Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 04:47 AM EDT

PDB ID	:	6NKN
Title	:	Time-resolved SFX structure of the PR intermediate of cytochrome c oxidase at room temperature
Authors	:	Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.
Deposited on	:	2019-01-07
Resolution	:	2.50 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

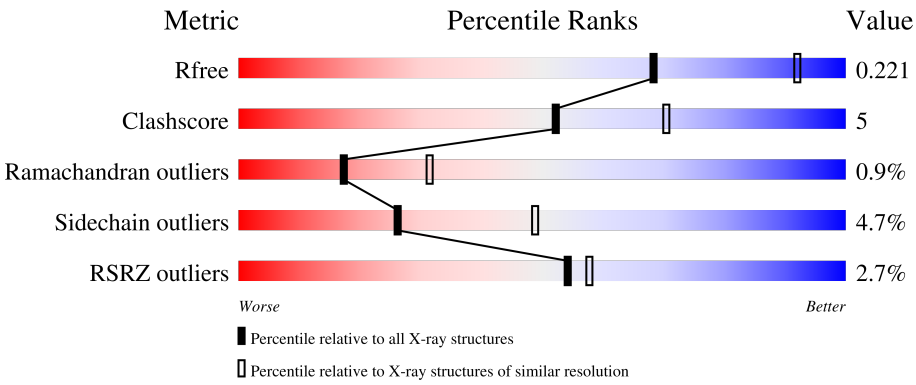
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	514	89% 10%
1	N	514	84% 15% •
2	B	227	% 80% 19% •
2	O	227	3% 77% 21% •
3	C	261	93% 6% •

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Mol	Chain	Length	Quality of chain
3	P	261	91% 8%
4	D	147	87% 10%
4	Q	147	5% 85% 10% 5%
5	E	109	2% 90% 6%
5	R	109	2% 89% 6%
6	F	98	5% 84% 9% 5%
6	S	98	5% 85% 10%
7	G	85	13% 75% 19% 5%
7	T	85	13% 73% 24%
8	H	85	5% 84% 8% 8%
8	U	85	7% 80% 12% 7%
9	I	73	5% 84% 15%
9	V	73	11% 85% 10% 5%
10	J	59	3% 92% 5%
10	W	59	8% 90% 7%
11	K	56	2% 82% 5% 12%
11	X	56	4% 59% 25% 12%
12	L	47	4% 87% 11%
12	Y	47	4% 79% 19%
13	M	46	4% 89% 7%
13	Z	46	11% 74% 20% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	A	604	X	-	-	-
17	HEA	A	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	N	605	X	-	-	-
17	HEA	N	606	X	-	-	-
26	CDL	N	601	-	-	X	-
7	TPO	G	11	-	-	-	X
9	SAC	I	1	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 31419 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, mitochondrial.

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	139	1160	755	190	211	4	0	0	0

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

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 subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	96	732	455	130	142	5	0	0	0
6	S	94	721	449	128	139	5	0	0	0

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

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 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	78	653	411	119	118	5	0	0	0
8	U	79	662	417	121	119	5	0	0	0

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

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 subunit 7A1, mitochondrial.

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 subunit 7B, mitochondrial.

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

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

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 subunit 8B, mitochondrial.

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

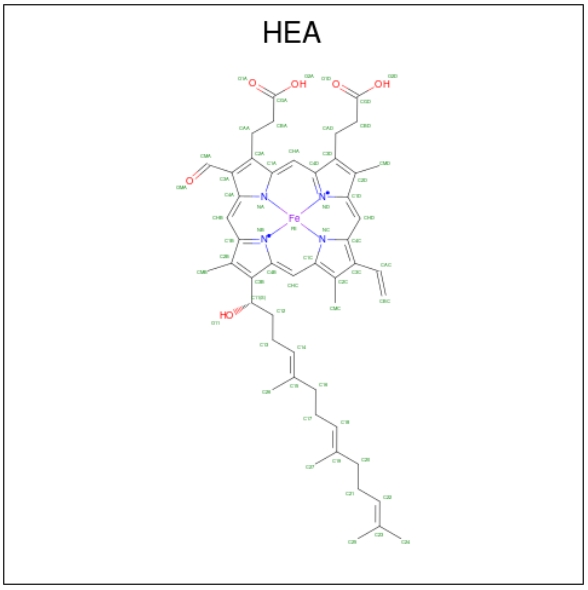
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

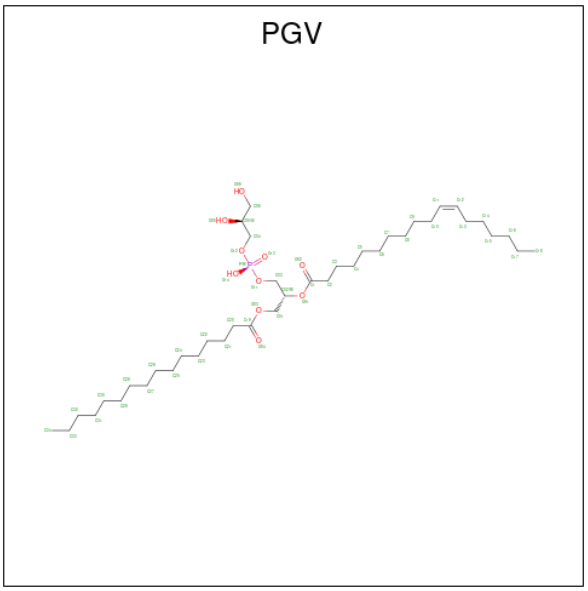
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
16	A	1	1	1	0	0
			Total	Na		
16	N	1	1	1	0	0

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



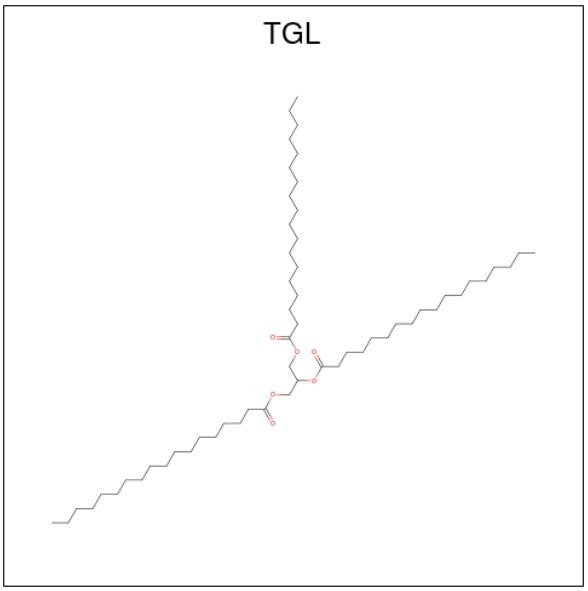
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
17	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	N	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
17	N	1	60	49	1	4	6	0	0

- 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	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	N	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	U	1	51	40	10	1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).

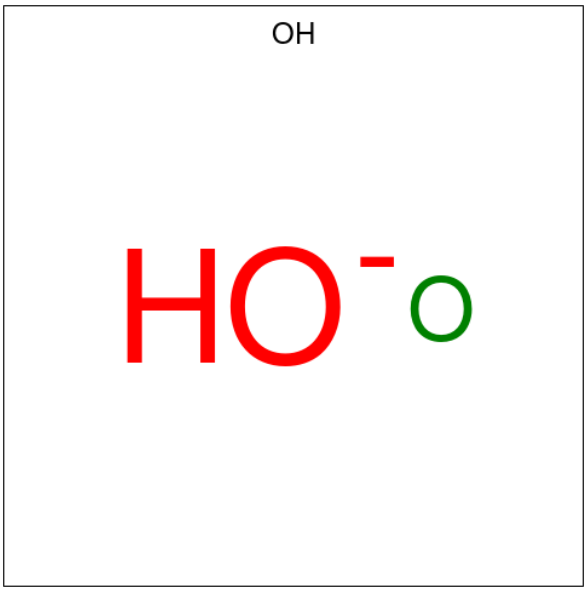


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	B	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

- Molecule 20 is OXYGEN ATOM (three-letter code: O) (formula: O).

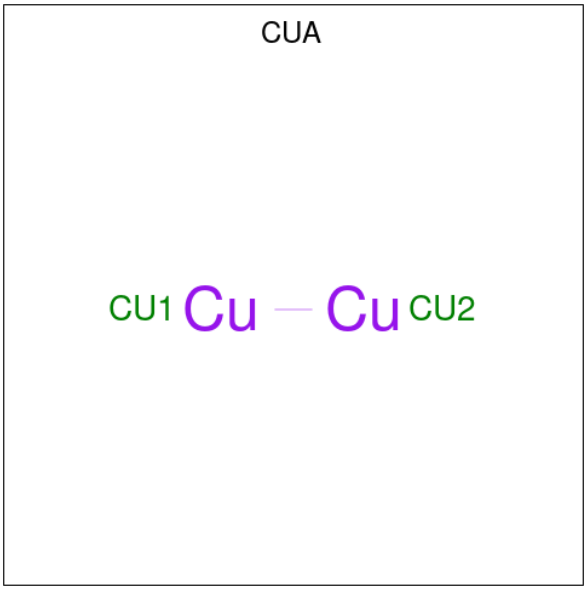
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	A	1	1	1	0	0
20	N	1	1	1	0	0

- Molecule 21 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



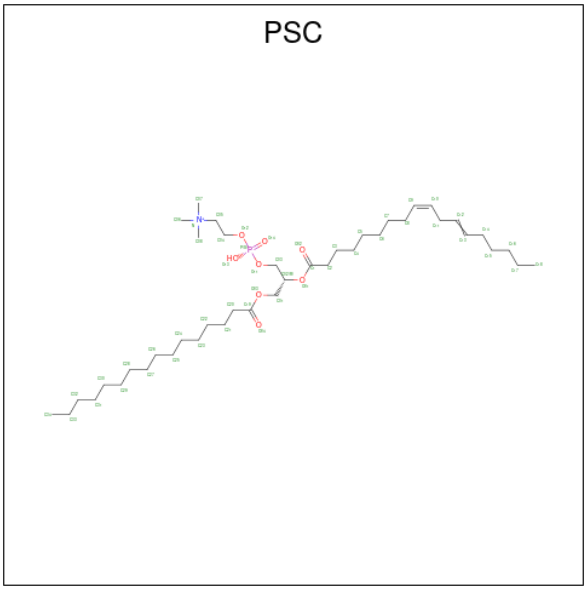
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total O 1 1	0	0
21	N	1	Total O 1 1	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



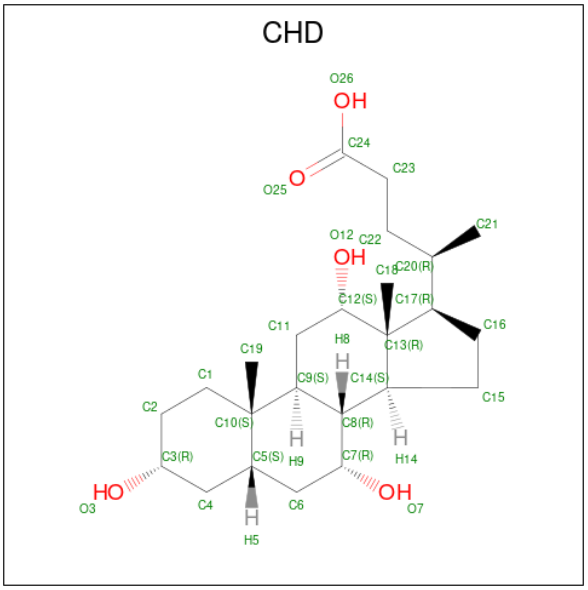
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 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: $C_{42}H_{81}NO_8P$).



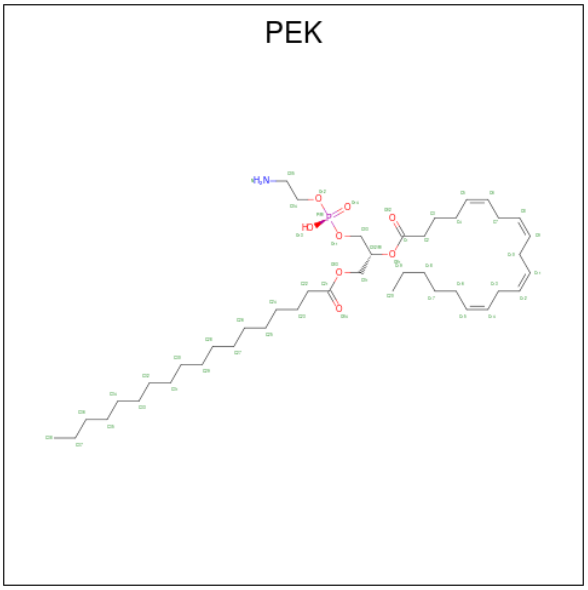
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
23	B	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
23	O	1	52	42	1	8	1	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
24	B	1	29	24	5		0	0
24	C	1	29	24	5		0	0
24	G	1	29	24	5		0	0
24	J	1	29	24	5		0	0
24	J	1	29	24	5		0	0
24	P	1	29	24	5		0	0
24	W	1	29	24	5		0	0
24	W	1	29	24	5		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
25	G	1	53	43	1	8	1	0	0
25	G	1	53	43	1	8	1	0	0

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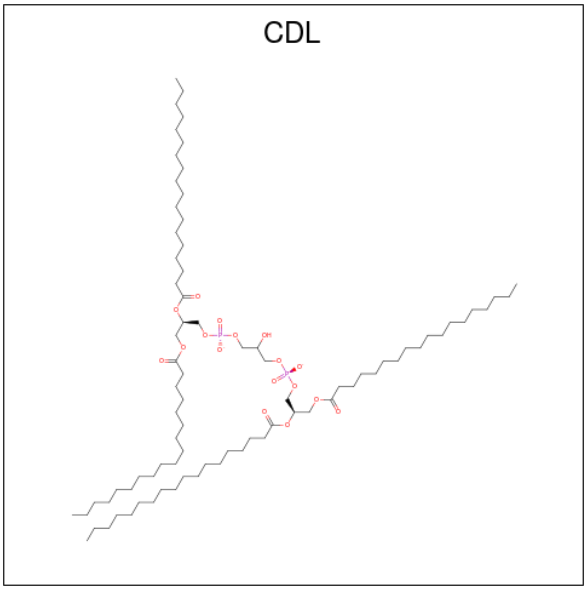
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
25	P	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	P	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
25	T	1	53	43	1	8	1	0	0

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

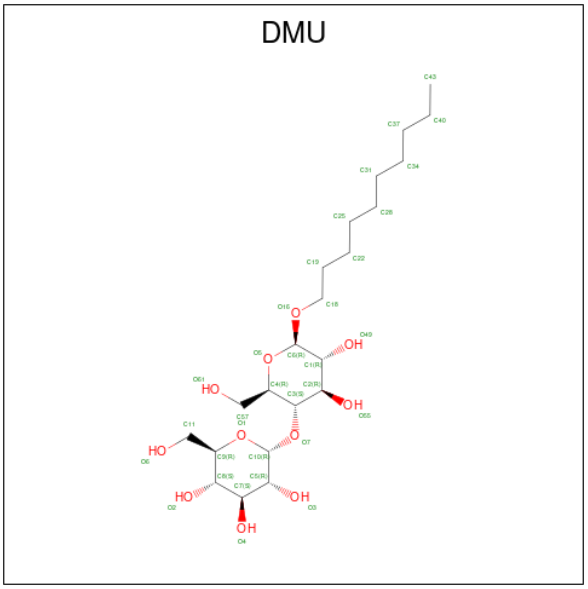


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
26	C	1	100	81	17	2	0	0
			Total	C	O	P		
26	N	1	100	81	17	2	0	0
			Total	C	O	P		
26	P	1	100	81	17	2	0	0
			Total	C	O	P		
26	T	1	100	81	17	2	0	0

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

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

- Molecule 28 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		
28	G	1	33	22	11	0	0
28	M	1	33	22	11	0	0
28	Q	1	33	22	11	0	0
28	T	1	33	22	11	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	A	152	152	152	0	0
29	B	102	102	102	0	0
29	C	58	58	58	0	0
29	D	45	45	45	0	0
29	E	26	26	26	0	0
29	F	36	36	36	0	0

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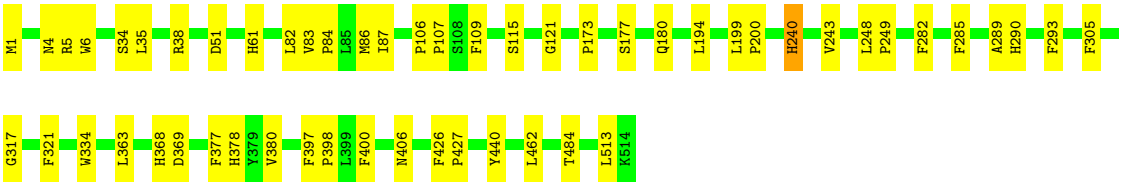
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	21	Total O 21 21	0	0
29	H	21	Total O 21 21	0	0
29	I	14	Total O 14 14	0	0
29	J	10	Total O 10 10	0	0
29	K	4	Total O 4 4	0	0
29	L	9	Total O 9 9	0	0
29	M	11	Total O 11 11	0	0
29	N	84	Total O 84 84	0	0
29	O	42	Total O 42 42	0	0
29	P	36	Total O 36 36	0	0
29	Q	18	Total O 18 18	0	0
29	R	11	Total O 11 11	0	0
29	S	22	Total O 22 22	0	0
29	T	15	Total O 15 15	0	0
29	U	7	Total O 7 7	0	0
29	V	8	Total O 8 8	0	0
29	W	7	Total O 7 7	0	0
29	X	6	Total O 6 6	0	0
29	Y	6	Total O 6 6	0	0
29	Z	1	Total O 1 1	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:

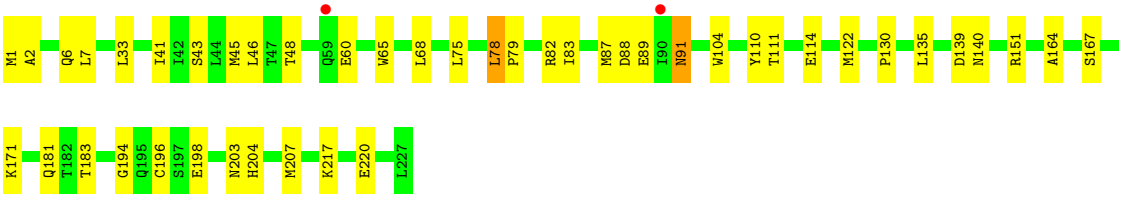


• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:

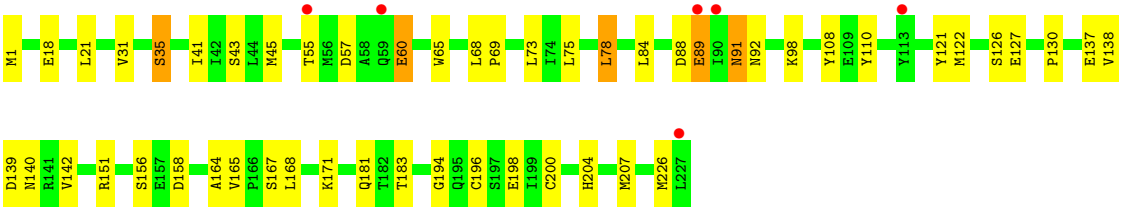
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



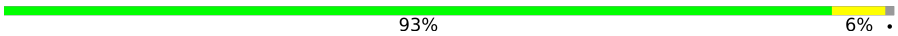
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



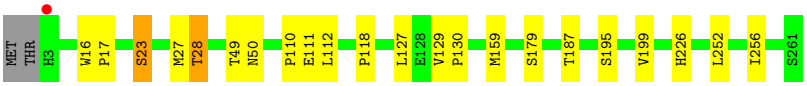
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



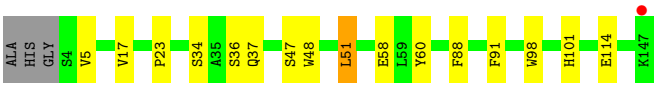
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



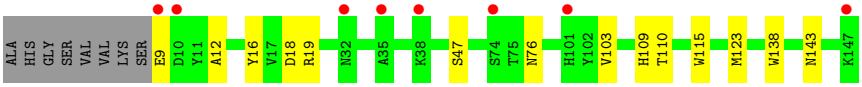
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



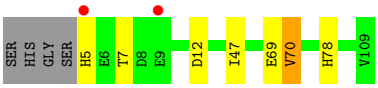
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



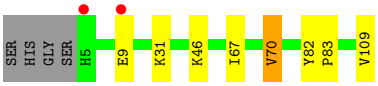
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



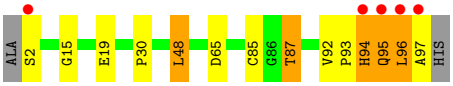
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



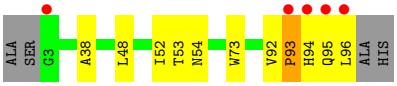
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



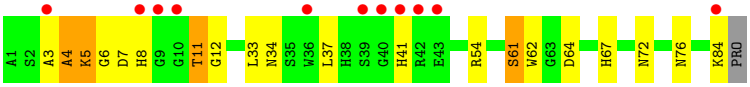
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



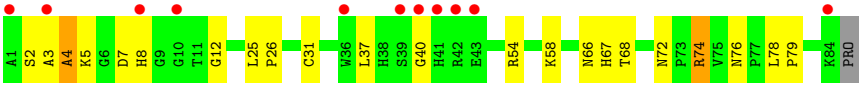
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



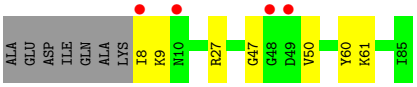
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:

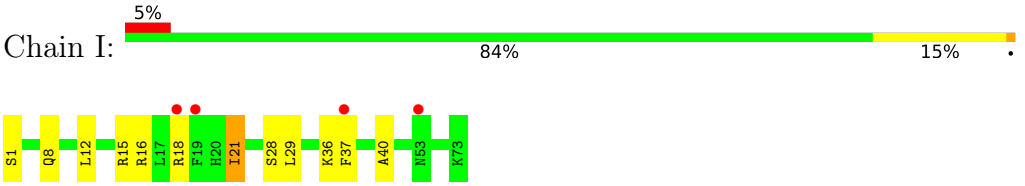


• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:

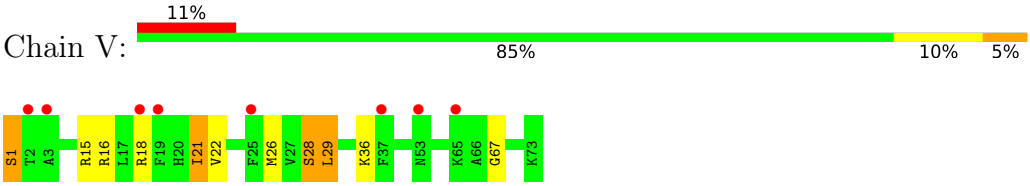
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



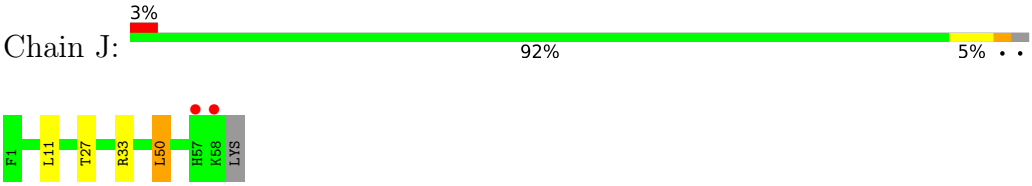
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



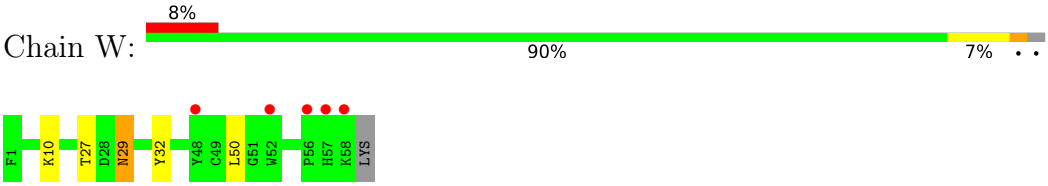
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



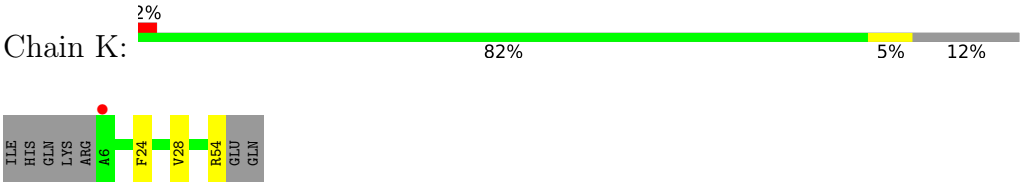
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



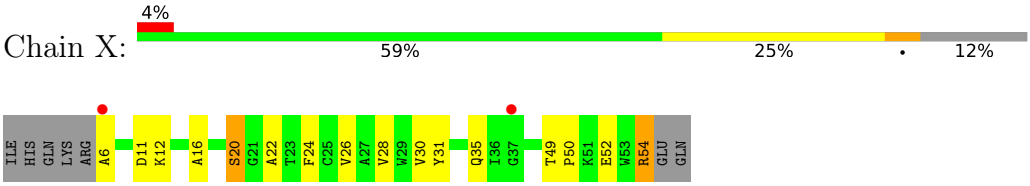
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



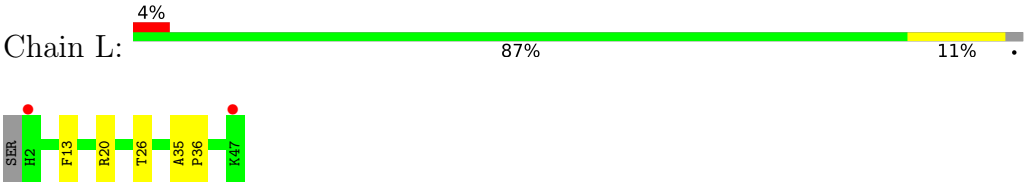
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:

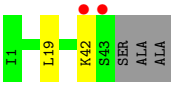


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:

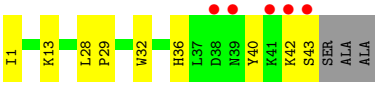
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	178.70Å 189.80Å 211.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.50 – 2.50 10.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (10.50-2.50) 100.0 (10.50-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.217 0.185 , 0.221	Depositor DCC
R_{free} test set	12143 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	31419	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: FME, ZN, TPO, OH, CUA, PGV, CHD, DMU, CDL, SAC, MG, NA, CU, HEA, TGL, O, PSC, PEK

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	0.66	0/4156	0.78	0/5678
1	N	0.74	0/4156	0.79	0/5678
2	B	0.69	1/1860 (0.1%)	0.85	0/2534
2	O	0.69	1/1860 (0.1%)	0.83	0/2534
3	C	0.64	0/2197	0.76	0/3005
3	P	0.70	0/2197	0.77	0/3005
4	D	0.68	0/1229	0.80	0/1658
4	Q	0.69	0/1194	0.76	0/1611
5	E	0.67	0/871	0.78	0/1182
5	R	0.68	0/871	0.76	0/1182
6	F	0.66	0/748	0.91	0/1016
6	S	0.68	0/737	0.85	0/1001
7	G	0.68	0/690	0.88	0/937
7	T	0.67	0/690	0.86	0/937
8	H	0.67	0/673	0.87	0/910
8	U	0.65	0/682	0.81	0/921
9	I	0.66	0/605	0.85	0/802
9	V	0.70	0/605	0.86	0/802
10	J	0.70	0/471	0.76	0/636
10	W	0.73	0/471	0.80	0/636
11	K	0.71	0/398	0.81	0/546
11	X	0.73	0/398	0.77	0/546
12	L	0.65	0/393	0.84	0/526
12	Y	0.71	0/393	0.80	0/526
13	M	0.62	0/345	0.76	0/470
13	Z	0.70	0/345	0.77	0/470
All	All	0.69	2/29235 (0.0%)	0.80	0/39749

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	1
6	F	0	1
6	S	0	1
9	V	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	7.49	1.37	1.23
2	O	198	GLU	C-O	5.13	1.33	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	368	HIS	Sidechain
6	F	93	PRO	Peptide
1	N	291	HIS	Sidechain
6	S	93	PRO	Peptide
9	V	1	SAC	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	29	0
1	N	4027	0	4001	49	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	26	0
3	C	2110	0	2027	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2110	0	2027	13	0
4	D	1195	0	1183	7	0
4	Q	1160	0	1142	13	0
5	E	852	0	845	4	0
5	R	852	0	845	2	0
6	F	732	0	713	8	0
6	S	721	0	703	4	0
7	G	675	0	643	10	0
7	T	675	0	643	17	0
8	H	653	0	610	1	0
8	U	662	0	623	4	0
9	I	601	0	612	5	0
9	V	601	0	613	9	0
10	J	460	0	459	4	0
10	W	460	0	459	3	0
11	K	384	0	366	1	0
11	X	384	0	366	9	0
12	L	380	0	380	7	0
12	Y	380	0	380	6	0
13	M	335	0	352	0	0
13	Z	335	0	352	4	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	2	0
17	N	120	0	108	9	0
18	A	153	0	228	5	0
18	C	51	0	76	0	0
18	N	102	0	152	1	0
18	P	51	0	76	0	0
18	U	51	0	76	0	0
19	A	63	0	109	1	0
19	B	63	0	110	10	0
19	L	63	0	110	12	0
19	N	126	0	220	20	0
19	Y	63	0	110	2	0
20	A	1	0	0	1	0
20	N	1	0	0	0	0
21	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	N	1	0	0	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	6	0
23	O	52	0	80	3	0
24	B	29	0	39	0	0
24	C	29	0	39	1	0
24	G	29	0	39	0	0
24	J	58	0	78	4	0
24	P	29	0	39	1	0
24	W	58	0	78	2	0
25	C	53	0	77	3	0
25	G	106	0	154	2	0
25	P	106	0	154	2	0
25	T	53	0	77	2	0
26	C	100	0	156	14	0
26	N	100	0	156	23	0
26	P	100	0	156	9	0
26	T	100	0	156	1	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	42	3	0
28	M	33	0	42	2	0
28	Q	33	0	42	0	0
28	T	33	0	42	0	0
29	A	152	0	0	3	0
29	B	102	0	0	4	0
29	C	58	0	0	2	0
29	D	45	0	0	1	0
29	E	26	0	0	0	0
29	F	36	0	0	2	0
29	G	21	0	0	4	0
29	H	21	0	0	1	0
29	I	14	0	0	0	0
29	J	10	0	0	3	0
29	K	4	0	0	0	0
29	L	9	0	0	0	0
29	M	11	0	0	1	0
29	N	84	0	0	3	0
29	O	42	0	0	1	0
29	P	36	0	0	0	0
29	Q	18	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	R	11	0	0	0	0
29	S	22	0	0	2	0
29	T	15	0	0	4	0
29	U	7	0	0	2	0
29	V	8	0	0	6	0
29	W	7	0	0	1	0
29	X	6	0	0	2	0
29	Y	6	0	0	1	0
29	Z	1	0	0	0	0
All	All	31419	0	31220	338	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 5.

All (338) 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)
19:N:607:TGL:OG1	29:N:701:HOH:O	1.67	1.11
12:L:20:ARG:HH22	19:L:101:TGL:HC52	1.12	1.06
4:Q:19:ARG:CD	29:Q:301:HOH:O	2.03	1.04
6:F:19:GLU:HG2	29:F:235:HOH:O	1.62	0.98
4:Q:19:ARG:HD3	29:Q:301:HOH:O	1.63	0.91
19:N:607:TGL:H272	19:N:607:TGL:H222	1.51	0.90
1:A:1:FME:HCN	1:A:4:ASN:HD22	1.40	0.86
19:A:609:TGL:H281	29:B:500:HOH:O	1.75	0.86
12:L:20:ARG:HH22	19:L:101:TGL:CC5	1.88	0.85
19:L:101:TGL:HC61	19:L:101:TGL:HC22	1.60	0.83
19:N:609:TGL:H192	19:N:609:TGL:H362	1.61	0.82
7:G:76:ASN:HD21	25:G:102:PEK:HN2	1.28	0.81
1:N:180:GLN:CD	29:N:708:HOH:O	2.19	0.81
12:Y:9:LYS:HG3	29:Y:204:HOH:O	1.79	0.80
17:A:605:HEA:HBC1	17:A:605:HEA:HMC1	1.61	0.80
12:L:20:ARG:NH2	19:L:101:TGL:HC52	1.93	0.80
1:A:35:LEU:HG	29:A:849:HOH:O	1.83	0.78
26:C:304:CDL:HB21	26:C:304:CDL:HB32	1.66	0.77
17:A:604:HEA:HBC1	17:A:604:HEA:HMC1	1.66	0.77
2:B:82:ARG:NH1	29:B:401:HOH:O	2.16	0.77
19:N:607:TGL:H301	19:N:607:TGL:H122	1.66	0.77
4:Q:9:GLU:HA	29:Q:317:HOH:O	1.84	0.76
25:P:302:PEK:HN2	7:T:76:ASN:HD21	1.34	0.76
26:N:601:CDL:H511	26:N:601:CDL:H231	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:32:TYR:CE2	29:W:201:HOH:O	2.40	0.74
1:N:334:TRP:CE3	19:N:609:TGL:HA31	2.23	0.74
7:G:72:ASN:H	7:G:76:ASN:HD22	1.32	0.73
12:L:13:PHE:HA	19:L:101:TGL:HC32	1.69	0.73
19:N:609:TGL:H231	19:N:609:TGL:HA71	1.73	0.71
19:N:607:TGL:HC61	29:Q:318:HOH:O	1.91	0.70
6:F:85:CYS:SG	6:F:87:THR:HG23	2.32	0.69
7:G:12:GLY:HA3	29:G:215:HOH:O	1.92	0.69
3:C:111:GLU:HB3	29:H:120:HOH:O	1.93	0.67
26:N:601:CDL:H782	26:N:601:CDL:C56	2.25	0.67
26:N:601:CDL:H782	26:N:601:CDL:C55	2.24	0.67
19:L:101:TGL:H202	19:L:101:TGL:C24	2.24	0.67
2:B:89:GLU:O	2:B:91:ASN:OD1	2.13	0.66
26:P:305:CDL:HB32	26:P:305:CDL:HB21	1.76	0.66
26:N:601:CDL:H181	26:N:601:CDL:HB32	1.79	0.65
26:N:601:CDL:H231	26:N:601:CDL:C51	2.26	0.65
7:T:5:LYS:HD2	25:T:102:PEK:H383	1.79	0.65
17:N:605:HEA:HMC1	17:N:605:HEA:HBC1	1.78	0.64
26:N:601:CDL:H782	26:N:601:CDL:C54	2.27	0.64
4:Q:109:HIS:HD2	29:Q:314:HOH:O	1.79	0.64
19:B:303:TGL:H212	19:B:303:TGL:H272	1.79	0.64
3:P:226:HIS:CE1	26:P:305:CDL:HB31	2.33	0.64
3:P:226:HIS:HE1	26:P:305:CDL:HB31	1.64	0.63
26:C:304:CDL:HA4	26:C:304:CDL:H122	1.80	0.62
1:N:60:ALA:O	1:N:64:VAL:HG23	1.99	0.62
24:W:102:CHD:H183	24:W:102:CHD:H222	1.80	0.62
19:L:101:TGL:HC61	19:L:101:TGL:CC2	2.28	0.62
20:A:610:O:O	21:A:611:OH:O	2.18	0.62
7:T:72:ASN:H	7:T:76:ASN:HD22	1.46	0.62
1:N:398:PRO:O	1:N:498:CYS:HB3	2.01	0.61
19:N:607:TGL:HA41	19:N:607:TGL:OA1	2.00	0.61
26:P:305:CDL:HA4	26:P:305:CDL:H122	1.83	0.60
23:B:302:PSC:O12	23:B:302:PSC:H072	2.02	0.60
26:C:304:CDL:H432	26:C:304:CDL:C38	2.32	0.60
26:N:601:CDL:H511	26:N:601:CDL:C23	2.31	0.60
3:C:67:PHE:HE2	26:C:304:CDL:H1	1.67	0.59
26:N:601:CDL:H372	2:O:78:LEU:HD12	1.83	0.59
26:N:601:CDL:H372	2:O:78:LEU:CD1	2.32	0.59
9:V:29:LEU:HD13	29:V:106:HOH:O	2.02	0.59
25:C:302:PEK:H383	26:N:601:CDL:H272	1.84	0.59
2:O:41:ILE:O	2:O:45:MET:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.83	0.59
26:N:601:CDL:H351	26:N:601:CDL:OA7	2.03	0.59
23:O:302:PSC:O12	29:O:401:HOH:O	2.17	0.58
19:N:607:TGL:H272	19:N:607:TGL:C22	2.27	0.58
2:O:164:ALA:O	2:O:194:GLY:HA3	2.03	0.58
2:B:7:LEU:HD11	19:B:303:TGL:H161	1.85	0.57
6:F:94:HIS:O	6:F:96:LEU:HD12	2.04	0.57
17:N:606:HEA:HMC1	17:N:606:HEA:HBC1	1.85	0.57
7:T:5:LYS:NZ	29:T:202:HOH:O	2.38	0.57
10:W:29:ASN:HD22	10:W:29:ASN:H	1.53	0.57
11:X:16:ALA:O	11:X:20:SER:OG	2.23	0.57
1:N:54:TYR:O	1:N:57:VAL:HB	2.05	0.57
19:B:303:TGL:H212	19:B:303:TGL:C26	2.33	0.57
2:O:130:PRO:HA	4:Q:115:TRP:CZ2	2.40	0.56
1:A:321:PHE:CD1	23:B:302:PSC:H341	2.40	0.56
24:P:301:CHD:H183	24:P:301:CHD:H212	1.86	0.56
19:N:607:TGL:HA21	19:N:607:TGL:HB21	1.86	0.56
4:Q:109:HIS:CD2	29:Q:314:HOH:O	2.54	0.56
18:A:606:PGV:H341	29:M:211:HOH:O	2.06	0.56
26:N:601:CDL:H752	26:N:601:CDL:H562	1.87	0.55
19:B:303:TGL:H212	19:B:303:TGL:C27	2.36	0.55
26:C:304:CDL:H192	26:C:304:CDL:H621	1.88	0.55
26:P:305:CDL:H391	26:P:305:CDL:H221	1.88	0.55
26:C:304:CDL:HB32	26:C:304:CDL:CB2	2.34	0.55
6:F:30:PRO:O	6:F:96:LEU:HD23	2.06	0.55
6:S:92:VAL:C	29:S:201:HOH:O	2.44	0.55
19:B:303:TGL:H212	19:B:303:TGL:C25	2.37	0.55
7:G:62:TRP:HB3	28:G:101:DMU:O61	2.07	0.55
6:F:48:LEU:HG	6:F:92:VAL:HG11	1.89	0.54
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.42	0.54
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.89	0.54
29:A:803:HOH:O	3:C:77:LYS:HD2	2.07	0.54
4:D:34:SER:H	4:D:37:GLN:NE2	2.05	0.54
7:T:31:CYS:SG	26:T:103:CDL:H532	2.49	0.53
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.08	0.53
24:J:101:CHD:H221	29:J:210:HOH:O	2.09	0.53
2:O:31:VAL:O	2:O:35:SER:OG	2.26	0.53
3:P:111:GLU:CG	29:U:206:HOH:O	2.57	0.53
1:A:87:ILE:O	1:A:173:PRO:HD3	2.08	0.53
2:B:41:ILE:HD13	23:B:302:PSC:H342	1.90	0.53
26:N:601:CDL:OA7	26:N:601:CDL:H321	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41:ILE:HD13	23:O:302:PSC:H342	1.90	0.53
19:B:303:TGL:H272	19:B:303:TGL:C21	2.39	0.53
1:A:289:ALA:HB3	1:A:305:PHE:CD2	2.45	0.52
1:A:400:PHE:HB3	19:L:101:TGL:H272	1.90	0.52
2:B:41:ILE:O	2:B:45:MET:HG2	2.09	0.52
26:C:304:CDL:OA3	26:C:304:CDL:O1	2.16	0.52
18:A:608:PGV:H032	29:C:451:HOH:O	2.08	0.52
26:C:304:CDL:H432	26:C:304:CDL:H382	1.91	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.44	0.52
3:P:187:THR:HB	7:T:68:THR:HG21	1.91	0.52
7:T:66:ASN:HD22	7:T:78:LEU:HD13	1.75	0.52
26:N:601:CDL:HB32	26:N:601:CDL:C18	2.41	0.52
9:V:29:LEU:HB2	29:V:106:HOH:O	2.10	0.51
1:N:146:THR:O	1:N:149:SER:HB3	2.10	0.51
19:N:609:TGL:H362	19:N:609:TGL:C19	2.38	0.51
12:Y:13:PHE:CE2	19:Y:101:TGL:HA72	2.45	0.51
1:A:406:ASN:HD21	18:A:606:PGV:H22	1.75	0.51
4:Q:109:HIS:CE1	4:Q:115:TRP:CZ3	2.99	0.51
1:N:334:TRP:CZ3	19:N:609:TGL:HA31	2.46	0.50
19:L:101:TGL:H202	19:L:101:TGL:H242	1.92	0.50
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.25	0.50
5:E:78:HIS:CD2	9:I:12:LEU:HD22	2.46	0.50
1:N:127:THR:HB	1:N:129:TYR:CE1	2.47	0.50
12:L:20:ARG:HH22	19:L:101:TGL:CC4	2.23	0.50
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.46	0.50
11:X:54:ARG:C	29:X:105:HOH:O	2.50	0.50
1:A:115:SER:O	1:A:121:GLY:HA2	2.12	0.49
1:A:177:SER:H	1:A:180:GLN:NE2	2.10	0.49
1:N:87:ILE:O	1:N:173:PRO:HD3	2.11	0.49
9:V:29:LEU:CB	29:V:106:HOH:O	2.60	0.49
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.94	0.49
19:Y:101:TGL:HA92	19:Y:101:TGL:H231	1.94	0.49
3:C:103:HIS:ND1	24:C:301:CHD:O26	2.37	0.49
7:G:61:SER:CB	29:G:201:HOH:O	2.59	0.49
1:N:309:THR:CG2	17:N:606:HEA:HMB2	2.42	0.49
11:X:22:ALA:O	11:X:26:VAL:HG23	2.12	0.49
26:N:601:CDL:H771	26:N:601:CDL:H571	1.94	0.48
2:O:98:LYS:HE2	8:U:62:SER:O	2.13	0.48
24:W:102:CHD:H183	24:W:102:CHD:C22	2.43	0.48
19:N:609:TGL:C36	9:V:16:ARG:HE	2.27	0.48
3:P:129:VAL:N	3:P:130:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:605:HEA:HHC	17:N:605:HEA:H122	1.95	0.48
9:I:36:LYS:HA	9:I:40:ALA:HB3	1.96	0.48
24:J:102:CHD:C18	24:J:102:CHD:H222	2.43	0.48
28:M:101:DMU:H30	28:M:101:DMU:O1	2.13	0.48
1:N:180:GLN:CG	29:N:708:HOH:O	2.57	0.48
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.48	0.48
19:N:607:TGL:CB9	19:N:607:TGL:H283	2.42	0.48
2:O:126:SER:O	2:O:126:SER:OG	2.27	0.48
1:N:378:HIS:CE1	17:N:605:HEA:NA	2.82	0.48
26:N:601:CDL:C37	2:O:78:LEU:HD12	2.44	0.48
19:N:607:TGL:H283	19:N:607:TGL:HB92	1.95	0.47
3:P:111:GLU:HG3	29:U:206:HOH:O	2.12	0.47
4:D:60:TYR:OH	5:E:69:GLU:OE1	2.29	0.47
1:N:251:PHE:HB3	1:N:319:LYS:HE2	1.96	0.47
1:N:467:LEU:O	1:N:471:ILE:HG13	2.15	0.47
1:A:440:TYR:HE1	2:B:204:HIS:CE1	2.33	0.47
1:N:52:GLN:O	1:N:56:VAL:HG23	2.13	0.47
4:Q:109:HIS:HE1	4:Q:115:TRP:CZ3	2.32	0.47
4:D:23:PRO:HG3	5:E:70:VAL:HG21	1.97	0.47
4:D:98:TRP:CE2	28:M:101:DMU:H11	2.49	0.47
1:A:240:HIS:O	1:A:243:VAL:HG22	2.14	0.47
10:J:50:LEU:HD22	10:J:50:LEU:O	2.14	0.47
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.79	0.47
7:G:61:SER:HB2	29:G:201:HOH:O	2.15	0.47
19:N:607:TGL:CC6	29:Q:318:HOH:O	2.55	0.47
11:X:6:ALA:N	29:X:101:HOH:O	2.47	0.47
19:B:303:TGL:H272	19:B:303:TGL:HA92	1.97	0.47
19:B:303:TGL:H302	19:B:303:TGL:H132	1.76	0.47
1:N:386:VAL:HG11	17:N:605:HEA:H261	1.97	0.47
4:D:34:SER:H	4:D:37:GLN:HE21	1.61	0.47
1:N:409:TRP:HA	1:N:412:ILE:HD12	1.97	0.47
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.97	0.46
4:D:88:PHE:O	4:D:91:PHE:HB3	2.15	0.46
1:N:177:SER:H	1:N:180:GLN:NE2	2.14	0.46
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.51	0.46
2:B:41:ILE:HD13	23:B:302:PSC:C34	2.45	0.46
2:O:18:GLU:O	2:O:21:LEU:HB2	2.16	0.46
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.98	0.46
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.98	0.46
4:Q:19:ARG:NE	29:Q:301:HOH:O	2.35	0.46
13:Z:1:ILE:HG23	13:Z:1:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:3:ALA:O	7:G:4:ALA:HB2	2.15	0.46
23:O:302:PSC:H343	23:O:302:PSC:H142	1.96	0.46
10:J:33:ARG:HD2	29:J:206:HOH:O	2.15	0.46
2:B:139:ASP:OD1	2:B:140:ASN:N	2.49	0.45
12:L:20:ARG:NH2	19:L:101:TGL:CC4	2.78	0.45
2:O:91:ASN:O	2:O:91:ASN:ND2	2.47	0.45
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.81	0.45
26:P:305:CDL:H241	26:P:305:CDL:H392	1.97	0.45
9:V:22:VAL:O	9:V:26:MET:HG2	2.17	0.45
1:N:426:PHE:N	1:N:427:PRO:CD	2.79	0.45
11:X:24:PHE:CE1	11:X:28:VAL:HG11	2.50	0.45
18:A:608:PGV:C03	29:C:451:HOH:O	2.64	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.17	0.45
19:B:303:TGL:H323	19:B:303:TGL:H121	1.97	0.45
3:C:226:HIS:HE1	26:C:304:CDL:HB31	1.82	0.45
1:N:383:MET:HA	1:N:387:PHE:CD1	2.50	0.45
26:N:601:CDL:H782	26:N:601:CDL:H562	1.97	0.45
3:P:112:LEU:HD22	3:P:118:PRO:HB3	1.98	0.45
26:N:601:CDL:H571	26:N:601:CDL:C78	2.46	0.45
1:A:199:LEU:N	1:A:200:PRO:CD	2.79	0.45
3:C:217:VAL:HG21	26:C:304:CDL:H561	1.99	0.45
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.99	0.45
2:O:126:SER:O	2:O:127:GLU:HG3	2.16	0.45
5:E:12:ASP:HA	5:E:47:ILE:HD11	1.97	0.45
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.99	0.45
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.99	0.45
1:N:148:PHE:CD1	3:P:28:THR:HG22	2.52	0.45
7:T:58:LYS:HG2	29:T:204:HOH:O	2.17	0.45
12:Y:36:PRO:O	12:Y:40:VAL:HG23	2.17	0.45
2:O:151:ARG:HE	2:O:181:GLN:NE2	2.15	0.45
1:N:38:ARG:HD2	17:N:605:HEA:OMA	2.17	0.45
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.99	0.44
28:G:101:DMU:C57	28:G:101:DMU:H36	2.47	0.44
1:N:75:ILE:O	1:N:79:GLY:HA3	2.17	0.44
9:V:29:LEU:HD22	29:V:106:HOH:O	2.16	0.44
6:F:65:ASP:HB2	29:F:224:HOH:O	2.17	0.44
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.99	0.44
2:O:108:TYR:CE2	2:O:142:VAL:HG21	2.52	0.44
7:T:66:ASN:HD21	7:T:79:PRO:HD2	1.82	0.44
1:A:5:ARG:HG2	1:A:6:TRP:NE1	2.32	0.44
1:N:435:GLY:O	1:N:437:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:498:CYS:HA	1:N:499:PRO:HA	1.87	0.44
5:R:67:ILE:O	5:R:70:VAL:HG12	2.16	0.44
1:N:2:PHE:CD1	1:N:2:PHE:C	2.91	0.44
19:B:303:TGL:HC52	19:B:303:TGL:HC82	1.74	0.44
25:C:302:PEK:H383	26:N:601:CDL:C27	2.48	0.44
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.82	0.44
19:N:609:TGL:H363	9:V:16:ARG:HE	1.82	0.44
1:A:397:PHE:N	1:A:398:PRO:CD	2.81	0.44
28:G:101:DMU:H36	28:G:101:DMU:H30	1.99	0.44
1:N:309:THR:HG22	17:N:606:HEA:HMB2	1.99	0.44
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.18	0.43
25:C:302:PEK:H032	29:G:213:HOH:O	2.18	0.43
26:C:304:CDL:HB21	26:C:304:CDL:CB3	2.43	0.43
1:N:195:LEU:HD23	1:N:245:ILE:HD13	1.99	0.43
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.86	0.43
26:N:601:CDL:H231	26:N:601:CDL:C52	2.48	0.43
12:Y:45:LEU:HD21	13:Z:40:TYR:CD1	2.54	0.43
1:N:31:THR:O	1:N:34:SER:OG	2.27	0.43
26:N:601:CDL:H231	26:N:601:CDL:H531	2.00	0.43
2:O:88:ASP:O	2:O:89:GLU:O	2.36	0.43
3:P:16:TRP:N	3:P:17:PRO:CD	2.81	0.43
26:P:305:CDL:HB32	26:P:305:CDL:CB2	2.45	0.43
2:B:83:ILE:O	2:B:87:MET:HG3	2.18	0.43
26:C:304:CDL:H432	26:C:304:CDL:H381	2.00	0.43
7:G:5:LYS:HG3	25:G:103:PEK:H383	2.00	0.43
2:O:121:TYR:O	2:O:138:VAL:HA	2.18	0.43
25:P:302:PEK:C05	7:T:76:ASN:HD21	2.30	0.43
1:A:426:PHE:N	1:A:427:PRO:CD	2.81	0.43
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.43
9:V:21:ILE:HD13	9:V:21:ILE:HA	1.90	0.43
9:V:67:GLY:HA2	29:V:103:HOH:O	2.19	0.43
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.54	0.43
1:N:83:VAL:HB	1:N:84:PRO:HD3	2.00	0.43
1:N:129:TYR:CZ	1:N:232:GLN:HG2	2.54	0.43
4:Q:138:TRP:CH2	11:X:50:PRO:CG	3.02	0.43
6:F:95:GLN:O	6:F:97:ALA:N	2.52	0.42
7:T:12:GLY:HA3	29:T:208:HOH:O	2.19	0.42
1:A:83:VAL:N	1:A:84:PRO:CD	2.82	0.42
19:L:101:TGL:H101	19:L:101:TGL:H131	1.89	0.42
1:N:381:LEU:O	1:N:386:VAL:HG23	2.19	0.42
1:N:495:LEU:HD12	1:N:495:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:607:TGL:H283	19:N:607:TGL:H111	2.02	0.42
3:P:195:SER:O	3:P:199:VAL:HG23	2.19	0.42
2:B:33:LEU:HD12	9:I:28:SER:HB3	2.00	0.42
2:B:48:THR:HB	9:I:16:ARG:CZ	2.49	0.42
1:N:236:TRP:HA	1:N:236:TRP:CE3	2.54	0.42
4:Q:76:ASN:ND2	11:X:11:ASP:OD1	2.53	0.42
24:J:101:CHD:H231	29:J:205:HOH:O	2.18	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.42
1:N:361:SER:OG	2:O:84:LEU:HD13	2.19	0.42
26:P:305:CDL:H241	26:P:305:CDL:C39	2.50	0.42
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.55	0.42
1:N:33:LEU:O	1:N:37:ILE:HG13	2.20	0.42
7:T:67:HIS:NE2	7:T:78:LEU:HD11	2.35	0.42
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.72	0.42
10:J:11:LEU:HD12	10:J:11:LEU:O	2.20	0.42
10:J:33:ARG:HG2	24:J:102:CHD:H151	2.01	0.42
11:X:26:VAL:O	11:X:30:VAL:HG23	2.20	0.42
2:B:111:THR:HA	2:B:114:GLU:O	2.20	0.41
4:Q:16:TYR:OH	4:Q:18:ASP:OD1	2.21	0.41
6:S:93:PRO:N	29:S:201:HOH:O	2.52	0.41
1:A:248:LEU:HB2	1:A:249:PRO:HD3	2.02	0.41
2:B:217:LYS:HG2	29:B:483:HOH:O	2.20	0.41
3:C:226:HIS:CE1	26:C:304:CDL:HB31	2.54	0.41
1:N:5:ARG:HG2	1:N:6:TRP:CE2	2.54	0.41
1:N:41:LEU:HD11	1:N:54:TYR:OH	2.21	0.41
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.19	0.41
3:P:23:SER:O	3:P:27:MET:HG3	2.20	0.41
26:P:305:CDL:H401	26:P:305:CDL:H432	1.81	0.41
7:T:12:GLY:CA	29:T:208:HOH:O	2.67	0.41
1:A:377:PHE:HA	1:A:380:VAL:HG22	2.02	0.41
2:B:151:ARG:HE	2:B:181:GLN:NE2	2.18	0.41
3:C:37:PHE:O	3:C:38:ASN:C	2.59	0.41
7:G:11:TPO:O	7:G:11:TPO:CG2	2.68	0.41
8:H:8:ILE:O	8:H:8:ILE:HG22	2.20	0.41
1:A:82:LEU:O	1:A:86:MET:HG3	2.20	0.41
19:N:607:TGL:HC61	29:V:107:HOH:O	2.20	0.41
7:T:72:ASN:OD1	7:T:74:ARG:HB2	2.20	0.41
1:A:290:HIS:HA	1:A:293:PHE:CZ	2.56	0.41
26:N:601:CDL:OB4	26:N:601:CDL:H1	2.18	0.41
1:A:106:PRO:HD2	1:A:107:PRO:HD2	2.03	0.41
18:A:606:PGV:H331	29:D:245:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:440:TYR:HE1	2:O:204:HIS:CE1	2.39	0.41
19:N:607:TGL:H111	19:N:607:TGL:C28	2.51	0.41
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.56	0.41
2:O:139:ASP:OD1	2:O:140:ASN:N	2.52	0.41
11:X:31:TYR:CD1	11:X:35:GLN:HG3	2.56	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.98	0.41
23:B:302:PSC:H063	23:B:302:PSC:P	2.61	0.41
10:W:29:ASN:H	10:W:29:ASN:ND2	2.19	0.41
1:A:317:GLY:HA3	29:A:754:HOH:O	2.21	0.41
1:A:377:PHE:CE1	1:A:378:HIS:CE1	3.08	0.41
26:N:601:CDL:H252	26:N:601:CDL:H222	1.79	0.41
3:P:252:LEU:CD2	3:P:256:ILE:HD12	2.51	0.41
13:Z:32:TRP:CD1	13:Z:36:HIS:CE1	3.09	0.41
2:O:122:MET:HA	2:O:137:GLU:O	2.21	0.40
2:B:122:MET:SD	2:B:135:LEU:HA	2.61	0.40
7:G:64:ASP:OD1	7:G:67:HIS:ND1	2.45	0.40
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.88	0.40
1:N:364:ASP:OD1	17:N:606:HEA:O1A	2.38	0.40
1:N:406:ASN:HD21	18:N:610:PGV:H22	1.85	0.40
2:O:69:PRO:O	2:O:73:LEU:HG	2.21	0.40
2:O:165:VAL:HG11	2:O:168:LEU:HD12	2.02	0.40
7:T:5:LYS:CD	25:T:102:PEK:H383	2.49	0.40
23:B:302:PSC:H011	23:B:302:PSC:H222	2.03	0.40
26:C:304:CDL:H831	26:C:304:CDL:H861	1.94	0.40
7:T:25:LEU:N	7:T:26:PRO:CD	2.84	0.40
11:K:24:PHE:O	11:K:28:VAL:HG12	2.21	0.40
2:B:220:GLU:CG	29:B:458:HOH:O	2.69	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%)	492 (96%)	19 (4%)	1 (0%)	47	68
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	47	68
2	B	225/227 (99%)	213 (95%)	12 (5%)	0	100	100
2	O	225/227 (99%)	210 (93%)	13 (6%)	2 (1%)	17	31
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	54
3	P	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
4	D	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	22	39
4	Q	137/147 (93%)	123 (90%)	13 (10%)	1 (1%)	22	39
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	94/98 (96%)	87 (93%)	3 (3%)	4 (4%)	2	3
6	S	92/98 (94%)	87 (95%)	3 (3%)	2 (2%)	6	10
7	G	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	1
7	T	81/85 (95%)	64 (79%)	12 (15%)	5 (6%)	1	1
8	H	76/85 (89%)	73 (96%)	1 (1%)	2 (3%)	5	8
8	U	77/85 (91%)	72 (94%)	3 (4%)	2 (3%)	5	8
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11	20
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	11	20
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	39 (83%)	7 (15%)	1 (2%)	7	11
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	3 (7%)	1 (2%)	6	10
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
All	All	3492/3614 (97%)	3293 (94%)	167 (5%)	32 (1%)	17	31

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	5	LYS
7	G	7	ASP

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Mol	Chain	Res	Type
7	G	37	LEU
2	O	89	GLU
6	S	94	HIS
7	T	4	ALA
7	T	7	ASP
7	T	37	LEU
3	C	38	ASN
4	D	5	VAL
6	F	96	LEU
8	H	47	GLY
9	I	37	PHE
6	S	95	GLN
7	T	3	ALA
7	T	40	GLY
9	V	28	SER
6	F	15	GLY
7	G	41	HIS
11	X	12	LYS
12	Y	28	PHE
1	A	51	ASP
8	H	9	LYS
1	N	119	GLU
2	O	60	GLU
8	U	8	ILE
6	F	94	HIS
6	F	95	GLN
7	G	6	GLY
4	Q	103	VAL
8	U	47	GLY

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%)	421 (99%)	5 (1%)	71	88
1	N	426/426 (100%)	412 (97%)	14 (3%)	38	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	210/210 (100%)	197 (94%)	13 (6%)	18	35
2	O	210/210 (100%)	191 (91%)	19 (9%)	9	19
3	C	224/226 (99%)	217 (97%)	7 (3%)	40	67
3	P	224/226 (99%)	217 (97%)	7 (3%)	40	67
4	D	128/129 (99%)	121 (94%)	7 (6%)	21	41
4	Q	123/129 (95%)	119 (97%)	4 (3%)	38	64
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	64
5	R	92/95 (97%)	87 (95%)	5 (5%)	22	42
6	F	80/81 (99%)	77 (96%)	3 (4%)	33	58
6	S	79/81 (98%)	74 (94%)	5 (6%)	18	34
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	19
7	T	67/68 (98%)	63 (94%)	4 (6%)	19	37
8	H	70/75 (93%)	66 (94%)	4 (6%)	20	39
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	29
9	I	57/57 (100%)	52 (91%)	5 (9%)	10	19
9	V	57/57 (100%)	51 (90%)	6 (10%)	7	13
10	J	49/50 (98%)	47 (96%)	2 (4%)	30	55
10	W	49/50 (98%)	45 (92%)	4 (8%)	11	22
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	72
11	X	39/46 (85%)	35 (90%)	4 (10%)	7	14
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	72
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	45
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	42
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	23
All	All	3031/3082 (98%)	2890 (95%)	141 (5%)	26	49

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	369	ASP
1	A	484	THR
1	A	513	LEU

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Mol	Chain	Res	Type
2	B	43	SER
2	B	60	GLU
2	B	65	TRP
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	88	ASP
2	B	91	ASN
2	B	110	TYR
2	B	130	PRO
2	B	167	SER
2	B	171	LYS
2	B	183	THR
3	C	33	MET
3	C	42	LEU
3	C	51	MET
3	C	127	LEU
3	C	159	MET
3	C	230	ASN
3	C	258	TRP
4	D	17	VAL
4	D	36	SER
4	D	47	SER
4	D	51	LEU
4	D	58	GLU
4	D	101	HIS
4	D	114	GLU
5	E	5	HIS
5	E	7	THR
5	E	70	VAL
6	F	2	SER
6	F	48	LEU
6	F	87	THR
7	G	8	HIS
7	G	33	LEU
7	G	34	ASN
7	G	54	ARG
7	G	61	SER
7	G	84	LYS
8	H	27	ARG
8	H	50	VAL
8	H	60	TYR

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Mol	Chain	Res	Type
8	H	61	LYS
9	I	8	GLN
9	I	15	ARG
9	I	18	ARG
9	I	21	ILE
9	I	29	LEU
10	J	27	THR
10	J	50	LEU
11	K	54	ARG
12	L	26	THR
13	M	19	LEU
13	M	42	LYS
1	N	9	SER
1	N	38	ARG
1	N	91	ASP
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	265	LYS
1	N	333	LYS
1	N	363	LEU
1	N	369	ASP
1	N	382	SER
1	N	455	SER
1	N	483	LEU
1	N	513	LEU
2	O	35	SER
2	O	43	SER
2	O	55	THR
2	O	57	ASP
2	O	60	GLU
2	O	65	TRP
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	92	ASN
2	O	110	TYR
2	O	156	SER
2	O	158	ASP
2	O	167	SER
2	O	171	LYS

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Mol	Chain	Res	Type
2	O	183	THR
2	O	200	CYS
2	O	226	MET
3	P	23	SER
3	P	28	THR
3	P	49	THR
3	P	50	ASN
3	P	127	LEU
3	P	159	MET
3	P	179	SER
4	Q	47	SER
4	Q	110	THR
4	Q	123	MET
4	Q	143	ASN
5	R	9	GLU
5	R	31	LYS
5	R	46	LYS
5	R	70	VAL
5	R	109	VAL
6	S	48	LEU
6	S	52	ILE
6	S	53	THR
6	S	54	ASN
6	S	96	LEU
7	T	2	SER
7	T	8	HIS
7	T	54	ARG
7	T	74	ARG
8	U	7	LYS
8	U	9	LYS
8	U	27	ARG
8	U	60	TYR
8	U	66	ILE
9	V	15	ARG
9	V	18	ARG
9	V	21	ILE
9	V	28	SER
9	V	29	LEU
9	V	36	LYS
10	W	10	LYS
10	W	27	THR
10	W	29	ASN

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Mol	Chain	Res	Type
10	W	50	LEU
11	X	20	SER
11	X	49	THR
11	X	52	GLU
11	X	54	ARG
12	Y	11	ILE
12	Y	26	THR
13	Z	13	LYS
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	32	ASN
4	D	37	GLN
5	E	78	HIS
5	E	94	ASN
6	F	80	GLN
7	G	76	ASN
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS

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Mol	Chain	Res	Type
5	R	94	ASN
6	S	54	ASN
7	T	34	ASN
7	T	66	ASN
7	T	76	ASN
8	U	31	GLN
8	U	32	ASN
8	U	37	HIS
10	W	29	ASN
13	Z	36	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	$\#\|Z\| > 2$
9	SAC	I	1	9	7,8,9	0.69	0	8,9,11	1.05	1 (12%)
7	TPO	T	11	7	8,10,11	0.91	0	10,14,16	0.81	0
1	FME	N	1	1	8,9,10	0.50	0	7,9,11	0.98	0
1	FME	A	1	1	8,9,10	0.48	0	7,9,11	0.96	0
7	TPO	G	11	7	8,10,11	1.30	1 (12%)	10,14,16	0.81	0
2	FME	O	1	2	8,9,10	0.44	0	7,9,11	1.63	2 (28%)
2	FME	B	1	2	8,9,10	0.56	0	7,9,11	2.08	2 (28%)
9	SAC	V	1	9	7,8,9	0.65	0	8,9,11	1.47	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.30	1.65	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-4.15	116.43	122.82
9	V	1	SAC	O-C-CA	-4.01	114.27	124.78
2	B	1	FME	C-CA-N	3.12	115.37	109.73
2	O	1	FME	CA-N-CN	-2.95	118.28	122.82
2	O	1	FME	C-CA-N	2.88	114.92	109.73
9	I	1	SAC	O-C-CA	-2.65	117.83	124.78

There are no chirality outliers.

All (26) 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
1	A	1	FME	C-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	C-CA-N-C1A
9	I	1	SAC	CB-CA-N-C1A
9	I	1	SAC	O-C-CA-CB
1	N	1	FME	O1-CN-N-CA

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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	CB-OG1-P-O1P
7	T	11	TPO	CB-OG1-P-O3P
9	V	1	SAC	C-CA-N-C1A
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	O-C-CA-CB
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	CA-CB-CG-SD
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C2A-C1A-N-CA
7	G	11	TPO	O-C-CA-CB
1	N	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
7	G	11	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 10 are monoatomic and 2 are modelled with single atom - 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	$\#\|Z\| > 2$
19	TGL	N	609	-	62,62,62	1.13	3 (4%)	65,65,65	1.03	5 (7%)
17	HEA	A	605	20,1	57,67,67	1.93	14 (24%)	61,103,103	2.31	22 (36%)
25	PEK	T	102	-	52,52,52	0.33	0	55,57,57	0.49	0
24	CHD	G	104	-	32,32,32	0.57	0	51,51,51	0.85	0
17	HEA	N	606	1	57,67,67	1.96	15 (26%)	61,103,103	2.37	22 (36%)
24	CHD	J	101	-	32,32,32	0.63	0	51,51,51	1.14	5 (9%)
24	CHD	W	101	-	32,32,32	0.56	0	51,51,51	0.71	0
24	CHD	P	301	-	32,32,32	0.62	0	51,51,51	0.75	0
18	PGV	A	608	-	50,50,50	1.18	2 (4%)	53,56,56	1.34	4 (7%)
23	PSC	O	302	-	51,51,51	0.31	0	57,59,59	0.39	0
24	CHD	J	102	-	32,32,32	0.77	0	51,51,51	1.27	4 (7%)
25	PEK	P	302	-	52,52,52	0.30	0	55,57,57	0.55	0
28	DMU	Q	201	-	34,34,34	1.06	2 (5%)	45,45,45	1.29	5 (11%)
18	PGV	C	303	-	50,50,50	0.85	2 (4%)	53,56,56	1.14	6 (11%)
26	CDL	T	103	-	99,99,99	1.01	4 (4%)	105,111,111	0.69	4 (3%)
19	TGL	N	607	-	62,62,62	1.06	4 (6%)	65,65,65	1.09	5 (7%)
19	TGL	B	303	-	62,62,62	1.01	4 (6%)	65,65,65	1.07	7 (10%)
19	TGL	L	101	-	62,62,62	1.11	5 (8%)	65,65,65	1.09	4 (6%)
18	PGV	U	101	-	50,50,50	1.12	2 (4%)	53,56,56	1.21	5 (9%)
18	PGV	N	610	-	50,50,50	1.06	2 (4%)	53,56,56	0.95	3 (5%)
18	PGV	A	606	-	50,50,50	1.10	2 (4%)	53,56,56	1.14	4 (7%)
19	TGL	A	609	-	62,62,62	1.13	4 (6%)	65,65,65	1.05	5 (7%)
25	PEK	P	303	-	52,52,52	0.38	0	55,57,57	0.56	0
18	PGV	P	304	-	50,50,50	0.94	2 (4%)	53,56,56	1.02	4 (7%)
22	CUA	O	301	2	0,1,1	-	-	-		
26	CDL	P	305	-	99,99,99	0.98	4 (4%)	105,111,111	0.87	5 (4%)
17	HEA	A	604	1	57,67,67	2.00	17 (29%)	61,103,103	2.28	26 (42%)
28	DMU	M	101	-	34,34,34	1.08	3 (8%)	45,45,45	1.50	8 (17%)
24	CHD	B	304	-	32,32,32	0.47	0	51,51,51	0.70	0
25	PEK	C	302	-	52,52,52	0.34	0	55,57,57	0.46	0
26	CDL	N	601	-	99,99,99	0.96	4 (4%)	105,111,111	0.71	2 (1%)
28	DMU	T	101	-	34,34,34	1.84	6 (17%)	45,45,45	1.58	6 (13%)
26	CDL	C	304	-	99,99,99	0.98	4 (4%)	105,111,111	0.81	4 (3%)
18	PGV	N	608	-	50,50,50	0.87	2 (4%)	53,56,56	1.08	4 (7%)
22	CUA	B	301	2	0,1,1	-	-	-		
25	PEK	G	102	-	52,52,52	0.33	0	55,57,57	0.57	0
18	PGV	A	607	-	50,50,50	0.85	2 (4%)	53,56,56	1.34	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	PEK	G	103	-	52,52,52	0.37	0	55,57,57	0.53	1 (1%)
24	CHD	C	301	-	32,32,32	0.64	1 (3%)	51,51,51	0.73	0
23	PSC	B	302	-	51,51,51	0.34	0	57,59,59	0.47	0
19	TGL	Y	101	-	62,62,62	1.09	4 (6%)	65,65,65	0.97	5 (7%)
17	HEA	N	605	1	57,67,67	1.96	14 (24%)	61,103,103	2.42	28 (45%)
24	CHD	W	102	-	32,32,32	0.69	0	51,51,51	1.04	4 (7%)
28	DMU	G	101	-	34,34,34	1.38	5 (14%)	45,45,45	1.71	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	N	609	-	-	42/65/65/65	-
17	HEA	A	605	20,1	3/3/7/16	5/32/76/76	-
25	PEK	T	102	-	-	30/56/56/56	-
24	CHD	G	104	-	-	4/9/74/74	0/4/4/4
17	HEA	N	606	1	3/3/7/16	5/32/76/76	-
24	CHD	J	101	-	-	4/9/74/74	1/4/4/4
24	CHD	W	101	-	-	2/9/74/74	1/4/4/4
24	CHD	P	301	-	-	3/9/74/74	0/4/4/4
18	PGV	A	608	-	-	26/55/55/55	-
23	PSC	O	302	-	-	31/55/55/55	-
24	CHD	J	102	-	-	6/9/74/74	0/4/4/4
25	PEK	P	302	-	-	21/56/56/56	-
28	DMU	Q	201	-	-	10/19/59/59	0/2/2/2
18	PGV	C	303	-	-	13/55/55/55	-
26	CDL	T	103	-	-	65/110/110/110	-
19	TGL	N	607	-	-	39/65/65/65	-
19	TGL	B	303	-	-	40/65/65/65	-
19	TGL	L	101	-	-	37/65/65/65	-
18	PGV	U	101	-	-	29/55/55/55	-
18	PGV	N	610	-	-	33/55/55/55	-
18	PGV	A	606	-	-	32/55/55/55	-
19	TGL	A	609	-	-	39/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	P	303	-	-	21/56/56/56	-
18	PGV	P	304	-	-	14/55/55/55	-
26	CDL	P	305	-	-	71/110/110/110	-
17	HEA	A	604	1	3/3/7/16	5/32/76/76	-
28	DMU	M	101	-	-	10/19/59/59	0/2/2/2
24	CHD	B	304	-	-	4/9/74/74	0/4/4/4
25	PEK	C	302	-	-	25/56/56/56	-
26	CDL	N	601	-	-	58/110/110/110	-
28	DMU	T	101	-	-	10/19/59/59	0/2/2/2
26	CDL	C	304	-	-	59/110/110/110	-
18	PGV	N	608	-	-	15/55/55/55	-
25	PEK	G	102	-	-	21/56/56/56	-
18	PGV	A	607	-	-	17/55/55/55	-
25	PEK	G	103	-	-	25/56/56/56	-
24	CHD	C	301	-	-	0/9/74/74	0/4/4/4
23	PSC	B	302	-	-	29/55/55/55	-
19	TGL	Y	101	-	-	32/65/65/65	-
17	HEA	N	605	1	3/3/7/16	5/32/76/76	-
24	CHD	W	102	-	-	6/9/74/74	0/4/4/4
28	DMU	G	101	-	-	12/19/59/59	0/2/2/2

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	101	DMU	O16-C6	6.46	1.51	1.40
17	N	606	HEA	C3B-C2B	6.00	1.48	1.34
17	N	605	HEA	C3B-C2B	5.68	1.47	1.34
18	A	608	PGV	O01-C1	5.49	1.49	1.34
18	A	606	PGV	O03-C19	5.15	1.48	1.33
17	A	604	HEA	C3C-C2C	5.15	1.47	1.40
18	U	101	PGV	O01-C1	5.07	1.48	1.34
19	N	609	TGL	OG2-CB1	5.05	1.48	1.34
17	A	605	HEA	C3B-C2B	5.03	1.46	1.34
17	N	605	HEA	C3C-C2C	5.01	1.47	1.40
17	A	605	HEA	CHC-C4B	4.93	1.47	1.35
19	B	303	TGL	OG2-CB1	4.83	1.47	1.34
17	A	604	HEA	CHD-C1D	4.80	1.47	1.35
17	A	604	HEA	C3B-C2B	4.80	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG1-CA1	4.76	1.47	1.33
19	N	609	TGL	OG3-CC1	4.75	1.47	1.33
17	A	604	HEA	C3D-C2D	4.71	1.46	1.36
19	L	101	TGL	OG2-CB1	4.66	1.47	1.34
18	U	101	PGV	O03-C19	4.65	1.46	1.33
19	A	609	TGL	OG2-CB1	4.62	1.47	1.34
18	A	608	PGV	O03-C19	4.60	1.46	1.33
18	P	304	PGV	O01-C1	4.55	1.47	1.34
17	A	604	HEA	CHC-C4B	4.54	1.46	1.35
18	A	606	PGV	O01-C1	4.54	1.47	1.34
18	N	610	PGV	O03-C19	4.52	1.46	1.33
19	A	609	TGL	OG3-CC1	4.51	1.46	1.33
17	A	605	HEA	C3D-C2D	4.51	1.46	1.36
17	N	605	HEA	CHD-C1D	4.47	1.46	1.35
26	T	103	CDL	OB8-CB7	4.45	1.46	1.33
26	T	103	CDL	OA8-CA7	4.44	1.46	1.33
28	Q	201	DMU	O16-C6	4.44	1.47	1.40
26	P	305	CDL	OA6-CA5	4.40	1.46	1.34
26	C	304	CDL	OA6-CA5	4.40	1.46	1.34
17	A	605	HEA	C1D-ND	-4.40	1.32	1.40
26	C	304	CDL	OA8-CA7	4.39	1.46	1.33
26	T	103	CDL	OA6-CA5	4.38	1.46	1.34
19	Y	101	TGL	OG3-CC1	4.37	1.46	1.33
26	P	305	CDL	OA8-CA7	4.37	1.46	1.33
17	N	606	HEA	C3C-C2C	4.36	1.46	1.40
26	N	601	CDL	OB6-CB5	4.35	1.46	1.34
26	P	305	CDL	OB6-CB5	4.31	1.46	1.34
26	C	304	CDL	OB6-CB5	4.31	1.46	1.34
17	N	606	HEA	C3A-C2A	4.31	1.46	1.40
26	N	601	CDL	OA8-CA7	4.27	1.45	1.33
18	N	610	PGV	O01-C1	4.27	1.46	1.34
19	A	609	TGL	OG1-CA1	4.26	1.45	1.33
26	N	601	CDL	OA6-CA5	4.21	1.46	1.34
28	M	101	DMU	O16-C6	4.20	1.47	1.40
26	N	601	CDL	OB8-CB7	4.19	1.45	1.33
19	Y	101	TGL	OG2-CB1	4.15	1.46	1.34
26	P	305	CDL	OB8-CB7	4.12	1.45	1.33
26	T	103	CDL	OB6-CB5	4.11	1.45	1.34
19	Y	101	TGL	OG1-CA1	4.04	1.45	1.33
17	N	606	HEA	C3D-C2D	4.04	1.45	1.36
19	N	607	TGL	OG3-CC1	4.02	1.45	1.33
26	C	304	CDL	OB8-CB7	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	101	DMU	O7-C10	3.95	1.52	1.41
17	A	605	HEA	C3C-C2C	3.91	1.45	1.40
19	N	607	TGL	OG2-CB1	3.89	1.45	1.34
19	N	609	TGL	OG1-CA1	3.88	1.44	1.33
17	N	606	HEA	CHC-C4B	3.87	1.44	1.35
17	N	605	HEA	C3D-C2D	3.86	1.44	1.36
17	A	604	HEA	C4B-C3B	3.81	1.51	1.44
17	A	604	HEA	C3A-C2A	3.78	1.45	1.40
17	N	605	HEA	C3A-C2A	3.76	1.45	1.40
17	N	605	HEA	CHC-C4B	3.76	1.44	1.35
18	N	608	PGV	O01-C1	3.74	1.44	1.34
18	P	304	PGV	O03-C19	3.72	1.44	1.33
17	A	605	HEA	CHD-C1D	3.69	1.44	1.35
28	G	101	DMU	O1-C10	3.65	1.51	1.41
18	N	608	PGV	O03-C19	3.65	1.44	1.33
17	N	606	HEA	C4B-NB	-3.63	1.34	1.40
19	N	607	TGL	OG1-CA1	3.62	1.43	1.33
17	N	605	HEA	C1D-ND	-3.61	1.34	1.40
17	N	606	HEA	CHD-C1D	3.60	1.44	1.35
18	A	607	PGV	O01-C1	3.55	1.44	1.34
18	C	303	PGV	O01-C1	3.55	1.44	1.34
17	N	606	HEA	C1D-ND	-3.51	1.34	1.40
17	N	605	HEA	C4B-NB	-3.47	1.34	1.40
19	B	303	TGL	OG1-CA1	3.46	1.43	1.33
19	N	607	TGL	OG2-CG2	-3.45	1.38	1.46
17	A	605	HEA	C3A-C2A	3.45	1.45	1.40
28	T	101	DMU	O1-C10	3.40	1.50	1.41
28	G	101	DMU	O7-C10	3.34	1.51	1.41
17	N	605	HEA	C2A-C1A	3.32	1.50	1.42
18	A	607	PGV	O03-C19	3.27	1.42	1.33
17	N	605	HEA	C4D-ND	-3.27	1.32	1.38
17	A	605	HEA	C4B-NB	-3.26	1.34	1.40
17	A	604	HEA	C1D-ND	-3.22	1.34	1.40
18	C	303	PGV	O03-C19	3.21	1.42	1.33
17	A	604	HEA	C4B-NB	-3.19	1.34	1.40
19	Y	101	TGL	OG2-CG2	-3.14	1.38	1.46
28	T	101	DMU	O7-C3	3.14	1.52	1.43
19	L	101	TGL	OG3-CC1	3.14	1.42	1.33
28	G	101	DMU	O16-C6	3.05	1.45	1.40
28	G	101	DMU	C10-C5	3.02	1.61	1.52
17	N	606	HEA	FE-ND	2.83	2.10	1.96
17	A	605	HEA	C1C-CHC	2.76	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG2-CG2	-2.76	1.39	1.46
19	A	609	TGL	OG2-CG2	-2.71	1.39	1.46
17	N	605	HEA	FE-ND	2.67	2.10	1.96
17	N	606	HEA	C4D-ND	-2.66	1.33	1.38
28	T	101	DMU	C2-C1	2.65	1.59	1.52
17	A	605	HEA	FE-NB	2.55	2.09	1.96
17	A	604	HEA	FE-NB	2.54	2.09	1.96
17	N	605	HEA	FE-NB	2.51	2.09	1.96
19	B	303	TGL	OC1-CC1	-2.48	1.15	1.22
17	A	604	HEA	C4D-ND	-2.41	1.33	1.38
28	G	101	DMU	O7-C3	2.40	1.50	1.43
17	N	606	HEA	FE-NB	2.35	2.08	1.96
17	N	606	HEA	C1C-CHC	2.31	1.47	1.41
28	M	101	DMU	O1-C9	2.31	1.49	1.44
17	N	605	HEA	C1C-CHC	2.30	1.47	1.41
17	A	605	HEA	CHA-C4D	2.27	1.47	1.41
19	L	101	TGL	OG3-CG3	-2.26	1.40	1.45
17	A	604	HEA	C1B-C2B	2.25	1.48	1.44
28	T	101	DMU	C2-C3	2.23	1.58	1.52
17	A	605	HEA	C1B-NB	-2.21	1.34	1.38
19	B	303	TGL	OG3-CC1	2.21	1.39	1.33
17	N	606	HEA	C2A-C1A	2.18	1.47	1.42
24	C	301	CHD	O26-C24	-2.17	1.23	1.30
17	A	605	HEA	C4C-NC	-2.15	1.31	1.36
17	A	604	HEA	FE-ND	2.14	2.07	1.96
17	A	604	HEA	C4C-CHD	2.12	1.46	1.41
17	N	606	HEA	CHB-C1B	2.10	1.47	1.41
17	A	604	HEA	C1B-NB	-2.08	1.34	1.38
28	M	101	DMU	O1-C10	2.08	1.47	1.41
17	A	604	HEA	C2A-C1A	2.06	1.47	1.42
17	N	605	HEA	C4C-CHD	2.04	1.46	1.41
17	A	605	HEA	C4D-C3D	2.03	1.48	1.45
17	A	604	HEA	CHB-C1B	2.03	1.46	1.41
17	N	606	HEA	C1B-NB	-2.03	1.34	1.38
28	Q	201	DMU	O7-C10	2.01	1.47	1.41

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	608	PGV	O01-C1-C2	6.28	125.04	111.50
17	N	606	HEA	C2D-C1D-ND	6.27	117.27	109.84
17	A	605	HEA	CAD-CBD-CGD	-6.09	100.50	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	606	HEA	C3D-C4D-ND	6.02	116.19	110.36
17	N	605	HEA	C3D-C4D-ND	6.00	116.17	110.36
28	T	101	DMU	O16-C6-C1	5.83	117.41	108.30
17	N	606	HEA	C1D-C2D-C3D	-5.70	100.96	106.96
17	A	605	HEA	C2D-C1D-ND	5.60	116.48	109.84
28	G	101	DMU	C10-O1-C9	5.55	124.57	113.69
17	N	605	HEA	C2D-C1D-ND	5.11	115.90	109.84
17	A	604	HEA	C2B-C1B-NB	5.11	116.01	109.88
18	A	606	PGV	O01-C1-C2	4.94	122.15	111.50
17	A	604	HEA	C3B-C4B-NB	4.93	115.68	109.84
17	A	605	HEA	C3C-C4C-NC	4.91	115.56	109.21
18	U	101	PGV	O01-C1-C2	4.87	121.99	111.50
17	A	605	HEA	C1D-C2D-C3D	-4.83	101.88	106.96
17	N	605	HEA	C1D-C2D-C3D	-4.78	101.93	106.96
24	J	102	CHD	C13-C17-C20	4.64	125.03	119.50
26	P	305	CDL	OA6-CA5-C11	4.63	121.48	111.50
17	A	605	HEA	C2B-C1B-NB	4.59	115.38	109.88
18	A	607	PGV	O03-C19-O04	-4.57	112.07	123.59
18	A	607	PGV	O03-C19-C20	4.54	126.17	111.91
26	C	304	CDL	OA6-CA5-C11	4.54	121.28	111.50
18	U	101	PGV	O03-C19-C20	4.47	125.92	111.91
17	N	606	HEA	C2B-C1B-NB	4.44	115.20	109.88
17	A	605	HEA	C3B-C4B-NB	4.44	115.10	109.84
17	A	604	HEA	C4A-CHB-C1B	4.44	128.41	122.56
17	N	606	HEA	CAD-CBD-CGD	-4.42	104.09	113.60
17	A	604	HEA	C3D-C4D-ND	4.37	114.59	110.36
17	N	606	HEA	C3B-C4B-NB	4.32	114.95	109.84
19	N	607	TGL	CG2-OG2-CB1	4.24	128.22	117.79
17	A	604	HEA	C1D-C2D-C3D	-4.21	102.53	106.96
28	T	101	DMU	C18-O16-C6	4.16	120.74	113.84
18	A	608	PGV	O03-C19-C20	4.16	124.95	111.91
17	N	605	HEA	OMA-CMA-C3A	-4.12	115.93	124.91
18	C	303	PGV	O01-C1-C2	4.10	120.34	111.50
17	A	605	HEA	C3D-C4D-ND	4.10	114.33	110.36
28	G	101	DMU	C10-O7-C3	4.06	128.00	117.96
17	N	605	HEA	C3B-C4B-NB	4.05	114.64	109.84
19	N	607	TGL	CG3-CG2-CG1	4.03	121.33	111.79
17	N	606	HEA	C3C-C4C-NC	4.02	114.41	109.21
18	A	607	PGV	O01-C1-C2	4.02	120.16	111.50
19	N	609	TGL	OG2-CB1-CB2	3.98	120.08	111.50
19	L	101	TGL	OG2-CG2-CG1	3.96	122.75	108.40
17	N	605	HEA	C2B-C1B-NB	3.95	114.61	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	W	102	CHD	C13-C17-C20	3.91	124.16	119.50
24	J	101	CHD	C10-C9-C8	3.85	115.96	111.82
17	N	606	HEA	C4D-CHA-C1A	3.82	127.61	122.56
17	A	604	HEA	CHA-C4D-C3D	-3.79	119.27	124.84
17	A	604	HEA	C2D-C1D-ND	3.75	114.28	109.84
18	N	610	PGV	O01-C1-C2	3.73	119.53	111.50
19	B	303	TGL	OG2-CB1-CB2	3.73	119.53	111.50
17	N	606	HEA	CMD-C2D-C1D	3.70	130.68	125.04
28	M	101	DMU	C18-O16-C6	3.68	119.94	113.84
17	N	605	HEA	C3C-C4C-NC	3.62	113.89	109.21
17	N	605	HEA	CHB-C1B-C2B	-3.58	119.39	124.98
17	A	605	HEA	CMD-C2D-C1D	3.56	130.46	125.04
19	A	609	TGL	OG2-CG2-CG1	3.42	120.79	108.40
19	A	609	TGL	CG2-OG2-CB1	-3.39	109.44	117.79
17	N	606	HEA	C1B-C2B-C3B	-3.39	102.75	106.80
18	A	608	PGV	O03-C19-O04	-3.34	115.17	123.59
17	A	604	HEA	CMB-C2B-C1B	3.29	130.04	125.04
19	N	607	TGL	OG2-CB1-CB2	3.29	118.58	111.50
28	M	101	DMU	C10-O1-C9	3.26	120.08	113.69
18	A	607	PGV	O01-C1-O02	-3.20	115.96	123.70
17	A	604	HEA	C4B-C3B-C2B	-3.20	101.95	107.41
17	N	605	HEA	CHA-C4D-C3D	-3.19	120.15	124.84
17	N	606	HEA	OMA-CMA-C3A	-3.18	117.98	124.91
18	N	608	PGV	O01-C1-C2	3.17	118.32	111.50
17	N	605	HEA	CMC-C2C-C3C	3.16	130.59	124.68
19	N	609	TGL	OG2-CG2-CG1	3.14	119.77	108.40
17	A	604	HEA	CMD-C2D-C1D	3.14	129.82	125.04
17	N	605	HEA	C17-C18-C19	-3.13	120.12	127.66
18	P	304	PGV	O01-C1-C2	3.10	118.18	111.50
19	L	101	TGL	OG2-CB1-CB2	3.09	118.17	111.50
17	N	605	HEA	CMD-C2D-C1D	3.08	129.74	125.04
17	N	605	HEA	C13-C12-C11	-3.06	109.76	114.35
28	G	101	DMU	O7-C10-C5	3.05	116.01	108.10
17	N	605	HEA	C4D-CHA-C1A	3.04	126.58	122.56
19	A	609	TGL	CG3-CG2-CG1	3.04	118.98	111.79
28	M	101	DMU	C11-C9-C8	-3.03	105.90	113.00
17	A	605	HEA	C4B-C3B-C2B	-3.02	102.24	107.41
17	N	606	HEA	CHB-C1B-C2B	-3.02	120.27	124.98
17	A	604	HEA	CHB-C1B-C2B	-3.00	120.29	124.98
26	P	305	CDL	OB6-CB5-C51	3.00	117.96	111.50
17	N	605	HEA	C26-C15-C16	2.99	120.31	115.27
17	A	605	HEA	CHB-C1B-C2B	-2.99	120.31	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	606	HEA	CHA-C4D-C3D	-2.99	120.45	124.84
17	A	604	HEA	C1B-C2B-C3B	-2.99	103.23	106.80
28	M	101	DMU	O1-C9-C11	2.98	113.84	106.44
19	A	609	TGL	OG3-CC1-CC2	2.97	121.23	111.91
24	J	102	CHD	C22-C23-C24	2.97	120.39	112.51
17	N	606	HEA	C1D-ND-C4D	-2.96	102.02	105.07
28	M	101	DMU	C8-C7-C5	-2.95	105.67	110.82
18	N	610	PGV	O03-C19-C20	2.95	121.16	111.91
17	N	606	HEA	CMC-C2C-C3C	2.94	130.19	124.68
18	A	607	PGV	O03-C01-C02	2.93	116.97	108.43
26	N	601	CDL	OA6-CA5-C11	2.90	117.76	111.50
17	N	606	HEA	C4B-C3B-C2B	-2.90	102.46	107.41
18	N	608	PGV	O03-C19-C20	2.89	120.97	111.91
19	Y	101	TGL	OG2-CG2-CG1	2.88	118.83	108.40
17	A	604	HEA	CHC-C4B-NB	-2.87	120.83	124.38
18	A	606	PGV	C02-O01-C1	2.87	124.86	117.79
18	C	303	PGV	O12-P-O13	-2.87	97.86	109.07
19	N	609	TGL	CG2-OG2-CB1	-2.87	110.73	117.79
26	T	103	CDL	OA6-CA5-C11	2.87	117.68	111.50
26	T	103	CDL	OB6-CB5-C51	2.86	117.67	111.50
18	N	608	PGV	O03-C01-C02	2.86	116.76	108.43
19	B	303	TGL	OG2-CG2-CG3	2.85	118.71	108.40
17	A	605	HEA	C4D-CHA-C1A	2.84	126.31	122.56
28	Q	201	DMU	C18-O16-C6	-2.84	109.13	113.84
17	A	605	HEA	C13-C12-C11	-2.83	110.10	114.35
17	N	605	HEA	C1B-C2B-C3B	-2.82	103.43	106.80
28	T	101	DMU	C10-O7-C3	2.82	124.94	117.96
17	N	605	HEA	C4B-C3B-C2B	-2.80	102.63	107.41
17	A	604	HEA	CMC-C2C-C3C	2.77	129.87	124.68
17	A	605	HEA	C1B-C2B-C3B	-2.77	103.49	106.80
17	N	605	HEA	C4D-C3D-C2D	-2.75	102.90	106.90
28	Q	201	DMU	O5-C6-O16	2.73	116.45	109.97
18	C	303	PGV	O01-C1-O02	-2.73	117.10	123.70
28	G	101	DMU	O16-C6-C1	2.73	112.56	108.30
17	N	606	HEA	C4A-CHB-C1B	2.73	126.16	122.56
17	A	605	HEA	C20-C19-C18	-2.71	115.63	121.12
17	A	605	HEA	CHA-C4D-C3D	-2.70	120.87	124.84
24	J	101	CHD	C14-C8-C9	-2.70	106.01	109.71
17	A	604	HEA	CBD-CAD-C3D	-2.67	105.20	112.63
17	A	604	HEA	C13-C14-C15	-2.67	121.24	127.66
19	N	609	TGL	OG2-CG2-CG3	2.66	118.03	108.40
17	A	605	HEA	CAD-C3D-C4D	2.65	129.29	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	101	TGL	CG3-CG2-CG1	2.65	118.05	111.79
28	Q	201	DMU	C7-C8-C9	2.63	114.93	110.24
19	Y	101	TGL	CG2-OG2-CB1	2.62	124.25	117.79
28	G	101	DMU	C2-C3-C4	-2.62	104.92	110.93
18	U	101	PGV	O03-C19-O04	-2.61	117.00	123.59
17	A	604	HEA	C26-C15-C16	2.60	119.65	115.27
17	A	605	HEA	C4A-CHB-C1B	2.60	125.99	122.56
17	N	605	HEA	O2D-CGD-CBD	2.60	122.39	114.03
28	T	101	DMU	C10-O1-C9	2.59	118.78	113.69
17	N	605	HEA	C12-C13-C14	-2.59	105.40	112.23
17	A	604	HEA	C17-C18-C19	-2.57	121.47	127.66
19	B	303	TGL	CG2-OG2-CB1	-2.56	111.49	117.79
17	A	604	HEA	C13-C12-C11	-2.55	110.51	114.35
17	A	605	HEA	CMC-C2C-C3C	2.55	129.44	124.68
17	N	605	HEA	O2A-CGA-O1A	-2.54	116.96	123.30
26	C	304	CDL	OA6-CA5-OA7	-2.51	117.64	123.70
17	A	605	HEA	C4D-C3D-C2D	-2.51	103.25	106.90
26	P	305	CDL	CB4-OB6-CB5	-2.50	111.62	117.79
19	Y	101	TGL	OG2-CB1-CB2	2.50	116.89	111.50
24	W	102	CHD	C16-C17-C13	-2.50	101.11	103.55
17	A	605	HEA	CHD-C1D-C2D	-2.47	119.89	126.72
17	A	604	HEA	OMA-CMA-C3A	-2.45	119.57	124.91
26	P	305	CDL	OA8-CA7-OA9	-2.44	117.42	123.59
17	N	605	HEA	O2A-CGA-CBA	2.43	121.85	114.03
19	L	101	TGL	OG3-CG3-CG2	2.42	115.47	108.43
28	Q	201	DMU	O1-C9-C8	2.42	114.08	109.69
28	G	101	DMU	O7-C3-C4	2.41	116.05	109.45
28	M	101	DMU	O1-C9-C8	2.40	114.06	109.69
17	A	605	HEA	C27-C19-C20	2.38	119.27	115.27
28	G	101	DMU	C6-O5-C4	-2.38	109.02	113.69
18	P	304	PGV	C03-C02-C01	-2.36	106.22	111.79
18	A	606	PGV	O03-C19-C20	2.35	119.28	111.91
24	W	102	CHD	C22-C20-C17	2.34	115.13	110.28
24	J	102	CHD	C22-C20-C17	2.32	115.09	110.28
18	P	304	PGV	O03-C19-O04	-2.32	117.73	123.59
18	U	101	PGV	O01-C1-O02	-2.31	118.11	123.70
17	N	606	HEA	O1D-CGD-CBD	-2.31	115.65	123.08
28	T	101	DMU	C1-C2-C3	2.31	114.95	109.68
18	N	610	PGV	O03-C19-O04	-2.30	117.78	123.59
17	A	604	HEA	C3C-C4C-NC	2.30	112.19	109.21
28	T	101	DMU	O1-C9-C11	2.30	112.15	106.44
17	N	606	HEA	C4D-C3D-C2D	-2.30	103.55	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	604	HEA	CHD-C1D-C2D	-2.29	120.38	126.72
24	J	102	CHD	C5-C6-C7	2.29	116.99	114.46
19	B	303	TGL	OG3-CG3-CG2	2.29	115.10	108.43
26	T	103	CDL	OA8-CA7-C31	2.29	119.09	111.91
17	A	604	HEA	C4D-C3D-C2D	-2.28	103.58	106.90
19	N	607	TGL	OG3-CC1-CC2	2.27	119.03	111.91
26	N	601	CDL	CA4-OA6-CA5	-2.26	112.22	117.79
17	N	606	HEA	CHD-C1D-C2D	-2.26	120.47	126.72
18	C	303	PGV	O03-C19-O04	-2.26	117.89	123.59
17	A	605	HEA	CMB-C2B-C1B	2.25	128.47	125.04
26	C	304	CDL	OA8-CA7-OA9	-2.25	117.92	123.59
28	M	101	DMU	C6-O5-C4	2.23	118.06	113.69
19	B	303	TGL	OG3-CC1-CC2	2.21	118.85	111.91
19	Y	101	TGL	OG1-CG1-CG2	-2.21	102.00	108.43
17	N	605	HEA	C21-C20-C19	-2.21	105.71	112.98
26	P	305	CDL	OA6-CA5-OA7	-2.21	118.37	123.70
24	W	102	CHD	C22-C23-C24	2.19	118.33	112.51
24	J	101	CHD	C9-C8-C7	2.19	114.49	111.88
28	G	101	DMU	C34-C31-C28	-2.18	103.35	114.42
17	N	605	HEA	CBD-CAD-C3D	-2.15	106.66	112.63
18	U	101	PGV	O03-C01-C02	2.15	114.68	108.43
26	C	304	CDL	OA8-CA7-C31	2.14	118.63	111.91
18	A	606	PGV	O03-C01-C02	2.14	114.67	108.43
17	A	604	HEA	C4D-CHA-C1A	2.14	125.38	122.56
17	A	604	HEA	CAD-C3D-C4D	2.14	128.39	124.66
18	C	303	PGV	C27-C26-C25	-2.13	103.60	114.42
18	N	608	PGV	C02-O01-C1	-2.13	112.54	117.79
24	J	101	CHD	C1-C2-C3	2.13	113.20	110.47
19	N	607	TGL	CG3-OG3-CC1	2.11	124.95	117.12
19	B	303	TGL	OB1-CB1-CB2	-2.11	115.49	123.73
18	P	304	PGV	O14-P-O13	2.11	122.67	112.24
17	N	606	HEA	O2D-CGD-CBD	2.10	120.77	114.03
17	N	605	HEA	CAA-CBA-CGA	-2.09	107.90	113.76
19	A	609	TGL	OG1-CG1-CG2	2.08	114.49	108.43
17	N	605	HEA	CAD-C3D-C4D	2.08	128.29	124.66
28	Q	201	DMU	C6-O5-C4	-2.08	109.61	113.69
19	B	303	TGL	OG3-CC1-OC1	-2.08	118.35	123.59
17	N	606	HEA	CAA-CBA-CGA	-2.07	107.96	113.76
17	N	605	HEA	CHC-C4B-NB	-2.07	121.83	124.38
25	G	103	PEK	O01-C1-C2	2.07	115.95	111.50
26	T	103	CDL	OA8-CA7-OA9	-2.05	118.42	123.59
18	C	303	PGV	C03-C02-C01	-2.05	106.94	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L	101	TGL	OG2-CG2-CG3	2.04	115.80	108.40
17	N	605	HEA	CHD-C1D-C2D	-2.04	121.07	126.72
28	M	101	DMU	O49-C1-C6	-2.04	105.10	110.05
28	G	101	DMU	O1-C10-C5	2.03	114.64	110.35
19	N	609	TGL	OG3-CC1-CC2	2.03	118.28	111.91
17	A	604	HEA	C25-C23-C22	-2.01	116.83	122.65
18	A	608	PGV	O01-C1-O02	-2.01	118.84	123.70
24	J	101	CHD	C11-C9-C8	-2.01	107.93	110.88

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	604	HEA	ND
17	A	604	HEA	NA
17	A	604	HEA	NB
17	A	605	HEA	ND
17	A	605	HEA	NA
17	A	605	HEA	NB
17	N	605	HEA	ND
17	N	605	HEA	NA
17	N	605	HEA	NB
17	N	606	HEA	ND
17	N	606	HEA	NA
17	N	606	HEA	NB

All (955) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
18	A	606	PGV	C02-C03-O11-P
18	A	606	PGV	C04-C05-C06-O06
18	A	606	PGV	O05-C05-C06-O06
18	A	606	PGV	O02-C1-O01-C02
18	A	606	PGV	C2-C1-O01-C02
18	A	606	PGV	O04-C19-O03-C01
18	A	606	PGV	C20-C19-O03-C01
18	A	607	PGV	C04-O12-P-O13
18	A	608	PGV	C05-C04-O12-P
18	N	610	PGV	C03-O11-P-O13
18	N	610	PGV	C04-C05-C06-O06
18	N	610	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
18	N	610	PGV	C20-C19-O03-C01
18	U	101	PGV	C03-O11-P-O13
18	U	101	PGV	O01-C02-C03-O11
18	U	101	PGV	O02-C1-O01-C02
18	U	101	PGV	C2-C1-O01-C02
19	L	101	TGL	CB2-CB1-OG2-CG2
19	N	607	TGL	OB1-CB1-OG2-CG2
23	B	302	PSC	C04-O12-P-O13
23	B	302	PSC	O12-C04-C05-N
23	B	302	PSC	C9-C10-C11-C12
23	O	302	PSC	C03-O11-P-O13
23	O	302	PSC	C04-O12-P-O14
23	O	302	PSC	O12-C04-C05-N
24	W	102	CHD	C13-C17-C20-C22
24	W	102	CHD	C16-C17-C20-C22
25	C	302	PEK	C03-O11-P-O13
25	C	302	PEK	C03-O11-P-O14
25	C	302	PEK	C04-O12-P-O11
25	C	302	PEK	C2-C1-O01-C02
25	G	103	PEK	C03-O11-P-O14
25	G	103	PEK	C04-O12-P-O11
25	G	103	PEK	C04-O12-P-O13
25	G	103	PEK	C04-O12-P-O14
25	G	103	PEK	O12-C04-C05-N
25	P	303	PEK	C03-O11-P-O13
25	P	303	PEK	C03-O11-P-O14
25	P	303	PEK	O02-C1-O01-C02
25	T	102	PEK	C03-O11-P-O13
25	T	102	PEK	C04-O12-P-O11
25	T	102	PEK	O12-C04-C05-N
26	C	304	CDL	C1-CA2-OA2-PA1
26	C	304	CDL	CA2-OA2-PA1-OA3
26	C	304	CDL	C11-CA5-OA6-CA4
26	C	304	CDL	CB3-OB5-PB2-OB3
26	N	601	CDL	CA3-OA5-PA1-OA3
26	N	601	CDL	C11-CA5-OA6-CA4
26	N	601	CDL	C1-CB2-OB2-PB2
26	P	305	CDL	CA2-C1-CB2-OB2
26	P	305	CDL	C1-CA2-OA2-PA1
26	P	305	CDL	CA2-OA2-PA1-OA4
26	P	305	CDL	OA7-CA5-OA6-CA4
26	P	305	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
26	P	305	CDL	CB3-OB5-PB2-OB3
26	P	305	CDL	C51-CB5-OB6-CB4
26	T	103	CDL	CA2-OA2-PA1-OA3
26	T	103	CDL	CA3-OA5-PA1-OA3
26	T	103	CDL	CA3-OA5-PA1-OA4
26	T	103	CDL	C11-CA5-OA6-CA4
26	T	103	CDL	C1-CB2-OB2-PB2
26	T	103	CDL	CB2-OB2-PB2-OB5
26	T	103	CDL	CB3-OB5-PB2-OB2
26	T	103	CDL	CB3-OB5-PB2-OB3
26	T	103	CDL	CB3-OB5-PB2-OB4
28	M	101	DMU	C19-C18-O16-C6
28	T	101	DMU	C1-C6-O16-C18
28	T	101	DMU	O5-C6-O16-C18
18	N	610	PGV	O04-C19-O03-C01
23	O	302	PSC	O04-C19-O03-C01
19	N	607	TGL	OA1-CA1-OG1-CG1
25	T	102	PEK	O04-C21-O03-C01
19	L	101	TGL	OB1-CB1-OG2-CG2
25	C	302	PEK	O02-C1-O01-C02
26	C	304	CDL	OA7-CA5-OA6-CA4
26	N	601	CDL	OA7-CA5-OA6-CA4
26	P	305	CDL	OB7-CB5-OB6-CB4
26	T	103	CDL	OA7-CA5-OA6-CA4
19	N	607	TGL	CA2-CA1-OG1-CG1
23	B	302	PSC	C20-C19-O03-C01
25	T	102	PEK	C22-C21-O03-C01
18	N	610	PGV	C2-C1-O01-C02
19	N	607	TGL	CB2-CB1-OG2-CG2
28	G	101	DMU	C5-C10-O7-C3
19	L	101	TGL	OA1-CA1-OG1-CG1
24	W	102	CHD	C16-C17-C20-C21
19	Y	101	TGL	CA2-CA1-OG1-CG1
23	O	302	PSC	C20-C19-O03-C01
26	C	304	CDL	C31-CA7-OA8-CA6
28	G	101	DMU	O6-C11-C9-O1
28	Q	201	DMU	O6-C11-C9-O1
23	B	302	PSC	O04-C19-O03-C01
26	C	304	CDL	OA9-CA7-OA8-CA6
24	J	102	CHD	C13-C17-C20-C22
18	A	606	PGV	O12-C04-C05-O05
18	U	101	PGV	O12-C04-C05-O05

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	CA2-CA1-OG1-CG1
25	P	303	PEK	C2-C1-O01-C02
19	N	607	TGL	CA3-CA4-CA5-CA6
19	Y	101	TGL	OA1-CA1-OG1-CG1
26	N	601	CDL	C80-C81-C82-C83
28	T	101	DMU	O5-C4-C57-O61
28	Q	201	DMU	O6-C11-C9-C8
28	G	101	DMU	O5-C4-C57-O61
28	G	101	DMU	O6-C11-C9-C8
28	M	101	DMU	O5-C6-O16-C18
28	Q	201	DMU	O5-C6-O16-C18
17	A	604	HEA	C15-C16-C17-C18
17	N	605	HEA	C15-C16-C17-C18
19	B	303	TGL	CC5-CC6-CC7-CC8
19	N	607	TGL	CA9-C20-C21-C22
19	N	609	TGL	CB9-C10-C11-C12
24	B	304	CHD	C17-C20-C22-C23
24	G	104	CHD	C17-C20-C22-C23
26	N	601	CDL	C71-C72-C73-C74
18	A	608	PGV	O12-C04-C05-C06
18	N	610	PGV	O12-C04-C05-C06
18	A	608	PGV	C20-C19-O03-C01
19	A	609	TGL	CC2-CC1-OG3-CG3
26	T	103	CDL	C31-CA7-OA8-CA6
28	G	101	DMU	C3-C4-C57-O61
28	Q	201	DMU	C3-C4-C57-O61
28	G	101	DMU	O1-C10-O7-C3
19	N	607	TGL	CA5-CA6-CA7-CA8
19	N	607	TGL	C13-C14-C29-C30
24	J	101	CHD	C17-C20-C22-C23
26	P	305	CDL	C40-C41-C42-C43
18	A	608	PGV	O12-C04-C05-O05
18	N	610	PGV	O12-C04-C05-O05
26	N	601	CDL	O1-C1-CB2-OB2
26	P	305	CDL	O1-C1-CB2-OB2
28	M	101	DMU	C1-C6-O16-C18
19	N	609	TGL	C19-C33-C34-C35
23	O	302	PSC	C2-C1-O01-C02
19	B	303	TGL	CB1-CB2-CB3-CB4
19	A	609	TGL	OC1-CC1-OG3-CG3
26	T	103	CDL	OA9-CA7-OA8-CA6
24	J	102	CHD	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	CC2-CC1-OG3-CG3
26	P	305	CDL	C31-CA7-OA8-CA6
24	B	304	CHD	C21-C20-C22-C23
24	J	101	CHD	C21-C20-C22-C23
19	N	609	TGL	C20-C21-C22-C23
26	P	305	CDL	C61-C62-C63-C64
26	N	601	CDL	CA5-C11-C12-C13
24	J	102	CHD	C13-C17-C20-C21
18	A	608	PGV	C1-C2-C3-C4
19	B	303	TGL	CA1-CA2-CA3-CA4
23	O	302	PSC	C19-C20-C21-C22
25	G	103	PEK	C1-C2-C3-C4
25	P	302	PEK	C1-C2-C3-C4
25	T	102	PEK	C1-C2-C3-C4
26	C	304	CDL	CA5-C11-C12-C13
26	N	601	CDL	CA7-C31-C32-C33
26	P	305	CDL	CB5-C51-C52-C53
28	T	101	DMU	C3-C4-C57-O61
19	A	609	TGL	CA2-CA1-OG1-CG1
26	P	305	CDL	C42-C43-C44-C45
19	Y	101	TGL	OB1-CB1-OG2-CG2
23	O	302	PSC	O02-C1-O01-C02
24	J	102	CHD	C21-C20-C22-C23
19	Y	101	TGL	CC1-CC2-CC3-CC4
26	C	304	CDL	CB7-C71-C72-C73
19	Y	101	TGL	CB2-CB1-OG2-CG2
18	A	608	PGV	O04-C19-O03-C01
28	T	101	DMU	C2-C3-O7-C10
26	P	305	CDL	CA5-C11-C12-C13
26	T	103	CDL	CB7-C71-C72-C73
28	Q	201	DMU	O16-C18-C19-C22
26	C	304	CDL	O1-C1-CB2-OB2
28	G	101	DMU	C2-C3-O7-C10
28	G	101	DMU	C4-C3-O7-C10
19	L	101	TGL	CC9-C15-C16-C17
26	C	304	CDL	C55-C56-C57-C58
26	N	601	CDL	C22-C23-C24-C25
19	L	101	TGL	CB3-CB4-CB5-CB6
19	N	609	TGL	OC1-CC1-OG3-CG3
26	P	305	CDL	OA9-CA7-OA8-CA6
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
18	N	610	PGV	C03-O11-P-O12
18	N	610	PGV	C04-O12-P-O11
23	O	302	PSC	C03-O11-P-O12
23	O	302	PSC	C04-O12-P-O11
25	C	302	PEK	C03-O11-P-O12
25	P	303	PEK	C03-O11-P-O12
25	T	102	PEK	C03-O11-P-O12
26	C	304	CDL	CA2-OA2-PA1-OA5
26	C	304	CDL	CB3-OB5-PB2-OB2
26	N	601	CDL	CA3-OA5-PA1-OA2
26	P	305	CDL	CA2-OA2-PA1-OA5
26	P	305	CDL	CA3-OA5-PA1-OA2
26	T	103	CDL	CA3-OA5-PA1-OA2
19	N	609	TGL	CC2-CC3-CC4-CC5
18	P	304	PGV	C20-C19-O03-C01
19	N	607	TGL	CC5-CC6-CC7-CC8
26	P	305	CDL	C43-C44-C45-C46
28	Q	201	DMU	O5-C4-C57-O61
24	W	102	CHD	C13-C17-C20-C21
18	A	606	PGV	O12-C04-C05-C06
26	C	304	CDL	CA2-C1-CB2-OB2
26	N	601	CDL	CA2-C1-CB2-OB2
25	G	102	PEK	C22-C21-O03-C01
25	P	302	PEK	C22-C21-O03-C01
19	A	609	TGL	C22-C23-C24-C25
19	N	607	TGL	CB6-CB7-CB8-CB9
19	N	607	TGL	C11-C10-CB9-CB8
25	T	102	PEK	C2-C1-O01-C02
18	N	610	PGV	C14-C15-C16-C17
19	A	609	TGL	CC9-C15-C16-C17
19	A	609	TGL	C18-C19-C33-C34
19	B	303	TGL	CA3-CA4-CA5-CA6
19	B	303	TGL	CB5-CB6-CB7-CB8
19	L	101	TGL	CA3-CA4-CA5-CA6
19	N	607	TGL	CB4-CB5-CB6-CB7
19	N	609	TGL	CC5-CC6-CC7-CC8
19	N	609	TGL	C23-C24-C25-C26
19	Y	101	TGL	CB6-CB7-CB8-CB9
19	Y	101	TGL	C16-C15-CC9-CC8
23	B	302	PSC	C26-C27-C28-C29
25	G	103	PEK	C29-C30-C31-C32
26	C	304	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	C	304	CDL	C71-C72-C73-C74
26	C	304	CDL	C74-C75-C76-C77
26	P	305	CDL	C22-C23-C24-C25
26	P	305	CDL	C73-C74-C75-C76
26	T	103	CDL	C59-C60-C61-C62
19	B	303	TGL	CC2-CC1-OG3-CG3
19	B	303	TGL	C20-C21-C22-C23
19	L	101	TGL	C11-C12-C13-C14
26	C	304	CDL	C15-C16-C17-C18
26	C	304	CDL	C59-C60-C61-C62
26	N	601	CDL	C41-C42-C43-C44
26	N	601	CDL	C58-C59-C60-C61
26	N	601	CDL	C79-C80-C81-C82
26	P	305	CDL	C63-C64-C65-C66
26	T	103	CDL	C78-C79-C80-C81
25	T	102	PEK	O02-C1-O01-C02
19	L	101	TGL	CA2-CA3-CA4-CA5
19	N	607	TGL	C23-C24-C25-C26
19	Y	101	TGL	C21-C22-C23-C24
25	G	102	PEK	C29-C30-C31-C32
26	N	601	CDL	C20-C21-C22-C23
26	N	601	CDL	C23-C24-C25-C26
26	P	305	CDL	C51-C52-C53-C54
26	T	103	CDL	C21-C22-C23-C24
26	T	103	CDL	C41-C42-C43-C44
18	N	608	PGV	C3-C4-C5-C6
18	P	304	PGV	C25-C26-C27-C28
19	B	303	TGL	C13-C14-C29-C30
19	Y	101	TGL	CC3-CC4-CC5-CC6
25	P	303	PEK	C25-C26-C27-C28
25	T	102	PEK	C25-C26-C27-C28
26	N	601	CDL	C16-C17-C18-C19
26	N	601	CDL	C39-C40-C41-C42
26	P	305	CDL	C14-C15-C16-C17
28	T	101	DMU	O6-C11-C9-C8
26	T	103	CDL	O1-C1-CA2-OA2
23	O	302	PSC	C29-C30-C31-C32
25	G	103	PEK	C31-C32-C33-C34
25	P	302	PEK	C25-C26-C27-C28
26	C	304	CDL	C39-C40-C41-C42
26	P	305	CDL	C82-C83-C84-C85
23	B	302	PSC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	P	303	PEK	C1-C2-C3-C4
19	N	607	TGL	C16-C15-CC9-CC8
26	N	601	CDL	C77-C78-C79-C80
26	P	305	CDL	C31-C32-C33-C34
26	T	103	CDL	C20-C21-C22-C23
18	P	304	PGV	O04-C19-O03-C01
18	A	607	PGV	C5-C6-C7-C8
18	N	608	PGV	C25-C26-C27-C28
19	A	609	TGL	C17-C18-C19-C33
19	B	303	TGL	CB7-CB8-CB9-C10
19	N	607	TGL	C20-C21-C22-C23
19	N	609	TGL	C15-C16-C17-C18
25	T	102	PEK	C29-C30-C31-C32
26	C	304	CDL	C20-C21-C22-C23
26	N	601	CDL	C53-C54-C55-C56
28	G	101	DMU	C22-C25-C28-C31
19	N	609	TGL	CB1-CB2-CB3-CB4
18	A	607	PGV	C7-C8-C9-C10
18	C	303	PGV	C7-C8-C9-C10
19	A	609	TGL	C13-C14-C29-C30
19	B	303	TGL	CB9-C10-C11-C12
19	Y	101	TGL	CB9-C10-C11-C12
26	P	305	CDL	C15-C16-C17-C18
19	A	609	TGL	OA1-CA1-OG1-CG1
18	A	606	PGV	C2-C3-C4-C5
18	A	606	PGV	C28-C29-C30-C31
18	P	304	PGV	C24-C25-C26-C27
19	A	609	TGL	C15-C16-C17-C18
19	Y	101	TGL	C22-C23-C24-C25
25	P	302	PEK	C24-C25-C26-C27
18	U	101	PGV	C04-C05-C06-O06
24	J	102	CHD	C16-C17-C20-C21
18	A	606	PGV	C4-C5-C6-C7
18	A	607	PGV	C22-C23-C24-C25
19	A	609	TGL	CC2-CC3-CC4-CC5
23	B	302	PSC	C3-C4-C5-C6
25	T	102	PEK	C16-C17-C18-C19
18	N	610	PGV	C12-C13-C14-C15
18	A	607	PGV	C19-C20-C21-C22
18	P	304	PGV	C1-C2-C3-C4
26	P	305	CDL	CB7-C71-C72-C73
18	A	606	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
18	N	610	PGV	C20-C21-C22-C23
18	U	101	PGV	C29-C30-C31-C32
19	A	609	TGL	CA3-CA4-CA5-CA6
19	A	609	TGL	CA7-CA8-CA9-C20
19	N	607	TGL	CB3-CB4-CB5-CB6
19	N	607	TGL	CC6-CC7-CC8-CC9
19	N	609	TGL	CB4-CB5-CB6-CB7
19	N	609	TGL	CB6-CB7-CB8-CB9
19	N	609	TGL	CC6-CC7-CC8-CC9
19	Y	101	TGL	CA2-CA3-CA4-CA5
19	Y	101	TGL	C13-C14-C29-C30
26	N	601	CDL	C21-C22-C23-C24
26	N	601	CDL	C73-C74-C75-C76
26	P	305	CDL	C23-C24-C25-C26
26	P	305	CDL	C71-C72-C73-C74
26	T	103	CDL	C72-C73-C74-C75
19	B	303	TGL	CA4-CA5-CA6-CA7
19	B	303	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	CB5-CB6-CB7-CB8
19	N	607	TGL	CC7-CC8-CC9-C15
25	C	302	PEK	C25-C26-C27-C28
26	P	305	CDL	C36-C37-C38-C39
26	P	305	CDL	C62-C63-C64-C65
26	T	103	CDL	C76-C77-C78-C79
28	Q	201	DMU	C19-C22-C25-C28
18	C	303	PGV	C22-C23-C24-C25
18	P	304	PGV	C7-C8-C9-C10
19	L	101	TGL	C23-C24-C25-C26
26	C	304	CDL	C14-C15-C16-C17
26	P	305	CDL	C17-C18-C19-C20
26	P	305	CDL	C38-C39-C40-C41
26	P	305	CDL	C41-C42-C43-C44
26	P	305	CDL	C76-C77-C78-C79
28	T	101	DMU	C4-C3-O7-C10
19	L	101	TGL	CB1-CB2-CB3-CB4
18	A	607	PGV	C25-C26-C27-C28
18	N	608	PGV	C6-C7-C8-C9
19	B	303	TGL	CC4-CC5-CC6-CC7
26	N	601	CDL	C42-C43-C44-C45
26	T	103	CDL	C71-CB7-OB8-CB6
18	A	607	PGV	C6-C7-C8-C9
25	G	102	PEK	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	N	601	CDL	C15-C16-C17-C18
19	L	101	TGL	CC7-CC8-CC9-C15
26	C	304	CDL	C80-C81-C82-C83
26	N	601	CDL	C35-C36-C37-C38
26	P	305	CDL	C37-C38-C39-C40
26	P	305	CDL	C72-C73-C74-C75
28	M	101	DMU	C19-C22-C25-C28
25	P	302	PEK	O04-C21-O03-C01
18	A	608	PGV	C29-C30-C31-C32
19	N	609	TGL	CA5-CA6-CA7-CA8
23	B	302	PSC	C29-C30-C31-C32
26	C	304	CDL	C33-C34-C35-C36
19	A	609	TGL	CG1-CG2-CG3-OG3
18	A	607	PGV	C26-C27-C28-C29
18	C	303	PGV	C23-C24-C25-C26
19	A	609	TGL	CA9-C20-C21-C22
26	T	103	CDL	C31-C32-C33-C34
19	L	101	TGL	CC1-CC2-CC3-CC4
18	A	608	PGV	C3-C4-C5-C6
26	T	103	CDL	C35-C36-C37-C38
18	A	608	PGV	C2-C1-O01-C02
19	N	607	TGL	CB2-CB3-CB4-CB5
26	T	103	CDL	C73-C74-C75-C76
18	N	610	PGV	O05-C05-C06-O06
18	U	101	PGV	O05-C05-C06-O06
19	L	101	TGL	C24-C25-C26-C27
19	Y	101	TGL	C24-C25-C26-C27
19	L	101	TGL	CC3-CC4-CC5-CC6
25	P	303	PEK	C28-C29-C30-C31
19	A	609	TGL	C11-C10-CB9-CB8
19	L	101	TGL	C22-C23-C24-C25
26	N	601	CDL	C74-C75-C76-C77
19	B	303	TGL	C23-C24-C25-C26
19	N	607	TGL	C16-C17-C18-C19
19	N	609	TGL	CA6-CA7-CA8-CA9
25	G	103	PEK	C24-C25-C26-C27
26	C	304	CDL	C60-C61-C62-C63
26	C	304	CDL	C76-C77-C78-C79
18	A	608	PGV	O02-C1-O01-C02
19	A	609	TGL	OB1-CB1-OG2-CG2
24	P	301	CHD	C13-C17-C20-C21
25	G	102	PEK	O04-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
19	B	303	TGL	C16-C15-CC9-CC8
19	B	303	TGL	C24-C25-C26-C27
19	N	607	TGL	CC4-CC5-CC6-CC7
25	G	102	PEK	C33-C34-C35-C36
26	N	601	CDL	C32-C33-C34-C35
26	T	103	CDL	C39-C40-C41-C42
18	A	608	PGV	C26-C27-C28-C29
18	A	608	PGV	C27-C28-C29-C30
28	M	101	DMU	O16-C18-C19-C22
19	B	303	TGL	CA2-CA1-OG1-CG1
26	N	601	CDL	C71-CB7-OB8-CB6
19	A	609	TGL	CB2-CB1-OG2-CG2
25	G	102	PEK	C2-C1-O01-C02
19	A	609	TGL	C16-C15-CC9-CC8
26	C	304	CDL	C52-C53-C54-C55
26	P	305	CDL	C58-C59-C60-C61
19	L	101	TGL	C11-C10-CB9-CB8
23	O	302	PSC	C21-C22-C23-C24
25	P	302	PEK	C26-C27-C28-C29
25	P	303	PEK	C24-C25-C26-C27
25	G	103	PEK	C27-C28-C29-C30
19	B	303	TGL	OC1-CC1-OG3-CG3
26	T	103	CDL	OB9-CB7-OB8-CB6
26	N	601	CDL	C82-C83-C84-C85
24	P	301	CHD	C16-C17-C20-C22
23	B	302	PSC	C6-C7-C8-C9
18	A	608	PGV	C22-C23-C24-C25
19	N	607	TGL	C21-C22-C23-C24
25	P	302	PEK	C27-C28-C29-C30
26	P	305	CDL	C21-C22-C23-C24
19	N	609	TGL	CA4-CA5-CA6-CA7
18	A	606	PGV	C30-C31-C32-C33
18	A	607	PGV	C24-C25-C26-C27
25	G	102	PEK	C31-C32-C33-C34
26	N	601	CDL	C54-C55-C56-C57
26	T	103	CDL	C13-C14-C15-C16
24	G	104	CHD	C21-C20-C22-C23
19	N	607	TGL	CC2-CC3-CC4-CC5
19	N	609	TGL	CC7-CC8-CC9-C15
26	C	304	CDL	C17-C18-C19-C20
26	C	304	CDL	C71-CB7-OB8-CB6
18	N	608	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
19	A	609	TGL	C19-C33-C34-C35
19	B	303	TGL	C16-C17-C18-C19
19	L	101	TGL	C16-C17-C18-C19
26	P	305	CDL	C74-C75-C76-C77
18	N	608	PGV	C19-C20-C21-C22
25	G	103	PEK	C2-C1-O01-C02
26	T	103	CDL	C51-CB5-OB6-CB4
18	A	608	PGV	O01-C02-C03-O11
18	N	608	PGV	C13-C14-C15-C16
19	N	609	TGL	CB3-CB4-CB5-CB6
28	G	101	DMU	C19-C22-C25-C28
18	N	608	PGV	C4-C5-C6-C7
25	G	103	PEK	O02-C1-O01-C02
26	T	103	CDL	OB7-CB5-OB6-CB4
19	B	303	TGL	OG1-CG1-CG2-OG2
19	N	609	TGL	C11-C10-CB9-CB8
19	Y	101	TGL	CA9-C20-C21-C22
19	B	303	TGL	CB4-CB5-CB6-CB7
25	T	102	PEK	C27-C28-C29-C30
18	A	606	PGV	C11-C10-C9-C8
25	T	102	PEK	C2-C3-C4-C5
18	A	608	PGV	C6-C7-C8-C9
26	N	601	CDL	C34-C35-C36-C37
25	G	103	PEK	C4-C5-C6-C7
18	N	610	PGV	C3-C4-C5-C6
19	N	607	TGL	C10-C11-C12-C13
19	N	609	TGL	CC4-CC5-CC6-CC7
19	A	609	TGL	CA5-CA6-CA7-CA8
19	Y	101	TGL	C11-C10-CB9-CB8
26	C	304	CDL	C16-C17-C18-C19
26	C	304	CDL	C79-C80-C81-C82
28	G	101	DMU	C18-C19-C22-C25
19	B	303	TGL	OA1-CA1-OG1-CG1
25	G	102	PEK	O02-C1-O01-C02
18	A	608	PGV	C7-C8-C9-C10
19	L	101	TGL	C21-C22-C23-C24
25	P	303	PEK	C23-C24-C25-C26
26	N	601	CDL	C60-C61-C62-C63
18	A	607	PGV	C04-O12-P-O11
18	U	101	PGV	C03-O11-P-O12
23	B	302	PSC	C04-O12-P-O11
26	N	601	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C22-C23-C24-C25
18	N	608	PGV	C7-C8-C9-C10
19	B	303	TGL	C18-C19-C33-C34
26	N	601	CDL	CB5-C51-C52-C53
19	N	609	TGL	C24-C25-C26-C27
26	N	601	CDL	OB9-CB7-OB8-CB6
28	M	101	DMU	C18-C19-C22-C25
18	N	610	PGV	C01-C02-C03-O11
26	N	601	CDL	OB5-CB3-CB4-CB6
26	P	305	CDL	C34-C35-C36-C37
19	N	609	TGL	CA1-CA2-CA3-CA4
26	C	304	CDL	C63-C64-C65-C66
19	B	303	TGL	C12-C13-C14-C29
19	B	303	TGL	C19-C33-C34-C35
25	T	102	PEK	C22-C23-C24-C25
18	A	606	PGV	C25-C26-C27-C28
19	B	303	TGL	CC6-CC7-CC8-CC9
18	A	606	PGV	C19-C20-C21-C22
18	A	608	PGV	C2-C3-C4-C5
18	C	303	PGV	C28-C29-C30-C31
25	T	102	PEK	C33-C34-C35-C36
26	T	103	CDL	C82-C83-C84-C85
18	A	607	PGV	C30-C31-C32-C33
19	L	101	TGL	C18-C19-C33-C34
26	T	103	CDL	C38-C39-C40-C41
26	T	103	CDL	C56-C57-C58-C59
18	A	606	PGV	O03-C01-C02-C03
18	N	610	PGV	O03-C01-C02-C03
19	A	609	TGL	OG1-CG1-CG2-CG3
25	P	302	PEK	O03-C01-C02-C03
26	C	304	CDL	CB3-CB4-CB6-OB8
18	A	608	PGV	C30-C31-C32-C33
18	N	610	PGV	C6-C7-C8-C9
19	L	101	TGL	C29-C30-C31-C32
19	L	101	TGL	C21-C20-CA9-CA8
19	N	607	TGL	C15-C16-C17-C18
23	O	302	PSC	C15-C16-C17-C18
25	P	303	PEK	C29-C30-C31-C32
26	T	103	CDL	C44-C45-C46-C47
18	U	101	PGV	C15-C16-C17-C18
23	B	302	PSC	C15-C16-C17-C18
23	B	302	PSC	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	T	103	CDL	C34-C35-C36-C37
18	A	608	PGV	C14-C15-C16-C17
19	B	303	TGL	CC2-CC3-CC4-CC5
28	T	101	DMU	C34-C37-C40-C43
18	N	610	PGV	C31-C32-C33-C34
25	G	102	PEK	C27-C28-C29-C30
26	N	601	CDL	C55-C56-C57-C58
25	C	302	PEK	C28-C29-C30-C31
25	T	102	PEK	C35-C36-C37-C38
26	N	601	CDL	C13-C14-C15-C16
26	C	304	CDL	C84-C85-C86-C87
19	B	303	TGL	C29-C30-C31-C32
25	T	102	PEK	C31-C32-C33-C34
18	A	608	PGV	C20-C21-C22-C23
19	Y	101	TGL	C25-C26-C27-C28
25	C	302	PEK	C16-C17-C18-C19
19	B	303	TGL	CA7-CA8-CA9-C20
23	O	302	PSC	C2-C3-C4-C5
26	N	601	CDL	C24-C25-C26-C27
25	P	303	PEK	C22-C21-O03-C01
26	T	103	CDL	C37-C38-C39-C40
28	M	101	DMU	C34-C37-C40-C43
25	P	303	PEK	O04-C21-O03-C01
18	N	608	PGV	C15-C16-C17-C18
23	O	302	PSC	C31-C32-C33-C34
25	T	102	PEK	O03-C01-C02-O01
26	N	601	CDL	OB6-CB4-CB6-OB8
26	T	103	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	C12-C13-C14-C29
23	O	302	PSC	C14-C15-C16-C17
26	N	601	CDL	C59-C60-C61-C62
26	T	103	CDL	C54-C55-C56-C57
26	C	304	CDL	OB9-CB7-OB8-CB6
18	P	304	PGV	C27-C28-C29-C30
19	N	609	TGL	C25-C26-C27-C28
26	N	601	CDL	C56-C57-C58-C59
26	T	103	CDL	C11-C12-C13-C14
28	M	101	DMU	C28-C31-C34-C37
18	P	304	PGV	C13-C14-C15-C16
19	N	609	TGL	CB2-CB3-CB4-CB5
26	N	601	CDL	C33-C34-C35-C36
26	P	305	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
19	N	607	TGL	C12-C13-C14-C29
23	B	302	PSC	C31-C32-C33-C34
26	C	304	CDL	C81-C82-C83-C84
26	N	601	CDL	C31-C32-C33-C34
18	U	101	PGV	C30-C31-C32-C33
26	C	304	CDL	C64-C65-C66-C67
18	A	608	PGV	C01-C02-C03-O11
18	U	101	PGV	C01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-CB6
25	C	302	PEK	C29-C30-C31-C32
26	T	103	CDL	C77-C78-C79-C80
26	T	103	CDL	O1-C1-CB2-OB2
19	L	101	TGL	CB2-CB3-CB4-CB5
19	A	609	TGL	C10-C11-C12-C13
19	B	303	TGL	C10-C11-C12-C13
25	C	302	PEK	C35-C36-C37-C38
18	U	101	PGV	C02-C03-O11-P
26	T	103	CDL	CB4-CB3-OB5-PB2
18	U	101	PGV	C23-C24-C25-C26
23	O	302	PSC	C27-C28-C29-C30
25	G	103	PEK	C33-C34-C35-C36
19	N	609	TGL	CA7-CA8-CA9-C20
19	B	303	TGL	OG1-CG1-CG2-CG3
23	B	302	PSC	O03-C01-C02-C03
23	O	302	PSC	O03-C01-C02-C03
25	C	302	PEK	O03-C01-C02-C03
25	G	102	PEK	O03-C01-C02-C03
18	N	610	PGV	C30-C31-C32-C33
18	C	303	PGV	C1-C2-C3-C4
19	L	101	TGL	CA9-C20-C21-C22
26	P	305	CDL	C54-C55-C56-C57
28	T	101	DMU	O6-C11-C9-O1
23	O	302	PSC	C9-C10-C11-C12
25	C	302	PEK	C6-C7-C8-C9
25	G	103	PEK	C6-C7-C8-C9
25	P	302	PEK	C11-C10-C9-C8
25	P	303	PEK	C6-C7-C8-C9
25	P	303	PEK	C11-C12-C13-C14
25	T	102	PEK	C6-C7-C8-C9
26	P	305	CDL	CB3-OB5-PB2-OB2
26	T	103	CDL	CA2-OA2-PA1-OA5
18	N	610	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	CB6-CB7-CB8-CB9
26	N	601	CDL	C11-C12-C13-C14
25	C	302	PEK	O01-C02-C03-O11
25	T	102	PEK	O01-C02-C03-O11
26	C	304	CDL	C35-C36-C37-C38
19	A	609	TGL	CC7-CC8-CC9-C15
19	L	101	TGL	CA4-CA5-CA6-CA7
19	N	607	TGL	OG2-CG2-CG3-OG3
25	C	302	PEK	O03-C01-C02-O01
26	P	305	CDL	OB6-CB4-CB6-OB8
18	N	608	PGV	O03-C19-C20-C21
26	P	305	CDL	C52-C51-CB5-OB6
19	B	303	TGL	C25-C26-C27-C28
25	T	102	PEK	C30-C31-C32-C33
26	T	103	CDL	CA2-C1-CB2-OB2
18	U	101	PGV	C31-C32-C33-C34
25	C	302	PEK	C34-C35-C36-C37
19	N	607	TGL	C18-C19-C33-C34
19	B	303	TGL	CA6-CA7-CA8-CA9
19	Y	101	TGL	C16-C17-C18-C19
18	N	610	PGV	C02-C03-O11-P
23	O	302	PSC	C02-C03-O11-P
23	B	302	PSC	C13-C14-C15-C16
25	T	102	PEK	C26-C27-C28-C29
26	T	103	CDL	C24-C25-C26-C27
26	T	103	CDL	C64-C65-C66-C67
26	C	304	CDL	C44-C45-C46-C47
26	P	305	CDL	C11-C12-C13-C14
19	Y	101	TGL	CB1-CB2-CB3-CB4
19	A	609	TGL	C33-C34-C35-C36
25	P	302	PEK	C22-C23-C24-C25
25	T	102	PEK	C01-C02-C03-O11
26	P	305	CDL	C59-C60-C61-C62
19	A	609	TGL	C21-C20-CA9-CA8
19	B	303	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	CC4-CC5-CC6-CC7
19	N	609	TGL	CG1-CG2-OG2-CB1
28	Q	201	DMU	C25-C28-C31-C34
18	C	303	PGV	C30-C31-C32-C33
18	U	101	PGV	C7-C8-C9-C10
25	P	303	PEK	C35-C36-C37-C38
18	N	610	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
19	N	607	TGL	CG1-CG2-CG3-OG3
25	T	102	PEK	O03-C01-C02-C03
26	P	305	CDL	CB3-CB4-CB6-OB8
18	N	610	PGV	O01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-OB6
19	L	101	TGL	C10-C11-C12-C13
25	G	102	PEK	C34-C35-C36-C37
26	C	304	CDL	C12-C13-C14-C15
26	C	304	CDL	C83-C84-C85-C86
19	B	303	TGL	OB1-CB1-OG2-CG2
19	N	609	TGL	OB1-CB1-OG2-CG2
19	A	609	TGL	CA2-CA3-CA4-CA5
26	C	304	CDL	C73-C74-C75-C76
26	P	305	CDL	C18-C19-C20-C21
19	N	609	TGL	CA3-CA4-CA5-CA6
18	A	606	PGV	O03-C01-C02-O01
23	O	302	PSC	O03-C01-C02-O01
25	G	102	PEK	O03-C01-C02-O01
26	N	601	CDL	C18-C19-C20-C21
19	N	609	TGL	CB2-CB1-OG2-CG2
25	G	103	PEK	C35-C36-C37-C38
26	N	601	CDL	C64-C65-C66-C67
28	M	101	DMU	C22-C25-C28-C31
18	C	303	PGV	C14-C15-C16-C17
18	A	608	PGV	C13-C14-C15-C16
23	B	302	PSC	C2-C3-C4-C5
19	L	101	TGL	CC2-CC3-CC4-CC5
18	P	304	PGV	C31-C32-C33-C34
19	N	609	TGL	C11-C12-C13-C14
25	G	102	PEK	C28-C29-C30-C31
25	G	103	PEK	C03-O11-P-O12
18	A	606	PGV	C05-C04-O12-P
18	C	303	PGV	C02-C03-O11-P
26	C	304	CDL	C42-C43-C44-C45
26	C	304	CDL	C75-C76-C77-C78
18	A	606	PGV	C03-O11-P-O14
18	N	610	PGV	C03-O11-P-O14
18	N	610	PGV	C04-O12-P-O13
18	U	101	PGV	C03-O11-P-O14
23	B	302	PSC	C04-O12-P-O14
23	O	302	PSC	C04-O12-P-O13
25	G	103	PEK	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
25	T	102	PEK	C03-O11-P-O14
25	T	102	PEK	C04-O12-P-O13
26	C	304	CDL	CA2-OA2-PA1-OA4
26	C	304	CDL	CB3-OB5-PB2-OB4
26	N	601	CDL	CA3-OA5-PA1-OA4
26	P	305	CDL	CA3-OA5-PA1-OA4
19	N	607	TGL	CC3-CC4-CC5-CC6
26	N	601	CDL	C75-C76-C77-C78
24	P	301	CHD	C16-C17-C20-C21
26	N	601	CDL	C62-C63-C64-C65
26	T	103	CDL	C43-C44-C45-C46
18	U	101	PGV	C24-C25-C26-C27
23	O	302	PSC	C05-C04-O12-P
19	N	609	TGL	C14-C29-C30-C31
19	L	101	TGL	CC6-CC7-CC8-CC9
19	N	609	TGL	C33-C34-C35-C36
18	N	610	PGV	C11-C10-C9-C8
18	N	610	PGV	C2-C3-C4-C5
18	U	101	PGV	O12-C04-C05-C06
18	A	607	PGV	C23-C24-C25-C26
19	B	303	TGL	C11-C12-C13-C14
26	C	304	CDL	OA5-CA3-CA4-OA6
26	P	305	CDL	OB5-CB3-CB4-OB6
26	T	103	CDL	C57-C58-C59-C60
25	P	303	PEK	C30-C31-C32-C33
26	C	304	CDL	C36-C37-C38-C39
25	P	302	PEK	C33-C34-C35-C36
19	L	101	TGL	CA7-CA8-CA9-C20
19	L	101	TGL	CG1-CG2-CG3-OG3
19	N	607	TGL	OG1-CG1-CG2-CG3
25	P	302	PEK	C16-C17-C18-C19
26	N	601	CDL	CB3-CB4-CB6-OB8
26	T	103	CDL	CB3-CB4-CB6-OB8
18	N	610	PGV	O03-C01-C02-O01
19	N	609	TGL	OG2-CG2-CG3-OG3
25	P	302	PEK	O03-C01-C02-O01
26	C	304	CDL	OB6-CB4-CB6-OB8
19	Y	101	TGL	C21-C20-CA9-CA8
19	Y	101	TGL	CB2-CB3-CB4-CB5
19	A	609	TGL	C24-C25-C26-C27
18	N	610	PGV	C26-C27-C28-C29
18	P	304	PGV	C02-C03-O11-P

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	C16-C15-CC9-CC8
19	A	609	TGL	C14-C29-C30-C31
19	B	303	TGL	C21-C20-CA9-CA8
28	Q	201	DMU	C34-C37-C40-C43
23	B	302	PSC	C28-C29-C30-C31
19	N	609	TGL	C29-C30-C31-C32
25	C	302	PEK	C10-C11-C12-C13
25	P	302	PEK	C10-C11-C12-C13
26	P	305	CDL	C35-C36-C37-C38
26	P	305	CDL	C13-C14-C15-C16
26	P	305	CDL	C24-C25-C26-C27
18	N	610	PGV	C03-C02-O01-C1
19	A	609	TGL	CG1-CG2-OG2-CB1
18	A	607	PGV	O03-C19-C20-C21
19	L	101	TGL	C33-C34-C35-C36
18	U	101	PGV	C3-C4-C5-C6
23	O	302	PSC	C3-C4-C5-C6
26	N	601	CDL	OB5-CB3-CB4-OB6
23	B	302	PSC	O03-C01-C02-O01
18	A	608	PGV	C04-O12-P-O11
18	U	101	PGV	C04-O12-P-O11
23	B	302	PSC	C03-O11-P-O12
26	N	601	CDL	CB2-OB2-PB2-OB5
19	N	609	TGL	C13-C14-C29-C30
28	M	101	DMU	C25-C28-C31-C34
18	N	608	PGV	C31-C32-C33-C34
26	P	305	CDL	C33-C34-C35-C36
18	U	101	PGV	C25-C26-C27-C28
18	A	606	PGV	C27-C28-C29-C30
19	N	607	TGL	C22-C23-C24-C25
26	T	103	CDL	C1-CA2-OA2-PA1
19	Y	101	TGL	C15-C16-C17-C18
23	O	302	PSC	C4-C5-C6-C7
18	N	610	PGV	C11-C12-C13-C14
19	N	607	TGL	C33-C34-C35-C36
18	U	101	PGV	C11-C10-C9-C8
23	O	302	PSC	C13-C14-C15-C16
17	N	605	HEA	CAA-CBA-CGA-O1A
19	B	303	TGL	CC7-CC8-CC9-C15
19	A	609	TGL	OG3-CC1-CC2-CC3
19	B	303	TGL	CA9-C20-C21-C22
23	B	302	PSC	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	C	302	PEK	C01-C02-C03-O11
26	P	305	CDL	OB5-CB3-CB4-CB6
26	C	304	CDL	C41-C42-C43-C44
17	A	605	HEA	CAD-CBD-CGD-O2D
26	P	305	CDL	C20-C21-C22-C23
19	A	609	TGL	CC1-CC2-CC3-CC4
24	B	304	CHD	C22-C23-C24-O26
24	G	104	CHD	C22-C23-C24-O26
25	G	102	PEK	C2-C3-C4-C5
23	O	302	PSC	C24-C25-C26-C27
24	W	102	CHD	C22-C23-C24-O26
26	C	304	CDL	CA4-CA3-OA5-PA1
24	W	102	CHD	C22-C23-C24-O25
23	O	302	PSC	C12-C13-C14-C15
26	T	103	CDL	C75-C76-C77-C78
25	C	302	PEK	C24-C25-C26-C27
25	P	303	PEK	C22-C23-C24-C25
25	C	302	PEK	C33-C34-C35-C36
26	P	305	CDL	C56-C57-C58-C59
25	P	302	PEK	C34-C35-C36-C37
17	A	605	HEA	CAA-CBA-CGA-O1A
19	N	609	TGL	C21-C20-CA9-CA8
19	Y	101	TGL	CC5-CC6-CC7-CC8
17	N	606	HEA	CAA-CBA-CGA-O1A
26	P	305	CDL	C19-C20-C21-C22
25	P	302	PEK	C15-C16-C17-C18
17	A	605	HEA	CAA-CBA-CGA-O2A
17	N	605	HEA	CAA-CBA-CGA-O2A
18	A	606	PGV	C03-C02-O01-C1
23	B	302	PSC	C01-C02-O01-C1
23	O	302	PSC	C03-C02-O01-C1
26	C	304	CDL	CA3-CA4-OA6-CA5
26	C	304	CDL	CA6-CA4-OA6-CA5
26	P	305	CDL	CA3-CA4-OA6-CA5
18	P	304	PGV	C9-C10-C11-C12
23	O	302	PSC	C7-C8-C9-C10
18	U	101	PGV	C1-C2-C3-C4
26	P	305	CDL	C60-C61-C62-C63
23	B	302	PSC	C10-C11-C12-C13
25	C	302	PEK	C11-C12-C13-C14
25	G	103	PEK	C11-C10-C9-C8
25	P	302	PEK	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	T	102	PEK	C12-C13-C14-C15
17	N	606	HEA	CAA-CBA-CGA-O2A
17	N	606	HEA	CAD-CBD-CGD-O2D
19	N	609	TGL	CC9-C15-C16-C17
18	N	608	PGV	C2-C3-C4-C5
28	G	101	DMU	C25-C28-C31-C34
19	B	303	TGL	CC1-CC2-CC3-CC4
17	N	606	HEA	CAD-CBD-CGD-O1D
24	G	104	CHD	C22-C23-C24-O25
19	N	607	TGL	CB1-CB2-CB3-CB4
26	C	304	CDL	OB7-CB5-OB6-CB4
26	P	305	CDL	C39-C40-C41-C42
25	G	102	PEK	C16-C17-C18-C19
25	G	102	PEK	C17-C18-C19-C20
25	G	103	PEK	O03-C01-C02-O01
25	P	302	PEK	C21-C22-C23-C24
19	N	607	TGL	CB9-C10-C11-C12
18	A	607	PGV	C4-C5-C6-C7
18	U	101	PGV	C20-C21-C22-C23
25	T	102	PEK	C24-C25-C26-C27
24	B	304	CHD	C22-C23-C24-O25
18	C	303	PGV	C21-C22-C23-C24
24	J	102	CHD	C16-C17-C20-C22
18	U	101	PGV	C22-C23-C24-C25
25	G	103	PEK	C16-C17-C18-C19
26	T	103	CDL	C79-C80-C81-C82
25	G	102	PEK	C21-C22-C23-C24
18	U	101	PGV	C4-C5-C6-C7
19	N	607	TGL	C24-C25-C26-C27
26	T	103	CDL	C58-C59-C60-C61
18	A	608	PGV	C31-C32-C33-C34
26	T	103	CDL	CA5-C11-C12-C13
26	C	304	CDL	OA5-CA3-CA4-CA6
19	Y	101	TGL	CB7-CB8-CB9-C10
26	P	305	CDL	C52-C53-C54-C55
18	A	606	PGV	O01-C1-C2-C3
19	A	609	TGL	CB2-CB3-CB4-CB5
17	A	605	HEA	CAD-CBD-CGD-O1D
18	N	608	PGV	C11-C10-C9-C8
26	T	103	CDL	C60-C61-C62-C63
19	N	609	TGL	CA2-CA3-CA4-CA5
26	T	103	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	OG3-CC1-CC2-CC3
19	Y	101	TGL	CC7-CC8-CC9-C15
17	N	606	HEA	C26-C15-C16-C17
26	T	103	CDL	C84-C85-C86-C87
25	G	102	PEK	O01-C1-C2-C3
26	T	103	CDL	C32-C31-CA7-OA8
19	Y	101	TGL	C12-C13-C14-C29
18	A	606	PGV	C7-C8-C9-C10
17	A	604	HEA	CAD-CBD-CGD-O1D
18	P	304	PGV	C28-C29-C30-C31
18	C	303	PGV	C11-C12-C13-C14
18	N	608	PGV	C9-C10-C11-C12
18	P	304	PGV	C11-C12-C13-C14
25	C	302	PEK	C3-C4-C5-C6
25	P	302	PEK	C3-C4-C5-C6
17	A	604	HEA	CAA-CBA-CGA-O1A
26	P	305	CDL	CA6-CA4-OA6-CA5
25	P	302	PEK	O01-C1-C2-C3
19	A	609	TGL	C16-C17-C18-C19
19	Y	101	TGL	OG3-CC1-CC2-CC3
26	C	304	CDL	C37-C38-C39-C40
18	N	608	PGV	C11-C12-C13-C14
25	G	103	PEK	C3-C4-C5-C6
25	T	102	PEK	C3-C4-C5-C6
17	N	605	HEA	C12-C11-C3B-C2B
19	Y	101	TGL	CB4-CB5-CB6-CB7
26	P	305	CDL	OA5-CA3-CA4-OA6
24	J	101	CHD	C22-C23-C24-O26
18	A	608	PGV	C23-C24-C25-C26
25	P	303	PEK	C33-C34-C35-C36
24	J	101	CHD	C22-C23-C24-O25
26	P	305	CDL	C52-C51-CB5-OB7
26	P	305	CDL	OA5-CA3-CA4-CA6
17	A	604	HEA	CAD-CBD-CGD-O2D
18	C	303	PGV	O03-C19-C20-C21
18	A	607	PGV	C15-C16-C17-C18
26	C	304	CDL	C54-C55-C56-C57
26	N	601	CDL	OB7-CB5-OB6-CB4
23	B	302	PSC	C14-C15-C16-C17
26	T	103	CDL	C74-C75-C76-C77
28	Q	201	DMU	C31-C34-C37-C40
19	L	101	TGL	C14-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	T	101	DMU	C25-C28-C31-C34
18	C	303	PGV	C9-C10-C11-C12
25	G	102	PEK	C14-C15-C16-C17
25	G	103	PEK	O03-C21-C22-C23
26	C	304	CDL	C51-CB5-OB6-CB4
18	P	304	PGV	C14-C15-C16-C17
19	N	609	TGL	OG1-CA1-CA2-CA3
17	A	604	HEA	CAA-CBA-CGA-O2A
19	A	609	TGL	CA6-CA7-CA8-CA9
19	Y	101	TGL	OC1-CC1-CC2-CC3
25	G	102	PEK	O02-C1-C2-C3
19	N	609	TGL	OC1-CC1-CC2-CC3
25	P	302	PEK	O02-C1-C2-C3
18	A	607	PGV	C9-C10-C11-C12
25	P	303	PEK	C3-C4-C5-C6
18	A	606	PGV	O02-C1-C2-C3
18	C	303	PGV	O04-C19-C20-C21
19	Y	101	TGL	CG1-CG2-CG3-OG3
26	N	601	CDL	C32-C31-CA7-OA8
26	N	601	CDL	C72-C73-C74-C75
26	T	103	CDL	C32-C31-CA7-OA9
25	G	103	PEK	C25-C26-C27-C28
19	A	609	TGL	OG2-CB1-CB2-CB3
25	G	103	PEK	O04-C21-C22-C23
23	B	302	PSC	C23-C24-C25-C26
26	T	103	CDL	C52-C53-C54-C55
18	A	607	PGV	C04-O12-P-O14
18	A	608	PGV	C03-O11-P-O13
18	U	101	PGV	C04-O12-P-O13
25	C	302	PEK	C04-O12-P-O13
26	P	305	CDL	CA3-OA5-PA1-OA3
26	T	103	CDL	CB2-OB2-PB2-OB4
26	C	304	CDL	OB5-CB3-CB4-CB6
25	C	302	PEK	O01-C1-C2-C3
19	A	609	TGL	CB6-CB7-CB8-CB9
19	Y	101	TGL	CA5-CA6-CA7-CA8
19	A	609	TGL	C23-C24-C25-C26
26	N	601	CDL	C52-C51-CB5-OB6
17	A	605	HEA	C26-C15-C16-C17
23	B	302	PSC	C05-C04-O12-P
19	A	609	TGL	C20-C21-C22-C23
19	Y	101	TGL	CC4-CC5-CC6-CC7

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Mol	Chain	Res	Type	Atoms
25	P	303	PEK	O01-C1-C2-C3
18	U	101	PGV	C28-C29-C30-C31
19	N	607	TGL	OG2-CB1-CB2-CB3
19	N	607	TGL	OG3-CC1-CC2-CC3
25	G	102	PEK	C02-C03-O11-P
18	N	610	PGV	O01-C1-C2-C3
19	L	101	TGL	OG3-CC1-CC2-CC3
23	B	302	PSC	O03-C19-C20-C21
25	C	302	PEK	O03-C21-C22-C23
24	W	101	CHD	C22-C23-C24-O25
23	B	302	PSC	C27-C28-C29-C30
19	N	607	TGL	CA6-CA7-CA8-CA9
23	O	302	PSC	C23-C24-C25-C26
26	P	305	CDL	C44-C45-C46-C47
18	A	606	PGV	C29-C30-C31-C32
17	N	605	HEA	CAD-CBD-CGD-O1D
24	W	101	CHD	C22-C23-C24-O26

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	J	101	CHD	C1-C10-C2-C3-C4-C5
24	W	101	CHD	C1-C10-C2-C3-C4-C5

31 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	609	TGL	7	0
17	A	605	HEA	1	0
25	T	102	PEK	2	0
17	N	606	HEA	4	0
24	J	101	CHD	2	0
24	P	301	CHD	1	0
18	A	608	PGV	2	0
23	O	302	PSC	3	0
24	J	102	CHD	2	0
25	P	302	PEK	2	0
26	T	103	CDL	1	0
19	N	607	TGL	13	0
19	B	303	TGL	10	0
19	L	101	TGL	12	0
18	N	610	PGV	1	0

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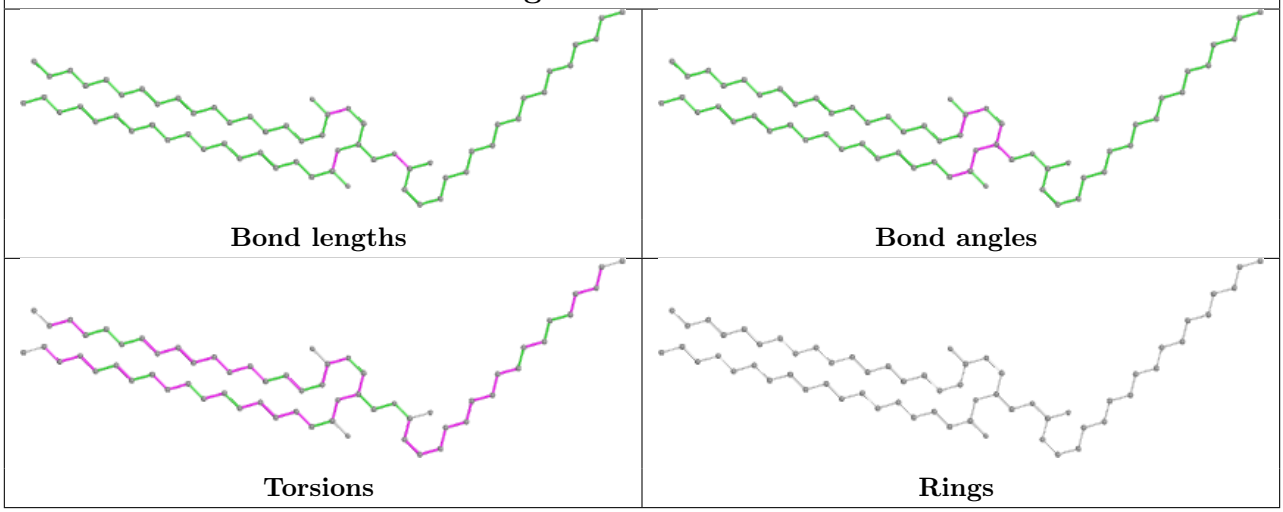
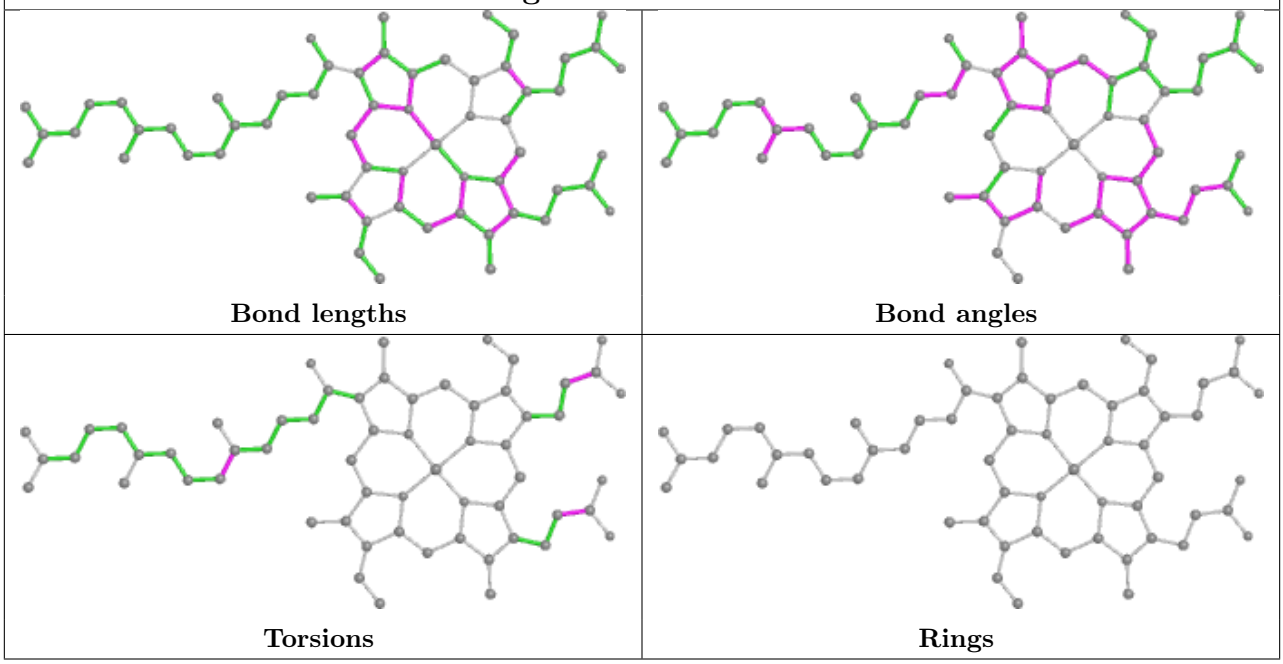
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	606	PGV	3	0
19	A	609	TGL	1	0
26	P	305	CDL	9	0
17	A	604	HEA	1	0
28	M	101	DMU	2	0
25	C	302	PEK	3	0
26	N	601	CDL	23	0
26	C	304	CDL	14	0
25	G	102	PEK	1	0
25	G	103	PEK	1	0
24	C	301	CHD	1	0
23	B	302	PSC	6	0
19	Y	101	TGL	2	0
17	N	605	HEA	5	0
24	W	102	CHD	2	0
28	G	101	DMU	3	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.

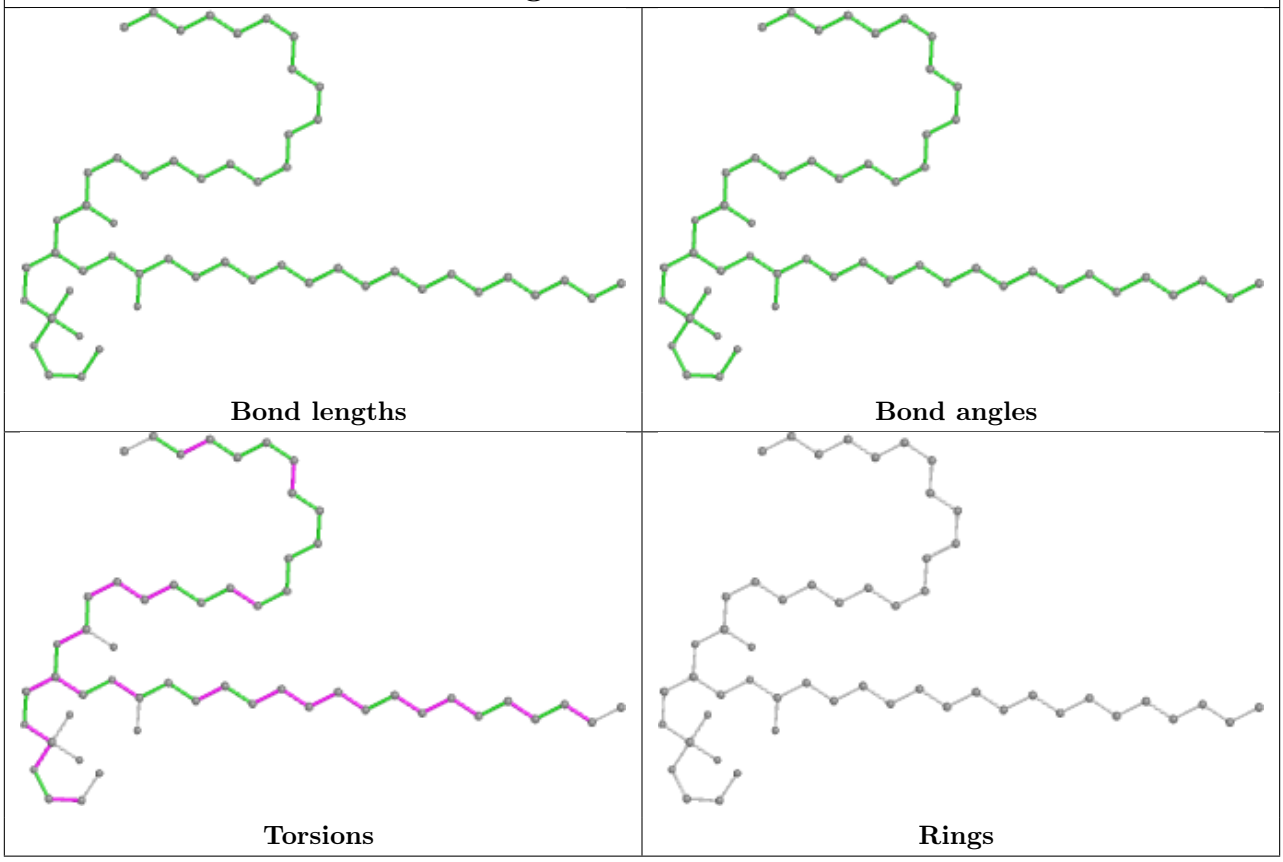
Ligand TGL N 609



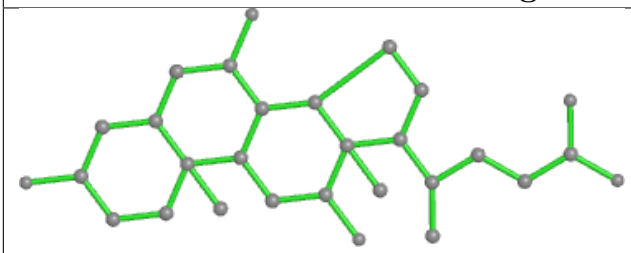
Ligand HEA A 605



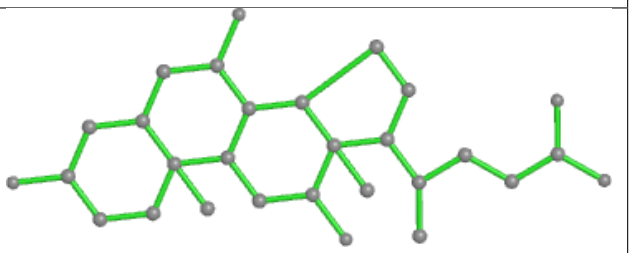
Ligand PEK T 102



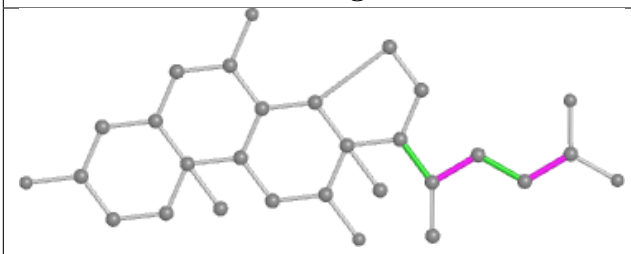
Ligand CHD G 104



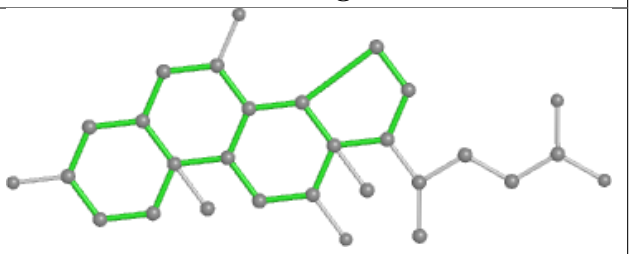
Bond lengths



Bond angles

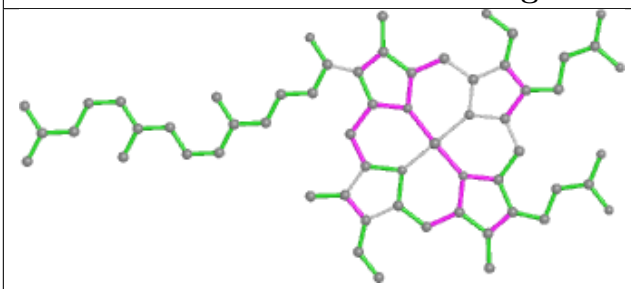


Torsions

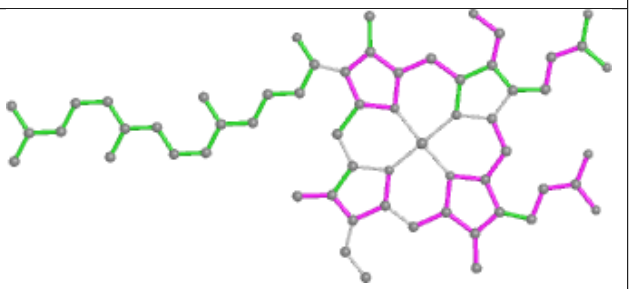


Rings

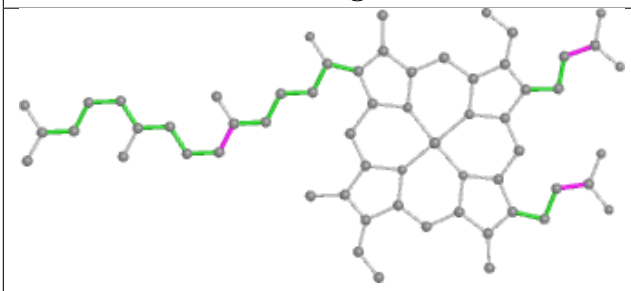
Ligand HEA N 606



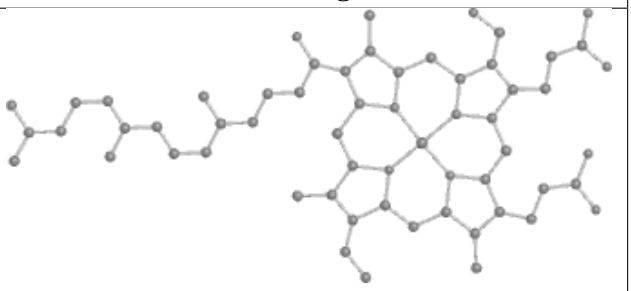
Bond lengths



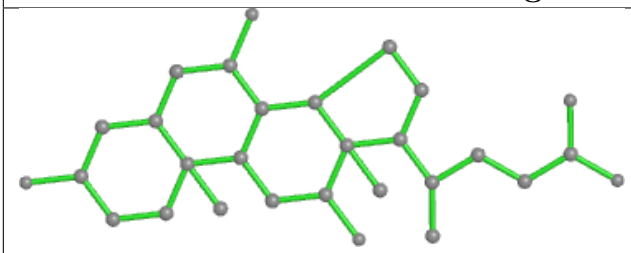
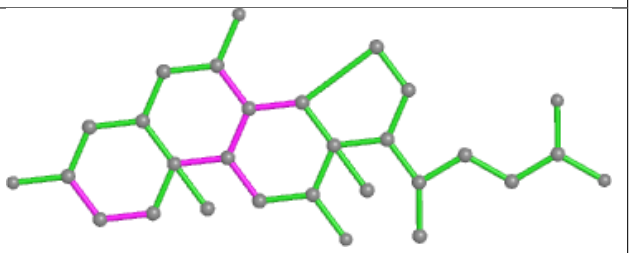
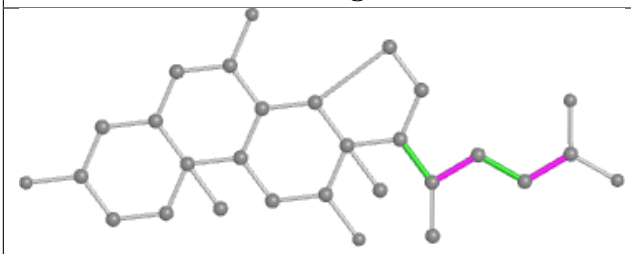
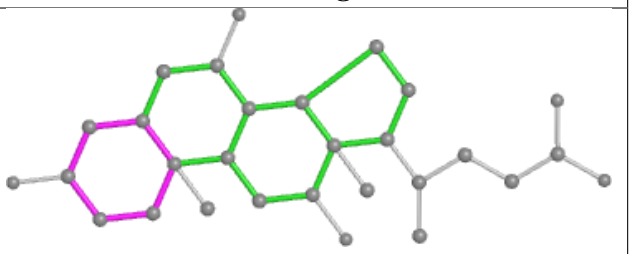
Bond angles

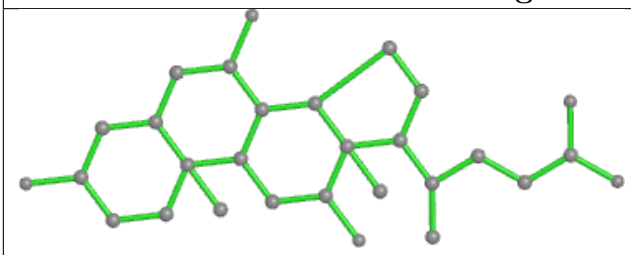
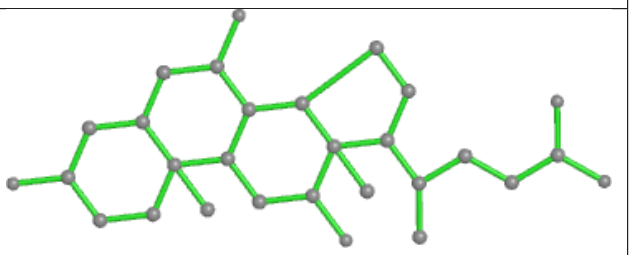
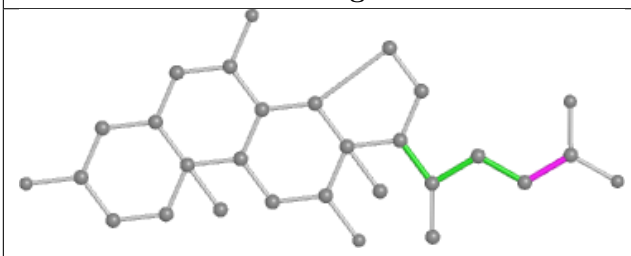
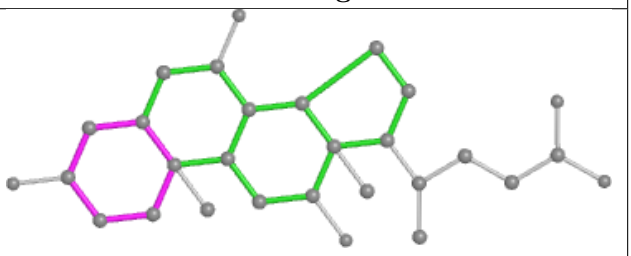


Torsions

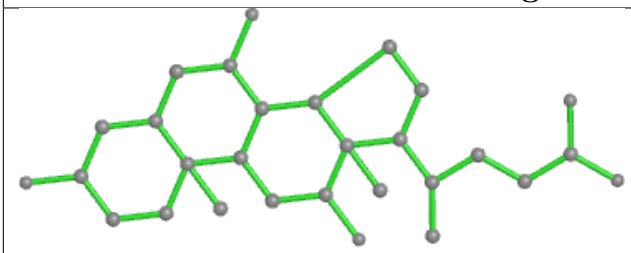


Rings

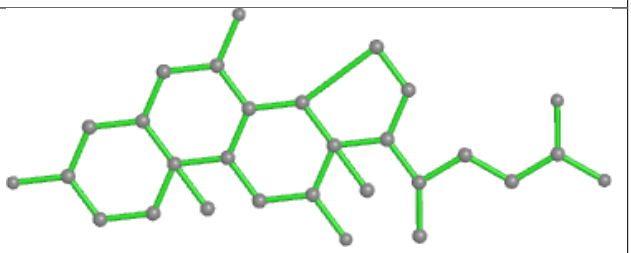
Ligand CHD J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD W 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

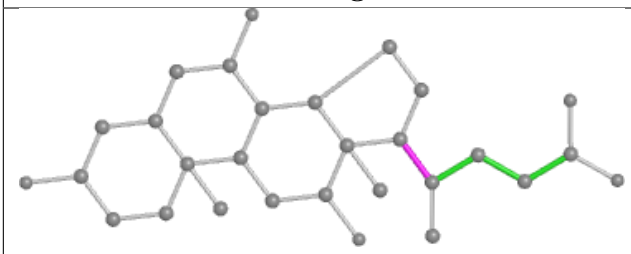
Ligand CHD P 301



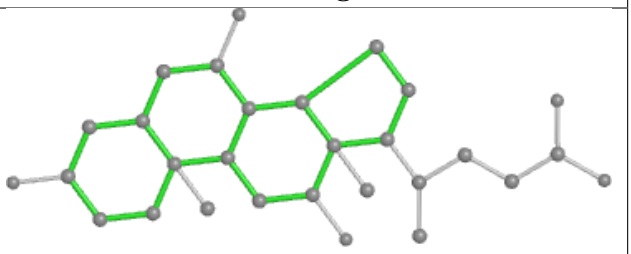
Bond lengths



Bond angles

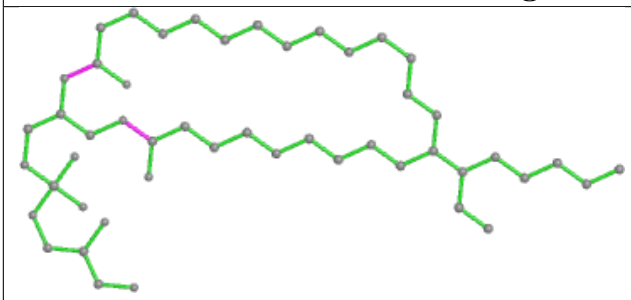


Torsions

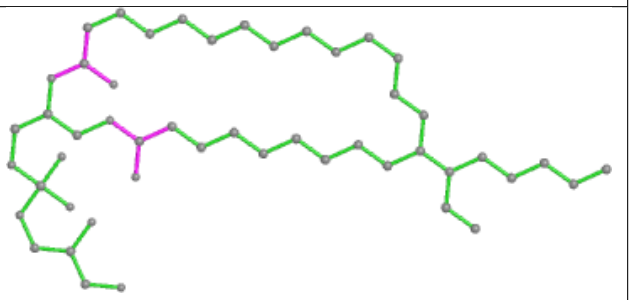


Rings

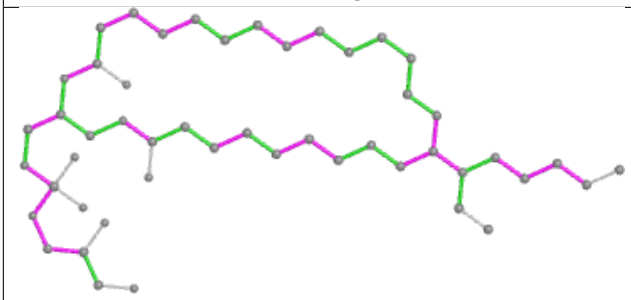
Ligand PGV A 608



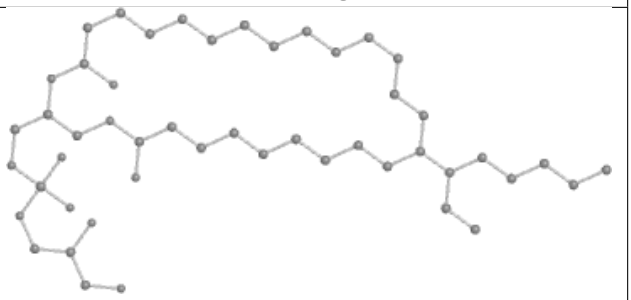
Bond lengths



Bond angles

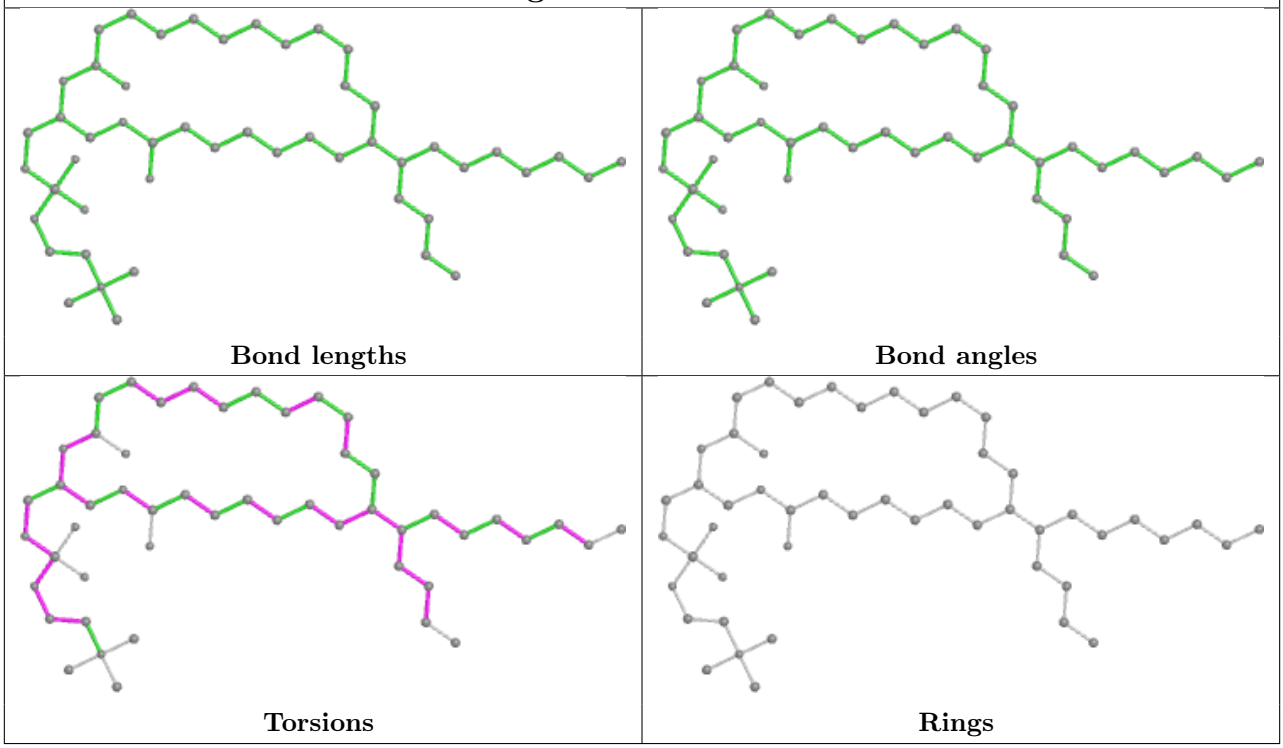


Torsions

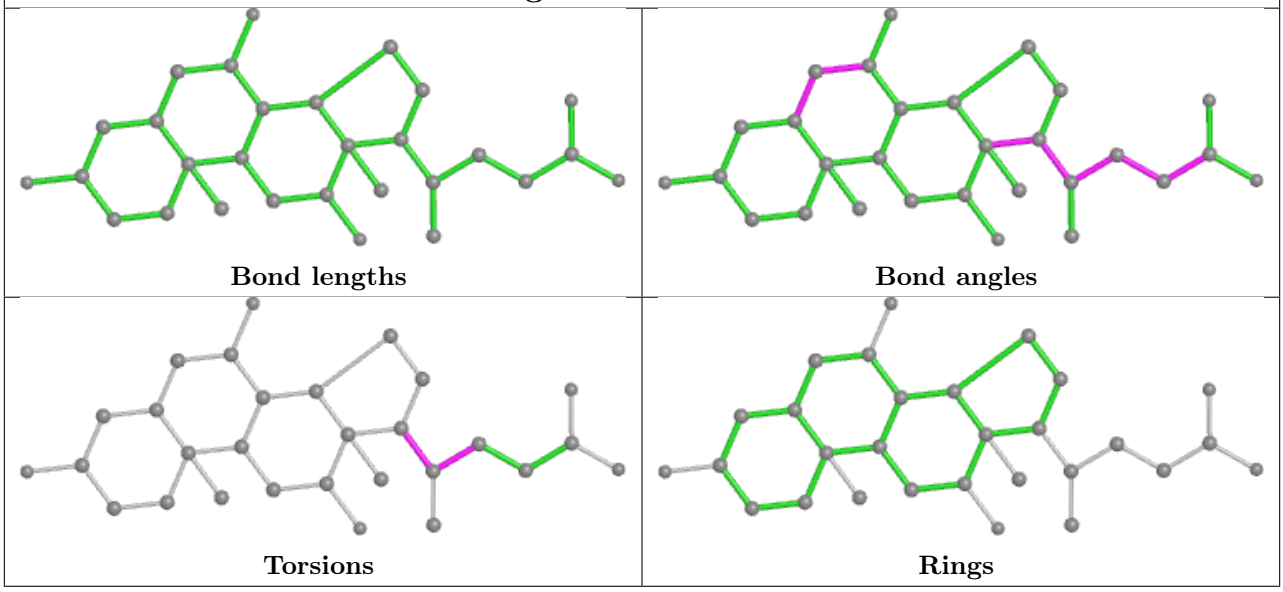


Rings

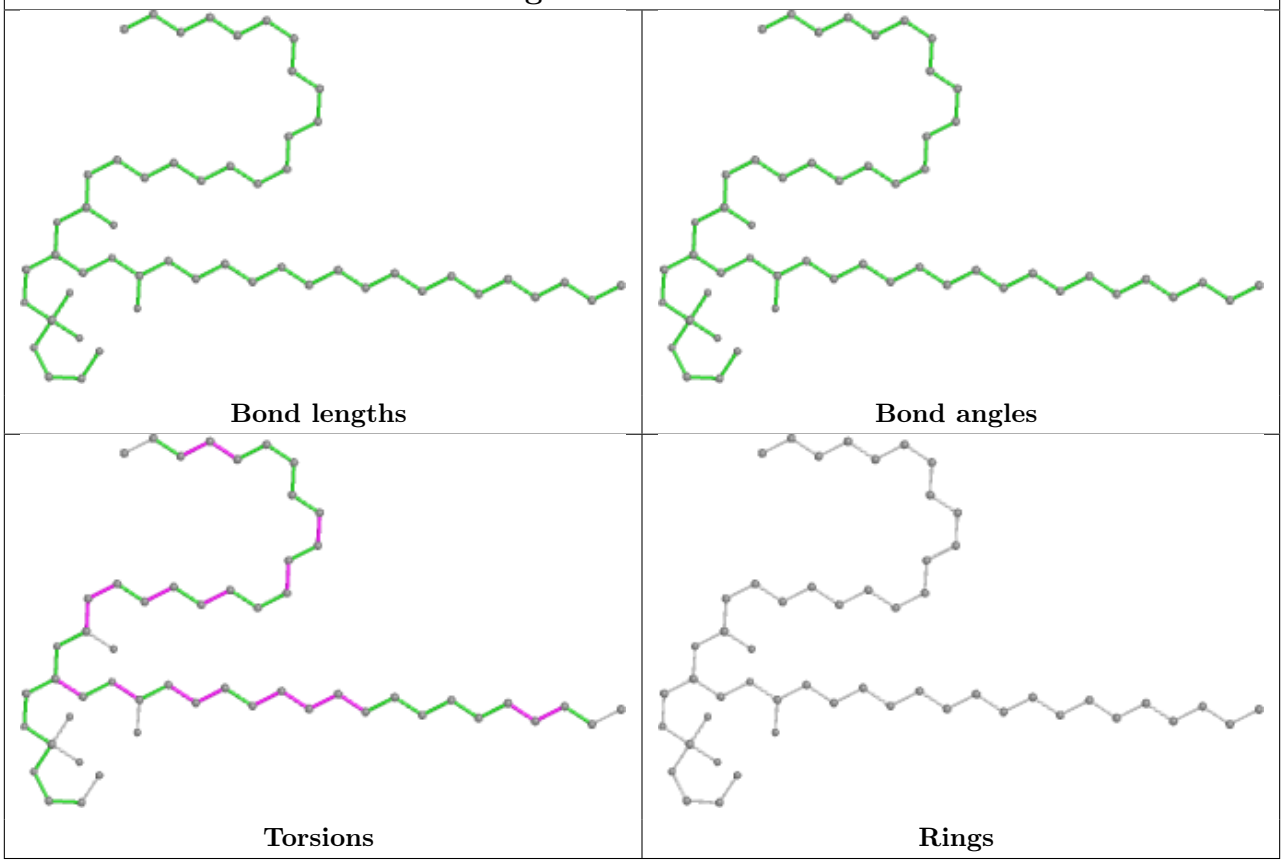
Ligand PSC O 302



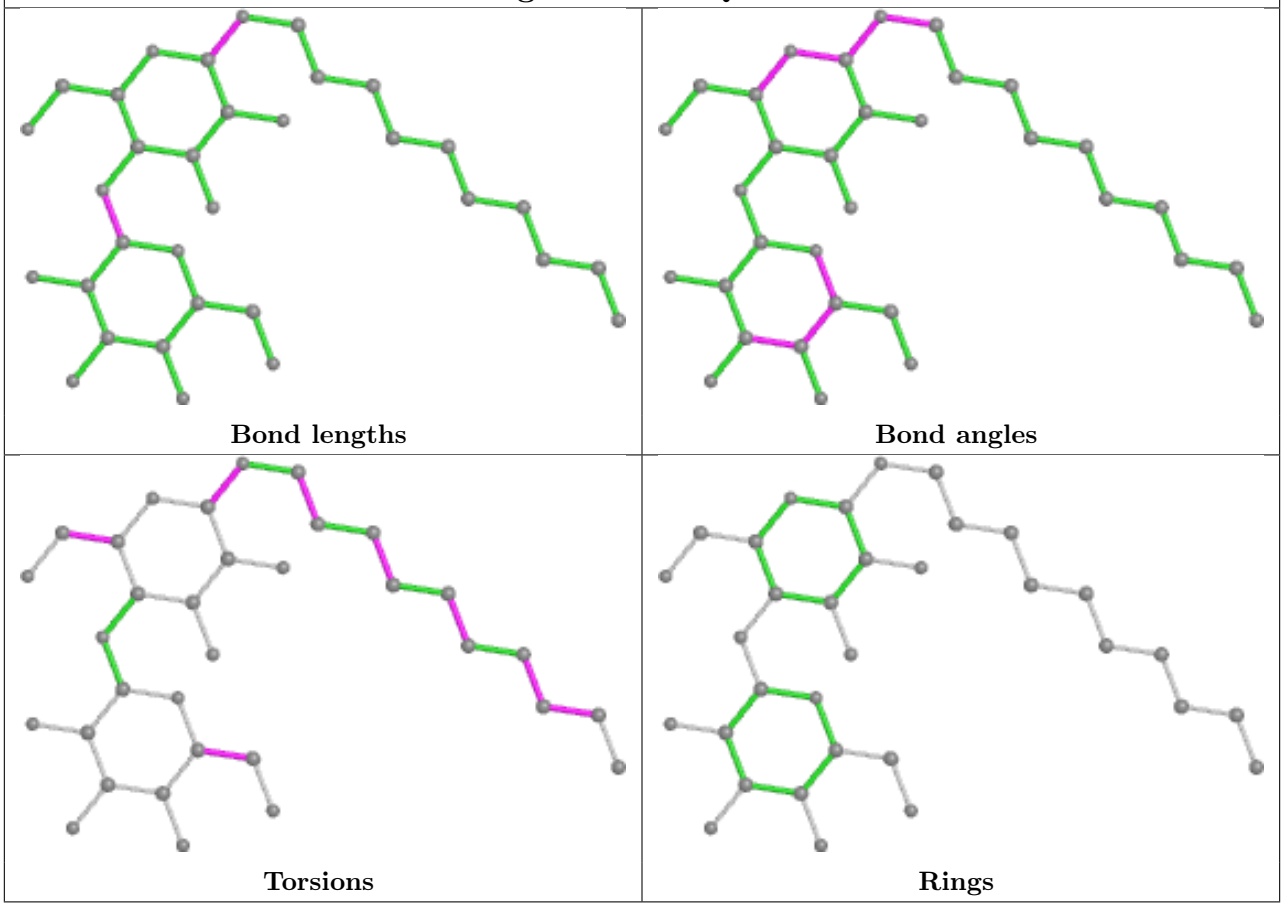
Ligand CHD J 102



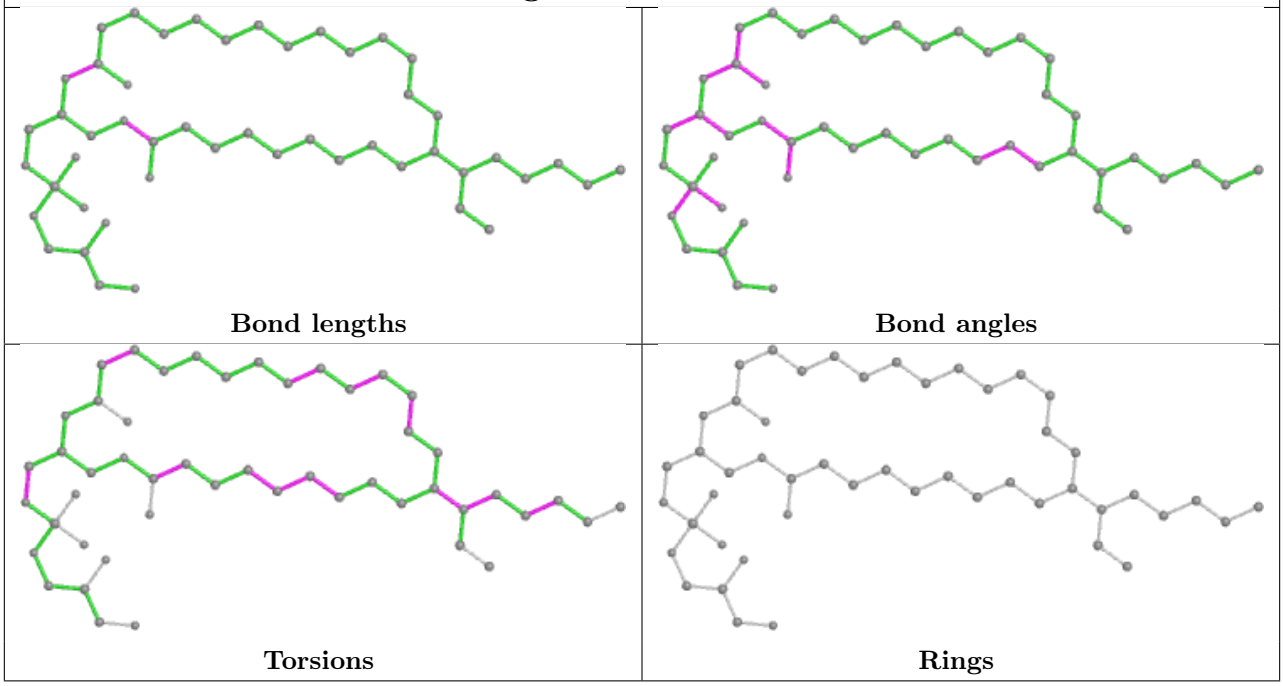
Ligand PEK P 302



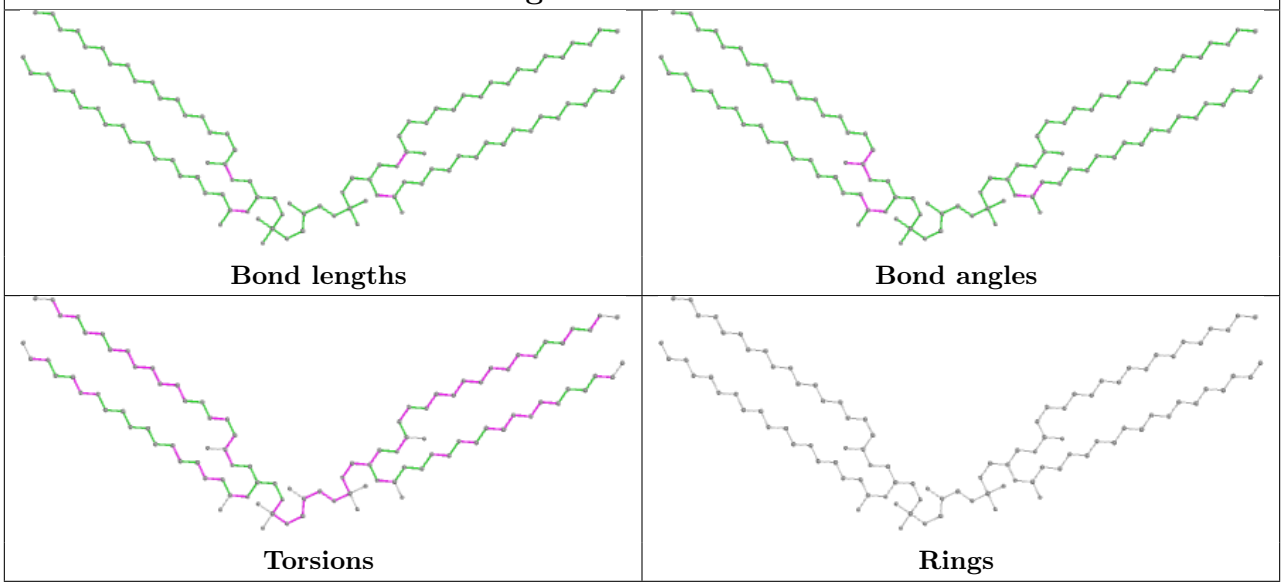
Ligand DMU Q 201



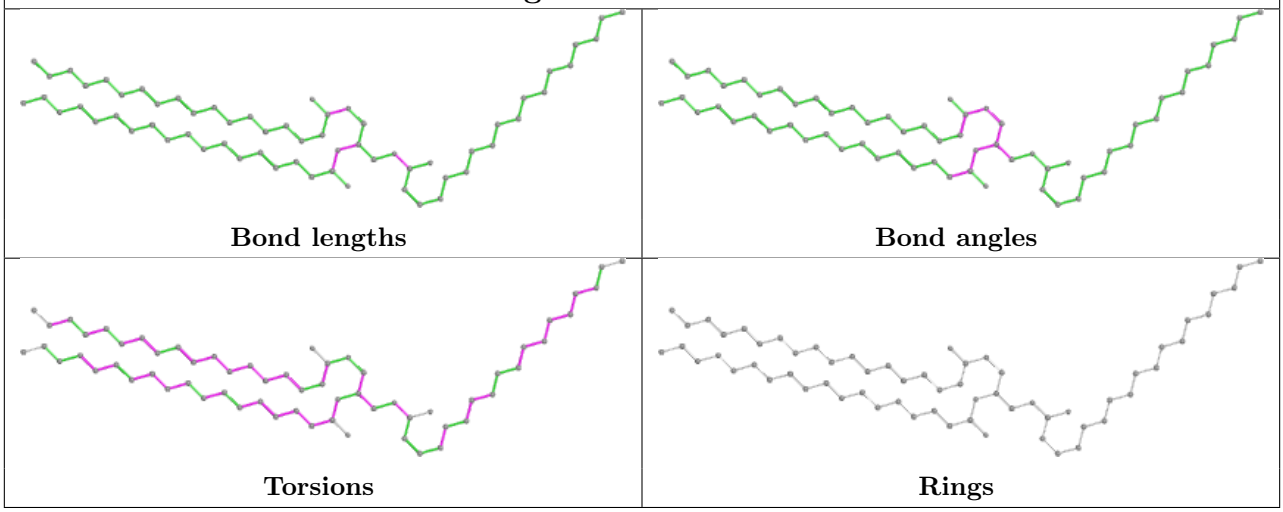
Ligand PGV C 303



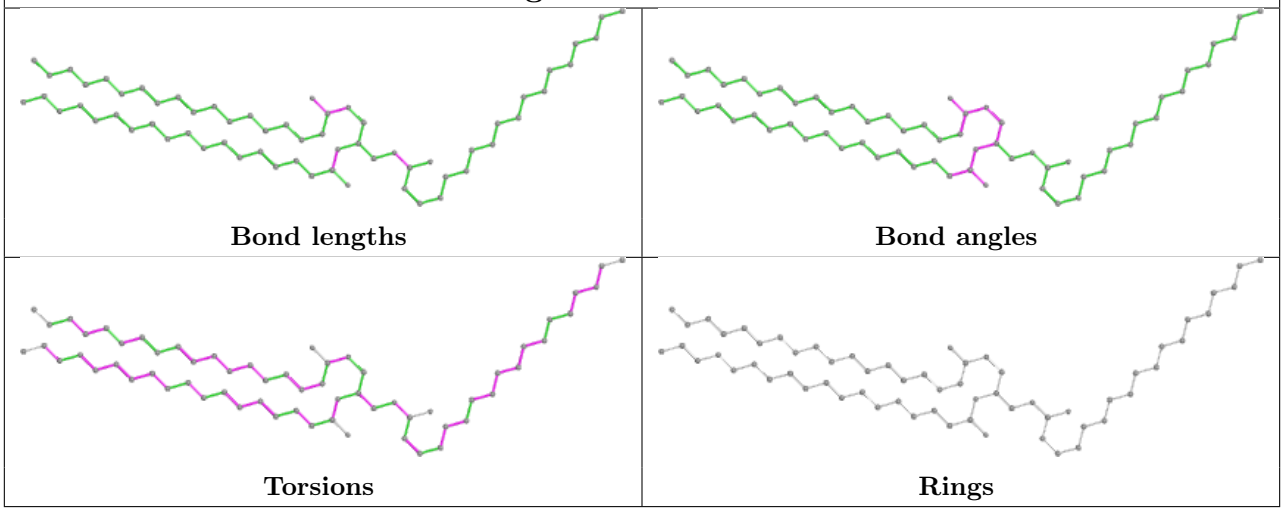
Ligand CDL T 103



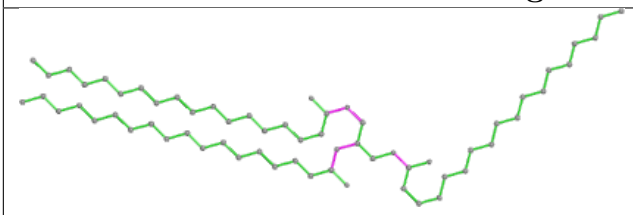
Ligand TGL N 607



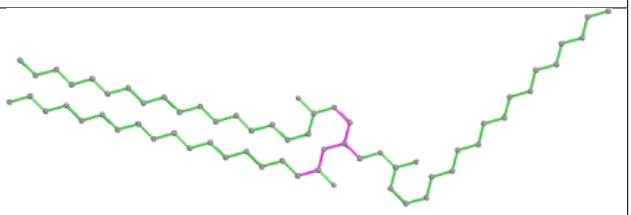
Ligand TGL B 303



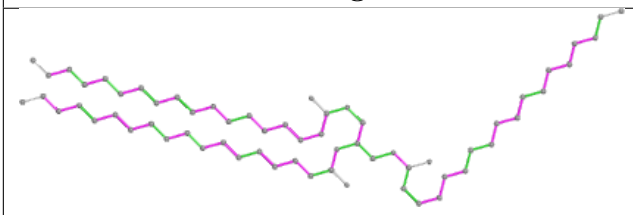
Ligand TGL L 101



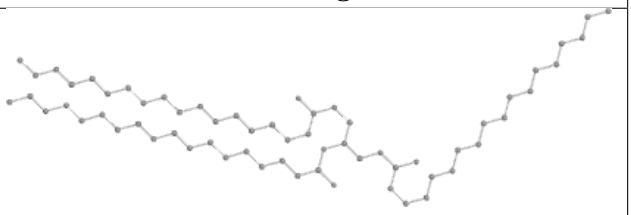
Bond lengths



Bond angles

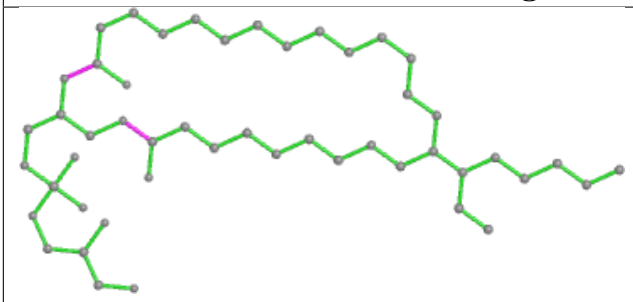


Torsions

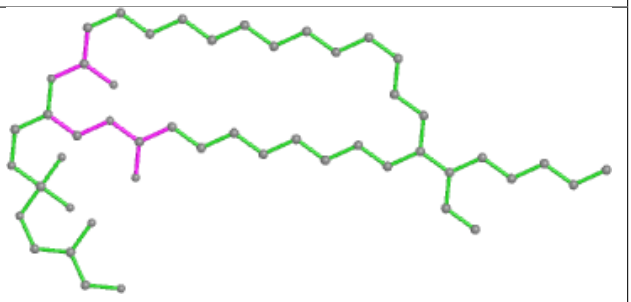


Rings

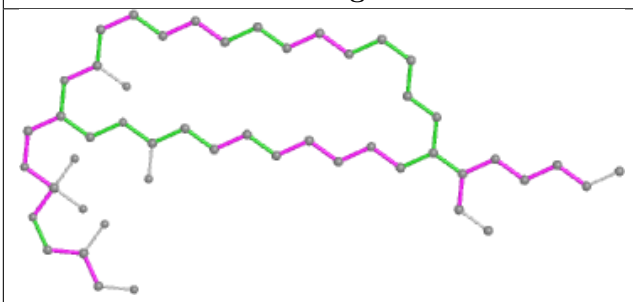
Ligand PGV U 101



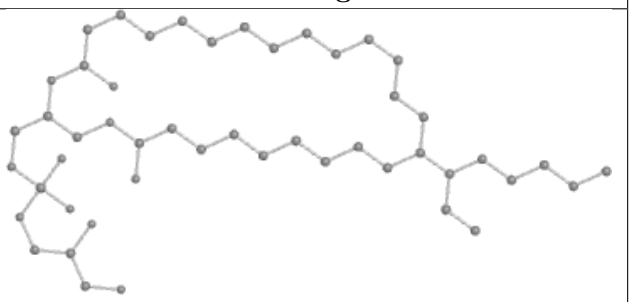
Bond lengths



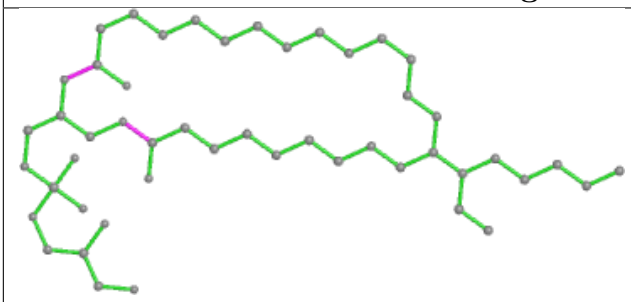
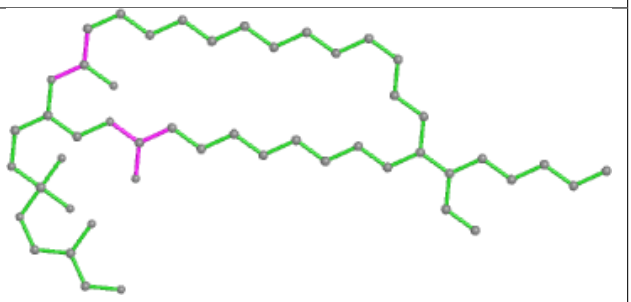
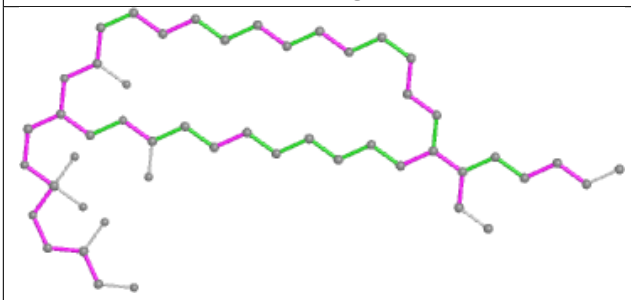
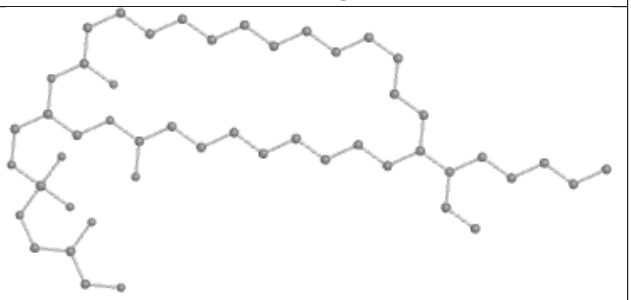
Bond angles

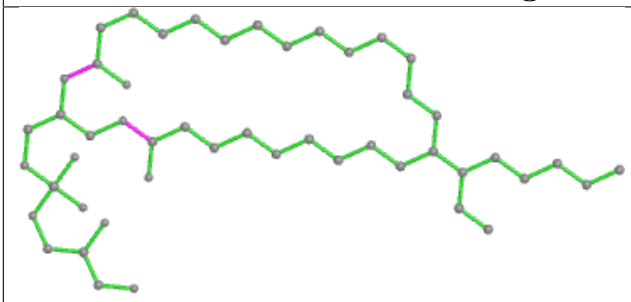
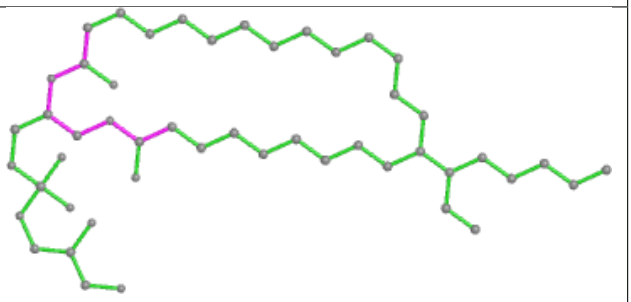
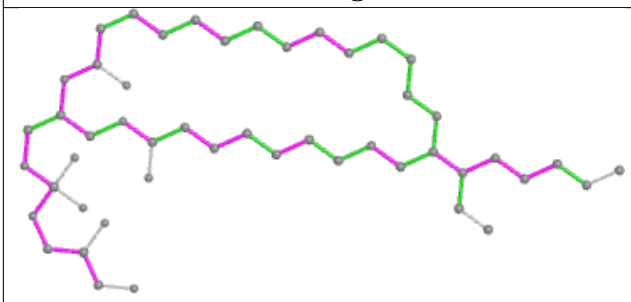
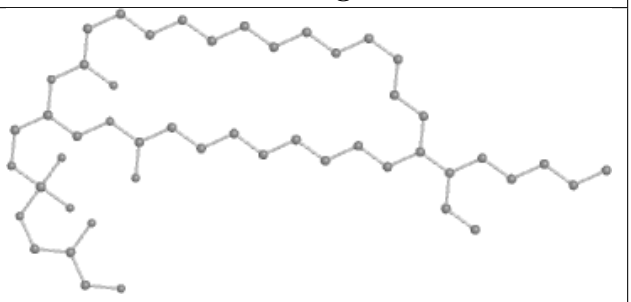


Torsions

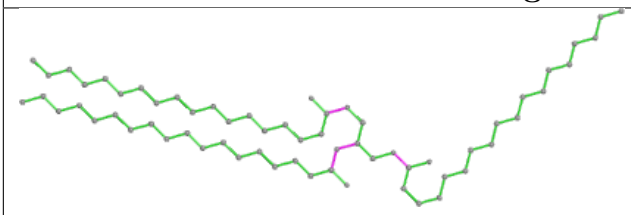


Rings

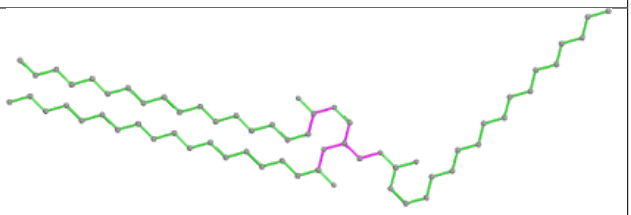
Ligand PGV N 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV A 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

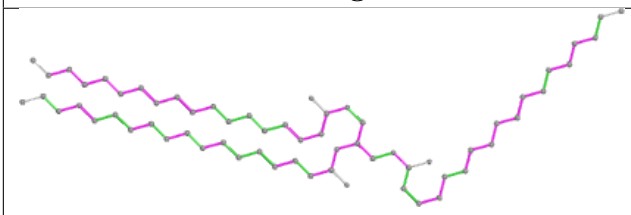
Ligand TGL A 609



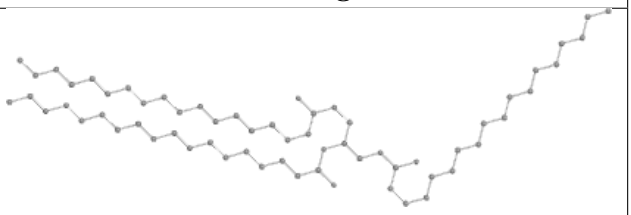
Bond lengths



Bond angles

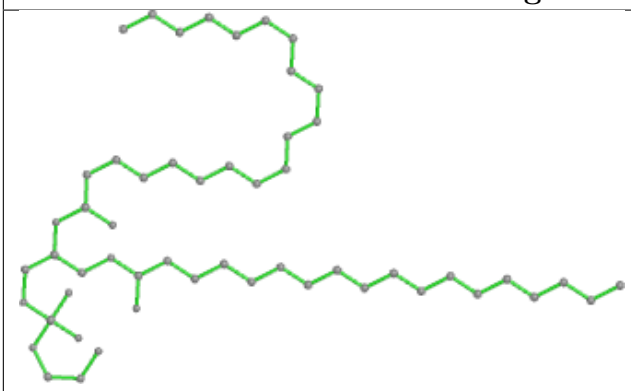


Torsions

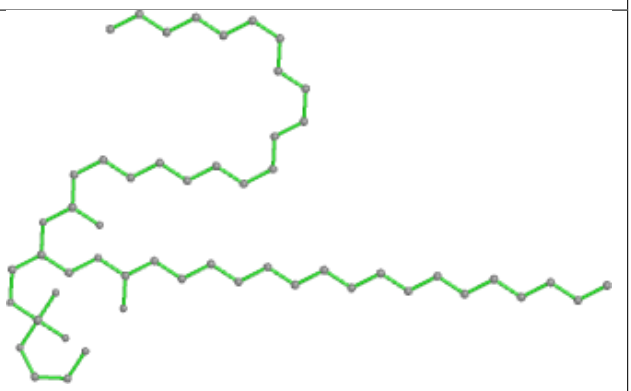


Rings

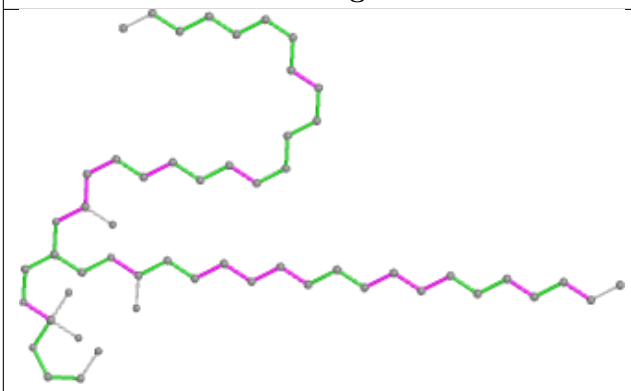
Ligand PEK P 303



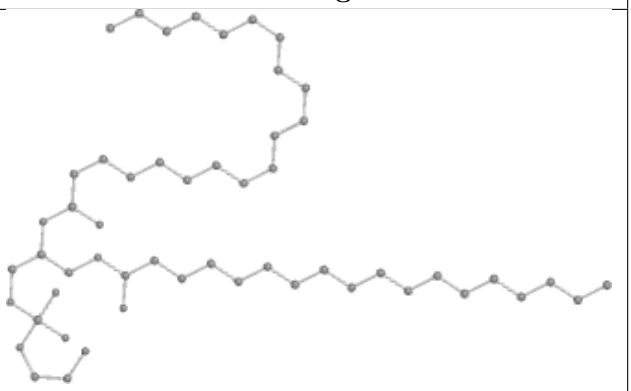
Bond lengths



Bond angles

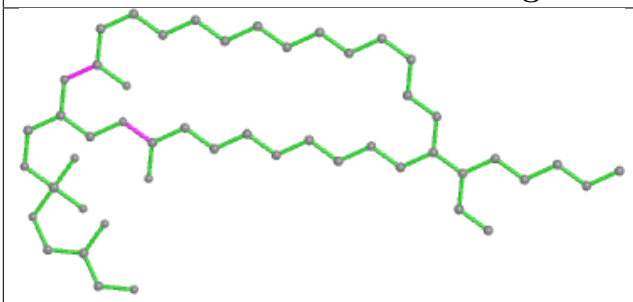


Torsions

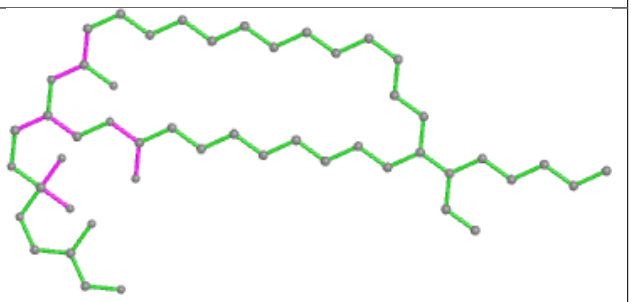


Rings

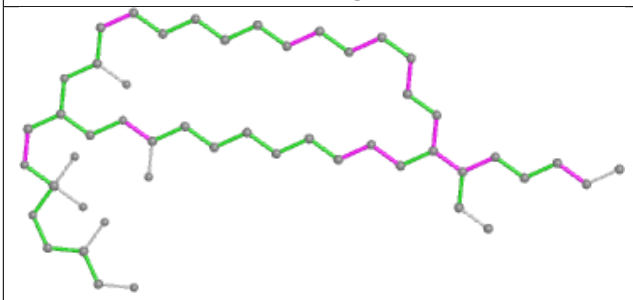
Ligand PGV P 304



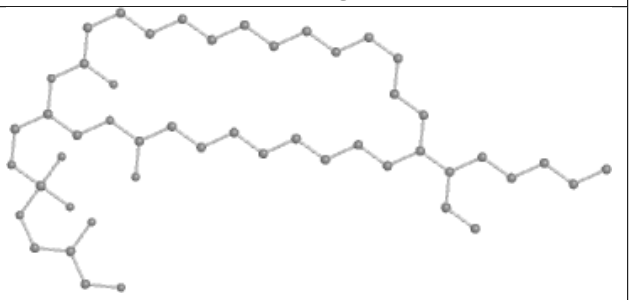
Bond lengths



Bond angles

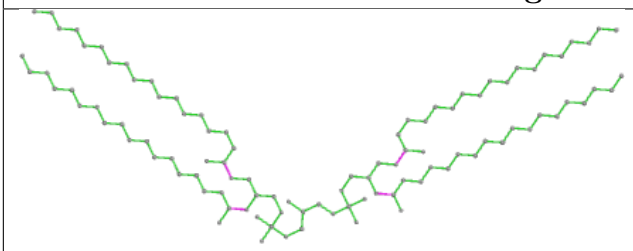


Torsions

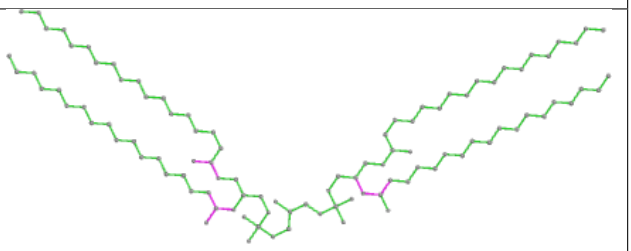


Rings

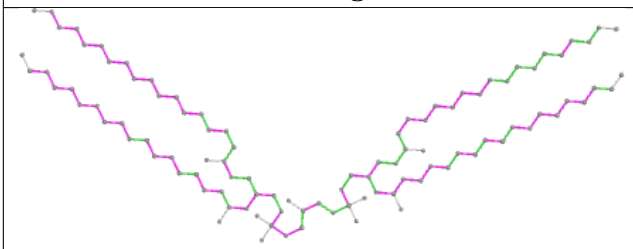
Ligand CDL P 305



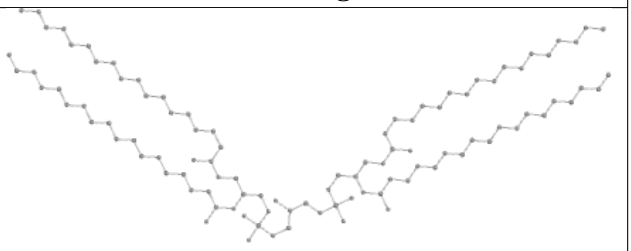
Bond lengths



Bond angles

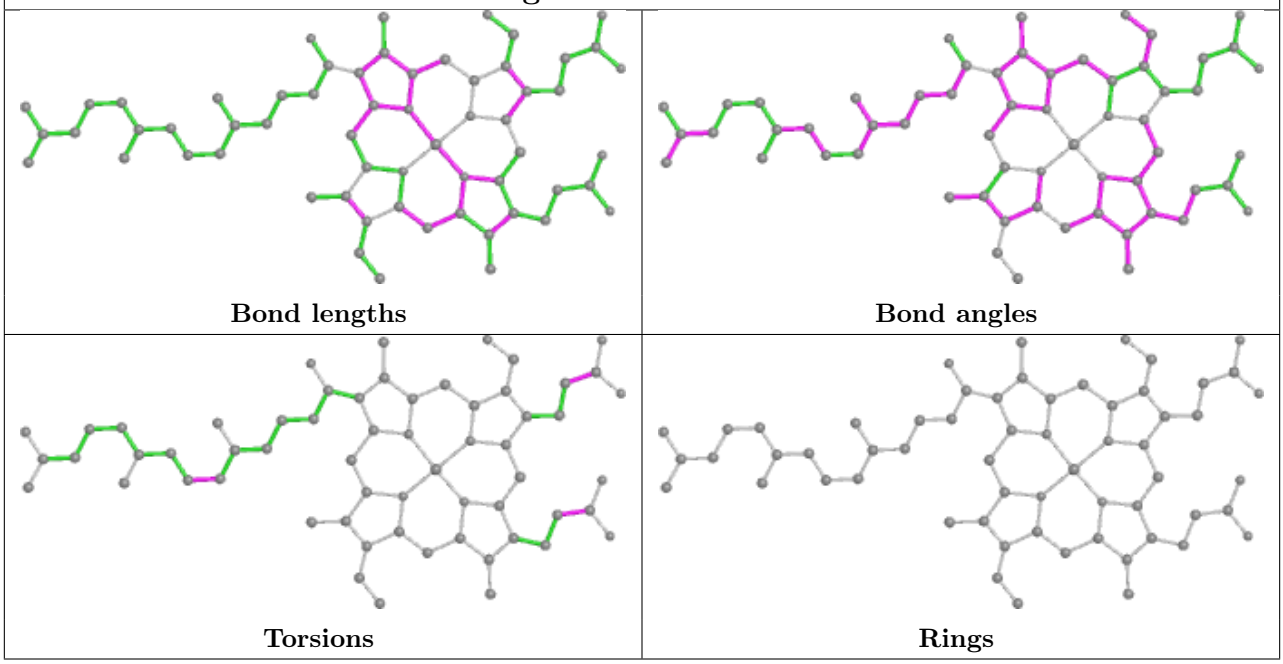


Torsions

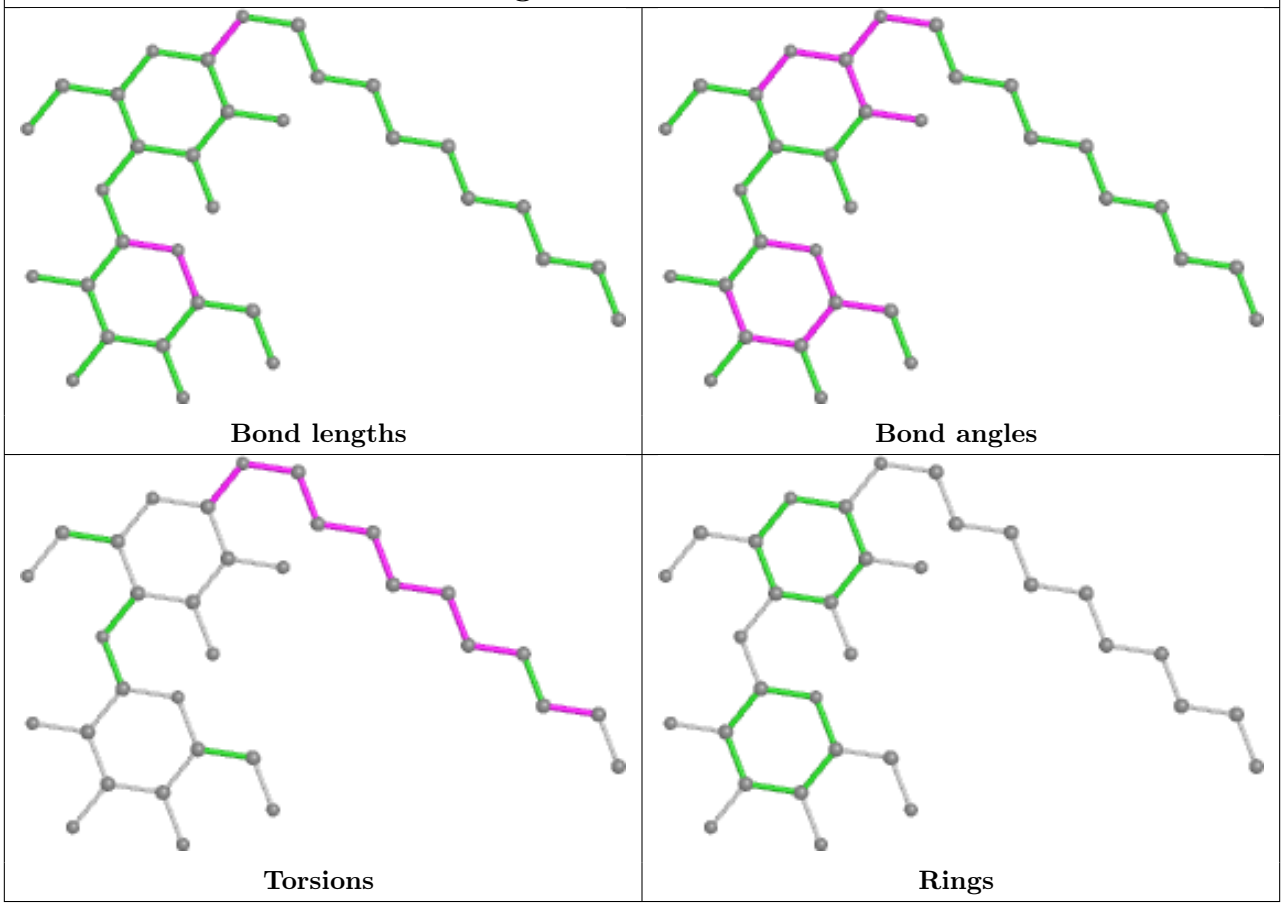


Rings

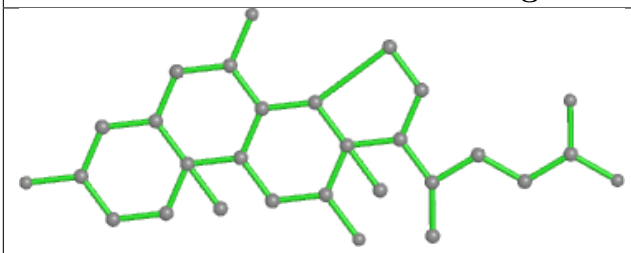
Ligand HEA A 604



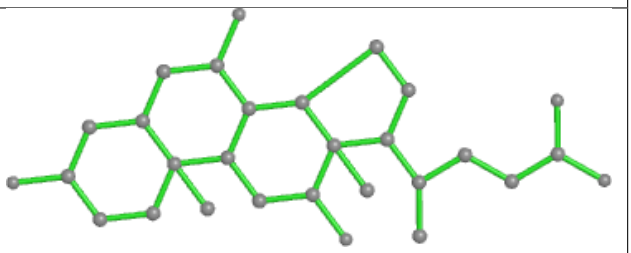
Ligand DMU M 101



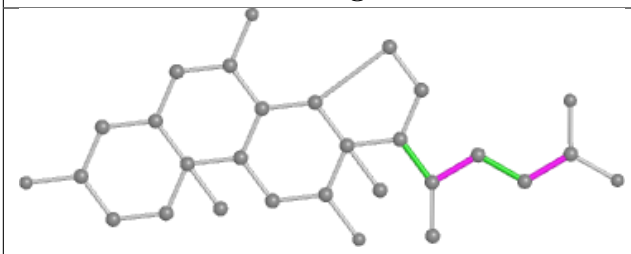
Ligand CHD B 304



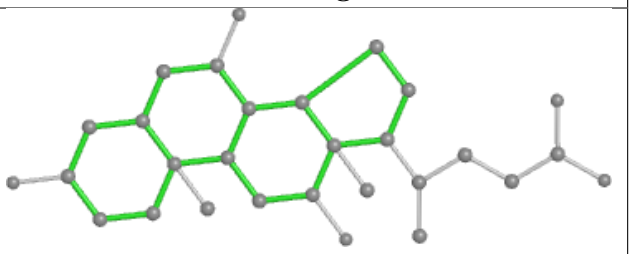
Bond lengths



Bond angles

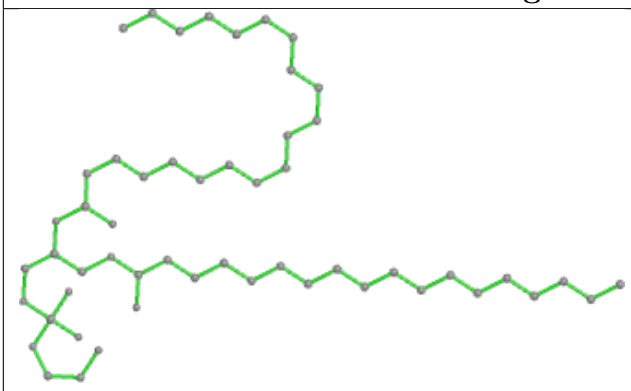


Torsions

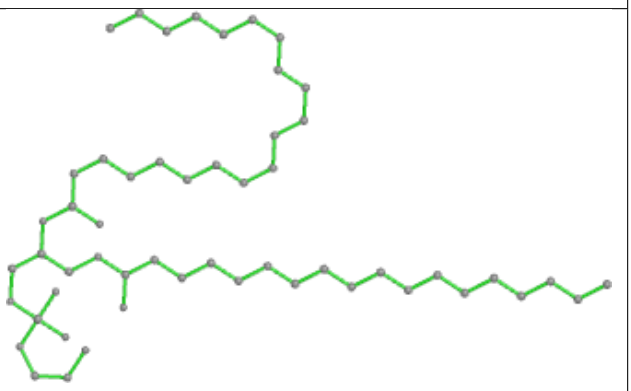


Rings

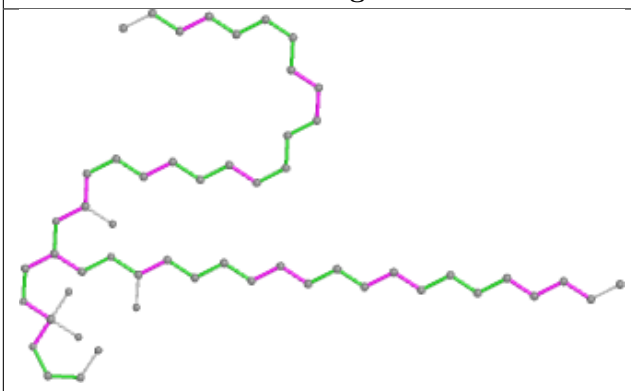
Ligand PEK C 302



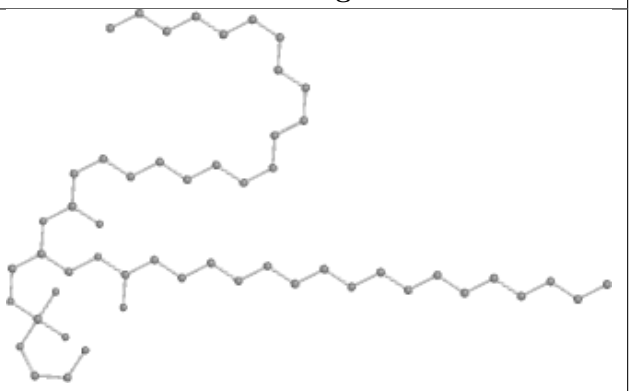
Bond lengths



Bond angles

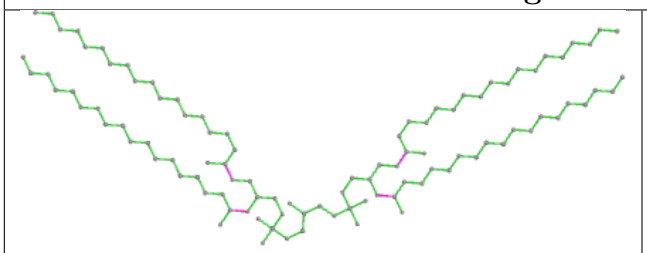


Torsions

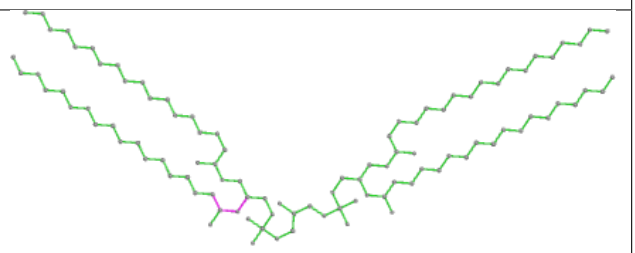


Rings

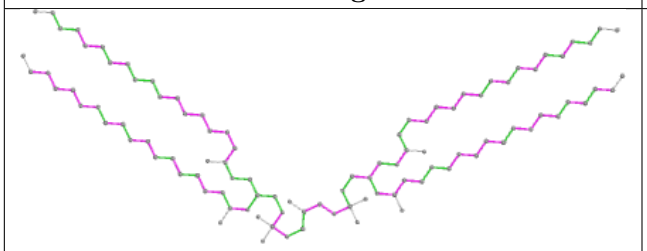
Ligand CDL N 601



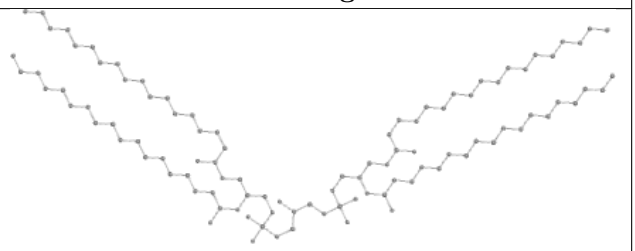
Bond lengths



Bond angles

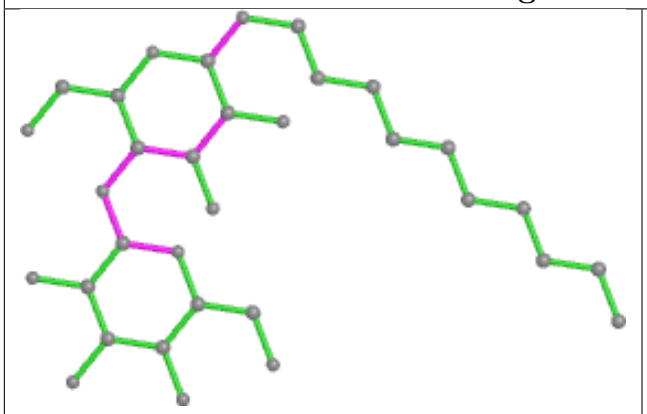


Torsions

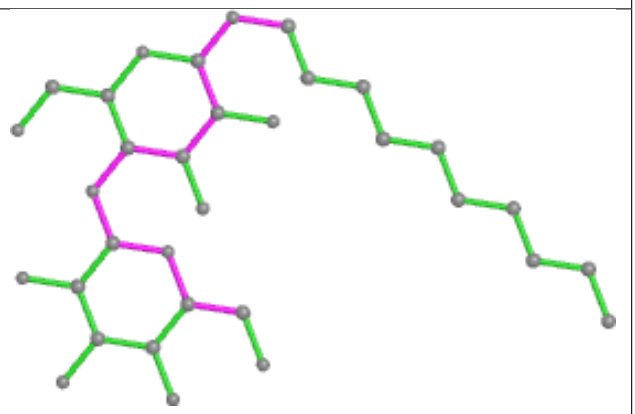


Rings

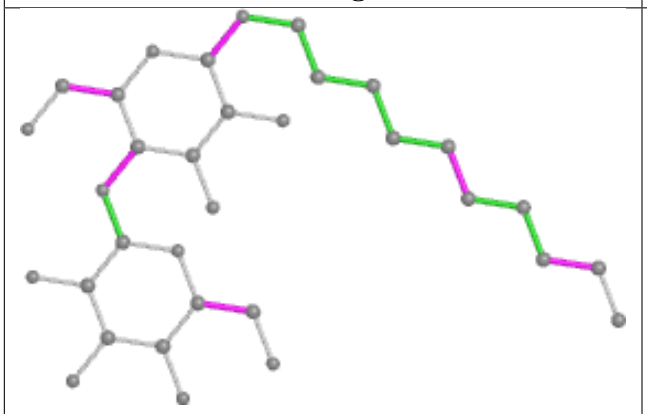
Ligand DMU T 101



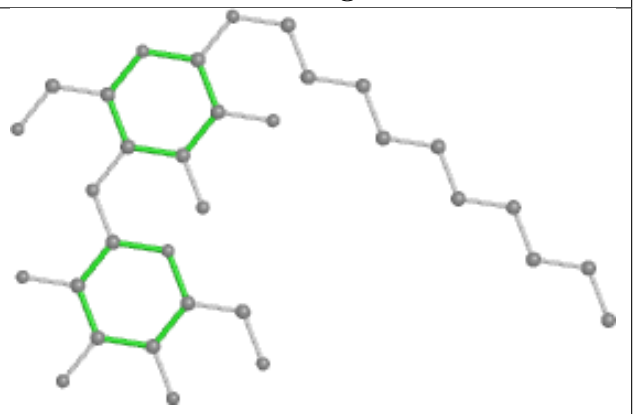
Bond lengths



Bond angles

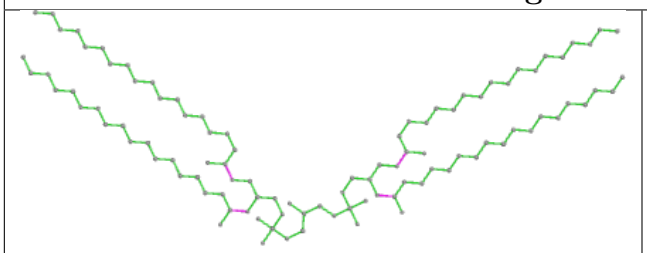


Torsions

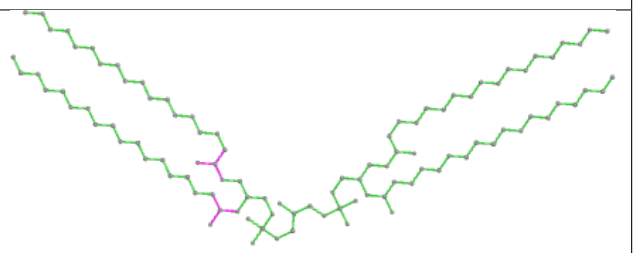


Rings

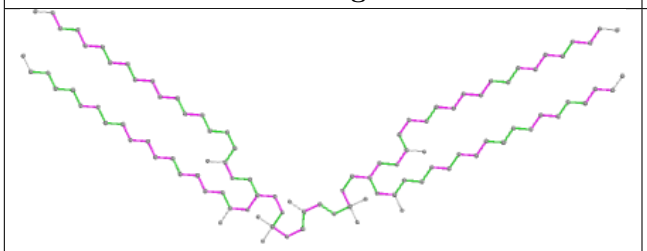
Ligand CDL C 304



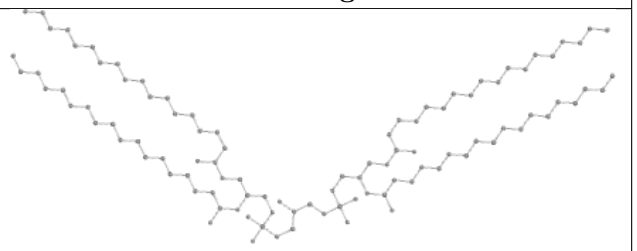
Bond lengths



Bond angles

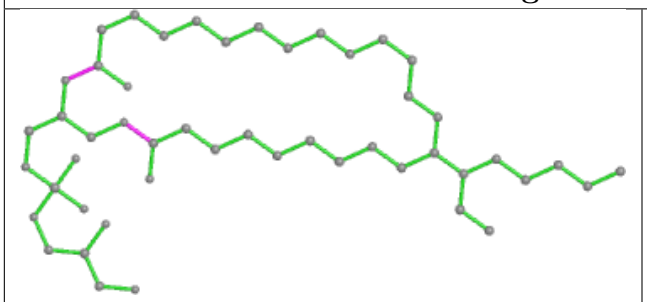


Torsions

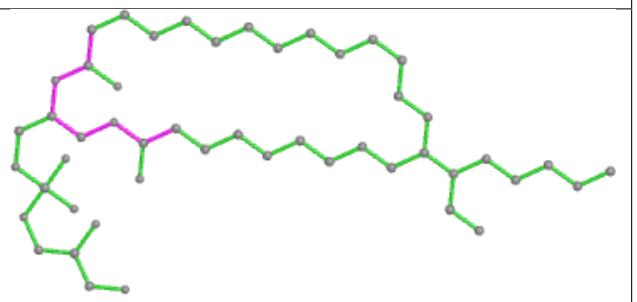


Rings

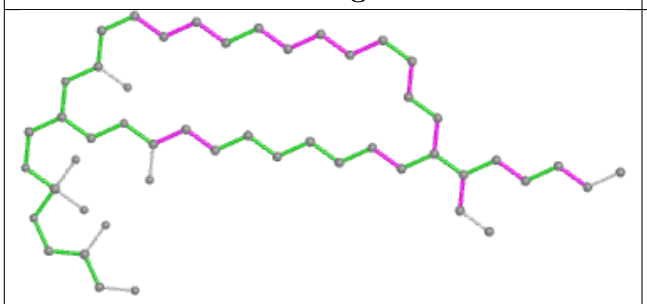
Ligand PGV N 608



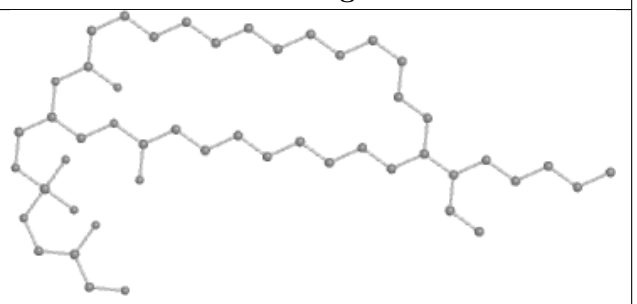
Bond lengths



Bond angles

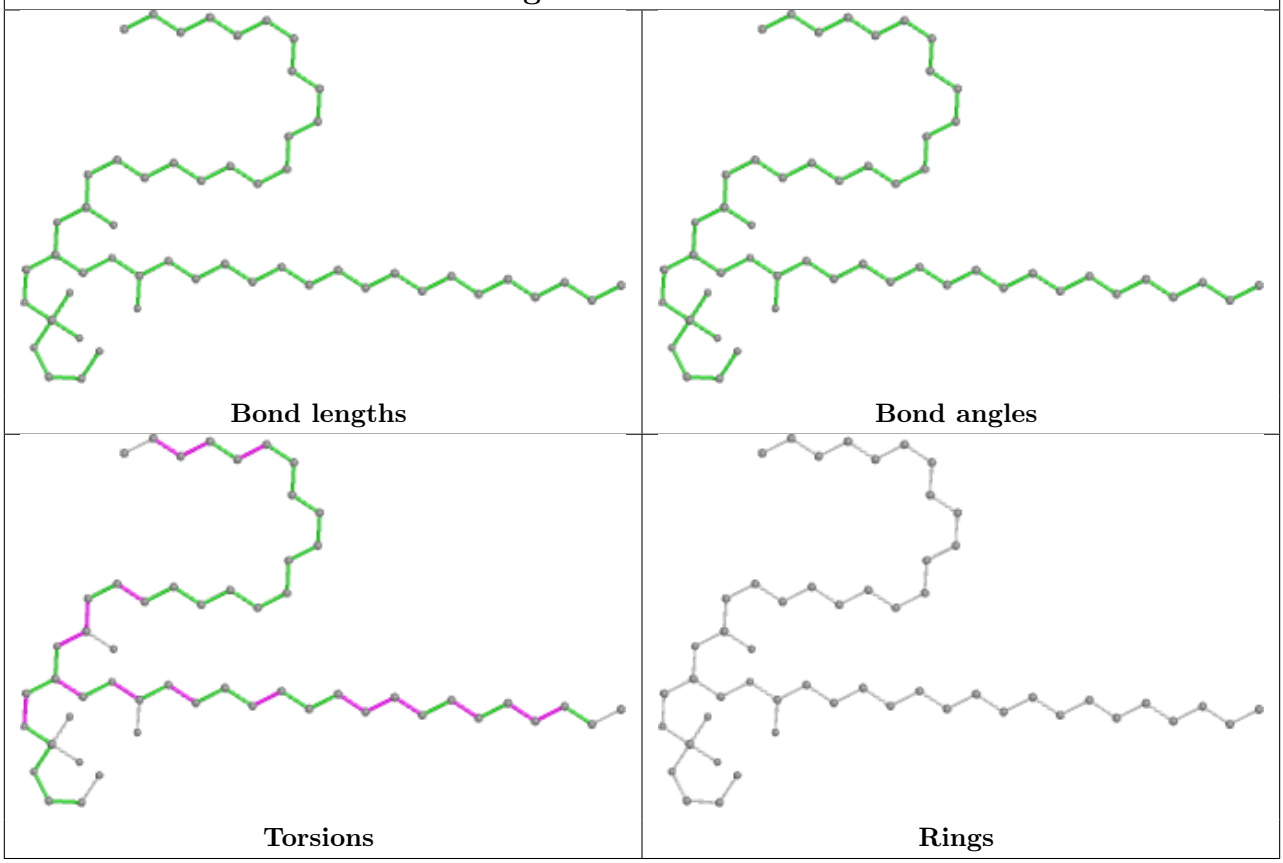


Torsions

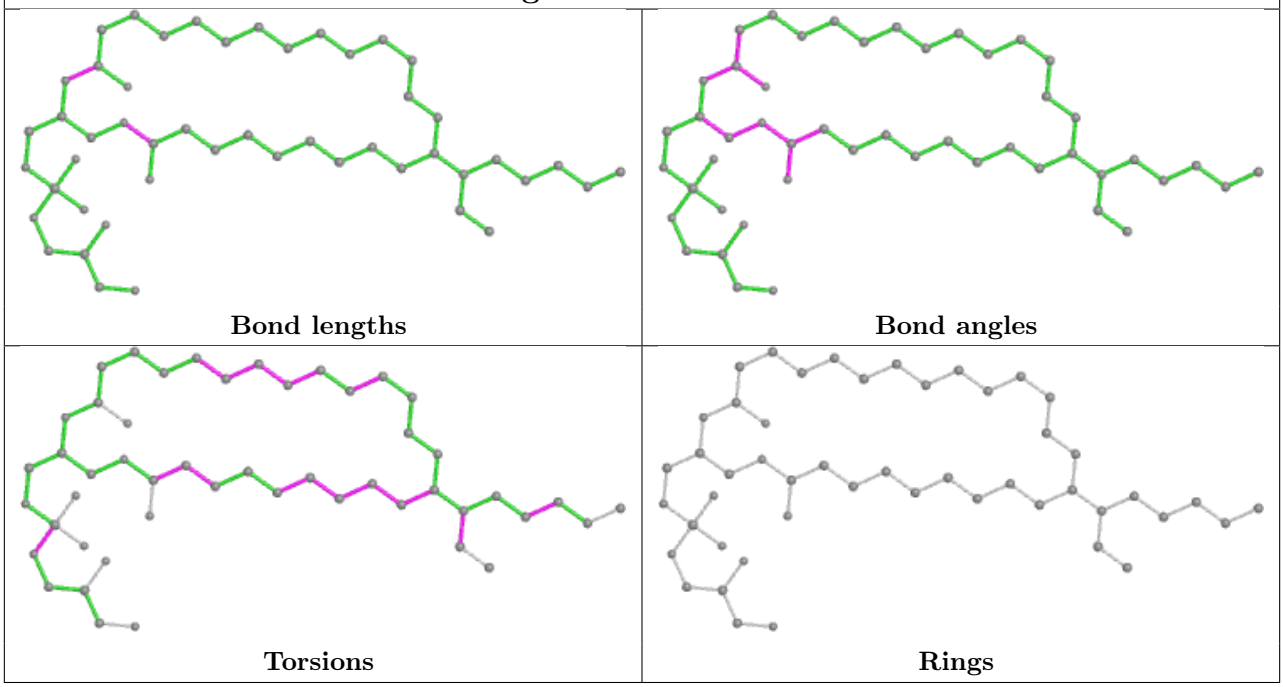


Rings

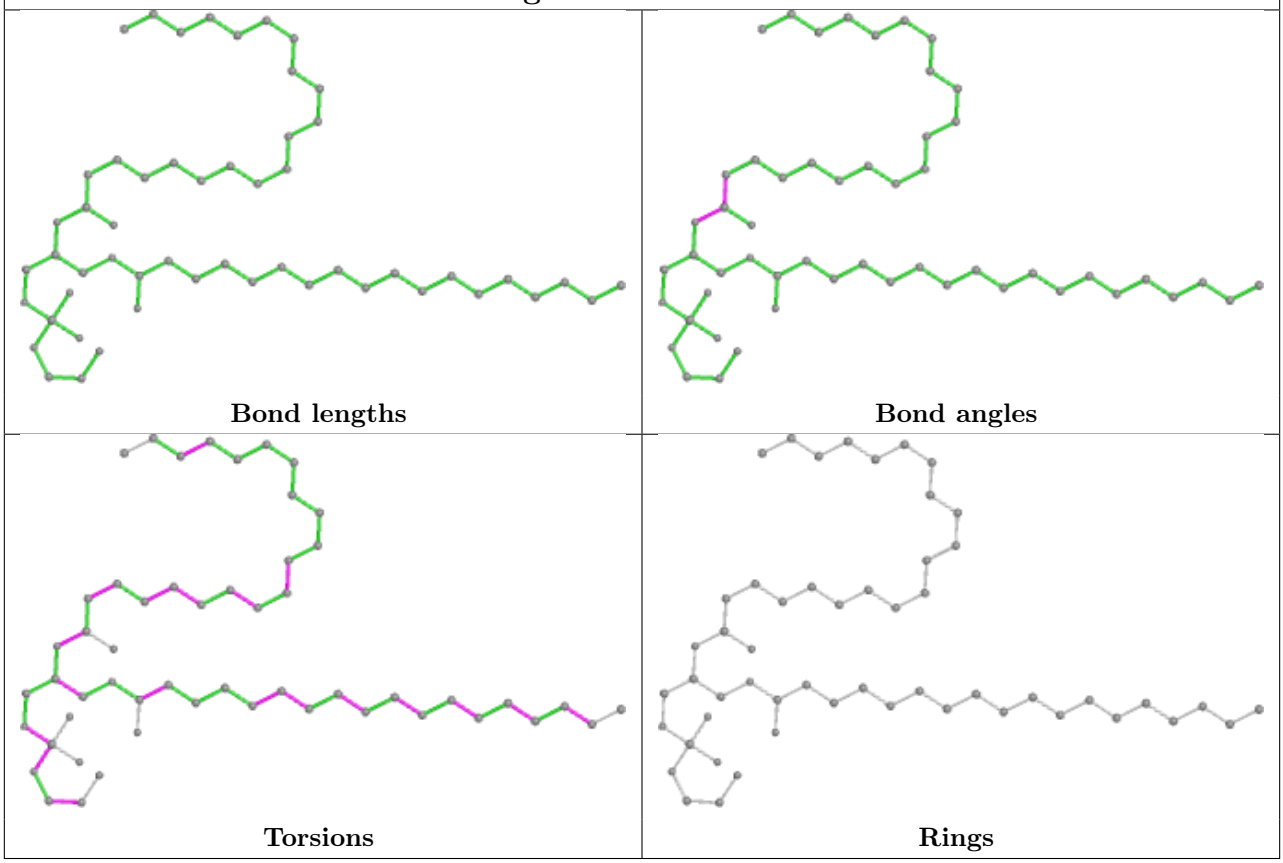
Ligand PEK G 102



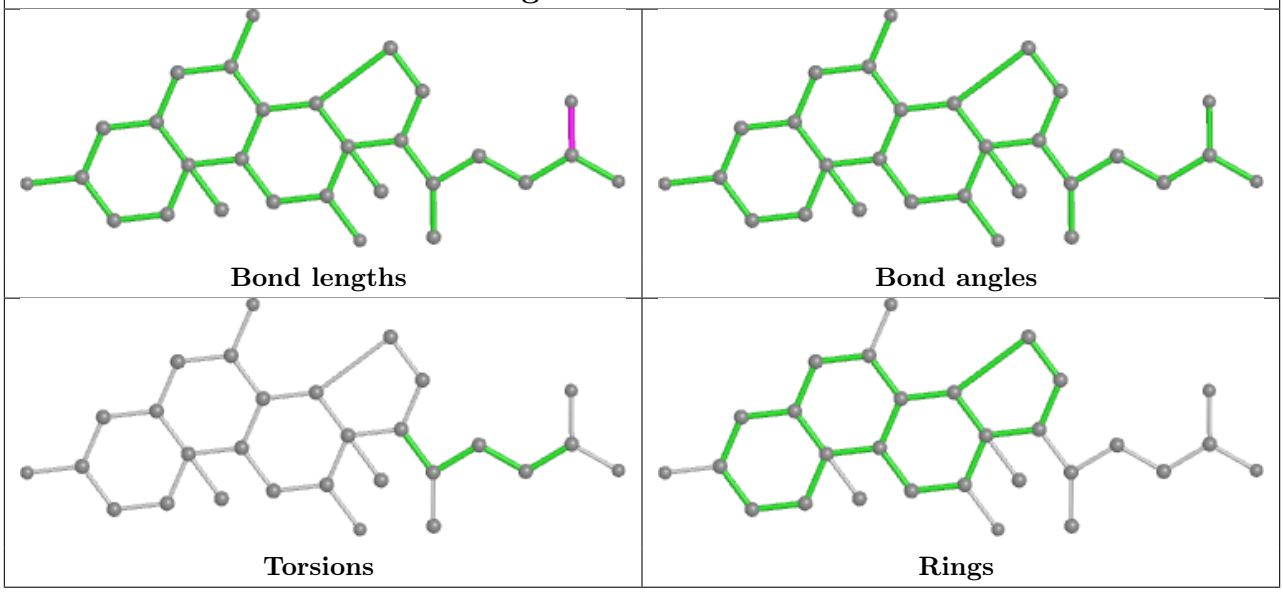
Ligand PGV A 607



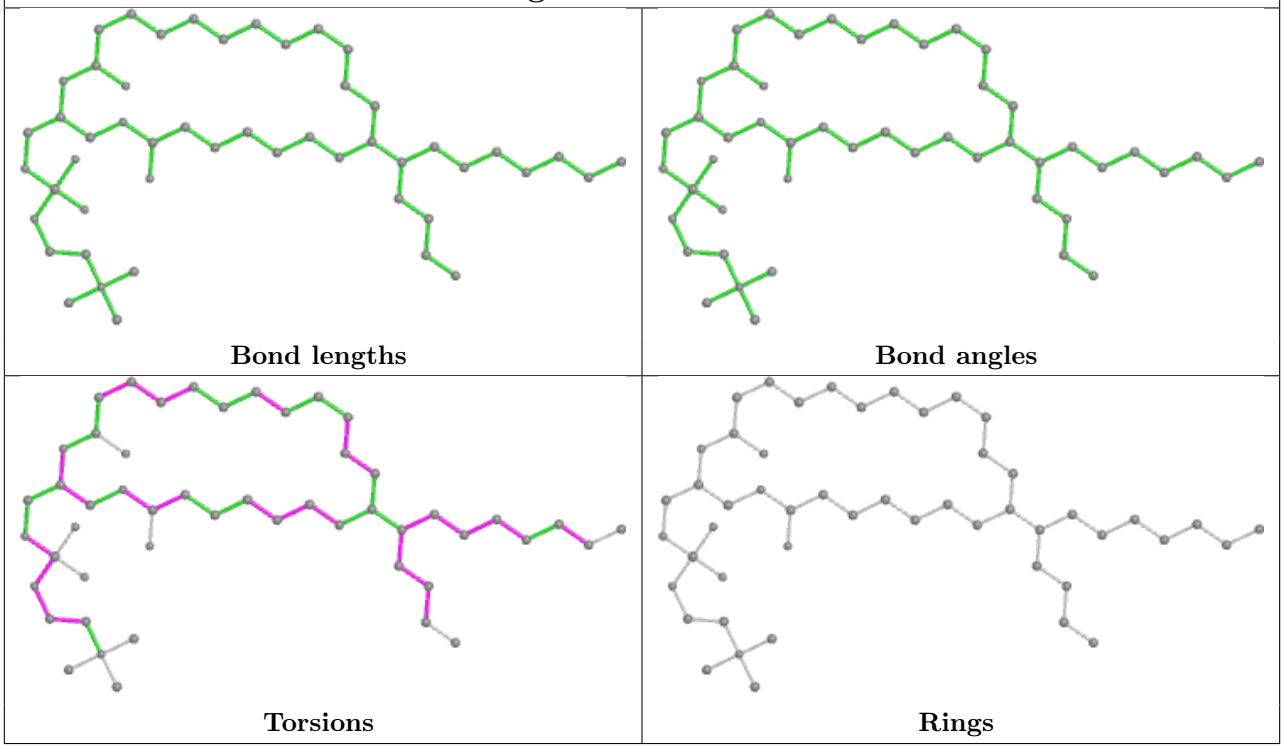
Ligand PEK G 103



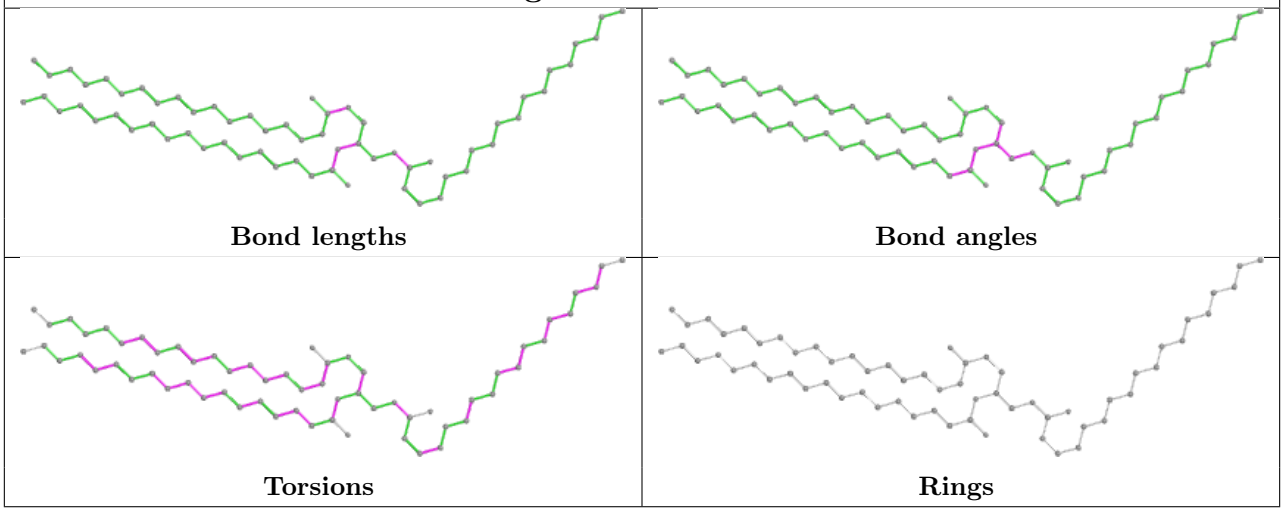
Ligand CHD C 301



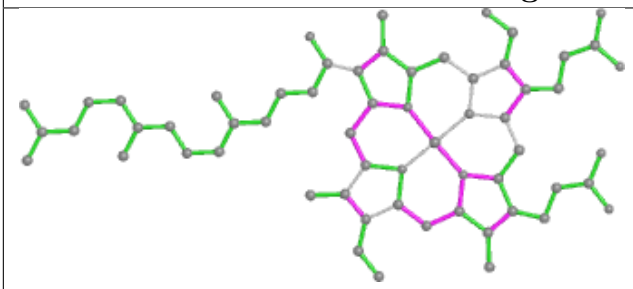
Ligand PSC B 302



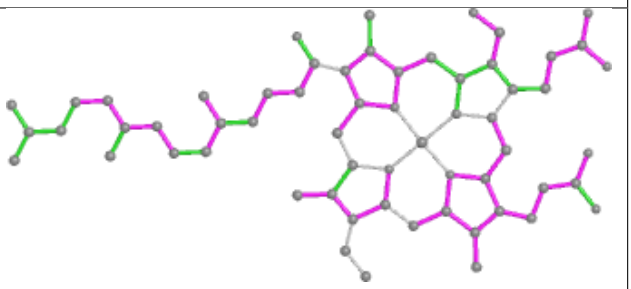
Ligand TGL Y 101



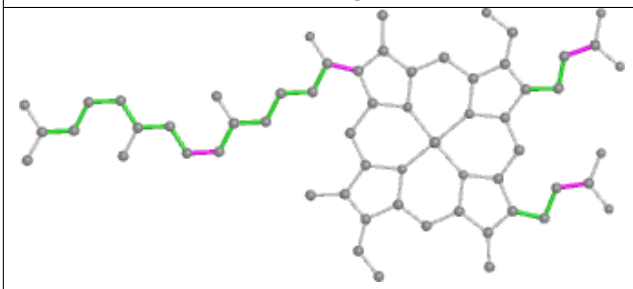
Ligand HEA N 605



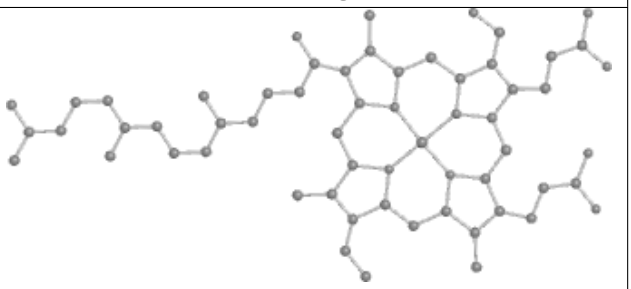
Bond lengths



Bond angles

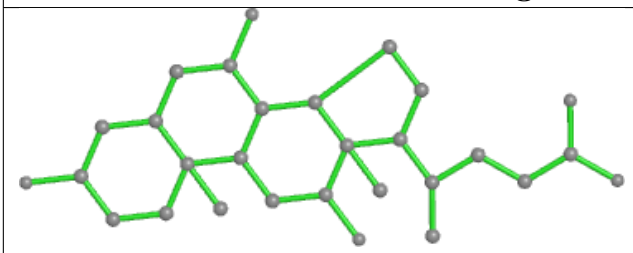


Torsions

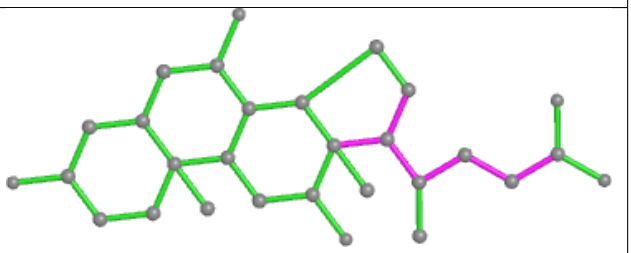


Rings

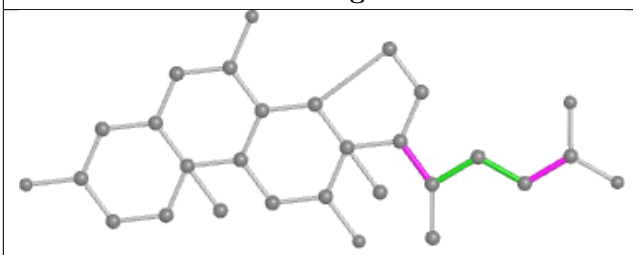
Ligand CHD W 102



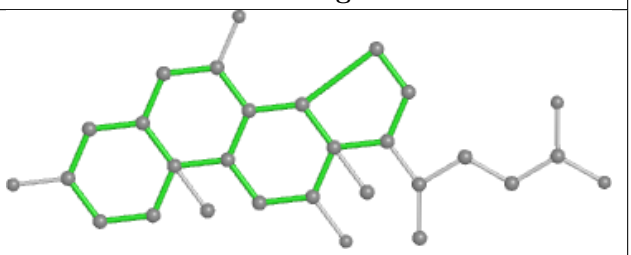
Bond lengths



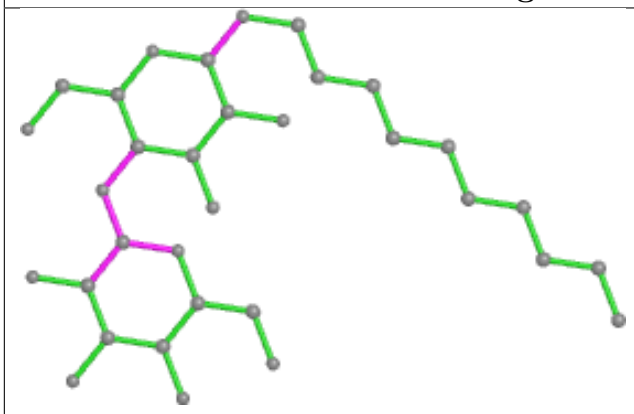
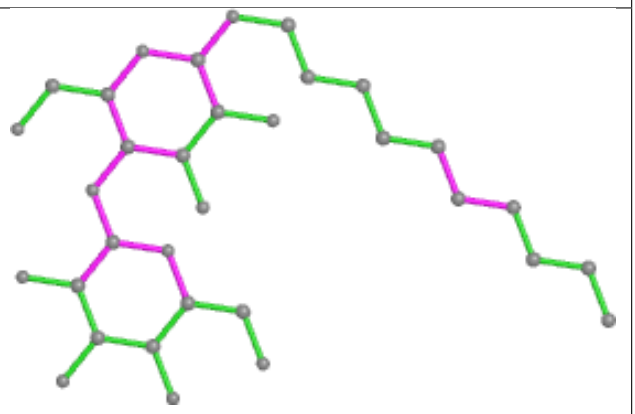
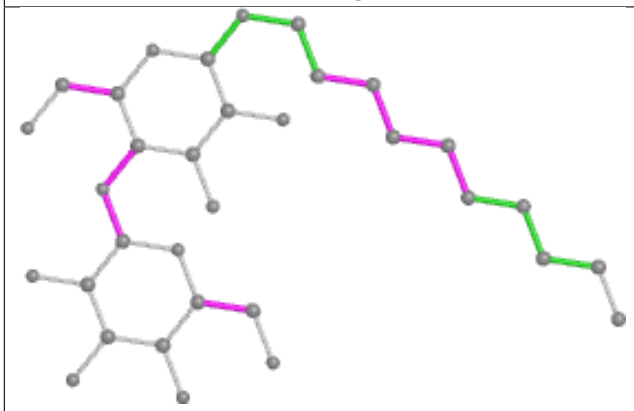
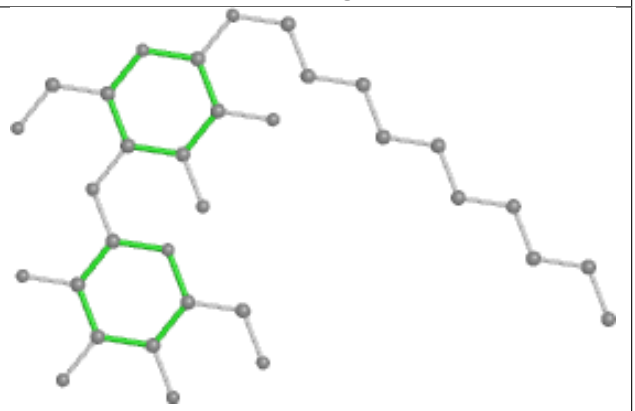
Bond angles



Torsions



Rings

Ligand DMU G 101	
 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%)	-1.12	0	100	100	35, 43, 55, 103	0
1	N	513/514 (99%)	-0.95	0	100	100	41, 57, 75, 129	0
2	B	226/227 (99%)	-0.83	2 (0%)	84	86	36, 50, 84, 158	0
2	O	226/227 (99%)	-0.46	6 (2%)	54	58	48, 70, 109, 160	0
3	C	259/261 (99%)	-0.97	0	100	100	39, 48, 66, 114	0
3	P	259/261 (99%)	-0.83	1 (0%)	92	93	45, 59, 86, 127	0
4	D	144/147 (97%)	-0.68	1 (0%)	87	89	43, 54, 81, 124	0
4	Q	139/147 (94%)	-0.01	8 (5%)	23	24	62, 86, 118, 135	0
5	E	105/109 (96%)	-0.68	2 (1%)	66	69	41, 54, 92, 147	0
5	R	105/109 (96%)	-0.36	2 (1%)	66	69	53, 73, 97, 152	0
6	F	96/98 (97%)	-0.37	5 (5%)	27	29	42, 55, 103, 145	0
6	S	94/98 (95%)	-0.24	5 (5%)	26	28	50, 70, 112, 153	0
7	G	83/85 (97%)	0.15	11 (13%)	3	2	44, 59, 156, 192	0
7	T	83/85 (97%)	0.25	11 (13%)	3	2	49, 74, 152, 192	0
8	H	78/85 (91%)	-0.29	4 (5%)	28	29	44, 59, 126, 160	0
8	U	79/85 (92%)	0.16	6 (7%)	13	14	51, 78, 144, 179	0
9	I	72/73 (98%)	-0.29	4 (5%)	24	25	50, 62, 95, 118	0
9	V	72/73 (98%)	0.17	8 (11%)	5	5	50, 82, 115, 137	0
10	J	58/59 (98%)	-0.19	2 (3%)	45	48	50, 62, 112, 160	0
10	W	58/59 (98%)	0.20	5 (8%)	10	10	64, 81, 124, 158	0
11	K	49/56 (87%)	-0.40	1 (2%)	65	68	41, 58, 78, 110	0
11	X	49/56 (87%)	0.27	2 (4%)	37	40	73, 86, 109, 144	0
12	L	46/47 (97%)	-0.78	2 (4%)	35	38	41, 49, 78, 137	0
12	Y	46/47 (97%)	-0.29	2 (4%)	35	38	56, 80, 108, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.53	2 (4%) 31 33	44, 51, 89, 143	0
13	Z	43/46 (93%)	0.34	5 (11%) 4 4	67, 81, 126, 158	0
All	All	3538/3614 (97%)	-0.60	97 (2%) 54 58	35, 58, 105, 192	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	40	GLY	13.8
13	Z	43	SER	8.6
7	T	10	GLY	8.3
7	T	40	GLY	8.1
7	T	8	HIS	7.8
7	G	3	ALA	7.7
2	O	59	GLN	7.5
8	U	8	ILE	7.4
7	G	8	HIS	7.2
10	W	58	LYS	7.1
7	G	41	HIS	7.0
5	R	5	HIS	6.3
2	O	90	ILE	5.6
7	T	41	HIS	5.6
13	Z	42	LYS	5.5
6	S	95	GLN	5.3
7	T	39	SER	5.2
5	E	5	HIS	5.1
7	G	39	SER	4.9
7	T	84	LYS	4.8
6	S	94	HIS	4.8
9	V	25	PHE	4.8
2	B	90	ILE	4.8
6	F	97	ALA	4.7
13	M	43	SER	4.6
7	T	3	ALA	4.6
8	H	8	ILE	4.6
9	I	37	PHE	4.5
10	J	58	LYS	4.5
6	F	2	SER	4.4
8	U	7	LYS	4.4
6	S	93	PRO	4.4
7	G	42	ARG	4.3
6	F	95	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
9	V	2	THR	4.3
10	J	57	HIS	4.3
10	W	57	HIS	4.2
9	V	37	PHE	4.2
8	H	10	ASN	4.1
8	U	10	ASN	4.0
12	Y	47	LYS	3.9
7	T	43	GLU	3.8
12	L	2	HIS	3.8
6	F	94	HIS	3.8
11	K	6	ALA	3.8
10	W	48	TYR	3.7
11	X	37	GLY	3.7
9	V	53	ASN	3.6
7	T	36	TRP	3.6
6	S	3	GLY	3.6
7	G	10	GLY	3.6
7	G	36	TRP	3.6
12	Y	2	HIS	3.5
2	O	113	TYR	3.5
7	T	42	ARG	3.4
2	B	59	GLN	3.4
6	S	96	LEU	3.4
11	X	6	ALA	3.4
13	Z	39	ASN	3.3
6	F	96	LEU	3.3
4	Q	35	ALA	3.3
4	Q	147	LYS	3.1
10	W	52	TRP	3.0
9	I	53	ASN	3.0
7	G	9	GLY	3.0
12	L	47	LYS	3.0
4	Q	101	HIS	2.9
4	Q	9	GLU	2.8
2	O	227	LEU	2.8
7	G	84	LYS	2.8
10	W	56	PRO	2.7
4	Q	32	ASN	2.7
2	O	89	GLU	2.7
9	V	3	ALA	2.6
13	Z	41	LYS	2.6
8	U	47	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
8	H	49	ASP	2.5
8	U	51	SER	2.5
13	Z	38	ASP	2.4
9	V	19	PHE	2.4
8	U	48	GLY	2.4
7	T	1	ALA	2.4
9	I	18	ARG	2.3
4	Q	38	LYS	2.3
2	O	55	THR	2.3
8	H	48	GLY	2.3
5	E	9	GLU	2.3
9	I	19	PHE	2.3
7	G	43	GLU	2.3
4	D	147	LYS	2.2
9	V	65	LYS	2.2
3	P	3	HIS	2.1
4	Q	10	ASP	2.1
13	M	42	LYS	2.1
5	R	9	GLU	2.1
9	V	18	ARG	2.1
4	Q	74	SER	2.1

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
9	SAC	V	1	9/10	0.40	0.78	140,158,175,179	0
7	TPO	G	11	11/12	0.67	0.40	116,142,176,188	0
9	SAC	I	1	9/10	0.69	0.60	128,141,151,154	0
7	TPO	T	11	11/12	0.79	0.35	139,157,180,188	0
1	FME	N	1	10/11	0.87	0.29	89,103,132,152	0
1	FME	A	1	10/11	0.94	0.17	69,80,105,120	0
2	FME	O	1	10/11	0.95	0.12	59,73,86,88	0
2	FME	B	1	10/11	0.97	0.11	48,54,56,64	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	G	103	53/53	0.62	0.28	78,133,201,215	0
28	DMU	T	101	33/33	0.66	0.29	117,166,199,205	0
25	PEK	P	303	53/53	0.69	0.25	78,129,162,178	0
18	PGV	N	610	51/51	0.70	0.29	67,113,153,166	0
26	CDL	T	103	100/100	0.72	0.22	86,134,181,206	0
25	PEK	C	302	53/53	0.72	0.23	80,123,194,208	0
23	PSC	B	302	52/52	0.74	0.27	78,132,259,284	0
18	PGV	A	608	51/51	0.74	0.28	76,120,154,156	0
18	PGV	U	101	51/51	0.75	0.28	75,119,151,156	0
19	TGL	N	609	63/63	0.76	0.21	91,125,149,159	0
25	PEK	T	102	53/53	0.76	0.24	72,147,234,241	0
28	DMU	G	101	33/33	0.77	0.27	101,139,187,198	0
19	TGL	A	609	63/63	0.77	0.20	75,106,129,133	0
23	PSC	O	302	52/52	0.78	0.25	73,139,232,252	0
24	CHD	W	102	29/29	0.78	0.26	98,143,157,162	0
18	PGV	A	606	51/51	0.78	0.22	53,107,152,185	0
26	CDL	N	601	100/100	0.81	0.18	90,125,171,189	0
19	TGL	Y	101	63/63	0.81	0.21	74,117,173,182	0
26	CDL	P	305	100/100	0.82	0.22	54,129,159,162	0
24	CHD	J	102	29/29	0.82	0.19	97,115,137,144	0
26	CDL	C	304	100/100	0.83	0.22	59,124,167,174	0
28	DMU	Q	201	33/33	0.84	0.18	96,111,126,131	0
19	TGL	N	607	63/63	0.86	0.18	53,109,152,162	0
19	TGL	L	101	63/63	0.87	0.17	58,95,149,160	0
19	TGL	B	303	63/63	0.88	0.18	47,99,151,158	0
24	CHD	J	101	29/29	0.89	0.17	89,107,119,123	0
24	CHD	W	101	29/29	0.89	0.18	102,115,125,128	0
28	DMU	M	101	33/33	0.91	0.12	56,65,83,87	0
16	NA	N	604	1/1	0.92	0.17	62,62,62,62	0
24	CHD	P	301	29/29	0.94	0.10	51,58,61,64	0
25	PEK	G	102	53/53	0.95	0.13	40,83,126,143	0
25	PEK	P	302	53/53	0.95	0.14	54,94,153,177	0

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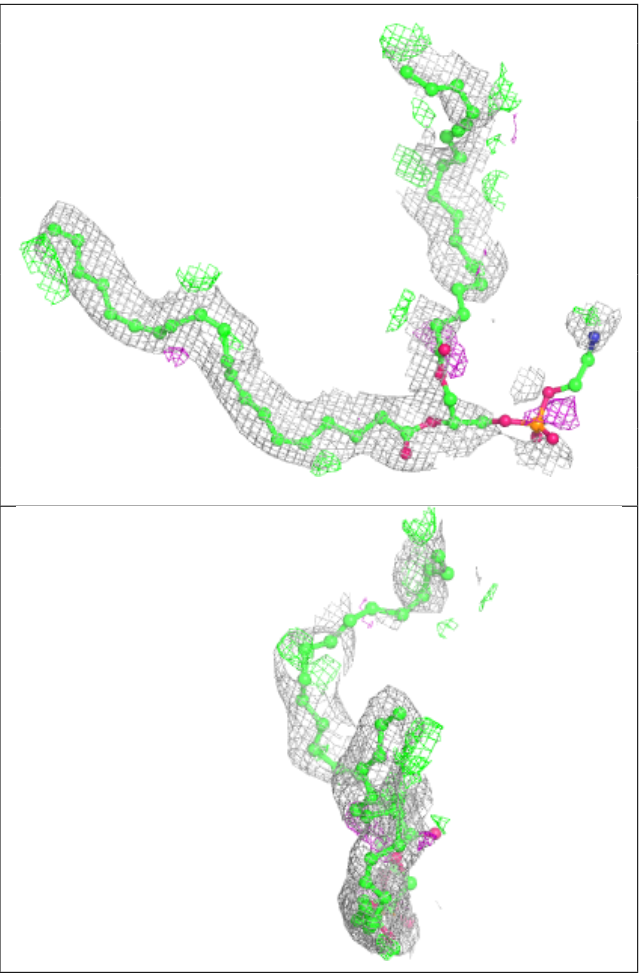
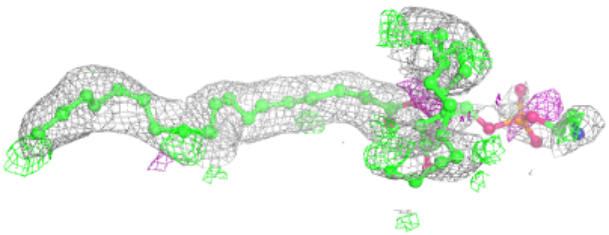
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CHD	C	301	29/29	0.96	0.09	41,48,54,61	0
24	CHD	G	104	29/29	0.96	0.09	45,52,60,66	0
15	MG	N	603	1/1	0.96	0.04	55,55,55,55	0
18	PGV	C	303	51/51	0.97	0.10	38,54,123,140	0
18	PGV	P	304	51/51	0.97	0.11	45,59,172,183	0
24	CHD	B	304	29/29	0.97	0.08	46,50,60,66	0
18	PGV	N	608	51/51	0.97	0.09	43,73,91,94	0
17	HEA	N	606	60/60	0.98	0.08	42,46,56,60	0
16	NA	A	603	1/1	0.98	0.04	45,45,45,45	0
18	PGV	A	607	51/51	0.98	0.09	32,68,86,90	0
22	CUA	O	301	2/2	0.98	0.04	59,59,59,61	0
17	HEA	A	604	60/60	0.98	0.07	32,39,75,81	0
17	HEA	A	605	60/60	0.98	0.07	32,39,51,55	0
17	HEA	N	605	60/60	0.98	0.08	45,56,74,86	0
15	MG	A	602	1/1	0.99	0.05	38,38,38,38	0
14	CU	A	601	1/1	0.99	0.02	46,46,46,46	0
22	CUA	B	301	2/2	0.99	0.03	42,42,42,45	0
27	ZN	F	101	1/1	0.99	0.02	58,58,58,58	0
20	O	N	611	1/1	1.00	0.05	50,50,50,50	0
27	ZN	S	101	1/1	1.00	0.01	64,64,64,64	0
21	OH	A	611	1/1	1.00	0.06	44,44,44,44	0
21	OH	N	612	1/1	1.00	0.05	64,64,64,64	0
14	CU	N	602	1/1	1.00	0.02	58,58,58,58	0
20	O	A	610	1/1	1.00	0.03	35,35,35,35	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 G 103:

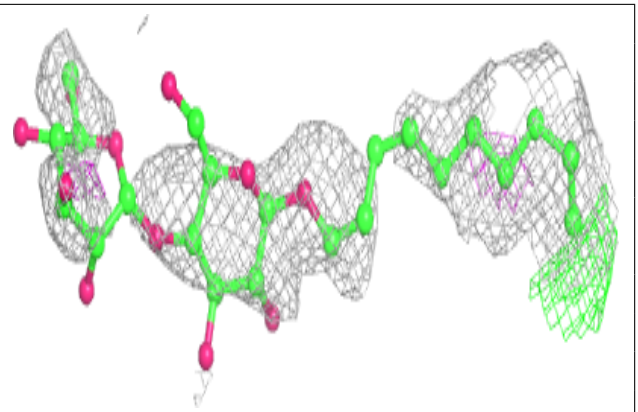
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

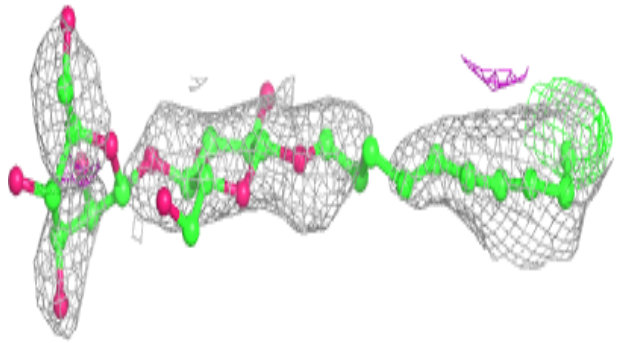


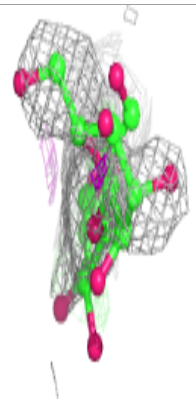


Electron density around DMU T 101:

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

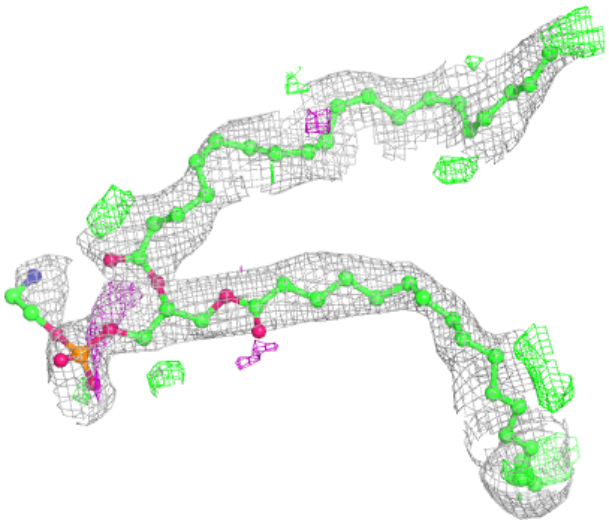


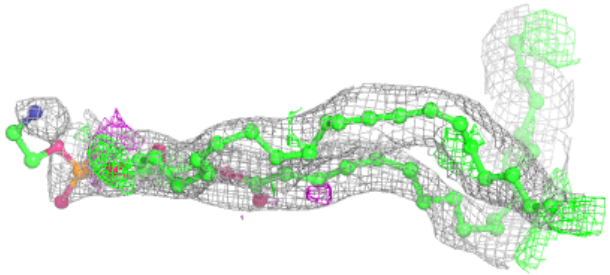


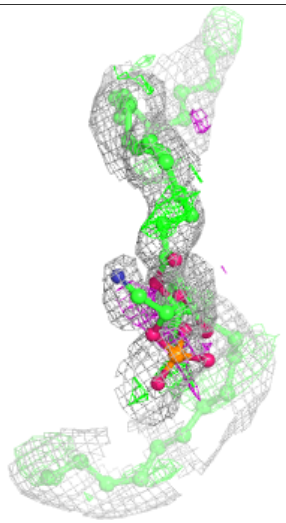


Electron density around PEK P 303:

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

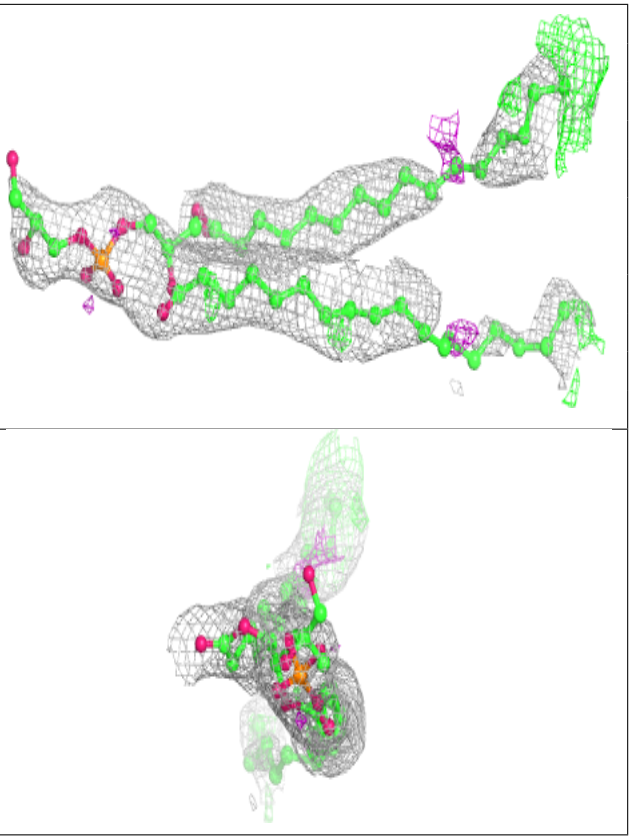


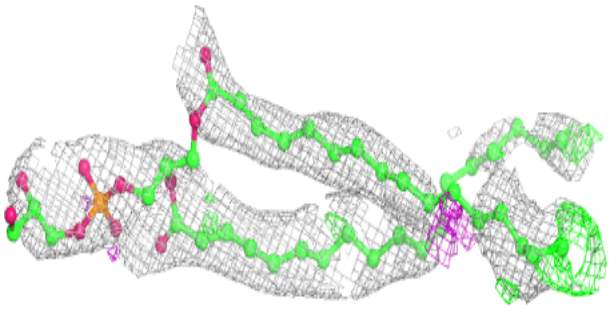




Electron density around PGV N 610:

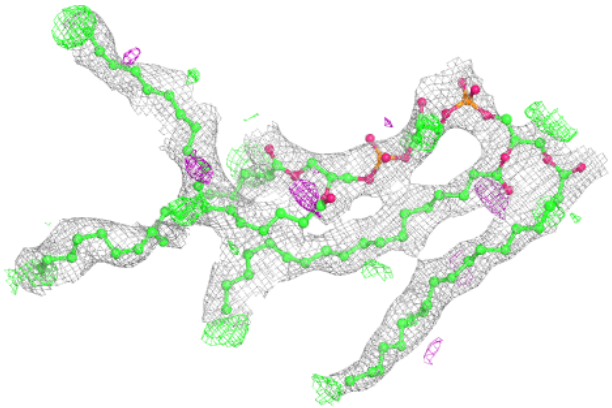
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

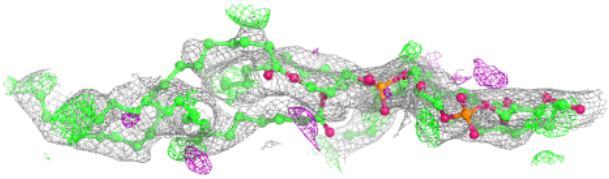


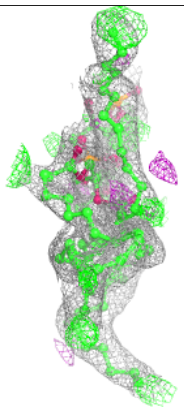


Electron density around CDL T 103:

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

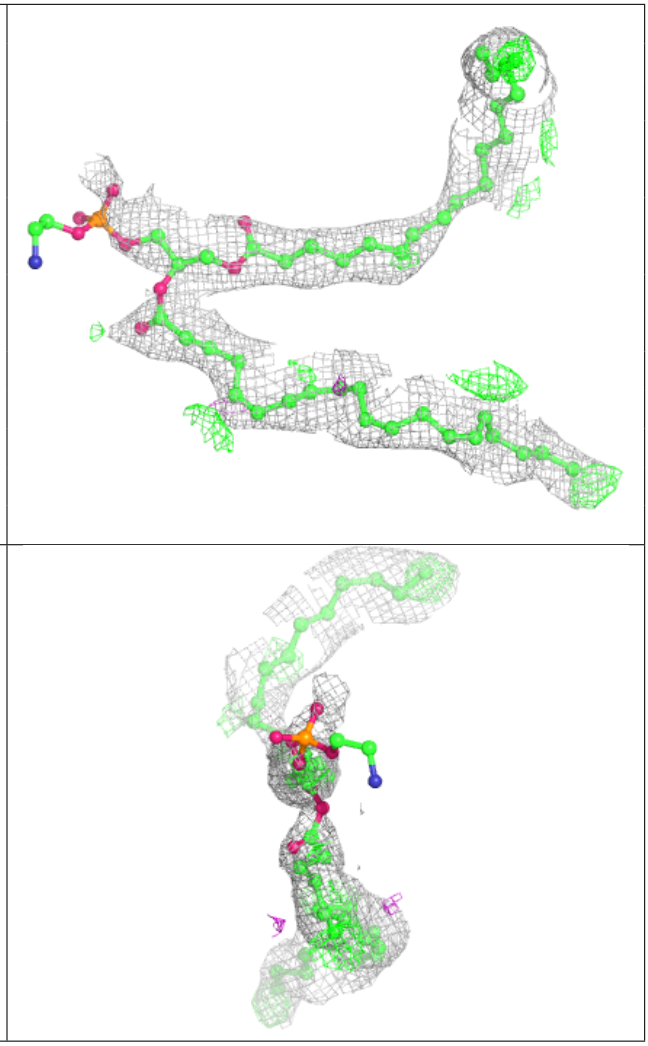






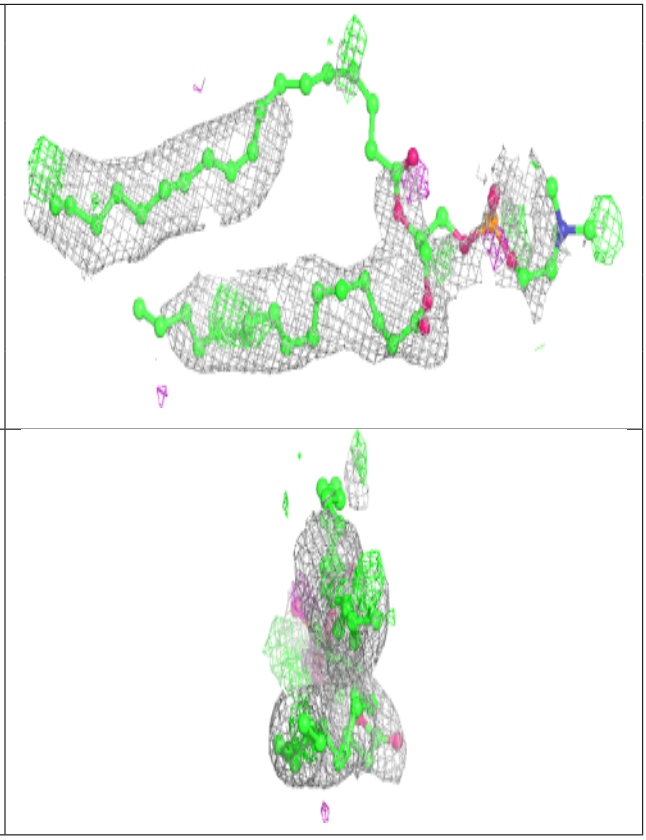
Electron density around PEK C 302:

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



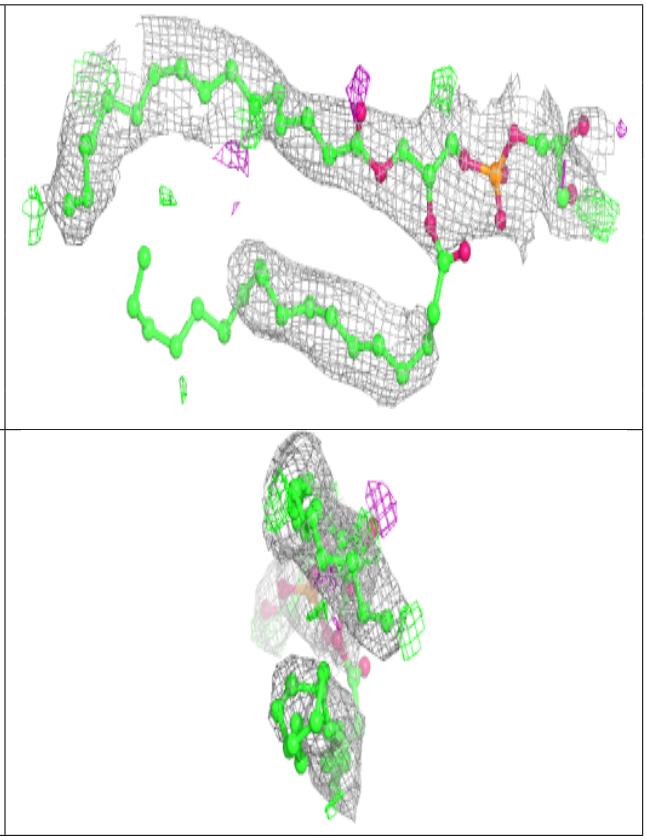
Electron density around PSC B 302:

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



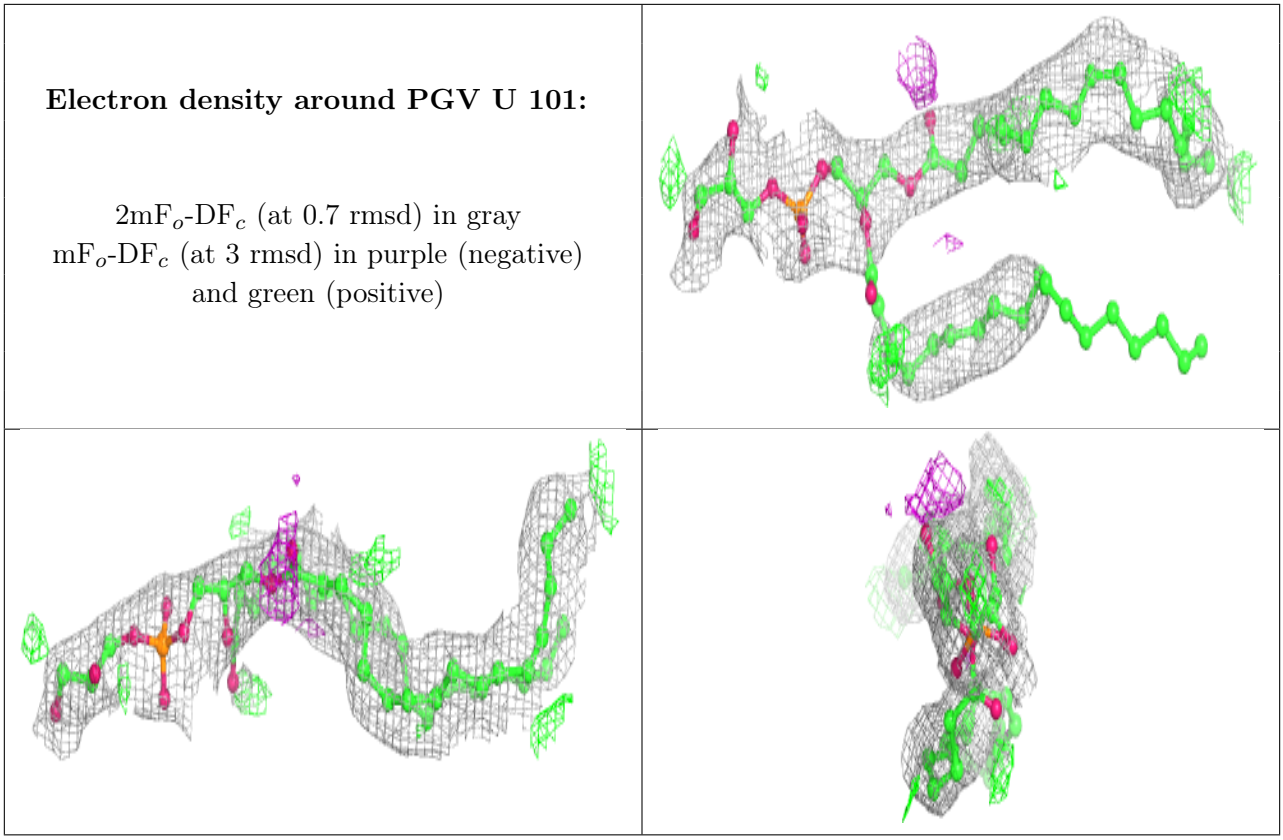
Electron density around PGV A 608:

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



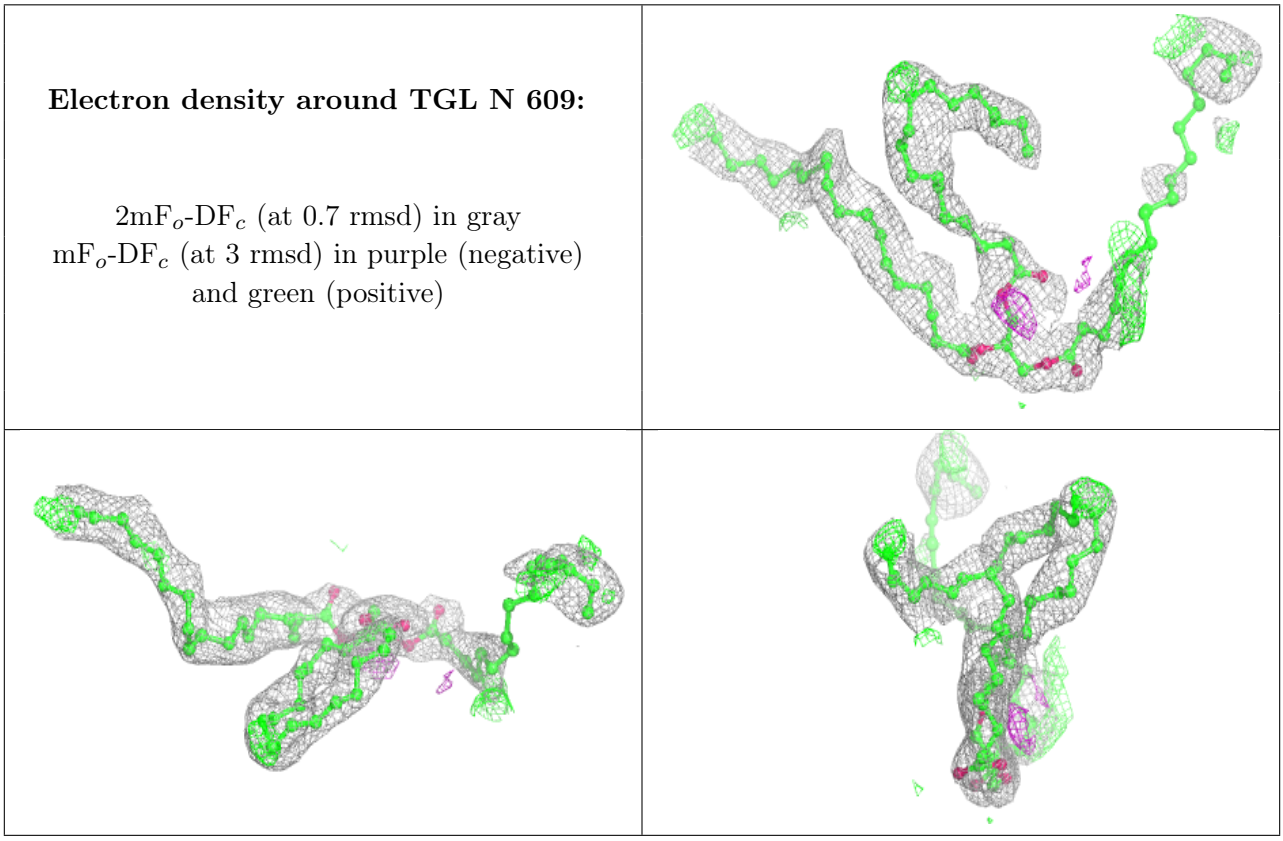
Electron density around PGV U 101:

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



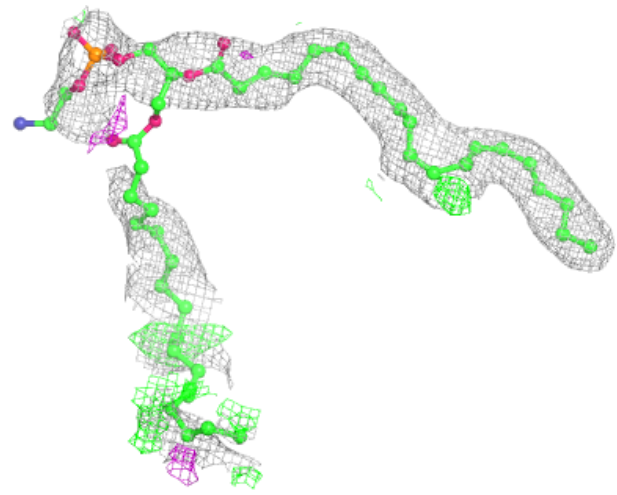
Electron density around TGL N 609:

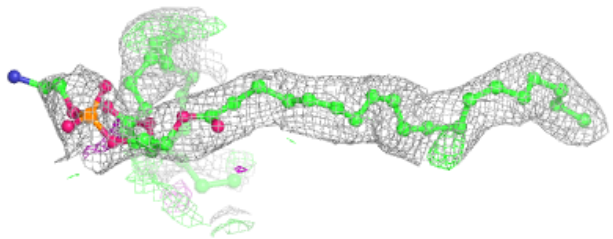
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

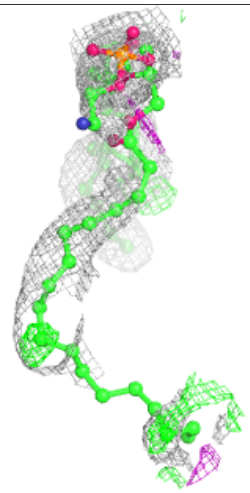


Electron density around PEK T 102:

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

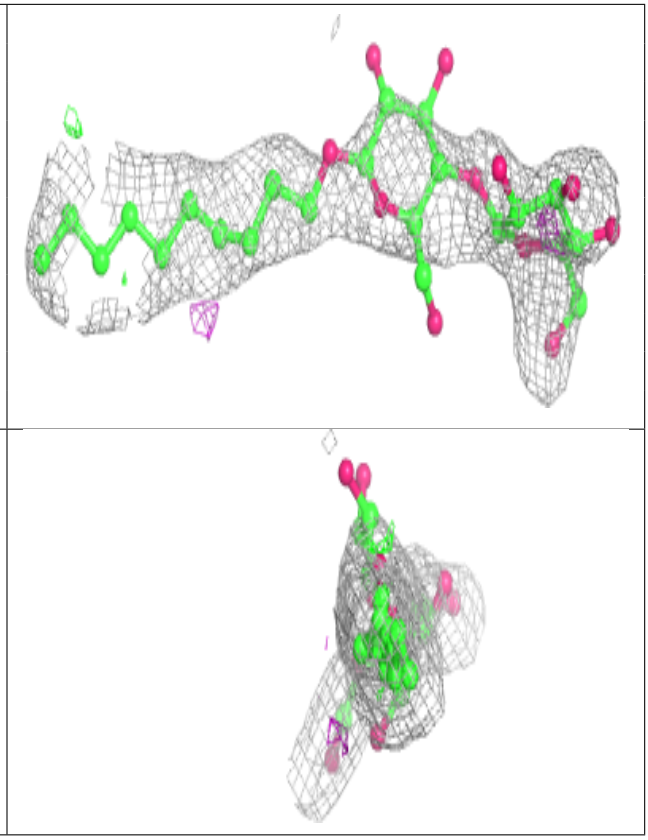






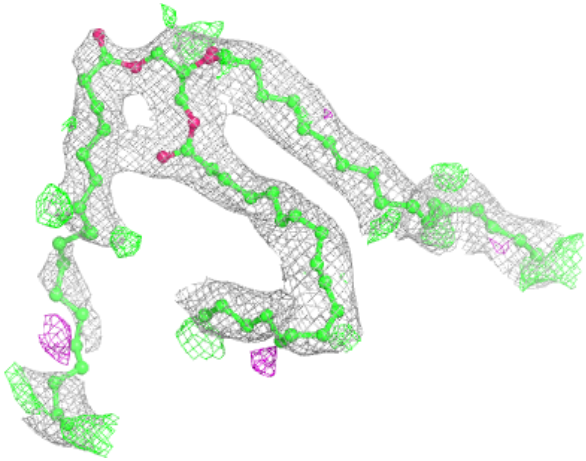
Electron density around DMU G 101:

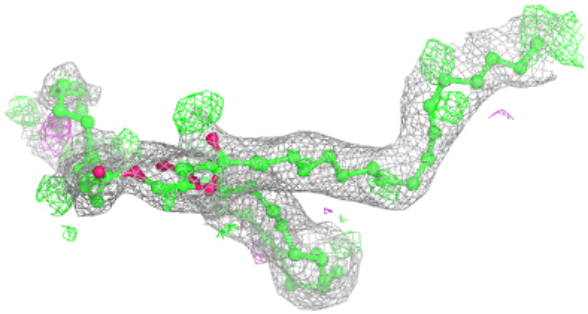
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

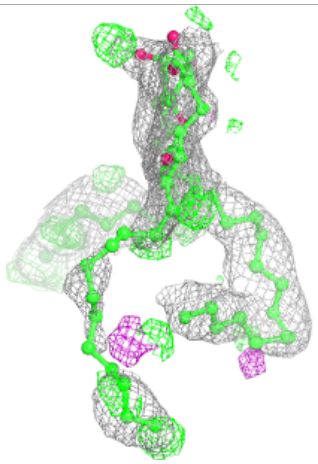


Electron density around TGL A 609:

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

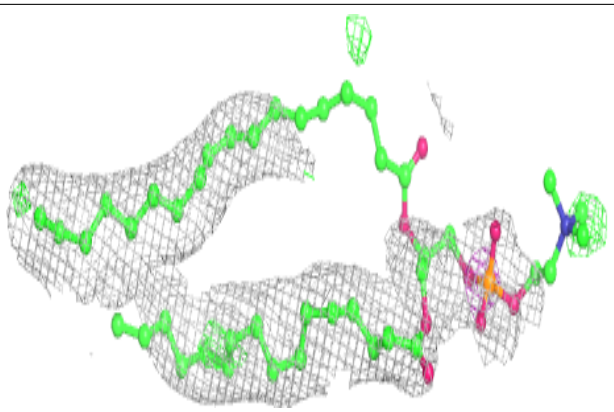


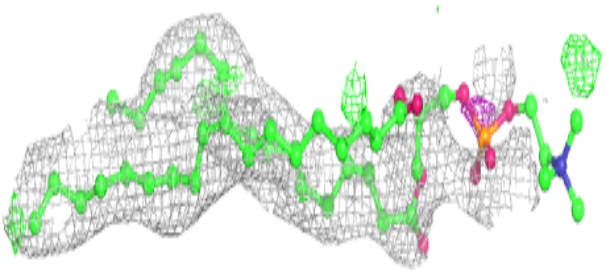


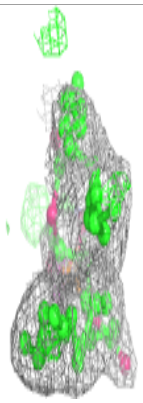


Electron density around PSC O 302:

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

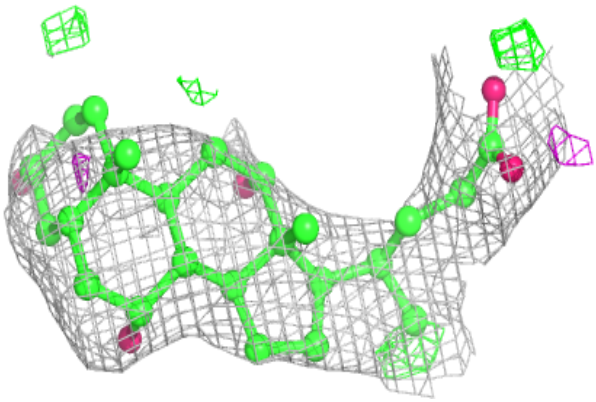


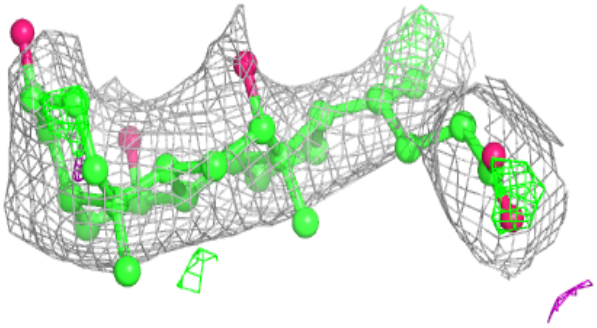


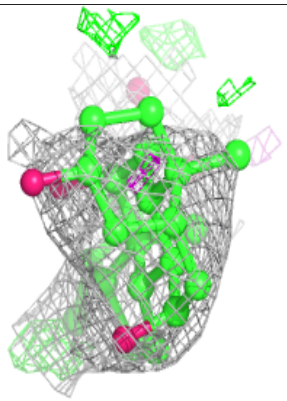


Electron density around CHD W 102:

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

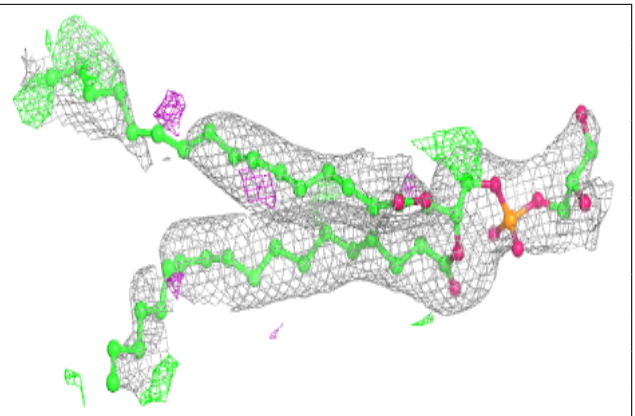


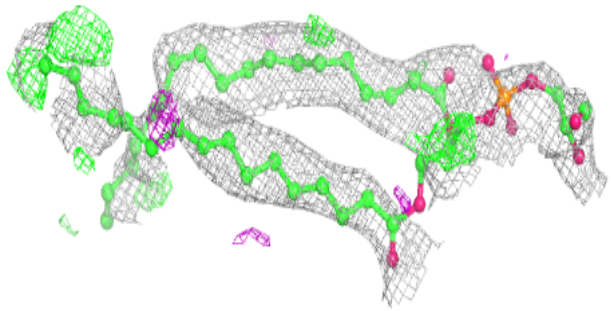


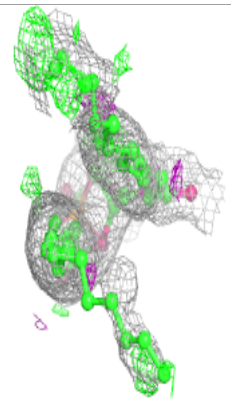


Electron density around PGV A 606:

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

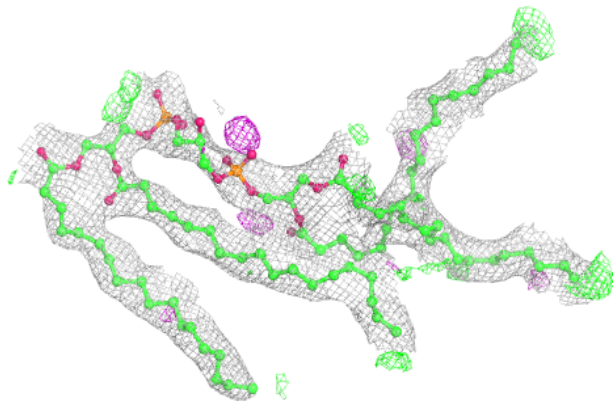


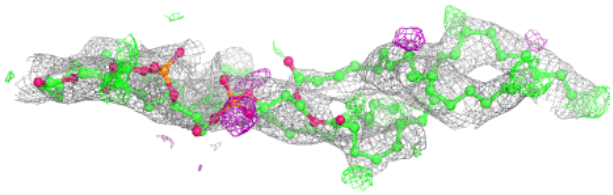


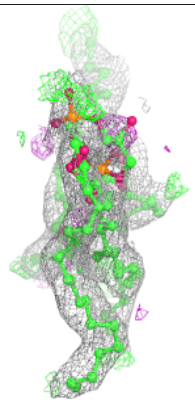


Electron density around CDL N 601:

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

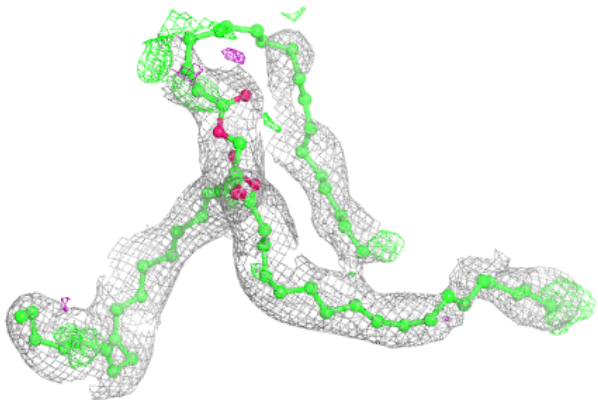


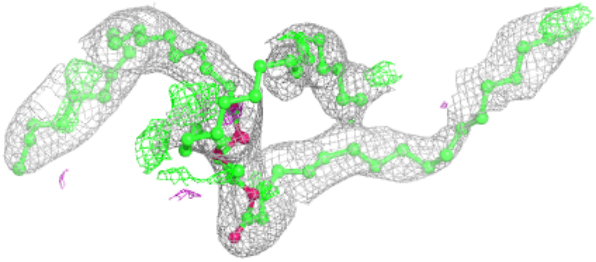


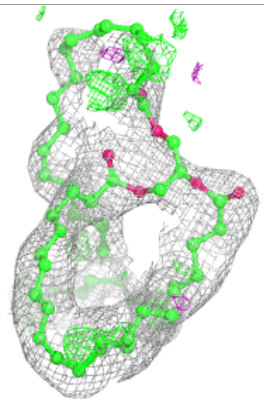


Electron density around TGL Y 101:

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

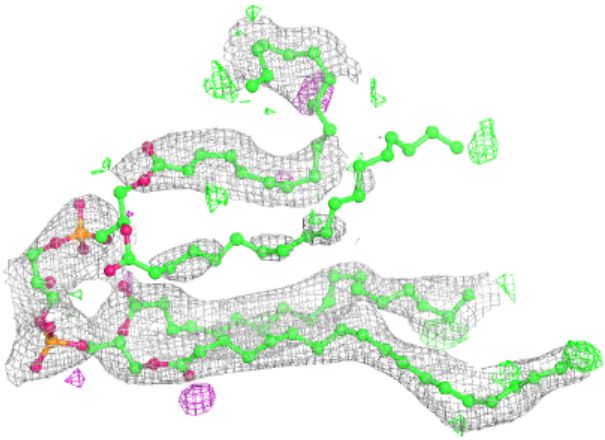


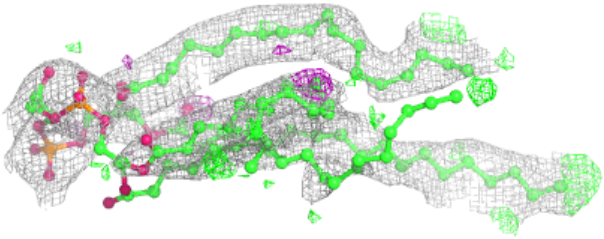


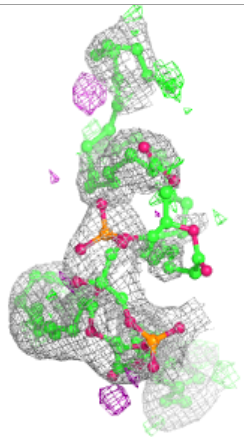


Electron density around CDL P 305:

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

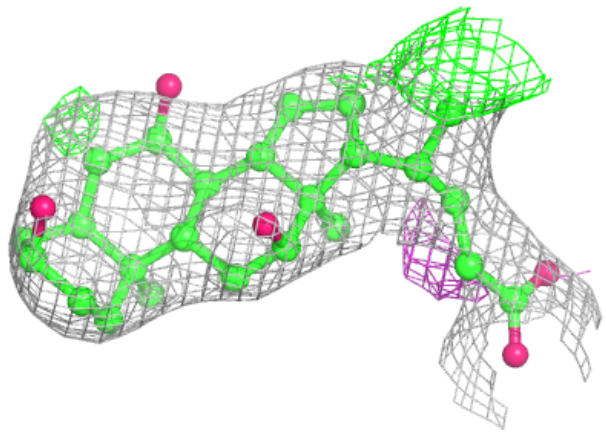


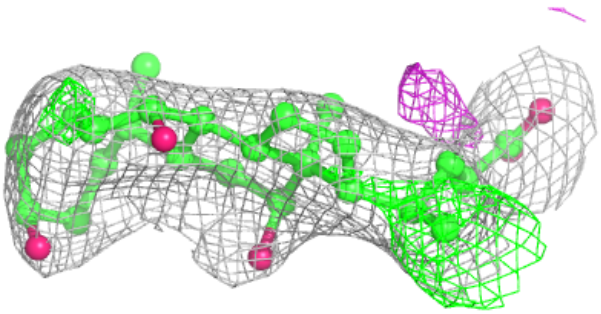


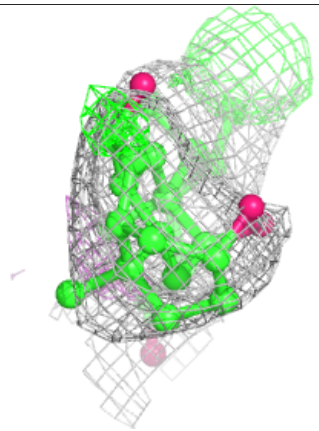


Electron density around CHD J 102:

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

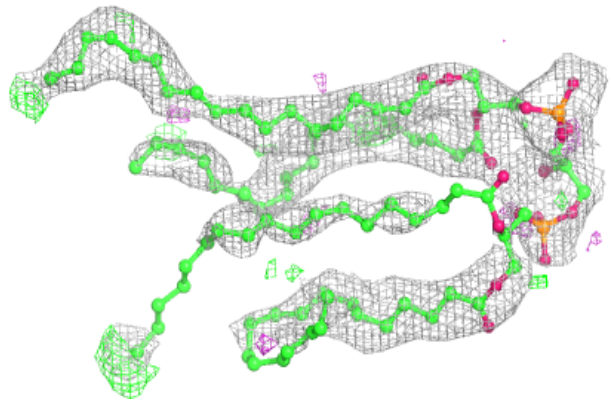


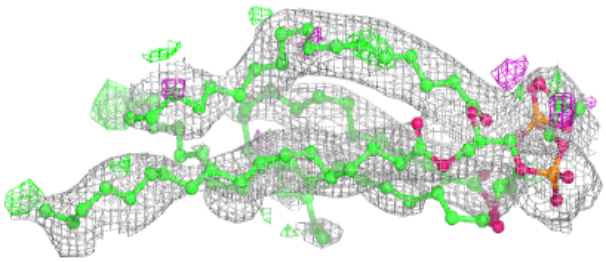


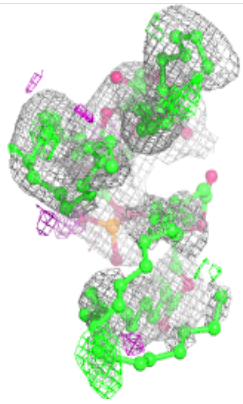


Electron density around CDL C 304:

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

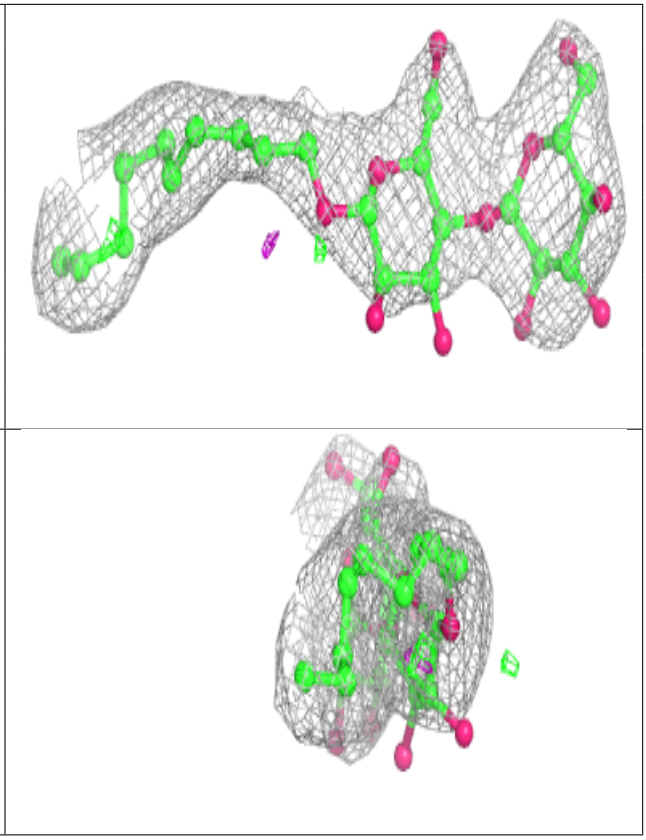






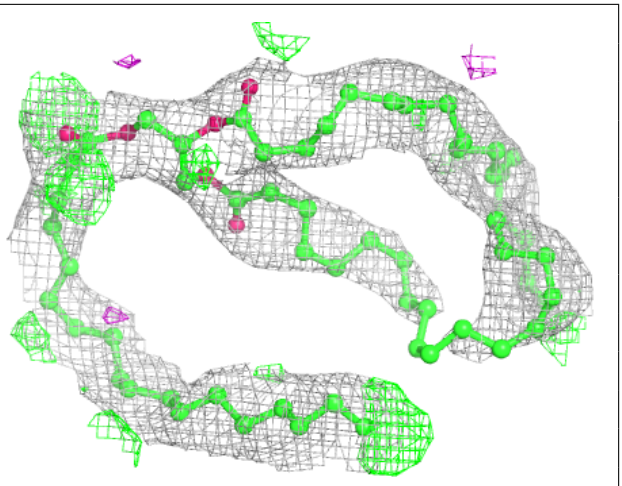
Electron density around DMU Q 201:

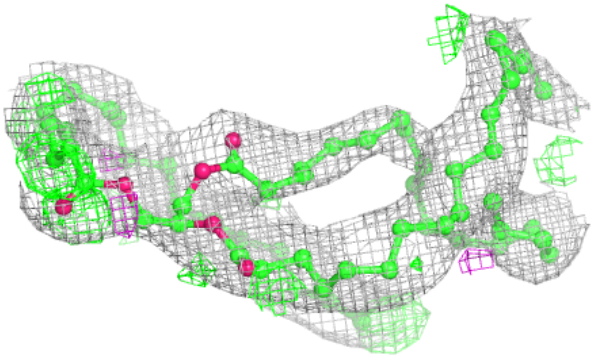
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

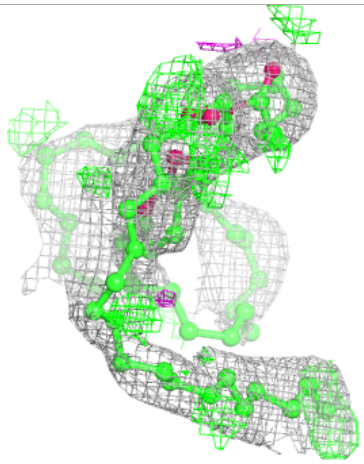


Electron density around TGL N 607:

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

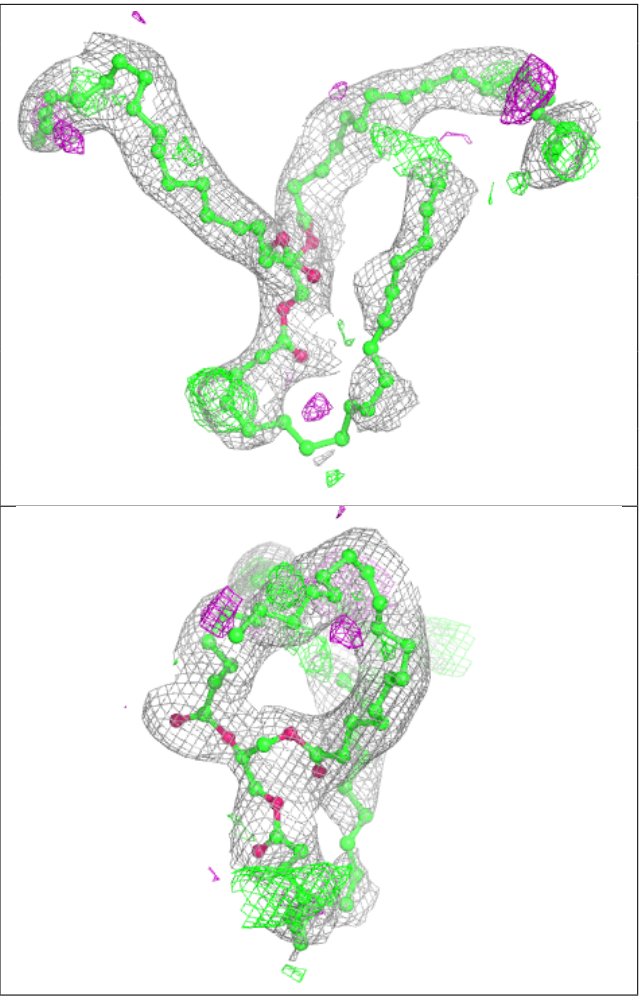






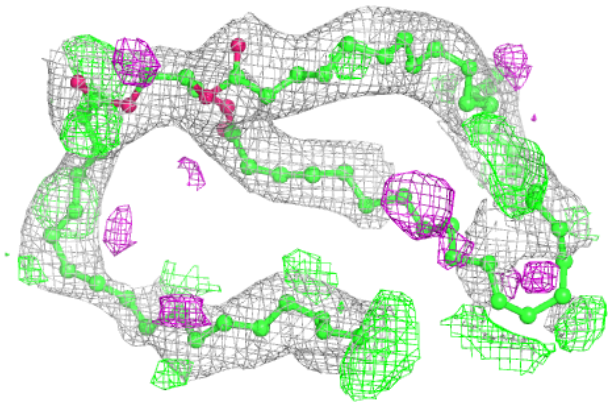
Electron density around TGL L 101:

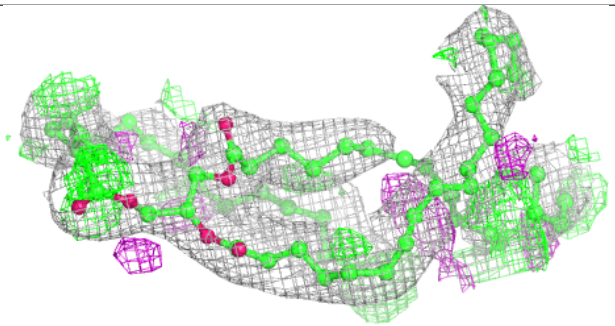
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

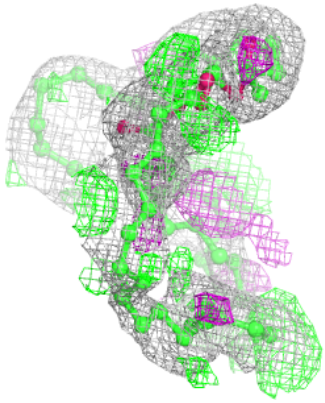


Electron density around TGL B 303:

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

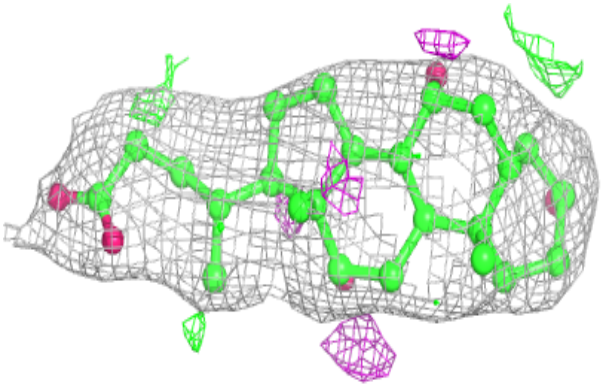


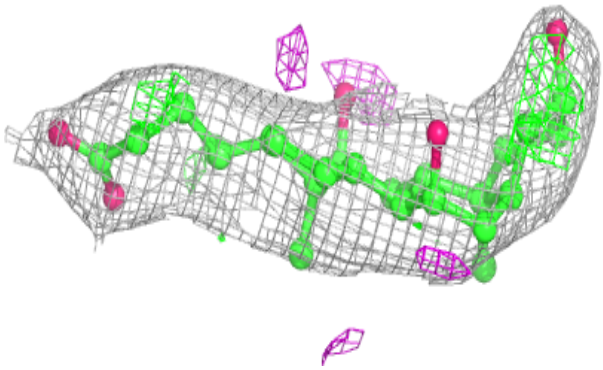


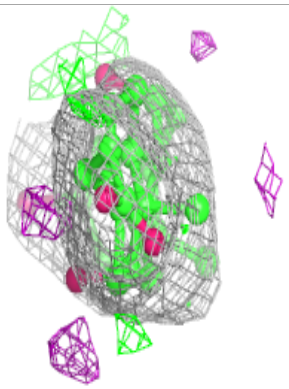


Electron density around CHD J 101:

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

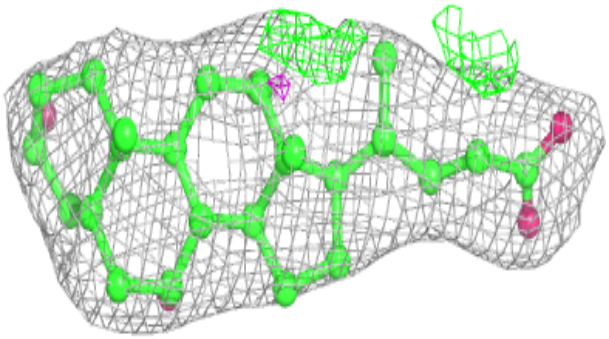


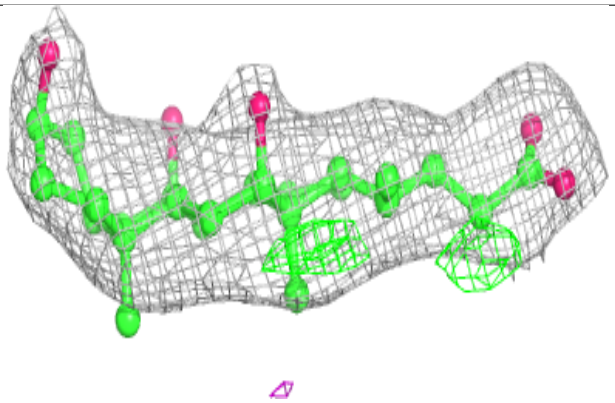


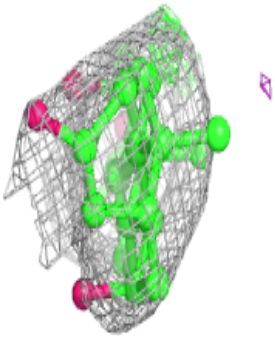


Electron density around CHD W 101:

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

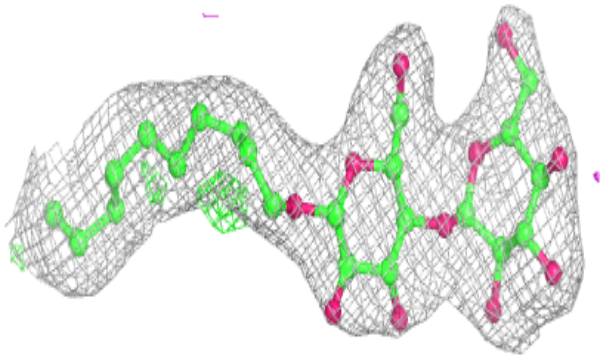


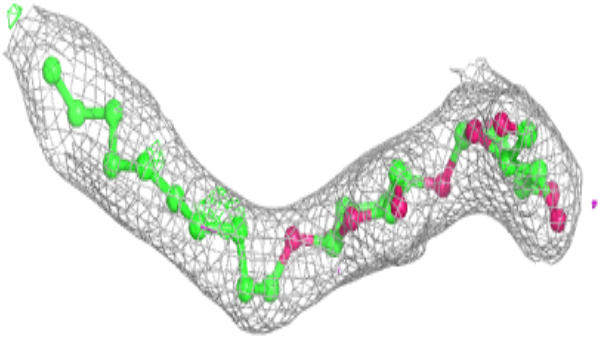


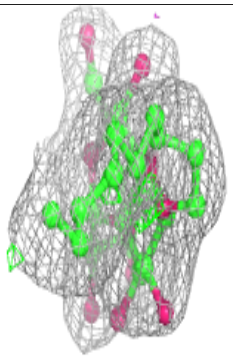


Electron density around DMU M 101:

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

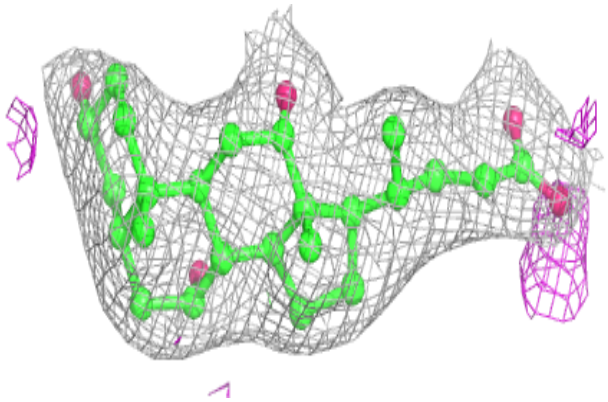


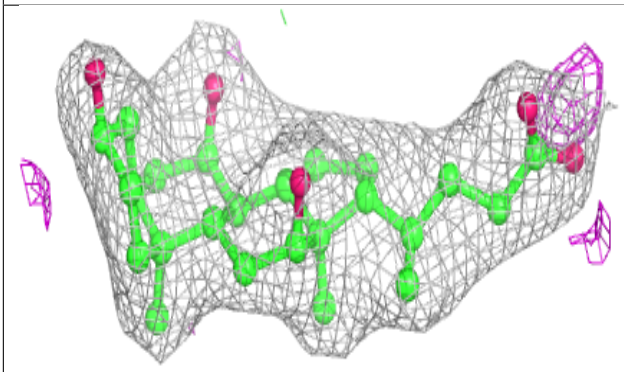


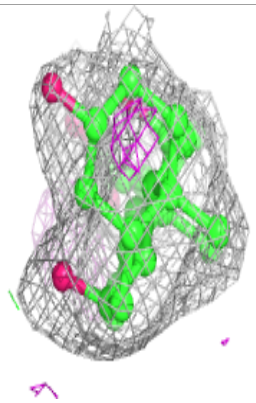


Electron density around CHD P 301:

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

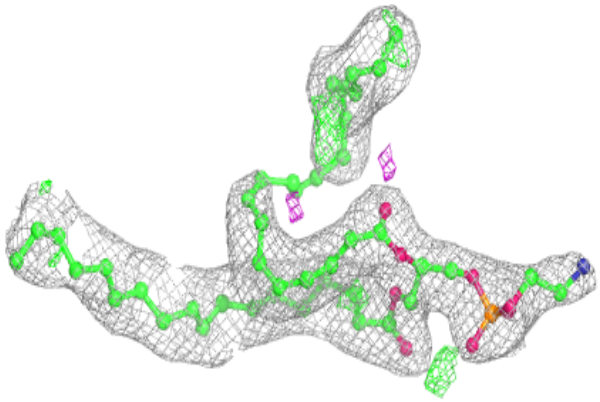


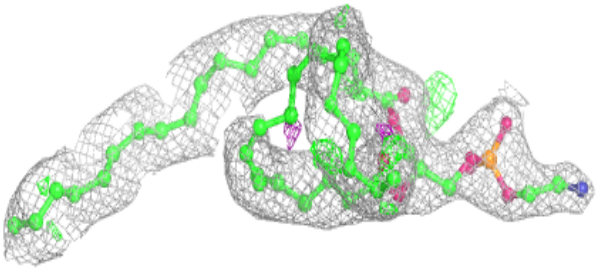


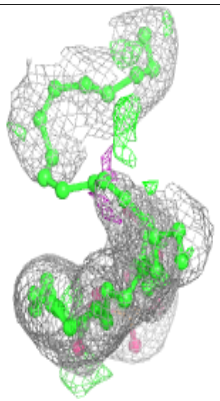


Electron density around PEK G 102:

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

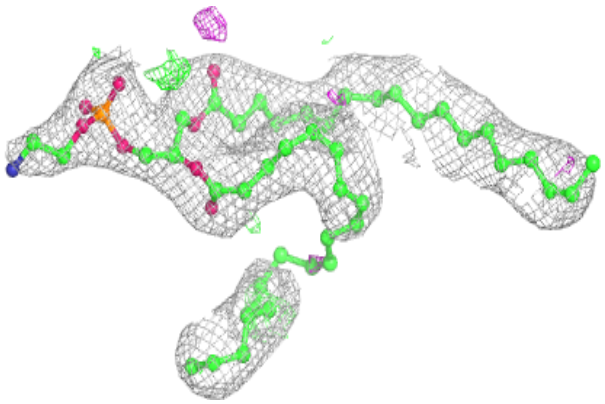


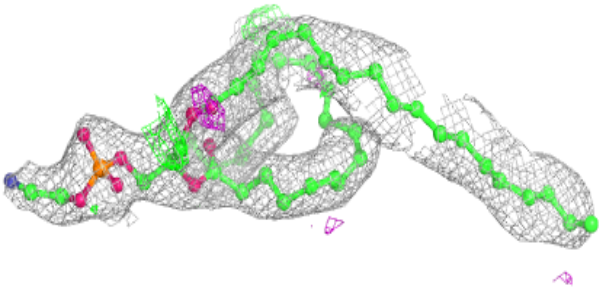


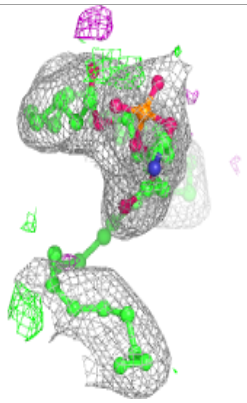


Electron density around PEK P 302:

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

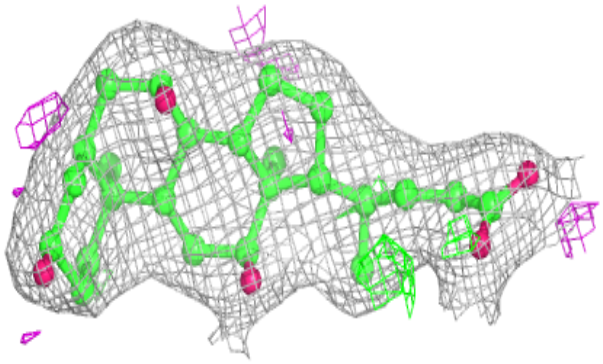


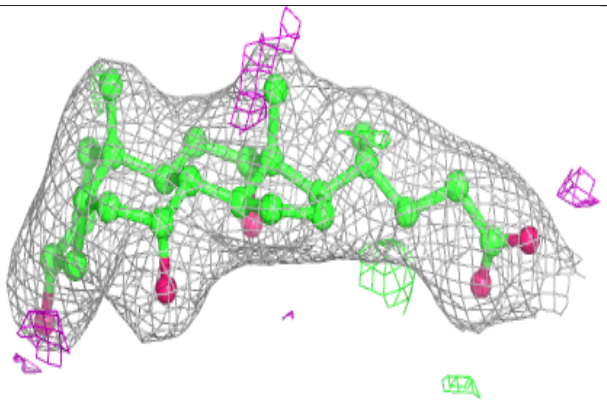


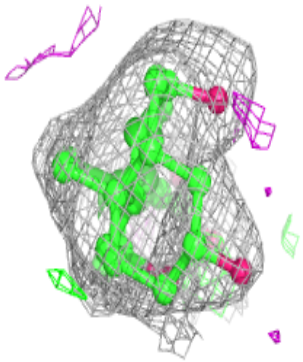


Electron density around CHD C 301:

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

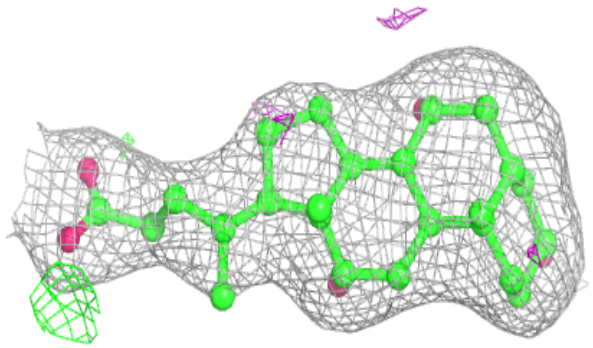


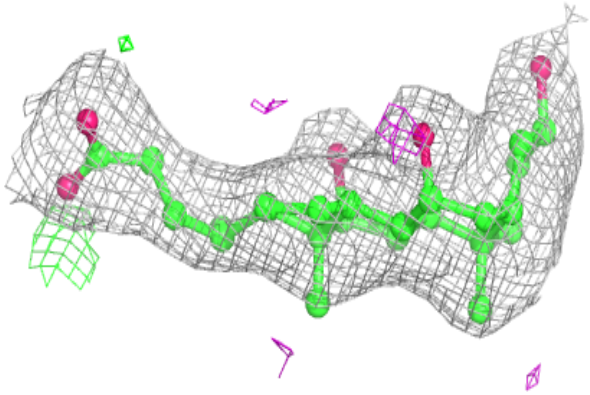


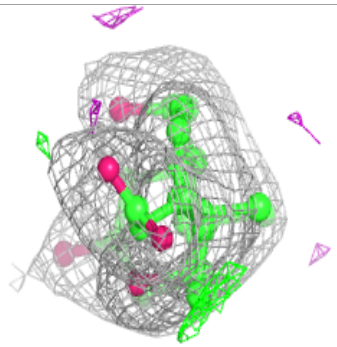


Electron density around CHD G 104:

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

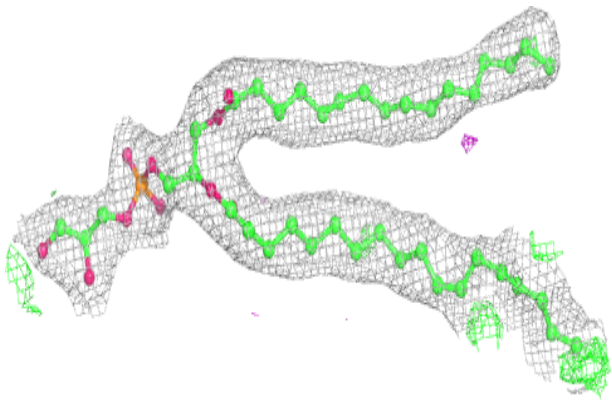


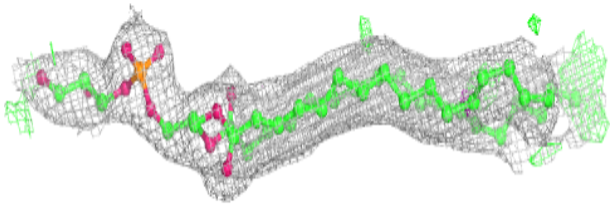


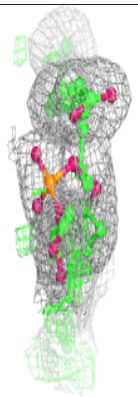


Electron density around PGV C 303:

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

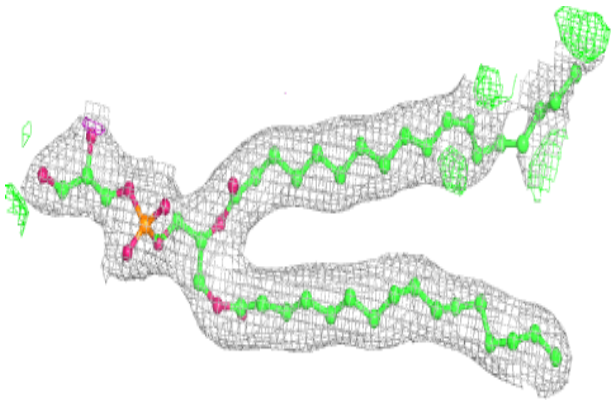


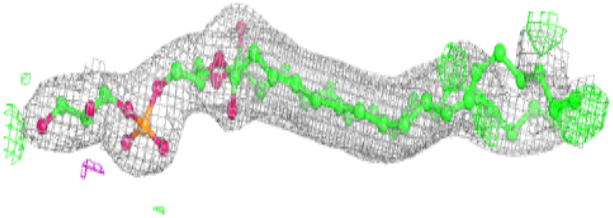


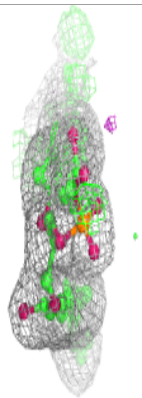


Electron density around PGV P 304:

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

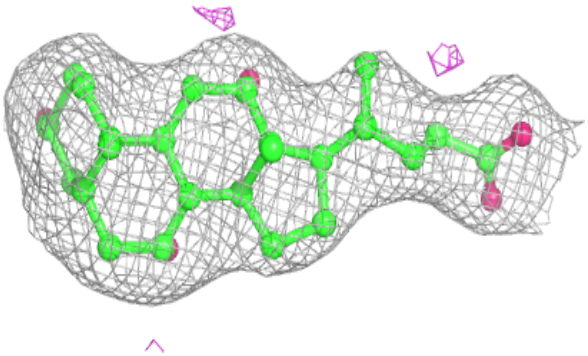


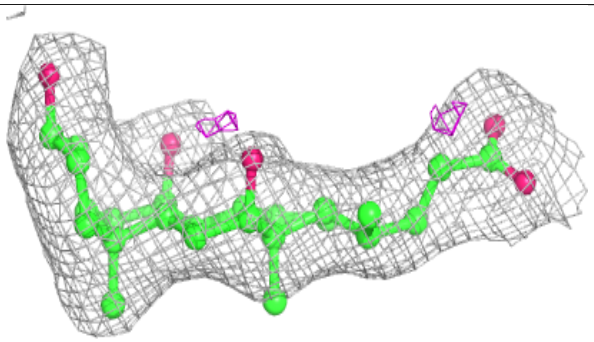


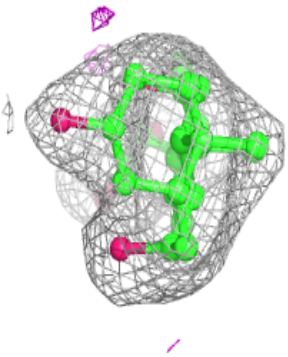


Electron density around CHD B 304:

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

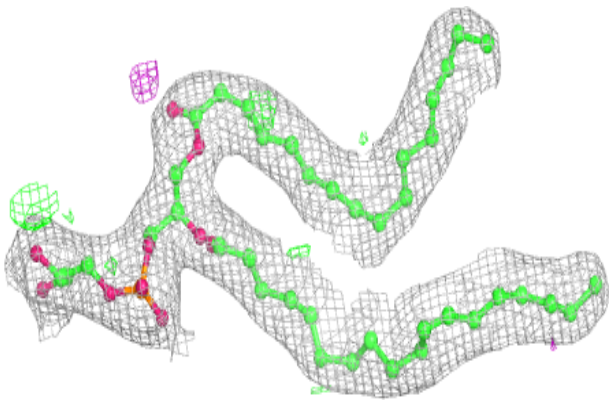


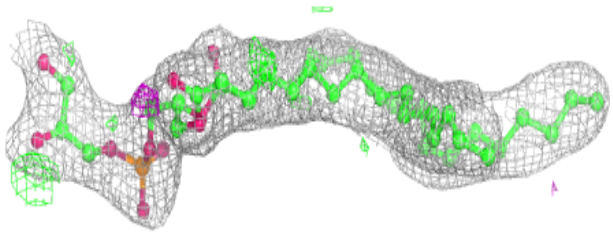


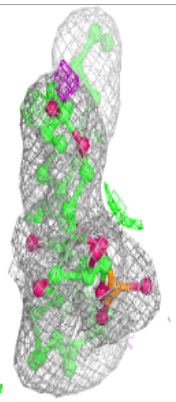


Electron density around PGV N 608:

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

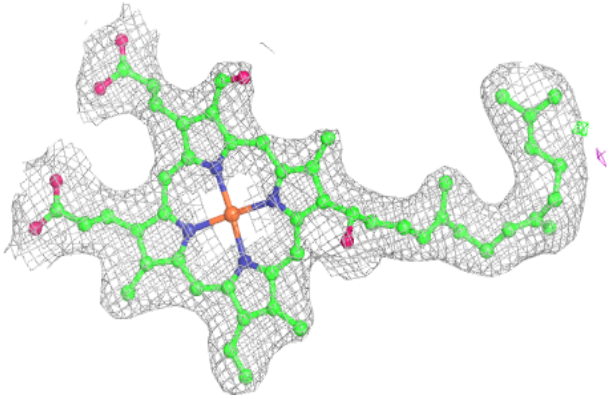


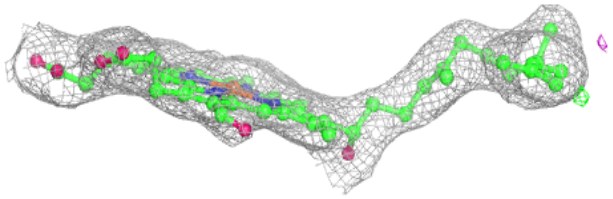


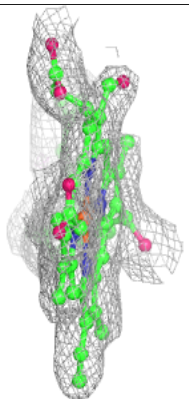


Electron density around HEA N 606:

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

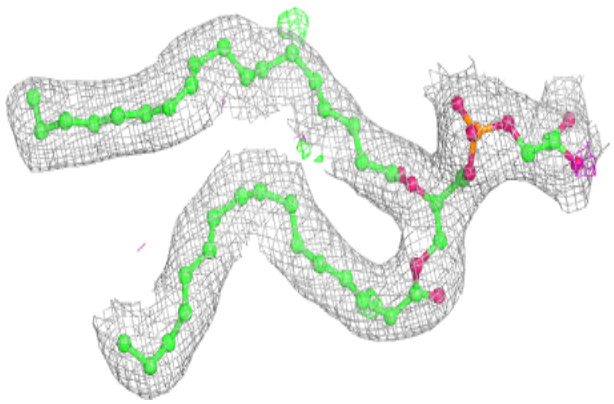


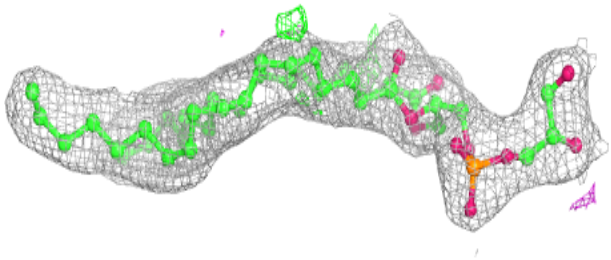


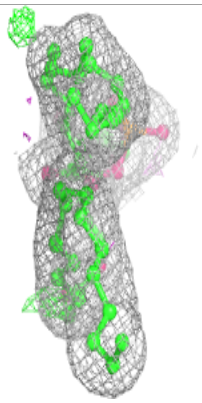


Electron density around PGV A 607:

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

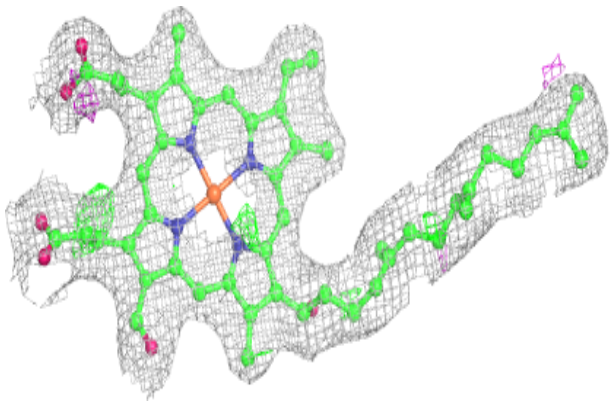


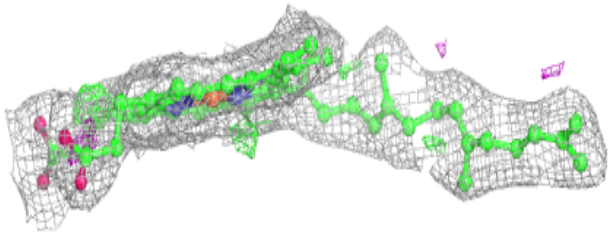


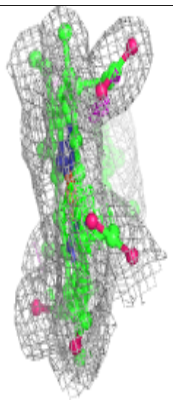


Electron density around HEA A 604:

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

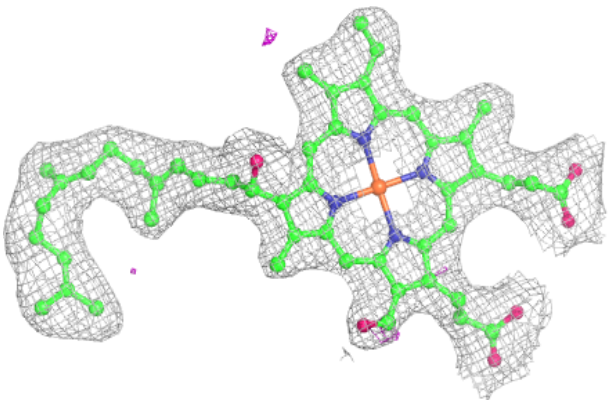


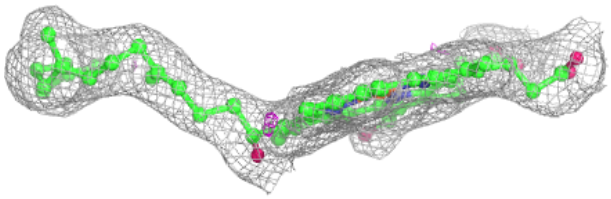


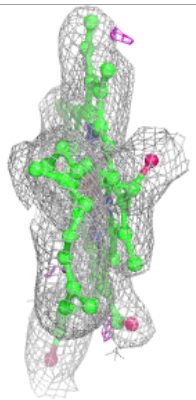


Electron density around HEA A 605:

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

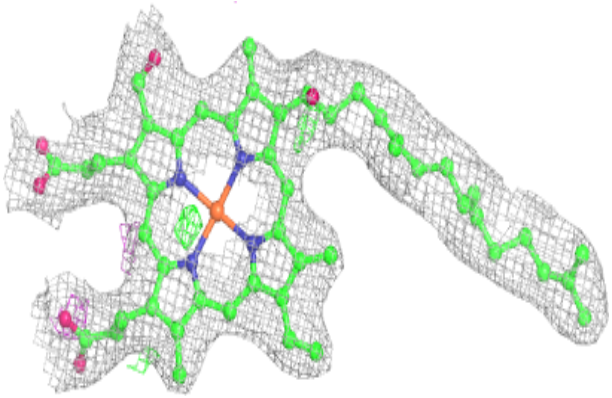


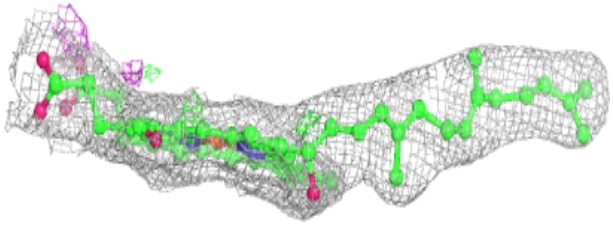


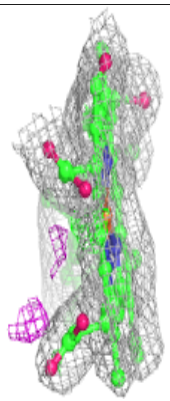


Electron density around HEA N 605:

$2mF_o$-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.