
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: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
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:H152	19:A:524:PGV:H321	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:524:PGV:P	19:A:524:PGV:H061	2.51	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
26:G:1263:PEK:H042	3:P:77:LYS:HZ1	1.77	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: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
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
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
6:S:52:ILE:C	6:S:94:HIS:CE1	2.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE22	1.61	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.31	0.45
27:G:269:CDL:H222	27:G:269:CDL:H252	1.73	0.45
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.97	0.45
1:N:472:ILE:HG21	21:N:1522:TGL:HA91	1.97	0.45
18:A:516:HEA:HBC1	18:A:516:HEA:HMC1	1.98	0.45
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.50	0.45
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
1:A:468:MET:CE	18:A:515:HEA:H212	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1:A:1:FME:HA	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:1:FME:HA	1:A:1:FME:HE2	2.00	0.44
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
3:C:116:TRP:HA	3:C:117:PRO:C	2.38	0.44
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.00	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
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
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:HA21	27:T:1269:CDL:H111	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:50:ASN:HD21	3:C:54:MET:HE1	1.83	0.43
2:O:13:THR:HG22	2:O:13:THR:O	2.18	0.43
4:Q:132:GLN:OE1	9:V:43:ARG:HD3	2.18	0.43
3:C:50:ASN:ND2	3:C:54:MET:CE	2.81	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
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
1:N:28:MET:HE2	18:N:515:HEA:H271	2.01	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
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.17	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
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
21:L:522:TGL:CC6	21:L:522:TGL:HC22	2.48	0.43
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:28:MET:HE3	18:A:515:HEA:H271	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.18	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
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
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:N:324:LEU:HD13	2:O:41:ILE:CG2	2.49	0.42
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
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
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
1:N:169:ILE:N	1:N:169:ILE:HD13	2.34	0.41
3:P:63:ARG:O	3:P:68:GLN:HG3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:486:ASP:OD2	4:D:19:ARG:HD3	2.20	0.41
3:C:159:MET:SD	3:C:159:MET:C	2.99	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
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:35:PHE:HA	7:G:61:SER:OG	2.21	0.41
4:D:9:GLU:H	4:D:9:GLU:CD	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:T:31:CYS:SG	27:T:1269:CDL:H551	2.61	0.40
3:C:50:ASN:HD21	3:C:54:MET:CE	2.33	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
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
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.22	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
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%)	12	21
2	O	225/227 (99%)	210 (93%)	12 (5%)	3 (1%)	12	21
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
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%)	15	28
5	R	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	14	26
6	S	91/98 (93%)	84 (92%)	5 (6%)	2 (2%)	6	10
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	0	0
7	T	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	1
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	3	3
8	U	73/85 (86%)	68 (93%)	4 (6%)	1 (1%)	11	20
9	I	69/73 (94%)	64 (93%)	4 (6%)	1 (1%)	11	20
9	V	69/73 (94%)	66 (96%)	2 (3%)	1 (1%)	11	20
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3478/3614 (96%)	3315 (95%)	132 (4%)	31 (1%)	17	31

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
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 (i)

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%)	416 (98%)	10 (2%)	50	76
1	N	426/426 (100%)	416 (98%)	10 (2%)	50	76
2	B	210/210 (100%)	199 (95%)	11 (5%)	23	44
2	O	210/210 (100%)	192 (91%)	18 (9%)	10	20
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	71
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	77
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	84
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	76
5	E	91/95 (96%)	89 (98%)	2 (2%)	52	77
5	R	91/95 (96%)	89 (98%)	2 (2%)	52	77
6	F	79/81 (98%)	76 (96%)	3 (4%)	33	58
6	S	79/81 (98%)	73 (92%)	6 (8%)	13	25
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	13
7	T	67/68 (98%)	63 (94%)	4 (6%)	19	37
8	H	67/75 (89%)	61 (91%)	6 (9%)	9	19
8	U	67/75 (89%)	62 (92%)	5 (8%)	13	26
9	I	56/57 (98%)	53 (95%)	3 (5%)	22	42
9	V	56/57 (98%)	52 (93%)	4 (7%)	14	28
10	J	48/50 (96%)	46 (96%)	2 (4%)	30	54
10	W	48/50 (96%)	45 (94%)	3 (6%)	18	34
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	72
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	45
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	72
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	72
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	12
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3022/3082 (98%)	2898 (96%)	124 (4%)	30 55

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	338	MET
1	A	369	ASP
1	A	377	PHE
1	A	382	SER
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
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	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	53	THR
6	F	87	THR
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU

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Mol	Chain	Res	Type
7	G	37	LEU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	27	ARG
8	H	29	CYS
8	H	40	GLU
8	H	51	SER
8	H	60	TYR
8	H	70	SER
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	27	THR
10	J	50	LEU
11	K	47	ARG
12	L	26	THR
13	M	13	LYS
13	M	34	LEU
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	180	GLN
1	N	338	MET
1	N	363	LEU
1	N	369	ASP
1	N	382	SER
1	N	484	THR
1	N	513	LEU
2	O	32	PHE
2	O	33	LEU
2	O	57	ASP
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER

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Mol	Chain	Res	Type
2	O	113	TYR
2	O	115	ASP
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	127	LEU
3	P	159	MET
3	P	230	ASN
4	Q	10	ASP
4	Q	121	LYS
4	Q	143	ASN
5	R	70	VAL
5	R	90	ARG
6	S	37	LYS
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	18	PHE
7	T	38	HIS
7	T	84	LYS
8	U	27	ARG
8	U	29	CYS
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	29	LEU
10	W	4	ARG
10	W	50	LEU
10	W	54	SER
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG

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Mol	Chain	Res	Type
13	Z	13	LYS
13	Z	38	ASP
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
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	149	HIS
4	D	37	GLN
4	D	109	HIS
5	E	78	HIS
5	E	94	ASN
7	G	76	ASN
8	H	22	ASN
9	I	8	GLN
10	J	29	ASN
11	K	35	GLN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	52	HIS
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
3	P	70	HIS
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS
4	Q	143	ASN

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Mol	Chain	Res	Type
5	R	78	HIS
5	R	94	ASN
6	S	94	HIS
7	T	66	ASN
7	T	71	HIS
7	T	76	ASN
11	X	35	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	2.87	3 (42%)
1	FME	N	1	1	8,9,10	0.57	0	7,9,11	3.28	3 (42%)
7	TPO	G	11	7	8,10,11	2.00	2 (25%)	10,14,16	1.38	3 (30%)
1	FME	A	1	1	8,9,10	0.70	0	7,9,11	2.49	3 (42%)
7	TPO	T	11	7	8,10,11	1.81	2 (25%)	10,14,16	1.66	2 (20%)
2	FME	B	1	2	8,9,10	0.85	0	7,9,11	3.35	2 (28%)

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
2	FME	O	1	2	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	6/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.40	1.65	1.59
7	T	11	TPO	P-O1P	3.23	1.61	1.50
7	G	11	TPO	P-O1P	2.83	1.59	1.50
7	T	11	TPO	P-OG1	2.57	1.64	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
2	O	1	FME	C-CA-N	4.17	117.26	109.73
7	T	11	TPO	CG2-CB-CA	4.07	121.20	113.16
1	N	1	FME	CE-SD-CG	3.98	114.07	100.40
1	A	1	FME	CE-SD-CG	3.97	114.05	100.40
2	B	1	FME	C-CA-N	3.87	116.71	109.73
1	A	1	FME	O1-CN-N	-2.51	118.66	125.27
7	G	11	TPO	O2P-P-OG1	2.46	117.03	105.99
1	N	1	FME	O-C-CA	-2.35	118.63	124.78
2	O	1	FME	CE-SD-CG	2.28	108.23	100.40
7	T	11	TPO	O-C-CA	-2.08	119.31	124.78
7	G	11	TPO	O-C-CA	-2.07	119.36	124.78
7	G	11	TPO	CG2-CB-CA	2.03	117.17	113.16

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
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
1	N	1	FME	CA-CB-CG-SD
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 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	3	0
1	N	1	FME	1	0
1	A	1	FME	3	0
7	T	11	TPO	1	0
2	B	1	FME	3	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	0.88	2 (4%)	53,56,56	1.02	3 (5%)
21	TGL	D	523	-	62,62,62	1.46	6 (9%)	65,65,65	1.47	13 (20%)
24	DMU	C	272	-	34,34,34	1.19	2 (5%)	45,45,45	3.27	23 (51%)
23	CHD	G	86	-	32,32,32	1.10	2 (6%)	51,51,51	5.01	33 (64%)
27	CDL	G	269	-	99,99,99	1.39	11 (11%)	105,111,111	1.25	10 (9%)
15	PER	N	520	14,18	0,1,1	-	-	-		
23	CHD	J	60	-	32,32,32	0.97	2 (6%)	51,51,51	4.89	33 (64%)
24	DMU	Z	1526	-	34,34,34	0.96	2 (5%)	45,45,45	3.13	19 (42%)
24	DMU	M	526	-	34,34,34	0.80	2 (5%)	45,45,45	3.08	23 (51%)
18	HEA	N	515	1	57,67,67	1.39	6 (10%)	61,103,103	2.07	16 (26%)
23	CHD	C	525	-	32,32,32	1.20	2 (6%)	51,51,51	4.89	35 (68%)
19	PGV	C	267	-	50,50,50	0.86	2 (4%)	53,56,56	1.18	4 (7%)
23	CHD	P	1271	-	32,32,32	0.84	0	51,51,51	4.89	30 (58%)
23	CHD	B	1086	-	32,32,32	1.22	3 (9%)	51,51,51	5.29	34 (66%)
24	DMU	P	1272	-	34,34,34	1.20	2 (5%)	45,45,45	3.19	22 (48%)
20	CUA	O	228	2	0,1,1	-	-	-		
21	TGL	N	1522	-	62,62,62	1.51	6 (9%)	65,65,65	1.36	9 (13%)
21	TGL	L	522	-	62,62,62	1.37	5 (8%)	65,65,65	1.48	7 (10%)
19	PGV	N	1266	-	50,50,50	0.94	3 (6%)	53,56,56	1.37	6 (11%)
22	PSC	B	230	-	51,51,51	1.29	3 (5%)	57,59,59	1.21	6 (10%)
19	PGV	N	1268	-	50,50,50	1.20	2 (4%)	53,56,56	1.36	5 (9%)
26	PEK	C	265	-	52,52,52	1.36	4 (7%)	55,57,57	1.24	4 (7%)
15	PER	A	520	14,18	0,1,1	-	-	-		
26	PEK	P	1265	-	52,52,52	1.53	4 (7%)	55,57,57	1.24	4 (7%)
22	PSC	O	1230	-	51,51,51	1.22	3 (5%)	57,59,59	1.07	2 (3%)
19	PGV	C	268	-	50,50,50	1.19	2 (4%)	53,56,56	1.31	4 (7%)
21	TGL	B	521	-	62,62,62	1.29	6 (9%)	65,65,65	1.68	10 (15%)
19	PGV	N	1524	-	50,50,50	1.13	2 (4%)	53,56,56	1.20	5 (9%)
21	TGL	N	1521	-	62,62,62	1.47	7 (11%)	65,65,65	1.60	13 (20%)
18	HEA	A	516	1,15	57,67,67	2.33	17 (29%)	61,103,103	4.27	33 (54%)
19	PGV	A	521	-	50,50,50	1.09	2 (4%)	53,56,56	1.26	5 (9%)
26	PEK	T	263	-	52,52,52	1.44	6 (11%)	55,57,57	1.35	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	PGV	A	524	-	50,50,50	1.18	2 (4%)	53,56,56	1.19	5 (9%)
18	HEA	N	516	1,15	57,67,67	1.62	14 (24%)	61,103,103	1.81	14 (22%)
27	CDL	P	1270	-	99,99,99	1.35	11 (11%)	105,111,111	1.28	12 (11%)
23	CHD	W	1060	-	32,32,32	1.14	3 (9%)	51,51,51	5.09	34 (66%)
21	TGL	O	1523	-	62,62,62	1.41	6 (9%)	65,65,65	1.22	9 (13%)
23	CHD	P	1525	-	32,32,32	0.95	1 (3%)	51,51,51	5.12	37 (72%)
27	CDL	C	270	-	99,99,99	1.36	13 (13%)	105,111,111	1.33	11 (10%)
26	PEK	G	264	-	52,52,52	0.97	3 (5%)	55,57,57	1.24	5 (9%)
23	CHD	C	271	-	32,32,32	0.85	0	51,51,51	4.76	33 (64%)
27	CDL	T	1269	-	99,99,99	1.34	11 (11%)	105,111,111	1.41	10 (9%)
18	HEA	A	515	1	57,67,67	1.42	10 (17%)	61,103,103	2.19	21 (34%)
26	PEK	G	1263	-	52,52,52	1.30	2 (3%)	55,57,57	1.23	5 (9%)
20	CUA	B	228	2	0,1,1	-	-	-		
26	PEK	P	1264	-	52,52,52	0.97	4 (7%)	55,57,57	1.51	7 (12%)

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	-
21	TGL	D	523	-	-	37/65/65/65	-
24	DMU	C	272	-	5/5/10/10	11/19/59/59	0/2/2/2
23	CHD	G	86	-	1/1/12/12	3/9/74/74	0/4/4/4
27	CDL	G	269	-	-	63/110/110/110	-
24	DMU	Z	1526	-	5/5/10/10	11/19/59/59	0/2/2/2
23	CHD	J	60	-	1/1/12/12	7/9/74/74	0/4/4/4
24	DMU	M	526	-	5/5/10/10	10/19/59/59	0/2/2/2
18	HEA	N	515	1	-	7/32/76/76	-
23	CHD	C	525	-	1/1/12/12	2/9/74/74	0/4/4/4
19	PGV	C	267	-	-	17/55/55/55	-
24	DMU	P	1272	-	5/5/10/10	12/19/59/59	0/2/2/2
23	CHD	P	1271	-	2/2/12/12	8/9/74/74	0/4/4/4
23	CHD	B	1086	-	1/1/12/12	3/9/74/74	0/4/4/4
21	TGL	N	1522	-	-	34/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	L	522	-	-	35/65/65/65	-
19	PGV	N	1266	-	-	14/55/55/55	-
22	PSC	B	230	-	-	28/55/55/55	-
19	PGV	N	1268	-	-	28/55/55/55	-
26	PEK	C	265	-	-	28/56/56/56	-
26	PEK	P	1265	-	-	28/56/56/56	-
22	PSC	O	1230	-	-	35/55/55/55	-
19	PGV	C	268	-	-	34/55/55/55	-
21	TGL	B	521	-	-	32/65/65/65	-
19	PGV	N	1524	-	-	36/55/55/55	-
21	TGL	N	1521	-	-	28/65/65/65	-
18	HEA	A	516	1,15	-	6/32/76/76	-
19	PGV	A	521	-	-	14/55/55/55	-
26	PEK	T	263	-	-	30/56/56/56	-
19	PGV	A	524	-	-	32/55/55/55	-
18	HEA	N	516	1,15	-	5/32/76/76	-
27	CDL	P	1270	-	-	62/110/110/110	-
23	CHD	W	1060	-	1/1/12/12	7/9/74/74	0/4/4/4
23	CHD	P	1525	-	1/1/12/12	2/9/74/74	0/4/4/4
21	TGL	O	1523	-	-	33/65/65/65	-
27	CDL	C	270	-	-	69/110/110/110	-
26	PEK	G	264	-	-	24/56/56/56	-
23	CHD	C	271	-	2/2/12/12	8/9/74/74	0/4/4/4
27	CDL	T	1269	-	-	62/110/110/110	-
18	HEA	A	515	1	-	7/32/76/76	-
26	PEK	G	1263	-	-	33/56/56/56	-
26	PEK	P	1264	-	-	26/56/56/56	-

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C4D-C3D	-6.68	1.33	1.45
26	T	263	PEK	O03-C21	6.01	1.50	1.33
19	A	524	PGV	O03-C19	5.74	1.50	1.33
21	N	1522	TGL	OG2-CB1	5.69	1.50	1.34
21	N	1522	TGL	OG1-CA1	5.66	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	523	TGL	OG3-CC1	5.56	1.49	1.33
18	A	516	HEA	C4B-NB	-5.55	1.30	1.40
19	N	1268	PGV	O01-C1	5.51	1.49	1.34
26	G	1263	PEK	O03-C21	5.49	1.49	1.33
21	L	522	TGL	OG1-CA1	5.43	1.49	1.33
18	A	516	HEA	CHD-C1D	5.41	1.48	1.35
27	P	1270	CDL	OA8-CA7	5.37	1.49	1.33
19	C	268	PGV	O01-C1	5.34	1.49	1.34
21	L	522	TGL	OG2-CB1	5.28	1.49	1.34
26	T	263	PEK	O01-C1	5.26	1.49	1.34
19	N	1524	PGV	O03-C19	5.25	1.48	1.33
18	A	516	HEA	FE-ND	5.25	2.22	1.96
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	5.24	1.49	1.34
26	C	265	PEK	O03-C21	5.23	1.48	1.33
22	B	230	PSC	O01-C1	5.20	1.49	1.34
26	P	1265	PEK	O03-C21	5.17	1.48	1.33
27	G	269	CDL	OA6-CA5	5.16	1.48	1.34
21	N	1521	TGL	OG1-CA1	5.13	1.48	1.33
27	T	1269	CDL	OB6-CB5	5.12	1.48	1.34
27	C	270	CDL	OA8-CA7	5.12	1.48	1.33
26	P	1265	PEK	O01-C1	5.04	1.48	1.34
27	G	269	CDL	OB8-CB7	5.02	1.48	1.33
21	D	523	TGL	OG1-CA1	4.97	1.47	1.33
27	T	1269	CDL	OB8-CB7	4.95	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	4.82	1.47	1.33
21	N	1521	TGL	OG2-CB1	4.80	1.47	1.34
26	C	265	PEK	O01-C1	4.76	1.47	1.34
27	P	1270	CDL	OB8-CB7	4.72	1.47	1.33
21	B	521	TGL	OG1-CA1	4.69	1.47	1.33
21	O	1523	TGL	OG3-CC1	4.69	1.47	1.33
18	A	516	HEA	C4B-C3B	-4.67	1.36	1.44
19	A	521	PGV	O03-C19	4.65	1.46	1.33
24	P	1272	DMU	O16-C6	4.63	1.48	1.40
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	4.58	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	521	TGL	OG2-CB1	4.56	1.47	1.34
18	A	516	HEA	CAA-C2A	4.49	1.60	1.52
27	C	270	CDL	OB8-CB7	4.44	1.46	1.33
18	N	516	HEA	CHD-C1D	4.37	1.46	1.35
21	N	1521	TGL	OG3-CC1	4.37	1.46	1.33
21	N	1522	TGL	OG3-CC1	4.36	1.46	1.33
18	A	516	HEA	C4D-ND	-4.36	1.29	1.38
19	C	268	PGV	O03-C19	4.36	1.46	1.33
19	N	1266	PGV	O03-C19	4.34	1.46	1.33
27	G	269	CDL	OA8-CA7	4.34	1.46	1.33
27	P	1270	CDL	OB6-CB5	4.34	1.46	1.34
19	N	1268	PGV	O03-C19	4.32	1.46	1.33
24	C	272	DMU	O16-C6	4.29	1.47	1.40
22	O	1230	PSC	O01-C1	4.24	1.46	1.34
27	T	1269	CDL	OA8-CA7	4.22	1.45	1.33
22	O	1230	PSC	C13-C12	4.18	1.56	1.31
19	N	1524	PGV	O01-C1	4.14	1.46	1.34
19	P	1267	PGV	O03-C19	4.03	1.45	1.33
27	C	270	CDL	OB6-CB5	4.00	1.45	1.34
22	B	230	PSC	C13-C12	3.96	1.54	1.31
26	G	264	PEK	O01-C1	3.95	1.45	1.34
19	A	524	PGV	O01-C1	3.92	1.45	1.34
22	O	1230	PSC	O03-C19	3.92	1.44	1.33
18	A	516	HEA	CHB-C1B	3.88	1.52	1.41
18	A	516	HEA	CHC-C4B	3.88	1.44	1.35
21	N	1521	TGL	CA6-CA5	3.81	1.73	1.51
19	C	267	PGV	O03-C19	3.79	1.44	1.33
21	L	522	TGL	OG3-CC1	3.73	1.44	1.33
26	P	1264	PEK	O01-C1	3.68	1.44	1.34
18	N	515	HEA	CHC-C4B	3.65	1.44	1.35
21	B	521	TGL	OG3-CC1	3.59	1.43	1.33
18	N	516	HEA	CHC-C4B	3.48	1.43	1.35
18	A	515	HEA	C1D-ND	-3.45	1.34	1.40
18	A	515	HEA	CHC-C4B	3.33	1.43	1.35
18	A	515	HEA	CHD-C1D	3.33	1.43	1.35
18	N	515	HEA	CHD-C1D	3.32	1.43	1.35
23	B	1086	CHD	C13-C14	-3.31	1.49	1.55
18	N	516	HEA	O11-C11	3.29	1.50	1.42
27	C	270	CDL	C59-C58	-3.21	1.33	1.51
21	L	522	TGL	C20-CA9	-3.21	1.33	1.51
21	N	1521	TGL	C10-CB9	-3.19	1.33	1.51
23	C	525	CHD	C18-C13	3.19	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	267	PGV	O01-C1	3.18	1.43	1.34
18	N	515	HEA	C4D-C3D	-3.17	1.39	1.45
21	L	522	TGL	C10-CB9	-3.15	1.33	1.51
24	Z	1526	DMU	C3-C4	-3.12	1.44	1.52
21	N	1522	TGL	C20-CA9	-3.09	1.34	1.51
26	P	1264	PEK	O03-C01	-3.09	1.38	1.45
27	P	1270	CDL	C59-C58	-3.05	1.34	1.51
27	P	1270	CDL	C62-C61	-3.03	1.34	1.51
27	G	269	CDL	C42-C41	-3.02	1.34	1.51
21	N	1522	TGL	C10-CB9	-3.00	1.34	1.51
27	G	269	CDL	C39-C38	-2.98	1.34	1.51
23	W	1060	CHD	C11-C9	2.97	1.58	1.53
21	D	523	TGL	C15-CC9	-2.97	1.34	1.51
27	G	269	CDL	C59-C58	-2.96	1.34	1.51
27	C	270	CDL	C79-C78	-2.96	1.34	1.51
18	N	515	HEA	C1D-ND	-2.96	1.35	1.40
21	B	521	TGL	C10-CB9	-2.93	1.35	1.51
21	O	1523	TGL	C15-CC9	-2.93	1.35	1.51
26	G	264	PEK	O03-C21	2.91	1.41	1.33
27	P	1270	CDL	C22-C21	-2.89	1.35	1.51
27	P	1270	CDL	C19-C18	-2.87	1.35	1.51
27	T	1269	CDL	C62-C61	-2.87	1.35	1.51
27	G	269	CDL	C19-C18	-2.86	1.35	1.51
21	N	1521	TGL	C20-CA9	-2.85	1.35	1.51
18	A	516	HEA	C1C-CHC	2.84	1.48	1.41
21	O	1523	TGL	C10-CB9	-2.83	1.35	1.51
27	T	1269	CDL	C19-C18	-2.83	1.35	1.51
27	C	270	CDL	C62-C61	-2.82	1.35	1.51
27	G	269	CDL	C62-C61	-2.81	1.35	1.51
27	C	270	CDL	C22-C21	-2.80	1.35	1.51
21	B	521	TGL	C20-CA9	-2.80	1.35	1.51
18	N	516	HEA	C4B-NB	-2.79	1.35	1.40
26	P	1265	PEK	C6-C5	2.78	1.47	1.31
27	T	1269	CDL	C42-C41	-2.78	1.36	1.51
19	N	1266	PGV	O01-C1	2.76	1.42	1.34
24	M	526	DMU	C3-C4	-2.74	1.45	1.52
18	A	516	HEA	C4C-NC	-2.73	1.30	1.36
18	N	515	HEA	C4B-NB	-2.73	1.35	1.40
27	C	270	CDL	C39-C38	-2.72	1.36	1.51
23	B	1086	CHD	C10-C5	-2.72	1.51	1.55
21	D	523	TGL	C20-CA9	-2.72	1.36	1.51
18	N	516	HEA	C1D-ND	-2.71	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
27	T	1269	CDL	C39-C38	-2.70	1.36	1.51
21	D	523	TGL	C10-CB9	-2.69	1.36	1.51
21	N	1522	TGL	C15-CC9	-2.66	1.36	1.51
18	A	516	HEA	C3A-CMA	2.66	1.52	1.46
27	T	1269	CDL	C59-C58	-2.65	1.36	1.51
27	C	270	CDL	C42-C41	-2.64	1.36	1.51
23	C	525	CHD	C13-C14	-2.64	1.51	1.55
18	A	515	HEA	C1B-NB	-2.61	1.33	1.38
27	C	270	CDL	C19-C18	-2.58	1.37	1.51
26	G	264	PEK	O03-C01	-2.58	1.39	1.45
27	C	270	CDL	C82-C81	-2.58	1.37	1.51
21	N	1521	TGL	C15-CC9	-2.55	1.37	1.51
21	O	1523	TGL	C20-CA9	-2.55	1.37	1.51
26	P	1264	PEK	O03-C21	2.54	1.40	1.33
26	C	265	PEK	C05-C04	2.52	1.60	1.50
23	W	1060	CHD	C20-C17	2.50	1.58	1.54
24	Z	1526	DMU	O16-C6	2.49	1.44	1.40
27	G	269	CDL	C82-C81	-2.48	1.37	1.51
27	T	1269	CDL	C22-C21	-2.47	1.37	1.51
18	A	516	HEA	C20-C19	2.46	1.56	1.51
21	B	521	TGL	C15-CC9	-2.46	1.37	1.51
18	N	516	HEA	C3D-C2D	2.44	1.41	1.36
27	P	1270	CDL	C39-C38	-2.44	1.37	1.51
23	P	1525	CHD	C13-C14	-2.43	1.51	1.55
27	T	1269	CDL	C82-C81	-2.41	1.38	1.51
24	C	272	DMU	O1-C10	2.41	1.48	1.41
18	A	516	HEA	C3C-CAC	2.38	1.52	1.47
18	N	516	HEA	C4B-C3B	-2.36	1.40	1.44
18	A	515	HEA	C4D-C3D	-2.35	1.41	1.45
18	A	516	HEA	OMA-CMA	2.34	1.29	1.21
18	A	515	HEA	C1D-C2D	-2.34	1.40	1.44
26	C	265	PEK	P-O12	2.32	1.68	1.59
18	A	515	HEA	C4B-NB	-2.31	1.36	1.40
18	N	516	HEA	C22-C23	2.30	1.39	1.32
23	G	86	CHD	C11-C9	2.29	1.57	1.53
18	A	515	HEA	FE-NB	2.29	2.08	1.96
18	N	516	HEA	FE-NB	2.29	2.08	1.96
18	N	516	HEA	C1B-NB	-2.28	1.34	1.38
18	A	515	HEA	O11-C11	2.28	1.47	1.42
18	A	516	HEA	CAD-C3D	2.26	1.57	1.51
18	N	516	HEA	C18-C19	2.25	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1086	CHD	C13-C12	-2.23	1.51	1.54
24	P	1272	DMU	O1-C10	2.20	1.47	1.41
23	G	86	CHD	C10-C5	-2.18	1.51	1.55
18	N	515	HEA	C3B-C2B	2.16	1.39	1.34
18	N	516	HEA	C3C-C2C	-2.15	1.37	1.40
27	C	270	CDL	OB6-CB4	-2.15	1.41	1.46
27	P	1270	CDL	C42-C41	-2.13	1.39	1.51
27	G	269	CDL	C22-C21	-2.12	1.39	1.51
26	T	263	PEK	C03-C02	2.12	1.57	1.50
26	P	1264	PEK	O01-C02	-2.12	1.41	1.46
18	N	516	HEA	C3B-C2B	2.12	1.39	1.34
24	M	526	DMU	O16-C6	2.11	1.43	1.40
26	T	263	PEK	C01-C02	2.10	1.57	1.50
26	T	263	PEK	P-O11	2.10	1.67	1.59
23	J	60	CHD	C11-C9	2.08	1.57	1.53
23	W	1060	CHD	O12-C12	2.05	1.47	1.43
18	A	516	HEA	C14-C15	2.04	1.37	1.33
18	A	515	HEA	C3D-C2D	2.04	1.41	1.36
23	J	60	CHD	O12-C12	2.03	1.47	1.43
27	P	1270	CDL	C82-C81	-2.03	1.40	1.51
26	T	263	PEK	C9-C8	2.02	1.43	1.31
19	N	1266	PGV	C01-C02	2.02	1.56	1.50
18	N	516	HEA	C4C-CHD	2.02	1.46	1.41

All (621) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	1086	CHD	C18-C13-C12	-13.92	94.89	109.07
23	C	271	CHD	C10-C9-C8	13.84	126.68	111.82
23	P	1271	CHD	C10-C9-C8	13.81	126.64	111.82
23	C	525	CHD	C6-C5-C10	13.26	126.73	112.66
23	P	1525	CHD	C6-C5-C10	12.43	125.86	112.66
23	C	525	CHD	C10-C9-C8	11.95	124.66	111.82
18	A	516	HEA	CMB-C2B-C1B	11.70	142.85	125.04
23	G	86	CHD	C6-C5-C10	11.45	124.82	112.66
23	B	1086	CHD	C10-C9-C8	11.17	123.81	111.82
23	P	1525	CHD	C1-C10-C5	10.94	123.94	107.77
23	B	1086	CHD	C1-C10-C5	10.83	123.78	107.77
18	A	516	HEA	CHA-C4D-C3D	-10.78	108.99	124.84
23	P	1271	CHD	C15-C14-C8	10.49	133.00	118.33
18	A	516	HEA	CMD-C2D-C1D	10.40	140.88	125.04
18	A	516	HEA	CMB-C2B-C3B	-10.33	110.64	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	1060	CHD	C13-C17-C20	10.31	131.81	119.50
23	P	1525	CHD	C14-C13-C12	10.26	116.95	107.40
23	B	1086	CHD	C14-C13-C12	10.25	116.94	107.40
23	J	60	CHD	C10-C9-C8	10.19	122.76	111.82
23	B	1086	CHD	C17-C13-C12	10.01	126.81	117.67
23	C	525	CHD	C1-C10-C5	9.95	122.48	107.77
23	G	86	CHD	C10-C9-C8	9.93	122.48	111.82
23	P	1525	CHD	C10-C9-C8	9.69	122.22	111.82
23	W	1060	CHD	C10-C9-C8	9.69	122.22	111.82
23	G	86	CHD	C18-C13-C12	-9.62	99.27	109.07
23	J	60	CHD	C15-C14-C13	9.62	112.99	103.55
23	G	86	CHD	C1-C10-C5	9.58	121.94	107.77
23	G	86	CHD	C17-C13-C12	9.44	126.28	117.67
23	C	271	CHD	C15-C14-C8	9.15	131.13	118.33
23	J	60	CHD	C16-C17-C13	9.14	112.52	103.55
18	A	516	HEA	C3D-C4D-ND	9.10	119.17	110.36
23	B	1086	CHD	C1-C2-C3	9.10	122.14	110.47
23	B	1086	CHD	C6-C5-C10	9.09	122.31	112.66
23	G	86	CHD	C14-C13-C12	9.07	115.85	107.40
23	B	1086	CHD	C19-C10-C9	-8.71	99.18	111.18
23	P	1525	CHD	C4-C3-C2	8.64	120.87	110.55
23	W	1060	CHD	C14-C8-C7	8.63	123.26	111.81
23	J	60	CHD	C13-C17-C20	8.54	129.69	119.50
24	C	272	DMU	O16-C6-C1	8.45	121.49	108.30
24	M	526	DMU	O1-C9-C8	8.43	125.01	109.69
18	A	516	HEA	CAD-C3D-C2D	8.43	143.58	127.88
23	C	525	CHD	C17-C13-C12	8.40	125.33	117.67
23	G	86	CHD	C19-C10-C9	-8.39	99.62	111.18
23	C	271	CHD	C11-C12-C13	8.38	119.85	111.24
23	W	1060	CHD	C6-C5-C4	-8.36	101.57	111.19
23	P	1525	CHD	C17-C13-C12	8.34	125.28	117.67
23	C	525	CHD	C4-C3-C2	8.28	120.44	110.55
23	P	1271	CHD	C4-C3-C2	8.16	120.29	110.55
23	G	86	CHD	C5-C4-C3	8.12	124.68	112.76
23	B	1086	CHD	C6-C7-C8	8.10	120.13	111.48
23	P	1271	CHD	C15-C14-C13	8.08	111.48	103.55
23	P	1525	CHD	C15-C14-C13	8.06	111.46	103.55
23	P	1525	CHD	C19-C10-C9	-7.97	100.20	111.18
23	W	1060	CHD	C4-C5-C10	7.95	121.10	112.66
24	P	1272	DMU	O16-C6-C1	7.95	120.71	108.30
23	C	525	CHD	C14-C13-C12	7.92	114.77	107.40
23	C	271	CHD	C5-C6-C7	7.91	123.19	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	1060	CHD	C15-C14-C13	7.86	111.26	103.55
23	C	271	CHD	C6-C7-C8	7.76	119.77	111.48
23	W	1060	CHD	C6-C7-C8	7.76	119.77	111.48
23	W	1060	CHD	C1-C2-C3	7.70	120.34	110.47
23	J	60	CHD	C1-C2-C3	7.69	120.34	110.47
23	P	1271	CHD	C6-C7-C8	7.61	119.60	111.48
23	P	1271	CHD	C5-C6-C7	7.57	122.81	114.46
23	J	60	CHD	C14-C8-C7	7.56	121.83	111.81
23	C	271	CHD	C15-C14-C13	7.42	110.83	103.55
23	P	1271	CHD	C1-C10-C5	7.38	118.68	107.77
23	P	1271	CHD	C11-C12-C13	7.36	118.81	111.24
18	A	515	HEA	C26-C15-C16	7.35	127.63	115.27
23	B	1086	CHD	C5-C4-C3	7.32	123.51	112.76
18	A	516	HEA	CAD-C3D-C4D	-7.23	112.02	124.66
23	J	60	CHD	C5-C6-C7	7.23	122.44	114.46
23	W	1060	CHD	C5-C6-C7	7.21	122.42	114.46
23	W	1060	CHD	C16-C17-C13	7.20	110.62	103.55
23	J	60	CHD	C4-C5-C10	7.18	120.28	112.66
23	C	525	CHD	C18-C13-C12	-7.18	101.76	109.07
23	W	1060	CHD	C11-C9-C10	7.15	121.10	113.73
23	C	271	CHD	C4-C5-C10	7.10	120.20	112.66
23	C	271	CHD	C1-C2-C3	7.04	119.50	110.47
23	B	1086	CHD	C18-C13-C17	-6.93	100.37	111.21
23	B	1086	CHD	C17-C13-C14	6.88	107.03	100.09
23	P	1271	CHD	C14-C8-C7	6.85	120.89	111.81
23	G	86	CHD	C18-C13-C17	-6.84	100.50	111.21
23	G	86	CHD	C1-C2-C3	6.81	119.21	110.47
24	Z	1526	DMU	O1-C9-C8	6.81	122.06	109.69
23	J	60	CHD	C6-C7-C8	6.76	118.69	111.48
23	P	1271	CHD	C16-C17-C13	6.70	110.13	103.55
18	A	516	HEA	CHA-C4D-ND	6.70	131.71	124.43
23	P	1271	CHD	C17-C13-C12	-6.68	111.57	117.67
23	C	271	CHD	C4-C3-C2	6.65	118.49	110.55
23	P	1271	CHD	C6-C5-C10	6.64	119.71	112.66
23	C	525	CHD	C19-C10-C9	-6.62	102.06	111.18
23	G	86	CHD	C15-C14-C13	6.62	110.04	103.55
23	W	1060	CHD	C9-C11-C12	6.62	123.04	114.30
23	C	271	CHD	C16-C17-C13	6.61	110.03	103.55
24	M	526	DMU	O5-C6-C1	6.58	124.28	110.35
23	C	271	CHD	C6-C5-C10	6.58	119.64	112.66
23	J	60	CHD	C6-C5-C10	6.55	119.61	112.66
23	C	525	CHD	C15-C14-C13	6.51	109.94	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J	60	CHD	C14-C13-C12	6.46	113.42	107.40
23	P	1525	CHD	C18-C13-C14	-6.44	101.13	111.21
23	W	1060	CHD	C6-C5-C10	6.42	119.48	112.66
23	C	271	CHD	C1-C10-C5	6.41	117.25	107.77
24	C	272	DMU	O1-C10-C5	6.39	123.88	110.35
24	P	1272	DMU	O1-C9-C8	6.39	121.30	109.69
23	W	1060	CHD	C4-C3-C2	6.38	118.17	110.55
23	C	525	CHD	C5-C4-C3	6.38	122.13	112.76
24	Z	1526	DMU	O5-C6-C1	6.37	123.84	110.35
23	W	1060	CHD	C11-C12-C13	6.35	117.76	111.24
23	P	1525	CHD	C18-C13-C12	-6.35	102.61	109.07
23	J	60	CHD	C5-C4-C3	6.33	122.06	112.76
23	P	1271	CHD	C11-C9-C8	6.32	120.13	110.88
23	G	86	CHD	C6-C7-C8	6.32	118.22	111.48
24	Z	1526	DMU	O1-C10-C5	6.29	123.66	110.35
18	N	515	HEA	C27-C19-C20	6.24	125.77	115.27
24	M	526	DMU	O1-C10-C5	6.20	123.46	110.35
23	W	1060	CHD	C9-C10-C5	6.19	117.28	108.58
23	C	271	CHD	C13-C17-C20	6.19	126.88	119.50
23	P	1525	CHD	C1-C2-C3	6.18	118.40	110.47
23	P	1525	CHD	C6-C5-C4	-6.18	104.08	111.19
23	W	1060	CHD	C15-C14-C8	6.17	126.96	118.33
24	P	1272	DMU	O1-C10-C5	6.17	123.41	110.35
24	C	272	DMU	O1-C9-C8	6.17	120.90	109.69
23	J	60	CHD	C9-C11-C12	6.17	122.45	114.30
24	Z	1526	DMU	O1-C9-C11	6.15	121.74	106.44
23	J	60	CHD	C4-C3-C2	6.15	117.89	110.55
24	C	272	DMU	C8-C7-C5	6.12	121.51	110.82
18	A	516	HEA	CAA-C2A-C3A	-6.08	111.86	126.86
23	J	60	CHD	C6-C5-C4	-6.04	104.23	111.19
23	C	271	CHD	C14-C8-C7	6.02	119.79	111.81
23	P	1271	CHD	C5-C4-C3	6.00	121.57	112.76
23	C	271	CHD	C2-C1-C10	5.97	123.03	112.78
24	P	1272	DMU	O5-C4-C3	5.97	122.34	109.75
19	N	1268	PGV	O01-C1-C2	5.97	124.36	111.50
23	B	1086	CHD	C9-C11-C12	5.96	122.17	114.30
23	W	1060	CHD	C5-C4-C3	5.93	121.47	112.76
23	P	1525	CHD	C5-C4-C3	5.93	121.47	112.76
23	G	86	CHD	C4-C3-C2	5.92	117.62	110.55
23	P	1271	CHD	C1-C2-C3	5.92	118.06	110.47
23	J	60	CHD	C1-C10-C5	5.91	116.51	107.77
23	C	525	CHD	C11-C12-C13	5.90	117.30	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J	60	CHD	C2-C1-C10	5.88	122.86	112.78
23	C	271	CHD	C5-C4-C3	5.86	121.37	112.76
23	W	1060	CHD	C2-C1-C10	5.84	122.80	112.78
24	Z	1526	DMU	O5-C4-C3	5.82	122.02	109.75
18	N	515	HEA	C26-C15-C16	5.82	125.06	115.27
23	C	525	CHD	C6-C7-C8	5.81	117.68	111.48
24	C	272	DMU	O5-C4-C3	5.78	121.95	109.75
23	P	1271	CHD	C4-C5-C10	5.75	118.77	112.66
23	G	86	CHD	C16-C17-C20	5.72	121.00	112.15
23	G	86	CHD	C17-C13-C14	5.70	105.84	100.09
18	A	516	HEA	OMA-CMA-C3A	5.70	137.32	124.91
23	G	86	CHD	C11-C9-C8	5.67	119.18	110.88
23	J	60	CHD	C11-C9-C10	5.67	119.58	113.73
18	N	515	HEA	C16-C17-C18	5.66	130.49	111.88
24	P	1272	DMU	C8-C7-C5	5.65	120.68	110.82
23	P	1271	CHD	C2-C1-C10	5.63	122.43	112.78
19	C	268	PGV	O01-C1-C2	5.62	123.61	111.50
21	B	521	TGL	CG2-OG2-CB1	5.62	131.62	117.79
23	J	60	CHD	C9-C10-C5	5.62	116.47	108.58
23	W	1060	CHD	C1-C10-C5	5.61	116.06	107.77
23	P	1525	CHD	C11-C9-C8	5.55	119.00	110.88
24	C	272	DMU	O5-C6-C1	5.54	122.08	110.35
23	P	1525	CHD	C18-C13-C17	-5.52	102.57	111.21
24	M	526	DMU	O16-C6-C1	5.52	116.92	108.30
23	P	1525	CHD	C6-C7-C8	5.52	117.37	111.48
22	B	230	PSC	O01-C1-C2	5.51	123.38	111.50
18	A	516	HEA	CBA-CAA-C2A	-5.50	103.33	112.60
23	C	525	CHD	C2-C1-C10	5.49	122.19	112.78
27	T	1269	CDL	OA6-CA5-C11	5.48	123.32	111.50
23	W	1060	CHD	C22-C20-C17	5.47	121.58	110.28
23	J	60	CHD	C11-C12-C13	5.45	116.84	111.24
23	J	60	CHD	C15-C14-C8	5.39	125.87	118.33
24	M	526	DMU	C2-C3-C4	5.39	123.28	110.93
23	W	1060	CHD	C14-C13-C12	5.38	112.41	107.40
23	J	60	CHD	C9-C8-C7	5.36	118.29	111.88
27	C	270	CDL	OA6-CA5-C11	5.34	123.02	111.50
23	C	525	CHD	C6-C5-C4	-5.33	105.06	111.19
26	T	263	PEK	O01-C1-C2	5.32	122.98	111.50
24	Z	1526	DMU	O5-C4-C57	5.31	119.65	106.44
24	P	1272	DMU	O5-C6-C1	5.30	121.57	110.35
23	C	271	CHD	C11-C9-C8	5.29	118.62	110.88
18	A	516	HEA	CHB-C1B-C2B	5.28	133.23	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	525	CHD	C18-C13-C17	-5.25	103.00	111.21
27	T	1269	CDL	OB6-CB5-C51	5.23	122.77	111.50
23	P	1525	CHD	C11-C12-C13	5.21	116.59	111.24
24	P	1272	DMU	O1-C9-C11	5.20	119.37	106.44
18	N	516	HEA	C27-C19-C20	5.20	124.02	115.27
18	A	516	HEA	CAA-CBA-CGA	-5.18	99.23	113.76
27	G	269	CDL	OA6-CA5-C11	5.16	122.62	111.50
18	A	515	HEA	C16-C17-C18	5.14	128.79	111.88
21	L	522	TGL	OG3-CC1-OC1	-5.13	110.66	123.59
23	G	86	CHD	O12-C12-C13	-5.12	102.37	111.03
24	M	526	DMU	O5-C4-C3	5.12	120.55	109.75
18	A	515	HEA	C4A-CHB-C1B	5.11	129.30	122.56
23	G	86	CHD	C11-C12-C13	5.09	116.47	111.24
26	G	1263	PEK	O01-C1-C2	5.08	122.45	111.50
23	W	1060	CHD	C19-C10-C5	-4.99	101.89	110.36
23	P	1271	CHD	C13-C17-C20	4.99	125.45	119.50
23	J	60	CHD	C18-C13-C12	-4.99	103.99	109.07
23	B	1086	CHD	C15-C14-C13	4.95	108.41	103.55
23	B	1086	CHD	O7-C7-C6	-4.94	97.68	109.94
19	N	1266	PGV	O03-C19-C20	4.94	127.42	111.91
27	P	1270	CDL	OA6-CA5-C11	4.94	122.14	111.50
24	C	272	DMU	O1-C9-C11	4.90	118.61	106.44
23	C	525	CHD	O12-C12-C13	-4.89	102.76	111.03
23	B	1086	CHD	C4-C3-C2	4.89	116.39	110.55
24	Z	1526	DMU	O16-C6-C1	4.87	115.91	108.30
23	C	525	CHD	C17-C13-C14	4.85	104.98	100.09
23	C	271	CHD	C16-C17-C20	4.84	119.63	112.15
18	A	516	HEA	CHB-C1B-NB	-4.78	119.24	124.43
19	N	1268	PGV	O03-C19-C20	4.78	126.90	111.91
23	P	1271	CHD	C18-C13-C12	-4.75	104.23	109.07
23	G	86	CHD	C6-C5-C4	-4.74	105.74	111.19
27	G	269	CDL	OB6-CB5-C51	4.73	121.69	111.50
24	Z	1526	DMU	C7-C8-C9	4.72	118.66	110.24
23	G	86	CHD	C2-C1-C10	4.71	120.86	112.78
18	A	516	HEA	CHD-C1D-ND	-4.69	118.58	124.38
23	P	1525	CHD	O7-C7-C6	-4.69	98.31	109.94
24	Z	1526	DMU	C2-C3-C4	4.66	121.61	110.93
23	C	271	CHD	C9-C11-C12	4.65	120.45	114.30
23	P	1525	CHD	C9-C8-C7	4.64	117.42	111.88
23	C	525	CHD	C11-C9-C8	4.62	117.64	110.88
23	W	1060	CHD	C18-C13-C12	-4.62	104.36	109.07
23	W	1060	CHD	C9-C8-C7	4.57	117.34	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	1060	CHD	C1-C10-C9	-4.55	104.20	111.35
21	N	1521	TGL	CG2-OG2-CB1	4.54	128.98	117.79
22	O	1230	PSC	O01-C1-C2	4.53	121.25	111.50
24	Z	1526	DMU	O7-C3-C2	4.49	119.23	107.28
23	P	1271	CHD	C16-C17-C20	4.49	119.09	112.15
24	Z	1526	DMU	C8-C7-C5	4.48	118.65	110.82
21	B	521	TGL	OG2-CG2-CG3	4.46	124.56	108.40
18	N	516	HEA	OMA-CMA-C3A	-4.46	115.19	124.91
19	C	268	PGV	O03-C19-C20	4.45	125.87	111.91
23	P	1525	CHD	C17-C13-C14	4.43	104.56	100.09
19	A	521	PGV	O03-C19-O04	-4.42	112.44	123.59
23	B	1086	CHD	C14-C8-C9	4.41	115.76	109.71
19	N	1266	PGV	O03-C19-O04	-4.40	112.48	123.59
26	C	265	PEK	O03-C21-C22	4.38	125.66	111.91
24	P	1272	DMU	C7-C8-C9	4.38	118.04	110.24
23	C	525	CHD	C18-C13-C14	-4.37	104.38	111.21
19	A	521	PGV	O03-C19-C20	4.36	125.58	111.91
23	P	1525	CHD	O12-C12-C11	-4.35	100.25	109.12
23	B	1086	CHD	C6-C5-C4	-4.35	106.18	111.19
26	P	1264	PEK	O03-C01-C02	-4.34	95.79	108.43
24	C	272	DMU	O5-C4-C57	4.31	117.14	106.44
24	M	526	DMU	O5-C4-C57	4.27	117.05	106.44
18	A	516	HEA	CMD-C2D-C3D	-4.27	114.53	126.12
23	B	1086	CHD	C11-C9-C10	4.26	118.12	113.73
18	N	516	HEA	CAD-CBD-CGD	-4.24	104.48	113.60
23	P	1525	CHD	C13-C17-C20	4.23	124.55	119.50
26	P	1264	PEK	C2-C3-C4	4.23	120.77	113.23
23	P	1271	CHD	C14-C13-C12	4.22	111.33	107.40
26	P	1265	PEK	O01-C1-C2	4.21	120.58	111.50
24	M	526	DMU	O1-C9-C11	4.19	116.86	106.44
21	D	523	TGL	OG3-CC1-CC2	4.18	125.01	111.91
23	C	525	CHD	C1-C2-C3	4.15	115.80	110.47
23	C	271	CHD	C19-C10-C1	-4.15	101.57	108.26
18	A	516	HEA	O11-C11-C12	-4.11	97.92	109.42
18	A	516	HEA	C3B-C4B-NB	4.11	114.70	109.84
24	C	272	DMU	C2-C3-C4	4.09	120.31	110.93
23	B	1086	CHD	C11-C9-C8	4.08	116.85	110.88
23	W	1060	CHD	C17-C13-C12	4.08	121.39	117.67
23	W	1060	CHD	O7-C7-C6	-4.06	99.87	109.94
24	M	526	DMU	C8-C7-C5	4.05	117.89	110.82
24	P	1272	DMU	O5-C4-C57	4.05	116.50	106.44
24	C	272	DMU	C7-C8-C9	4.04	117.45	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	M	526	DMU	C10-C5-C7	4.04	118.41	110.00
23	C	525	CHD	C9-C11-C12	4.04	119.63	114.30
23	C	525	CHD	C16-C17-C13	4.03	107.50	103.55
23	P	1271	CHD	C9-C11-C12	4.02	119.61	114.30
23	J	60	CHD	C19-C10-C5	-4.01	103.57	110.36
26	P	1264	PEK	C24-C23-C22	-4.00	98.80	113.19
19	N	1524	PGV	O01-C1-C2	4.00	120.12	111.50
26	C	265	PEK	O01-C1-C2	3.98	120.09	111.50
24	M	526	DMU	C7-C8-C9	3.97	117.32	110.24
23	C	271	CHD	C6-C5-C4	-3.96	106.63	111.19
23	C	525	CHD	C16-C17-C20	3.95	118.26	112.15
26	P	1264	PEK	O01-C1-O02	-3.92	114.23	123.70
24	C	272	DMU	O7-C3-C4	3.92	120.19	109.45
23	P	1525	CHD	C11-C9-C10	3.91	117.76	113.73
24	P	1272	DMU	C1-C2-C3	3.91	118.60	109.68
19	A	524	PGV	O03-C19-C20	3.90	124.15	111.91
23	P	1271	CHD	C9-C10-C5	3.90	114.05	108.58
23	P	1271	CHD	C19-C10-C5	-3.89	103.76	110.36
23	G	86	CHD	C9-C8-C7	3.88	116.52	111.88
26	P	1265	PEK	O03-C21-C22	3.88	124.09	111.91
23	B	1086	CHD	C19-C10-C5	-3.88	103.78	110.36
23	J	60	CHD	C22-C20-C17	3.87	118.27	110.28
26	G	264	PEK	O01-C1-O02	-3.86	114.36	123.70
23	P	1525	CHD	C1-C10-C9	-3.85	105.30	111.35
27	P	1270	CDL	OB8-CB7-C71	3.82	123.90	111.91
21	D	523	TGL	OG2-CB1-CB2	3.81	119.72	111.50
23	B	1086	CHD	C5-C6-C7	3.79	118.64	114.46
24	P	1272	DMU	C6-C1-C2	3.79	117.88	110.00
24	P	1272	DMU	C2-C3-C4	3.78	119.59	110.93
24	P	1272	DMU	O7-C10-C5	3.78	117.88	108.10
21	B	521	TGL	OG2-CB1-CB2	3.77	119.64	111.50
21	L	522	TGL	OG3-CC1-CC2	3.76	123.72	111.91
18	N	516	HEA	C4A-CHB-C1B	3.76	127.52	122.56
24	C	272	DMU	C10-O1-C9	3.76	121.06	113.69
19	N	1524	PGV	O03-C19-C20	3.75	123.69	111.91
23	P	1525	CHD	C22-C20-C17	-3.75	102.54	110.28
27	T	1269	CDL	OB8-CB6-CB4	3.75	119.34	108.43
23	C	525	CHD	C14-C8-C9	3.72	114.82	109.71
24	Z	1526	DMU	C6-C1-C2	3.68	117.65	110.00
26	C	265	PEK	O03-C21-O04	-3.67	114.33	123.59
23	P	1525	CHD	C16-C17-C13	3.66	107.14	103.55
24	P	1272	DMU	C10-O1-C9	3.66	120.87	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	264	PEK	O01-C1-C2	3.66	119.38	111.50
18	N	515	HEA	C12-C13-C14	-3.66	102.58	112.23
21	N	1521	TGL	OG1-CG1-CG2	3.65	119.07	108.43
26	T	263	PEK	O03-C01-C02	3.64	119.04	108.43
24	C	272	DMU	C6-C1-C2	3.63	117.56	110.00
24	Z	1526	DMU	C10-C5-C7	3.62	117.53	110.00
24	P	1272	DMU	O7-C3-C4	3.62	119.36	109.45
23	P	1525	CHD	C9-C11-C12	3.60	119.06	114.30
23	B	1086	CHD	C1-C10-C9	-3.59	105.72	111.35
21	N	1522	TGL	OG2-CB1-CB2	3.58	119.22	111.50
21	N	1521	TGL	OG1-CA1-CA2	3.58	123.14	111.91
24	C	272	DMU	O7-C10-C5	3.57	117.36	108.10
23	G	86	CHD	C15-C14-C8	3.57	123.32	118.33
23	G	86	CHD	C14-C8-C9	3.57	114.61	109.71
21	D	523	TGL	OG1-CG1-CG2	3.55	118.77	108.43
24	C	272	DMU	C1-C2-C3	3.55	117.78	109.68
23	C	271	CHD	C9-C10-C5	3.55	113.56	108.58
21	N	1521	TGL	OG2-CB1-CB2	3.54	119.14	111.50
23	G	86	CHD	C9-C11-C12	3.54	118.98	114.30
23	G	86	CHD	C18-C13-C14	-3.54	105.68	111.21
21	O	1523	TGL	OG3-CC1-CC2	3.53	123.00	111.91
18	A	515	HEA	C2D-C1D-ND	3.53	114.03	109.84
19	C	267	PGV	O01-C1-C2	3.53	119.10	111.50
23	G	86	CHD	C11-C9-C10	3.52	117.35	113.73
23	P	1525	CHD	C14-C8-C9	3.49	114.50	109.71
26	G	1263	PEK	O03-C21-C22	3.49	122.86	111.91
18	A	516	HEA	CMC-C2C-C1C	3.48	133.82	128.46
23	P	1271	CHD	C19-C10-C9	-3.47	106.41	111.18
21	L	522	TGL	OG1-CA1-CA2	3.46	122.77	111.91
23	J	60	CHD	C11-C9-C8	3.46	115.94	110.88
27	T	1269	CDL	C83-C82-C81	3.44	131.88	114.42
21	N	1521	TGL	CG3-OG3-CC1	3.43	129.84	117.12
18	N	516	HEA	C4D-CHA-C1A	3.43	127.09	122.56
23	J	60	CHD	C1-C10-C9	-3.43	105.96	111.35
21	N	1521	TGL	CA6-CA5-CA4	-3.43	97.02	114.42
27	C	270	CDL	OA8-CA7-C31	3.42	122.64	111.91
21	B	521	TGL	OG1-CA1-CA2	3.41	122.61	111.91
23	G	86	CHD	C1-C10-C9	-3.40	106.01	111.35
24	C	272	DMU	O4-C7-C5	3.38	118.17	110.35
18	N	515	HEA	C4A-CHB-C1B	3.38	127.02	122.56
18	A	515	HEA	C12-C13-C14	-3.38	103.32	112.23
23	C	525	CHD	C13-C17-C20	3.38	123.53	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1525	CHD	C23-C22-C20	-3.38	108.35	114.52
23	C	525	CHD	C15-C14-C8	3.37	123.05	118.33
27	T	1269	CDL	OA6-CA5-OA7	-3.36	115.57	123.70
23	C	271	CHD	C17-C13-C14	3.36	103.48	100.09
18	A	515	HEA	CMC-C2C-C3C	3.36	130.96	124.68
21	L	522	TGL	CC3-CC2-CC1	3.33	125.74	113.62
21	N	1521	TGL	OG2-CG2-CG3	3.33	120.45	108.40
26	T	263	PEK	O03-C21-C22	3.31	122.30	111.91
24	C	272	DMU	C6-O5-C4	3.30	120.16	113.69
22	O	1230	PSC	O01-C1-O02	-3.30	115.73	123.70
24	M	526	DMU	O7-C10-C5	-3.29	99.56	108.10
21	N	1522	TGL	OG1-CA1-CA2	3.28	122.21	111.91
23	P	1271	CHD	C17-C13-C14	3.27	103.39	100.09
23	G	86	CHD	O12-C12-C11	-3.24	102.52	109.12
18	A	515	HEA	C26-C15-C14	-3.24	115.36	123.68
21	B	521	TGL	CG3-OG3-CC1	3.24	129.12	117.12
18	N	515	HEA	C21-C20-C19	-3.24	102.33	112.98
26	P	1264	PEK	O01-C1-C2	3.23	118.46	111.50
23	J	60	CHD	C21-C20-C22	3.22	115.42	110.36
23	B	1086	CHD	C18-C13-C14	-3.22	106.18	111.21
23	C	271	CHD	C18-C13-C12	-3.22	105.79	109.07
24	P	1272	DMU	C6-O5-C4	3.20	119.97	113.69
23	C	525	CHD	C11-C9-C10	3.20	117.03	113.73
23	P	1525	CHD	C2-C1-C10	3.20	118.27	112.78
24	C	272	DMU	C11-C9-C8	3.19	120.49	113.00
24	M	526	DMU	C6-C1-C2	3.19	116.65	110.00
23	C	525	CHD	C9-C8-C7	3.19	115.69	111.88
23	P	1525	CHD	O12-C12-C13	-3.18	105.65	111.03
27	P	1270	CDL	OA8-CA7-C31	3.18	121.87	111.91
24	P	1272	DMU	O16-C18-C19	3.17	120.69	109.56
18	N	515	HEA	C27-C19-C18	-3.17	115.55	123.68
19	N	1268	PGV	O03-C19-O04	-3.16	115.62	123.59
18	A	515	HEA	CMC-C2C-C1C	-3.15	123.62	128.46
18	A	515	HEA	C3B-C4B-NB	3.14	113.56	109.84
18	A	516	HEA	CHC-C4B-C3B	-3.14	117.71	125.80
24	Z	1526	DMU	O5-C6-O16	3.14	117.41	109.97
18	A	515	HEA	C2B-C1B-NB	3.13	113.64	109.88
27	P	1270	CDL	OB8-CB7-OB9	-3.13	115.69	123.59
18	N	515	HEA	O2D-CGD-O1D	-3.12	115.52	123.30
27	C	270	CDL	OB8-CB7-C71	3.12	121.69	111.91
24	M	526	DMU	C57-C4-C3	3.12	122.39	113.33
27	C	270	CDL	OB8-CB7-OB9	-3.11	115.75	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	O	1523	TGL	OG2-CB1-CB2	3.11	118.20	111.50
23	G	86	CHD	O7-C7-C6	-3.10	102.26	109.94
21	N	1522	TGL	OG3-CC1-OC1	-3.10	115.78	123.59
26	G	264	PEK	O03-C01-C02	-3.08	99.47	108.43
24	Z	1526	DMU	O55-C2-C3	3.07	118.09	109.94
21	D	523	TGL	C21-C20-CA9	3.07	130.02	114.42
23	C	271	CHD	C14-C13-C12	3.07	110.26	107.40
24	C	272	DMU	O7-C3-C2	3.06	115.43	107.28
19	N	1266	PGV	O01-C1-O02	-3.06	116.30	123.70
24	C	272	DMU	C18-O16-C6	3.06	118.92	113.84
26	G	1263	PEK	O03-C01-C02	3.06	117.34	108.43
18	N	516	HEA	C20-C19-C18	-3.02	115.00	121.12
23	J	60	CHD	C16-C17-C20	3.02	116.81	112.15
21	D	523	TGL	CG3-OG3-CC1	2.99	128.18	117.12
21	B	521	TGL	OG3-CC1-OC1	-2.98	116.08	123.59
18	A	515	HEA	C1D-C2D-C3D	-2.98	103.83	106.96
23	P	1525	CHD	C16-C17-C20	2.98	116.75	112.15
23	P	1525	CHD	C15-C14-C8	2.97	122.49	118.33
26	P	1265	PEK	C7-C6-C5	-2.97	98.48	123.57
23	C	271	CHD	O7-C7-C6	-2.96	102.59	109.94
23	B	1086	CHD	C11-C12-C13	2.96	114.28	111.24
23	B	1086	CHD	C16-C17-C20	2.95	116.71	112.15
19	C	268	PGV	O03-C19-O04	-2.93	116.19	123.59
23	B	1086	CHD	O12-C12-C13	-2.93	106.07	111.03
26	G	264	PEK	C24-C23-C22	-2.92	102.68	113.19
23	B	1086	CHD	C16-C17-C13	2.92	106.42	103.55
21	N	1521	TGL	CG1-OG1-CA1	-2.91	106.33	117.12
23	C	271	CHD	C22-C23-C24	-2.91	104.78	112.51
27	T	1269	CDL	OA8-CA7-C31	2.91	121.03	111.91
19	A	521	PGV	O01-C1-C2	2.89	117.73	111.50
23	P	1271	CHD	C22-C23-C24	-2.88	104.87	112.51
18	A	516	HEA	C3C-C4C-NC	2.88	112.93	109.21
23	P	1525	CHD	C19-C10-C5	-2.87	105.49	110.36
19	A	524	PGV	C01-O03-C19	2.87	127.75	117.12
19	A	524	PGV	O01-C1-C2	2.87	117.69	111.50
23	P	1525	CHD	C5-C6-C7	2.87	117.62	114.46
24	Z	1526	DMU	C1-C2-C3	2.85	116.20	109.68
21	N	1522	TGL	OG3-CC1-CC2	2.85	120.86	111.91
24	Z	1526	DMU	C10-O1-C9	2.85	119.28	113.69
23	B	1086	CHD	C15-C14-C8	2.84	122.31	118.33
23	G	86	CHD	C16-C17-C13	2.83	106.33	103.55
26	T	263	PEK	C02-O01-C1	2.83	124.75	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	1060	CHD	C16-C17-C20	2.82	116.52	112.15
24	M	526	DMU	C6-O5-C4	2.82	119.22	113.69
26	P	1265	PEK	O03-C21-O04	-2.81	116.50	123.59
23	W	1060	CHD	C18-C13-C14	-2.81	106.82	111.21
19	N	1524	PGV	C01-O03-C19	2.78	127.42	117.12
27	T	1269	CDL	OA8-CA7-OA9	-2.77	116.61	123.59
18	A	516	HEA	C13-C14-C15	-2.76	121.00	127.66
18	A	516	HEA	O2A-CGA-CBA	2.76	122.90	114.03
18	A	516	HEA	C16-C15-C14	2.76	126.70	121.12
24	M	526	DMU	C1-C2-C3	2.75	115.97	109.68
18	A	515	HEA	CAA-C2A-C3A	2.75	133.65	126.86
18	A	516	HEA	O2D-CGD-CBD	2.75	122.86	114.03
19	N	1266	PGV	O03-C01-C02	2.74	116.40	108.43
24	M	526	DMU	C10-O7-C3	2.73	124.71	117.96
24	P	1272	DMU	O5-C6-O16	2.72	116.42	109.97
27	G	269	CDL	OA6-CA5-OA7	-2.72	117.12	123.70
23	W	1060	CHD	C13-C14-C8	2.72	118.21	114.74
21	L	522	TGL	OG1-CG1-CG2	2.72	116.34	108.43
24	P	1272	DMU	C11-C9-C8	2.69	119.31	113.00
24	P	1272	DMU	C57-C4-C3	2.69	121.14	113.33
19	N	1268	PGV	C03-C02-C01	-2.69	105.43	111.79
24	P	1272	DMU	C10-C5-C7	2.68	115.58	110.00
18	N	515	HEA	O1A-CGA-CBA	-2.68	114.47	123.08
23	C	525	CHD	O7-C7-C6	-2.67	103.32	109.94
26	P	1264	PEK	C3-C2-C1	-2.66	103.93	113.62
23	W	1060	CHD	C11-C9-C8	2.66	114.77	110.88
23	P	1271	CHD	O7-C7-C6	-2.65	103.37	109.94
21	O	1523	TGL	OG1-CA1-CA2	2.64	120.20	111.91
18	N	516	HEA	CHB-C1B-NB	2.64	127.29	124.43
24	M	526	DMU	O7-C3-C2	2.63	114.28	107.28
21	N	1522	TGL	OG1-CG1-CG2	2.62	116.06	108.43
18	N	515	HEA	C1D-C2D-C3D	-2.60	104.22	106.96
24	C	272	DMU	C57-C4-C3	2.60	120.89	113.33
18	N	516	HEA	C3C-C4C-NC	2.60	112.57	109.21
19	C	267	PGV	O03-C19-O04	-2.58	117.08	123.59
27	T	1269	CDL	C82-C81-C80	2.57	127.47	114.42
21	O	1523	TGL	OG1-CA1-OA1	-2.57	117.11	123.59
23	P	1271	CHD	C6-C5-C4	-2.57	108.23	111.19
23	C	525	CHD	C5-C6-C7	2.57	117.29	114.46
18	A	516	HEA	C1D-ND-C4D	-2.56	102.43	105.07
23	P	1271	CHD	C19-C10-C1	-2.55	104.15	108.26
24	Z	1526	DMU	O7-C10-C5	-2.55	101.49	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	1521	TGL	CA7-CA6-CA5	-2.53	101.58	114.42
21	N	1522	TGL	CG1-OG1-CA1	2.53	126.48	117.12
18	A	515	HEA	C20-C21-C22	-2.52	103.59	111.88
18	A	515	HEA	C25-C23-C22	-2.52	115.36	122.65
21	O	1523	TGL	C21-C20-CA9	2.51	127.19	114.42
23	P	1525	CHD	O3-C3-C4	2.50	114.83	109.85
18	N	516	HEA	C2D-C1D-ND	2.50	112.80	109.84
23	G	86	CHD	C5-C6-C7	2.49	117.21	114.46
19	A	521	PGV	O12-P-O13	2.49	118.80	109.07
24	Z	1526	DMU	C6-O5-C4	2.49	118.57	113.69
19	P	1267	PGV	O03-C19-O04	-2.48	117.33	123.59
27	G	269	CDL	OA8-CA7-C31	2.47	119.65	111.91
22	B	230	PSC	O01-C1-O02	-2.47	117.74	123.70
18	N	516	HEA	C1D-C2D-C3D	-2.47	104.36	106.96
21	N	1521	TGL	CB7-CB6-CB5	-2.47	101.90	114.42
23	C	271	CHD	C19-C10-C5	-2.46	106.19	110.36
21	B	521	TGL	OG3-CC1-CC2	2.45	119.60	111.91
21	D	523	TGL	OG1-CA1-CA2	2.45	119.59	111.91
19	N	1524	PGV	C02-O01-C1	2.44	123.80	117.79
27	G	269	CDL	OB8-CB7-OB9	-2.44	117.43	123.59
23	J	60	CHD	C17-C13-C12	2.44	119.89	117.67
18	A	515	HEA	CHC-C4B-NB	-2.44	121.37	124.38
23	G	86	CHD	C19-C10-C5	-2.44	106.23	110.36
27	P	1270	CDL	OA8-CA6-CA4	2.44	115.53	108.43
21	D	523	TGL	CG2-OG2-CB1	2.43	123.78	117.79
18	N	515	HEA	CHB-C1B-C2B	-2.43	121.18	124.98
27	C	270	CDL	C52-C51-CB5	-2.42	104.82	113.62
23	J	60	CHD	C13-C14-C8	2.41	117.81	114.74
27	C	270	CDL	OA8-CA6-CA4	2.41	115.44	108.43
27	G	269	CDL	CA6-OA8-CA7	2.40	126.02	117.12
27	T	1269	CDL	C43-C42-C41	2.40	126.61	114.42
18	N	516	HEA	CHA-C4D-C3D	-2.39	121.32	124.84
27	C	270	CDL	C39-C38-C37	2.39	126.57	114.42
26	T	263	PEK	C01-O03-C21	2.38	125.95	117.12
21	N	1521	TGL	OG3-CC1-CC2	2.38	119.39	111.91
21	B	521	TGL	OG1-CG1-CG2	2.38	115.36	108.43
18	A	516	HEA	CHC-C4B-NB	2.38	127.32	124.38
18	A	516	HEA	C17-C16-C15	2.37	120.79	112.98
21	O	1523	TGL	OG2-CG2-CG3	2.37	116.99	108.40
21	D	523	TGL	C11-C10-CB9	2.37	126.45	114.42
19	A	524	PGV	C02-O01-C1	2.37	123.62	117.79
23	B	1086	CHD	C2-C1-C10	2.37	116.84	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	N	1524	PGV	O03-C19-O04	-2.37	117.62	123.59
21	N	1522	TGL	C15-CC9-CC8	2.36	126.40	114.42
27	P	1270	CDL	C78-C77-C76	-2.35	102.51	114.42
21	N	1522	TGL	C24-C23-C22	-2.35	102.51	114.42
23	C	271	CHD	O12-C12-C11	-2.34	104.37	109.12
27	G	269	CDL	OB8-CB7-C71	2.34	119.24	111.91
23	J	60	CHD	O7-C7-C6	-2.33	104.15	109.94
27	P	1270	CDL	OB6-CB5-C51	2.33	116.53	111.50
24	M	526	DMU	O7-C3-C4	2.33	115.84	109.45
24	C	272	DMU	O5-C6-O16	2.33	115.49	109.97
27	C	270	CDL	OA8-CA7-OA9	-2.33	117.71	123.59
21	D	523	TGL	C10-CB9-CB8	2.33	126.24	114.42
18	A	515	HEA	OMA-CMA-C3A	-2.32	119.84	124.91
18	A	516	HEA	CMC-C2C-C3C	-2.31	120.36	124.68
19	N	1266	PGV	C15-C14-C13	-2.30	103.75	113.79
21	B	521	TGL	CG1-OG1-CA1	-2.30	108.59	117.12
27	P	1270	CDL	OA8-CA7-OA9	-2.29	117.81	123.59
21	N	1522	TGL	CB9-CB8-CB7	-2.28	102.84	114.42
23	C	271	CHD	C13-C14-C8	2.28	117.65	114.74
23	W	1060	CHD	C19-C10-C1	-2.28	104.58	108.26
18	A	516	HEA	O1A-CGA-CBA	-2.28	115.75	123.08
24	M	526	DMU	O7-C10-O1	-2.27	104.34	110.67
18	N	516	HEA	CHA-C4D-ND	2.27	126.89	124.43
21	L	522	TGL	OG2-CB1-CB2	2.26	116.38	111.50
21	D	523	TGL	C20-CA9-CA8	2.26	125.91	114.42
18	A	516	HEA	O1D-CGD-CBD	-2.26	115.82	123.08
23	C	525	CHD	C22-C23-C24	-2.26	106.51	112.51
19	N	1268	PGV	O02-C1-C2	-2.25	114.94	123.73
23	C	525	CHD	O3-C3-C4	2.25	114.33	109.85
18	A	516	HEA	C1D-C2D-C3D	-2.25	104.59	106.96
18	N	515	HEA	C2B-C1B-NB	2.25	112.57	109.88
27	P	1270	CDL	OA6-CA5-OA7	-2.24	118.28	123.70
19	P	1267	PGV	O03-C19-C20	2.24	118.94	111.91
27	C	270	CDL	CA6-CA4-CA3	-2.24	106.49	111.79
21	N	1521	TGL	OG1-CA1-OA1	-2.24	117.94	123.59
21	O	1523	TGL	CG3-OG3-CC1	2.24	125.41	117.12
21	B	521	TGL	CB7-CB6-CB5	-2.22	103.14	114.42
26	T	263	PEK	O01-C1-O02	-2.22	118.33	123.70
18	N	515	HEA	C2D-C1D-ND	2.22	112.47	109.84
27	C	270	CDL	OA6-CA5-OA7	-2.22	118.34	123.70
21	D	523	TGL	CG3-CG2-CG1	-2.20	106.58	111.79
24	M	526	DMU	O5-C6-O16	2.19	115.17	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1525	CHD	O7-C7-C8	-2.18	104.54	109.43
21	O	1523	TGL	OG3-CC1-OC1	-2.18	118.08	123.59
18	N	515	HEA	C26-C15-C14	-2.18	118.08	123.68
24	M	526	DMU	C11-C9-C8	2.18	118.11	113.00
27	G	269	CDL	OA8-CA7-OA9	-2.17	118.12	123.59
26	P	1264	PEK	O01-C02-C01	-2.17	100.55	108.40
27	P	1270	CDL	C39-C38-C37	2.16	125.41	114.42
23	C	271	CHD	C18-C13-C17	-2.16	107.83	111.21
18	A	516	HEA	C4A-CHB-C1B	2.16	125.41	122.56
23	C	525	CHD	C1-C10-C9	-2.15	107.97	111.35
18	A	515	HEA	C13-C12-C11	2.15	117.58	114.35
27	G	269	CDL	CB6-OB8-CB7	2.15	125.08	117.12
23	C	525	CHD	C19-C10-C5	-2.15	106.72	110.36
24	C	272	DMU	C10-C5-C7	2.14	114.45	110.00
23	C	271	CHD	C19-C10-C9	-2.13	108.24	111.18
27	P	1270	CDL	C20-C19-C18	2.13	125.24	114.42
23	B	1086	CHD	O7-C7-C8	-2.13	104.67	109.43
27	T	1269	CDL	CA4-OA6-CA5	-2.13	112.55	117.79
21	O	1523	TGL	C11-C10-CB9	2.13	125.22	114.42
18	N	515	HEA	C16-C15-C14	-2.13	116.81	121.12
26	G	1263	PEK	O01-C1-O02	-2.12	118.57	123.70
18	A	515	HEA	O2D-CGD-O1D	-2.12	118.03	123.30
19	A	524	PGV	O01-C02-C01	2.11	116.05	108.40
19	P	1267	PGV	C27-C26-C25	-2.11	103.71	114.42
21	D	523	TGL	CC3-CC2-CC1	-2.11	105.96	113.62
26	G	264	PEK	C3-C2-C1	-2.10	105.97	113.62
21	N	1521	TGL	C15-CC9-CC8	2.10	125.09	114.42
23	B	1086	CHD	C14-C8-C7	2.09	114.58	111.81
27	G	269	CDL	C83-C82-C81	2.09	125.05	114.42
23	B	1086	CHD	O25-C24-C23	-2.09	116.38	123.08
22	B	230	PSC	C3-C2-C1	2.08	121.20	113.62
23	C	271	CHD	C23-C22-C20	-2.08	110.72	114.52
24	P	1272	DMU	O4-C7-C5	2.08	115.16	110.35
21	L	522	TGL	CG2-OG2-CB1	2.08	122.91	117.79
26	G	1263	PEK	C01-O03-C21	2.08	124.81	117.12
24	M	526	DMU	O55-C2-C1	2.07	115.14	110.35
23	C	525	CHD	C22-C20-C17	-2.06	106.02	110.28
22	B	230	PSC	O03-C19-C20	2.06	118.39	111.91
19	N	1266	PGV	C01-O03-C19	-2.06	109.48	117.12
27	P	1270	CDL	O1-C1-CA2	-2.06	102.33	109.56
23	W	1060	CHD	C23-C22-C20	-2.05	110.77	114.52
26	C	265	PEK	C01-O03-C21	2.04	124.69	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	N	516	HEA	C4B-NB-C1B	2.04	107.18	105.07
21	D	523	TGL	OC1-CC1-CC2	-2.04	115.77	123.73
18	N	516	HEA	CBA-CAA-C2A	-2.04	109.17	112.60
18	A	515	HEA	C4B-C3B-C2B	-2.04	103.93	107.41
19	C	267	PGV	C27-C26-C25	-2.04	104.08	114.42
23	G	86	CHD	C13-C14-C8	2.04	117.34	114.74
19	C	268	PGV	O03-C01-C02	2.04	114.36	108.43
22	B	230	PSC	C32-C31-C30	-2.03	104.10	114.42
22	B	230	PSC	C29-C28-C27	-2.03	104.11	114.42
27	C	270	CDL	C57-C56-C55	-2.03	104.11	114.42
18	A	515	HEA	C16-C15-C14	-2.03	117.01	121.12
26	T	263	PEK	O04-C21-C22	-2.03	115.81	123.73
18	N	515	HEA	C3D-C4D-ND	2.02	112.32	110.36
19	A	521	PGV	C26-C25-C24	-2.02	104.15	114.42
19	C	267	PGV	O03-C19-C20	2.02	118.24	111.91
18	A	515	HEA	C3C-C4C-NC	2.02	111.82	109.21
23	J	60	CHD	C19-C10-C1	-2.01	105.02	108.26
23	B	1086	CHD	O12-C12-C11	-2.01	105.03	109.12

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	C9
23	C	271	CHD	C14
23	G	86	CHD	C9
23	J	60	CHD	C17
23	P	1525	CHD	C9
23	P	1271	CHD	C9
23	P	1271	CHD	C14
23	W	1060	CHD	C17
24	C	272	DMU	C2
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C5
24	M	526	DMU	C2
24	M	526	DMU	C9
24	M	526	DMU	C4
24	M	526	DMU	C5
24	M	526	DMU	C6

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Mol	Chain	Res	Type	Atom
24	P	1272	DMU	C2
24	P	1272	DMU	C6
24	P	1272	DMU	C9
24	P	1272	DMU	C4
24	P	1272	DMU	C5
24	Z	1526	DMU	C2
24	Z	1526	DMU	C9
24	Z	1526	DMU	C4
24	Z	1526	DMU	C5
24	Z	1526	DMU	C6

All (984) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	515	HEA	C14-C15-C16-C17
18	A	515	HEA	C26-C15-C16-C17
18	A	515	HEA	C16-C17-C18-C19
18	N	515	HEA	C14-C15-C16-C17
18	N	515	HEA	C26-C15-C16-C17
18	N	515	HEA	C16-C17-C18-C19
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	C04-C05-C06-O06
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-C05-C06-O06
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	B	230	PSC	C11-C10-C9-C8
22	O	1230	PSC	C03-O11-P-O14
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

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Mol	Chain	Res	Type	Atoms
23	J	60	CHD	C16-C17-C20-C22
23	P	1271	CHD	C16-C17-C20-C22
23	W	1060	CHD	C13-C17-C20-C22
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22
24	C	272	DMU	O5-C6-O16-C18
26	C	265	PEK	C03-O11-P-O13
26	C	265	PEK	C04-O12-P-O11
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	1264	PEK	C13-C14-C15-C16
26	P	1265	PEK	C04-O12-P-O14
26	P	1265	PEK	O12-C04-C05-N
26	P	1265	PEK	C13-C14-C15-C16
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-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-OB3
27	P	1270	CDL	CA2-C1-CB2-OB2
27	P	1270	CDL	CA2-OA2-PA1-OA3
27	P	1270	CDL	C11-CA5-OA6-CA4
27	T	1269	CDL	O1-C1-CA2-OA2
27	T	1269	CDL	C1-CB2-OB2-PB2
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
23	C	271	CHD	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
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
21	L	522	TGL	OA1-CA1-OG1-CG1
21	N	1522	TGL	OA1-CA1-OG1-CG1
21	D	523	TGL	C21-C20-CA9-CA8
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
19	P	1267	PGV	C10-C11-C12-C13
26	C	265	PEK	C4-C5-C6-C7
26	C	265	PEK	C13-C14-C15-C16
26	G	264	PEK	C13-C14-C15-C16
26	G	1263	PEK	C4-C5-C6-C7
26	G	1263	PEK	C10-C11-C12-C13
26	P	1265	PEK	C4-C5-C6-C7
26	P	1265	PEK	C10-C11-C12-C13
26	T	263	PEK	C4-C5-C6-C7
26	T	263	PEK	C7-C8-C9-C10
26	T	263	PEK	C13-C14-C15-C16
21	N	1522	TGL	CC3-CC4-CC5-CC6
27	C	270	CDL	OA7-CA5-OA6-CA4
21	N	1522	TGL	C21-C20-CA9-CA8
27	C	270	CDL	O1-C1-CB2-OB2
27	P	1270	CDL	O1-C1-CB2-OB2
27	P	1270	CDL	C20-C21-C22-C23
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
24	Z	1526	DMU	O6-C11-C9-O1
21	O	1523	TGL	C11-C10-CB9-CB8

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Mol	Chain	Res	Type	Atoms
24	M	526	DMU	C19-C22-C25-C28
27	T	1269	CDL	C80-C81-C82-C83
21	D	523	TGL	C11-C10-CB9-CB8
26	G	1263	PEK	C28-C29-C30-C31
27	G	269	CDL	C15-C16-C17-C18
27	G	269	CDL	C22-C23-C24-C25
27	C	270	CDL	C20-C21-C22-C23
21	L	522	TGL	CA2-CA1-OG1-CG1
21	N	1522	TGL	CA2-CA1-OG1-CG1
27	G	269	CDL	OA7-CA5-OA6-CA4
27	T	1269	CDL	C73-C74-C75-C76
21	O	1523	TGL	OA1-CA1-OG1-CG1
22	B	230	PSC	O04-C19-O03-C01
22	O	1230	PSC	O04-C19-O03-C01
27	T	1269	CDL	OA9-CA7-OA8-CA6
24	M	526	DMU	O5-C6-O16-C18
24	P	1272	DMU	O5-C6-O16-C18
24	Z	1526	DMU	O5-C6-O16-C18
21	B	521	TGL	CA2-CA1-OG1-CG1
22	B	230	PSC	C20-C21-C22-C23
24	Z	1526	DMU	C19-C22-C25-C28
19	A	524	PGV	O12-C04-C05-C06
27	C	270	CDL	CA2-C1-CB2-OB2
27	G	269	CDL	CA2-C1-CB2-OB2
19	C	268	PGV	O02-C1-O01-C02
21	L	522	TGL	OB1-CB1-OG2-CG2
21	N	1521	TGL	CC2-CC1-OG3-CG3
27	G	269	CDL	C31-CA7-OA8-CA6
24	Z	1526	DMU	O5-C4-C57-O61
24	C	272	DMU	O6-C11-C9-C8
21	B	521	TGL	C21-C20-CA9-CA8
27	C	270	CDL	C83-C84-C85-C86
27	T	1269	CDL	C15-C16-C17-C18
23	P	1271	CHD	C17-C20-C22-C23
26	T	263	PEK	C28-C29-C30-C31
21	L	522	TGL	CC3-CC4-CC5-CC6
23	P	1271	CHD	C21-C20-C22-C23
24	P	1272	DMU	C1-C6-O16-C18
21	N	1521	TGL	CA2-CA1-OG1-CG1
24	M	526	DMU	O5-C4-C57-O61
26	G	264	PEK	C1-C2-C3-C4
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	C	272	DMU	C3-C4-C57-O61
24	P	1272	DMU	C3-C4-C57-O61
24	P	1272	DMU	O6-C11-C9-C8
22	O	1230	PSC	C11-C10-C9-C8
26	C	265	PEK	C7-C8-C9-C10
26	C	265	PEK	C10-C11-C12-C13
27	G	269	CDL	C40-C41-C42-C43
23	J	60	CHD	C13-C17-C20-C21
21	N	1521	TGL	OC1-CC1-OG3-CG3
19	A	524	PGV	C19-C20-C21-C22
21	N	1521	TGL	CA1-CA2-CA3-CA4
27	G	269	CDL	CA5-C11-C12-C13
27	G	269	CDL	CA7-C31-C32-C33
27	T	1269	CDL	CA5-C11-C12-C13
23	C	271	CHD	C17-C20-C22-C23
21	B	521	TGL	CC2-CC1-OG3-CG3
21	B	521	TGL	CA9-C20-C21-C22
27	T	1269	CDL	C40-C41-C42-C43
27	T	1269	CDL	OA7-CA5-OA6-CA4
24	C	272	DMU	O16-C18-C19-C22
21	N	1522	TGL	CB1-CB2-CB3-CB4
26	P	1264	PEK	C1-C2-C3-C4
27	P	1270	CDL	CB7-C71-C72-C73
24	M	526	DMU	O6-C11-C9-C8
19	N	1268	PGV	C2-C1-O01-C02
27	P	1270	CDL	C51-CB5-OB6-CB4
21	D	523	TGL	C16-C15-CC9-CC8
23	C	271	CHD	C21-C20-C22-C23
24	M	526	DMU	O6-C11-C9-O1
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	1521	TGL	OB1-CB1-OG2-CG2
21	B	521	TGL	CG2-CG3-OG3-CC1
22	O	1230	PSC	C20-C21-C22-C23
23	P	1271	CHD	C13-C17-C20-C21
21	B	521	TGL	OC1-CC1-OG3-CG3
27	C	270	CDL	CB7-C71-C72-C73
27	C	270	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C04-O12-P-O11
22	O	1230	PSC	C03-O11-P-O12
26	C	265	PEK	C03-O11-P-O12
26	T	263	PEK	C03-O11-P-O12
27	C	270	CDL	CA3-OA5-PA1-OA2
27	C	270	CDL	CB2-OB2-PB2-OB5
27	G	269	CDL	CB3-OB5-PB2-OB2
27	P	1270	CDL	CA2-OA2-PA1-OA5
27	P	1270	CDL	CA3-OA5-PA1-OA2
27	P	1270	CDL	CB2-OB2-PB2-OB5
27	T	1269	CDL	CB3-OB5-PB2-OB2
21	L	522	TGL	CB1-CB2-CB3-CB4
23	W	1060	CHD	C13-C17-C20-C21
22	O	1230	PSC	C1-C2-C3-C4
19	C	268	PGV	O12-C04-C05-C06
19	N	1268	PGV	O12-C04-C05-C06
27	T	1269	CDL	CA2-C1-CB2-OB2
19	N	1268	PGV	O02-C1-O01-C02
27	P	1270	CDL	OB7-CB5-OB6-CB4
24	P	1272	DMU	O16-C18-C19-C22
27	G	269	CDL	C59-C60-C61-C62
24	C	272	DMU	C4-C3-O7-C10
19	C	268	PGV	C12-C13-C14-C15
21	O	1523	TGL	CB5-CB6-CB7-CB8
26	G	264	PEK	C25-C26-C27-C28
27	C	270	CDL	C76-C77-C78-C79
21	N	1521	TGL	CB2-CB1-OG2-CG2
19	N	1266	PGV	C23-C24-C25-C26
21	B	521	TGL	C14-C29-C30-C31
21	D	523	TGL	C19-C33-C34-C35
26	G	1263	PEK	C31-C32-C33-C34
27	C	270	CDL	C73-C74-C75-C76
27	C	270	CDL	C82-C83-C84-C85
27	P	1270	CDL	C58-C59-C60-C61
19	A	524	PGV	C24-C25-C26-C27
19	C	268	PGV	C20-C21-C22-C23
19	C	268	PGV	C24-C25-C26-C27
19	C	268	PGV	C30-C31-C32-C33
19	P	1267	PGV	C13-C14-C15-C16
21	D	523	TGL	CB3-CB4-CB5-CB6
21	D	523	TGL	CB5-CB6-CB7-CB8
21	L	522	TGL	CA7-CA8-CA9-C20

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Mol	Chain	Res	Type	Atoms
21	N	1521	TGL	CA5-CA6-CA7-CA8
21	O	1523	TGL	CC4-CC5-CC6-CC7
19	A	521	PGV	C6-C7-C8-C9
19	N	1524	PGV	C4-C5-C6-C7
19	N	1266	PGV	C5-C6-C7-C8
19	N	1268	PGV	C13-C14-C15-C16
27	P	1270	CDL	C72-C73-C74-C75
27	P	1270	CDL	C73-C74-C75-C76
27	T	1269	CDL	C60-C61-C62-C63
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	N	1522	TGL	CA5-CA6-CA7-CA8
21	N	1522	TGL	CB4-CB5-CB6-CB7
26	G	264	PEK	C31-C32-C33-C34
26	T	263	PEK	C25-C26-C27-C28
27	C	270	CDL	C72-C73-C74-C75
21	L	522	TGL	CB9-C10-C11-C12
21	N	1521	TGL	CA6-CA7-CA8-CA9
21	N	1522	TGL	CA7-CA8-CA9-C20
24	Z	1526	DMU	C28-C31-C34-C37
26	C	265	PEK	C16-C17-C18-C19
26	C	265	PEK	C25-C26-C27-C28
26	G	1263	PEK	C25-C26-C27-C28
27	C	270	CDL	C59-C60-C61-C62
27	P	1270	CDL	C15-C16-C17-C18
19	N	1266	PGV	C6-C7-C8-C9
19	N	1266	PGV	C7-C8-C9-C10
19	N	1268	PGV	C26-C27-C28-C29
21	L	522	TGL	CB6-CB7-CB8-CB9
21	L	522	TGL	C21-C22-C23-C24
21	N	1522	TGL	C24-C25-C26-C27
26	T	263	PEK	C31-C32-C33-C34
27	C	270	CDL	C42-C43-C44-C45
19	A	524	PGV	C20-C21-C22-C23
19	A	521	PGV	C5-C6-C7-C8
19	N	1524	PGV	C22-C23-C24-C25
21	O	1523	TGL	C17-C18-C19-C33
22	B	230	PSC	C24-C25-C26-C27
26	G	1263	PEK	C29-C30-C31-C32
27	C	270	CDL	C57-C58-C59-C60
19	C	267	PGV	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
21	D	523	TGL	CB1-CB2-CB3-CB4
19	N	1268	PGV	C25-C26-C27-C28
19	N	1268	PGV	C27-C28-C29-C30
21	L	522	TGL	C24-C25-C26-C27
21	N	1522	TGL	CC4-CC5-CC6-CC7
21	O	1523	TGL	C15-C16-C17-C18
26	G	1263	PEK	C33-C34-C35-C36
27	C	270	CDL	C36-C37-C38-C39
27	G	269	CDL	C81-C82-C83-C84
27	P	1270	CDL	C36-C37-C38-C39
27	P	1270	CDL	C79-C80-C81-C82
21	N	1521	TGL	OA1-CA1-OG1-CG1
19	N	1268	PGV	C24-C25-C26-C27
26	G	264	PEK	C29-C30-C31-C32
27	G	269	CDL	C61-C62-C63-C64
27	G	269	CDL	C62-C63-C64-C65
27	P	1270	CDL	C11-C12-C13-C14
21	B	521	TGL	OB1-CB1-OG2-CG2
19	N	1268	PGV	C14-C15-C16-C17
21	O	1523	TGL	CB2-CB3-CB4-CB5
26	P	1265	PEK	C25-C26-C27-C28
26	T	263	PEK	C29-C30-C31-C32
27	C	270	CDL	C11-C12-C13-C14
27	G	269	CDL	C82-C83-C84-C85
19	N	1268	PGV	C11-C10-C9-C8
21	B	521	TGL	CB1-CB2-CB3-CB4
21	O	1523	TGL	CB1-CB2-CB3-CB4
19	C	268	PGV	C13-C14-C15-C16
21	D	523	TGL	C10-C11-C12-C13
22	B	230	PSC	C26-C27-C28-C29
22	O	1230	PSC	C5-C6-C7-C8
24	M	526	DMU	C25-C28-C31-C34
24	P	1272	DMU	C19-C22-C25-C28
26	G	1263	PEK	C16-C17-C18-C19
26	G	1263	PEK	C27-C28-C29-C30
26	P	1264	PEK	C16-C17-C18-C19
27	C	270	CDL	C13-C14-C15-C16
27	G	269	CDL	C13-C14-C15-C16
27	G	269	CDL	C56-C57-C58-C59
21	N	1521	TGL	C15-C16-C17-C18
21	N	1522	TGL	C12-C13-C14-C29
21	N	1522	TGL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C23-C24-C25-C26
24	P	1272	DMU	C28-C31-C34-C37
27	G	269	CDL	C54-C55-C56-C57
21	L	522	TGL	CC9-C15-C16-C17
21	N	1521	TGL	C16-C17-C18-C19
21	O	1523	TGL	C18-C19-C33-C34
24	Z	1526	DMU	C25-C28-C31-C34
26	C	265	PEK	C32-C33-C34-C35
27	G	269	CDL	C79-C80-C81-C82
27	P	1270	CDL	C42-C43-C44-C45
27	P	1270	CDL	C51-C52-C53-C54
21	N	1521	TGL	CB1-CB2-CB3-CB4
22	B	230	PSC	C1-C2-C3-C4
26	P	1265	PEK	C1-C2-C3-C4
21	L	522	TGL	CC6-CC7-CC8-CC9
26	T	263	PEK	C27-C28-C29-C30
26	T	263	PEK	C30-C31-C32-C33
27	C	270	CDL	C74-C75-C76-C77
27	C	270	CDL	C78-C79-C80-C81
27	P	1270	CDL	C59-C60-C61-C62
19	A	521	PGV	C7-C8-C9-C10
21	N	1522	TGL	C10-C11-C12-C13
19	C	268	PGV	C14-C15-C16-C17
21	L	522	TGL	CA3-CA4-CA5-CA6
27	G	269	CDL	C73-C74-C75-C76
21	N	1521	TGL	C13-C14-C29-C30
21	N	1522	TGL	CC6-CC7-CC8-CC9
21	N	1522	TGL	CC9-C15-C16-C17
26	P	1264	PEK	C26-C27-C28-C29
27	C	270	CDL	C38-C39-C40-C41
27	C	270	CDL	C41-C42-C43-C44
19	A	524	PGV	C22-C23-C24-C25
21	D	523	TGL	CB2-CB3-CB4-CB5
21	N	1522	TGL	CA2-CA3-CA4-CA5
27	T	1269	CDL	C72-C73-C74-C75
27	P	1270	CDL	CA5-C11-C12-C13
19	N	1268	PGV	C30-C31-C32-C33
21	N	1521	TGL	CA4-CA5-CA6-CA7
27	C	270	CDL	C51-C52-C53-C54
21	B	521	TGL	CA5-CA6-CA7-CA8
26	P	1265	PEK	C29-C30-C31-C32
27	P	1270	CDL	C13-C14-C15-C16

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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	N	1266	PGV	C29-C30-C31-C32
27	C	270	CDL	C61-C62-C63-C64
19	A	524	PGV	C11-C10-C9-C8
19	C	268	PGV	C11-C10-C9-C8
19	N	1524	PGV	C11-C10-C9-C8
26	C	265	PEK	C15-C16-C17-C18
26	G	264	PEK	C27-C28-C29-C30
24	C	272	DMU	C19-C22-C25-C28
27	T	1269	CDL	C36-C37-C38-C39
27	C	270	CDL	C75-C76-C77-C78
27	G	269	CDL	C72-C73-C74-C75
19	A	521	PGV	C30-C31-C32-C33
21	L	522	TGL	CC2-CC3-CC4-CC5
27	C	270	CDL	C15-C16-C17-C18
27	T	1269	CDL	C23-C24-C25-C26
19	A	521	PGV	C4-C5-C6-C7
21	D	523	TGL	CA9-C20-C21-C22
21	L	522	TGL	C17-C18-C19-C33
22	O	1230	PSC	C29-C30-C31-C32
24	P	1272	DMU	C22-C25-C28-C31
26	P	1264	PEK	C25-C26-C27-C28
21	D	523	TGL	CC6-CC7-CC8-CC9
22	B	230	PSC	C29-C30-C31-C32
19	C	268	PGV	C26-C27-C28-C29
19	N	1524	PGV	C24-C25-C26-C27
21	L	522	TGL	C10-C11-C12-C13
26	G	1263	PEK	C26-C27-C28-C29
19	P	1267	PGV	C1-C2-C3-C4
21	L	522	TGL	C25-C26-C27-C28
21	N	1521	TGL	CB9-C10-C11-C12
27	G	269	CDL	C35-C36-C37-C38
27	G	269	CDL	C36-C37-C38-C39
19	N	1524	PGV	C14-C15-C16-C17
27	C	270	CDL	C40-C41-C42-C43
22	B	230	PSC	C11-C12-C13-C14
19	N	1268	PGV	C12-C13-C14-C15
26	P	1264	PEK	C15-C16-C17-C18
26	P	1265	PEK	C15-C16-C17-C18
19	N	1268	PGV	C20-C19-O03-C01
26	C	265	PEK	C22-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
27	T	1269	CDL	C71-CB7-OB8-CB6
22	O	1230	PSC	C23-C24-C25-C26
21	B	521	TGL	C15-C16-C17-C18
21	N	1521	TGL	CA3-CA4-CA5-CA6
21	O	1523	TGL	CC6-CC7-CC8-CC9
27	G	269	CDL	CB7-C71-C72-C73
21	N	1521	TGL	C14-C29-C30-C31
24	C	272	DMU	C22-C25-C28-C31
26	P	1264	PEK	C24-C25-C26-C27
27	P	1270	CDL	C74-C75-C76-C77
27	T	1269	CDL	C62-C63-C64-C65
22	B	230	PSC	C27-C28-C29-C30
27	C	270	CDL	C32-C33-C34-C35
27	T	1269	CDL	C77-C78-C79-C80
19	N	1266	PGV	C4-C5-C6-C7
21	B	521	TGL	C16-C17-C18-C19
26	P	1264	PEK	C31-C32-C33-C34
27	P	1270	CDL	C60-C61-C62-C63
19	N	1524	PGV	C19-C20-C21-C22
19	N	1266	PGV	C19-C20-C21-C22
21	B	521	TGL	CB2-CB1-OG2-CG2
27	C	270	CDL	C51-CB5-OB6-CB4
27	G	269	CDL	C78-C79-C80-C81
21	D	523	TGL	C17-C18-C19-C33
26	C	265	PEK	C34-C35-C36-C37
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
22	O	1230	PSC	C04-C05-N-C08
27	C	270	CDL	C71-C72-C73-C74
27	P	1270	CDL	C35-C36-C37-C38
27	T	1269	CDL	C71-C72-C73-C74
27	T	1269	CDL	C11-C12-C13-C14
27	T	1269	CDL	C31-C32-C33-C34
19	C	268	PGV	C29-C30-C31-C32
21	L	522	TGL	C20-C21-C22-C23
21	O	1523	TGL	CB3-CB4-CB5-CB6
26	G	264	PEK	C16-C17-C18-C19
26	G	264	PEK	C24-C25-C26-C27
21	L	522	TGL	CC4-CC5-CC6-CC7
26	C	265	PEK	O04-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
19	N	1268	PGV	C22-C23-C24-C25
21	N	1522	TGL	CB6-CB7-CB8-CB9
27	P	1270	CDL	C71-C72-C73-C74
27	T	1269	CDL	C55-C56-C57-C58
19	A	524	PGV	C03-O11-P-O12
19	N	1524	PGV	C04-O12-P-O11
22	O	1230	PSC	C04-O12-P-O11
27	C	270	CDL	OA5-CA3-CA4-CA6
27	C	270	CDL	OB5-CB3-CB4-CB6
19	C	267	PGV	C24-C25-C26-C27
21	O	1523	TGL	CA9-C20-C21-C22
26	P	1265	PEK	C24-C25-C26-C27
24	P	1272	DMU	C4-C3-O7-C10
19	P	1267	PGV	C22-C23-C24-C25
22	O	1230	PSC	C27-C28-C29-C30
26	C	265	PEK	C29-C30-C31-C32
19	N	1268	PGV	O04-C19-O03-C01
24	M	526	DMU	C3-C4-C57-O61
21	N	1521	TGL	CA9-C20-C21-C22
21	N	1522	TGL	C11-C12-C13-C14
26	G	1263	PEK	C30-C31-C32-C33
27	G	269	CDL	C37-C38-C39-C40
19	N	1524	PGV	C2-C3-C4-C5
19	A	521	PGV	C19-C20-C21-C22
24	Z	1526	DMU	C22-C25-C28-C31
27	C	270	CDL	C19-C20-C21-C22
27	G	269	CDL	C44-C45-C46-C47
19	A	524	PGV	O03-C01-C02-C03
19	C	267	PGV	C30-C31-C32-C33
21	N	1521	TGL	OG1-CG1-CG2-CG3
22	O	1230	PSC	C26-C27-C28-C29
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
26	P	1264	PEK	C7-C8-C9-C10
26	C	265	PEK	C22-C23-C24-C25
27	G	269	CDL	C33-C34-C35-C36
27	T	1269	CDL	C64-C65-C66-C67
27	P	1270	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
21	L	522	TGL	CA2-CA3-CA4-CA5
21	N	1522	TGL	C29-C30-C31-C32
19	C	268	PGV	C31-C32-C33-C34
26	P	1264	PEK	C27-C28-C29-C30
27	G	269	CDL	C55-C56-C57-C58
19	A	521	PGV	C12-C13-C14-C15
19	N	1524	PGV	C12-C13-C14-C15
19	P	1267	PGV	C25-C26-C27-C28
21	L	522	TGL	C21-C20-CA9-CA8
27	P	1270	CDL	C41-C42-C43-C44
27	P	1270	CDL	C55-C56-C57-C58
19	P	1267	PGV	C23-C24-C25-C26
19	P	1267	PGV	C31-C32-C33-C34
26	T	263	PEK	C26-C27-C28-C29
21	N	1521	TGL	CB3-CB4-CB5-CB6
24	P	1272	DMU	C34-C37-C40-C43
27	G	269	CDL	CB5-C51-C52-C53
19	C	267	PGV	C7-C8-C9-C10
19	P	1267	PGV	C15-C16-C17-C18
21	D	523	TGL	C15-C16-C17-C18
21	D	523	TGL	C33-C34-C35-C36
21	N	1522	TGL	C16-C15-CC9-CC8
24	C	272	DMU	O5-C4-C57-O61
21	B	521	TGL	C25-C26-C27-C28
26	G	264	PEK	C32-C33-C34-C35
27	P	1270	CDL	C44-C45-C46-C47
27	T	1269	CDL	OB9-CB7-OB8-CB6
19	C	268	PGV	O01-C02-C03-O11
19	C	268	PGV	C10-C11-C12-C13
22	O	1230	PSC	C04-C05-N-C07
27	G	269	CDL	C75-C76-C77-C78
19	C	268	PGV	C25-C26-C27-C28
24	C	272	DMU	C1-C6-O16-C18
19	C	267	PGV	C25-C26-C27-C28
22	O	1230	PSC	O03-C01-C02-O01
21	B	521	TGL	CB9-C10-C11-C12
21	N	1522	TGL	C22-C23-C24-C25
26	G	264	PEK	C26-C27-C28-C29
27	C	270	CDL	OB7-CB5-OB6-CB4
26	G	264	PEK	C17-C18-C19-C20
27	G	269	CDL	C64-C65-C66-C67
26	C	265	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
21	N	1522	TGL	CB5-CB6-CB7-CB8
19	N	1524	PGV	C28-C29-C30-C31
21	O	1523	TGL	C19-C33-C34-C35
26	G	264	PEK	C34-C35-C36-C37
27	T	1269	CDL	C54-C55-C56-C57
21	D	523	TGL	C13-C14-C29-C30
27	T	1269	CDL	C44-C45-C46-C47
19	C	267	PGV	C31-C32-C33-C34
27	T	1269	CDL	CB2-C1-CA2-OA2
24	M	526	DMU	C28-C31-C34-C37
24	M	526	DMU	C34-C37-C40-C43
26	P	1265	PEK	C22-C21-O03-C01
27	P	1270	CDL	C31-CA7-OA8-CA6
19	N	1268	PGV	C10-C11-C12-C13
26	G	264	PEK	C10-C11-C12-C13
27	T	1269	CDL	CA7-C31-C32-C33
21	D	523	TGL	C16-C17-C18-C19
22	O	1230	PSC	C21-C22-C23-C24
27	P	1270	CDL	C57-C58-C59-C60
27	P	1270	CDL	C61-C62-C63-C64
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
27	T	1269	CDL	C21-C22-C23-C24
19	C	267	PGV	C13-C14-C15-C16
19	P	1267	PGV	C7-C8-C9-C10
24	P	1272	DMU	C25-C28-C31-C34
21	B	521	TGL	C13-C14-C29-C30
19	A	521	PGV	C31-C32-C33-C34
19	C	267	PGV	C22-C23-C24-C25
27	C	270	CDL	C77-C78-C79-C80
19	A	524	PGV	C05-C04-O12-P
27	C	270	CDL	CA4-CA3-OA5-PA1
21	N	1522	TGL	C21-C22-C23-C24
26	P	1265	PEK	C22-C23-C24-C25
27	T	1269	CDL	C13-C14-C15-C16
24	M	526	DMU	C19-C18-O16-C6
24	Z	1526	DMU	C19-C18-O16-C6
27	T	1269	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
21	B	521	TGL	CA6-CA7-CA8-CA9
21	B	521	TGL	C20-C21-C22-C23
21	O	1523	TGL	C16-C15-CC9-CC8
27	G	269	CDL	C42-C43-C44-C45
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
19	C	267	PGV	C15-C16-C17-C18
21	D	523	TGL	CB6-CB7-CB8-CB9
27	G	269	CDL	C31-C32-C33-C34
19	N	1524	PGV	C10-C11-C12-C13
26	P	1264	PEK	C10-C11-C12-C13
26	T	263	PEK	C10-C11-C12-C13
27	G	269	CDL	C80-C81-C82-C83
27	C	270	CDL	C55-C56-C57-C58
27	C	270	CDL	C58-C59-C60-C61
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	B	521	TGL	C16-C15-CC9-CC8
22	O	1230	PSC	C31-C32-C33-C34
19	A	524	PGV	O05-C05-C06-O06
19	N	1268	PGV	O01-C02-C03-O11
26	G	1263	PEK	O01-C02-C03-O11
27	C	270	CDL	OB5-CB3-CB4-OB6
19	C	268	PGV	C23-C24-C25-C26
19	A	521	PGV	C29-C30-C31-C32
27	C	270	CDL	C84-C85-C86-C87
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
21	D	523	TGL	CA2-CA1-OG1-CG1
19	N	1268	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	L	522	TGL	C29-C30-C31-C32
27	P	1270	CDL	C22-C23-C24-C25
21	O	1523	TGL	C12-C13-C14-C29
21	O	1523	TGL	C33-C34-C35-C36
27	T	1269	CDL	C82-C83-C84-C85
26	G	1263	PEK	C21-C22-C23-C24
27	G	269	CDL	CB4-CB3-OB5-PB2
26	P	1264	PEK	C2-C3-C4-C5
21	L	522	TGL	OG1-CA1-CA2-CA3
21	L	522	TGL	CC5-CC6-CC7-CC8
22	B	230	PSC	C31-C32-C33-C34
26	P	1265	PEK	O04-C21-O03-C01
21	D	523	TGL	CB9-C10-C11-C12
26	G	1263	PEK	C32-C33-C34-C35
27	C	270	CDL	C80-C81-C82-C83
27	G	269	CDL	C39-C40-C41-C42
19	A	524	PGV	C25-C26-C27-C28
26	T	263	PEK	C01-C02-C03-O11
27	P	1270	CDL	OA5-CA3-CA4-CA6
21	L	522	TGL	CB7-CB8-CB9-C10
21	B	521	TGL	CA3-CA4-CA5-CA6
26	P	1264	PEK	C32-C33-C34-C35
27	G	269	CDL	C14-C15-C16-C17
27	P	1270	CDL	C43-C44-C45-C46
21	B	521	TGL	C22-C23-C24-C25
27	T	1269	CDL	C33-C34-C35-C36
19	N	1524	PGV	C6-C7-C8-C9
26	P	1264	PEK	C30-C31-C32-C33
21	N	1521	TGL	CB4-CB5-CB6-CB7
19	A	524	PGV	C03-C02-O01-C1
19	N	1524	PGV	C03-C02-O01-C1
21	D	523	TGL	CG3-CG2-OG2-CB1
27	G	269	CDL	C71-CB7-OB8-CB6
19	C	267	PGV	C28-C29-C30-C31
26	C	265	PEK	C1-C2-C3-C4
22	O	1230	PSC	O03-C01-C02-C03
27	G	269	CDL	CA3-CA4-CA6-OA8
19	N	1266	PGV	C31-C32-C33-C34
27	P	1270	CDL	OA5-CA3-CA4-OA6
27	T	1269	CDL	OA5-CA3-CA4-OA6
19	A	524	PGV	C10-C11-C12-C13
19	N	1524	PGV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C26-C27-C28-C29
27	C	270	CDL	OA6-CA4-CA6-OA8
27	C	270	CDL	OB6-CB4-CB6-OB8
19	A	524	PGV	C26-C27-C28-C29
19	A	524	PGV	C28-C29-C30-C31
21	D	523	TGL	OA1-CA1-OG1-CG1
27	P	1270	CDL	OA9-CA7-OA8-CA6
26	P	1264	PEK	C29-C30-C31-C32
27	T	1269	CDL	C19-C20-C21-C22
22	O	1230	PSC	C04-C05-N-C06
27	C	270	CDL	CA5-C11-C12-C13
26	P	1264	PEK	C17-C18-C19-C20
19	C	268	PGV	O04-C19-O03-C01
19	C	268	PGV	C20-C19-O03-C01
27	T	1269	CDL	C79-C80-C81-C82
19	N	1268	PGV	C04-O12-P-O11
26	P	1265	PEK	C04-O12-P-O11
27	T	1269	CDL	CB2-OB2-PB2-OB5
19	N	1524	PGV	O12-C04-C05-O05
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
27	T	1269	CDL	CB4-CB3-OB5-PB2
21	N	1521	TGL	C18-C19-C33-C34
21	O	1523	TGL	CA5-CA6-CA7-CA8
27	C	270	CDL	C35-C36-C37-C38
19	A	524	PGV	C03-O11-P-O14
19	C	268	PGV	C04-O12-P-O14
19	N	1524	PGV	C04-O12-P-O13
22	O	1230	PSC	C03-O11-P-O13
22	O	1230	PSC	C04-O12-P-O13
26	C	265	PEK	C03-O11-P-O14
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
21	O	1523	TGL	CA6-CA7-CA8-CA9
26	G	1263	PEK	C17-C18-C19-C20
22	B	230	PSC	C3-C4-C5-C6
24	Z	1526	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
18	A	516	HEA	C3B-C11-C12-C13
21	N	1522	TGL	C17-C18-C19-C33
26	T	263	PEK	C21-C22-C23-C24
21	N	1522	TGL	CB2-CB3-CB4-CB5
27	G	269	CDL	C24-C25-C26-C27
26	G	264	PEK	O02-C1-O01-C02
18	A	516	HEA	C2A-CAA-CBA-CGA
26	P	1265	PEK	O01-C02-C03-O11
27	C	270	CDL	OA5-CA3-CA4-OA6
27	P	1270	CDL	OB5-CB3-CB4-OB6
19	C	268	PGV	C15-C16-C17-C18
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	C2-C1-O01-C02
27	P	1270	CDL	C84-C85-C86-C87
27	T	1269	CDL	C16-C17-C18-C19
26	C	265	PEK	C30-C31-C32-C33
23	C	271	CHD	C13-C17-C20-C21
21	O	1523	TGL	CB6-CB7-CB8-CB9
22	O	1230	PSC	C22-C23-C24-C25
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
27	C	270	CDL	C34-C35-C36-C37
27	T	1269	CDL	C39-C40-C41-C42
21	B	521	TGL	CC5-CC6-CC7-CC8
19	N	1268	PGV	C4-C5-C6-C7
19	A	521	PGV	O03-C19-C20-C21
27	G	269	CDL	OB9-CB7-OB8-CB6
21	D	523	TGL	C24-C25-C26-C27
19	N	1266	PGV	C30-C31-C32-C33
26	P	1265	PEK	C23-C24-C25-C26
21	D	523	TGL	CA7-CA8-CA9-C20
26	C	265	PEK	C23-C24-C25-C26
19	P	1267	PGV	C24-C25-C26-C27
26	G	264	PEK	C4-C5-C6-C7
27	G	269	CDL	O1-C1-CA2-OA2
23	C	271	CHD	C13-C17-C20-C22
21	N	1522	TGL	CB3-CB4-CB5-CB6

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Mol	Chain	Res	Type	Atoms
27	T	1269	CDL	C24-C25-C26-C27
22	O	1230	PSC	C03-C02-O01-C1
19	N	1268	PGV	C01-C02-C03-O11
22	B	230	PSC	C01-C02-C03-O11
26	G	1263	PEK	C01-C02-C03-O11
27	P	1270	CDL	C81-C82-C83-C84
19	N	1524	PGV	O03-C19-C20-C21
19	N	1266	PGV	O03-C19-C20-C21
21	L	522	TGL	OG2-CB1-CB2-CB3
19	A	521	PGV	C9-C10-C11-C12
19	C	268	PGV	C05-C04-O12-P
27	C	270	CDL	C1-CA2-OA2-PA1
27	P	1270	CDL	CA4-CA3-OA5-PA1
21	B	521	TGL	CB3-CB4-CB5-CB6
26	T	263	PEK	O01-C02-C03-O11
19	A	524	PGV	C7-C8-C9-C10
19	C	268	PGV	C3-C4-C5-C6
27	G	269	CDL	C20-C21-C22-C23
23	G	86	CHD	C17-C20-C22-C23
19	P	1267	PGV	C30-C31-C32-C33
21	D	523	TGL	OG2-CG2-CG3-OG3
19	N	1268	PGV	C23-C24-C25-C26
21	O	1523	TGL	C13-C14-C29-C30
27	T	1269	CDL	C75-C76-C77-C78
19	N	1524	PGV	C03-O11-P-O12
27	C	270	CDL	CA2-OA2-PA1-OA5
27	G	269	CDL	CB2-OB2-PB2-OB5
21	N	1521	TGL	C20-C21-C22-C23
26	P	1265	PEK	C33-C34-C35-C36
27	C	270	CDL	C81-C82-C83-C84
27	P	1270	CDL	C34-C35-C36-C37
19	N	1266	PGV	C9-C10-C11-C12
27	T	1269	CDL	C58-C59-C60-C61
26	G	1263	PEK	C02-C03-O11-P
19	P	1267	PGV	C9-C10-C11-C12
21	N	1521	TGL	C11-C10-CB9-CB8
24	C	272	DMU	C25-C28-C31-C34
23	W	1060	CHD	C17-C20-C22-C23
26	P	1264	PEK	C34-C35-C36-C37
19	A	524	PGV	C21-C22-C23-C24
23	J	60	CHD	C22-C23-C24-O25
19	C	268	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	T	1269	CDL	OB5-CB3-CB4-CB6
27	T	1269	CDL	C53-C54-C55-C56
26	T	263	PEK	C33-C34-C35-C36
21	D	523	TGL	CC3-CC4-CC5-CC6
27	G	269	CDL	OB6-CB4-CB6-OB8
27	P	1270	CDL	C16-C17-C18-C19
19	C	268	PGV	C02-C03-O11-P
18	A	516	HEA	CAA-CBA-CGA-O1A
18	N	516	HEA	CAA-CBA-CGA-O1A
23	G	86	CHD	C22-C23-C24-O25
19	N	1524	PGV	C9-C10-C11-C12
22	O	1230	PSC	C7-C8-C9-C10
27	C	270	CDL	C31-CA7-OA8-CA6
19	N	1524	PGV	C20-C21-C22-C23
21	O	1523	TGL	CB7-CB8-CB9-C10
19	C	267	PGV	C12-C13-C14-C15
23	W	1060	CHD	C22-C23-C24-O25
19	A	521	PGV	C28-C29-C30-C31
19	N	1268	PGV	C7-C8-C9-C10
21	O	1523	TGL	C14-C29-C30-C31
19	N	1524	PGV	O12-C04-C05-C06
21	O	1523	TGL	OG1-CG1-CG2-CG3
23	J	60	CHD	C17-C20-C22-C23
23	B	1086	CHD	C22-C23-C24-O26
26	P	1265	PEK	C7-C8-C9-C10
21	O	1523	TGL	CC2-CC3-CC4-CC5
26	T	263	PEK	C22-C23-C24-C25
26	G	264	PEK	C23-C24-C25-C26
21	N	1521	TGL	CC5-CC6-CC7-CC8
21	B	521	TGL	CG3-CG2-OG2-CB1
18	N	516	HEA	CAA-CBA-CGA-O2A
23	C	271	CHD	C22-C23-C24-O25
23	P	1271	CHD	C22-C23-C24-O25
19	C	267	PGV	C29-C30-C31-C32
22	O	1230	PSC	C25-C26-C27-C28
22	B	230	PSC	C03-O11-P-O12
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

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Mol	Chain	Res	Type	Atoms
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	B	1086	CHD	C22-C23-C24-O25
23	J	60	CHD	C22-C23-C24-O26
23	P	1271	CHD	C22-C23-C24-O26
26	T	263	PEK	C34-C35-C36-C37
27	G	269	CDL	OA5-CA3-CA4-CA6
23	B	1086	CHD	C17-C20-C22-C23
19	A	521	PGV	C23-C24-C25-C26
27	C	270	CDL	C52-C53-C54-C55
23	W	1060	CHD	C22-C23-C24-O26
18	N	516	HEA	CAD-CBD-CGD-O1D
21	B	521	TGL	CB4-CB5-CB6-CB7
18	A	516	HEA	CAA-CBA-CGA-O2A
27	G	269	CDL	C23-C24-C25-C26
21	D	523	TGL	CA5-CA6-CA7-CA8
21	L	522	TGL	CA5-CA6-CA7-CA8
19	C	268	PGV	C19-C20-C21-C22
27	C	270	CDL	C24-C25-C26-C27
19	A	524	PGV	C31-C32-C33-C34
18	N	516	HEA	CAD-CBD-CGD-O2D
27	P	1270	CDL	C18-C19-C20-C21
19	N	1266	PGV	C20-C21-C22-C23
26	P	1265	PEK	C32-C33-C34-C35
21	L	522	TGL	C16-C17-C18-C19
26	G	264	PEK	C3-C4-C5-C6
21	B	521	TGL	OG1-CG1-CG2-CG3
18	A	515	HEA	CAD-CBD-CGD-O1D
23	C	271	CHD	C22-C23-C24-O26
18	A	516	HEA	CAD-CBD-CGD-O2D
23	G	86	CHD	C22-C23-C24-O26
21	N	1522	TGL	OG2-CB1-CB2-CB3
27	T	1269	CDL	C35-C36-C37-C38
19	A	521	PGV	C11-C12-C13-C14
26	G	1263	PEK	C3-C4-C5-C6
23	C	525	CHD	C22-C23-C24-O26
27	C	270	CDL	C62-C63-C64-C65
27	G	269	CDL	C71-C72-C73-C74
21	O	1523	TGL	CB9-C10-C11-C12
21	N	1521	TGL	C29-C30-C31-C32
21	O	1523	TGL	OG2-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
27	T	1269	CDL	OB6-CB4-CB6-OB8
21	B	521	TGL	OG1-CA1-CA2-CA3
24	C	272	DMU	C5-C10-O7-C3
18	A	516	HEA	CAD-CBD-CGD-O1D
19	N	1266	PGV	C11-C12-C13-C14
21	D	523	TGL	CA1-CA2-CA3-CA4
21	N	1522	TGL	OG3-CC1-CC2-CC3
22	O	1230	PSC	O01-C1-C2-C3
18	A	515	HEA	CAA-CBA-CGA-O1A
27	G	269	CDL	CA2-OA2-PA1-OA5
22	B	230	PSC	C04-C05-N-C08
22	B	230	PSC	O01-C1-C2-C3
27	P	1270	CDL	C75-C76-C77-C78
18	N	515	HEA	CAA-CBA-CGA-O1A
18	N	515	HEA	CAD-CBD-CGD-O1D
27	C	270	CDL	C53-C54-C55-C56
19	C	267	PGV	C9-C10-C11-C12
26	C	265	PEK	C35-C36-C37-C38
23	P	1525	CHD	C22-C23-C24-O26
21	O	1523	TGL	CG1-CG2-OG2-CB1
22	B	230	PSC	C03-C02-O01-C1
27	T	1269	CDL	C56-C57-C58-C59
19	C	268	PGV	C21-C22-C23-C24
21	B	521	TGL	C12-C13-C14-C29
26	P	1264	PEK	C28-C29-C30-C31
26	P	1264	PEK	O01-C1-C2-C3
19	N	1268	PGV	C6-C7-C8-C9
27	T	1269	CDL	C37-C38-C39-C40
26	G	1263	PEK	C15-C16-C17-C18
19	C	267	PGV	C05-C04-O12-P
21	B	521	TGL	CB6-CB7-CB8-CB9
26	T	263	PEK	C23-C24-C25-C26
18	A	515	HEA	CAD-CBD-CGD-O2D
23	P	1525	CHD	C22-C23-C24-O25
23	C	525	CHD	C22-C23-C24-O25
26	P	1264	PEK	C14-C15-C16-C17
26	T	263	PEK	O02-C1-O01-C02
18	A	515	HEA	CAA-CBA-CGA-O2A
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	OG1-CA1-CA2-CA3

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Mol	Chain	Res	Type	Atoms
26	G	1263	PEK	O01-C1-C2-C3
21	D	523	TGL	OG1-CG1-CG2-OG2
19	C	267	PGV	O04-C19-O03-C01
18	N	515	HEA	CAA-CBA-CGA-O2A
18	N	515	HEA	CAD-CBD-CGD-O2D
21	O	1523	TGL	OG3-CC1-CC2-CC3
27	P	1270	CDL	C32-C31-CA7-OA8
19	N	1268	PGV	C31-C32-C33-C34
24	Z	1526	DMU	C18-C19-C22-C25
27	G	269	CDL	C18-C19-C20-C21
21	N	1522	TGL	C11-C10-CB9-CB8
27	T	1269	CDL	C20-C21-C22-C23
21	L	522	TGL	OG3-CC1-CC2-CC3
21	N	1522	TGL	OG1-CA1-CA2-CA3
21	D	523	TGL	CC4-CC5-CC6-CC7
27	G	269	CDL	C63-C64-C65-C66
27	C	270	CDL	OA9-CA7-OA8-CA6
21	D	523	TGL	C21-C22-C23-C24
21	D	523	TGL	C29-C30-C31-C32
21	L	522	TGL	CB4-CB5-CB6-CB7
26	P	1265	PEK	C26-C27-C28-C29
26	T	263	PEK	C3-C4-C5-C6
26	P	1265	PEK	C34-C35-C36-C37
21	D	523	TGL	C12-C13-C14-C29
21	N	1522	TGL	OC1-CC1-CC2-CC3
26	P	1264	PEK	O02-C1-C2-C3
26	G	264	PEK	O01-C1-C2-C3
26	T	263	PEK	C2-C1-O01-C02
27	T	1269	CDL	C63-C64-C65-C66
21	L	522	TGL	CG1-CG2-CG3-OG3
27	T	1269	CDL	CB3-CB4-CB6-OB8
22	B	230	PSC	O02-C1-C2-C3
26	G	1263	PEK	O02-C1-C2-C3
26	T	263	PEK	O01-C1-C2-C3
27	T	1269	CDL	OB7-CB5-OB6-CB4
26	P	1264	PEK	C3-C4-C5-C6
19	N	1266	PGV	C04-O12-P-O13
22	B	230	PSC	C03-O11-P-O13
26	C	265	PEK	C04-O12-P-O13
27	C	270	CDL	CA2-OA2-PA1-OA4
27	G	269	CDL	CA2-OA2-PA1-OA3
27	G	269	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
27	P	1270	CDL	CB2-OB2-PB2-OB3
19	N	1524	PGV	O01-C1-C2-C3
27	T	1269	CDL	CB7-C71-C72-C73
21	B	521	TGL	OA1-CA1-CA2-CA3
19	A	524	PGV	C14-C15-C16-C17
26	G	264	PEK	C15-C16-C17-C18
18	N	516	HEA	C3B-C11-C12-C13
22	O	1230	PSC	C05-C04-O12-P
21	L	522	TGL	C15-C16-C17-C18
21	L	522	TGL	C19-C33-C34-C35
27	G	269	CDL	C32-C33-C34-C35
27	C	270	CDL	C64-C65-C66-C67
27	G	269	CDL	C58-C59-C60-C61
24	Z	1526	DMU	C34-C37-C40-C43
26	P	1265	PEK	C31-C32-C33-C34
22	O	1230	PSC	O02-C1-C2-C3
26	T	263	PEK	O02-C1-C2-C3
19	N	1524	PGV	C25-C26-C27-C28
27	C	270	CDL	C37-C38-C39-C40
26	G	264	PEK	O02-C1-C2-C3
27	P	1270	CDL	C83-C84-C85-C86
19	A	524	PGV	O01-C1-C2-C3
27	P	1270	CDL	C12-C11-CA5-OA6
22	B	230	PSC	C7-C8-C9-C10
26	P	1265	PEK	C14-C15-C16-C17
21	O	1523	TGL	OC1-CC1-CC2-CC3
24	P	1272	DMU	C5-C10-O7-C3
21	L	522	TGL	OC1-CC1-CC2-CC3
21	D	523	TGL	OG3-CC1-CC2-CC3
27	P	1270	CDL	C32-C31-CA7-OA9
27	P	1270	CDL	C12-C11-CA5-OA7
27	G	269	CDL	C52-C51-CB5-OB6

There are no ring outliers.

40 monomers are involved in 244 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	1267	PGV	5	0
21	D	523	TGL	5	0
24	C	272	DMU	2	0
23	G	86	CHD	2	0
27	G	269	CDL	17	0

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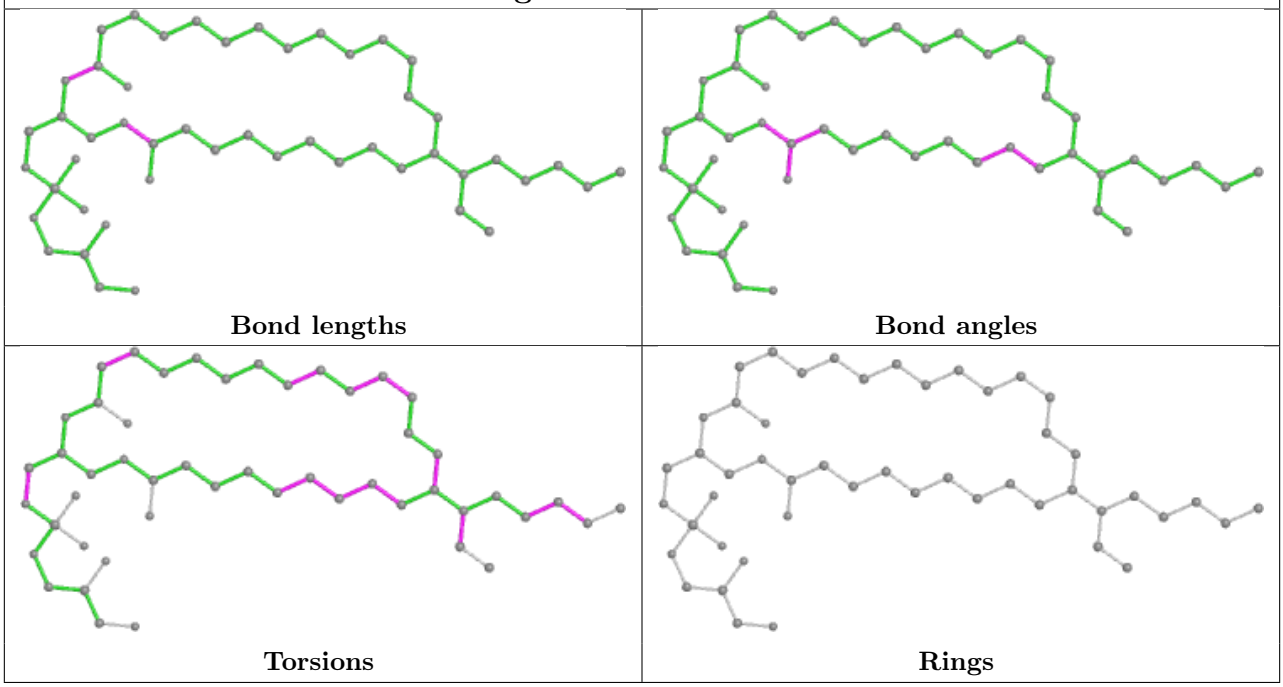
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	520	PER	1	0
23	J	60	CHD	2	0
24	Z	1526	DMU	2	0
18	N	515	HEA	7	0
19	C	267	PGV	3	0
23	P	1271	CHD	3	0
24	P	1272	DMU	3	0
21	N	1522	TGL	19	0
21	L	522	TGL	13	0
19	N	1266	PGV	1	0
22	B	230	PSC	13	0
19	N	1268	PGV	2	0
26	C	265	PEK	4	0
15	A	520	PER	1	0
26	P	1265	PEK	8	0
22	O	1230	PSC	12	0
19	C	268	PGV	2	0
21	B	521	TGL	10	0
19	N	1524	PGV	9	0
21	N	1521	TGL	7	0
18	A	516	HEA	5	0
26	T	263	PEK	14	0
19	A	524	PGV	5	0
18	N	516	HEA	1	0
27	P	1270	CDL	9	0
23	W	1060	CHD	1	0
21	O	1523	TGL	6	0
23	P	1525	CHD	2	0
27	C	270	CDL	13	0
26	G	264	PEK	4	0
23	C	271	CHD	4	0
27	T	1269	CDL	17	0
18	A	515	HEA	7	0
26	G	1263	PEK	12	0
26	P	1264	PEK	5	0

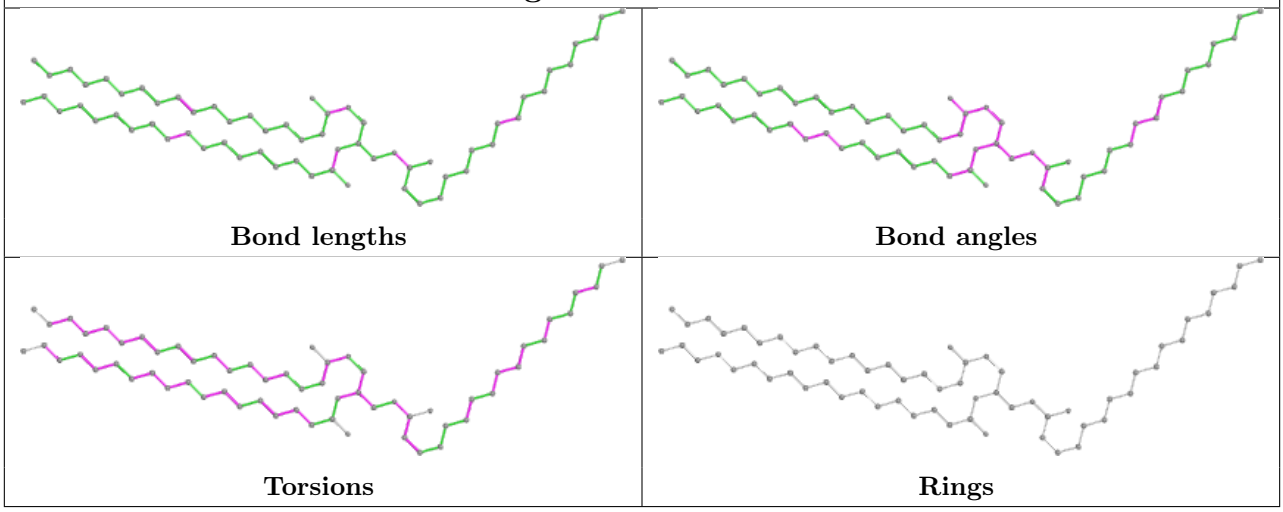
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

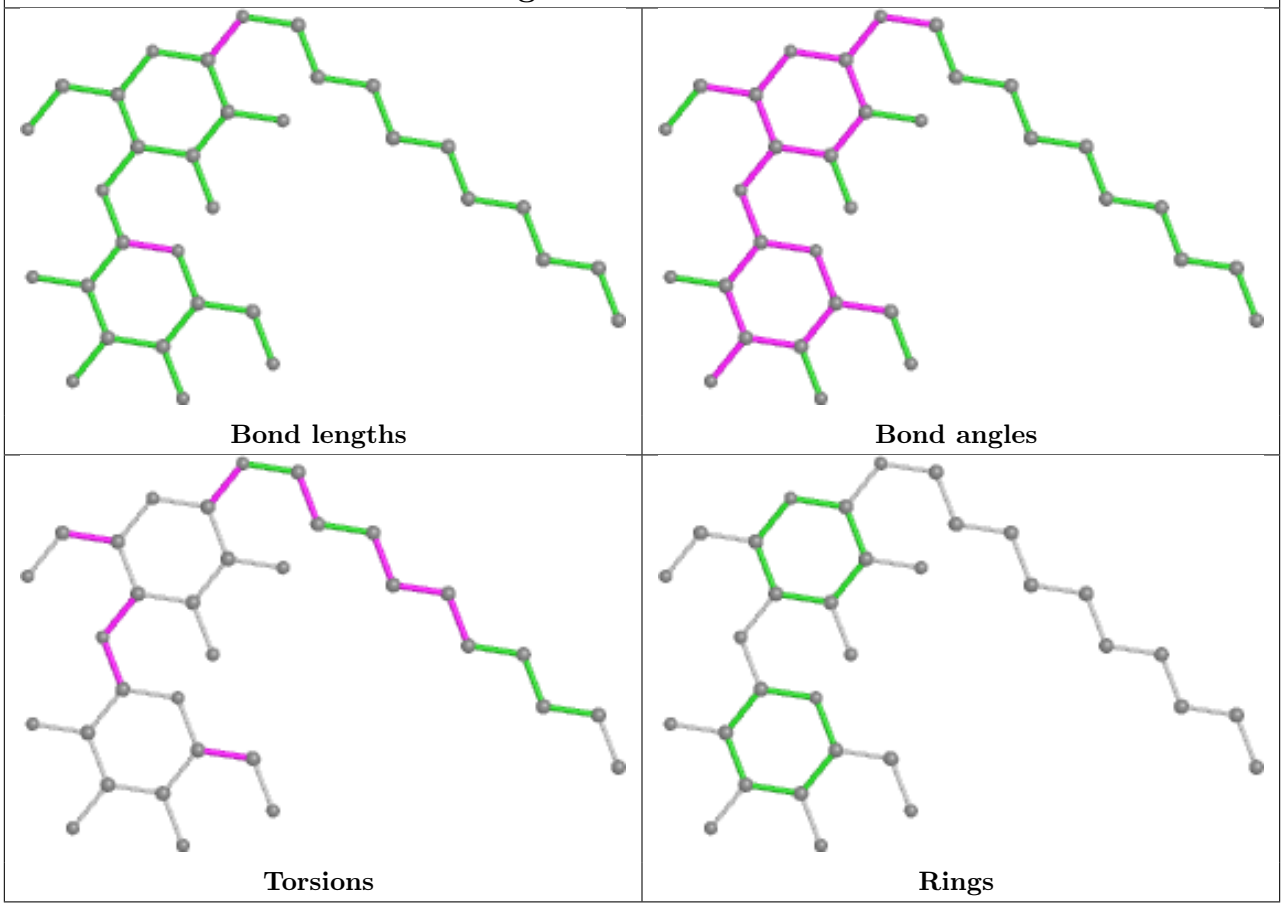
Ligand PGV P 1267



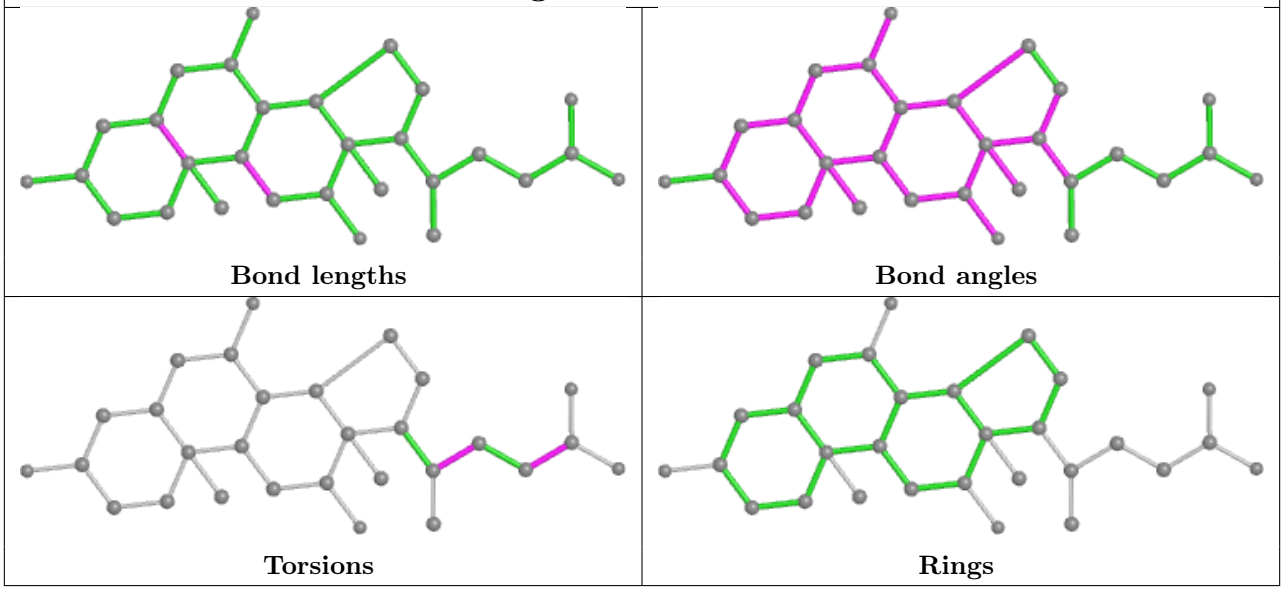
Ligand TGL D 523



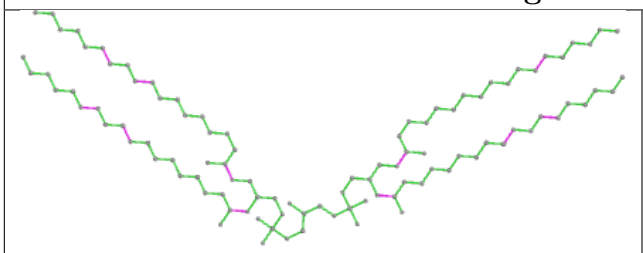
Ligand DMU C 272



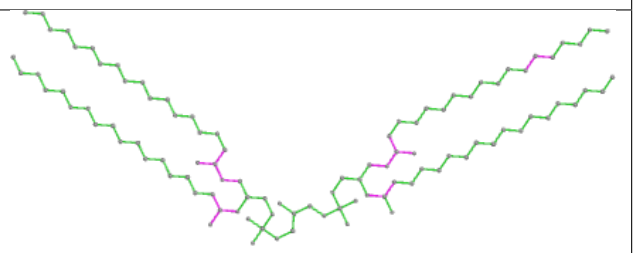
Ligand CHD G 86



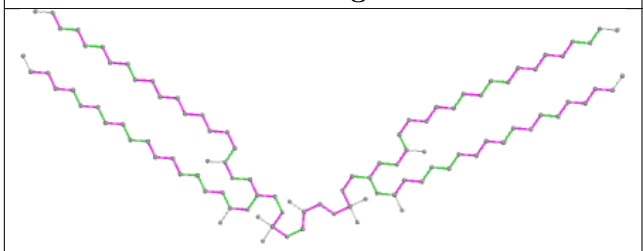
Ligand CDL G 269



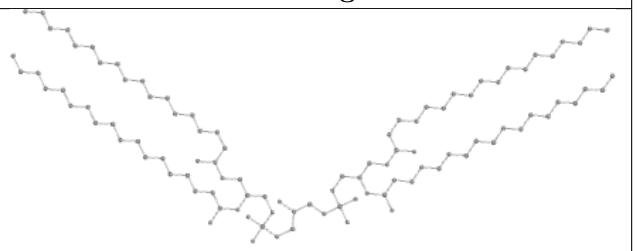
Bond lengths



Bond angles

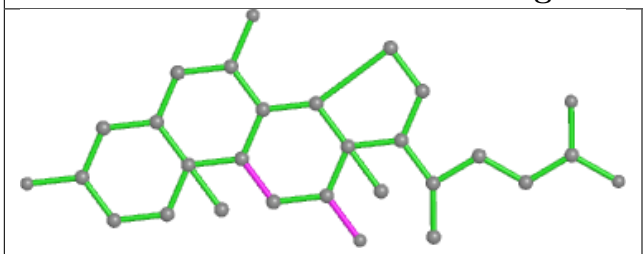


Torsions

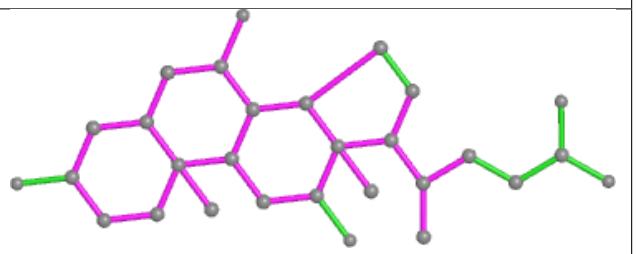


Rings

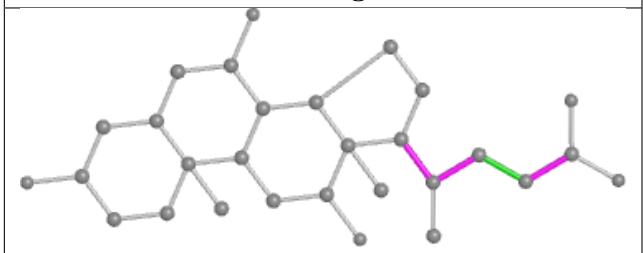
Ligand CHD J 60



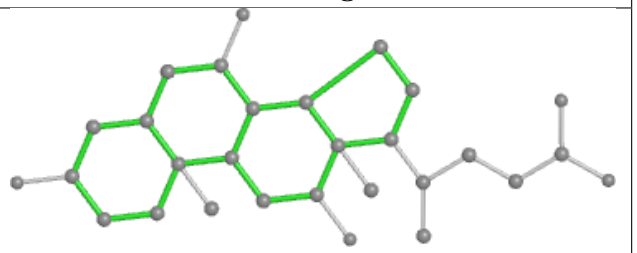
Bond lengths



Bond angles

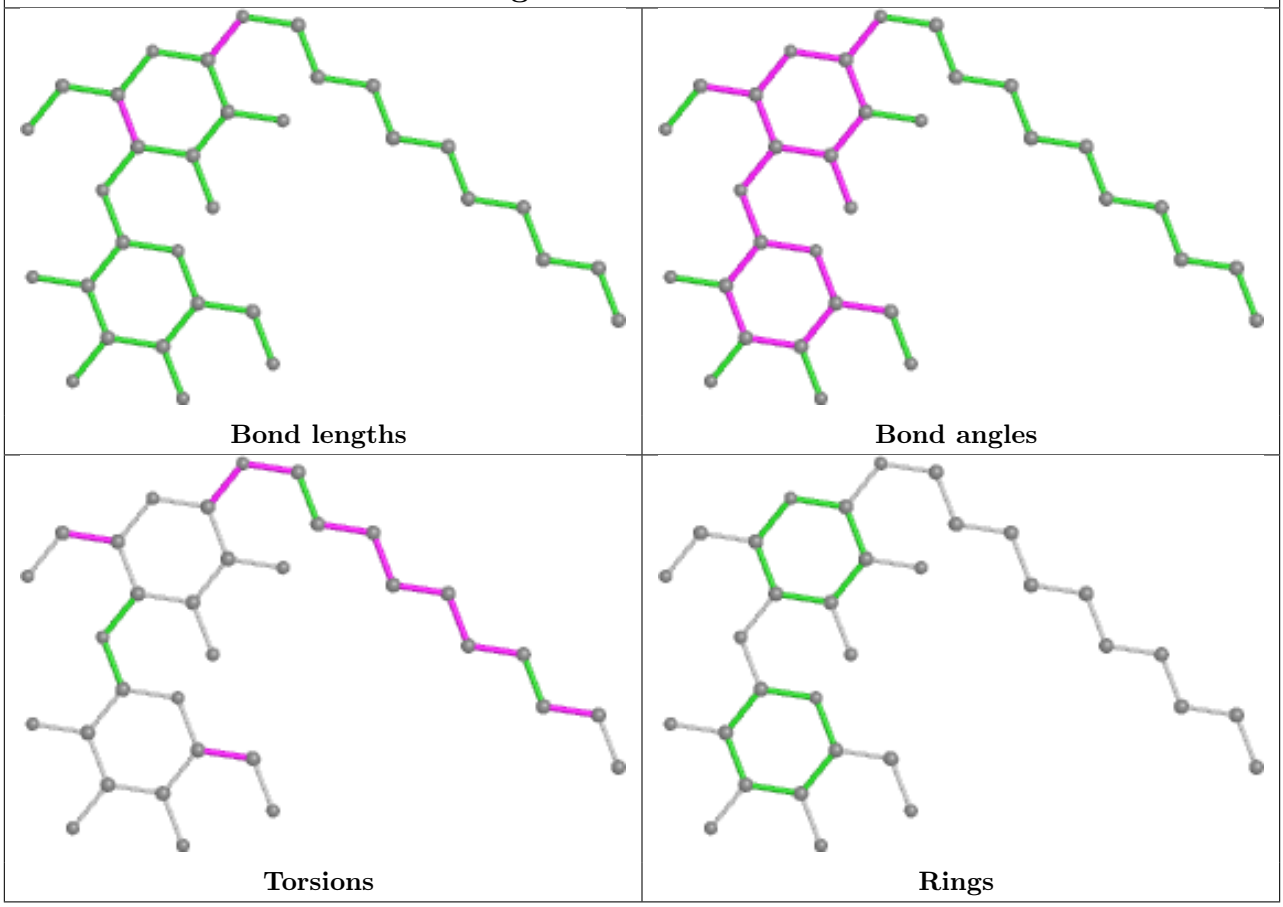


Torsions

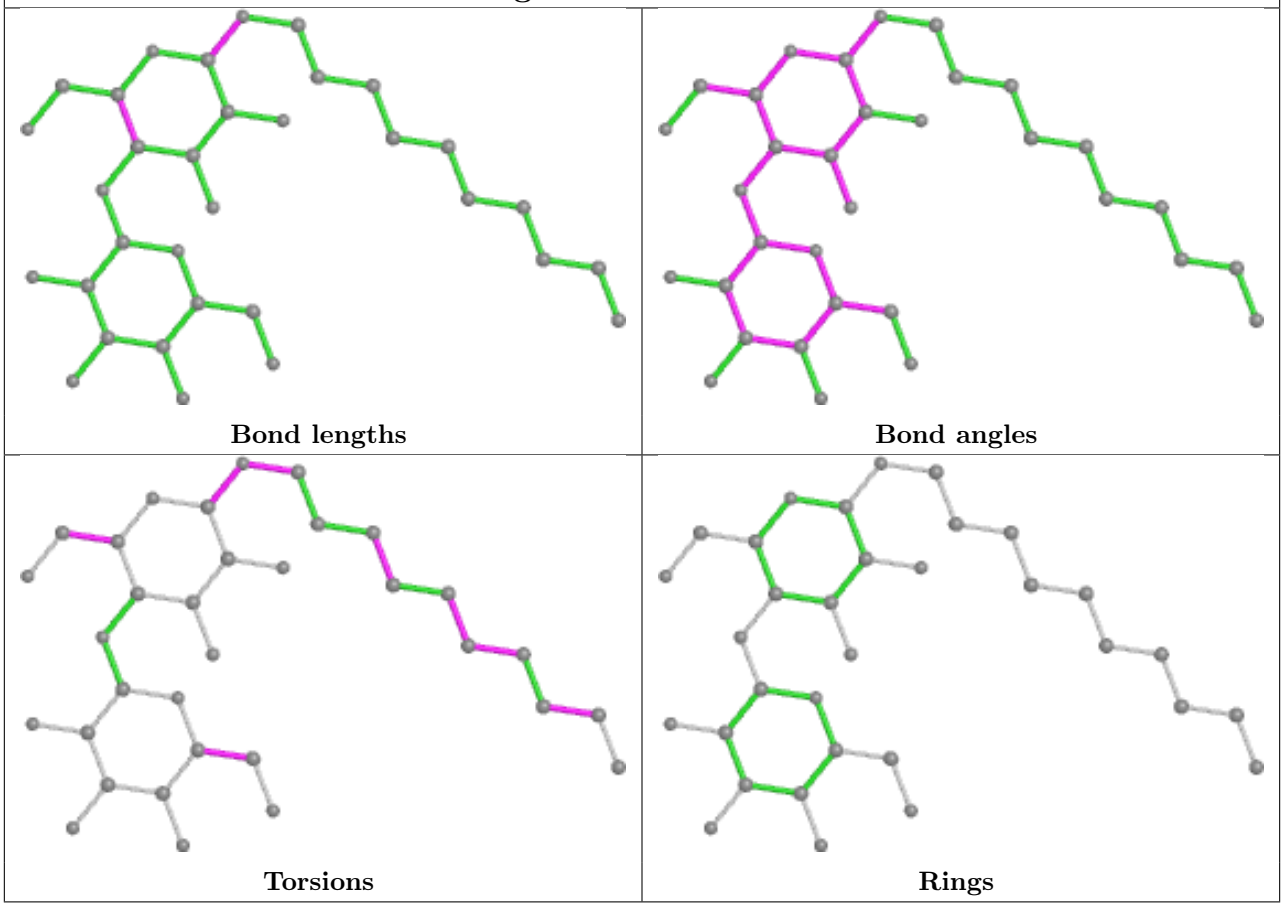


Rings

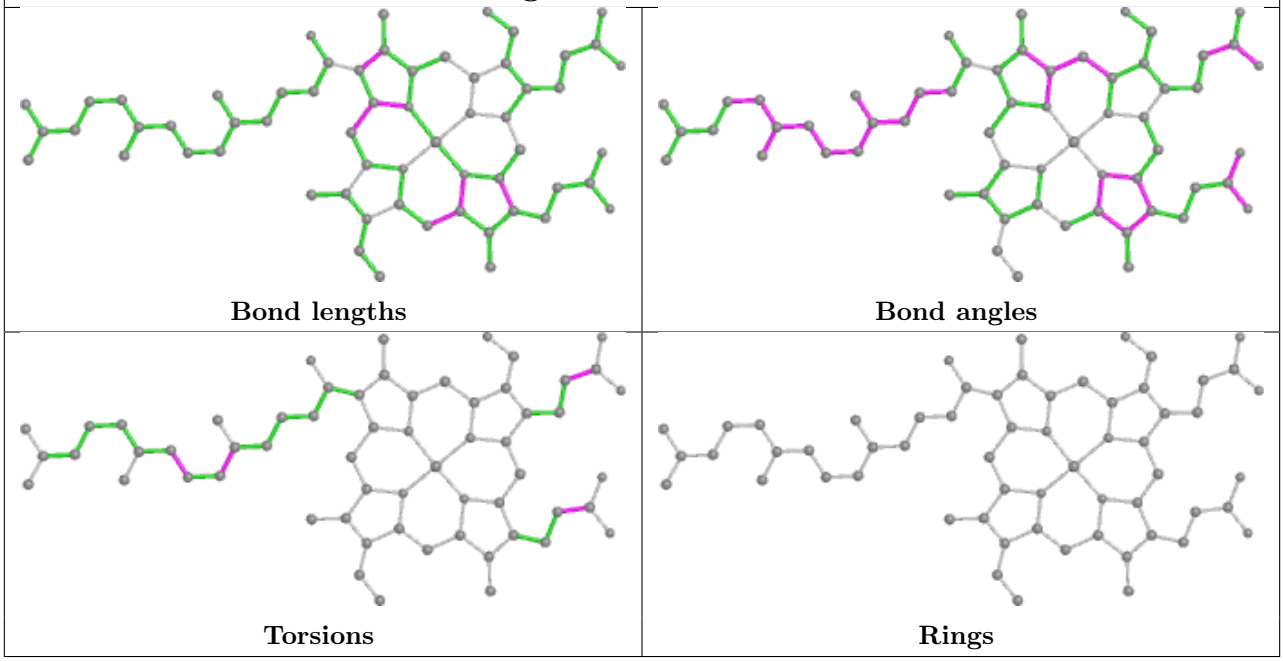
Ligand DMU Z 1526



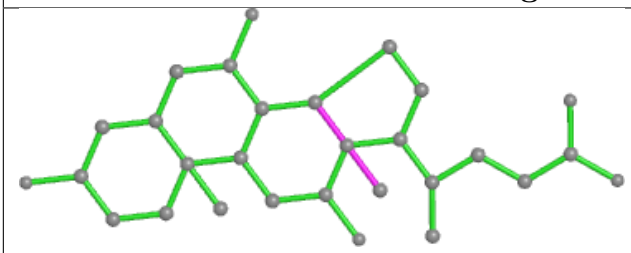
Ligand DMU M 526



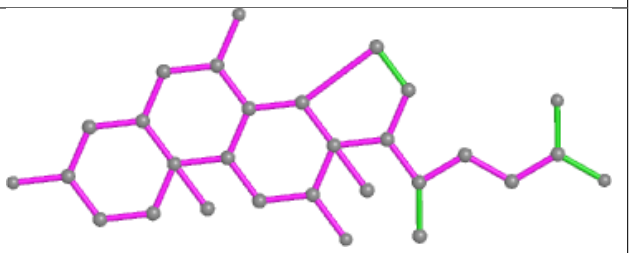
Ligand HEA N 515



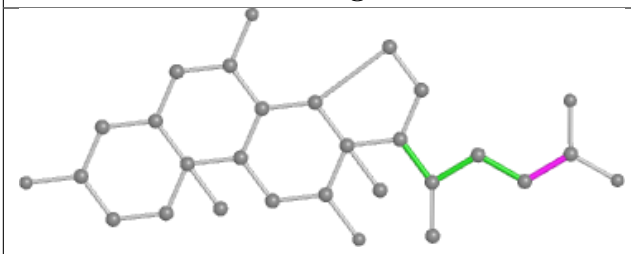
Ligand CHD C 525



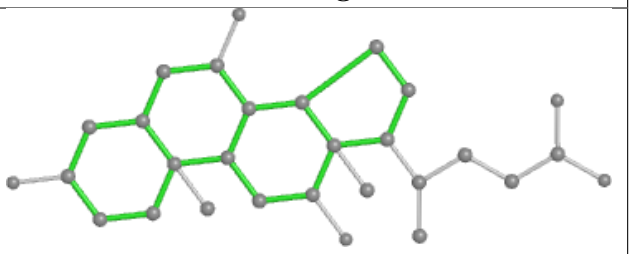
Bond lengths



Bond angles

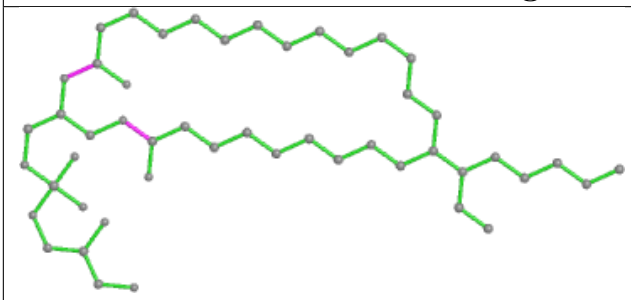


Torsions

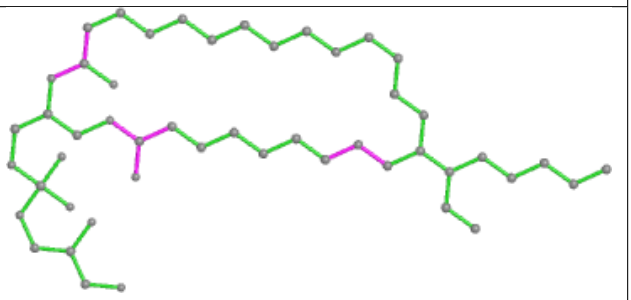


Rings

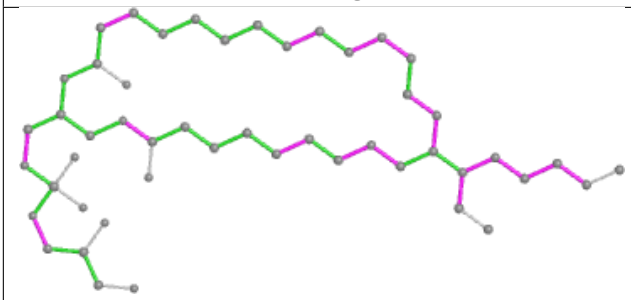
Ligand PGV C 267



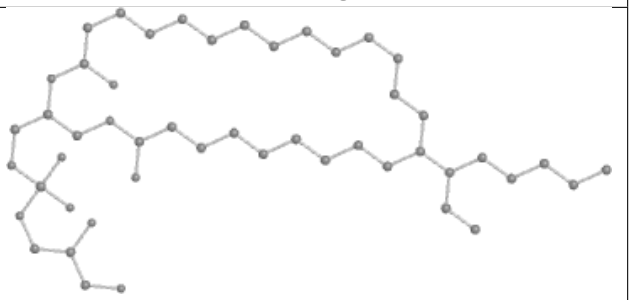
Bond lengths



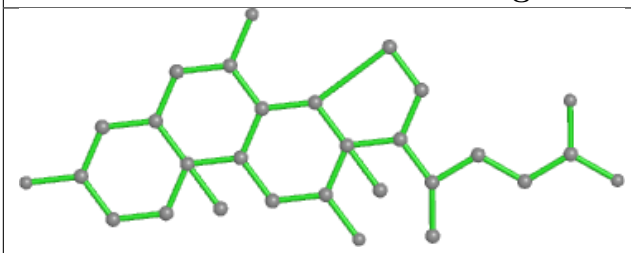
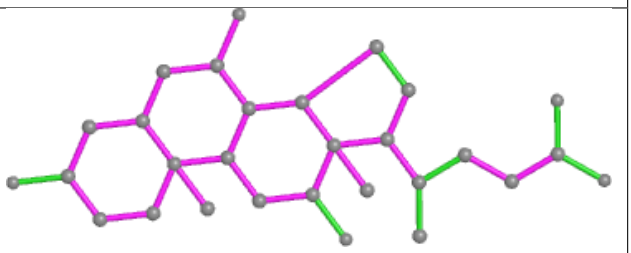
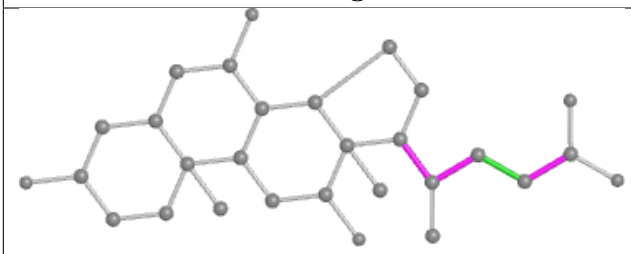
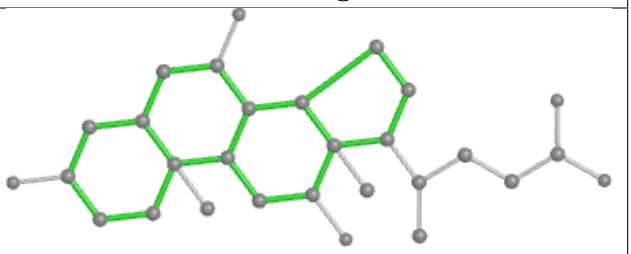
Bond angles

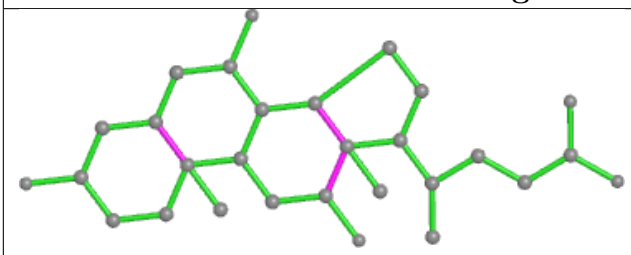
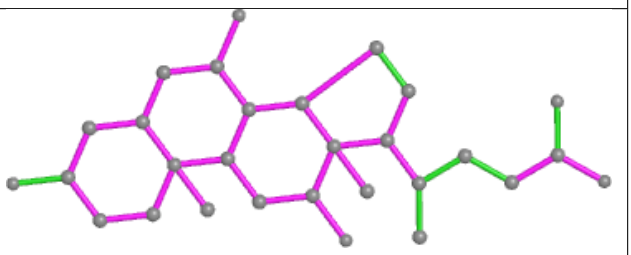
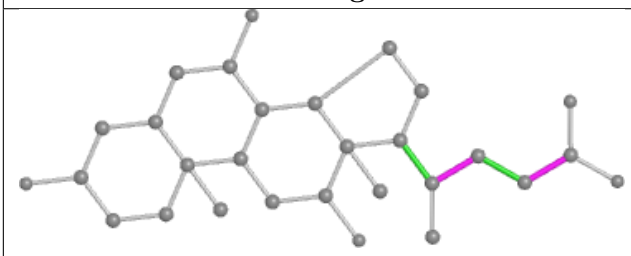
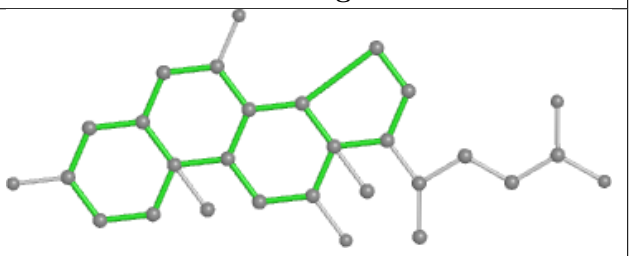


Torsions

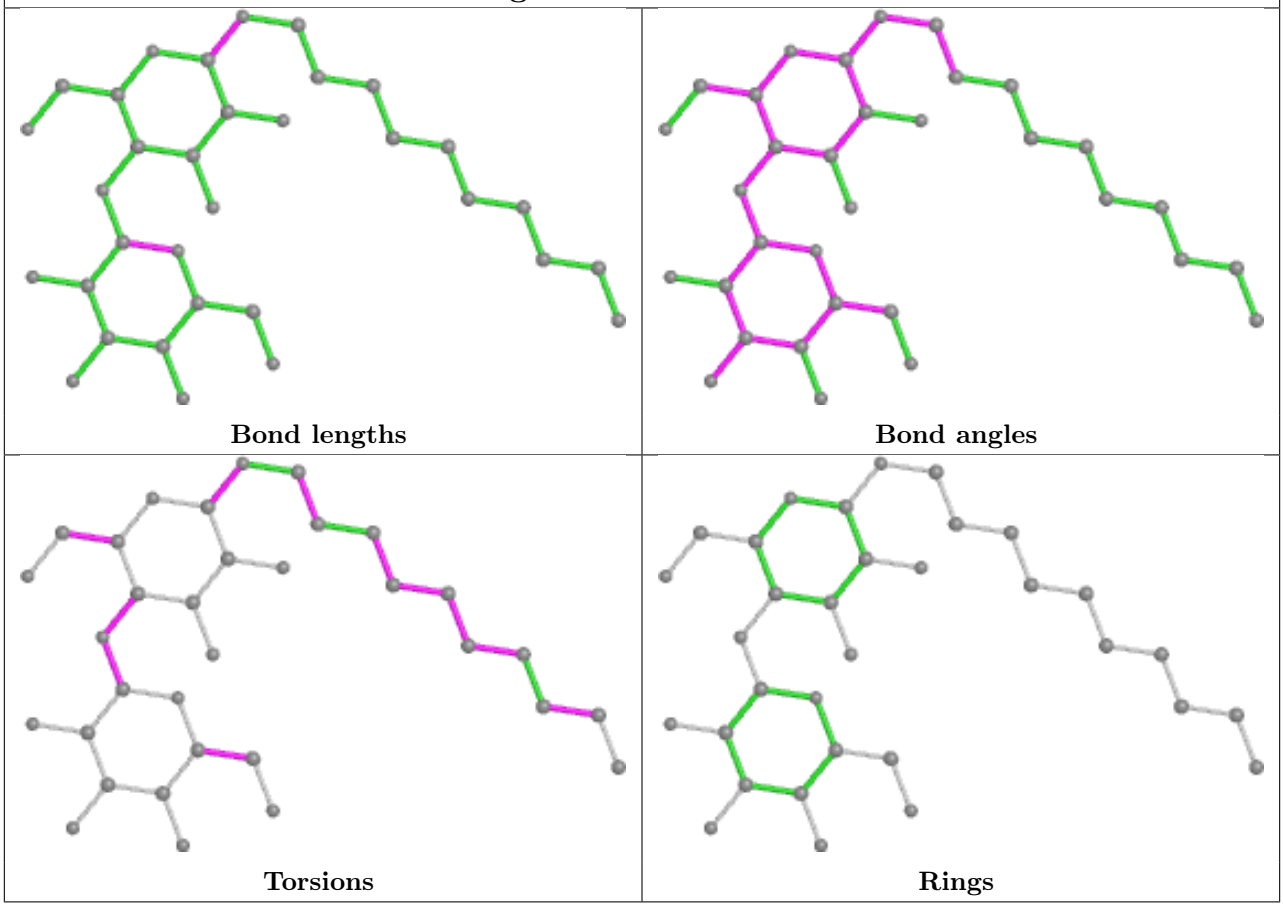


Rings

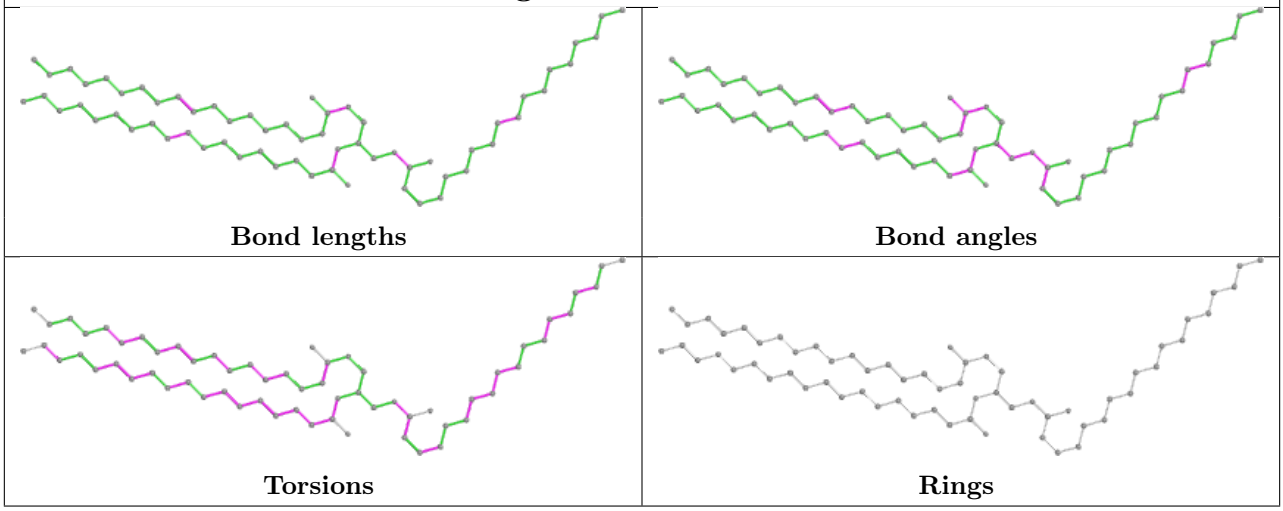
Ligand CHD P 1271	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD B 1086	
 Bond lengths	 Bond angles
 Torsions	 Rings

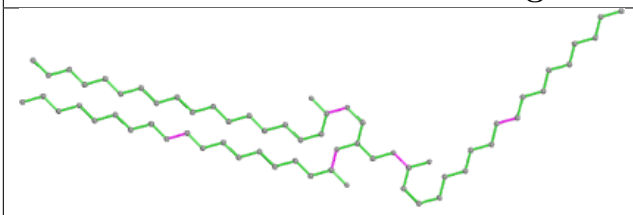
Ligand DMU P 1272



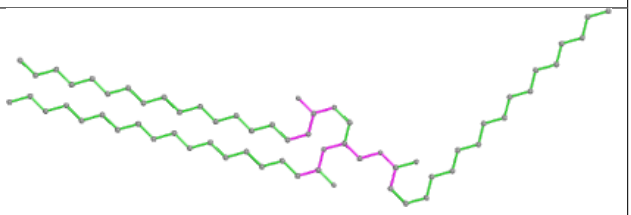
Ligand TGL N 1522



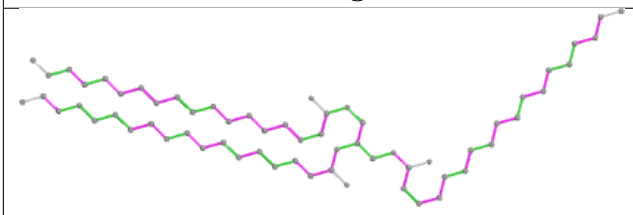
Ligand TGL L 522



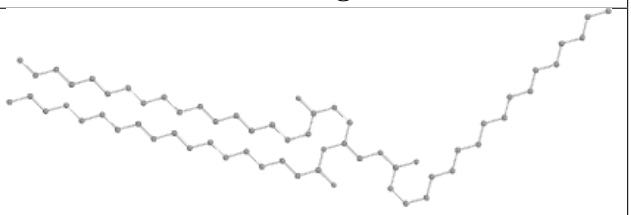
Bond lengths



Bond angles

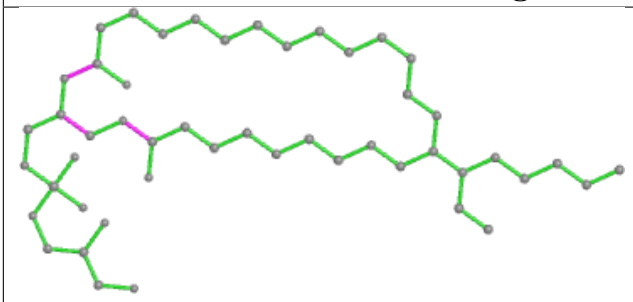


Torsions

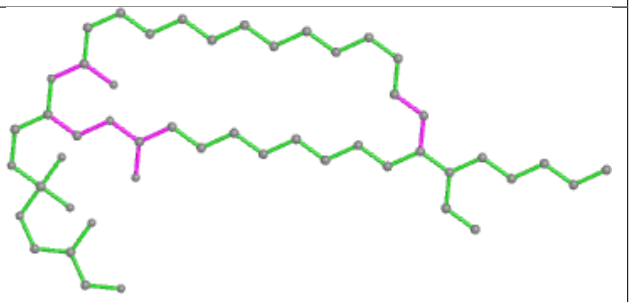


Rings

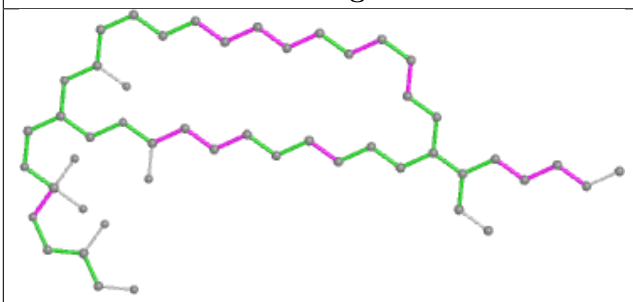
Ligand PGV N 1266



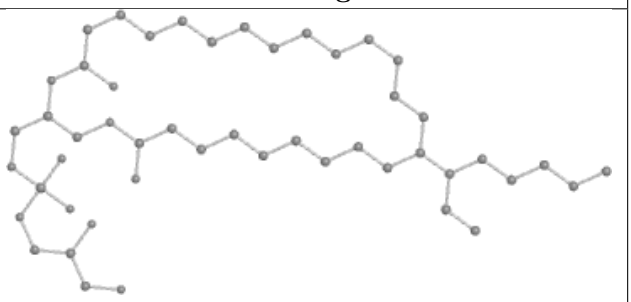
Bond lengths



Bond angles

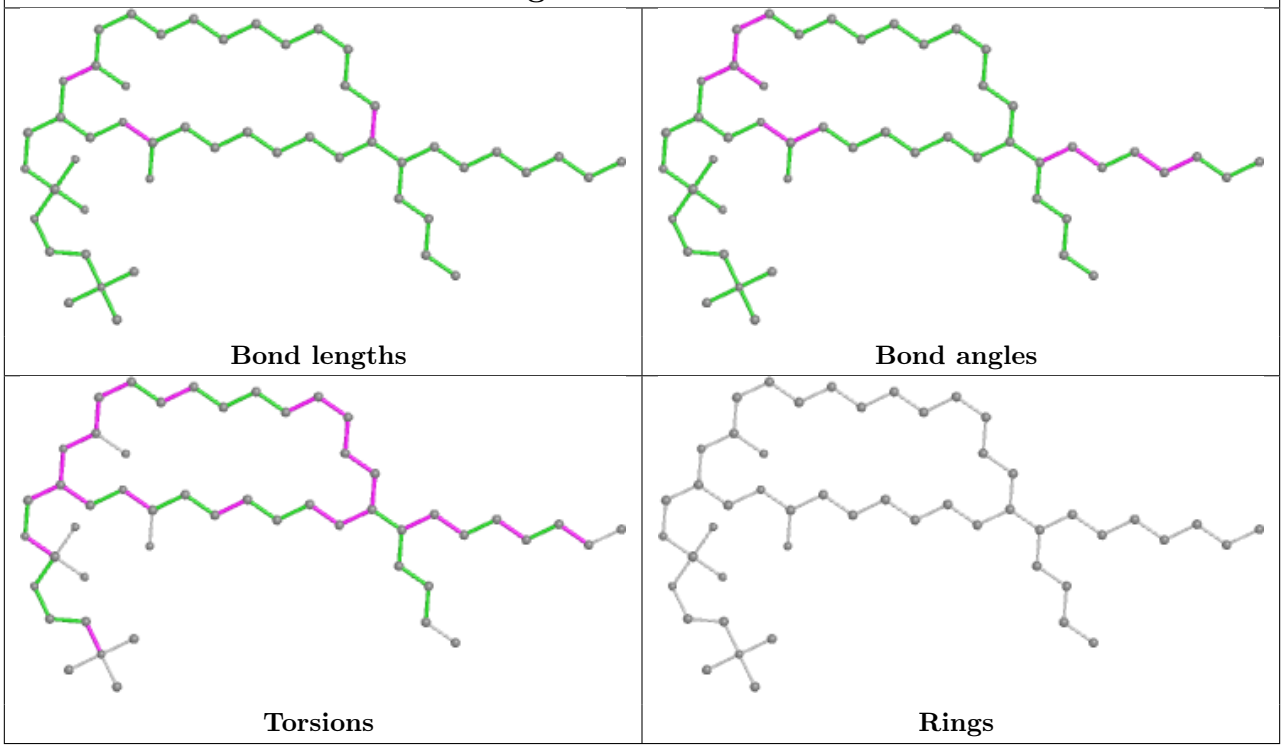


Torsions

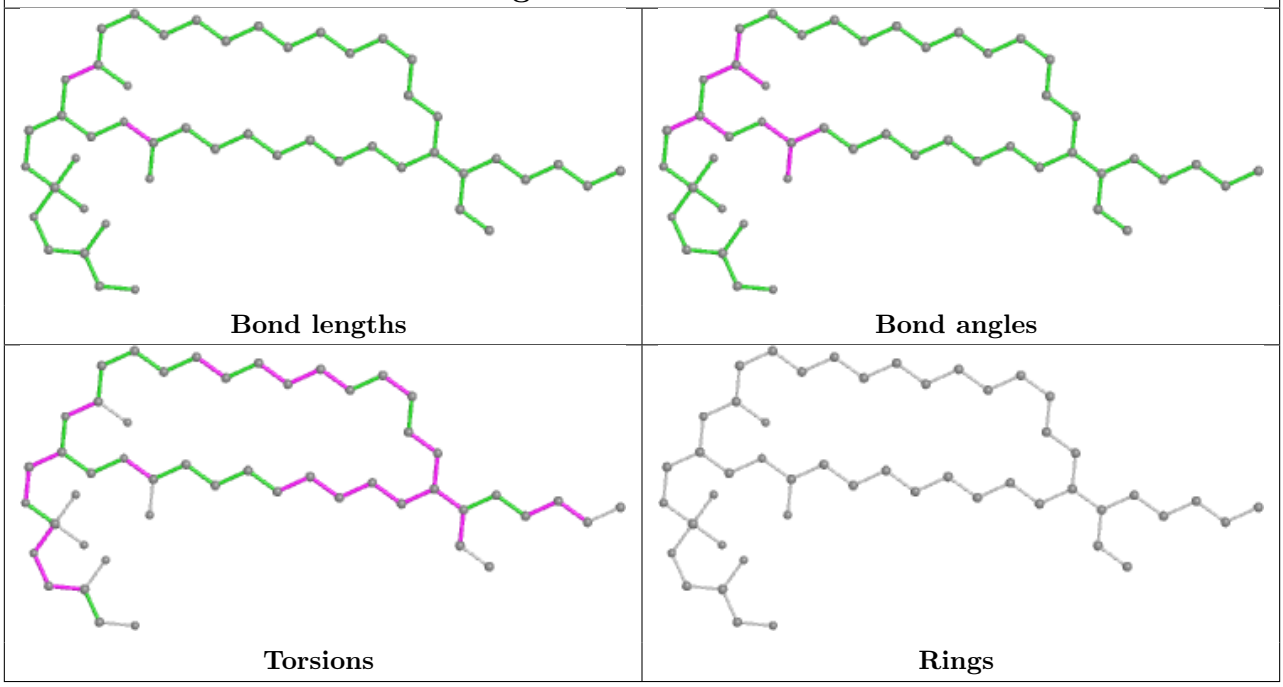


Rings

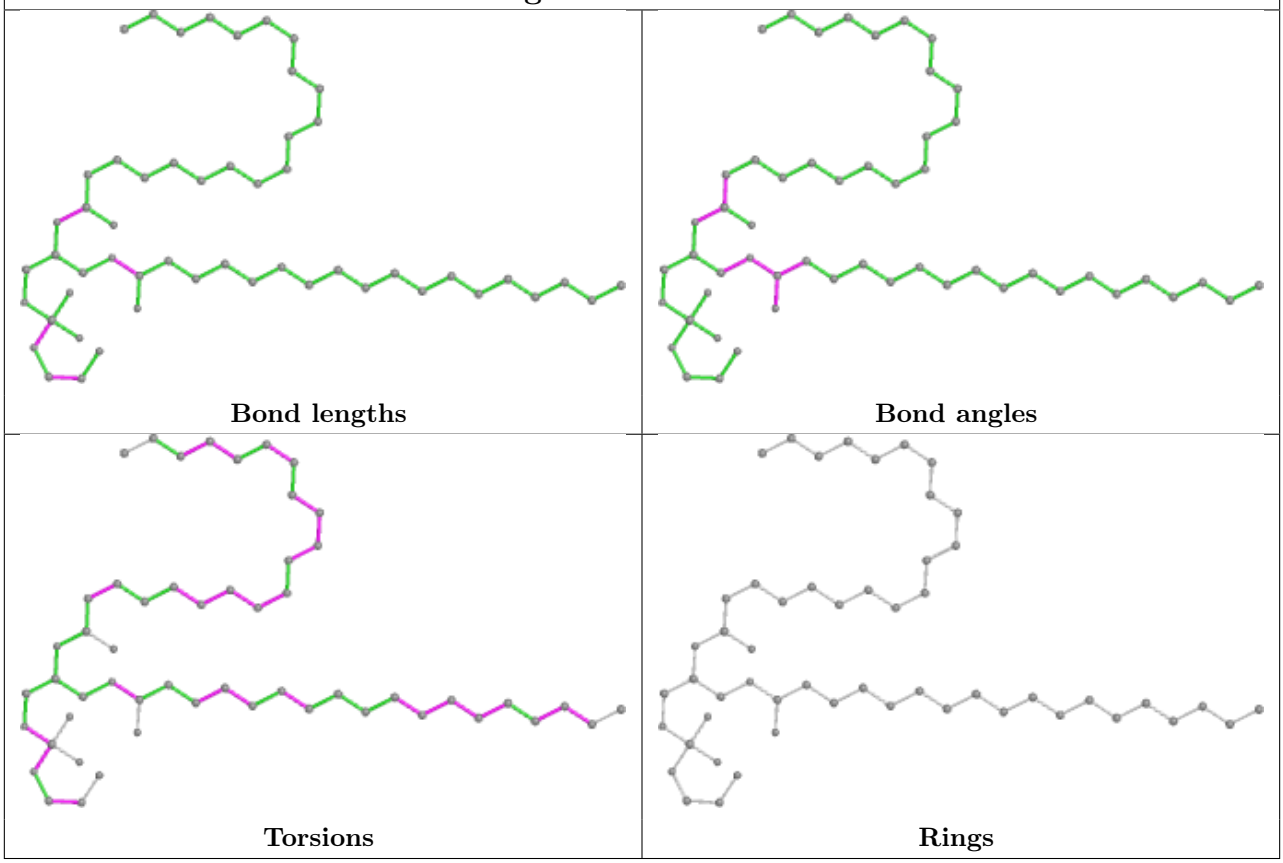
Ligand PSC B 230



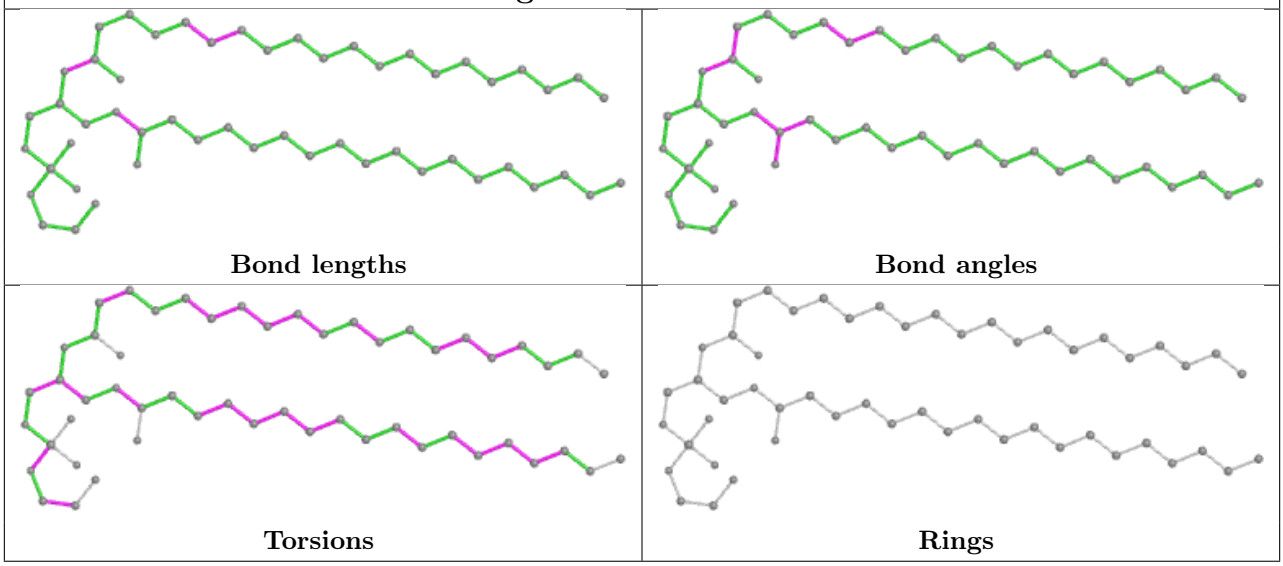
Ligand PGV N 1268



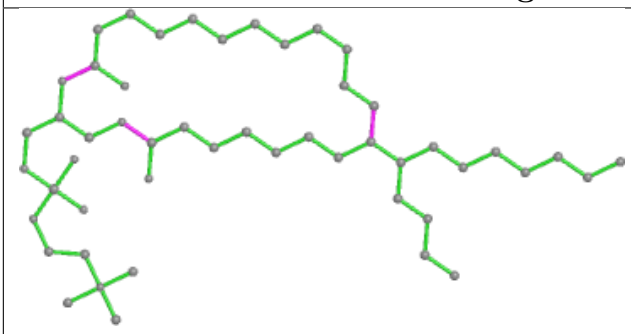
Ligand PEK C 265



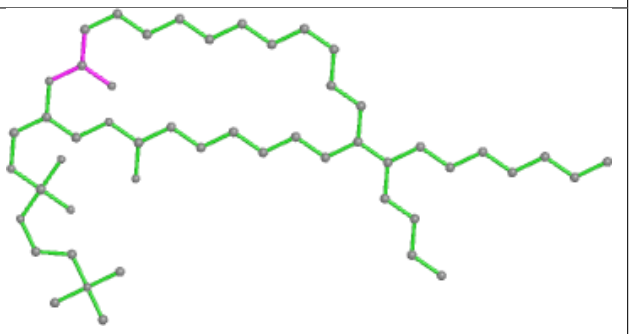
Ligand PEK P 1265



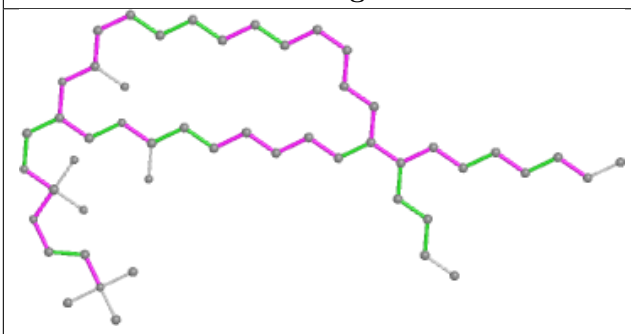
Ligand PSC O 1230



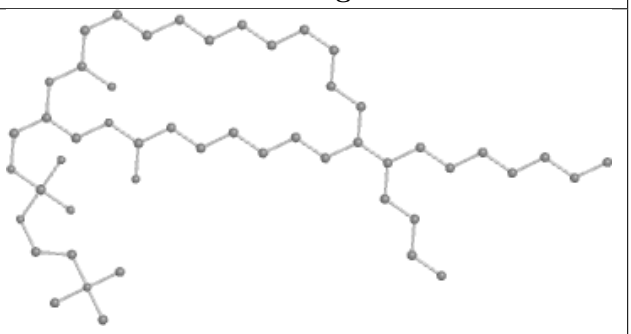
Bond lengths



Bond angles

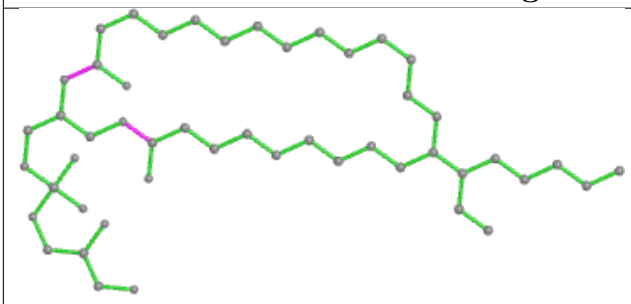


Torsions



Rings

Ligand PGV C 268



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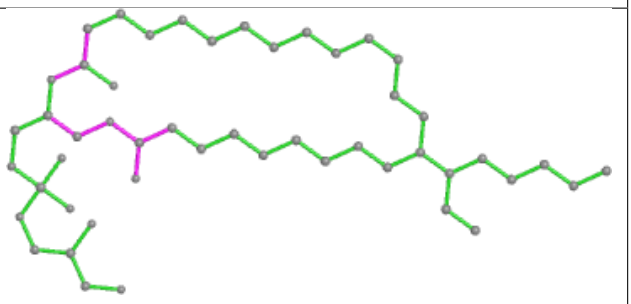
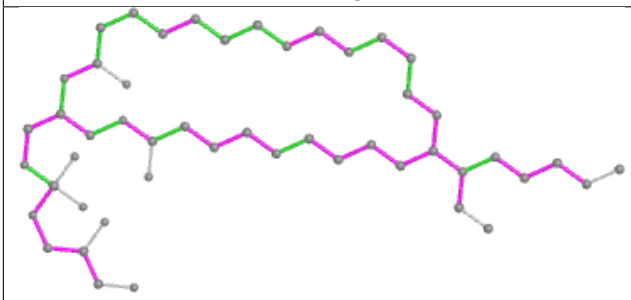
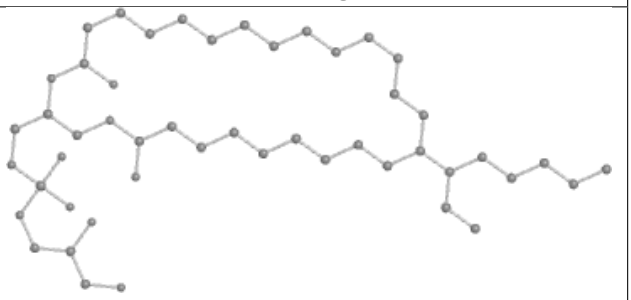


Bond angles

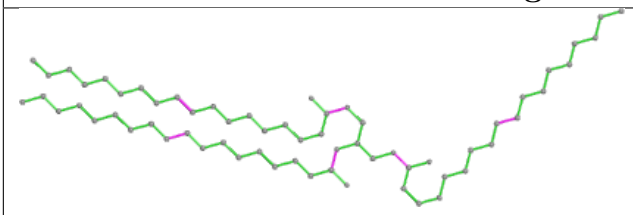


Torsions

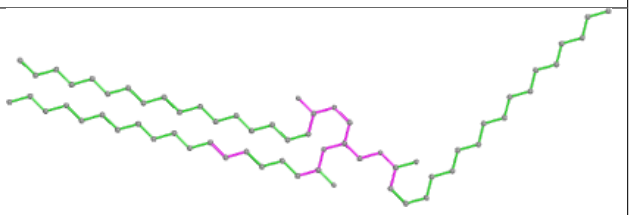


Rings

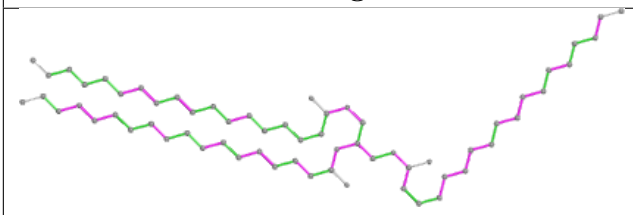
Ligand TGL B 521



Bond lengths



Bond angles



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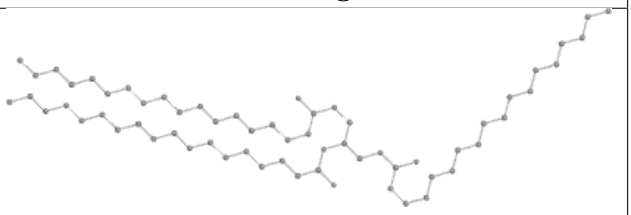
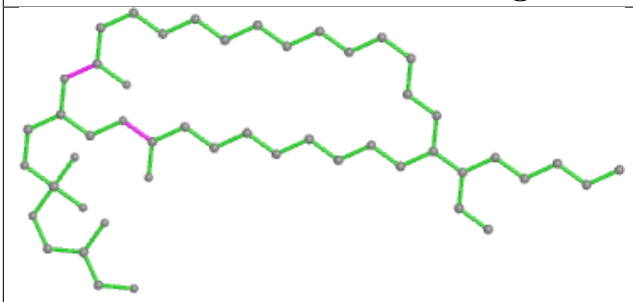


Rings

Ligand PGV N 1524



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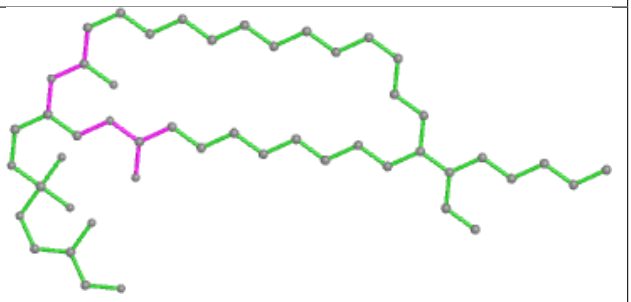
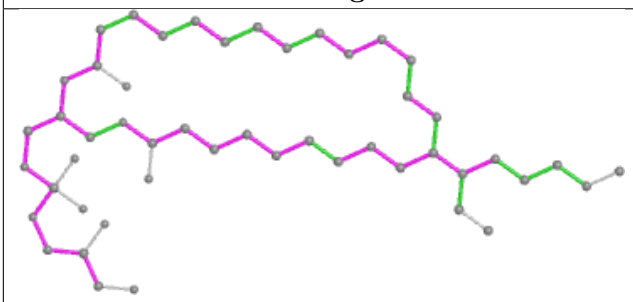
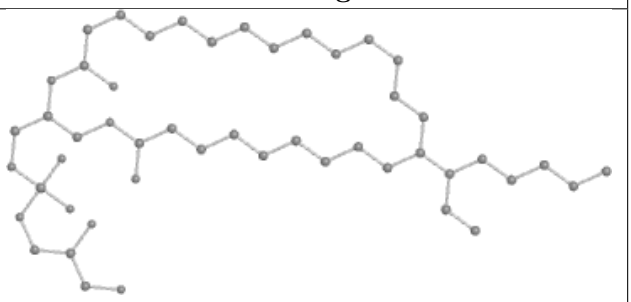


Bond angles

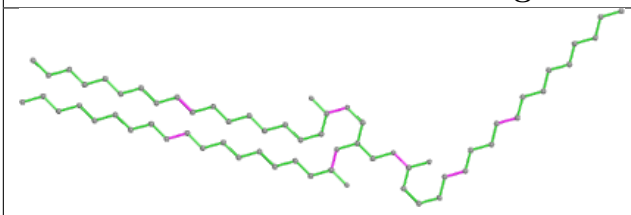


Torsions

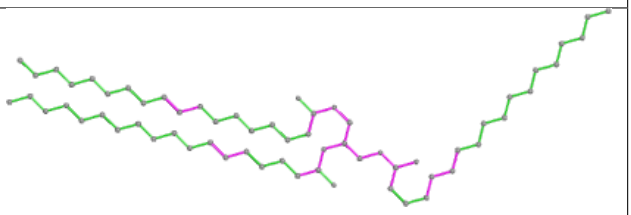


Rings

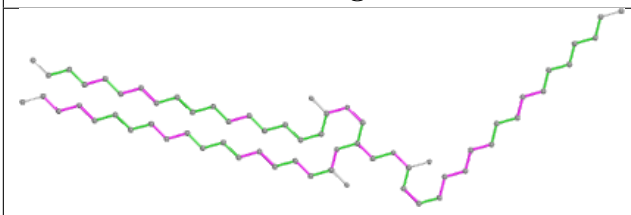
Ligand TGL N 1521



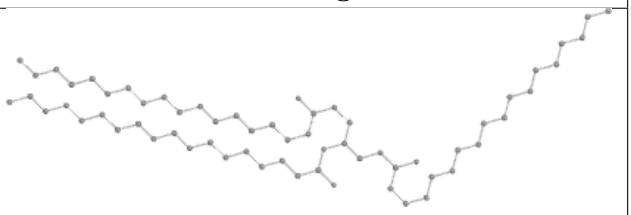
Bond lengths



Bond angles

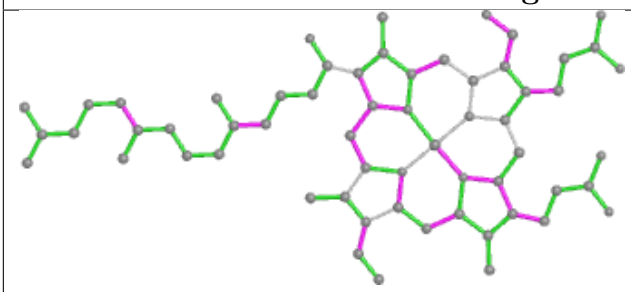


Torsions

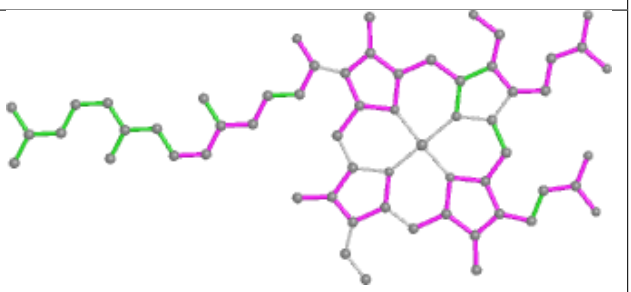


Rings

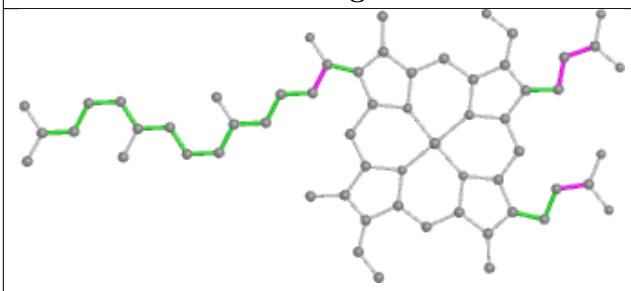
Ligand HEA A 516



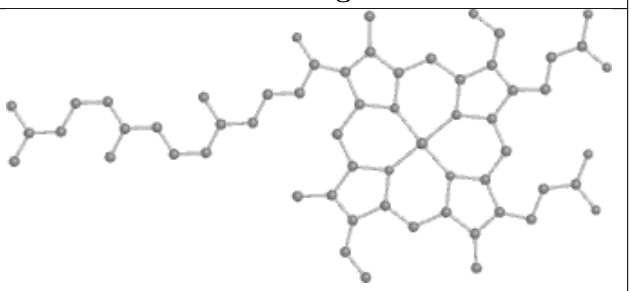
Bond lengths



Bond angles

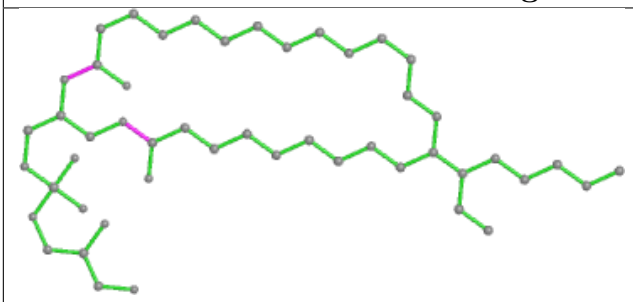


Torsions

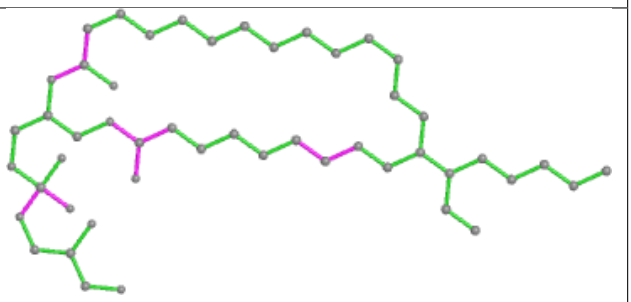


Rings

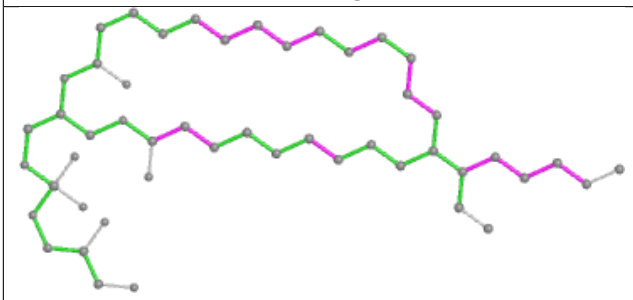
Ligand PGV A 521



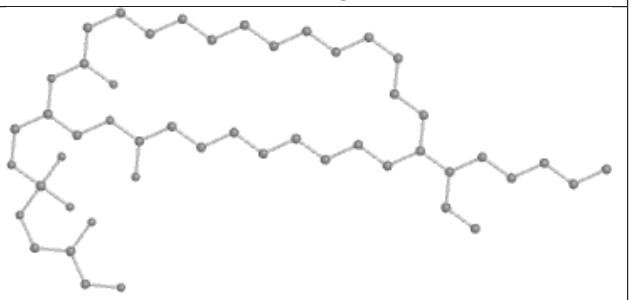
Bond lengths



Bond angles

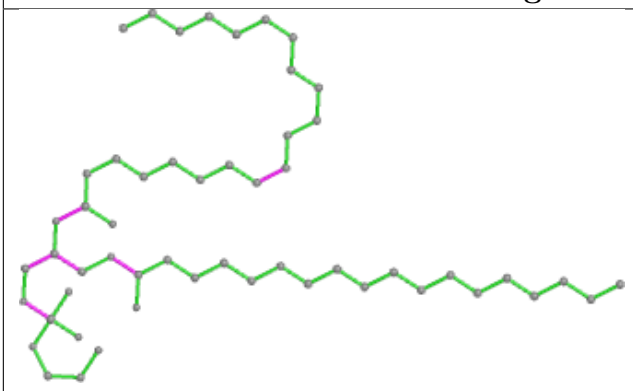


Torsions

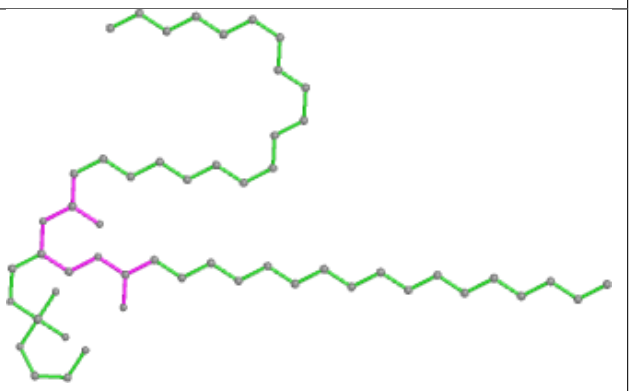


Rings

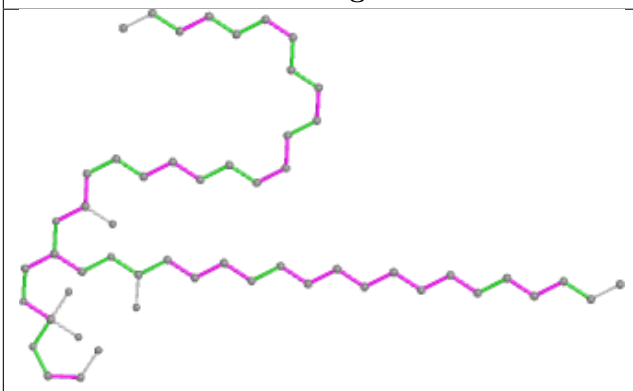
Ligand PEK T 263



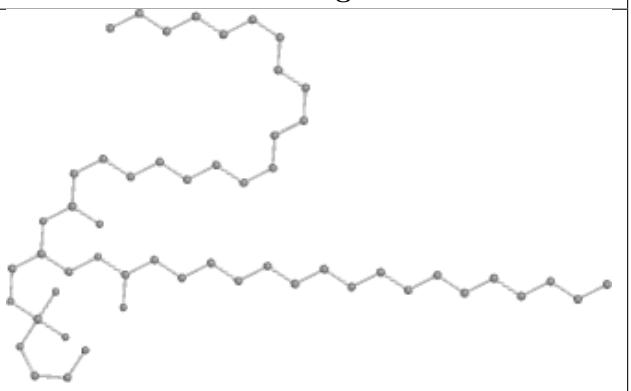
Bond lengths



Bond angles

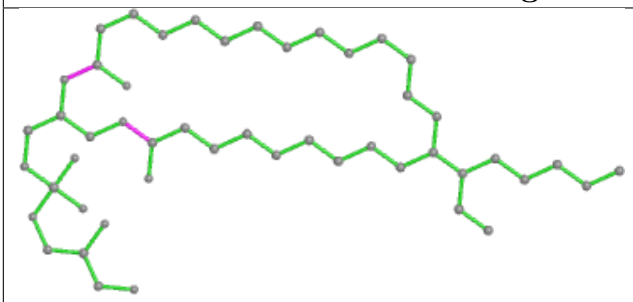


Torsions

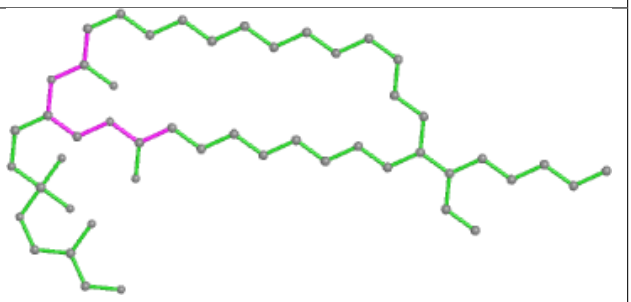


Rings

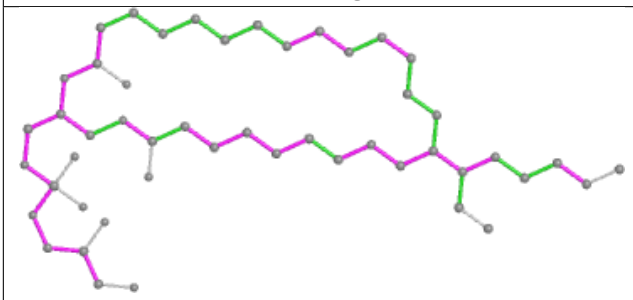
Ligand PGV A 524



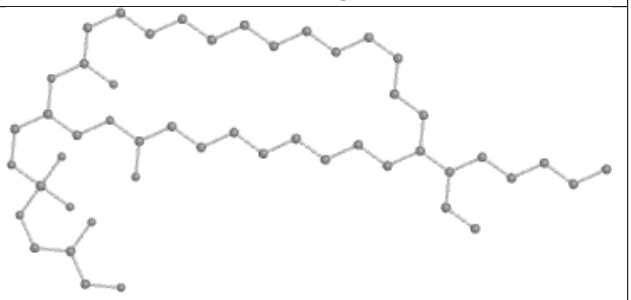
Bond lengths



Bond angles

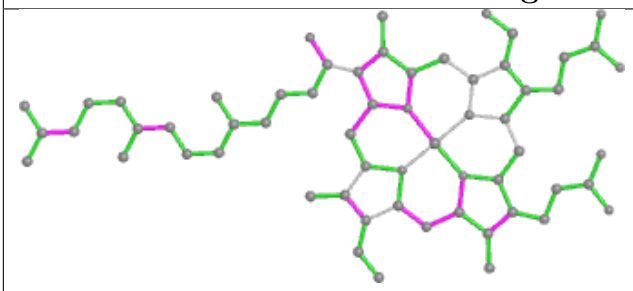


Torsions

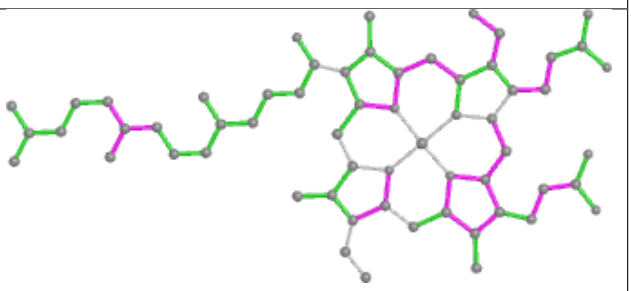


Rings

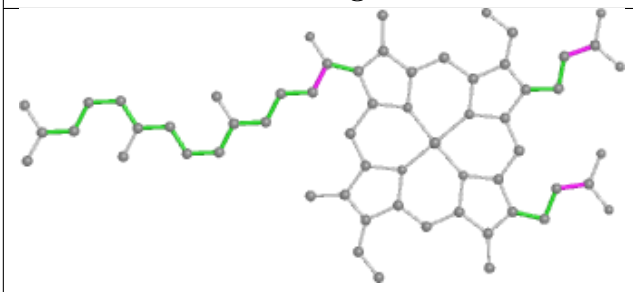
Ligand HEA N 516



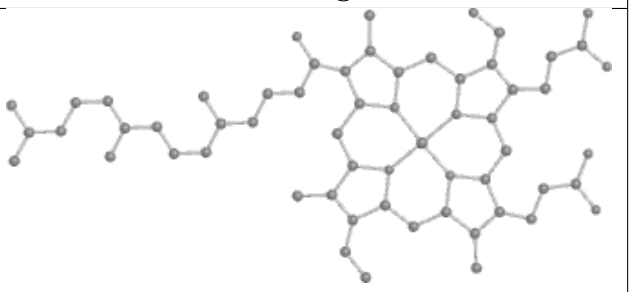
Bond lengths



Bond angles

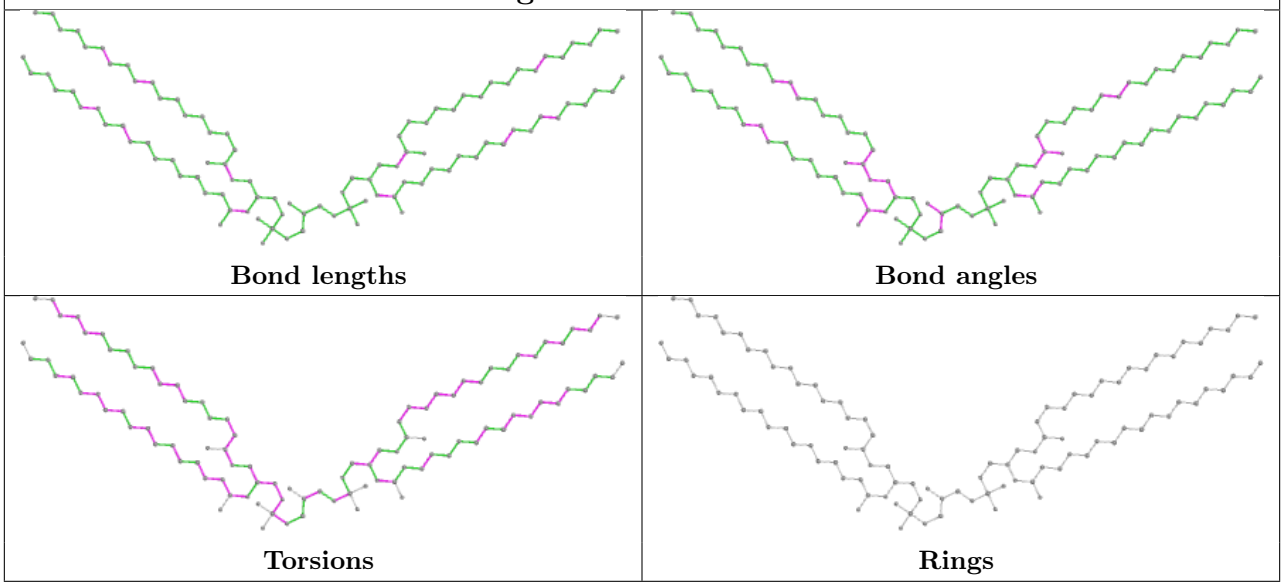


Torsions

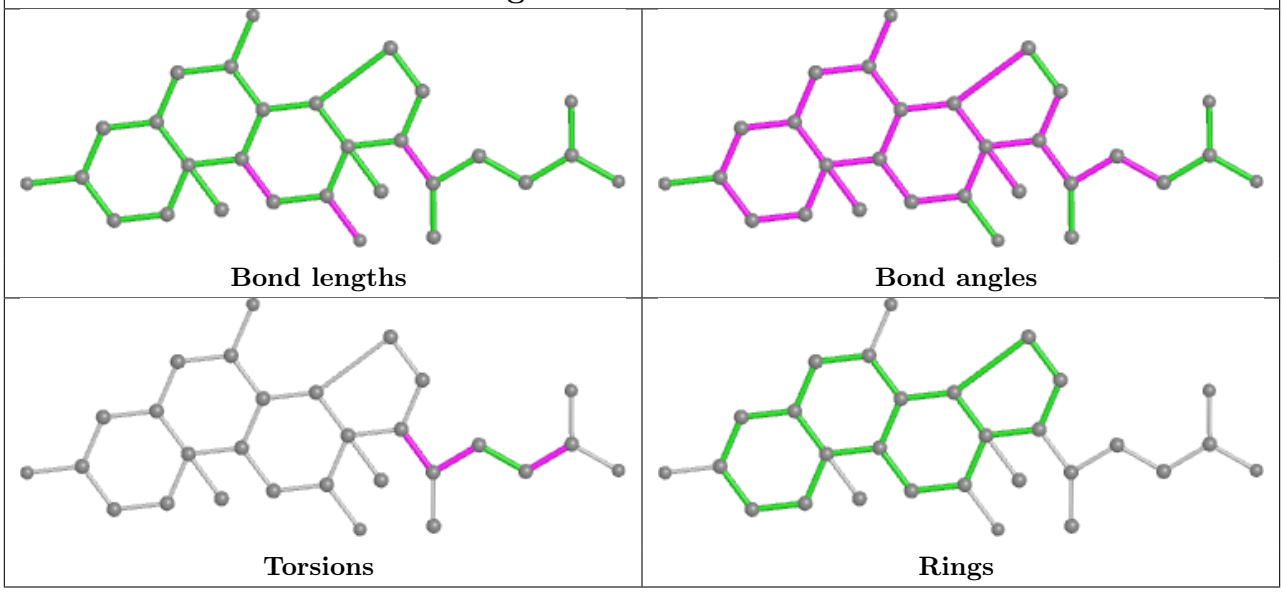


Rings

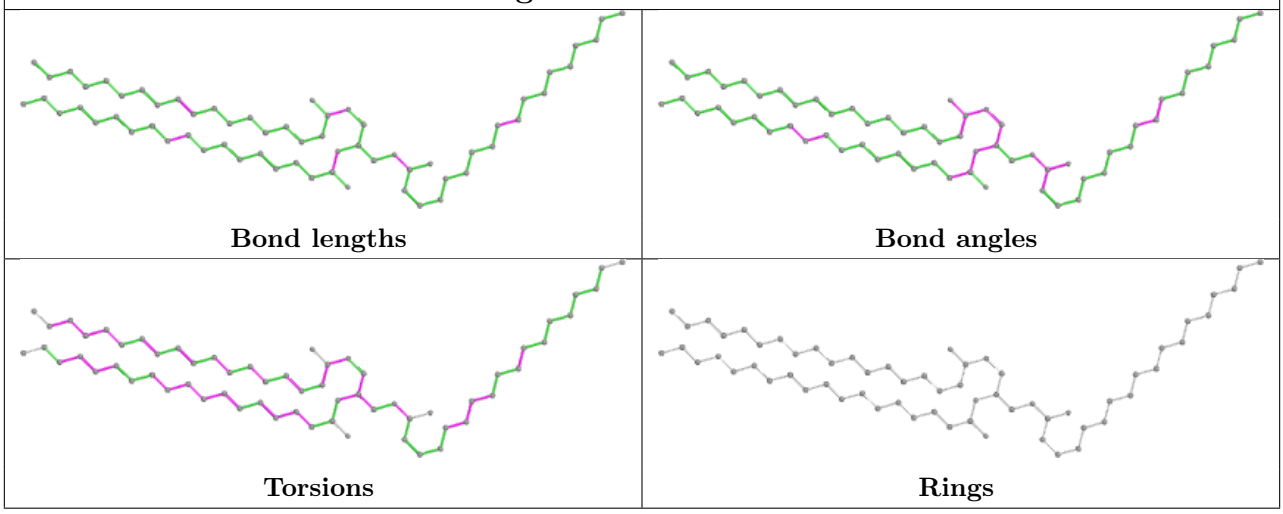
Ligand CDL P 1270



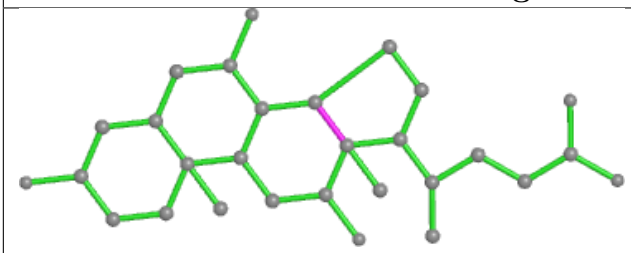
Ligand CHD W 1060



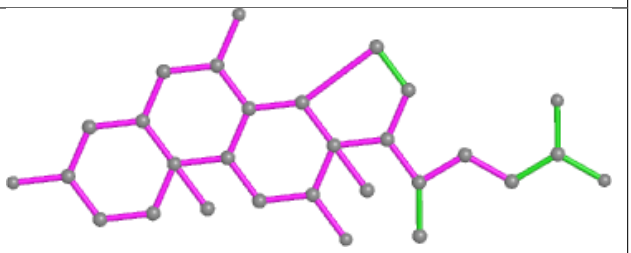
Ligand TGL O 1523



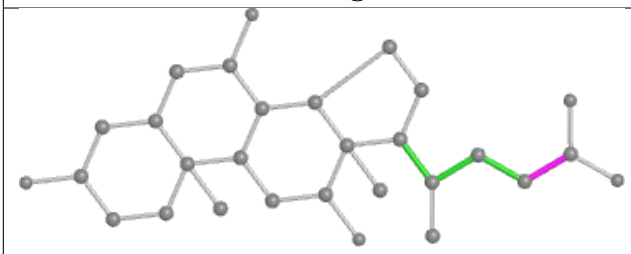
Ligand CHD P 1525



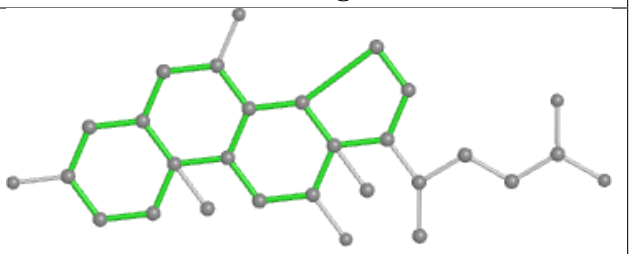
Bond lengths



Bond angles

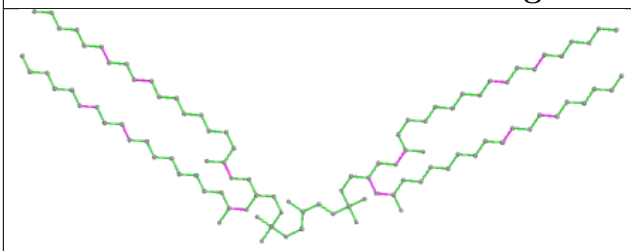


Torsions

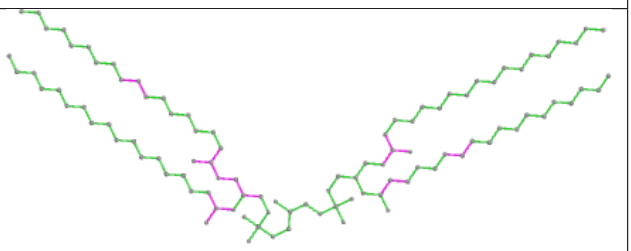


Rings

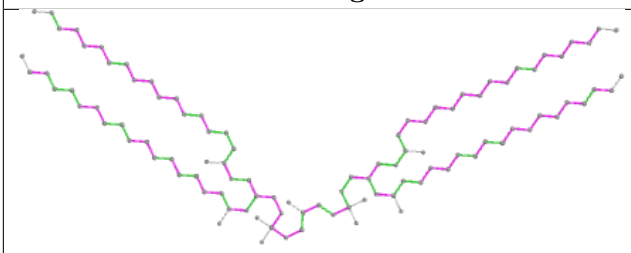
Ligand CDL C 270



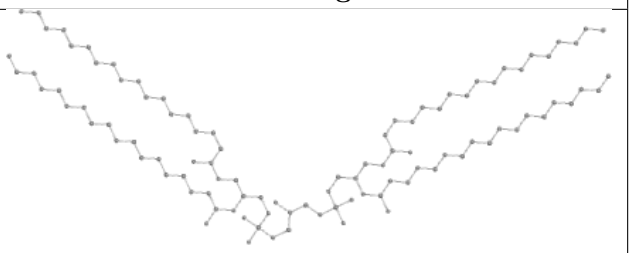
Bond lengths



Bond angles

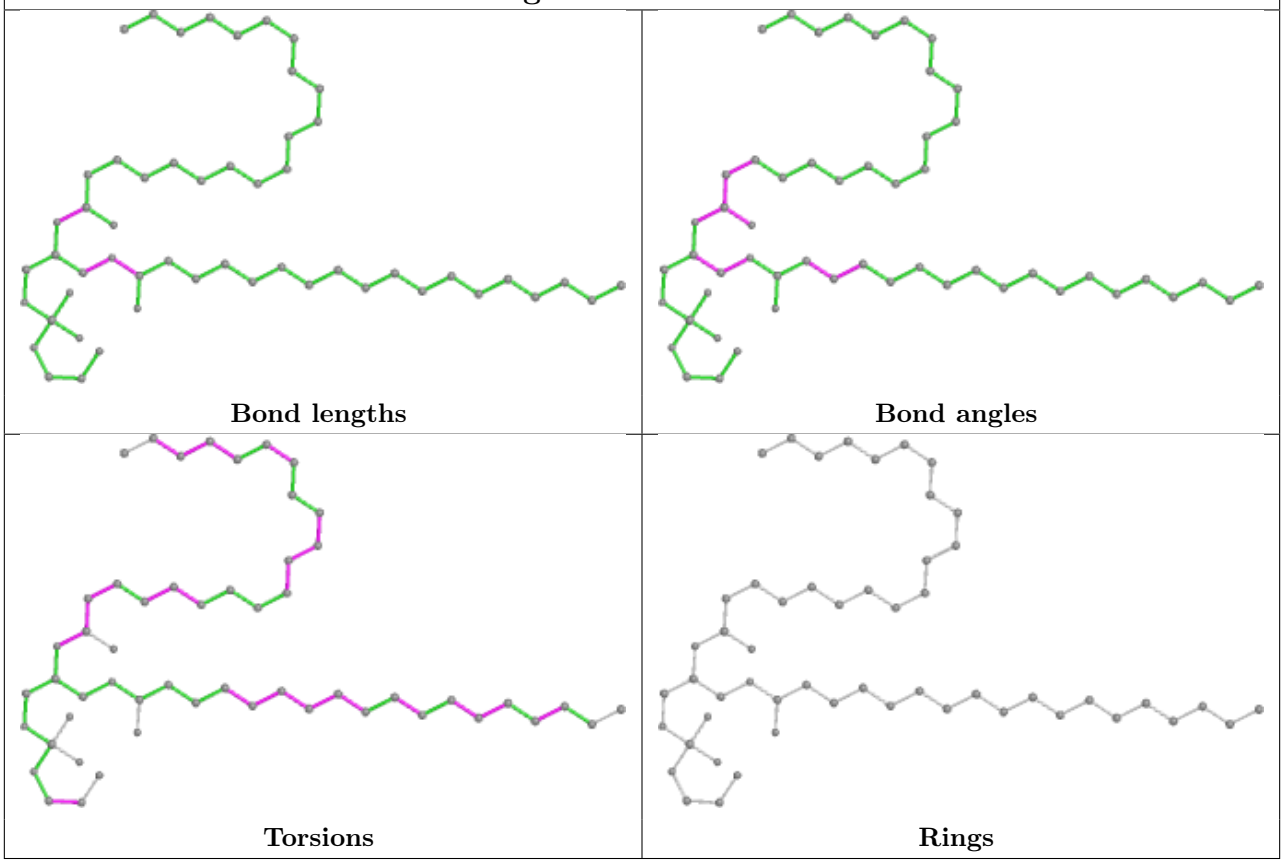


Torsions

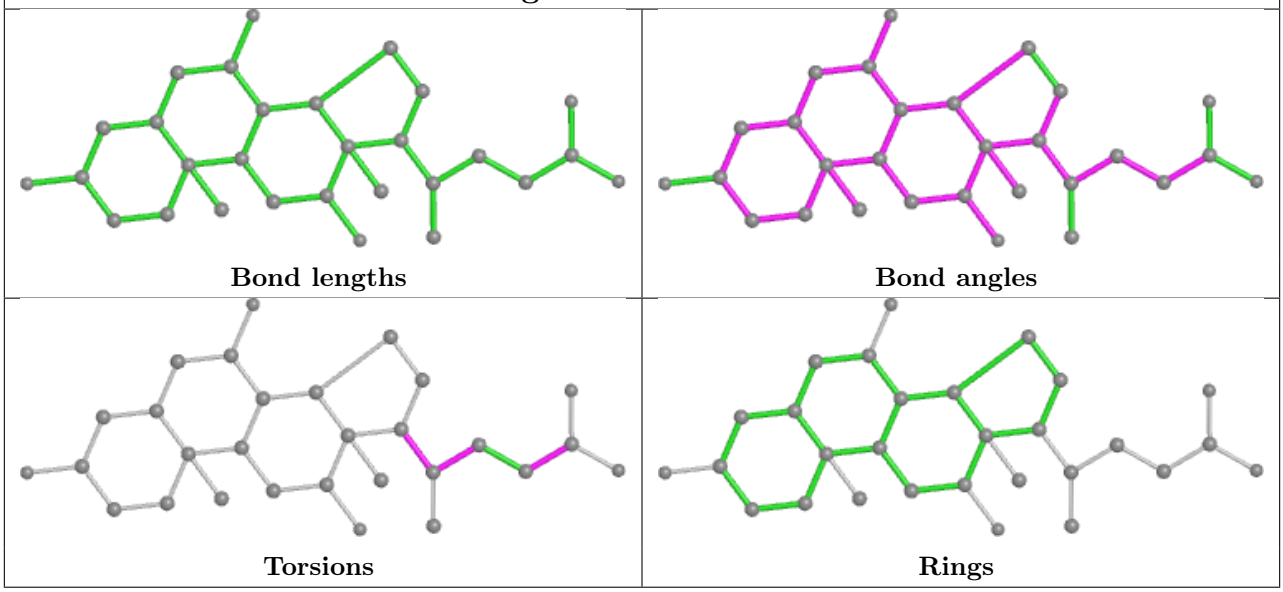


Rings

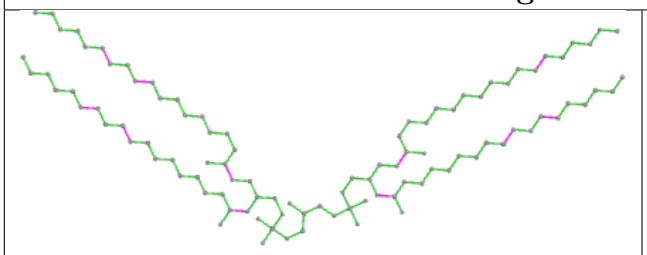
Ligand PEK G 264



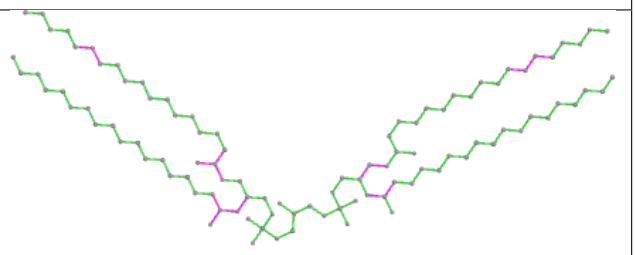
Ligand CHD C 271



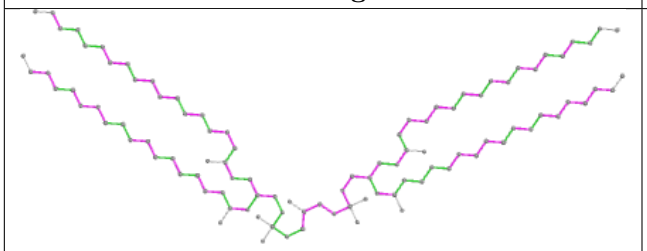
Ligand CDL T 1269



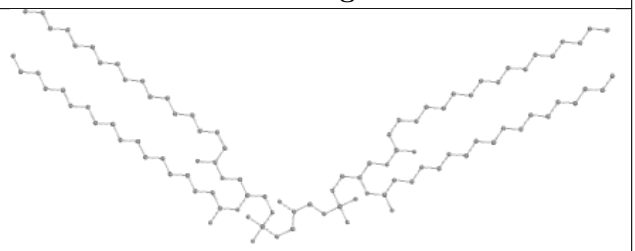
Bond lengths



Bond angles

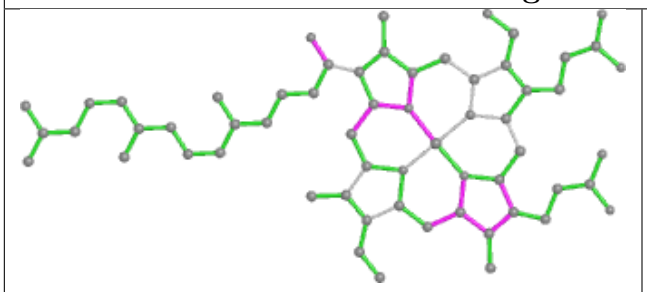


Torsions

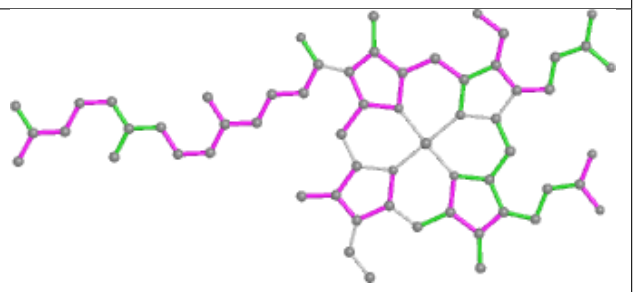


Rings

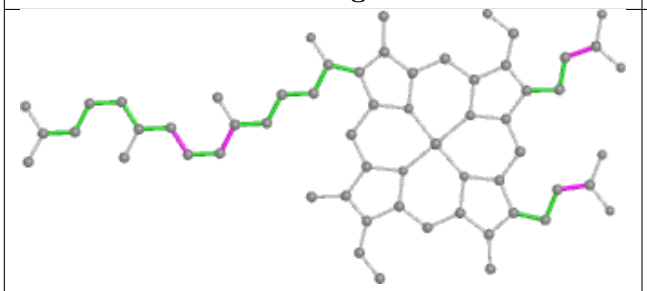
Ligand HEA A 515



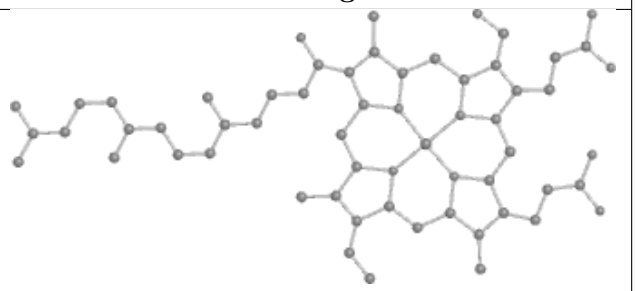
Bond lengths



Bond angles

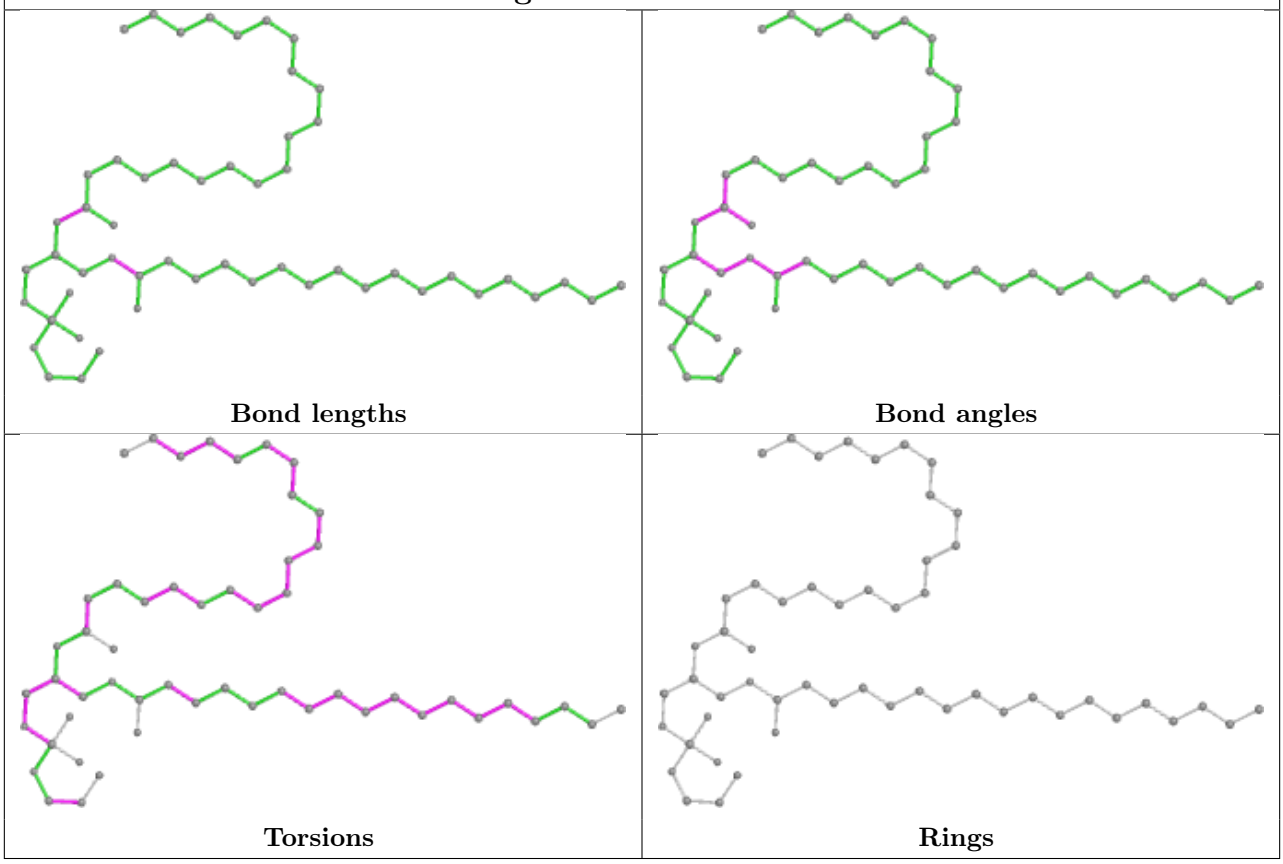


Torsions

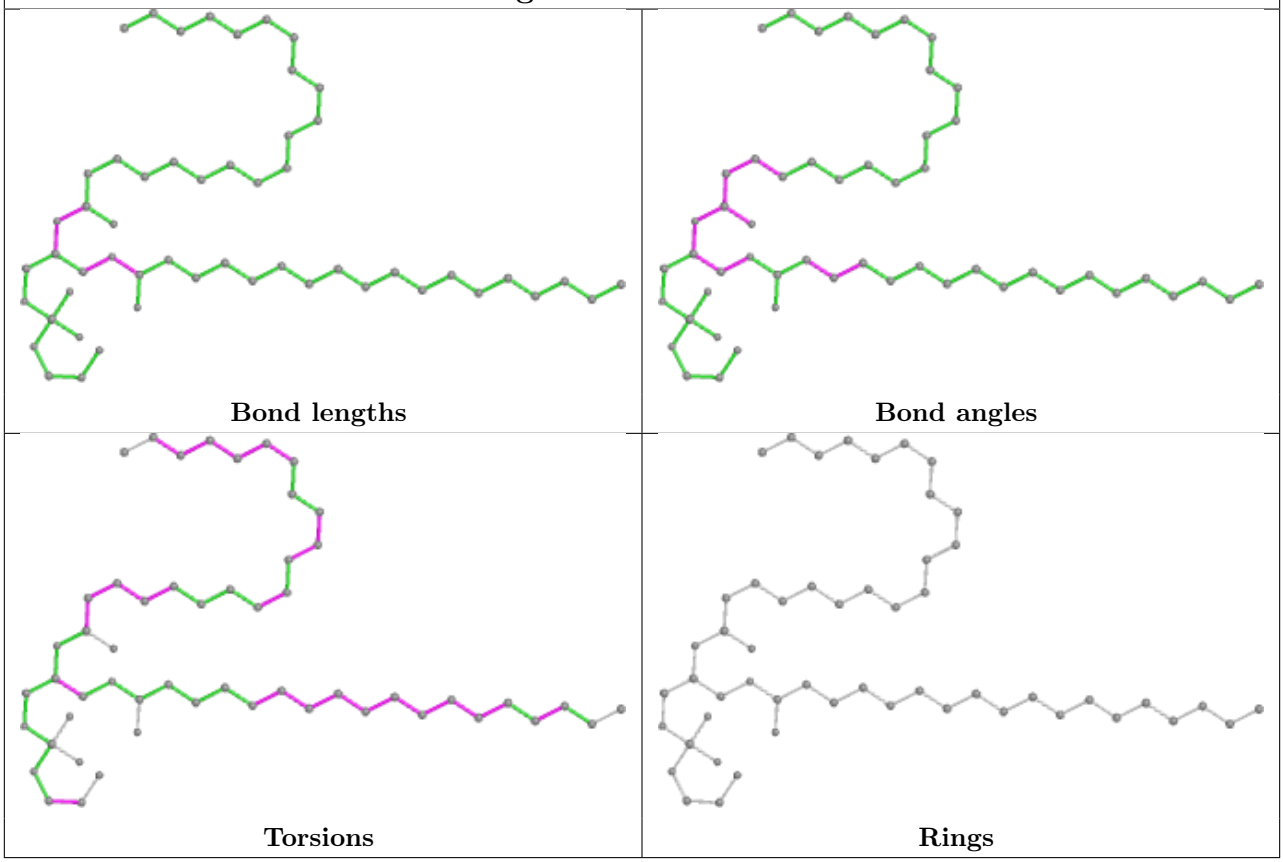


Rings

Ligand PEK G 1263



Ligand PEK P 1264



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.65	0 100 100	11, 17, 25, 51	0
1	N	513/514 (99%)	-0.66	1 (0%) 95 95	15, 23, 33, 56	0
2	B	226/227 (99%)	-0.78	0 100 100	12, 22, 49, 86	0
2	O	226/227 (99%)	-0.54	5 (2%) 62 65	20, 30, 60, 84	0
3	C	259/261 (99%)	-0.91	0 100 100	13, 21, 34, 58	0
3	P	259/261 (99%)	-0.84	1 (0%) 92 93	16, 24, 40, 64	0
4	D	144/147 (97%)	-0.64	0 100 100	14, 26, 48, 70	0
4	Q	144/147 (97%)	0.33	12 (8%) 11 11	27, 41, 63, 105	0
5	E	104/109 (95%)	-0.71	3 (2%) 51 55	18, 27, 54, 75	0
5	R	104/109 (95%)	-0.33	1 (0%) 82 84	23, 35, 57, 77	0
6	F	93/98 (94%)	-0.25	3 (3%) 47 51	15, 27, 49, 94	0
6	S	93/98 (94%)	0.03	4 (4%) 35 38	20, 33, 55, 102	0
7	G	83/85 (97%)	0.15	13 (15%) 2 1	15, 28, 99, 105	0
7	T	83/85 (97%)	0.34	15 (18%) 1 1	17, 33, 98, 102	0
8	H	75/85 (88%)	-0.20	3 (4%) 38 41	18, 29, 70, 78	0
8	U	75/85 (88%)	-0.06	3 (4%) 38 41	24, 34, 72, 79	0
9	I	71/73 (97%)	0.09	6 (8%) 10 10	21, 34, 60, 65	0
9	V	71/73 (97%)	0.29	4 (5%) 24 25	23, 45, 60, 70	0
10	J	57/59 (96%)	-0.29	5 (8%) 10 10	19, 32, 59, 82	0
10	W	57/59 (96%)	0.20	8 (14%) 2 2	25, 37, 68, 92	0
11	K	49/56 (87%)	-0.34	0 100 100	19, 31, 43, 50	0
11	X	49/56 (87%)	0.83	6 (12%) 4 3	33, 42, 59, 71	0
12	L	46/47 (97%)	-0.61	1 (2%) 62 65	17, 26, 48, 74	0
12	Y	46/47 (97%)	-0.28	2 (4%) 35 38	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%)	-0.28	5 (11%)	4	4	15, 24, 72, 97	0
13	Z	43/46 (93%)	0.26	5 (11%)	4	4	28, 36, 89, 106	0
All	All	3526/3614 (97%)	-0.45	106 (3%)	50	53	11, 26, 57, 106	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	17.7
4	Q	6	VAL	10.2
4	Q	4	SER	9.8
4	Q	8	SER	9.5
13	Z	43	SER	7.7
6	S	96	LEU	7.3
7	T	39	SER	7.0
4	Q	7	LYS	6.9
6	S	94	HIS	6.6
7	G	40	GLY	6.5
7	T	3	ALA	6.3
6	F	96	LEU	6.1
7	T	1	ALA	5.6
13	Z	41	LYS	5.2
11	X	6	ALA	5.2
7	G	8	HIS	5.1
13	Z	42	LYS	5.0
10	W	52	TRP	5.0
6	F	95	GLN	5.0
10	W	57	HIS	4.8
5	R	109	VAL	4.7
7	G	3	ALA	4.7
10	W	56	PRO	4.7
7	G	5	LYS	4.7
9	I	37	PHE	4.6
11	X	13	TYR	4.6
13	M	43	SER	4.6
7	T	2	SER	4.5
12	Y	47	LYS	4.4
4	Q	35	ALA	4.3
7	G	42	ARG	4.3
7	T	40	GLY	4.3
7	T	5	LYS	4.2
13	Z	39	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
6	S	95	GLN	4.0
4	Q	147	LYS	3.9
7	T	8	HIS	3.9
8	U	44	THR	3.9
6	S	93	PRO	3.9
13	Z	40	TYR	3.8
7	G	2	SER	3.7
6	F	94	HIS	3.7
10	W	1	PHE	3.7
11	X	7	PRO	3.6
9	V	37	PHE	3.6
13	M	42	LYS	3.6
7	T	42	ARG	3.5
7	G	36	TRP	3.4
8	H	47	GLY	3.4
2	O	113	TYR	3.3
1	N	513	LEU	3.3
7	T	36	TRP	3.3
7	T	10	GLY	3.2
8	U	47	GLY	3.1
7	T	4	ALA	3.0
7	T	84	LYS	3.0
2	O	59	GLN	3.0
2	O	226	MET	3.0
11	X	23	THR	3.0
7	G	4	ALA	2.9
8	H	44	THR	2.9
9	I	26	MET	2.9
7	G	84	LYS	2.9
13	M	39	ASN	2.9
9	I	33	THR	2.8
10	J	52	TRP	2.8
9	I	34	PHE	2.8
12	Y	45	LEU	2.8
9	I	30	GLY	2.8
5	E	7	THR	2.7
8	U	49	ASP	2.7
12	L	2	HIS	2.7
9	I	25	PHE	2.7
5	E	109	VAL	2.6
7	G	1	ALA	2.6
13	M	38	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	217	LYS	2.6
7	G	7	ASP	2.6
3	P	3	HIS	2.6
7	G	9	GLY	2.5
9	V	33	THR	2.5
9	V	30	GLY	2.5
13	M	40	TYR	2.4
4	Q	142	LYS	2.4
4	Q	51	LEU	2.4
7	T	41	HIS	2.3
7	G	41	HIS	2.3
10	J	1	PHE	2.2
11	X	16	ALA	2.2
10	W	55	PHE	2.2
7	T	12	GLY	2.2
4	Q	9	GLU	2.2
5	E	9	GLU	2.2
10	J	55	PHE	2.2
10	J	56	PRO	2.2
2	O	227	LEU	2.2
7	T	43	GLU	2.1
8	H	45	ALA	2.1
10	W	4	ARG	2.1
4	Q	33	LEU	2.1
4	Q	58	GLU	2.1
10	W	48	TYR	2.0
10	W	2	GLU	2.0
10	J	57	HIS	2.0
11	X	12	LYS	2.0
9	V	34	PHE	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	G	11	11/12	0.51	0.33	74,81,102,102	0
7	TPO	T	11	11/12	0.59	0.36	74,80,100,101	0
1	FME	N	1	10/11	0.92	0.18	48,50,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	A	1	10/11	0.92	0.19	44,46,62,65	0
2	FME	O	1	10/11	0.96	0.12	30,31,37,38	0
2	FME	B	1	10/11	0.98	0.13	19,21,26,33	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	0.58	0.40	74,102,105,106	0
26	PEK	C	265	53/53	0.59	0.33	39,87,101,104	0
24	DMU	C	272	33/33	0.62	0.35	64,101,103,105	0
26	PEK	T	263	53/53	0.64	0.38	35,81,112,112	0
21	TGL	N	1522	63/63	0.66	0.34	25,66,80,81	0
26	PEK	G	1263	53/53	0.67	0.37	46,88,115,116	0
23	CHD	J	60	29/29	0.68	0.48	95,98,101,103	0
27	CDL	P	1270	100/100	0.71	0.34	44,89,104,105	0
23	CHD	W	1060	29/29	0.72	0.50	97,100,102,103	0
26	PEK	P	1265	53/53	0.72	0.30	32,83,103,103	0
27	CDL	T	1269	100/100	0.72	0.27	43,76,109,113	0
27	CDL	G	269	100/100	0.73	0.31	42,77,109,113	0
25	UNX	P	1262	1/1	0.74	0.30	29,29,29,29	0
22	PSC	O	1230	52/52	0.74	0.28	38,82,113,115	0
19	PGV	N	1268	51/51	0.76	0.29	62,89,99,101	0
21	TGL	O	1523	63/63	0.77	0.23	34,64,86,90	0
19	PGV	C	268	51/51	0.77	0.26	53,87,97,98	0
22	PSC	B	230	52/52	0.79	0.31	31,86,112,114	0
21	TGL	L	522	63/63	0.79	0.28	25,61,74,78	0
27	CDL	C	270	100/100	0.80	0.30	40,86,103,105	0
19	PGV	N	1524	51/51	0.81	0.29	36,68,102,102	0
19	PGV	A	524	51/51	0.81	0.26	30,65,100,103	0
21	TGL	D	523	63/63	0.81	0.23	38,57,83,86	0
21	TGL	N	1521	63/63	0.82	0.23	43,63,85,90	0
24	DMU	Z	1526	33/33	0.82	0.23	32,50,66,68	0

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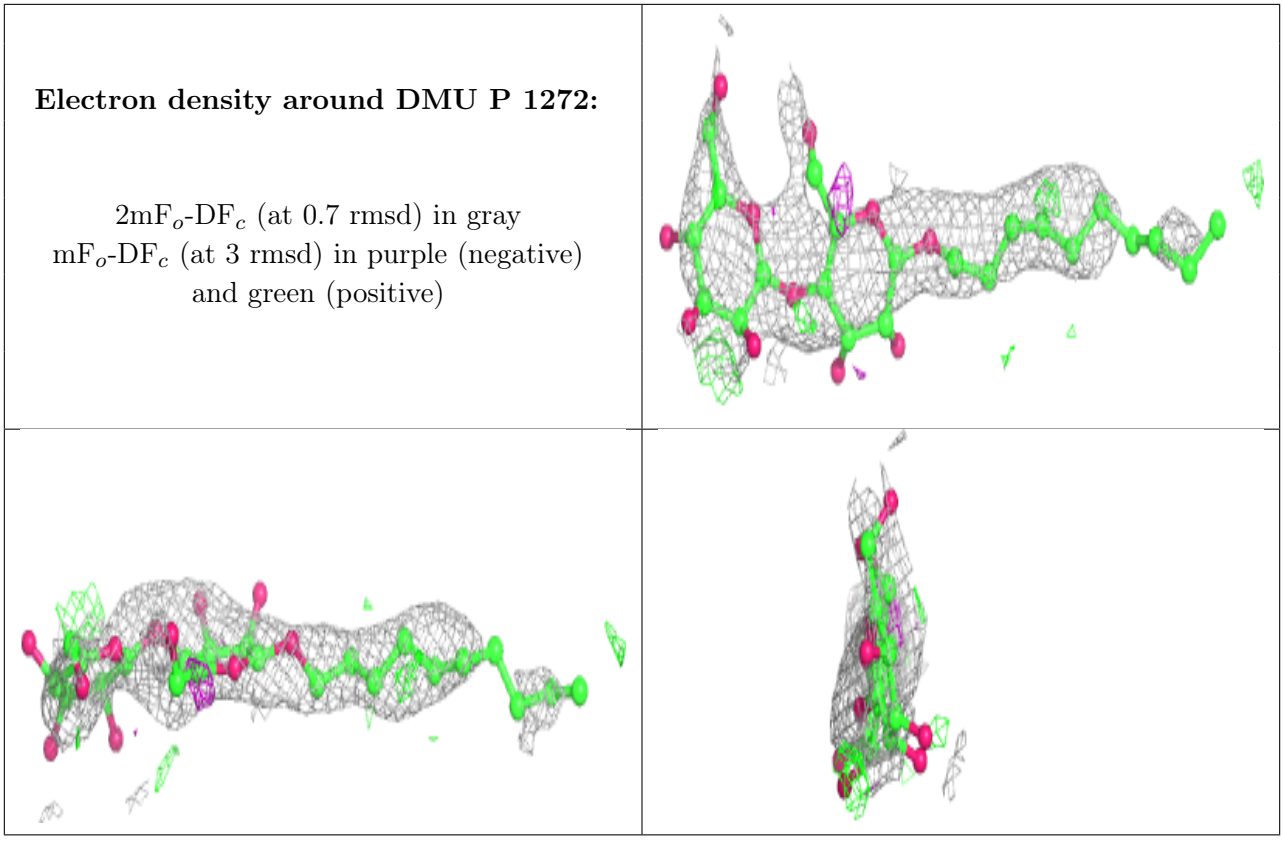
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	UNX	C	262	1/1	0.82	0.21	26,26,26,26	0
23	CHD	P	1271	29/29	0.82	0.27	74,82,84,84	0
21	TGL	B	521	63/63	0.84	0.24	31,58,87,89	0
16	MG	N	1518	1/1	0.85	0.13	26,26,26,26	0
23	CHD	C	271	29/29	0.86	0.31	71,83,86,86	0
24	DMU	M	526	33/33	0.91	0.16	15,38,57,59	0
26	PEK	P	1264	53/53	0.94	0.20	20,37,65,65	0
23	CHD	P	1525	29/29	0.95	0.10	17,27,31,35	0
23	CHD	C	525	29/29	0.96	0.10	14,24,31,33	0
17	NA	A	519	1/1	0.96	0.07	16,16,16,16	0
16	MG	A	518	1/1	0.96	0.08	21,21,21,21	0
26	PEK	G	264	53/53	0.96	0.18	15,31,57,58	0
19	PGV	C	267	51/51	0.96	0.18	13,24,55,58	0
19	PGV	P	1267	51/51	0.96	0.18	16,28,59,60	0
17	NA	N	1519	1/1	0.97	0.04	24,24,24,24	0
23	CHD	B	1086	29/29	0.97	0.10	11,20,27,33	0
23	CHD	G	86	29/29	0.98	0.08	17,21,25,26	0
20	CUA	O	228	2/2	0.98	0.07	25,25,25,26	0
18	HEA	N	516	60/60	0.98	0.12	9,20,26,28	0
15	PER	N	520	2/2	0.98	0.13	13,13,13,13	0
19	PGV	N	1266	51/51	0.98	0.20	15,28,50,52	0
19	PGV	A	521	51/51	0.98	0.18	12,24,48,57	0
18	HEA	N	515	60/60	0.98	0.17	14,25,37,39	0
18	HEA	A	516	60/60	0.99	0.12	9,16,24,27	0
15	PER	A	520	2/2	0.99	0.17	8,8,8,10	0
20	CUA	B	228	2/2	0.99	0.09	17,17,17,18	0
18	HEA	A	515	60/60	0.99	0.16	8,17,40,45	0
28	ZN	S	99	1/1	0.99	0.05	28,28,28,28	0
14	CU	N	517	1/1	1.00	0.10	18,18,18,18	0
28	ZN	F	99	1/1	1.00	0.07	26,26,26,26	0
14	CU	A	517	1/1	1.00	0.09	17,17,17,17	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.

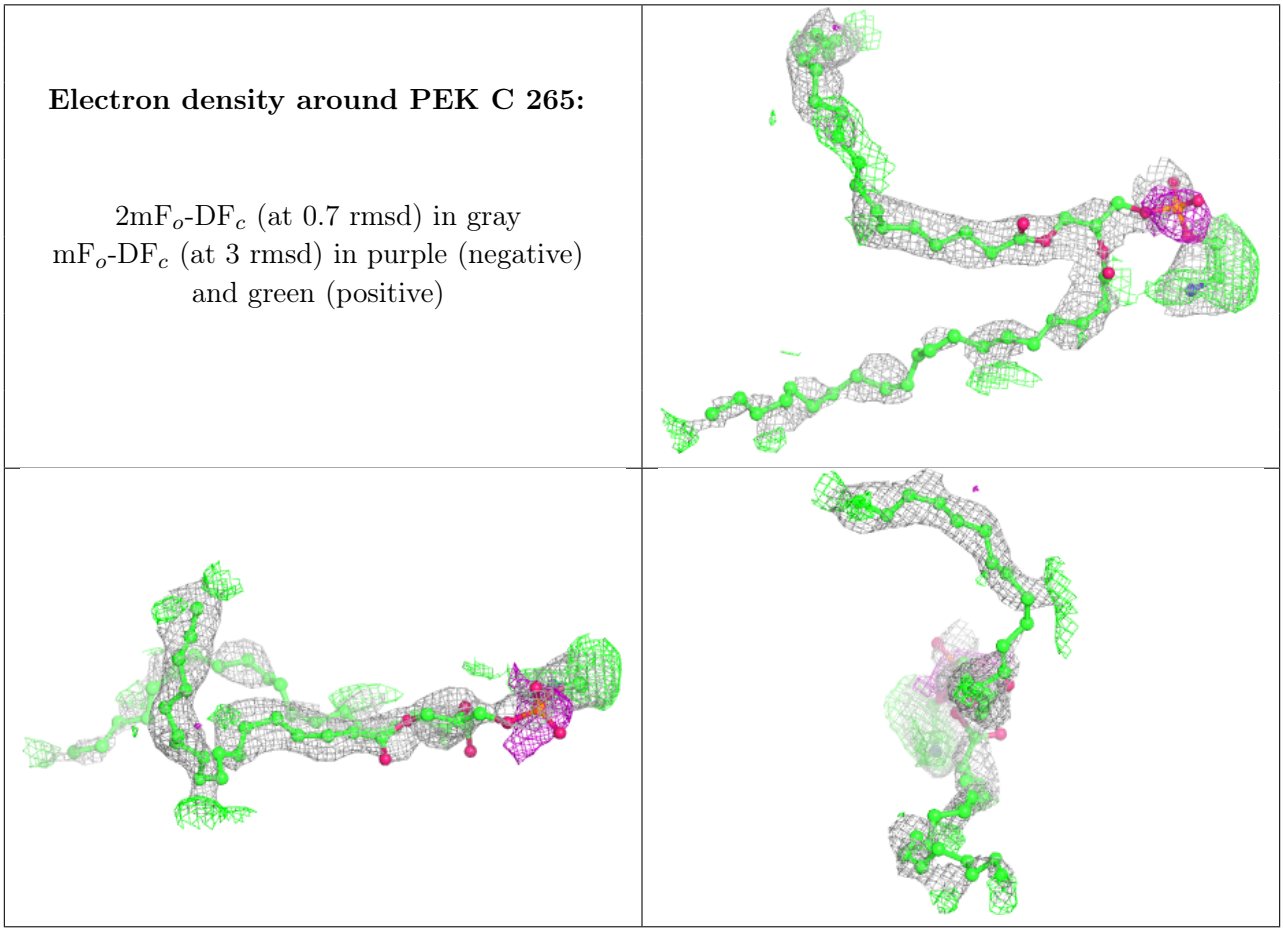
Electron density around DMU P 1272:

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



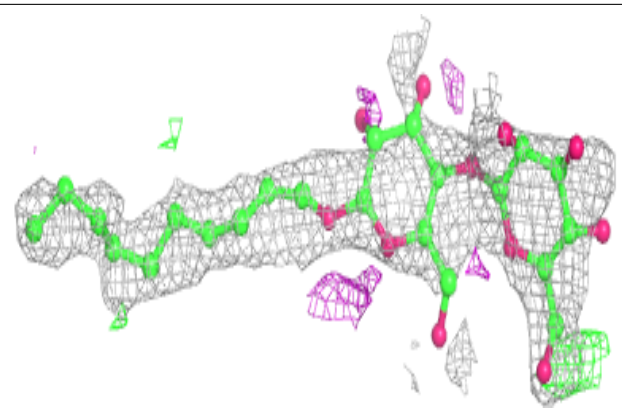
Electron density around PEK C 265:

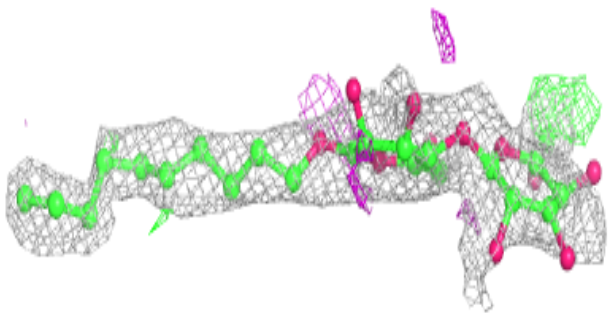
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

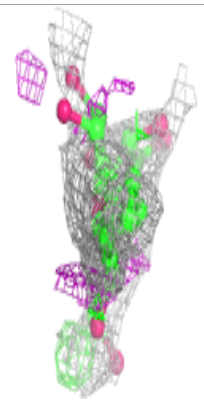


Electron density around DMU C 272:

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

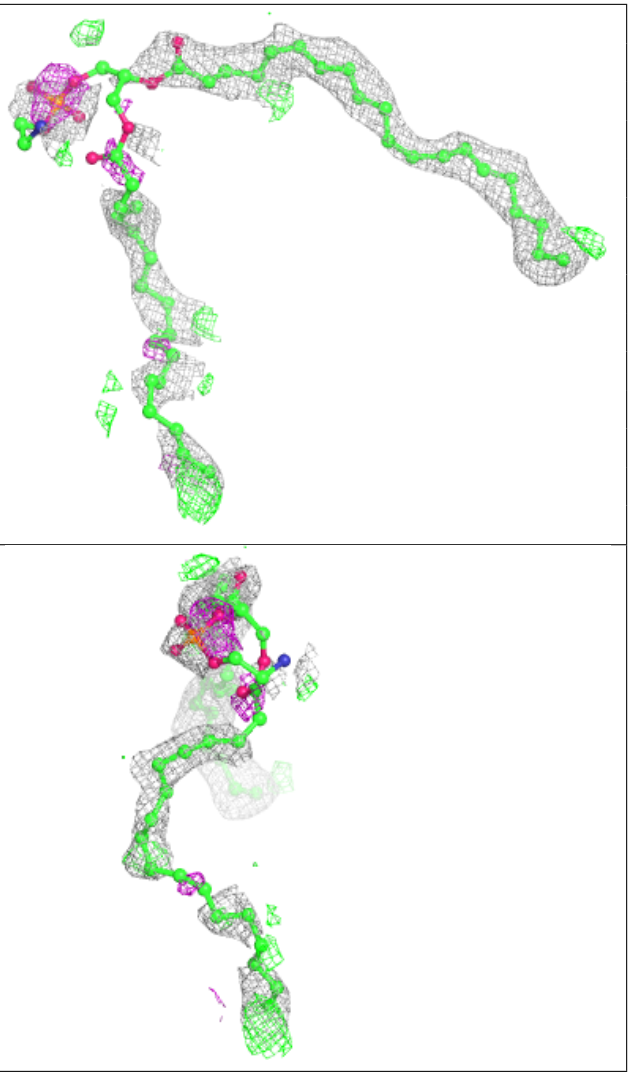






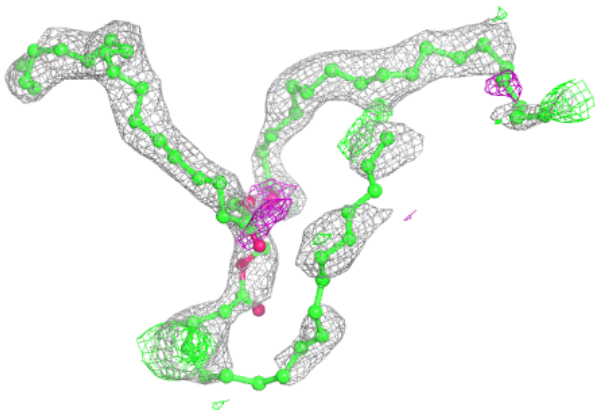
Electron density around PEK T 263:

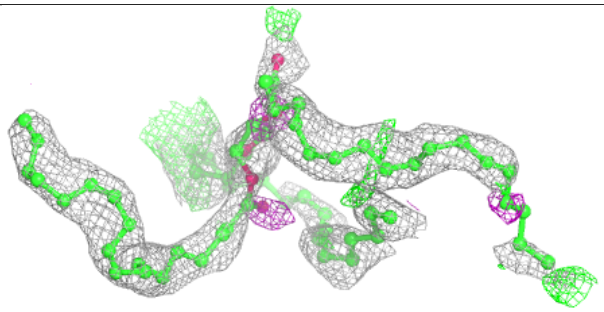
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

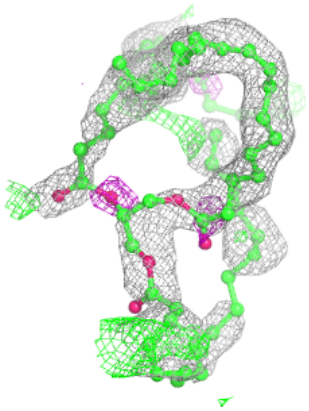


Electron density around TGL N 1522:

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

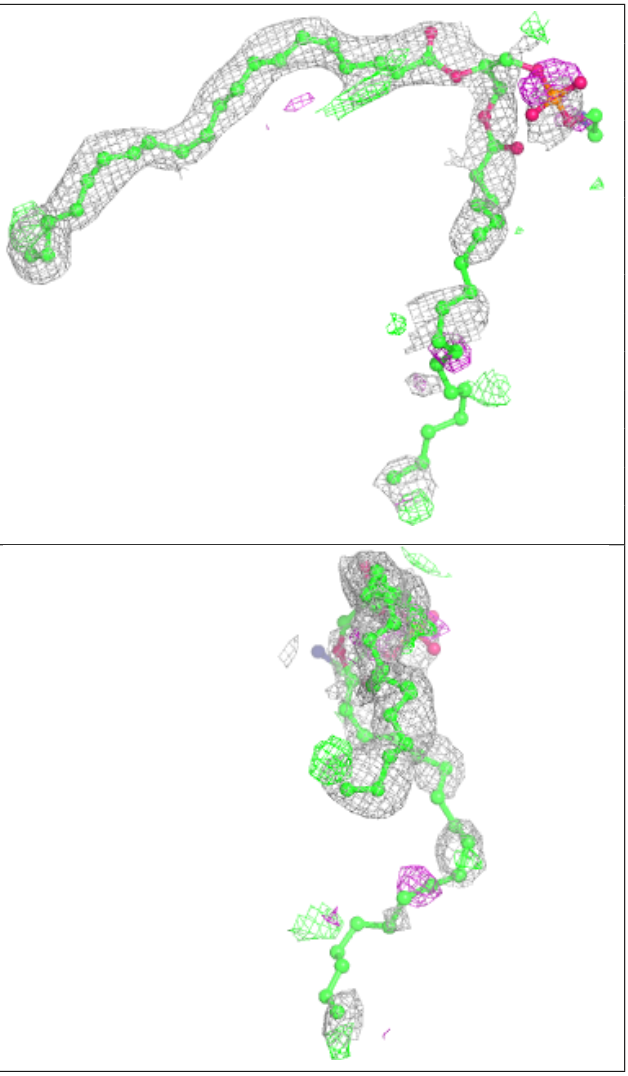






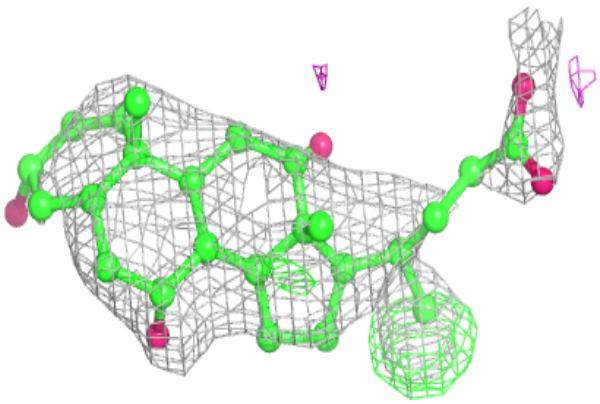
Electron density around PEK G 1263:

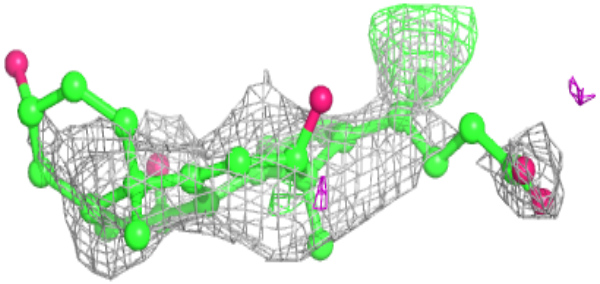
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

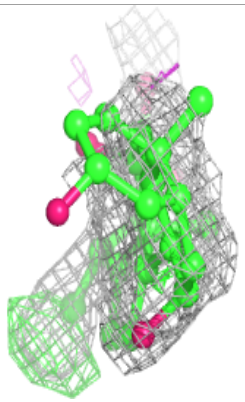


Electron density around CHD J 60:

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

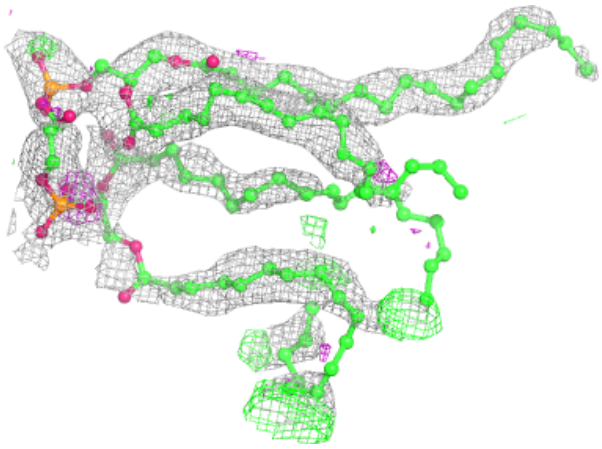


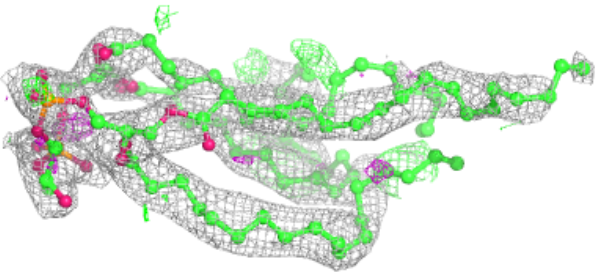


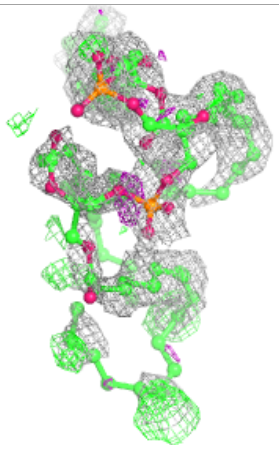


Electron density around CDL P 1270:

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

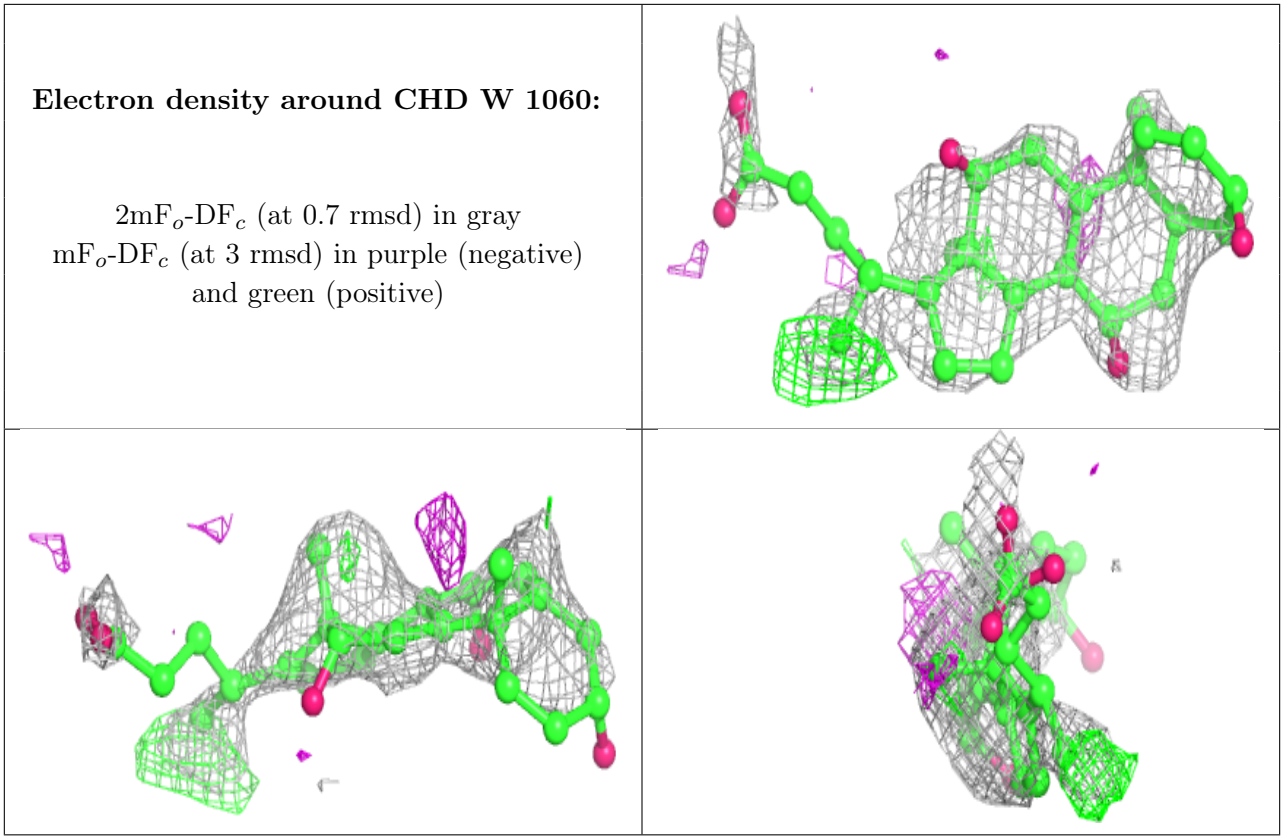






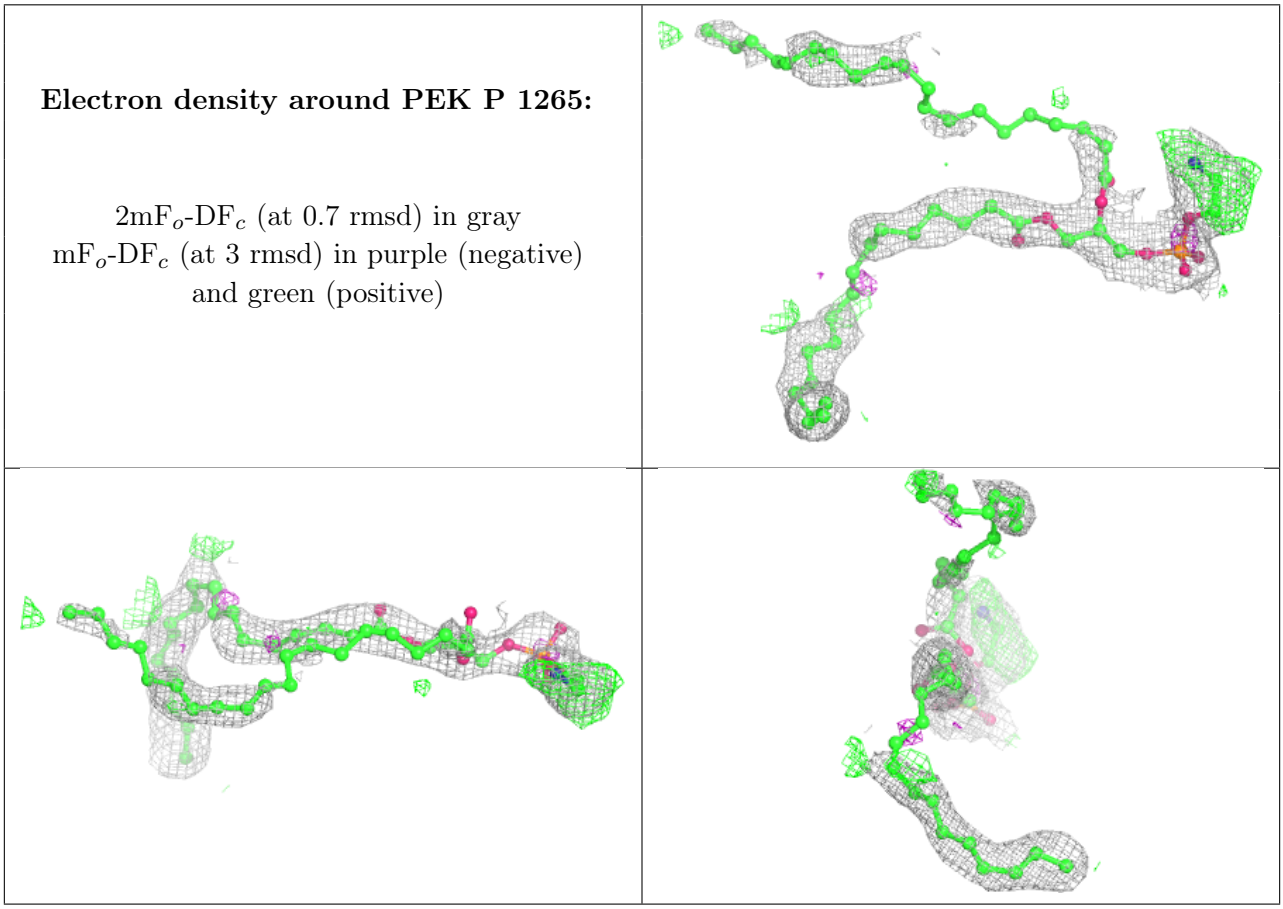
Electron density around CHD W 1060:

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



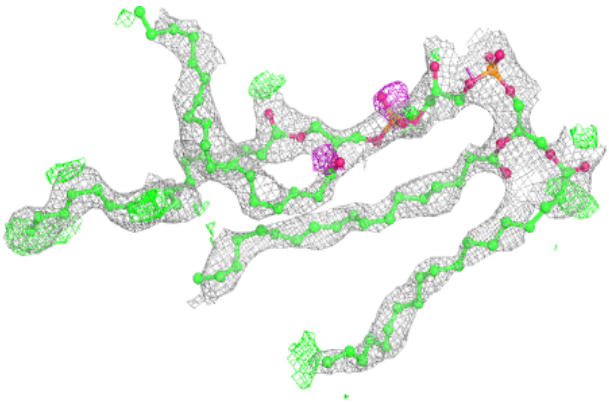
Electron density around PEK P 1265:

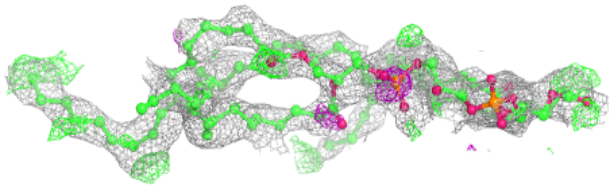
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CDL T 1269:

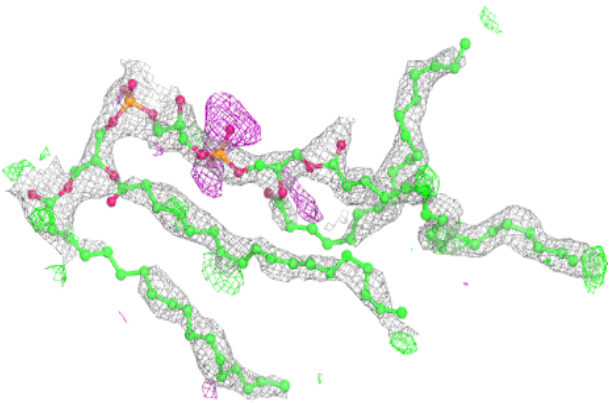
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

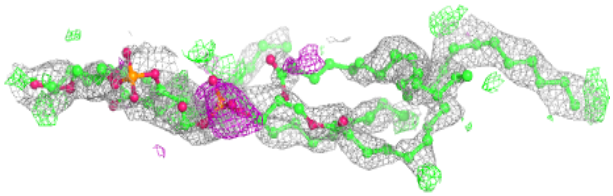


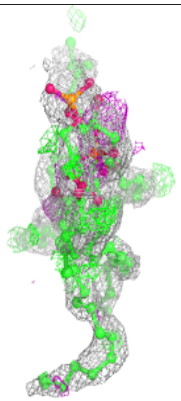


Electron density around CDL G 269:

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

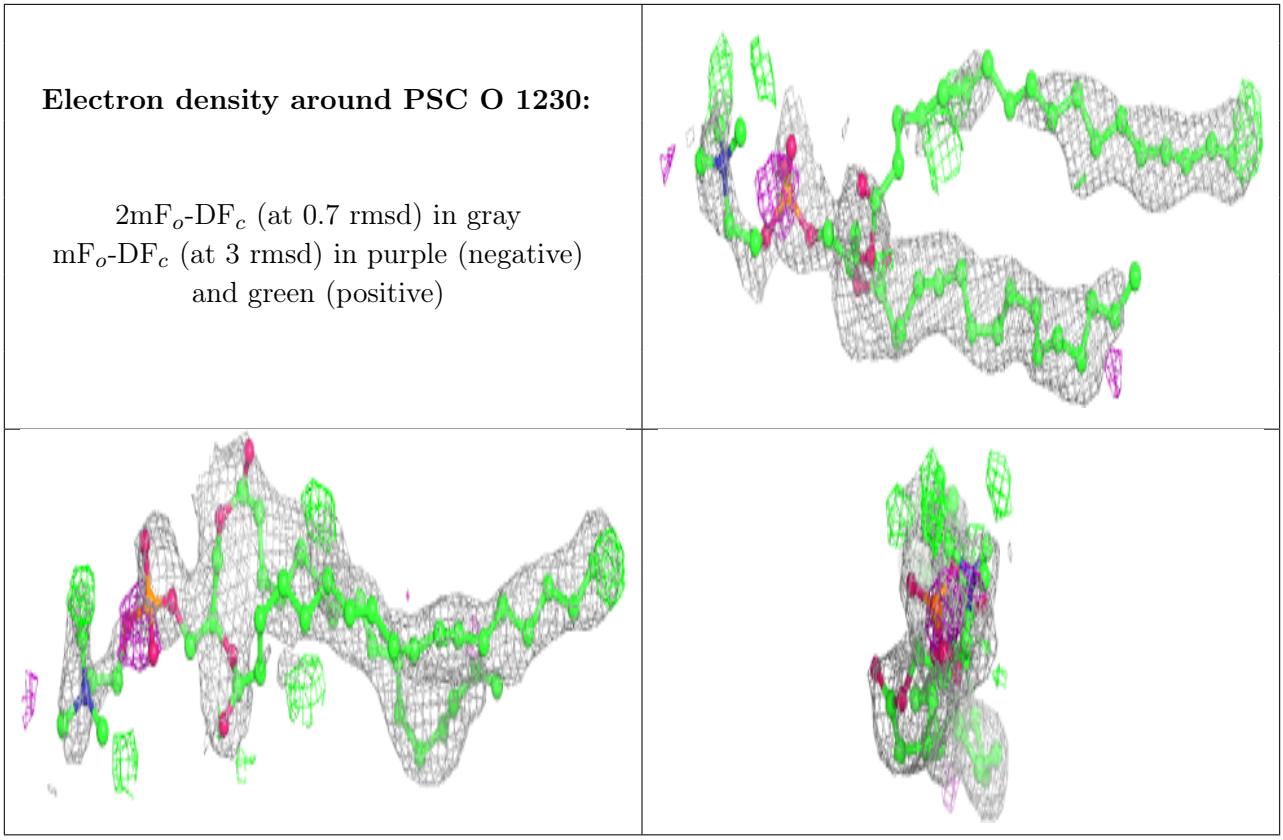






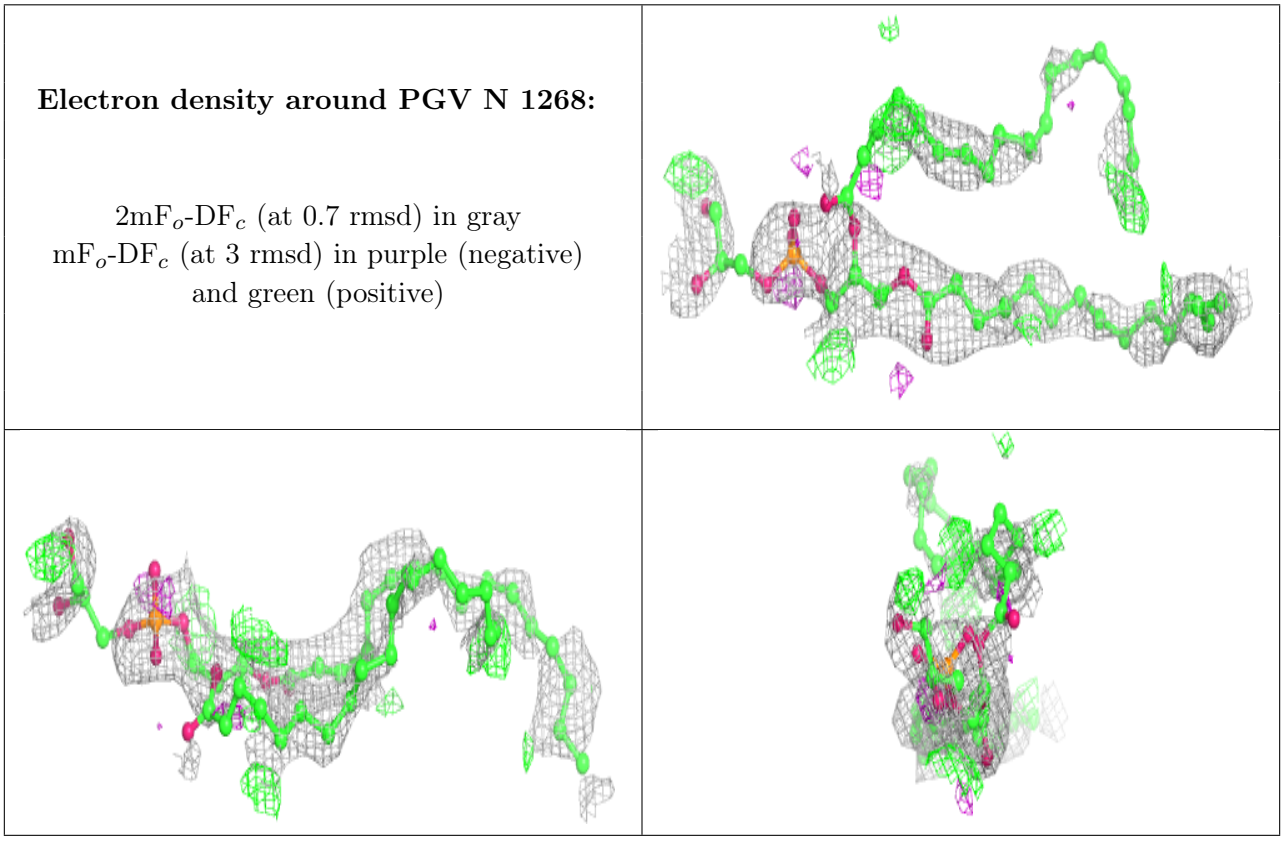
Electron density around PSC O 1230:

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



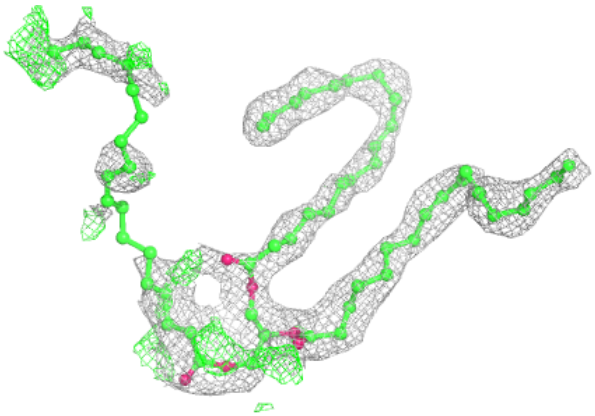
Electron density around PGV N 1268:

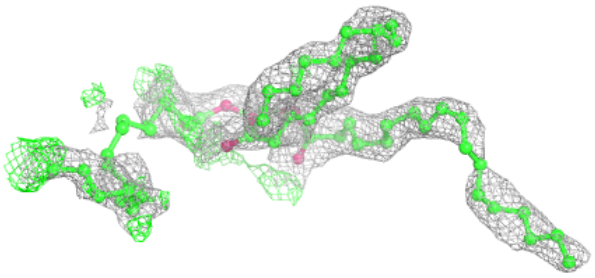
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

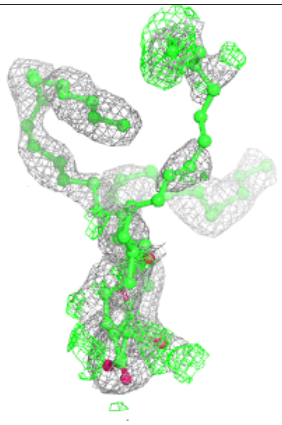


Electron density around TGL O 1523:

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

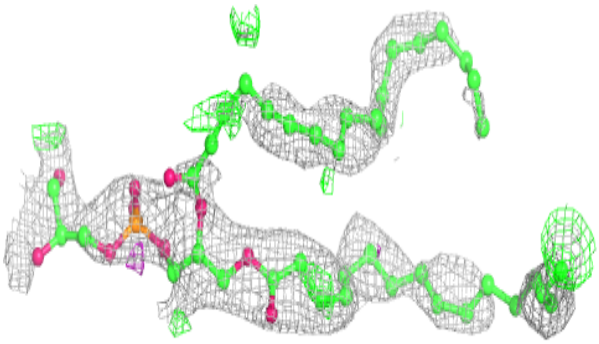


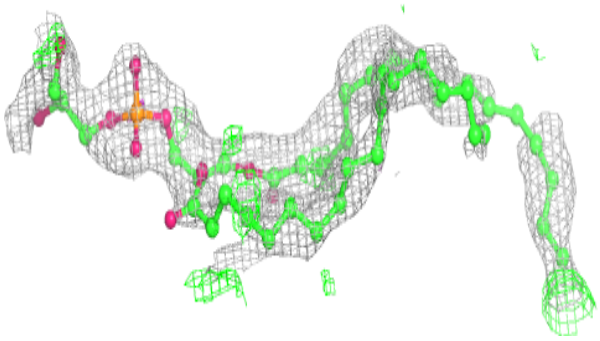


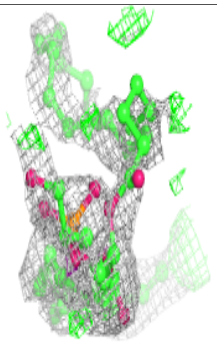


Electron density around PGV C 268:

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

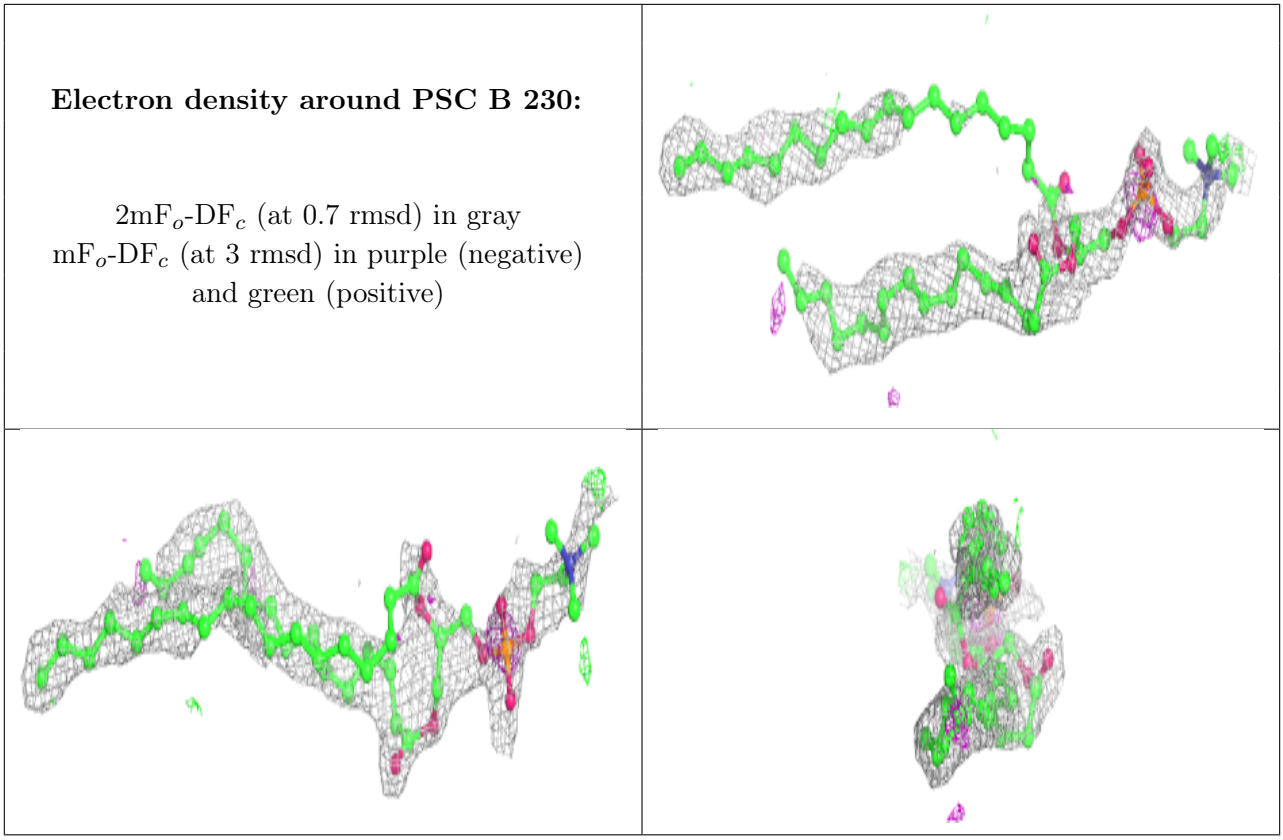






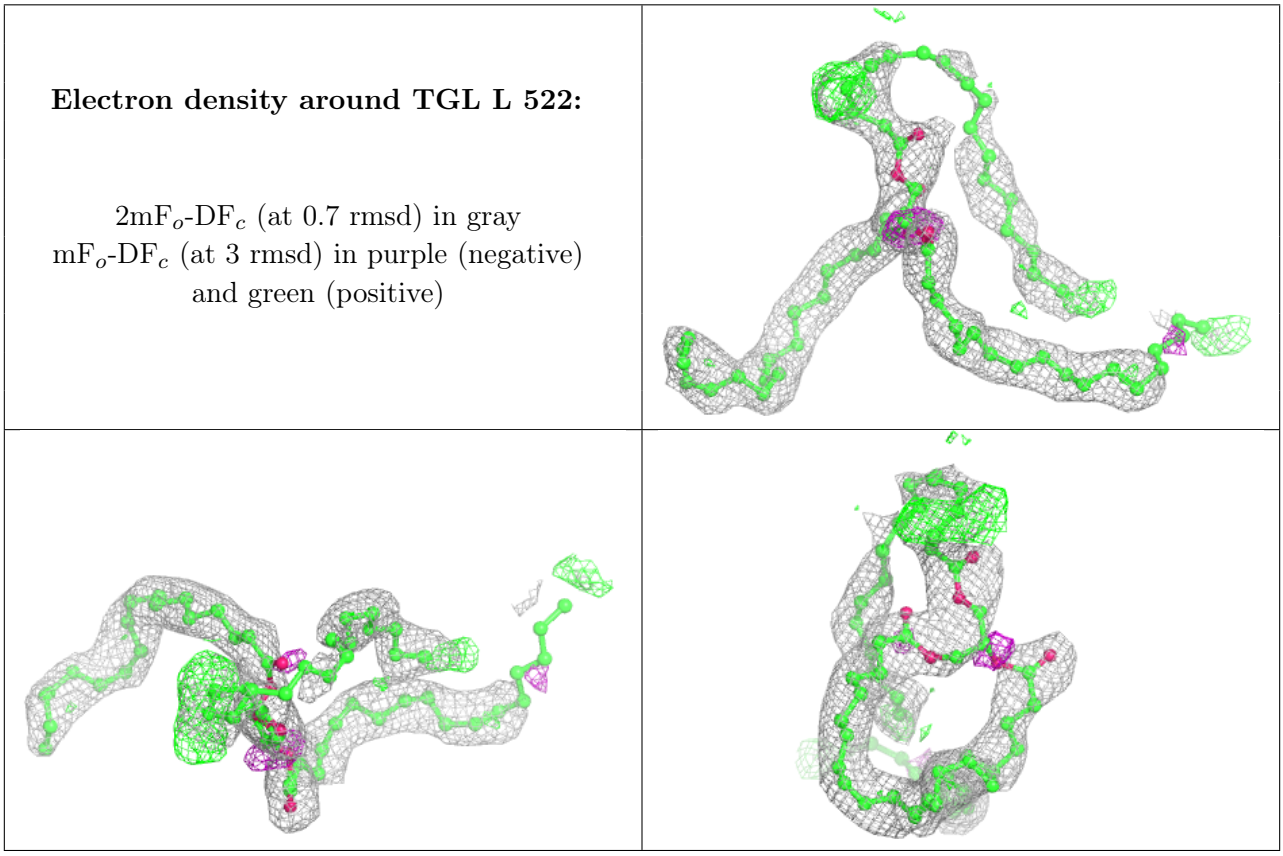
Electron density around PSC B 230:

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



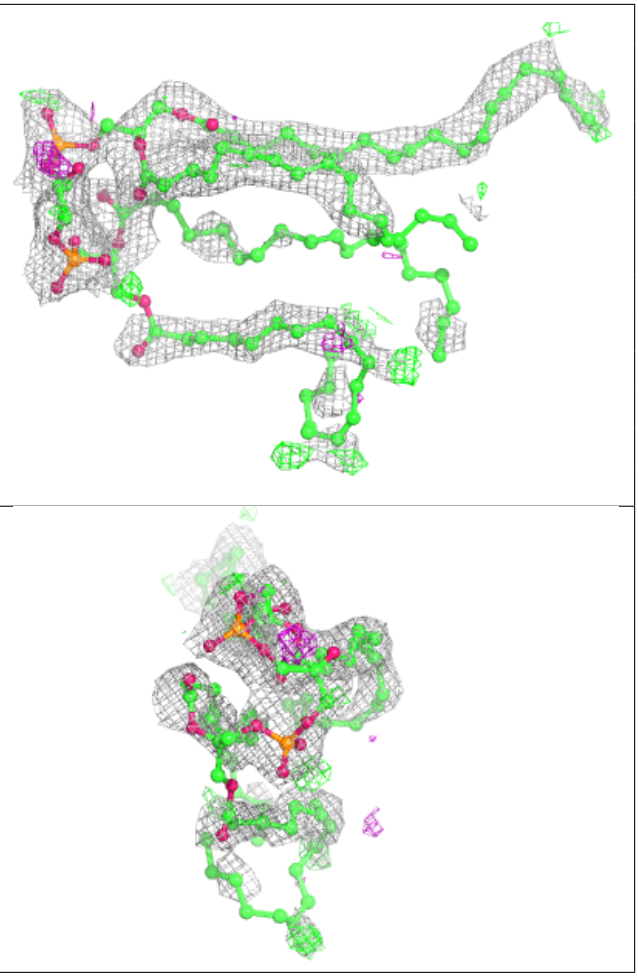
Electron density around TGL L 522:

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



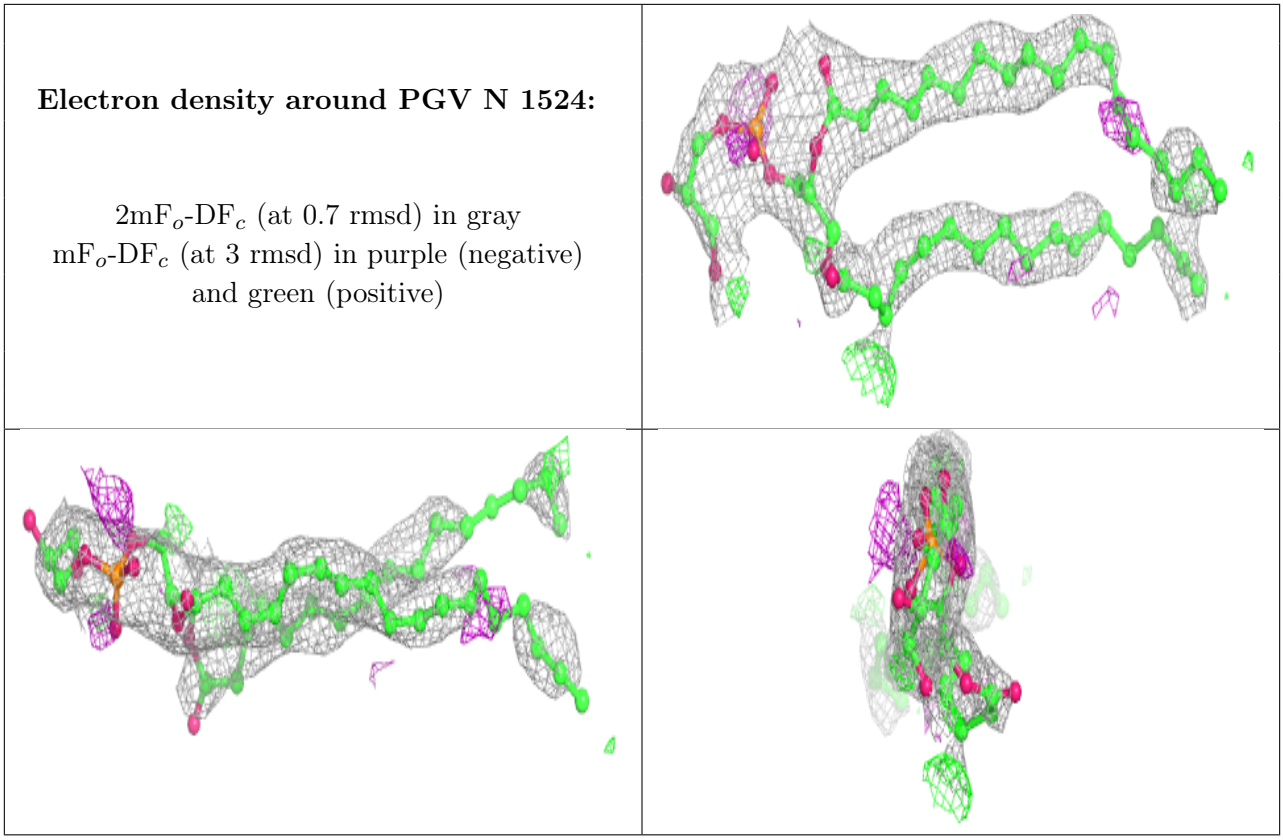
Electron density around CDL C 270:

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



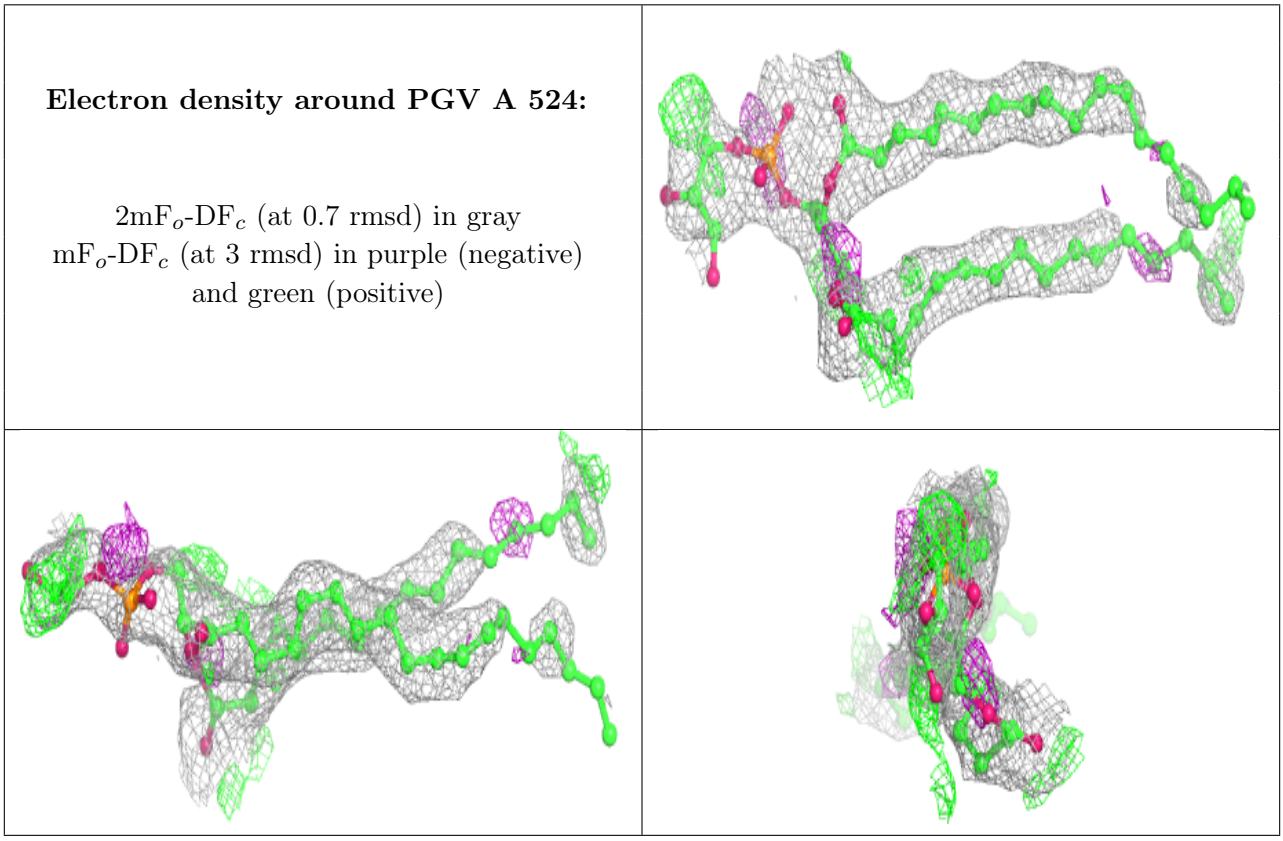
Electron density around PGV N 1524:

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



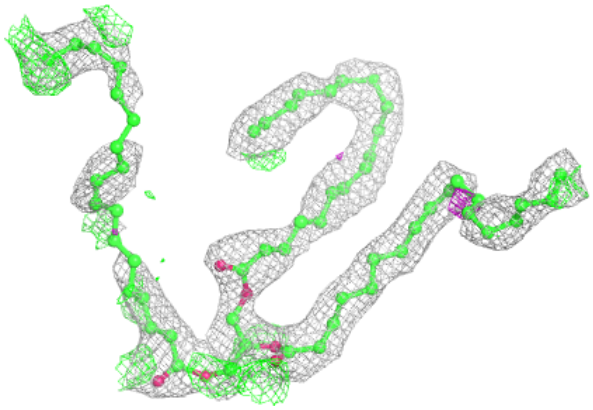
Electron density around PGV A 524:

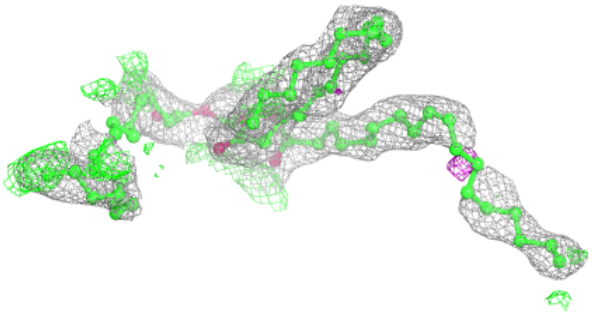
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TGL D 523:

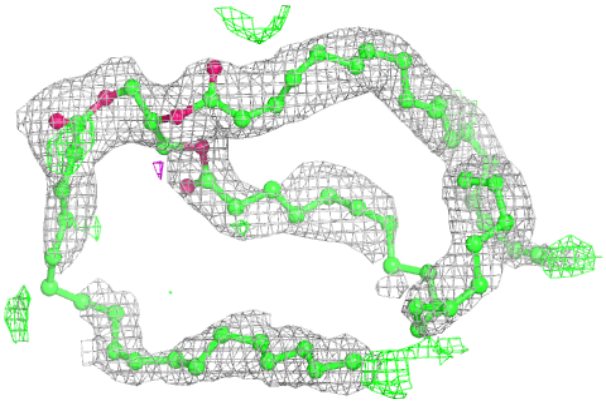
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

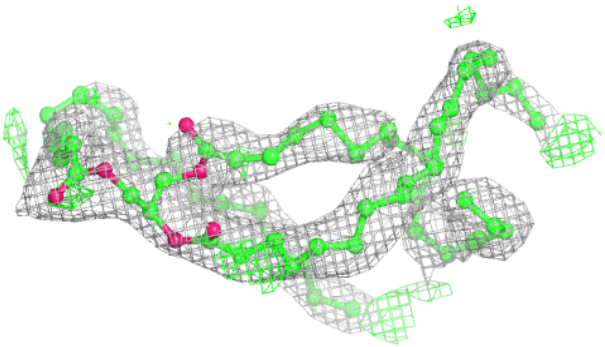


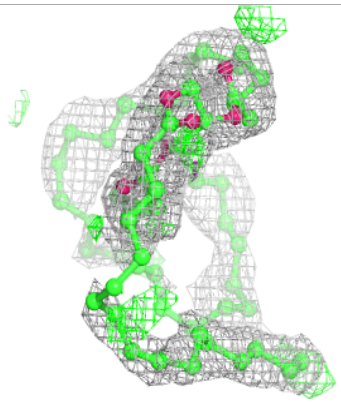


Electron density around TGL N 1521:

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

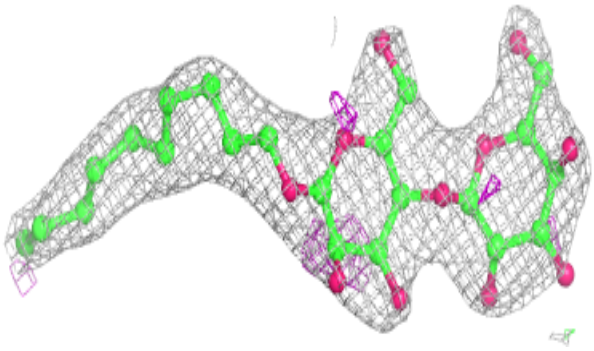


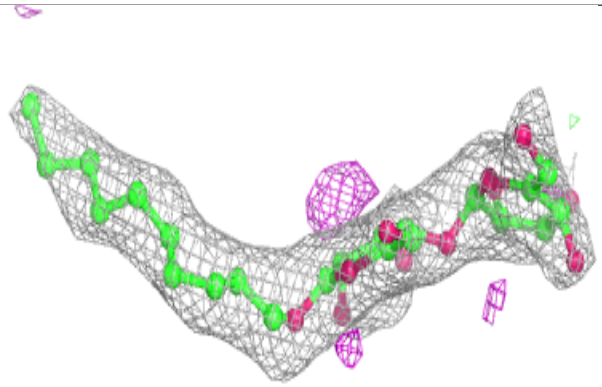


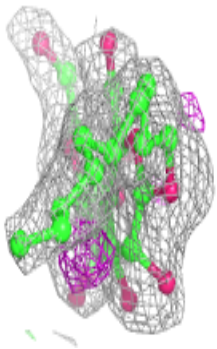


Electron density around DMU Z 1526:

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

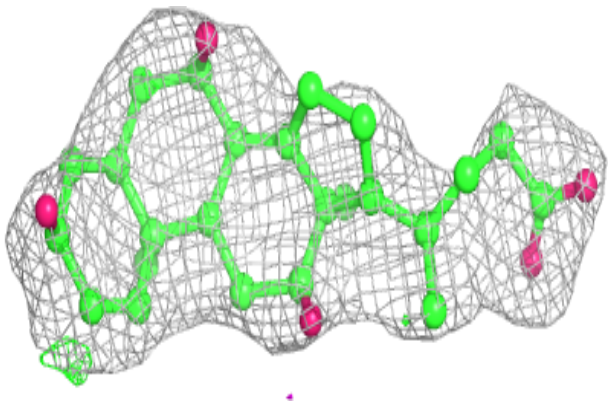


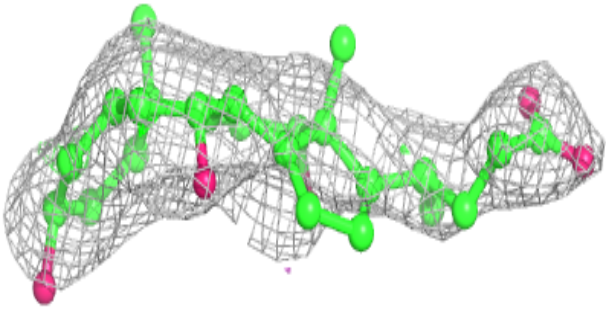


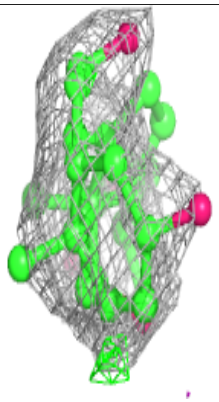


Electron density around CHD P 1271:

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

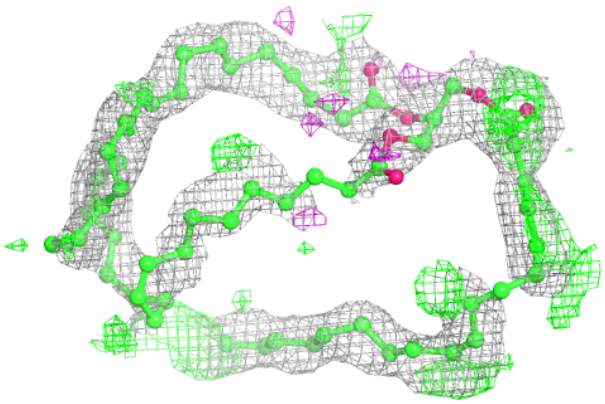


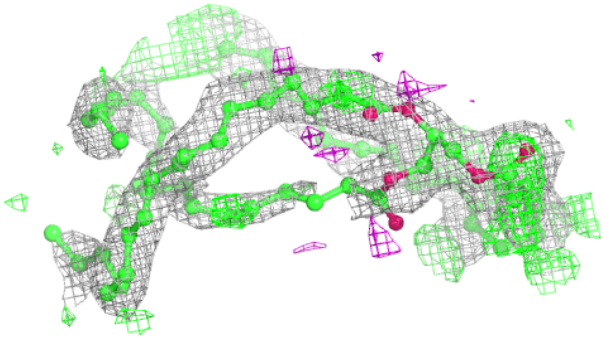


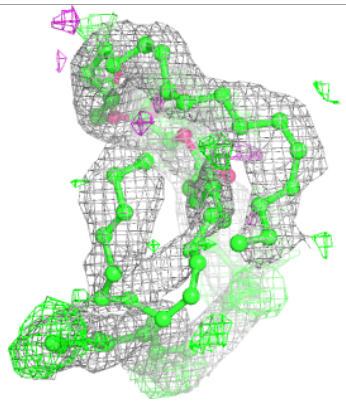


Electron density around TGL B 521:

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

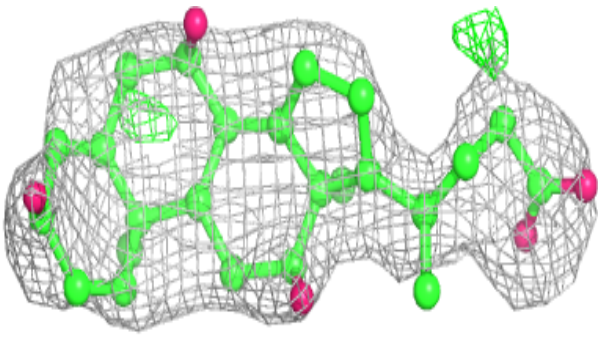


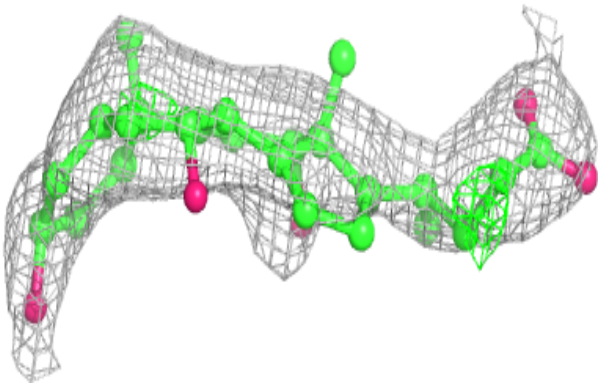


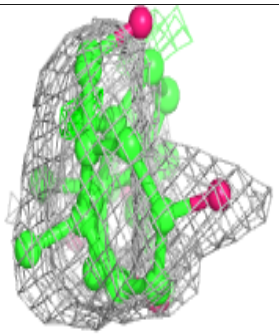


Electron density around CHD C 271:

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

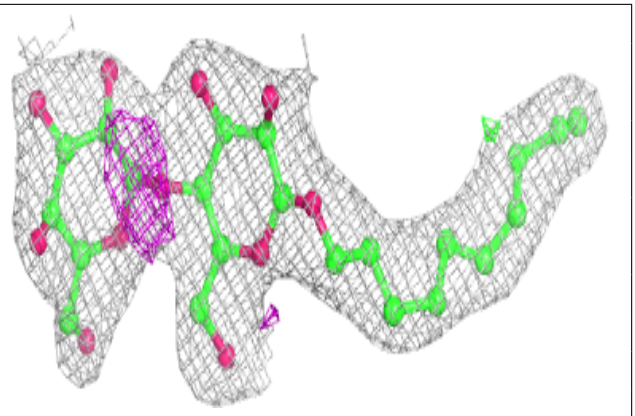


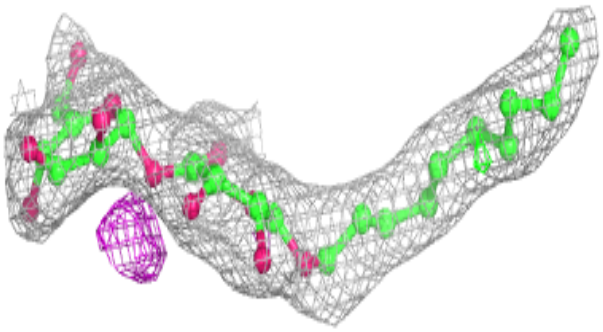


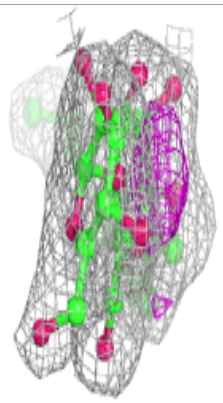


Electron density around DMU M 526:

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

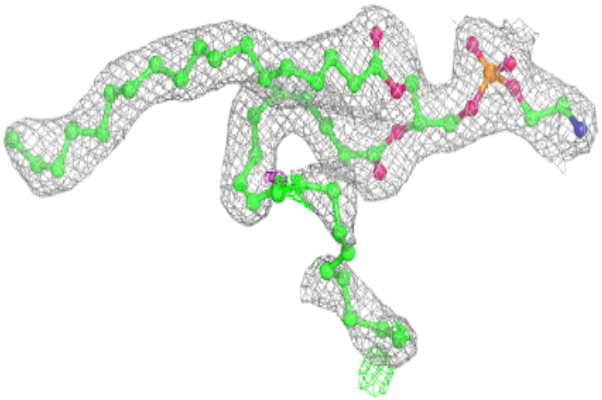


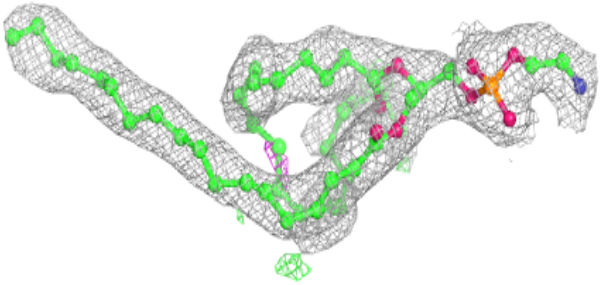


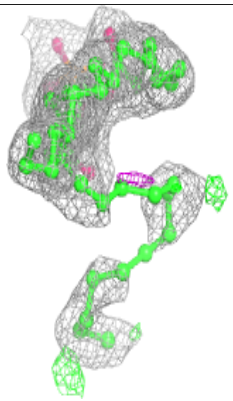


Electron density around PEK P 1264:

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

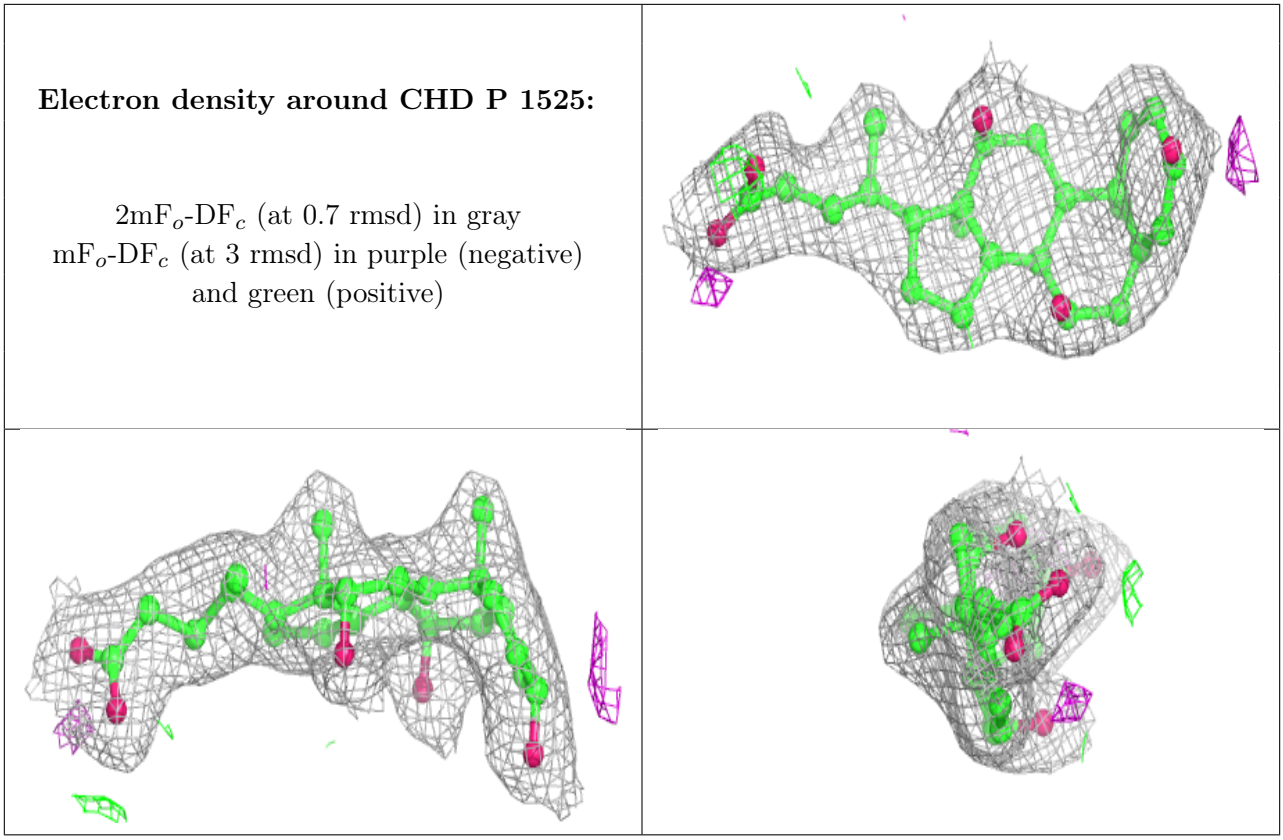






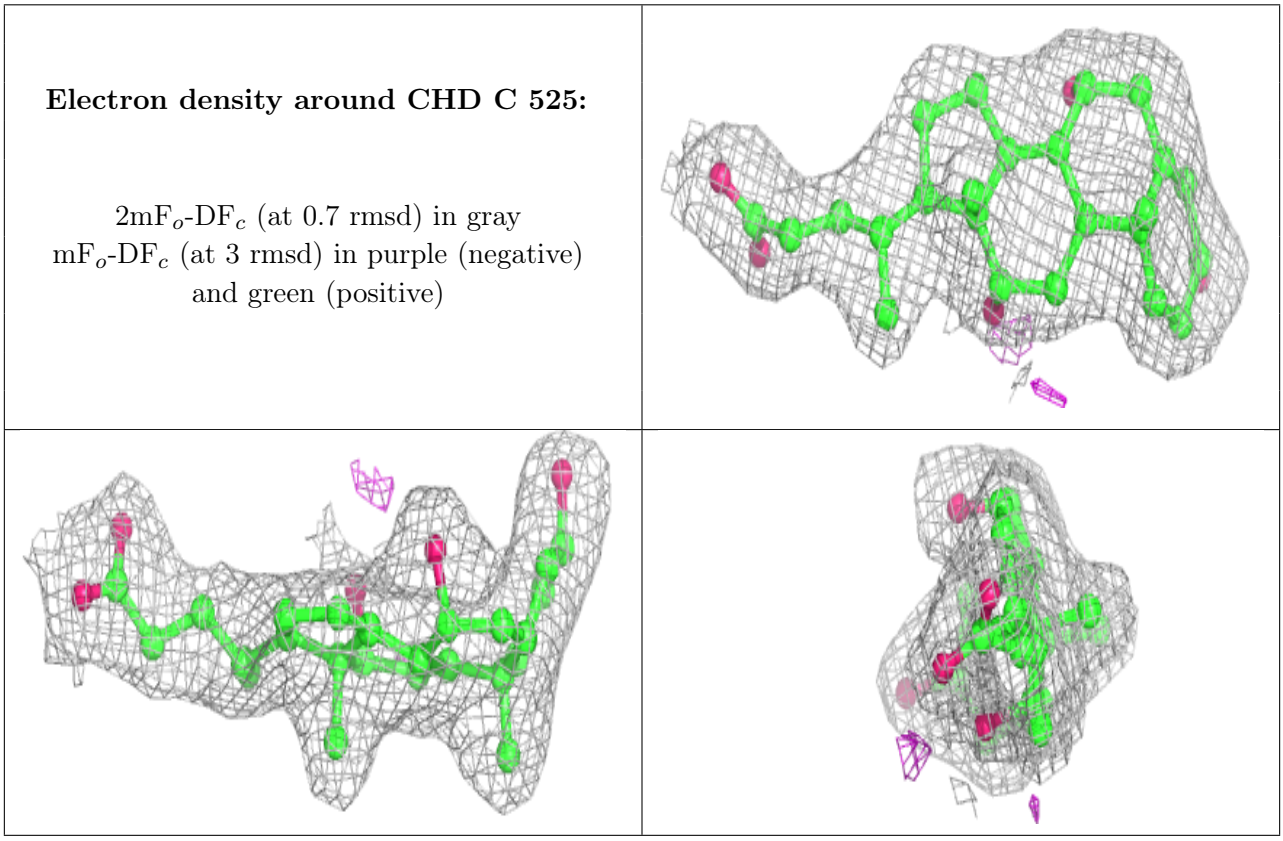
Electron density around CHD P 1525:

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



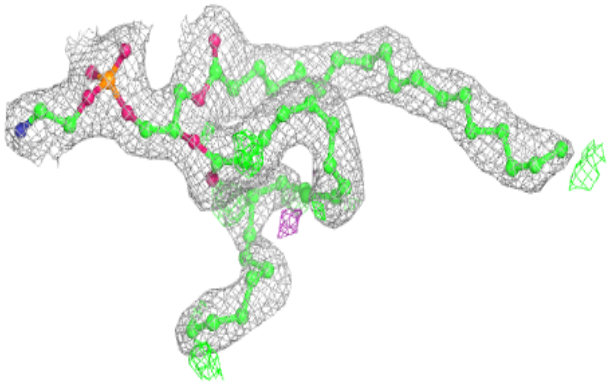
Electron density around CHD C 525:

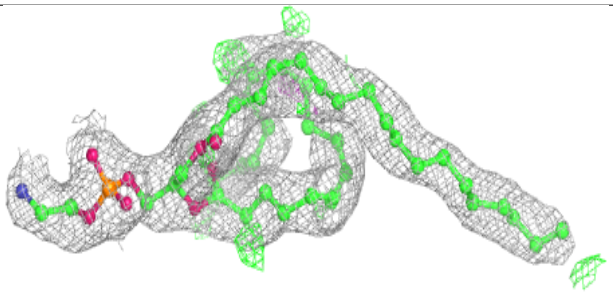
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEK G 264:

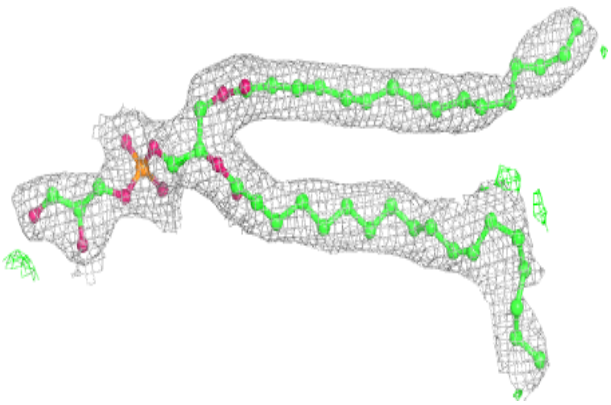
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

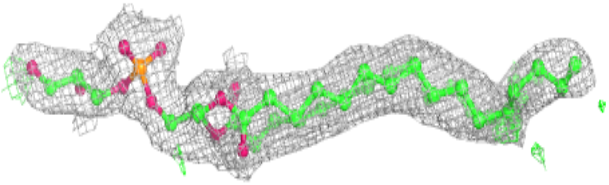


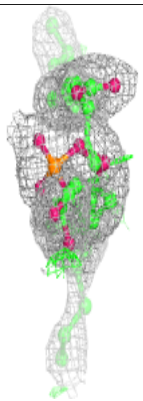


Electron density around PGV C 267:

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

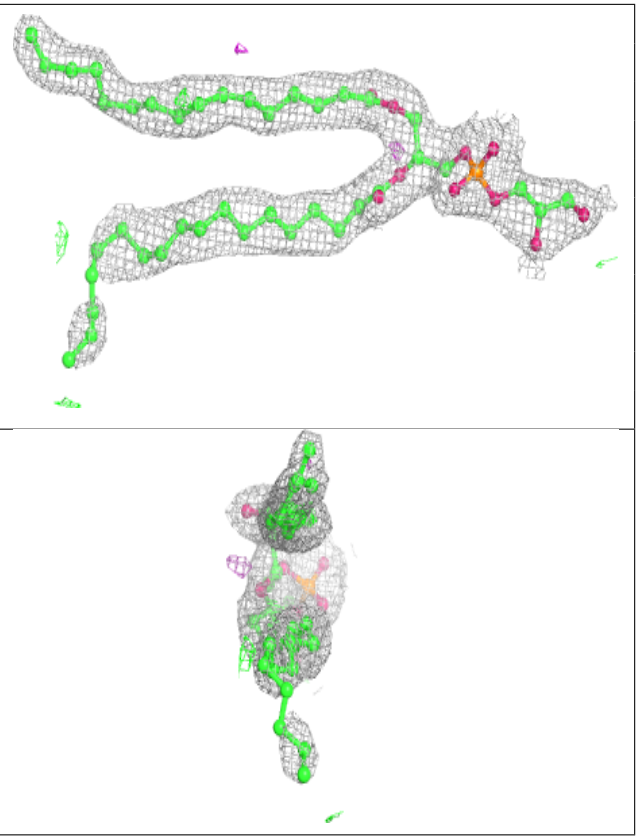






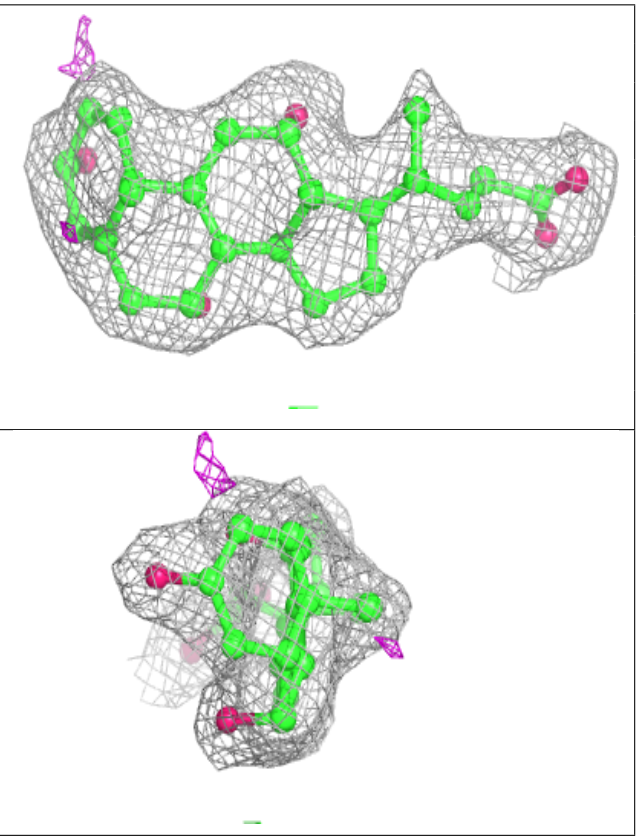
Electron density around PGV P 1267:

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



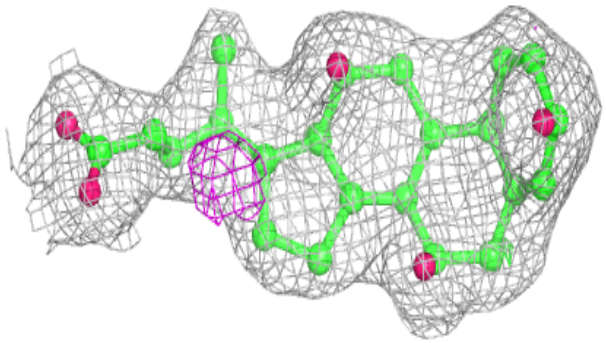
Electron density around CHD B 1086:

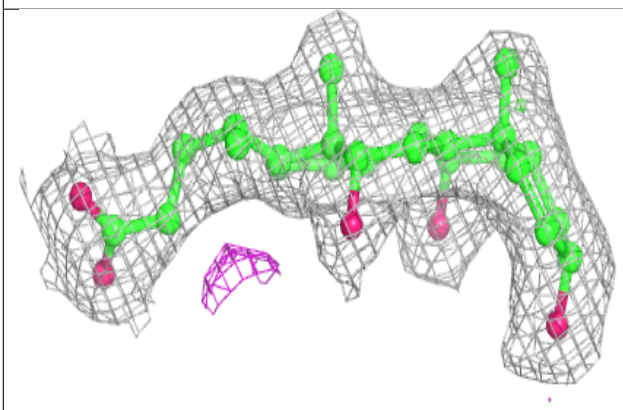
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

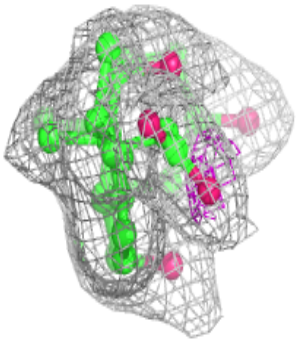


Electron density around CHD G 86:

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

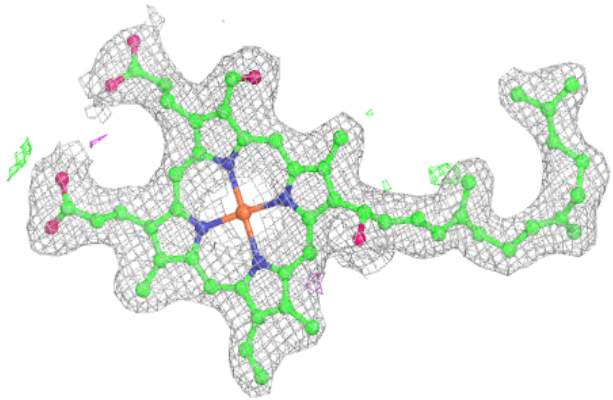


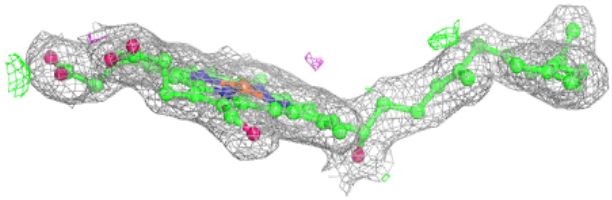


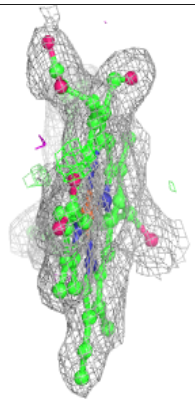


Electron density around HEA N 516:

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

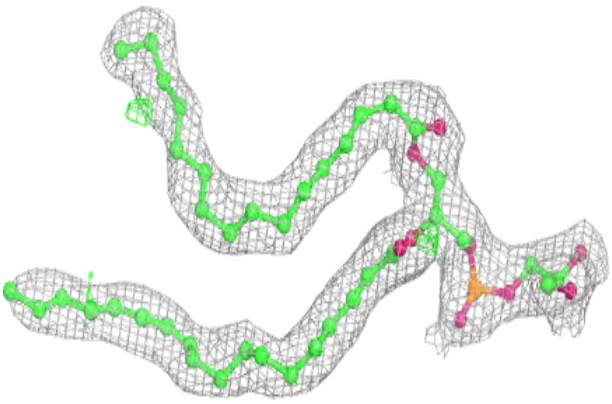


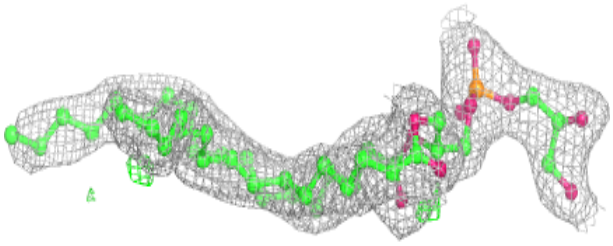


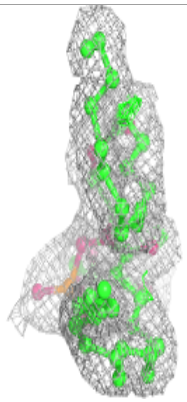


Electron density around PGV N 1266:

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

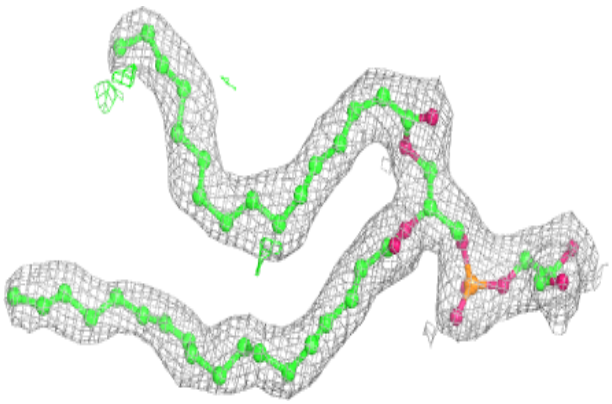


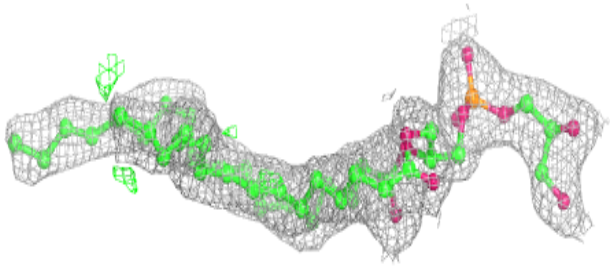


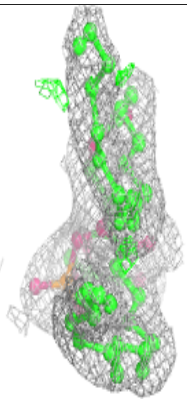


Electron density around PGV A 521:

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

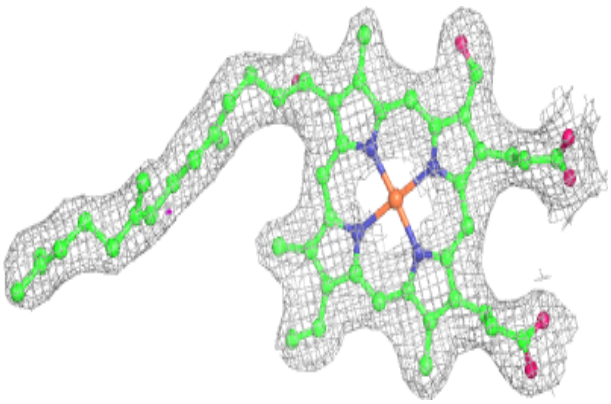


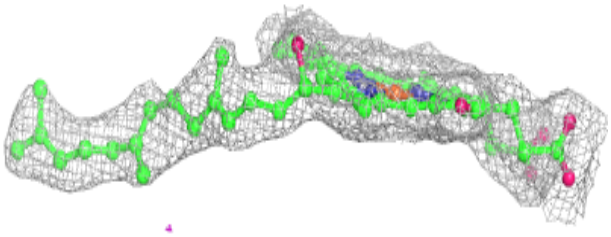


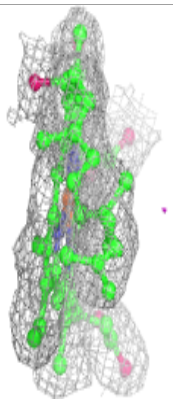


Electron density around HEA N 515:

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

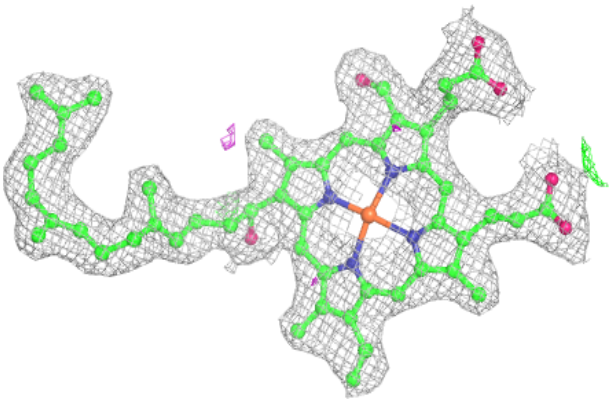


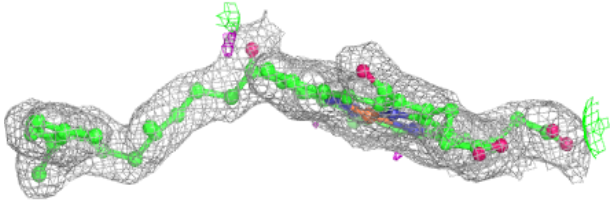


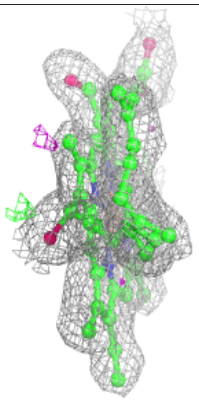


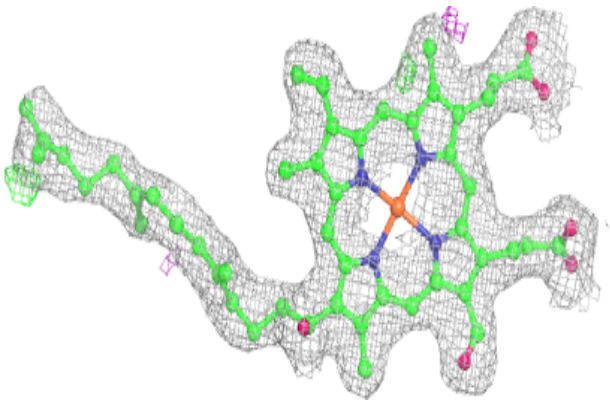
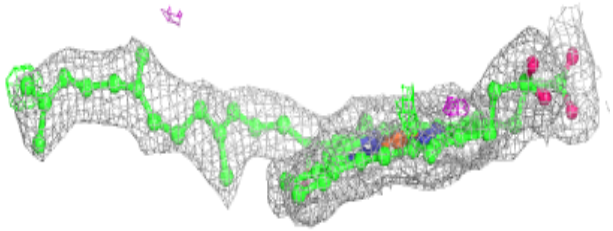
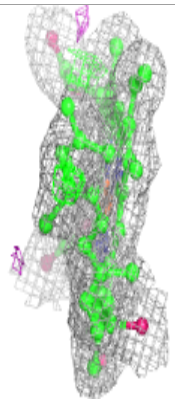
Electron density around HEA A 516:

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







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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.