Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 05:07 PM EDT

PDB ID	:	2DYR
Title	:	Bovine heart cytochrome C oxidase at the fully oxidized state
Authors	:	Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2006-09-16
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

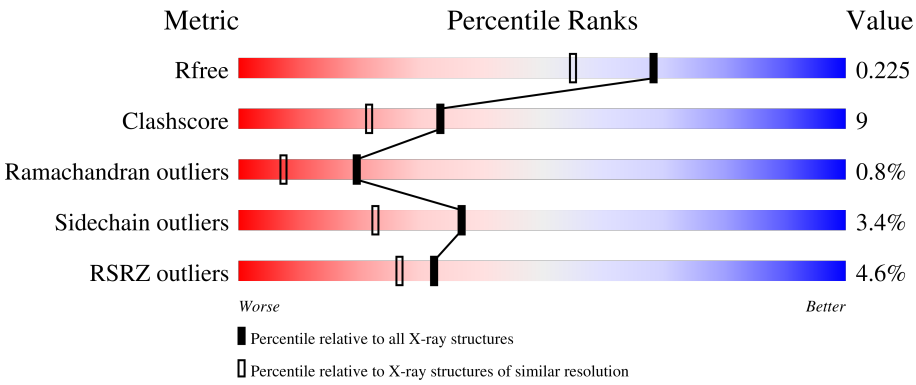
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	87% 13% •
1	N	514	84% 16% •
2	B	227	% 81% 17% •
2	O	227	4% 75% 22% •
3	C	261	90% 10% •

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Mol	Chain	Length	Quality of chain
3	P	261	%, 88%, 11%
4	D	147	2%, 88%, 10%
4	Q	147	12%, 82%, 16%
5	E	109	2%, 84%, 11%
5	R	109	11%, 73%, 21%
6	F	98	8%, 81%, 14%, 5%
6	S	98	8%, 83%, 13%
7	G	85	20%, 69%, 21%, 8%
7	T	85	20%, 74%, 16%, 8%
8	H	85	13%, 85%, 6%, 7%
8	U	85	12%, 73%, 19%, 7%
9	I	73	7%, 85%, 14%
9	V	73	10%, 81%, 19%
10	J	59	8%, 86%, 10%
10	W	59	14%, 92%, 5%
11	K	56	2%, 80%, 7%, 12%
11	X	56	9%, 80%, 5%, 12%
12	L	47	4%, 83%, 15%
12	Y	47	2%, 81%, 15%
13	M	46	9%, 74%, 17%, 7%
13	Z	46	11%, 67%, 24%, 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
20	TGL	L	522	-	-	X	-
22	CHD	C	271	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
23	DMU	C	272	X	-	-	-
23	DMU	M	526	X	-	-	-
23	DMU	P	1272	X	-	-	-
23	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-
9	SAC	V	1	-	X	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 32735 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 polypeptide Va.

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

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

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

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

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	79	662	417	121	119	5	0	0	0
8	U	79	662	417	121	119	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	73	601	390	107	100	4	0	0	0
9	V	73	601	390	107	100	4	0	0	0

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

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

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

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

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 polypeptide VIIc.

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 VIII-heart.

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

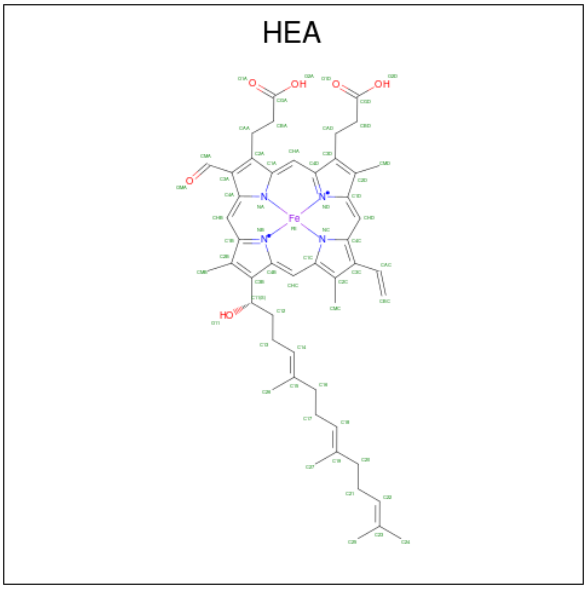
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

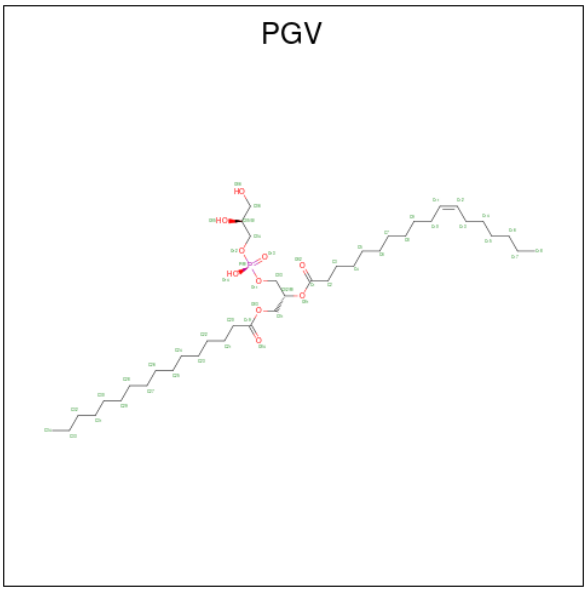
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
16	A	1	1	1	0	0
			Total	Na		
16	N	1	1	1	0	0

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



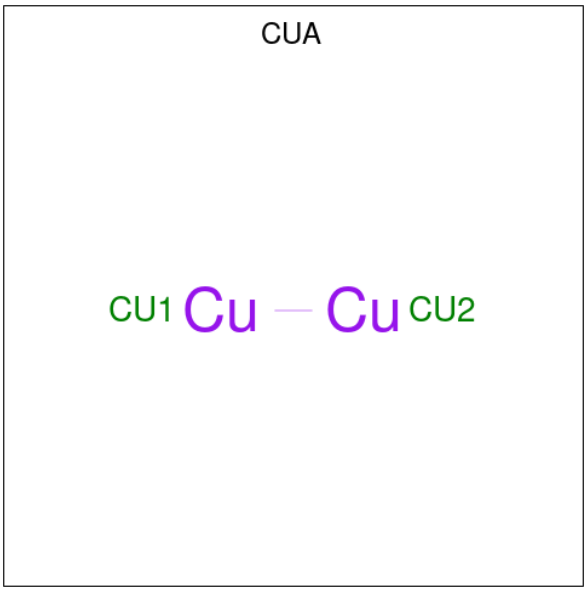
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
17	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	N	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	N	1	60	49	1	4	6	0	0

- Molecule 18 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



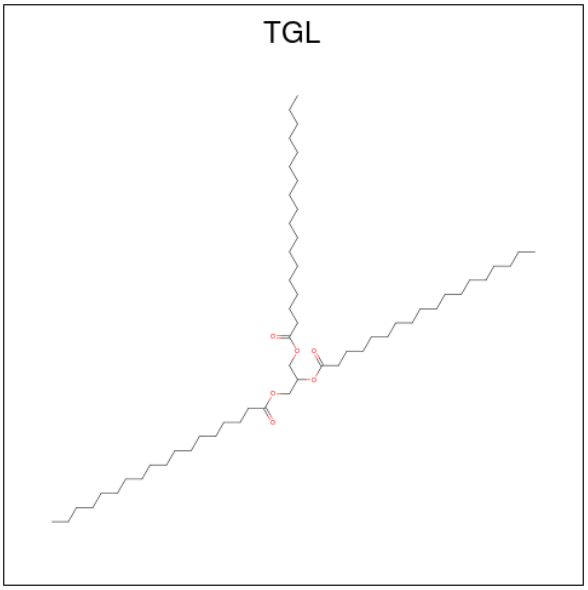
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	A	1	51	40	10	1	0	0
			Total	C	O	P		
18	A	1	51	40	10	1	0	0
			Total	C	O	P		
18	C	1	51	40	10	1	0	0
			Total	C	O	P		
18	C	1	51	40	10	1	0	0
			Total	C	O	P		
18	N	1	51	40	10	1	0	0
			Total	C	O	P		
18	P	1	51	40	10	1	0	0
			Total	C	O	P		
18	P	1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

- Molecule 19 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



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

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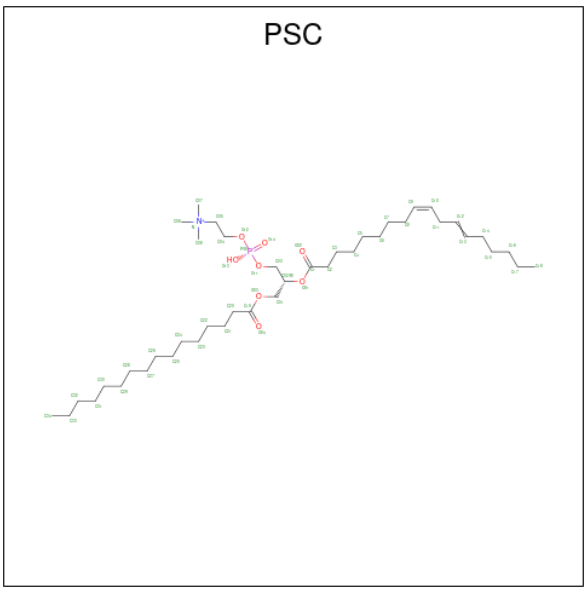
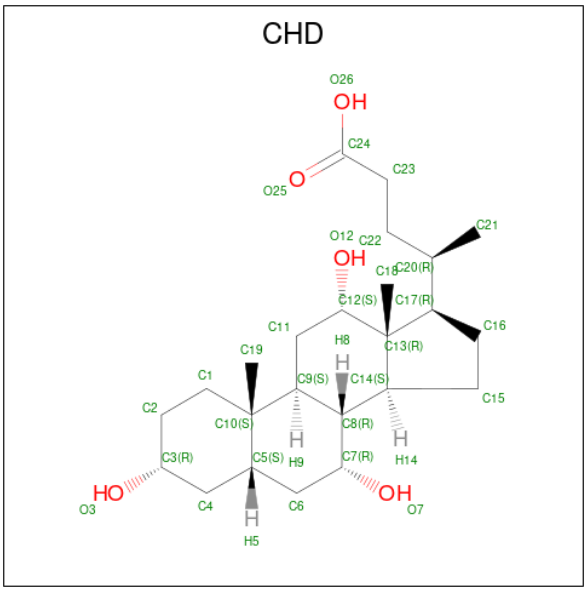
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	L	1	63	57	6	0	0
			Total	C	O		
20	N	1	63	57	6	0	0
			Total	C	O		
20	N	1	63	57	6	0	0
			Total	C	O		
20	Q	1	63	57	6	0	0

- Molecule 21 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: $C_{42}H_{81}NO_8P$).



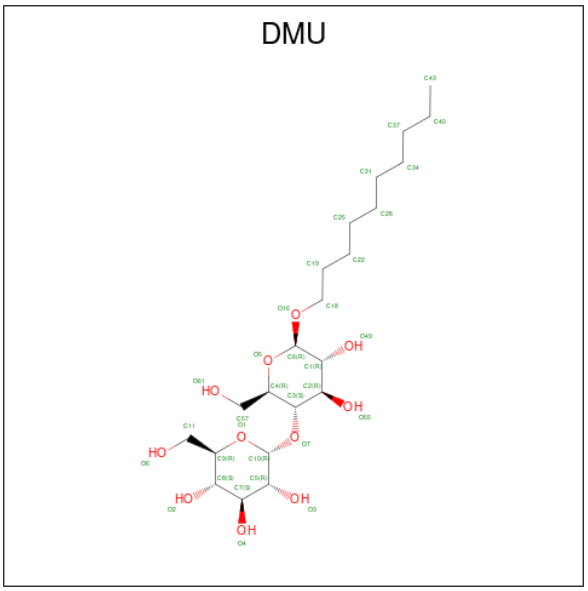
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
21	B	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
21	O	1	52	42	1	8	1	0	0

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

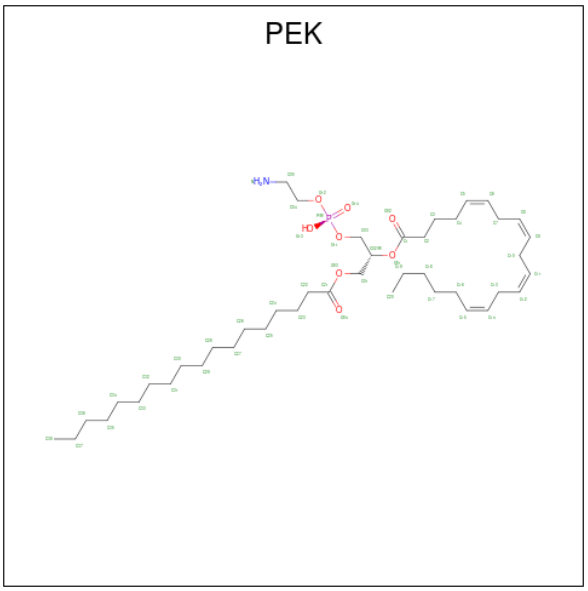


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
23	C	1	33	22	11	0	0
			Total	C	O		
23	M	1	33	22	11	0	0
			Total	C	O		
23	P	1	33	22	11	0	0
			Total	C	O		
23	Z	1	33	22	11	0	0

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

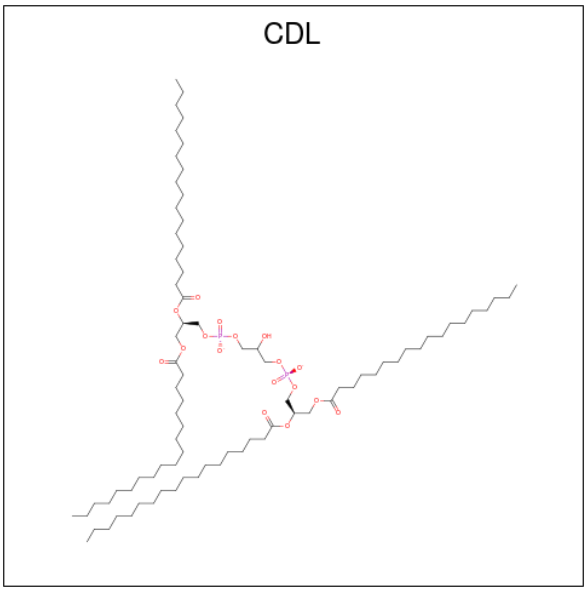
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
24	C	1	1	1	0	0
			Total	X		
24	P	1	1	1	0	0

- Molecule 25 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		
25	C	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	C	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	G	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	P	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	P	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	T	1	53	43	1	8	1	0	0

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	243	Total	O	0	0
			243	243		
28	B	186	Total	O	0	0
			186	186		
28	C	127	Total	O	0	0
			127	127		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
28	D	109	109	109	0	0
			Total	O		
28	E	67	67	67	0	0
			Total	O		
28	F	85	85	85	0	0
			Total	O		
28	G	57	57	57	0	0
			Total	O		
28	H	66	66	66	0	0
			Total	O		
28	I	58	58	58	0	0
			Total	O		
28	J	21	21	21	0	0
			Total	O		
28	K	38	38	38	0	0
			Total	O		
28	L	22	22	22	0	0
			Total	O		
28	M	27	27	27	0	0
			Total	O		
28	N	212	212	212	0	0
			Total	O		
28	O	152	152	152	0	0
			Total	O		
28	P	120	120	120	0	0
			Total	O		
28	Q	75	75	75	0	0
			Total	O		
28	R	32	32	32	0	0
			Total	O		
28	S	53	53	53	0	0
			Total	O		
28	T	59	59	59	0	0
			Total	O		
28	U	62	62	62	0	0
			Total	O		
28	V	33	33	33	0	0
			Total	O		
28	W	18	18	18	0	0
			Total	O		
28	X	29	29	29	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
28	Y	31	31	31	0	0
			Total	O		
28	Z	21	21	21	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

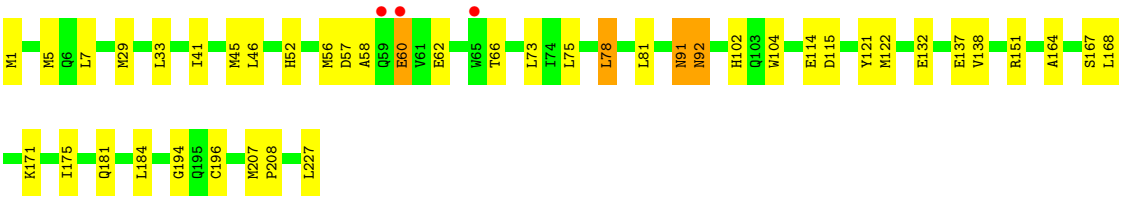
Chain A:

• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:

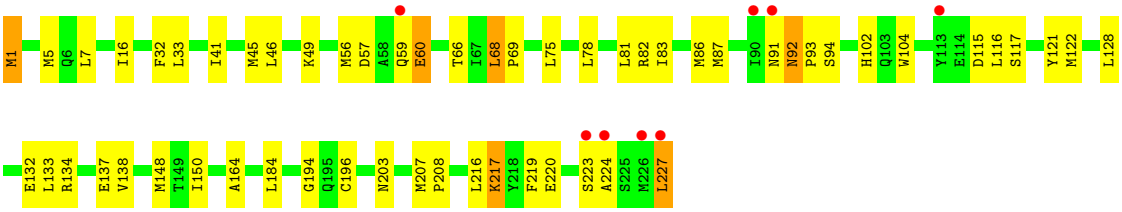
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:

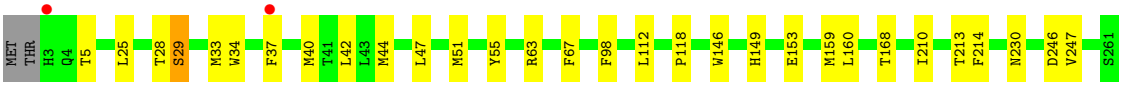


- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:

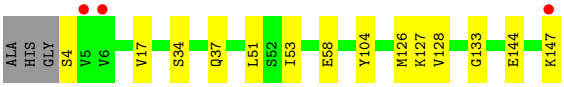
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



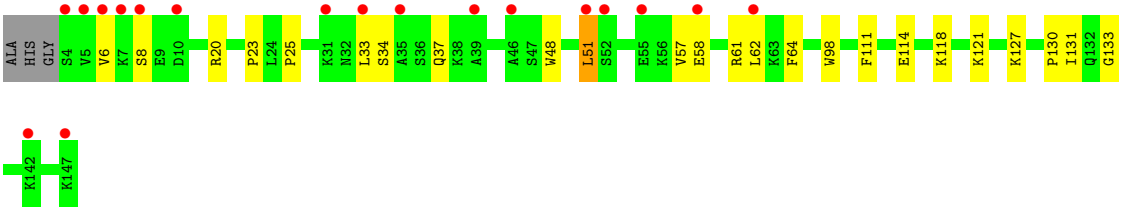
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



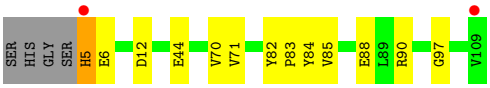
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



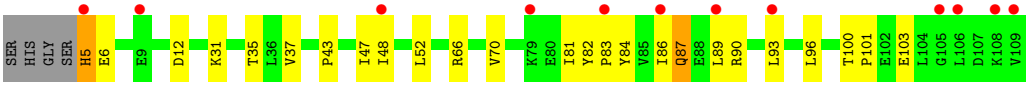
- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:



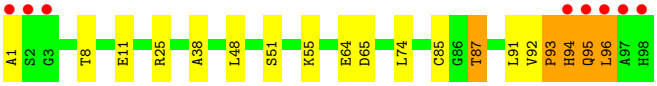
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:



• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:

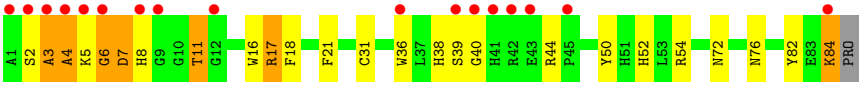


• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:

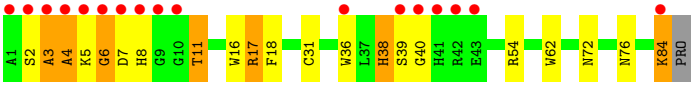
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:



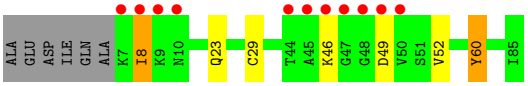
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:



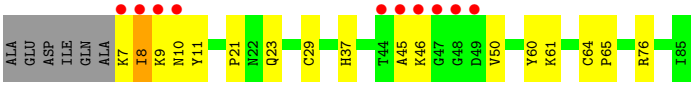
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:



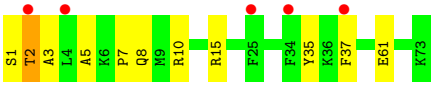
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:



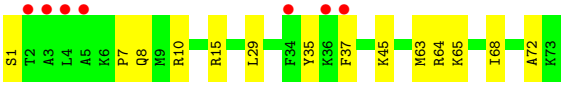
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



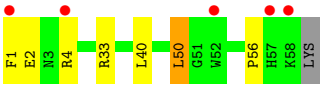
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



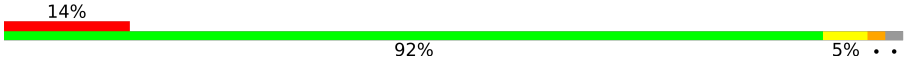
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

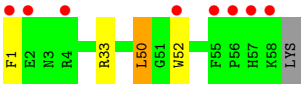
Chain J:



• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

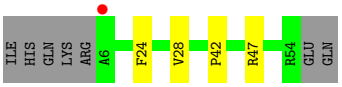
Chain W:





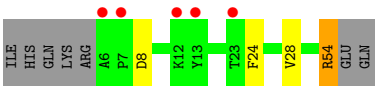
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



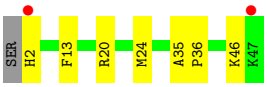
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:



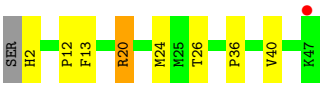
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:



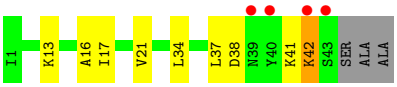
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



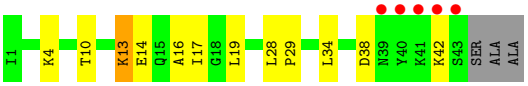
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

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	182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 68.19 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 98.9 (68.19-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.202 , 0.227 0.203 , 0.225	Depositor DCC
R_{free} test set	22992 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32735	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: CUA, TGL, HEA, ZN, PSC, NA, CHD, FME, MG, CU, SAC, PEK, PGV, TPO, UNX, DMU, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.49	0/4156	0.67	0/5678
1	N	0.48	0/4156	0.65	0/5678
2	B	0.48	0/1860	0.76	0/2534
2	O	0.50	0/1860	0.79	1/2534 (0.0%)
3	C	0.51	0/2197	0.58	0/3005
3	P	0.48	0/2197	0.61	0/3005
4	D	0.47	0/1229	0.66	1/1658 (0.1%)
4	Q	0.50	0/1229	0.65	1/1658 (0.1%)
5	E	0.50	0/871	0.66	0/1182
5	R	0.48	0/871	0.68	0/1182
6	F	0.47	0/765	0.83	3/1038 (0.3%)
6	S	0.47	0/765	0.87	3/1038 (0.3%)
7	G	0.51	0/690	0.70	1/937 (0.1%)
7	T	0.53	0/690	0.70	1/937 (0.1%)
8	H	0.47	0/682	0.68	0/921
8	U	0.48	0/682	0.67	0/921
9	I	0.52	0/605	0.59	0/802
9	V	0.51	0/605	0.62	0/802
10	J	0.45	0/471	0.60	0/636
10	W	0.46	0/471	0.63	0/636
11	K	0.48	0/398	0.66	0/546
11	X	0.47	0/398	0.65	0/546
12	L	0.48	0/393	0.55	0/526
12	Y	0.53	0/393	0.57	0/526
13	M	0.46	0/345	0.62	0/470
13	Z	0.45	0/345	0.62	0/470
All	All	0.49	0/29324	0.67	11/39866 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
8	U	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	94	HIS	N-CA-C	7.74	131.91	111.00
6	F	94	HIS	N-CA-C	7.14	130.29	111.00
4	D	133	GLY	N-CA-C	5.67	127.28	113.10
2	O	227	LEU	CA-CB-CG	5.64	128.28	115.30
4	Q	133	GLY	N-CA-C	5.61	127.12	113.10
6	F	93	PRO	N-CA-C	5.47	126.31	112.10
6	S	54	ASN	CB-CA-C	-5.35	99.69	110.40
7	G	6	GLY	N-CA-C	5.29	126.33	113.10
7	T	6	GLY	N-CA-C	5.26	126.25	113.10
6	F	95	GLN	N-CA-C	5.07	124.70	111.00
6	S	93	PRO	N-CA-C	5.01	125.12	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
8	U	11	TYR	Sidechain

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	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4027	0	4001	74	0
2	B	1824	0	1833	28	0
2	O	1824	0	1833	39	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	29	0
4	D	1195	0	1183	10	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	6	0
5	R	852	0	845	15	0
6	F	748	0	728	12	0
6	S	748	0	728	15	0
7	G	675	0	644	26	0
7	T	675	0	644	28	0
8	H	662	0	623	4	0
8	U	662	0	623	9	0
9	I	601	0	613	6	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	4	0
11	K	384	0	366	3	0
11	X	384	0	366	6	0
12	L	380	0	380	14	0
12	Y	380	0	380	9	0
13	M	335	0	352	6	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	3	0
17	N	120	0	108	4	0
18	A	102	0	152	7	0
18	C	102	0	152	7	0
18	N	51	0	76	2	0
18	P	102	0	152	8	0
18	Z	51	0	76	4	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	B	63	0	110	10	0
20	D	63	0	110	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	L	63	0	110	23	0
20	N	126	0	220	30	0
20	Q	63	0	110	6	0
21	B	52	0	80	13	0
21	O	52	0	80	12	0
22	B	29	0	39	0	0
22	C	58	0	78	2	0
22	J	29	0	39	2	0
22	O	29	0	39	1	0
22	P	58	0	78	2	0
22	W	29	0	39	2	0
23	C	33	0	36	2	0
23	M	33	0	36	0	0
23	P	33	0	36	7	0
23	Z	33	0	36	1	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	11	0
25	G	53	0	77	7	0
25	P	106	0	154	12	0
25	T	53	0	77	8	0
26	C	100	0	156	16	0
26	G	100	0	156	21	0
26	P	100	0	156	13	0
26	T	100	0	156	21	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	243	0	0	4	0
28	B	186	0	0	4	0
28	C	127	0	0	2	0
28	D	109	0	0	4	0
28	E	67	0	0	0	0
28	F	85	0	0	1	0
28	G	57	0	0	2	0
28	H	66	0	0	1	0
28	I	58	0	0	3	0
28	J	21	0	0	1	0
28	K	38	0	0	0	0
28	L	22	0	0	2	0
28	M	27	0	0	2	0
28	N	212	0	0	3	0
28	O	152	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	P	120	0	0	3	0
28	Q	75	0	0	3	0
28	R	32	0	0	0	0
28	S	53	0	0	1	0
28	T	59	0	0	2	0
28	U	62	0	0	3	0
28	V	33	0	0	2	0
28	W	18	0	0	0	0
28	X	29	0	0	1	0
28	Y	31	0	0	2	0
28	Z	21	0	0	2	0
All	All	32735	0	31294	534	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 (534) 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)
7:G:84:LYS:H	7:G:84:LYS:HD2	1.17	1.05
7:T:84:LYS:HD2	7:T:84:LYS:H	1.19	1.02
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.24	1.01
21:O:1230:PSC:H142	21:O:1230:PSC:H343	1.42	1.01
21:B:230:PSC:H343	21:B:230:PSC:H142	1.42	1.01
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.21	0.98
7:T:72:ASN:H	7:T:76:ASN:HD22	1.16	0.94
4:D:34:SER:H	4:D:37:GLN:HE21	1.14	0.93
26:P:1270:CDL:H191	26:P:1270:CDL:H642	1.51	0.92
26:C:270:CDL:H191	26:C:270:CDL:H642	1.51	0.91
7:G:72:ASN:H	7:G:76:ASN:HD22	1.19	0.90
10:W:33:ARG:HG2	22:W:1060:CHD:H152	1.53	0.90
26:G:269:CDL:H541	26:G:269:CDL:H231	1.53	0.90
2:O:224:ALA:O	2:O:227:LEU:HG	1.72	0.89
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.53	0.89
20:B:521:TGL:H281	20:B:521:TGL:H102	1.55	0.88
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.56	0.88
20:N:1521:TGL:H281	20:N:1521:TGL:H102	1.54	0.88
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.55	0.88
6:F:85:CYS:SG	6:F:87:THR:HG23	2.14	0.87
25:C:264:PEK:H161	25:C:264:PEK:H102	1.57	0.86
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.16	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:472:ILE:HG21	20:N:1522:TGL:HA92	1.58	0.85
7:G:5:LYS:HB3	1:N:278:MET:SD	2.16	0.85
1:A:472:ILE:HG21	20:L:522:TGL:HA92	1.59	0.84
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.59	0.84
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.58	0.83
2:O:41:ILE:HD13	21:O:1230:PSC:H342	1.60	0.83
6:S:53:THR:HA	6:S:94:HIS:CE1	2.14	0.83
12:L:20:ARG:HH22	20:L:522:TGL:HC61	1.45	0.82
28:C:4863:HOH:O	6:F:1:ALA:HB2	1.79	0.81
7:G:31:CYS:SG	26:G:269:CDL:H532	2.21	0.80
12:L:24:MET:SD	20:L:522:TGL:H162	2.21	0.80
20:L:522:TGL:HC62	20:L:522:TGL:HC22	1.64	0.80
21:O:1230:PSC:H071	9:V:10:ARG:HE	1.47	0.80
1:A:278:MET:SD	7:T:5:LYS:HB3	2.22	0.79
20:N:1521:TGL:H102	20:N:1521:TGL:C28	2.12	0.79
7:T:84:LYS:H	7:T:84:LYS:CD	1.95	0.79
26:G:269:CDL:H622	18:P:1268:PGV:H152	1.64	0.78
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.66	0.77
20:B:521:TGL:H102	20:B:521:TGL:C28	2.15	0.77
4:D:34:SER:H	4:D:37:GLN:NE2	1.84	0.76
20:N:1522:TGL:HC62	20:N:1522:TGL:HC22	1.66	0.76
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.68	0.76
1:N:321:PHE:CD2	21:O:1230:PSC:H341	2.20	0.75
20:B:521:TGL:H241	20:B:521:TGL:H201	1.69	0.74
3:P:246:ASP:HB2	28:P:4502:HOH:O	1.87	0.74
25:C:264:PEK:HN2	7:G:76:ASN:HD21	1.37	0.73
20:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.69	0.73
12:L:13:PHE:HA	20:L:522:TGL:HC31	1.70	0.73
20:N:1521:TGL:H241	20:N:1521:TGL:H201	1.68	0.73
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.70	0.73
26:G:269:CDL:H522	26:G:269:CDL:H202	1.70	0.72
3:P:34:TRP:CZ2	23:P:1272:DMU:H29	2.25	0.72
20:N:1522:TGL:H242	20:N:1522:TGL:H202	1.72	0.71
12:L:20:ARG:HH12	20:L:522:TGL:HC61	1.55	0.71
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.72	0.70
20:L:522:TGL:H242	20:L:522:TGL:H202	1.72	0.70
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.73	0.70
1:N:334:TRP:CZ3	20:Q:1523:TGL:HA51	2.27	0.70
2:B:41:ILE:HD13	21:B:230:PSC:H342	1.74	0.70
18:C:268:PGV:H152	26:T:1269:CDL:H622	1.74	0.69
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PHE:CD2	21:B:230:PSC:H341	2.27	0.69
25:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.39	0.69
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.75	0.69
18:Z:1524:PGV:H152	18:Z:1524:PGV:H321	1.74	0.69
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.75	0.68
1:N:449:MET:SD	2:O:5:MET:HG2	2.33	0.68
21:B:230:PSC:C07	9:I:10:ARG:HH21	2.06	0.67
10:J:33:ARG:HG2	22:J:60:CHD:H152	1.77	0.67
4:Q:114:GLU:HG2	28:Q:4443:HOH:O	1.95	0.67
1:N:1:FME:HCN	1:N:4:ASN:H	1.60	0.67
7:G:72:ASN:H	7:G:76:ASN:ND2	1.93	0.67
18:A:524:PGV:H152	18:A:524:PGV:H321	1.77	0.67
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.76	0.66
18:P:1267:PGV:H161	18:P:1267:PGV:H12	1.76	0.66
6:S:52:ILE:O	6:S:94:HIS:NE2	2.29	0.66
6:S:85:CYS:SG	6:S:87:THR:HG23	2.35	0.66
5:R:89:LEU:O	5:R:93:LEU:HG	1.95	0.66
21:O:1230:PSC:C07	9:V:10:ARG:HE	2.08	0.66
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.26	0.66
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.78	0.66
12:L:20:ARG:NH2	20:L:522:TGL:HC61	2.11	0.65
4:Q:58:GLU:O	4:Q:62:LEU:HG	1.96	0.65
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.77	0.65
13:Z:19:LEU:HD23	18:Z:1524:PGV:H322	1.78	0.65
1:A:334:TRP:CZ3	20:D:523:TGL:HA51	2.31	0.65
26:C:270:CDL:H642	26:C:270:CDL:C19	2.25	0.65
1:A:472:ILE:HG21	20:L:522:TGL:CA9	2.26	0.64
18:C:267:PGV:H12	18:C:267:PGV:H161	1.77	0.64
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.62	0.64
26:G:269:CDL:H541	26:G:269:CDL:C23	2.26	0.64
26:P:1270:CDL:H112	28:P:5001:HOH:O	1.97	0.64
7:G:84:LYS:HD2	7:G:84:LYS:N	2.01	0.64
7:G:84:LYS:H	7:G:84:LYS:CD	2.00	0.64
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.80	0.64
3:C:34:TRP:CZ2	23:C:272:DMU:H29	2.33	0.64
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.62	0.63
18:C:267:PGV:H182	26:C:270:CDL:H673	1.79	0.63
1:N:472:ILE:HG21	20:N:1522:TGL:CA9	2.26	0.63
1:N:472:ILE:HD13	20:N:1522:TGL:HA91	1.80	0.62
2:O:217:LYS:HA	2:O:217:LYS:HE2	1.80	0.62
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:1268:PGV:H062	28:U:4465:HOH:O	1.99	0.62
26:G:269:CDL:H511	26:G:269:CDL:H172	1.80	0.62
6:S:52:ILE:O	6:S:94:HIS:CE1	2.52	0.62
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.82	0.62
2:B:92:ASN:HB3	28:B:5097:HOH:O	1.99	0.61
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.65	0.61
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.35	0.61
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.81	0.61
21:B:230:PSC:H072	9:I:10:ARG:HH21	1.65	0.61
3:P:210:ILE:HG23	18:P:1267:PGV:H102	1.82	0.61
20:B:521:TGL:HC22	28:I:2381:HOH:O	2.00	0.61
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.28	0.60
26:G:269:CDL:H231	26:G:269:CDL:C54	2.30	0.60
1:A:17:THR:OG1	20:L:522:TGL:H281	2.01	0.60
18:C:267:PGV:H172	26:C:270:CDL:H662	1.82	0.60
20:N:1521:TGL:H161	2:O:7:LEU:HD11	1.84	0.60
20:N:1521:TGL:HC92	28:O:4466:HOH:O	2.02	0.60
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.83	0.60
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.67	0.60
9:V:65:LYS:O	11:X:54:ARG:NH1	2.34	0.60
1:A:282:PHE:HA	7:T:4:ALA:CB	2.32	0.59
1:N:113:LEU:CD1	20:N:1522:TGL:H292	2.32	0.59
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.02	0.59
7:T:17:ARG:HD2	28:T:3307:HOH:O	2.02	0.59
3:P:34:TRP:HZ2	23:P:1272:DMU:H29	1.67	0.59
12:L:20:ARG:NH1	20:L:522:TGL:HC61	2.18	0.59
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.02	0.59
6:F:92:VAL:HG23	6:F:92:VAL:O	2.03	0.58
21:B:230:PSC:H222	21:B:230:PSC:H21	1.85	0.58
6:F:25:ARG:HD2	28:F:4173:HOH:O	2.03	0.58
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.32	0.58
1:A:430:PHE:HE1	20:B:521:TGL:HB21	1.69	0.58
20:N:1522:TGL:H162	12:Y:24:MET:SD	2.43	0.58
20:B:521:TGL:H222	20:B:521:TGL:HA82	1.86	0.58
3:C:210:ILE:HG23	18:C:267:PGV:H102	1.86	0.58
12:L:20:ARG:HH22	20:L:522:TGL:CC6	2.16	0.58
8:U:50:VAL:HG21	28:U:5105:HOH:O	2.04	0.58
18:A:525:PGV:H182	3:C:28:THR:HG22	1.84	0.57
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.68	0.57
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.87	0.57
6:S:53:THR:HA	6:S:94:HIS:HE1	1.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41:ILE:CD1	21:O:1230:PSC:H342	2.34	0.57
21:O:1230:PSC:H21	21:O:1230:PSC:H222	1.85	0.57
25:C:265:PEK:C38	26:G:269:CDL:H273	2.35	0.57
7:G:17:ARG:HD2	28:G:2307:HOH:O	2.04	0.57
1:N:112:LEU:HG	28:N:3073:HOH:O	2.04	0.57
1:A:1:FME:HE2	1:A:1:FME:HA	1.85	0.56
20:Q:1523:TGL:HC21	20:Q:1523:TGL:HG11	1.85	0.56
1:A:321:PHE:CZ	21:B:230:PSC:H171	2.40	0.56
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.86	0.56
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.88	0.56
6:S:76:LYS:HE3	6:S:93:PRO:HG3	1.87	0.56
12:Y:20:ARG:NH1	28:Y:4492:HOH:O	2.39	0.56
9:I:5:ALA:O	9:I:7:PRO:HD3	2.04	0.56
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.69	0.56
1:N:321:PHE:CZ	21:O:1230:PSC:H171	2.41	0.56
20:N:1521:TGL:H222	20:N:1521:TGL:HA82	1.87	0.56
1:A:1:FME:HCN	1:A:4:ASN:H	1.70	0.56
26:C:270:CDL:H431	28:J:5157:HOH:O	2.05	0.56
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.87	0.56
6:F:93:PRO:HB2	6:F:94:HIS:ND1	2.21	0.56
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.88	0.55
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.89	0.55
1:A:113:LEU:CD1	20:L:522:TGL:H292	2.37	0.55
7:T:84:LYS:HD2	7:T:84:LYS:N	2.05	0.55
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.05	0.55
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.72	0.55
7:T:72:ASN:N	7:T:76:ASN:HD22	1.97	0.55
18:A:524:PGV:H062	28:M:2158:HOH:O	2.05	0.55
18:A:524:PGV:H311	13:M:16:ALA:HA	1.88	0.55
26:G:269:CDL:H212	1:N:311:ILE:HD12	1.89	0.55
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.88	0.55
2:O:57:ASP:H	21:O:1230:PSC:H201	1.72	0.55
1:N:87:ILE:O	1:N:173:PRO:HD3	2.07	0.54
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.37	0.54
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.54
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.90	0.54
20:D:523:TGL:HC21	20:D:523:TGL:HG11	1.90	0.54
20:L:522:TGL:HC21	20:L:522:TGL:OA1	2.06	0.54
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.42	0.54
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.41	0.54
21:B:230:PSC:H12	21:B:230:PSC:H322	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:265:PEK:H383	26:G:269:CDL:H273	1.88	0.54
1:N:430:PHE:HE1	20:N:1521:TGL:HB21	1.73	0.54
3:C:34:TRP:HZ2	23:C:272:DMU:H29	1.71	0.54
4:D:58:GLU:HG3	28:D:4047:HOH:O	2.07	0.54
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.43	0.54
2:B:56:MET:HG2	21:B:230:PSC:H211	1.88	0.54
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.42	0.54
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.43	0.54
13:Z:16:ALA:HA	18:Z:1524:PGV:H311	1.90	0.54
17:A:515:HEA:HBC1	17:A:515:HEA:HMC1	1.89	0.54
2:O:59:GLN:O	2:O:59:GLN:HG3	2.08	0.54
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.90	0.54
18:N:1266:PGV:H182	3:P:28:THR:HG22	1.90	0.54
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.37	0.54
18:P:1267:PGV:H182	26:P:1270:CDL:H673	1.88	0.54
20:N:1522:TGL:HC21	20:N:1522:TGL:OA1	2.09	0.53
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.91	0.53
9:V:15:ARG:HD2	28:V:4894:HOH:O	2.08	0.53
1:A:407:ASP:O	1:A:411:LYS:HG3	2.09	0.53
3:C:213:THR:HG23	26:C:270:CDL:H762	1.90	0.53
5:E:84:TYR:O	5:E:88:GLU:HG2	2.09	0.53
1:A:406:ASN:HD21	18:A:524:PGV:C2	2.21	0.53
18:P:1267:PGV:H172	26:P:1270:CDL:H662	1.91	0.53
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.23	0.53
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.91	0.53
26:G:269:CDL:H322	26:G:269:CDL:HA62	1.90	0.52
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.91	0.52
6:S:51:SER:O	6:S:94:HIS:N	2.42	0.52
28:A:4756:HOH:O	8:H:23:GLN:HG3	2.08	0.52
25:C:264:PEK:H102	25:C:264:PEK:C16	2.36	0.52
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.44	0.52
21:O:1230:PSC:H322	21:O:1230:PSC:H12	1.91	0.52
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.90	0.52
7:G:3:ALA:O	7:G:4:ALA:HB2	2.10	0.52
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.75	0.52
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.74	0.52
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.57	0.52
1:N:28:MET:HE2	17:N:515:HEA:H271	1.92	0.52
20:N:1521:TGL:HC22	28:Q:3381:HOH:O	2.09	0.52
1:A:472:ILE:HD13	20:L:522:TGL:HA91	1.92	0.51
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:40:LEU:HD12	22:J:60:CHD:H183	1.90	0.51
1:N:488:THR:HB	1:N:495:LEU:HD13	1.92	0.51
20:N:1522:TGL:H202	20:N:1522:TGL:C24	2.40	0.51
6:F:64:GLU:O	6:F:65:ASP:HB2	2.11	0.51
20:N:1521:TGL:HB91	2:O:32:PHE:HE2	1.75	0.51
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.92	0.51
1:N:347:LEU:HD13	1:N:383:MET:SD	2.49	0.51
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.10	0.51
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.10	0.51
8:H:49:ASP:O	8:H:52:VAL:HG22	2.11	0.51
10:W:1:PHE:HD1	10:W:1:PHE:H1	1.55	0.51
1:A:136:LEU:HB2	28:A:4733:HOH:O	2.11	0.51
7:G:2:SER:O	25:G:1263:PEK:H322	2.10	0.51
7:T:72:ASN:H	7:T:76:ASN:ND2	1.98	0.51
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.93	0.50
1:N:400:PHE:HB3	20:N:1522:TGL:H283	1.93	0.50
1:N:407:ASP:O	1:N:411:LYS:HG3	2.12	0.50
6:S:52:ILE:O	6:S:94:HIS:CD2	2.64	0.50
12:L:24:MET:HG3	28:L:5077:HOH:O	2.11	0.50
1:A:87:ILE:O	1:A:173:PRO:HD3	2.11	0.50
3:C:51:MET:SD	26:C:270:CDL:C62	3.00	0.50
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.92	0.50
12:Y:2:HIS:N	28:Y:5165:HOH:O	2.45	0.50
28:B:4821:HOH:O	25:P:1265:PEK:H031	2.11	0.50
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.42	0.50
1:N:52:GLN:O	1:N:56:VAL:HG23	2.12	0.50
4:D:127:LYS:HD2	28:I:2389:HOH:O	2.11	0.49
1:A:488:THR:HB	1:A:495:LEU:HD13	1.94	0.49
7:G:2:SER:OG	25:G:1263:PEK:H301	2.12	0.49
20:L:522:TGL:H202	20:L:522:TGL:C24	2.39	0.49
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.49
11:K:24:PHE:O	11:K:28:VAL:HG12	2.12	0.49
7:T:3:ALA:O	7:T:4:ALA:HB2	2.12	0.49
1:A:1:FME:HA	1:A:1:FME:CE	2.42	0.49
5:R:48:ILE:O	5:R:52:LEU:HG	2.12	0.49
10:J:1:PHE:H1	10:J:1:PHE:HD1	1.60	0.49
13:M:42:LYS:HA	13:M:42:LYS:CE	2.42	0.49
1:A:449:MET:SD	2:B:5:MET:HG2	2.53	0.49
3:P:34:TRP:CE2	23:P:1272:DMU:H29	2.46	0.49
1:A:379:TYR:O	1:A:383:MET:HB2	2.12	0.49
18:P:1268:PGV:H101	28:P:4808:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:365:ILE:HD11	28:N:4705:HOH:O	2.12	0.49
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.93	0.49
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.78	0.48
4:D:17:VAL:HG12	28:D:4051:HOH:O	2.13	0.48
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.01	0.48
1:N:484:THR:HB	28:Z:5071:HOH:O	2.13	0.48
2:B:58:ALA:O	2:B:62:GLU:HG3	2.13	0.48
3:C:51:MET:SD	26:C:270:CDL:H622	2.53	0.48
1:N:17:THR:OG1	20:N:1522:TGL:H281	2.13	0.48
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
5:R:81:ILE:HG12	9:V:7:PRO:HG2	1.94	0.48
11:K:42:PRO:HG2	11:K:47:ARG:NE	2.29	0.48
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.94	0.48
6:F:51:SER:O	6:F:94:HIS:N	2.46	0.48
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.49	0.48
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.44	0.48
2:O:1:FME:SD	2:O:133:LEU:CD1	3.02	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
25:C:265:PEK:H383	26:G:269:CDL:C27	2.44	0.48
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.95	0.48
1:N:379:TYR:O	1:N:383:MET:HB2	2.14	0.47
6:S:52:ILE:C	6:S:94:HIS:CE1	2.88	0.47
20:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.95	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.12	0.47
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.96	0.47
2:O:220:GLU:O	2:O:223:SER:HB2	2.14	0.47
2:B:114:GLU:HB3	28:B:4063:HOH:O	2.13	0.47
3:P:34:TRP:NE1	23:P:1272:DMU:H29	2.30	0.47
3:P:213:THR:HG23	26:P:1270:CDL:H762	1.96	0.47
6:S:92:VAL:O	6:S:92:VAL:HG23	2.14	0.47
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.63	0.47
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.47
1:A:383:MET:O	1:A:387:PHE:HB2	2.15	0.47
4:D:34:SER:N	4:D:37:GLN:HE21	1.96	0.47
7:G:5:LYS:CD	1:N:278:MET:HB3	2.44	0.47
2:O:56:MET:HG2	21:O:1230:PSC:H211	1.97	0.47
18:Z:1524:PGV:H062	28:Z:3158:HOH:O	2.15	0.47
1:A:222:PRO:HD2	28:B:4914:HOH:O	2.15	0.47
1:A:52:GLN:O	1:A:56:VAL:HG23	2.15	0.47
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.97	0.47
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:HD21	18:A:524:PGV:H21	1.80	0.46
10:W:50:LEU:O	10:W:50:LEU:HD22	2.16	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.97	0.46
25:C:264:PEK:H32	25:C:264:PEK:H71	1.98	0.46
1:A:365:ILE:HD11	28:H:4750:HOH:O	2.16	0.46
22:P:1271:CHD:H112	22:P:1271:CHD:H12A	1.68	0.46
1:A:311:ILE:HD12	26:T:1269:CDL:H212	1.98	0.46
1:A:278:MET:HB3	7:T:5:LYS:HD3	1.98	0.46
25:G:1263:PEK:H132	3:P:247:VAL:HG11	1.97	0.46
1:N:28:MET:CE	17:N:515:HEA:H271	2.46	0.46
2:O:216:LEU:O	2:O:219:PHE:HB3	2.16	0.46
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.97	0.46
6:F:55:LYS:HA	6:F:74:LEU:O	2.15	0.46
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.33	0.46
18:P:1267:PGV:H12	18:P:1267:PGV:C16	2.43	0.46
6:S:55:LYS:HA	6:S:74:LEU:O	2.15	0.46
26:G:269:CDL:H221	1:N:286:ILE:CD1	2.46	0.46
6:S:87:THR:HG21	28:S:3337:HOH:O	2.16	0.46
7:T:2:SER:OG	25:T:263:PEK:H301	2.15	0.46
7:T:38:HIS:CE1	26:T:1269:CDL:H111	2.51	0.46
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.98	0.46
26:C:270:CDL:H352	26:C:270:CDL:H162	1.97	0.46
7:G:4:ALA:CB	1:N:282:PHE:HA	2.46	0.46
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.98	0.46
1:A:422:ASN:HB3	20:B:521:TGL:H242	1.98	0.46
9:I:5:ALA:N	28:I:4913:HOH:O	2.36	0.46
2:O:41:ILE:O	2:O:45:MET:HG2	2.15	0.46
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.14	0.46
26:T:1269:CDL:H382	28:T:5116:HOH:O	2.15	0.46
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.16	0.45
7:G:7:ASP:O	1:N:169:ILE:HD12	2.16	0.45
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.81	0.45
2:B:52:HIS:HE1	21:B:230:PSC:H02	1.80	0.45
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.17	0.45
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.98	0.45
2:O:46:LEU:HD12	20:Q:1523:TGL:H271	1.97	0.45
18:C:267:PGV:H12	18:C:267:PGV:C16	2.44	0.45
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.46	0.45
1:A:240:HIS:O	1:A:243:VAL:HG22	2.16	0.45
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.81	0.45
1:A:113:LEU:HD12	20:L:522:TGL:H292	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.45
1:N:54:TYR:HB2	28:N:3111:HOH:O	2.15	0.45
20:N:1522:TGL:HB31	20:N:1522:TGL:HB61	1.80	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.45
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.52	0.45
2:B:7:LEU:HD11	20:B:521:TGL:H161	1.99	0.45
21:B:230:PSC:H062	21:B:230:PSC:H042	1.81	0.45
3:C:246:ASP:HB2	28:C:4590:HOH:O	2.17	0.45
20:D:523:TGL:H212	20:D:523:TGL:H242	1.66	0.45
7:G:38:HIS:CE1	26:G:269:CDL:H111	2.52	0.45
2:O:1:FME:SD	2:O:133:LEU:HD11	2.57	0.45
26:P:1270:CDL:H352	26:P:1270:CDL:H162	1.99	0.45
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.99	0.45
10:J:50:LEU:HD22	10:J:50:LEU:O	2.17	0.45
1:N:177:SER:H	1:N:180:GLN:NE2	2.15	0.45
3:P:25:LEU:O	3:P:29:SER:HB2	2.17	0.45
1:A:513:LEU:HD22	1:A:513:LEU:HA	1.79	0.45
23:P:1272:DMU:H25	25:P:1264:PEK:H341	1.99	0.45
28:O:4738:HOH:O	8:U:61:LYS:HD3	2.17	0.45
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.38	0.45
26:P:1270:CDL:H202	26:P:1270:CDL:H171	1.79	0.45
7:T:84:LYS:CD	7:T:84:LYS:N	2.73	0.44
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.32	0.44
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.98	0.44
5:E:71:VAL:HG11	5:E:85:VAL:HG11	2.00	0.44
3:P:34:TRP:HE1	23:P:1272:DMU:H29	1.82	0.44
26:G:269:CDL:H122	2:O:81:LEU:HD13	1.99	0.44
12:L:20:ARG:CZ	20:L:522:TGL:HC61	2.47	0.44
1:N:350:VAL:HG13	20:N:1521:TGL:HB81	1.99	0.44
2:O:83:ILE:O	2:O:87:MET:HG3	2.18	0.44
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.99	0.44
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.32	0.44
20:Q:1523:TGL:H212	20:Q:1523:TGL:H242	1.67	0.44
8:U:37:HIS:CD2	8:U:76:ARG:CZ	3.00	0.44
26:C:270:CDL:H672	26:C:270:CDL:H641	1.85	0.44
2:O:102:HIS:O	2:O:104:TRP:HA	2.18	0.44
25:P:1265:PEK:H383	26:T:1269:CDL:C27	2.47	0.44
11:X:8:ASP:HB2	28:X:5081:HOH:O	2.17	0.44
3:C:191:GLY:HA3	28:G:2161:HOH:O	2.17	0.44
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.48	0.44
22:W:1060:CHD:H212	22:W:1060:CHD:H161	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:344:PHE:CD1	1:N:344:PHE:C	2.90	0.44
5:R:31:LYS:HE2	5:R:35:THR:OG1	2.17	0.44
1:A:377:PHE:CD1	17:A:516:HEA:HAD1	2.53	0.44
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.31	0.44
2:O:56:MET:HA	21:O:1230:PSC:H202	1.99	0.44
7:T:31:CYS:HG	26:T:1269:CDL:H532	1.80	0.44
9:V:45:LYS:HB3	28:V:5052:HOH:O	2.17	0.44
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.00	0.43
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.76	0.43
20:B:521:TGL:H201	20:B:521:TGL:C24	2.45	0.43
5:E:5:HIS:HB3	5:E:6:GLU:H	1.56	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.00	0.43
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.83	0.43
2:B:41:ILE:O	2:B:45:MET:HG2	2.18	0.43
4:Q:98:TRP:CD2	23:Z:1526:DMU:H10	2.53	0.43
5:R:100:THR:HB	5:R:101:PRO:HD2	2.00	0.43
8:U:7:LYS:O	8:U:8:ILE:HG22	2.17	0.43
7:G:44:ARG:HD2	7:G:82:TYR:CE1	2.52	0.43
7:T:2:SER:O	25:T:263:PEK:H322	2.18	0.43
20:L:522:TGL:HB31	20:L:522:TGL:HB61	1.79	0.43
2:B:91:ASN:HD22	2:B:92:ASN:N	2.17	0.43
2:O:116:LEU:HD12	2:O:117:SER:N	2.34	0.43
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.19	0.43
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.01	0.43
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.54	0.43
13:M:17:ILE:O	13:M:21:VAL:HG23	2.18	0.43
11:X:24:PHE:O	11:X:28:VAL:HG12	2.19	0.43
26:C:270:CDL:H202	26:C:270:CDL:H171	1.79	0.43
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.01	0.43
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.49	0.43
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.34	0.43
3:C:168:THR:CG2	25:C:265:PEK:H14	2.49	0.43
1:N:76:GLY:O	1:N:80:ASN:HB2	2.19	0.43
1:N:449:MET:SD	2:O:5:MET:CG	3.06	0.43
3:P:40:MET:O	3:P:44:MET:HG2	2.19	0.43
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	2.01	0.43
20:N:1522:TGL:H272	20:N:1522:TGL:H231	2.00	0.42
5:R:82:TYR:N	5:R:83:PRO:CD	2.82	0.42
5:R:86:ILE:HD13	5:R:86:ILE:HA	1.83	0.42
3:C:51:MET:HB3	26:C:270:CDL:H622	2.00	0.42
26:G:269:CDL:H571	26:G:269:CDL:H601	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:522:TGL:H231	20:L:522:TGL:H272	2.01	0.42
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.86	0.42
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.19	0.42
1:A:298:ASP:HB3	28:A:2387:HOH:O	2.20	0.42
20:D:523:TGL:HC31	28:D:4745:HOH:O	2.18	0.42
12:Y:20:ARG:NH1	12:Y:20:ARG:HB3	2.34	0.42
1:N:177:SER:H	1:N:180:GLN:HE21	1.67	0.42
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.48	0.42
3:P:149:HIS:O	3:P:153:GLU:HG3	2.19	0.42
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.55	0.42
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.55	0.42
2:O:121:TYR:O	2:O:138:VAL:HA	2.19	0.42
3:P:51:MET:SD	26:P:1270:CDL:C62	3.07	0.42
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.19	0.42
1:N:112:LEU:HD23	1:N:112:LEU:C	2.39	0.42
1:A:306:THR:O	1:A:310:MET:HG3	2.20	0.42
3:C:210:ILE:HD13	18:C:267:PGV:H301	2.02	0.42
12:L:20:ARG:HH22	20:L:522:TGL:HC32	1.85	0.42
25:P:1264:PEK:H71	25:P:1264:PEK:H32	2.01	0.42
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.84	0.42
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.20	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.42
1:N:400:PHE:HB3	20:N:1522:TGL:C28	2.50	0.42
23:P:1272:DMU:H30	7:T:62:TRP:HB3	2.01	0.42
1:A:400:PHE:HB3	20:L:522:TGL:H283	2.02	0.42
21:B:230:PSC:H251	21:B:230:PSC:H221	1.77	0.42
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.20	0.42
1:N:169:ILE:HD11	1:N:189:MET:SD	2.59	0.42
1:N:426:PHE:CZ	20:N:1521:TGL:HA62	2.55	0.42
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.82	0.42
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.54	0.41
8:U:9:LYS:HB3	8:U:10:ASN:H	1.57	0.41
22:C:271:CHD:H112	22:C:271:CHD:H12A	1.67	0.41
9:V:64:ARG:HD3	9:V:72:ALA:HB1	2.01	0.41
3:C:212:SER:O	3:C:216:ILE:HG13	2.21	0.41
10:J:2:GLU:HB2	10:J:4:ARG:NH1	2.35	0.41
1:N:422:ASN:HB3	20:N:1521:TGL:H242	2.02	0.41
13:M:41:LYS:NZ	28:M:5113:HOH:O	2.53	0.41
2:O:1:FME:SD	2:O:133:LEU:HD13	2.61	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.88	0.41
5:R:84:TYR:O	5:R:87:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.50	0.41
3:C:127:LEU:HG	26:G:269:CDL:OB3	2.20	0.41
28:D:4059:HOH:O	5:E:97:GLY:HA2	2.20	0.41
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.02	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.97	0.41
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.34	0.41
1:A:406:ASN:HD21	18:A:524:PGV:H22	1.84	0.41
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.03	0.41
25:G:1263:PEK:H182	3:P:98:PHE:CD2	2.56	0.41
1:N:398:PRO:HA	1:N:403:TYR:O	2.20	0.41
26:G:269:CDL:H762	26:G:269:CDL:H732	1.98	0.41
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.56	0.41
1:N:430:PHE:CE1	20:N:1521:TGL:HB21	2.54	0.41
22:O:229:CHD:H12	22:O:229:CHD:H212	2.02	0.41
4:Q:64:PHE:CE1	5:R:66:ARG:HB2	2.56	0.41
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.03	0.41
1:A:416:ILE:HG22	1:A:464:ALA:HB2	2.02	0.41
2:B:57:ASP:H	21:B:230:PSC:H201	1.86	0.41
2:B:102:HIS:O	2:B:104:TRP:HA	2.21	0.41
3:C:22:LEU:O	3:C:26:LEU:HG	2.21	0.41
3:C:168:THR:HG22	25:C:265:PEK:H14	2.03	0.41
26:C:270:CDL:H602	26:C:270:CDL:H572	1.91	0.41
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.02	0.41
8:H:60:TYR:CD1	8:H:60:TYR:C	2.93	0.41
1:N:105:LEU:HD23	1:N:105:LEU:HA	1.88	0.41
4:Q:118:LYS:HE3	28:Q:4443:HOH:O	2.21	0.41
1:A:112:LEU:HG	28:A:2073:HOH:O	2.19	0.41
9:V:35:TYR:C	9:V:37:PHE:H	2.25	0.41
20:D:523:TGL:HC22	20:D:523:TGL:HC51	1.93	0.40
12:L:20:ARG:HH12	20:L:522:TGL:CC6	2.30	0.40
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.20	0.40
25:T:263:PEK:H282	25:T:263:PEK:H312	1.84	0.40
2:B:121:TYR:O	2:B:138:VAL:HA	2.21	0.40
4:D:53:ILE:HD13	4:D:53:ILE:HA	1.88	0.40
1:N:172:LYS:HB2	1:N:172:LYS:HE2	1.92	0.40
5:R:100:THR:OG1	5:R:103:GLU:HG3	2.21	0.40
8:U:50:VAL:O	8:U:50:VAL:HG12	2.21	0.40
26:C:270:CDL:H602	26:C:270:CDL:H632	1.69	0.40
9:I:2:THR:HG23	9:I:3:ALA:O	2.21	0.40
3:P:47:LEU:O	3:P:51:MET:HG2	2.21	0.40
20:Q:1523:TGL:HG11	20:Q:1523:TGL:CC2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:45:ALA:HB2	28:U:5144:HOH:O	2.20	0.40
12:L:46:LYS:HG3	28:L:4932:HOH:O	2.22	0.40
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.56	0.40
20:N:1521:TGL:H201	20:N:1521:TGL:C24	2.44	0.40
18:N:1266:PGV:H251	18:N:1266:PGV:H42	2.04	0.40
6:S:53:THR:CA	6:S:94:HIS:CE1	2.96	0.40
7:T:2:SER:O	7:T:3:ALA:HB3	2.21	0.40
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.02	0.40
1:A:310:MET:HB3	2:B:73:LEU:HD22	2.03	0.40
1:A:430:PHE:CE1	20:B:521:TGL:HB21	2.52	0.40
3:C:247:VAL:HG11	25:T:263:PEK:H132	2.02	0.40
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.02	0.40
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	2.03	0.40
1:N:397:PHE:HB3	1:N:398:PRO:HD3	2.03	0.40
2:O:59:GLN:O	2:O:59:GLN:CG	2.69	0.40
2:O:150:ILE:HD12	2:O:184:LEU:HD22	2.04	0.40
20:Q:1523:TGL:HC22	20:Q:1523:TGL:HC51	1.92	0.40
5:R:5:HIS:HB3	5:R:6:GLU:H	1.57	0.40
11:X:54:ARG:HG3	11:X:54:ARG:HH21	1.87	0.40
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.20	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%)	497 (97%)	15 (3%)	0	100 100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100 100
2	B	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	17 6
2	O	225/227 (99%)	208 (92%)	15 (7%)	2 (1%)	17 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	5 (5%)	2 (2%)	7	1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	0
7	G	81/85 (95%)	67 (83%)	7 (9%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	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%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3350 (96%)	127 (4%)	27 (1%)	19	7

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA

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Mol	Chain	Res	Type
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	60	GLU
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
2	O	60	GLU
7	T	3	ALA
8	U	8	ILE
8	H	46	LYS
7	T	40	GLY
6	F	96	LEU
7	G	6	GLY
6	S	96	LEU
7	T	6	GLY
8	U	46	LYS
2	O	92	ASN
2	B	92	ASN

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%)	417 (98%)	9 (2%)	53	42
1	N	426/426 (100%)	414 (97%)	12 (3%)	43	30
2	B	210/210 (100%)	201 (96%)	9 (4%)	29	14
2	O	210/210 (100%)	199 (95%)	11 (5%)	23	10
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	48
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	39
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	54
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	23
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	23
6	F	81/81 (100%)	79 (98%)	2 (2%)	47	34
6	S	81/81 (100%)	78 (96%)	3 (4%)	34	19
7	G	67/68 (98%)	62 (92%)	5 (8%)	13	4
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	2
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	15
8	U	71/75 (95%)	68 (96%)	3 (4%)	30	15
9	I	57/57 (100%)	52 (91%)	5 (9%)	10	3
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	21
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	44
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	44
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	32
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	32
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	10
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	1
All	All	3040/3082 (99%)	2936 (97%)	104 (3%)	37	22

All (104) 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	241	PRO
1	A	338	MET
1	A	369	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU

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Mol	Chain	Res	Type
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	5	HIS
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	87	THR
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS
8	H	60	TYR
9	I	2	THR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
12	L	2	HIS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO

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Mol	Chain	Res	Type
1	N	338	MET
1	N	369	ASP
1	N	484	THR
1	N	504	THR
1	N	513	LEU
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	148	MET
2	O	217	LYS
3	P	29	SER
3	P	33	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	51	LEU
4	Q	121	LYS
5	R	5	HIS
5	R	87	GLN
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	95	GLN
7	T	17	ARG
7	T	18	PHE
7	T	36	TRP
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	21	PRO
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	29	LEU
10	W	50	LEU

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Mol	Chain	Res	Type
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	91	ASN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
7	G	76	ASN
9	I	8	GLN
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	181	GLN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
7	T	76	ASN
10	W	57	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	O	1	2	8,9,10	0.67	0	7,9,11	1.81	2 (28%)
1	FME	N	1	1	8,9,10	0.75	0	7,9,11	1.68	2 (28%)
9	SAC	V	1	9	7,8,9	2.75	2 (28%)	8,9,11	3.18	5 (62%)
2	FME	B	1	2	8,9,10	0.85	0	7,9,11	2.43	2 (28%)
1	FME	A	1	1	8,9,10	0.66	0	7,9,11	1.20	1 (14%)
7	TPO	G	11	7	8,10,11	1.53	1 (12%)	10,14,16	1.03	0
7	TPO	T	11	7	8,10,11	1.30	1 (12%)	10,14,16	1.05	0
9	SAC	I	1	9	7,8,9	2.55	2 (28%)	8,9,11	2.99	4 (50%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.27	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.12	1.34	1.23
9	V	1	SAC	CA-N	4.56	1.52	1.46
9	I	1	SAC	CA-N	4.11	1.52	1.46
7	G	11	TPO	CB-CA	2.94	1.60	1.53
7	T	11	TPO	CB-CA	2.47	1.59	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	CA-N-C1A	-6.81	110.59	123.15
9	I	1	SAC	CA-N-C1A	-6.06	111.98	123.15
2	B	1	FME	C-CA-N	4.41	117.69	109.73
2	B	1	FME	CA-N-CN	-4.41	116.05	122.82
1	N	1	FME	CA-N-CN	-3.73	117.09	122.82
2	O	1	FME	C-CA-N	3.68	116.37	109.73
9	I	1	SAC	C-CA-N	-3.64	103.16	109.73
9	I	1	SAC	CB-CA-N	3.49	118.37	110.55
9	V	1	SAC	C-CA-N	-3.23	103.90	109.73
9	V	1	SAC	C2A-C1A-N	2.88	120.97	116.10
9	V	1	SAC	CB-CA-N	2.70	116.60	110.55
2	O	1	FME	CA-N-CN	-2.69	118.68	122.82
1	A	1	FME	CA-N-CN	-2.43	119.08	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.22	117.94	122.06
9	I	1	SAC	C2A-C1A-N	2.16	119.75	116.10
1	N	1	FME	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	CB-CA-N-C1A
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
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
7	T	11	TPO	O-C-CA-CB
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
7	G	11	TPO	CB-OG1-P-O3P
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	CB-CG-SD-CE
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 9 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	G	11	TPO	1	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 44 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	$\#\|Z\| > 2$
17	HEA	N	515	1	57,67,67	1.14	3 (5%)	61,103,103	1.26	8 (13%)
17	HEA	N	516	1	57,67,67	1.12	1 (1%)	61,103,103	1.35	10 (16%)
18	PGV	C	268	-	50,50,50	1.22	3 (6%)	53,56,56	0.81	1 (1%)
18	PGV	Z	1524	-	50,50,50	1.04	3 (6%)	53,56,56	0.90	1 (1%)
22	CHD	C	525	-	32,32,32	0.85	1 (3%)	51,51,51	1.65	12 (23%)
22	CHD	O	229	-	32,32,32	0.84	0	51,51,51	1.84	13 (25%)
21	PSC	O	1230	-	51,51,51	1.13	3 (5%)	57,59,59	0.87	1 (1%)
25	PEK	G	1263	-	52,52,52	1.81	11 (21%)	55,57,57	1.19	4 (7%)
23	DMU	C	272	-	34,34,34	3.01	8 (23%)	45,45,45	4.01	19 (42%)
18	PGV	C	267	-	50,50,50	0.82	1 (2%)	53,56,56	0.84	2 (3%)
25	PEK	C	265	-	52,52,52	1.59	10 (19%)	55,57,57	1.10	6 (10%)
25	PEK	P	1265	-	52,52,52	1.63	11 (21%)	55,57,57	1.08	6 (10%)
23	DMU	Z	1526	-	34,34,34	3.18	8 (23%)	45,45,45	4.18	19 (42%)
18	PGV	A	525	-	50,50,50	0.88	2 (4%)	53,56,56	0.74	2 (3%)
22	CHD	W	1060	-	32,32,32	0.96	2 (6%)	51,51,51	3.19	26 (50%)
17	HEA	A	516	1	57,67,67	1.17	4 (7%)	61,103,103	1.33	7 (11%)
23	DMU	P	1272	-	34,34,34	3.01	9 (26%)	45,45,45	4.00	19 (42%)
20	TGL	Q	1523	-	62,62,62	0.80	2 (3%)	65,65,65	1.26	9 (13%)
17	HEA	A	515	1	57,67,67	1.07	4 (7%)	61,103,103	1.26	7 (11%)
22	CHD	B	1086	-	32,32,32	0.73	0	51,51,51	1.79	15 (29%)
20	TGL	N	1521	-	62,62,62	0.71	1 (1%)	65,65,65	1.40	10 (15%)
22	CHD	P	1271	-	32,32,32	0.79	0	51,51,51	3.54	22 (43%)
21	PSC	B	230	-	51,51,51	1.16	3 (5%)	57,59,59	0.86	1 (1%)
22	CHD	C	271	-	32,32,32	0.82	0	51,51,51	3.60	21 (41%)
18	PGV	A	524	-	50,50,50	1.07	3 (6%)	53,56,56	0.93	2 (3%)
20	TGL	N	1522	-	62,62,62	1.15	4 (6%)	65,65,65	1.70	13 (20%)
22	CHD	P	1525	-	32,32,32	0.86	0	51,51,51	1.59	8 (15%)
22	CHD	J	60	-	32,32,32	0.89	1 (3%)	51,51,51	3.20	25 (49%)
25	PEK	C	264	-	52,52,52	1.40	4 (7%)	55,57,57	1.02	3 (5%)
25	PEK	P	1264	-	52,52,52	1.39	4 (7%)	55,57,57	1.05	3 (5%)
23	DMU	M	526	-	34,34,34	3.22	8 (23%)	45,45,45	4.23	19 (42%)
25	PEK	T	263	-	52,52,52	1.83	12 (23%)	55,57,57	1.20	4 (7%)
19	CUA	B	228	2	0,1,1	-	-	-		
19	CUA	O	228	2	0,1,1	-	-	-		
26	CDL	G	269	-	99,99,99	0.91	5 (5%)	105,111,111	0.96	7 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	TGL	L	522	-	62,62,62	1.11	4 (6%)	65,65,65	1.72	13 (20%)
26	CDL	P	1270	-	99,99,99	0.81	3 (3%)	105,111,111	0.95	6 (5%)
20	TGL	D	523	-	62,62,62	0.76	1 (1%)	65,65,65	1.28	9 (13%)
18	PGV	P	1267	-	50,50,50	0.84	1 (2%)	53,56,56	0.82	1 (1%)
26	CDL	C	270	-	99,99,99	0.78	3 (3%)	105,111,111	0.97	6 (5%)
18	PGV	N	1266	-	50,50,50	0.92	2 (4%)	53,56,56	0.77	3 (5%)
18	PGV	P	1268	-	50,50,50	1.25	4 (8%)	53,56,56	0.83	1 (1%)
20	TGL	B	521	-	62,62,62	0.67	0	65,65,65	1.41	11 (16%)
26	CDL	T	1269	-	99,99,99	0.88	5 (5%)	105,111,111	0.97	7 (6%)

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
17	HEA	N	515	1	-	7/32/76/76	-
17	HEA	N	516	1	-	6/32/76/76	-
18	PGV	C	268	-	-	34/55/55/55	-
18	PGV	Z	1524	-	-	32/55/55/55	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4
21	PSC	O	1230	-	-	40/55/55/55	-
25	PEK	G	1263	-	-	27/56/56/56	-
23	DMU	C	272	-	6/6/10/10	8/19/59/59	0/2/2/2
18	PGV	C	267	-	-	17/55/55/55	-
25	PEK	C	265	-	-	22/56/56/56	-
25	PEK	P	1265	-	-	23/56/56/56	-
23	DMU	Z	1526	-	5/5/10/10	8/19/59/59	0/2/2/2
22	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
18	PGV	A	525	-	-	13/55/55/55	-
17	HEA	A	516	1	-	5/32/76/76	-
23	DMU	P	1272	-	6/6/10/10	8/19/59/59	0/2/2/2
20	TGL	Q	1523	-	-	14/65/65/65	-
17	HEA	A	515	1	-	8/32/76/76	-
22	CHD	B	1086	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	P	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
20	TGL	N	1521	-	-	14/65/65/65	-
21	PSC	B	230	-	-	40/55/55/55	-
22	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4
18	PGV	A	524	-	-	33/55/55/55	-
20	TGL	N	1522	-	-	16/65/65/65	-
22	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
22	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
25	PEK	C	264	-	-	21/56/56/56	-
25	PEK	P	1264	-	-	21/56/56/56	-
23	DMU	M	526	-	5/5/10/10	8/19/59/59	0/2/2/2
25	PEK	T	263	-	-	27/56/56/56	-
26	CDL	G	269	-	-	62/110/110/110	-
20	TGL	L	522	-	-	16/65/65/65	-
26	CDL	P	1270	-	-	69/110/110/110	-
20	TGL	D	523	-	-	14/65/65/65	-
18	PGV	P	1267	-	-	17/55/55/55	-
26	CDL	C	270	-	-	70/110/110/110	-
18	PGV	N	1266	-	-	14/55/55/55	-
18	PGV	P	1268	-	-	35/55/55/55	-
20	TGL	B	521	-	-	14/65/65/65	-
26	CDL	T	1269	-	-	62/110/110/110	-

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	1526	DMU	O7-C3	-8.03	1.23	1.43
23	M	526	DMU	O7-C3	-7.98	1.23	1.43
23	M	526	DMU	O16-C6	-7.34	1.27	1.40
23	Z	1526	DMU	O16-C6	-7.27	1.27	1.40
23	M	526	DMU	O1-C9	-7.23	1.26	1.44
23	P	1272	DMU	O1-C9	-7.15	1.27	1.44
23	C	272	DMU	O16-C6	-6.98	1.28	1.40
23	Z	1526	DMU	O1-C9	-6.96	1.27	1.44
23	P	1272	DMU	O16-C6	-6.84	1.28	1.40
23	C	272	DMU	O1-C9	-6.84	1.27	1.44
23	P	1272	DMU	O7-C3	-6.63	1.26	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	272	DMU	O7-C3	-6.60	1.26	1.43
23	M	526	DMU	O5-C4	-6.53	1.28	1.44
23	Z	1526	DMU	O5-C4	-6.47	1.28	1.44
23	C	272	DMU	O16-C18	-6.45	1.25	1.43
23	P	1272	DMU	O16-C18	-6.41	1.25	1.43
23	M	526	DMU	O16-C18	-6.13	1.25	1.43
23	Z	1526	DMU	O7-C10	-5.98	1.24	1.41
23	M	526	DMU	O7-C10	-5.97	1.25	1.41
23	M	526	DMU	O1-C10	-5.86	1.27	1.41
23	Z	1526	DMU	O16-C18	-5.85	1.26	1.43
23	Z	1526	DMU	O1-C10	-5.81	1.27	1.41
23	C	272	DMU	O5-C4	-5.36	1.31	1.44
23	P	1272	DMU	O5-C4	-5.26	1.31	1.44
23	C	272	DMU	O1-C10	-5.22	1.28	1.41
23	P	1272	DMU	O1-C10	-5.18	1.28	1.41
23	C	272	DMU	O7-C10	-5.15	1.27	1.41
23	P	1272	DMU	O7-C10	-5.11	1.27	1.41
20	N	1522	TGL	OG2-CB1	5.05	1.48	1.34
20	L	522	TGL	OG2-CB1	4.94	1.48	1.34
23	C	272	DMU	O5-C6	-4.81	1.29	1.41
23	P	1272	DMU	O5-C6	-4.69	1.29	1.41
25	G	1263	PEK	C12-C11	4.68	1.58	1.31
25	C	264	PEK	C15-C14	4.63	1.58	1.31
25	P	1264	PEK	C12-C11	4.62	1.58	1.31
23	M	526	DMU	O5-C6	-4.60	1.30	1.41
25	T	263	PEK	C12-C11	4.52	1.58	1.31
25	P	1264	PEK	C15-C14	4.50	1.57	1.31
25	T	263	PEK	C6-C5	4.50	1.57	1.31
25	G	1263	PEK	C6-C5	4.49	1.57	1.31
25	C	264	PEK	C12-C11	4.48	1.57	1.31
18	P	1268	PGV	C12-C11	4.40	1.57	1.31
25	T	263	PEK	O03-C21	4.39	1.46	1.33
23	Z	1526	DMU	O5-C6	-4.37	1.30	1.41
25	P	1265	PEK	C12-C11	4.37	1.57	1.31
18	C	268	PGV	C12-C11	4.35	1.57	1.31
25	C	265	PEK	C9-C8	4.33	1.56	1.31
25	C	265	PEK	C12-C11	4.31	1.56	1.31
25	C	265	PEK	C15-C14	4.26	1.56	1.31
25	G	1263	PEK	O03-C21	4.26	1.45	1.33
21	O	1230	PSC	C10-C9	4.25	1.56	1.31
25	P	1265	PEK	C15-C14	4.20	1.56	1.31
25	P	1265	PEK	C9-C8	4.19	1.56	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	1263	PEK	C15-C14	4.19	1.56	1.31
21	B	230	PSC	C10-C9	4.18	1.56	1.31
18	P	1268	PGV	O01-C1	4.17	1.46	1.34
25	T	263	PEK	C15-C14	4.12	1.55	1.31
25	P	1265	PEK	C6-C5	4.12	1.55	1.31
21	O	1230	PSC	C13-C12	4.11	1.55	1.31
21	B	230	PSC	C13-C12	4.08	1.55	1.31
25	C	264	PEK	C6-C5	4.08	1.55	1.31
25	C	264	PEK	C9-C8	4.08	1.55	1.31
25	T	263	PEK	C9-C8	4.08	1.55	1.31
25	P	1264	PEK	C9-C8	4.05	1.55	1.31
25	P	1264	PEK	C6-C5	4.04	1.55	1.31
25	G	1263	PEK	C9-C8	4.02	1.55	1.31
18	N	1266	PGV	C12-C11	3.99	1.54	1.31
25	C	265	PEK	C6-C5	3.97	1.54	1.31
18	Z	1524	PGV	C12-C11	3.95	1.54	1.31
20	N	1522	TGL	OG1-CA1	3.92	1.44	1.33
18	A	524	PGV	C12-C11	3.85	1.54	1.31
18	A	525	PGV	C12-C11	3.82	1.53	1.31
25	G	1263	PEK	C01-C02	3.67	1.61	1.50
26	T	1269	CDL	CB6-CB4	3.64	1.61	1.50
18	C	268	PGV	O01-C1	3.61	1.44	1.34
25	G	1263	PEK	C03-C02	3.53	1.61	1.50
25	T	263	PEK	C01-C02	3.42	1.61	1.50
18	A	524	PGV	O03-C19	3.42	1.43	1.33
26	G	269	CDL	CB6-CB4	3.37	1.61	1.50
25	T	263	PEK	C03-C02	3.35	1.61	1.50
17	A	516	HEA	C3A-C2A	-3.35	1.35	1.40
17	N	515	HEA	C3A-CMA	-3.31	1.38	1.46
18	P	1267	PGV	C12-C11	3.22	1.50	1.31
18	C	267	PGV	C12-C11	3.20	1.50	1.31
17	N	516	HEA	C3A-CMA	-3.14	1.39	1.46
20	L	522	TGL	OG1-CA1	3.07	1.42	1.33
22	W	1060	CHD	C13-C17	3.04	1.60	1.55
25	T	263	PEK	O01-C1	2.99	1.42	1.34
18	Z	1524	PGV	O03-C19	2.93	1.41	1.33
17	A	515	HEA	C3A-CMA	-2.93	1.39	1.46
20	L	522	TGL	CG1-CG2	2.90	1.59	1.50
25	T	263	PEK	C2-C1	2.85	1.59	1.50
25	T	263	PEK	P-O11	2.84	1.70	1.59
25	P	1265	PEK	O03-C21	2.84	1.41	1.33
26	P	1270	CDL	CA6-CA4	2.78	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	1522	TGL	CG1-CG2	2.67	1.58	1.50
26	G	269	CDL	OA6-CA5	2.65	1.41	1.34
25	C	265	PEK	C03-C02	2.64	1.58	1.50
22	J	60	CHD	C13-C17	2.64	1.60	1.55
25	G	1263	PEK	P-O11	2.58	1.69	1.59
25	P	1265	PEK	C22-C21	2.58	1.58	1.50
25	P	1265	PEK	C03-C02	2.55	1.58	1.50
26	G	269	CDL	CB3-CB4	2.53	1.58	1.50
25	G	1263	PEK	O01-C1	2.53	1.41	1.34
17	A	516	HEA	C3C-C2C	-2.53	1.36	1.40
25	C	265	PEK	C22-C21	2.53	1.58	1.50
26	C	270	CDL	CA6-CA4	2.50	1.58	1.50
21	B	230	PSC	C2-C1	2.48	1.58	1.50
20	N	1521	TGL	OG2-CB1	2.47	1.41	1.34
17	A	516	HEA	C3A-CMA	-2.47	1.40	1.46
17	N	515	HEA	C3A-C2A	-2.44	1.37	1.40
17	A	515	HEA	CHC-C4B	2.44	1.41	1.35
18	P	1268	PGV	C2-C1	2.43	1.57	1.50
25	P	1265	PEK	P-O11	2.41	1.69	1.59
17	A	516	HEA	C20-C19	2.40	1.56	1.51
26	G	269	CDL	CA6-CA4	2.40	1.58	1.50
26	T	1269	CDL	C11-CA5	2.40	1.57	1.50
20	Q	1523	TGL	OG2-CB1	2.40	1.41	1.34
25	C	265	PEK	O03-C21	2.38	1.40	1.33
25	P	1265	PEK	C01-C02	2.36	1.57	1.50
18	C	268	PGV	C04-C05	2.36	1.59	1.51
26	T	1269	CDL	CB3-CB4	2.36	1.57	1.50
25	T	263	PEK	C22-C21	2.35	1.57	1.50
17	N	515	HEA	C1C-NC	2.34	1.41	1.36
26	P	1270	CDL	CA3-CA4	2.33	1.57	1.50
25	C	265	PEK	C01-C02	2.32	1.57	1.50
26	P	1270	CDL	OA8-CA7	2.31	1.40	1.33
25	G	1263	PEK	C22-C21	2.31	1.57	1.50
26	C	270	CDL	CA3-CA4	2.27	1.57	1.50
25	C	265	PEK	P-O11	2.27	1.68	1.59
25	P	1265	PEK	O01-C1	2.25	1.40	1.34
21	O	1230	PSC	C2-C1	2.24	1.57	1.50
25	P	1265	PEK	P-O12	2.22	1.68	1.59
26	G	269	CDL	C11-CA5	2.19	1.57	1.50
22	C	525	CHD	C10-C9	-2.17	1.52	1.56
26	T	1269	CDL	OA6-CA5	2.17	1.40	1.34
26	C	270	CDL	OA8-CA7	2.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	524	PGV	C20-C19	2.14	1.57	1.50
25	G	1263	PEK	C2-C1	2.14	1.57	1.50
18	N	1266	PGV	C01-C02	2.13	1.57	1.50
20	L	522	TGL	CG3-CG2	2.13	1.57	1.50
25	T	263	PEK	P-O12	2.12	1.67	1.59
17	A	515	HEA	C1C-NC	2.09	1.40	1.36
20	D	523	TGL	OG1-CA1	2.08	1.39	1.33
20	N	1522	TGL	CC2-CC1	2.08	1.56	1.50
22	W	1060	CHD	C20-C17	2.08	1.58	1.54
17	A	515	HEA	CMB-C2B	2.05	1.55	1.50
18	P	1268	PGV	C04-C05	2.05	1.58	1.51
18	Z	1524	PGV	C20-C19	2.05	1.56	1.50
20	Q	1523	TGL	OG1-CA1	2.04	1.39	1.33
26	T	1269	CDL	CA6-CA4	2.04	1.57	1.50
25	C	265	PEK	P-O12	2.03	1.67	1.59
18	A	525	PGV	C20-C19	2.02	1.56	1.50
23	P	1272	DMU	C3-C4	2.02	1.58	1.52

All (382) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	271	CHD	C17-C13-C14	10.46	110.64	100.09
22	P	1271	CHD	C10-C9-C8	10.23	122.80	111.82
23	C	272	DMU	C1-C2-C3	10.05	132.62	109.68
22	P	1271	CHD	C17-C13-C14	9.94	110.12	100.09
23	P	1272	DMU	C1-C2-C3	9.93	132.34	109.68
22	C	271	CHD	C10-C9-C8	9.78	122.32	111.82
23	Z	1526	DMU	C1-C2-C3	9.69	131.80	109.68
23	M	526	DMU	C1-C2-C3	9.62	131.64	109.68
22	P	1271	CHD	C17-C13-C12	-9.53	108.97	117.67
23	M	526	DMU	C10-C5-C7	9.51	129.80	110.00
22	C	271	CHD	C17-C13-C12	-9.47	109.02	117.67
22	J	60	CHD	C17-C13-C14	9.46	109.63	100.09
23	Z	1526	DMU	C10-C5-C7	9.38	129.53	110.00
22	W	1060	CHD	C17-C13-C14	9.12	109.29	100.09
23	P	1272	DMU	O16-C6-C1	8.88	122.16	108.30
23	C	272	DMU	O16-C6-C1	8.79	122.02	108.30
23	C	272	DMU	C6-O5-C4	8.69	130.74	113.69
23	P	1272	DMU	C6-O5-C4	8.46	130.29	113.69
22	C	271	CHD	C19-C10-C9	-8.40	99.61	111.18
23	C	272	DMU	O5-C4-C3	8.36	127.38	109.75
23	P	1272	DMU	O5-C4-C3	8.35	127.36	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	526	DMU	C6-O5-C4	8.14	129.67	113.69
23	C	272	DMU	O1-C9-C11	8.12	126.62	106.44
23	Z	1526	DMU	C6-O5-C4	8.01	129.41	113.69
22	P	1271	CHD	C19-C10-C9	-7.77	100.48	111.18
23	P	1272	DMU	O1-C9-C11	7.75	125.70	106.44
23	M	526	DMU	O1-C9-C8	7.62	123.54	109.69
23	Z	1526	DMU	O5-C4-C3	7.56	125.69	109.75
23	C	272	DMU	O7-C3-C4	7.47	129.92	109.45
23	Z	1526	DMU	O1-C9-C11	7.31	124.61	106.44
23	P	1272	DMU	O7-C3-C4	7.28	129.39	109.45
23	Z	1526	DMU	O1-C9-C8	7.22	122.80	109.69
23	M	526	DMU	O5-C4-C3	7.19	124.92	109.75
23	M	526	DMU	C8-C7-C5	-7.15	98.34	110.82
22	W	1060	CHD	C13-C17-C20	7.13	128.00	119.50
23	M	526	DMU	O5-C4-C57	6.95	123.72	106.44
23	M	526	DMU	O1-C9-C11	6.94	123.70	106.44
23	Z	1526	DMU	C8-C7-C5	-6.91	98.76	110.82
22	J	60	CHD	C13-C17-C20	6.89	127.72	119.50
23	M	526	DMU	O7-C3-C2	6.84	125.48	107.28
23	M	526	DMU	C7-C8-C9	6.84	122.44	110.24
23	Z	1526	DMU	C7-C8-C9	6.73	122.25	110.24
23	Z	1526	DMU	O5-C4-C57	6.67	123.02	106.44
23	M	526	DMU	C18-O16-C6	6.55	124.69	113.84
23	Z	1526	DMU	O7-C3-C2	6.42	124.35	107.28
23	P	1272	DMU	C18-O16-C6	6.39	124.44	113.84
23	P	1272	DMU	O1-C9-C8	6.32	121.18	109.69
22	J	60	CHD	C10-C9-C8	6.32	118.60	111.82
22	W	1060	CHD	C10-C9-C8	6.30	118.58	111.82
22	P	1271	CHD	C1-C10-C5	6.13	116.84	107.77
22	C	271	CHD	C1-C10-C5	6.10	116.79	107.77
23	Z	1526	DMU	C18-O16-C6	6.00	123.79	113.84
23	C	272	DMU	C18-O16-C6	5.97	123.73	113.84
23	C	272	DMU	O1-C9-C8	5.92	120.44	109.69
23	Z	1526	DMU	O5-C6-O16	5.91	123.97	109.97
22	W	1060	CHD	C6-C5-C10	5.78	118.80	112.66
22	J	60	CHD	C6-C5-C10	5.72	118.73	112.66
22	C	271	CHD	C9-C8-C7	5.65	118.63	111.88
22	J	60	CHD	C4-C3-C2	5.60	117.24	110.55
22	W	1060	CHD	C15-C14-C8	-5.60	110.50	118.33
22	P	1271	CHD	C9-C8-C7	5.56	118.53	111.88
23	P	1272	DMU	O5-C4-C57	5.55	120.25	106.44
23	C	272	DMU	O5-C4-C57	5.54	120.21	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	J	60	CHD	C15-C14-C8	-5.47	110.69	118.33
22	W	1060	CHD	C9-C8-C7	5.33	118.25	111.88
22	J	60	CHD	C9-C8-C7	5.31	118.23	111.88
22	W	1060	CHD	C4-C3-C2	5.31	116.90	110.55
23	P	1272	DMU	O7-C3-C2	5.30	121.37	107.28
23	M	526	DMU	O5-C6-C1	5.27	121.50	110.35
23	M	526	DMU	O5-C6-O16	5.24	122.39	109.97
22	J	60	CHD	C1-C10-C5	5.22	115.49	107.77
23	C	272	DMU	O7-C3-C2	5.21	121.15	107.28
22	P	1525	CHD	C13-C17-C20	5.16	125.65	119.50
23	Z	1526	DMU	O5-C6-C1	5.15	121.25	110.35
22	P	1271	CHD	C15-C14-C8	-5.11	111.19	118.33
23	C	272	DMU	O7-C10-C5	5.09	121.28	108.10
22	C	271	CHD	C15-C14-C8	-5.05	111.28	118.33
22	C	271	CHD	C19-C10-C1	-5.04	100.14	108.26
23	P	1272	DMU	O7-C10-C5	5.02	121.11	108.10
22	P	1271	CHD	C19-C10-C1	-4.93	100.32	108.26
22	W	1060	CHD	C1-C10-C5	4.92	115.04	107.77
23	M	526	DMU	O16-C6-C1	4.83	115.85	108.30
20	L	522	TGL	C12-C11-C10	-4.76	90.25	114.42
20	L	522	TGL	CB9-CB8-CB7	-4.74	90.36	114.42
20	N	1522	TGL	CB9-CB8-CB7	-4.73	90.40	114.42
22	C	271	CHD	C14-C13-C12	4.69	111.77	107.40
22	C	271	CHD	C4-C5-C10	4.68	117.63	112.66
22	C	525	CHD	C13-C17-C20	4.65	125.04	119.50
20	N	1522	TGL	C12-C11-C10	-4.62	90.97	114.42
22	J	60	CHD	C18-C13-C14	-4.62	103.98	111.21
23	Z	1526	DMU	O7-C3-C4	4.57	121.98	109.45
23	M	526	DMU	O7-C10-C5	4.44	119.59	108.10
22	P	1271	CHD	C14-C13-C12	4.38	111.48	107.40
22	W	1060	CHD	C18-C13-C14	-4.38	104.36	111.21
22	C	271	CHD	C4-C3-C2	4.37	115.77	110.55
22	W	1060	CHD	C11-C12-C13	4.31	115.67	111.24
22	P	1271	CHD	C4-C5-C10	4.26	117.18	112.66
20	B	521	TGL	CG2-OG2-CB1	4.23	128.21	117.79
23	P	1272	DMU	C10-O1-C9	4.20	121.94	113.69
23	Z	1526	DMU	O7-C10-C5	4.19	118.97	108.10
20	B	521	TGL	CG1-OG1-CA1	-4.19	101.61	117.12
20	L	522	TGL	C15-CC9-CC8	4.18	135.65	114.42
20	N	1521	TGL	CG2-OG2-CB1	4.18	128.07	117.79
23	C	272	DMU	C10-O1-C9	4.17	121.88	113.69
22	W	1060	CHD	C5-C6-C7	4.16	119.05	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	N	1521	TGL	CG1-OG1-CA1	-4.16	101.72	117.12
20	N	1522	TGL	C15-CC9-CC8	4.12	135.36	114.42
23	C	272	DMU	O7-C10-O1	4.12	122.18	110.67
22	J	60	CHD	C11-C12-C13	4.12	115.47	111.24
23	C	272	DMU	C2-C3-C4	-4.09	101.55	110.93
23	P	1272	DMU	O5-C6-C1	4.08	118.99	110.35
25	T	263	PEK	O03-C01-C02	4.04	120.19	108.43
23	P	1272	DMU	O7-C10-O1	4.02	121.89	110.67
25	G	1263	PEK	O03-C01-C02	4.01	120.11	108.43
22	O	229	CHD	C10-C9-C8	4.01	116.12	111.82
23	Z	1526	DMU	O16-C6-C1	4.00	114.55	108.30
23	M	526	DMU	O7-C3-C4	4.00	120.40	109.45
23	C	272	DMU	O5-C6-C1	3.98	118.77	110.35
22	J	60	CHD	C5-C6-C7	3.96	118.83	114.46
20	L	522	TGL	CC3-CC2-CC1	3.96	128.02	113.62
22	C	525	CHD	C14-C13-C12	-3.95	103.73	107.40
22	P	1271	CHD	C4-C3-C2	3.94	115.25	110.55
23	P	1272	DMU	C2-C3-C4	-3.92	101.93	110.93
25	G	1263	PEK	C02-O01-C1	3.87	127.32	117.79
22	B	1086	CHD	C16-C17-C13	-3.79	99.84	103.55
20	N	1522	TGL	C16-C15-CC9	3.78	133.62	114.42
25	T	263	PEK	P-O11-C03	3.78	143.84	121.68
20	N	1522	TGL	CC3-CC2-CC1	3.77	127.34	113.62
22	O	229	CHD	C5-C6-C7	3.76	118.61	114.46
20	L	522	TGL	C16-C15-CC9	3.75	133.48	114.42
25	G	1263	PEK	P-O11-C03	3.73	143.57	121.68
22	W	1060	CHD	C2-C1-C10	3.71	119.14	112.78
22	P	1271	CHD	C1-C10-C9	3.69	117.15	111.35
25	T	263	PEK	C02-O01-C1	3.68	126.86	117.79
22	C	271	CHD	C1-C10-C9	3.68	117.14	111.35
22	J	60	CHD	C17-C13-C12	-3.67	114.31	117.67
22	W	1060	CHD	C17-C13-C12	-3.67	114.31	117.67
22	P	1525	CHD	C15-C14-C8	-3.62	113.27	118.33
22	O	229	CHD	C5-C4-C3	3.61	118.06	112.76
23	C	272	DMU	O5-C6-O16	3.60	118.51	109.97
20	D	523	TGL	CG3-OG3-CC1	3.58	130.36	117.12
20	N	1522	TGL	C11-C10-CB9	3.55	132.47	114.42
23	M	526	DMU	C10-O7-C3	3.55	126.76	117.96
22	P	1271	CHD	C5-C4-C3	3.54	117.96	112.76
22	W	1060	CHD	C5-C4-C3	3.54	117.96	112.76
23	P	1272	DMU	O5-C6-O16	3.52	118.32	109.97
22	B	1086	CHD	C15-C14-C8	-3.50	113.44	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	229	CHD	C14-C13-C12	-3.50	104.15	107.40
22	J	60	CHD	C2-C1-C10	3.49	118.77	112.78
22	B	1086	CHD	C14-C13-C12	-3.49	104.16	107.40
22	O	229	CHD	C16-C17-C13	-3.45	100.17	103.55
22	O	229	CHD	C15-C14-C8	-3.45	113.51	118.33
22	C	271	CHD	C18-C13-C14	-3.42	105.85	111.21
22	P	1271	CHD	C5-C6-C7	3.42	118.23	114.46
22	B	1086	CHD	C1-C2-C3	3.41	114.84	110.47
20	L	522	TGL	C11-C10-CB9	3.41	131.71	114.42
25	C	265	PEK	P-O11-C03	3.40	141.61	121.68
18	A	524	PGV	C02-O01-C1	3.39	126.14	117.79
20	Q	1523	TGL	CG3-OG3-CC1	3.35	129.54	117.12
22	C	525	CHD	C15-C14-C8	-3.33	113.67	118.33
25	P	1265	PEK	P-O11-C03	3.32	141.16	121.68
22	J	60	CHD	C5-C4-C3	3.31	117.62	112.76
22	J	60	CHD	C19-C10-C9	-3.31	106.62	111.18
20	D	523	TGL	OG1-CG1-CG2	3.28	117.97	108.43
22	B	1086	CHD	C15-C14-C13	-3.27	100.35	103.55
22	J	60	CHD	C11-C9-C10	3.24	117.07	113.73
26	P	1270	CDL	PA1-OA5-CA3	3.22	140.59	121.68
22	B	1086	CHD	O3-C3-C4	-3.22	103.44	109.85
22	C	271	CHD	C5-C4-C3	3.20	117.46	112.76
18	Z	1524	PGV	C02-O01-C1	3.16	125.58	117.79
23	C	272	DMU	C8-C7-C5	3.16	116.34	110.82
23	P	1272	DMU	C8-C7-C5	3.15	116.32	110.82
22	W	1060	CHD	C11-C9-C10	3.12	116.95	113.73
22	J	60	CHD	C1-C2-C3	3.09	114.43	110.47
22	W	1060	CHD	C19-C10-C9	-3.07	106.95	111.18
26	C	270	CDL	PA1-OA5-CA3	3.07	139.69	121.68
22	B	1086	CHD	C10-C9-C8	3.07	115.11	111.82
22	C	271	CHD	C5-C6-C7	3.06	117.84	114.46
22	P	1525	CHD	C14-C8-C9	-3.03	105.55	109.71
20	Q	1523	TGL	CG1-OG1-CA1	-3.02	105.94	117.12
22	B	1086	CHD	C1-C10-C5	3.01	112.22	107.77
22	P	1271	CHD	C18-C13-C14	-3.00	106.52	111.21
22	W	1060	CHD	C1-C2-C3	2.98	114.29	110.47
26	G	269	CDL	C22-C21-C20	2.98	129.53	114.42
22	B	1086	CHD	C19-C10-C1	-2.97	103.47	108.26
17	A	515	HEA	C27-C19-C18	-2.97	116.06	123.68
26	T	1269	CDL	C22-C21-C20	2.96	129.44	114.42
22	C	271	CHD	C6-C5-C10	2.96	115.80	112.66
22	P	1525	CHD	C5-C6-C7	2.96	117.72	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	525	CHD	C5-C6-C7	2.95	117.71	114.46
17	N	515	HEA	C27-C19-C18	-2.94	116.14	123.68
23	Z	1526	DMU	C2-C3-C4	-2.93	104.21	110.93
17	N	516	HEA	C27-C19-C20	2.93	120.20	115.27
22	P	1525	CHD	C14-C13-C12	-2.92	104.68	107.40
22	C	525	CHD	C10-C9-C8	2.92	114.95	111.82
22	W	1060	CHD	C16-C15-C14	2.91	110.89	105.13
22	O	229	CHD	C1-C10-C5	2.90	112.06	107.77
22	P	1271	CHD	C6-C5-C10	2.90	115.74	112.66
26	C	270	CDL	OB6-CB5-C51	-2.88	105.29	111.50
20	L	522	TGL	CG2-OG2-CB1	2.87	124.85	117.79
22	J	60	CHD	C16-C15-C14	2.86	110.80	105.13
22	W	1060	CHD	C14-C13-C12	2.86	110.06	107.40
22	J	60	CHD	C4-C5-C10	2.84	115.67	112.66
20	D	523	TGL	CG1-OG1-CA1	-2.83	106.63	117.12
22	J	60	CHD	C15-C16-C17	2.83	110.75	105.13
22	C	525	CHD	C2-C1-C10	2.82	117.62	112.78
23	Z	1526	DMU	O7-C10-O1	2.82	118.55	110.67
23	Z	1526	DMU	C10-O7-C3	2.81	124.93	117.96
17	A	516	HEA	C27-C19-C20	2.81	120.00	115.27
22	J	60	CHD	C14-C13-C12	2.81	110.02	107.40
23	P	1272	DMU	O1-C10-C5	2.81	116.29	110.35
20	N	1522	TGL	CG2-OG2-CB1	2.80	124.68	117.79
20	Q	1523	TGL	OG2-CG2-CG3	2.80	118.52	108.40
20	Q	1523	TGL	OG1-CG1-CG2	2.79	116.56	108.43
22	P	1525	CHD	C1-C2-C3	2.79	114.05	110.47
20	B	521	TGL	CG3-CG2-CG1	2.78	118.36	111.79
26	T	1269	CDL	C23-C22-C21	2.77	128.48	114.42
17	A	516	HEA	CMC-C2C-C3C	2.77	129.85	124.68
21	B	230	PSC	C01-O03-C19	-2.76	106.89	117.12
22	W	1060	CHD	C4-C5-C10	2.76	115.59	112.66
22	W	1060	CHD	C15-C16-C17	2.75	110.59	105.13
22	C	271	CHD	C15-C16-C17	2.75	110.58	105.13
20	L	522	TGL	CC4-CC3-CC2	2.75	123.07	113.19
17	A	516	HEA	CMB-C2B-C3B	-2.75	125.11	130.34
20	D	523	TGL	CB3-CB2-CB1	2.74	123.59	113.62
25	C	265	PEK	C24-C23-C22	2.72	122.96	113.19
22	P	1271	CHD	C15-C16-C17	2.71	110.51	105.13
23	M	526	DMU	C2-C3-C4	-2.71	104.71	110.93
26	G	269	CDL	C23-C22-C21	2.71	128.19	114.42
21	O	1230	PSC	C01-O03-C19	-2.70	107.11	117.12
22	C	525	CHD	C14-C8-C9	-2.70	106.00	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	271	CHD	O12-C12-C13	2.70	115.59	111.03
20	N	1522	TGL	CC4-CC3-CC2	2.68	122.82	113.19
22	O	229	CHD	C15-C14-C13	-2.68	100.93	103.55
25	P	1264	PEK	C3-C2-C1	-2.67	103.91	113.62
22	C	271	CHD	C16-C15-C14	2.67	110.42	105.13
22	O	229	CHD	C1-C2-C3	2.67	113.89	110.47
20	N	1522	TGL	C10-CB9-CB8	2.65	127.89	114.42
25	C	265	PEK	C11-C10-C9	2.65	125.05	112.02
22	C	271	CHD	C1-C2-C3	2.64	113.86	110.47
25	P	1265	PEK	C11-C10-C9	2.64	125.04	112.02
17	N	516	HEA	CHA-C4D-C3D	-2.64	120.95	124.84
20	L	522	TGL	C10-CB9-CB8	2.62	127.72	114.42
22	P	1271	CHD	C1-C2-C3	2.62	113.83	110.47
18	P	1267	PGV	C9-C10-C11	-2.61	97.48	112.43
23	C	272	DMU	O1-C10-C5	2.60	115.85	110.35
17	N	515	HEA	C17-C18-C19	-2.59	121.42	127.66
23	C	272	DMU	C10-O7-C3	2.59	124.36	117.96
20	N	1521	TGL	CG3-CG2-CG1	2.59	117.90	111.79
25	C	264	PEK	O03-C21-C22	-2.58	103.80	111.91
18	C	267	PGV	C9-C10-C11	-2.58	97.65	112.43
23	P	1272	DMU	C10-O7-C3	2.58	124.34	117.96
26	G	269	CDL	C20-C19-C18	2.56	127.43	114.42
26	C	270	CDL	OA8-CA6-CA4	2.56	115.88	108.43
18	P	1268	PGV	O03-C01-C02	2.55	115.86	108.43
17	N	516	HEA	C3C-C4C-NC	2.55	112.50	109.21
22	J	60	CHD	C14-C8-C7	2.55	115.19	111.81
22	C	525	CHD	C16-C17-C13	-2.54	101.06	103.55
22	O	229	CHD	O3-C3-C4	-2.54	104.79	109.85
22	P	1271	CHD	C16-C15-C14	2.54	110.16	105.13
22	O	229	CHD	C19-C10-C1	-2.53	104.19	108.26
22	W	1060	CHD	C14-C8-C7	2.53	115.16	111.81
20	N	1522	TGL	C13-C12-C11	2.52	127.24	114.42
26	C	270	CDL	OB6-CB5-OB7	2.52	129.78	123.70
18	C	268	PGV	O03-C01-C02	2.51	115.75	108.43
25	C	264	PEK	C3-C2-C1	-2.51	104.49	113.62
20	B	521	TGL	CA8-CA7-CA6	-2.51	101.70	114.42
26	C	270	CDL	C52-C51-CB5	-2.49	104.57	113.62
20	Q	1523	TGL	CB3-CB2-CB1	2.49	122.67	113.62
25	P	1265	PEK	C24-C23-C22	2.49	122.13	113.19
26	P	1270	CDL	OB6-CB5-C51	-2.49	106.14	111.50
25	P	1264	PEK	O03-C21-C22	-2.48	104.12	111.91
26	T	1269	CDL	C20-C19-C18	2.48	127.01	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	523	TGL	OG2-CG2-CG3	2.48	117.36	108.40
22	P	1271	CHD	O12-C12-C13	2.45	115.17	111.03
22	O	229	CHD	C14-C8-C9	-2.45	106.35	109.71
22	B	1086	CHD	C14-C8-C9	-2.45	106.35	109.71
22	B	1086	CHD	C9-C11-C12	2.45	117.53	114.30
22	B	1086	CHD	C5-C4-C3	2.43	116.32	112.76
18	N	1266	PGV	C01-O03-C19	-2.43	108.14	117.12
22	P	1525	CHD	C1-C10-C5	2.42	111.35	107.77
20	N	1521	TGL	CA8-CA7-CA6	-2.42	102.13	114.42
26	P	1270	CDL	CB6-OB8-CB7	-2.42	108.16	117.12
25	P	1265	PEK	P-O12-C04	2.42	133.48	121.59
17	N	515	HEA	C4D-CHA-C1A	2.40	125.72	122.56
20	D	523	TGL	OG2-CG2-CG1	2.40	117.08	108.40
26	P	1270	CDL	OA8-CA6-CA4	2.39	115.39	108.43
26	P	1270	CDL	C52-C51-CB5	-2.37	105.01	113.62
20	B	521	TGL	CA3-CA2-CA1	-2.36	105.02	113.62
17	N	515	HEA	C13-C14-C15	-2.36	121.97	127.66
20	L	522	TGL	C20-CA9-CA8	2.36	126.41	114.42
17	N	515	HEA	CMC-C2C-C3C	2.35	129.08	124.68
20	N	1522	TGL	C20-CA9-CA8	2.35	126.37	114.42
17	N	516	HEA	CHA-C4D-ND	2.35	126.98	124.43
20	L	522	TGL	C13-C12-C11	2.35	126.33	114.42
20	D	523	TGL	CB4-CB3-CB2	2.34	121.60	113.19
17	A	515	HEA	C13-C14-C15	-2.34	122.03	127.66
22	J	60	CHD	C19-C10-C1	-2.34	104.50	108.26
25	C	265	PEK	P-O12-C04	2.33	133.06	121.59
26	C	270	CDL	CB6-OB8-CB7	-2.32	108.54	117.12
20	Q	1523	TGL	OG2-CG2-CG1	2.31	116.77	108.40
20	Q	1523	TGL	CB4-CB3-CB2	2.31	121.50	113.19
17	A	516	HEA	C21-C20-C19	2.31	120.58	112.98
17	N	516	HEA	C21-C20-C19	2.31	120.57	112.98
25	P	1264	PEK	O03-C21-O04	2.31	129.41	123.59
20	D	523	TGL	CG2-OG2-CB1	2.31	123.47	117.79
25	T	263	PEK	P-O12-C04	2.30	132.90	121.59
23	M	526	DMU	O7-C10-O1	2.30	117.09	110.67
26	P	1270	CDL	OB6-CB5-OB7	2.29	129.25	123.70
17	A	516	HEA	CMC-C2C-C1C	-2.29	124.94	128.46
20	L	522	TGL	OG1-CG1-CG2	2.29	115.10	108.43
20	N	1521	TGL	CA3-CA2-CA1	-2.28	105.31	113.62
26	T	1269	CDL	OB8-CB6-CB4	2.28	115.07	108.43
26	T	1269	CDL	C19-C18-C17	2.27	125.97	114.42
17	A	515	HEA	CMC-C2C-C3C	2.27	128.93	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	N	1521	TGL	CG3-OG3-CC1	2.27	125.51	117.12
22	W	1060	CHD	C18-C13-C12	-2.26	106.76	109.07
17	N	516	HEA	C1D-ND-C4D	-2.26	102.74	105.07
18	N	1266	PGV	O03-C01-C02	2.26	115.00	108.43
20	B	521	TGL	CG3-OG3-CC1	2.26	125.47	117.12
22	C	525	CHD	C19-C10-C9	-2.25	108.09	111.18
18	A	525	PGV	O01-C1-C2	-2.24	106.67	111.50
20	L	522	TGL	CC7-CC6-CC5	2.23	125.75	114.42
26	G	269	CDL	C19-C18-C17	2.23	125.73	114.42
20	N	1522	TGL	OG1-CG1-CG2	2.23	114.91	108.43
18	C	267	PGV	O01-C1-C2	-2.20	106.77	111.50
25	C	264	PEK	O03-C21-O04	2.19	129.13	123.59
22	O	229	CHD	C9-C11-C12	2.19	117.19	114.30
20	N	1521	TGL	OG2-CG2-CG3	2.19	116.32	108.40
26	G	269	CDL	OB8-CB6-CB4	2.18	114.77	108.43
17	N	516	HEA	C26-C15-C16	2.17	118.92	115.27
25	C	265	PEK	O03-C01-C02	2.17	114.75	108.43
20	N	1521	TGL	C10-CB9-CB8	2.17	125.42	114.42
22	C	525	CHD	C15-C14-C13	-2.16	101.43	103.55
22	B	1086	CHD	C5-C6-C7	2.16	116.84	114.46
22	W	1060	CHD	C19-C10-C5	-2.16	106.70	110.36
26	T	1269	CDL	OB8-CB7-C71	-2.15	105.15	111.91
20	Q	1523	TGL	CG2-OG2-CB1	2.15	123.09	117.79
20	N	1521	TGL	CA6-CA5-CA4	-2.15	103.50	114.42
17	N	515	HEA	C20-C19-C18	2.15	125.47	121.12
18	N	1266	PGV	O01-C1-C2	-2.15	106.87	111.50
25	P	1265	PEK	O03-C01-C02	2.13	114.65	108.43
17	A	515	HEA	C27-C19-C20	2.13	118.86	115.27
25	G	1263	PEK	P-O12-C04	2.13	132.08	121.59
17	A	515	HEA	C17-C18-C19	-2.13	122.54	127.66
22	P	1271	CHD	C11-C12-C13	2.12	113.42	111.24
26	G	269	CDL	OB8-CB7-C71	-2.12	105.24	111.91
20	B	521	TGL	CA6-CA5-CA4	-2.11	103.69	114.42
20	B	521	TGL	OG1-CG1-CG2	2.11	114.58	108.43
22	J	60	CHD	C9-C11-C12	2.11	117.09	114.30
22	C	525	CHD	C1-C10-C5	2.11	110.88	107.77
22	J	60	CHD	C19-C10-C5	-2.11	106.79	110.36
20	D	523	TGL	CA3-CA2-CA1	-2.10	105.97	113.62
25	C	265	PEK	C2-C3-C4	2.10	116.97	113.23
17	A	515	HEA	C2D-C1D-ND	2.10	112.33	109.84
17	N	516	HEA	C4B-NB-C1B	-2.10	102.91	105.07
17	N	516	HEA	C2D-C1D-ND	2.09	112.31	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Q	1523	TGL	CA3-CA2-CA1	-2.09	106.03	113.62
20	B	521	TGL	C10-CB9-CB8	2.09	125.02	114.42
22	C	525	CHD	C1-C2-C3	2.09	113.14	110.47
17	A	516	HEA	C4A-CHB-C1B	2.09	125.31	122.56
22	W	1060	CHD	C19-C10-C1	-2.08	104.91	108.26
22	C	271	CHD	C14-C8-C7	2.08	114.56	111.81
20	B	521	TGL	OG2-CG2-CG3	2.07	115.90	108.40
18	A	525	PGV	C01-O03-C19	-2.07	109.47	117.12
20	B	521	TGL	CB9-CB8-CB7	-2.06	103.95	114.42
22	P	1525	CHD	C2-C1-C10	2.06	116.31	112.78
25	P	1265	PEK	C2-C3-C4	2.05	116.89	113.23
17	A	515	HEA	C4A-CHB-C1B	2.04	125.25	122.56
26	T	1269	CDL	C83-C82-C81	2.04	124.79	114.42
22	B	1086	CHD	C14-C8-C7	2.03	114.50	111.81
22	B	1086	CHD	C17-C13-C14	2.03	102.14	100.09
20	N	1522	TGL	CC7-CC6-CC5	2.03	124.72	114.42
17	N	515	HEA	C4A-CHB-C1B	2.02	125.23	122.56
17	N	516	HEA	C3B-C4B-NB	2.02	112.23	109.84
17	N	515	HEA	C26-C15-C14	-2.02	118.49	123.68
20	N	1521	TGL	OG1-CG1-CG2	2.02	114.31	108.43
26	G	269	CDL	C80-C79-C78	2.01	124.64	114.42
22	W	1060	CHD	C9-C11-C12	2.01	116.95	114.30
22	P	1271	CHD	C14-C8-C7	2.01	114.47	111.81
18	A	524	PGV	P-O12-C04	2.00	133.42	121.68
17	A	516	HEA	C3C-C4C-NC	2.00	111.80	109.21

All (42) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	271	CHD	C12
22	C	271	CHD	C3
22	C	271	CHD	C8
22	C	271	CHD	C14
22	C	271	CHD	C9
22	J	60	CHD	C12
22	J	60	CHD	C8
22	J	60	CHD	C17
22	J	60	CHD	C14
22	J	60	CHD	C9
22	P	1271	CHD	C12
22	P	1271	CHD	C3
22	P	1271	CHD	C8

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Mol	Chain	Res	Type	Atom
22	P	1271	CHD	C14
22	P	1271	CHD	C9
22	W	1060	CHD	C12
22	W	1060	CHD	C8
22	W	1060	CHD	C17
22	W	1060	CHD	C14
22	W	1060	CHD	C9
23	C	272	DMU	C5
23	C	272	DMU	C4
23	C	272	DMU	C6
23	C	272	DMU	C10
23	C	272	DMU	C9
23	C	272	DMU	C2
23	M	526	DMU	C5
23	M	526	DMU	C4
23	M	526	DMU	C6
23	M	526	DMU	C9
23	M	526	DMU	C2
23	P	1272	DMU	C5
23	P	1272	DMU	C4
23	P	1272	DMU	C6
23	P	1272	DMU	C10
23	P	1272	DMU	C9
23	P	1272	DMU	C2
23	Z	1526	DMU	C5
23	Z	1526	DMU	C4
23	Z	1526	DMU	C6
23	Z	1526	DMU	C9
23	Z	1526	DMU	C2

All (865) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	524	PGV	C04-O12-P-O11
18	A	524	PGV	C04-O12-P-O13
18	A	524	PGV	C04-O12-P-O14
18	A	524	PGV	C02-C03-O11-P
18	A	524	PGV	C05-C04-O12-P
18	A	524	PGV	O02-C1-O01-C02
18	A	524	PGV	C20-C19-O03-C01
18	C	268	PGV	C04-O12-P-O11
18	C	268	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
18	C	268	PGV	C04-O12-P-O14
18	P	1268	PGV	C04-O12-P-O11
18	P	1268	PGV	C04-O12-P-O13
18	P	1268	PGV	C04-O12-P-O14
18	Z	1524	PGV	C04-O12-P-O11
18	Z	1524	PGV	C04-O12-P-O13
18	Z	1524	PGV	C04-O12-P-O14
18	Z	1524	PGV	C02-C03-O11-P
18	Z	1524	PGV	C05-C04-O12-P
18	Z	1524	PGV	O02-C1-O01-C02
18	Z	1524	PGV	C20-C19-O03-C01
21	B	230	PSC	C03-O11-P-O14
21	B	230	PSC	C04-O12-P-O14
21	B	230	PSC	O02-C1-O01-C02
21	O	1230	PSC	C03-O11-P-O14
21	O	1230	PSC	C04-O12-P-O14
22	J	60	CHD	C16-C17-C20-C21
22	J	60	CHD	C16-C17-C20-C22
22	W	1060	CHD	C16-C17-C20-C21
22	W	1060	CHD	C16-C17-C20-C22
23	M	526	DMU	O5-C6-O16-C18
23	Z	1526	DMU	O5-C6-O16-C18
25	C	265	PEK	C03-O11-P-O13
25	C	265	PEK	C04-O12-P-O11
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C04-O12-P-O14
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
25	P	1265	PEK	C03-O11-P-O13
25	P	1265	PEK	C04-O12-P-O11
25	P	1265	PEK	C04-O12-P-O13
25	P	1265	PEK	C04-O12-P-O14
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
26	C	270	CDL	CA2-C1-CB2-OB2
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
26	G	269	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
26	P	1270	CDL	CA2-C1-CB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	T	1269	CDL	OB6-CB4-CB6-OB8
18	A	524	PGV	O04-C19-O03-C01
18	Z	1524	PGV	O04-C19-O03-C01
20	D	523	TGL	OC1-CC1-OG3-CG3
20	Q	1523	TGL	OC1-CC1-OG3-CG3
20	B	521	TGL	OB1-CB1-OG2-CG2
20	N	1521	TGL	OB1-CB1-OG2-CG2
21	O	1230	PSC	O02-C1-O01-C02
26	C	270	CDL	OA7-CA5-OA6-CA4
18	A	524	PGV	C2-C1-O01-C02
18	Z	1524	PGV	C2-C1-O01-C02
26	C	270	CDL	C40-C41-C42-C43
26	C	270	CDL	C57-C58-C59-C60
26	C	270	CDL	C60-C61-C62-C63
26	C	270	CDL	C80-C81-C82-C83
26	G	269	CDL	C17-C18-C19-C20
26	G	269	CDL	C20-C21-C22-C23
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	C57-C58-C59-C60
26	G	269	CDL	C77-C78-C79-C80
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C60-C61-C62-C63
26	P	1270	CDL	C80-C81-C82-C83
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C77-C78-C79-C80
20	D	523	TGL	CC2-CC1-OG3-CG3
20	Q	1523	TGL	CC2-CC1-OG3-CG3
26	G	269	CDL	C31-CA7-OA8-CA6
26	T	1269	CDL	C31-CA7-OA8-CA6
23	C	272	DMU	O6-C11-C9-O1
23	P	1272	DMU	O6-C11-C9-O1
20	B	521	TGL	C16-C15-CC9-CC8
20	N	1521	TGL	C16-C15-CC9-CC8
26	C	270	CDL	C20-C21-C22-C23
26	C	270	CDL	C77-C78-C79-C80
26	P	1270	CDL	C20-C21-C22-C23
26	P	1270	CDL	C77-C78-C79-C80
26	T	1269	CDL	C40-C41-C42-C43
26	T	1269	CDL	C60-C61-C62-C63
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C80-C81-C82-C83
26	T	1269	CDL	C80-C81-C82-C83
26	P	1270	CDL	OA7-CA5-OA6-CA4
20	B	521	TGL	OA1-CA1-OG1-CG1
20	N	1521	TGL	OA1-CA1-OG1-CG1
20	N	1522	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	OA9-CA7-OA8-CA6
20	N	1522	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C37-C38-C39-C40
26	G	269	CDL	C60-C61-C62-C63
26	P	1270	CDL	C37-C38-C39-C40
26	T	1269	CDL	C37-C38-C39-C40
20	L	522	TGL	C21-C20-CA9-CA8
26	P	1270	CDL	C17-C18-C19-C20
18	P	1268	PGV	O12-C04-C05-O05
26	G	269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CA2-OA2
26	C	270	CDL	C17-C18-C19-C20
20	L	522	TGL	OA1-CA1-OG1-CG1
23	M	526	DMU	O6-C11-C9-C8
20	B	521	TGL	CB2-CB1-OG2-CG2
20	N	1521	TGL	CB2-CB1-OG2-CG2
20	Q	1523	TGL	C21-C20-CA9-CA8
23	Z	1526	DMU	O6-C11-C9-C8
20	D	523	TGL	C21-C20-CA9-CA8

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Mol	Chain	Res	Type	Atoms
20	D	523	TGL	C11-C10-CB9-CB8
20	Q	1523	TGL	C11-C10-CB9-CB8
20	Q	1523	TGL	C16-C15-CC9-CC8
20	B	521	TGL	C21-C20-CA9-CA8
20	B	521	TGL	C11-C10-CB9-CB8
20	D	523	TGL	C16-C15-CC9-CC8
20	L	522	TGL	C11-C10-CB9-CB8
20	N	1521	TGL	C21-C20-CA9-CA8
20	N	1521	TGL	C11-C10-CB9-CB8
20	N	1522	TGL	C11-C10-CB9-CB8
20	L	522	TGL	C16-C15-CC9-CC8
20	N	1522	TGL	C16-C15-CC9-CC8
20	B	521	TGL	CA2-CA1-OG1-CG1
20	N	1521	TGL	CA2-CA1-OG1-CG1
20	N	1522	TGL	CA2-CA1-OG1-CG1
18	A	524	PGV	O12-C04-C05-C06
18	Z	1524	PGV	O12-C04-C05-C06
26	G	269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CB2-C1-CA2-OA2
20	D	523	TGL	CA2-CA1-OG1-CG1
20	L	522	TGL	CA2-CA1-OG1-CG1
20	Q	1523	TGL	CA2-CA1-OG1-CG1
21	B	230	PSC	C20-C19-O03-C01
21	O	1230	PSC	C20-C19-O03-C01
22	J	60	CHD	C13-C17-C20-C22
22	W	1060	CHD	C13-C17-C20-C22
26	C	270	CDL	O1-C1-CB2-OB2
26	G	269	CDL	O1-C1-CB2-OB2
26	P	1270	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CB2-OB2
23	C	272	DMU	C1-C6-O16-C18
23	P	1272	DMU	C1-C6-O16-C18
25	G	1263	PEK	C28-C29-C30-C31
25	T	263	PEK	C28-C29-C30-C31
21	B	230	PSC	C1-C2-C3-C4
21	O	1230	PSC	C1-C2-C3-C4
25	C	265	PEK	C21-C22-C23-C24
25	P	1265	PEK	C21-C22-C23-C24
23	M	526	DMU	O5-C4-C57-O61
22	W	1060	CHD	C21-C20-C22-C23
21	O	1230	PSC	C20-C21-C22-C23
18	Z	1524	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
21	B	230	PSC	C20-C21-C22-C23
18	P	1268	PGV	O05-C05-C06-O06
18	A	524	PGV	C19-C20-C21-C22
23	P	1272	DMU	O5-C4-C57-O61
23	Z	1526	DMU	O5-C4-C57-O61
20	L	522	TGL	CC3-CC4-CC5-CC6
21	B	230	PSC	C2-C1-O01-C02
21	O	1230	PSC	C2-C1-O01-C02
20	D	523	TGL	OA1-CA1-OG1-CG1
20	Q	1523	TGL	OA1-CA1-OG1-CG1
23	C	272	DMU	O5-C4-C57-O61
22	P	1271	CHD	C17-C20-C22-C23
22	W	1060	CHD	C17-C20-C22-C23
22	C	271	CHD	C21-C20-C22-C23
22	J	60	CHD	C21-C20-C22-C23
22	P	1271	CHD	C21-C20-C22-C23
21	B	230	PSC	O04-C19-O03-C01
23	Z	1526	DMU	O16-C18-C19-C22
18	P	1268	PGV	C1-C2-C3-C4
26	P	1270	CDL	CB7-C71-C72-C73
18	C	268	PGV	O12-C04-C05-O05
20	N	1522	TGL	CC3-CC4-CC5-CC6
22	J	60	CHD	C13-C17-C20-C21
22	W	1060	CHD	C13-C17-C20-C21
21	O	1230	PSC	O04-C19-O03-C01
26	C	270	CDL	CB7-C71-C72-C73
22	C	271	CHD	C17-C20-C22-C23
22	J	60	CHD	C17-C20-C22-C23
23	M	526	DMU	O16-C18-C19-C22
26	T	1269	CDL	C11-CA5-OA6-CA4
21	B	230	PSC	C22-C23-C24-C25
25	G	1263	PEK	C03-O11-P-O12
25	T	263	PEK	C03-O11-P-O12
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CB2-OB2-PB2-OB5
26	G	269	CDL	CB3-OB5-PB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB3-OB5-PB2-OB2
18	C	268	PGV	C1-C2-C3-C4
25	T	263	PEK	C1-C2-C3-C4
18	C	268	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
18	P	1268	PGV	O12-C04-C05-C06
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA2-C1-CB2-OB2
26	G	269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OA7-CA5-OA6-CA4
26	G	269	CDL	CA5-C11-C12-C13
26	G	269	CDL	C73-C74-C75-C76
26	T	1269	CDL	C73-C74-C75-C76
23	C	272	DMU	C3-C4-C57-O61
23	P	1272	DMU	C3-C4-C57-O61
21	O	1230	PSC	C22-C23-C24-C25
26	P	1270	CDL	C51-C52-C53-C54
18	C	268	PGV	C2-C1-O01-C02
18	P	1268	PGV	C2-C1-O01-C02
26	G	269	CDL	C11-CA5-OA6-CA4
18	C	268	PGV	C22-C23-C24-C25
18	N	1266	PGV	C6-C7-C8-C9
18	P	1268	PGV	C22-C23-C24-C25
18	Z	1524	PGV	C4-C5-C6-C7
21	B	230	PSC	C2-C3-C4-C5
21	B	230	PSC	C29-C30-C31-C32
21	O	1230	PSC	C2-C3-C4-C5
26	C	270	CDL	C13-C14-C15-C16
18	A	524	PGV	C4-C5-C6-C7
18	A	525	PGV	C6-C7-C8-C9
18	C	268	PGV	C13-C14-C15-C16
18	P	1268	PGV	C13-C14-C15-C16
21	O	1230	PSC	C29-C30-C31-C32
25	P	1265	PEK	C25-C26-C27-C28
25	T	263	PEK	C29-C30-C31-C32
26	C	270	CDL	C51-C52-C53-C54
26	C	270	CDL	C59-C60-C61-C62
26	P	1270	CDL	C13-C14-C15-C16
26	P	1270	CDL	C59-C60-C61-C62
18	P	1268	PGV	O02-C1-O01-C02
25	C	265	PEK	C25-C26-C27-C28
25	G	1263	PEK	C29-C30-C31-C32
18	N	1266	PGV	C29-C30-C31-C32
23	Z	1526	DMU	C25-C28-C31-C34
26	P	1270	CDL	C16-C17-C18-C19
26	T	1269	CDL	C72-C73-C74-C75
18	A	524	PGV	O12-C04-C05-O05

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Mol	Chain	Res	Type	Atoms
18	Z	1524	PGV	O12-C04-C05-O05
18	A	525	PGV	C23-C24-C25-C26
18	N	1266	PGV	C23-C24-C25-C26
23	M	526	DMU	C25-C28-C31-C34
26	C	270	CDL	C16-C17-C18-C19
26	G	269	CDL	C72-C73-C74-C75
26	T	1269	CDL	C58-C59-C60-C61
25	C	264	PEK	C1-C2-C3-C4
25	G	1263	PEK	C1-C2-C3-C4
26	T	1269	CDL	CA5-C11-C12-C13
18	A	525	PGV	C29-C30-C31-C32
18	C	268	PGV	C3-C4-C5-C6
18	C	268	PGV	C24-C25-C26-C27
18	P	1268	PGV	C3-C4-C5-C6
18	P	1268	PGV	C24-C25-C26-C27
25	C	264	PEK	C23-C24-C25-C26
26	G	269	CDL	C58-C59-C60-C61
26	C	270	CDL	C55-C56-C57-C58
25	P	1264	PEK	C1-C2-C3-C4
26	P	1270	CDL	CA5-C11-C12-C13
18	C	267	PGV	C7-C8-C9-C10
25	G	1263	PEK	C27-C28-C29-C30
25	P	1264	PEK	C23-C24-C25-C26
26	G	269	CDL	C13-C14-C15-C16
26	T	1269	CDL	C13-C14-C15-C16
18	N	1266	PGV	C5-C6-C7-C8
18	P	1267	PGV	C7-C8-C9-C10
25	P	1265	PEK	C31-C32-C33-C34
26	P	1270	CDL	C55-C56-C57-C58
18	C	268	PGV	C04-C05-C06-O06
18	P	1268	PGV	C04-C05-C06-O06
18	C	268	PGV	O02-C1-O01-C02
18	A	525	PGV	C5-C6-C7-C8
25	C	265	PEK	C31-C32-C33-C34
25	T	263	PEK	C27-C28-C29-C30
26	C	270	CDL	CA5-C11-C12-C13
18	C	268	PGV	C27-C28-C29-C30
20	L	522	TGL	CB4-CB5-CB6-CB7
26	T	1269	CDL	C56-C57-C58-C59
23	C	272	DMU	O5-C6-O16-C18
23	P	1272	DMU	O5-C6-O16-C18
18	C	267	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	P	1267	PGV	C22-C23-C24-C25
18	P	1268	PGV	C27-C28-C29-C30
25	P	1265	PEK	C16-C17-C18-C19
26	C	270	CDL	C74-C75-C76-C77
26	G	269	CDL	C56-C57-C58-C59
18	A	524	PGV	C22-C23-C24-C25
18	Z	1524	PGV	C28-C29-C30-C31
20	N	1522	TGL	CB4-CB5-CB6-CB7
25	C	265	PEK	C16-C17-C18-C19
26	C	270	CDL	C72-C73-C74-C75
26	P	1270	CDL	C75-C76-C77-C78
18	A	524	PGV	C28-C29-C30-C31
18	A	525	PGV	C7-C8-C9-C10
18	N	1266	PGV	C7-C8-C9-C10
18	Z	1524	PGV	C22-C23-C24-C25
25	P	1264	PEK	C22-C23-C24-C25
26	P	1270	CDL	C72-C73-C74-C75
25	C	264	PEK	C22-C21-O03-C01
26	C	270	CDL	C75-C76-C77-C78
25	C	264	PEK	C22-C23-C24-C25
25	P	1264	PEK	C31-C32-C33-C34
26	P	1270	CDL	C74-C75-C76-C77
26	G	269	CDL	C79-C80-C81-C82
26	T	1269	CDL	C79-C80-C81-C82
25	C	264	PEK	O03-C01-C02-C03
25	P	1264	PEK	O03-C01-C02-C03
26	T	1269	CDL	C43-C44-C45-C46
25	C	264	PEK	C31-C32-C33-C34
25	T	263	PEK	C25-C26-C27-C28
25	C	264	PEK	C16-C17-C18-C19
25	G	1263	PEK	C25-C26-C27-C28
25	P	1264	PEK	C16-C17-C18-C19
18	C	268	PGV	O05-C05-C06-O06
25	G	1263	PEK	C26-C27-C28-C29
25	T	263	PEK	C26-C27-C28-C29
26	P	1270	CDL	C73-C74-C75-C76
21	B	230	PSC	C13-C14-C15-C16
20	B	521	TGL	OC1-CC1-OG3-CG3
23	C	272	DMU	C25-C28-C31-C34
26	G	269	CDL	C43-C44-C45-C46
23	P	1272	DMU	C25-C28-C31-C34
26	C	270	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C71-C72-C73-C74
20	N	1521	TGL	OC1-CC1-OG3-CG3
25	P	1264	PEK	O04-C21-O03-C01
26	C	270	CDL	C71-C72-C73-C74
18	P	1267	PGV	C25-C26-C27-C28
26	C	270	CDL	C36-C37-C38-C39
25	C	264	PEK	O04-C21-O03-C01
18	A	524	PGV	C5-C6-C7-C8
18	C	267	PGV	C25-C26-C27-C28
18	Z	1524	PGV	C24-C25-C26-C27
26	G	269	CDL	C53-C54-C55-C56
21	O	1230	PSC	C04-C05-N-C08
18	A	524	PGV	C24-C25-C26-C27
18	C	268	PGV	C25-C26-C27-C28
18	P	1268	PGV	C25-C26-C27-C28
26	P	1270	CDL	C36-C37-C38-C39
25	P	1264	PEK	C22-C21-O03-C01
26	P	1270	CDL	C51-CB5-OB6-CB4
18	P	1268	PGV	C28-C29-C30-C31
26	G	269	CDL	C21-C22-C23-C24
17	A	515	HEA	C21-C22-C23-C25
18	Z	1524	PGV	C5-C6-C7-C8
20	B	521	TGL	CB6-CB7-CB8-CB9
20	N	1522	TGL	CC2-CC3-CC4-CC5
26	P	1270	CDL	C11-C12-C13-C14
18	C	268	PGV	C12-C13-C14-C15
18	P	1268	PGV	C12-C13-C14-C15
21	O	1230	PSC	C13-C14-C15-C16
26	C	270	CDL	OB7-CB5-OB6-CB4
26	P	1270	CDL	OB7-CB5-OB6-CB4
26	G	269	CDL	CB5-C51-C52-C53
26	T	1269	CDL	CB5-C51-C52-C53
18	C	268	PGV	C28-C29-C30-C31
20	L	522	TGL	CC2-CC3-CC4-CC5
26	T	1269	CDL	C21-C22-C23-C24
26	T	1269	CDL	C53-C54-C55-C56
23	Z	1526	DMU	C22-C25-C28-C31
26	C	270	CDL	C11-C12-C13-C14
26	P	1270	CDL	C32-C33-C34-C35
25	C	265	PEK	C29-C30-C31-C32
21	B	230	PSC	C14-C15-C16-C17
21	B	230	PSC	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
21	O	1230	PSC	C14-C15-C16-C17
26	C	270	CDL	C32-C33-C34-C35
26	C	270	CDL	C51-CB5-OB6-CB4
26	C	270	CDL	C18-C19-C20-C21
26	P	1270	CDL	C18-C19-C20-C21
18	P	1267	PGV	C23-C24-C25-C26
21	O	1230	PSC	C27-C28-C29-C30
23	M	526	DMU	C22-C25-C28-C31
18	C	267	PGV	C23-C24-C25-C26
20	N	1521	TGL	CB6-CB7-CB8-CB9
25	G	1263	PEK	O03-C01-C02-O01
25	T	263	PEK	O03-C01-C02-O01
26	C	270	CDL	C63-C64-C65-C66
21	B	230	PSC	C04-C05-N-C08
26	C	270	CDL	C61-C62-C63-C64
26	P	1270	CDL	C63-C64-C65-C66
18	A	524	PGV	C12-C13-C14-C15
18	C	268	PGV	C11-C10-C9-C8
18	P	1268	PGV	C11-C10-C9-C8
25	G	1263	PEK	C2-C3-C4-C5
25	G	1263	PEK	C15-C16-C17-C18
21	B	230	PSC	C24-C25-C26-C27
21	O	1230	PSC	C24-C25-C26-C27
25	P	1265	PEK	C29-C30-C31-C32
26	P	1270	CDL	C61-C62-C63-C64
26	T	1269	CDL	C33-C34-C35-C36
23	Z	1526	DMU	C3-C4-C57-O61
26	G	269	CDL	C33-C34-C35-C36
21	B	230	PSC	C03-O11-P-O12
21	O	1230	PSC	C03-O11-P-O12
21	O	1230	PSC	C04-O12-P-O11
25	C	265	PEK	C03-O11-P-O12
25	P	1265	PEK	C03-O11-P-O12
21	O	1230	PSC	C23-C24-C25-C26
21	B	230	PSC	C23-C24-C25-C26
20	N	1522	TGL	CC2-CC1-OG3-CG3
25	G	1263	PEK	C01-C02-C03-O11
25	T	263	PEK	C01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-CB6
26	P	1270	CDL	OB5-CB3-CB4-CB6
26	T	1269	CDL	OA5-CA3-CA4-CA6
25	C	264	PEK	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
18	C	268	PGV	C30-C31-C32-C33
18	P	1268	PGV	C30-C31-C32-C33
18	Z	1524	PGV	C12-C13-C14-C15
25	T	263	PEK	C2-C3-C4-C5
26	G	269	CDL	C82-C83-C84-C85
26	C	270	CDL	C64-C65-C66-C67
26	P	1270	CDL	C64-C65-C66-C67
25	P	1265	PEK	C32-C33-C34-C35
21	B	230	PSC	O03-C01-C02-C03
21	O	1230	PSC	O03-C01-C02-C03
25	G	1263	PEK	O03-C01-C02-C03
25	T	263	PEK	O03-C01-C02-C03
26	C	270	CDL	CB3-CB4-CB6-OB8
26	G	269	CDL	CB3-CB4-CB6-OB8
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CB3-CB4-CB6-OB8
18	C	268	PGV	C31-C32-C33-C34
18	C	268	PGV	C14-C15-C16-C17
26	P	1270	CDL	C44-C45-C46-C47
18	P	1268	PGV	C14-C15-C16-C17
26	T	1269	CDL	C82-C83-C84-C85
26	C	270	CDL	C44-C45-C46-C47
18	C	267	PGV	C11-C10-C9-C8
18	P	1267	PGV	C11-C10-C9-C8
18	C	267	PGV	C15-C16-C17-C18
25	C	265	PEK	C32-C33-C34-C35
25	P	1264	PEK	C24-C25-C26-C27
26	C	270	CDL	C84-C85-C86-C87
26	P	1270	CDL	C84-C85-C86-C87
18	P	1267	PGV	C15-C16-C17-C18
18	P	1268	PGV	C31-C32-C33-C34
26	T	1269	CDL	C35-C36-C37-C38
20	B	521	TGL	CC2-CC1-OG3-CG3
20	N	1521	TGL	CC2-CC1-OG3-CG3
26	C	270	CDL	C38-C39-C40-C41
26	G	269	CDL	C35-C36-C37-C38
18	A	524	PGV	C03-C02-O01-C1
18	Z	1524	PGV	C03-C02-O01-C1
23	C	272	DMU	C34-C37-C40-C43
23	P	1272	DMU	C34-C37-C40-C43
18	P	1267	PGV	C13-C14-C15-C16
26	P	1270	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C38-C39-C40-C41
20	L	522	TGL	CC2-CC1-OG3-CG3
26	C	270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	OA5-CA3-CA4-OA6
18	C	267	PGV	C13-C14-C15-C16
18	P	1268	PGV	C5-C6-C7-C8
25	T	263	PEK	C34-C35-C36-C37
26	C	270	CDL	C34-C35-C36-C37
21	B	230	PSC	O03-C01-C02-O01
25	G	1263	PEK	C16-C17-C18-C19
17	N	515	HEA	C21-C22-C23-C25
18	C	268	PGV	C5-C6-C7-C8
26	G	269	CDL	C52-C53-C54-C55
26	P	1270	CDL	C42-C43-C44-C45
18	C	268	PGV	C26-C27-C28-C29
18	N	1266	PGV	C30-C31-C32-C33
25	C	264	PEK	C25-C26-C27-C28
25	G	1263	PEK	C34-C35-C36-C37
26	T	1269	CDL	C52-C53-C54-C55
21	B	230	PSC	C3-C4-C5-C6
26	G	269	CDL	C41-C42-C43-C44
25	P	1264	PEK	C25-C26-C27-C28
18	P	1268	PGV	C26-C27-C28-C29
25	C	264	PEK	C24-C25-C26-C27
26	P	1270	CDL	C78-C79-C80-C81
26	T	1269	CDL	C19-C20-C21-C22
26	T	1269	CDL	C71-C72-C73-C74
26	T	1269	CDL	C31-C32-C33-C34
25	G	1263	PEK	C22-C21-O03-C01
26	G	269	CDL	C31-C32-C33-C34
26	C	270	CDL	C42-C43-C44-C45
21	O	1230	PSC	C04-C05-N-C07
26	G	269	CDL	OA5-CA3-CA4-CA6
21	O	1230	PSC	C3-C4-C5-C6
26	C	270	CDL	C78-C79-C80-C81
26	T	1269	CDL	C41-C42-C43-C44
25	T	263	PEK	C16-C17-C18-C19
26	G	269	CDL	C44-C45-C46-C47
26	G	269	CDL	C71-C72-C73-C74
26	T	1269	CDL	C44-C45-C46-C47
18	A	525	PGV	C30-C31-C32-C33
26	G	269	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C39-C40-C41-C42
26	C	270	CDL	C43-C44-C45-C46
25	T	263	PEK	C22-C21-O03-C01
25	C	264	PEK	C17-C18-C19-C20
25	P	1264	PEK	C17-C18-C19-C20
18	Z	1524	PGV	O03-C01-C02-C03
26	G	269	CDL	CA3-CA4-CA6-OA8
26	T	1269	CDL	CA3-CA4-CA6-OA8
20	N	1522	TGL	OB1-CB1-OG2-CG2
26	P	1270	CDL	C39-C40-C41-C42
18	P	1268	PGV	C4-C5-C6-C7
26	P	1270	CDL	C43-C44-C45-C46
25	G	1263	PEK	O04-C21-O03-C01
21	B	230	PSC	C04-O12-P-O11
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
25	C	265	PEK	C11-C12-C13-C14
25	G	1263	PEK	C6-C7-C8-C9
25	P	1264	PEK	C5-C6-C7-C8
25	P	1264	PEK	C9-C10-C11-C12
25	P	1265	PEK	C11-C12-C13-C14
25	T	263	PEK	C6-C7-C8-C9
18	C	268	PGV	C4-C5-C6-C7
18	C	268	PGV	C20-C19-O03-C01
25	T	263	PEK	C15-C16-C17-C18
25	T	263	PEK	O04-C21-O03-C01
18	A	524	PGV	C20-C21-C22-C23
18	C	268	PGV	C15-C16-C17-C18
21	O	1230	PSC	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
23	M	526	DMU	C3-C4-C57-O61
20	L	522	TGL	OB1-CB1-OG2-CG2
18	C	268	PGV	C23-C24-C25-C26
25	G	1263	PEK	C02-C03-O11-P
25	T	263	PEK	C02-C03-O11-P
18	P	1268	PGV	C23-C24-C25-C26
18	P	1268	PGV	C15-C16-C17-C18
25	P	1264	PEK	C35-C36-C37-C38
18	C	268	PGV	O04-C19-O03-C01
26	G	269	CDL	C14-C15-C16-C17
18	P	1267	PGV	C31-C32-C33-C34
18	C	267	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
18	P	1267	PGV	C20-C21-C22-C23
25	P	1264	PEK	C26-C27-C28-C29
18	C	267	PGV	C31-C32-C33-C34
25	C	264	PEK	C26-C27-C28-C29
25	G	1263	PEK	C30-C31-C32-C33
18	P	1268	PGV	C20-C19-O03-C01
18	A	525	PGV	C25-C26-C27-C28
25	T	263	PEK	C30-C31-C32-C33
18	A	524	PGV	O03-C01-C02-C03
26	T	1269	CDL	CB4-CB3-OB5-PB2
26	C	270	CDL	OB5-CB3-CB4-OB6
26	P	1270	CDL	OB5-CB3-CB4-OB6
22	C	271	CHD	C13-C17-C20-C21
21	B	230	PSC	C31-C32-C33-C34
26	T	1269	CDL	C14-C15-C16-C17
18	P	1268	PGV	O04-C19-O03-C01
18	N	1266	PGV	C25-C26-C27-C28
26	P	1270	CDL	OB6-CB4-CB6-OB8
20	B	521	TGL	C12-C13-C14-C29
22	P	1271	CHD	C13-C17-C20-C21
21	O	1230	PSC	C31-C32-C33-C34
18	Z	1524	PGV	C20-C21-C22-C23
26	T	1269	CDL	C36-C37-C38-C39
23	P	1272	DMU	C22-C25-C28-C31
26	G	269	CDL	C24-C25-C26-C27
25	C	265	PEK	C30-C31-C32-C33
20	B	521	TGL	CG2-CG3-OG3-CC1
26	C	270	CDL	CA3-OA5-PA1-OA2
26	G	269	CDL	CB2-OB2-PB2-OB5
26	P	1270	CDL	CA3-OA5-PA1-OA2
26	T	1269	CDL	CB2-OB2-PB2-OB5
25	P	1265	PEK	C30-C31-C32-C33
18	C	267	PGV	C02-C03-O11-P
18	P	1267	PGV	C02-C03-O11-P
26	G	269	CDL	CB4-CB3-OB5-PB2
20	N	1521	TGL	C12-C13-C14-C29
26	G	269	CDL	C36-C37-C38-C39
21	B	230	PSC	C03-O11-P-O13
21	B	230	PSC	C04-O12-P-O13
21	B	230	PSC	C04-C05-N-C07
21	O	1230	PSC	C03-O11-P-O13
21	O	1230	PSC	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
21	O	1230	PSC	C04-C05-N-C06
25	C	265	PEK	C03-O11-P-O14
25	G	1263	PEK	C03-O11-P-O13
25	P	1265	PEK	C03-O11-P-O14
25	T	263	PEK	C03-O11-P-O13
17	N	515	HEA	C15-C16-C17-C18
22	C	271	CHD	C13-C17-C20-C22
20	N	1522	TGL	CC5-CC6-CC7-CC8
18	Z	1524	PGV	C26-C27-C28-C29
20	Q	1523	TGL	CA9-C20-C21-C22
20	N	1522	TGL	CC7-CC8-CC9-C15
23	C	272	DMU	C22-C25-C28-C31
26	C	270	CDL	C52-C53-C54-C55
18	C	267	PGV	C24-C25-C26-C27
18	N	1266	PGV	C26-C27-C28-C29
25	T	263	PEK	O01-C02-C03-O11
26	C	270	CDL	C24-C25-C26-C27
26	G	269	CDL	C64-C65-C66-C67
26	P	1270	CDL	C24-C25-C26-C27
22	P	1271	CHD	C13-C17-C20-C22
18	P	1267	PGV	C24-C25-C26-C27
20	D	523	TGL	CA9-C20-C21-C22
26	T	1269	CDL	C12-C13-C14-C15
21	B	230	PSC	C04-C05-N-C06
26	T	1269	CDL	C64-C65-C66-C67
25	C	264	PEK	C32-C33-C34-C35
18	A	524	PGV	O03-C01-C02-O01
18	Z	1524	PGV	O03-C01-C02-O01
20	D	523	TGL	OG2-CG2-CG3-OG3
20	Q	1523	TGL	OG2-CG2-CG3-OG3
25	C	264	PEK	O03-C01-C02-O01
25	P	1264	PEK	O03-C01-C02-O01
26	G	269	CDL	OA6-CA4-CA6-OA8
26	T	1269	CDL	OA6-CA4-CA6-OA8
26	G	269	CDL	C12-C13-C14-C15
18	A	524	PGV	C26-C27-C28-C29
22	P	1271	CHD	C16-C17-C20-C22
20	L	522	TGL	CC7-CC8-CC9-C15
17	A	515	HEA	C15-C16-C17-C18
25	C	264	PEK	C27-C28-C29-C30
25	C	265	PEK	C17-C18-C19-C20
25	P	1264	PEK	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
17	N	515	HEA	C17-C18-C19-C27
26	G	269	CDL	CB7-C71-C72-C73
25	P	1265	PEK	C17-C18-C19-C20
26	T	1269	CDL	C24-C25-C26-C27
22	C	271	CHD	C16-C17-C20-C22
25	G	1263	PEK	C21-C22-C23-C24
25	T	263	PEK	C21-C22-C23-C24
26	P	1270	CDL	C52-C53-C54-C55
26	G	269	CDL	C38-C39-C40-C41
20	Q	1523	TGL	CG1-CG2-OG2-CB1
21	B	230	PSC	C03-C02-O01-C1
21	O	1230	PSC	C03-C02-O01-C1
26	C	270	CDL	OA5-CA3-CA4-CA6
26	P	1270	CDL	OA5-CA3-CA4-CA6
20	N	1521	TGL	CG2-CG3-OG3-CC1
25	G	1263	PEK	O01-C02-C03-O11
26	T	1269	CDL	OA5-CA3-CA4-OA6
18	A	525	PGV	C26-C27-C28-C29
21	O	1230	PSC	C4-C5-C6-C7
20	L	522	TGL	CC5-CC6-CC7-CC8
18	A	524	PGV	C03-O11-P-O12
18	Z	1524	PGV	C03-O11-P-O12
21	B	230	PSC	C4-C5-C6-C7
26	G	269	CDL	C11-C12-C13-C14
18	A	525	PGV	C9-C10-C11-C12
18	N	1266	PGV	C9-C10-C11-C12
25	T	263	PEK	C32-C33-C34-C35
25	G	1263	PEK	C32-C33-C34-C35
22	P	1271	CHD	C16-C17-C20-C21
21	B	230	PSC	C15-C16-C17-C18
25	P	1264	PEK	C32-C33-C34-C35
26	T	1269	CDL	C38-C39-C40-C41
26	T	1269	CDL	C59-C60-C61-C62
18	Z	1524	PGV	C11-C10-C9-C8
26	T	1269	CDL	C11-C12-C13-C14
18	A	525	PGV	C19-C20-C21-C22
22	C	271	CHD	C16-C17-C20-C21
18	C	267	PGV	C14-C15-C16-C17
17	A	516	HEA	CAA-CBA-CGA-O1A
18	A	524	PGV	C11-C10-C9-C8
25	C	264	PEK	C3-C4-C5-C6
21	O	1230	PSC	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	P	1267	PGV	C14-C15-C16-C17
18	P	1268	PGV	O03-C01-C02-O01
18	C	267	PGV	C05-C04-O12-P
26	C	270	CDL	C1-CA2-OA2-PA1
18	P	1268	PGV	C7-C8-C9-C10
18	A	524	PGV	C25-C26-C27-C28
26	G	269	CDL	C59-C60-C61-C62
22	C	271	CHD	C22-C23-C24-O25
18	A	525	PGV	O03-C19-C20-C21
17	N	516	HEA	CAA-CBA-CGA-O1A
17	N	516	HEA	CAA-CBA-CGA-O2A
22	O	229	CHD	C22-C23-C24-O25
18	C	268	PGV	C7-C8-C9-C10
17	A	516	HEA	CAD-CBD-CGD-O1D
17	N	516	HEA	CAD-CBD-CGD-O1D
22	B	1086	CHD	C22-C23-C24-O26
20	D	523	TGL	CG1-CG2-OG2-CB1
18	P	1267	PGV	C11-C12-C13-C14
18	C	267	PGV	C1-C2-C3-C4
26	T	1269	CDL	CB7-C71-C72-C73
21	B	230	PSC	C9-C10-C11-C12
21	O	1230	PSC	C9-C10-C11-C12
25	C	265	PEK	C5-C6-C7-C8
25	C	265	PEK	C12-C13-C14-C15
25	P	1265	PEK	C5-C6-C7-C8
25	P	1265	PEK	C12-C13-C14-C15
17	A	515	HEA	CAD-CBD-CGD-O1D
22	P	1271	CHD	C22-C23-C24-O25
26	P	1270	CDL	C1-CA2-OA2-PA1
20	N	1522	TGL	OC1-CC1-OG3-CG3
22	B	1086	CHD	C22-C23-C24-O25
22	O	229	CHD	C22-C23-C24-O26
18	P	1268	PGV	C01-C02-C03-O11
17	N	516	HEA	CAD-CBD-CGD-O2D
26	C	270	CDL	C41-C42-C43-C44
17	A	516	HEA	CAA-CBA-CGA-O2A
26	P	1270	CDL	C22-C23-C24-C25
18	A	524	PGV	C7-C8-C9-C10
18	C	268	PGV	O03-C01-C02-O01
25	C	265	PEK	O03-C01-C02-O01
25	P	1265	PEK	O03-C01-C02-O01
25	P	1264	PEK	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
18	Z	1524	PGV	C7-C8-C9-C10
21	B	230	PSC	C11-C12-C13-C14
21	O	1230	PSC	C11-C12-C13-C14
17	A	516	HEA	CAD-CBD-CGD-O2D
22	C	271	CHD	C22-C23-C24-O26
22	P	1271	CHD	C22-C23-C24-O26
25	C	265	PEK	C3-C4-C5-C6
25	P	1265	PEK	C3-C4-C5-C6
18	N	1266	PGV	C19-C20-C21-C22
18	N	1266	PGV	O03-C19-C20-C21
26	G	269	CDL	C15-C16-C17-C18
17	N	515	HEA	CAD-CBD-CGD-O1D
18	C	267	PGV	C11-C12-C13-C14
18	A	524	PGV	C04-C05-C06-O06
18	Z	1524	PGV	C04-C05-C06-O06
21	O	1230	PSC	C7-C8-C9-C10
26	G	269	CDL	OA5-CA3-CA4-OA6
17	N	516	HEA	C2D-C3D-CAD-CBD
18	A	525	PGV	C31-C32-C33-C34
20	L	522	TGL	OG2-CB1-CB2-CB3
20	N	1522	TGL	OG2-CB1-CB2-CB3
23	Z	1526	DMU	C34-C37-C40-C43
26	T	1269	CDL	CA7-C31-C32-C33
26	C	270	CDL	C22-C23-C24-C25
18	Z	1524	PGV	C25-C26-C27-C28
26	T	1269	CDL	C39-C40-C41-C42
18	A	524	PGV	C01-C02-C03-O11
18	C	268	PGV	C01-C02-C03-O11
26	T	1269	CDL	C22-C23-C24-C25
26	P	1270	CDL	C52-C51-CB5-OB6
26	G	269	CDL	C39-C40-C41-C42
26	P	1270	CDL	C41-C42-C43-C44
25	C	264	PEK	O01-C1-C2-C3
25	P	1264	PEK	O01-C1-C2-C3
17	A	515	HEA	C21-C22-C23-C24
18	C	267	PGV	C9-C10-C11-C12
18	Z	1524	PGV	O01-C1-C2-C3
21	B	230	PSC	O03-C19-C20-C21
21	O	1230	PSC	O03-C19-C20-C21
26	P	1270	CDL	C56-C57-C58-C59
25	P	1265	PEK	C35-C36-C37-C38
26	G	269	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	N	1266	PGV	C31-C32-C33-C34
20	L	522	TGL	CB5-CB6-CB7-CB8
18	A	525	PGV	C11-C12-C13-C14
18	P	1267	PGV	C9-C10-C11-C12
21	B	230	PSC	C7-C8-C9-C10
21	B	230	PSC	C12-C13-C14-C15
25	T	263	PEK	C3-C4-C5-C6
22	C	525	CHD	C22-C23-C24-O26
20	B	521	TGL	CG1-CG2-OG2-CB1
20	N	1522	TGL	CB5-CB6-CB7-CB8
18	A	524	PGV	O01-C1-C2-C3
26	C	270	CDL	C52-C51-CB5-OB6
20	Q	1523	TGL	C21-C22-C23-C24
22	J	60	CHD	C22-C23-C24-O25
22	P	1525	CHD	C22-C23-C24-O26
22	W	1060	CHD	C22-C23-C24-O25
26	C	270	CDL	C76-C77-C78-C79
18	N	1266	PGV	C11-C12-C13-C14
25	G	1263	PEK	C3-C4-C5-C6
25	G	1263	PEK	C14-C15-C16-C17
26	C	270	CDL	C32-C31-CA7-OA8
26	P	1270	CDL	C32-C31-CA7-OA8
26	P	1270	CDL	C76-C77-C78-C79
20	D	523	TGL	C21-C22-C23-C24
26	P	1270	CDL	C83-C84-C85-C86
21	O	1230	PSC	C12-C13-C14-C15
22	J	60	CHD	C22-C23-C24-O26
22	W	1060	CHD	C22-C23-C24-O26
20	L	522	TGL	OG3-CC1-CC2-CC3
25	C	265	PEK	C35-C36-C37-C38
21	B	230	PSC	C26-C27-C28-C29
17	A	515	HEA	CAA-CBA-CGA-O1A
17	N	515	HEA	CAA-CBA-CGA-O1A
18	Z	1524	PGV	C9-C10-C11-C12
25	T	263	PEK	C14-C15-C16-C17
26	C	270	CDL	C56-C57-C58-C59
20	D	523	TGL	OG2-CB1-CB2-CB3
20	N	1522	TGL	OG3-CC1-CC2-CC3
17	A	515	HEA	CAD-CBD-CGD-O2D
26	P	1270	CDL	C12-C11-CA5-OA6
17	A	516	HEA	C2D-C3D-CAD-CBD
26	T	1269	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	Q	1523	TGL	OG2-CB1-CB2-CB3
22	P	1525	CHD	C22-C23-C24-O25
26	C	270	CDL	C32-C31-CA7-OA9
23	M	526	DMU	C34-C37-C40-C43
21	O	1230	PSC	C26-C27-C28-C29
22	C	525	CHD	C22-C23-C24-O25
26	G	269	CDL	CA7-C31-C32-C33
17	N	515	HEA	CAD-CBD-CGD-O2D
26	P	1270	CDL	C32-C31-CA7-OA9
18	N	1266	PGV	C24-C25-C26-C27
21	O	1230	PSC	O04-C19-C20-C21
18	P	1268	PGV	C2-C3-C4-C5
26	C	270	CDL	C82-C83-C84-C85
26	P	1270	CDL	C82-C83-C84-C85
20	L	522	TGL	OC1-CC1-OG3-CG3
18	A	524	PGV	C9-C10-C11-C12
20	D	523	TGL	OC1-CC1-CC2-CC3
20	Q	1523	TGL	OB1-CB1-CB2-CB3
21	B	230	PSC	O04-C19-C20-C21
18	C	267	PGV	C29-C30-C31-C32
20	D	523	TGL	OB1-CB1-CB2-CB3
21	B	230	PSC	O01-C1-C2-C3
26	C	270	CDL	C12-C11-CA5-OA6
18	C	268	PGV	C02-C03-O11-P
18	P	1267	PGV	C05-C04-O12-P
18	P	1268	PGV	C02-C03-O11-P
18	P	1267	PGV	C29-C30-C31-C32
18	A	524	PGV	O02-C1-C2-C3
25	P	1264	PEK	O02-C1-C2-C3
18	A	524	PGV	C03-O11-P-O13
18	Z	1524	PGV	C03-O11-P-O13
20	Q	1523	TGL	OC1-CC1-CC2-CC3
20	N	1521	TGL	OG1-CA1-CA2-CA3
18	Z	1524	PGV	O02-C1-C2-C3
25	C	264	PEK	O02-C1-C2-C3
25	P	1265	PEK	C34-C35-C36-C37
26	C	270	CDL	C83-C84-C85-C86
26	C	270	CDL	C19-C20-C21-C22
17	A	515	HEA	CAA-CBA-CGA-O2A
20	N	1521	TGL	CG1-CG2-OG2-CB1
21	B	230	PSC	C05-C04-O12-P
21	O	1230	PSC	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
21	B	230	PSC	O02-C1-C2-C3
21	O	1230	PSC	O02-C1-C2-C3
26	P	1270	CDL	C52-C51-CB5-OB7
20	B	521	TGL	OG1-CA1-CA2-CA3
21	O	1230	PSC	O01-C1-C2-C3
17	N	515	HEA	CAA-CBA-CGA-O2A
18	P	1267	PGV	C21-C22-C23-C24
18	P	1268	PGV	O01-C02-C03-O11
17	N	516	HEA	C4D-C3D-CAD-CBD
25	C	265	PEK	O03-C21-C22-C23
25	P	1265	PEK	O03-C21-C22-C23
25	C	265	PEK	O04-C21-C22-C23
25	P	1265	PEK	O04-C21-C22-C23
26	C	270	CDL	C52-C51-CB5-OB7
18	C	268	PGV	C2-C3-C4-C5
17	A	515	HEA	C17-C18-C19-C27

There are no ring outliers.

37 monomers are involved in 249 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	515	HEA	4	0
18	C	268	PGV	1	0
18	Z	1524	PGV	4	0
22	O	229	CHD	1	0
21	O	1230	PSC	12	0
25	G	1263	PEK	7	0
23	C	272	DMU	2	0
18	C	267	PGV	6	0
25	C	265	PEK	6	0
25	P	1265	PEK	6	0
23	Z	1526	DMU	1	0
18	A	525	PGV	1	0
22	W	1060	CHD	2	0
17	A	516	HEA	1	0
23	P	1272	DMU	7	0
20	Q	1523	TGL	6	0
17	A	515	HEA	2	0
20	N	1521	TGL	14	0
22	P	1271	CHD	2	0
21	B	230	PSC	13	0
22	C	271	CHD	2	0

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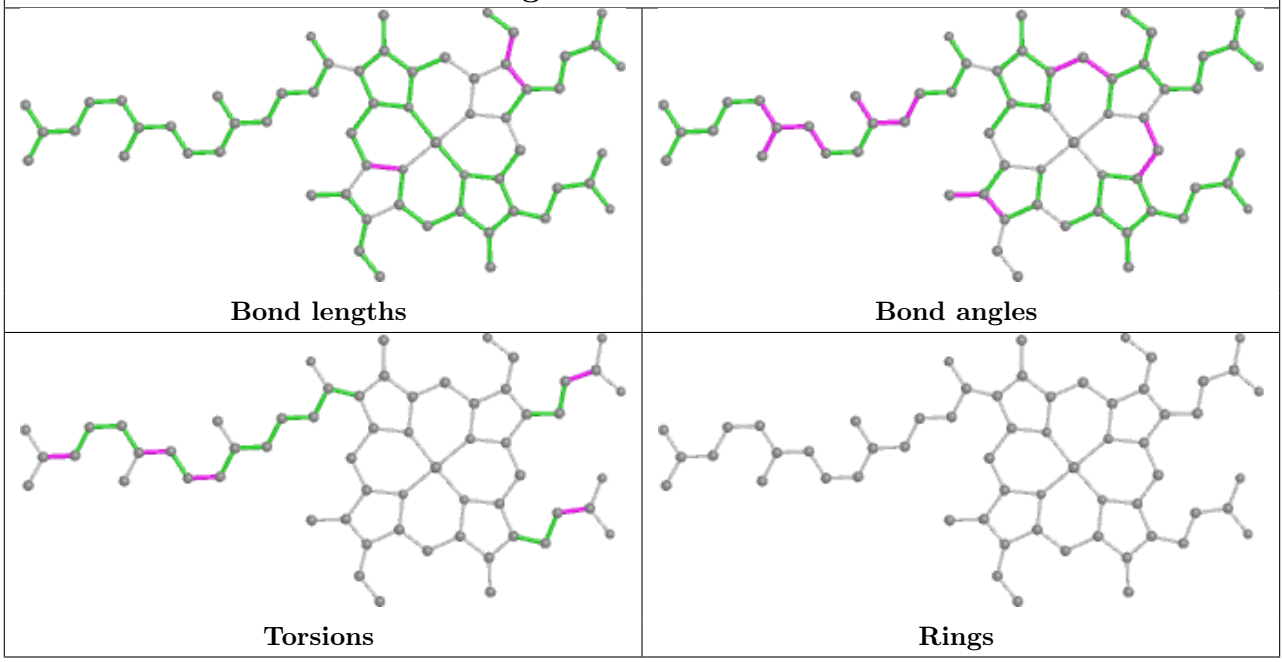
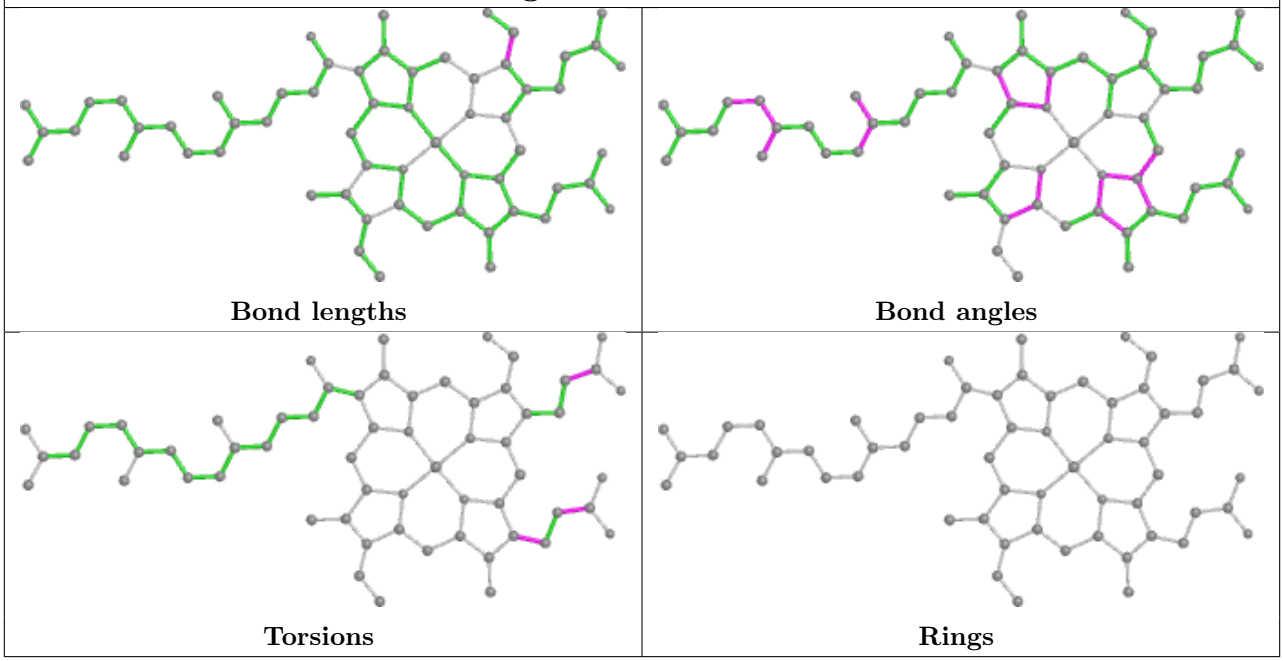
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	524	PGV	6	0
20	N	1522	TGL	16	0
22	J	60	CHD	2	0
25	C	264	PEK	5	0
25	P	1264	PEK	6	0
25	T	263	PEK	8	0
26	G	269	CDL	21	0
20	L	522	TGL	23	0
26	P	1270	CDL	13	0
20	D	523	TGL	5	0
18	P	1267	PGV	5	0
26	C	270	CDL	16	0
18	N	1266	PGV	2	0
18	P	1268	PGV	3	0
20	B	521	TGL	10	0
26	T	1269	CDL	21	0

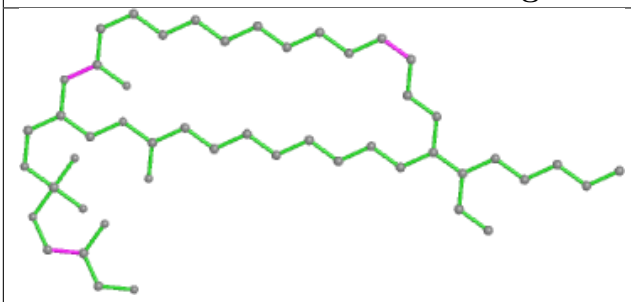
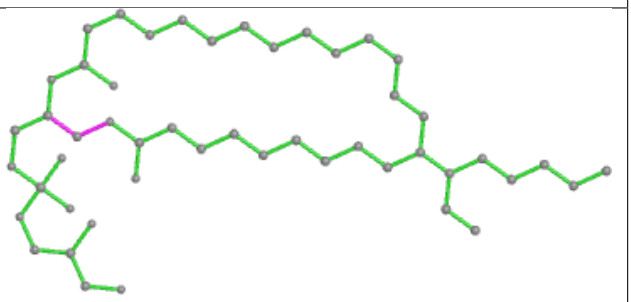
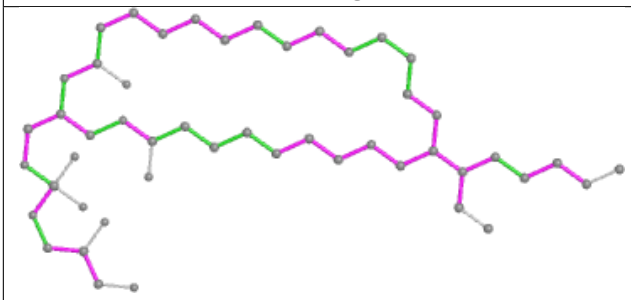
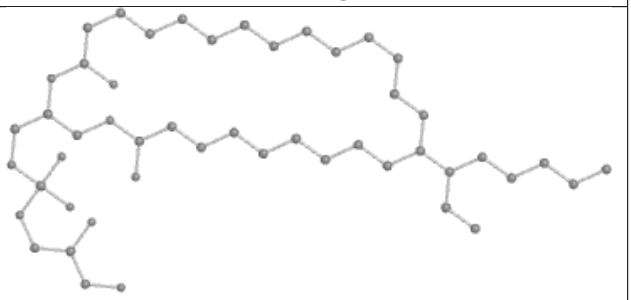
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

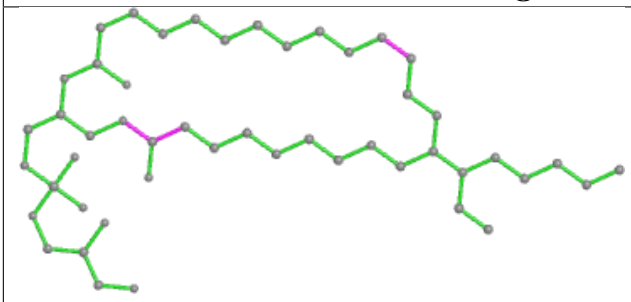
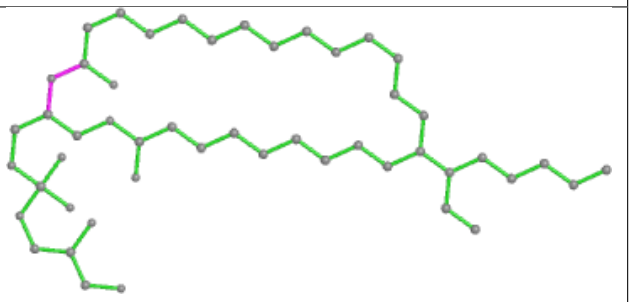
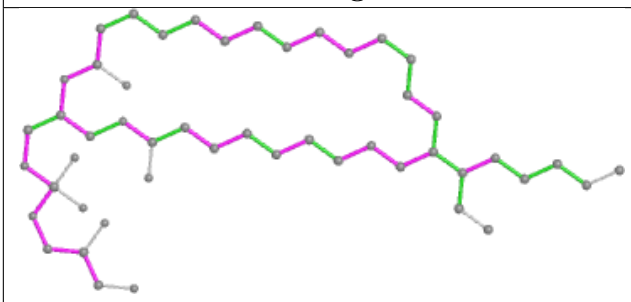
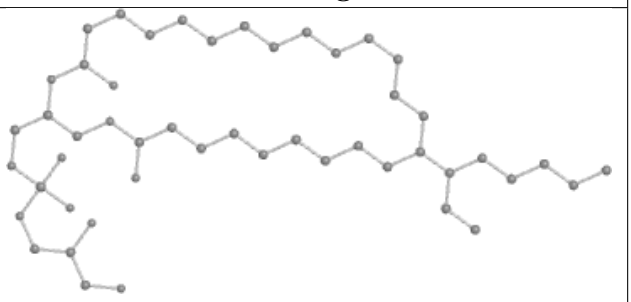
Ligand HEA N 515



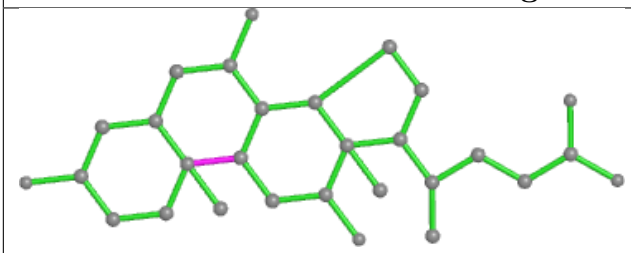
Ligand HEA N 516



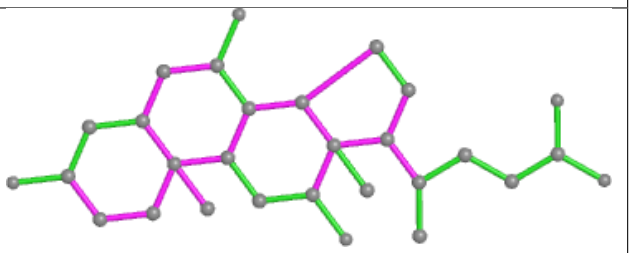
Ligand PGV C 268	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV Z 1524	
 Bond lengths	 Bond angles
 Torsions	 Rings

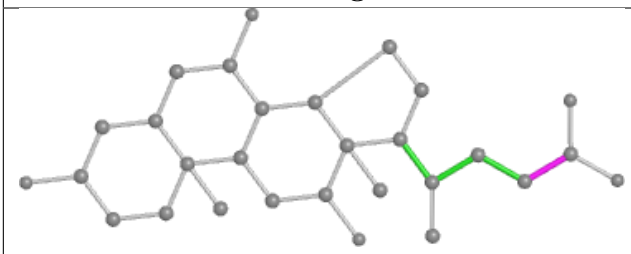
Ligand CHD C 525



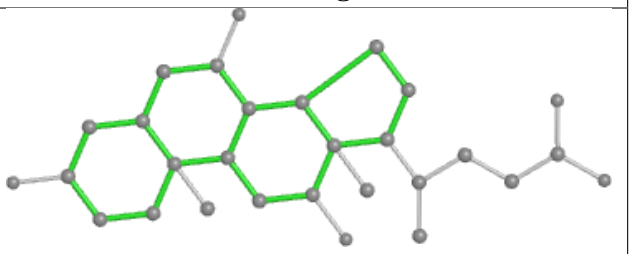
Bond lengths



Bond angles

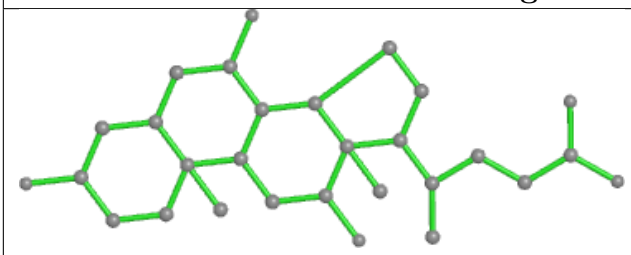


Torsions

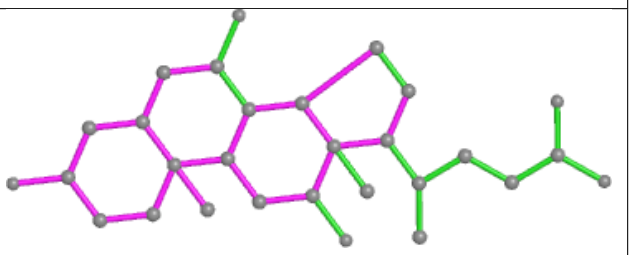


Rings

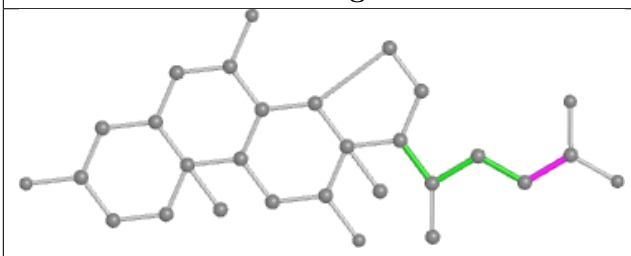
Ligand CHD O 229



Bond lengths



Bond angles



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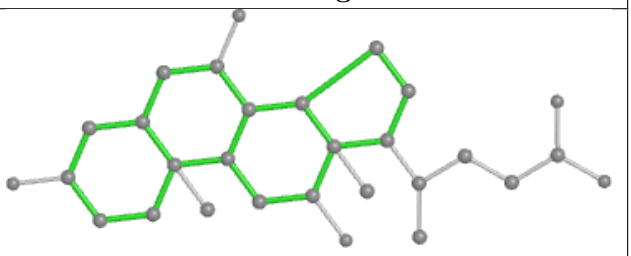
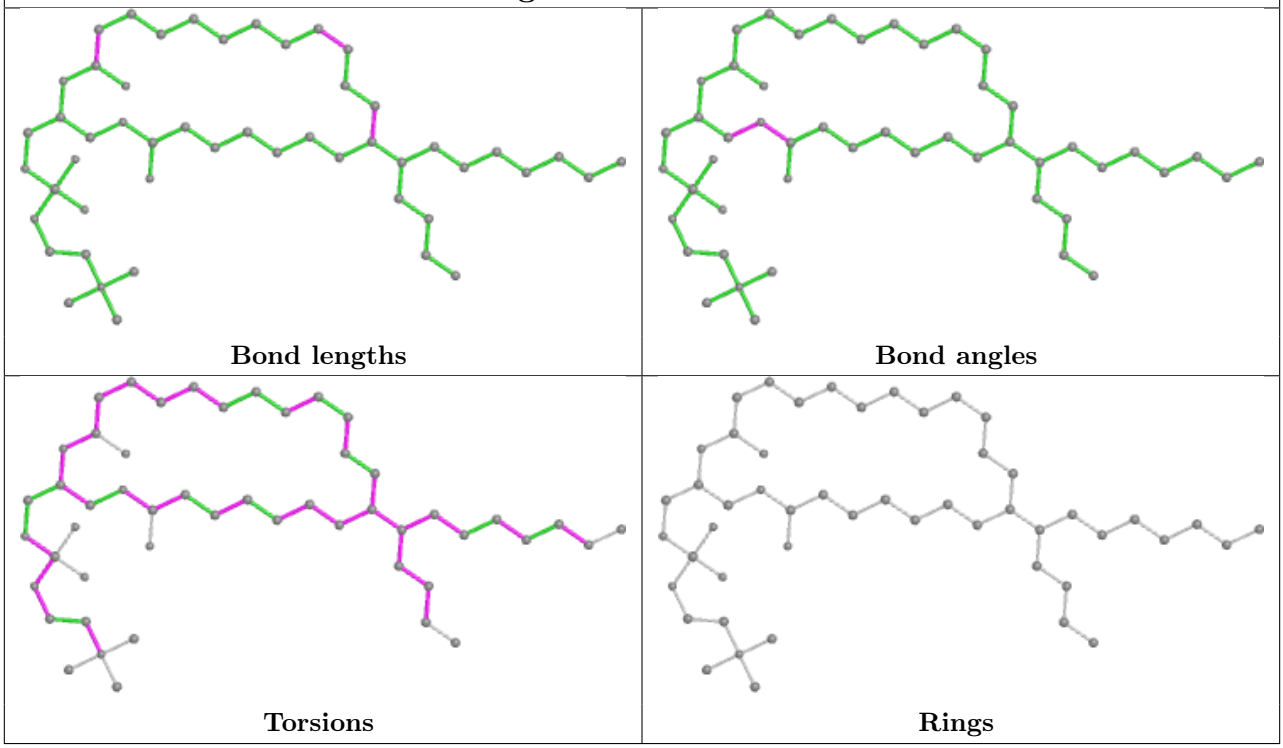
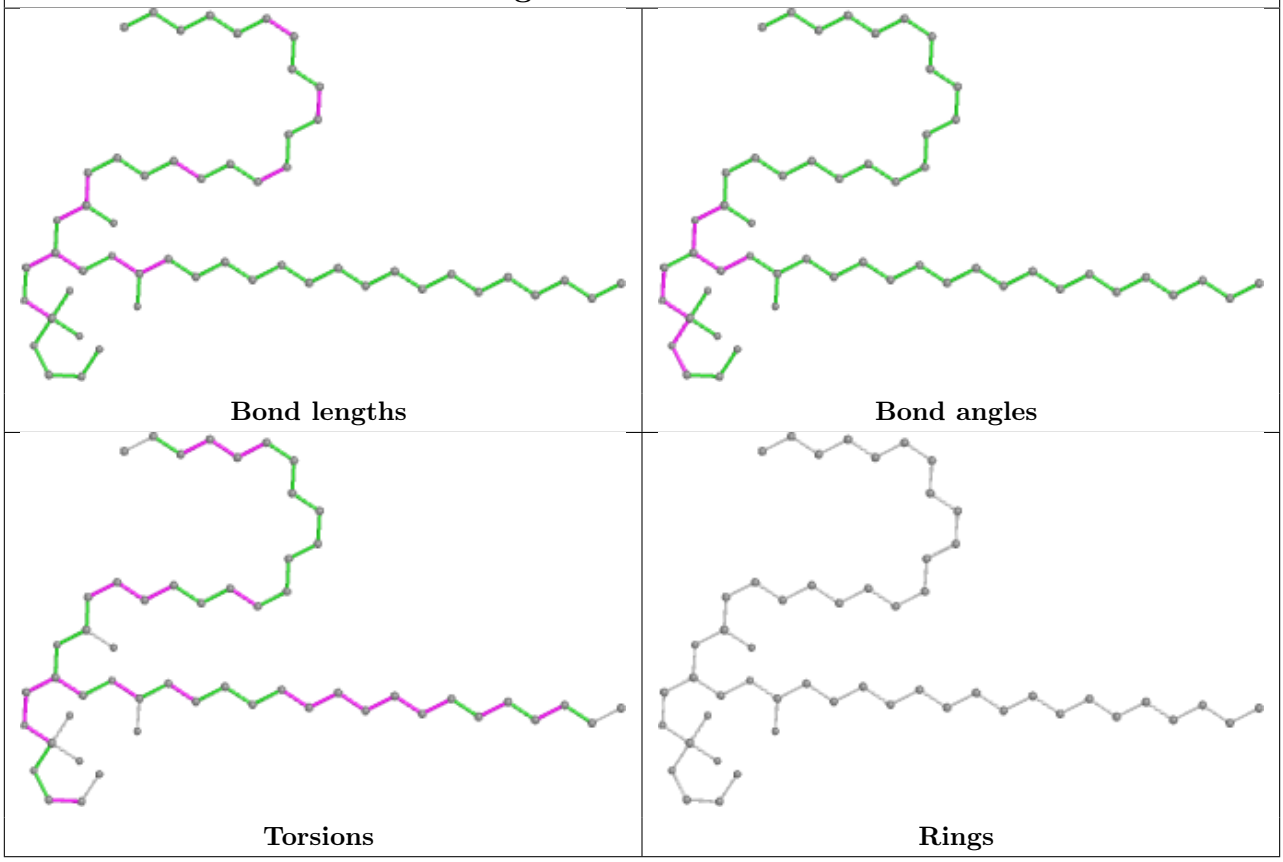


Rings

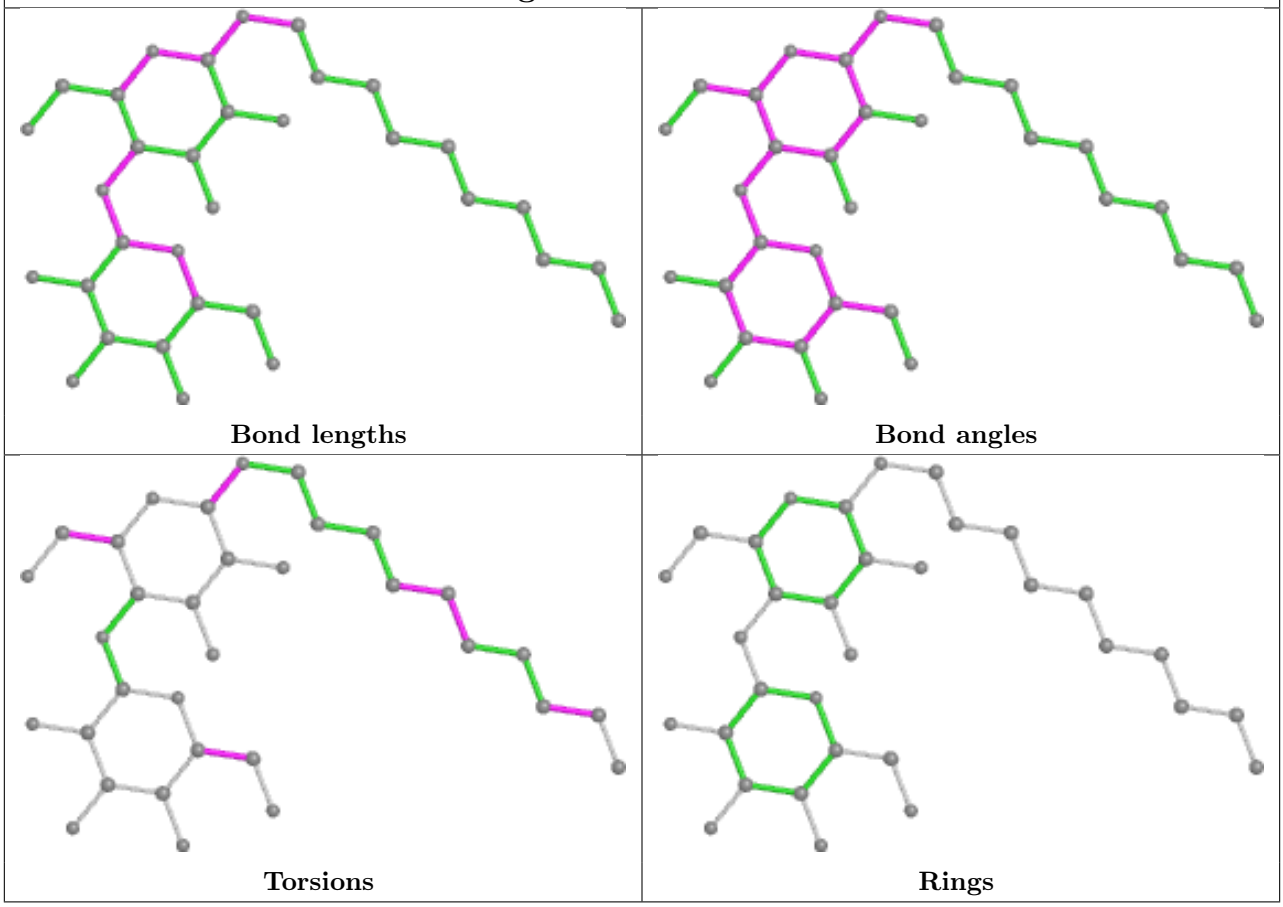
Ligand PSC O 1230



Ligand PEK G 1263



Ligand DMU C 272



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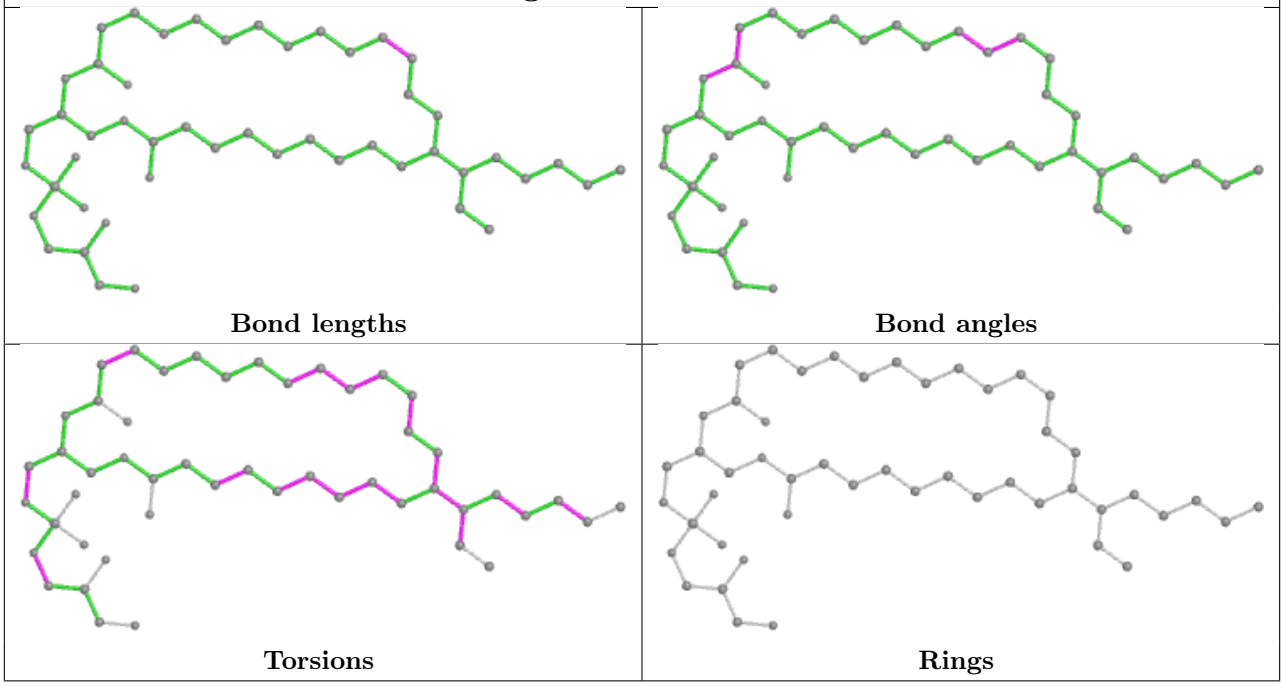

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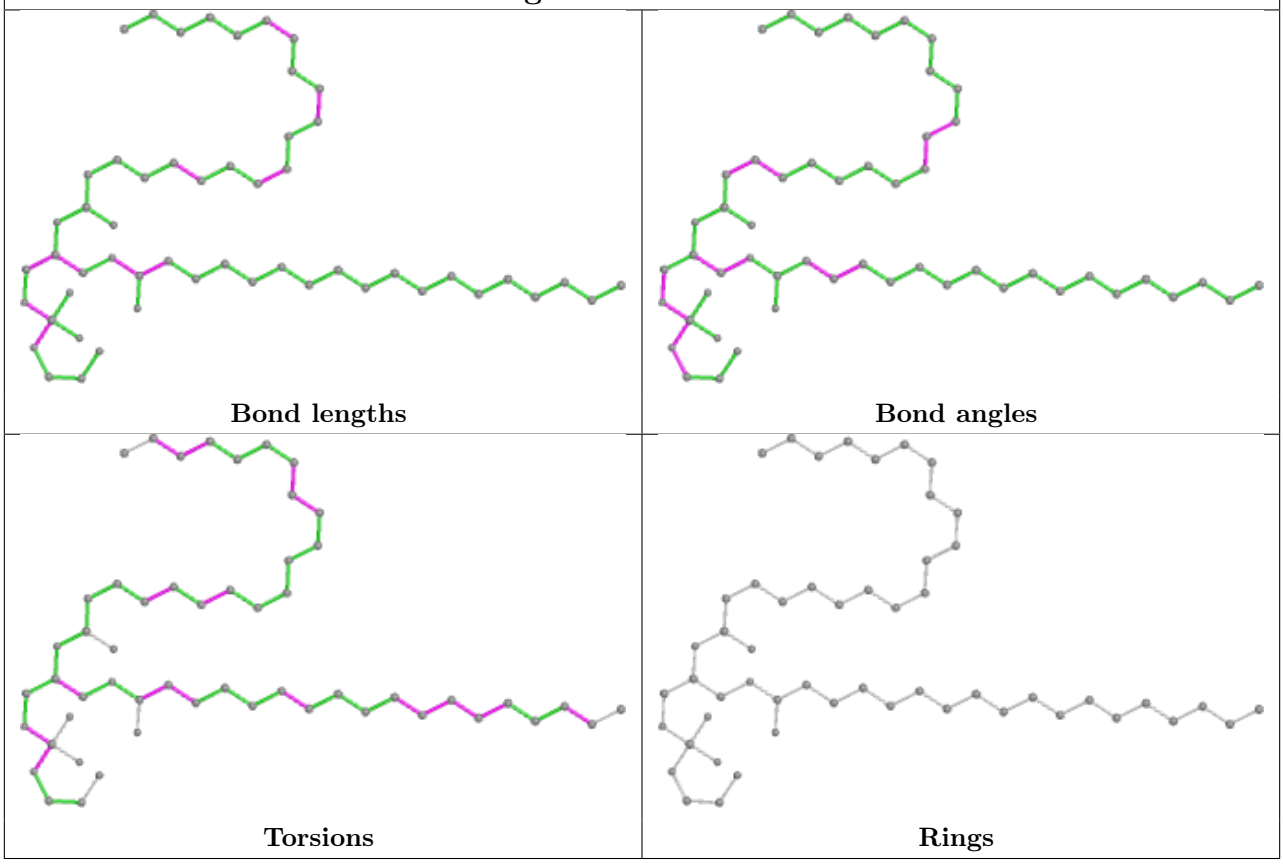

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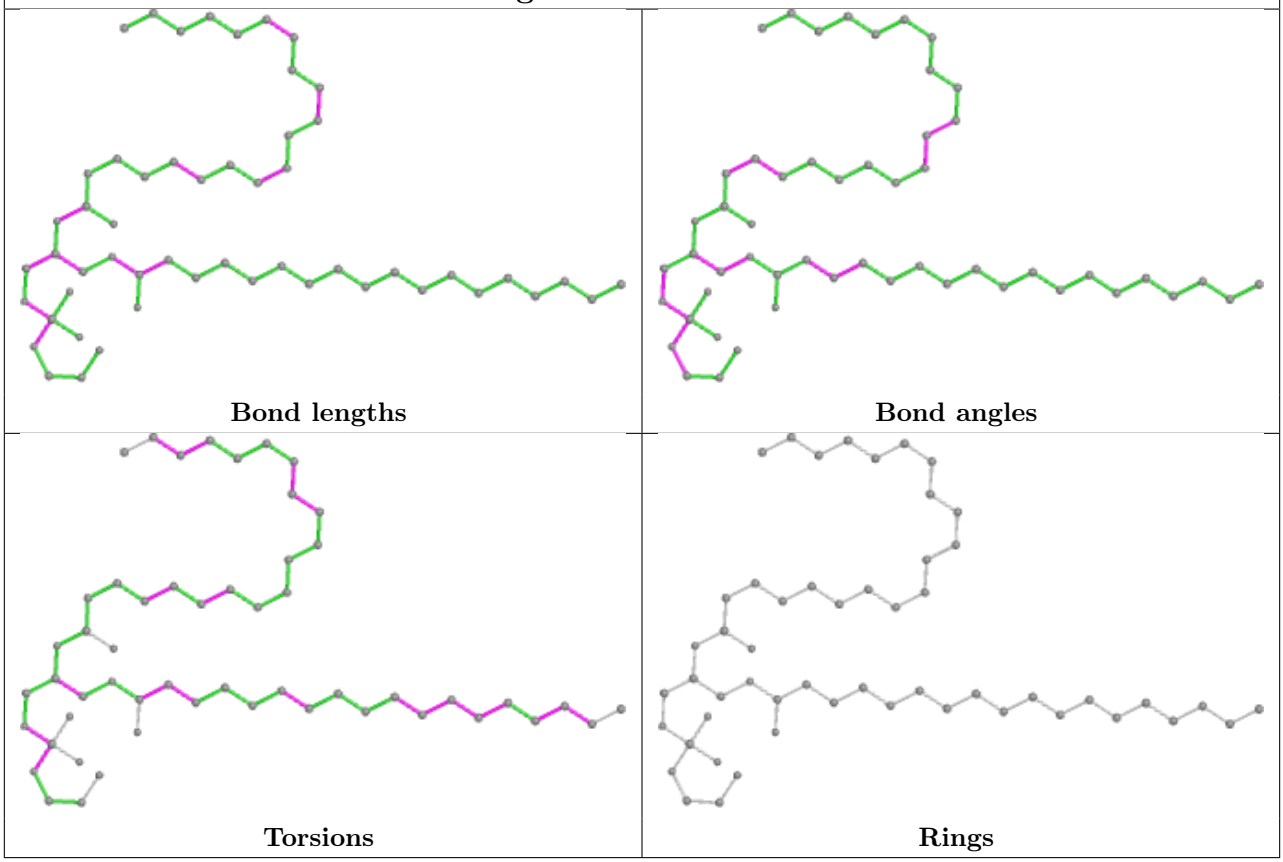

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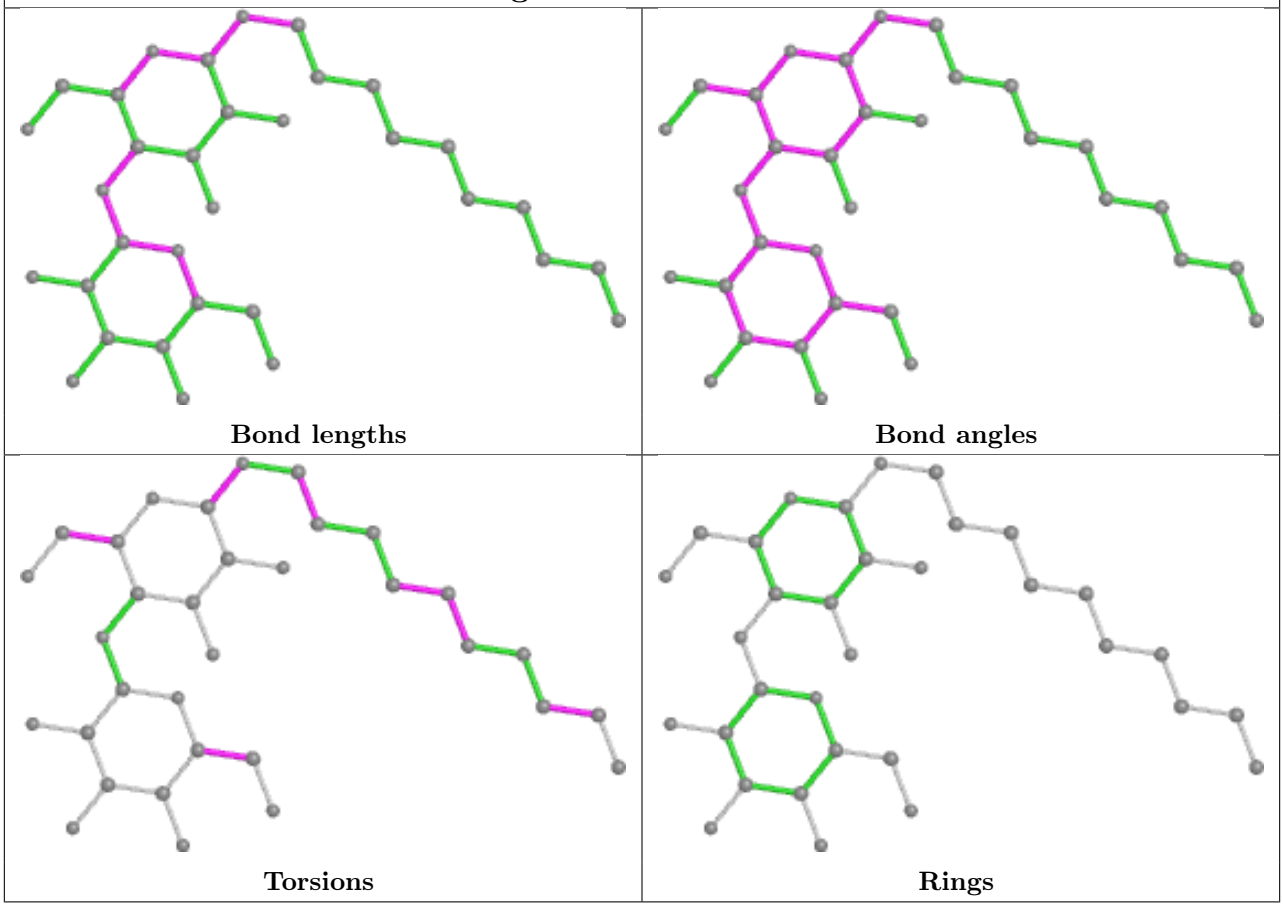
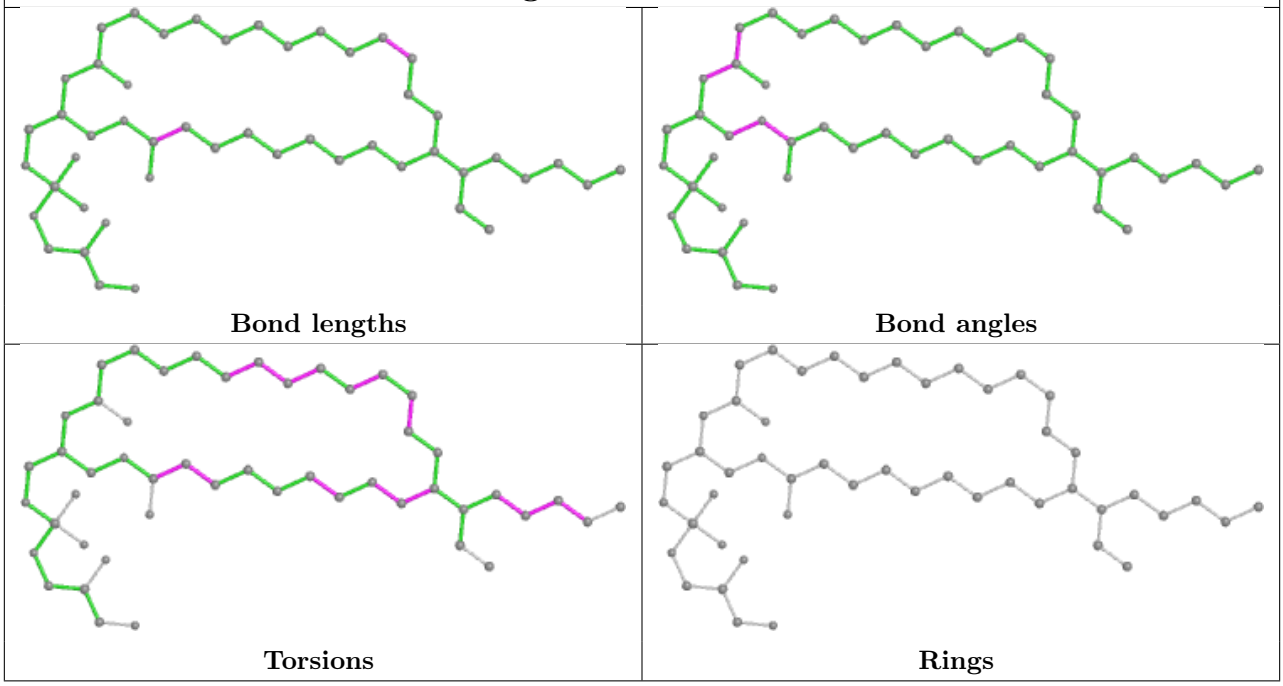
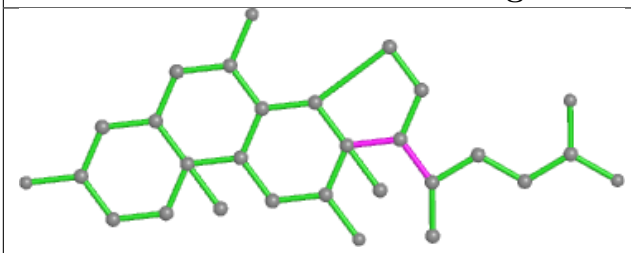


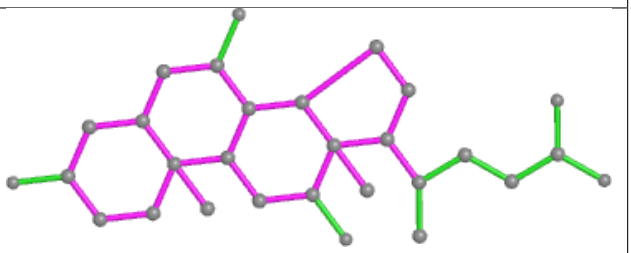
Ligand PGV A 525



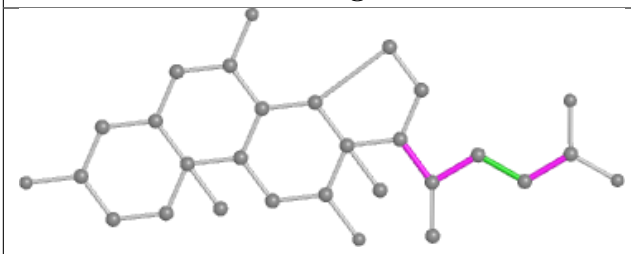
Ligand CHD W 1060



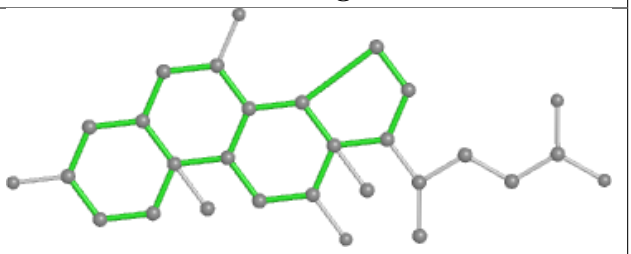
Bond lengths



Bond angles

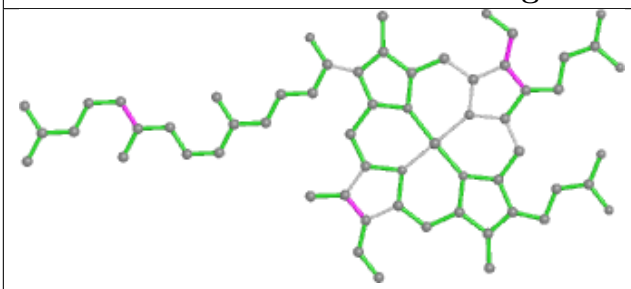


Torsions



Rings

Ligand HEA A 516



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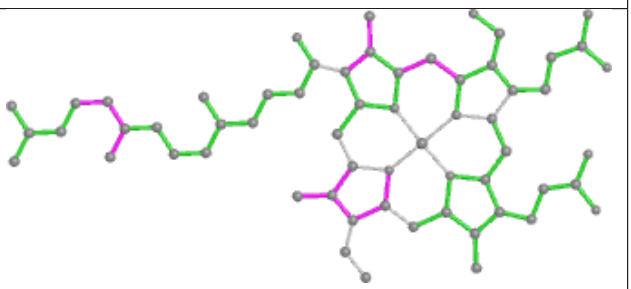
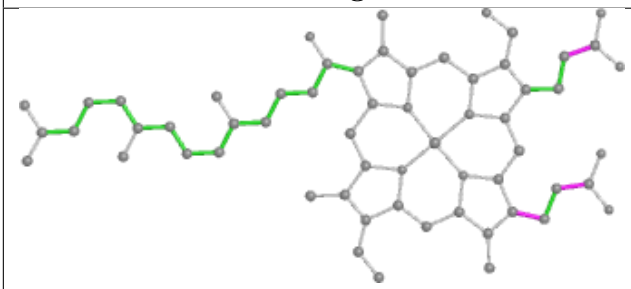


Bond angles



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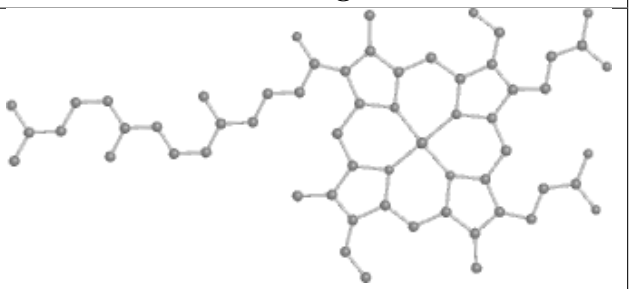
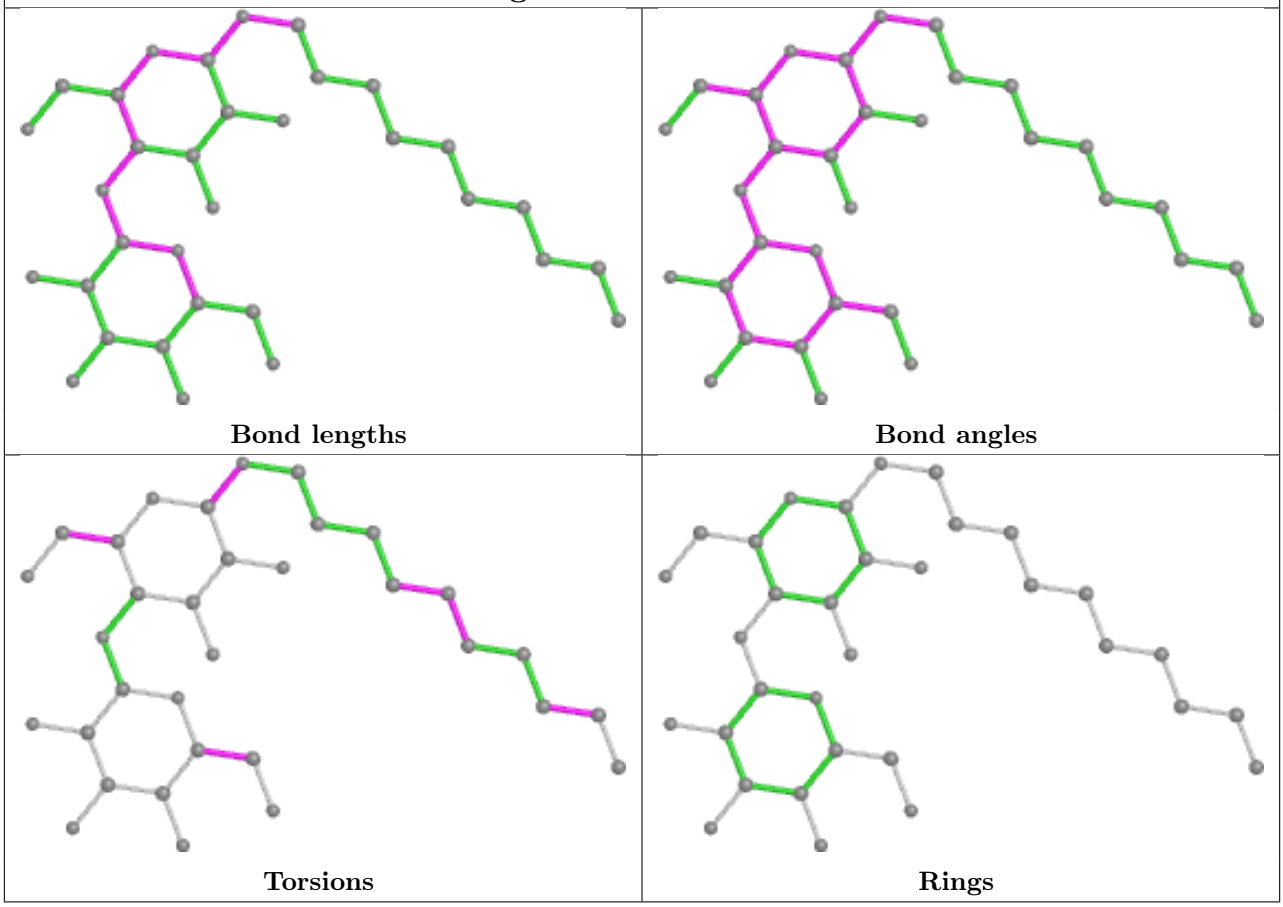
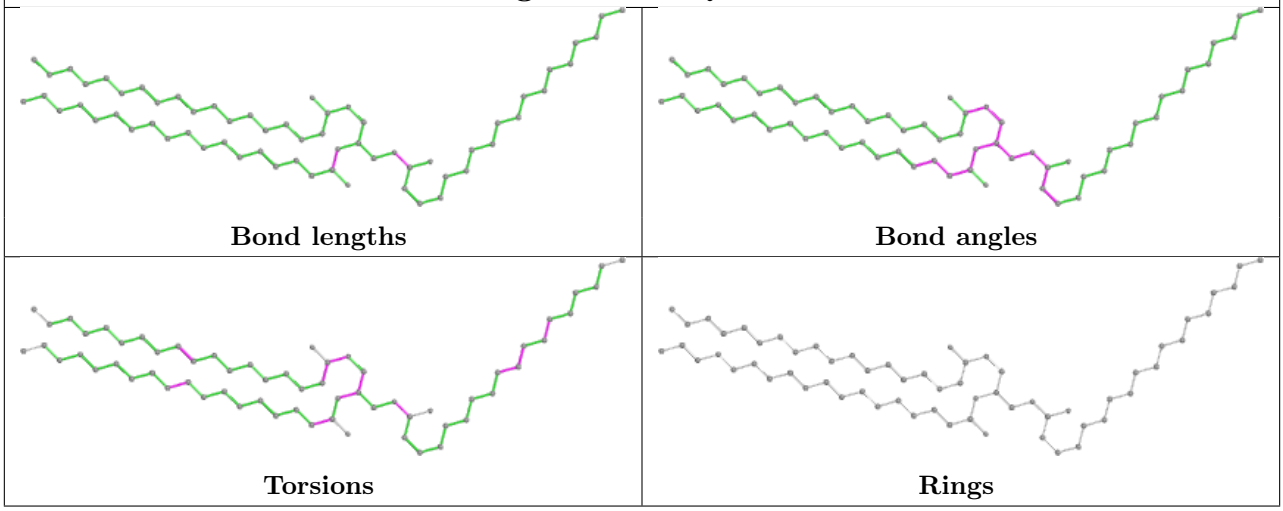


Rings

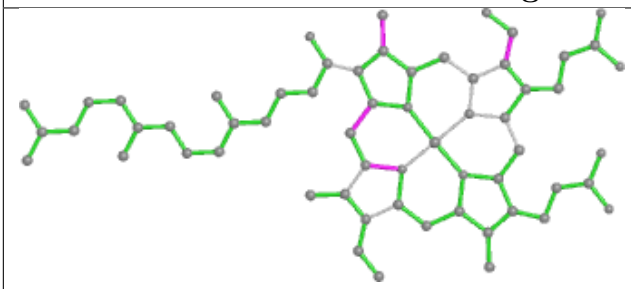
Ligand DMU P 1272



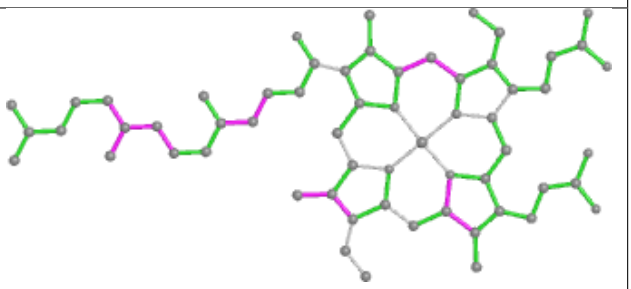
Ligand TGL Q 1523



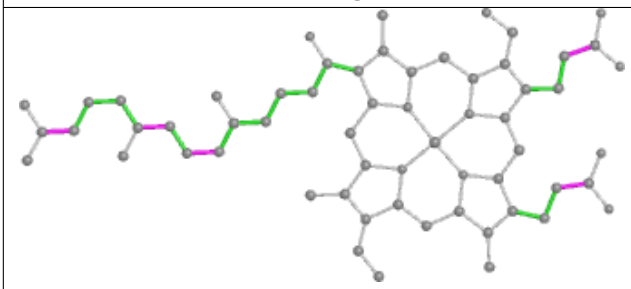
Ligand HEA A 515



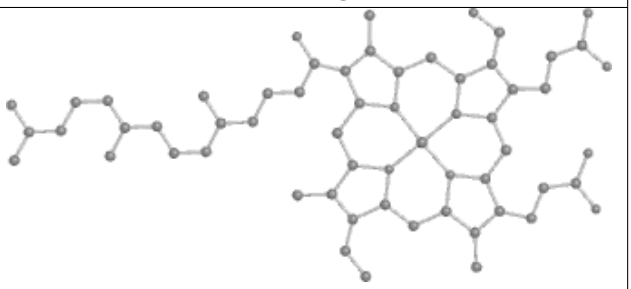
Bond lengths



Bond angles

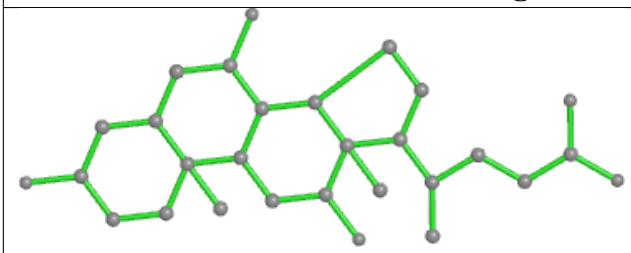


Torsions



Rings

Ligand CHD B 1086



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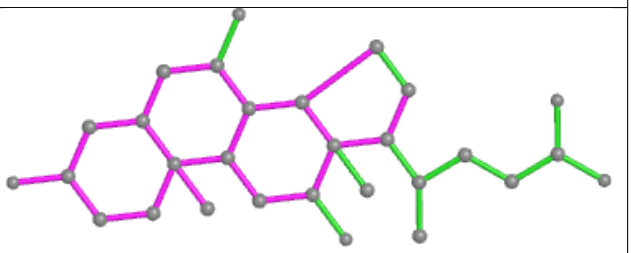
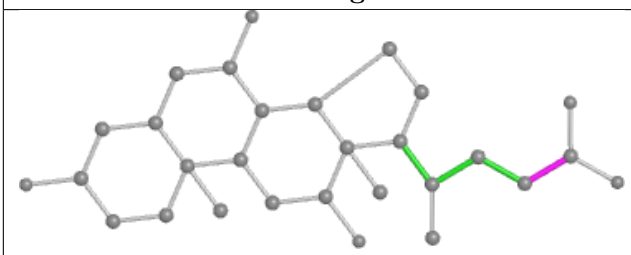
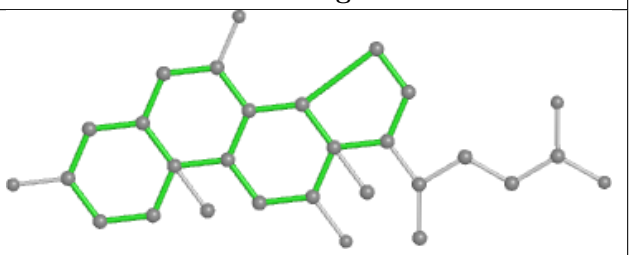


Bond angles

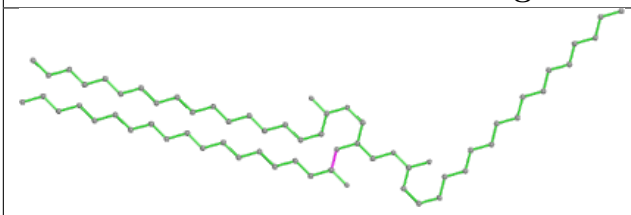


Torsions



Rings

Ligand TGL N 1521



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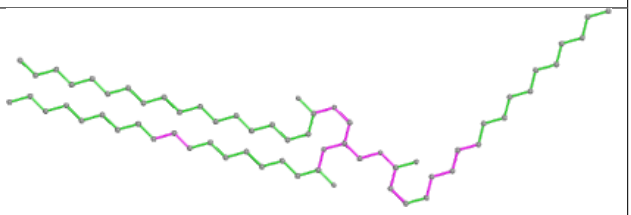
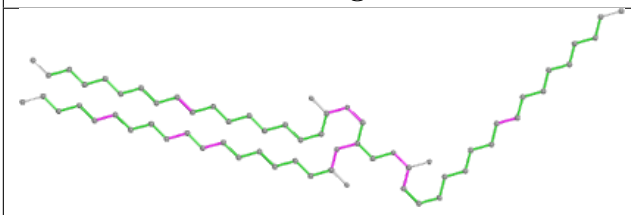
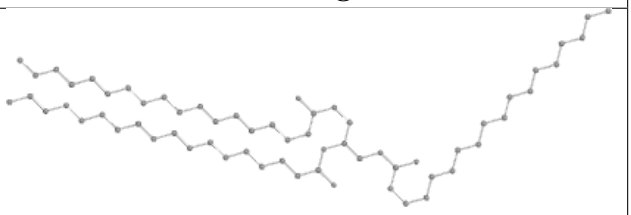


Bond angles

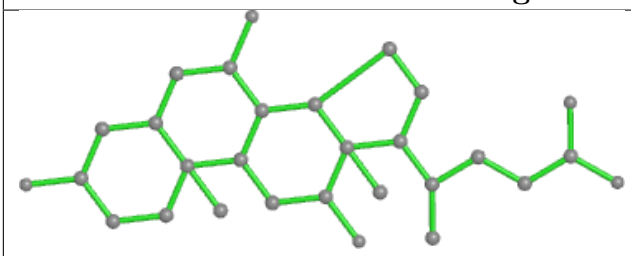


Torsions



Rings

Ligand CHD P 1271



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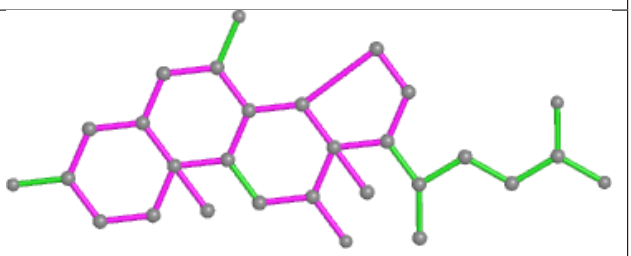
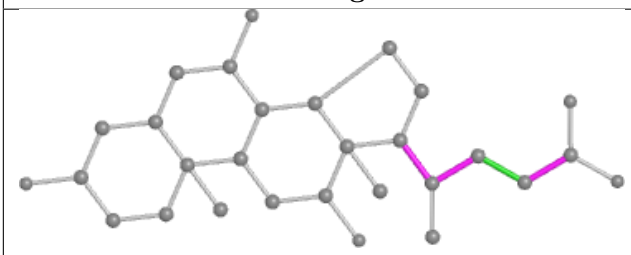


Bond angles



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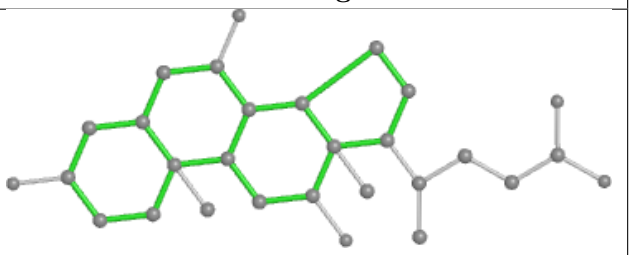
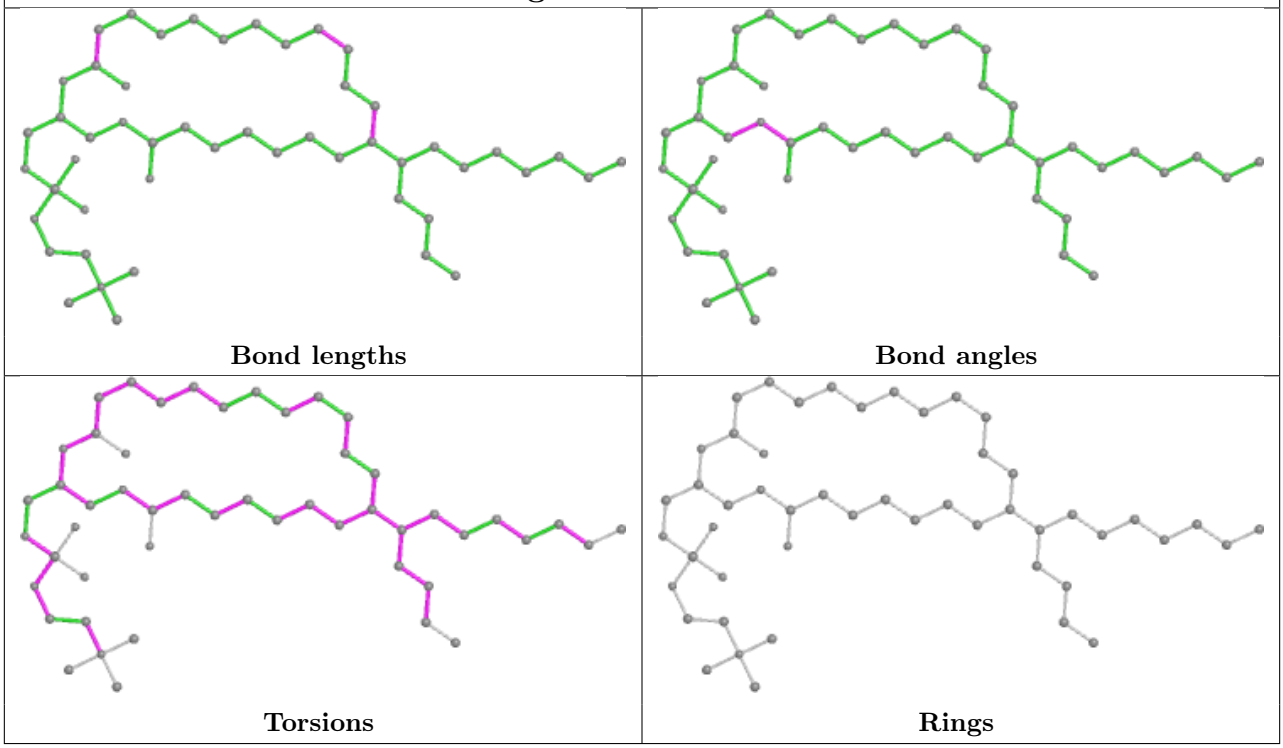
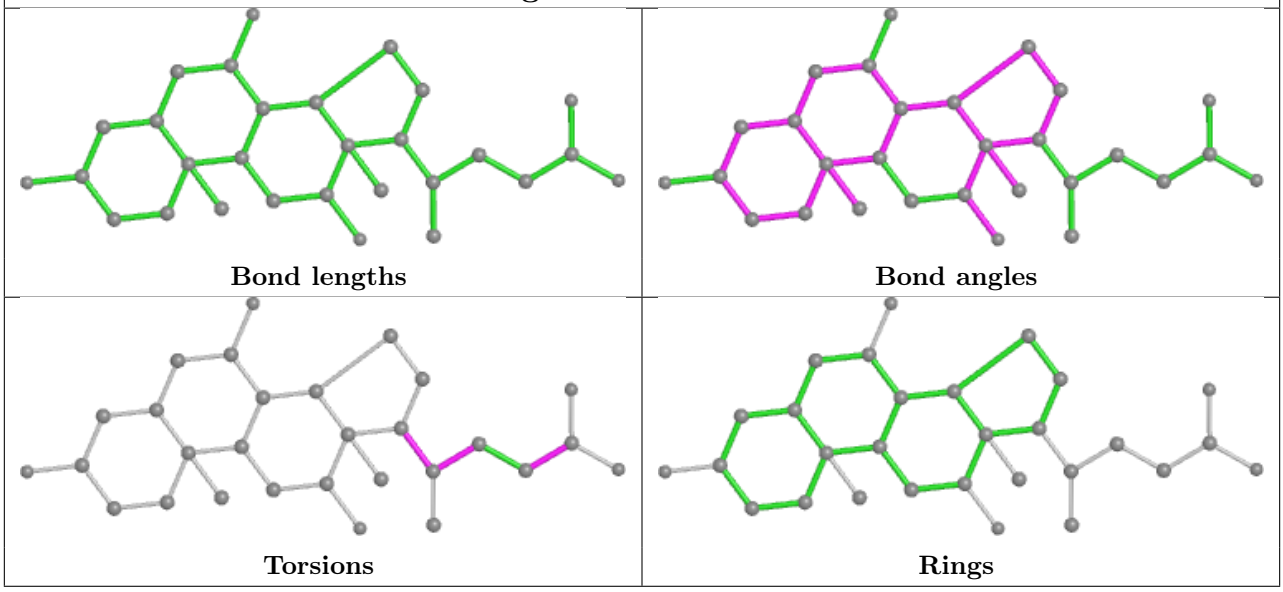


Rings

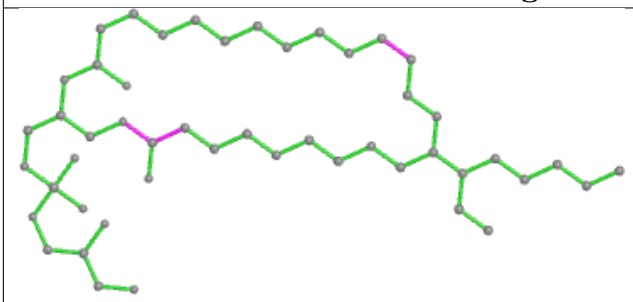
Ligand PSC B 230



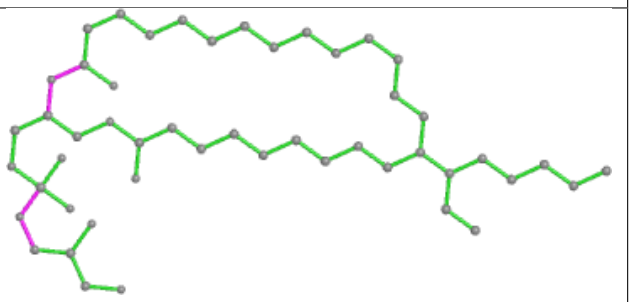
Ligand CHD C 271



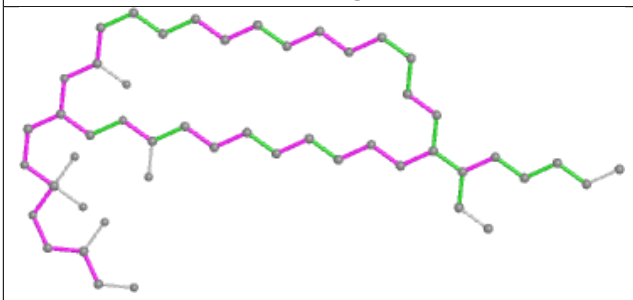
Ligand PGV A 524



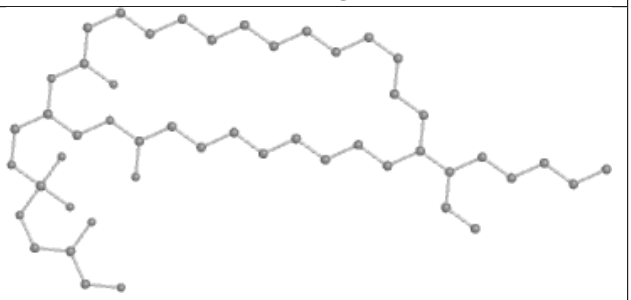
Bond lengths



Bond angles

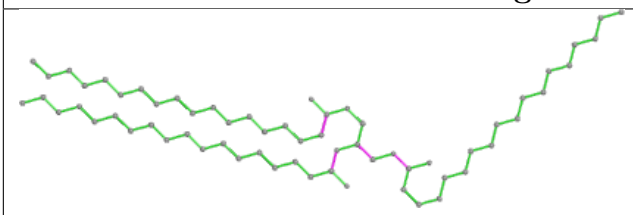


Torsions

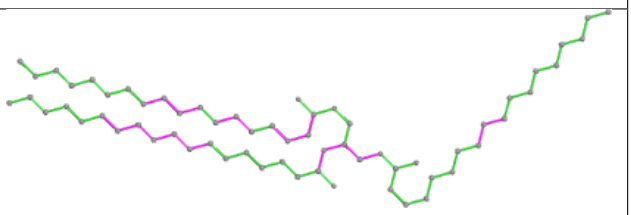


Rings

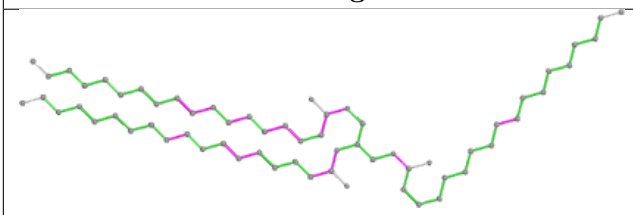
Ligand TGL N 1522



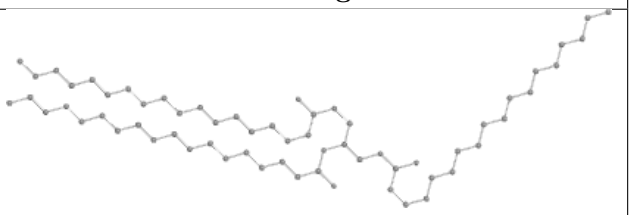
Bond lengths



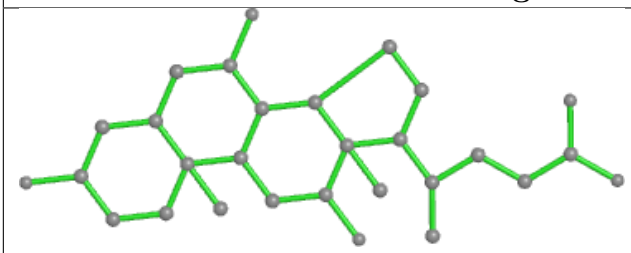
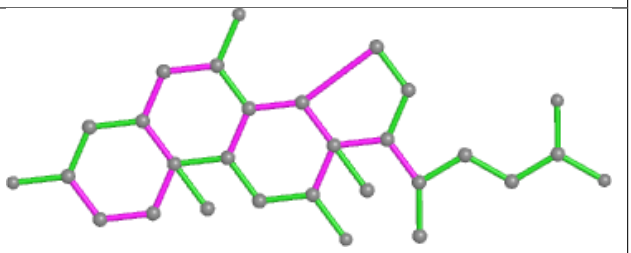
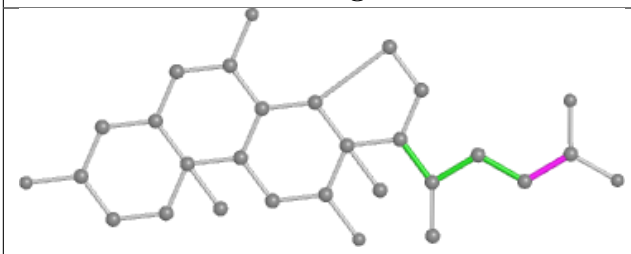
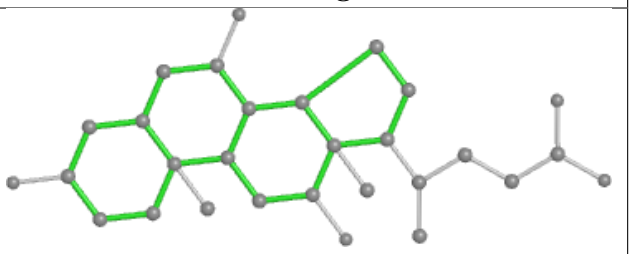
Bond angles

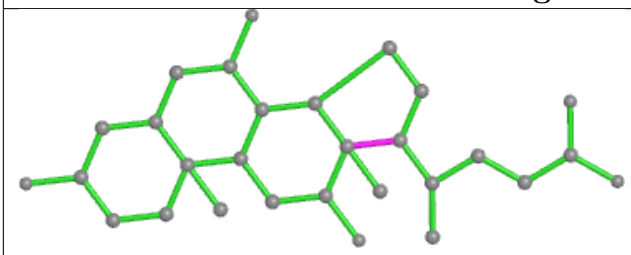
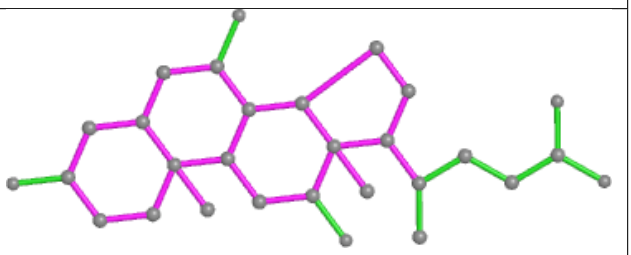
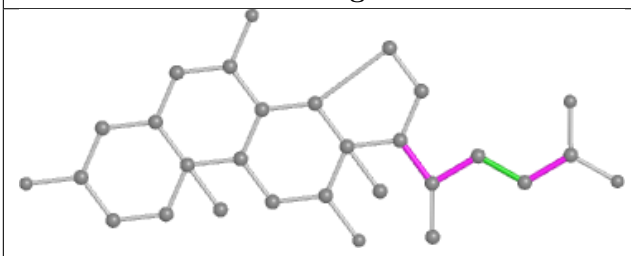
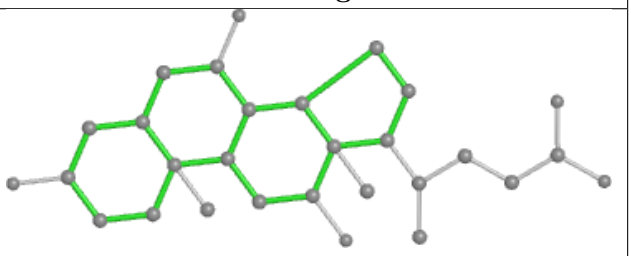


Torsions

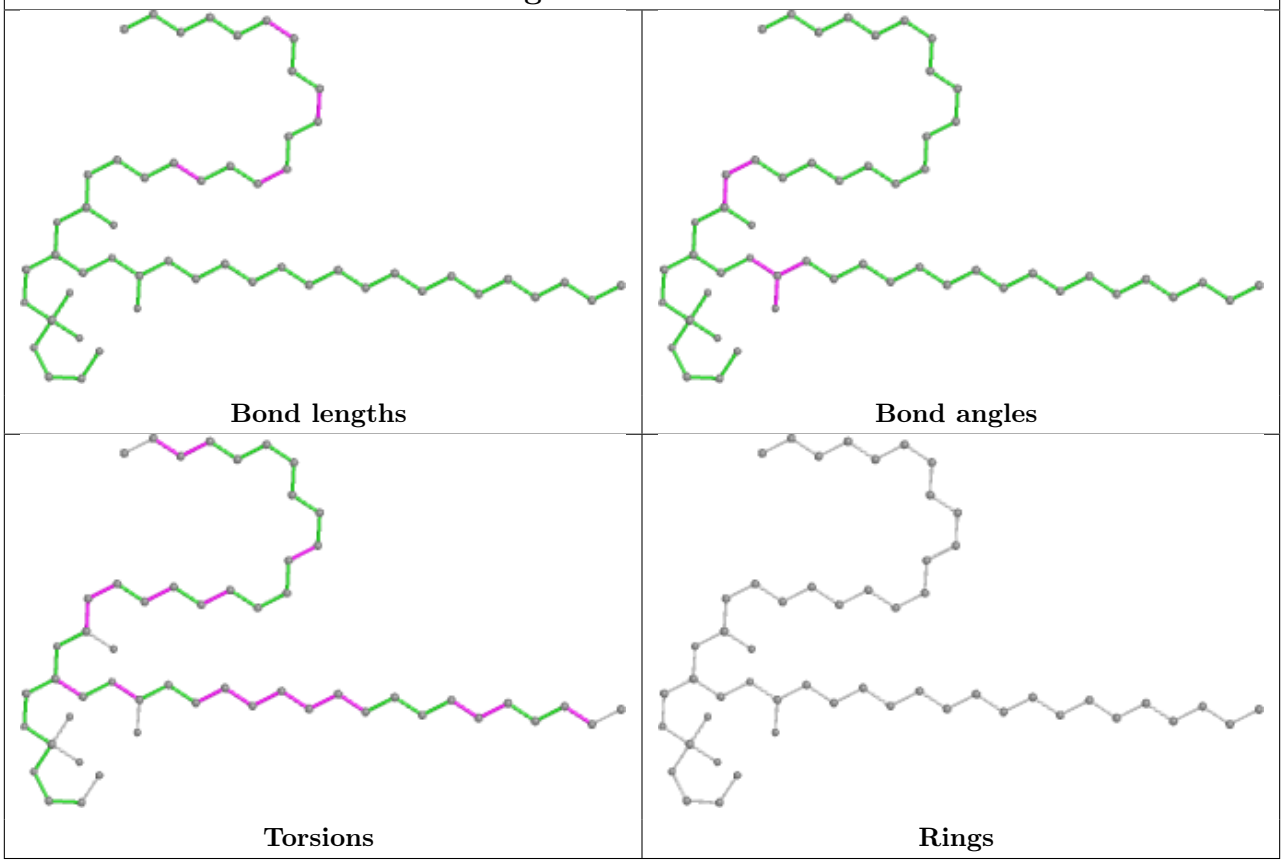


Rings

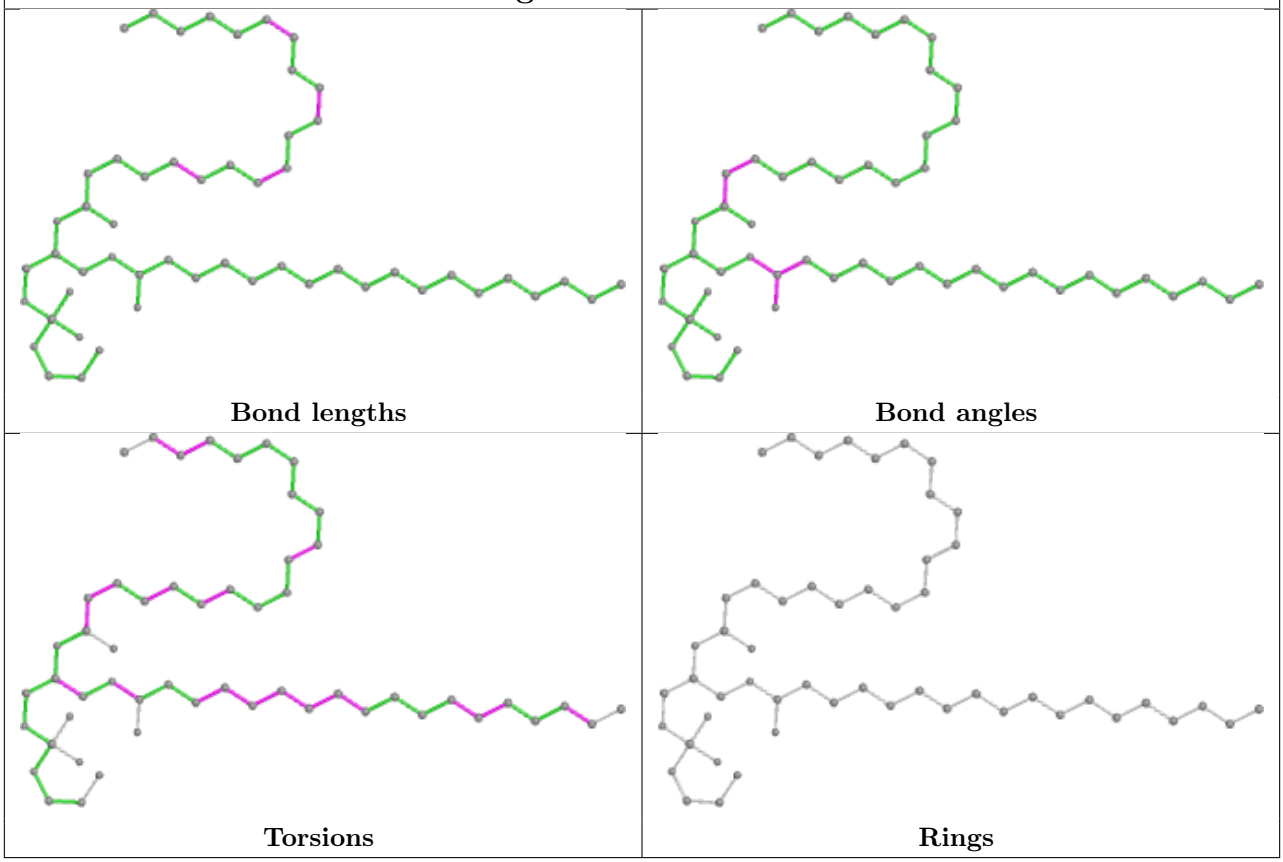
Ligand CHD P 1525	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD J 60	
 Bond lengths	 Bond angles
 Torsions	 Rings

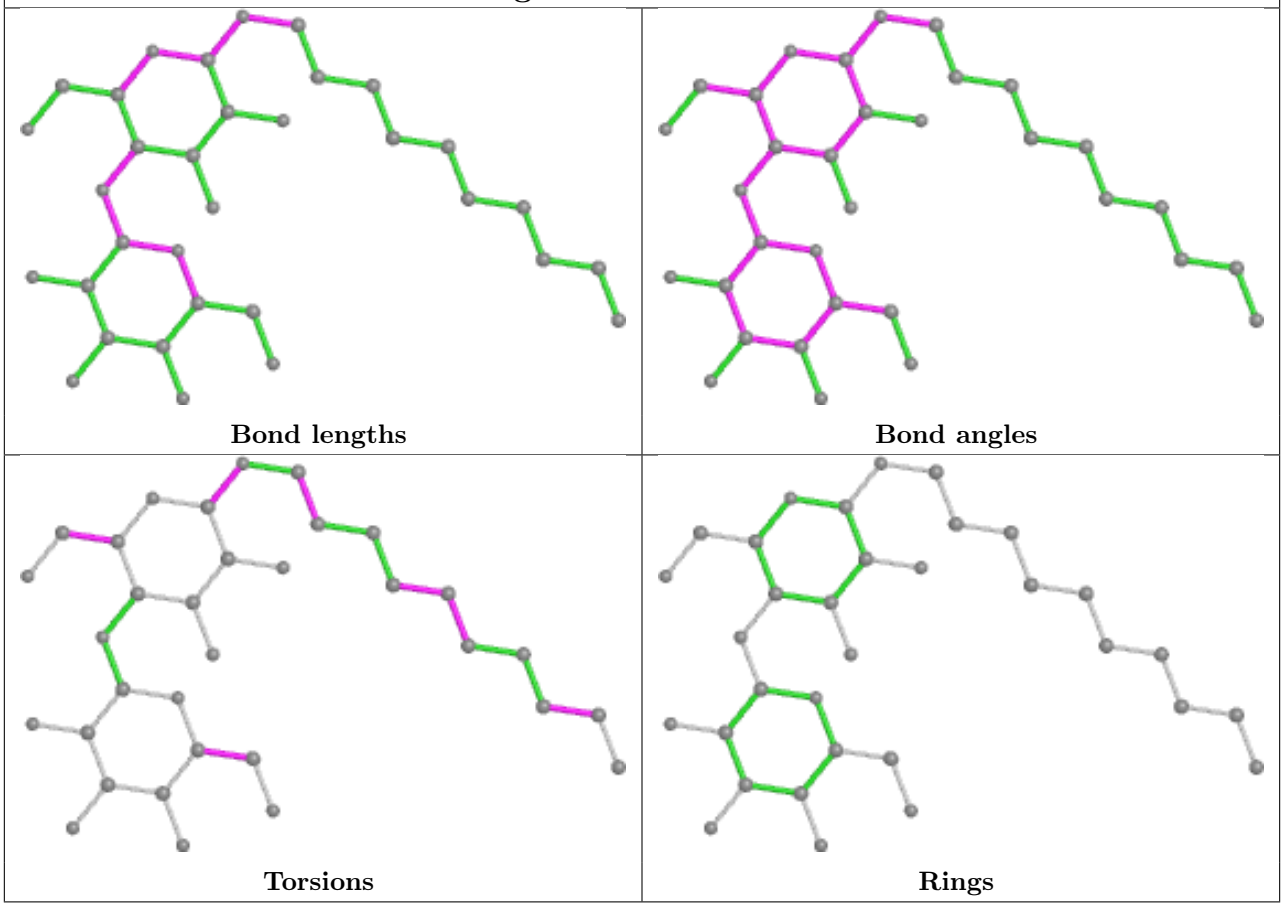
Ligand PEK C 264



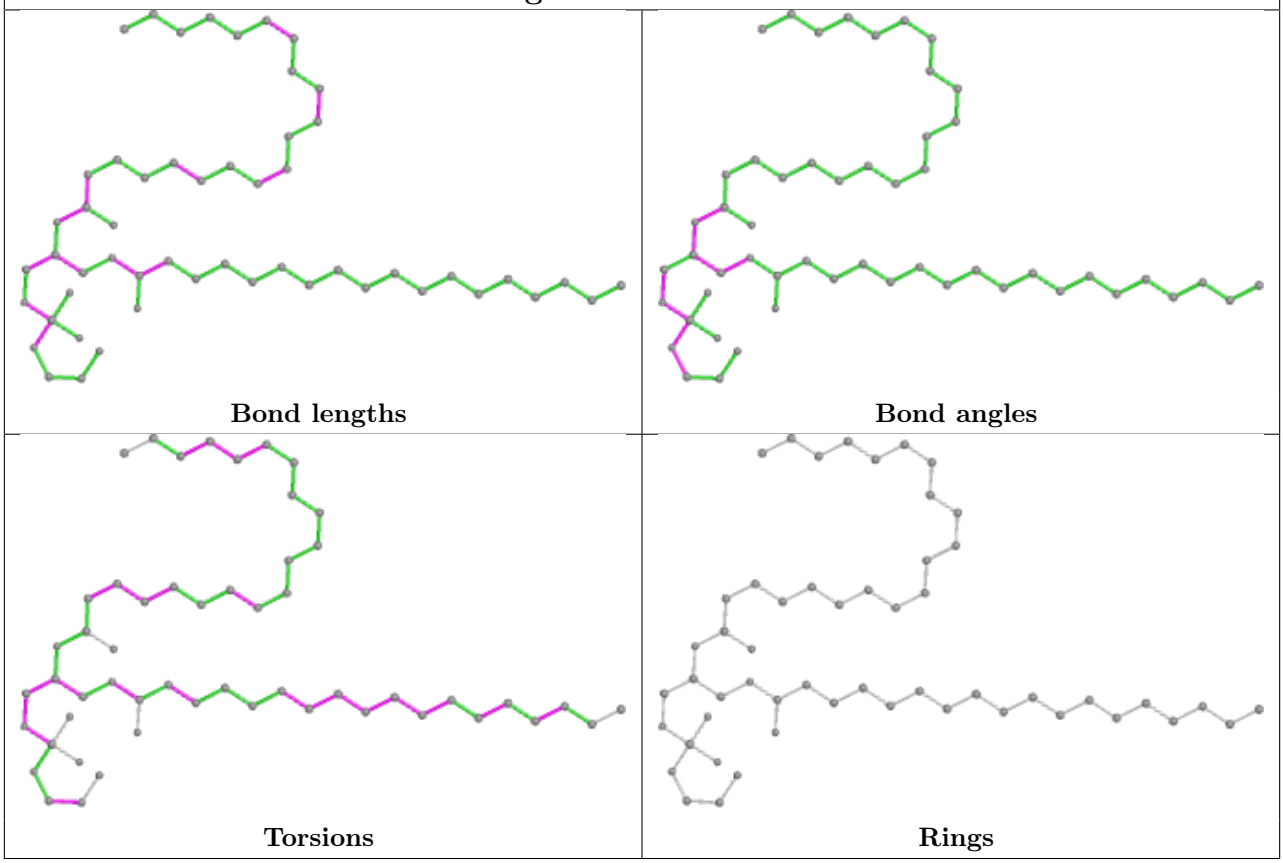
Ligand PEK P 1264



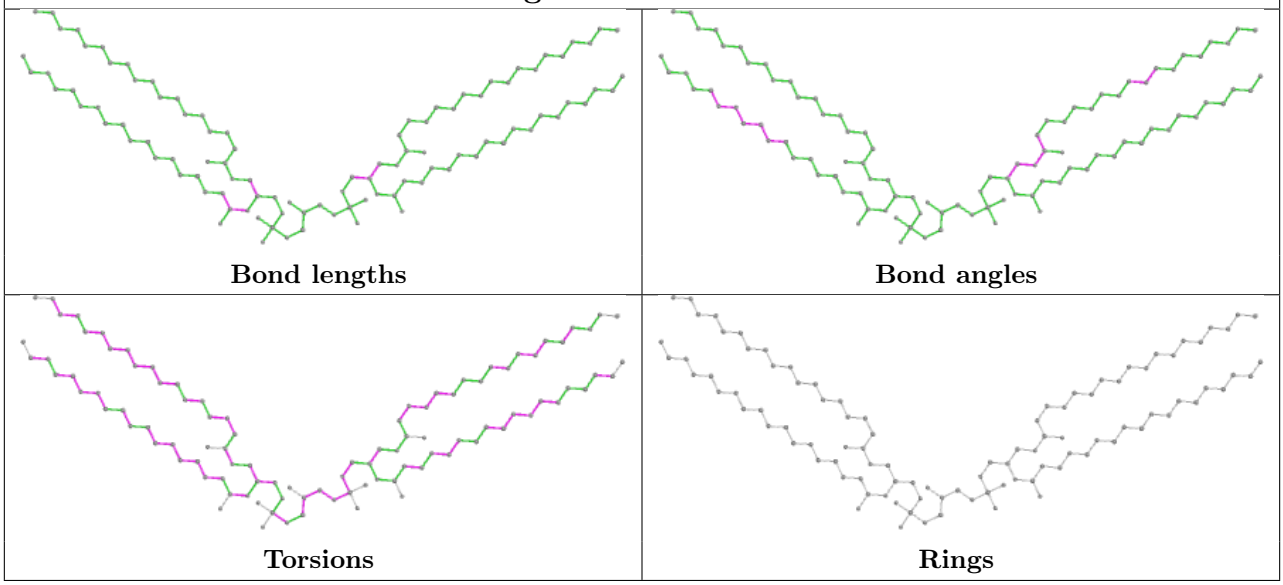
Ligand DMU M 526



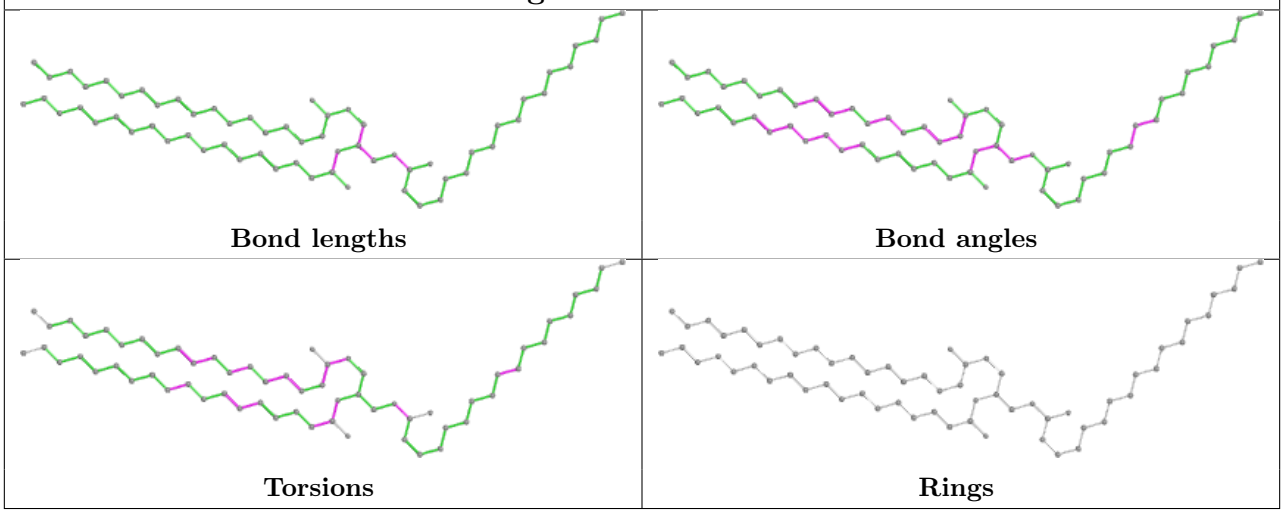
Ligand PEK T 263



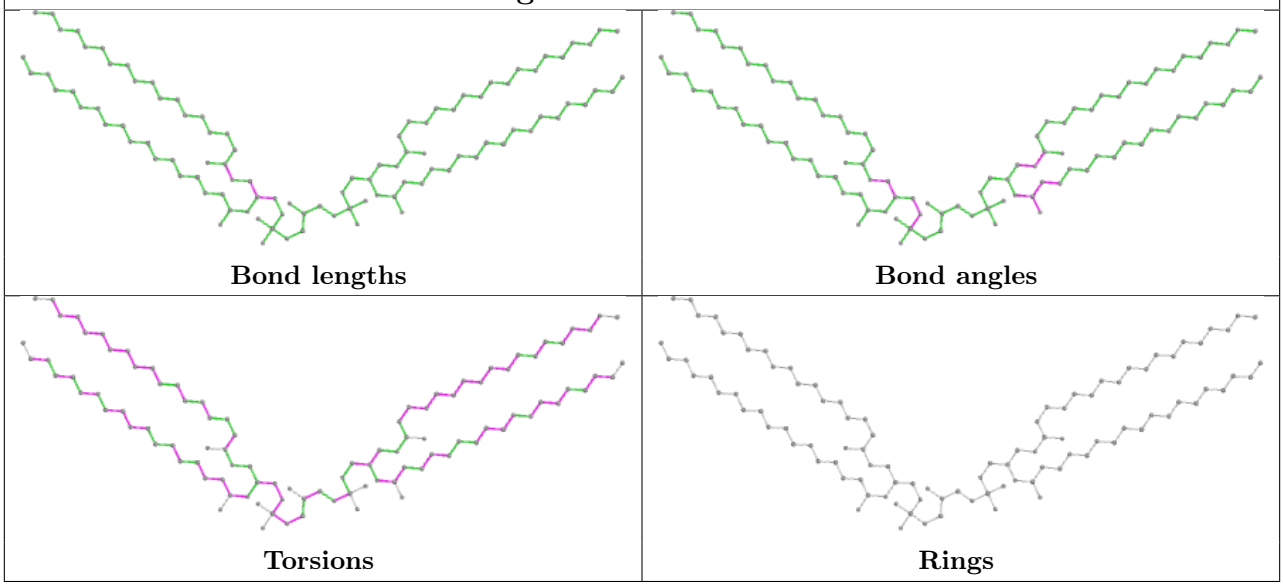
Ligand CDL G 269



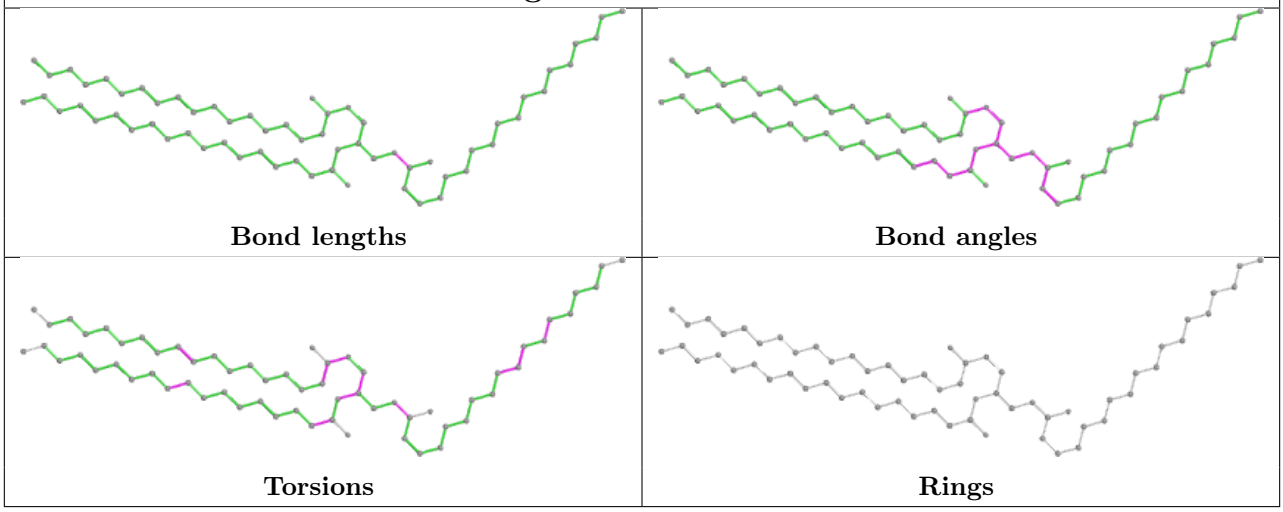
Ligand TGL L 522



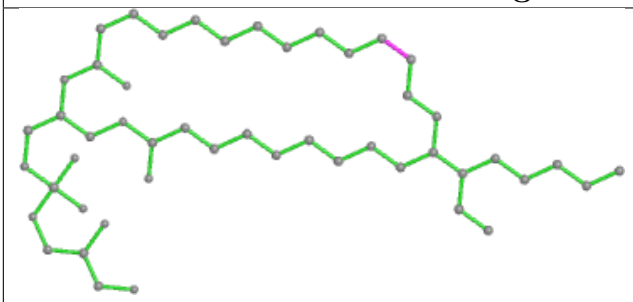
Ligand CDL P 1270



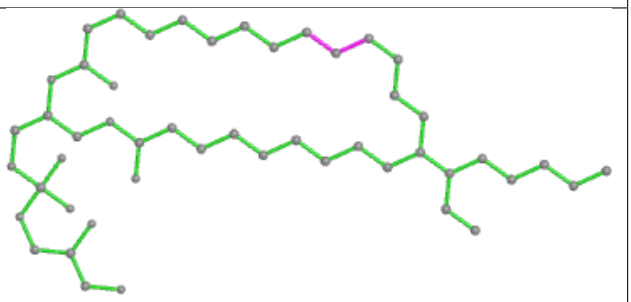
Ligand TGL D 523



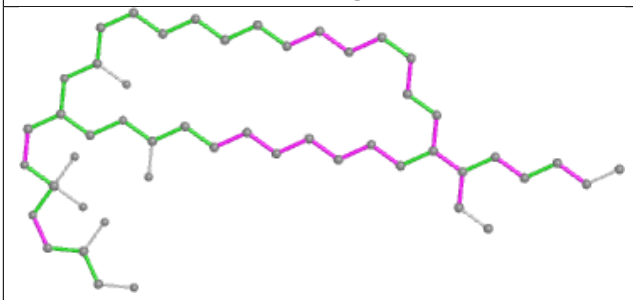
Ligand PGV P 1267



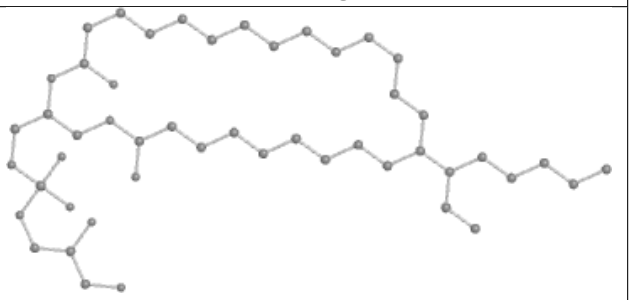
Bond lengths



Bond angles

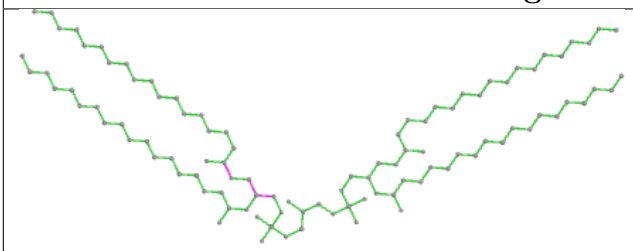


Torsions

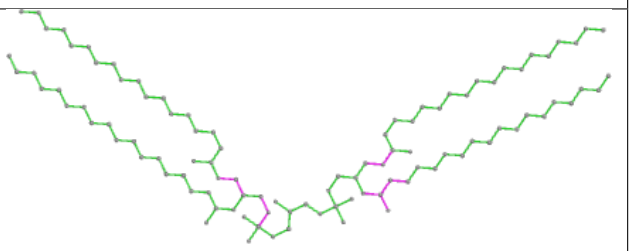


Rings

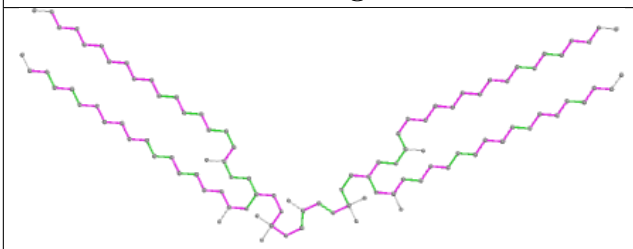
Ligand CDL C 270



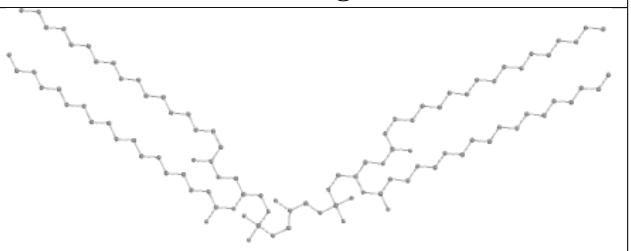
Bond lengths



Bond angles

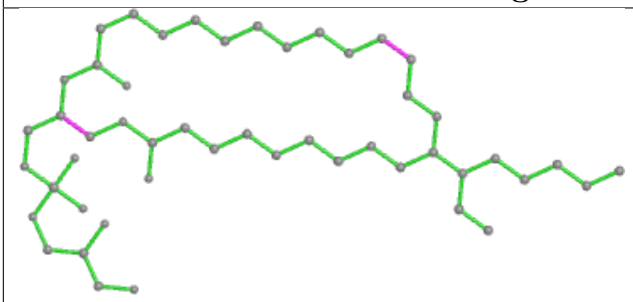


Torsions

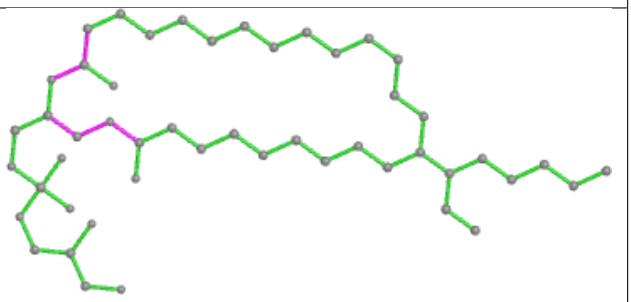


Rings

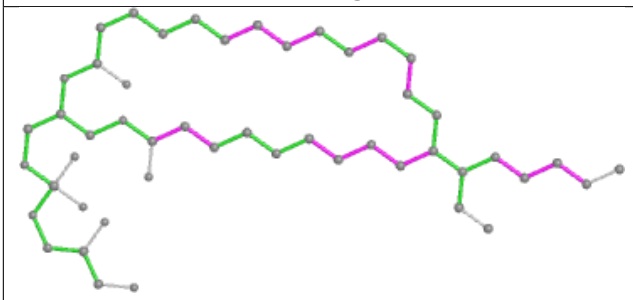
Ligand PGV N 1266



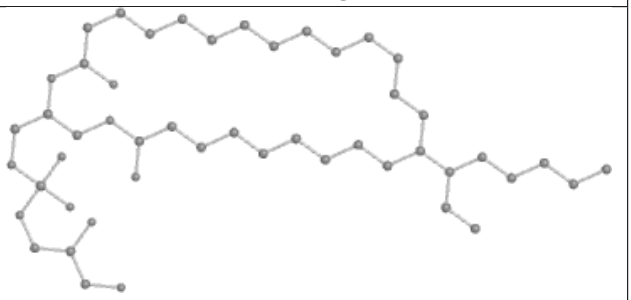
Bond lengths



Bond angles

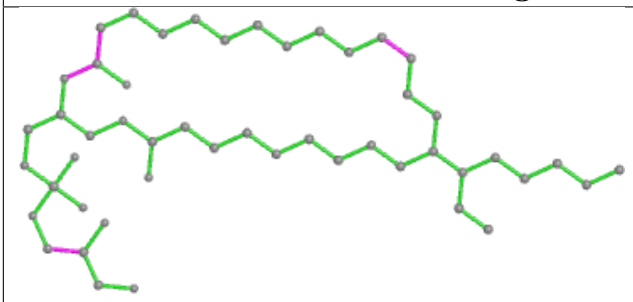


Torsions

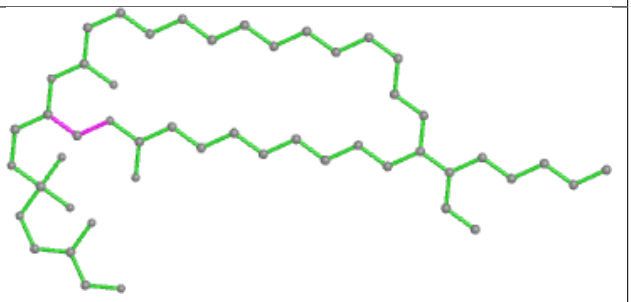


Rings

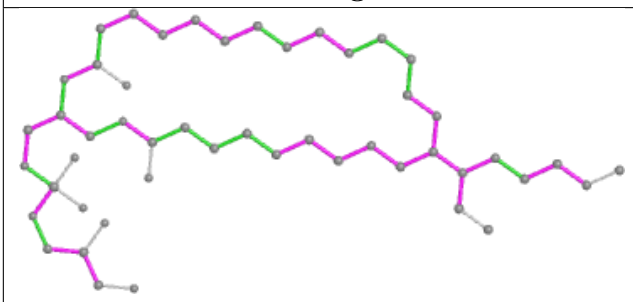
Ligand PGV P 1268



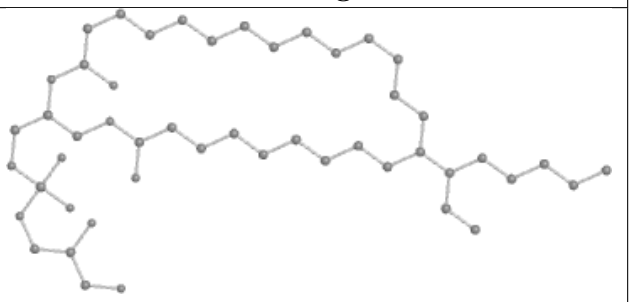
Bond lengths



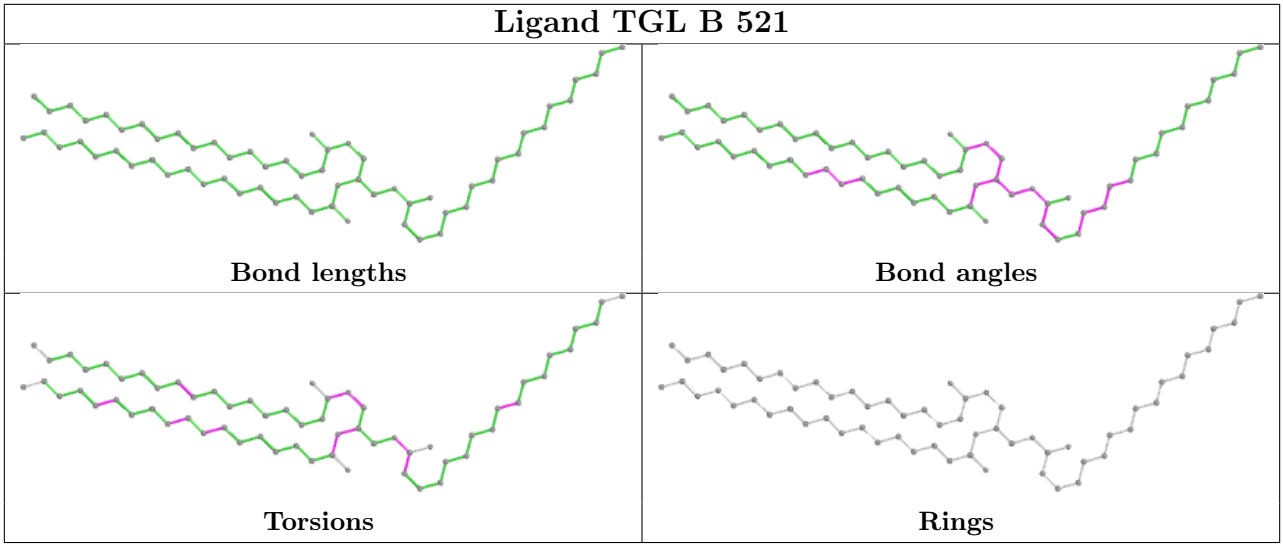
Bond angles

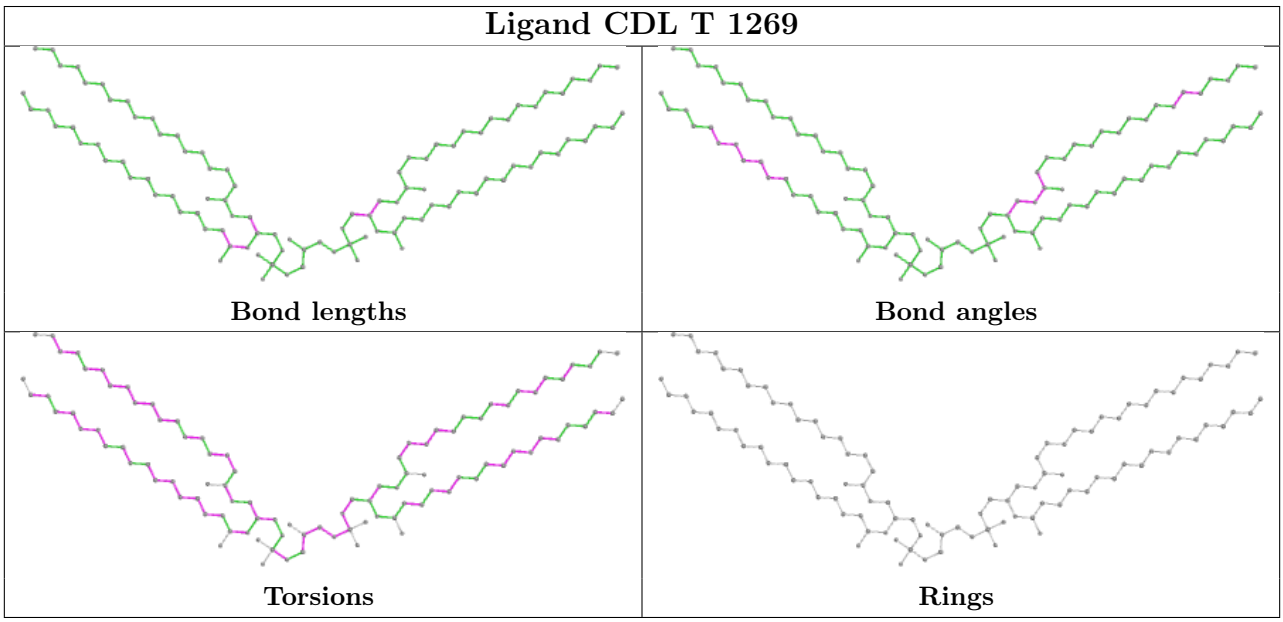


Torsions



Rings





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%)	-0.23	0	100	100	16, 22, 31, 72	0
1	N	513/514 (99%)	-0.27	1 (0%)	95	93	17, 24, 34, 66	0
2	B	226/227 (99%)	-0.50	3 (1%)	77	74	18, 29, 52, 90	0
2	O	226/227 (99%)	-0.22	8 (3%)	44	38	22, 32, 61, 84	0
3	C	259/261 (99%)	-0.53	1 (0%)	92	90	19, 25, 39, 70	0
3	P	259/261 (99%)	-0.47	2 (0%)	86	84	19, 26, 40, 74	0
4	D	144/147 (97%)	-0.33	3 (2%)	63	59	21, 31, 57, 86	0
4	Q	144/147 (97%)	1.00	18 (12%)	3	2	28, 42, 65, 100	0
5	E	105/109 (96%)	-0.05	2 (1%)	66	63	22, 31, 59, 101	0
5	R	105/109 (96%)	0.76	12 (11%)	5	3	25, 39, 71, 102	0
6	F	98/98 (100%)	0.23	8 (8%)	11	9	20, 32, 88, 110	0
6	S	98/98 (100%)	0.23	8 (8%)	11	9	20, 31, 93, 106	0
7	G	83/85 (97%)	0.78	17 (20%)	1	0	23, 34, 99, 107	0
7	T	83/85 (97%)	0.84	17 (20%)	1	0	23, 36, 102, 109	0
8	H	79/85 (92%)	0.22	11 (13%)	2	2	23, 35, 90, 108	0
8	U	79/85 (92%)	0.39	10 (12%)	3	2	27, 39, 91, 110	0
9	I	72/73 (98%)	0.31	5 (6%)	16	13	25, 44, 65, 85	0
9	V	72/73 (98%)	0.62	7 (9%)	7	6	24, 49, 68, 94	0
10	J	58/59 (98%)	0.34	5 (8%)	10	8	26, 36, 72, 99	0
10	W	58/59 (98%)	0.44	8 (13%)	2	2	26, 38, 75, 106	0
11	K	49/56 (87%)	-0.16	1 (2%)	65	61	26, 36, 50, 66	0
11	X	49/56 (87%)	0.79	5 (10%)	6	5	35, 41, 60, 76	0
12	L	46/47 (97%)	-0.39	2 (4%)	35	29	22, 28, 52, 87	0
12	Y	46/47 (97%)	-0.31	1 (2%)	62	57	26, 34, 65, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.10	4 (9%)	8	6	23, 28, 75, 103	0
13	Z	43/46 (93%)	0.31	5 (11%)	4	3	31, 36, 80, 106	0
All	All	3550/3614 (98%)	-0.04	164 (4%)	32	26	16, 29, 64, 110	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	25.6
4	Q	6	VAL	24.6
4	Q	4	SER	19.0
6	S	97	ALA	16.9
6	F	98	HIS	12.0
6	F	96	LEU	11.9
6	S	94	HIS	11.8
6	F	1	ALA	11.7
6	F	97	ALA	9.6
10	W	58	LYS	9.5
6	F	2	SER	8.9
6	S	98	HIS	8.8
13	Z	43	SER	8.8
4	Q	8	SER	8.8
9	V	3	ALA	8.7
7	G	1	ALA	8.4
6	S	1	ALA	8.3
5	R	5	HIS	8.2
8	U	7	LYS	8.1
5	R	109	VAL	7.7
6	S	96	LEU	7.6
8	U	8	ILE	7.5
6	F	95	GLN	7.4
7	T	3	ALA	7.3
10	J	58	LYS	7.3
7	T	1	ALA	7.3
7	T	42	ARG	7.1
7	T	5	LYS	7.0
10	J	1	PHE	6.9
7	T	4	ALA	6.8
7	G	5	LYS	6.6
5	R	79	LYS	6.5
7	T	36	TRP	6.2
7	G	4	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
2	O	226	MET	6.1
10	W	1	PHE	6.1
9	V	2	THR	6.1
9	I	37	PHE	6.1
8	H	7	LYS	6.0
7	T	2	SER	6.0
8	U	44	THR	5.9
5	E	5	HIS	5.9
7	G	3	ALA	5.8
2	O	227	LEU	5.8
7	G	2	SER	5.8
7	T	8	HIS	5.7
10	W	57	HIS	5.7
11	X	6	ALA	5.5
6	S	2	SER	5.5
13	M	43	SER	5.4
4	Q	35	ALA	5.3
9	V	5	ALA	5.2
2	O	113	TYR	5.0
6	F	94	HIS	4.8
4	Q	7	LYS	4.8
9	V	37	PHE	4.7
8	H	47	GLY	4.7
8	U	48	GLY	4.6
13	Z	42	LYS	4.5
7	T	39	SER	4.5
7	T	84	LYS	4.5
7	G	42	ARG	4.4
4	Q	147	LYS	4.4
8	H	46	LYS	4.4
8	H	8	ILE	4.4
7	T	6	GLY	4.3
4	Q	58	GLU	4.3
5	R	108	LYS	4.3
8	H	44	THR	4.2
7	G	36	TRP	4.2
4	Q	51	LEU	4.2
7	G	6	GLY	4.2
8	H	45	ALA	4.2
12	Y	47	LYS	4.1
8	U	9	LYS	4.0
4	D	6	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
13	Z	41	LYS	3.9
7	T	9	GLY	3.9
6	S	95	GLN	3.9
8	U	46	LYS	3.8
1	N	513	LEU	3.7
12	L	2	HIS	3.7
8	U	47	GLY	3.6
2	O	59	GLN	3.6
11	X	7	PRO	3.6
11	X	13	TYR	3.5
3	P	3	HIS	3.5
7	G	84	LYS	3.5
2	O	91	ASN	3.4
2	B	59	GLN	3.4
7	G	8	HIS	3.4
4	Q	33	LEU	3.4
7	G	39	SER	3.3
8	H	48	GLY	3.3
9	I	2	THR	3.2
4	Q	39	ALA	3.1
9	V	4	LEU	3.1
10	J	57	HIS	3.1
7	T	10	GLY	3.1
4	D	5	VAL	3.1
13	M	39	ASN	3.0
13	M	40	TYR	3.0
5	E	109	VAL	3.0
7	G	41	HIS	3.0
13	Z	40	TYR	3.0
6	F	3	GLY	2.9
7	G	40	GLY	2.9
7	T	40	GLY	2.9
5	R	86	ILE	2.8
10	W	55	PHE	2.8
8	U	45	ALA	2.8
5	R	9	GLU	2.8
11	K	6	ALA	2.8
8	H	9	LYS	2.8
8	U	10	ASN	2.8
10	W	52	TRP	2.7
9	I	4	LEU	2.7
5	R	83	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	O	90	ILE	2.7
4	Q	46	ALA	2.6
8	H	10	ASN	2.6
7	T	41	HIS	2.6
2	O	223	SER	2.5
4	D	147	LYS	2.5
12	L	47	LYS	2.5
10	J	4	ARG	2.5
9	V	36	LYS	2.5
10	J	52	TRP	2.5
4	Q	10	ASP	2.4
5	R	105	GLY	2.4
7	G	9	GLY	2.4
8	H	49	ASP	2.4
5	R	93	LEU	2.4
7	T	43	GLU	2.4
13	M	42	LYS	2.4
5	R	89	LEU	2.4
5	R	106	LEU	2.4
7	G	12	GLY	2.4
7	G	45	PRO	2.4
8	H	50	VAL	2.4
6	S	93	PRO	2.3
13	Z	39	ASN	2.3
2	B	65	TRP	2.3
7	G	43	GLU	2.3
7	T	7	ASP	2.3
2	B	60	GLU	2.2
2	O	224	ALA	2.2
10	W	2	GLU	2.2
10	W	56	PRO	2.2
11	X	23	THR	2.2
10	W	4	ARG	2.1
11	X	12	LYS	2.1
3	C	3	HIS	2.1
5	R	48	ILE	2.1
4	Q	55	GLU	2.1
9	I	25	PHE	2.1
4	Q	52	SER	2.1
3	P	37	PHE	2.1
9	I	34	PHE	2.0
9	V	34	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
4	Q	31	LYS	2.0
8	U	49	ASP	2.0
4	Q	62	LEU	2.0
4	Q	142	LYS	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	0.38	0.37	77,85,107,108	0
9	SAC	V	1	9/10	0.51	0.49	99,100,104,104	0
7	TPO	T	11	11/12	0.53	0.31	76,84,110,112	0
9	SAC	I	1	9/10	0.69	0.39	93,97,99,99	0
1	FME	A	1	10/11	0.83	0.15	40,45,66,72	0
1	FME	N	1	10/11	0.90	0.16	39,43,65,69	0
2	FME	B	1	10/11	0.93	0.14	23,31,39,50	0
2	FME	O	1	10/11	0.93	0.15	37,38,47,53	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
25	PEK	T	263	53/53	0.50	0.40	45,83,100,103	0
25	PEK	P	1265	53/53	0.52	0.33	46,89,107,109	0
25	PEK	C	265	53/53	0.52	0.29	44,88,103,104	0
23	DMU	P	1272	33/33	0.56	0.39	73,96,104,105	0
23	DMU	C	272	33/33	0.58	0.39	71,97,102,104	0
21	PSC	O	1230	52/52	0.59	0.34	48,80,111,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	CDL	G	269	100/100	0.59	0.32	61,83,101,105	0
26	CDL	T	1269	100/100	0.59	0.32	54,84,97,105	0
21	PSC	B	230	52/52	0.61	0.35	48,84,113,116	0
25	PEK	G	1263	53/53	0.61	0.39	46,83,99,101	0
18	PGV	C	268	51/51	0.62	0.39	65,84,103,106	0
20	TGL	N	1522	63/63	0.63	0.32	42,67,79,82	0
22	CHD	W	1060	29/29	0.64	0.40	98,104,106,108	0
26	CDL	P	1270	100/100	0.67	0.37	42,88,101,105	0
20	TGL	Q	1523	63/63	0.67	0.23	45,70,80,84	0
18	PGV	P	1268	51/51	0.69	0.37	65,84,104,106	0
20	TGL	L	522	63/63	0.71	0.30	34,65,79,81	0
22	CHD	J	60	29/29	0.73	0.37	98,104,107,109	0
20	TGL	D	523	63/63	0.73	0.23	47,65,79,82	0
26	CDL	C	270	100/100	0.73	0.38	44,87,100,106	0
18	PGV	A	524	51/51	0.74	0.26	35,71,101,104	0
22	CHD	C	271	29/29	0.76	0.26	87,95,96,97	0
22	CHD	P	1271	29/29	0.78	0.28	89,95,98,101	0
18	PGV	Z	1524	51/51	0.78	0.27	38,71,101,104	0
20	TGL	N	1521	63/63	0.78	0.24	49,67,84,86	0
20	TGL	B	521	63/63	0.80	0.23	49,64,85,90	0
24	UNX	C	262	1/1	0.86	0.27	47,47,47,47	0
23	DMU	Z	1526	33/33	0.89	0.19	40,49,61,64	0
24	UNX	P	1262	1/1	0.90	0.44	43,43,43,43	0
23	DMU	M	526	33/33	0.92	0.12	32,42,55,58	0
16	NA	N	1519	1/1	0.93	0.07	30,30,30,30	0
25	PEK	P	1264	53/53	0.95	0.13	25,44,68,72	0
25	PEK	C	264	53/53	0.96	0.12	10,44,70,73	0
16	NA	A	519	1/1	0.96	0.06	27,27,27,27	0
15	MG	N	1518	1/1	0.96	0.10	26,26,26,26	0
18	PGV	P	1267	51/51	0.96	0.12	23,34,59,61	0
22	CHD	P	1525	29/29	0.96	0.10	20,27,31,34	0
18	PGV	C	267	51/51	0.97	0.10	20,34,58,62	0
18	PGV	A	525	51/51	0.97	0.11	21,36,56,63	0
22	CHD	B	1086	29/29	0.97	0.07	20,24,30,37	0
22	CHD	C	525	29/29	0.97	0.12	21,27,30,33	0
18	PGV	N	1266	51/51	0.97	0.11	20,38,55,64	0
19	CUA	O	228	2/2	0.98	0.08	26,26,26,27	0
22	CHD	O	229	29/29	0.98	0.07	19,22,28,32	0
17	HEA	N	515	60/60	0.98	0.11	18,24,41,43	0
17	HEA	N	516	60/60	0.99	0.10	17,20,29,31	0
19	CUA	B	228	2/2	0.99	0.08	19,19,19,22	0
17	HEA	A	515	60/60	0.99	0.11	12,20,44,45	0

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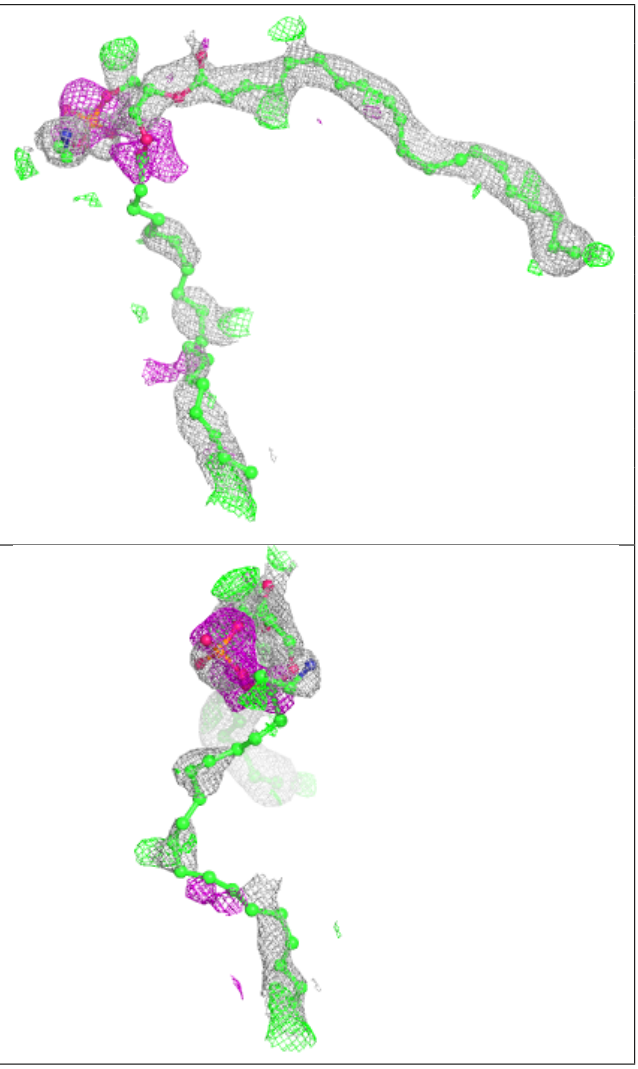
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	HEA	A	516	60/60	0.99	0.10	15,18,29,29	0
15	MG	A	518	1/1	0.99	0.10	20,20,20,20	0
27	ZN	F	99	1/1	0.99	0.06	25,25,25,25	0
27	ZN	S	99	1/1	0.99	0.06	27,27,27,27	0
14	CU	A	517	1/1	1.00	0.09	20,20,20,20	0
14	CU	N	517	1/1	1.00	0.09	21,21,21,21	0

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.

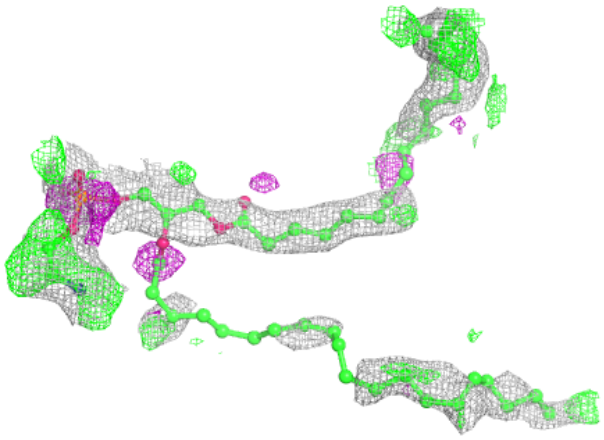
Electron density around PEK T 263:

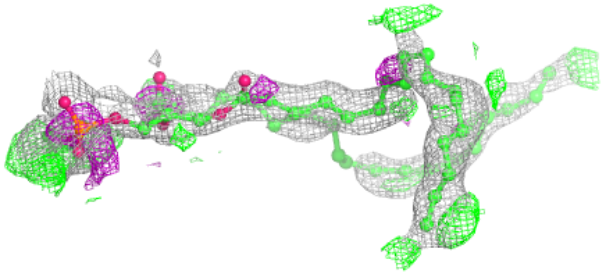
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEK P 1265:

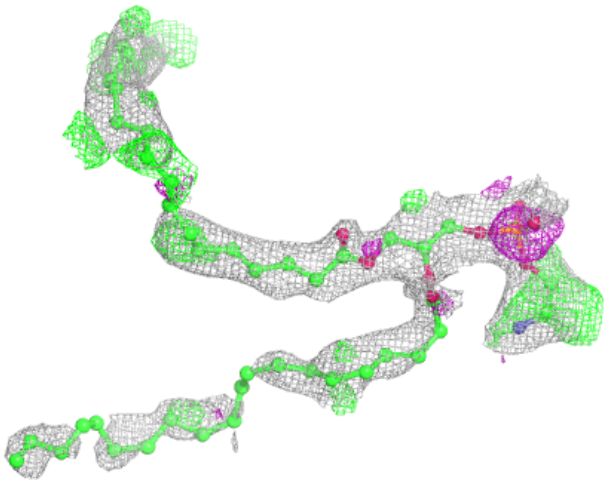
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

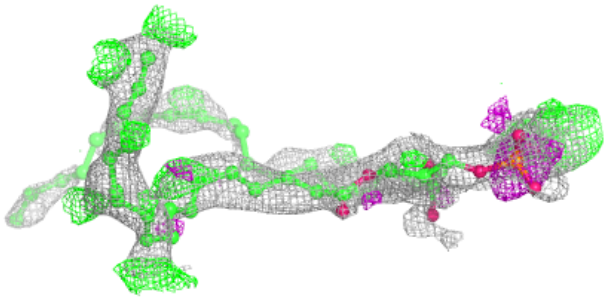


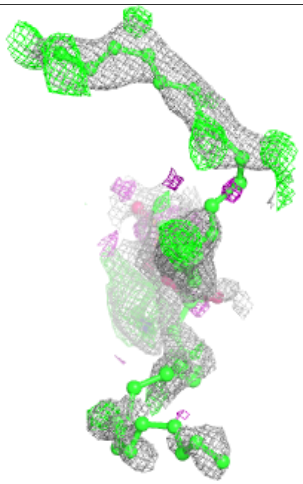


Electron density around PEK C 265:

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

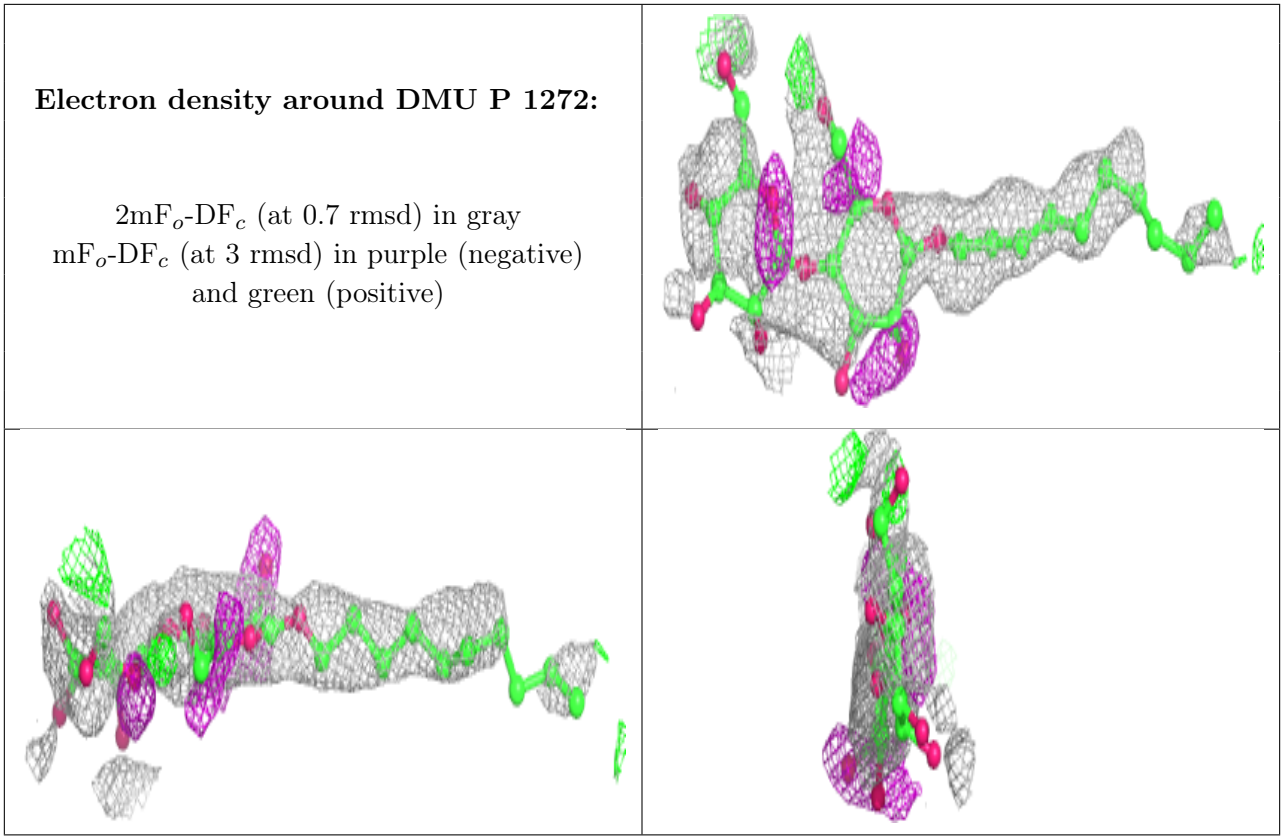






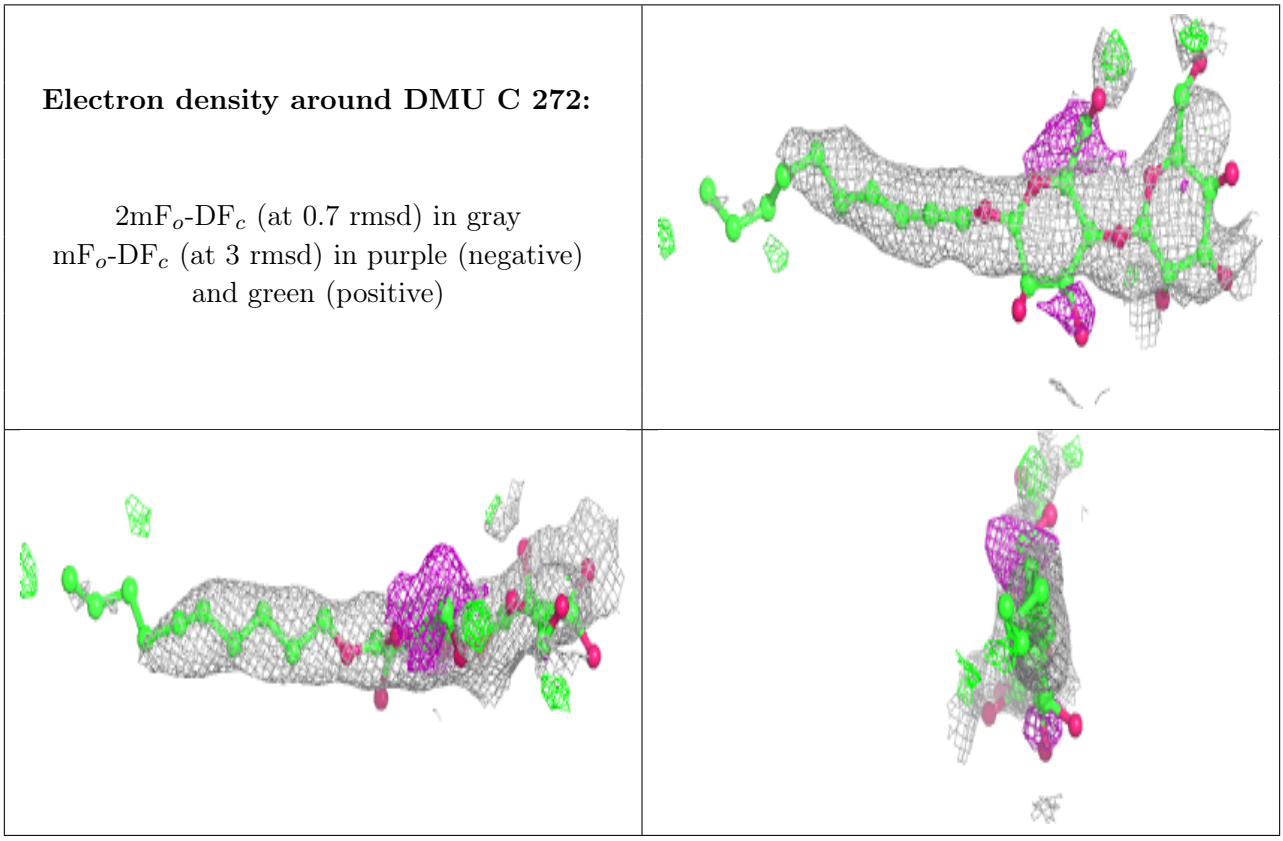
Electron density around DMU P 1272:

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



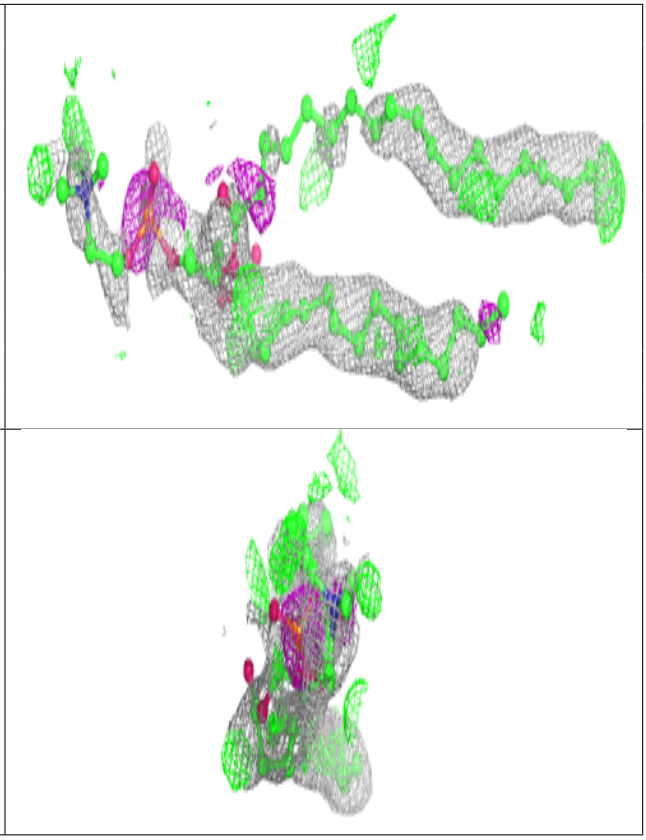
Electron density around DMU C 272:

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



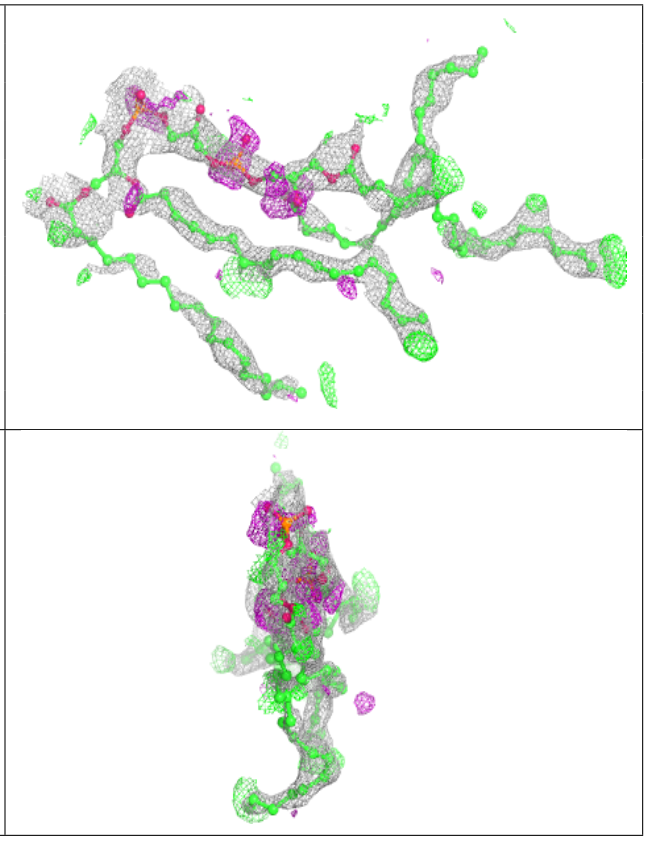
Electron density around PSC O 1230:

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



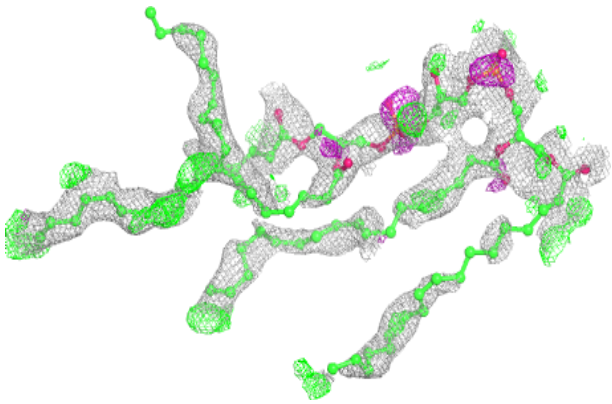
Electron density around CDL G 269:

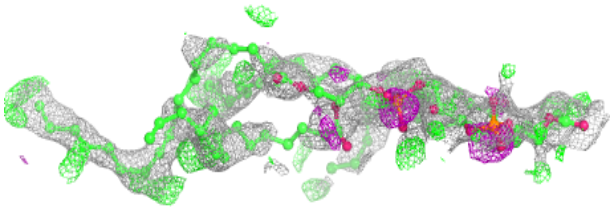
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

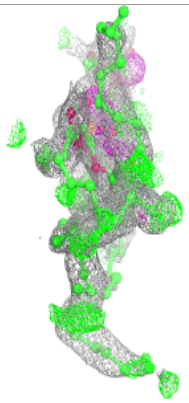


Electron density around CDL T 1269:

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

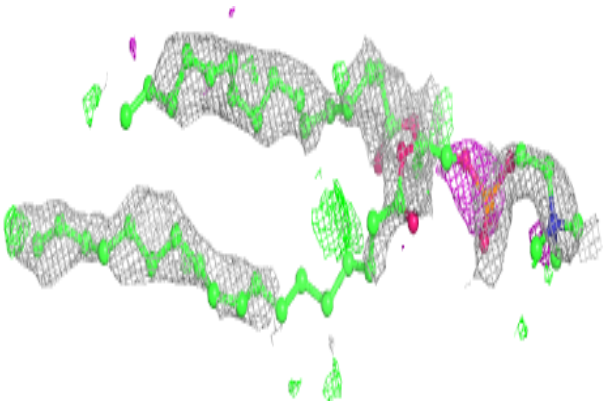


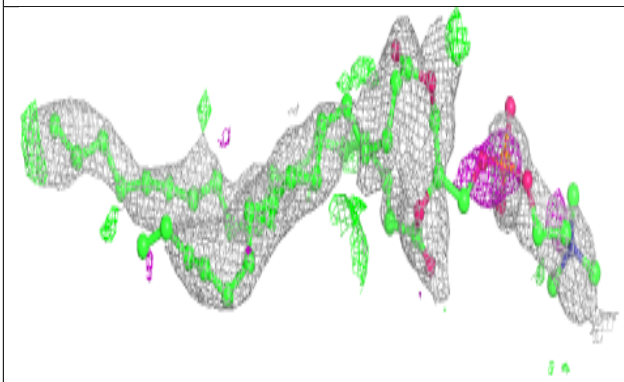


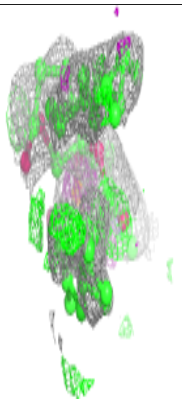


Electron density around PSC B 230:

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

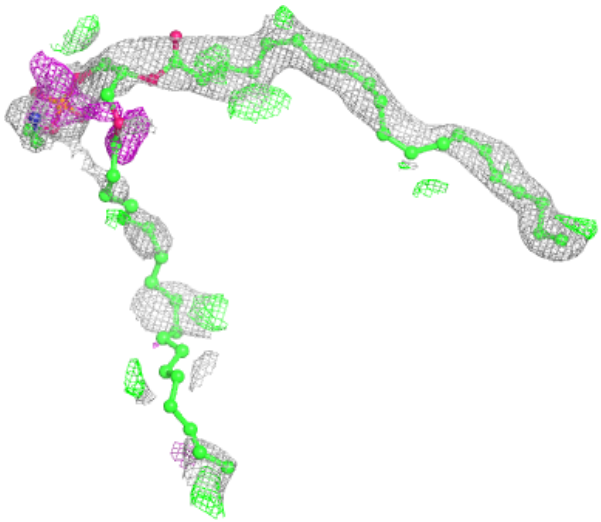


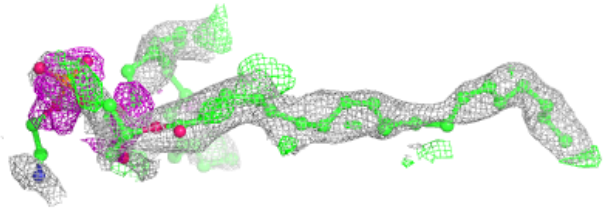


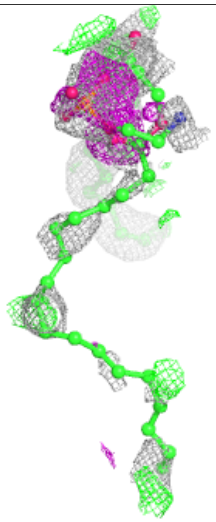


Electron density around PEK G 1263:

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

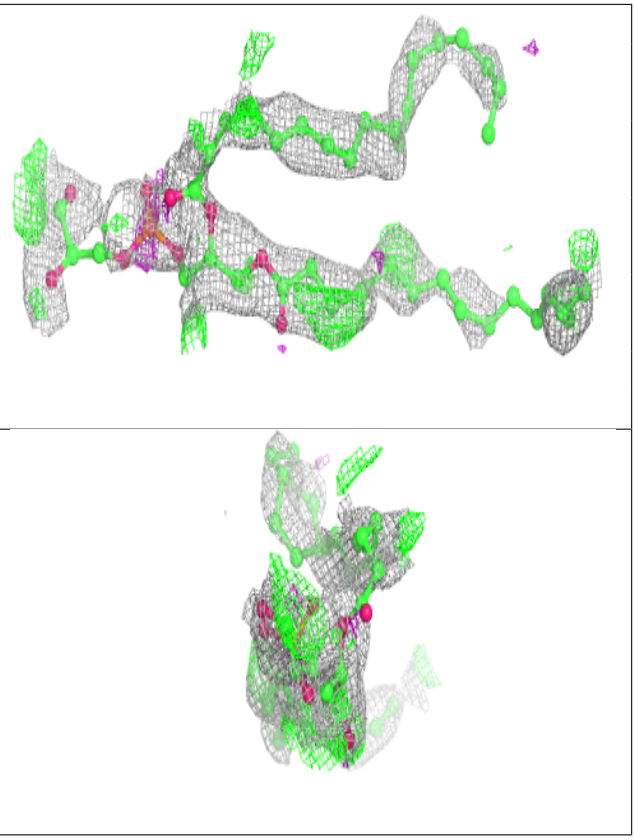






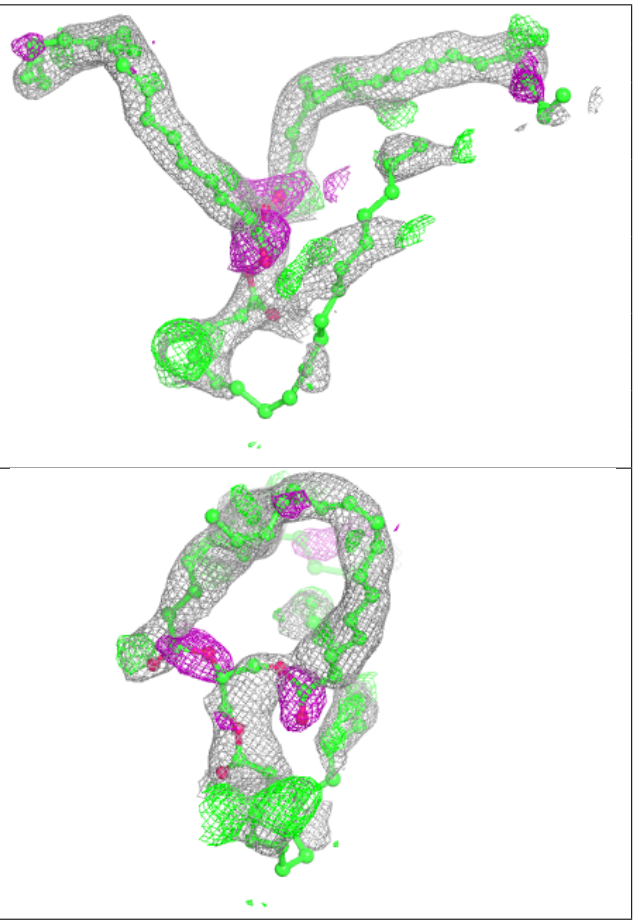
Electron density around PGV C 268:

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



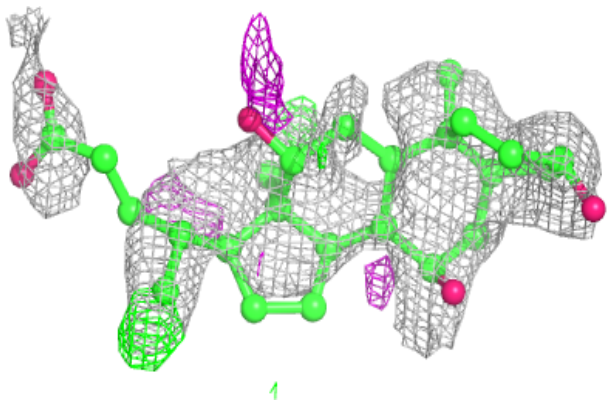
Electron density around TGL N 1522:

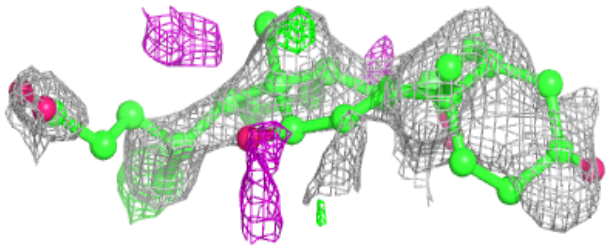
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

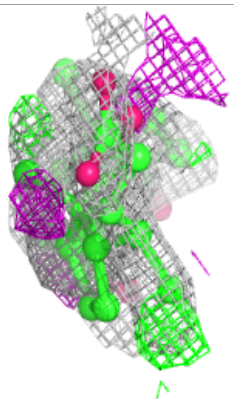


Electron density around CHD W 1060:

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

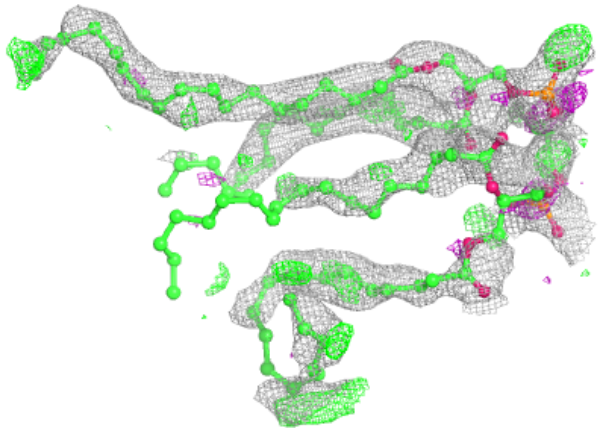


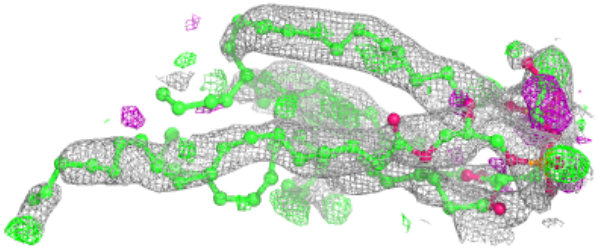


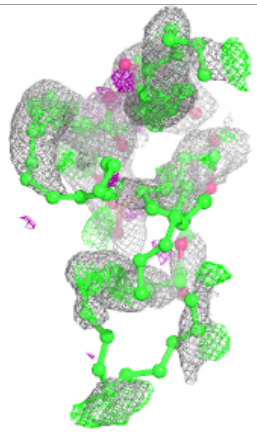


Electron density around CDL P 1270:

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

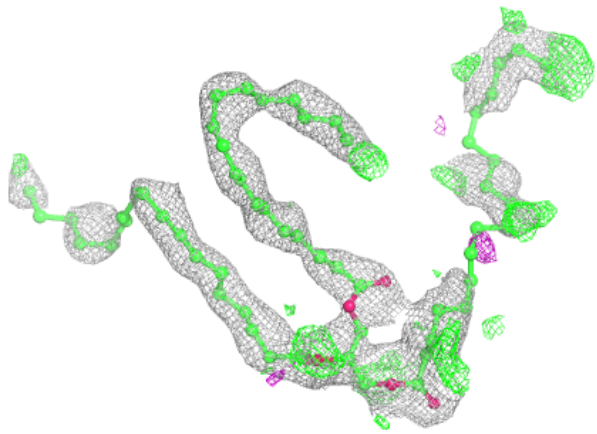


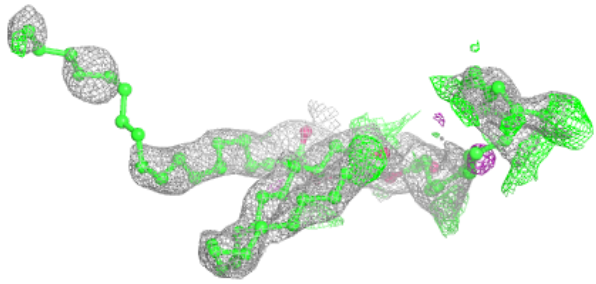


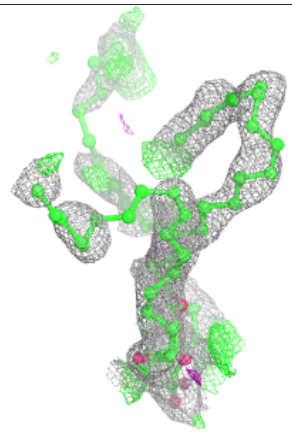


Electron density around TGL Q 1523:

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

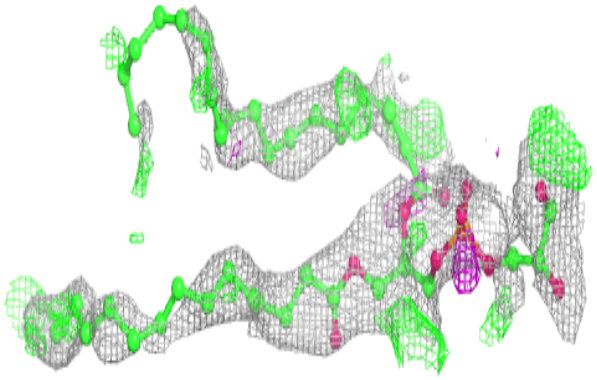


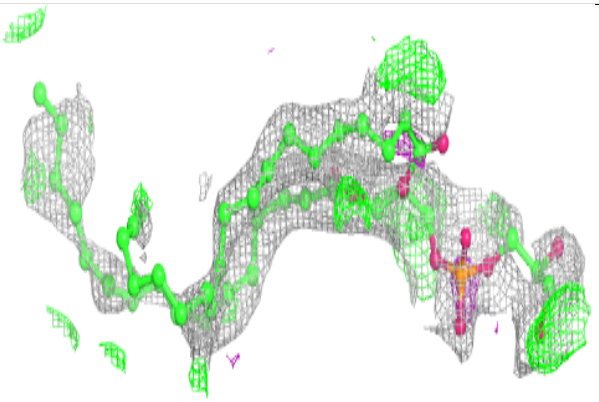


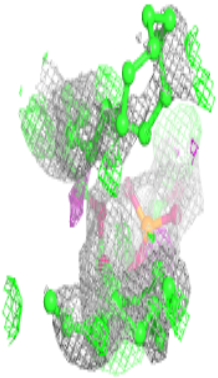


Electron density around PGV P 1268:

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

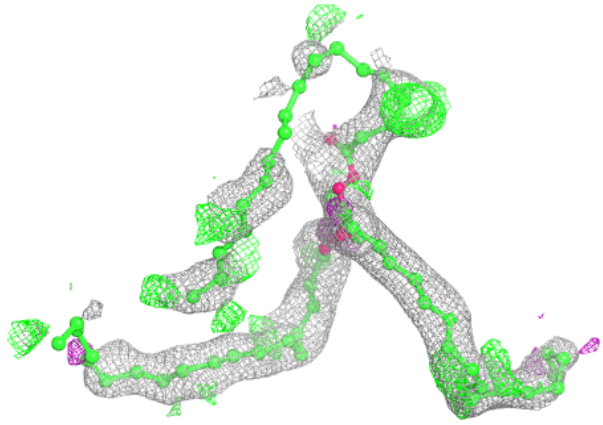


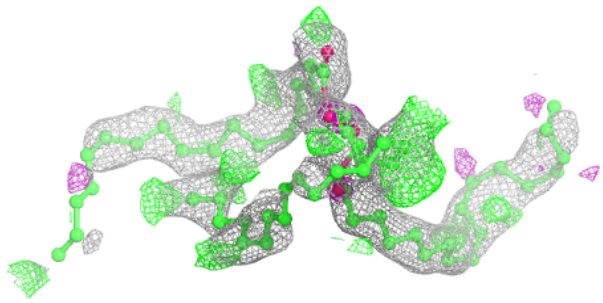


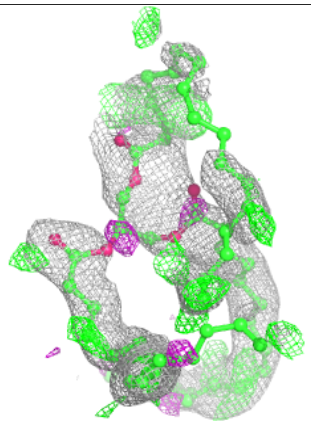


Electron density around TGL L 522:

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

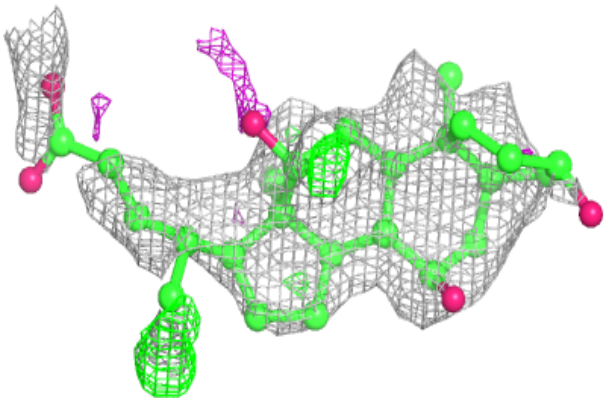


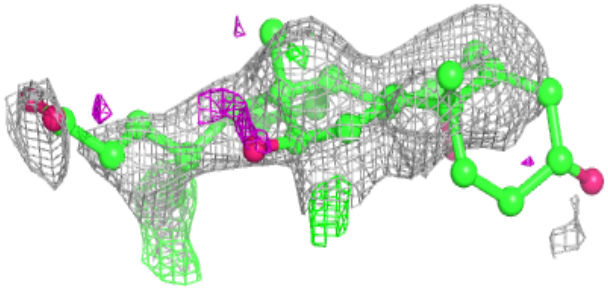


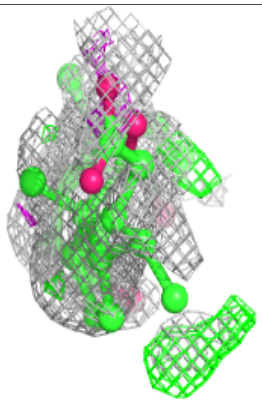


Electron density around CHD J 60:

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

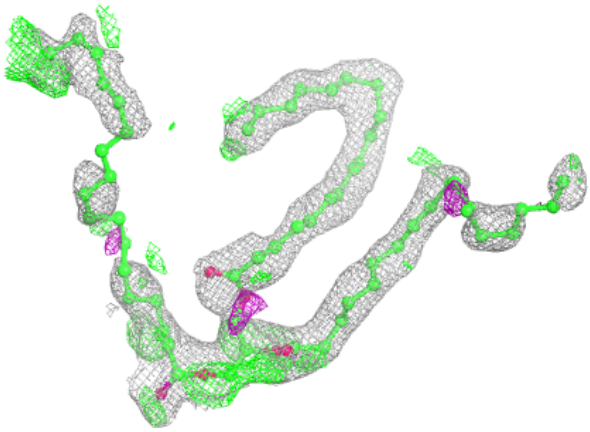


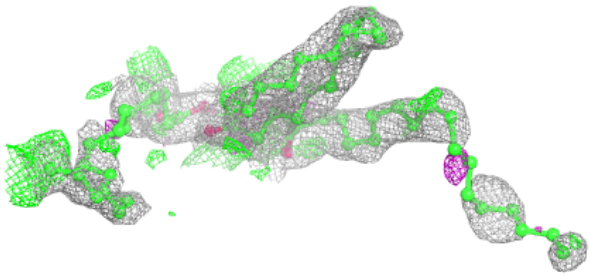


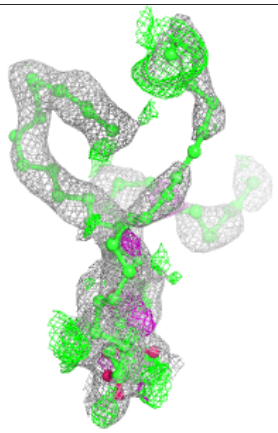


Electron density around TGL D 523:

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

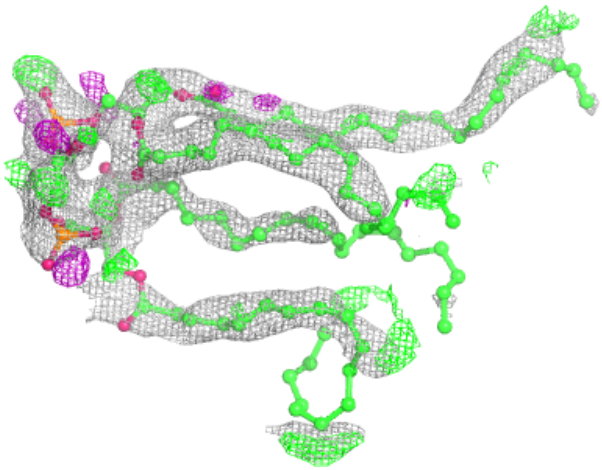


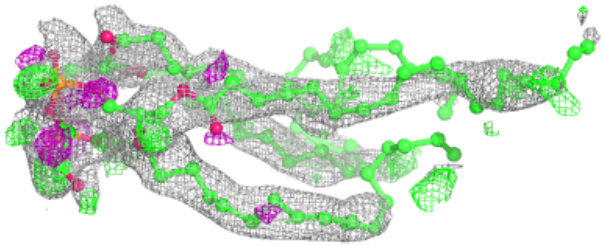


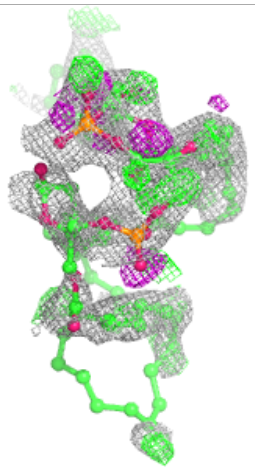


Electron density around CDL C 270:

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

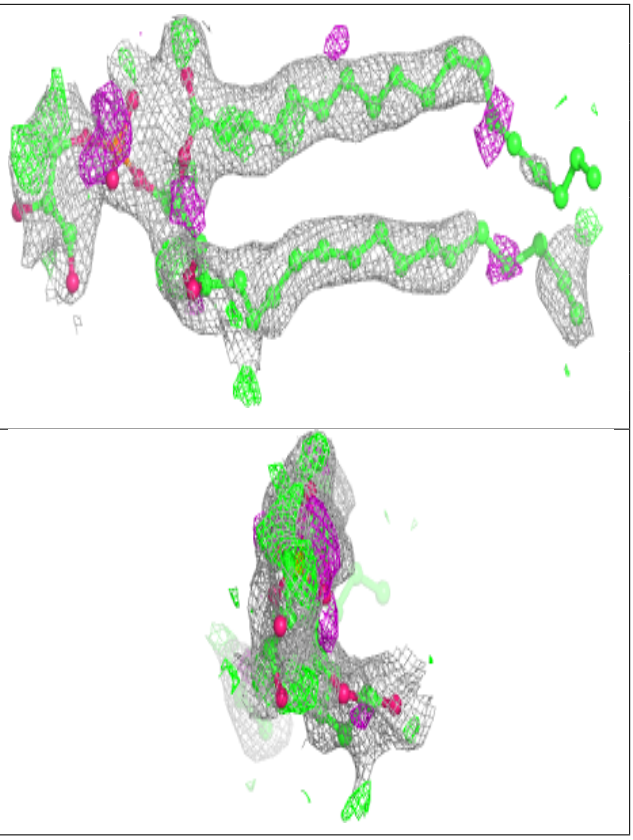






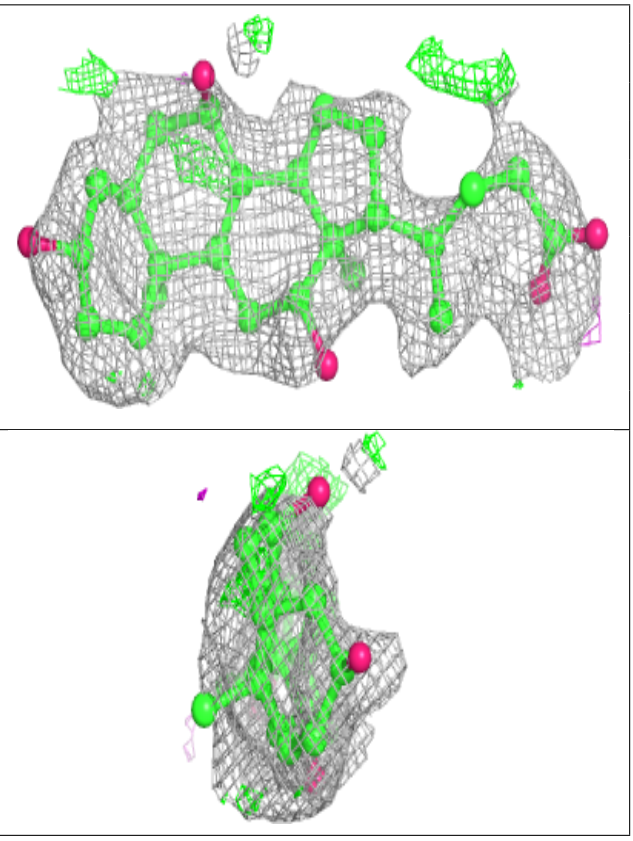
Electron density around PGV A 524:

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



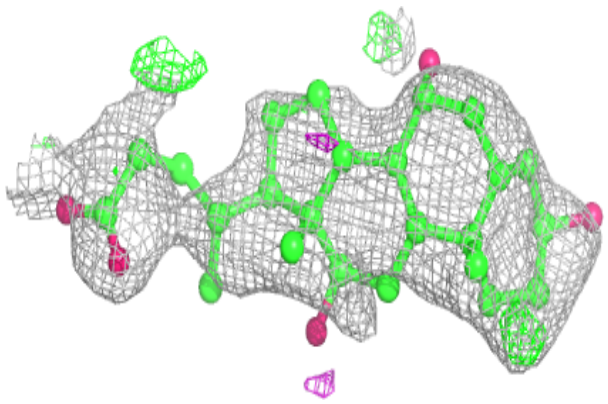
Electron density around CHD C 271:

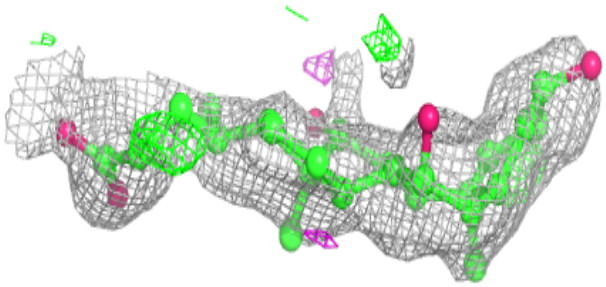
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

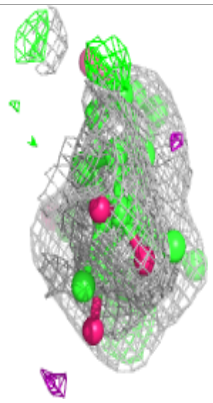


Electron density around CHD P 1271:

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

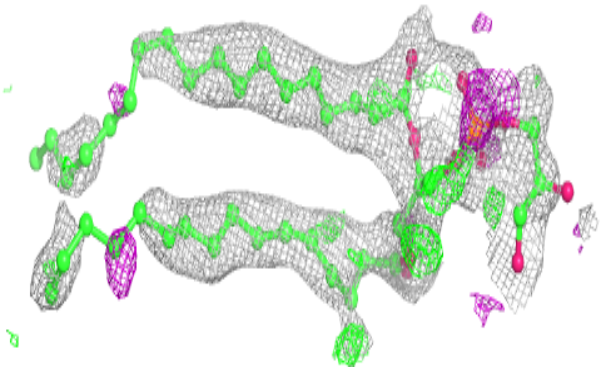


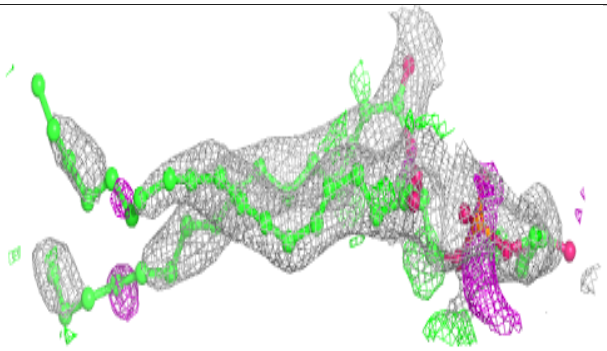


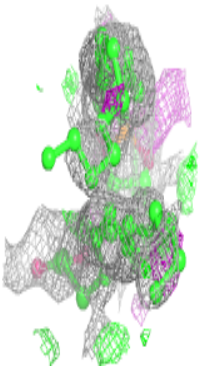


Electron density around PGV Z 1524:

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

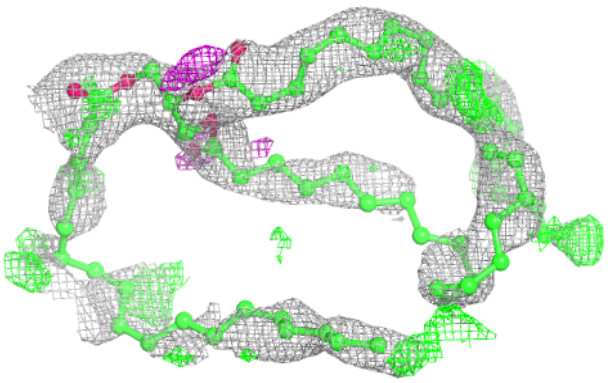


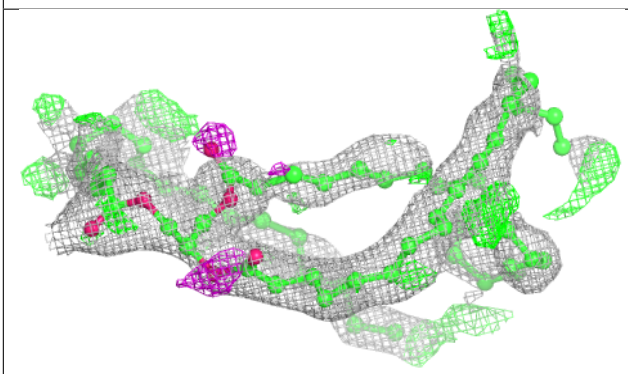


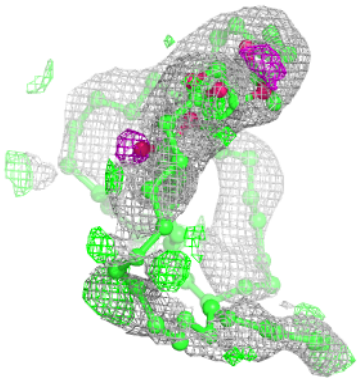


Electron density around TGL N 1521:

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

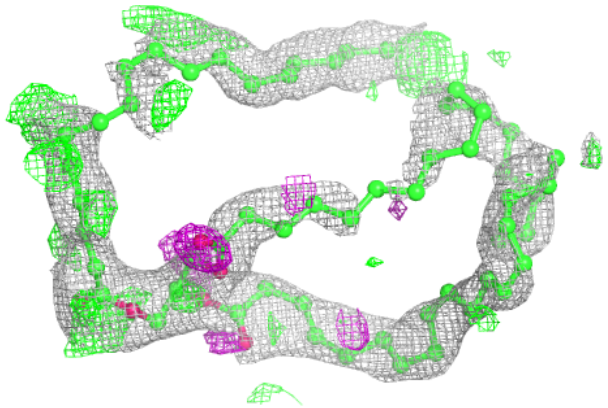


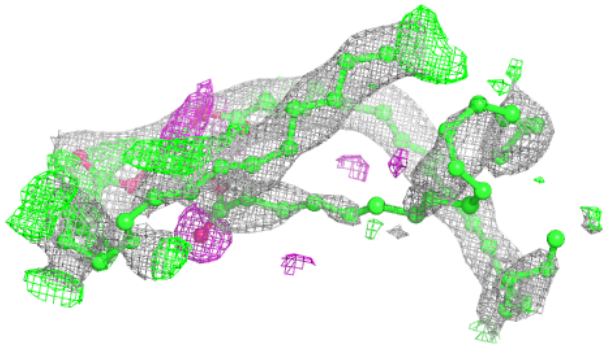


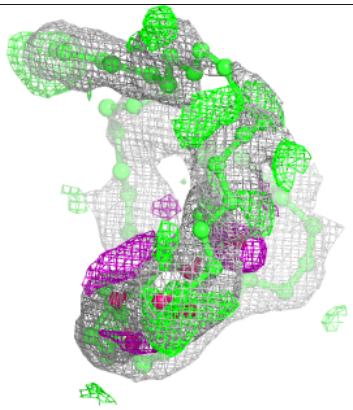


Electron density around TGL B 521:

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

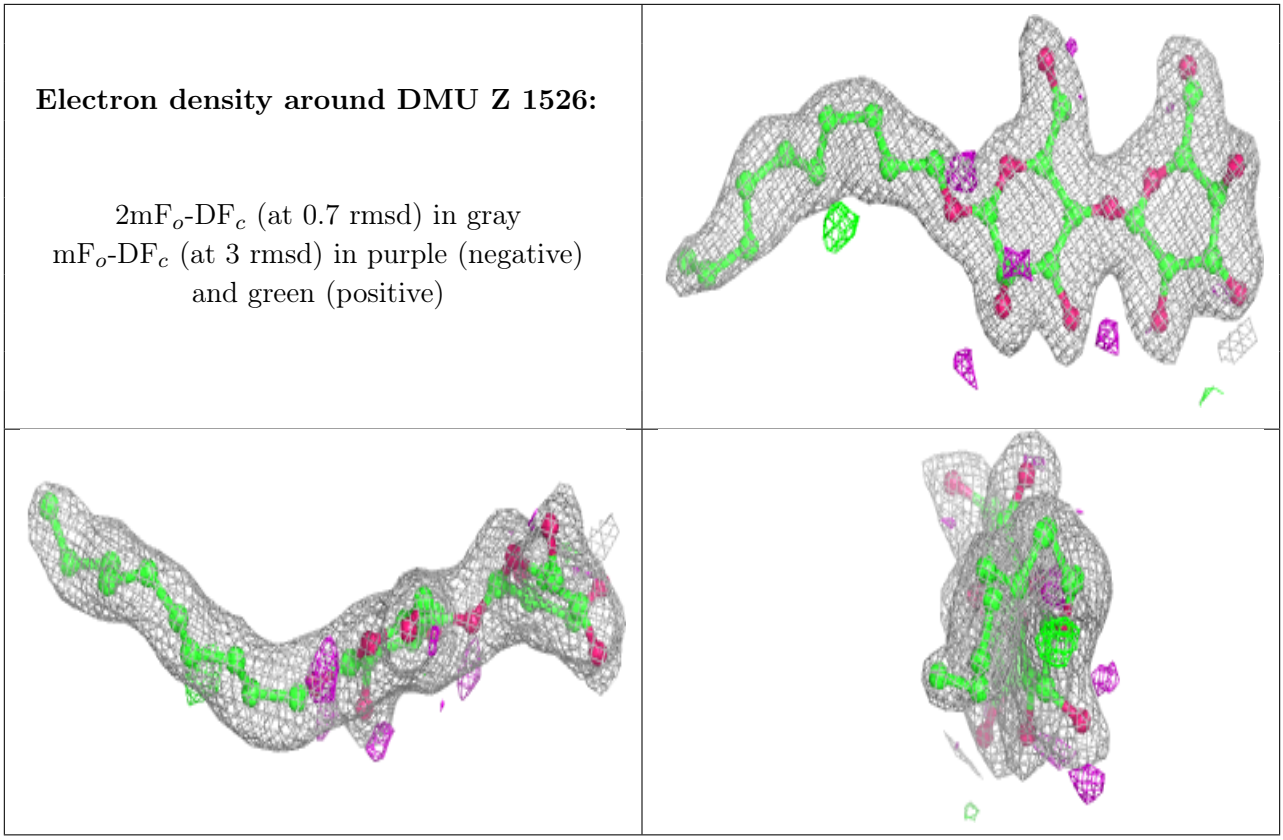






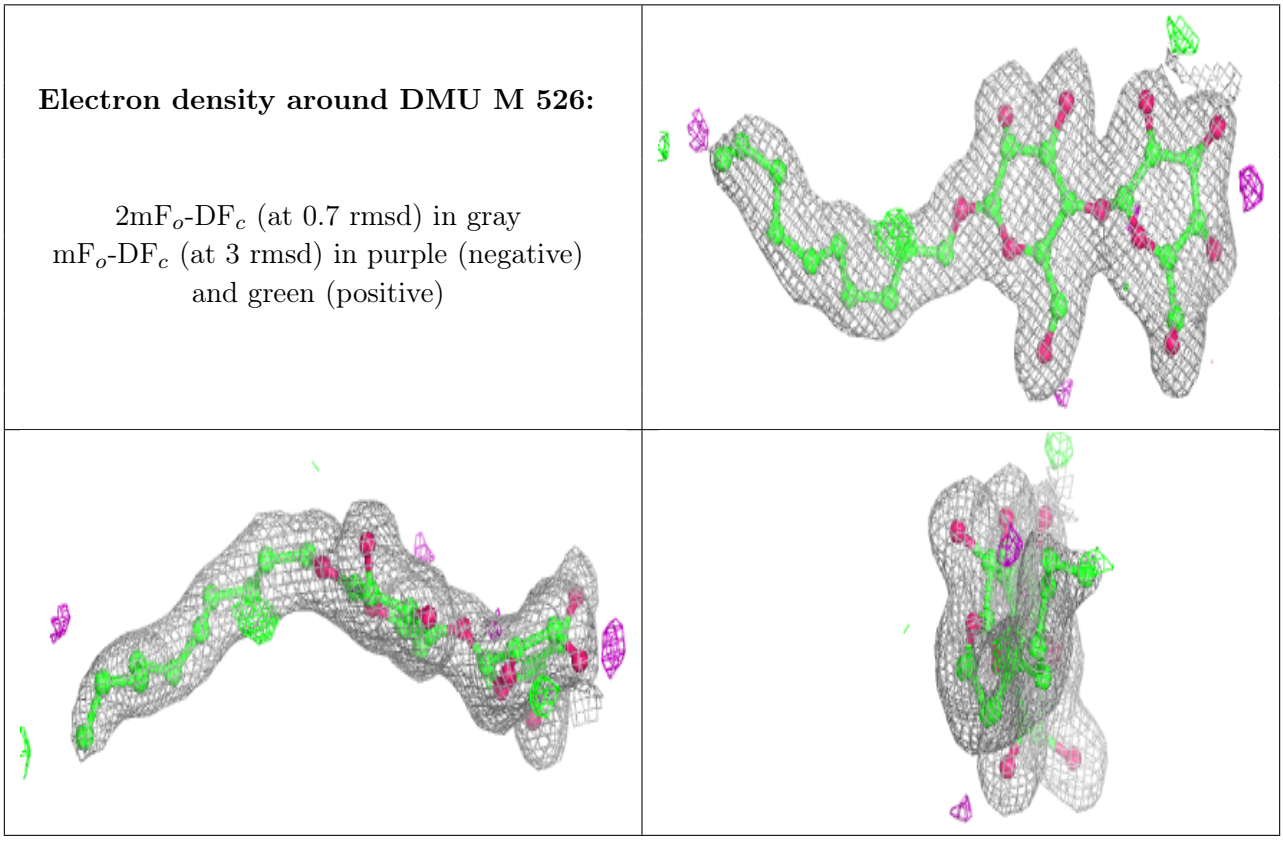
Electron density around DMU Z 1526:

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



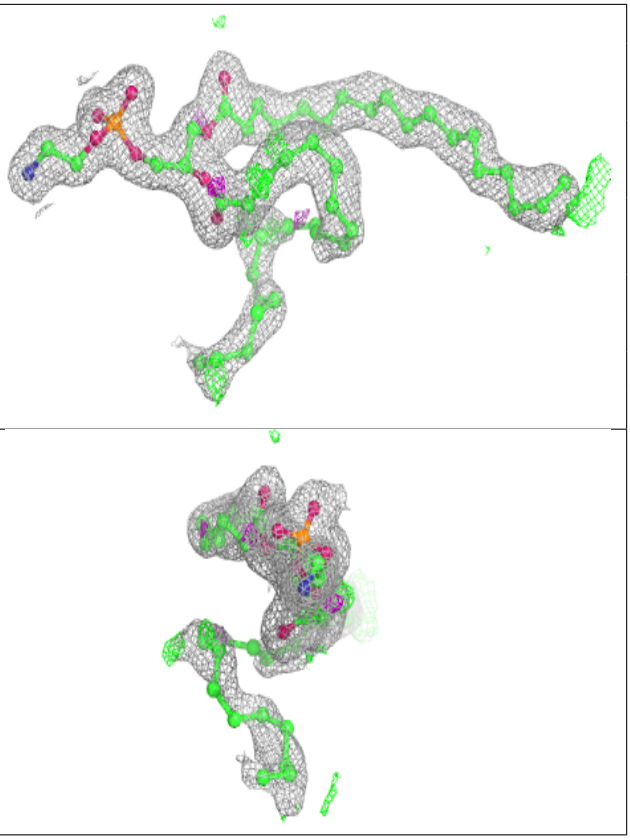
Electron density around DMU M 526:

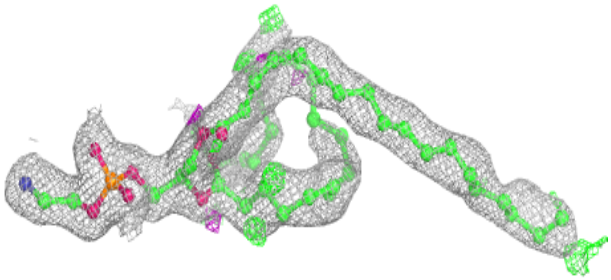
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEK P 1264:

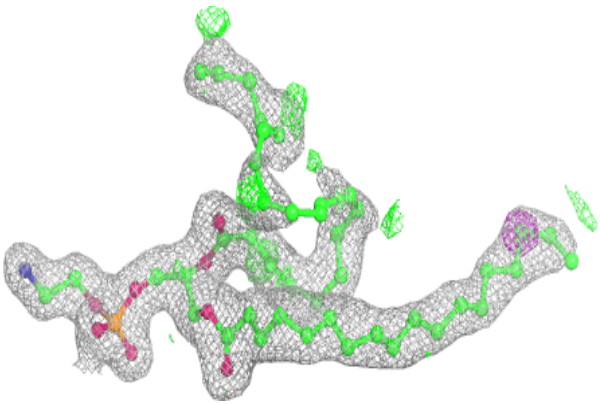
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

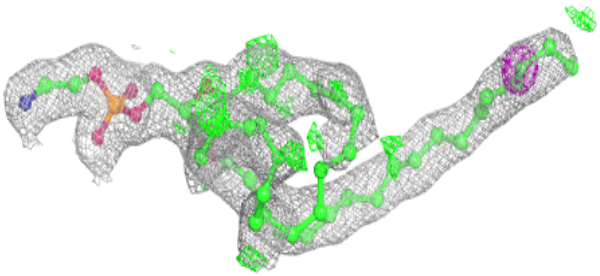


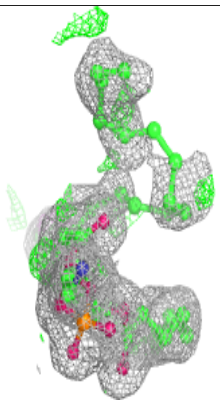


Electron density around PEK C 264:

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

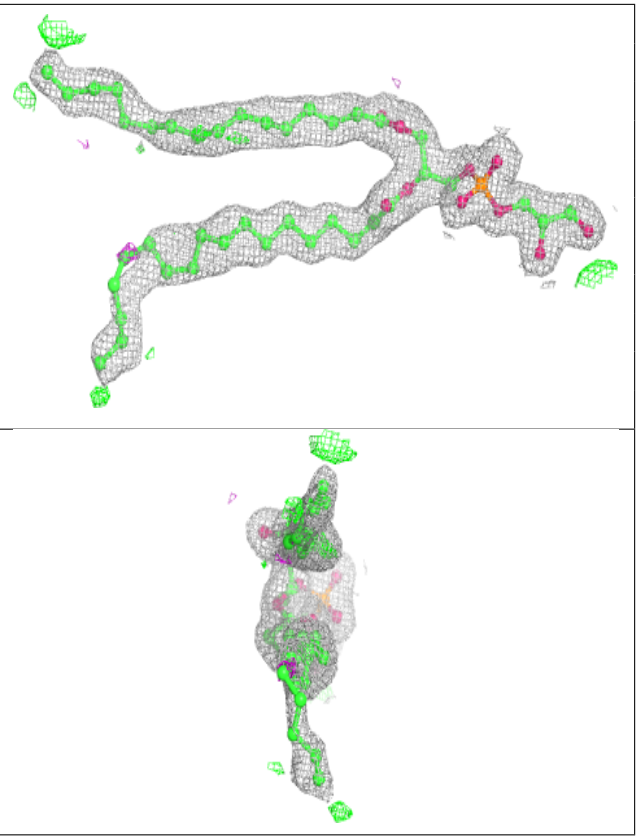






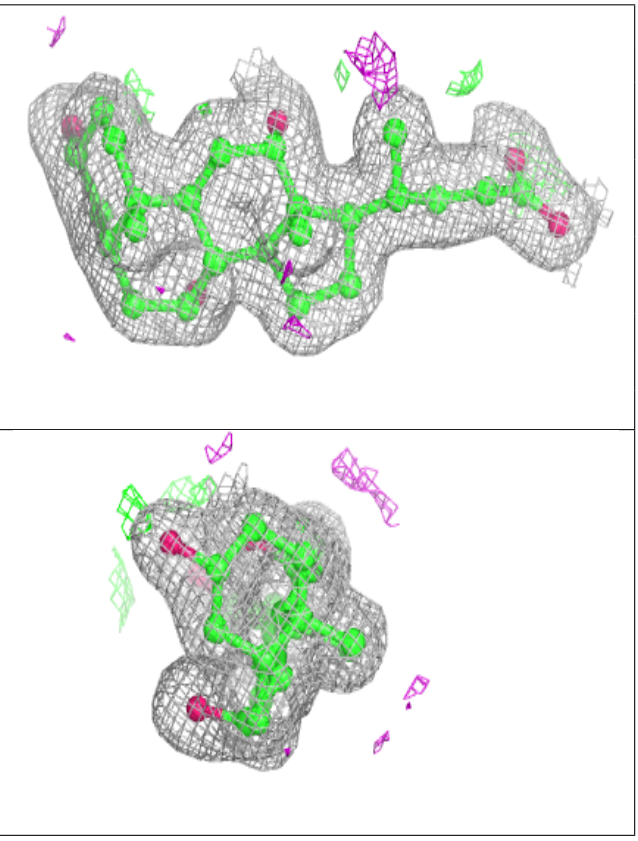
Electron density around PGV P 1267:

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



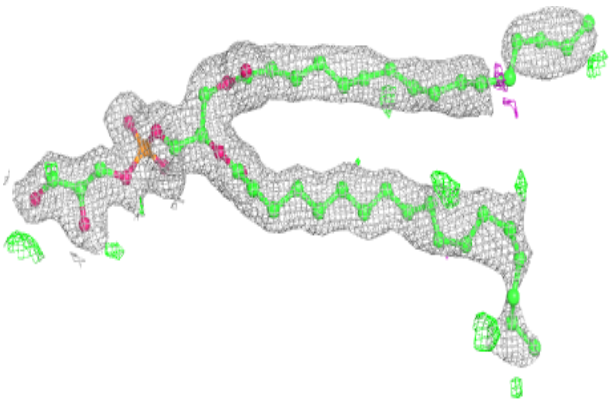
Electron density around CHD P 1525:

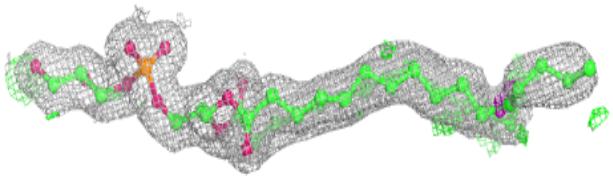
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

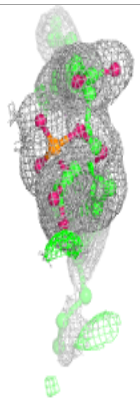


Electron density around PGV C 267:

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

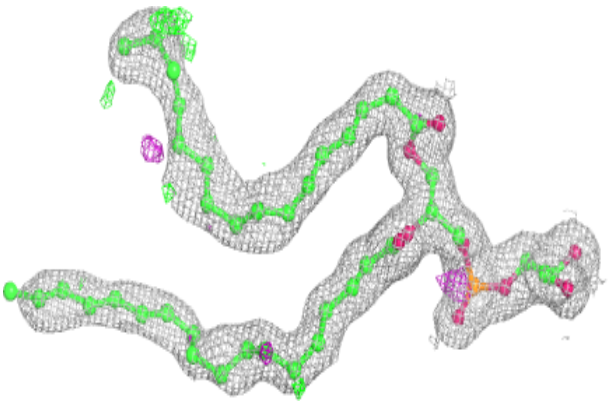


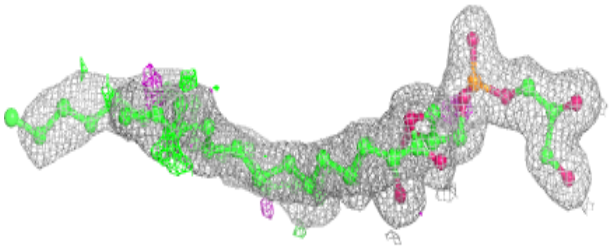


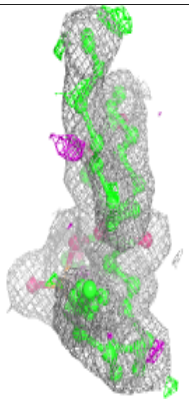


Electron density around PGV A 525:

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

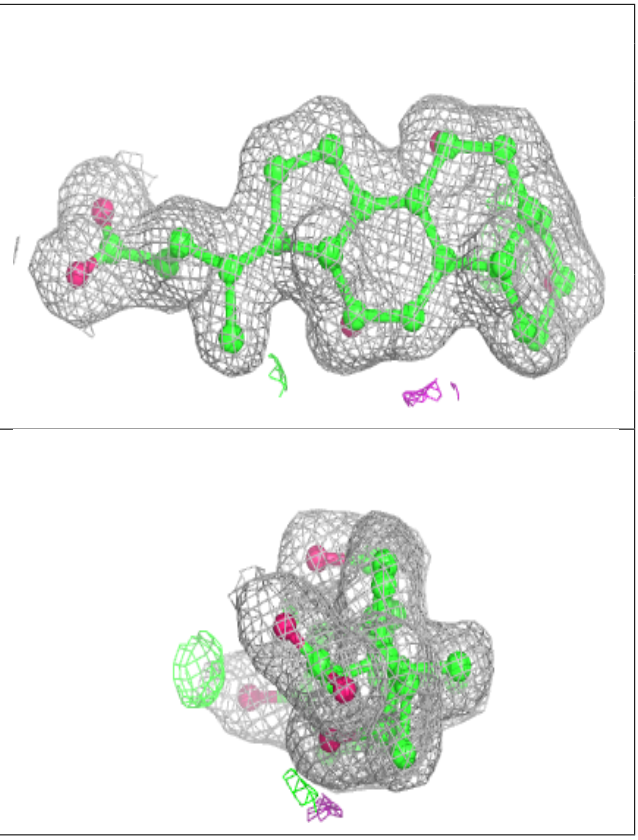






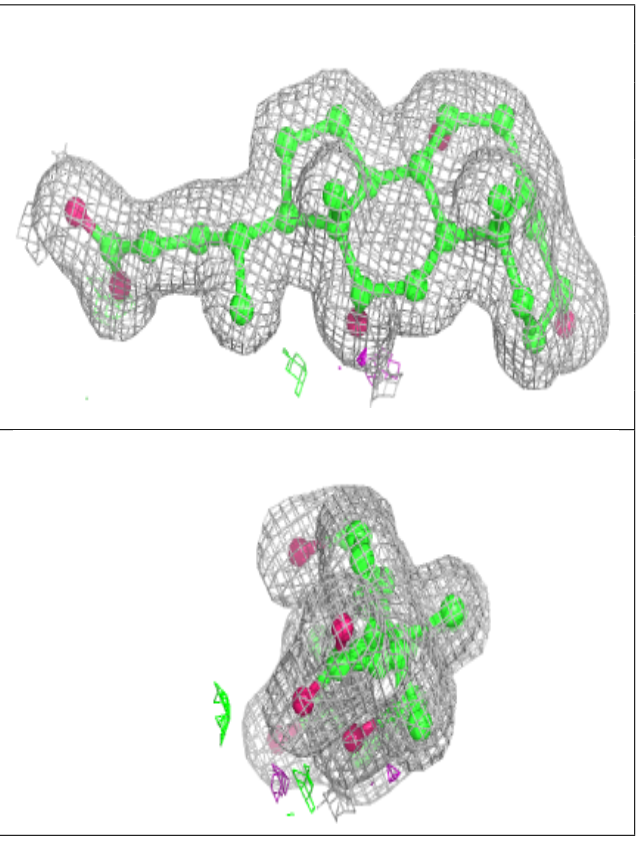
Electron density around CHD B 1086:

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



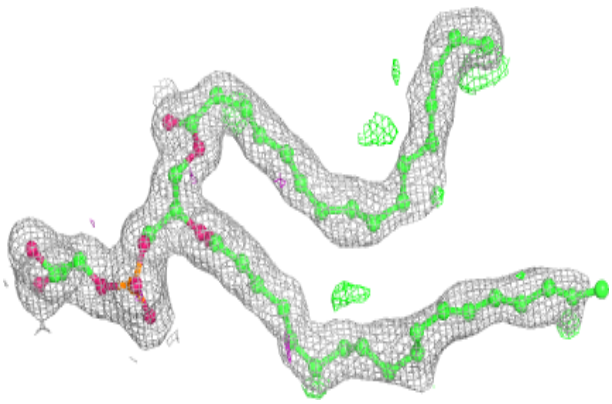
Electron density around CHD C 525:

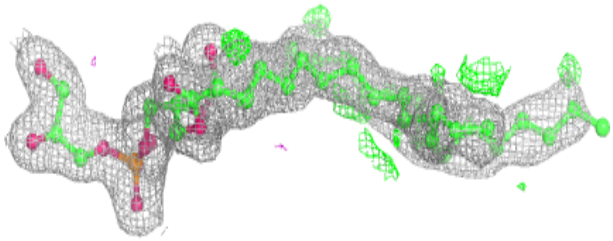
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

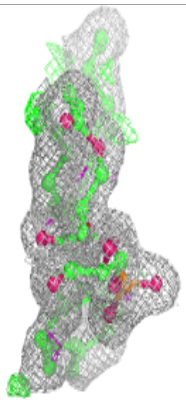


Electron density around PGV N 1266:

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

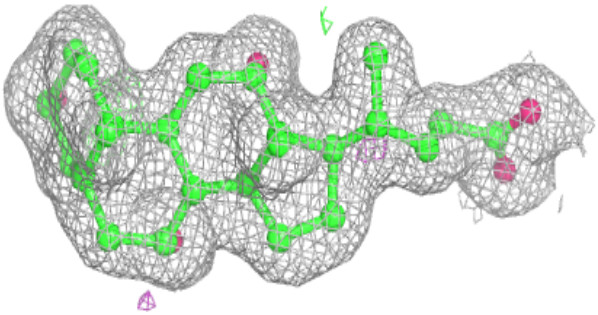


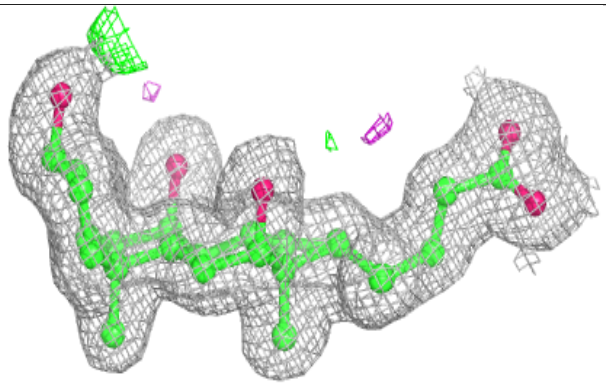


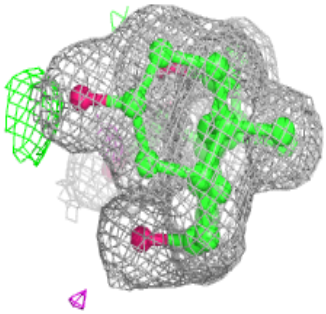


Electron density around CHD O 229:

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

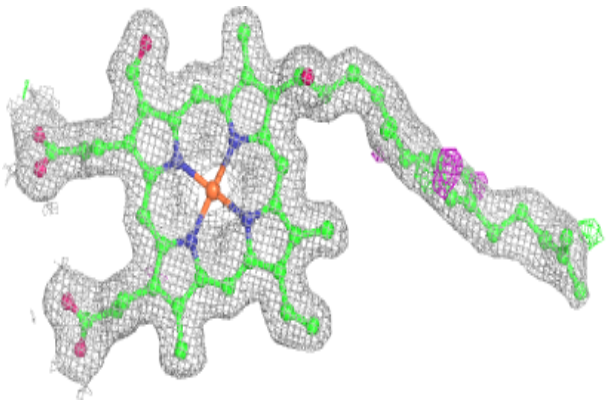


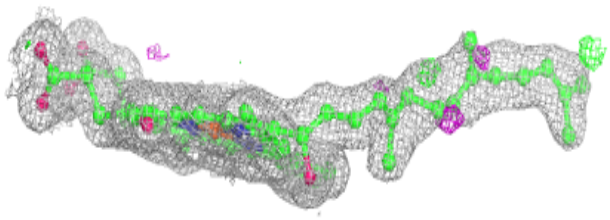


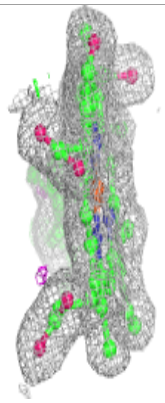


Electron density around HEA N 515:

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

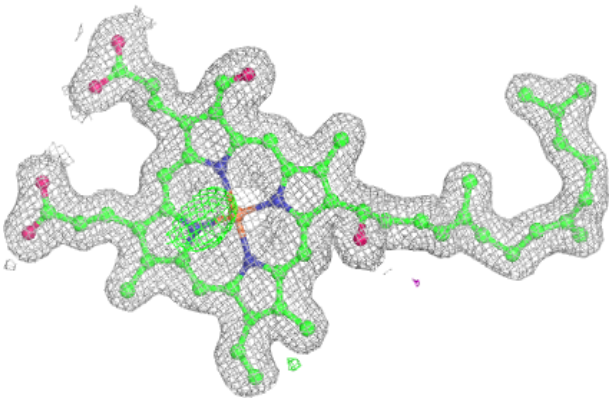


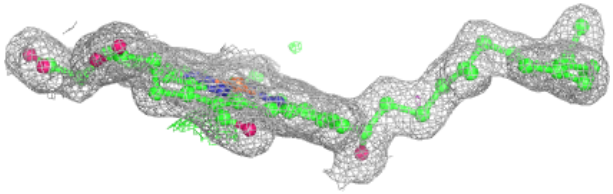


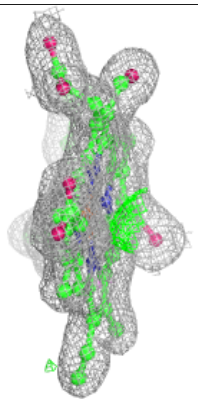


Electron density around HEA N 516:

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

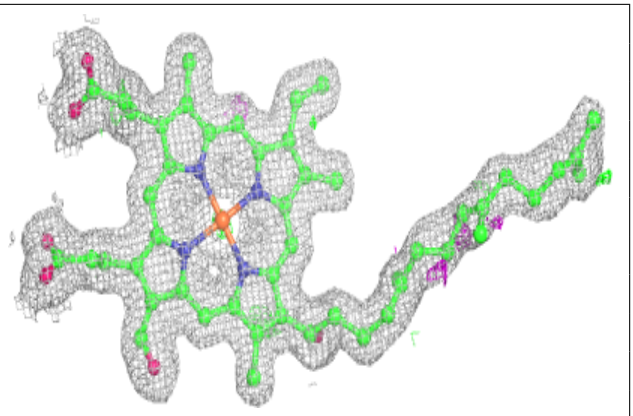


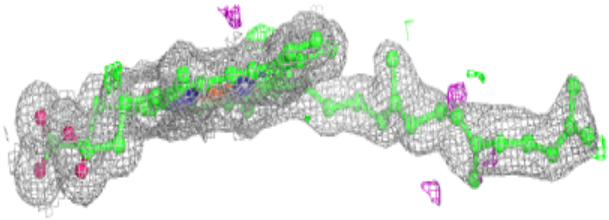


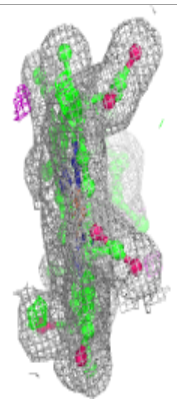


Electron density around HEA A 515:

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

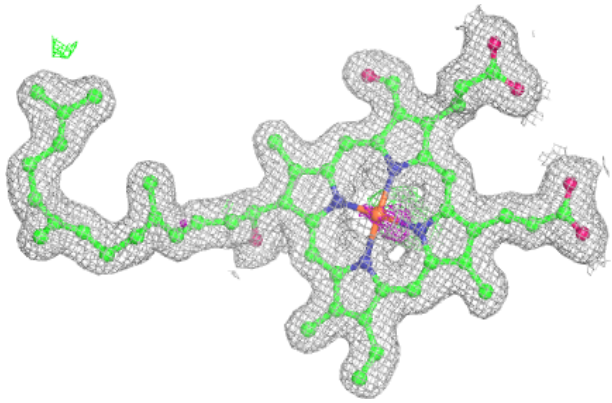


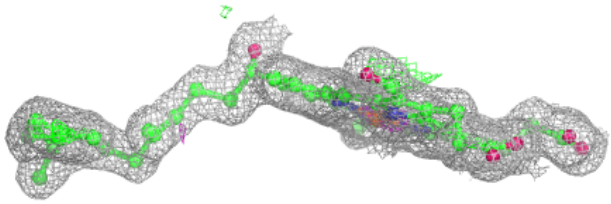


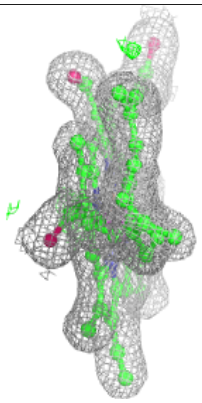


Electron density around HEA A 516:

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







6.5 Other polymers (i)

There are no such residues in this entry.