Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2023 – 02:20 PM EDT

PDB ID	:	8GBT
Title	:	Time-resolve SFX structure of a photoproduct of carbon monoxide complex of bovine cytochrome c oxidase
Authors	:	Ishigami, I.; Yeh, S.-R.; Rousseau, D.L.
Deposited on	:	2023-02-28
Resolution	:	2.80 Å(reported)

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

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

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

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

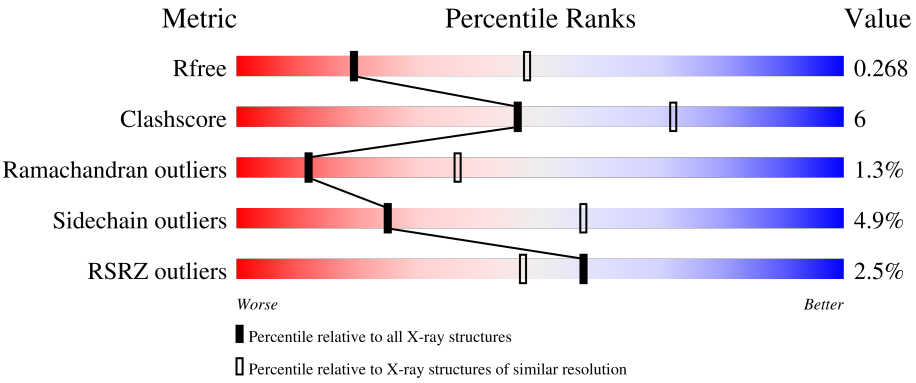
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	514	87% 13%
1	N	514	% 77% 22%
2	B	227	% 80% 18%
2	O	227	2% 78% 21%
3	C	261	85% 14%

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Mol	Chain	Length	Quality of chain
3	P	261	80% 19%
4	D	147	78% 18%
4	Q	147	5% 82% 14%
5	E	109	80% 17%
5	R	109	2% 82% 15%
6	F	98	6% 83% 15%
6	S	98	8% 81% 17%
7	G	85	15% 67% 28%
7	T	85	11% 75% 19% 5%
8	H	85	4% 78% 13% 7%
8	U	85	6% 79% 13% 7%
9	I	73	81% 18%
9	V	73	7% 79% 16%
10	J	59	3% 90% 7%
10	W	59	7% 81% 17%
11	K	56	82% 12%
11	X	56	7% 59% 23% 12%
12	L	47	89% 9%
12	Y	47	2% 77% 21%
13	M	46	2% 83% 11% 7%
13	Z	46	7% 61% 30% 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
19	PGV	Z	101	-	-	-	X
25	PSC	R	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	PEK	G	106	-	-	-	X
27	PEK	T	103	-	-	-	X
28	DMU	G	102	X	-	-	X
28	DMU	M	102	X	-	-	-
28	DMU	Q	201	X	-	-	-
28	DMU	T	102	X	-	-	X
29	SAC	I	102	-	-	-	X
29	SAC	V	101	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 30981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

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

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

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

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

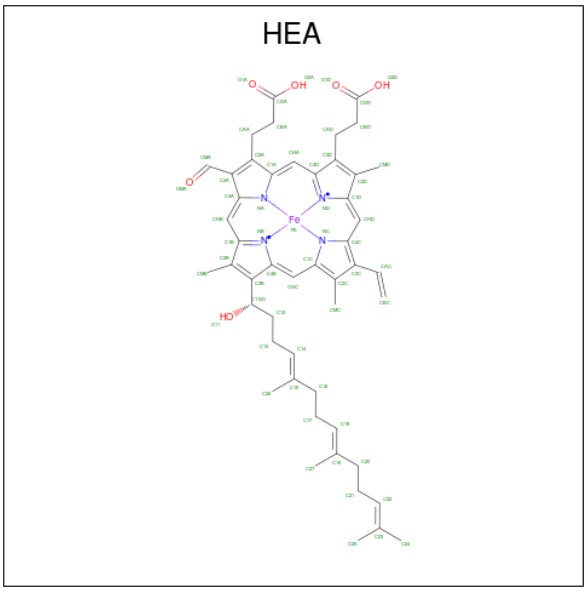
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

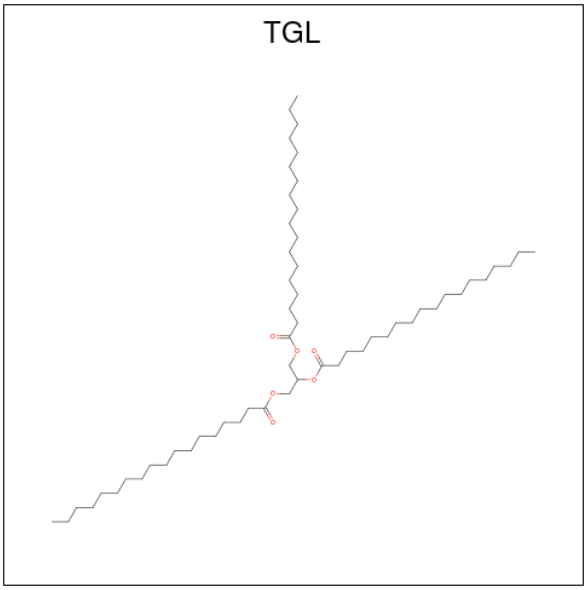
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

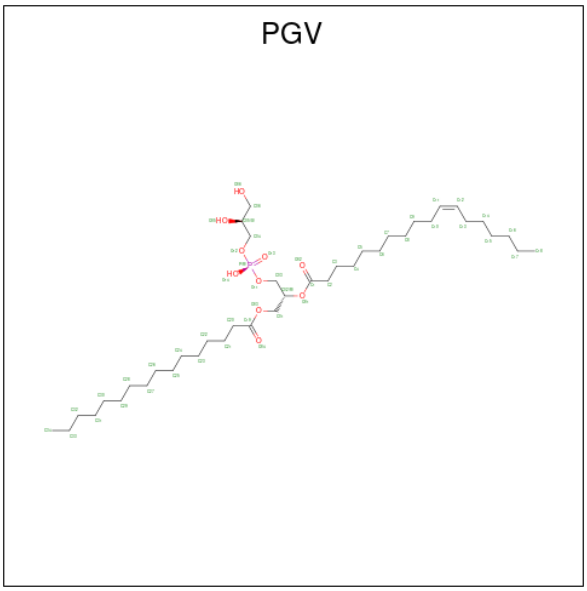
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



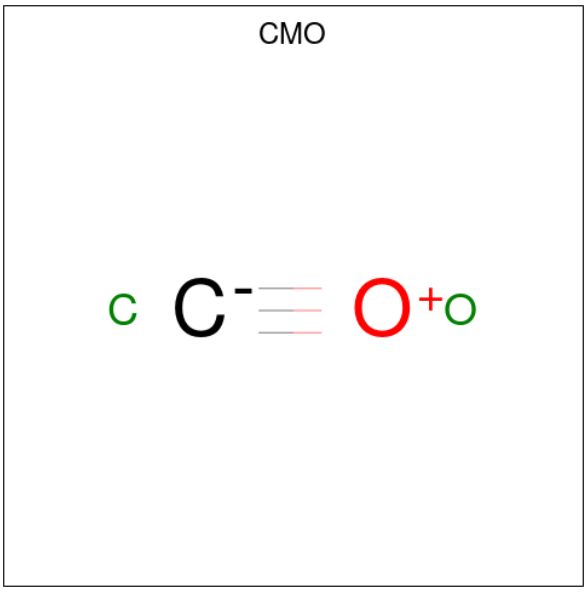
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 63 57 6	0	0
18	I	1	Total C O 63 57 6	0	0
18	L	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	Y	1	Total C O 63 57 6	0	0

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



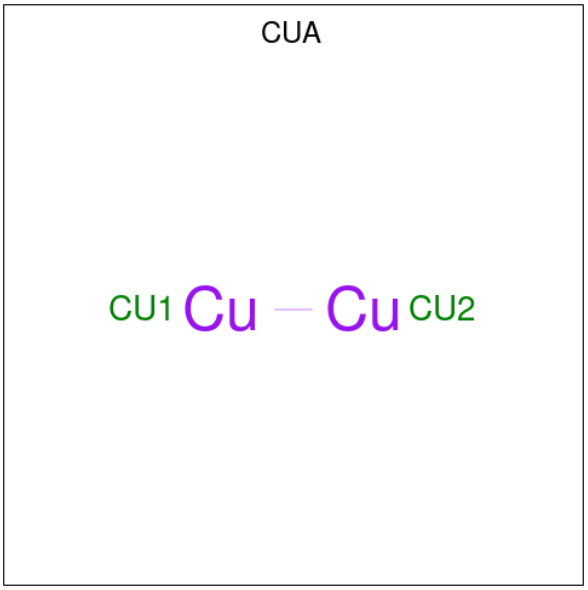
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	M	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	U	1	Total	C	O	P	0	0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

- Molecule 20 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



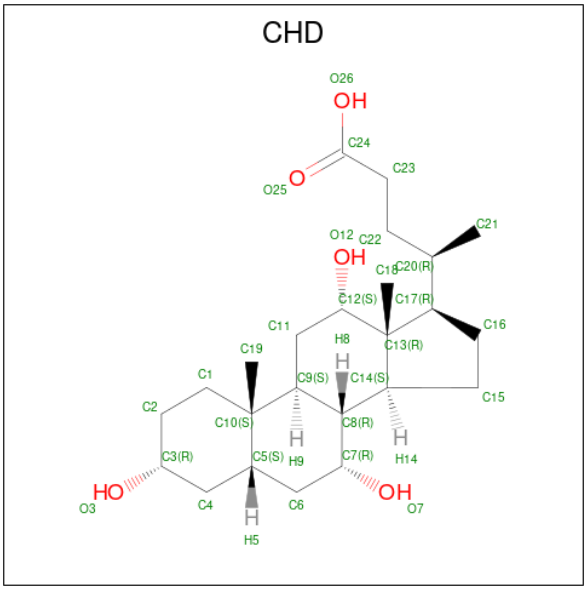
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 2 1 1	0	0
20	N	1	Total C O 2 1 1	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



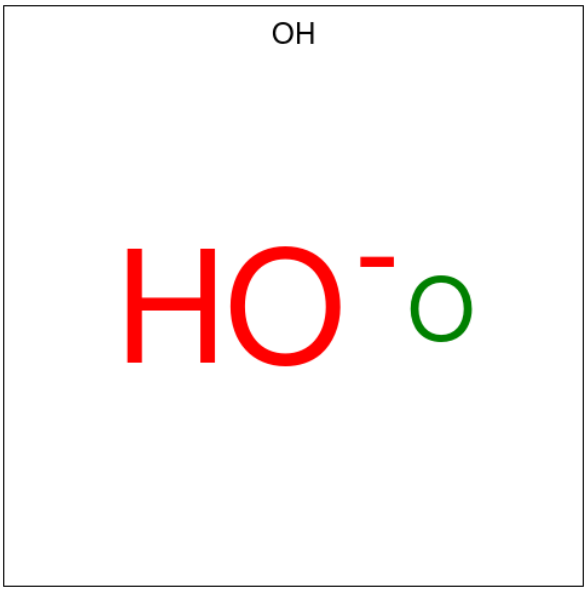
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

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



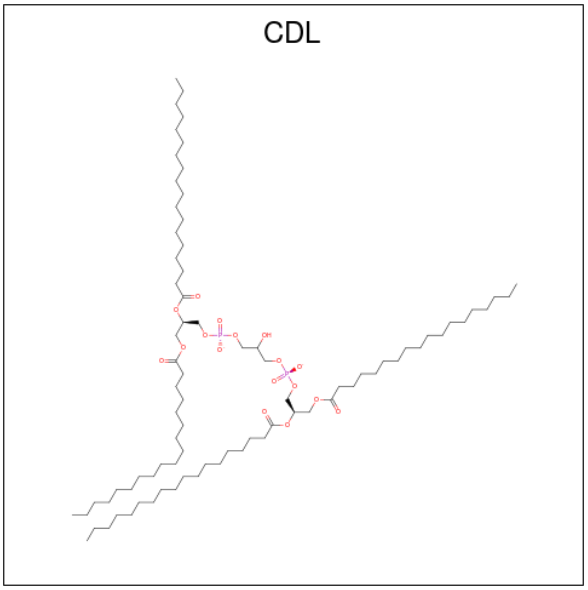
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	N	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0

- Molecule 23 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total O 1 1	0	1
23	P	1	Total O 1 1	0	1

- Molecule 24 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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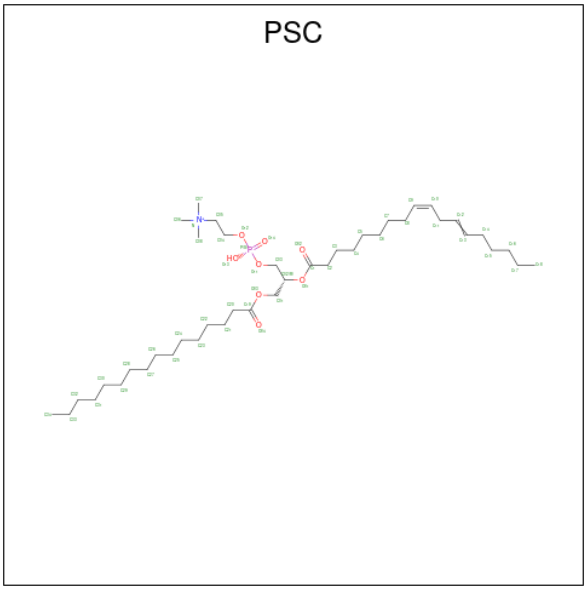
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	P	1	Total	C	O	P	0	0
			100	81	17	2		
24	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 25 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: $C_{42}H_{81}NO_8P$) (labeled as "Ligand of Interest" by depositor).

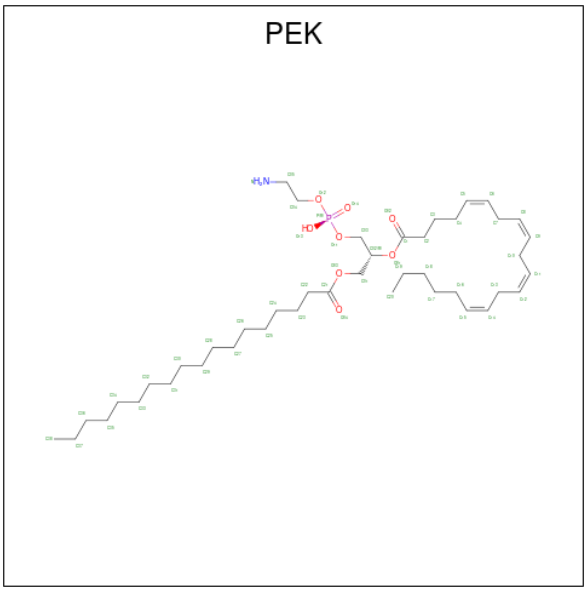


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

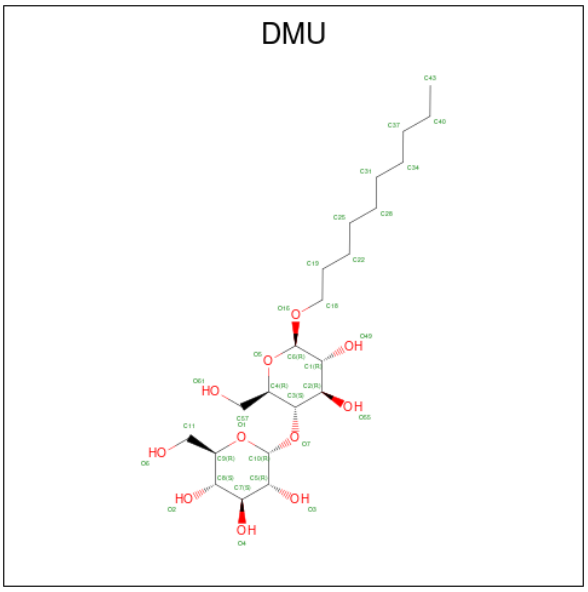
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	F	1	Total	Zn	0	0
			1	1		
26	S	1	Total	Zn	0	0
			1	1		

- Molecule 27 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: $C_{43}H_{78}NO_8P$).



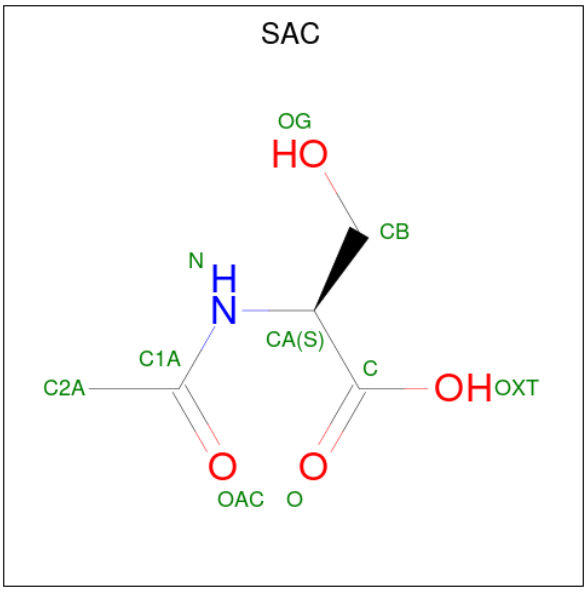
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is N-ACETYL-SERINE (three-letter code: SAC) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	1	Total C N O 9 5 1 3	0	0
29	V	1	Total C N O 9 5 1 3	0	0

- Molecule 30 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	43	Total O 43 43	0	0
30	B	21	Total O 21 21	0	0
30	C	23	Total O 23 23	0	0
30	D	11	Total O 11 11	0	0
30	E	10	Total O 10 10	0	0
30	F	7	Total O 7 7	0	0
30	G	11	Total O 11 11	0	0
30	H	1	Total O 1 1	0	0
30	I	2	Total O 2 2	0	0
30	K	4	Total O 4 4	0	0
30	L	4	Total O 4 4	0	0
30	M	3	Total O 3 3	0	0
30	N	31	Total O 31 31	0	0
30	O	21	Total O 21 21	0	0
30	P	12	Total O 12 12	0	0
30	Q	7	Total O 7 7	0	0
30	R	8	Total O 8 8	0	0
30	S	5	Total O 5 5	0	0

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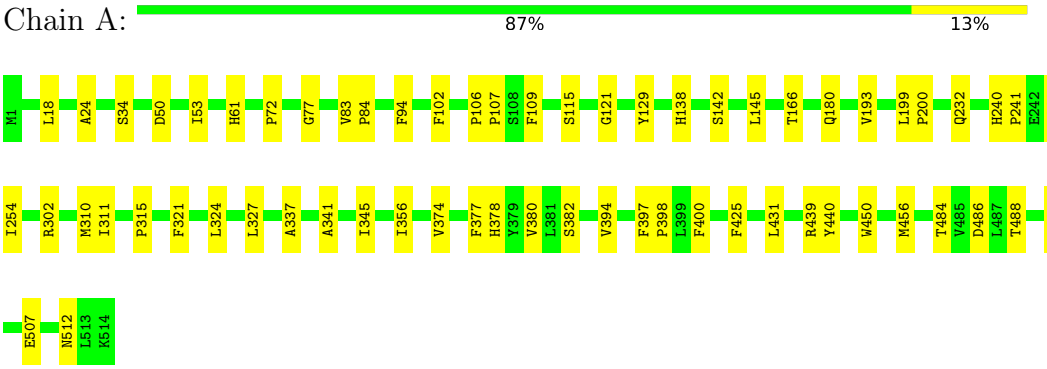
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	T	7	Total O 7 7	0	0
30	U	1	Total O 1 1	0	0
30	V	8	Total O 8 8	0	0
30	W	1	Total O 1 1	0	0
30	Y	2	Total O 2 2	0	0
30	Z	2	Total O 2 2	0	0

3 Residue-property plots

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

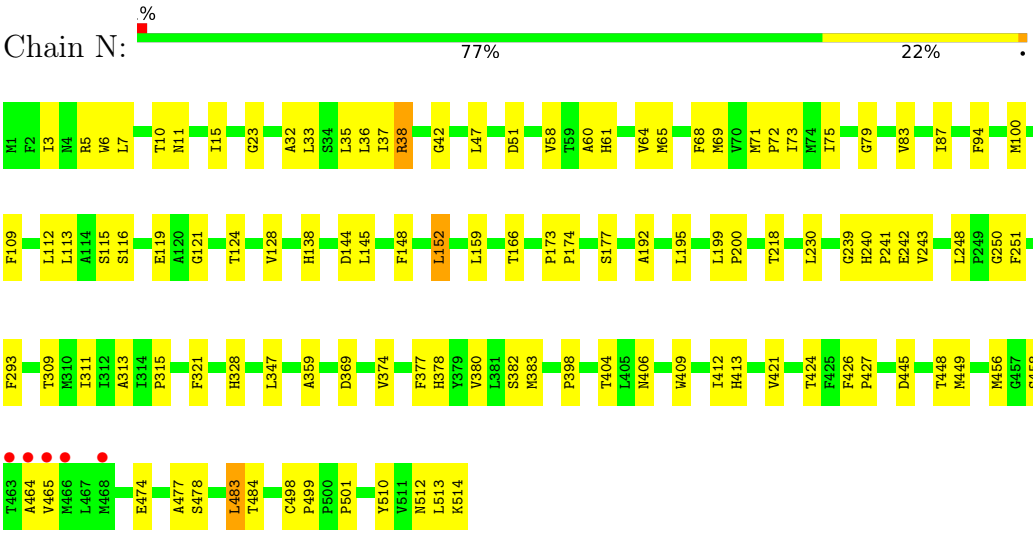
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



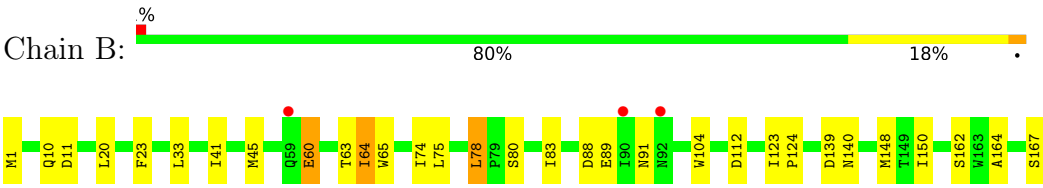
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:

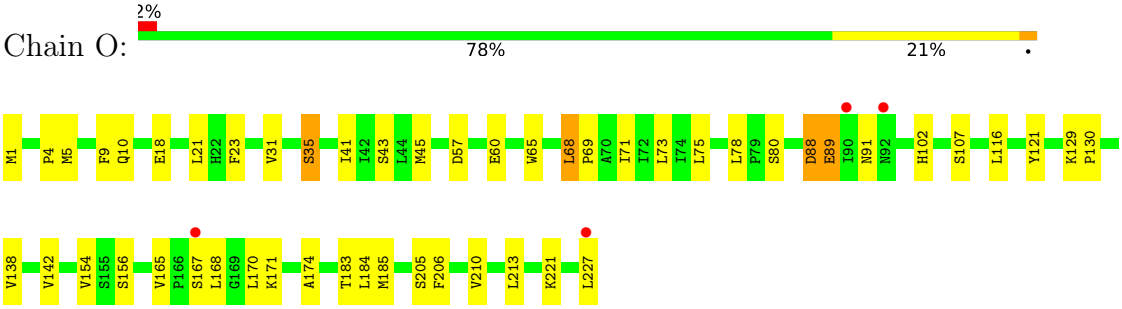


• Molecule 2: Cytochrome c oxidase subunit 2

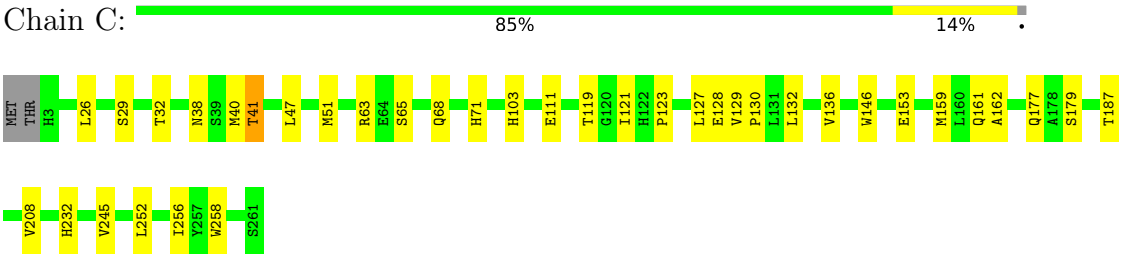
Chain B:



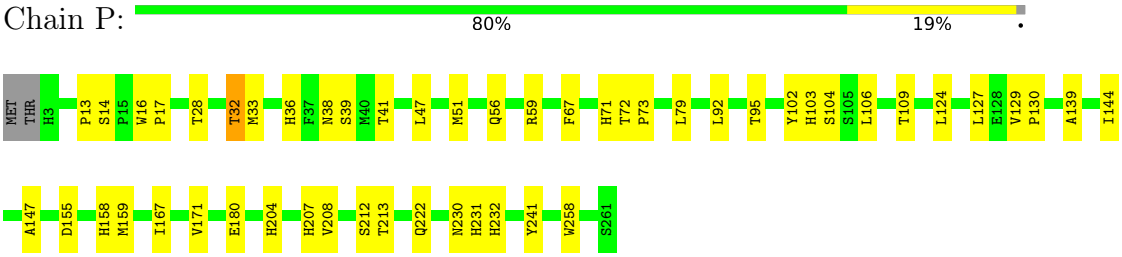
• Molecule 2: Cytochrome c oxidase subunit 2



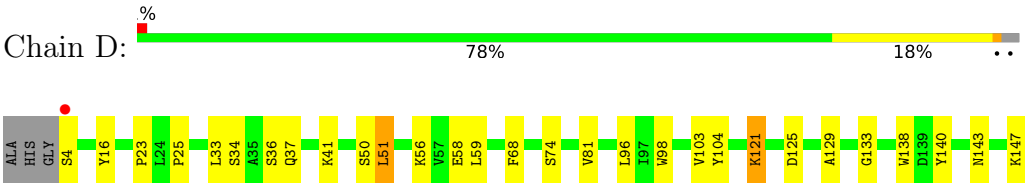
• Molecule 3: Cytochrome c oxidase subunit 3



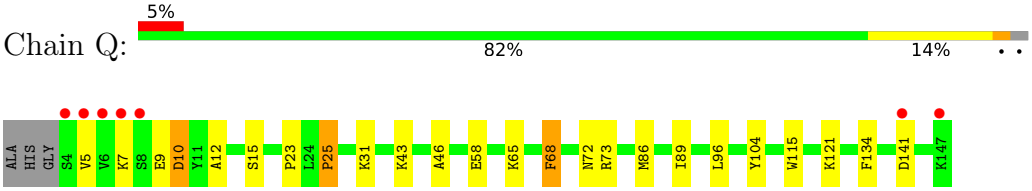
• Molecule 3: Cytochrome c oxidase subunit 3



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

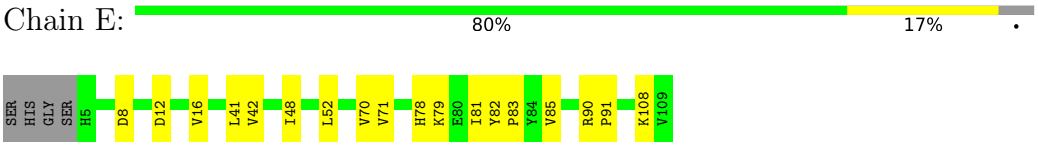


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



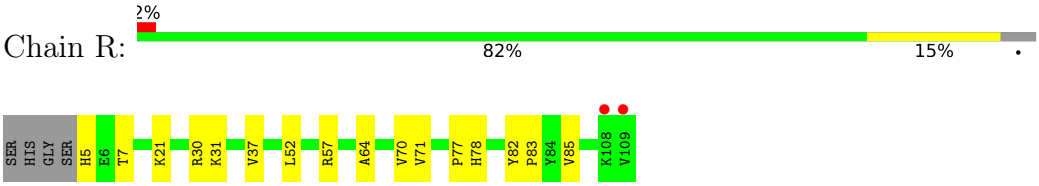
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



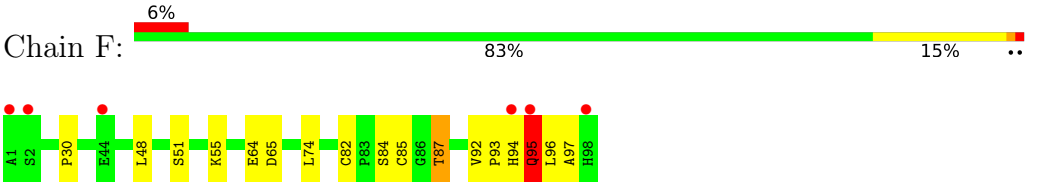
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



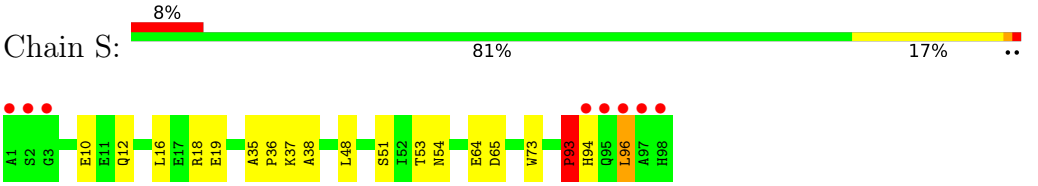
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



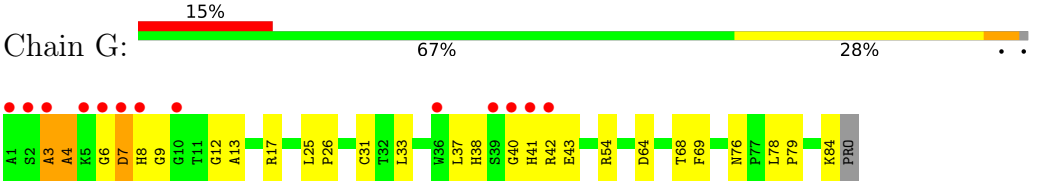
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



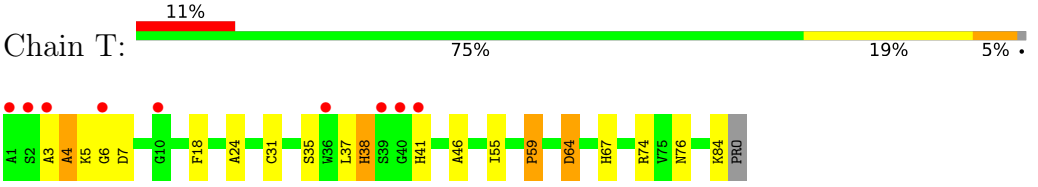
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



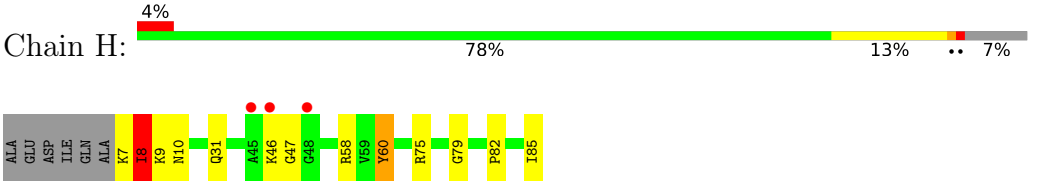
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



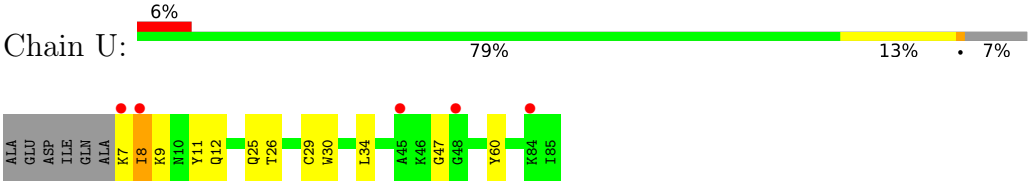
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



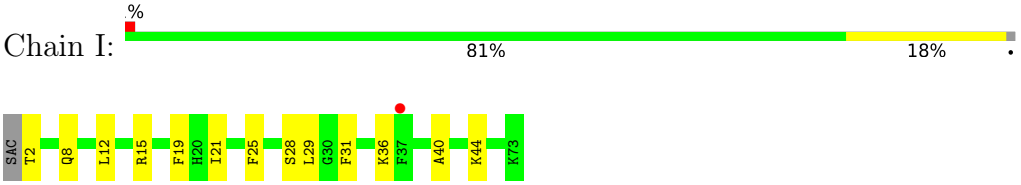
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



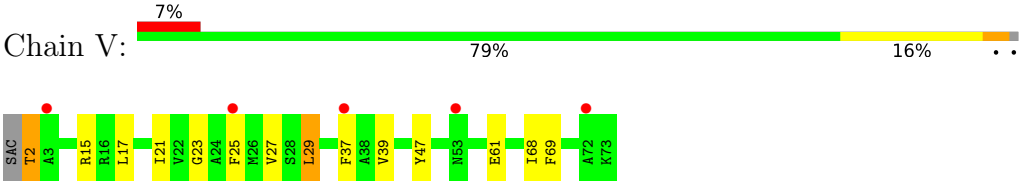
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



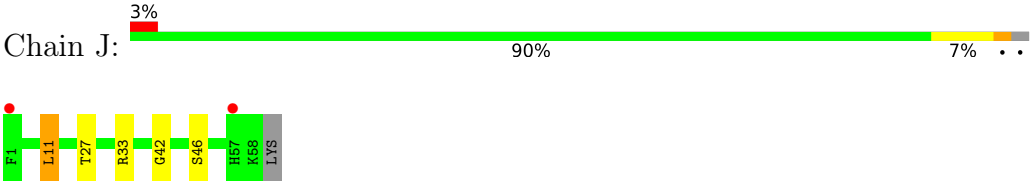
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



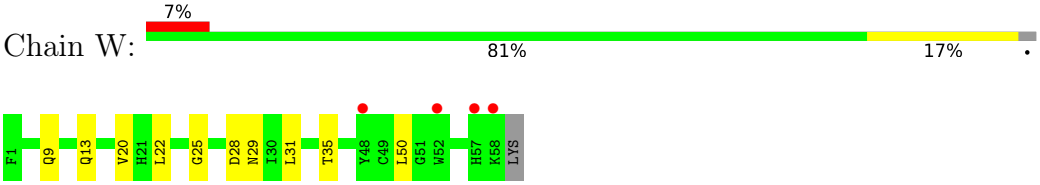
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



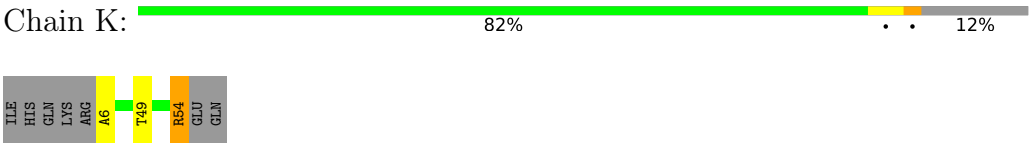
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



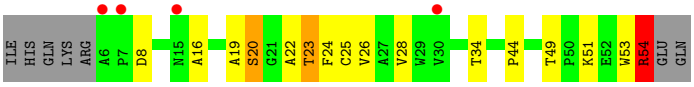
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



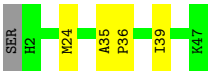
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



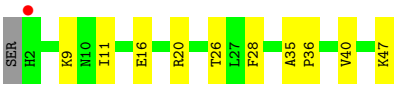
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



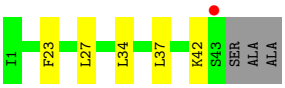
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



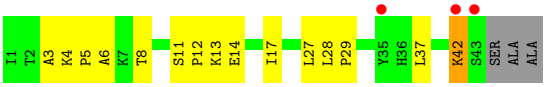
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	178.30Å 189.00Å 209.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.00 – 2.80 31.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.00-2.80) 99.4 (31.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.269 0.227 , 0.268	Depositor DCC
R_{free} test set	8688 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	30981	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, SAC, PGV, CDL, DMU, PEK, TGL, CUA, NA, HEA, CU, CHD, TPO, OH, MG, ZN, CMO, PSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.66	0/4156	0.78	0/5678
1	N	0.69	0/4156	0.78	0/5678
2	B	0.65	0/1860	0.82	0/2534
2	O	0.67	0/1860	0.81	0/2534
3	C	0.64	0/2197	0.75	0/3005
3	P	0.66	0/2197	0.75	0/3005
4	D	0.66	0/1229	0.78	0/1658
4	Q	0.66	0/1229	0.77	0/1658
5	E	0.64	0/871	0.78	0/1182
5	R	0.66	0/871	0.76	0/1182
6	F	0.64	0/765	0.86	0/1038
6	S	0.67	0/765	0.85	0/1038
7	G	0.65	0/690	0.84	0/937
7	T	0.66	0/690	0.85	0/937
8	H	0.64	0/682	0.80	0/921
8	U	0.64	0/682	0.80	0/921
9	I	0.67	0/605	0.86	0/802
9	V	0.66	0/605	0.82	0/802
10	J	0.65	0/471	0.79	0/636
10	W	0.68	0/471	0.77	0/636
11	K	0.67	0/398	0.74	0/546
11	X	0.68	0/398	0.83	1/546 (0.2%)
12	L	0.63	0/393	0.78	0/526
12	Y	0.66	0/393	0.76	0/526
13	M	0.63	0/345	0.74	0/470
13	Z	0.66	0/345	0.77	0/470
All	All	0.66	0/29324	0.79	1/39866 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	S	0	1
7	G	0	1
7	T	0	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	X	54	ARG	NE-CZ-NH2	5.59	123.10	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
7	G	12	GLY	Peptide
6	S	93	PRO	Peptide
7	T	5	LYS	Peptide
7	T	6	GLY	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	43	0
1	N	4027	0	4001	84	0
2	B	1824	0	1833	23	0
2	O	1824	0	1833	26	0
3	C	2110	0	2027	23	0
3	P	2110	0	2027	30	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	852	0	845	13	0
5	R	852	0	845	8	0
6	F	748	0	728	11	0
6	S	748	0	728	8	0
7	G	675	0	644	14	0
7	T	675	0	644	8	0
8	H	662	0	623	13	0
8	U	662	0	623	5	0
9	I	592	0	604	4	0
9	V	592	0	604	9	0
10	J	460	0	459	6	0
10	W	460	0	459	5	0
11	K	384	0	366	2	0
11	X	384	0	366	10	0
12	L	380	0	380	2	0
12	Y	380	0	380	4	0
13	M	335	0	352	2	0
13	Z	335	0	352	12	0
14	A	120	0	108	7	0
14	N	120	0	108	9	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	1	0	0	0	0
17	N	1	0	0	0	0
18	A	63	0	110	2	0
18	I	63	0	110	1	0
18	L	63	0	110	1	0
18	N	126	0	220	1	0
18	Y	63	0	110	0	0
19	A	51	0	76	0	0
19	C	102	0	152	2	0
19	M	51	0	76	0	0
19	N	51	0	76	1	0
19	P	51	0	76	2	0
19	U	51	0	76	2	0
19	Z	51	0	76	3	0
20	A	2	0	0	1	0
20	N	2	0	0	0	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	29	0	39	0	0
22	C	58	0	78	3	0
22	G	29	0	39	1	0
22	J	29	0	39	4	0
22	N	29	0	39	5	0
22	P	58	0	78	3	0
23	C	1	0	0	1	0
23	P	1	0	0	1	0
24	C	100	0	156	2	0
24	G	100	0	156	7	0
24	P	100	0	156	0	0
24	T	100	0	156	6	0
25	E	52	0	80	10	0
25	R	52	0	80	3	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	G	159	0	231	6	0
27	P	53	0	77	2	0
27	T	106	0	154	1	0
28	G	33	0	42	0	0
28	M	33	0	42	0	0
28	Q	33	0	42	2	0
28	T	33	0	41	0	0
29	I	9	0	8	2	0
29	V	9	0	8	0	0
30	A	43	0	0	1	0
30	B	21	0	0	2	0
30	C	23	0	0	8	0
30	D	11	0	0	0	0
30	E	10	0	0	0	0
30	F	7	0	0	0	0
30	G	11	0	0	2	0
30	H	1	0	0	0	0
30	I	2	0	0	0	0
30	K	4	0	0	2	0
30	L	4	0	0	0	0
30	M	3	0	0	0	0
30	N	31	0	0	3	0
30	O	21	0	0	7	0
30	P	12	0	0	0	0
30	Q	7	0	0	2	0
30	R	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	S	5	0	0	0	0
30	T	7	0	0	0	0
30	U	1	0	0	1	0
30	V	8	0	0	2	0
30	W	1	0	0	0	0
30	Y	2	0	0	0	0
30	Z	2	0	0	3	0
All	All	30981	0	31315	390	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 6.

All (390) 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)
18:N:608:TGL:CC1	30:N:701:HOH:O	2.24	0.85
3:P:47:LEU:O	3:P:51:MET:HG2	1.79	0.81
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.65	0.77
30:C:412:HOH:O	10:J:46:SER:CB	2.34	0.75
7:G:76:ASN:HD21	27:G:101:PEK:HN2	1.35	0.75
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.68	0.75
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.71	0.73
3:P:232:HIS:NE2	23:P:301[H]:OH:O	2.23	0.72
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.72	0.72
11:X:19:ALA:O	11:X:23:THR:OG1	2.09	0.70
9:V:37:PHE:HB2	30:V:205:HOH:O	1.91	0.70
30:C:412:HOH:O	10:J:46:SER:HB2	1.92	0.70
2:O:88:ASP:O	2:O:89:GLU:O	2.11	0.69
1:A:240:HIS:O	1:A:243:VAL:HG22	1.93	0.69
6:F:85:CYS:SG	6:F:87:THR:HG22	2.33	0.69
3:C:103:HIS:ND1	22:C:301:CHD:O26	2.25	0.68
2:B:41:ILE:O	2:B:45:MET:HG2	1.94	0.67
1:A:321:PHE:CD1	25:E:201:PSC:H341	2.30	0.66
1:N:445:ASP:O	1:N:448:THR:OG1	2.09	0.66
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.76	0.66
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.78	0.66
5:E:8:ASP:OD1	25:E:201:PSC:H081	1.95	0.66
30:O:407:HOH:O	4:Q:115:TRP:CH2	2.49	0.66
22:J:101:CHD:H222	22:J:101:CHD:H183	1.76	0.65
29:I:102:SAC:C	29:I:102:SAC:OAC	2.45	0.65
3:C:47:LEU:O	3:C:51:MET:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.79	0.64
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.32	0.64
10:J:33:ARG:HG2	22:J:101:CHD:H151	1.80	0.63
2:O:130:PRO:HA	30:O:407:HOH:O	1.99	0.62
14:A:602:HEA:NA	20:A:608:CMO:C	2.62	0.62
6:F:95:GLN:O	6:F:97:ALA:N	2.26	0.62
1:N:144:ASP:OD2	3:P:36:HIS:NE2	2.20	0.62
2:B:41:ILE:HD13	25:E:201:PSC:H342	1.81	0.62
2:O:102:HIS:NE2	2:O:107:SER:OG	2.29	0.61
28:Q:201:DMU:H19	30:Z:201:HOH:O	2.01	0.61
2:B:33:LEU:HD12	9:I:28:SER:HB3	1.83	0.61
8:H:85:ILE:HG22	8:H:85:ILE:OXT	2.01	0.60
2:O:121:TYR:O	2:O:138:VAL:HA	2.00	0.60
12:Y:36:PRO:O	12:Y:40:VAL:HG23	2.02	0.59
2:O:41:ILE:O	2:O:45:MET:HG2	2.03	0.59
10:W:31:LEU:O	10:W:35:THR:OG1	2.19	0.59
11:X:54:ARG:CG	11:X:54:ARG:HH21	2.16	0.59
4:D:16:TYR:CE2	4:D:25:PRO:HG2	2.37	0.59
9:I:2:THR:N	29:I:102:SAC:O	2.36	0.59
1:N:112:LEU:HD23	1:N:112:LEU:O	2.02	0.59
3:C:63:ARG:HE	24:C:305:CDL:HA22	1.68	0.58
5:E:78:HIS:CD2	9:I:12:LEU:HD22	2.38	0.58
8:H:8:ILE:HG23	8:H:8:ILE:O	2.04	0.58
1:N:128:VAL:HG12	1:N:128:VAL:O	2.04	0.58
5:E:90:ARG:HB3	5:E:91:PRO:HD3	1.84	0.58
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.39	0.58
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.85	0.57
1:A:321:PHE:CE1	25:E:201:PSC:H341	2.39	0.57
8:H:31:GLN:HE21	8:H:31:GLN:HA	1.70	0.57
30:O:407:HOH:O	4:Q:115:TRP:CZ2	2.57	0.57
24:C:305:CDL:H112	30:C:420:HOH:O	2.05	0.56
3:P:67:PHE:HA	10:W:9:GLN:HG2	1.86	0.56
30:C:412:HOH:O	10:J:46:SER:HB3	2.00	0.56
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.04	0.56
3:C:26:LEU:HD21	10:J:42:GLY:C	2.26	0.56
6:F:30:PRO:O	6:F:96:LEU:HD21	2.05	0.56
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.87	0.56
1:N:409:TRP:HA	1:N:412:ILE:HD12	1.88	0.56
7:G:76:ASN:ND2	27:G:101:PEK:HN2	2.02	0.55
10:W:25:GLY:O	10:W:29:ASN:ND2	2.38	0.55
22:N:609:CHD:C22	22:N:609:CHD:H183	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:10:GLN:NE2	2:O:167:SER:OG	2.40	0.55
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.06	0.55
22:P:306:CHD:H151	22:P:306:CHD:O7	2.06	0.55
1:N:113:LEU:O	1:N:116:SER:OG	2.19	0.55
1:N:406:ASN:HD21	19:Z:101:PGV:C2	2.18	0.55
27:P:303:PEK:HN2	7:T:76:ASN:HD21	1.55	0.55
22:J:101:CHD:H183	22:J:101:CHD:C22	2.37	0.55
2:B:139:ASP:OD1	2:B:140:ASN:N	2.39	0.54
1:N:398:PRO:O	1:N:498:CYS:HB3	2.07	0.54
3:C:29:SER:HB2	30:C:412:HOH:O	2.07	0.54
7:G:7:ASP:O	7:G:8:HIS:HB2	2.08	0.54
1:N:230:LEU:HB2	3:P:103:HIS:CD2	2.42	0.54
1:N:60:ALA:O	1:N:64:VAL:HG23	2.07	0.54
1:N:321:PHE:CD1	25:R:201:PSC:H341	2.42	0.54
1:A:145:LEU:HD21	3:C:32:THR:HG21	1.90	0.54
3:C:29:SER:CB	30:C:412:HOH:O	2.56	0.54
2:O:165:VAL:HG11	2:O:168:LEU:HD12	1.90	0.54
1:A:507:GLU:OE1	6:F:51:SER:HA	2.07	0.53
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.44	0.53
9:V:23:GLY:O	9:V:27:VAL:HG23	2.09	0.53
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.90	0.53
6:F:55:LYS:HA	6:F:74:LEU:O	2.08	0.53
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.90	0.53
1:N:58:VAL:O	1:N:61:HIS:HB3	2.09	0.53
1:A:24:ALA:HB2	14:A:601:HEA:H252	1.89	0.53
1:A:199:LEU:N	1:A:200:PRO:CD	2.72	0.52
19:U:101:PGV:H62	19:U:101:PGV:H21	1.91	0.52
6:S:51:SER:O	6:S:93:PRO:HA	2.09	0.52
2:O:41:ILE:HD13	25:R:201:PSC:H342	1.92	0.52
6:F:92:VAL:HG23	6:F:92:VAL:O	2.10	0.52
1:N:347:LEU:HD13	1:N:383:MET:HB3	1.92	0.52
1:N:449:MET:SD	2:O:5:MET:HG3	2.50	0.52
3:C:232:HIS:NE2	23:C:302[H]:OH:O	2.41	0.52
1:A:400:PHE:HB3	18:L:101:TGL:H283	1.90	0.51
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.92	0.51
3:C:153:GLU:OE1	7:G:13:ALA:N	2.35	0.51
2:O:69:PRO:HG2	30:O:408:HOH:O	2.09	0.51
1:A:488:THR:HB	1:A:495:LEU:HD13	1.92	0.51
7:G:31:CYS:SG	24:G:104:CDL:H532	2.50	0.51
4:Q:89:ILE:HG23	30:Q:301:HOH:O	2.10	0.51
1:A:83:VAL:HB	1:A:84:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:60:TYR:CD1	8:H:60:TYR:C	2.84	0.51
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.91	0.51
1:N:51:ASP:OD2	2:O:206:PHE:HE2	1.93	0.51
9:V:68:ILE:HG13	9:V:69:PHE:N	2.25	0.51
1:N:248:LEU:O	1:N:251:PHE:HB2	2.10	0.51
3:P:144:ILE:O	3:P:147:ALA:HB3	2.10	0.51
3:C:40:MET:O	3:C:41:THR:C	2.48	0.51
3:P:231:HIS:CD2	19:P:304:PGV:O14	2.64	0.51
2:B:78:LEU:HD12	24:T:104:CDL:H351	1.93	0.50
1:N:313:ALA:HB3	2:O:73:LEU:HD11	1.93	0.50
5:E:90:ARG:HB3	5:E:91:PRO:CD	2.41	0.50
3:P:72:THR:HB	3:P:73:PRO:CD	2.42	0.50
27:G:103:PEK:H381	24:G:104:CDL:H272	1.93	0.50
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.92	0.50
9:V:2:THR:HB	30:V:203:HOH:O	2.12	0.50
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.50
3:P:67:PHE:O	10:W:13:GLN:NE2	2.28	0.50
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.94	0.50
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.93	0.49
25:E:201:PSC:C14	25:E:201:PSC:H343	2.42	0.49
1:N:230:LEU:HB2	3:P:103:HIS:HD2	1.76	0.49
19:N:607:PGV:H51	19:N:607:PGV:H251	1.93	0.49
5:E:8:ASP:HA	25:E:201:PSC:H081	1.94	0.49
2:O:142:VAL:HG23	2:O:210:VAL:O	2.13	0.49
1:A:324:LEU:O	1:A:327:LEU:HB2	2.13	0.49
2:B:183:THR:HG23	30:B:401:HOH:O	2.10	0.49
4:D:121:LYS:HE3	4:D:125:ASP:OD2	2.13	0.49
1:A:106:PRO:HB2	1:A:107:PRO:CD	2.41	0.49
1:N:33:LEU:O	1:N:37:ILE:HG13	2.12	0.49
1:N:359:ALA:HA	14:N:602:HEA:OMA	2.12	0.49
2:O:68:LEU:HA	30:O:416:HOH:O	2.13	0.49
3:P:16:TRP:N	3:P:17:PRO:HD2	2.28	0.49
9:V:68:ILE:HD11	9:V:69:PHE:CE1	2.48	0.49
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.48	0.48
25:E:201:PSC:H343	25:E:201:PSC:H151	1.95	0.48
9:I:36:LYS:HA	9:I:40:ALA:HB3	1.95	0.48
6:S:12:GLN:O	6:S:12:GLN:HG2	2.12	0.48
1:N:424:THR:HG21	14:N:601:HEA:HMB2	1.93	0.48
2:O:170:LEU:HD11	2:O:184:LEU:HG	1.96	0.48
2:B:74:ILE:HG22	2:B:78:LEU:HD22	1.96	0.48
3:P:155:ASP:OD2	3:P:158:HIS:ND1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:PHE:N	1:A:398:PRO:CD	2.77	0.48
1:N:483:LEU:HD23	13:Z:4:LYS:CG	2.43	0.48
3:P:124:LEU:HD13	3:P:180:GLU:OE1	2.13	0.48
1:A:378:HIS:O	1:A:382:SER:HB3	2.14	0.48
4:Q:43:LYS:O	4:Q:46:ALA:HB3	2.13	0.48
11:X:24:PHE:O	11:X:28:VAL:HG12	2.13	0.48
22:C:306:CHD:H183	22:C:306:CHD:H212	1.96	0.48
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.48
4:Q:68:PHE:O	4:Q:72:ASN:HB2	2.14	0.48
3:C:161:GLN:OE1	27:G:103:PEK:H21	2.14	0.47
1:N:152:LEU:HD21	3:P:28:THR:HG21	1.96	0.47
8:U:30:TRP:CZ2	8:U:34:LEU:HD11	2.50	0.47
13:Z:14:GLU:O	13:Z:17:ILE:N	2.47	0.47
1:N:483:LEU:HD23	13:Z:4:LYS:HG3	1.96	0.47
2:O:154:VAL:CG1	2:O:174:ALA:HB2	2.45	0.47
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.45	0.47
3:P:204:HIS:O	3:P:208:VAL:HG23	2.15	0.47
7:T:31:CYS:SG	24:T:104:CDL:H542	2.55	0.47
11:X:8:ASP:OD1	11:X:8:ASP:C	2.53	0.47
1:N:218:THR:CG2	7:T:55:ILE:HG21	2.45	0.47
22:N:609:CHD:H183	22:N:609:CHD:H222	1.97	0.47
3:P:129:VAL:N	3:P:130:PRO:CD	2.78	0.47
1:A:115:SER:HB2	1:A:142:SER:O	2.15	0.47
1:N:38:ARG:NH1	30:N:703:HOH:O	2.48	0.47
1:N:406:ASN:HD21	19:Z:101:PGV:H22	1.79	0.47
5:R:77:PRO:HG2	5:R:78:HIS:CD2	2.50	0.47
4:D:23:PRO:HG3	5:E:70:VAL:HG21	1.96	0.46
2:O:31:VAL:O	2:O:35:SER:OG	2.33	0.46
11:X:16:ALA:O	11:X:20:SER:OG	2.31	0.46
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.97	0.46
1:A:311:ILE:O	1:A:315:PRO:HD2	2.15	0.46
2:O:71:ILE:HD12	30:O:416:HOH:O	2.15	0.46
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.69	0.46
22:P:306:CHD:H183	22:P:306:CHD:H212	1.98	0.46
1:A:380:VAL:HG21	14:A:602:HEA:C3C	2.45	0.46
11:K:54:ARG:C	30:K:104:HOH:O	2.54	0.46
28:Q:201:DMU:H14	30:Z:201:HOH:O	2.16	0.46
1:A:129:TYR:CE1	1:A:232:GLN:HG2	2.51	0.46
1:N:383:MET:HG2	1:N:421:VAL:HG21	1.98	0.46
3:P:92:LEU:O	3:P:95:THR:HB	2.15	0.46
1:A:250:GLY:O	1:A:254:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:GLN:HA	8:H:31:GLN:NE2	2.30	0.46
4:D:68:PHE:CZ	5:E:70:VAL:HG23	2.51	0.46
5:E:42:VAL:HG21	5:E:81:ILE:HG21	1.98	0.46
1:N:112:LEU:HD23	1:N:112:LEU:C	2.36	0.46
25:R:201:PSC:H142	25:R:201:PSC:H343	1.98	0.46
4:D:98:TRP:CZ3	4:D:103:VAL:CG2	2.99	0.46
22:P:306:CHD:O7	22:P:306:CHD:C15	2.63	0.46
8:U:11:TYR:N	30:U:201:HOH:O	2.48	0.46
8:H:8:ILE:O	8:H:8:ILE:CG2	2.64	0.46
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.50	0.45
27:G:103:PEK:H321	24:G:104:CDL:H473	1.98	0.45
8:H:46:LYS:HE2	8:U:8:ILE:HG21	1.98	0.45
1:N:378:HIS:CE1	14:N:601:HEA:NA	2.84	0.45
3:P:16:TRP:N	3:P:17:PRO:CD	2.80	0.45
2:B:20:LEU:HD23	2:B:83:ILE:HG21	1.99	0.45
1:N:240:HIS:O	1:N:243:VAL:HG22	2.15	0.45
1:N:250:GLY:O	1:N:254:ILE:HG12	2.16	0.45
2:O:154:VAL:HG12	2:O:174:ALA:HA	1.97	0.45
3:P:102:TYR:O	3:P:106:LEU:HB2	2.16	0.45
1:A:456:MET:HG2	4:D:96:LEU:HD13	1.99	0.45
1:N:404:THR:HG21	13:Z:3:ALA:HB2	1.97	0.45
27:P:303:PEK:C05	7:T:76:ASN:HD21	2.28	0.45
1:N:100:MET:CE	1:N:159:LEU:HD12	2.47	0.45
1:A:302:ARG:HD2	30:A:730:HOH:O	2.15	0.45
19:C:303:PGV:C11	30:C:422:HOH:O	2.64	0.45
24:G:104:CDL:HA61	30:G:202:HOH:O	2.16	0.45
1:N:71:MET:SD	1:N:242:GLU:OE1	2.75	0.45
7:G:3:ALA:O	7:G:4:ALA:CB	2.65	0.45
24:G:104:CDL:H571	24:G:104:CDL:H771	1.98	0.45
13:M:23:PHE:O	13:M:27:LEU:HG	2.17	0.45
5:E:12:ASP:O	5:E:16:VAL:HG23	2.17	0.45
10:W:22:LEU:HA	10:W:28:ASP:HB3	1.99	0.45
8:H:85:ILE:OXT	8:H:85:ILE:CG2	2.65	0.45
1:A:72:PRO:O	1:A:77:GLY:N	2.49	0.45
1:A:440:TYR:CE2	2:B:205:SER:HA	2.52	0.45
2:B:200:CYS:SG	2:B:204:HIS:HA	2.57	0.45
1:A:50:ASP:HB3	1:A:53:ILE:HD12	1.97	0.45
18:A:606:TGL:HG32	18:A:606:TGL:OB1	2.16	0.45
2:B:123:ILE:HG22	2:B:124:PRO:O	2.17	0.45
4:D:33:LEU:HA	4:D:37:GLN:HE21	1.82	0.45
1:N:474:GLU:OE1	1:N:478:SER:OG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:609:CHD:H183	22:N:609:CHD:H221	1.99	0.45
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.98	0.45
3:C:187:THR:HB	7:G:68:THR:HG21	1.98	0.44
7:G:69:PHE:CD2	27:G:101:PEK:H221	2.52	0.44
1:N:510:TYR:CE2	6:S:36:PRO:HG3	2.52	0.44
3:P:71:HIS:CE1	3:P:79:LEU:HD11	2.52	0.44
24:T:104:CDL:H531	24:T:104:CDL:H201	1.98	0.44
1:A:374:VAL:HA	1:A:377:PHE:CE2	2.52	0.44
2:B:214:VAL:HB	2:B:215:PRO:CD	2.47	0.44
1:N:174:PRO:HB2	6:S:35:ALA:HB2	2.00	0.44
1:N:239:GLY:O	1:N:242:GLU:HB3	2.17	0.44
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.44
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.18	0.44
25:E:201:PSC:H212	25:E:201:PSC:H011	1.98	0.44
7:G:17:ARG:HD3	30:G:204:HOH:O	2.16	0.44
1:N:380:VAL:HG21	14:N:602:HEA:C3C	2.47	0.44
2:O:129:LYS:HB3	2:O:130:PRO:CD	2.47	0.44
1:A:18:LEU:HB3	1:A:102:PHE:CE1	2.52	0.44
1:A:439:ARG:HB3	2:B:199:ILE:HD12	1.99	0.44
6:F:85:CYS:SG	6:F:87:THR:CG2	3.05	0.44
24:G:104:CDL:H241	24:G:104:CDL:H542	2.00	0.44
24:G:104:CDL:H711	30:N:721:HOH:O	2.18	0.44
22:N:609:CHD:H9	22:N:609:CHD:O3	2.17	0.44
1:A:378:HIS:CG	1:A:425:PHE:CE1	3.05	0.44
1:N:68:PHE:HE2	1:N:112:LEU:HD12	1.82	0.44
3:C:252:LEU:HD22	3:C:256:ILE:HD12	2.00	0.43
25:E:201:PSC:H072	25:E:201:PSC:H042	1.86	0.43
1:N:192:ALA:HA	1:N:195:LEU:HD12	2.00	0.43
2:B:78:LEU:CD1	24:T:104:CDL:H351	2.48	0.43
27:T:101:PEK:H381	24:T:104:CDL:H273	2.00	0.43
1:N:461:SER:O	1:N:465:VAL:HG23	2.18	0.43
18:A:606:TGL:HB52	4:D:81:VAL:HG11	2.00	0.43
1:N:413:HIS:CD2	1:N:464:ALA:O	2.71	0.43
6:S:53:THR:OG1	6:S:54:ASN:N	2.50	0.43
9:V:21:ILE:HD13	9:V:21:ILE:HA	1.93	0.43
1:N:10:THR:HG23	3:P:13:PRO:HA	2.01	0.43
7:T:64:ASP:OD1	7:T:67:HIS:ND1	2.51	0.43
19:U:101:PGV:H21	19:U:101:PGV:C6	2.48	0.43
11:X:54:ARG:HH21	11:X:54:ARG:HG2	1.83	0.43
6:F:82:CYS:SG	6:F:84:SER:HB3	2.58	0.43
1:N:5:ARG:HG2	1:N:6:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:36:LEU:HD13	12:Y:40:VAL:HG21	2.01	0.43
6:S:16:LEU:O	6:S:19:GLU:HB2	2.18	0.43
1:N:38:ARG:HD2	14:N:601:HEA:OMA	2.19	0.43
1:N:406:ASN:HD21	19:Z:101:PGV:H21	1.83	0.43
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.43
1:N:65:MET:O	1:N:69:MET:HB3	2.19	0.43
5:E:41:LEU:O	5:E:41:LEU:HD12	2.19	0.43
25:E:201:PSC:H343	25:E:201:PSC:H142	2.00	0.43
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.00	0.43
1:N:94:PHE:CZ	1:N:166:THR:HG21	2.53	0.43
1:N:218:THR:HG21	7:T:55:ILE:HG21	2.01	0.43
1:N:240:HIS:O	1:N:241:PRO:C	2.57	0.43
1:N:328:HIS:CE1	9:V:17:LEU:HD22	2.54	0.43
22:N:609:CHD:C22	22:N:609:CHD:C18	2.97	0.43
5:R:52:LEU:HD22	5:R:64:ALA:HB1	2.01	0.43
9:V:25:PHE:CZ	9:V:29:LEU:HD13	2.54	0.43
2:B:11:ASP:HB2	4:D:129:ALA:HA	2.00	0.42
5:E:71:VAL:HG11	5:E:85:VAL:HG11	2.01	0.42
22:J:101:CHD:C22	22:J:101:CHD:C18	2.96	0.42
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.54	0.42
1:A:94:PHE:CZ	1:A:166:THR:HG21	2.54	0.42
2:B:63:THR:O	2:B:64:ILE:C	2.57	0.42
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.50	0.42
4:D:33:LEU:CD1	4:D:41:LYS:HG3	2.49	0.42
10:J:11:LEU:HD12	10:J:11:LEU:O	2.18	0.42
1:N:199:LEU:N	1:N:200:PRO:CD	2.82	0.42
3:P:213:THR:HG21	19:P:304:PGV:H11	2.00	0.42
7:G:42:ARG:O	7:G:43:GLU:C	2.57	0.42
1:N:115:SER:O	1:N:121:GLY:HA2	2.19	0.42
30:O:407:HOH:O	4:Q:115:TRP:CZ3	2.70	0.42
14:A:601:HEA:OMA	14:A:601:HEA:HHB	2.19	0.42
6:F:92:VAL:O	6:F:92:VAL:CG2	2.66	0.42
1:N:145:LEU:HG	3:P:32:THR:HG21	2.02	0.42
11:X:22:ALA:O	11:X:26:VAL:HG23	2.18	0.42
2:B:150:ILE:HD12	2:B:184:LEU:HD22	2.02	0.42
1:N:105:LEU:HB2	1:N:106:PRO:HD3	2.02	0.42
1:N:311:ILE:O	1:N:315:PRO:HD2	2.19	0.42
2:O:4:PRO:HG2	11:X:44:PRO:HD3	2.01	0.42
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.02	0.42
1:A:377:PHE:HB2	14:A:602:HEA:HMD3	2.02	0.42
3:C:121:ILE:O	3:C:123:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:309:THR:CG2	14:N:602:HEA:HMB2	2.49	0.42
1:N:426:PHE:N	1:N:427:PRO:CD	2.83	0.42
13:Z:27:LEU:HA	30:Z:201:HOH:O	2.19	0.42
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.90	0.42
7:G:64:ASP:OD1	7:G:64:ASP:N	2.52	0.42
3:P:72:THR:HB	3:P:73:PRO:HD2	2.01	0.42
13:Z:11:SER:O	13:Z:12:PRO:C	2.57	0.42
11:K:6:ALA:N	30:K:101:HOH:O	2.52	0.42
1:N:456:MET:HG2	4:Q:96:LEU:HD13	2.01	0.42
1:A:498:CYS:HA	1:A:499:PRO:HA	1.89	0.42
3:C:132:LEU:O	3:C:136:VAL:HG23	2.20	0.42
7:G:25:LEU:O	7:G:26:PRO:C	2.58	0.42
1:N:477:ALA:O	13:Z:8:THR:OG1	2.37	0.42
8:U:25:GLN:O	8:U:26:THR:C	2.58	0.42
1:A:397:PHE:N	1:A:398:PRO:HD3	2.35	0.42
1:N:460:ILE:HG12	30:Q:301:HOH:O	2.19	0.42
3:P:56:GLN:O	3:P:59:ARG:HB3	2.20	0.42
8:H:9:LYS:HG3	8:H:10:ASN:N	2.35	0.41
1:A:102:PHE:CD2	1:A:102:PHE:C	2.93	0.41
14:N:602:HEA:H243	2:O:69:PRO:HB3	2.02	0.41
3:P:167:ILE:O	3:P:171:VAL:HG23	2.20	0.41
5:R:71:VAL:HG11	5:R:85:VAL:HG11	2.02	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.83	0.41
1:N:11:ASN:O	1:N:15:ILE:HG13	2.21	0.41
2:O:213:LEU:N	2:O:213:LEU:HD22	2.35	0.41
30:B:421:HOH:O	24:T:104:CDL:H312	2.20	0.41
1:N:75:ILE:O	1:N:79:GLY:HA3	2.20	0.41
1:N:87:ILE:O	1:N:173:PRO:HD3	2.20	0.41
5:R:37:VAL:CG1	5:R:70:VAL:HG21	2.50	0.41
3:P:139:ALA:HA	7:T:24:ALA:HB1	2.01	0.41
1:N:83:VAL:O	1:N:87:ILE:HG12	2.21	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.82	0.41
2:B:164:ALA:HA	2:B:170:LEU:O	2.20	0.41
4:D:138:TRP:HD1	4:D:140:TYR:CD1	2.39	0.41
4:Q:121:LYS:HG2	11:X:53:TRP:HD1	1.84	0.41
1:A:356:ILE:HD13	1:A:356:ILE:HA	1.93	0.41
3:C:119:THR:HG21	8:H:82:PRO:HA	2.02	0.41
22:G:105:CHD:O7	22:G:105:CHD:H41	2.21	0.41
1:N:3:ILE:O	1:N:7:LEU:HB2	2.20	0.41
1:N:290:HIS:HA	1:N:293:PHE:CZ	2.56	0.41
4:Q:86:MET:O	11:X:25:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:30:TRP:CE2	8:U:34:LEU:HD11	2.55	0.41
2:B:112:ASP:O	8:H:58:ARG:NH2	2.53	0.41
3:C:63:ARG:O	3:C:68:GLN:HG3	2.20	0.41
6:F:95:GLN:C	6:F:97:ALA:N	2.73	0.41
1:N:47:LEU:HD11	13:Z:37:LEU:HD12	2.03	0.41
1:N:144:ASP:O	1:N:148:PHE:CD2	2.73	0.41
2:O:18:GLU:OE2	9:V:47:TYR:HB3	2.21	0.41
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.56	0.41
5:R:37:VAL:HG11	5:R:70:VAL:HG21	2.03	0.41
2:B:162:SER:HB3	2:B:197:SER:C	2.41	0.41
4:D:129:ALA:HB1	4:D:133:GLY:HA3	2.03	0.41
5:E:48:ILE:O	5:E:52:LEU:HG	2.20	0.41
8:H:9:LYS:HG3	8:H:10:ASN:H	1.86	0.41
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.21	0.41
1:A:193:VAL:CG1	7:T:4:ALA:HA	2.51	0.40
1:N:100:MET:HE2	1:N:159:LEU:HD12	2.03	0.40
3:P:222:GLN:HA	3:P:222:GLN:OE1	2.20	0.40
13:Z:5:PRO:O	13:Z:6:ALA:C	2.60	0.40
4:D:37:GLN:O	4:D:41:LYS:HG2	2.21	0.40
4:D:51:LEU:HB3	4:D:56:LYS:HG3	2.03	0.40
6:F:64:GLU:O	6:F:65:ASP:HB2	2.22	0.40
13:Z:28:LEU:HB2	13:Z:29:PRO:CD	2.47	0.40
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.03	0.40
1:A:341:ALA:O	1:A:345:ILE:HG13	2.21	0.40
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.57	0.40
22:C:301:CHD:H212	22:C:301:CHD:H183	2.03	0.40
19:C:303:PGV:C12	30:C:422:HOH:O	2.68	0.40
12:L:35:ALA:O	12:L:39:ILE:HG13	2.21	0.40
4:D:59:LEU:HD23	4:D:59:LEU:HA	1.98	0.40
8:H:75:ARG:O	8:H:79:GLY:N	2.52	0.40
18:I:101:TGL:H252	18:I:101:TGL:H222	1.96	0.40
4:Q:25:PRO:O	5:R:30:ARG:NE	2.54	0.40
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.95	0.40
1:N:35:LEU:HD23	1:N:458:SER:HB2	2.04	0.40
5:R:21:LYS:O	5:R:57:ARG:NH2	2.53	0.40
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.91	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%)	481 (94%)	31 (6%)	0	100 100
1	N	512/514 (100%)	471 (92%)	39 (8%)	2 (0%)	34 66
2	B	225/227 (99%)	206 (92%)	17 (8%)	2 (1%)	17 46
2	O	225/227 (99%)	204 (91%)	20 (9%)	1 (0%)	34 66
3	C	257/261 (98%)	240 (93%)	14 (5%)	3 (1%)	13 39
3	P	257/261 (98%)	240 (93%)	16 (6%)	1 (0%)	34 66
4	D	142/147 (97%)	132 (93%)	9 (6%)	1 (1%)	22 53
4	Q	142/147 (97%)	120 (84%)	17 (12%)	5 (4%)	3 12
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100 100
5	R	103/109 (94%)	94 (91%)	9 (9%)	0	100 100
6	F	96/98 (98%)	84 (88%)	10 (10%)	2 (2%)	7 23
6	S	96/98 (98%)	80 (83%)	11 (12%)	5 (5%)	2 6
7	G	81/85 (95%)	60 (74%)	13 (16%)	8 (10%)	0 1
7	T	81/85 (95%)	60 (74%)	13 (16%)	8 (10%)	0 1
8	H	77/85 (91%)	62 (80%)	13 (17%)	2 (3%)	5 18
8	U	77/85 (91%)	61 (79%)	13 (17%)	3 (4%)	3 10
9	I	70/73 (96%)	61 (87%)	9 (13%)	0	100 100
9	V	70/73 (96%)	61 (87%)	8 (11%)	1 (1%)	11 34
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
10	W	56/59 (95%)	50 (89%)	6 (11%)	0	100 100
11	K	47/56 (84%)	40 (85%)	7 (15%)	0	100 100
11	X	47/56 (84%)	38 (81%)	9 (19%)	0	100 100
12	L	44/47 (94%)	40 (91%)	4 (9%)	0	100 100
12	Y	44/47 (94%)	39 (89%)	3 (7%)	2 (4%)	2 8
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	Z	41/46 (89%)	31 (76%)	9 (22%)	1 (2%)	6 20
All	All	3502/3614 (97%)	3146 (90%)	309 (9%)	47 (1%)	12 36

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	3	ALA
7	G	4	ALA
7	G	7	ASP
8	H	8	ILE
2	O	89	GLU
4	Q	65	LYS
6	S	94	HIS
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
12	Y	16	GLU
3	C	38	ASN
3	C	128	GLU
7	G	37	LEU
7	G	41	HIS
8	H	47	GLY
1	N	119	GLU
6	S	96	LEU
7	T	37	LEU
7	T	38	HIS
8	U	8	ILE
8	U	9	LYS
8	U	47	GLY
3	C	41	THR
6	F	95	GLN
7	G	9	GLY
4	Q	25	PRO
6	S	10	GLU
7	T	41	HIS
12	Y	28	PHE
13	Z	42	LYS
4	D	34	SER
7	G	40	GLY
6	S	64	GLU
7	T	46	ALA

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Mol	Chain	Res	Type
1	N	501	PRO
4	Q	134	PHE
6	S	93	PRO
7	T	59	PRO
2	B	60	GLU
3	P	39	SER
4	Q	141	ASP
7	G	6	GLY
4	Q	5	VAL
2	B	64	ILE
9	V	39	VAL

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%)	419 (98%)	7 (2%)	62	88
1	N	426/426 (100%)	414 (97%)	12 (3%)	43	77
2	B	210/210 (100%)	196 (93%)	14 (7%)	16	43
2	O	210/210 (100%)	192 (91%)	18 (9%)	10	30
3	C	224/226 (99%)	219 (98%)	5 (2%)	52	83
3	P	224/226 (99%)	212 (95%)	12 (5%)	22	53
4	D	128/129 (99%)	118 (92%)	10 (8%)	12	35
4	Q	128/129 (99%)	121 (94%)	7 (6%)	21	52
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	83
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	72
6	F	81/81 (100%)	78 (96%)	3 (4%)	34	68
6	S	81/81 (100%)	76 (94%)	5 (6%)	18	47
7	G	67/68 (98%)	63 (94%)	4 (6%)	19	48
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	21
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	U	71/75 (95%)	67 (94%)	4 (6%)	21 51
9	I	57/57 (100%)	49 (86%)	8 (14%)	3 11
9	V	57/57 (100%)	53 (93%)	4 (7%)	15 40
10	J	49/50 (98%)	47 (96%)	2 (4%)	30 64
10	W	49/50 (98%)	47 (96%)	2 (4%)	30 64
11	K	39/46 (85%)	37 (95%)	2 (5%)	24 55
11	X	39/46 (85%)	33 (85%)	6 (15%)	2 8
12	L	39/40 (98%)	38 (97%)	1 (3%)	46 79
12	Y	39/40 (98%)	34 (87%)	5 (13%)	4 13
13	M	37/38 (97%)	35 (95%)	2 (5%)	22 53
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22 53
All	All	3040/3082 (99%)	2890 (95%)	150 (5%)	25 57

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	310	MET
1	A	484	THR
1	A	486	ASP
1	A	512	ASN
2	B	10	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	88	ASP
2	B	89	GLU
2	B	91	ASN
2	B	148	MET
2	B	167	SER
2	B	171	LYS
2	B	183	THR
2	B	202	SER
2	B	205	SER
3	C	111	GLU

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Mol	Chain	Res	Type
3	C	127	LEU
3	C	159	MET
3	C	179	SER
3	C	258	TRP
4	D	4	SER
4	D	36	SER
4	D	50	SER
4	D	51	LEU
4	D	58	GLU
4	D	74	SER
4	D	104	TYR
4	D	121	LYS
4	D	143	ASN
4	D	147	LYS
5	E	79	LYS
5	E	108	LYS
6	F	48	LEU
6	F	87	THR
6	F	95	GLN
7	G	33	LEU
7	G	38	HIS
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	19	PHE
9	I	21	ILE
9	I	25	PHE
9	I	29	LEU
9	I	31	PHE
9	I	44	LYS
10	J	11	LEU
10	J	27	THR
11	K	49	THR
11	K	54	ARG
12	L	24	MET
13	M	34	LEU
13	M	42	LYS
1	N	38	ARG

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Mol	Chain	Res	Type
1	N	109	PHE
1	N	124	THR
1	N	138	HIS
1	N	152	LEU
1	N	177	SER
1	N	369	ASP
1	N	382	SER
1	N	483	LEU
1	N	484	THR
1	N	512	ASN
1	N	513	LEU
2	O	35	SER
2	O	43	SER
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	88	ASP
2	O	91	ASN
2	O	116	LEU
2	O	156	SER
2	O	171	LYS
2	O	183	THR
2	O	185	MET
2	O	205	SER
2	O	221	LYS
2	O	227	LEU
3	P	14	SER
3	P	32	THR
3	P	33	MET
3	P	38	ASN
3	P	41	THR
3	P	104	SER
3	P	109	THR
3	P	127	LEU
3	P	159	MET
3	P	212	SER
3	P	230	ASN
3	P	258	TRP
4	Q	9	GLU

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Mol	Chain	Res	Type
4	Q	10	ASP
4	Q	15	SER
4	Q	31	LYS
4	Q	58	GLU
4	Q	68	PHE
4	Q	73	ARG
5	R	5	HIS
5	R	7	THR
5	R	31	LYS
6	S	18	ARG
6	S	37	LYS
6	S	48	LEU
6	S	65	ASP
6	S	96	LEU
7	T	18	PHE
7	T	35	SER
7	T	38	HIS
7	T	59	PRO
7	T	64	ASP
7	T	74	ARG
7	T	84	LYS
8	U	7	LYS
8	U	12	GLN
8	U	29	CYS
8	U	60	TYR
9	V	2	THR
9	V	15	ARG
9	V	29	LEU
9	V	61	GLU
10	W	20	VAL
10	W	50	LEU
11	X	20	SER
11	X	23	THR
11	X	34	THR
11	X	49	THR
11	X	51	LYS
11	X	54	ARG
12	Y	9	LYS
12	Y	11	ILE
12	Y	20	ARG
12	Y	26	THR
12	Y	47	LYS

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Mol	Chain	Res	Type
13	Z	13	LYS
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	512	ASN
3	C	68	GLN
3	C	149	HIS
3	C	158	HIS
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
5	E	78	HIS
5	E	94	ASN
7	G	76	ASN
8	H	31	GLN
8	H	32	ASN
10	J	57	HIS
1	N	178	GLN
1	N	328	HIS
2	O	10	GLN
2	O	181	GLN
2	O	203	ASN
3	P	149	HIS
3	P	161	GLN
3	P	230	ASN
4	Q	37	GLN
5	R	78	HIS
5	R	94	ASN
7	T	76	ASN
8	U	12	GLN
8	U	32	ASN
10	W	29	ASN
10	W	57	HIS
12	Y	42	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	TPO	T	11	7	8,10,11	0.83	0	10,14,16	0.79	0
2	FME	O	1	2	8,9,10	0.43	0	7,9,11	1.47	2 (28%)
1	FME	A	1	1	8,9,10	0.45	0	7,9,11	0.90	0
7	TPO	G	11	7	8,10,11	0.76	0	10,14,16	0.81	0
1	FME	N	1	1	8,9,10	0.51	0	7,9,11	0.84	0
2	FME	B	1	2	8,9,10	0.60	0	7,9,11	1.57	2 (28%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-3.22	117.87	122.82
2	O	1	FME	CA-N-CN	-2.95	118.29	122.82
2	O	1	FME	C-CA-N	2.24	113.77	109.73
2	B	1	FME	C-CA-N	2.05	113.42	109.73

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 58 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 48 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	$\#\|Z\|>2$
27	PEK	P	303	-	52,52,52	0.29	0	55,57,57	0.40	0
29	SAC	I	102	-	7,8,9	0.55	0	8,9,11	1.06	1 (12%)
18	TGL	N	608	-	62,62,62	0.32	0	65,65,65	0.50	1 (1%)
21	CUA	O	301	2	0,1,1	-	-	-		
28	DMU	Q	201	-	34,34,34	0.73	1 (2%)	45,45,45	1.37	7 (15%)
22	CHD	C	306	-	32,32,32	0.56	0	51,51,51	0.85	2 (3%)
21	CUA	B	301	2	0,1,1	-	-	-		
22	CHD	J	101	-	32,32,32	0.61	0	51,51,51	0.93	3 (5%)
18	TGL	I	101	-	62,62,62	0.35	0	65,65,65	0.50	1 (1%)
22	CHD	C	301	-	32,32,32	0.58	0	51,51,51	0.74	0
27	PEK	G	101	-	52,52,52	0.31	0	55,57,57	0.35	0
27	PEK	T	101	-	52,52,52	0.31	0	55,57,57	0.36	0
22	CHD	N	609	-	32,32,32	0.62	0	51,51,51	1.24	8 (15%)
18	TGL	N	606	-	62,62,62	0.28	0	65,65,65	0.28	0
24	CDL	P	305	-	99,99,99	0.31	0	105,111,111	0.39	1 (0%)
19	PGV	C	304	-	50,50,50	0.35	0	53,56,56	0.64	1 (1%)
22	CHD	G	105	-	32,32,32	0.62	0	51,51,51	1.00	2 (3%)
19	PGV	C	303	-	50,50,50	0.30	0	53,56,56	0.55	1 (1%)
22	CHD	P	306	-	32,32,32	0.67	0	51,51,51	1.34	7 (13%)
22	CHD	P	302	-	32,32,32	0.55	0	51,51,51	0.76	1 (1%)
19	PGV	Z	101	-	50,50,50	0.35	0	53,56,56	0.47	0
19	PGV	A	607	-	50,50,50	0.32	0	53,56,56	0.49	0
25	PSC	E	201	-	51,51,51	0.30	0	57,59,59	0.42	0
22	CHD	B	302	-	32,32,32	0.59	0	51,51,51	0.80	1 (1%)
28	DMU	G	102	-	34,34,34	0.73	1 (2%)	45,45,45	1.05	4 (8%)
19	PGV	U	101	-	50,50,50	0.36	0	53,56,56	0.63	1 (1%)
28	DMU	M	102	-	34,34,34	0.77	1 (2%)	45,45,45	1.62	12 (26%)
27	PEK	G	106	-	52,52,52	0.32	0	55,57,57	0.44	0
24	CDL	T	104	-	99,99,99	0.32	0	105,111,111	0.45	1 (0%)
19	PGV	M	101	-	50,50,50	0.38	0	53,56,56	0.58	2 (3%)
27	PEK	T	103	-	52,52,52	0.36	0	55,57,57	0.49	0
18	TGL	A	606	-	62,62,62	0.36	0	65,65,65	0.48	0
28	DMU	T	102	-	34,34,34	0.92	1 (2%)	45,45,45	1.85	7 (15%)
29	SAC	V	101	-	7,8,9	0.55	0	8,9,11	0.94	1 (12%)
14	HEA	A	602	1,20	57,67,67	1.92	14 (24%)	61,103,103	2.53	27 (44%)
24	CDL	C	305	-	99,99,99	0.30	0	105,111,111	0.32	0
27	PEK	G	103	-	52,52,52	0.31	0	55,57,57	0.41	0
18	TGL	Y	101	-	62,62,62	0.28	0	65,65,65	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	HEA	A	601	1	57,67,67	2.02	15 (26%)	61,103,103	2.39	21 (34%)
19	PGV	N	607	-	50,50,50	0.33	0	53,56,56	0.40	0
24	CDL	G	104	-	99,99,99	0.33	0	105,111,111	0.49	1 (0%)
18	TGL	L	101	-	62,62,62	0.34	0	65,65,65	0.54	1 (1%)
14	HEA	N	602	1,20	57,67,67	2.01	15 (26%)	61,103,103	2.56	28 (45%)
25	PSC	R	201	-	51,51,51	0.29	0	57,59,59	0.43	0
20	CMO	A	608	14	0,1,1	-	-	-		
14	HEA	N	601	1	57,67,67	1.99	17 (29%)	61,103,103	2.43	26 (42%)
19	PGV	P	304	-	50,50,50	0.29	0	53,56,56	0.43	0
20	CMO	N	610	14	0,1,1	-	-	-		

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
27	PEK	P	303	-	-	19/56/56/56	-
29	SAC	I	102	-	-	3/7/8/10	-
18	TGL	N	608	-	-	26/65/65/65	-
28	DMU	Q	201	-	2/2/10/10	8/19/59/59	0/2/2/2
22	CHD	C	306	-	-	3/9/74/74	1/4/4/4
22	CHD	J	101	-	-	6/9/74/74	0/4/4/4
18	TGL	I	101	-	-	29/65/65/65	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
27	PEK	G	101	-	-	18/56/56/56	-
27	PEK	T	101	-	-	27/56/56/56	-
22	CHD	N	609	-	-	4/9/74/74	0/4/4/4
18	TGL	N	606	-	-	30/65/65/65	-
24	CDL	P	305	-	-	55/110/110/110	-
19	PGV	C	304	-	-	27/55/55/55	-
22	CHD	G	105	-	-	4/9/74/74	0/4/4/4
19	PGV	C	303	-	-	16/55/55/55	-
22	CHD	P	306	-	-	3/9/74/74	0/4/4/4
22	CHD	P	302	-	-	3/9/74/74	0/4/4/4
19	PGV	Z	101	-	-	26/55/55/55	-
19	PGV	A	607	-	-	18/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSC	E	201	-	-	29/55/55/55	-
22	CHD	B	302	-	-	5/9/74/74	0/4/4/4
28	DMU	G	102	-	2/2/10/10	9/19/59/59	0/2/2/2
28	DMU	M	102	-	2/2/10/10	9/19/59/59	0/2/2/2
19	PGV	U	101	-	-	34/55/55/55	-
27	PEK	G	106	-	-	32/56/56/56	-
24	CDL	T	104	-	-	58/110/110/110	-
19	PGV	M	101	-	-	32/55/55/55	-
27	PEK	T	103	-	-	29/56/56/56	-
18	TGL	A	606	-	-	34/65/65/65	-
28	DMU	T	102	-	3/3/10/10	8/19/59/59	0/2/2/2
29	SAC	V	101	-	-	1/7/8/10	-
14	HEA	A	602	1,20	-	5/32/76/76	-
24	CDL	C	305	-	-	60/110/110/110	-
27	PEK	G	103	-	-	26/56/56/56	-
18	TGL	Y	101	-	-	32/65/65/65	-
14	HEA	A	601	1	-	6/32/76/76	-
19	PGV	N	607	-	-	24/55/55/55	-
24	CDL	G	104	-	-	55/110/110/110	-
18	TGL	L	101	-	-	35/65/65/65	-
14	HEA	N	602	1,20	-	8/32/76/76	-
25	PSC	R	201	-	-	22/55/55/55	-
14	HEA	N	601	1	-	5/32/76/76	-
19	PGV	P	304	-	-	21/55/55/55	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C3B-C2B	6.04	1.48	1.34
14	N	601	HEA	C3B-C2B	5.83	1.47	1.34
14	N	602	HEA	C3C-C2C	5.75	1.48	1.40
14	N	601	HEA	CHD-C1D	4.95	1.47	1.35
14	A	601	HEA	C3D-C2D	4.82	1.47	1.36
14	N	602	HEA	C3B-C2B	4.70	1.45	1.34
14	N	602	HEA	C3A-C2A	4.63	1.46	1.40
14	A	601	HEA	C3C-C2C	4.60	1.46	1.40
14	N	601	HEA	C3D-C2D	4.58	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4B-NB	-4.58	1.32	1.40
14	A	601	HEA	C1D-ND	-4.51	1.32	1.40
14	A	601	HEA	CHC-C4B	4.48	1.46	1.35
14	A	602	HEA	CHC-C4B	4.45	1.46	1.35
14	N	602	HEA	C3D-C2D	4.39	1.46	1.36
14	A	602	HEA	C3C-C2C	4.28	1.46	1.40
14	A	602	HEA	C3A-C2A	4.11	1.46	1.40
14	N	601	HEA	CHC-C4B	4.08	1.45	1.35
14	N	602	HEA	CHD-C1D	4.08	1.45	1.35
14	A	602	HEA	C3D-C2D	4.00	1.45	1.36
14	N	601	HEA	C3C-C2C	3.99	1.45	1.40
14	A	602	HEA	C1D-ND	-3.95	1.33	1.40
14	A	601	HEA	CHD-C1D	3.92	1.45	1.35
14	N	602	HEA	CHC-C4B	3.92	1.45	1.35
14	A	602	HEA	C3B-C2B	3.69	1.43	1.34
14	N	602	HEA	C4B-NB	-3.65	1.34	1.40
14	N	601	HEA	C4B-NB	-3.63	1.34	1.40
14	A	602	HEA	CHD-C1D	3.60	1.44	1.35
14	A	601	HEA	C4D-ND	-3.50	1.31	1.38
14	N	601	HEA	C3A-C2A	3.43	1.45	1.40
28	T	102	DMU	O16-C6	3.42	1.46	1.40
14	N	602	HEA	C1D-ND	-3.41	1.34	1.40
14	A	602	HEA	C1B-NB	-3.39	1.31	1.38
28	M	102	DMU	O16-C6	3.35	1.45	1.40
28	Q	201	DMU	O16-C6	3.02	1.45	1.40
28	G	102	DMU	O16-C6	2.96	1.45	1.40
14	N	602	HEA	FE-ND	2.91	2.11	1.96
14	A	601	HEA	C4B-NB	-2.87	1.35	1.40
14	A	602	HEA	C2A-C1A	2.85	1.49	1.42
14	A	601	HEA	C3A-C2A	2.85	1.44	1.40
14	N	602	HEA	C4D-C3D	2.82	1.49	1.45
14	N	601	HEA	FE-ND	2.81	2.10	1.96
14	N	601	HEA	C1B-C2B	2.75	1.49	1.44
14	A	601	HEA	FE-NB	2.72	2.10	1.96
14	N	601	HEA	FE-NB	2.70	2.10	1.96
14	A	601	HEA	C4B-C3B	2.60	1.49	1.44
14	A	601	HEA	C1C-CHC	2.58	1.48	1.41
14	N	602	HEA	C1B-NB	-2.57	1.33	1.38
14	A	601	HEA	C2A-C1A	2.57	1.48	1.42
14	N	601	HEA	C2A-C1A	2.49	1.48	1.42
14	A	602	HEA	CHA-C4D	2.40	1.48	1.41
14	N	602	HEA	C1D-C2D	2.39	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	FE-ND	2.38	2.08	1.96
14	N	601	HEA	C1B-NB	-2.37	1.33	1.38
14	A	602	HEA	FE-NB	2.36	2.08	1.96
14	N	601	HEA	C1D-ND	-2.34	1.36	1.40
14	A	601	HEA	C1B-NB	-2.33	1.34	1.38
14	N	602	HEA	C2A-C1A	2.32	1.47	1.42
14	A	601	HEA	C1B-C2B	2.27	1.49	1.44
14	N	602	HEA	FE-NB	2.22	2.07	1.96
14	N	601	HEA	C4D-ND	-2.20	1.34	1.38
14	N	601	HEA	C1D-C2D	2.17	1.48	1.44
14	N	601	HEA	C1C-CHC	2.13	1.46	1.41
14	N	602	HEA	C4D-ND	-2.13	1.34	1.38
14	A	602	HEA	C1C-CHC	2.01	1.46	1.41
14	N	601	HEA	C4C-CHD	2.00	1.46	1.41

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C3B-C4B-NB	6.90	118.01	109.84
14	A	602	HEA	CAD-CBD-CGD	-6.68	99.22	113.60
14	N	602	HEA	C3D-C4D-ND	6.66	116.81	110.36
14	N	602	HEA	C2D-C1D-ND	6.44	117.47	109.84
14	A	601	HEA	C1D-C2D-C3D	-6.02	100.63	106.96
14	A	601	HEA	C2D-C1D-ND	6.02	116.97	109.84
28	T	102	DMU	C2-C3-C4	-5.83	97.57	110.93
28	T	102	DMU	O55-C2-C1	5.80	123.77	110.35
14	A	601	HEA	C3B-C4B-NB	5.67	116.56	109.84
14	A	602	HEA	C3B-C4B-NB	5.54	116.40	109.84
14	A	601	HEA	C3D-C4D-ND	5.53	115.71	110.36
14	N	601	HEA	C3D-C4D-ND	5.50	115.69	110.36
14	A	602	HEA	C2B-C1B-NB	5.31	116.25	109.88
22	P	306	CHD	C4-C5-C10	4.92	117.89	112.66
14	N	602	HEA	C1D-C2D-C3D	-4.89	101.81	106.96
14	A	602	HEA	C2D-C1D-ND	4.87	115.61	109.84
14	A	602	HEA	C3D-C4D-ND	4.85	115.06	110.36
14	N	602	HEA	C3B-C4B-NB	4.70	115.41	109.84
14	N	601	HEA	C2D-C1D-ND	4.58	115.27	109.84
28	T	102	DMU	O16-C6-C1	4.57	115.44	108.30
14	N	602	HEA	CAD-C3D-C4D	4.54	132.60	124.66
14	A	602	HEA	CMB-C2B-C1B	4.51	131.90	125.04
14	N	601	HEA	CBA-CAA-C2A	4.50	120.19	112.60
14	A	601	HEA	C2B-C1B-NB	4.47	115.23	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C1D-C2D-C3D	-4.38	102.35	106.96
14	A	601	HEA	C3C-C4C-NC	4.38	114.87	109.21
14	A	601	HEA	C13-C12-C11	-4.19	108.05	114.35
14	A	602	HEA	C3C-C4C-NC	4.16	114.58	109.21
28	M	102	DMU	C6-O5-C4	4.10	121.73	113.69
14	A	602	HEA	C1D-C2D-C3D	-4.06	102.69	106.96
14	N	601	HEA	C4B-C3B-C2B	-4.05	100.49	107.41
28	Q	201	DMU	C6-C1-C2	3.98	118.29	110.00
14	N	602	HEA	C3C-C4C-NC	3.98	114.35	109.21
14	N	602	HEA	CMB-C2B-C1B	3.98	131.09	125.04
28	T	102	DMU	O55-C2-C3	3.96	120.44	109.94
14	A	602	HEA	C4A-CHB-C1B	3.93	127.74	122.56
22	P	306	CHD	C5-C6-C7	-3.86	110.20	114.46
14	N	602	HEA	CMD-C2D-C1D	3.83	130.87	125.04
14	A	601	HEA	C4B-C3B-C2B	-3.75	101.01	107.41
14	N	601	HEA	C2B-C1B-NB	3.71	114.33	109.88
14	N	602	HEA	C4D-CHA-C1A	3.71	127.45	122.56
14	N	601	HEA	C3C-C4C-NC	3.71	114.00	109.21
14	A	602	HEA	C1B-C2B-C3B	-3.67	102.41	106.80
22	P	306	CHD	C1-C10-C5	3.67	113.20	107.77
14	A	601	HEA	C4A-CHB-C1B	3.65	127.37	122.56
19	C	304	PGV	O01-C1-C2	3.62	119.30	111.50
22	J	101	CHD	C13-C17-C20	3.59	123.78	119.50
14	A	602	HEA	C13-C12-C11	-3.53	109.05	114.35
22	N	609	CHD	C13-C17-C20	3.52	123.70	119.50
14	N	601	HEA	CAA-CBA-CGA	-3.46	104.06	113.76
14	N	602	HEA	C4A-CHB-C1B	3.44	127.10	122.56
14	N	602	HEA	C2B-C1B-NB	3.41	113.97	109.88
18	L	101	TGL	OG2-CB1-CB2	3.39	118.81	111.50
14	N	602	HEA	CAD-CBD-CGD	-3.36	106.38	113.60
28	M	102	DMU	C8-C7-C5	3.34	116.66	110.82
14	A	601	HEA	OMA-CMA-C3A	-3.34	117.64	124.91
14	A	601	HEA	CHA-C4D-C3D	-3.33	119.95	124.84
14	A	602	HEA	CMD-C2D-C1D	3.32	130.09	125.04
14	N	602	HEA	C1D-ND-C4D	-3.30	101.66	105.07
28	Q	201	DMU	C18-O16-C6	3.27	119.26	113.84
14	A	602	HEA	OMA-CMA-C3A	-3.27	117.79	124.91
14	N	601	HEA	CMB-C2B-C1B	3.24	129.98	125.04
14	N	602	HEA	C4D-C3D-C2D	-3.20	102.24	106.90
14	N	601	HEA	CHB-C1B-NB	-3.17	120.99	124.43
14	N	602	HEA	C4B-C3B-C2B	-3.15	102.03	107.41
14	N	602	HEA	CBA-CAA-C2A	3.15	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	U	101	PGV	O01-C1-C2	3.13	118.24	111.50
24	G	104	CDL	OB6-CB5-C51	3.12	118.23	111.50
14	A	602	HEA	C4D-CHA-C1A	3.12	126.67	122.56
14	N	601	HEA	OMA-CMA-C3A	-3.10	118.15	124.91
14	N	601	HEA	C4A-CHB-C1B	3.08	126.62	122.56
28	M	102	DMU	C6-C1-C2	3.05	116.34	110.00
14	A	602	HEA	CHA-C4D-C3D	-3.00	120.43	124.84
14	N	601	HEA	CMD-C2D-C1D	2.98	129.58	125.04
14	A	602	HEA	C4B-C3B-C2B	-2.97	102.34	107.41
14	N	602	HEA	CMC-C2C-C3C	2.96	130.22	124.68
14	N	601	HEA	CMC-C2C-C3C	2.94	130.18	124.68
22	G	105	CHD	C5-C4-C3	2.92	117.04	112.76
28	G	102	DMU	C6-O5-C4	2.88	119.34	113.69
28	Q	201	DMU	C2-C3-C4	-2.88	104.33	110.93
14	N	601	HEA	C4D-CHA-C1A	2.85	126.32	122.56
14	N	601	HEA	CAD-CBD-CGD	-2.84	107.50	113.60
14	N	601	HEA	CHC-C4B-C3B	-2.84	118.50	125.80
14	N	602	HEA	CMB-C2B-C3B	-2.83	124.95	130.34
14	A	601	HEA	C1B-C2B-C3B	-2.72	103.55	106.80
28	T	102	DMU	C1-C2-C3	2.68	115.79	109.68
22	N	609	CHD	C1-C2-C3	2.66	113.88	110.47
14	A	602	HEA	C4D-C3D-C2D	-2.66	103.02	106.90
18	N	608	TGL	OG2-CB1-CB2	2.66	117.23	111.50
22	C	306	CHD	C10-C9-C8	2.66	114.67	111.82
14	N	602	HEA	OMA-CMA-C3A	-2.65	119.13	124.91
14	A	602	HEA	C27-C19-C20	2.65	119.72	115.27
28	M	102	DMU	C7-C8-C9	2.62	114.92	110.24
28	Q	201	DMU	O5-C6-C1	2.62	115.89	110.35
22	J	101	CHD	C16-C17-C13	-2.61	100.99	103.55
14	A	601	HEA	C4D-C3D-C2D	-2.60	103.10	106.90
28	M	102	DMU	O7-C3-C2	2.58	114.15	107.28
14	N	601	HEA	C1B-C2B-C3B	-2.57	103.73	106.80
14	A	601	HEA	CAA-CBA-CGA	-2.55	106.60	113.76
29	I	102	SAC	O-C-CA	-2.55	118.09	124.78
14	A	602	HEA	CMC-C2C-C3C	2.53	129.42	124.68
14	N	602	HEA	CHA-C4D-C3D	-2.52	121.13	124.84
22	N	609	CHD	C5-C4-C3	2.50	116.43	112.76
22	G	105	CHD	C4-C3-C2	2.49	113.52	110.55
28	T	102	DMU	O7-C3-C4	2.48	116.25	109.45
14	N	601	HEA	C4D-C3D-C2D	-2.48	103.28	106.90
14	A	601	HEA	CHD-C1D-C2D	-2.47	119.89	126.72
14	N	601	HEA	C17-C18-C19	-2.46	121.73	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	CHA-C4D-C3D	-2.46	121.22	124.84
14	A	602	HEA	CAD-C3D-C4D	2.45	128.94	124.66
28	M	102	DMU	O5-C4-C3	2.45	114.91	109.75
22	N	609	CHD	C4-C5-C10	2.44	115.25	112.66
14	A	602	HEA	CMB-C2B-C3B	-2.44	125.69	130.34
22	P	306	CHD	C2-C1-C10	2.44	116.96	112.78
29	V	101	SAC	O-C-CA	-2.43	118.41	124.78
18	I	101	TGL	OG2-CB1-CB2	2.42	116.72	111.50
14	A	602	HEA	C4B-NB-C1B	-2.39	102.60	105.07
14	N	602	HEA	C1B-C2B-C3B	-2.39	103.95	106.80
22	P	306	CHD	C4-C3-C2	-2.38	107.71	110.55
14	N	601	HEA	O2D-CGD-CBD	2.38	121.69	114.03
14	N	602	HEA	O2D-CGD-CBD	2.38	121.67	114.03
24	T	104	CDL	OB6-CB5-C51	2.37	116.60	111.50
14	A	601	HEA	CMC-C2C-C3C	2.37	129.10	124.68
14	A	601	HEA	C13-C14-C15	-2.36	121.98	127.66
28	Q	201	DMU	C7-C8-C9	2.36	114.44	110.24
14	A	602	HEA	CHD-C1D-C2D	-2.36	120.20	126.72
14	A	602	HEA	CHB-C1B-NB	-2.35	121.88	124.43
14	N	602	HEA	CHD-C1D-C2D	-2.35	120.23	126.72
22	N	609	CHD	C16-C17-C13	-2.33	101.27	103.55
28	M	102	DMU	O2-C8-C7	-2.33	104.97	110.35
28	T	102	DMU	C6-O5-C4	2.33	118.25	113.69
14	A	601	HEA	CMD-C2D-C1D	2.30	128.54	125.04
28	M	102	DMU	C18-O16-C6	2.30	117.65	113.84
28	Q	201	DMU	O5-C4-C57	2.29	112.13	106.44
14	A	602	HEA	CHC-C4B-C3B	-2.29	119.91	125.80
22	N	609	CHD	C4-C3-C2	2.28	113.27	110.55
14	A	601	HEA	CBD-CAD-C3D	-2.27	106.32	112.63
28	M	102	DMU	O3-C5-C7	2.24	115.54	110.35
14	N	602	HEA	CAA-CBA-CGA	-2.24	107.47	113.76
14	A	601	HEA	C4D-CHA-C1A	2.23	125.50	122.56
14	N	602	HEA	CHA-C4D-ND	-2.22	122.02	124.43
19	M	101	PGV	O01-C1-C2	2.21	116.27	111.50
22	B	302	CHD	C16-C17-C13	-2.20	101.39	103.55
22	J	101	CHD	C22-C23-C24	2.20	118.34	112.51
28	G	102	DMU	C1-C2-C3	2.19	114.69	109.68
14	A	602	HEA	CAA-CBA-CGA	-2.19	107.61	113.76
28	G	102	DMU	O1-C9-C8	-2.19	105.72	109.69
22	P	302	CHD	C16-C17-C13	-2.17	101.42	103.55
19	M	101	PGV	C02-O01-C1	2.16	123.11	117.79
28	M	102	DMU	C57-C4-C3	-2.16	107.05	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601	HEA	C17-C18-C19	-2.16	122.47	127.66
22	N	609	CHD	C17-C13-C14	-2.13	97.94	100.09
28	G	102	DMU	O1-C9-C11	2.13	111.73	106.44
14	N	601	HEA	CMB-C2B-C3B	-2.13	126.29	130.34
28	M	102	DMU	O7-C3-C4	-2.11	103.67	109.45
14	N	601	HEA	CAD-C3D-C4D	2.08	128.29	124.66
28	Q	201	DMU	C6-O5-C4	2.08	117.76	113.69
22	C	306	CHD	C1-C2-C3	2.07	113.12	110.47
24	P	305	CDL	OA6-CA5-C11	2.06	115.94	111.50
14	N	602	HEA	C13-C12-C11	-2.05	111.26	114.35
22	P	306	CHD	C10-C9-C8	2.04	114.01	111.82
14	N	602	HEA	O2A-CGA-CBA	2.03	120.56	114.03
14	A	602	HEA	CHB-C1B-C2B	-2.03	121.81	124.98
28	M	102	DMU	C10-C5-C7	2.03	114.22	110.00
14	N	602	HEA	CHC-C4B-C3B	-2.02	120.59	125.80
22	N	609	CHD	C10-C9-C8	2.02	113.99	111.82
14	N	601	HEA	C17-C16-C15	-2.02	106.35	112.98
22	P	306	CHD	C1-C10-C9	-2.01	108.19	111.35
19	C	303	PGV	O01-C1-C2	2.01	115.83	111.50

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	G	102	DMU	C6
28	G	102	DMU	C5
28	M	102	DMU	C6
28	M	102	DMU	C5
28	Q	201	DMU	C6
28	Q	201	DMU	C5
28	T	102	DMU	C6
28	T	102	DMU	C2
28	T	102	DMU	C5

All (906) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	I	101	TGL	CB2-CB1-OG2-CG2
18	L	101	TGL	CB2-CB1-OG2-CG2
19	A	607	PGV	C04-O12-P-O13
19	C	303	PGV	C04-C05-C06-O06
19	C	304	PGV	C04-O12-P-O11
19	C	304	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
19	M	101	PGV	C03-O11-P-O14
19	M	101	PGV	O02-C1-O01-C02
19	P	304	PGV	C04-C05-C06-O06
19	U	101	PGV	C03-O11-P-O12
19	U	101	PGV	C03-O11-P-O13
19	U	101	PGV	C03-O11-P-O14
19	U	101	PGV	C04-O12-P-O14
19	U	101	PGV	O12-C04-C05-C06
19	U	101	PGV	O12-C04-C05-O05
19	U	101	PGV	C2-C1-O01-C02
19	Z	101	PGV	C03-O11-P-O14
19	Z	101	PGV	O02-C1-O01-C02
19	Z	101	PGV	C2-C1-O01-C02
19	Z	101	PGV	O04-C19-O03-C01
22	J	101	CHD	C13-C17-C20-C22
22	J	101	CHD	C16-C17-C20-C21
22	J	101	CHD	C16-C17-C20-C22
22	N	609	CHD	C13-C17-C20-C22
22	N	609	CHD	C16-C17-C20-C21
24	C	305	CDL	CA2-OA2-PA1-OA3
24	C	305	CDL	C11-CA5-OA6-CA4
24	G	104	CDL	CB2-OB2-PB2-OB4
24	G	104	CDL	CB3-OB5-PB2-OB3
24	P	305	CDL	CA2-OA2-PA1-OA4
24	P	305	CDL	OA7-CA5-OA6-CA4
24	P	305	CDL	C11-CA5-OA6-CA4
24	P	305	CDL	CB3-OB5-PB2-OB3
24	P	305	CDL	OB7-CB5-OB6-CB4
24	P	305	CDL	C51-CB5-OB6-CB4
24	T	104	CDL	CA2-OA2-PA1-OA3
24	T	104	CDL	CA2-OA2-PA1-OA4
24	T	104	CDL	CA2-OA2-PA1-OA5
24	T	104	CDL	CB2-OB2-PB2-OB5
24	T	104	CDL	CB3-OB5-PB2-OB3
24	T	104	CDL	OB6-CB4-CB6-OB8
25	E	201	PSC	O12-C04-C05-N
25	R	201	PSC	O12-C04-C05-N
27	G	103	PEK	C04-O12-P-O13
27	G	103	PEK	O12-C04-C05-N
27	G	103	PEK	C2-C1-O01-C02
27	G	106	PEK	C03-O11-P-O12
27	G	106	PEK	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
27	G	106	PEK	C03-O11-P-O14
27	G	106	PEK	C04-O12-P-O13
27	G	106	PEK	O12-C04-C05-N
27	G	106	PEK	C2-C1-O01-C02
27	P	303	PEK	C9-C10-C11-C12
27	T	101	PEK	C03-O11-P-O12
27	T	101	PEK	C03-O11-P-O13
27	T	101	PEK	C03-O11-P-O14
27	T	101	PEK	C04-O12-P-O11
27	T	103	PEK	C03-O11-P-O14
27	T	103	PEK	C04-O12-P-O13
27	T	103	PEK	O12-C04-C05-N
28	M	102	DMU	O5-C6-O16-C18
28	M	102	DMU	C19-C18-O16-C6
28	Q	201	DMU	O5-C6-O16-C18
28	Q	201	DMU	C19-C18-O16-C6
29	I	102	SAC	C-CA-N-C1A
29	I	102	SAC	C-CA-CB-OG
29	V	101	SAC	C-CA-N-C1A
18	A	606	TGL	OC1-CC1-OG3-CG3
18	A	606	TGL	CC2-CC1-OG3-CG3
19	M	101	PGV	O04-C19-O03-C01
24	G	104	CDL	OA9-CA7-OA8-CA6
22	N	609	CHD	C16-C17-C20-C22
18	I	101	TGL	OB1-CB1-OG2-CG2
18	L	101	TGL	OB1-CB1-OG2-CG2
19	U	101	PGV	O02-C1-O01-C02
24	C	305	CDL	OA7-CA5-OA6-CA4
24	G	104	CDL	OA7-CA5-OA6-CA4
25	E	201	PSC	O02-C1-O01-C02
27	G	103	PEK	O02-C1-O01-C02
27	G	106	PEK	O02-C1-O01-C02
18	L	101	TGL	CA2-CA1-OG1-CG1
19	M	101	PGV	C20-C19-O03-C01
24	T	104	CDL	C31-CA7-OA8-CA6
19	M	101	PGV	C2-C1-O01-C02
24	G	104	CDL	C11-CA5-OA6-CA4
24	T	104	CDL	C11-CA5-OA6-CA4
19	Z	101	PGV	C20-C19-O03-C01
24	G	104	CDL	C31-CA7-OA8-CA6
27	T	103	PEK	C22-C21-O03-C01
24	T	104	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
18	A	606	TGL	OA1-CA1-OG1-CG1
18	L	101	TGL	OA1-CA1-OG1-CG1
24	T	104	CDL	OA9-CA7-OA8-CA6
24	T	104	CDL	OB9-CB7-OB8-CB6
25	E	201	PSC	O04-C19-O03-C01
24	G	104	CDL	O1-C1-CA2-OA2
24	P	305	CDL	O1-C1-CA2-OA2
18	A	606	TGL	CA2-CA1-OG1-CG1
24	G	104	CDL	C71-CB7-OB8-CB6
25	R	201	PSC	C20-C19-O03-C01
25	E	201	PSC	C2-C1-O01-C02
24	T	104	CDL	C22-C23-C24-C25
28	G	102	DMU	O5-C4-C57-O61
22	B	302	CHD	C17-C20-C22-C23
24	T	104	CDL	C71-CB7-OB8-CB6
25	E	201	PSC	C20-C19-O03-C01
24	T	104	CDL	C52-C53-C54-C55
24	C	305	CDL	CA4-CA3-OA5-PA1
24	T	104	CDL	C1-CB2-OB2-PB2
24	G	104	CDL	OB9-CB7-OB8-CB6
25	R	201	PSC	O04-C19-O03-C01
27	T	103	PEK	O04-C21-O03-C01
28	T	102	DMU	C5-C10-O7-C3
18	Y	101	TGL	CA2-CA1-OG1-CG1
27	T	101	PEK	C22-C21-O03-C01
22	C	306	CHD	C17-C20-C22-C23
22	G	105	CHD	C17-C20-C22-C23
22	P	306	CHD	C17-C20-C22-C23
18	Y	101	TGL	OA1-CA1-OG1-CG1
24	C	305	CDL	C51-CB5-OB6-CB4
19	A	607	PGV	O12-C04-C05-C06
19	Z	101	PGV	O12-C04-C05-C06
24	C	305	CDL	CB2-C1-CA2-OA2
24	P	305	CDL	CB2-C1-CA2-OA2
22	P	306	CHD	C21-C20-C22-C23
18	N	606	TGL	CC2-CC1-OG3-CG3
19	C	304	PGV	C20-C19-O03-C01
19	Z	101	PGV	C19-C20-C21-C22
19	C	304	PGV	O12-C04-C05-O05
22	G	105	CHD	C21-C20-C22-C23
24	P	305	CDL	CA5-C11-C12-C13
28	T	102	DMU	O1-C10-O7-C3

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Mol	Chain	Res	Type	Atoms
19	C	304	PGV	O04-C19-O03-C01
22	C	306	CHD	C21-C20-C22-C23
18	A	606	TGL	CB1-CB2-CB3-CB4
18	N	606	TGL	CC2-CC3-CC4-CC5
19	C	303	PGV	O05-C05-C06-O06
19	P	304	PGV	O05-C05-C06-O06
19	Z	101	PGV	O05-C05-C06-O06
18	L	101	TGL	CB1-CB2-CB3-CB4
18	Y	101	TGL	CA1-CA2-CA3-CA4
19	M	101	PGV	C19-C20-C21-C22
27	G	101	PEK	C1-C2-C3-C4
24	C	305	CDL	OB7-CB5-OB6-CB4
19	U	101	PGV	C1-C2-C3-C4
24	T	104	CDL	CA5-C11-C12-C13
22	N	609	CHD	C13-C17-C20-C21
28	M	102	DMU	O16-C18-C19-C22
18	N	608	TGL	CB1-CB2-CB3-CB4
25	E	201	PSC	C19-C20-C21-C22
18	A	606	TGL	C21-C22-C23-C24
19	Z	101	PGV	O12-C04-C05-O05
22	J	101	CHD	C13-C17-C20-C21
27	T	101	PEK	O04-C21-O03-C01
18	N	606	TGL	OC1-CC1-OG3-CG3
24	G	104	CDL	C51-CB5-OB6-CB4
19	M	101	PGV	C03-O11-P-O12
19	U	101	PGV	C04-O12-P-O11
19	Z	101	PGV	C03-O11-P-O12
24	C	305	CDL	CA2-OA2-PA1-OA5
24	C	305	CDL	CA3-OA5-PA1-OA2
24	G	104	CDL	CB2-OB2-PB2-OB5
24	P	305	CDL	CA2-OA2-PA1-OA5
24	P	305	CDL	CB2-OB2-PB2-OB5
27	G	103	PEK	C03-O11-P-O12
27	G	103	PEK	C04-O12-P-O11
27	G	106	PEK	C04-O12-P-O11
27	T	103	PEK	C03-O11-P-O12
27	T	103	PEK	C04-O12-P-O11
18	N	608	TGL	CA1-CA2-CA3-CA4
19	C	304	PGV	O12-C04-C05-C06
18	N	608	TGL	OB1-CB1-OG2-CG2
24	G	104	CDL	OB7-CB5-OB6-CB4
18	I	101	TGL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	L	101	TGL	CA5-CA6-CA7-CA8
18	N	606	TGL	C16-C15-CC9-CC8
24	C	305	CDL	C37-C38-C39-C40
24	C	305	CDL	C42-C43-C44-C45
24	P	305	CDL	C16-C17-C18-C19
24	T	104	CDL	C55-C56-C57-C58
24	T	104	CDL	C75-C76-C77-C78
18	N	608	TGL	CB2-CB1-OG2-CG2
27	T	103	PEK	C2-C1-O01-C02
18	A	606	TGL	C19-C33-C34-C35
18	L	101	TGL	C16-C15-CC9-CC8
18	N	608	TGL	CA4-CA5-CA6-CA7
18	N	608	TGL	C13-C14-C29-C30
19	P	304	PGV	C30-C31-C32-C33
19	Z	101	PGV	C4-C5-C6-C7
24	G	104	CDL	C80-C81-C82-C83
24	P	305	CDL	C56-C57-C58-C59
25	R	201	PSC	C5-C6-C7-C8
27	P	303	PEK	C26-C27-C28-C29
27	G	106	PEK	C22-C21-O03-C01
18	I	101	TGL	CC7-CC8-CC9-C15
18	N	608	TGL	C17-C18-C19-C33
18	N	608	TGL	C14-C29-C30-C31
18	Y	101	TGL	C16-C15-CC9-CC8
24	P	305	CDL	C41-C42-C43-C44
24	P	305	CDL	C81-C82-C83-C84
25	E	201	PSC	C5-C6-C7-C8
28	Q	201	DMU	C19-C22-C25-C28
18	I	101	TGL	CG1-CG2-OG2-CB1
19	M	101	PGV	C03-C02-O01-C1
18	A	606	TGL	OB1-CB1-OG2-CG2
27	T	101	PEK	O02-C1-O01-C02
27	T	103	PEK	O02-C1-O01-C02
18	I	101	TGL	CA4-CA5-CA6-CA7
18	N	606	TGL	CB9-C10-C11-C12
18	Y	101	TGL	C14-C29-C30-C31
19	A	607	PGV	C5-C6-C7-C8
19	A	607	PGV	C7-C8-C9-C10
19	N	607	PGV	C6-C7-C8-C9
19	P	304	PGV	C20-C21-C22-C23
24	C	305	CDL	C11-C12-C13-C14
24	P	305	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	E	201	PSC	C4-C5-C6-C7
25	E	201	PSC	C29-C30-C31-C32
27	G	101	PEK	C24-C25-C26-C27
19	U	101	PGV	C02-C03-O11-P
18	I	101	TGL	C13-C14-C29-C30
18	L	101	TGL	CC3-CC4-CC5-CC6
18	Y	101	TGL	CB5-CB6-CB7-CB8
24	C	305	CDL	C71-C72-C73-C74
27	G	101	PEK	C23-C24-C25-C26
27	G	103	PEK	C32-C33-C34-C35
19	A	607	PGV	O12-C04-C05-O05
19	M	101	PGV	O12-C04-C05-O05
24	C	305	CDL	O1-C1-CA2-OA2
18	A	606	TGL	CA6-CA7-CA8-CA9
18	I	101	TGL	CC5-CC6-CC7-CC8
19	C	304	PGV	C29-C30-C31-C32
24	C	305	CDL	C16-C17-C18-C19
24	T	104	CDL	C17-C18-C19-C20
27	T	101	PEK	C28-C29-C30-C31
28	M	102	DMU	C25-C28-C31-C34
18	L	101	TGL	CC1-CC2-CC3-CC4
27	G	106	PEK	C21-C22-C23-C24
28	G	102	DMU	C1-C6-O16-C18
18	Y	101	TGL	C22-C23-C24-C25
19	P	304	PGV	C28-C29-C30-C31
24	C	305	CDL	C12-C13-C14-C15
24	C	305	CDL	C81-C82-C83-C84
27	T	103	PEK	C24-C25-C26-C27
18	N	608	TGL	CC7-CC8-CC9-C15
19	C	303	PGV	C13-C14-C15-C16
19	U	101	PGV	C24-C25-C26-C27
24	C	305	CDL	C35-C36-C37-C38
24	P	305	CDL	C15-C16-C17-C18
24	T	104	CDL	C61-C62-C63-C64
18	N	606	TGL	CC9-C15-C16-C17
18	N	606	TGL	C23-C24-C25-C26
18	N	608	TGL	CC3-CC4-CC5-CC6
18	Y	101	TGL	C11-C10-CB9-CB8
18	Y	101	TGL	C11-C12-C13-C14
19	M	101	PGV	C2-C3-C4-C5
19	P	304	PGV	C7-C8-C9-C10
19	U	101	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	U	101	PGV	C29-C30-C31-C32
24	C	305	CDL	C79-C80-C81-C82
24	G	104	CDL	C14-C15-C16-C17
24	G	104	CDL	C37-C38-C39-C40
24	T	104	CDL	C18-C19-C20-C21
24	T	104	CDL	C19-C20-C21-C22
28	T	102	DMU	C28-C31-C34-C37
18	A	606	TGL	CB9-C10-C11-C12
18	I	101	TGL	C21-C20-CA9-CA8
19	M	101	PGV	C4-C5-C6-C7
19	M	101	PGV	C24-C25-C26-C27
19	P	304	PGV	C22-C23-C24-C25
24	C	305	CDL	C40-C41-C42-C43
24	T	104	CDL	C72-C73-C74-C75
27	G	106	PEK	C16-C17-C18-C19
28	Q	201	DMU	C25-C28-C31-C34
19	Z	101	PGV	C04-C05-C06-O06
28	T	102	DMU	O5-C4-C57-O61
27	T	101	PEK	C2-C1-O01-C02
18	N	608	TGL	CB9-C10-C11-C12
24	T	104	CDL	C20-C21-C22-C23
27	T	101	PEK	C29-C30-C31-C32
27	T	103	PEK	C34-C35-C36-C37
28	G	102	DMU	C3-C4-C57-O61
22	B	302	CHD	C21-C20-C22-C23
19	M	101	PGV	C12-C13-C14-C15
18	A	606	TGL	CA2-CA3-CA4-CA5
18	I	101	TGL	CC3-CC4-CC5-CC6
18	L	101	TGL	C11-C12-C13-C14
18	N	608	TGL	CA7-CA8-CA9-C20
18	Y	101	TGL	CA9-C20-C21-C22
19	C	304	PGV	C14-C15-C16-C17
19	U	101	PGV	C23-C24-C25-C26
24	P	305	CDL	C35-C36-C37-C38
24	P	305	CDL	C79-C80-C81-C82
24	T	104	CDL	C35-C36-C37-C38
25	R	201	PSC	C14-C15-C16-C17
25	R	201	PSC	C23-C24-C25-C26
25	R	201	PSC	C27-C28-C29-C30
25	R	201	PSC	C29-C30-C31-C32
27	G	103	PEK	C23-C24-C25-C26
27	P	303	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	G	106	PEK	C01-C02-C03-O11
18	I	101	TGL	CB4-CB5-CB6-CB7
18	L	101	TGL	C11-C10-CB9-CB8
18	L	101	TGL	C20-C21-C22-C23
18	N	606	TGL	C13-C14-C29-C30
19	A	607	PGV	C29-C30-C31-C32
19	U	101	PGV	C20-C21-C22-C23
24	C	305	CDL	C53-C54-C55-C56
27	G	101	PEK	C32-C33-C34-C35
27	P	303	PEK	O12-C04-C05-N
18	A	606	TGL	CC6-CC7-CC8-CC9
18	I	101	TGL	C17-C18-C19-C33
18	L	101	TGL	C13-C14-C29-C30
18	N	608	TGL	CC5-CC6-CC7-CC8
18	Y	101	TGL	CA3-CA4-CA5-CA6
19	C	303	PGV	C20-C21-C22-C23
24	P	305	CDL	C54-C55-C56-C57
24	T	104	CDL	C13-C14-C15-C16
27	T	101	PEK	C22-C23-C24-C25
28	Q	201	DMU	C28-C31-C34-C37
27	G	106	PEK	C1-C2-C3-C4
18	A	606	TGL	CB2-CB3-CB4-CB5
19	N	607	PGV	C23-C24-C25-C26
24	C	305	CDL	C83-C84-C85-C86
27	T	101	PEK	C25-C26-C27-C28
19	C	304	PGV	C30-C31-C32-C33
25	E	201	PSC	C26-C27-C28-C29
18	L	101	TGL	C17-C18-C19-C33
18	N	606	TGL	C16-C17-C18-C19
19	A	607	PGV	C6-C7-C8-C9
24	C	305	CDL	C55-C56-C57-C58
24	G	104	CDL	C63-C64-C65-C66
25	R	201	PSC	C21-C22-C23-C24
27	T	101	PEK	C23-C24-C25-C26
27	G	106	PEK	O04-C21-O03-C01
18	N	608	TGL	C21-C20-CA9-CA8
19	C	304	PGV	C24-C25-C26-C27
19	N	607	PGV	C3-C4-C5-C6
19	P	304	PGV	C13-C14-C15-C16
24	C	305	CDL	C60-C61-C62-C63
24	P	305	CDL	C59-C60-C61-C62
18	A	606	TGL	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
18	L	101	TGL	C21-C22-C23-C24
19	C	303	PGV	C14-C15-C16-C17
24	T	104	CDL	C60-C61-C62-C63
24	T	104	CDL	C62-C63-C64-C65
27	G	103	PEK	C25-C26-C27-C28
19	A	607	PGV	C12-C13-C14-C15
27	T	103	PEK	C15-C16-C17-C18
18	N	608	TGL	CB6-CB7-CB8-CB9
18	Y	101	TGL	C23-C24-C25-C26
19	C	304	PGV	C13-C14-C15-C16
28	G	102	DMU	C25-C28-C31-C34
19	C	303	PGV	C1-C2-C3-C4
19	U	101	PGV	C22-C23-C24-C25
24	P	305	CDL	C17-C18-C19-C20
18	A	606	TGL	C12-C13-C14-C29
24	G	104	CDL	C79-C80-C81-C82
18	N	608	TGL	C20-C21-C22-C23
18	N	606	TGL	CB2-CB1-OG2-CG2
18	L	101	TGL	CB5-CB6-CB7-CB8
19	Z	101	PGV	C2-C3-C4-C5
27	T	103	PEK	C16-C17-C18-C19
24	T	104	CDL	C37-C38-C39-C40
19	C	304	PGV	C11-C10-C9-C8
18	Y	101	TGL	OB1-CB1-OG2-CG2
19	N	607	PGV	O02-C1-O01-C02
18	N	606	TGL	CA6-CA7-CA8-CA9
24	P	305	CDL	C13-C14-C15-C16
24	T	104	CDL	C34-C35-C36-C37
18	N	606	TGL	C17-C18-C19-C33
19	U	101	PGV	C3-C4-C5-C6
18	Y	101	TGL	CB4-CB5-CB6-CB7
18	Y	101	TGL	C15-C16-C17-C18
28	G	102	DMU	O5-C6-O16-C18
18	A	606	TGL	C16-C17-C18-C19
18	Y	101	TGL	CB2-CB1-OG2-CG2
19	N	607	PGV	C2-C1-O01-C02
24	G	104	CDL	OA5-CA3-CA4-OA6
18	Y	101	TGL	C21-C22-C23-C24
27	P	303	PEK	C28-C29-C30-C31
18	N	606	TGL	OB1-CB1-OG2-CG2
18	L	101	TGL	CA3-CA4-CA5-CA6
18	L	101	TGL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	G	106	PEK	O03-C01-C02-O01
27	T	103	PEK	O03-C01-C02-O01
18	A	606	TGL	CC4-CC5-CC6-CC7
19	C	304	PGV	C21-C22-C23-C24
24	C	305	CDL	C59-C60-C61-C62
24	P	305	CDL	C73-C74-C75-C76
25	E	201	PSC	C20-C21-C22-C23
18	N	608	TGL	CB3-CB4-CB5-CB6
19	C	304	PGV	C23-C24-C25-C26
19	N	607	PGV	C14-C15-C16-C17
24	C	305	CDL	C17-C18-C19-C20
24	G	104	CDL	C40-C41-C42-C43
19	C	304	PGV	C12-C13-C14-C15
19	M	101	PGV	C11-C10-C9-C8
19	N	607	PGV	C19-C20-C21-C22
24	T	104	CDL	C33-C34-C35-C36
27	T	101	PEK	C24-C25-C26-C27
27	T	103	PEK	C25-C26-C27-C28
18	L	101	TGL	C12-C13-C14-C29
18	I	101	TGL	CA5-CA6-CA7-CA8
19	C	304	PGV	C5-C6-C7-C8
24	G	104	CDL	C18-C19-C20-C21
24	G	104	CDL	C33-C34-C35-C36
19	C	304	PGV	C22-C23-C24-C25
19	Z	101	PGV	C6-C7-C8-C9
24	P	305	CDL	C74-C75-C76-C77
24	G	104	CDL	CB3-OB5-PB2-OB2
19	C	303	PGV	C7-C8-C9-C10
19	M	101	PGV	C02-C03-O11-P
24	G	104	CDL	C1-CB2-OB2-PB2
24	C	305	CDL	C62-C63-C64-C65
27	G	106	PEK	C27-C28-C29-C30
24	P	305	CDL	OB5-CB3-CB4-CB6
24	T	104	CDL	OA5-CA3-CA4-CA6
18	L	101	TGL	C16-C17-C18-C19
18	N	606	TGL	CB2-CB3-CB4-CB5
27	G	106	PEK	C26-C27-C28-C29
19	M	101	PGV	C13-C14-C15-C16
19	Z	101	PGV	C24-C25-C26-C27
24	G	104	CDL	C13-C14-C15-C16
24	G	104	CDL	C36-C37-C38-C39
24	T	104	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	T	104	CDL	C57-C58-C59-C60
24	C	305	CDL	C71-CB7-OB8-CB6
19	M	101	PGV	O12-C04-C05-C06
18	N	606	TGL	CA9-C20-C21-C22
19	A	607	PGV	C4-C5-C6-C7
18	A	606	TGL	C23-C24-C25-C26
18	Y	101	TGL	CA5-CA6-CA7-CA8
24	G	104	CDL	C31-C32-C33-C34
24	G	104	CDL	C61-C62-C63-C64
18	A	606	TGL	CG1-CG2-CG3-OG3
19	U	101	PGV	O03-C01-C02-C03
24	C	305	CDL	CA3-CA4-CA6-OA8
24	C	305	CDL	CB3-CB4-CB6-OB8
24	G	104	CDL	CA3-CA4-CA6-OA8
25	E	201	PSC	O03-C01-C02-C03
18	A	606	TGL	C29-C30-C31-C32
14	N	602	HEA	C4D-C3D-CAD-CBD
19	M	101	PGV	C15-C16-C17-C18
24	C	305	CDL	C73-C74-C75-C76
24	T	104	CDL	C16-C17-C18-C19
24	P	305	CDL	CB5-C51-C52-C53
18	I	101	TGL	C25-C26-C27-C28
18	L	101	TGL	CB3-CB4-CB5-CB6
18	L	101	TGL	C22-C23-C24-C25
27	T	101	PEK	C2-C3-C4-C5
27	T	101	PEK	C15-C16-C17-C18
27	T	103	PEK	C2-C3-C4-C5
24	G	104	CDL	C16-C17-C18-C19
18	N	606	TGL	CC4-CC5-CC6-CC7
19	P	304	PGV	C14-C15-C16-C17
24	G	104	CDL	C24-C25-C26-C27
18	Y	101	TGL	CB1-CB2-CB3-CB4
19	P	304	PGV	C20-C19-O03-C01
27	P	303	PEK	C22-C21-O03-C01
19	C	303	PGV	C15-C16-C17-C18
19	Z	101	PGV	C03-C02-O01-C1
14	A	601	HEA	C11-C12-C13-C14
27	G	103	PEK	C17-C18-C19-C20
19	M	101	PGV	C1-C2-C3-C4
18	L	101	TGL	CC4-CC5-CC6-CC7
24	C	305	CDL	OB9-CB7-OB8-CB6
19	Z	101	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
27	T	103	PEK	O01-C02-C03-O11
19	N	607	PGV	O03-C19-C20-C21
18	L	101	TGL	CC5-CC6-CC7-CC8
29	I	102	SAC	N-CA-CB-OG
19	U	101	PGV	C5-C6-C7-C8
24	G	104	CDL	C15-C16-C17-C18
19	U	101	PGV	C27-C28-C29-C30
24	T	104	CDL	C77-C78-C79-C80
27	P	303	PEK	C2-C3-C4-C5
24	C	305	CDL	C72-C73-C74-C75
18	N	606	TGL	OG2-CG2-CG3-OG3
18	Y	101	TGL	CC2-CC3-CC4-CC5
19	U	101	PGV	C31-C32-C33-C34
27	P	303	PEK	O04-C21-O03-C01
19	N	607	PGV	C7-C8-C9-C10
19	U	101	PGV	C7-C8-C9-C10
27	G	101	PEK	C34-C35-C36-C37
14	N	602	HEA	C2D-C3D-CAD-CBD
27	G	106	PEK	C33-C34-C35-C36
27	T	101	PEK	C34-C35-C36-C37
18	N	608	TGL	CB5-CB6-CB7-CB8
19	U	101	PGV	C30-C31-C32-C33
24	P	305	CDL	C61-C62-C63-C64
18	I	101	TGL	C19-C33-C34-C35
19	C	304	PGV	C3-C4-C5-C6
18	I	101	TGL	C29-C30-C31-C32
25	E	201	PSC	C22-C23-C24-C25
27	T	101	PEK	C35-C36-C37-C38
19	U	101	PGV	C25-C26-C27-C28
24	C	305	CDL	C13-C14-C15-C16
24	G	104	CDL	C76-C77-C78-C79
24	G	104	CDL	C59-C60-C61-C62
28	T	102	DMU	C2-C3-O7-C10
24	C	305	CDL	OA5-CA3-CA4-CA6
24	C	305	CDL	OB5-CB3-CB4-CB6
24	G	104	CDL	OA5-CA3-CA4-CA6
24	G	104	CDL	C43-C44-C45-C46
28	Q	201	DMU	O16-C18-C19-C22
19	C	303	PGV	C22-C23-C24-C25
19	C	304	PGV	C25-C26-C27-C28
27	G	106	PEK	C22-C23-C24-C25
24	T	104	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
18	I	101	TGL	C21-C22-C23-C24
27	G	101	PEK	C16-C17-C18-C19
24	C	305	CDL	C22-C23-C24-C25
24	T	104	CDL	C58-C59-C60-C61
19	P	304	PGV	O04-C19-O03-C01
24	T	104	CDL	C36-C37-C38-C39
19	C	304	PGV	C26-C27-C28-C29
24	P	305	CDL	CA3-CA4-CA6-OA8
24	P	305	CDL	CB3-CB4-CB6-OB8
24	T	104	CDL	CA3-CA4-CA6-OA8
24	T	104	CDL	CB3-CB4-CB6-OB8
27	G	106	PEK	O03-C01-C02-C03
27	T	103	PEK	O03-C01-C02-C03
28	T	102	DMU	C19-C22-C25-C28
18	A	606	TGL	CC7-CC8-CC9-C15
19	A	607	PGV	C21-C22-C23-C24
18	A	606	TGL	CC5-CC6-CC7-CC8
19	C	303	PGV	C26-C27-C28-C29
19	P	304	PGV	C25-C26-C27-C28
19	U	101	PGV	C2-C3-C4-C5
25	E	201	PSC	C9-C10-C11-C12
25	E	201	PSC	C10-C11-C12-C13
25	R	201	PSC	C9-C10-C11-C12
25	R	201	PSC	C10-C11-C12-C13
27	G	101	PEK	C11-C10-C9-C8
27	G	103	PEK	C5-C6-C7-C8
27	G	103	PEK	C9-C10-C11-C12
27	G	106	PEK	C5-C6-C7-C8
27	G	106	PEK	C6-C7-C8-C9
27	G	106	PEK	C11-C10-C9-C8
27	G	106	PEK	C9-C10-C11-C12
27	G	106	PEK	C12-C13-C14-C15
27	T	101	PEK	C11-C10-C9-C8
27	T	101	PEK	C9-C10-C11-C12
27	T	101	PEK	C12-C13-C14-C15
27	T	103	PEK	C11-C10-C9-C8
27	T	103	PEK	C9-C10-C11-C12
27	T	101	PEK	C17-C18-C19-C20
18	A	606	TGL	CB4-CB5-CB6-CB7
24	C	305	CDL	OA5-CA3-CA4-OA6
24	P	305	CDL	OA5-CA3-CA4-OA6
27	G	103	PEK	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
27	G	106	PEK	O01-C02-C03-O11
24	T	104	CDL	C84-C85-C86-C87
19	P	304	PGV	C19-C20-C21-C22
28	G	102	DMU	C22-C25-C28-C31
19	N	607	PGV	C31-C32-C33-C34
25	E	201	PSC	C31-C32-C33-C34
28	G	102	DMU	C34-C37-C40-C43
24	T	104	CDL	C73-C74-C75-C76
28	M	102	DMU	C4-C3-O7-C10
18	A	606	TGL	OG2-CG2-CG3-OG3
19	M	101	PGV	O03-C01-C02-O01
27	G	103	PEK	O03-C01-C02-O01
19	P	304	PGV	C31-C32-C33-C34
24	G	104	CDL	C17-C18-C19-C20
18	A	606	TGL	CA9-C20-C21-C22
25	E	201	PSC	C27-C28-C29-C30
24	G	104	CDL	C73-C74-C75-C76
19	Z	101	PGV	C02-C03-O11-P
24	C	305	CDL	C1-CA2-OA2-PA1
27	G	103	PEK	C02-C03-O11-P
18	N	606	TGL	CA4-CA5-CA6-CA7
27	G	106	PEK	C25-C26-C27-C28
27	P	303	PEK	C29-C30-C31-C32
18	Y	101	TGL	C29-C30-C31-C32
24	P	305	CDL	C83-C84-C85-C86
19	N	607	PGV	C15-C16-C17-C18
18	N	608	TGL	C15-C16-C17-C18
27	G	103	PEK	C01-C02-C03-O11
24	P	305	CDL	C51-C52-C53-C54
18	I	101	TGL	C16-C17-C18-C19
19	A	607	PGV	C22-C23-C24-C25
19	M	101	PGV	C6-C7-C8-C9
18	L	101	TGL	CB4-CB5-CB6-CB7
18	I	101	TGL	CA3-CA4-CA5-CA6
19	M	101	PGV	C21-C22-C23-C24
24	G	104	CDL	C12-C13-C14-C15
24	T	104	CDL	C38-C39-C40-C41
25	R	201	PSC	C4-C5-C6-C7
27	G	103	PEK	C29-C30-C31-C32
19	M	101	PGV	C14-C15-C16-C17
24	T	104	CDL	C79-C80-C81-C82
18	A	606	TGL	CG3-CG2-OG2-CB1

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Mol	Chain	Res	Type	Atoms
18	N	606	TGL	CG1-CG2-OG2-CB1
18	N	608	TGL	CG1-CG2-OG2-CB1
27	G	103	PEK	C34-C35-C36-C37
28	M	102	DMU	C28-C31-C34-C37
19	C	304	PGV	C6-C7-C8-C9
18	I	101	TGL	CA2-CA1-OG1-CG1
19	A	607	PGV	C13-C14-C15-C16
24	G	104	CDL	C56-C57-C58-C59
18	N	608	TGL	C11-C12-C13-C14
24	G	104	CDL	C78-C79-C80-C81
24	C	305	CDL	CA5-C11-C12-C13
19	M	101	PGV	O03-C01-C02-C03
25	E	201	PSC	C02-C03-O11-P
25	R	201	PSC	O03-C01-C02-C03
27	P	303	PEK	O03-C01-C02-C03
24	P	305	CDL	OB5-CB3-CB4-OB6
19	C	304	PGV	C27-C28-C29-C30
27	P	303	PEK	C24-C25-C26-C27
28	M	102	DMU	C2-C3-O7-C10
27	T	101	PEK	C32-C33-C34-C35
19	N	607	PGV	C25-C26-C27-C28
18	I	101	TGL	OG2-CG2-CG3-OG3
19	U	101	PGV	O03-C01-C02-O01
18	N	606	TGL	C14-C29-C30-C31
25	R	201	PSC	C6-C7-C8-C9
27	G	103	PEK	C24-C25-C26-C27
24	C	305	CDL	C32-C33-C34-C35
18	Y	101	TGL	C25-C26-C27-C28
24	G	104	CDL	C20-C21-C22-C23
24	G	104	CDL	C72-C73-C74-C75
25	R	201	PSC	C3-C4-C5-C6
18	I	101	TGL	OA1-CA1-OG1-CG1
19	P	304	PGV	C2-C3-C4-C5
27	P	303	PEK	C35-C36-C37-C38
24	T	104	CDL	C78-C79-C80-C81
19	N	607	PGV	C04-C05-C06-O06
27	T	101	PEK	C30-C31-C32-C33
19	P	304	PGV	C1-C2-C3-C4
18	L	101	TGL	C23-C24-C25-C26
19	Z	101	PGV	C12-C13-C14-C15
25	E	201	PSC	C03-O11-P-O12
25	R	201	PSC	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
18	I	101	TGL	CB7-CB8-CB9-C10
25	E	201	PSC	C2-C3-C4-C5
19	C	303	PGV	C02-C03-O11-P
19	P	304	PGV	C02-C03-O11-P
24	P	305	CDL	C1-CA2-OA2-PA1
18	Y	101	TGL	CB2-CB3-CB4-CB5
19	C	304	PGV	C04-O12-P-O14
24	C	305	CDL	CA2-OA2-PA1-OA4
24	C	305	CDL	CA3-OA5-PA1-OA3
24	G	104	CDL	CB3-OB5-PB2-OB4
24	P	305	CDL	CB2-OB2-PB2-OB3
24	P	305	CDL	CB2-OB2-PB2-OB4
24	T	104	CDL	CB2-OB2-PB2-OB4
27	G	103	PEK	C03-O11-P-O14
27	G	106	PEK	C04-O12-P-O14
27	T	101	PEK	C04-O12-P-O13
27	T	103	PEK	C03-O11-P-O13
27	T	103	PEK	C04-O12-P-O14
24	T	104	CDL	C80-C81-C82-C83
19	M	101	PGV	C01-C02-C03-O11
24	P	305	CDL	OA5-CA3-CA4-CA6
27	T	103	PEK	C01-C02-C03-O11
24	C	305	CDL	C51-C52-C53-C54
19	Z	101	PGV	C15-C16-C17-C18
24	P	305	CDL	C31-C32-C33-C34
28	Q	201	DMU	C34-C37-C40-C43
25	R	201	PSC	C05-C04-O12-P
27	T	101	PEK	C16-C17-C18-C19
27	P	303	PEK	C17-C18-C19-C20
18	L	101	TGL	CA1-CA2-CA3-CA4
24	G	104	CDL	CB2-C1-CA2-OA2
18	Y	101	TGL	C17-C18-C19-C33
14	A	601	HEA	O11-C11-C3B-C2B
24	C	305	CDL	OB5-CB3-CB4-OB6
24	T	104	CDL	OA5-CA3-CA4-OA6
18	N	608	TGL	C12-C13-C14-C29
19	N	607	PGV	C2-C3-C4-C5
19	N	607	PGV	C27-C28-C29-C30
19	N	607	PGV	C28-C29-C30-C31
25	E	201	PSC	C04-C05-N-C07
24	C	305	CDL	CB7-C71-C72-C73
27	G	103	PEK	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
27	G	106	PEK	C32-C33-C34-C35
28	Q	201	DMU	C22-C25-C28-C31
24	P	305	CDL	OA6-CA4-CA6-OA8
24	P	305	CDL	OB6-CB4-CB6-OB8
25	R	201	PSC	O03-C01-C02-O01
24	G	104	CDL	C52-C53-C54-C55
19	U	101	PGV	C21-C22-C23-C24
27	G	103	PEK	C30-C31-C32-C33
27	P	303	PEK	C27-C28-C29-C30
24	T	104	CDL	C64-C65-C66-C67
22	P	302	CHD	C16-C17-C20-C22
19	N	607	PGV	C22-C23-C24-C25
24	P	305	CDL	C52-C53-C54-C55
24	G	104	CDL	C52-C51-CB5-OB6
19	C	303	PGV	C27-C28-C29-C30
19	Z	101	PGV	C14-C15-C16-C17
24	C	305	CDL	C44-C45-C46-C47
27	G	101	PEK	C17-C18-C19-C20
19	A	607	PGV	C9-C10-C11-C12
24	P	305	CDL	C20-C21-C22-C23
18	A	606	TGL	C11-C10-CB9-CB8
19	Z	101	PGV	C22-C23-C24-C25
24	T	104	CDL	C74-C75-C76-C77
27	P	303	PEK	C32-C33-C34-C35
18	A	606	TGL	CB7-CB8-CB9-C10
18	A	606	TGL	C11-C12-C13-C14
18	L	101	TGL	CA7-CA8-CA9-C20
24	G	104	CDL	C23-C24-C25-C26
25	E	201	PSC	C04-C05-N-C08
19	A	607	PGV	C26-C27-C28-C29
19	N	607	PGV	C4-C5-C6-C7
22	P	302	CHD	C13-C17-C20-C21
24	C	305	CDL	OA6-CA4-CA6-OA8
24	C	305	CDL	OB6-CB4-CB6-OB8
24	G	104	CDL	OA6-CA4-CA6-OA8
25	E	201	PSC	O03-C01-C02-O01
24	C	305	CDL	C54-C55-C56-C57
19	A	607	PGV	C03-O11-P-O12
19	A	607	PGV	C04-O12-P-O11
19	Z	101	PGV	C04-O12-P-O11
24	G	104	CDL	CA3-OA5-PA1-OA2
24	T	104	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
25	R	201	PSC	C03-O11-P-O12
27	G	103	PEK	C21-C22-C23-C24
18	I	101	TGL	C15-C16-C17-C18
18	Y	101	TGL	CB9-C10-C11-C12
24	P	305	CDL	C22-C23-C24-C25
18	Y	101	TGL	C16-C17-C18-C19
24	T	104	CDL	C43-C44-C45-C46
27	G	101	PEK	C27-C28-C29-C30
19	P	304	PGV	C27-C28-C29-C30
24	C	305	CDL	C41-C42-C43-C44
27	P	303	PEK	C02-C03-O11-P
19	N	607	PGV	C11-C12-C13-C14
27	T	103	PEK	C3-C4-C5-C6
18	Y	101	TGL	CC6-CC7-CC8-CC9
14	A	601	HEA	CAD-CBD-CGD-O1D
19	N	607	PGV	C24-C25-C26-C27
19	M	101	PGV	C11-C12-C13-C14
27	G	101	PEK	O04-C21-O03-C01
14	A	602	HEA	CAA-CBA-CGA-O1A
19	C	303	PGV	C11-C10-C9-C8
22	P	302	CHD	C16-C17-C20-C21
27	G	101	PEK	C10-C11-C12-C13
22	B	302	CHD	C22-C23-C24-O25
22	G	105	CHD	C22-C23-C24-O25
18	L	101	TGL	CA9-C20-C21-C22
22	C	306	CHD	C13-C17-C20-C21
27	P	303	PEK	C22-C23-C24-C25
27	P	303	PEK	C14-C15-C16-C17
18	N	606	TGL	CB3-CB4-CB5-CB6
19	Z	101	PGV	C5-C6-C7-C8
18	L	101	TGL	CB2-CB3-CB4-CB5
24	P	305	CDL	C58-C59-C60-C61
14	A	601	HEA	CAA-CBA-CGA-O1A
22	B	302	CHD	C22-C23-C24-O26
22	J	101	CHD	C22-C23-C24-O26
18	N	606	TGL	C12-C13-C14-C29
18	N	606	TGL	OG1-CA1-CA2-CA3
24	C	305	CDL	C56-C57-C58-C59
24	T	104	CDL	C51-C52-C53-C54
28	M	102	DMU	C19-C22-C25-C28
14	N	601	HEA	CAA-CBA-CGA-O1A
25	E	201	PSC	C01-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
19	N	607	PGV	C5-C6-C7-C8
25	E	201	PSC	C04-C05-N-C06
24	P	305	CDL	C36-C37-C38-C39
24	G	104	CDL	CB7-C71-C72-C73
18	A	606	TGL	C20-C21-C22-C23
24	P	305	CDL	C76-C77-C78-C79
27	G	101	PEK	C9-C10-C11-C12
27	T	103	PEK	C12-C13-C14-C15
14	N	601	HEA	CAA-CBA-CGA-O2A
22	J	101	CHD	C22-C23-C24-O25
18	L	101	TGL	CB6-CB7-CB8-CB9
19	M	101	PGV	C05-C04-O12-P
24	C	305	CDL	C23-C24-C25-C26
19	C	304	PGV	O01-C02-C03-O11
14	A	601	HEA	CAD-CBD-CGD-O2D
25	E	201	PSC	C6-C7-C8-C9
19	Z	101	PGV	C01-C02-C03-O11
22	G	105	CHD	C22-C23-C24-O26
27	P	303	PEK	C30-C31-C32-C33
18	N	608	TGL	CC9-C15-C16-C17
19	P	304	PGV	C24-C25-C26-C27
18	A	606	TGL	C24-C25-C26-C27
18	I	101	TGL	C11-C10-CB9-CB8
19	A	607	PGV	C3-C4-C5-C6
14	A	602	HEA	CAA-CBA-CGA-O2A
24	C	305	CDL	C24-C25-C26-C27
24	G	104	CDL	C55-C56-C57-C58
27	T	103	PEK	C17-C18-C19-C20
19	U	101	PGV	O04-C19-O03-C01
18	A	606	TGL	CB6-CB7-CB8-CB9
19	C	304	PGV	O01-C1-C2-C3
28	T	102	DMU	C25-C28-C31-C34
27	G	106	PEK	C14-C15-C16-C17
27	T	101	PEK	O01-C02-C03-O11
22	B	302	CHD	C20-C22-C23-C24
24	C	305	CDL	C31-C32-C33-C34
19	C	303	PGV	C25-C26-C27-C28
25	R	201	PSC	C12-C13-C14-C15
18	N	608	TGL	C16-C17-C18-C19
19	N	607	PGV	O04-C19-C20-C21
18	L	101	TGL	OG2-CB1-CB2-CB3
24	G	104	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
24	T	104	CDL	CB2-C1-CA2-OA2
24	C	305	CDL	C12-C11-CA5-OA6
14	A	602	HEA	CAD-CBD-CGD-O1D
14	A	602	HEA	CAD-CBD-CGD-O2D
27	G	101	PEK	C22-C21-O03-C01
27	G	101	PEK	C22-C23-C24-C25
18	I	101	TGL	OG1-CA1-CA2-CA3
19	U	101	PGV	O01-C1-C2-C3
24	P	305	CDL	C12-C11-CA5-OA6
27	G	103	PEK	O04-C21-O03-C01
18	N	606	TGL	OA1-CA1-OG1-CG1
19	M	101	PGV	C9-C10-C11-C12
19	N	607	PGV	C9-C10-C11-C12
19	P	304	PGV	C9-C10-C11-C12
27	G	101	PEK	C31-C32-C33-C34
28	T	102	DMU	C4-C3-O7-C10
24	C	305	CDL	C58-C59-C60-C61
18	Y	101	TGL	OG2-CB1-CB2-CB3
14	N	602	HEA	C26-C15-C16-C17
19	C	303	PGV	C9-C10-C11-C12
27	G	106	PEK	C3-C4-C5-C6
27	T	103	PEK	C35-C36-C37-C38
14	N	602	HEA	CAA-CBA-CGA-O1A
18	N	606	TGL	CA2-CA1-OG1-CG1
18	N	606	TGL	OG3-CC1-CC2-CC3
27	G	101	PEK	O01-C1-C2-C3
27	T	103	PEK	O01-C1-C2-C3
14	A	601	HEA	CAA-CBA-CGA-O2A
14	N	602	HEA	CAD-CBD-CGD-O1D
18	N	606	TGL	C29-C30-C31-C32
24	P	305	CDL	CB7-C71-C72-C73
27	G	103	PEK	C14-C15-C16-C17
19	M	101	PGV	O01-C1-C2-C3
19	C	304	PGV	C01-C02-C03-O11
22	C	301	CHD	C22-C23-C24-O26
18	L	101	TGL	OG3-CC1-CC2-CC3
24	T	104	CDL	C52-C51-CB5-OB6
27	G	103	PEK	C22-C21-O03-C01
24	C	305	CDL	C82-C83-C84-C85
14	N	601	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAD-CBD-CGD-O2D
24	G	104	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
18	Y	101	TGL	CA6-CA7-CA8-CA9
14	N	602	HEA	CAA-CBA-CGA-O2A
19	N	607	PGV	O05-C05-C06-O06
18	Y	101	TGL	OG1-CA1-CA2-CA3
28	M	102	DMU	O6-C11-C9-C8
14	N	602	HEA	C14-C15-C16-C17
18	I	101	TGL	CC4-CC5-CC6-CC7
19	C	303	PGV	C11-C12-C13-C14
19	U	101	PGV	C26-C27-C28-C29
18	N	606	TGL	OG2-CB1-CB2-CB3
22	P	306	CHD	C20-C22-C23-C24
25	E	201	PSC	C12-C13-C14-C15
18	I	101	TGL	OA1-CA1-CA2-CA3
14	A	602	HEA	C26-C15-C16-C17
18	N	606	TGL	OC1-CC1-CC2-CC3
28	G	102	DMU	C2-C3-O7-C10
19	U	101	PGV	O02-C1-C2-C3
27	T	103	PEK	O02-C1-C2-C3
28	G	102	DMU	C4-C3-O7-C10
19	P	304	PGV	C11-C12-C13-C14
19	Z	101	PGV	C11-C12-C13-C14
18	Y	101	TGL	OB1-CB1-CB2-CB3
24	C	305	CDL	C12-C11-CA5-OA7
18	N	606	TGL	CG1-CG2-CG3-OG3
24	C	305	CDL	C18-C19-C20-C21
24	P	305	CDL	C62-C63-C64-C65
24	T	104	CDL	OB7-CB5-OB6-CB4
24	G	104	CDL	CB4-CB3-OB5-PB2
24	G	104	CDL	C32-C31-CA7-OA9
18	I	101	TGL	C16-C15-CC9-CC8
24	P	305	CDL	CB3-OB5-PB2-OB4
24	T	104	CDL	CB3-OB5-PB2-OB4
25	E	201	PSC	C03-O11-P-O13
25	R	201	PSC	C03-O11-P-O14
18	L	101	TGL	OC1-CC1-CC2-CC3
19	M	101	PGV	O02-C1-C2-C3
24	P	305	CDL	C12-C11-CA5-OA7
18	N	608	TGL	C21-C22-C23-C24
19	A	607	PGV	C11-C10-C9-C8
14	N	601	HEA	CAD-CBD-CGD-O2D
18	A	606	TGL	CC3-CC4-CC5-CC6
14	N	601	HEA	C26-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	P	305	CDL	C14-C15-C16-C17
25	R	201	PSC	C22-C23-C24-C25
22	C	301	CHD	C22-C23-C24-O25
25	E	201	PSC	C05-C04-O12-P
27	G	101	PEK	C05-C04-O12-P
27	G	101	PEK	O02-C1-C2-C3
18	N	608	TGL	CB2-CB3-CB4-CB5
24	P	305	CDL	C32-C31-CA7-OA8
27	G	106	PEK	O01-C1-C2-C3
18	L	101	TGL	C21-C20-CA9-CA8
19	M	101	PGV	O03-C19-C20-C21
19	C	304	PGV	C2-C3-C4-C5
24	P	305	CDL	C80-C81-C82-C83
18	Y	101	TGL	OA1-CA1-CA2-CA3
19	U	101	PGV	C20-C19-O03-C01
18	A	606	TGL	C15-C16-C17-C18
19	U	101	PGV	C4-C5-C6-C7
19	M	101	PGV	O04-C19-C20-C21

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	C	306	CHD	C1-C10-C2-C3-C4-C5

31 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	P	303	PEK	2	0
29	I	102	SAC	2	0
18	N	608	TGL	1	0
28	Q	201	DMU	2	0
22	C	306	CHD	1	0
22	J	101	CHD	4	0
18	I	101	TGL	1	0
22	C	301	CHD	2	0
27	G	101	PEK	3	0
27	T	101	PEK	1	0
22	N	609	CHD	5	0
22	G	105	CHD	1	0
19	C	303	PGV	2	0
22	P	306	CHD	3	0
19	Z	101	PGV	3	0

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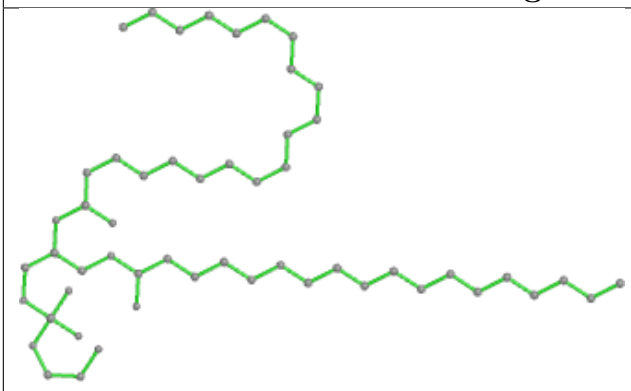
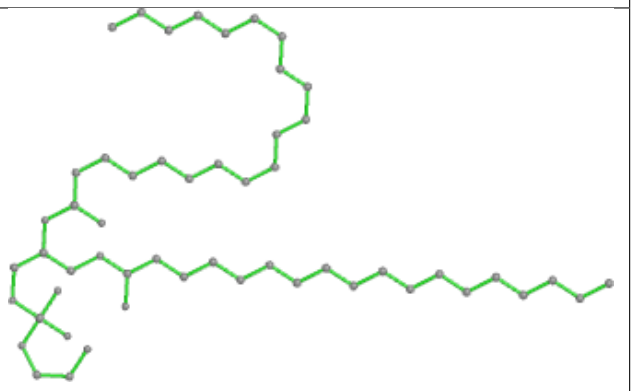
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	E	201	PSC	10	0
19	U	101	PGV	2	0
24	T	104	CDL	6	0
18	A	606	TGL	2	0
14	A	602	HEA	4	0
24	C	305	CDL	2	0
27	G	103	PEK	3	0
14	A	601	HEA	3	0
19	N	607	PGV	1	0
24	G	104	CDL	7	0
18	L	101	TGL	1	0
14	N	602	HEA	5	0
25	R	201	PSC	3	0
20	A	608	CMO	1	0
14	N	601	HEA	4	0
19	P	304	PGV	2	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.

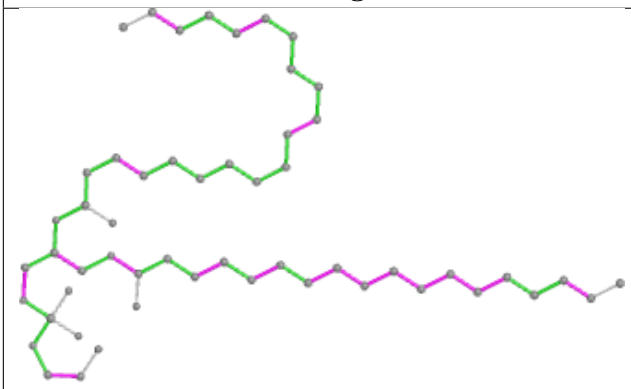
Ligand PEK P 303



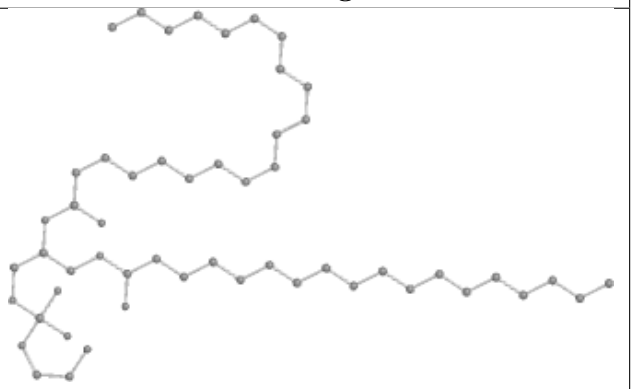
Bond lengths



Bond angles

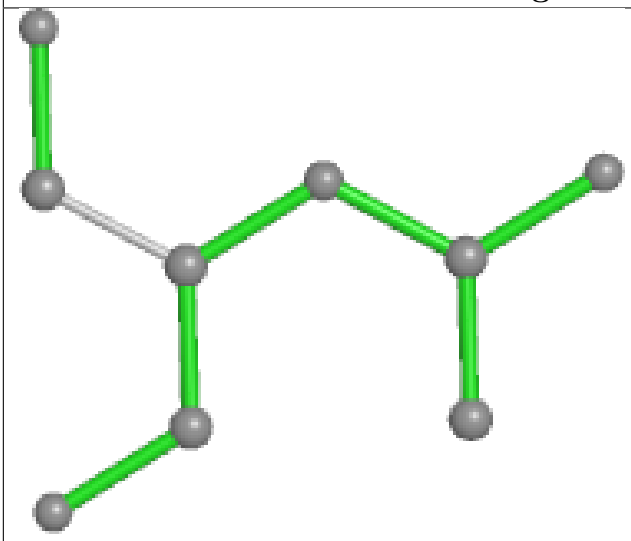


Torsions



Rings

Ligand SAC I 102



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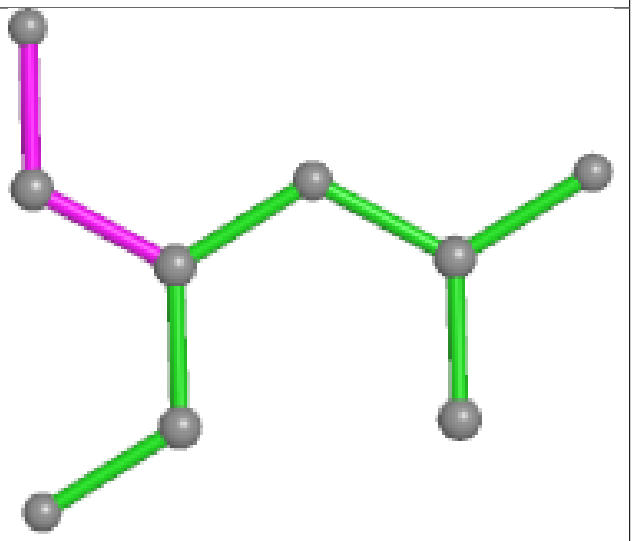
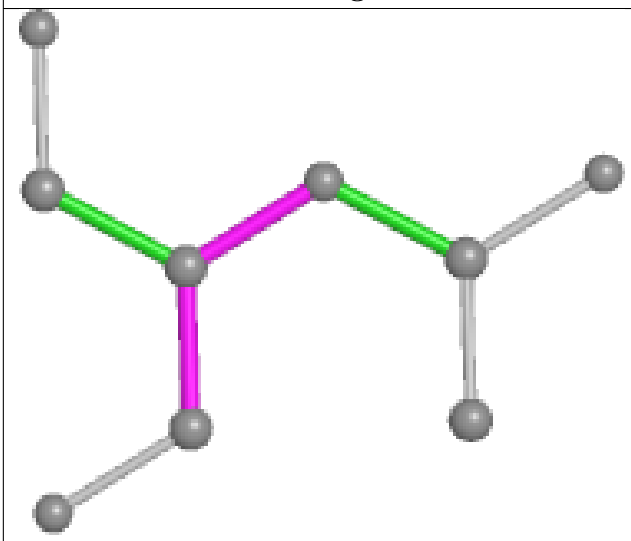


Bond angles



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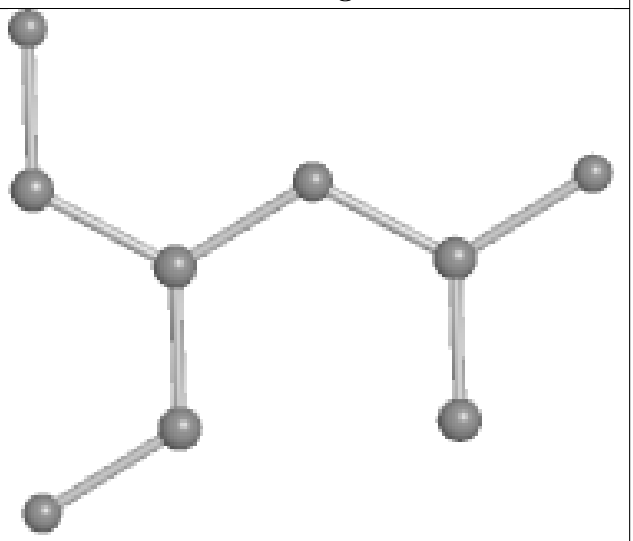
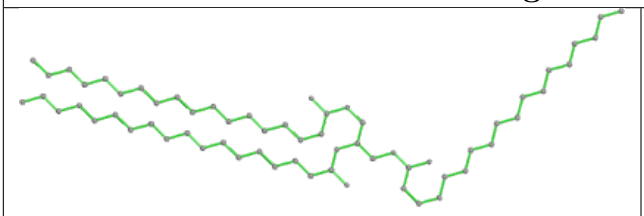


Rings

Ligand TGL N 608



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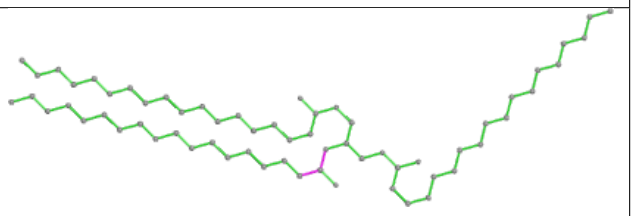
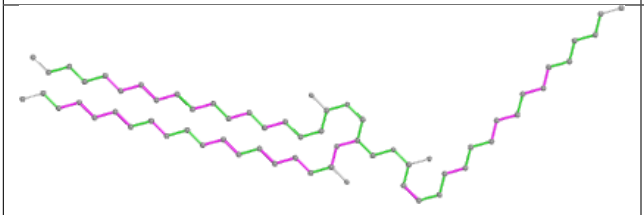
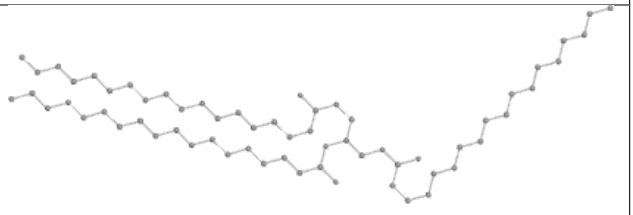


Bond angles

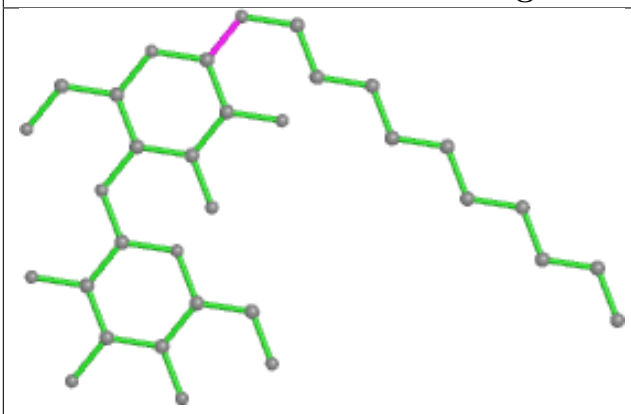


Torsions



Rings

Ligand DMU Q 201



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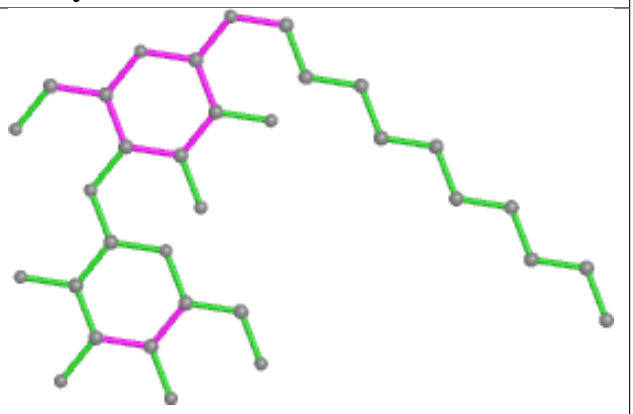
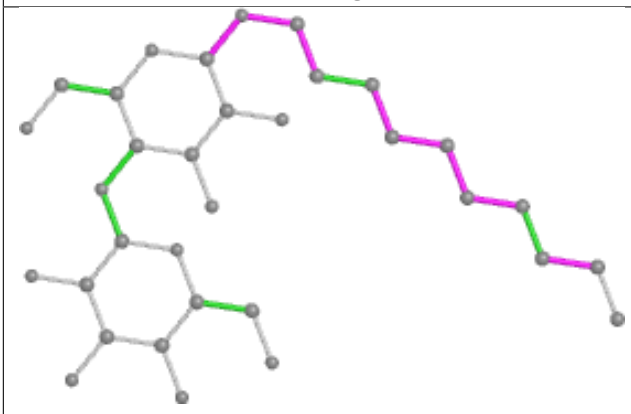
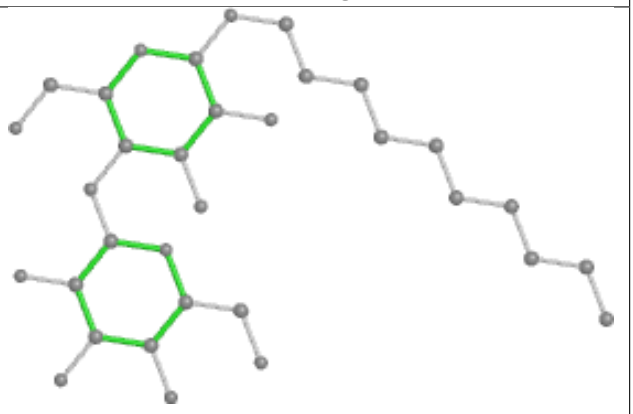


Bond angles

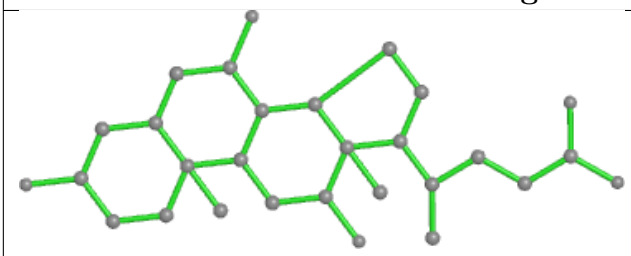


Torsions



Rings

Ligand CHD C 306



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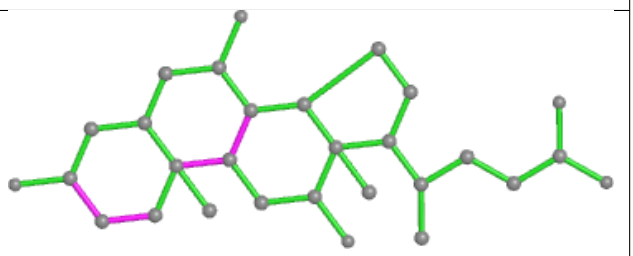
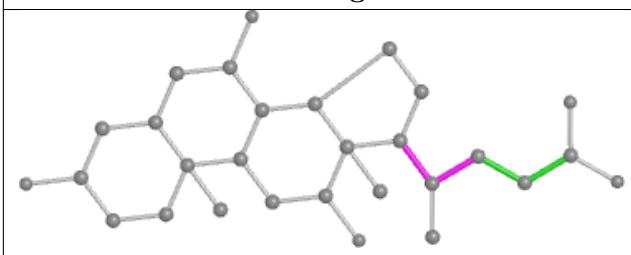


Bond angles



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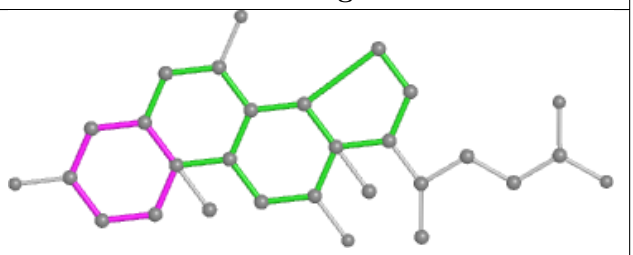
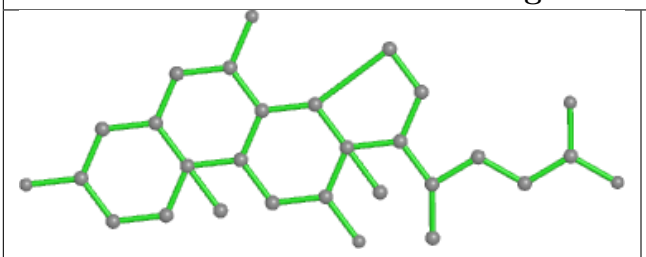


Rings

Ligand CHD J 101



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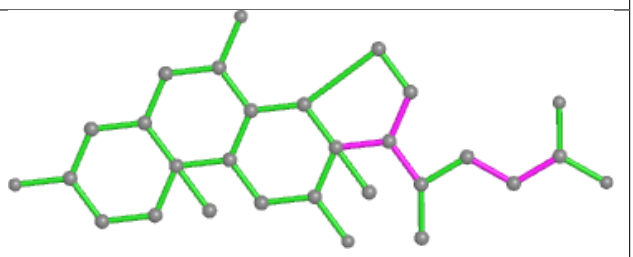

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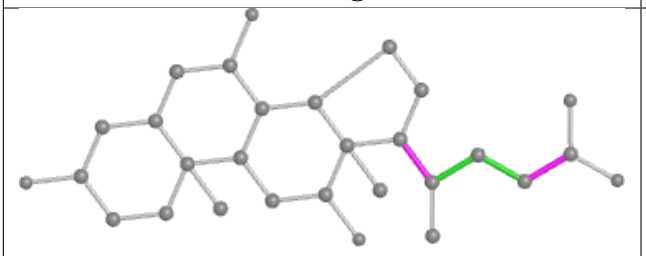

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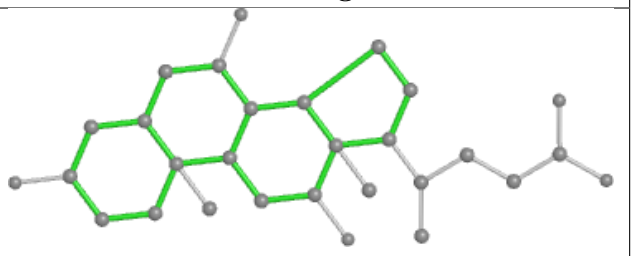
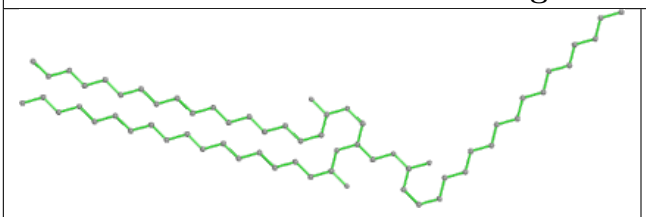


Rings

Ligand TGL I 101



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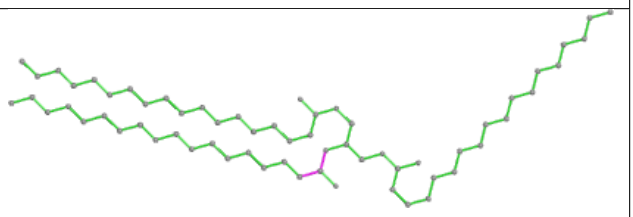

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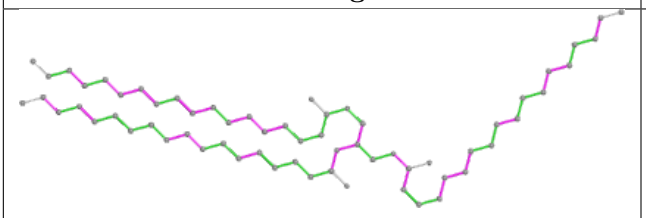

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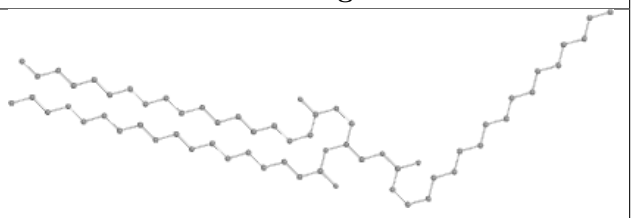
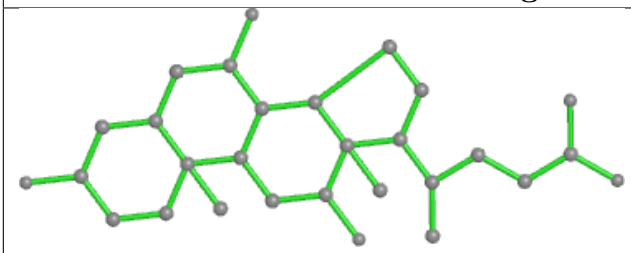


Rings

Ligand CHD C 301



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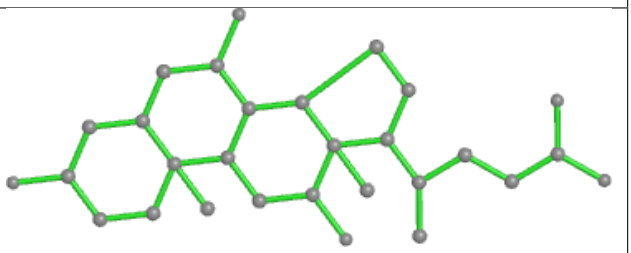

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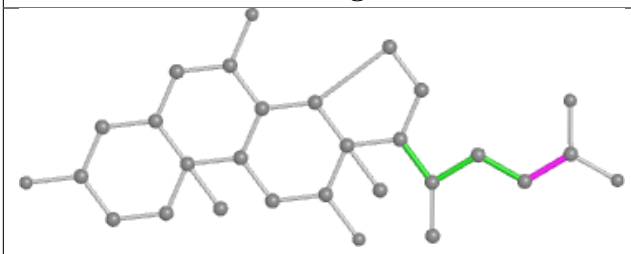

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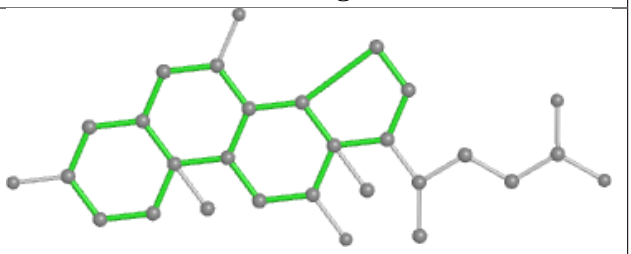
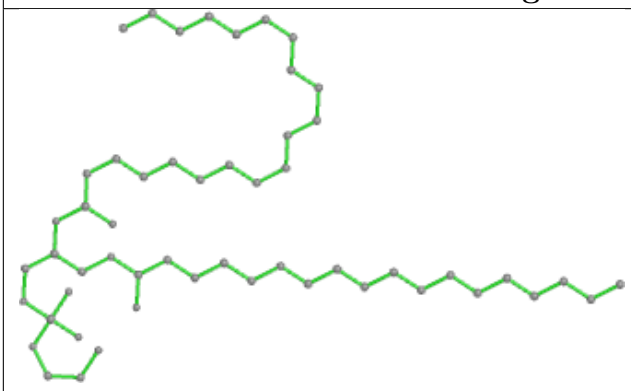


Rings

Ligand PEK G 101



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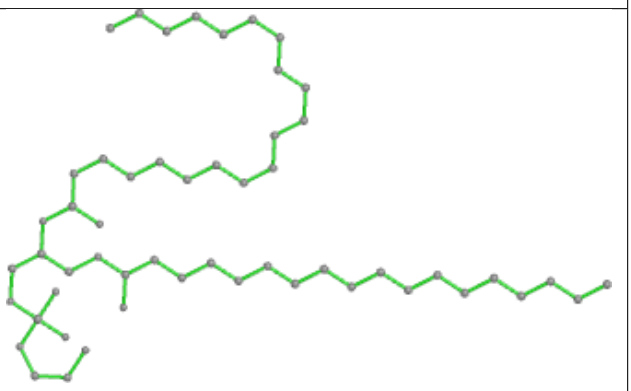
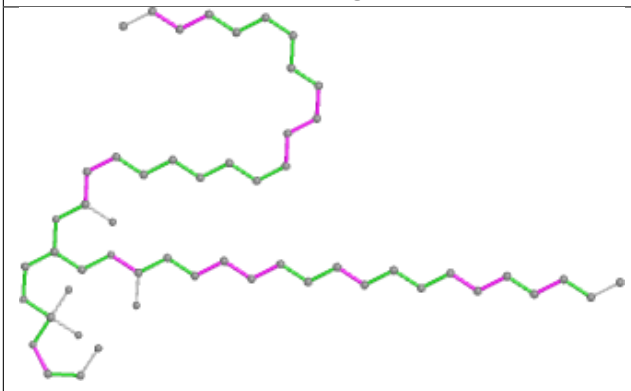
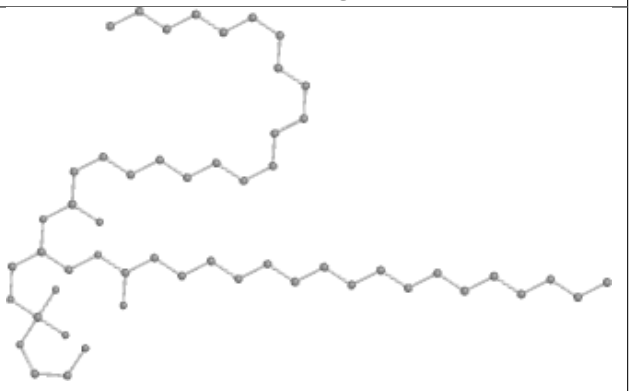


Bond angles

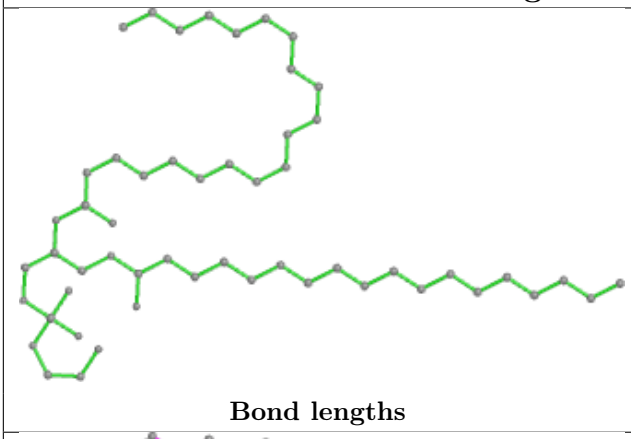


Torsions



Rings

Ligand PEK T 101



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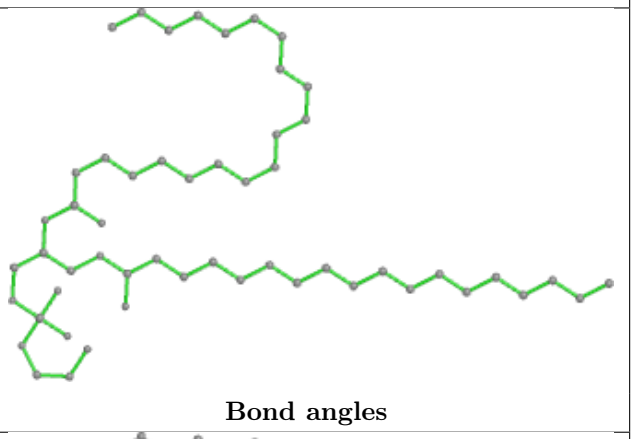
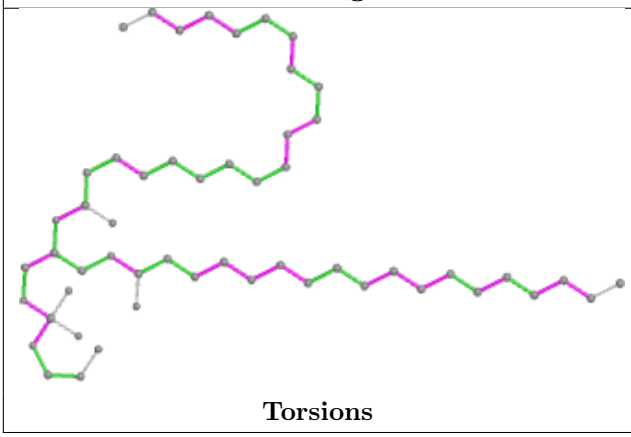


Bond angles



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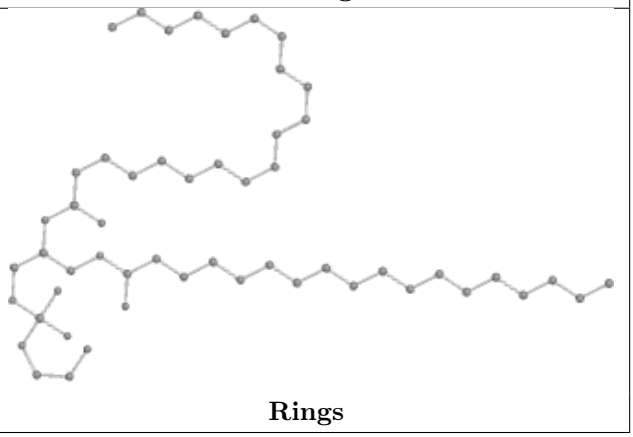
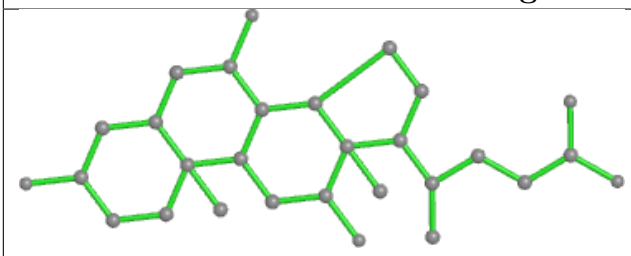


Rings

Ligand CHD N 609



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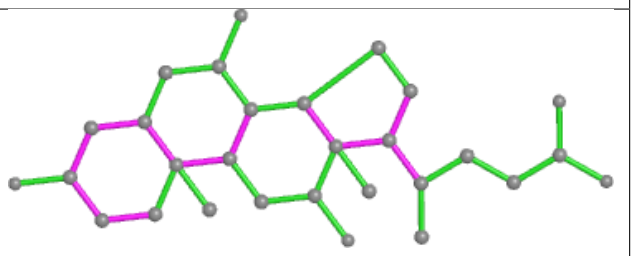
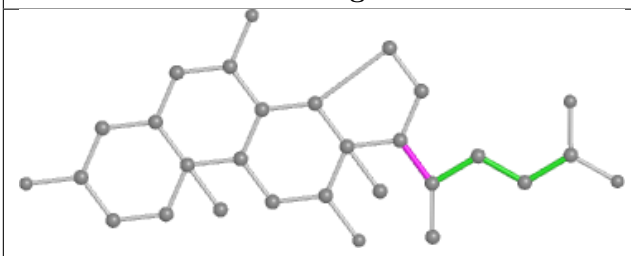
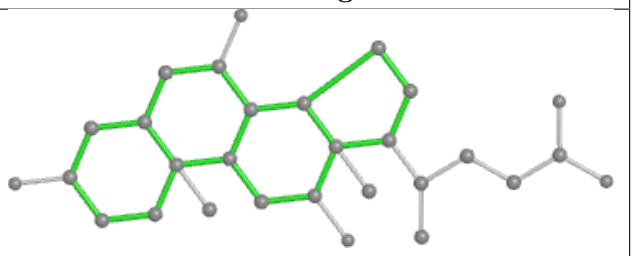


Bond angles

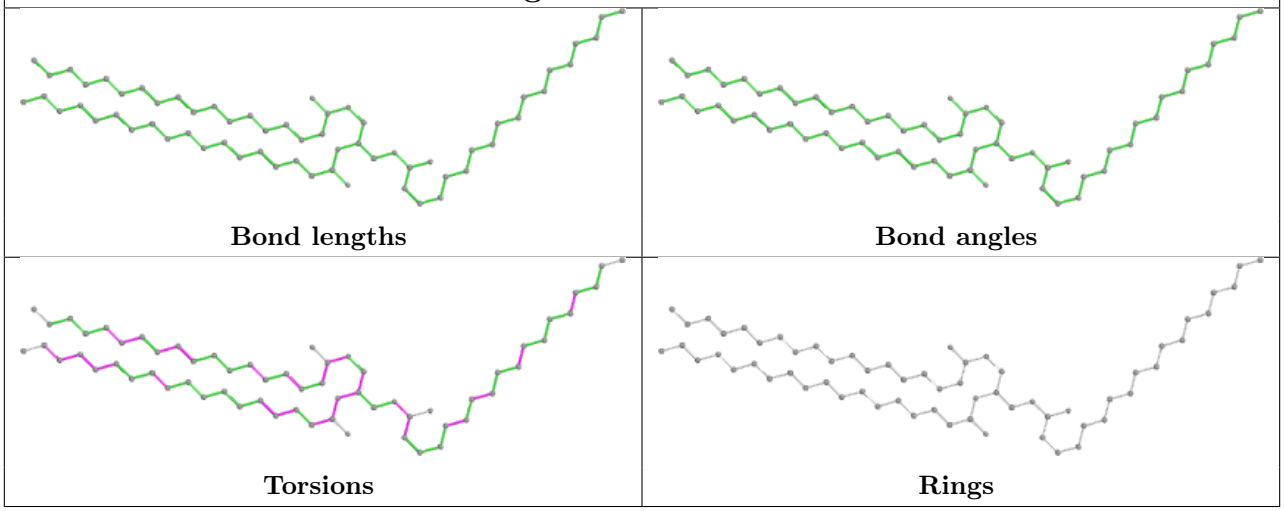


Torsions

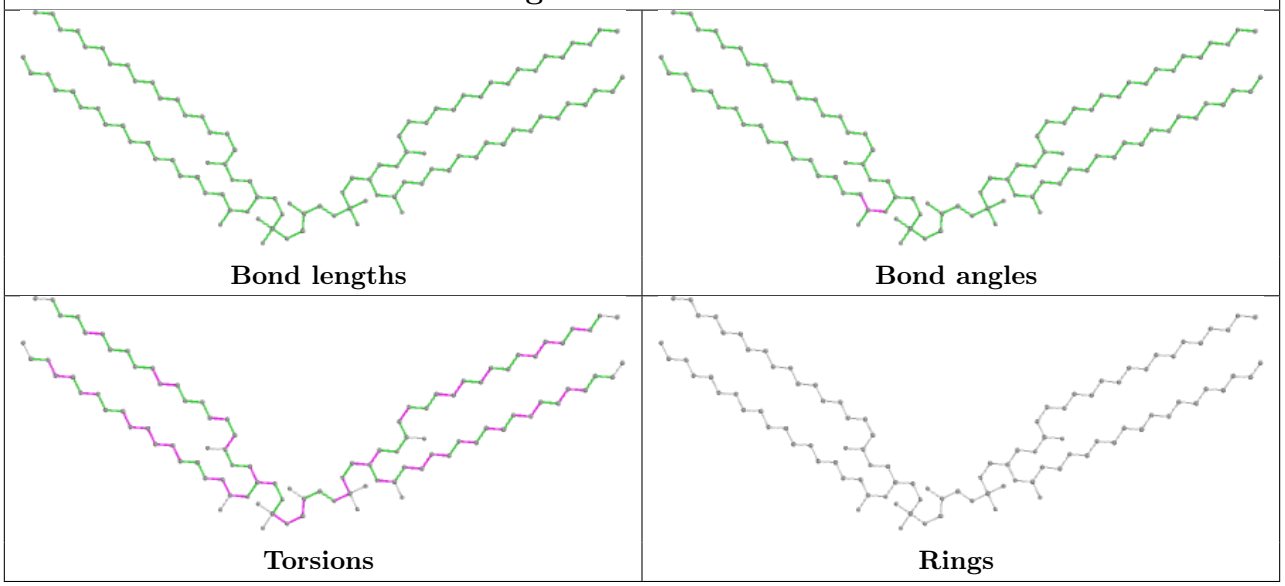


Rings

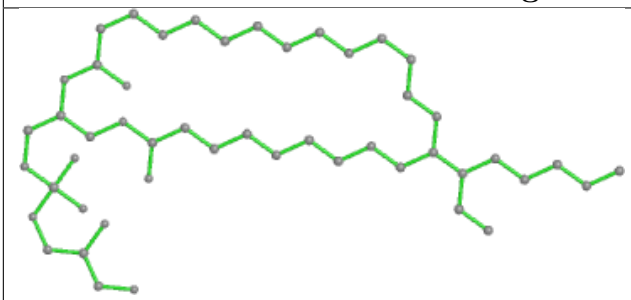
Ligand TGL N 606



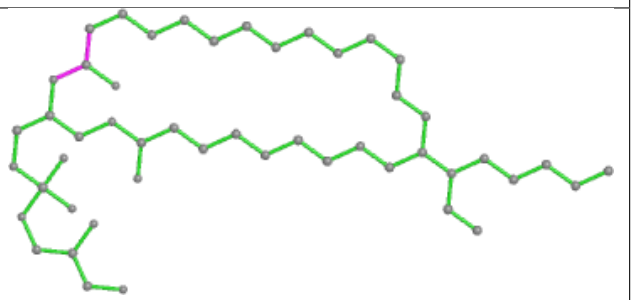
Ligand CDL P 305



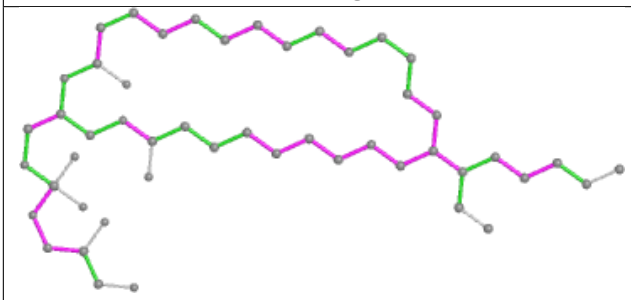
Ligand PGV C 304



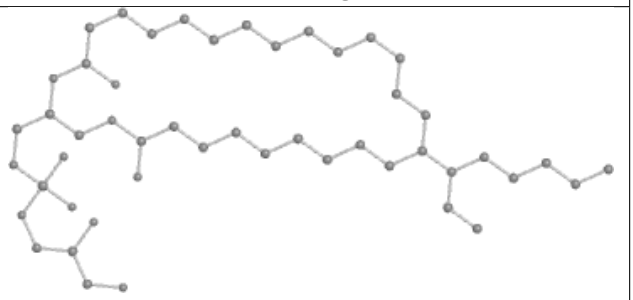
Bond lengths



Bond angles

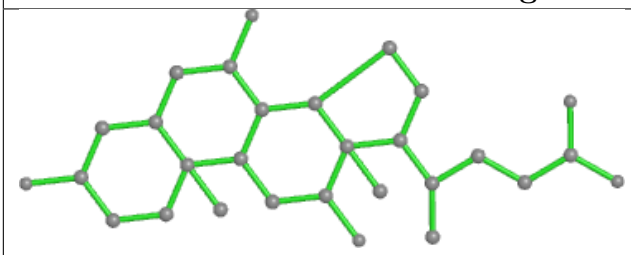


Torsions

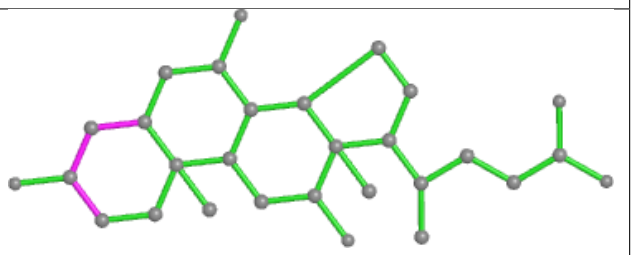


Rings

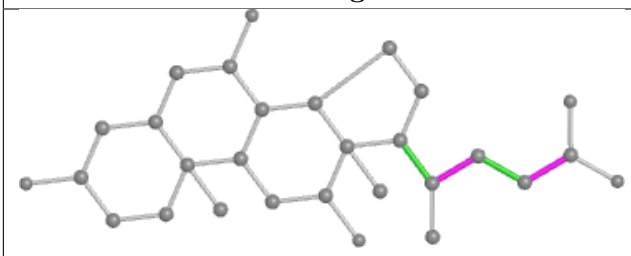
Ligand CHD G 105



Bond lengths



Bond angles



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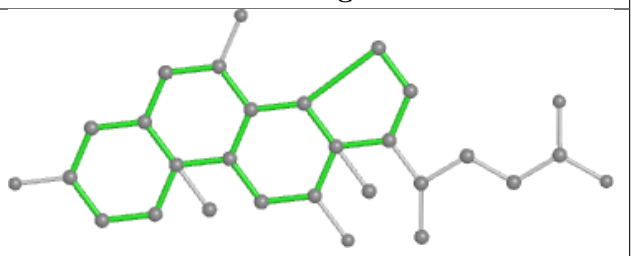
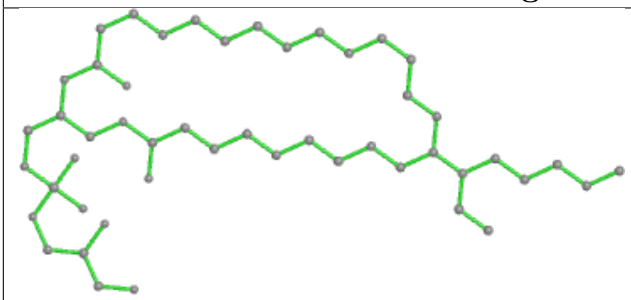


Rings

Ligand PGV C 303



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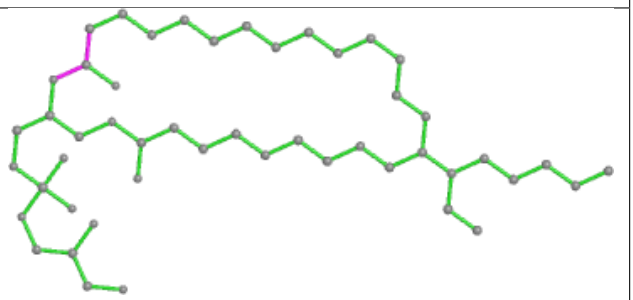
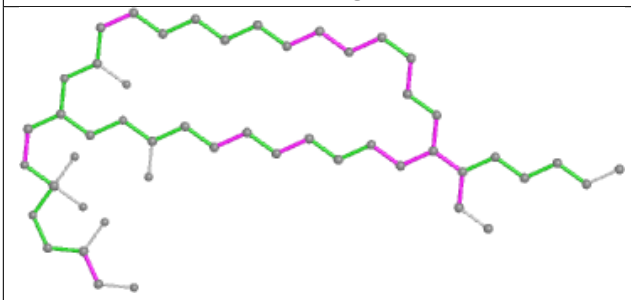


Bond angles



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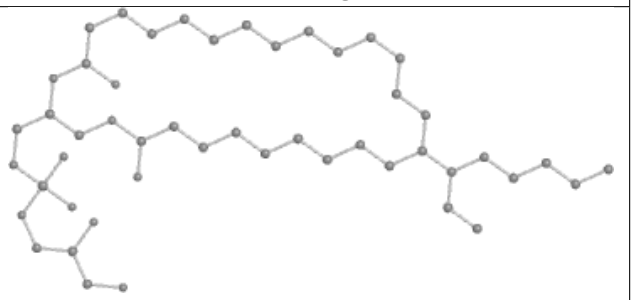
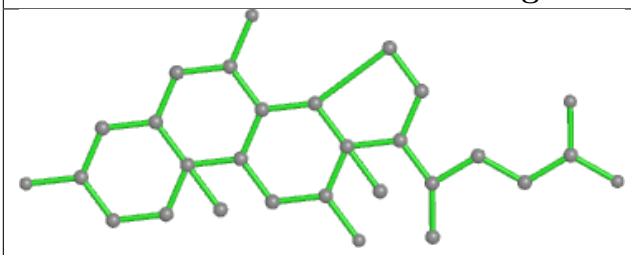


Rings

Ligand CHD P 306



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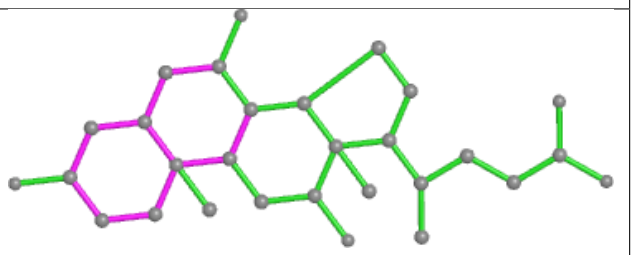

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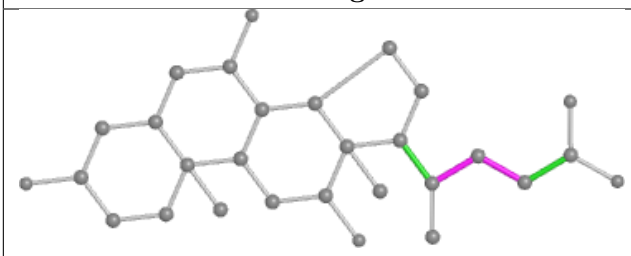

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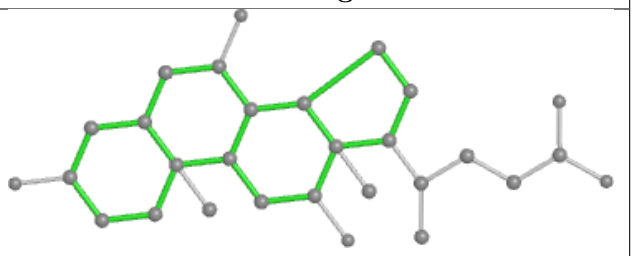
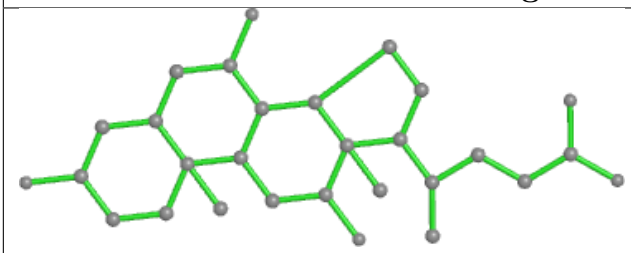


Rings

Ligand CHD P 302



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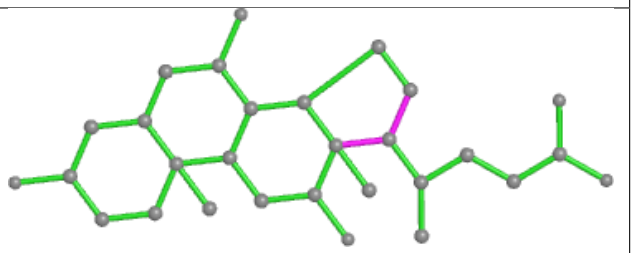

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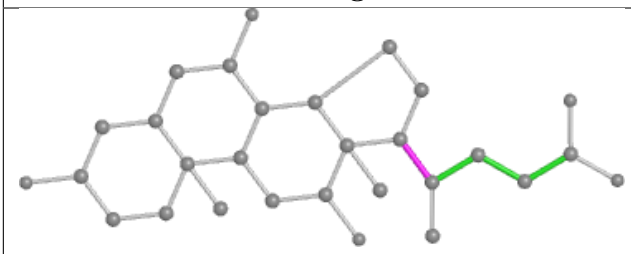

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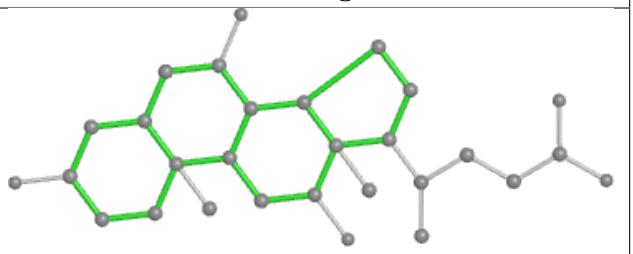
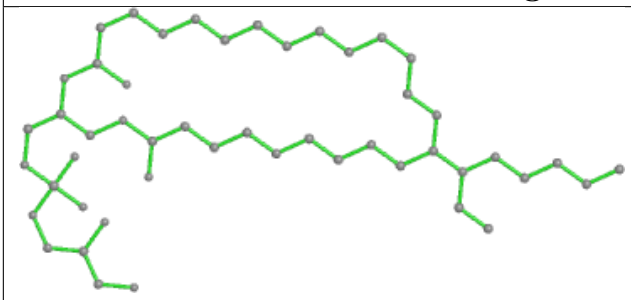


Rings

Ligand PGV Z 101



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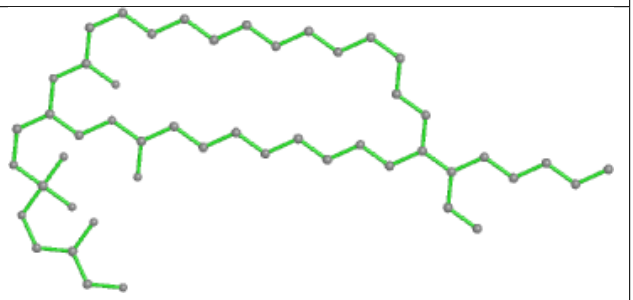
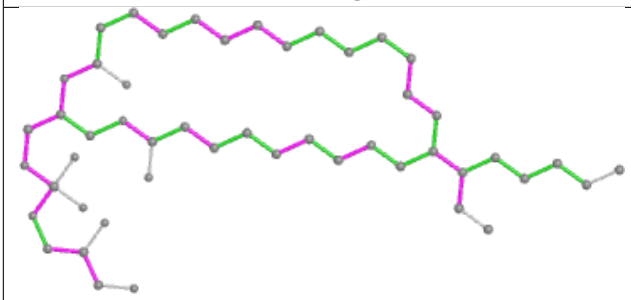


Bond angles



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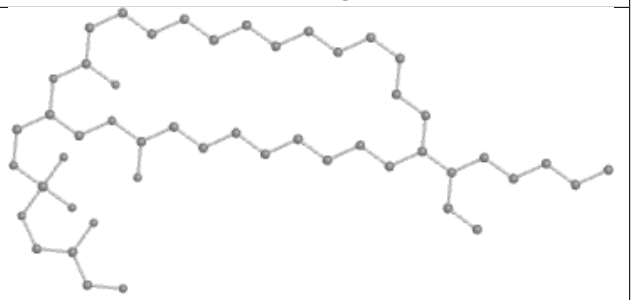
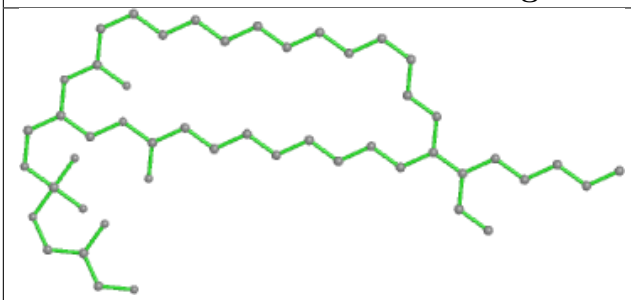


Rings

Ligand PGV A 607



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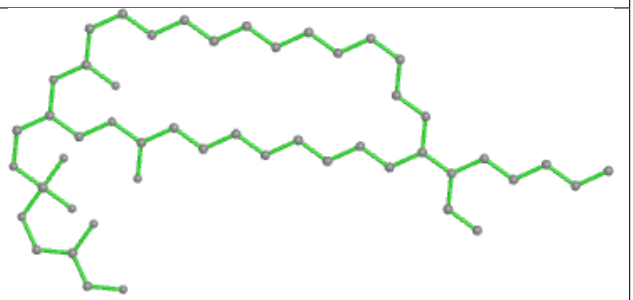
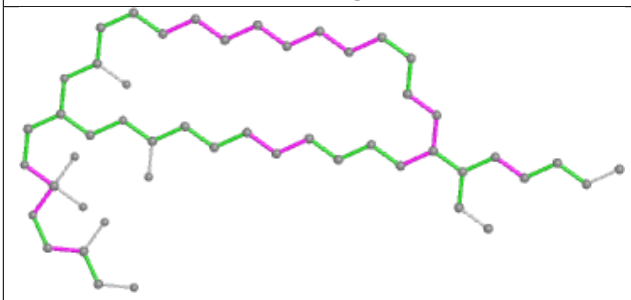


Bond angles



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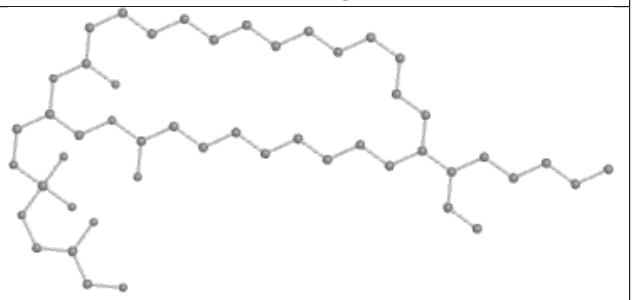
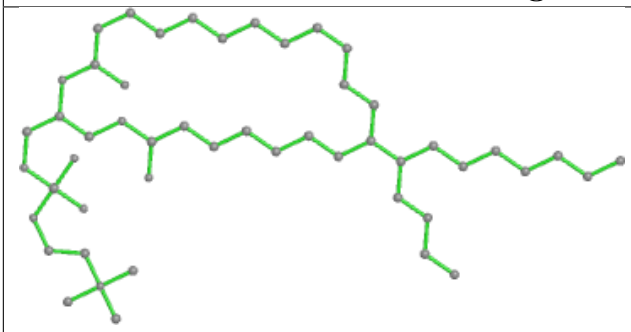


Rings

Ligand PSC E 201



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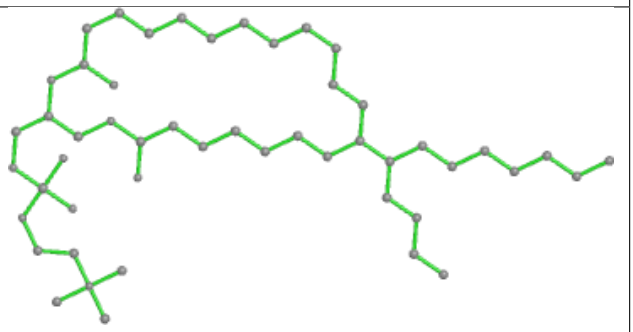
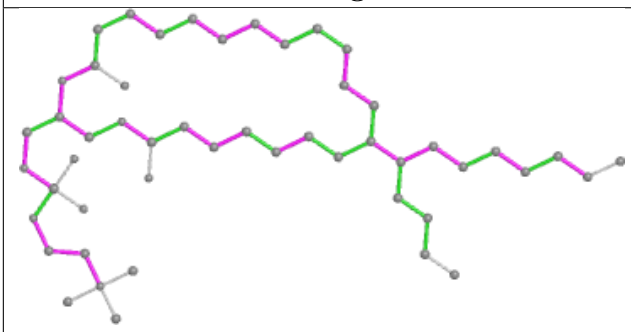


Bond angles



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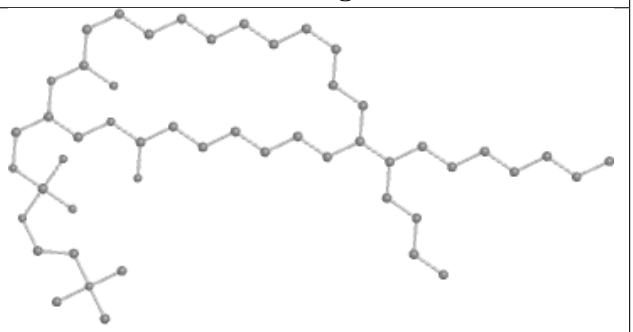
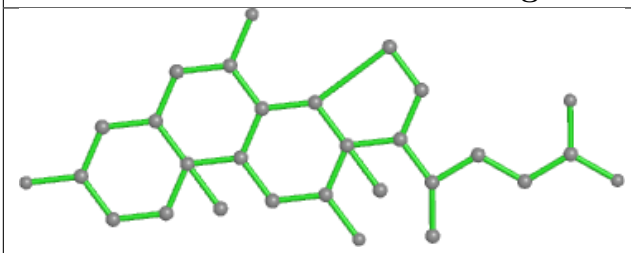


Rings

Ligand CHD B 302



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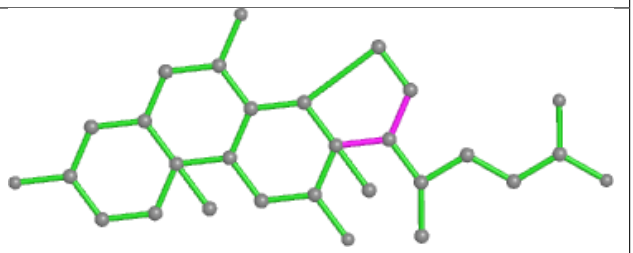
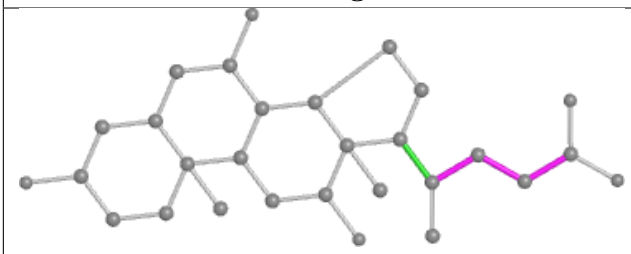


Bond angles



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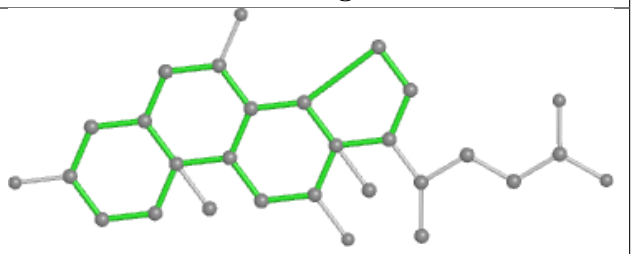
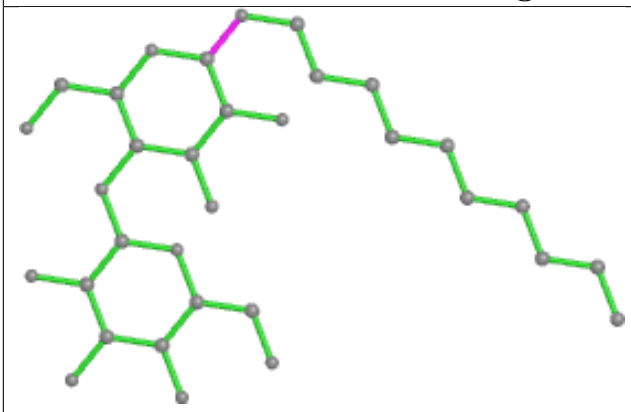


Rings

Ligand DMU G 102



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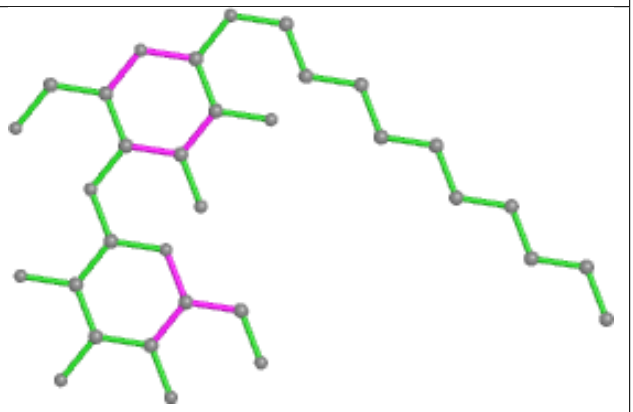
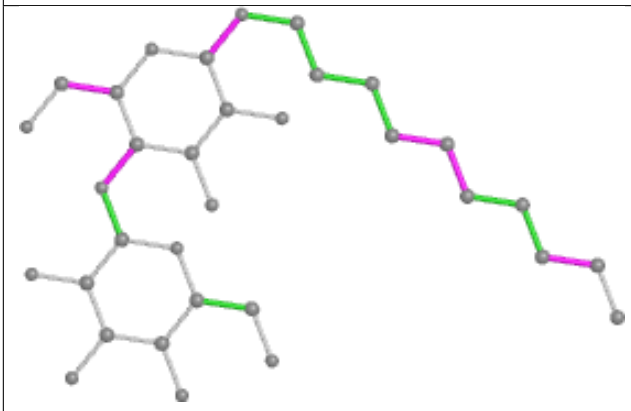


Bond angles



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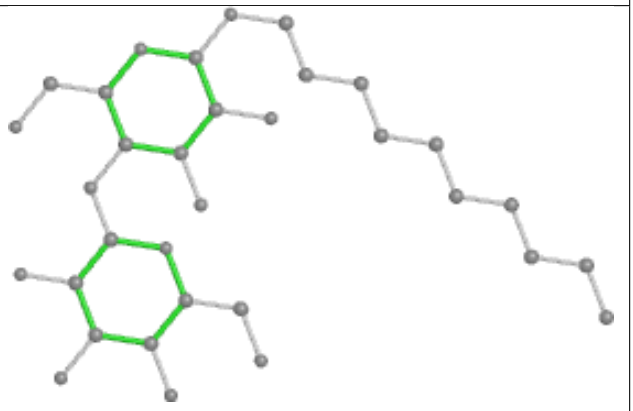
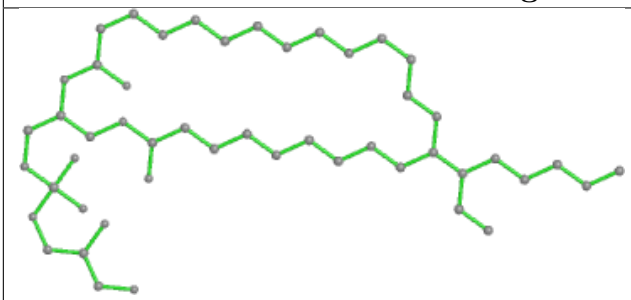


Rings

Ligand PGV U 101



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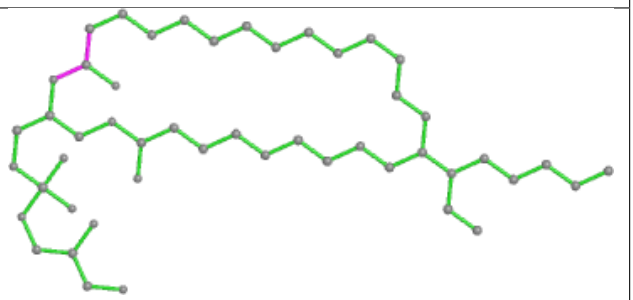
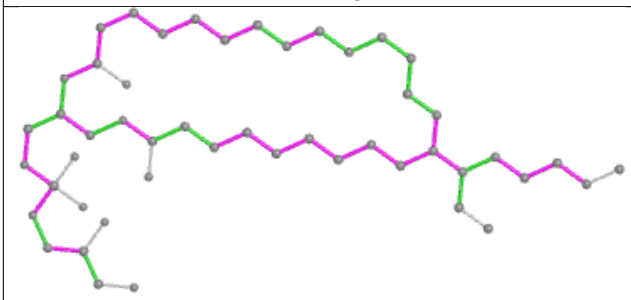


Bond angles



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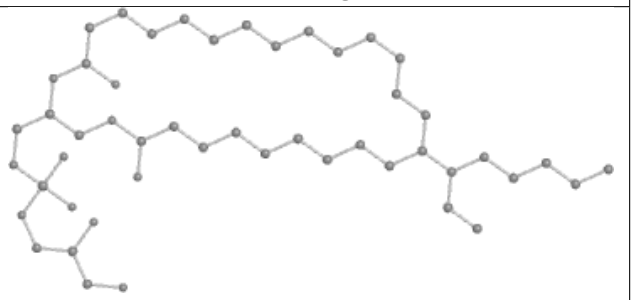
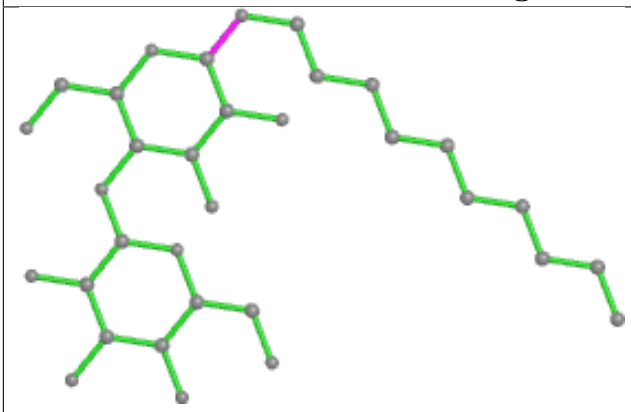


Rings

Ligand DMU M 102



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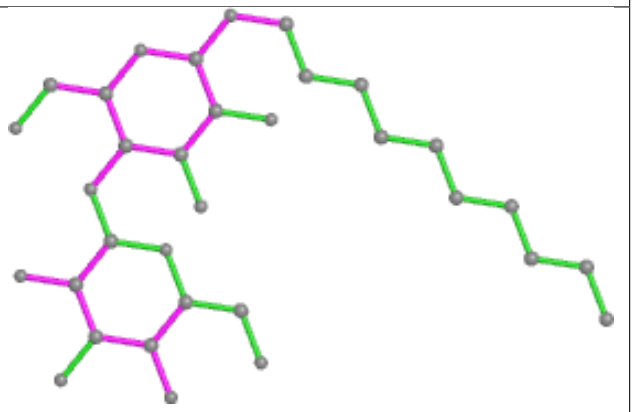
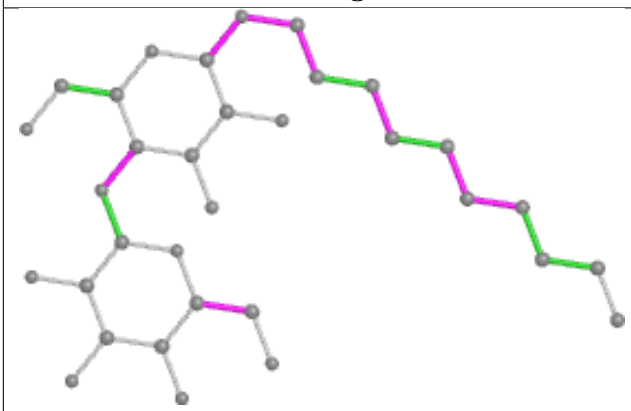


Bond angles



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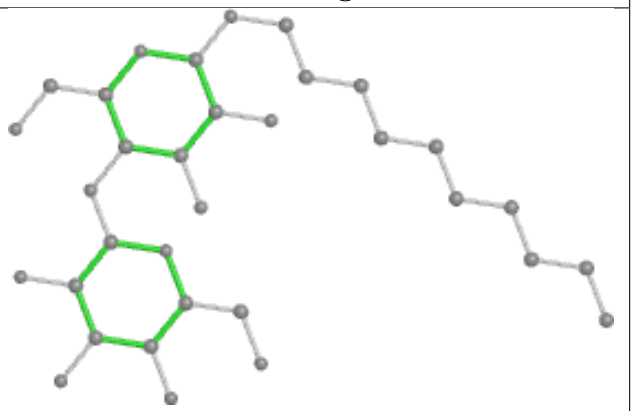
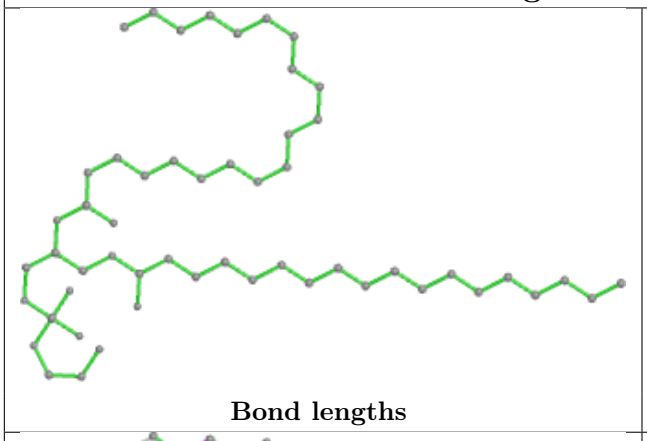


Rings

Ligand PEK G 106



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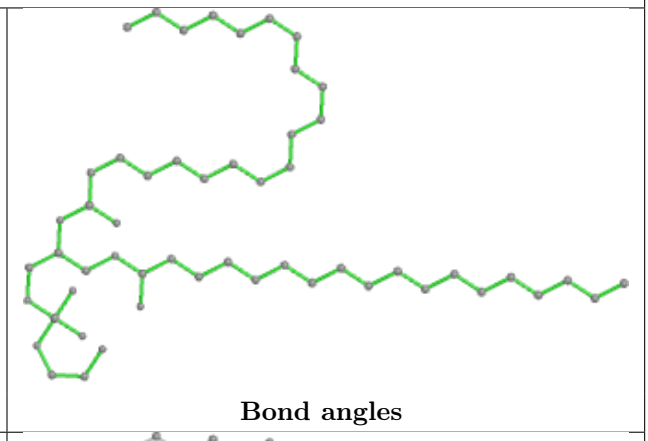
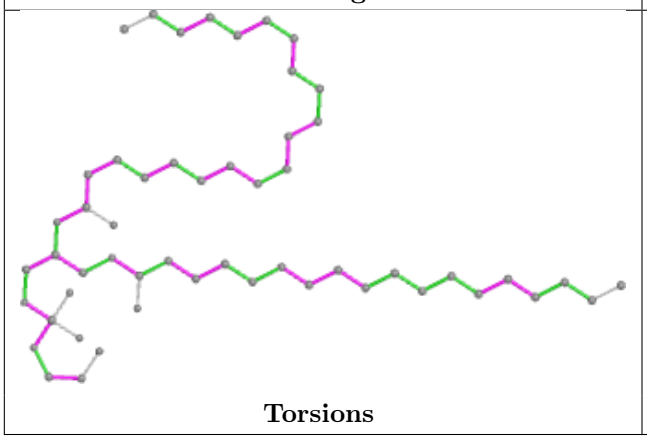


Bond angles



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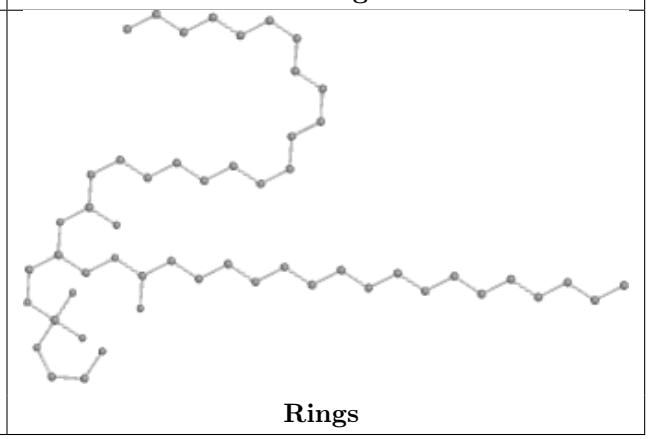
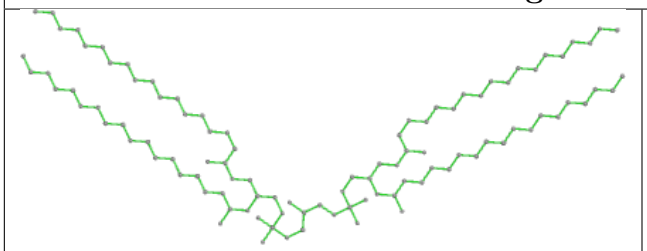


Rings

Ligand CDL T 104



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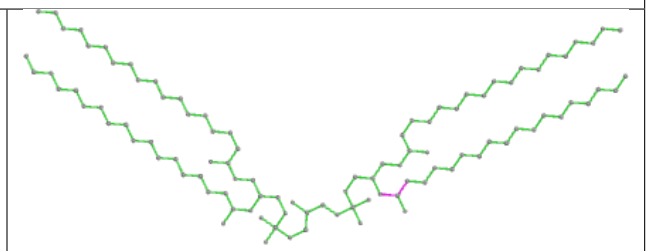
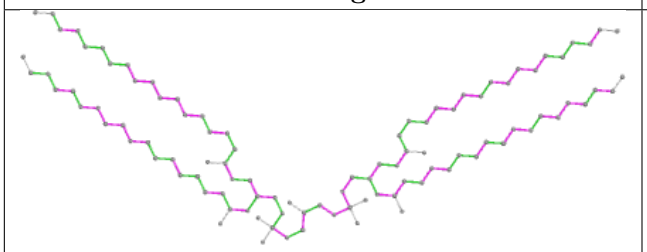


Bond angles



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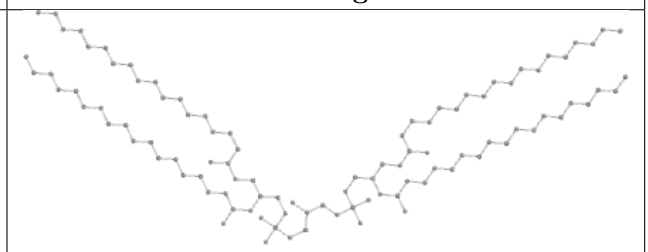
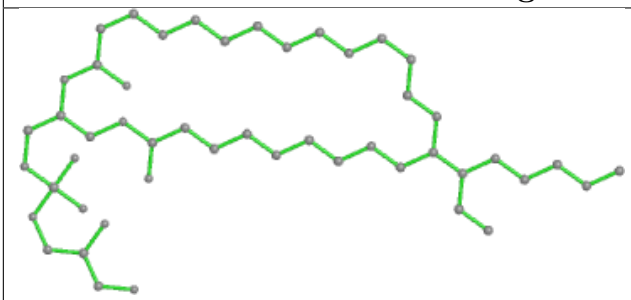


Rings

Ligand PGV M 101



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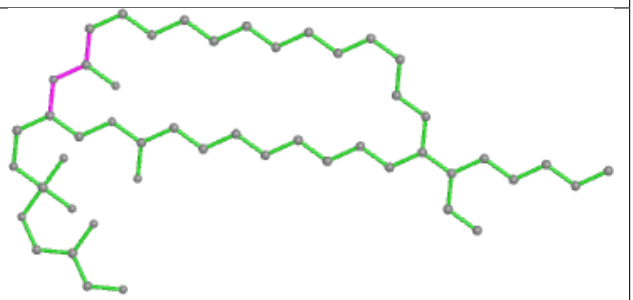
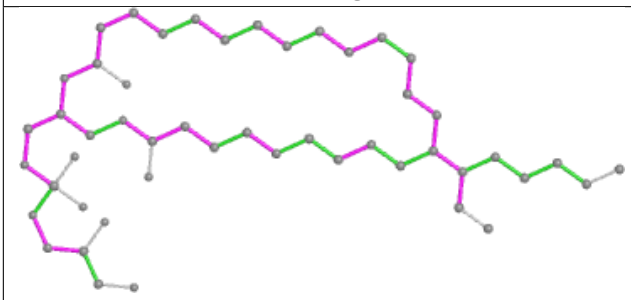


Bond angles



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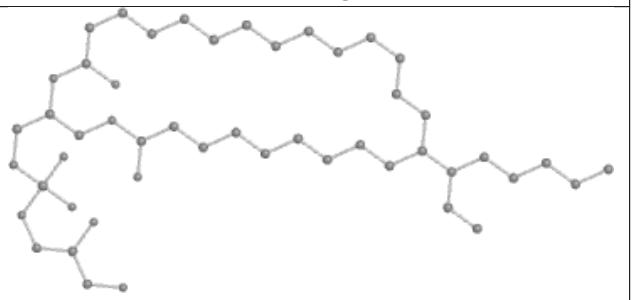
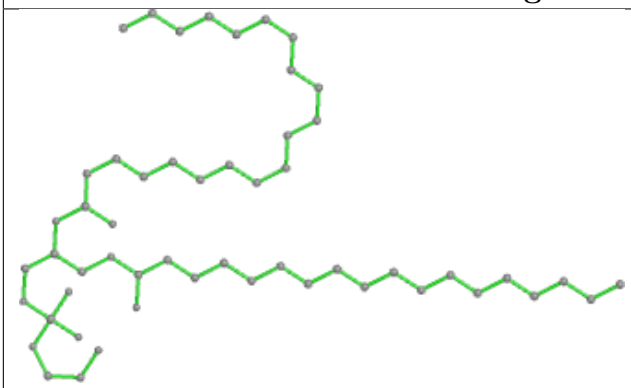
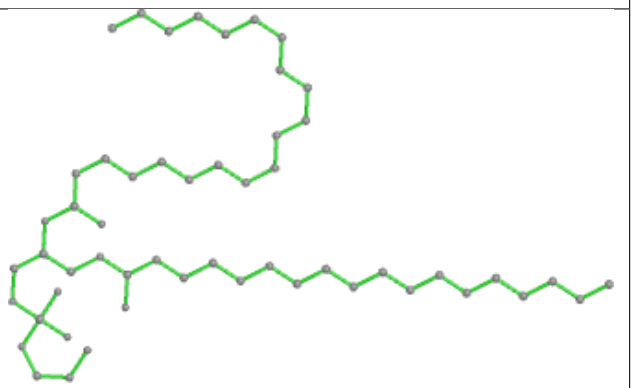


Rings

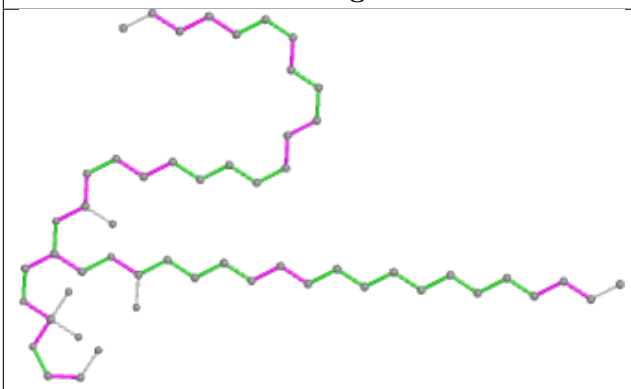
Ligand PEK T 103



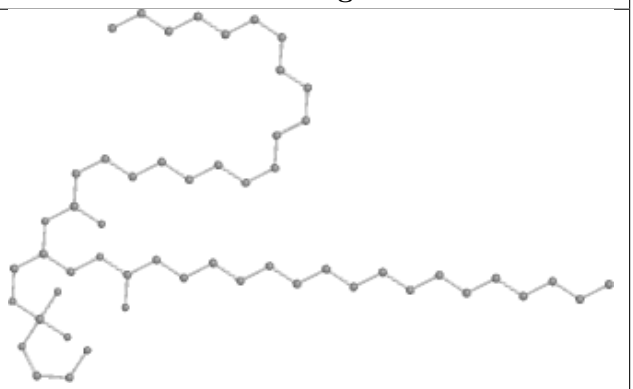
Bond lengths



Bond angles

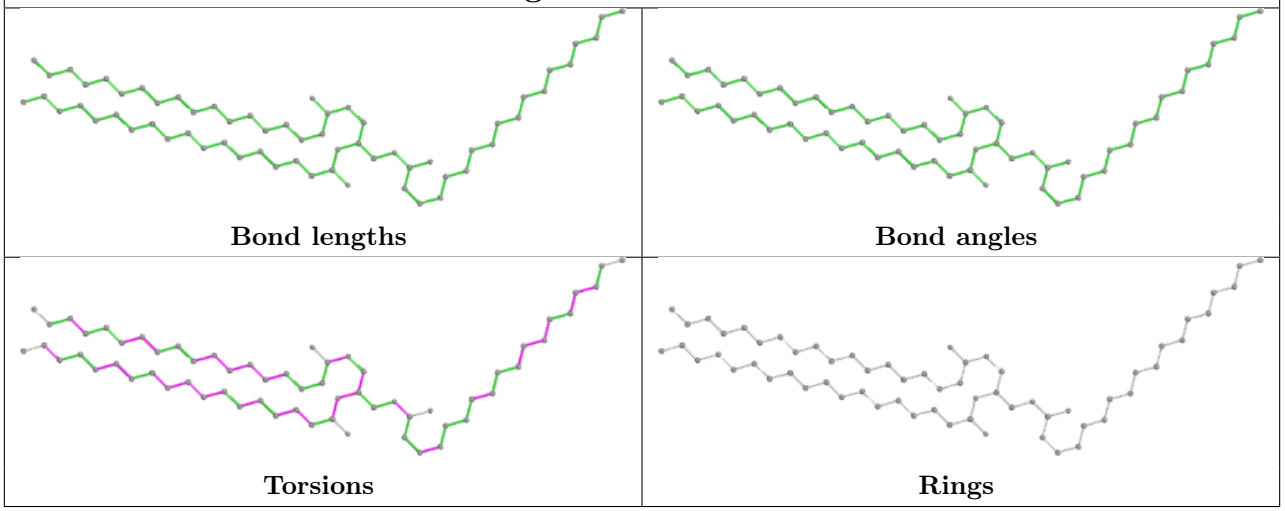


Torsions

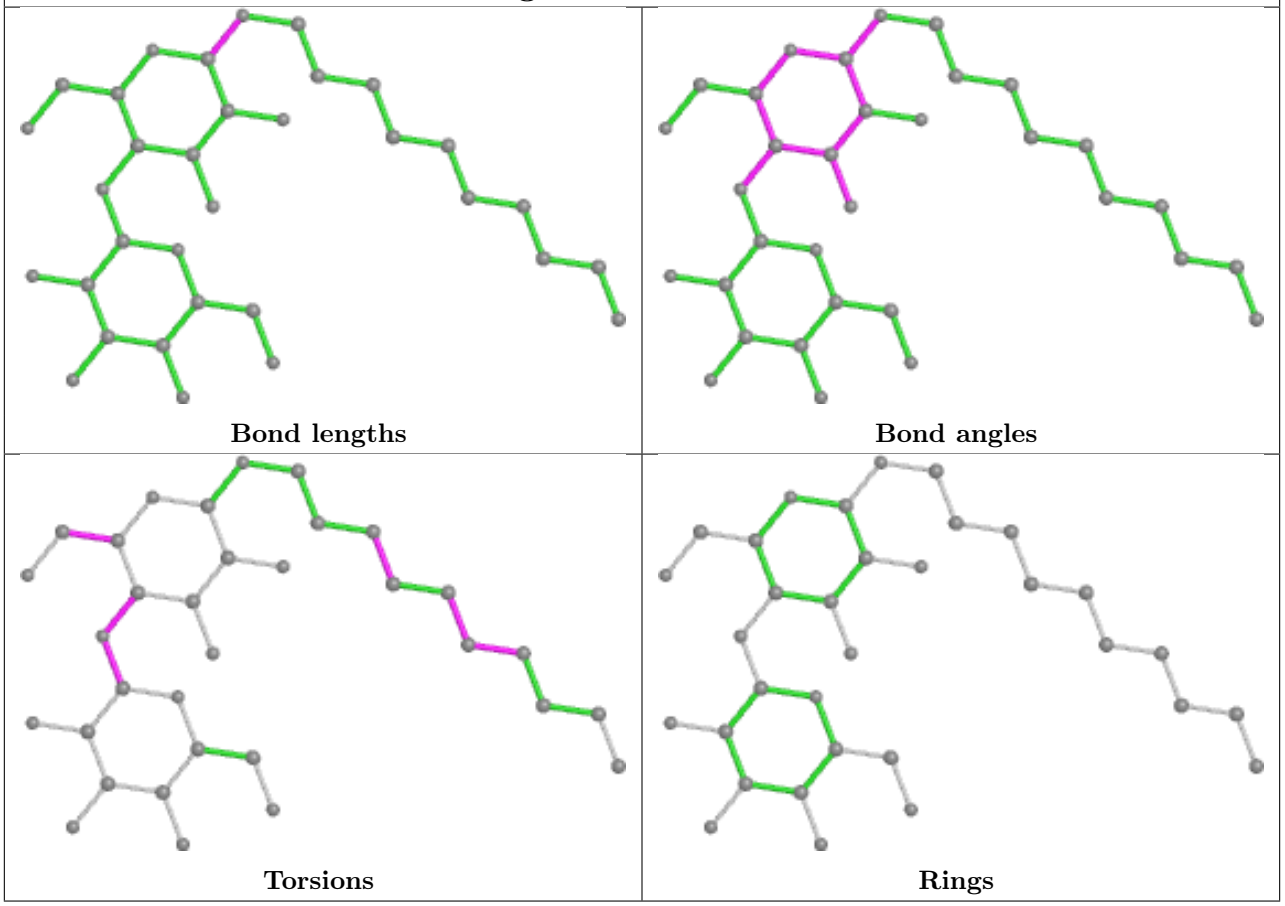


Rings

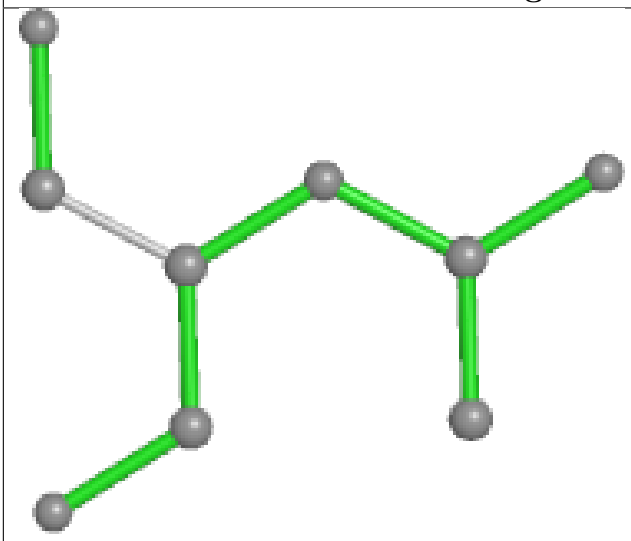
Ligand TGL A 606



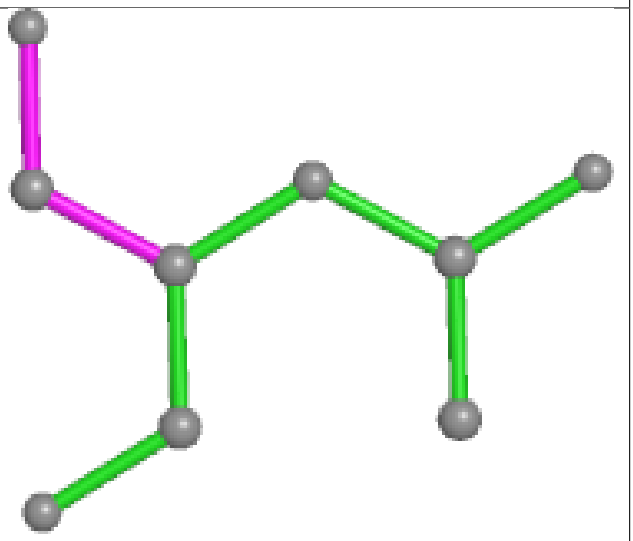
Ligand DMU T 102



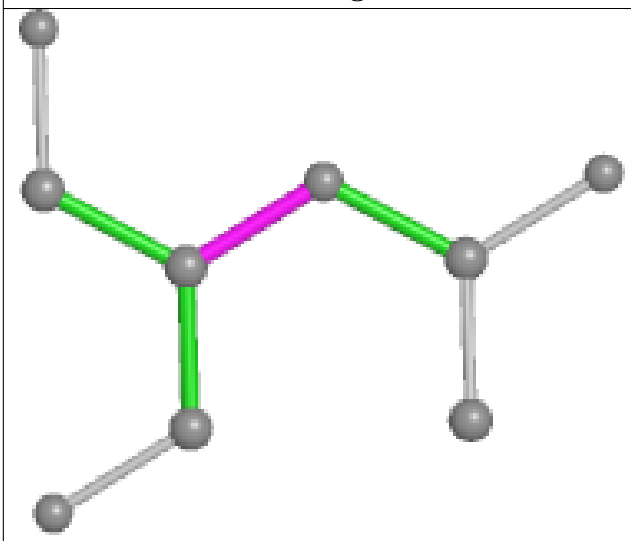
Ligand SAC V 101



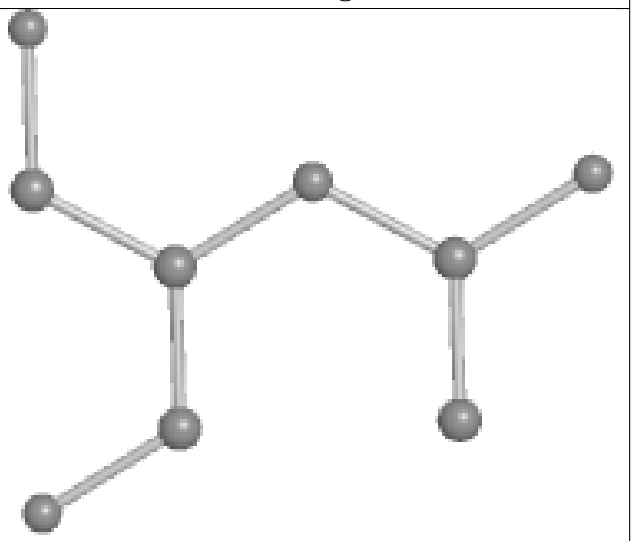
Bond lengths



Bond angles

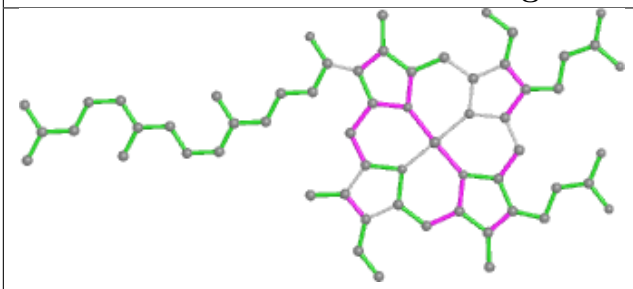


Torsions

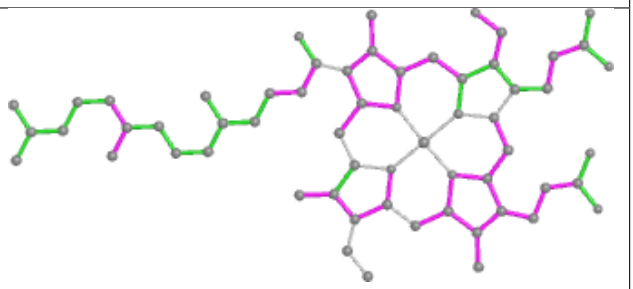


Rings

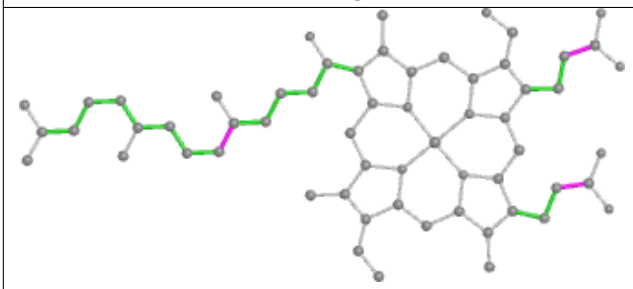
Ligand HEA A 602



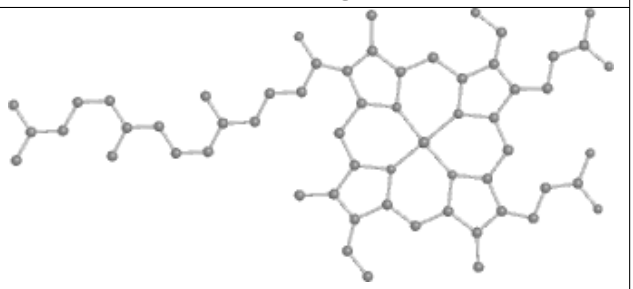
Bond lengths



Bond angles

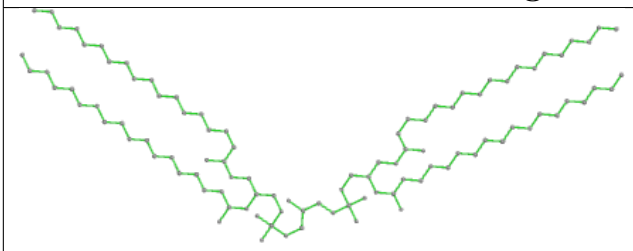


Torsions

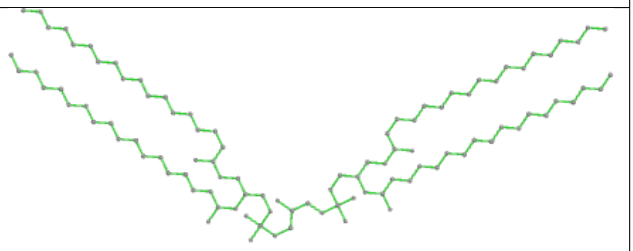


Rings

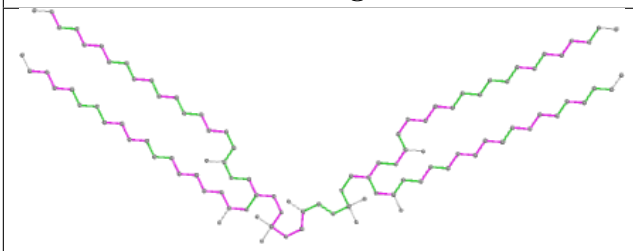
Ligand CDL C 305



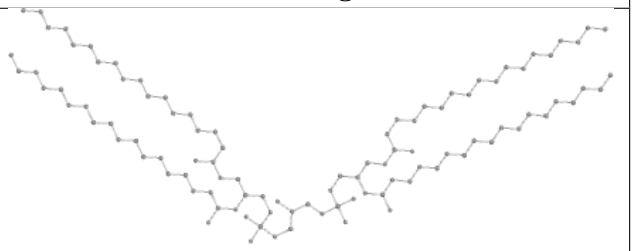
Bond lengths



Bond angles

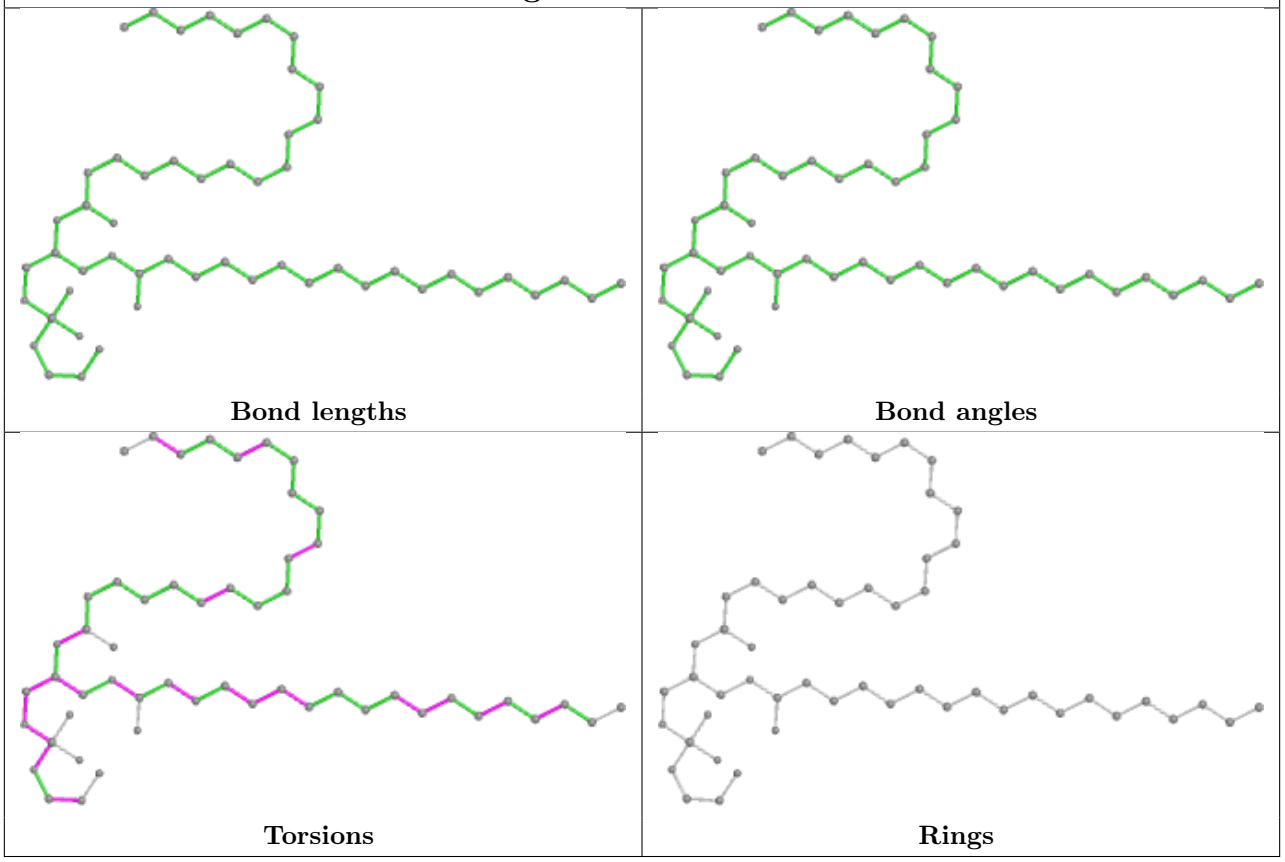


Torsions

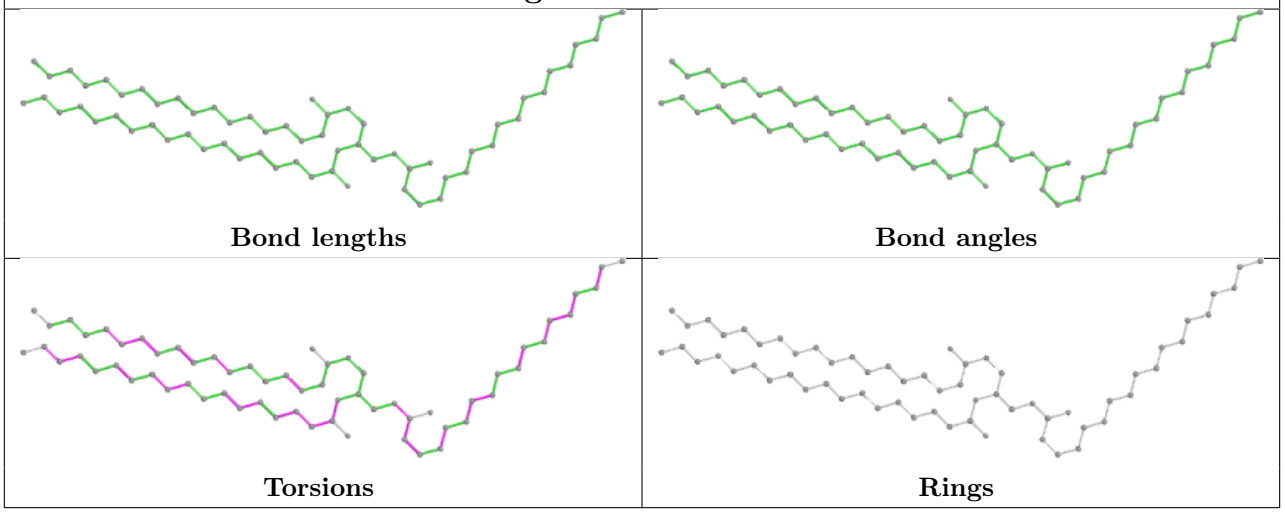


Rings

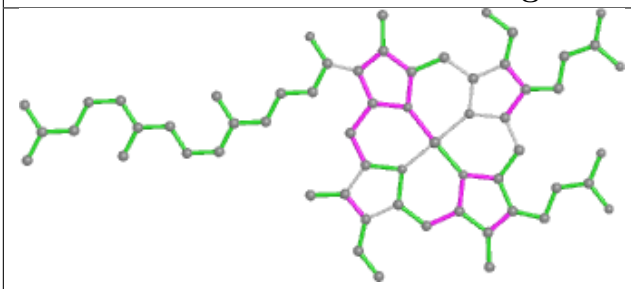
Ligand PEK G 103



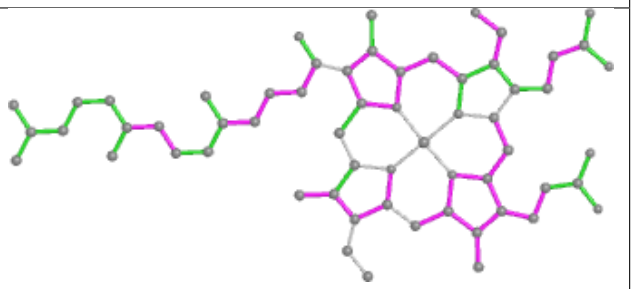
Ligand TGL Y 101



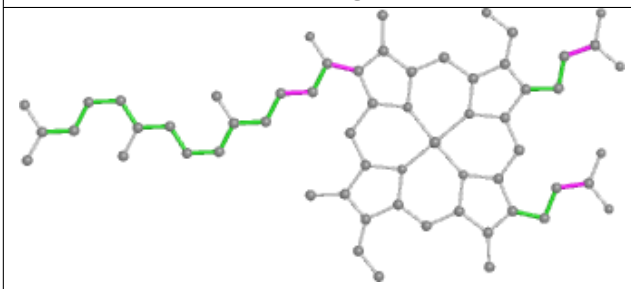
Ligand HEA A 601



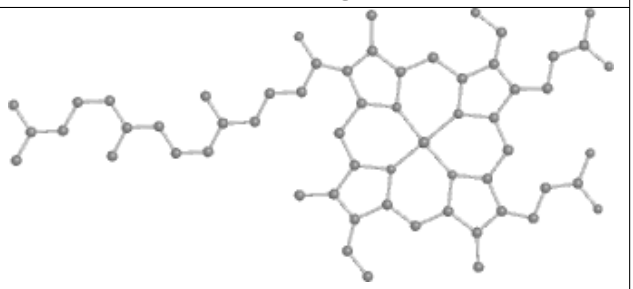
Bond lengths



Bond angles

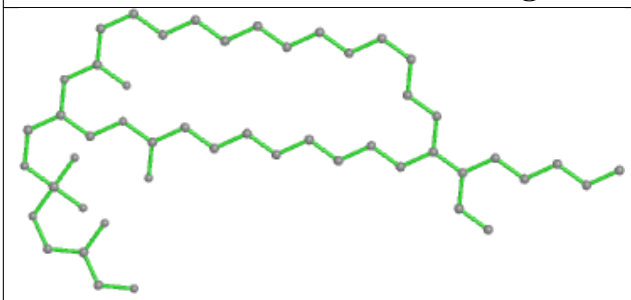


Torsions

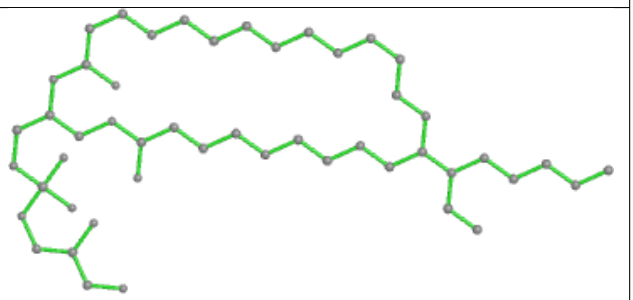


Rings

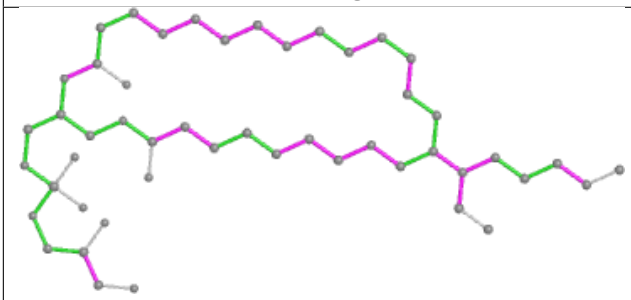
Ligand PGV N 607



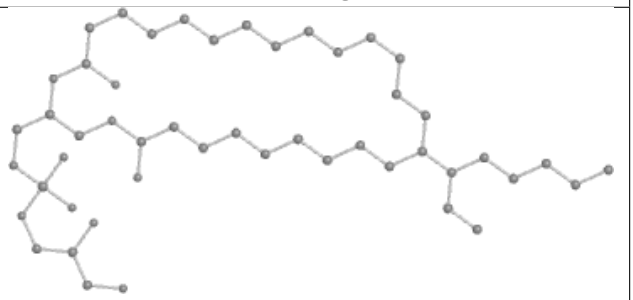
Bond lengths



Bond angles

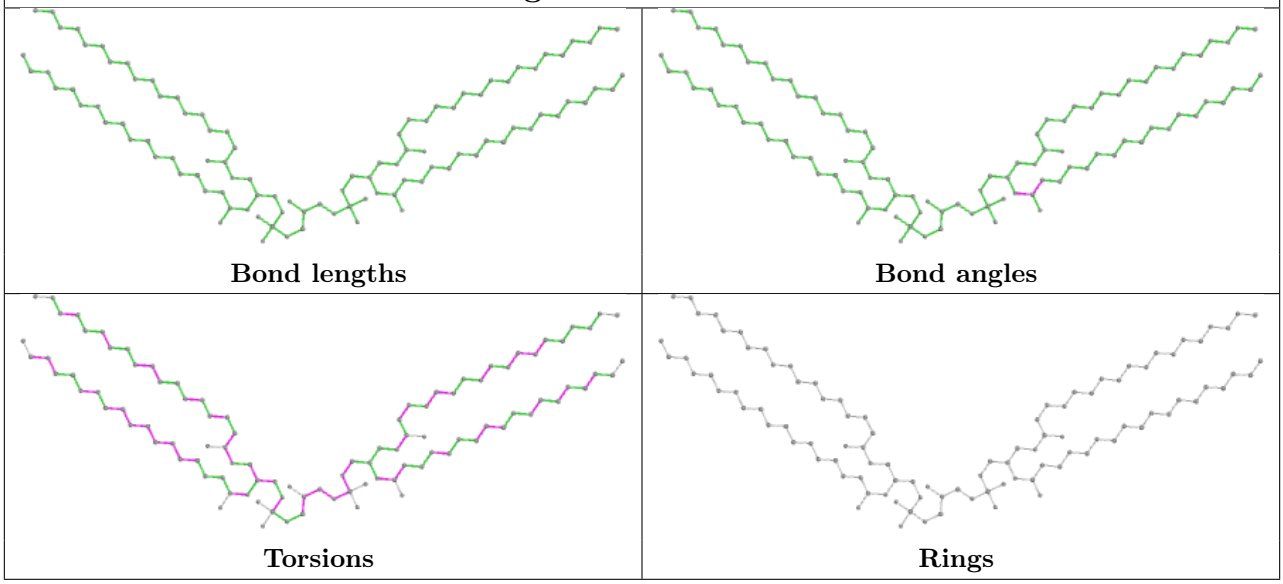


Torsions

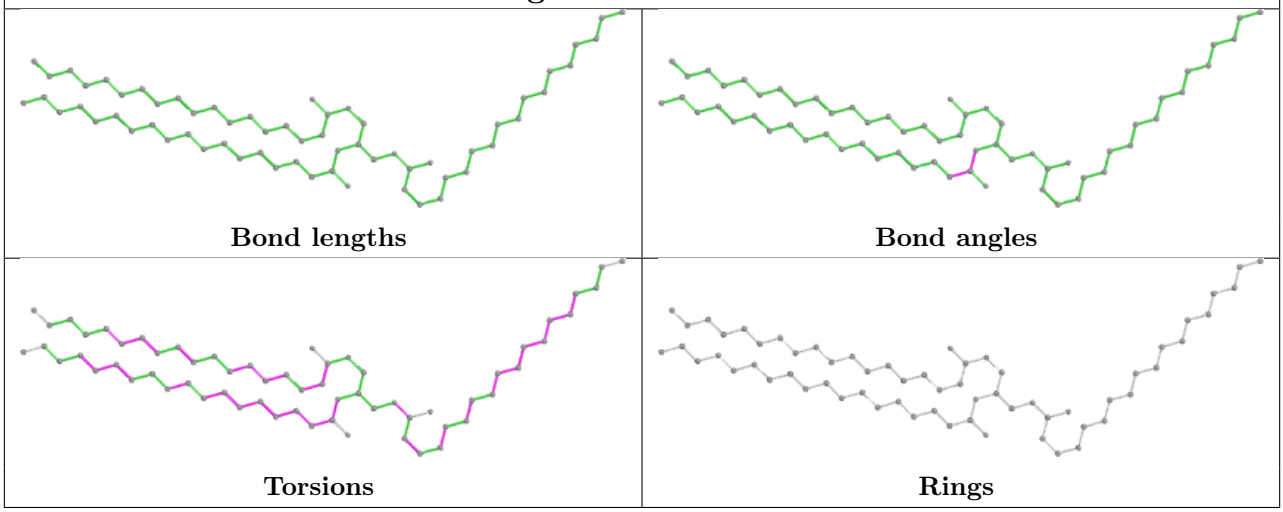


Rings

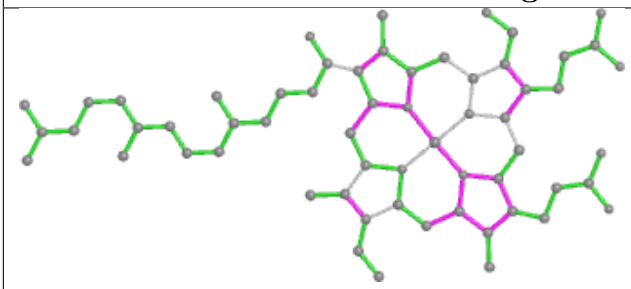
Ligand CDL G 104



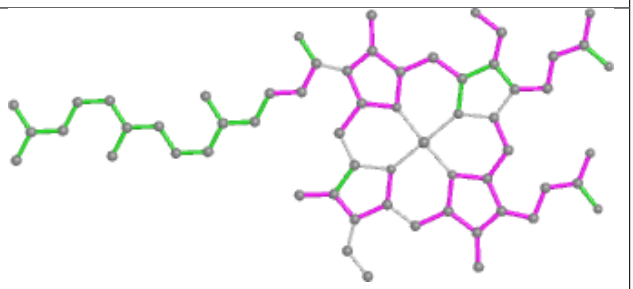
Ligand TGL L 101



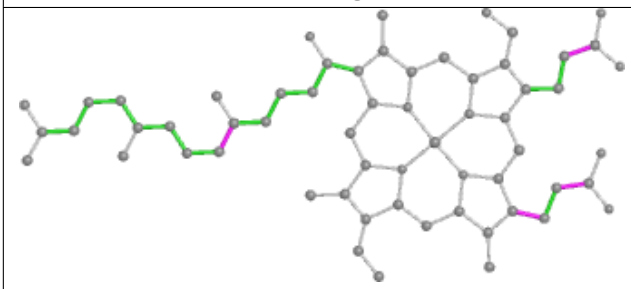
Ligand HEA N 602



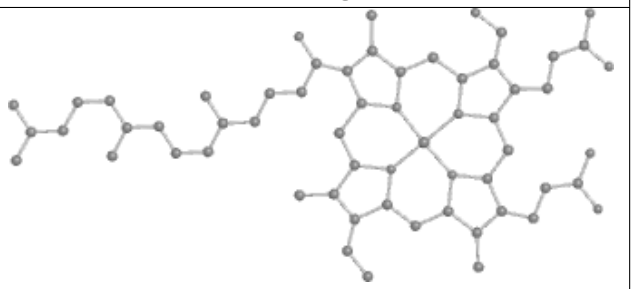
Bond lengths



Bond angles

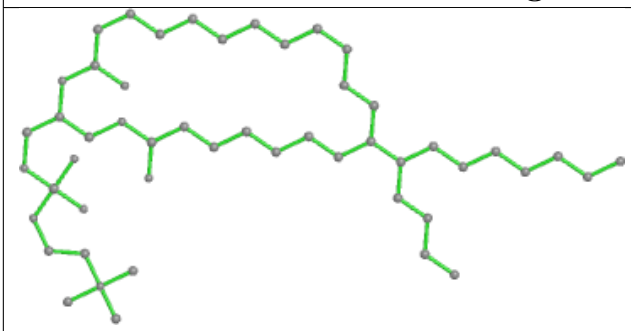


Torsions

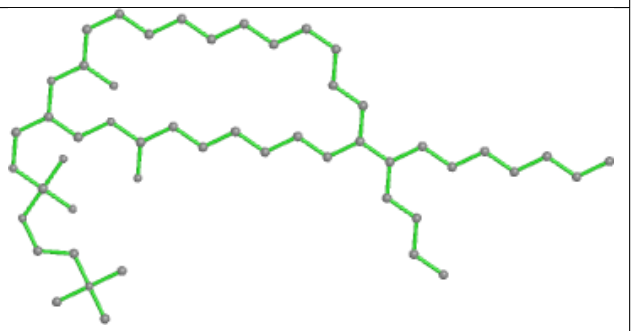


Rings

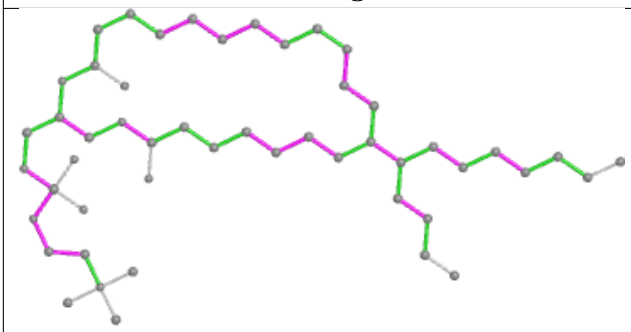
Ligand PSC R 201



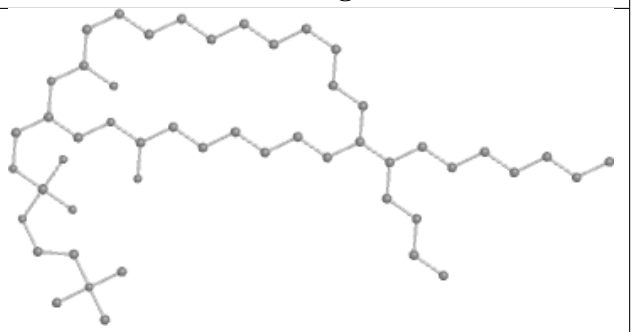
Bond lengths



Bond angles

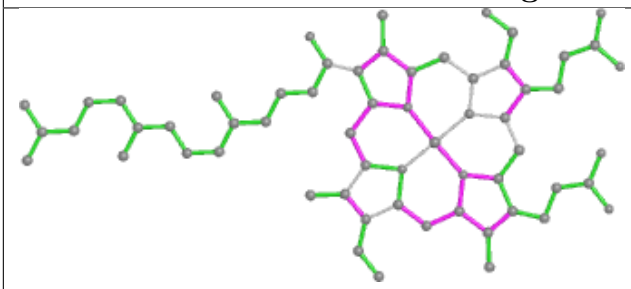


Torsions

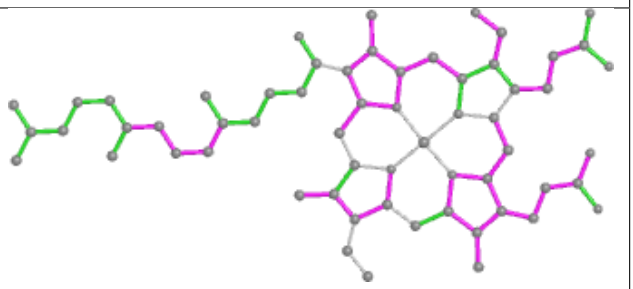


Rings

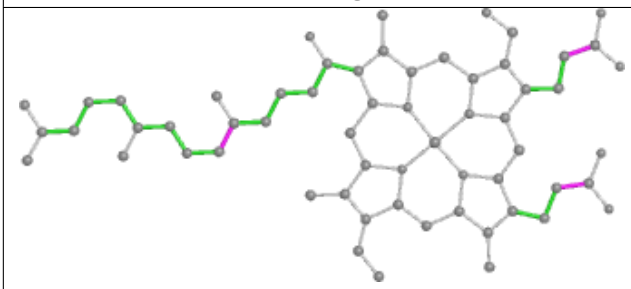
Ligand HEA N 601



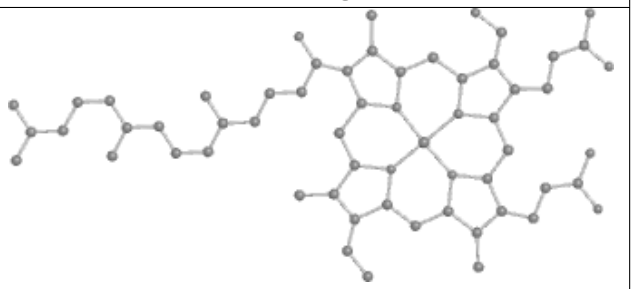
Bond lengths



Bond angles

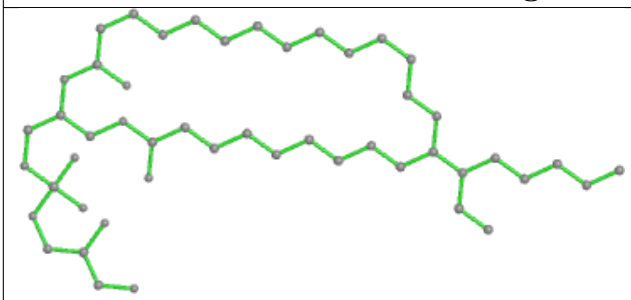


Torsions

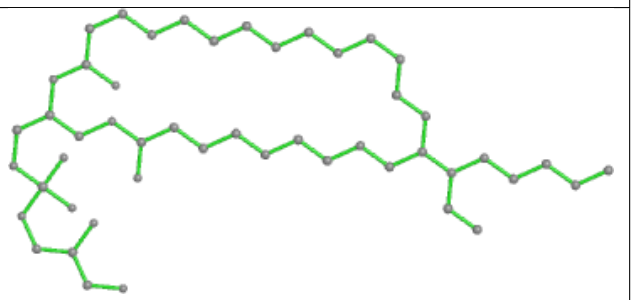


Rings

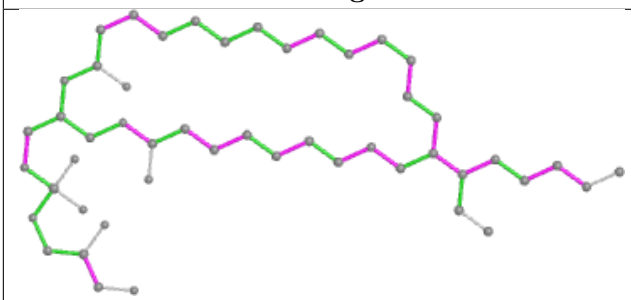
Ligand PGV P 304



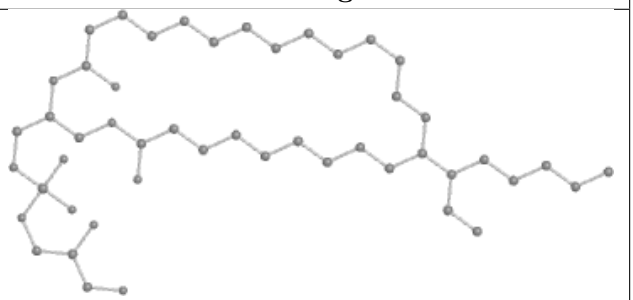
Bond lengths



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	-0.80	0 100 100	27, 39, 52, 90	0
1	N	513/514 (99%)	-0.65	7 (1%) 75 70	37, 52, 69, 92	0
2	B	226/227 (99%)	-0.65	3 (1%) 77 72	32, 47, 75, 138	0
2	O	226/227 (99%)	-0.48	4 (1%) 68 61	42, 63, 94, 133	0
3	C	259/261 (99%)	-0.73	0 100 100	33, 45, 62, 101	0
3	P	259/261 (99%)	-0.67	0 100 100	37, 54, 78, 112	0
4	D	144/147 (97%)	-0.55	1 (0%) 87 84	40, 50, 76, 98	0
4	Q	144/147 (97%)	0.01	7 (4%) 29 20	54, 75, 108, 166	0
5	E	105/109 (96%)	-0.81	0 100 100	36, 50, 82, 135	0
5	R	105/109 (96%)	-0.47	2 (1%) 66 59	47, 68, 89, 118	0
6	F	98/98 (100%)	-0.17	6 (6%) 21 13	38, 55, 121, 165	0
6	S	98/98 (100%)	-0.12	8 (8%) 11 6	46, 64, 138, 178	0
7	G	83/85 (97%)	0.06	13 (15%) 2 1	39, 55, 142, 158	0
7	T	83/85 (97%)	0.31	9 (10%) 5 3	44, 67, 146, 162	0
8	H	79/85 (92%)	-0.31	3 (3%) 40 30	42, 58, 119, 149	0
8	U	79/85 (92%)	-0.03	5 (6%) 20 12	49, 72, 132, 149	0
9	I	72/73 (98%)	-0.40	1 (1%) 75 70	45, 58, 90, 101	0
9	V	72/73 (98%)	-0.05	5 (6%) 16 10	51, 76, 104, 122	0
10	J	58/59 (98%)	-0.45	2 (3%) 45 35	44, 58, 94, 122	0
10	W	58/59 (98%)	-0.29	4 (6%) 16 10	55, 73, 111, 142	0
11	K	49/56 (87%)	-0.27	0 100 100	45, 56, 74, 101	0
11	X	49/56 (87%)	0.16	4 (8%) 11 6	54, 78, 97, 110	0
12	L	46/47 (97%)	-0.84	0 100 100	36, 47, 73, 108	0
12	Y	46/47 (97%)	-0.56	1 (2%) 62 52	51, 69, 105, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.33	1 (2%) 60 51	34, 49, 87, 132	0
13	Z	43/46 (93%)	-0.02	3 (6%) 16 9	58, 71, 108, 147	0
All	All	3550/3614 (98%)	-0.50	89 (2%) 57 47	27, 54, 96, 178	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	98	HIS	11.5
4	Q	4	SER	8.1
6	F	94	HIS	8.0
13	M	43	SER	7.7
7	T	40	GLY	7.6
7	T	39	SER	7.5
6	F	1	ALA	7.1
7	T	41	HIS	7.0
4	Q	6	VAL	6.7
7	G	2	SER	6.4
6	S	1	ALA	6.4
4	Q	5	VAL	6.3
6	S	96	LEU	6.0
7	T	6	GLY	5.7
4	Q	7	LYS	5.7
7	T	3	ALA	5.5
7	T	1	ALA	5.5
7	G	40	GLY	5.3
2	O	227	LEU	5.0
4	Q	8	SER	5.0
6	S	98	HIS	4.9
6	S	97	ALA	4.8
6	S	95	GLN	4.7
2	O	90	ILE	4.5
8	H	45	ALA	4.5
6	S	2	SER	4.4
7	G	41	HIS	4.3
2	B	90	ILE	4.3
7	T	36	TRP	4.3
13	Z	43	SER	4.3
7	G	3	ALA	4.1
7	G	39	SER	4.0
4	Q	147	LYS	3.9
8	U	45	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
7	G	1	ALA	3.8
10	J	57	HIS	3.7
10	W	57	HIS	3.7
7	T	10	GLY	3.6
8	U	7	LYS	3.5
4	D	4	SER	3.4
6	F	2	SER	3.3
8	U	48	GLY	3.3
10	W	58	LYS	3.2
2	B	59	GLN	3.1
11	X	30	VAL	3.1
11	X	7	PRO	3.0
9	I	37	PHE	2.9
8	H	46	LYS	2.9
12	Y	2	HIS	2.9
7	G	5	LYS	2.9
1	N	463	THR	2.8
13	Z	42	LYS	2.8
8	U	8	ILE	2.8
1	N	464	ALA	2.7
9	V	53	ASN	2.6
5	R	108	LYS	2.6
7	T	2	SER	2.6
7	G	10	GLY	2.5
10	J	1	PHE	2.5
1	N	465	VAL	2.5
7	G	36	TRP	2.5
2	O	167	SER	2.5
1	N	466	MET	2.5
1	N	461	SER	2.5
5	R	109	VAL	2.5
7	G	42	ARG	2.5
8	U	84	LYS	2.5
1	N	462	LEU	2.5
9	V	25	PHE	2.4
7	G	7	ASP	2.4
11	X	6	ALA	2.4
4	Q	141	ASP	2.4
7	G	8	HIS	2.3
2	B	92	ASN	2.3
10	W	48	TYR	2.3
9	V	3	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
9	V	37	PHE	2.3
2	O	92	ASN	2.2
10	W	52	TRP	2.2
13	Z	35	TYR	2.2
1	N	468	MET	2.2
8	H	48	GLY	2.2
11	X	15	ASN	2.2
6	S	94	HIS	2.2
6	S	3	GLY	2.1
7	G	6	GLY	2.1
9	V	72	ALA	2.1
6	F	44	GLU	2.1
6	F	95	GLN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.79	0.32	130,155,173,179	0
7	TPO	T	11	11/12	0.84	0.27	128,139,156,165	0
1	FME	N	1	10/11	0.93	0.37	85,93,132,138	0
1	FME	A	1	10/11	0.93	0.26	62,73,99,106	0
2	FME	O	1	10/11	0.97	0.16	50,65,73,73	0
2	FME	B	1	10/11	0.97	0.22	49,51,53,61	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, 95^{th} 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
28	DMU	G	102	33/33	0.52	0.53	73,155,175,175	0
29	SAC	V	101	9/10	0.54	0.64	106,135,145,154	0
16	MG	A	604	1/1	0.60	0.15	47,47,47,47	0
28	DMU	T	102	33/33	0.66	0.51	94,128,165,185	0
18	TGL	Y	101	63/63	0.66	0.39	70,110,161,176	0
29	SAC	I	102	9/10	0.68	0.40	117,130,135,138	0
27	PEK	G	106	53/53	0.69	0.47	65,140,205,219	0
24	CDL	C	305	100/100	0.70	0.40	70,120,150,154	0
27	PEK	T	101	53/53	0.73	0.32	61,101,157,172	0
24	CDL	P	305	100/100	0.75	0.36	68,117,159,183	0
25	PSC	R	201	52/52	0.75	0.42	78,119,219,243	0
18	TGL	L	101	63/63	0.76	0.32	57,97,131,136	0
27	PEK	T	103	53/53	0.76	0.48	73,135,200,205	0
18	TGL	N	606	63/63	0.77	0.29	79,107,126,129	0
24	CDL	G	104	100/100	0.78	0.36	90,126,183,224	0
27	PEK	G	103	53/53	0.78	0.29	85,102,150,159	0
25	PSC	E	201	52/52	0.78	0.37	64,109,198,208	0
19	PGV	Z	101	51/51	0.79	0.42	65,104,165,168	0
19	PGV	C	304	51/51	0.79	0.26	75,99,134,148	0
19	PGV	M	101	51/51	0.80	0.37	64,99,161,175	0
24	CDL	T	104	100/100	0.80	0.32	72,118,184,209	0
18	TGL	N	608	63/63	0.82	0.27	47,95,138,152	0
22	CHD	N	609	29/29	0.82	0.36	108,129,146,153	0
18	TGL	A	606	63/63	0.83	0.23	66,95,108,110	0
19	PGV	U	101	51/51	0.84	0.29	74,112,145,159	0
28	DMU	Q	201	33/33	0.85	0.34	70,96,112,116	0
18	TGL	I	101	63/63	0.85	0.24	39,95,134,150	0
23	OH	C	302[H]	1/1	0.86	0.24	24,24,24,24	0
22	CHD	J	101	29/29	0.89	0.39	75,108,123,130	0
22	CHD	C	306	29/29	0.91	0.33	75,86,97,110	0
28	DMU	M	102	33/33	0.92	0.21	45,60,78,79	0
27	PEK	P	303	53/53	0.93	0.31	60,78,128,137	0
17	NA	N	605	1/1	0.95	0.16	63,63,63,63	0
16	MG	N	604	1/1	0.95	0.13	39,39,39,39	0
22	CHD	P	302	29/29	0.95	0.12	42,47,50,51	0
27	PEK	G	101	53/53	0.95	0.23	43,69,117,125	0
22	CHD	P	306	29/29	0.95	0.30	80,89,94,99	0
22	CHD	G	105	29/29	0.96	0.17	42,45,51,54	0
19	PGV	P	304	51/51	0.96	0.28	42,57,136,153	0
22	CHD	C	301	29/29	0.96	0.10	35,38,41,41	0
14	HEA	N	601	60/60	0.96	0.16	39,48,61,72	0
19	PGV	N	607	51/51	0.97	0.21	45,63,74,85	0
21	CUA	B	301	2/2	0.97	0.05	41,41,41,46	0

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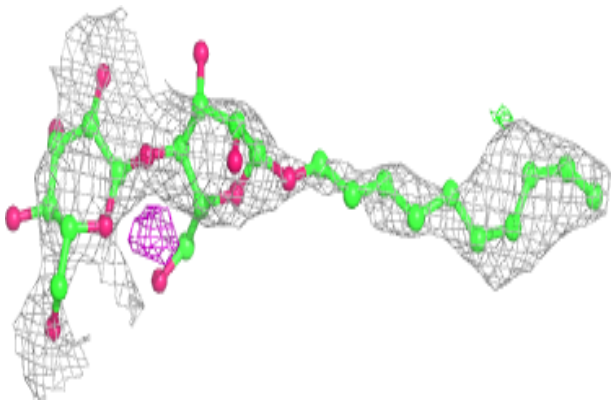
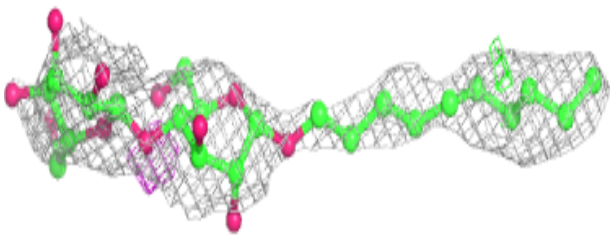
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CUA	O	301	2/2	0.97	0.05	62,62,62,63	0
22	CHD	B	302	29/29	0.97	0.14	36,45,51,62	0
14	HEA	A	602	60/60	0.97	0.12	24,34,48,55	0
19	PGV	C	303	51/51	0.97	0.25	35,50,110,115	0
14	HEA	N	602	60/60	0.98	0.14	34,39,55,56	0
14	HEA	A	601	60/60	0.98	0.13	27,36,56,59	0
26	ZN	S	101	1/1	0.98	0.05	67,67,67,67	0
19	PGV	A	607	51/51	0.98	0.21	34,54,72,86	0
23	OH	P	301[H]	1/1	0.98	0.30	24,24,24,24	0
15	CU	N	603	1/1	0.99	0.08	55,55,55,55	0
17	NA	A	605	1/1	0.99	0.13	38,38,38,38	0
20	CMO	A	608	2/2	0.99	0.10	33,33,33,36	0
20	CMO	N	610	2/2	0.99	0.14	56,56,56,56	0
15	CU	A	603	1/1	0.99	0.07	44,44,44,44	0
26	ZN	F	101	1/1	1.00	0.05	67,67,67,67	0

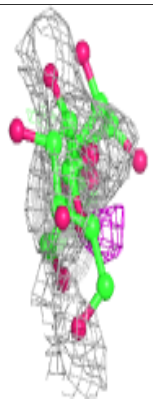
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU 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)

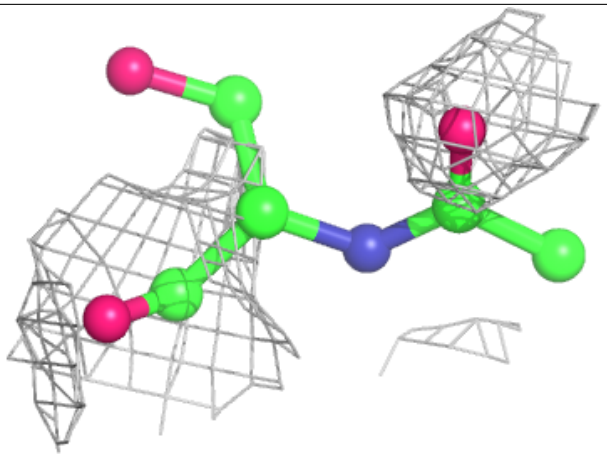


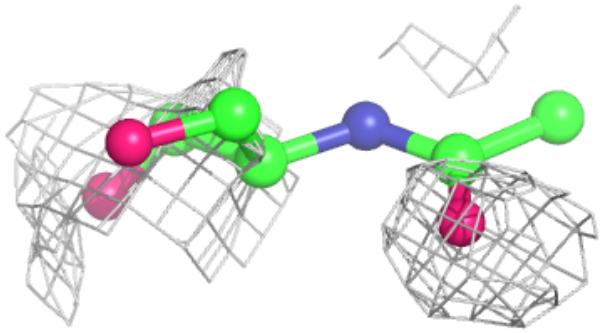


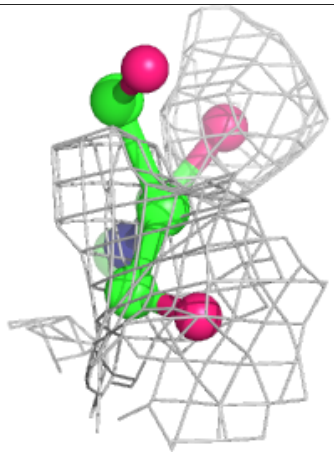


Electron density around SAC V 101:

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

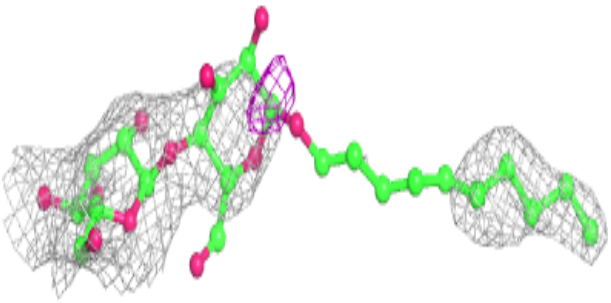


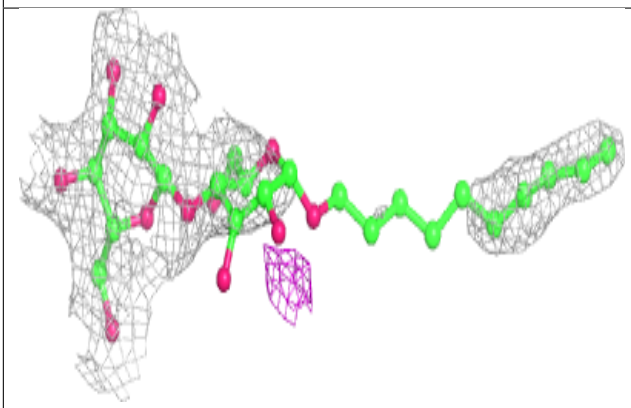


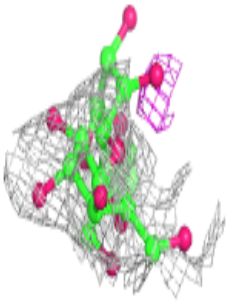


Electron density around DMU T 102:

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

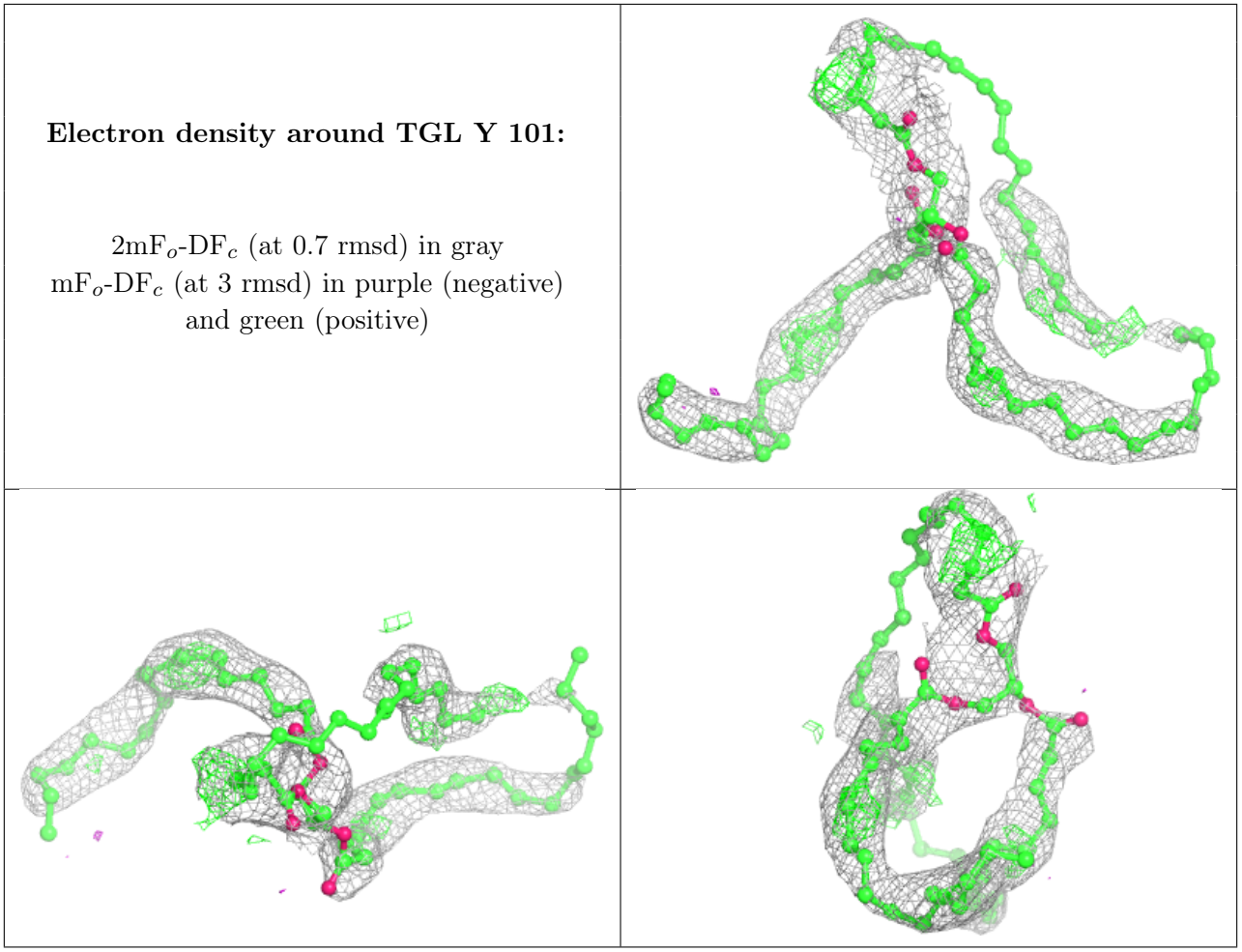






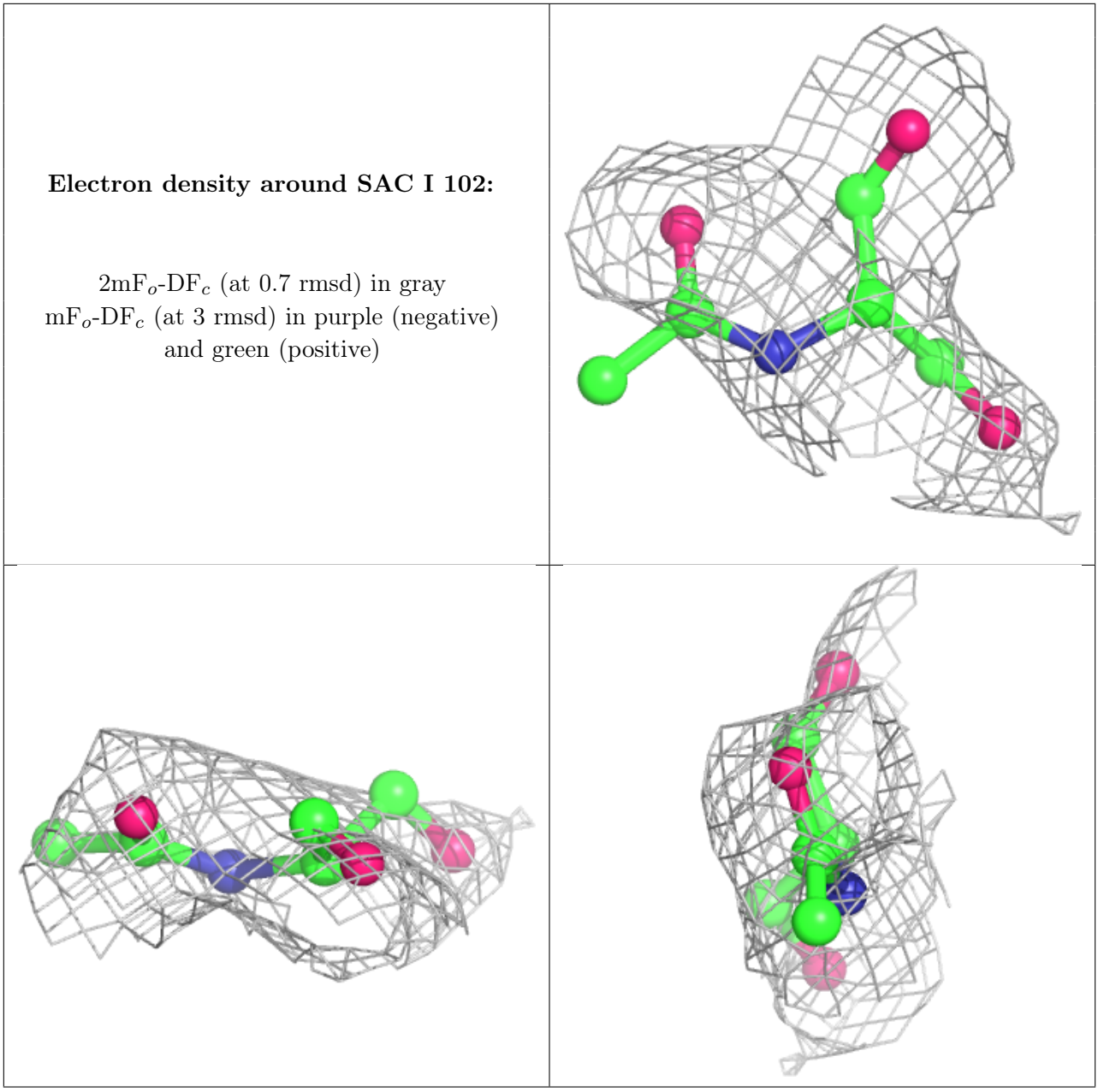
Electron density around TGL Y 101:

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



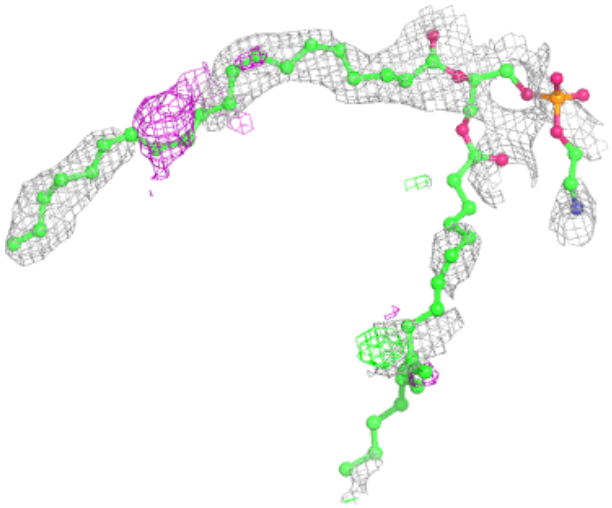
Electron density around SAC I 102:

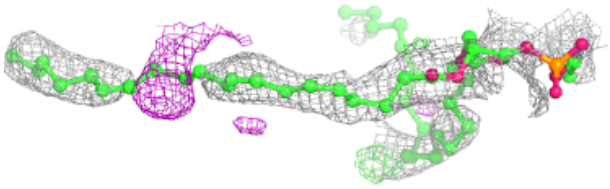
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

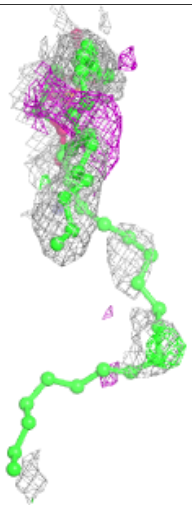


Electron density around PEK G 106:

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

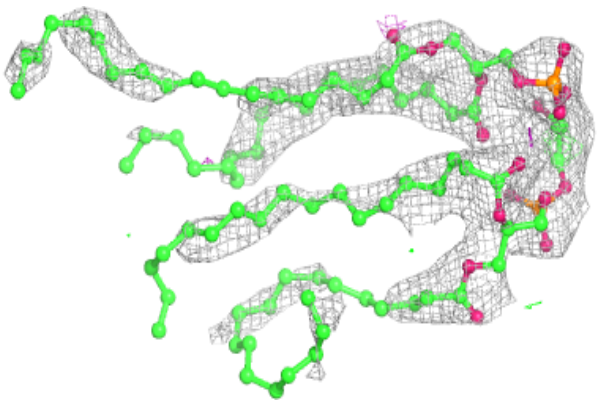


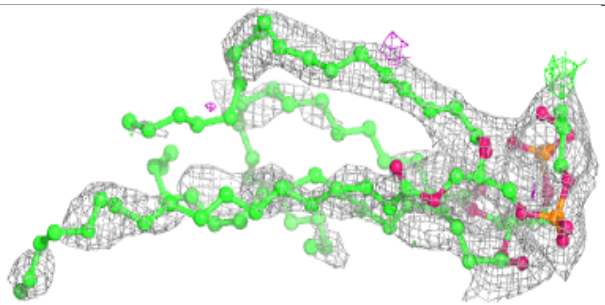


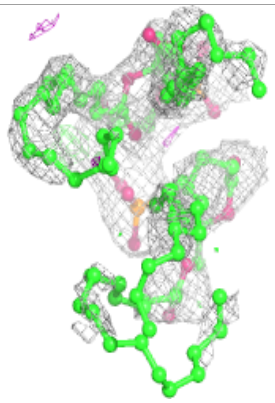


Electron density around CDL C 305:

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

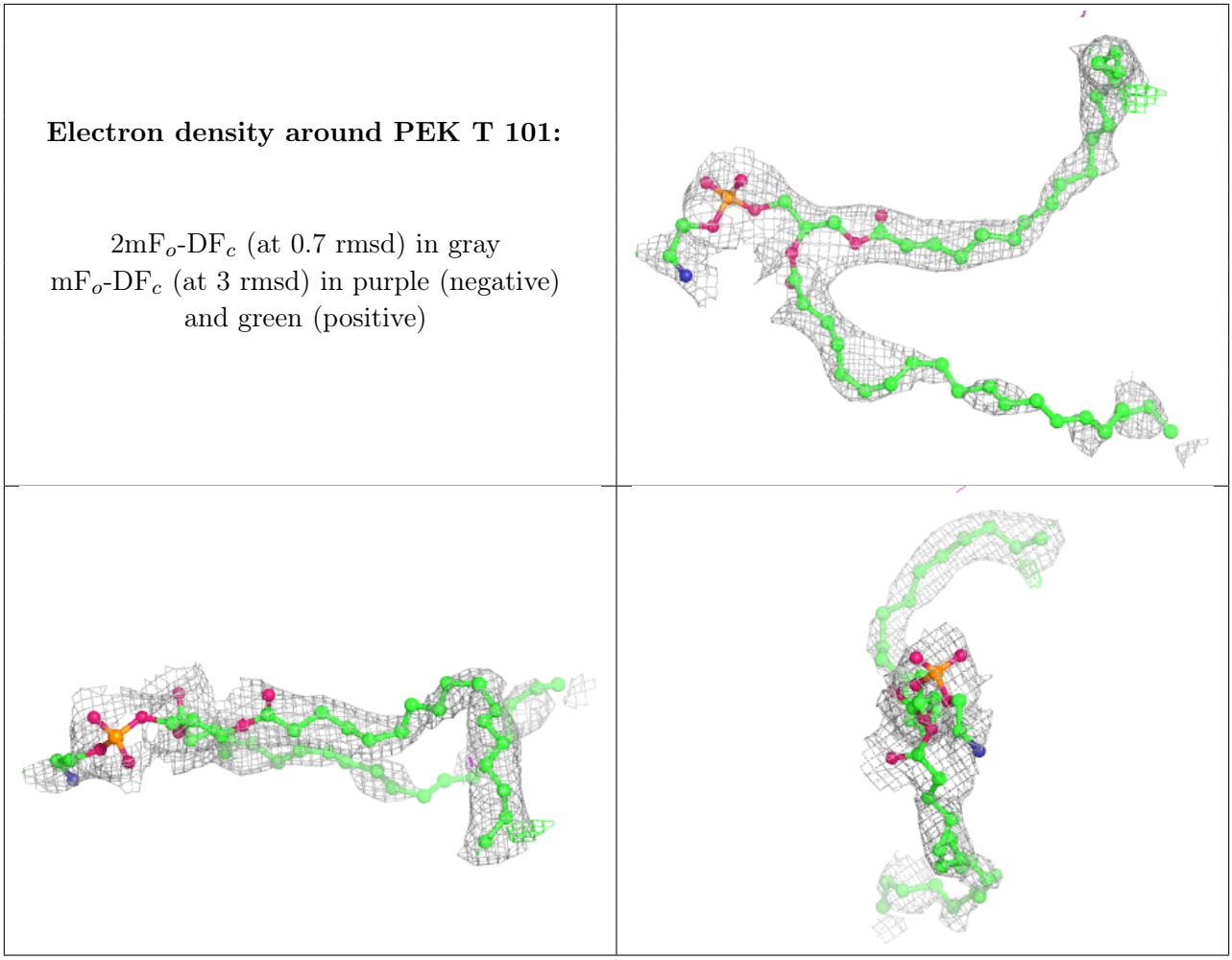






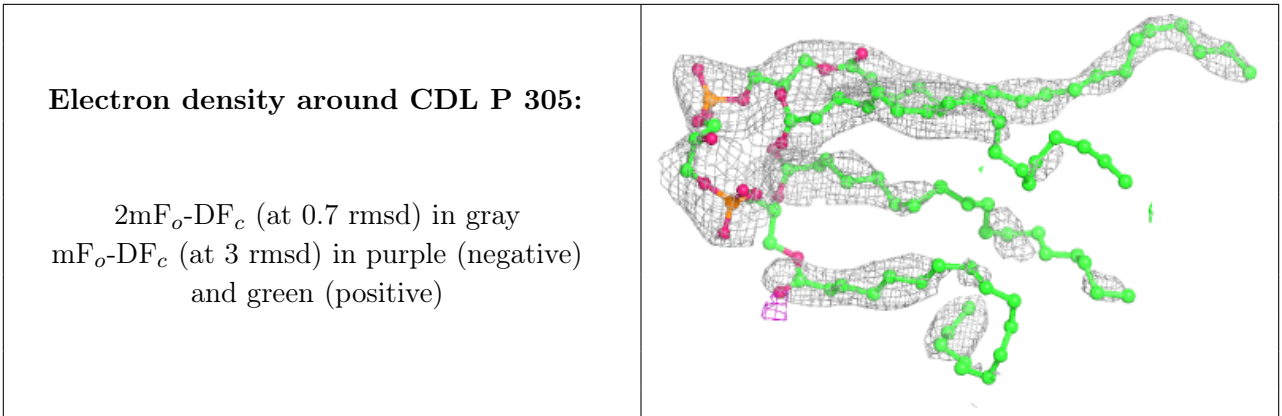
Electron density around PEK T 101:

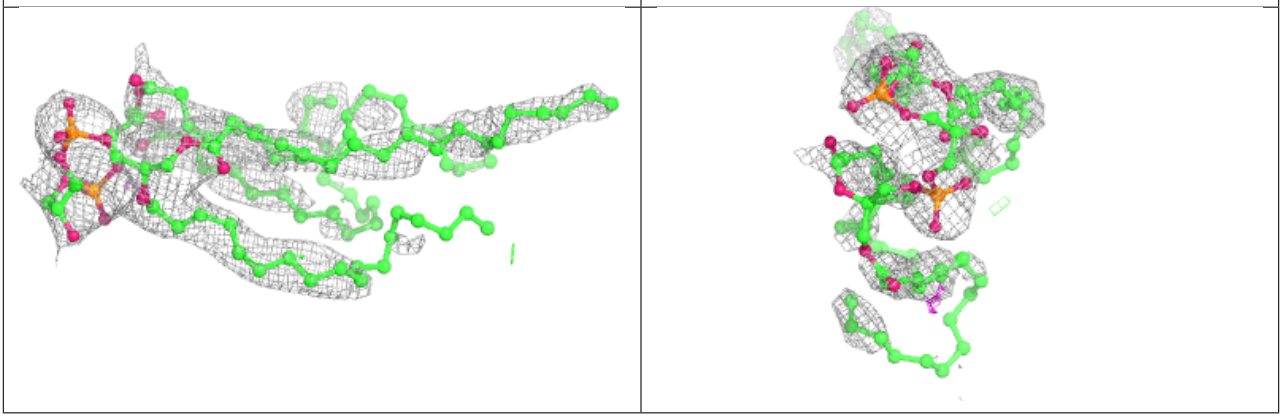
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CDL P 305:

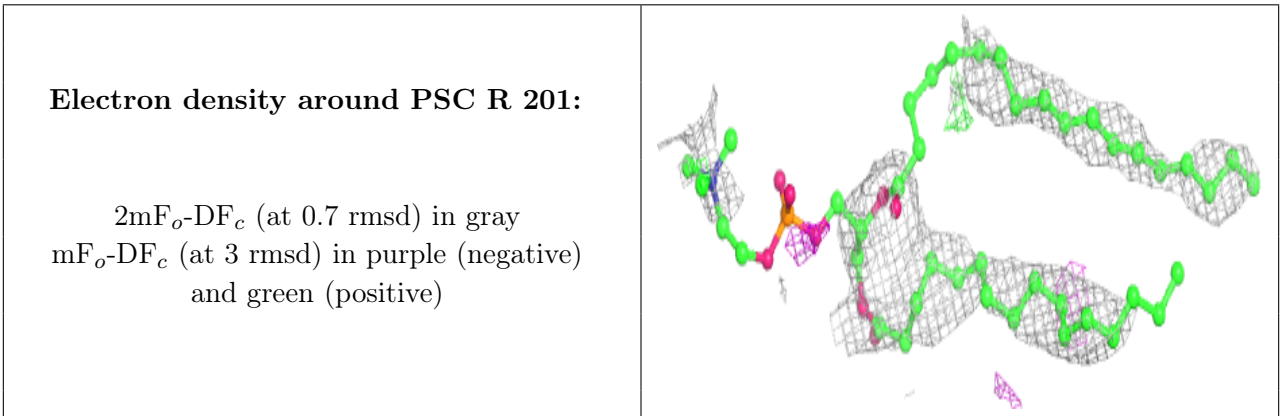
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

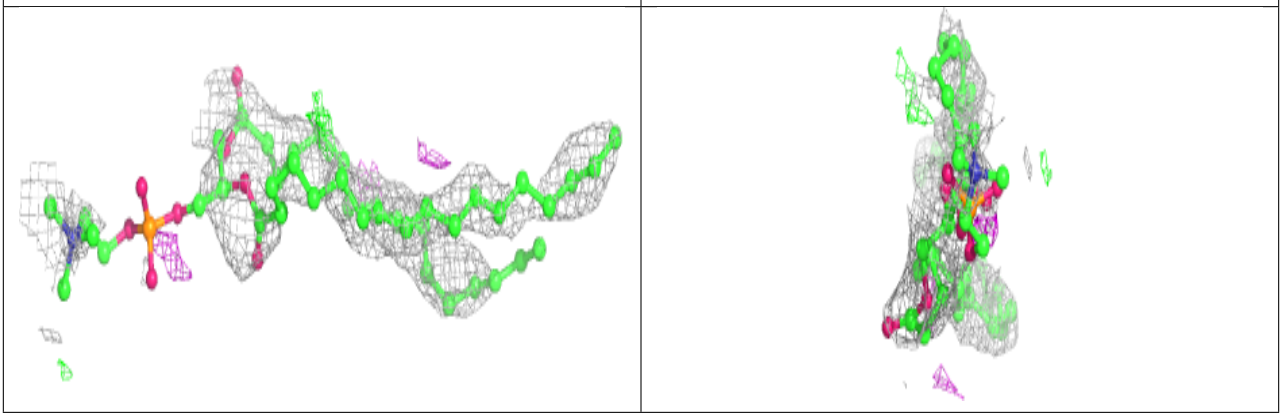




Electron density around PSC R 201:

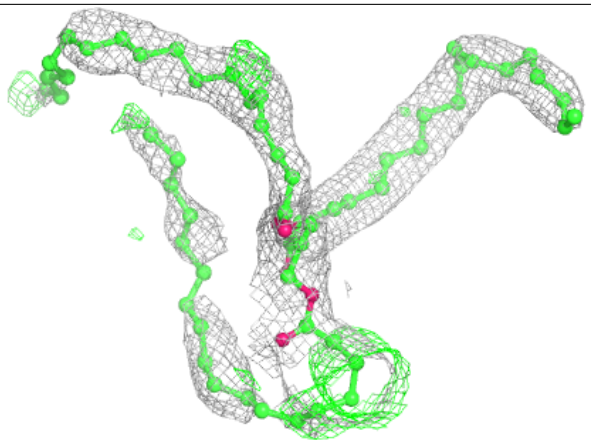
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

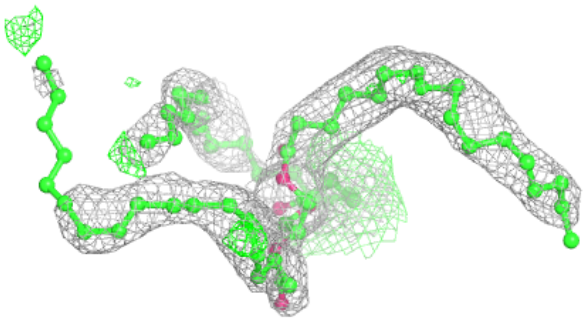


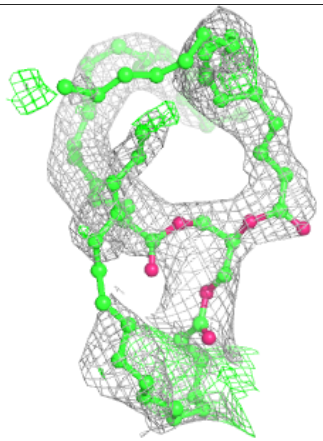


Electron density around TGL L 101:

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

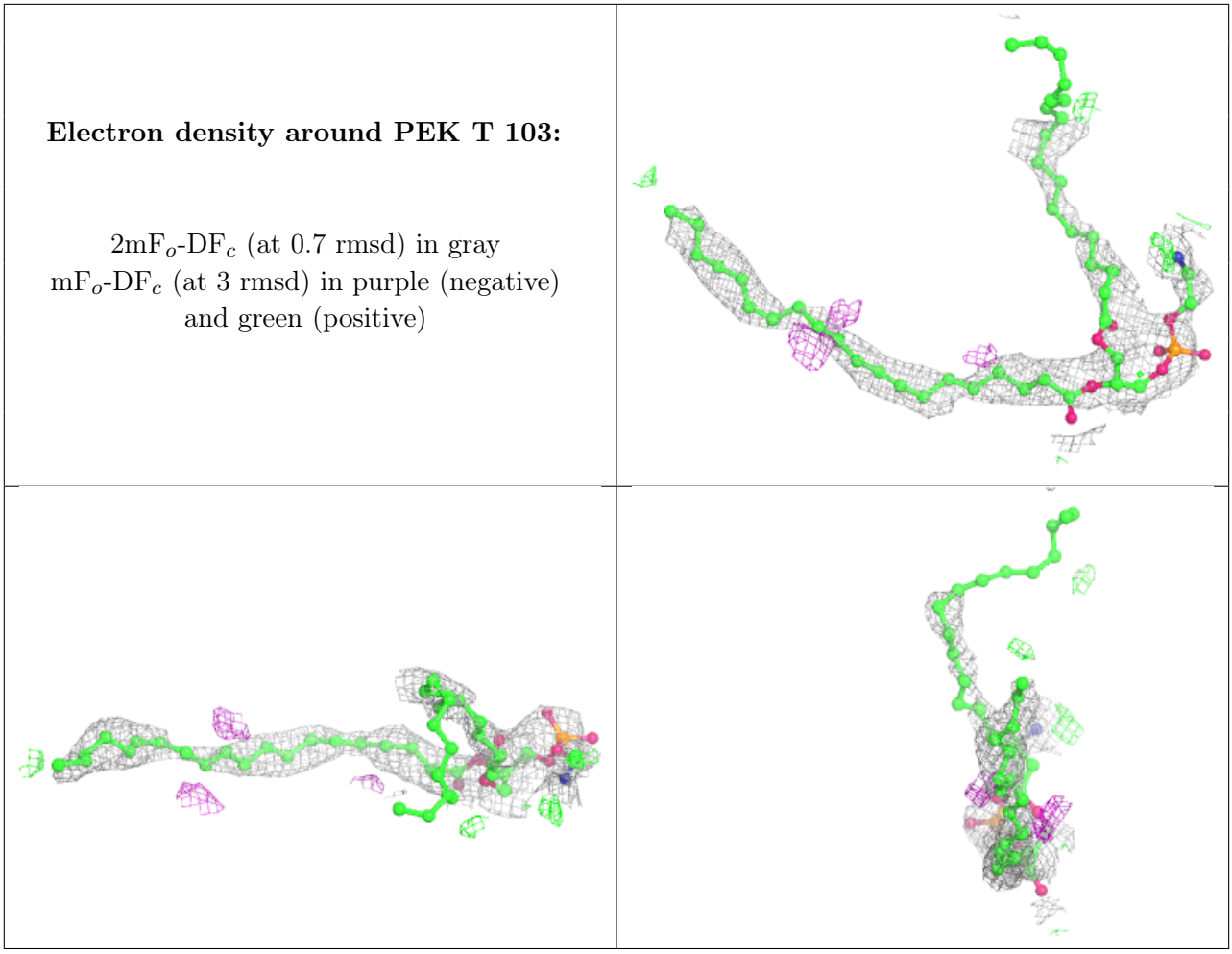






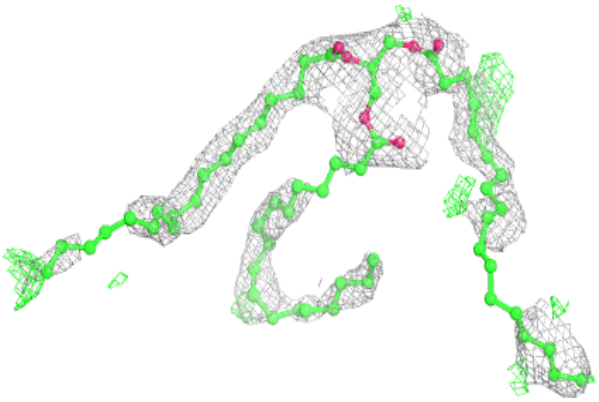
Electron density around PEK T 103:

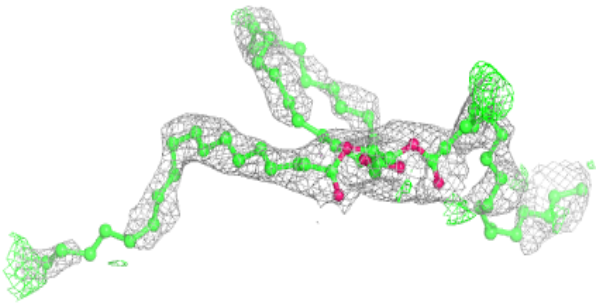
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

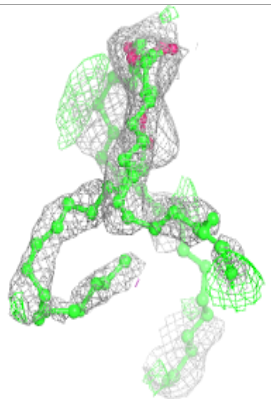


Electron density around TGL N 606:

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

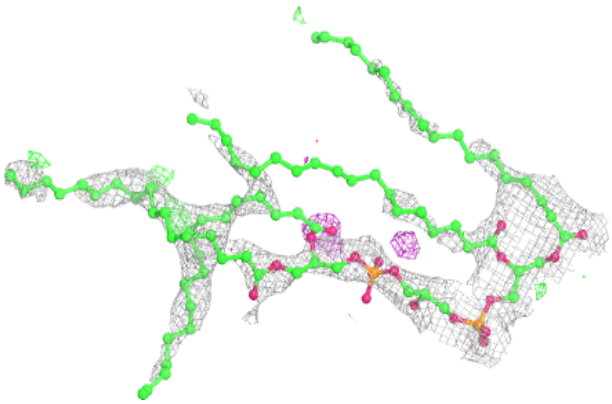


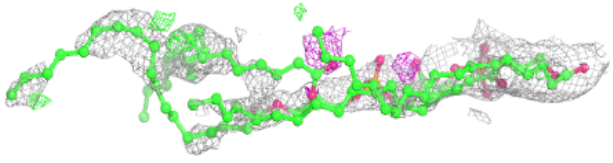


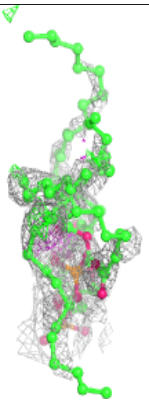


Electron density around CDL G 104:

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

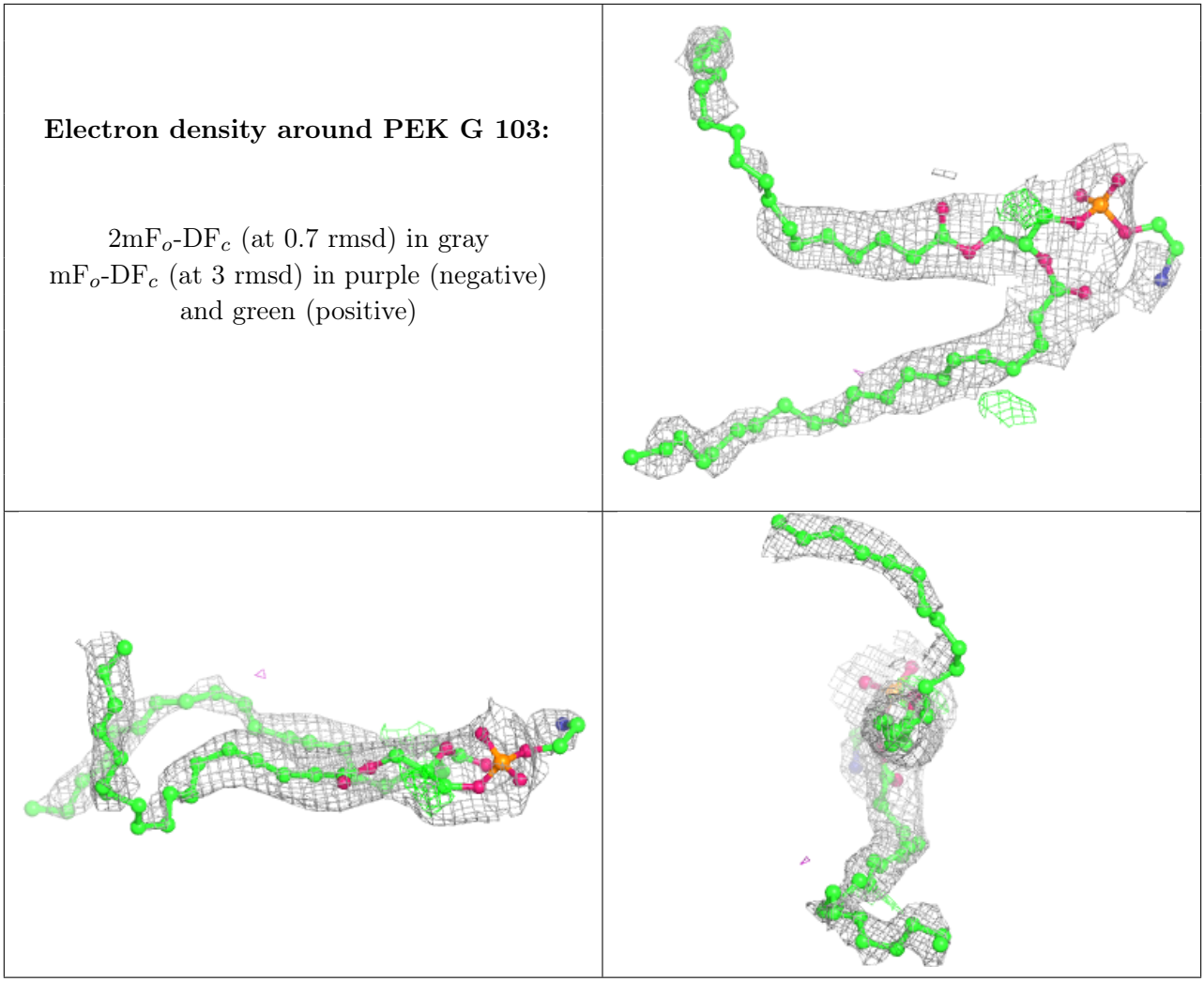






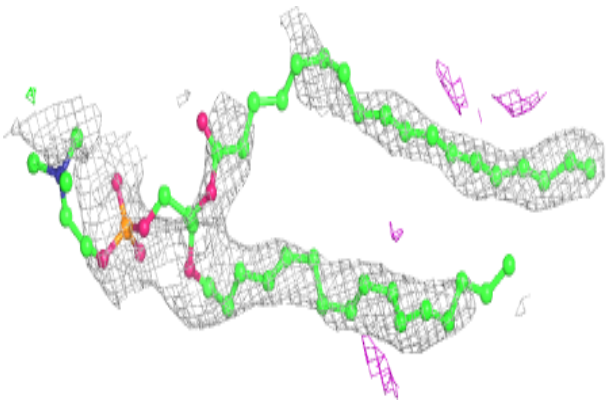
Electron density around PEK G 103:

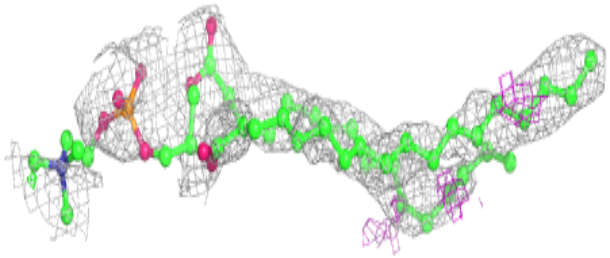
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

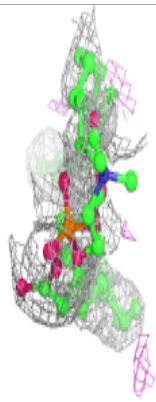


Electron density around PSC E 201:

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

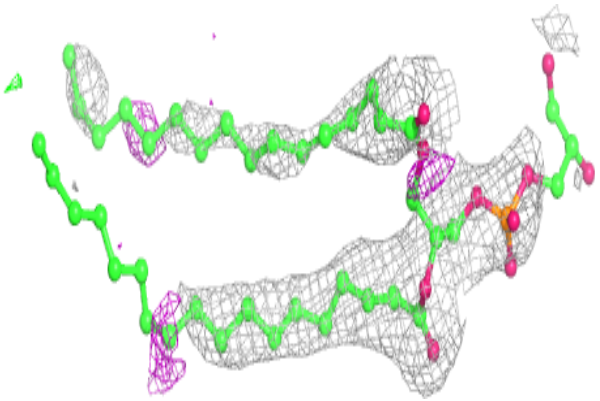


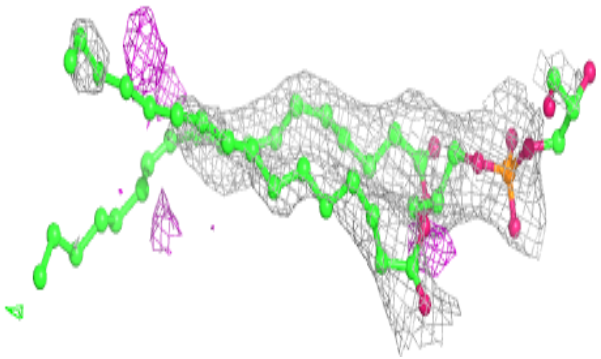


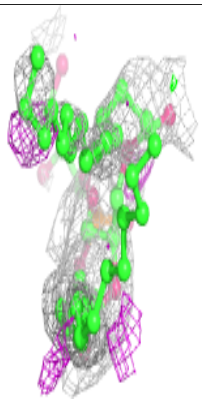


Electron density around PGV Z 101:

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

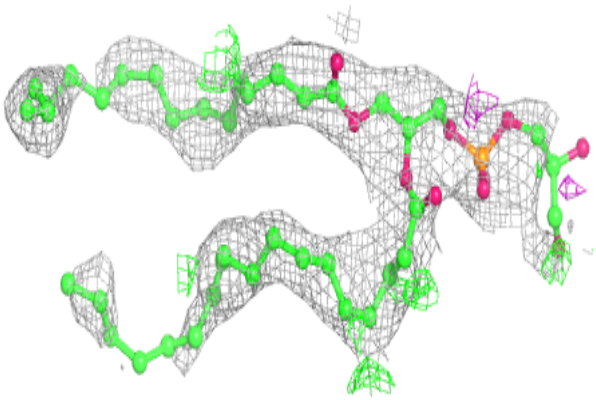


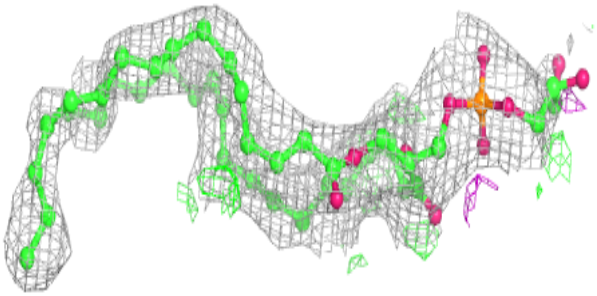


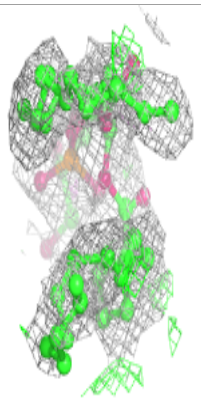


Electron density around PGV C 304:

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

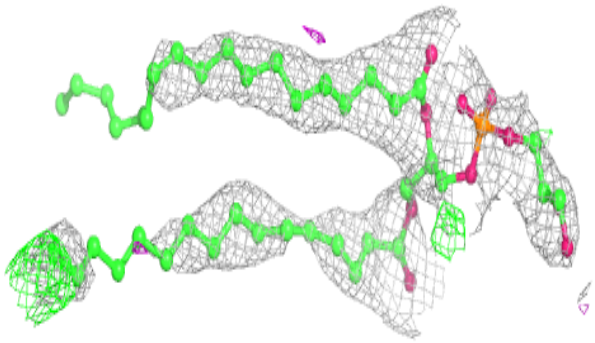


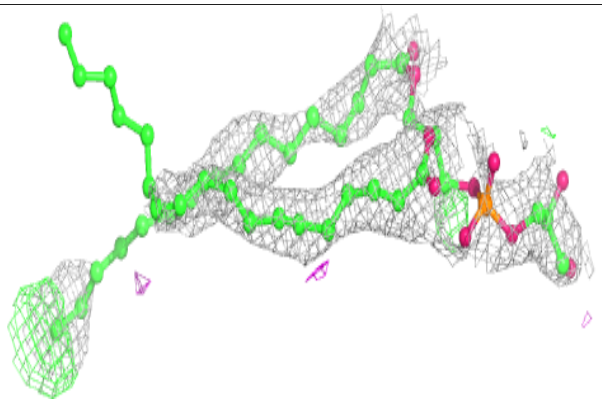


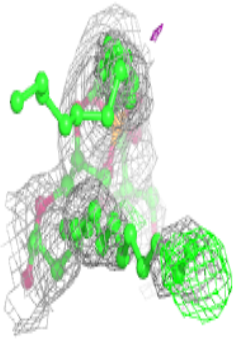


Electron density around PGV M 101:

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

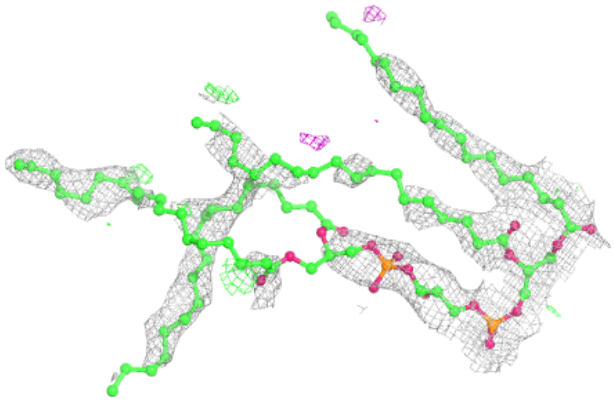


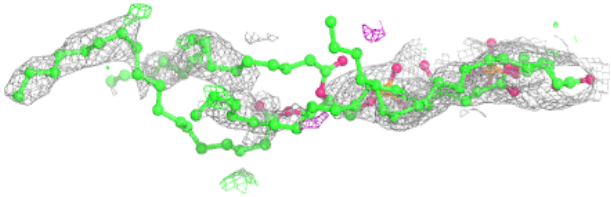


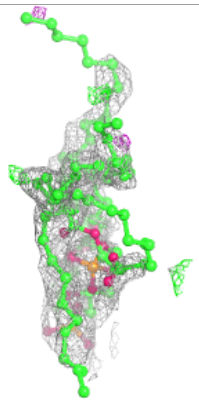


Electron density around CDL T 104:

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

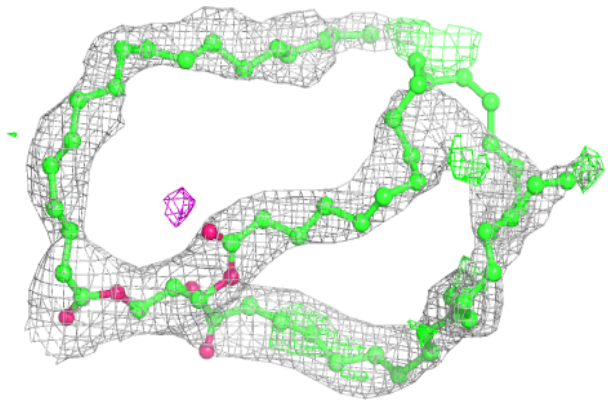


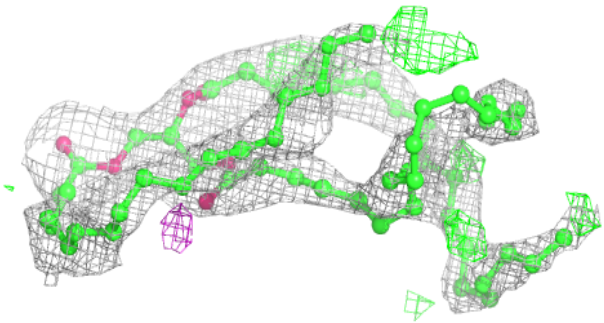


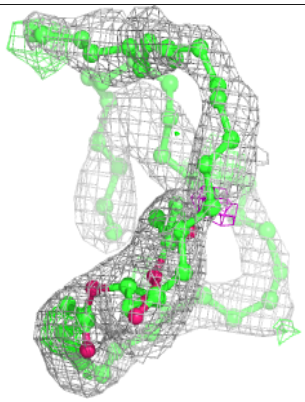


Electron density around TGL N 608:

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

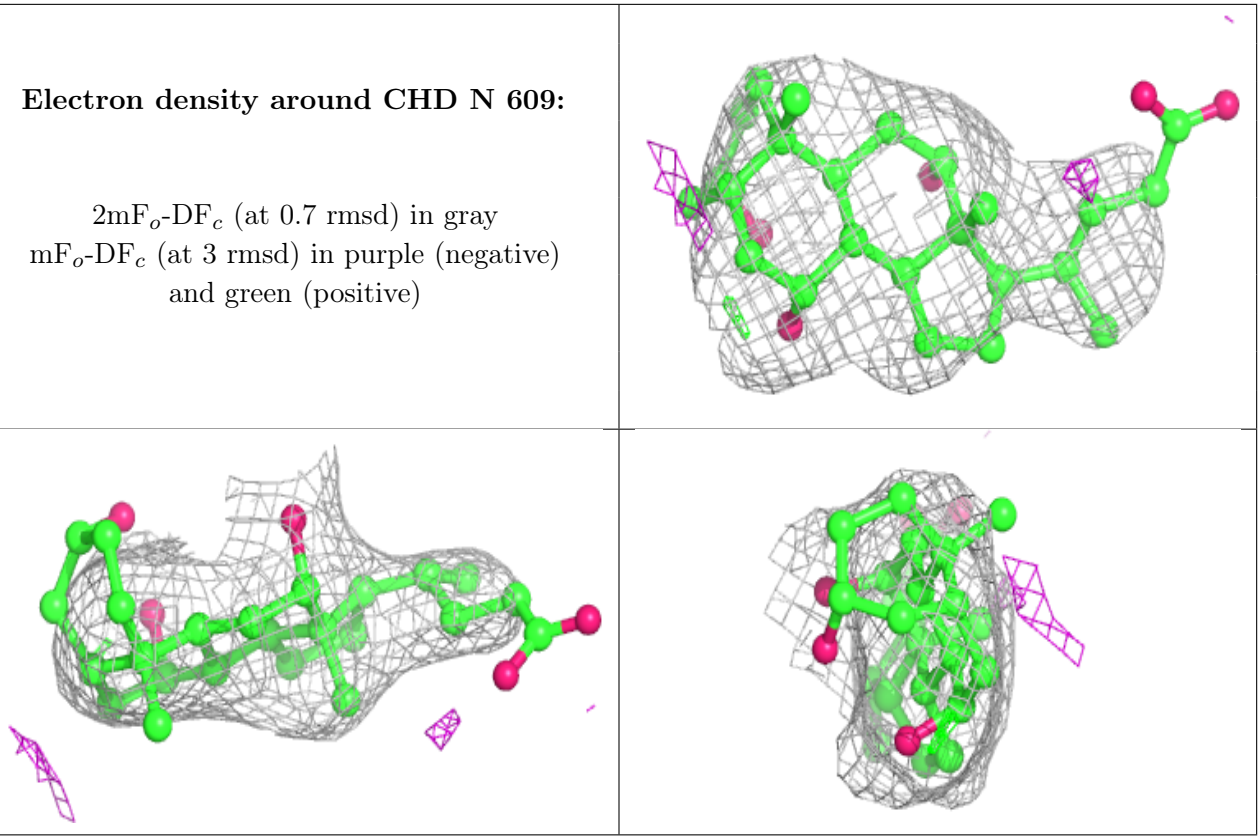






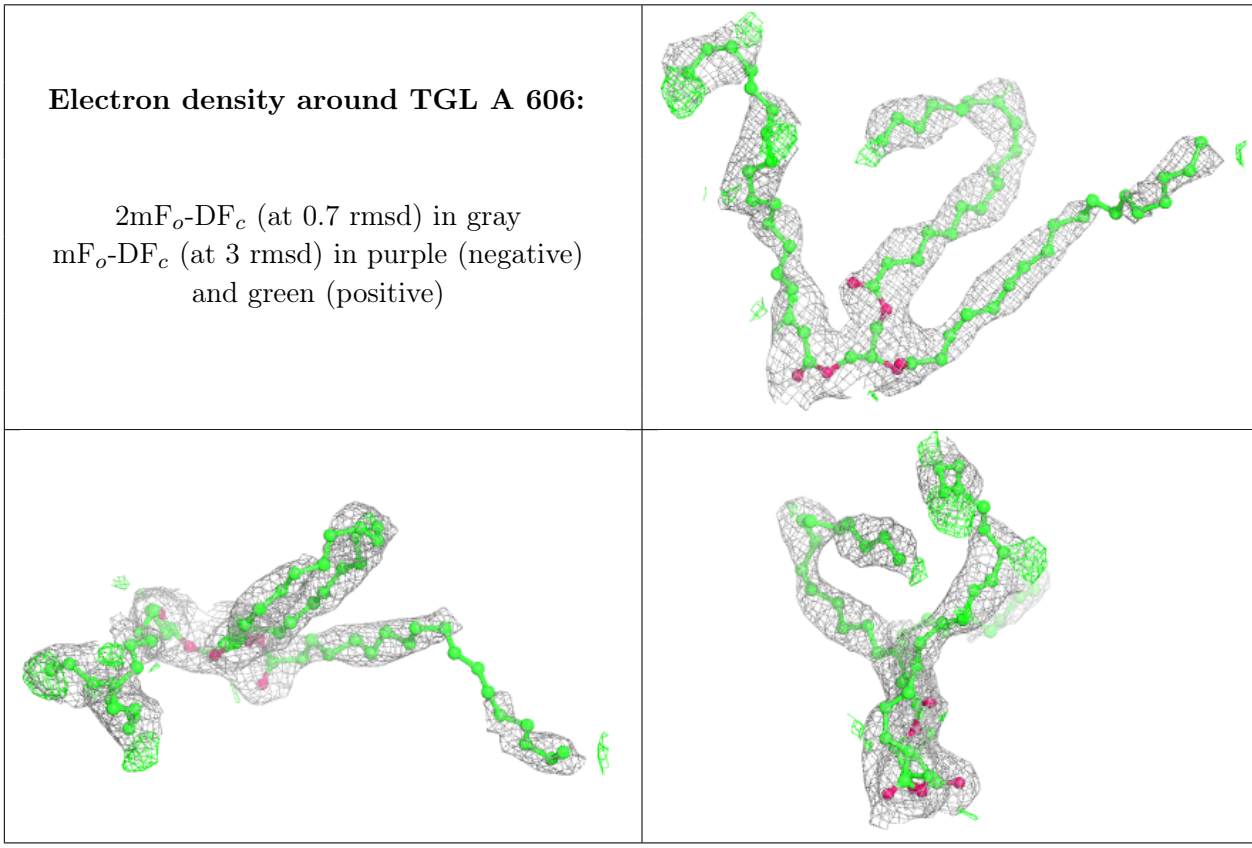
Electron density around CHD N 609:

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



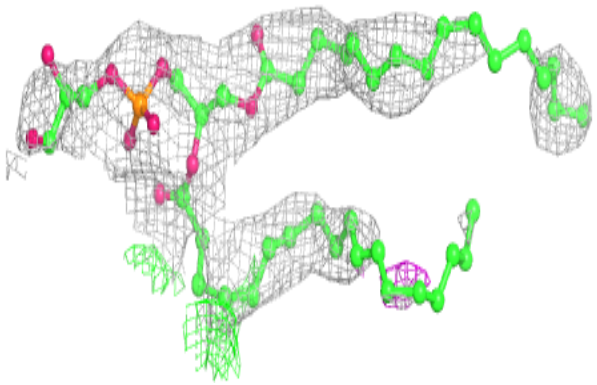
Electron density around TGL A 606:

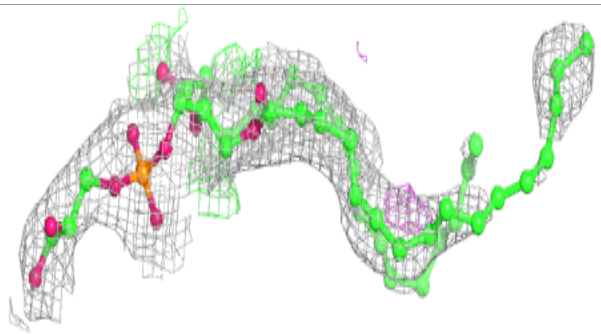
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

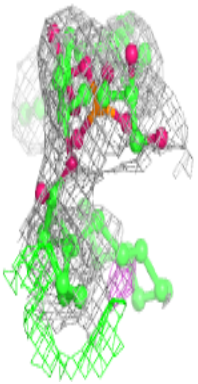


Electron density around PGV U 101:

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

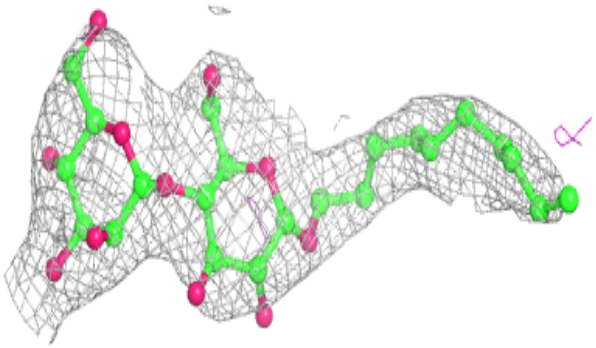


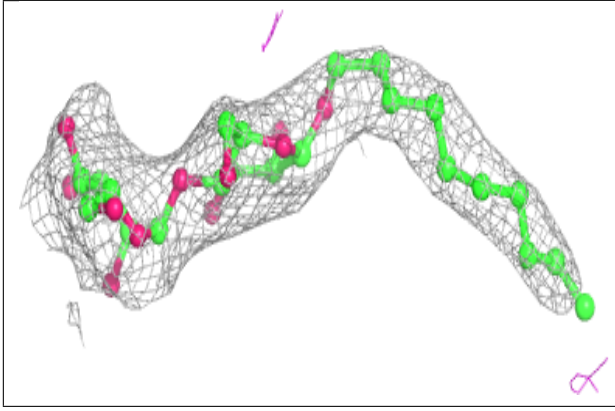


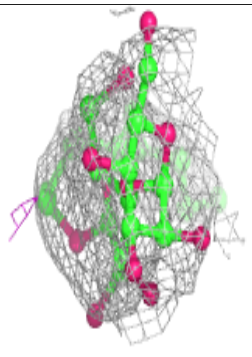


Electron density around DMU Q 201:

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

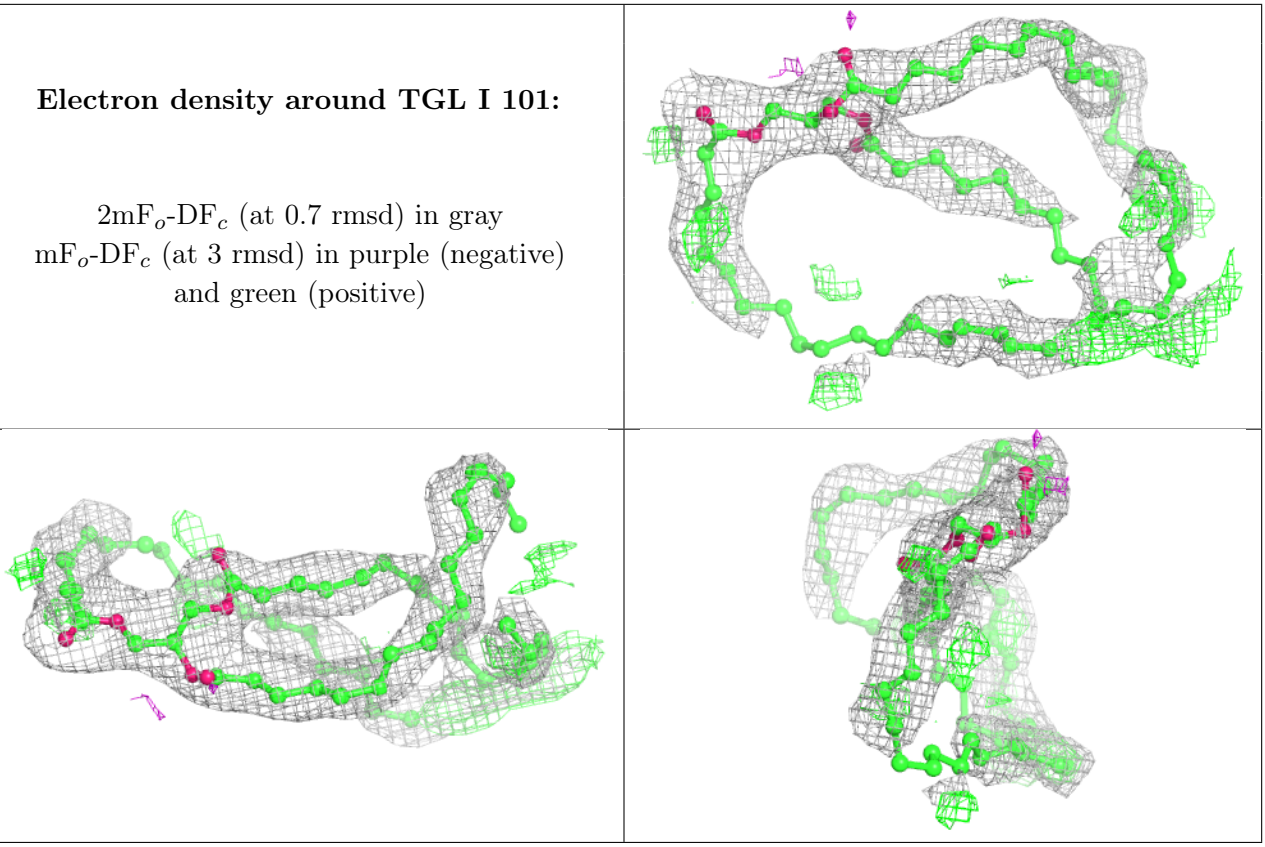






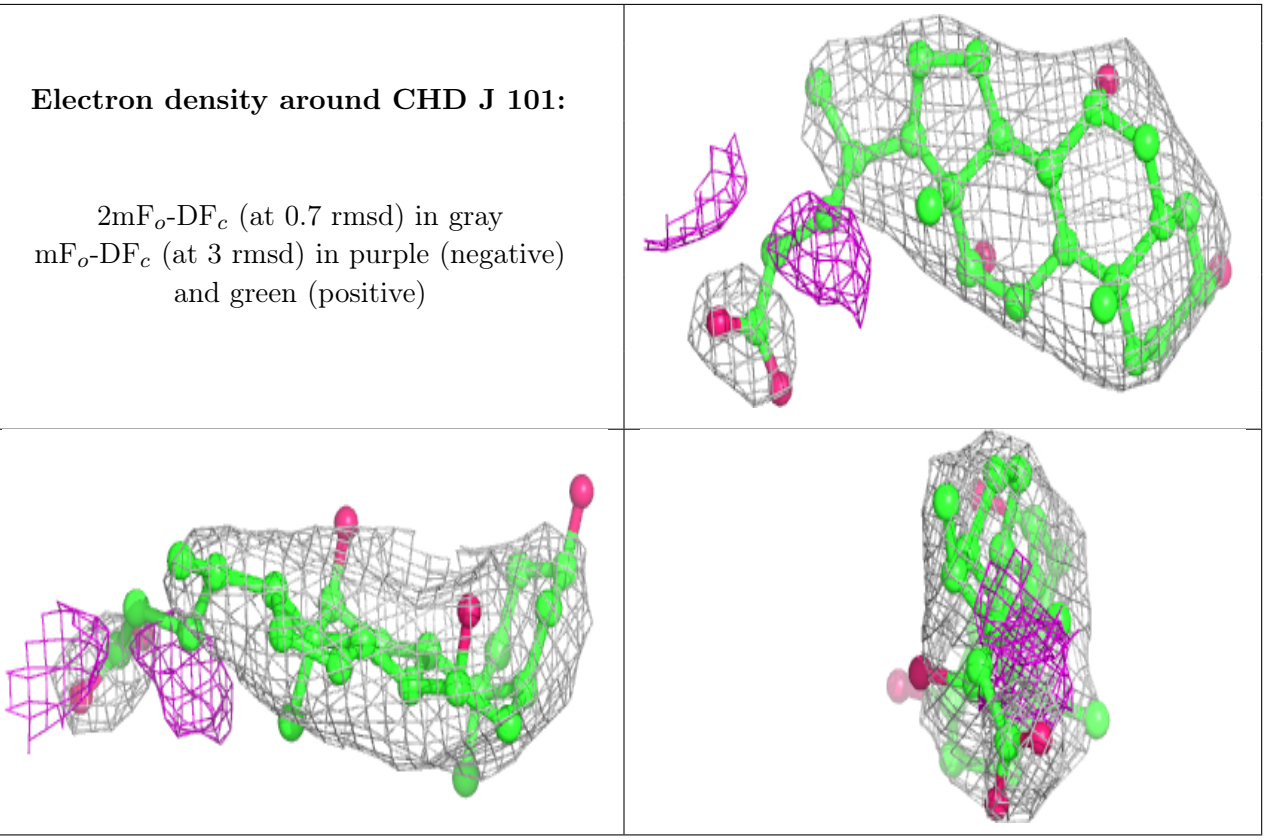
Electron density around TGL I 101:

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



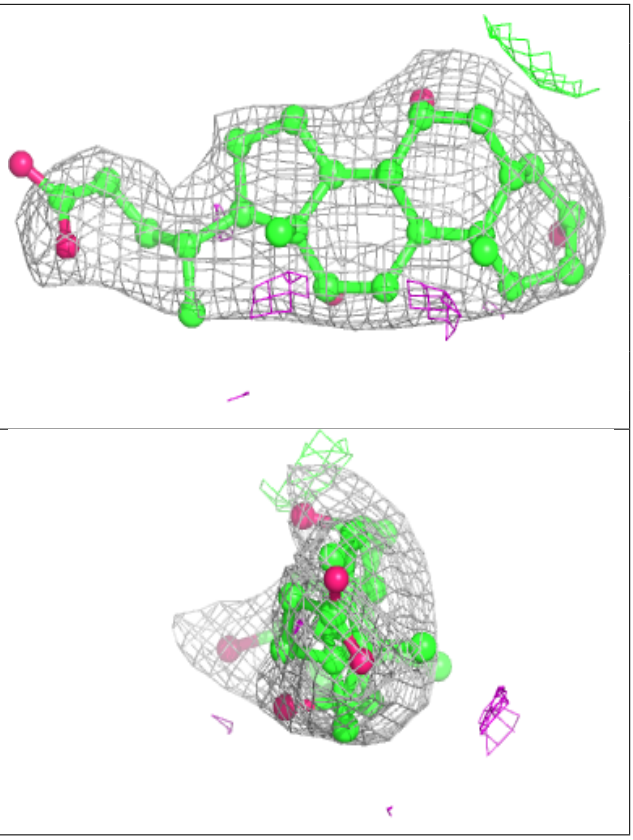
Electron density around CHD J 101:

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



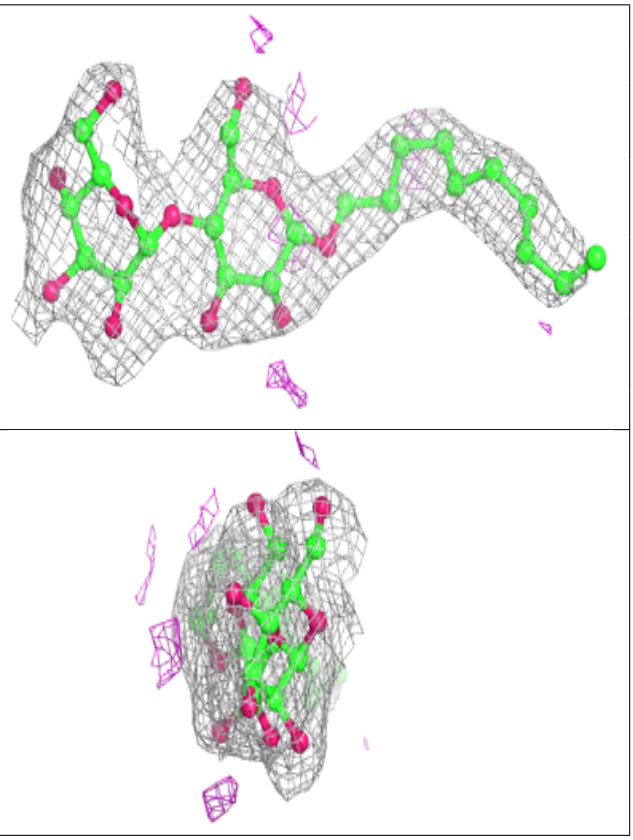
Electron density around CHD C 306:

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



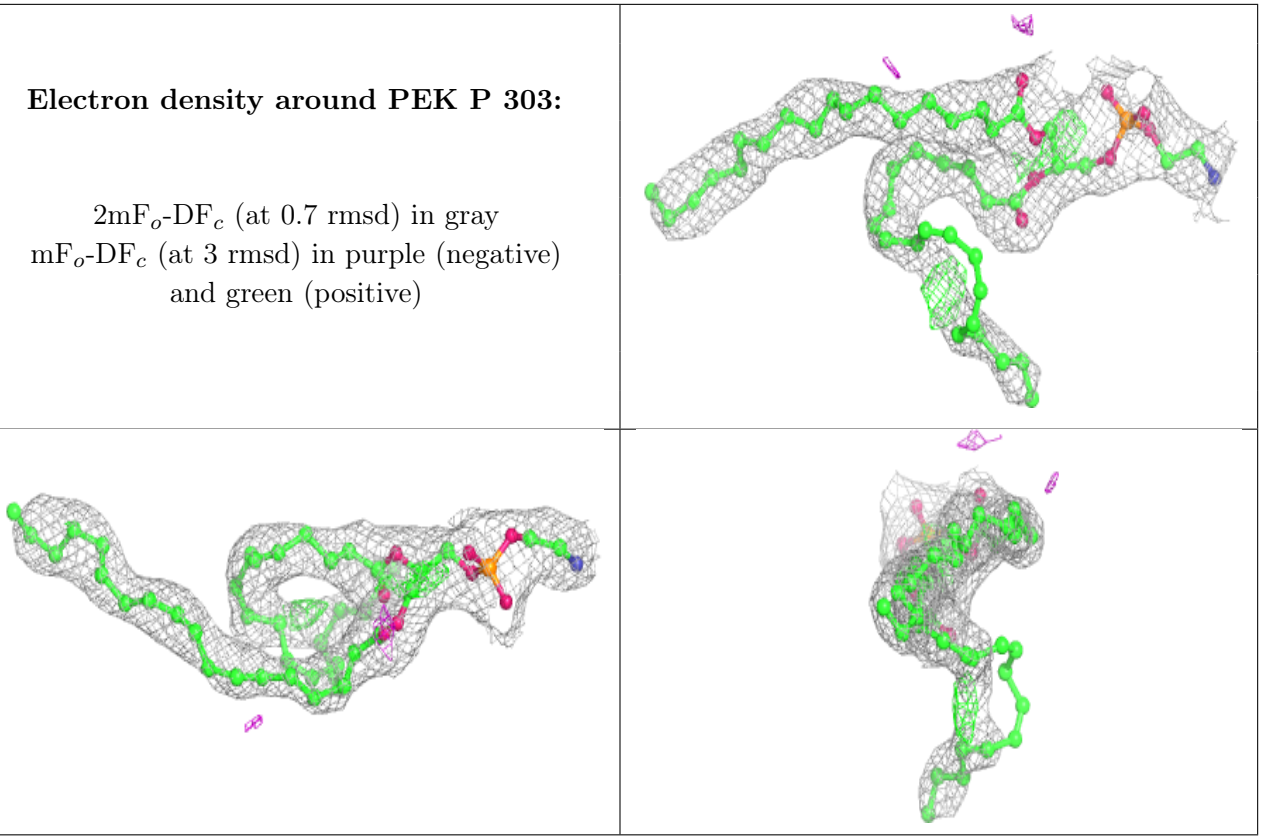
Electron density around DMU M 102:

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



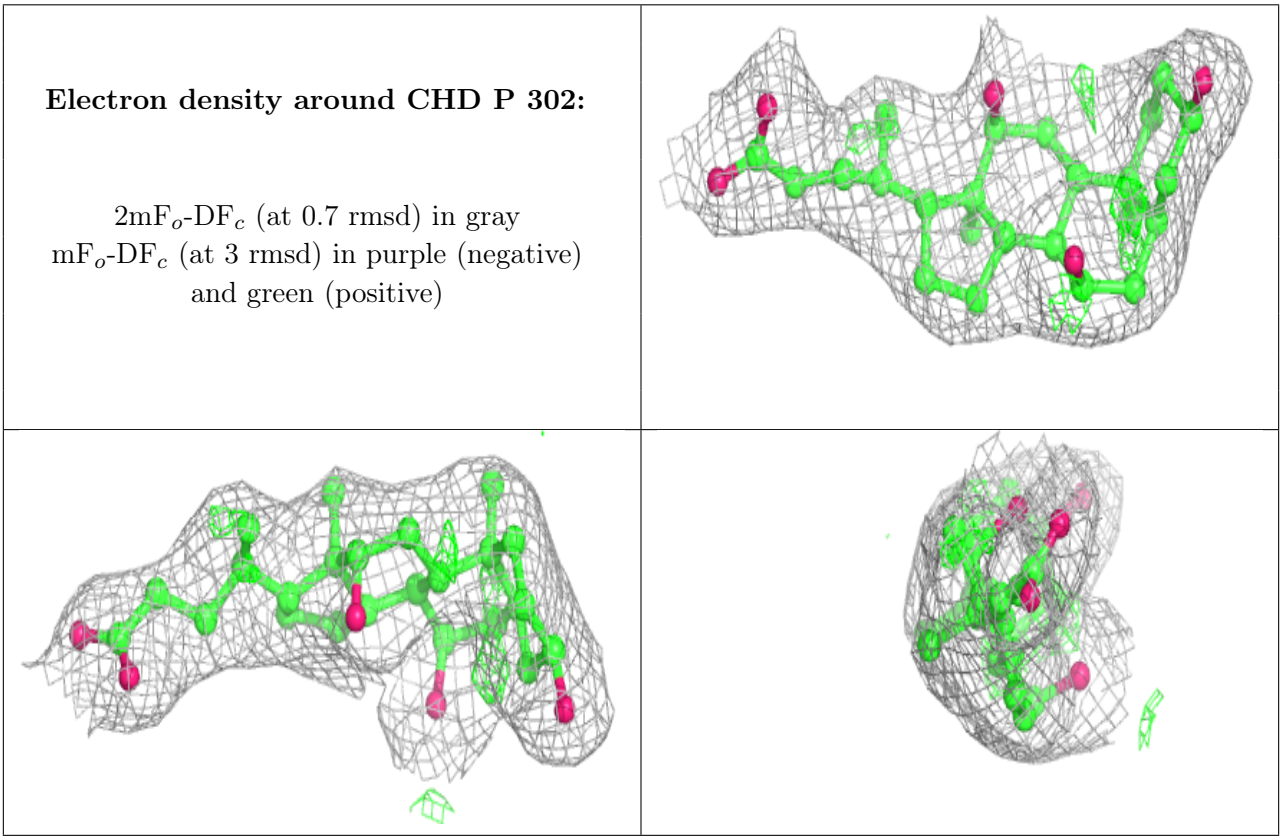
Electron density around PEK P 303:

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



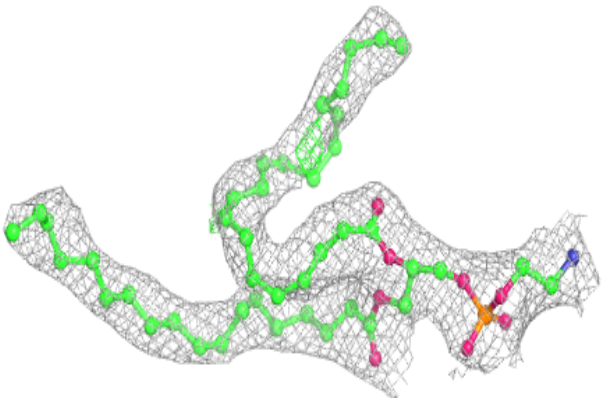
Electron density around CHD P 302:

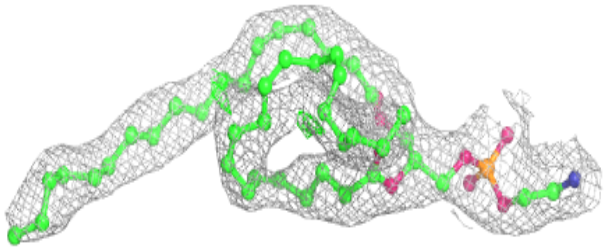
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

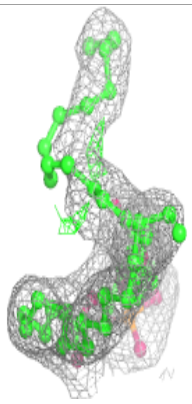


Electron density around PEK G 101:

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

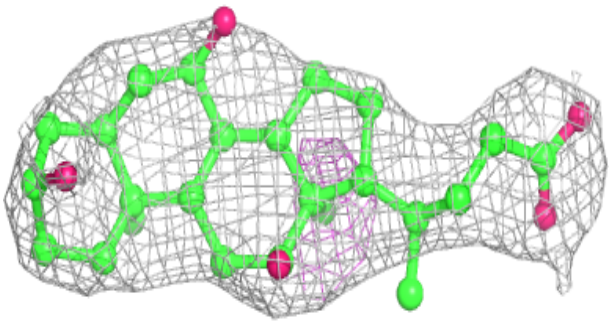


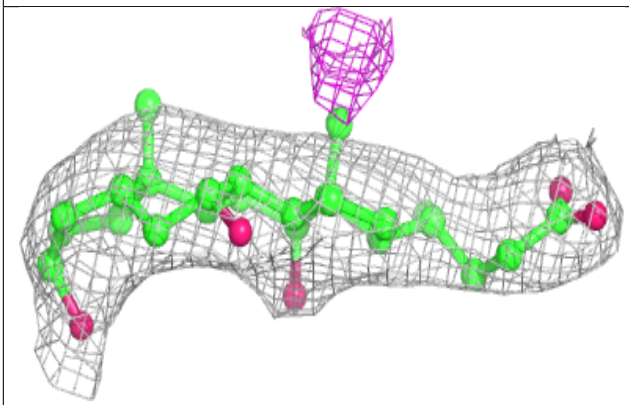


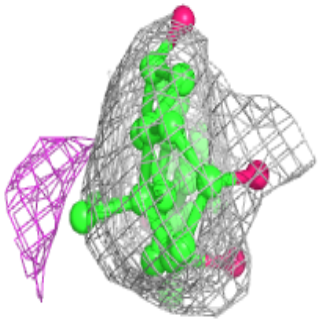


Electron density around CHD P 306:

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

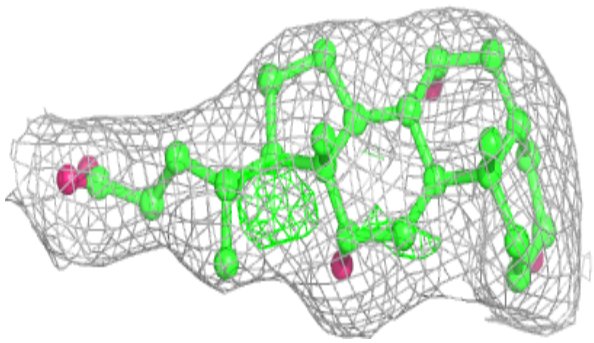


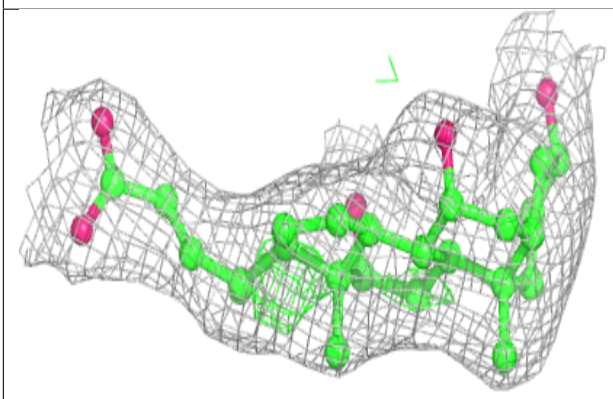


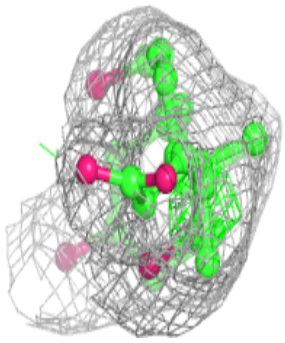


Electron density around CHD G 105:

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

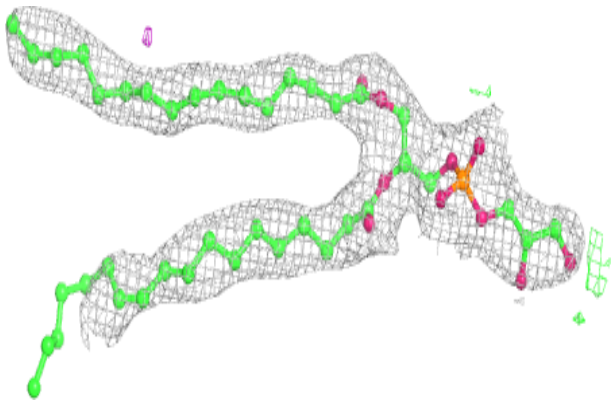


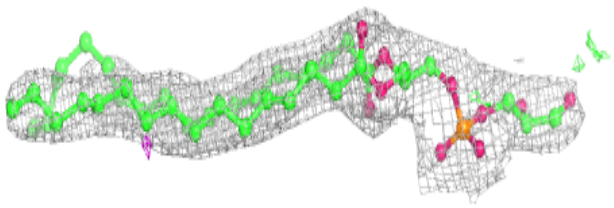


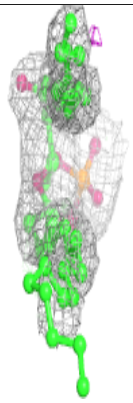


Electron density around PGV P 304:

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

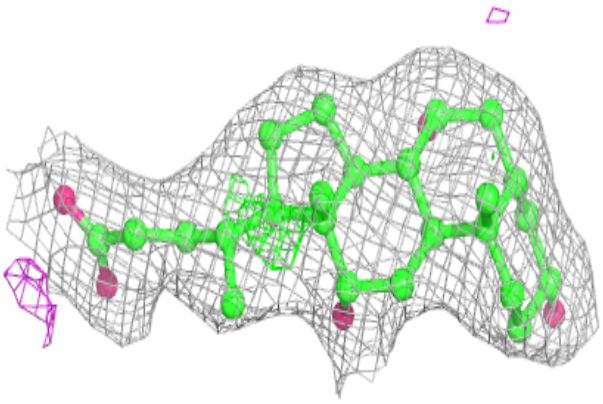


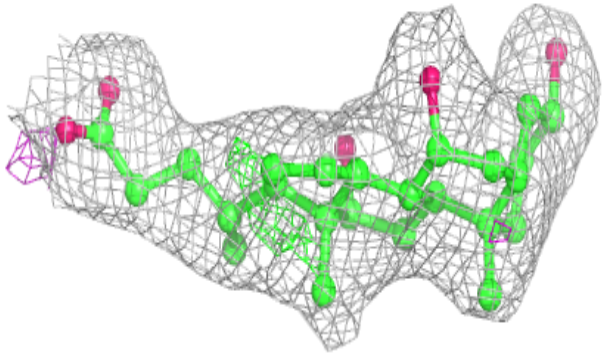


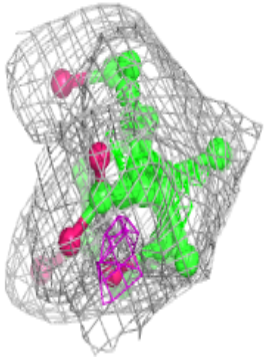


Electron density around CHD C 301:

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

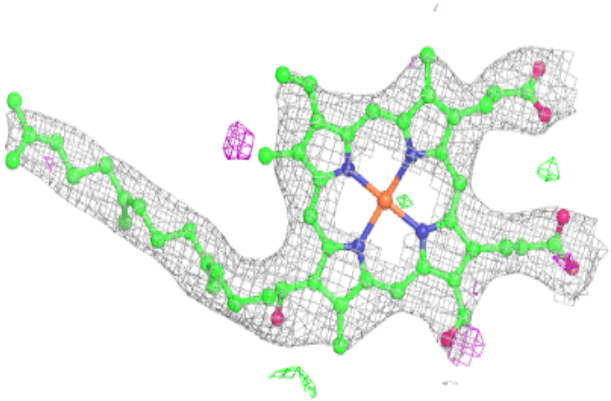


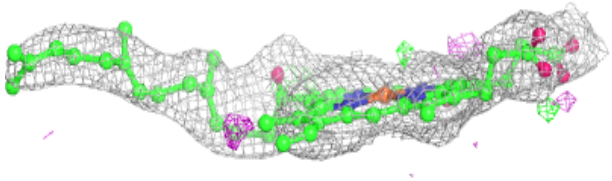


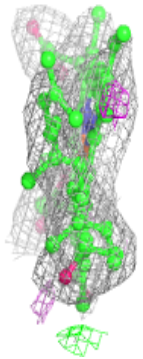


Electron density around HEA N 601:

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

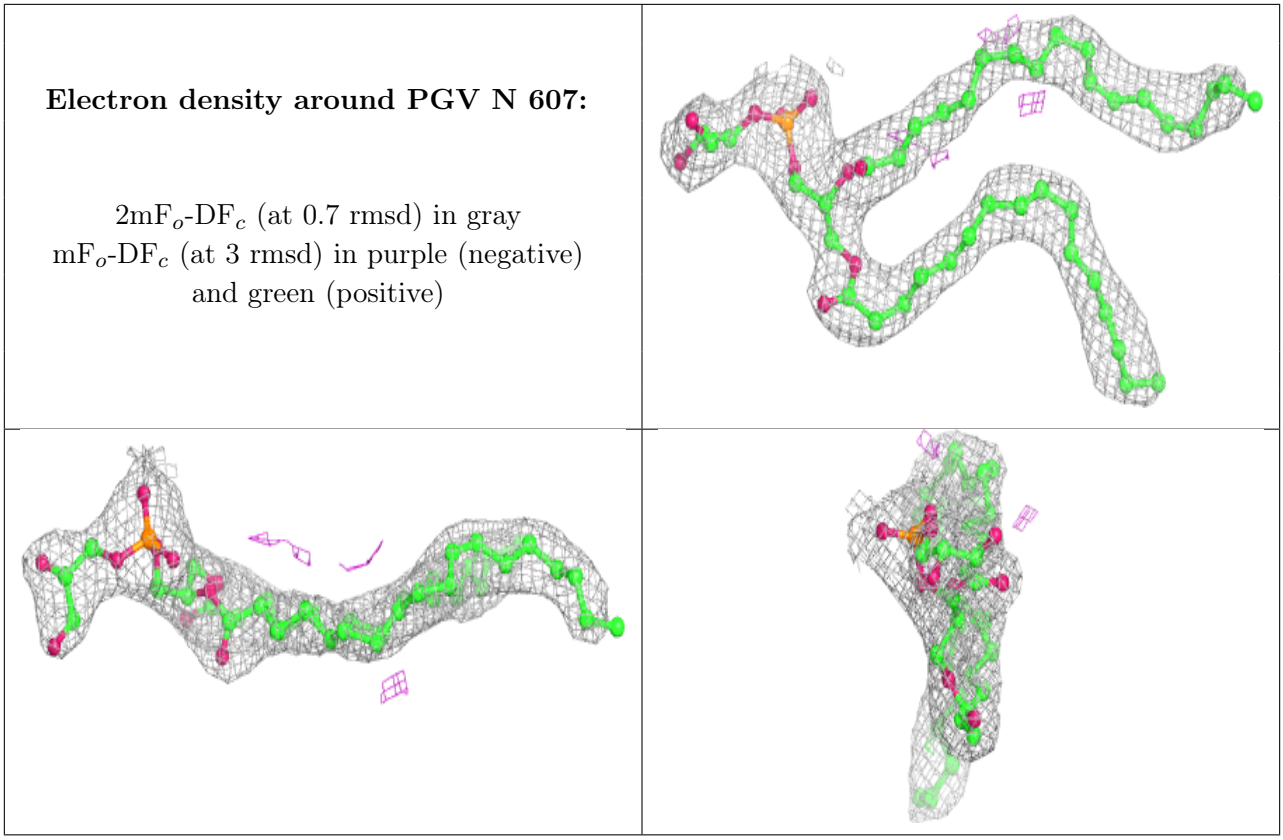






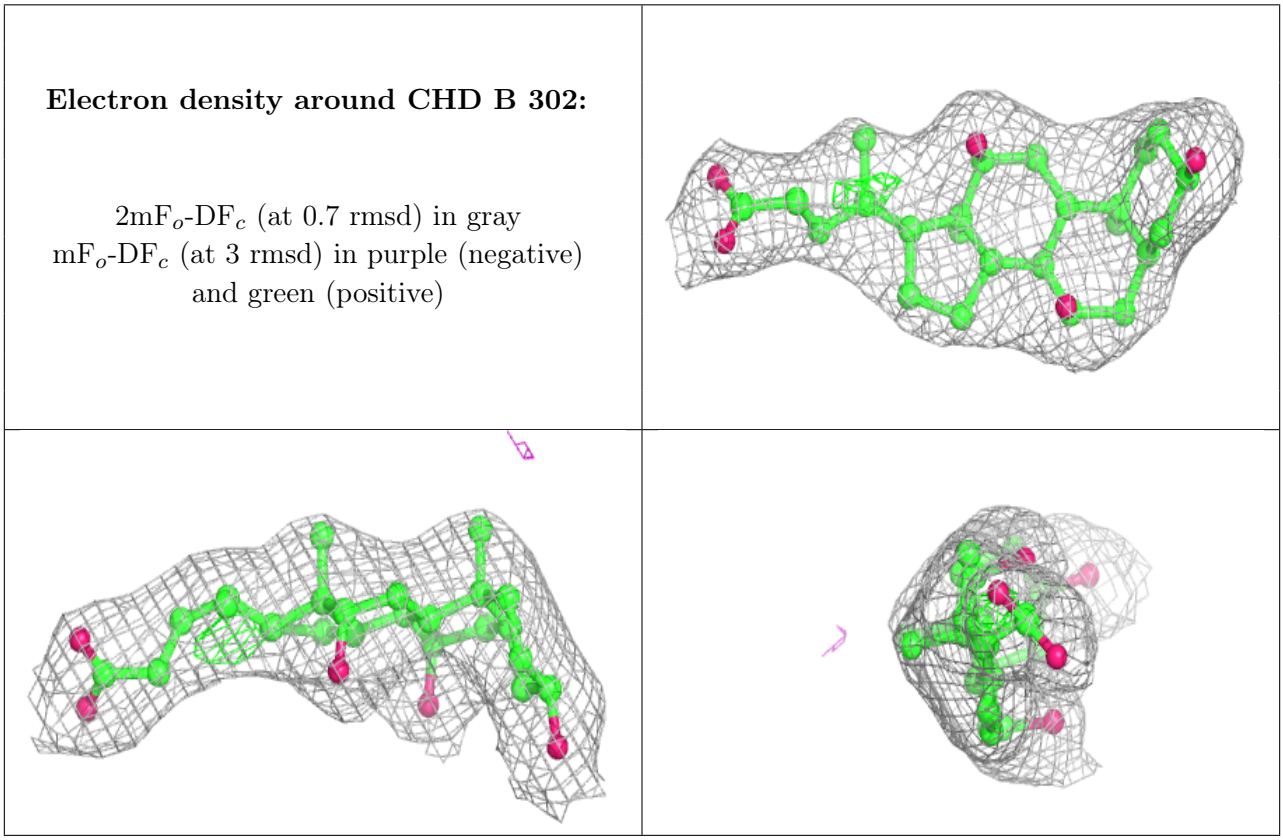
Electron density around PGV N 607:

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



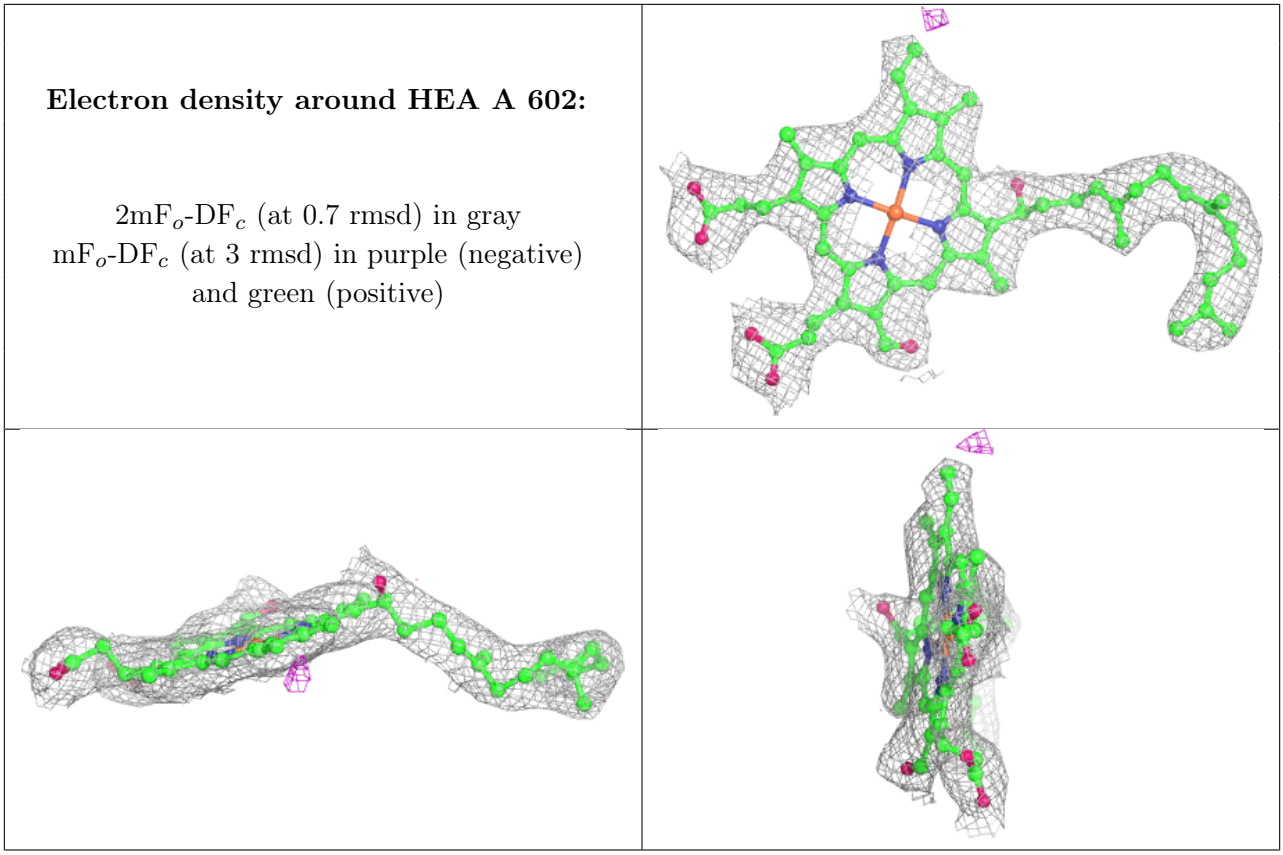
Electron density around CHD B 302:

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



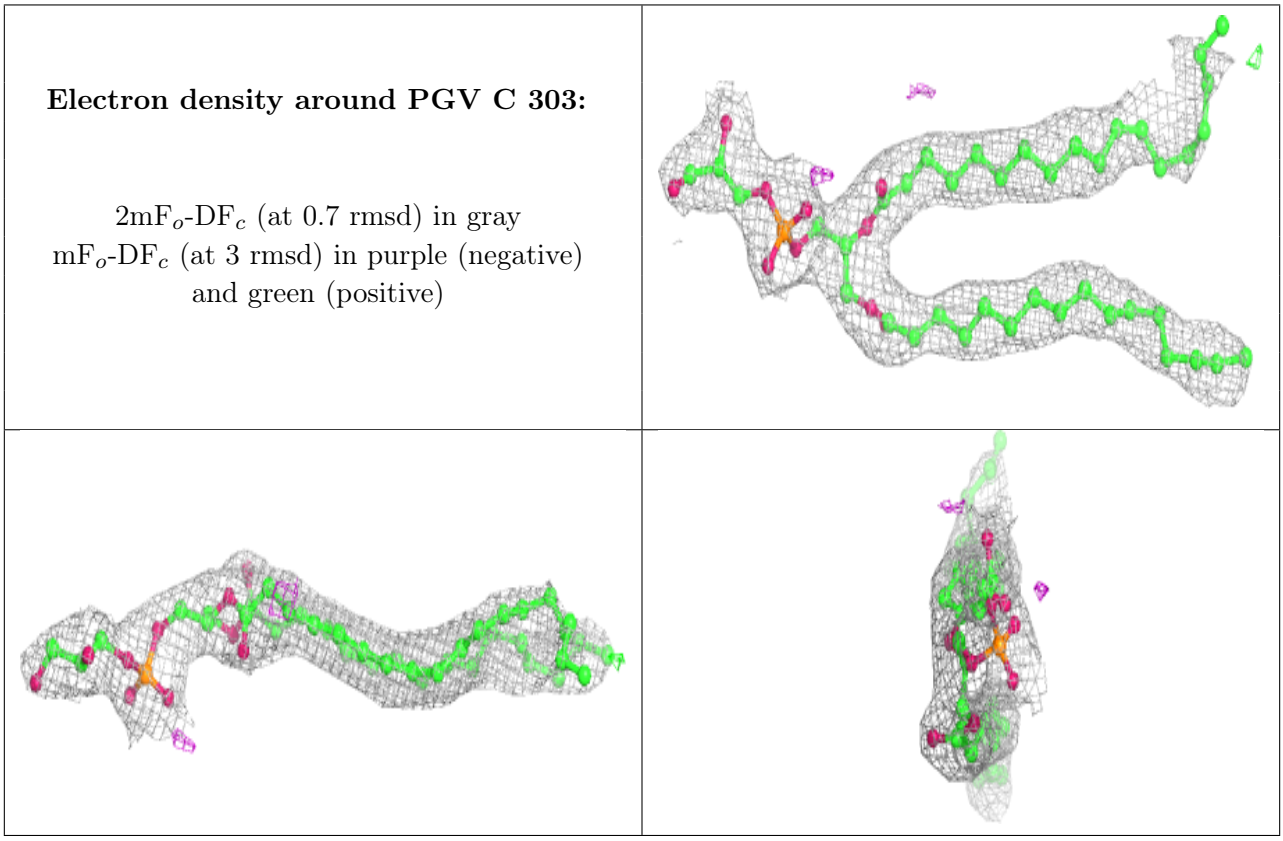
Electron density around HEA A 602:

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



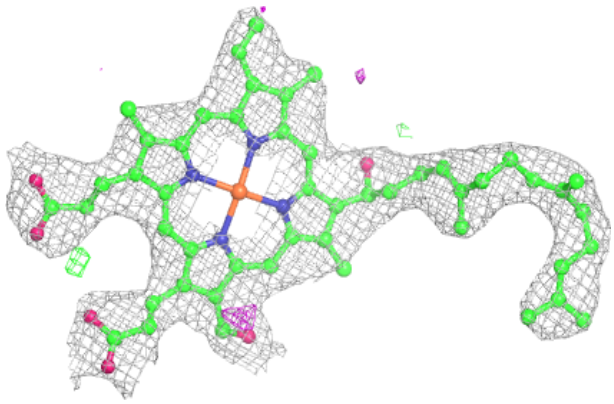
Electron density around PGV C 303:

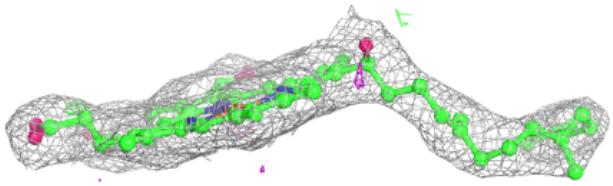
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

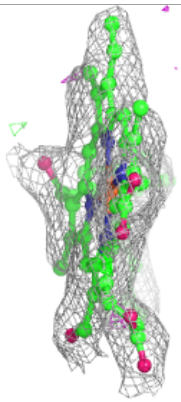


Electron density around HEA N 602:

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

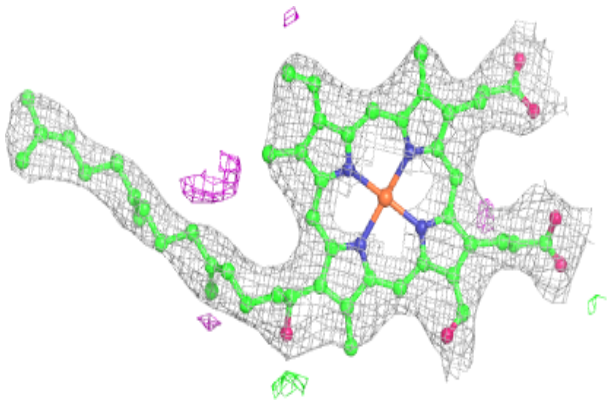


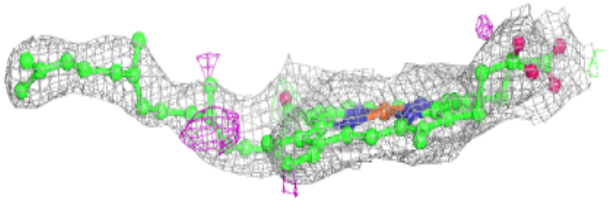


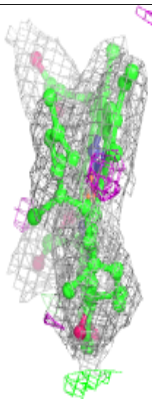


Electron density around HEA A 601:

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

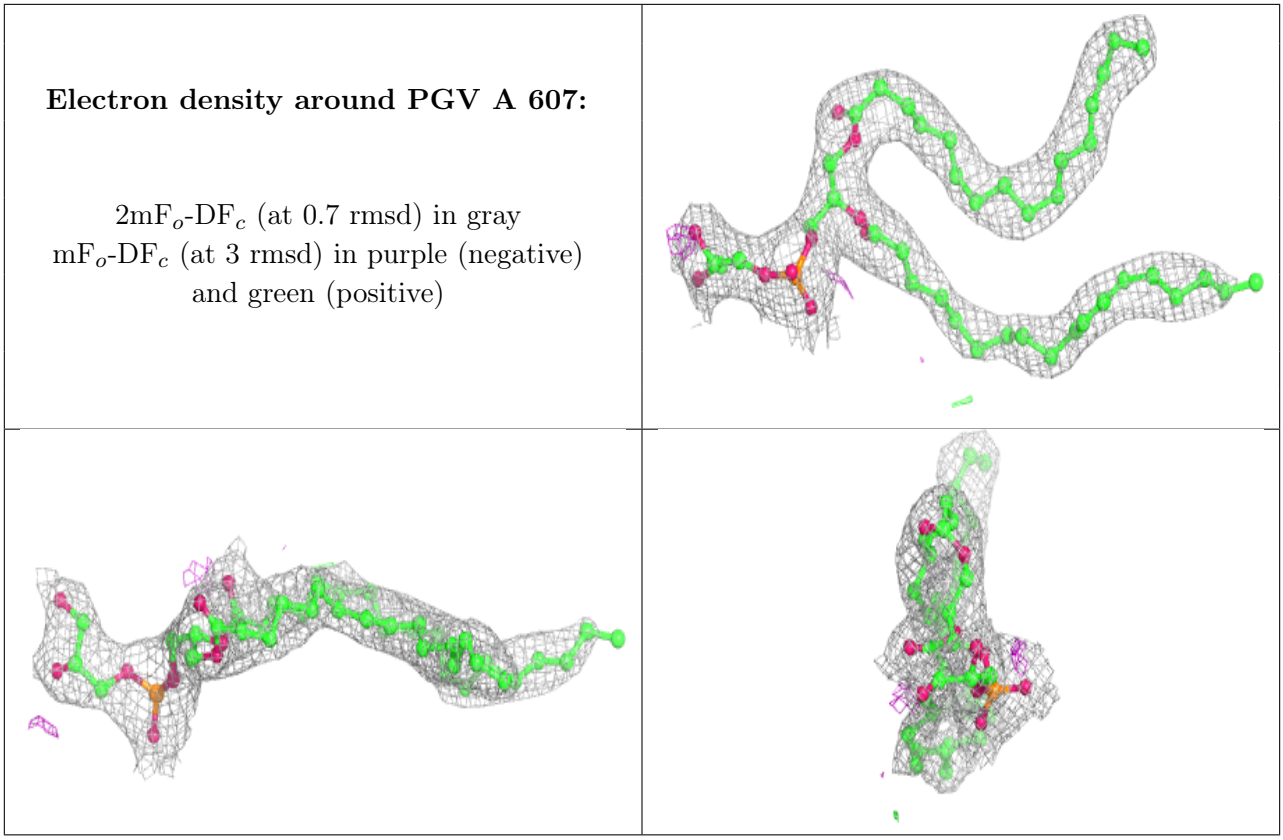






Electron density around PGV A 607:

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



6.5 Other polymers (i)

There are no such residues in this entry.