Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2021 – 04:25 PM EST

PDB ID	:	3X2Q
Title	:	X-ray structure of cyanide-bound bovine heart cytochrome c oxidase in the fully oxidized state at 2.0 angstrom resolution
Authors	:	Yano, N.; Muramoto, K.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on	:	2014-12-26
Resolution	:	2.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

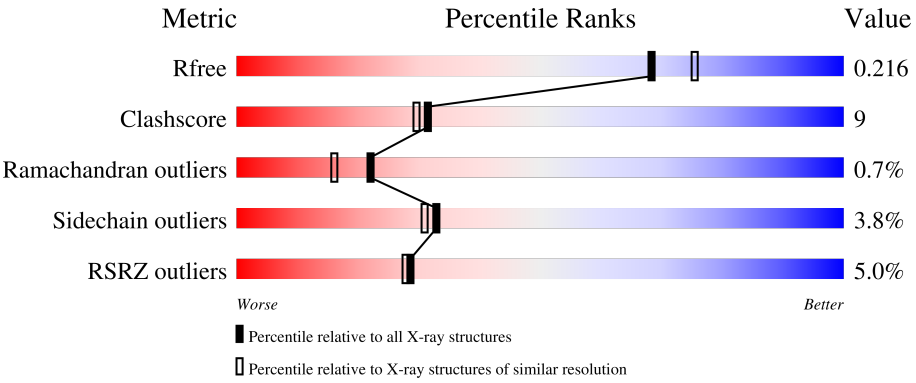
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	81% 17%
1	N	514	84% 14%
2	B	227	78% 20%
2	O	227	79% 19%
3	C	261	83% 16%

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Mol	Chain	Length	Quality of chain
3	P	261	2% 84% 14%
4	D	147	% 79% 16%
4	Q	147	14% 82% 12%
5	E	109	2% 82% 13%
5	R	109	4% 86% 7%
6	F	98	8% 79% 18%
6	S	98	10% 76% 17% 7%
7	G	85	19% 71% 18% 11%
7	T	85	20% 68% 19% 12%
8	H	85	9% 76% 12% 7%
8	U	85	11% 74% 14% 7%
9	I	73	4% 86% 8% 5%
9	V	73	11% 84% 14%
10	J	59	14% 90% 7%
10	W	59	14% 93%
11	K	56	79% 9% 12%
11	X	56	32% 77% 9% 12%
12	L	47	79% 17%
12	Y	47	2% 77% 19%
13	M	46	11% 74% 17% 7%
13	Z	46	17% 78% 15% 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
15	HEA	A	602	X	-	-	-
15	HEA	A	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	N	602	X	-	-	-
15	HEA	N	603	X	-	-	-
20	PGV	C	307	-	-	-	X
20	PGV	P	302	-	-	-	X
22	CHD	C	304	-	-	-	X
24	CDL	G	103	-	-	X	-
24	CDL	T	102	-	-	X	-
25	PEK	G	104	-	-	-	X
25	PEK	T	101	-	-	X	X
28	DMU	P	301	-	-	-	X
9	SAC	V	1	-	X	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 32060 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	3	0
			4051	2708	626	681	36			
1	N	514	Total	C	N	O	S	0	3	0
			4051	2708	626	681	36			

- 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	3	0
			2134	1427	339	353	15			
3	P	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			

- 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	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	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			

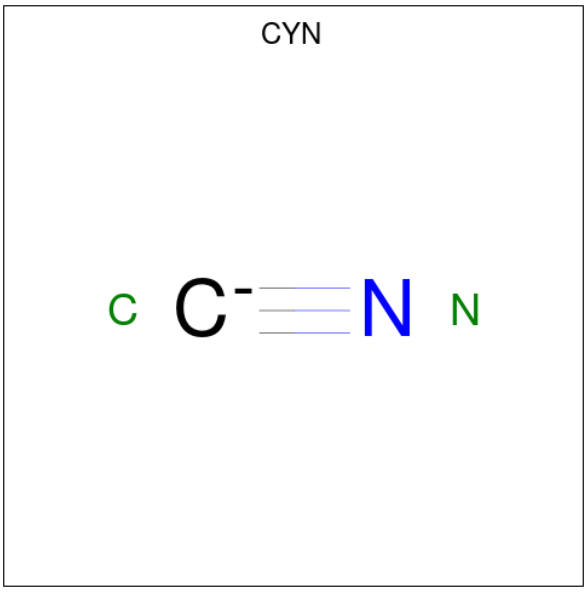
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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.

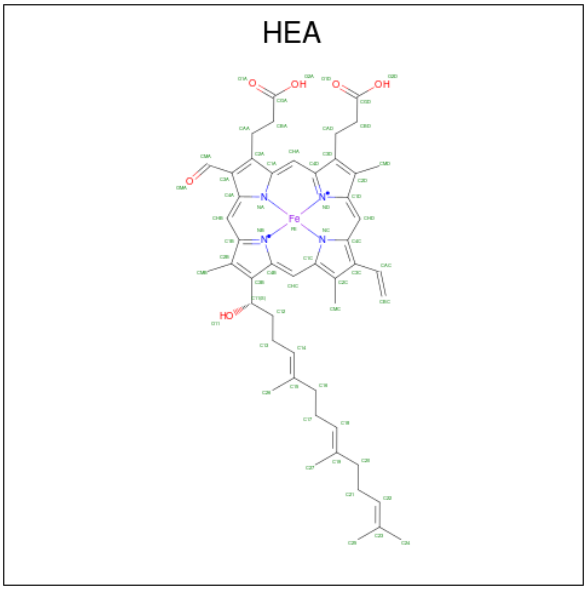
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 15 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

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

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

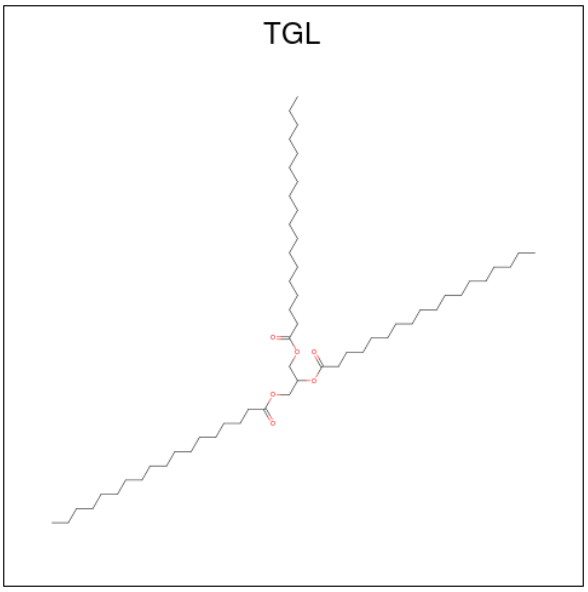
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

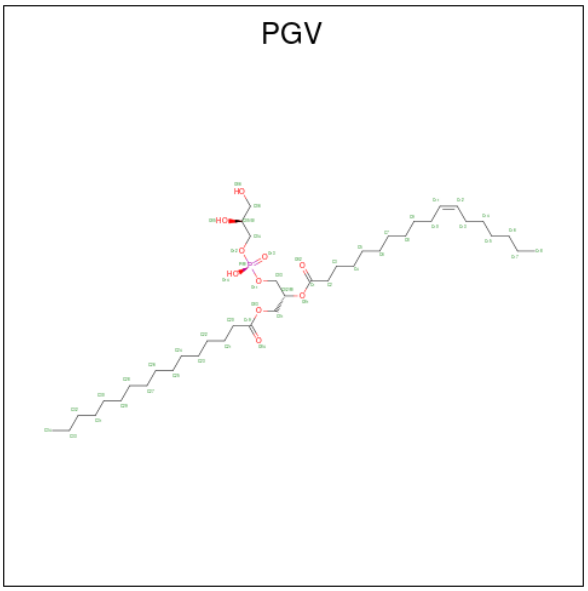
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

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



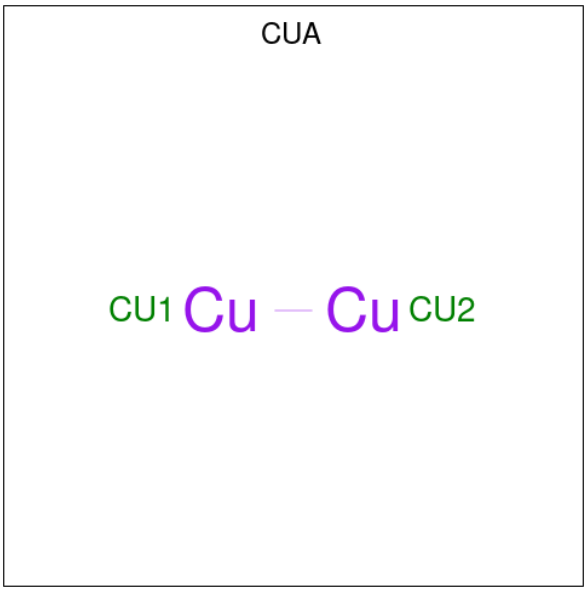
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	Q	1	Total C O 63 57 6	0	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



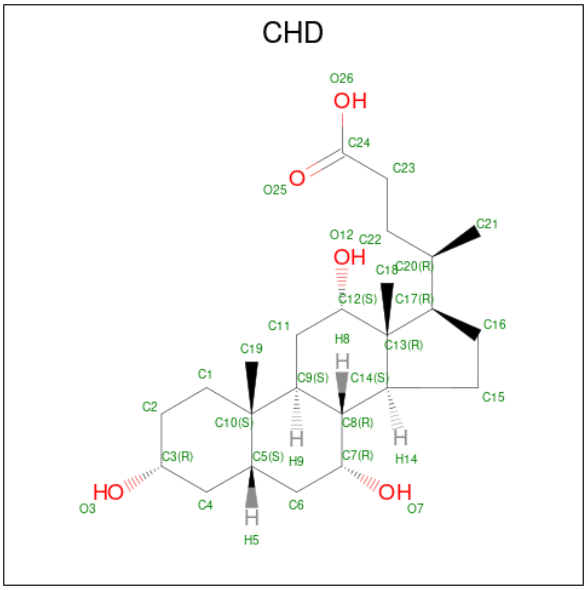
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- 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

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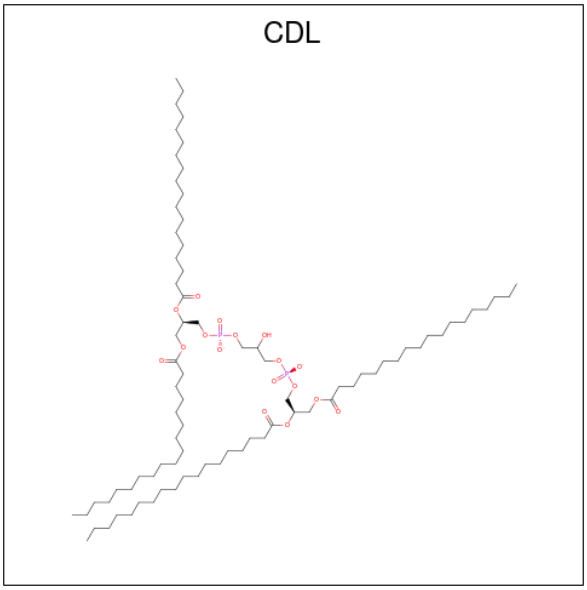
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- 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
24	P	1	Total C O P 100 81 17 2	0	0

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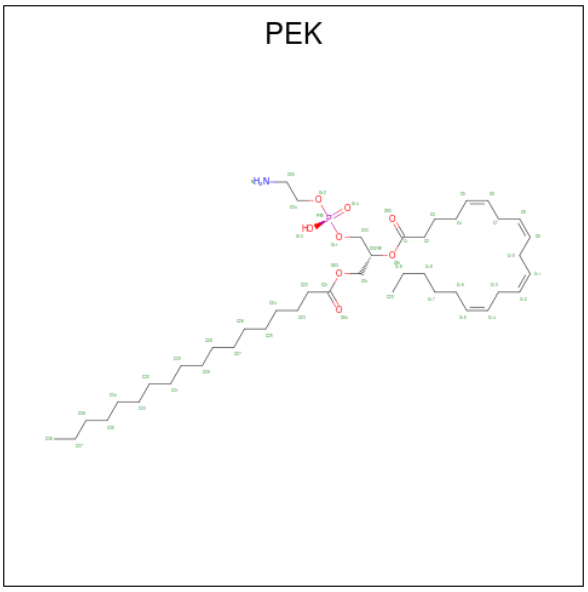
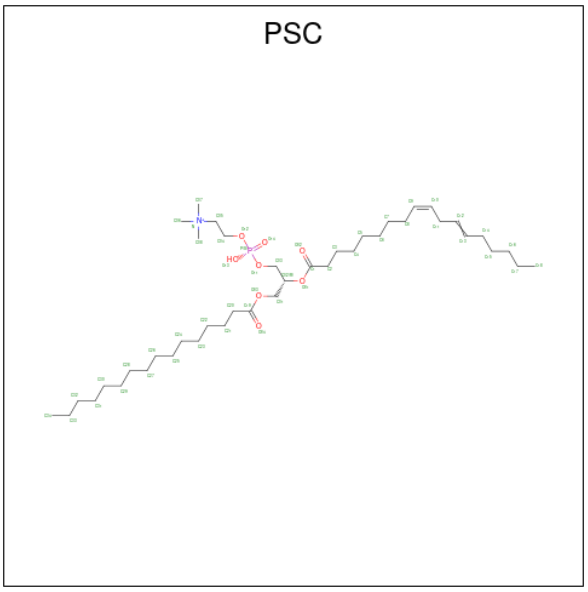
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

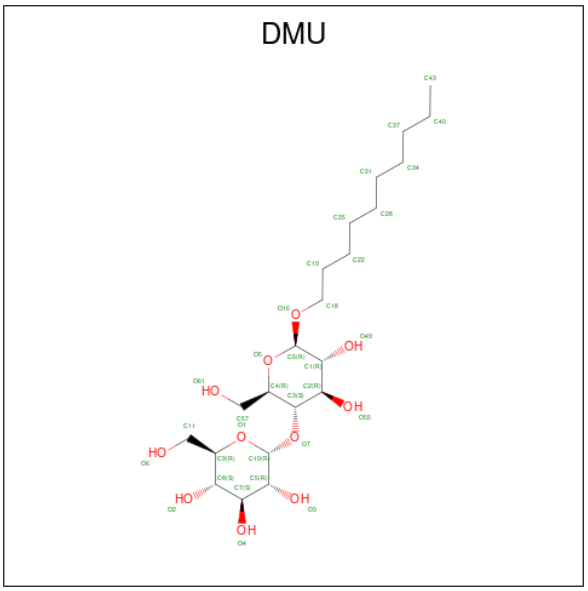


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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	P	1	Total C O 33 22 11	0	0
28	Z	1	Total C O 33 22 11	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	188	Total O 188 188	0	0
29	B	121	Total O 121 121	0	0
29	C	77	Total O 77 77	0	0
29	D	78	Total O 78 78	0	0
29	E	58	Total O 58 58	0	0
29	F	58	Total O 58 58	0	0
29	G	27	Total O 27 27	0	0
29	H	34	Total O 34 34	0	0

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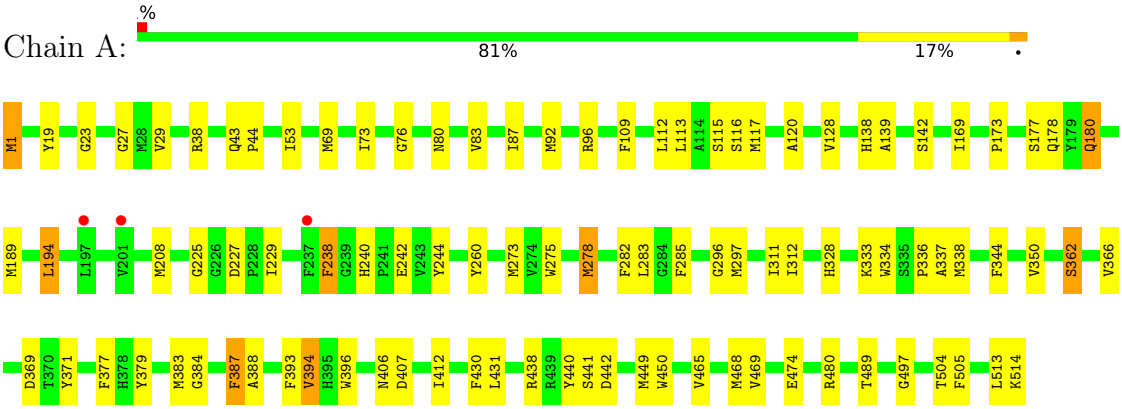
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	29	Total O 29 29	0	0
29	J	15	Total O 15 15	0	0
29	K	20	Total O 20 20	0	0
29	L	16	Total O 16 16	0	0
29	M	14	Total O 14 14	0	0
29	N	156	Total O 156 156	0	0
29	O	91	Total O 91 91	0	0
29	P	76	Total O 76 76	0	0
29	Q	46	Total O 46 46	0	0
29	R	42	Total O 42 42	0	0
29	S	38	Total O 38 38	0	0
29	T	23	Total O 23 23	0	0
29	U	28	Total O 28 28	0	0
29	V	14	Total O 14 14	0	0
29	W	4	Total O 4 4	0	0
29	X	15	Total O 15 15	0	0
29	Y	11	Total O 11 11	0	0
29	Z	7	Total O 7 7	0	0

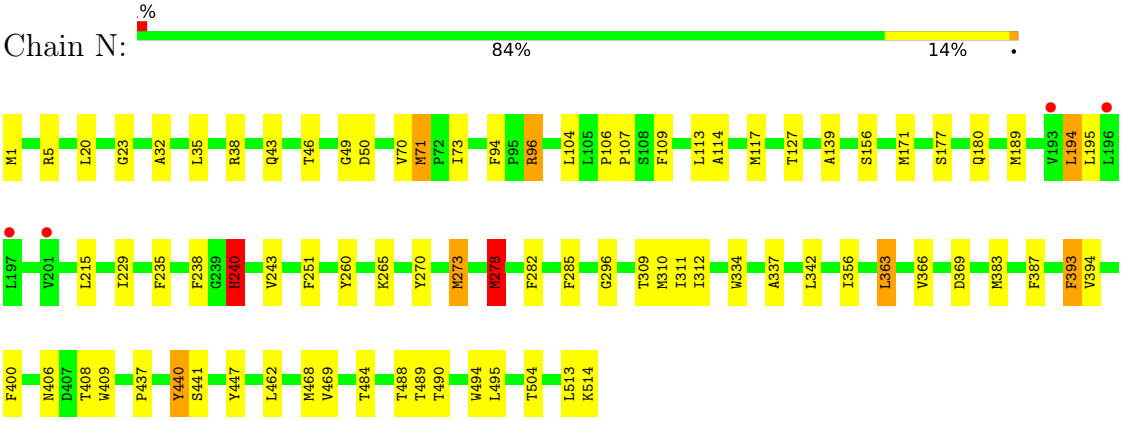
3 Residue-property plots (i)

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

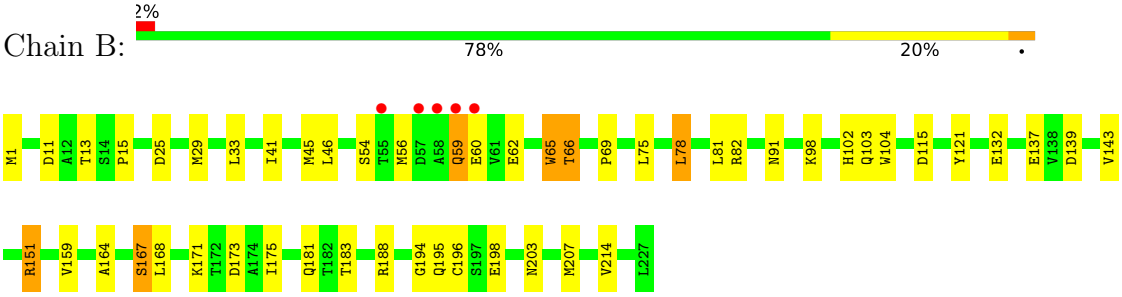
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

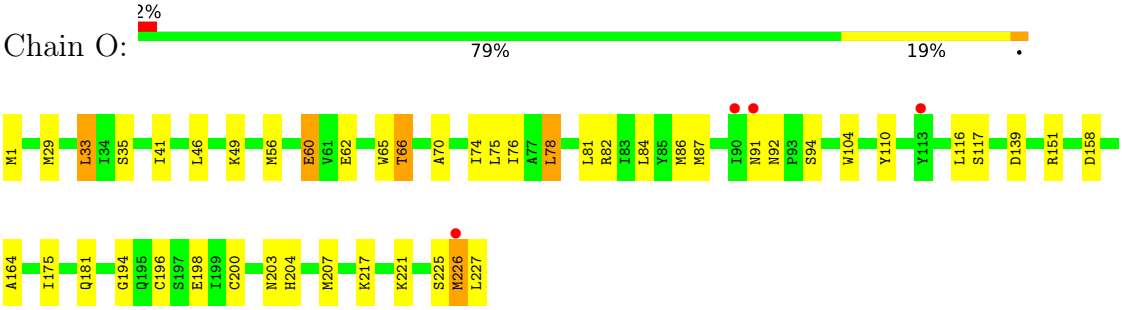


• Molecule 2: Cytochrome c oxidase subunit 2



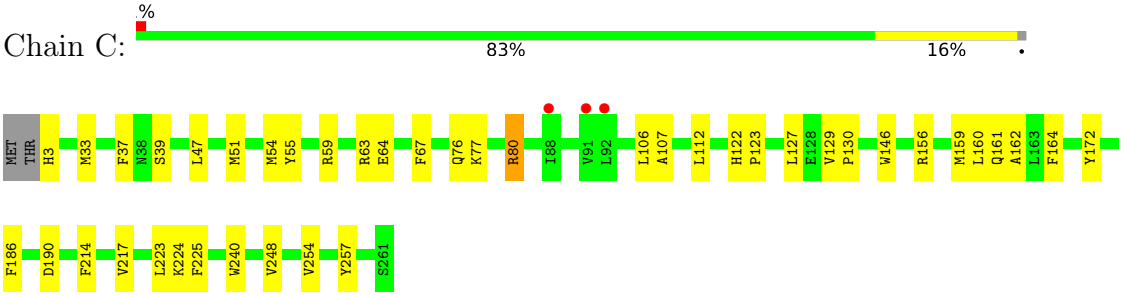
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



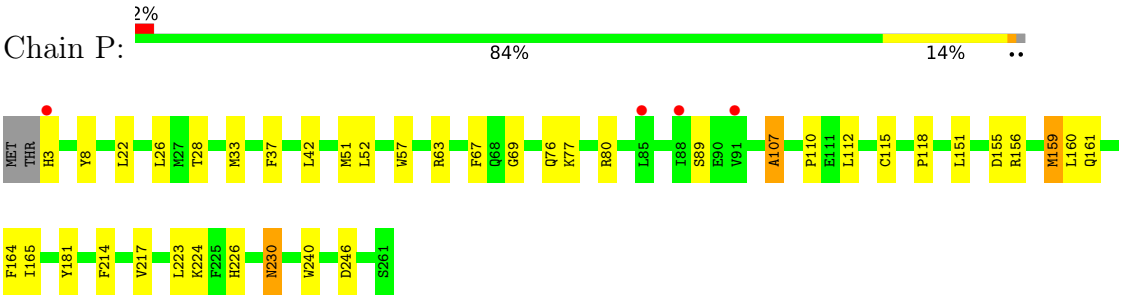
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



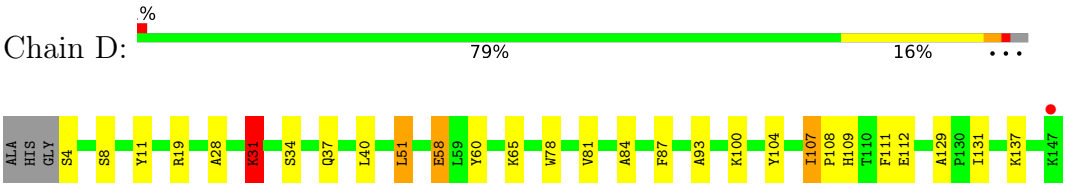
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



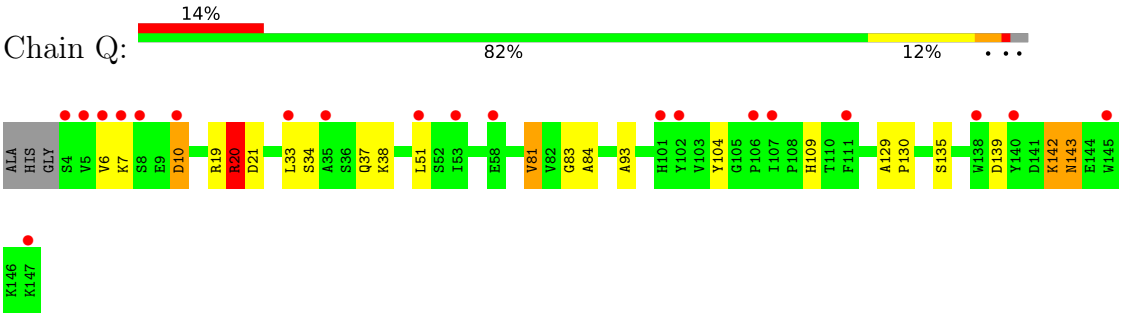
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



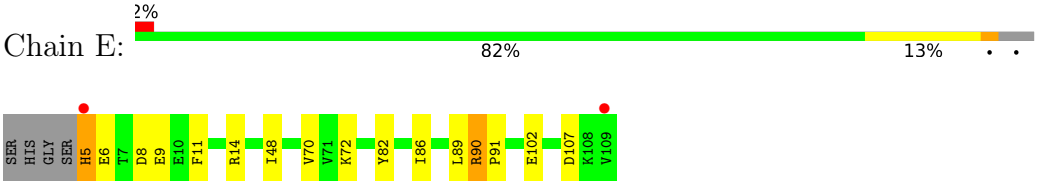
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



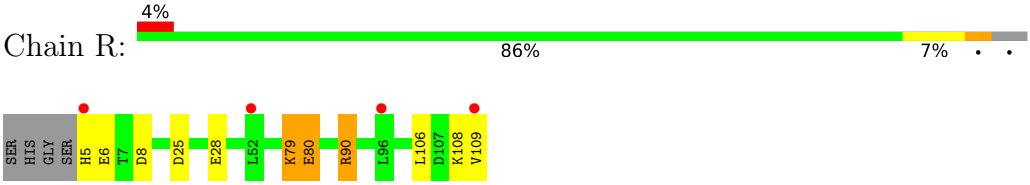
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



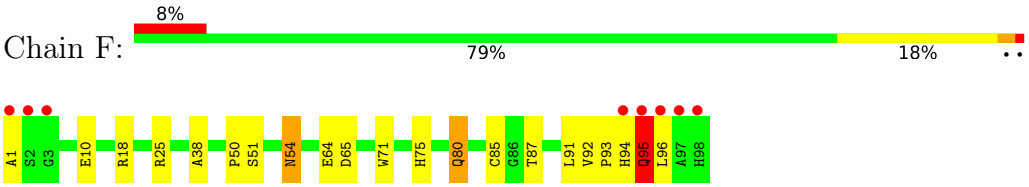
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



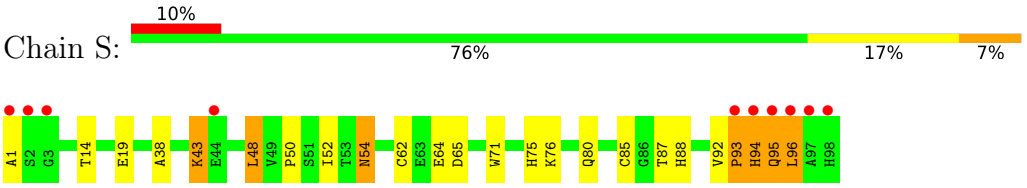
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



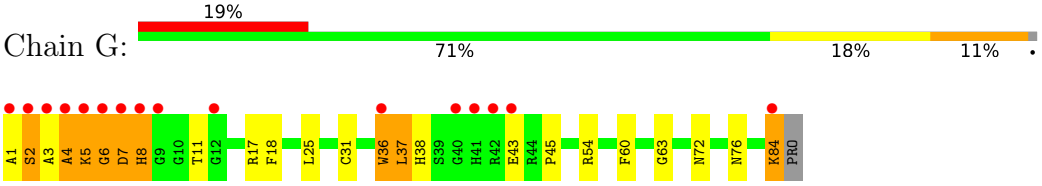
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



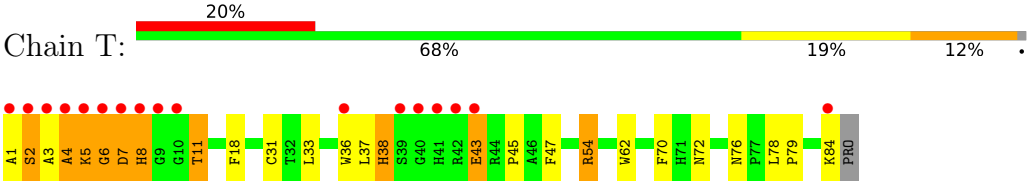
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



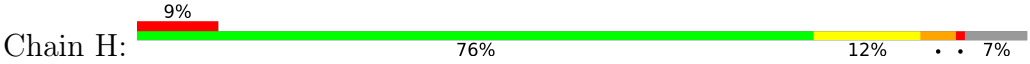
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

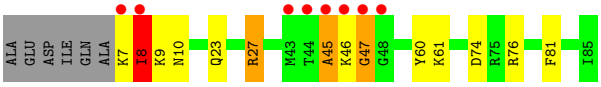
Chain T:



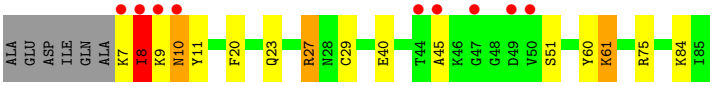
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:

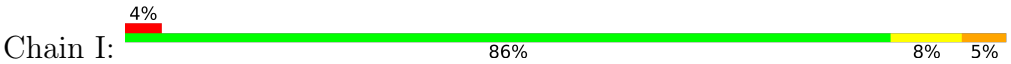


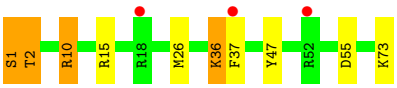


• Molecule 8: Cytochrome c oxidase subunit 6B1

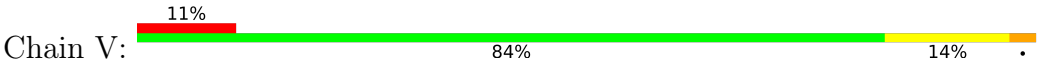


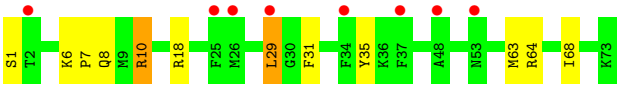
• Molecule 9: Cytochrome c oxidase subunit 6C



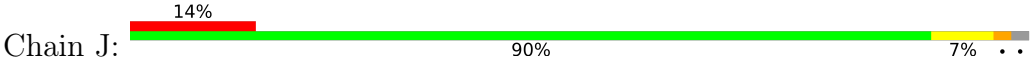


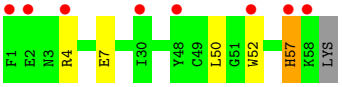
• Molecule 9: Cytochrome c oxidase subunit 6C



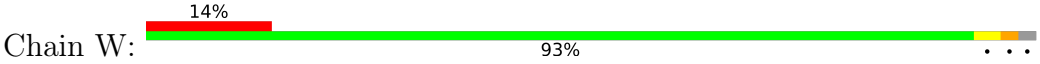


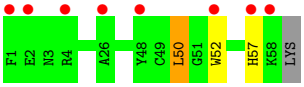
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



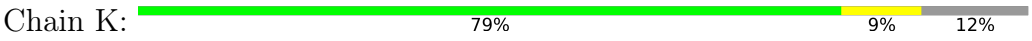


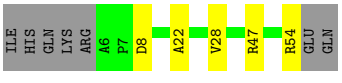
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial





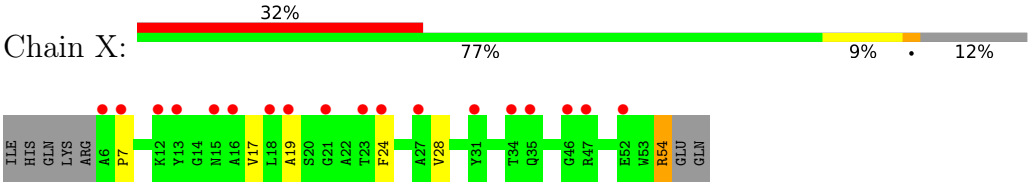
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial





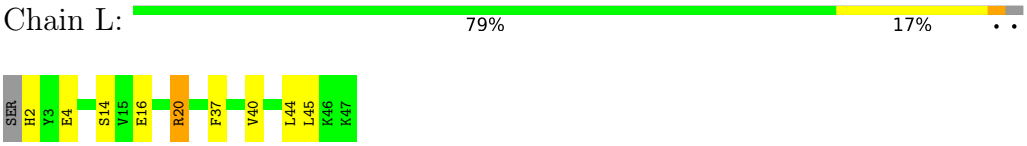
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



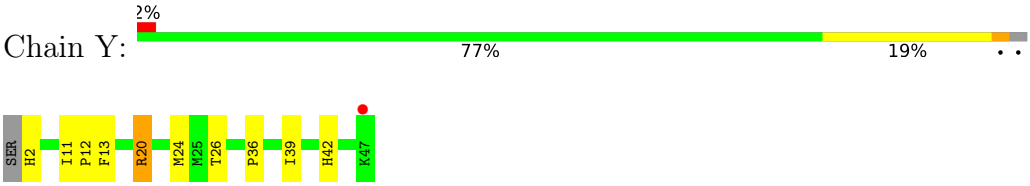
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



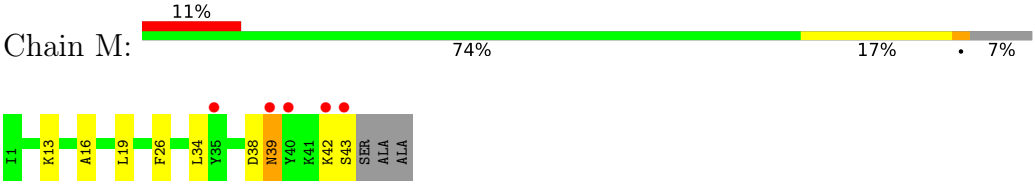
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



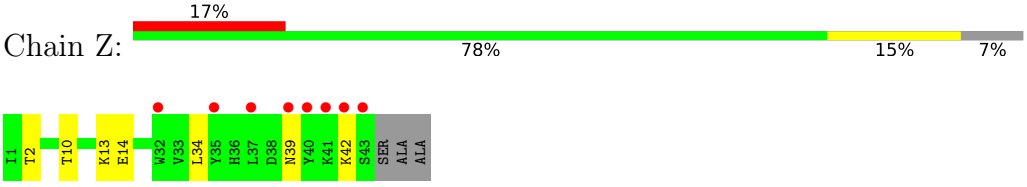
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	183.68Å 206.68Å 178.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 81.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.00) 99.9 (81.64-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.214 0.189 , 0.216	Depositor DCC
R_{free} test set	22864 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32060	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.51	29/4180 (0.7%)	1.15	18/5710 (0.3%)
1	N	1.34	15/4180 (0.4%)	0.99	10/5710 (0.2%)
2	B	1.45	11/1860 (0.6%)	1.16	13/2534 (0.5%)
2	O	1.14	3/1860 (0.2%)	1.01	3/2534 (0.1%)
3	C	1.35	5/2221 (0.2%)	0.96	1/3035 (0.0%)
3	P	1.31	6/2221 (0.3%)	0.93	2/3035 (0.1%)
4	D	1.48	10/1229 (0.8%)	1.14	6/1658 (0.4%)
4	Q	1.03	1/1229 (0.1%)	0.92	3/1658 (0.2%)
5	E	1.27	3/871 (0.3%)	1.11	3/1182 (0.3%)
5	R	1.15	3/871 (0.3%)	0.97	2/1182 (0.2%)
6	F	1.31	0/765	1.08	2/1038 (0.2%)
6	S	1.20	0/765	1.02	0/1038
7	G	1.33	3/690 (0.4%)	1.01	4/937 (0.4%)
7	T	1.31	4/690 (0.6%)	1.07	2/937 (0.2%)
8	H	1.26	1/682 (0.1%)	1.01	3/921 (0.3%)
8	U	1.04	0/682	0.91	1/921 (0.1%)
9	I	1.36	0/605	1.11	2/802 (0.2%)
9	V	1.09	0/605	1.06	3/802 (0.4%)
10	J	1.21	0/471	0.94	0/636
10	W	1.07	0/471	0.92	0/636
11	K	1.38	1/398 (0.3%)	1.11	2/546 (0.4%)
11	X	1.07	1/398 (0.3%)	0.85	0/546
12	L	1.38	3/393 (0.8%)	1.02	1/526 (0.2%)
12	Y	1.16	0/393	0.82	0/526
13	M	1.38	2/345 (0.6%)	1.04	0/470
13	Z	1.05	0/345	0.87	0/470
All	All	1.32	101/29420 (0.3%)	1.03	81/39990 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	6

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	80	GLU	CG-CD	9.50	1.66	1.51
2	B	167	SER	CB-OG	-8.83	1.30	1.42
1	A	371	TYR	CD1-CE1	8.27	1.51	1.39
7	T	36	TRP	CB-CG	8.23	1.65	1.50
5	R	80	GLU	CB-CG	8.14	1.67	1.52
7	G	36	TRP	CB-CG	7.93	1.64	1.50
2	O	198	GLU	C-O	7.50	1.37	1.23
1	A	139	ALA	CA-CB	7.40	1.68	1.52
1	N	70	VAL	CB-CG2	7.32	1.68	1.52
1	N	260	TYR	CE1-CZ	7.21	1.48	1.38
1	A	242	GLU	CG-CD	7.10	1.62	1.51
3	P	181	TYR	CD1-CE1	7.02	1.49	1.39
1	N	139	ALA	CA-CB	6.95	1.67	1.52
1	A	393	PHE	CE1-CZ	6.94	1.50	1.37
1	A	275	TRP	CG-CD1	6.93	1.46	1.36
11	X	19	ALA	CA-CB	6.93	1.67	1.52
13	M	26	PHE	CE2-CZ	6.88	1.50	1.37
4	D	112	GLU	CG-CD	6.78	1.62	1.51
4	D	31	LYS	CD-CE	6.75	1.68	1.51
13	M	16	ALA	CA-CB	6.66	1.66	1.52
1	A	377	PHE	CE2-CZ	6.60	1.49	1.37
3	P	115	CYS	CB-SG	6.43	1.93	1.82
2	B	143	VAL	CB-CG2	6.43	1.66	1.52
1	A	244	TYR	CE1-CZ	6.41	1.46	1.38
2	B	214	VAL	CB-CG1	6.31	1.66	1.52
4	D	100	LYS	CD-CE	6.29	1.67	1.51
1	N	273	MET	CB-CG	6.28	1.71	1.51
3	P	57	TRP	CB-CG	6.27	1.61	1.50
5	E	70	VAL	CB-CG2	6.24	1.66	1.52
1	N	189	MET	CB-CG	6.23	1.71	1.51

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	102	GLU	CB-CG	6.14	1.63	1.52
12	L	4	GLU	CG-CD	6.13	1.61	1.51
11	K	22	ALA	CA-CB	6.12	1.65	1.52
4	D	11	TYR	CB-CG	6.06	1.60	1.51
2	B	121	TYR	CE2-CZ	6.03	1.46	1.38
5	E	9	GLU	CG-CD	6.01	1.60	1.51
2	B	159	VAL	CB-CG2	5.97	1.65	1.52
1	A	19	TYR	CD2-CE2	5.97	1.48	1.39
3	C	64	GLU	CG-CD	5.92	1.60	1.51
2	B	59	GLN	CG-CD	5.90	1.64	1.51
1	A	465	VAL	CB-CG1	5.87	1.65	1.52
8	H	81	PHE	CE2-CZ	5.87	1.48	1.37
1	N	494	TRP	CZ3-CH2	5.87	1.49	1.40
4	D	19	ARG	CZ-NH2	5.85	1.40	1.33
3	C	172	TYR	CD2-CE2	5.83	1.48	1.39
1	A	505	PHE	CE2-CZ	5.78	1.48	1.37
4	D	104	TYR	CD1-CE1	5.76	1.48	1.39
1	A	388	ALA	CA-CB	5.75	1.64	1.52
1	A	441	SER	C-O	5.74	1.34	1.23
2	B	198	GLU	CD-OE1	-5.71	1.19	1.25
2	B	198	GLU	CB-CG	5.71	1.62	1.52
7	T	47	PHE	CE1-CZ	5.68	1.48	1.37
1	A	396	TRP	CE3-CZ3	5.67	1.48	1.38
1	A	83	VAL	CB-CG2	5.66	1.64	1.52
3	C	257	TYR	CE2-CZ	5.64	1.45	1.38
1	N	251	PHE	CE2-CZ	5.62	1.48	1.37
1	N	366	VAL	CB-CG1	-5.56	1.41	1.52
3	P	107	ALA	CA-CB	5.53	1.64	1.52
4	D	28	ALA	CA-CB	5.53	1.64	1.52
1	A	238	PHE	CE2-CZ	5.52	1.47	1.37
1	A	394	VAL	CB-CG2	-5.51	1.41	1.52
1	N	94	PHE	CD1-CE1	5.50	1.50	1.39
3	C	240	TRP	CG-CD1	5.46	1.44	1.36
1	A	260	TYR	CD2-CE2	5.46	1.47	1.39
2	B	98	LYS	CD-CE	5.40	1.64	1.51
5	R	80	GLU	CD-OE1	5.40	1.31	1.25
1	A	387	PHE	CD2-CE2	5.37	1.50	1.39
7	T	5	LYS	CB-CG	5.33	1.67	1.52
2	O	110	TYR	CD1-CE1	5.32	1.47	1.39
1	A	120	ALA	CA-CB	5.31	1.63	1.52
1	A	128	VAL	CB-CG1	5.31	1.64	1.52
3	C	225	PHE	CD2-CE2	5.29	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	60	GLU	CG-CD	5.28	1.59	1.51
1	A	469	VAL	CB-CG1	5.25	1.63	1.52
1	N	447	TYR	CD2-CE2	5.25	1.47	1.39
3	P	89	SER	CB-OG	5.24	1.49	1.42
4	Q	81	VAL	CB-CG1	5.20	1.63	1.52
12	L	37	PHE	CE2-CZ	5.20	1.47	1.37
4	D	100	LYS	CE-NZ	5.18	1.62	1.49
1	A	260	TYR	CE2-CZ	5.18	1.45	1.38
1	A	362	SER	CB-OG	-5.17	1.35	1.42
1	A	29	VAL	CB-CG1	5.14	1.63	1.52
1	N	270	TYR	CD1-CE1	5.12	1.47	1.39
2	B	159	VAL	CB-CG1	5.12	1.63	1.52
7	G	60	PHE	CE1-CZ	5.11	1.47	1.37
7	T	70	PHE	CG-CD2	5.10	1.46	1.38
3	P	240	TRP	CE3-CZ3	5.10	1.47	1.38
4	D	87	PHE	CD2-CE2	5.09	1.49	1.39
7	G	5	LYS	CB-CG	5.08	1.66	1.52
1	A	497	GLY	C-O	5.07	1.31	1.23
1	A	92	MET	CB-CG	5.07	1.67	1.51
4	D	60	TYR	CG-CD1	5.06	1.45	1.39
2	B	198	GLU	C-O	5.05	1.32	1.23
1	N	469	VAL	CB-CG2	5.05	1.63	1.52
1	N	440	TYR	CD2-CE2	5.03	1.46	1.39
1	N	393	PHE	CE1-CZ	5.03	1.47	1.37
12	L	16	GLU	CG-CD	5.03	1.59	1.51
1	A	371	TYR	CD2-CE2	5.02	1.46	1.39
1	A	379	TYR	CG-CD1	5.02	1.45	1.39
1	A	474	GLU	CB-CG	5.01	1.61	1.52
1	N	441	SER	C-O	5.01	1.32	1.23

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	MET	CG-SD-CE	-19.27	69.37	100.20
4	D	19	ARG	NE-CZ-NH1	-13.36	113.62	120.30
1	A	96	ARG	NE-CZ-NH2	-11.58	114.51	120.30
4	Q	20	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	278	MET	CG-SD-CE	-9.12	85.61	100.20
5	E	90	ARG	NE-CZ-NH1	9.08	124.84	120.30
9	V	10	ARG	NE-CZ-NH2	-8.69	115.96	120.30
11	K	47	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	N	5	ARG	NE-CZ-NH2	-8.25	116.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	90	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	N	278	MET	CG-SD-CE	-8.11	87.22	100.20
7	T	33	LEU	CA-CB-CG	8.04	133.78	115.30
1	A	208	MET	CG-SD-CE	7.98	112.96	100.20
6	F	18	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	194	LEU	CB-CG-CD2	7.19	123.22	111.00
1	N	194	LEU	CB-CG-CD2	7.16	123.17	111.00
4	D	19	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	N	71	MET	CG-SD-CE	-7.02	88.97	100.20
1	A	227	ASP	CB-CG-OD2	6.88	124.49	118.30
5	E	107	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	366	VAL	CG1-CB-CG2	-6.85	99.94	110.90
3	C	80	ARG	CG-CD-NE	-6.82	97.48	111.80
1	A	480	ARG	NE-CZ-NH2	-6.70	116.95	120.30
5	R	90	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	227	ASP	CB-CG-OD1	-6.42	112.52	118.30
2	B	188	ARG	NE-CZ-NH2	-6.34	117.13	120.30
9	V	10	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	168	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	A	407	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	189	MET	CA-CB-CG	-6.24	102.70	113.30
2	B	25	ASP	CB-CG-OD1	6.01	123.71	118.30
2	B	198	GLU	OE1-CD-OE2	-6.01	116.08	123.30
1	A	438	ARG	NE-CZ-NH2	5.96	123.28	120.30
2	B	139	ASP	CB-CG-OD2	5.95	123.66	118.30
2	B	151	ARG	NE-CZ-NH1	5.92	123.26	120.30
3	P	155	ASP	CB-CG-OD1	5.92	123.62	118.30
2	B	65	TRP	CB-CA-C	5.85	122.11	110.40
1	N	189	MET	CA-CB-CG	-5.83	103.39	113.30
8	H	76	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	480	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	244	TYR	CA-CB-CG	-5.74	102.50	113.40
8	H	27	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	96	ARG	NE-CZ-NH1	5.69	123.14	120.30
9	I	55	ASP	CB-CG-OD1	5.68	123.41	118.30
4	D	65	LYS	CD-CE-NZ	-5.67	98.66	111.70
1	N	96	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	P	80	ARG	CG-CD-NE	-5.66	99.91	111.80
4	D	137	LYS	CD-CE-NZ	-5.62	98.77	111.70
2	B	173	ASP	CB-CG-OD1	5.57	123.31	118.30
2	B	167	SER	CB-CA-C	-5.51	99.63	110.10
1	A	438	ARG	NE-CZ-NH1	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	74	ASP	CB-CG-OD1	5.44	123.20	118.30
4	Q	20	ARG	CG-CD-NE	-5.40	100.46	111.80
7	G	7	ASP	N-CA-C	5.39	125.55	111.00
6	F	18	ARG	NE-CZ-NH1	5.33	122.96	120.30
7	G	8	HIS	N-CA-C	5.31	125.34	111.00
11	K	47	ARG	CD-NE-CZ	5.29	131.01	123.60
2	O	139	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	442	ASP	CB-CG-OD2	5.27	123.04	118.30
4	D	51	LEU	CA-CB-CG	5.26	127.40	115.30
2	B	151	ARG	NE-CZ-NH2	-5.22	117.69	120.30
9	V	64	ARG	NE-CZ-NH1	-5.18	117.71	120.30
8	U	75	ARG	NE-CZ-NH2	-5.13	117.73	120.30
7	G	17	ARG	NE-CZ-NH1	-5.13	117.74	120.30
2	B	102	HIS	CB-CA-C	-5.12	100.15	110.40
7	G	6	GLY	N-CA-C	5.12	125.90	113.10
2	B	11	ASP	CB-CG-OD2	5.11	122.89	118.30
4	D	107	ILE	CB-CG1-CD1	-5.10	99.61	113.90
9	I	10	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	O	226	MET	CG-SD-CE	5.09	108.35	100.20
1	N	50	ASP	CB-CG-OD2	5.08	122.88	118.30
4	Q	20	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	N	5	ARG	CG-CD-NE	-5.07	101.16	111.80
5	R	90	ARG	CG-CD-NE	-5.06	101.17	111.80
1	N	363	LEU	CB-CG-CD2	5.04	119.58	111.00
7	T	54	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	B	82	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	N	240	HIS	N-CA-CB	5.03	119.66	110.60
2	O	158	ASP	CB-CG-OD1	5.02	122.82	118.30
12	L	20	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	449	MET	CA-CB-CG	-5.00	104.80	113.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
10	W	57	HIS	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	4051	0	4029	55	0
1	N	4051	0	4029	56	0
2	B	1824	0	1833	26	0
2	O	1824	0	1833	31	0
3	C	2134	0	2051	31	0
3	P	2134	0	2051	36	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	11	0
5	R	852	0	845	8	0
6	F	748	0	728	16	0
6	S	748	0	728	29	0
7	G	675	0	643	27	0
7	T	675	0	643	45	0
8	H	662	0	623	7	0
8	U	662	0	623	12	0
9	I	601	0	613	12	0
9	V	601	0	613	10	0
10	J	460	0	459	4	0
10	W	460	0	459	2	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	10	0
12	Y	380	0	380	15	0
13	M	335	0	352	2	0
13	Z	335	0	352	2	0
14	A	2	0	0	0	0
14	N	2	0	0	0	0
15	A	120	0	108	9	0
15	N	120	0	108	8	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	1	0	0	1	0
18	N	1	0	0	0	0
19	A	63	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	12	0
19	L	63	0	110	14	0
19	N	126	0	220	22	0
19	Q	63	0	110	2	0
20	A	102	0	152	8	0
20	C	102	0	152	5	0
20	N	102	0	152	10	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	2	0
22	C	58	0	78	6	0
22	O	29	0	39	1	0
22	P	58	0	78	8	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	100	0	156	17	0
24	G	100	0	156	26	0
24	P	100	0	156	20	0
24	T	100	0	156	27	0
25	C	53	0	77	6	0
25	G	106	0	154	13	0
25	P	106	0	154	13	0
25	T	53	0	77	22	0
26	E	52	0	80	16	0
26	O	52	0	80	17	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	41	4	0
28	M	33	0	42	0	0
28	P	33	0	42	3	0
28	Z	33	0	42	0	0
29	A	188	0	0	10	0
29	B	121	0	0	3	0
29	C	77	0	0	1	0
29	D	78	0	0	4	0
29	E	58	0	0	2	0
29	F	58	0	0	4	0
29	G	27	0	0	3	0
29	H	34	0	0	0	0
29	I	29	0	0	4	0
29	J	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	20	0	0	1	0
29	L	16	0	0	2	0
29	M	14	0	0	0	0
29	N	156	0	0	3	0
29	O	91	0	0	3	0
29	P	76	0	0	9	0
29	Q	46	0	0	4	0
29	R	42	0	0	1	0
29	S	38	0	0	3	0
29	T	23	0	0	2	0
29	U	28	0	0	3	0
29	V	14	0	0	0	0
29	W	4	0	0	0	0
29	X	15	0	0	1	0
29	Y	11	0	0	0	0
29	Z	7	0	0	0	0
All	All	32060	0	31341	561	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (561) 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)
25:P:309:PEK:H383	24:T:102:CDL:C27	1.43	1.46
1:A:297:MET:SD	1:A:297:MET:CE	2.04	1.45
25:C:306:PEK:H383	24:G:103:CDL:C27	1.49	1.38
1:A:312[A]:ILE:HD12	29:A:740:HOH:O	1.21	1.31
6:S:43:LYS:H	6:S:43:LYS:CD	1.43	1.26
6:F:95:GLN:HA	29:F:256:HOH:O	1.34	1.25
19:N:610:TGL:HC32	12:Y:20:ARG:NH2	1.53	1.22
24:G:103:CDL:H541	24:G:103:CDL:H241	1.25	1.17
12:L:20:ARG:HH22	19:L:101:TGL:HC32	1.08	1.16
12:L:20:ARG:NH2	19:L:101:TGL:HC32	1.60	1.15
1:A:27:GLY:HA3	15:A:602:HEA:C27	1.78	1.13
25:C:306:PEK:H383	24:G:103:CDL:H273	1.18	1.12
26:E:201:PSC:H072	9:I:10:ARG:HH21	1.10	1.12
19:L:101:TGL:HC62	19:L:101:TGL:HC22	1.32	1.08
25:P:309:PEK:C38	24:T:102:CDL:C27	2.31	1.08
7:G:45:PRO:HD2	29:G:221:HOH:O	1.53	1.08
8:U:9:LYS:HG3	8:U:10:ASN:H	1.14	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:309:PEK:H383	24:T:102:CDL:H272	1.33	1.07
3:P:67:PHE:HE1	24:P:306:CDL:H1	1.15	1.06
25:P:309:PEK:H383	24:T:102:CDL:H273	1.10	1.06
6:S:43:LYS:H	6:S:43:LYS:HD3	1.21	1.05
7:T:5:LYS:HB2	25:T:101:PEK:H362	1.05	1.04
24:G:103:CDL:H241	24:G:103:CDL:C54	1.86	1.04
2:B:41:ILE:HD13	26:E:201:PSC:H342	1.36	1.04
19:L:101:TGL:OC1	19:L:101:TGL:HC41	1.53	1.02
6:S:43:LYS:H	6:S:43:LYS:HD2	1.23	1.01
1:A:27:GLY:HA3	15:A:602:HEA:H273	1.38	1.01
7:G:5:LYS:HG3	25:G:104:PEK:H383	1.38	1.01
6:S:85:CYS:SG	6:S:87:THR:HG23	2.01	1.00
20:P:305:PGV:H182	24:P:306:CDL:H671	1.43	0.98
25:C:306:PEK:C38	24:G:103:CDL:H273	1.94	0.97
6:S:43:LYS:CD	6:S:43:LYS:N	2.26	0.96
25:C:306:PEK:H383	24:G:103:CDL:H271	1.47	0.95
6:S:43:LYS:HE2	29:S:220:HOH:O	1.65	0.95
25:C:306:PEK:C38	24:G:103:CDL:C27	2.44	0.94
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.30	0.94
24:G:103:CDL:H541	24:G:103:CDL:C24	1.97	0.94
24:P:306:CDL:OB9	24:P:306:CDL:H522	1.68	0.94
1:N:400:PHE:HB3	19:N:610:TGL:H283	1.48	0.93
18:A:606:NA:NA	29:A:709:HOH:O	1.41	0.93
28:G:101:DMU:H36	28:G:101:DMU:H30	1.47	0.93
7:T:5:LYS:CD	25:T:101:PEK:H371	1.98	0.93
26:E:201:PSC:C07	9:I:10:ARG:HH21	1.83	0.92
25:P:304:PEK:H71	25:P:304:PEK:H32	1.51	0.92
3:C:67:PHE:HE1	24:C:303:CDL:H1	1.32	0.92
3:P:3:HIS:HB3	29:P:456:HOH:O	1.71	0.91
7:T:31:CYS:SG	24:T:102:CDL:H532	2.12	0.90
7:T:5:LYS:HB2	25:T:101:PEK:C36	1.99	0.90
7:T:5:LYS:HD2	25:T:101:PEK:H371	1.52	0.89
3:C:63:ARG:HE	24:C:303:CDL:HA22	1.37	0.89
6:S:75:HIS:H	6:S:80:GLN:HE22	1.15	0.89
15:N:602:HEA:C16	15:N:602:HEA:H273	2.00	0.89
19:N:610:TGL:HC32	12:Y:20:ARG:HH22	1.39	0.88
1:A:27:GLY:CA	15:A:602:HEA:H273	2.03	0.88
6:F:85:CYS:SG	6:F:87:THR:HG23	2.14	0.88
20:N:607:PGV:H02	20:N:607:PGV:O14	1.71	0.88
19:L:101:TGL:HC62	19:L:101:TGL:CC2	2.03	0.86
6:S:19:GLU:HG2	29:S:232:HOH:O	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:PHE:CE1	24:P:306:CDL:H1	2.08	0.86
1:N:117[A]:MET:HE2	12:Y:42:HIS:CD2	2.09	0.86
7:T:5:LYS:HD2	25:T:101:PEK:C38	2.06	0.86
19:N:610:TGL:HC32	12:Y:20:ARG:HH21	1.33	0.86
25:P:309:PEK:C38	24:T:102:CDL:H273	2.02	0.85
29:P:463:HOH:O	6:S:96:LEU:HD13	1.77	0.85
25:P:309:PEK:C38	24:T:102:CDL:H272	2.00	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.25	0.84
26:E:201:PSC:H072	9:I:10:ARG:NH2	1.92	0.83
6:F:75:HIS:H	6:F:80:GLN:HE22	1.26	0.83
3:P:160:LEU:HD13	22:P:307:CHD:H181	1.59	0.83
20:P:305:PGV:H182	24:P:306:CDL:C67	2.08	0.83
7:T:2:SER:OG	25:T:101:PEK:H301	1.78	0.82
19:L:101:TGL:OA1	19:L:101:TGL:OG3	1.97	0.82
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.80	0.82
29:P:475:HOH:O	6:S:1:ALA:HB2	1.80	0.82
1:A:406:ASN:HD21	20:A:609:PGV:H22	1.44	0.82
1:A:27:GLY:HA3	15:A:602:HEA:H271	1.59	0.82
7:T:5:LYS:HD2	25:T:101:PEK:C37	2.09	0.81
8:U:9:LYS:HG3	8:U:10:ASN:N	1.93	0.81
1:A:297:MET:HB2	29:A:884:HOH:O	1.80	0.81
24:T:102:CDL:H111	24:T:102:CDL:HA21	1.63	0.80
7:G:72:ASN:H	7:G:76:ASN:HD22	1.27	0.79
24:P:306:CDL:H652	29:P:468:HOH:O	1.81	0.79
25:P:304:PEK:HN2	7:T:76:ASN:HD21	1.31	0.78
6:F:54:ASN:H	6:F:54:ASN:HD22	1.31	0.78
6:F:1:ALA:HB2	29:F:251:HOH:O	1.82	0.78
28:G:101:DMU:H30	28:G:101:DMU:C10	2.13	0.78
3:C:161:GLN:HE22	25:C:306:PEK:H22	1.48	0.78
8:U:7:LYS:O	8:U:8:ILE:HB	1.83	0.78
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.20	0.77
20:P:305:PGV:H172	29:P:468:HOH:O	1.84	0.77
4:D:34:SER:H	4:D:37:GLN:HE21	1.34	0.76
19:D:201:TGL:CG3	29:D:323:HOH:O	2.33	0.75
7:T:45:PRO:HD2	29:T:223:HOH:O	1.85	0.75
6:S:43:LYS:HD2	6:S:43:LYS:N	1.91	0.75
1:A:278:MET:HB3	7:T:5:LYS:HG2	1.69	0.75
7:T:37:LEU:CD2	24:T:102:CDL:H361	2.16	0.75
3:C:160:LEU:HD13	22:C:304:CHD:H181	1.69	0.75
5:E:8:ASP:HA	26:E:201:PSC:H071	1.69	0.75
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:64:GLU:O	6:F:65:ASP:HB2	1.86	0.74
19:N:610:TGL:H231	19:N:610:TGL:HA92	1.68	0.74
8:H:9:LYS:O	8:H:10:ASN:HB2	1.87	0.74
2:O:56:MET:HA	26:O:303:PSC:H202	1.69	0.74
1:N:513:LEU:O	1:N:514:LYS:HB2	1.88	0.74
15:N:602:HEA:H273	15:N:602:HEA:H161	1.69	0.74
12:L:2:HIS:CD2	29:L:209:HOH:O	2.40	0.74
20:A:609:PGV:C01	20:A:609:PGV:H221	2.17	0.74
19:N:610:TGL:H161	12:Y:24:MET:SD	2.28	0.74
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.53	0.73
8:H:45:ALA:O	8:H:47:GLY:N	2.18	0.73
7:T:5:LYS:CB	25:T:101:PEK:H362	2.01	0.73
4:Q:34:SER:O	4:Q:38:LYS:HG3	1.88	0.73
4:D:81:VAL:HG11	19:D:201:TGL:HB52	1.70	0.72
9:I:26:MET:HE3	29:I:128:HOH:O	1.89	0.72
1:N:117[A]:MET:HE3	12:Y:39:ILE:HG23	1.71	0.72
7:T:31:CYS:SG	24:T:102:CDL:H551	2.29	0.72
9:I:1:SAC:OAC	9:I:2:THR:HG22	1.89	0.72
2:O:217:LYS:HG3	29:O:485:HOH:O	1.88	0.72
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.72	0.71
8:U:9:LYS:CG	8:U:10:ASN:H	1.98	0.71
8:U:20:PHE:CE2	8:U:27:ARG:HG2	2.26	0.71
3:P:165:ILE:HG12	25:P:309:PEK:H102	1.72	0.71
4:Q:109:HIS:HD2	29:Q:338:HOH:O	1.72	0.71
24:T:102:CDL:HA21	24:T:102:CDL:C11	2.20	0.71
15:N:602:HEA:HBC1	15:N:602:HEA:HMC1	1.73	0.70
6:S:43:LYS:HD3	6:S:43:LYS:N	1.99	0.70
1:A:312[A]:ILE:CD1	29:A:740:HOH:O	2.01	0.70
7:G:5:LYS:HB2	25:G:104:PEK:H362	1.74	0.70
7:G:38:HIS:CE1	24:G:103:CDL:H111	2.27	0.70
1:N:273:MET:HE2	29:N:735:HOH:O	1.92	0.70
24:C:303:CDL:H242	24:C:303:CDL:H661	1.73	0.70
8:H:7:LYS:O	8:H:8:ILE:HB	1.91	0.70
26:O:303:PSC:H212	26:O:303:PSC:O01	1.92	0.70
7:G:76:ASN:HD21	25:G:102:PEK:HN2	1.38	0.69
19:N:609:TGL:H122	19:N:609:TGL:H302	1.74	0.69
24:C:303:CDL:OB9	24:C:303:CDL:H521	1.92	0.69
2:O:41:ILE:HD13	26:O:303:PSC:H342	1.75	0.69
3:C:63:ARG:HE	24:C:303:CDL:CA2	2.05	0.69
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.75	0.68
1:A:468:MET:HG3	29:A:735:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:609:PGV:H221	20:A:609:PGV:H012	1.73	0.68
26:O:303:PSC:C07	9:V:10:ARG:HH21	2.07	0.67
1:A:27:GLY:CA	15:A:602:HEA:C27	2.66	0.67
3:P:107:ALA:HB2	20:P:302:PGV:H031	1.77	0.67
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.93	0.67
20:A:609:PGV:C06	29:A:822:HOH:O	2.43	0.67
3:P:63:ARG:HE	24:P:306:CDL:CA2	2.07	0.67
24:T:102:CDL:H541	24:T:102:CDL:H231	1.76	0.67
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.77	0.66
3:P:246:ASP:HB2	29:P:428:HOH:O	1.94	0.66
2:B:183:THR:HG22	29:B:424:HOH:O	1.96	0.66
1:N:406:ASN:HD21	20:N:607:PGV:H21	1.58	0.66
7:T:37:LEU:HD21	24:T:102:CDL:H361	1.78	0.66
24:C:303:CDL:HB22	24:C:303:CDL:PA1	2.35	0.66
7:G:45:PRO:CD	29:G:221:HOH:O	2.26	0.66
7:G:3:ALA:HB1	25:G:104:PEK:H382	1.78	0.66
3:P:63:ARG:HE	24:P:306:CDL:HA22	1.58	0.66
26:E:201:PSC:C07	9:I:10:ARG:NH2	2.55	0.66
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.76	0.66
7:T:5:LYS:HD3	25:T:101:PEK:H371	1.78	0.66
24:G:103:CDL:H541	24:G:103:CDL:C23	2.25	0.65
24:G:103:CDL:H571	24:G:103:CDL:H792	1.77	0.65
26:O:303:PSC:H212	26:O:303:PSC:C02	2.26	0.65
1:N:117[A]:MET:CE	12:Y:42:HIS:CD2	2.79	0.65
24:G:103:CDL:H241	24:G:103:CDL:H542	1.77	0.65
3:P:160:LEU:HD13	22:P:307:CHD:C18	2.27	0.65
1:N:117[B]:MET:HE3	10:W:50:LEU:HD21	1.77	0.64
1:N:177:SER:H	1:N:180:GLN:NE2	1.94	0.64
19:L:101:TGL:OC1	19:L:101:TGL:CC4	2.36	0.64
26:O:303:PSC:H072	9:V:10:ARG:HH21	1.63	0.64
24:G:103:CDL:H201	1:N:311:ILE:CD1	2.27	0.64
19:N:609:TGL:H111	2:O:35:SER:HB3	1.80	0.64
24:P:306:CDL:H672	24:P:306:CDL:H262	1.79	0.64
29:O:452:HOH:O	8:U:61:LYS:HD3	1.98	0.64
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.63	0.64
7:G:5:LYS:CG	25:G:104:PEK:H383	2.19	0.64
1:N:177:SER:H	1:N:180:GLN:HE21	1.46	0.64
1:A:406:ASN:HD21	20:A:609:PGV:C2	2.11	0.63
2:B:78:LEU:HD12	24:T:102:CDL:H352	1.80	0.63
4:D:34:SER:H	4:D:37:GLN:NE2	1.95	0.63
3:P:3:HIS:HD2	29:P:465:HOH:O	1.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D:201:TGL:HA91	19:D:201:TGL:C24	2.29	0.63
5:E:11:PHE:CB	26:E:201:PSC:H073	2.28	0.62
19:D:201:TGL:HG32	29:D:323:HOH:O	1.98	0.62
6:S:94:HIS:CD2	6:S:95:GLN:H	2.16	0.62
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.80	0.62
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.81	0.62
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.80	0.62
19:D:201:TGL:HA91	19:D:201:TGL:H242	1.81	0.62
26:O:303:PSC:C22	26:O:303:PSC:H21	2.30	0.61
8:U:9:LYS:O	8:U:10:ASN:HB2	2.01	0.61
7:T:8:HIS:CD2	25:T:101:PEK:H252	2.36	0.61
5:E:11:PHE:HB3	26:E:201:PSC:H073	1.83	0.61
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.01	0.61
7:G:72:ASN:H	7:G:76:ASN:ND2	1.96	0.61
1:A:273:MET:HE2	29:A:738:HOH:O	2.00	0.61
19:A:607:TGL:H252	19:A:607:TGL:HA91	1.82	0.60
29:N:790:HOH:O	4:Q:20:ARG:HG2	2.01	0.60
7:T:3:ALA:HB3	25:T:101:PEK:H361	1.83	0.60
19:L:101:TGL:CA9	19:L:101:TGL:H231	2.31	0.60
1:A:311:ILE:CD1	24:T:102:CDL:H201	2.32	0.60
19:N:610:TGL:CC3	12:Y:20:ARG:HH22	2.14	0.59
26:O:303:PSC:H071	5:R:8:ASP:HA	1.84	0.59
6:S:64:GLU:O	6:S:65:ASP:HB2	2.02	0.59
7:T:3:ALA:O	7:T:4:ALA:CB	2.50	0.59
1:N:309:THR:O	1:N:312[B]:ILE:HG22	2.02	0.59
2:B:41:ILE:HD13	26:E:201:PSC:C34	2.23	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.67	0.59
3:P:224:LYS:CD	24:P:306:CDL:HB31	2.32	0.59
5:E:91:PRO:HD2	29:E:335:HOH:O	2.03	0.59
5:R:79:LYS:HE2	29:R:219:HOH:O	2.03	0.59
19:A:607:TGL:H101	19:A:607:TGL:C28	2.33	0.58
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.84	0.58
20:A:609:PGV:H311	13:M:19:LEU:HD23	1.85	0.58
20:C:302:PGV:H182	24:C:303:CDL:H671	1.85	0.58
4:D:40:LEU:HD22	4:D:58:GLU:HG2	1.85	0.58
11:K:8:ASP:HB2	29:K:108:HOH:O	2.03	0.58
11:X:54:ARG:HD3	29:X:114:HOH:O	2.03	0.58
24:G:103:CDL:H541	24:G:103:CDL:H231	1.85	0.58
1:A:1:FME:CE	1:A:1:FME:HA	2.33	0.58
20:C:302:PGV:H172	24:C:303:CDL:H651	1.85	0.58
6:F:1:ALA:HB3	6:S:65:ASP:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.69	0.58
2:B:62:GLU:O	2:B:66:THR:HB	2.04	0.58
1:A:513:LEU:O	1:A:514:LYS:HB2	2.05	0.57
9:I:15:ARG:HD3	29:I:122:HOH:O	2.04	0.57
24:P:306:CDL:PA1	24:P:306:CDL:HB22	2.44	0.57
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.03	0.57
1:A:430:PHE:HE1	19:A:607:TGL:HB21	1.69	0.57
20:N:608:PGV:H182	3:P:28:THR:HG22	1.86	0.57
2:O:225:SER:C	2:O:227:LEU:H	2.06	0.57
19:D:201:TGL:HG32	19:D:201:TGL:OB1	2.04	0.57
5:E:90:ARG:HD2	29:E:347:HOH:O	2.04	0.57
9:I:26:MET:HG3	29:I:128:HOH:O	2.03	0.57
26:O:303:PSC:H061	5:R:8:ASP:OD1	2.05	0.57
1:N:468:MET:HG3	29:N:732:HOH:O	2.04	0.57
24:G:103:CDL:H112	24:G:103:CDL:HA21	1.87	0.56
3:C:67:PHE:CE1	24:C:303:CDL:H1	2.25	0.56
26:O:303:PSC:H343	26:O:303:PSC:H142	1.88	0.56
24:T:102:CDL:H342	24:T:102:CDL:OA7	2.06	0.56
7:G:38:HIS:HE1	24:G:103:CDL:H111	1.69	0.56
10:J:7:GLU:HG3	29:J:110:HOH:O	2.04	0.56
3:P:164:PHE:CD1	22:P:307:CHD:H192	2.40	0.56
1:A:334:TRP:HB2	19:D:201:TGL:HG11	1.88	0.56
7:T:2:SER:OG	25:T:101:PEK:C30	2.53	0.56
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.05	0.56
7:T:37:LEU:HD23	24:T:102:CDL:H361	1.88	0.56
3:C:59:ARG:HG3	24:C:303:CDL:H511	1.88	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
7:T:5:LYS:HD2	25:T:101:PEK:H383	1.88	0.55
7:T:72:ASN:H	7:T:76:ASN:ND2	2.01	0.55
5:E:8:ASP:HA	26:E:201:PSC:C07	2.36	0.55
6:F:54:ASN:HB3	29:F:226:HOH:O	2.06	0.55
3:P:33[A]:MET:HE1	3:P:42:LEU:N	2.12	0.55
20:N:607:PGV:H011	20:N:607:PGV:C21	2.37	0.55
2:O:29:MET:HG3	9:V:35:TYR:CD2	2.42	0.55
20:A:609:PGV:H221	20:A:609:PGV:H011	1.89	0.55
20:A:609:PGV:H152	20:A:609:PGV:H321	1.87	0.54
26:O:303:PSC:H21	26:O:303:PSC:H221	1.89	0.54
3:C:106:LEU:HD13	20:C:307:PGV:H22	1.88	0.54
1:N:310:MET:CE	1:N:356:ILE:HG23	2.37	0.54
12:L:2:HIS:CG	29:L:209:HOH:O	2.57	0.54
7:G:63:GLY:H	28:G:101:DMU:H34	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:161:GLN:HE22	25:P:309:PEK:H22	1.73	0.54
24:P:306:CDL:H642	24:P:306:CDL:H242	1.89	0.54
5:E:72:LYS:HB2	5:E:82:TYR:CD2	2.43	0.54
7:T:38:HIS:HE2	24:T:102:CDL:H111	1.73	0.54
1:N:117[A]:MET:HE2	12:Y:42:HIS:HD2	1.67	0.54
4:Q:7:LYS:HB2	4:Q:10:ASP:OD1	2.06	0.54
24:G:103:CDL:H511	24:G:103:CDL:H181	1.89	0.53
3:C:164:PHE:CD1	22:C:304:CHD:H192	2.43	0.53
7:G:31:CYS:SG	24:G:103:CDL:H532	2.48	0.53
25:G:104:PEK:H051	3:P:77:LYS:HZ1	1.73	0.53
8:U:9:LYS:HG3	29:U:123:HOH:O	2.07	0.53
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.89	0.53
2:B:13:THR:OG1	2:B:167:SER:HB3	2.08	0.53
26:E:201:PSC:O13	26:E:201:PSC:H083	2.09	0.53
19:N:609:TGL:C12	19:N:609:TGL:C30	2.86	0.53
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.43	0.53
7:G:3:ALA:O	7:G:4:ALA:HB2	2.08	0.53
1:N:383:MET:O	1:N:387:PHE:HB2	2.07	0.53
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.08	0.53
6:S:54:ASN:HD22	6:S:54:ASN:C	2.11	0.53
15:A:602:HEA:HHC	15:A:602:HEA:H122	1.91	0.53
15:N:602:HEA:HHC	15:N:602:HEA:H122	1.91	0.52
3:C:107:ALA:HB2	20:C:307:PGV:H031	1.90	0.52
20:N:607:PGV:H011	20:N:607:PGV:H211	1.91	0.52
2:O:56:MET:CA	26:O:303:PSC:H202	2.39	0.52
3:P:156:ARG:HE	22:P:307:CHD:C24	2.22	0.52
7:T:2:SER:O	25:T:101:PEK:H322	2.10	0.52
6:F:64:GLU:O	6:F:65:ASP:CB	2.53	0.52
28:P:301:DMU:H30	7:T:62:TRP:HB3	1.91	0.52
4:D:31:LYS:NZ	29:D:359:HOH:O	2.26	0.52
19:N:610:TGL:CC3	12:Y:20:ARG:NH2	2.47	0.52
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.75	0.52
3:C:156:ARG:HE	22:C:304:CHD:C24	2.22	0.52
3:C:254:VAL:CG2	24:G:103:CDL:H672	2.40	0.52
4:D:109:HIS:HD2	29:D:314:HOH:O	1.93	0.52
25:P:304:PEK:H102	25:P:304:PEK:H161	1.92	0.51
3:P:224:LYS:HD3	24:P:306:CDL:HB31	1.92	0.51
4:D:131:ILE:HD13	9:I:47:TYR:CE2	2.45	0.51
24:C:303:CDL:HB22	24:C:303:CDL:OA5	2.10	0.51
2:O:164:ALA:O	2:O:194:GLY:HA3	2.10	0.51
15:A:603:HEA:HBC1	15:A:603:HEA:HMC1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:MET:HG2	26:E:201:PSC:H211	1.92	0.51
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.92	0.51
1:A:76:GLY:O	1:A:80:ASN:HB2	2.11	0.51
1:A:112:LEU:HG	29:A:742:HOH:O	2.11	0.51
1:A:311:ILE:HD12	24:T:102:CDL:H201	1.91	0.51
19:N:610:TGL:HG11	12:Y:12:PRO:HG2	1.93	0.51
26:O:303:PSC:H212	26:O:303:PSC:C01	2.41	0.51
26:O:303:PSC:H21	26:O:303:PSC:H222	1.91	0.51
8:H:9:LYS:O	8:H:10:ASN:CB	2.57	0.50
2:B:41:ILE:CD1	26:E:201:PSC:H342	2.26	0.50
19:D:201:TGL:CG3	19:D:201:TGL:OB1	2.59	0.50
12:L:14:SER:H	19:L:101:TGL:HC31	1.75	0.50
8:U:51:SER:HB2	29:U:122:HOH:O	2.10	0.50
15:N:603:HEA:HMC1	15:N:603:HEA:HBC1	1.92	0.50
19:N:610:TGL:HC31	12:Y:13:PHE:HA	1.93	0.50
7:G:3:ALA:O	7:G:4:ALA:CB	2.59	0.50
26:E:201:PSC:H212	26:E:201:PSC:O01	2.12	0.50
25:G:102:PEK:H71	25:G:102:PEK:H32	1.94	0.50
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.93	0.50
22:C:305:CHD:H152	20:C:307:PGV:H11	1.93	0.50
7:G:3:ALA:CB	25:G:104:PEK:H382	2.40	0.50
1:N:20:LEU:HB3	19:N:610:TGL:H221	1.92	0.50
2:B:56:MET:HA	26:E:201:PSC:H202	1.94	0.50
12:L:20:ARG:HH22	19:L:101:TGL:CC3	2.01	0.50
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.94	0.50
2:O:41:ILE:CD1	26:O:303:PSC:H342	2.41	0.49
3:C:33[A]:MET:HG2	3:C:39:SER:HB3	1.94	0.49
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.57	0.49
3:C:224:LYS:CD	24:C:303:CDL:HB31	2.42	0.49
6:S:48:LEU:HG	6:S:92:VAL:HG11	1.94	0.49
1:A:169:ILE:HD12	7:T:7:ASP:O	2.12	0.49
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.49
7:G:5:LYS:CB	25:G:104:PEK:H362	2.43	0.49
1:A:328:HIS:HB2	2:B:45:MET:SD	2.53	0.49
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.48	0.49
3:C:217:VAL:HG22	24:C:303:CDL:H732	1.95	0.49
3:C:254:VAL:HG23	24:G:103:CDL:H672	1.94	0.49
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.43	0.49
1:A:177:SER:H	1:A:180:GLN:HE21	1.61	0.49
8:H:7:LYS:O	8:H:8:ILE:CB	2.61	0.49
9:I:73:LYS:HB3	29:I:121:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.13	0.48
3:C:55:TYR:CE1	24:C:303:CDL:H532	2.48	0.48
5:E:5:HIS:HB3	5:E:6:GLU:HG2	1.95	0.48
6:F:50:PRO:HG2	29:F:244:HOH:O	2.13	0.48
9:I:1:SAC:OAC	9:I:2:THR:CG2	2.59	0.48
6:S:19:GLU:CG	29:S:232:HOH:O	2.49	0.48
28:G:101:DMU:H36	28:G:101:DMU:C57	2.30	0.48
19:N:609:TGL:H302	19:N:609:TGL:C12	2.40	0.48
19:N:610:TGL:HA22	12:Y:13:PHE:HB3	1.96	0.48
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.96	0.48
7:G:2:SER:O	25:G:104:PEK:H321	2.13	0.48
2:B:66:THR:HG21	22:B:302:CHD:H3	1.94	0.48
3:P:224:LYS:HD2	24:P:306:CDL:HB31	1.95	0.48
29:A:855:HOH:O	3:C:77:LYS:HE3	2.12	0.48
20:N:607:PGV:H22	20:N:607:PGV:H221	1.95	0.48
7:T:1:ALA:N	29:T:222:HOH:O	2.47	0.48
3:P:52:LEU:HD21	24:P:306:CDL:H411	1.96	0.47
6:S:94:HIS:CD2	6:S:95:GLN:N	2.82	0.47
12:L:20:ARG:HH21	19:L:101:TGL:HC32	1.69	0.47
6:S:94:HIS:HD2	6:S:95:GLN:H	1.60	0.47
1:A:383:MET:O	1:A:387:PHE:HB2	2.14	0.47
19:A:607:TGL:H101	19:A:607:TGL:H281	1.96	0.47
24:T:102:CDL:H592	24:T:102:CDL:H561	1.63	0.47
1:N:106:PRO:N	1:N:107:PRO:HD2	2.30	0.47
6:S:52:ILE:O	6:S:94:HIS:CE1	2.67	0.47
4:Q:109:HIS:CD2	29:Q:338:HOH:O	2.56	0.47
26:O:303:PSC:H343	26:O:303:PSC:C14	2.44	0.47
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.96	0.47
19:N:609:TGL:H101	19:N:609:TGL:C28	2.44	0.47
7:T:8:HIS:CE1	25:T:101:PEK:H332	2.49	0.47
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.97	0.46
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.96	0.46
13:M:39:ASN:O	13:M:43:SER:HB2	2.15	0.46
29:O:456:HOH:O	4:Q:129:ALA:HB2	2.15	0.46
10:J:52:TRP:O	10:J:57:HIS:HE1	1.98	0.46
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.98	0.46
24:T:102:CDL:H631	24:T:102:CDL:H662	1.69	0.46
26:E:201:PSC:H62	26:E:201:PSC:H241	1.98	0.46
3:P:164:PHE:CE1	22:P:307:CHD:H192	2.50	0.46
1:A:177:SER:H	1:A:180:GLN:NE2	2.14	0.46
3:C:248:VAL:HG22	25:T:101:PEK:H15	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:63:ARG:HE	24:P:306:CDL:HA21	1.80	0.46
6:S:43:LYS:HD2	6:S:88:HIS:CE1	2.51	0.46
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.51	0.45
6:S:75:HIS:H	6:S:80:GLN:NE2	1.99	0.45
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.99	0.45
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.45
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.52	0.45
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.34	0.45
3:P:22:LEU:O	3:P:26:LEU:HG	2.16	0.45
1:A:283:LEU:HB2	1:A:312[B]:ILE:HD12	1.99	0.45
24:G:103:CDL:H332	2:O:78:LEU:HD12	1.99	0.45
1:A:113:LEU:HB3	1:A:117[B]:MET:CE	2.46	0.45
1:A:178:GLN:CB	7:T:7:ASP:OD2	2.65	0.45
6:F:92:VAL:HG23	6:F:92:VAL:O	2.16	0.45
19:L:101:TGL:HC22	19:L:101:TGL:CC6	2.23	0.45
4:Q:93:ALA:HB3	11:X:28:VAL:HG22	1.98	0.45
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.45
15:N:602:HEA:H172	15:N:602:HEA:H272	1.31	0.45
24:G:103:CDL:H561	24:G:103:CDL:H592	1.69	0.44
24:G:103:CDL:H452	2:O:70:ALA:HB1	1.99	0.44
5:R:106:LEU:HD23	5:R:106:LEU:HA	1.79	0.44
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.99	0.44
1:N:240:HIS:O	1:N:243:VAL:HG22	2.18	0.44
1:N:488:THR:HB	1:N:495:LEU:HD13	1.98	0.44
3:P:51[B]:MET:HB3	24:P:306:CDL:H381	2.00	0.44
1:N:310:MET:HE3	1:N:356:ILE:HG23	1.99	0.44
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.98	0.44
25:P:304:PEK:H32	25:P:304:PEK:C7	2.31	0.44
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.44
2:B:41:ILE:O	2:B:45:MET:HG2	2.17	0.44
1:N:127:THR:HG22	1:N:235:PHE:CE2	2.53	0.44
22:P:307:CHD:H112	22:P:307:CHD:H12A	1.84	0.44
24:T:102:CDL:H122	24:T:102:CDL:H362	2.00	0.44
1:N:409:TRP:CE2	20:N:607:PGV:H61	2.53	0.44
20:N:607:PGV:H011	20:N:607:PGV:H221	1.99	0.44
26:O:303:PSC:O02	26:O:303:PSC:H031	2.17	0.44
7:T:3:ALA:HB1	25:T:101:PEK:H382	2.00	0.44
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.83	0.44
1:N:437:PRO:HG2	1:N:440:TYR:CE1	2.53	0.44
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
7:T:31:CYS:HG	24:T:102:CDL:H532	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:29:LEU:HD12	9:V:29:LEU:HA	1.81	0.43
1:A:116:SER:HB3	29:A:746:HOH:O	2.17	0.43
19:D:201:TGL:H132	19:D:201:TGL:H302	1.72	0.43
7:G:5:LYS:HB3	1:N:278:MET:SD	2.58	0.43
24:P:306:CDL:HB21	24:P:306:CDL:OB6	2.18	0.43
4:Q:143:ASN:ND2	29:Q:309:HOH:O	2.50	0.43
24:T:102:CDL:H541	24:T:102:CDL:C23	2.43	0.43
3:C:54:MET:HE3	24:C:303:CDL:H612	2.00	0.43
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.91	0.43
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.00	0.43
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.00	0.43
19:N:609:TGL:H111	2:O:35:SER:CB	2.48	0.43
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.43
24:T:102:CDL:H111	24:T:102:CDL:CA2	2.43	0.43
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.99	0.43
15:A:603:HEA:H243	2:B:69:PRO:HB3	2.00	0.43
22:C:304:CHD:H12A	22:C:304:CHD:H112	1.77	0.43
24:G:103:CDL:H351	2:O:81:LEU:HD12	2.01	0.43
22:B:302:CHD:H212	22:B:302:CHD:H12	2.00	0.43
1:N:393:PHE:CD1	15:N:602:HEA:H241	2.53	0.43
7:T:3:ALA:HB1	25:T:101:PEK:C38	2.49	0.43
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.00	0.43
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.18	0.43
19:N:609:TGL:H122	19:N:609:TGL:C30	2.43	0.43
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.54	0.43
2:B:81:LEU:HD13	24:T:102:CDL:H121	2.00	0.43
5:E:48:ILE:HG21	5:E:89:LEU:HD11	2.00	0.43
24:G:103:CDL:H662	24:G:103:CDL:H631	1.78	0.43
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.18	0.43
11:X:24:PHE:O	11:X:28:VAL:HG12	2.19	0.43
3:C:122:HIS:HA	3:C:123:PRO:HD3	1.88	0.43
4:D:107:ILE:HB	4:D:108:PRO:CD	2.48	0.43
3:P:217:VAL:HG22	24:P:306:CDL:H732	2.01	0.43
5:R:108:LYS:HB2	5:R:108:LYS:NZ	2.34	0.43
1:A:430:PHE:CE1	19:A:607:TGL:HB21	2.52	0.42
3:C:223:LEU:HD21	22:C:304:CHD:H183	2.02	0.42
19:L:101:TGL:H231	19:L:101:TGL:HA91	1.99	0.42
4:Q:139:ASP:OD2	4:Q:142:LYS:HG3	2.19	0.42
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.00	0.42
1:N:113:LEU:HD13	19:N:610:TGL:H292	2.01	0.42
3:P:69:GLY:HA3	6:S:14:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:G:103:CDL:H182	24:G:103:CDL:H152	1.69	0.42
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.42
3:P:230:ASN:HB2	29:P:459:HOH:O	2.19	0.42
7:T:3:ALA:CB	25:T:101:PEK:H382	2.50	0.42
25:T:101:PEK:H282	25:T:101:PEK:H312	1.73	0.42
3:C:37:PHE:CD1	10:J:52:TRP:HZ3	2.36	0.42
3:C:76:GLN:NE2	3:C:80:ARG:HH21	2.17	0.42
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.66	0.42
3:P:226:HIS:CE1	24:P:306:CDL:HB32	2.55	0.42
7:T:2:SER:HG	25:T:101:PEK:H301	1.81	0.42
7:T:38:HIS:ND1	7:T:38:HIS:N	2.68	0.42
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.01	0.42
2:B:69:PRO:HG2	29:B:474:HOH:O	2.19	0.42
9:V:6:LYS:HA	9:V:7:PRO:HD3	1.87	0.42
2:O:116:LEU:HD12	2:O:117:SER:N	2.34	0.42
1:A:297:MET:CE	1:A:297:MET:CB	2.97	0.42
15:A:602:HEA:HBC1	15:A:602:HEA:HMC1	2.01	0.42
2:B:78:LEU:CD1	24:T:102:CDL:H352	2.47	0.42
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.42
6:F:54:ASN:H	6:F:54:ASN:ND2	2.07	0.42
7:G:3:ALA:HB3	25:G:104:PEK:H361	2.01	0.42
19:L:101:TGL:CA9	19:L:101:TGL:C23	2.97	0.42
1:N:114:ALA:HA	1:N:117[B]:MET:HE3	2.01	0.42
1:N:408:THR:HB	20:N:607:PGV:H51	2.01	0.42
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.85	0.42
12:L:45:LEU:HD23	12:L:45:LEU:HA	1.83	0.42
1:N:310:MET:HE1	2:O:76:ILE:HG21	2.02	0.42
3:P:76:GLN:NE2	29:P:414:HOH:O	2.47	0.42
28:P:301:DMU:H30	7:T:62:TRP:CB	2.48	0.42
2:B:29:MET:SD	9:I:36:LYS:HE3	2.60	0.42
4:D:93:ALA:HB3	11:K:28:VAL:HG22	2.00	0.42
1:N:309:THR:HG22	15:N:603:HEA:HMB2	2.02	0.42
1:N:215:LEU:HD11	25:P:304:PEK:H271	2.02	0.41
28:P:301:DMU:C57	7:T:62:TRP:HB3	2.50	0.41
6:S:95:GLN:HG3	6:S:96:LEU:H	1.85	0.41
9:V:18:ARG:HH11	9:V:18:ARG:CG	2.32	0.41
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.01	0.41
3:C:224:LYS:HD2	24:C:303:CDL:HB31	2.01	0.41
25:G:104:PEK:H341	29:G:227:HOH:O	2.18	0.41
8:H:8:ILE:HG23	8:H:8:ILE:O	2.20	0.41
19:N:609:TGL:C28	19:N:609:TGL:C10	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.01	0.41
22:O:302:CHD:H12	22:O:302:CHD:H212	2.02	0.41
1:A:412:ILE:HG12	4:D:84:ALA:HB3	2.01	0.41
7:G:1:ALA:N	20:P:302:PGV:H321	2.35	0.41
1:N:43:GLN:OE1	4:Q:104:TYR:HB3	2.20	0.41
2:O:82:ARG:HH11	2:O:86:MET:HE3	1.85	0.41
10:J:4:ARG:HD3	10:J:7:GLU:OE2	2.20	0.41
5:R:5:HIS:CD2	5:R:6:GLU:HG2	2.55	0.41
1:A:334:TRP:CB	19:D:201:TGL:HG11	2.50	0.41
3:C:3:HIS:N	29:C:475:HOH:O	2.52	0.41
3:C:186:PHE:HA	3:C:190:ASP:OD2	2.19	0.41
7:G:84:LYS:H	7:G:84:LYS:HD2	1.86	0.41
19:N:610:TGL:H272	12:Y:11:ILE:CG2	2.50	0.41
2:O:62:GLU:O	2:O:66:THR:HB	2.21	0.41
2:O:74:ILE:HG22	2:O:78:LEU:HD22	2.02	0.41
19:Q:201:TGL:OB1	29:Q:308:HOH:O	2.22	0.41
1:N:342:LEU:HD13	2:O:46:LEU:HD11	2.03	0.41
2:O:29:MET:HG3	9:V:35:TYR:CG	2.56	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
24:C:303:CDL:H222	24:C:303:CDL:H641	2.02	0.41
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.51	0.41
7:G:5:LYS:HG3	25:G:104:PEK:C38	2.28	0.41
1:N:35:LEU:HD11	1:N:462:LEU:HD13	2.02	0.41
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.03	0.41
2:O:200:CYS:SG	2:O:204:HIS:HA	2.61	0.41
1:A:169:ILE:CD1	7:T:7:ASP:O	2.69	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
7:T:11:TPO:HA	7:T:11:TPO:O2P	2.21	0.41
8:U:9:LYS:CG	29:U:123:HOH:O	2.66	0.41
1:A:115:SER:HB2	1:A:142:SER:O	2.20	0.41
1:A:489:THR:HA	6:F:71:TRP:O	2.21	0.41
29:B:490:HOH:O	4:D:129:ALA:HB2	2.21	0.41
12:L:44:LEU:HD23	12:L:44:LEU:HA	1.87	0.41
1:N:104:LEU:HB2	1:N:156:SER:HB2	2.03	0.41
3:P:223:LEU:HD21	22:P:307:CHD:H183	2.03	0.41
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	2.03	0.41
7:T:6:GLY:O	25:T:101:PEK:H311	2.21	0.41
2:B:103:GLN:HA	2:B:104:TRP:HA	1.88	0.41
22:P:308:CHD:H12	22:P:308:CHD:H212	2.03	0.41
7:G:37:LEU:HD23	7:G:38:HIS:ND1	2.37	0.40
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:81:VAL:HG11	19:Q:201:TGL:HB51	2.03	0.40
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.51	0.40
1:A:350:VAL:HG13	19:A:607:TGL:HB81	2.04	0.40
5:E:86:ILE:O	5:E:90:ARG:HG2	2.22	0.40
1:N:46:THR:HG23	1:N:49:GLY:O	2.21	0.40
20:N:607:PGV:H92	4:Q:84:ALA:HB2	2.02	0.40
5:R:79:LYS:N	5:R:79:LYS:HD2	2.35	0.40
1:A:344:PHE:CD1	1:A:344:PHE:C	2.95	0.40
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.21	0.40
2:O:84:LEU:HA	2:O:87:MET:HE2	2.03	0.40
4:Q:33:LEU:HB2	4:Q:38:LYS:HE2	2.02	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	515/514 (100%)	502 (98%)	12 (2%)	1 (0%)	47 44
1	N	515/514 (100%)	501 (97%)	14 (3%)	0	100 100
2	B	225/227 (99%)	216 (96%)	9 (4%)	0	100 100
2	O	225/227 (99%)	218 (97%)	6 (3%)	1 (0%)	34 30
3	C	260/261 (100%)	256 (98%)	4 (2%)	0	100 100
3	P	260/261 (100%)	255 (98%)	5 (2%)	0	100 100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100 100
4	Q	142/147 (97%)	132 (93%)	10 (7%)	0	100 100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100 100
5	R	103/109 (94%)	103 (100%)	0	0	100 100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	7 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	S	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	4 1
7	G	81/85 (95%)	70 (86%)	6 (7%)	5 (6%)	1 0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	1 0
8	H	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	2 0
8	U	77/85 (91%)	71 (92%)	2 (3%)	4 (5%)	2 0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100 100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100 100
10	J	56/59 (95%)	56 (100%)	0	0	100 100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
13	M	41/46 (89%)	41 (100%)	0	0	100 100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100 100
All	All	3516/3614 (97%)	3386 (96%)	105 (3%)	25 (1%)	22 16

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
8	H	8	ILE
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	8	ILE
6	F	95	GLN
7	G	37	LEU
7	T	43	GLU
8	U	45	ALA
8	H	47	GLY

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Mol	Chain	Res	Type
6	S	95	GLN
8	U	11	TYR
7	G	8	HIS
7	T	6	GLY
7	G	6	GLY
8	U	10	ASN
1	A	384	GLY
2	O	92	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	429/426 (101%)	418 (97%)	11 (3%)	46 48
1	N	429/426 (101%)	421 (98%)	8 (2%)	57 61
2	B	210/210 (100%)	198 (94%)	12 (6%)	20 16
2	O	210/210 (100%)	200 (95%)	10 (5%)	25 22
3	C	227/226 (100%)	224 (99%)	3 (1%)	69 74
3	P	227/226 (100%)	223 (98%)	4 (2%)	59 63
4	D	128/129 (99%)	123 (96%)	5 (4%)	32 30
4	Q	128/129 (99%)	122 (95%)	6 (5%)	26 22
5	E	92/95 (97%)	91 (99%)	1 (1%)	73 78
5	R	92/95 (97%)	88 (96%)	4 (4%)	29 26
6	F	81/81 (100%)	77 (95%)	4 (5%)	25 21
6	S	81/81 (100%)	77 (95%)	4 (5%)	25 21
7	G	67/68 (98%)	61 (91%)	6 (9%)	9 6
7	T	67/68 (98%)	61 (91%)	6 (9%)	9 6
8	H	71/75 (95%)	67 (94%)	4 (6%)	21 17
8	U	71/75 (95%)	64 (90%)	7 (10%)	8 4
9	I	57/57 (100%)	54 (95%)	3 (5%)	22 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	V	57/57 (100%)	55 (96%)	2 (4%)	36 35
10	J	49/50 (98%)	48 (98%)	1 (2%)	55 58
10	W	49/50 (98%)	48 (98%)	1 (2%)	55 58
11	K	39/46 (85%)	38 (97%)	1 (3%)	46 48
11	X	39/46 (85%)	37 (95%)	2 (5%)	24 19
12	L	39/40 (98%)	39 (100%)	0	100 100
12	Y	39/40 (98%)	36 (92%)	3 (8%)	13 8
13	M	37/38 (97%)	32 (86%)	5 (14%)	4 2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6 3
All	All	3052/3082 (99%)	2935 (96%)	117 (4%)	33 31

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	333	LYS
1	A	336	PRO
1	A	338	MET
1	A	362	SER
1	A	369	ASP
1	A	504	THR
2	B	15	PRO
2	B	33	LEU
2	B	54	SER
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	127	LEU
3	C	159	MET

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Mol	Chain	Res	Type
3	C	214	PHE
4	D	4	SER
4	D	8	SER
4	D	31	LYS
4	D	51	LEU
4	D	58	GLU
5	E	5	HIS
6	F	54	ASN
6	F	80	GLN
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	18	PHE
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	27	ARG
8	H	60	TYR
8	H	61	LYS
9	I	2	THR
9	I	36	LYS
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	96	ARG
1	N	109	PHE
1	N	238	PHE
1	N	278	MET
1	N	363	LEU
1	N	369	ASP
1	N	504	THR
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP

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Mol	Chain	Res	Type
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	221	LYS
2	O	226	MET
3	P	110	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	6	VAL
4	Q	10	ASP
4	Q	20	ARG
4	Q	51	LEU
4	Q	142	LYS
4	Q	143	ASN
5	R	79	LYS
5	R	80	GLU
5	R	90	ARG
5	R	109	VAL
6	S	43	LYS
6	S	48	LEU
6	S	50	PRO
6	S	54	ASN
7	T	2	SER
7	T	18	PHE
7	T	38	HIS
7	T	43	GLU
7	T	54	ARG
7	T	84	LYS
8	U	8	ILE
8	U	27	ARG
8	U	29	CYS
8	U	40	GLU
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	8	GLN
9	V	29	LEU
10	W	50	LEU
11	X	7	PRO

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Mol	Chain	Res	Type
11	X	54	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	39	ASN
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	503	HIS
2	B	22	HIS
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
3	C	149	HIS
3	C	161	GLN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
7	G	76	ASN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
2	O	10	GLN
2	O	52	HIS
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN

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Mol	Chain	Res	Type
3	P	68	GLN
4	Q	37	GLN
4	Q	143	ASN
5	R	5	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	76	ASN
11	X	35	GLN
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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SAC	V	1	9	7,8,9	2.37	2 (28%)	8,9,11	2.61	5 (62%)
7	TPO	G	11	7	8,10,11	1.71	2 (25%)	10,14,16	1.45	2 (20%)
1	FME	N	1	1	8,9,10	1.57	1 (12%)	7,9,11	6.39	3 (42%)
9	SAC	I	1	9	7,8,9	3.34	2 (28%)	8,9,11	3.80	5 (62%)
2	FME	B	1	2	8,9,10	2.18	2 (25%)	7,9,11	8.37	4 (57%)
7	TPO	T	11	7	8,10,11	2.06	2 (25%)	10,14,16	1.72	1 (10%)
1	FME	A	1	1	8,9,10	1.28	1 (12%)	7,9,11	6.05	3 (42%)
2	FME	O	1	2	8,9,10	1.02	1 (12%)	7,9,11	4.61	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	8.08	1.41	1.23
2	B	1	FME	CA-N	4.75	1.53	1.46
9	V	1	SAC	OAC-C1A	4.46	1.33	1.23
9	V	1	SAC	CA-N	4.04	1.52	1.46
1	N	1	FME	CA-N	3.56	1.51	1.46
7	T	11	TPO	P-O1P	3.31	1.61	1.50
9	I	1	SAC	CA-N	3.18	1.50	1.46
7	G	11	TPO	P-O1P	3.07	1.60	1.50
7	T	11	TPO	P-OG1	2.87	1.64	1.59
2	B	1	FME	O1-CN	-2.64	1.14	1.22
1	A	1	FME	O1-CN	-2.43	1.15	1.22
2	O	1	FME	O1-CN	-2.05	1.16	1.22
7	G	11	TPO	O-C	2.02	1.28	1.19

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-20.20	91.75	122.82
1	N	1	FME	CA-N-CN	-16.07	98.11	122.82
1	A	1	FME	CA-N-CN	-15.24	99.38	122.82
2	O	1	FME	CA-N-CN	-10.62	106.50	122.82
9	I	1	SAC	C2A-C1A-N	-7.75	102.98	116.10
2	B	1	FME	O1-CN-N	6.58	142.60	125.27
2	B	1	FME	CG-CB-CA	-5.33	98.15	112.95
9	I	1	SAC	OAC-C1A-N	4.90	130.95	121.95
7	T	11	TPO	CG2-CB-CA	4.39	121.83	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	1	SAC	OG-CB-CA	-4.24	100.16	110.97
1	N	1	FME	O1-CN-N	3.97	135.74	125.27
1	A	1	FME	CE-SD-CG	3.80	113.47	100.40
9	V	1	SAC	CA-N-C1A	3.78	130.13	123.15
2	O	1	FME	C-CA-N	3.52	116.09	109.73
9	V	1	SAC	C-CA-N	3.44	115.94	109.73
9	V	1	SAC	C2A-C1A-N	3.33	121.74	116.10
7	G	11	TPO	CG2-CB-CA	3.31	119.70	113.16
2	O	1	FME	CG-CB-CA	-3.04	104.50	112.95
9	I	1	SAC	CA-N-C1A	-2.84	117.91	123.15
1	N	1	FME	CE-SD-CG	2.66	109.52	100.40
9	V	1	SAC	CB-CA-N	-2.61	104.69	110.55
2	O	1	FME	O1-CN-N	-2.57	118.51	125.27
2	B	1	FME	O-C-CA	-2.52	118.17	124.78
1	A	1	FME	CG-CB-CA	-2.27	106.64	112.95
9	V	1	SAC	OAC-C1A-N	-2.16	117.98	121.95
9	I	1	SAC	OAC-C1A-C2A	2.15	126.05	122.06
7	G	11	TPO	O2P-P-OG1	2.06	115.21	105.99

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1	SAC	2	0
7	T	11	TPO	1	0
1	A	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CHD	C	305	-	29,32,32	1.19	3 (10%)	48,51,51	1.86	11 (22%)
15	HEA	A	602	1	44,67,67	1.65	8 (18%)	37,103,103	2.70	10 (27%)
26	PSC	O	303	-	51,51,51	1.20	3 (5%)	57,59,59	1.32	5 (8%)
19	TGL	N	610	-	62,62,62	1.53	6 (9%)	65,65,65	1.66	16 (24%)
28	DMU	G	101	-	34,34,34	0.86	2 (5%)	45,45,45	2.44	13 (28%)
20	PGV	A	608	-	50,50,50	0.96	2 (4%)	53,56,56	1.43	5 (9%)
22	CHD	B	302	-	29,32,32	1.09	3 (10%)	48,51,51	1.72	9 (18%)
25	PEK	T	101	-	52,52,52	1.22	2 (3%)	55,57,57	1.27	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	TGL	A	607	-	62,62,62	1.36	7 (11%)	65,65,65	2.25	16 (24%)
20	PGV	P	305	-	50,50,50	0.89	2 (4%)	53,56,56	1.14	5 (9%)
15	HEA	N	603	1	44,67,67	1.19	3 (6%)	37,103,103	2.36	15 (40%)
14	CYN	N	601	16	0,1,1	0.00	-	-		
25	PEK	G	102	-	52,52,52	0.97	3 (5%)	55,57,57	1.64	8 (14%)
20	PGV	N	608	-	50,50,50	1.03	3 (6%)	53,56,56	1.28	4 (7%)
15	HEA	N	602	1	44,67,67	1.10	3 (6%)	37,103,103	2.65	11 (29%)
14	CYN	A	601	16	0,1,1	0.00	-	-		
21	CUA	B	301	2	0,1,1	0.00	-	-		
24	CDL	G	103	-	99,99,99	1.42	12 (12%)	105,111,111	1.41	17 (16%)
20	PGV	N	607	-	50,50,50	1.02	2 (4%)	53,56,56	1.56	6 (11%)
28	DMU	P	301	-	34,34,34	0.94	1 (2%)	45,45,45	2.37	12 (26%)
19	TGL	L	101	-	62,62,62	1.52	7 (11%)	65,65,65	1.66	14 (21%)
21	CUA	O	301	2	0,1,1	0.00	-	-		
15	HEA	A	603	1	44,67,67	1.21	6 (13%)	37,103,103	2.42	11 (29%)
28	DMU	Z	101	-	34,34,34	0.65	0	45,45,45	1.89	10 (22%)
24	CDL	C	303	-	99,99,99	1.41	13 (13%)	105,111,111	1.42	12 (11%)
20	PGV	C	307	-	50,50,50	1.43	4 (8%)	53,56,56	1.43	7 (13%)
20	PGV	A	609	-	50,50,50	1.23	2 (4%)	53,56,56	1.46	9 (16%)
20	PGV	P	302	-	50,50,50	1.15	2 (4%)	53,56,56	1.23	3 (5%)
19	TGL	D	201	-	62,62,62	1.44	7 (11%)	65,65,65	1.46	14 (21%)
22	CHD	O	302	-	29,32,32	1.09	3 (10%)	48,51,51	1.68	8 (16%)
28	DMU	M	101	-	34,34,34	0.60	0	45,45,45	1.94	12 (26%)
25	PEK	P	304	-	52,52,52	0.84	2 (3%)	55,57,57	1.74	9 (16%)
22	CHD	C	304	-	29,32,32	0.68	0	48,51,51	2.75	22 (45%)
25	PEK	G	104	-	52,52,52	1.12	2 (3%)	55,57,57	1.16	6 (10%)
20	PGV	C	302	-	50,50,50	0.92	3 (6%)	53,56,56	1.09	4 (7%)
22	CHD	P	308	-	29,32,32	1.16	3 (10%)	48,51,51	1.96	18 (37%)
24	CDL	T	102	-	99,99,99	1.36	12 (12%)	105,111,111	1.36	12 (11%)
19	TGL	Q	201	-	62,62,62	1.32	6 (9%)	65,65,65	1.46	9 (13%)
26	PSC	E	201	-	51,51,51	1.29	3 (5%)	57,59,59	1.23	4 (7%)
22	CHD	P	307	-	29,32,32	0.72	0	48,51,51	3.10	23 (47%)
25	PEK	P	309	-	52,52,52	1.20	2 (3%)	55,57,57	1.18	4 (7%)
24	CDL	P	306	-	99,99,99	1.41	12 (12%)	105,111,111	1.38	10 (9%)
25	PEK	C	306	-	52,52,52	1.14	2 (3%)	55,57,57	1.20	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	TGL	N	609	-	62,62,62	1.29	6 (9%)	65,65,65	1.45	10 (15%)

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
22	CHD	C	305	-	-	0/7/74/74	0/4/4/4
15	HEA	A	602	1	2/2/7/16	2/24/76/76	-
26	PSC	O	303	-	-	35/55/55/55	-
19	TGL	N	610	-	-	35/65/65/65	-
28	DMU	G	101	-	-	12/19/59/59	0/2/2/2
20	PGV	A	608	-	-	10/55/55/55	-
22	CHD	B	302	-	-	0/7/74/74	0/4/4/4
25	PEK	T	101	-	-	38/56/56/56	-
19	TGL	A	607	-	-	36/65/65/65	-
20	PGV	P	305	-	-	16/55/55/55	-
15	HEA	N	603	1	2/2/7/16	0/24/76/76	-
25	PEK	G	102	-	-	24/56/56/56	-
20	PGV	N	608	-	-	12/55/55/55	-
15	HEA	N	602	1	3/3/7/16	3/24/76/76	-
24	CDL	G	103	-	-	56/110/110/110	-
20	PGV	N	607	-	-	31/55/55/55	-
28	DMU	P	301	-	-	7/19/59/59	0/2/2/2
19	TGL	L	101	-	-	35/65/65/65	-
15	HEA	A	603	1	2/2/7/16	1/24/76/76	-
28	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
24	CDL	C	303	-	-	69/110/110/110	-
20	PGV	C	307	-	-	31/55/55/55	-
20	PGV	A	609	-	-	33/55/55/55	-
20	PGV	P	302	-	-	35/55/55/55	-
19	TGL	D	201	-	-	40/65/65/65	-
22	CHD	O	302	-	-	0/7/74/74	0/4/4/4
28	DMU	M	101	-	-	7/19/59/59	0/2/2/2
25	PEK	P	304	-	-	26/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	C	304	-	-	3/7/74/74	0/4/4/4
25	PEK	G	104	-	-	34/56/56/56	-
20	PGV	C	302	-	-	16/55/55/55	-
22	CHD	P	308	-	-	0/7/74/74	0/4/4/4
24	CDL	T	102	-	-	56/110/110/110	-
19	TGL	Q	201	-	-	37/65/65/65	-
26	PSC	E	201	-	-	37/55/55/55	-
22	CHD	P	307	-	-	7/7/74/74	0/4/4/4
25	PEK	P	309	-	-	22/56/56/56	-
24	CDL	P	306	-	-	74/110/110/110	-
25	PEK	C	306	-	-	31/56/56/56	-
19	TGL	N	609	-	-	33/65/65/65	-

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	610	TGL	OG2-CB1	6.08	1.51	1.34
20	C	307	PGV	O01-C1	6.07	1.51	1.34
19	L	101	TGL	OG2-CB1	5.99	1.51	1.34
20	C	307	PGV	O03-C19	5.84	1.50	1.33
24	P	306	CDL	OA8-CA7	5.43	1.49	1.33
19	N	610	TGL	OG3-CC1	5.42	1.49	1.33
19	A	607	TGL	OG1-CA1	5.32	1.48	1.33
19	L	101	TGL	OG3-CC1	5.25	1.48	1.33
25	C	306	PEK	O01-C1	5.21	1.49	1.34
25	P	309	PEK	O01-C1	5.21	1.49	1.34
19	D	201	TGL	OG1-CA1	5.20	1.48	1.33
24	C	303	CDL	OA8-CA7	5.20	1.48	1.33
24	G	103	CDL	OB6-CB5	5.19	1.48	1.34
25	T	101	PEK	O03-C21	5.18	1.48	1.33
20	P	302	PGV	O01-C1	5.14	1.48	1.34
24	G	103	CDL	OB8-CB7	5.11	1.48	1.33
19	L	101	TGL	OG1-CA1	5.11	1.48	1.33
19	N	609	TGL	OG2-CB1	5.10	1.48	1.34
19	N	610	TGL	OG1-CA1	5.09	1.48	1.33
19	D	201	TGL	OG3-CC1	5.06	1.48	1.33
24	T	102	CDL	OA6-CA5	5.05	1.48	1.34
25	T	101	PEK	O01-C1	5.05	1.48	1.34
26	E	201	PSC	O03-C19	5.03	1.48	1.33
20	A	609	PGV	O03-C19	5.01	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	103	CDL	OA6-CA5	4.98	1.48	1.34
25	G	104	PEK	O03-C21	4.97	1.47	1.33
26	E	201	PSC	O01-C1	4.96	1.48	1.34
25	P	309	PEK	O03-C21	4.94	1.47	1.33
19	Q	201	TGL	OG2-CB1	4.94	1.48	1.34
20	A	609	PGV	O01-C1	4.93	1.48	1.34
24	T	102	CDL	OB8-CB7	4.85	1.47	1.33
25	C	306	PEK	O03-C21	4.81	1.47	1.33
19	A	607	TGL	OG2-CB1	4.77	1.47	1.34
24	C	303	CDL	OA6-CA5	4.74	1.47	1.34
24	T	102	CDL	OB6-CB5	4.73	1.47	1.34
19	N	609	TGL	OG1-CA1	4.64	1.46	1.33
20	P	302	PGV	O03-C19	4.60	1.46	1.33
24	P	306	CDL	OB6-CB5	4.56	1.47	1.34
24	P	306	CDL	OA6-CA5	4.55	1.47	1.34
26	O	303	PSC	O01-C1	4.54	1.47	1.34
19	Q	201	TGL	OG1-CA1	4.53	1.46	1.33
25	G	104	PEK	O01-C1	4.52	1.47	1.34
20	N	608	PGV	O03-C19	4.42	1.46	1.33
24	C	303	CDL	OB8-CB7	4.41	1.46	1.33
24	P	306	CDL	OB8-CB7	4.39	1.46	1.33
20	A	608	PGV	O03-C19	4.38	1.46	1.33
15	A	602	HEA	C3B-C11	-4.38	1.49	1.52
19	Q	201	TGL	OG3-CC1	4.36	1.46	1.33
19	D	201	TGL	OG2-CB1	4.34	1.46	1.34
24	G	103	CDL	OA8-CA7	4.28	1.45	1.33
15	A	602	HEA	C27-C19	4.24	1.61	1.50
26	O	303	PSC	O03-C19	4.23	1.45	1.33
28	P	301	DMU	O16-C6	4.09	1.47	1.40
20	N	607	PGV	O03-C19	4.01	1.45	1.33
20	N	607	PGV	O01-C1	4.01	1.45	1.34
24	C	303	CDL	OB6-CB5	4.01	1.45	1.34
26	E	201	PSC	C13-C12	3.92	1.54	1.31
26	O	303	PSC	C13-C12	3.88	1.54	1.31
19	L	101	TGL	C20-CA9	-3.84	1.30	1.51
15	A	602	HEA	O11-C11	3.84	1.51	1.42
20	P	305	PGV	O03-C19	3.74	1.44	1.33
25	G	102	PEK	O01-C1	3.62	1.44	1.34
19	A	607	TGL	OG3-CC1	3.56	1.43	1.33
15	N	603	HEA	C3B-C11	-3.54	1.50	1.52
20	C	302	PGV	O03-C19	3.52	1.43	1.33
19	N	609	TGL	OG3-CC1	3.51	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	610	TGL	C20-CA9	-3.48	1.32	1.51
24	C	303	CDL	C59-C58	-3.47	1.32	1.51
24	G	103	CDL	C59-C58	-3.42	1.32	1.51
19	N	609	TGL	C10-CB9	-3.39	1.32	1.51
24	P	306	CDL	C59-C58	-3.33	1.32	1.51
24	C	303	CDL	C79-C78	-3.32	1.32	1.51
24	T	102	CDL	OA8-CA7	3.31	1.43	1.33
19	N	610	TGL	C10-CB9	-3.31	1.33	1.51
25	P	304	PEK	O03-C01	-3.30	1.37	1.45
24	T	102	CDL	C59-C58	-3.27	1.33	1.51
24	T	102	CDL	C42-C41	-3.26	1.33	1.51
15	A	602	HEA	C3A-C2A	-3.22	1.35	1.40
24	T	102	CDL	C62-C61	-3.21	1.33	1.51
24	C	303	CDL	C62-C61	-3.21	1.33	1.51
24	P	306	CDL	C79-C78	-3.20	1.33	1.51
24	P	306	CDL	C82-C81	-3.19	1.33	1.51
20	A	608	PGV	O01-C1	3.17	1.43	1.34
19	A	607	TGL	C10-CB9	-3.17	1.33	1.51
24	G	103	CDL	C62-C61	-3.16	1.33	1.51
28	G	101	DMU	O16-C6	3.15	1.45	1.40
24	P	306	CDL	C62-C61	-3.13	1.34	1.51
20	C	302	PGV	O01-C1	3.08	1.43	1.34
19	N	609	TGL	C20-CA9	-3.06	1.34	1.51
24	P	306	CDL	C19-C18	-3.04	1.34	1.51
19	A	607	TGL	C20-CA9	-3.03	1.34	1.51
24	C	303	CDL	C82-C81	-3.02	1.34	1.51
24	P	306	CDL	C22-C21	-3.01	1.34	1.51
19	Q	201	TGL	C20-CA9	-3.00	1.34	1.51
15	A	602	HEA	CMC-C2C	3.00	1.57	1.51
24	T	102	CDL	C19-C18	-2.99	1.34	1.51
24	C	303	CDL	C22-C21	-2.99	1.34	1.51
24	P	306	CDL	C39-C38	-2.98	1.34	1.51
24	C	303	CDL	C19-C18	-2.97	1.34	1.51
24	G	103	CDL	C42-C41	-2.95	1.35	1.51
24	G	103	CDL	C19-C18	-2.95	1.35	1.51
19	D	201	TGL	C15-CC9	-2.94	1.35	1.51
24	T	102	CDL	C39-C38	-2.93	1.35	1.51
19	L	101	TGL	C10-CB9	-2.93	1.35	1.51
24	T	102	CDL	C79-C78	-2.89	1.35	1.51
15	A	603	HEA	C3C-C2C	-2.89	1.36	1.40
22	C	305	CHD	C8-C9	2.88	1.59	1.53
24	T	102	CDL	C82-C81	-2.87	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	103	CDL	C22-C21	-2.86	1.35	1.51
24	C	303	CDL	C39-C38	-2.85	1.35	1.51
19	Q	201	TGL	C10-CB9	-2.85	1.35	1.51
25	G	102	PEK	O03-C21	2.84	1.41	1.33
24	C	303	CDL	C42-C41	-2.80	1.35	1.51
19	Q	201	TGL	C15-CC9	-2.79	1.35	1.51
22	P	308	CHD	C8-C7	2.79	1.58	1.53
24	G	103	CDL	C39-C38	-2.78	1.36	1.51
24	T	102	CDL	C22-C21	-2.77	1.36	1.51
15	N	602	HEA	C3C-C2C	-2.77	1.36	1.40
19	D	201	TGL	C20-CA9	-2.77	1.36	1.51
15	N	602	HEA	C12-C13	2.76	1.62	1.53
15	A	602	HEA	C12-C13	2.75	1.62	1.53
19	N	609	TGL	C15-CC9	-2.74	1.36	1.51
15	N	603	HEA	C12-C13	2.74	1.62	1.53
15	A	603	HEA	C12-C13	2.73	1.62	1.53
24	G	103	CDL	C82-C81	-2.71	1.36	1.51
19	D	201	TGL	OB1-CB1	2.65	1.30	1.22
19	L	101	TGL	C15-CC9	-2.65	1.36	1.51
24	G	103	CDL	C79-C78	-2.64	1.36	1.51
15	A	603	HEA	O11-C11	2.64	1.48	1.42
19	D	201	TGL	C10-CB9	-2.63	1.36	1.51
20	N	608	PGV	O01-C1	2.63	1.41	1.34
24	P	306	CDL	C42-C41	-2.62	1.36	1.51
19	N	610	TGL	C15-CC9	-2.61	1.36	1.51
22	O	302	CHD	C11-C9	2.58	1.58	1.53
22	B	302	CHD	C6-C7	2.57	1.57	1.52
19	A	607	TGL	C15-CC9	-2.51	1.37	1.51
22	B	302	CHD	C4-C3	2.51	1.56	1.51
22	P	308	CHD	C6-C5	2.50	1.57	1.53
15	A	602	HEA	C1C-CHC	2.48	1.47	1.41
22	O	302	CHD	C11-C12	2.41	1.57	1.53
25	P	304	PEK	O01-C1	2.41	1.41	1.34
19	L	101	TGL	CG3-CG2	2.40	1.58	1.50
25	G	102	PEK	O03-C01	-2.39	1.39	1.45
22	O	302	CHD	C6-C7	2.35	1.56	1.52
22	P	308	CHD	C6-C7	2.32	1.56	1.52
20	C	307	PGV	P-O11	2.31	1.68	1.59
19	A	607	TGL	OC1-CC1	-2.31	1.15	1.22
22	B	302	CHD	C19-C10	2.28	1.58	1.54
20	P	305	PGV	O01-C1	2.28	1.40	1.34
15	A	603	HEA	OMA-CMA	2.26	1.29	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	305	CHD	C8-C14	2.25	1.58	1.53
28	G	101	DMU	O1-C10	2.22	1.47	1.41
15	N	602	HEA	C3B-C11	-2.21	1.51	1.52
20	C	307	PGV	C03-C02	2.21	1.57	1.50
15	A	602	HEA	C1A-C2A	-2.20	1.37	1.42
22	C	305	CHD	C4-C5	2.18	1.57	1.53
15	A	603	HEA	C18-C19	2.17	1.38	1.33
24	C	303	CDL	OB6-CB4	-2.14	1.41	1.46
15	N	603	HEA	C3C-C2C	-2.13	1.37	1.40
15	A	603	HEA	C16-C15	2.07	1.55	1.51
20	N	608	PGV	P-O13	2.04	1.58	1.50
20	C	302	PGV	P-O14	-2.00	1.45	1.55

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	602	HEA	C20-C19-C18	-10.50	99.87	121.12
15	N	602	HEA	C17-C18-C19	-10.18	103.15	127.66
28	P	301	DMU	O16-C6-C1	9.15	122.58	108.30
19	A	607	TGL	CG2-OG2-CB1	8.90	139.70	117.79
15	A	603	HEA	C13-C12-C11	-8.34	101.82	114.35
28	G	101	DMU	O1-C9-C11	8.11	126.60	106.44
22	P	307	CHD	C6-C7-C8	8.01	120.03	111.48
28	P	301	DMU	C18-O16-C6	7.48	126.25	113.84
19	A	607	TGL	OG2-CB1-CB2	7.43	127.52	111.50
22	C	304	CHD	C6-C5-C4	-7.19	102.91	111.19
25	G	102	PEK	C2-C3-C4	6.83	125.41	113.23
22	P	307	CHD	C14-C13-C12	6.57	113.52	107.40
25	P	304	PEK	C2-C3-C4	6.46	124.75	113.23
22	P	307	CHD	C6-C5-C10	6.35	119.40	112.66
28	G	101	DMU	C8-C7-C5	-6.23	99.94	110.82
19	Q	201	TGL	OG2-CB1-CB2	6.20	124.86	111.50
15	A	602	HEA	C27-C19-C18	6.16	139.47	123.68
15	N	603	HEA	C1B-C2B-C3B	-6.10	102.75	107.00
22	P	307	CHD	C18-C13-C12	-5.96	103.00	109.07
24	C	303	CDL	OA6-CA5-C11	5.81	124.03	111.50
28	M	101	DMU	O2-C8-C9	-5.80	94.89	109.30
22	P	308	CHD	C23-C22-C20	-5.57	107.22	114.72
24	P	306	CDL	OA6-CA5-C11	5.57	123.50	111.50
28	G	101	DMU	C7-C8-C9	-5.38	100.65	110.24
15	N	603	HEA	CAD-CBD-CGD	-5.37	103.66	112.67
19	L	101	TGL	OG3-CC1-CC2	5.35	128.71	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	103	CDL	OA6-CA5-C11	5.34	123.02	111.50
15	A	603	HEA	C20-C19-C18	-5.31	110.38	121.12
22	B	302	CHD	C18-C13-C12	-5.30	103.67	109.07
25	T	101	PEK	O01-C1-C2	5.29	122.90	111.50
28	Z	101	DMU	C8-C7-C5	-5.28	101.61	110.82
24	T	102	CDL	OB6-CB5-C51	5.26	122.83	111.50
20	N	607	PGV	O01-C1-C2	5.22	122.76	111.50
20	N	607	PGV	C3-C2-C1	-5.19	94.76	113.62
15	N	602	HEA	C27-C19-C18	-5.14	110.48	123.68
24	T	102	CDL	OA6-CA5-C11	5.12	122.54	111.50
19	N	609	TGL	OG2-CB1-CB2	5.10	122.49	111.50
24	G	103	CDL	OB6-CB5-C51	5.10	122.49	111.50
20	P	302	PGV	O01-C1-C2	5.08	122.46	111.50
22	P	307	CHD	C6-C5-C4	-5.03	105.40	111.19
15	A	602	HEA	C25-C23-C24	5.02	125.69	114.60
22	P	307	CHD	C14-C8-C7	4.96	118.38	111.81
20	C	307	PGV	O01-C1-C2	4.95	122.18	111.50
22	C	304	CHD	C10-C9-C8	4.91	117.09	111.82
20	A	608	PGV	O03-C19-O04	-4.89	111.24	123.59
25	G	104	PEK	O01-C1-C2	4.89	122.03	111.50
26	O	303	PSC	O01-C1-C2	4.88	122.01	111.50
15	A	603	HEA	CAD-CBD-CGD	-4.87	104.51	112.67
22	P	307	CHD	C14-C8-C9	-4.77	103.16	109.71
22	C	304	CHD	C14-C8-C7	4.74	118.09	111.81
25	P	304	PEK	O01-C1-O02	-4.73	112.26	123.70
15	N	603	HEA	C13-C12-C11	-4.73	107.24	114.35
19	A	607	TGL	OG1-CA1-CA2	4.72	126.74	111.91
20	A	608	PGV	O03-C19-C20	4.71	126.69	111.91
22	C	304	CHD	C19-C10-C1	-4.65	100.76	108.26
15	N	602	HEA	C3C-C4C-NC	4.58	115.13	109.21
28	Z	101	DMU	C7-C8-C9	-4.57	102.09	110.24
22	C	304	CHD	C15-C14-C8	4.56	124.71	118.33
19	A	607	TGL	OG3-CC1-OC1	-4.55	112.10	123.59
26	E	201	PSC	O01-C1-C2	4.51	121.23	111.50
25	G	102	PEK	C24-C23-C22	-4.51	96.97	113.19
20	C	307	PGV	O03-C19-C20	4.51	126.05	111.91
22	B	302	CHD	C6-C7-C8	4.51	116.29	111.48
25	C	306	PEK	O01-C1-C2	4.50	121.21	111.50
22	C	304	CHD	C1-C10-C5	4.50	114.43	107.77
25	P	309	PEK	O01-C1-C2	4.49	121.17	111.50
15	N	602	HEA	C16-C17-C18	4.48	126.61	111.88
22	C	305	CHD	C1-C2-C3	-4.47	104.74	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	101	DMU	O3-C5-C7	4.45	120.63	110.35
20	P	302	PGV	O03-C19-C20	4.42	125.77	111.91
22	C	304	CHD	C4-C5-C10	4.39	117.32	112.66
25	P	304	PEK	O03-C01-C02	-4.37	95.71	108.43
19	N	610	TGL	CG2-OG2-CB1	4.36	128.53	117.79
15	A	603	HEA	C27-C19-C20	4.31	122.53	115.27
22	C	305	CHD	C5-C4-C3	-4.31	106.43	112.76
24	C	303	CDL	OB8-CB7-C71	4.29	125.37	111.91
15	N	602	HEA	C27-C19-C20	4.28	122.47	115.27
19	N	610	TGL	OG2-CB1-CB2	4.28	120.72	111.50
19	A	607	TGL	OG3-CG3-CG2	4.26	120.84	108.43
28	M	101	DMU	O1-C9-C8	4.26	117.42	109.69
20	A	609	PGV	C02-O01-C1	4.24	128.24	117.79
19	A	607	TGL	OB1-CB1-CB2	-4.21	107.29	123.73
22	P	307	CHD	C15-C14-C8	4.20	124.20	118.33
19	L	101	TGL	CG2-OG2-CB1	4.18	128.08	117.79
26	O	303	PSC	O03-C19-C20	4.14	124.89	111.91
20	N	608	PGV	O03-C19-O04	-4.12	113.20	123.59
20	N	608	PGV	O03-C19-C20	4.10	124.79	111.91
24	P	306	CDL	OB8-CB7-C71	4.10	124.76	111.91
15	N	603	HEA	C27-C19-C20	4.09	122.16	115.27
22	P	307	CHD	C2-C1-C10	4.09	119.80	112.78
22	C	305	CHD	C22-C23-C24	-4.09	104.81	113.59
19	L	101	TGL	OG2-CB1-CB2	4.07	120.28	111.50
22	O	302	CHD	O12-C12-C13	-4.06	104.16	111.03
15	N	603	HEA	C26-C15-C16	4.05	122.08	115.27
22	P	307	CHD	C9-C8-C7	4.04	116.71	111.88
19	D	201	TGL	OG2-CB1-CB2	4.04	120.20	111.50
25	P	309	PEK	O03-C21-C22	4.02	124.52	111.91
19	A	607	TGL	OG3-CC1-CC2	3.96	124.34	111.91
22	P	307	CHD	C5-C6-C7	3.96	118.83	114.46
19	A	607	TGL	CG3-OG3-CC1	3.92	131.63	117.12
20	A	609	PGV	O01-C1-C2	3.89	119.88	111.50
22	C	304	CHD	C14-C8-C9	-3.87	104.40	109.71
22	P	307	CHD	C10-C9-C8	3.87	115.97	111.82
20	A	609	PGV	O03-C19-C20	3.83	123.93	111.91
22	P	307	CHD	C1-C10-C5	3.81	113.41	107.77
19	N	609	TGL	CG2-OG2-CB1	3.81	127.17	117.79
28	G	101	DMU	C18-O16-C6	3.79	120.12	113.84
22	C	305	CHD	C11-C12-C13	3.78	115.13	111.24
22	P	308	CHD	C1-C10-C5	3.78	113.36	107.77
28	M	101	DMU	C18-O16-C6	-3.77	107.58	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	P	301	DMU	O5-C6-C1	-3.76	102.39	110.35
22	O	302	CHD	C6-C5-C4	-3.75	106.88	111.19
22	C	304	CHD	C6-C7-C8	3.74	115.48	111.48
22	P	307	CHD	C19-C10-C9	-3.74	106.03	111.18
28	P	301	DMU	C8-C7-C5	-3.72	104.33	110.82
28	Z	101	DMU	O1-C9-C11	3.72	115.67	106.44
22	C	304	CHD	C18-C13-C12	-3.69	105.31	109.07
22	C	304	CHD	C6-C5-C10	3.68	116.57	112.66
15	A	602	HEA	C17-C18-C19	3.68	136.52	127.66
19	D	201	TGL	OG1-CA1-CA2	3.66	123.41	111.91
22	B	302	CHD	C13-C14-C8	-3.66	110.06	114.74
28	Z	101	DMU	O49-C1-C2	-3.65	101.92	110.35
22	C	305	CHD	C9-C8-C7	3.63	116.22	111.88
22	B	302	CHD	C22-C23-C24	-3.62	105.81	113.59
28	G	101	DMU	O16-C6-C1	3.60	113.93	108.30
22	O	302	CHD	C9-C8-C7	3.60	116.18	111.88
28	M	101	DMU	O3-C5-C7	3.59	118.65	110.35
22	P	308	CHD	C21-C20-C22	-3.59	104.73	110.36
28	G	101	DMU	O7-C10-C5	3.59	117.40	108.10
15	A	603	HEA	CAA-CBA-CGA	-3.57	106.68	112.67
28	P	301	DMU	C10-O1-C9	3.56	120.68	113.69
19	N	610	TGL	OG1-CA1-CA2	3.55	123.04	111.91
19	A	607	TGL	OG2-CG2-CG1	3.54	121.23	108.40
25	G	102	PEK	O03-C01-C02	-3.53	98.15	108.43
22	C	304	CHD	C14-C13-C12	3.53	110.69	107.40
20	A	608	PGV	O01-C1-C2	3.53	119.10	111.50
19	N	609	TGL	OG3-CC1-OC1	-3.52	114.70	123.59
28	M	101	DMU	O1-C9-C11	3.50	115.13	106.44
22	C	304	CHD	C5-C4-C3	3.49	117.88	112.76
20	N	607	PGV	O03-C19-C20	3.47	122.79	111.91
15	A	602	HEA	C20-C21-C22	-3.45	100.54	111.88
19	L	101	TGL	CB4-CB3-CB2	-3.45	100.81	113.19
22	P	307	CHD	C23-C22-C20	-3.44	110.08	114.72
28	G	101	DMU	C6-O5-C4	3.44	120.44	113.69
22	C	304	CHD	C15-C14-C13	3.44	106.93	103.55
24	G	103	CDL	OA6-CA5-OA7	-3.43	115.41	123.70
24	C	303	CDL	OB8-CB7-OB9	-3.41	115.00	123.59
22	P	308	CHD	C11-C12-C13	3.40	114.74	111.24
22	C	305	CHD	C15-C14-C13	3.39	106.88	103.55
22	C	304	CHD	C22-C23-C24	-3.39	106.31	113.59
19	Q	201	TGL	OG3-CC1-CC2	3.38	122.51	111.91
25	P	309	PEK	O03-C21-O04	-3.37	115.09	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	N	602	HEA	C1B-C2B-C3B	3.35	109.33	107.00
20	C	307	PGV	O03-C01-C02	3.35	118.17	108.43
28	P	301	DMU	C7-C8-C9	-3.34	104.28	110.24
20	N	607	PGV	O01-C02-C03	3.34	120.49	108.40
20	N	607	PGV	O03-C19-O04	-3.31	115.23	123.59
24	P	306	CDL	OB8-CB7-OB9	-3.30	115.26	123.59
25	G	102	PEK	O01-C1-O02	-3.29	115.76	123.70
25	G	104	PEK	O03-C21-C22	3.29	122.22	111.91
28	Z	101	DMU	O1-C9-C8	3.28	115.66	109.69
22	O	302	CHD	O7-C7-C6	3.27	118.06	109.94
19	A	607	TGL	CB3-CB2-CB1	-3.27	101.73	113.62
25	C	306	PEK	O03-C21-C22	3.26	122.14	111.91
26	E	201	PSC	C02-O01-C1	3.26	125.81	117.79
25	P	304	PEK	C01-O03-C21	3.21	129.00	117.12
28	P	301	DMU	C11-C9-C8	3.20	120.51	113.00
15	A	602	HEA	C27-C19-C20	3.19	120.64	115.27
22	P	307	CHD	C19-C10-C1	-3.18	103.14	108.26
19	N	610	TGL	OG3-CC1-CC2	3.18	121.88	111.91
20	P	305	PGV	O12-P-O13	-3.16	96.70	109.07
24	T	102	CDL	OA6-CA5-OA7	-3.16	116.06	123.70
19	Q	201	TGL	OG1-CA1-CA2	3.16	121.82	111.91
28	Z	101	DMU	O16-C6-C1	3.14	113.21	108.30
15	A	602	HEA	C1B-C2B-C3B	-3.14	104.81	107.00
22	C	304	CHD	C23-C22-C20	-3.14	110.50	114.72
19	Q	201	TGL	OG1-CA1-OA1	-3.13	115.69	123.59
19	L	101	TGL	OG1-CA1-CA2	3.11	121.67	111.91
24	P	306	CDL	OA6-CA5-OA7	-3.11	116.20	123.70
22	O	302	CHD	C11-C9-C8	3.09	115.41	110.88
19	L	101	TGL	OG3-CC1-OC1	-3.09	115.80	123.59
20	P	302	PGV	O03-C19-O04	-3.06	115.86	123.59
15	N	603	HEA	C17-C18-C19	3.06	135.03	127.66
15	A	602	HEA	C4B-C3B-C2B	-3.05	104.73	106.87
20	N	608	PGV	O01-C1-O02	-3.05	116.33	123.70
22	P	308	CHD	C11-C9-C8	3.02	115.30	110.88
25	P	304	PEK	C24-C23-C22	-3.02	102.33	113.19
24	T	102	CDL	OA8-CA7-OA9	-3.02	115.97	123.59
19	N	610	TGL	CG3-OG3-CC1	3.01	128.27	117.12
22	P	308	CHD	C15-C14-C13	3.01	106.50	103.55
26	O	303	PSC	O01-C1-O02	-3.00	116.45	123.70
24	G	103	CDL	CB6-OB8-CB7	3.00	128.23	117.12
25	T	101	PEK	O01-C1-O02	-2.99	116.47	123.70
22	P	307	CHD	C22-C23-C24	-2.99	107.16	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	E	201	PSC	O03-C19-C20	2.98	121.27	111.91
22	P	307	CHD	C9-C10-C5	2.98	112.77	108.58
22	C	304	CHD	C5-C6-C7	2.98	117.75	114.46
15	N	602	HEA	C13-C14-C15	-2.97	120.50	127.66
19	Q	201	TGL	OG3-CC1-OC1	-2.95	116.14	123.59
19	D	201	TGL	CG2-OG2-CB1	2.95	125.05	117.79
19	D	201	TGL	OG1-CA1-OA1	-2.95	116.15	123.59
19	D	201	TGL	C10-CB9-CB8	2.94	129.37	114.42
28	P	301	DMU	O3-C5-C10	2.94	117.19	110.05
15	N	602	HEA	C20-C19-C18	2.93	127.04	121.12
22	C	305	CHD	C23-C22-C20	-2.93	110.78	114.72
28	G	101	DMU	C10-C5-C7	2.92	116.09	110.00
20	A	609	PGV	O03-C19-O04	-2.91	116.24	123.59
24	P	306	CDL	OB6-CB5-C51	2.90	117.75	111.50
22	B	302	CHD	C17-C13-C12	2.89	120.31	117.67
15	N	603	HEA	OMA-CMA-C3A	-2.88	118.64	124.91
19	N	609	TGL	OG1-CA1-CA2	2.88	120.94	111.91
25	P	304	PEK	C30-C29-C28	-2.87	99.84	114.42
22	P	307	CHD	C11-C12-C13	2.87	114.19	111.24
28	M	101	DMU	O5-C4-C57	2.87	113.56	106.44
25	T	101	PEK	O03-C21-C22	2.87	120.90	111.91
19	D	201	TGL	OG3-CC1-CC2	2.86	120.89	111.91
24	C	303	CDL	OB6-CB5-C51	2.86	117.67	111.50
19	D	201	TGL	CG1-OG1-CA1	2.86	127.70	117.12
22	P	308	CHD	C22-C20-C17	-2.85	104.40	110.28
24	G	103	CDL	OA8-CA7-C31	2.84	120.83	111.91
15	N	602	HEA	CBA-CAA-C2A	2.84	117.71	112.48
19	Q	201	TGL	CG3-OG3-CC1	2.84	127.63	117.12
15	A	602	HEA	CAA-CBA-CGA	-2.83	107.92	112.67
22	P	307	CHD	C15-C14-C13	2.82	106.32	103.55
24	C	303	CDL	C54-C53-C52	-2.82	100.12	114.42
19	Q	201	TGL	OG2-CG2-CG3	2.81	118.58	108.40
19	N	610	TGL	OG1-CG1-CG2	2.81	116.62	108.43
28	P	301	DMU	C1-C2-C3	2.81	116.10	109.68
19	N	610	TGL	C25-C24-C23	-2.79	100.25	114.42
25	C	306	PEK	C2-C3-C4	-2.79	108.25	113.23
24	G	103	CDL	C43-C42-C41	2.79	128.58	114.42
24	C	303	CDL	OA8-CA7-C31	2.77	120.59	111.91
28	P	301	DMU	O1-C9-C11	2.76	113.31	106.44
19	L	101	TGL	OG1-CG1-CG2	2.76	116.47	108.43
19	N	609	TGL	CG3-OG3-CC1	2.76	127.33	117.12
25	G	102	PEK	C26-C25-C24	-2.74	100.52	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	201	TGL	CG3-OG3-CC1	2.73	127.25	117.12
24	P	306	CDL	CB6-CB4-CB3	-2.73	105.32	111.79
28	M	101	DMU	O7-C10-C5	2.73	115.18	108.10
25	T	101	PEK	C01-O03-C21	2.73	127.23	117.12
19	N	610	TGL	C26-C25-C24	-2.72	100.64	114.42
24	T	102	CDL	OB8-CB6-CB4	2.71	116.33	108.43
28	Z	101	DMU	C28-C25-C22	-2.71	100.69	114.42
24	T	102	CDL	CA6-CA4-CA3	-2.70	105.40	111.79
28	Z	101	DMU	O5-C4-C57	2.70	113.15	106.44
22	P	307	CHD	C16-C17-C13	2.70	106.20	103.55
28	Z	101	DMU	O3-C5-C7	2.70	116.58	110.35
24	C	303	CDL	OA6-CA5-OA7	-2.70	117.19	123.70
20	A	609	PGV	C8-C9-C10	-2.69	102.05	113.79
22	C	305	CHD	C5-C6-C7	-2.69	111.49	114.46
22	O	302	CHD	C14-C8-C7	2.68	115.37	111.81
19	N	610	TGL	OG3-CC1-OC1	-2.68	116.82	123.59
22	C	305	CHD	C9-C11-C12	-2.68	110.76	114.30
24	T	102	CDL	C83-C82-C81	2.66	127.93	114.42
22	P	308	CHD	C6-C5-C4	-2.66	108.13	111.19
20	A	608	PGV	O03-C01-C02	2.65	116.16	108.43
22	C	304	CHD	C19-C10-C9	-2.65	107.53	111.18
19	N	609	TGL	OG3-CC1-CC2	2.65	120.22	111.91
20	C	302	PGV	C22-C21-C20	-2.65	103.68	113.19
24	G	103	CDL	OB8-CB7-C71	2.64	120.20	111.91
24	G	103	CDL	OB8-CB6-CB4	2.64	116.12	108.43
19	A	607	TGL	C15-CC9-CC8	2.64	127.81	114.42
19	N	610	TGL	CC3-CC2-CC1	2.64	123.20	113.62
22	C	304	CHD	C16-C17-C20	2.63	116.22	112.15
24	P	306	CDL	OA8-CA7-C31	2.61	120.10	111.91
24	T	102	CDL	OA8-CA7-C31	2.60	120.07	111.91
15	N	603	HEA	C21-C20-C19	2.60	121.52	112.98
22	P	308	CHD	C5-C4-C3	-2.60	108.95	112.76
20	C	302	PGV	O03-C19-O04	-2.59	117.05	123.59
15	N	602	HEA	CAD-C3D-C2D	2.57	134.63	127.25
22	P	308	CHD	C22-C23-C24	-2.56	108.09	113.59
20	N	607	PGV	C5-C4-C3	-2.56	101.44	114.42
24	P	306	CDL	C53-C52-C51	-2.56	104.00	113.19
19	N	609	TGL	OB1-CB1-CB2	-2.55	113.77	123.73
19	D	201	TGL	C11-C10-CB9	2.55	127.38	114.42
25	P	304	PEK	C28-C27-C26	-2.55	101.48	114.42
22	B	302	CHD	C6-C5-C4	-2.54	108.26	111.19
19	D	201	TGL	OG3-CC1-OC1	-2.54	117.18	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	308	CHD	C4-C5-C10	-2.53	109.97	112.66
22	P	307	CHD	C5-C4-C3	-2.52	109.05	112.76
15	N	603	HEA	C20-C19-C18	-2.52	116.01	121.12
24	G	103	CDL	C83-C82-C81	2.51	127.19	114.42
19	L	101	TGL	OG3-CG3-CG2	2.50	115.72	108.43
22	P	308	CHD	C6-C5-C10	2.50	115.31	112.66
28	M	101	DMU	C7-C8-C9	-2.50	105.78	110.24
24	C	303	CDL	C52-C51-CB5	-2.49	104.56	113.62
28	M	101	DMU	O7-C3-C4	-2.48	102.66	109.45
15	A	603	HEA	C1B-C2B-C3B	-2.46	105.28	107.00
22	C	304	CHD	C4-C3-C2	2.45	113.48	110.55
24	P	306	CDL	C42-C41-C40	2.45	126.88	114.42
20	A	609	PGV	O01-C02-C03	2.45	117.28	108.40
19	N	609	TGL	CB3-CB2-CB1	-2.44	104.73	113.62
20	P	305	PGV	C03-C02-C01	-2.44	106.01	111.79
19	L	101	TGL	OB1-CB1-CB2	-2.44	114.22	123.73
15	A	603	HEA	C12-C11-C3B	-2.44	106.18	112.56
24	C	303	CDL	C39-C38-C37	2.44	126.79	114.42
22	O	302	CHD	C15-C16-C17	2.43	109.95	105.13
25	G	104	PEK	O01-C1-O02	-2.43	117.84	123.70
28	P	301	DMU	O7-C10-C5	2.41	114.34	108.10
24	C	303	CDL	CB4-OB6-CB5	-2.41	111.86	117.79
15	A	602	HEA	C3C-C4C-NC	2.39	112.30	109.21
25	P	304	PEK	C03-C02-C01	-2.39	106.14	111.79
19	L	101	TGL	C26-C25-C24	-2.39	102.31	114.42
22	P	307	CHD	C21-C20-C17	2.39	116.57	112.92
15	A	603	HEA	C3C-C4C-NC	2.38	112.29	109.21
15	N	603	HEA	CMC-C2C-C3C	2.38	129.13	124.68
22	C	305	CHD	C15-C14-C8	2.37	121.64	118.33
25	G	104	PEK	O03-C01-C02	2.37	115.33	108.43
22	C	304	CHD	C21-C20-C17	2.37	116.55	112.92
19	A	607	TGL	CB7-CB6-CB5	-2.36	102.43	114.42
20	A	609	PGV	O03-C01-C02	2.36	115.30	108.43
28	Z	101	DMU	O2-C8-C9	-2.36	103.45	109.30
15	N	603	HEA	CAA-CBA-CGA	-2.36	108.72	112.67
19	Q	201	TGL	OG2-CB1-OB1	-2.35	118.02	123.70
20	P	305	PGV	C8-C9-C10	-2.35	103.54	113.79
20	N	608	PGV	O01-C1-C2	2.34	116.55	111.50
19	N	610	TGL	OG3-CG3-CG2	2.34	115.24	108.43
19	L	101	TGL	OG1-CA1-OA1	-2.34	117.69	123.59
20	A	609	PGV	C01-O03-C19	2.34	125.77	117.12
22	P	308	CHD	C16-C15-C14	-2.33	100.52	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	101	DMU	O1-C10-C5	2.32	115.27	110.35
15	A	603	HEA	CAA-C2A-C3A	-2.32	121.14	126.86
20	C	307	PGV	O01-C02-C03	2.31	116.78	108.40
25	P	304	PEK	O01-C1-C2	2.31	116.47	111.50
15	N	603	HEA	C12-C13-C14	-2.30	106.16	112.23
25	G	102	PEK	C25-C24-C23	-2.30	102.75	114.42
24	G	103	CDL	OB8-CB7-OB9	-2.30	117.79	123.59
20	A	608	PGV	O01-C1-O02	-2.29	118.16	123.70
22	P	308	CHD	C16-C17-C20	2.29	115.69	112.15
25	C	306	PEK	C01-O03-C21	2.29	125.59	117.12
22	B	302	CHD	C10-C9-C8	2.29	114.27	111.82
19	L	101	TGL	C15-CC9-CC8	2.28	126.02	114.42
15	N	603	HEA	CAA-C2A-C3A	2.27	132.47	126.86
25	T	101	PEK	O03-C01-C02	2.27	115.04	108.43
19	N	610	TGL	C15-CC9-CC8	2.27	125.94	114.42
25	T	101	PEK	O03-C21-O04	-2.26	117.88	123.59
24	G	103	CDL	C79-C78-C77	2.26	125.91	114.42
22	C	304	CHD	C16-C17-C13	2.26	105.77	103.55
22	O	302	CHD	C15-C14-C13	2.26	105.77	103.55
24	T	102	CDL	OB8-CB7-C71	2.25	118.98	111.91
19	L	101	TGL	CA3-CA2-CA1	-2.25	105.43	113.62
15	A	603	HEA	OMA-CMA-C3A	2.25	129.81	124.91
20	C	302	PGV	C8-C9-C10	-2.24	104.02	113.79
24	T	102	CDL	C82-C81-C80	2.24	125.81	114.42
24	G	103	CDL	C82-C81-C80	2.24	125.81	114.42
20	C	302	PGV	O06-C06-C05	-2.24	99.46	110.20
19	A	607	TGL	OG1-CA1-OA1	-2.24	117.94	123.59
25	G	104	PEK	O03-C21-O04	-2.23	117.95	123.59
22	P	308	CHD	C17-C13-C14	-2.23	97.84	100.09
24	T	102	CDL	CB6-OB8-CB7	2.21	125.31	117.12
25	T	101	PEK	C2-C3-C4	2.21	117.17	113.23
24	G	103	CDL	C40-C39-C38	2.21	125.64	114.42
19	N	610	TGL	OB1-CB1-CB2	-2.20	115.15	123.73
22	P	308	CHD	C11-C9-C10	-2.20	111.46	113.73
28	P	301	DMU	O1-C10-C5	2.20	115.00	110.35
25	G	104	PEK	C01-O03-C21	2.19	125.23	117.12
19	N	610	TGL	OG1-CA1-OA1	-2.18	118.08	123.59
25	G	102	PEK	C11-C10-C9	2.18	122.75	112.02
25	P	309	PEK	O03-C01-C02	2.17	114.76	108.43
28	M	101	DMU	C28-C25-C22	-2.17	103.42	114.42
22	C	305	CHD	C14-C8-C9	2.16	112.68	109.71
19	A	607	TGL	OA1-CA1-CA2	-2.16	115.31	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	E	201	PSC	C08-N-C06	2.16	114.52	108.97
28	G	101	DMU	C10-O1-C9	2.15	117.92	113.69
19	D	201	TGL	C21-C20-CA9	2.15	125.36	114.42
22	P	308	CHD	C16-C17-C13	2.15	105.66	103.55
22	B	302	CHD	C14-C8-C9	2.14	112.64	109.71
24	G	103	CDL	C80-C79-C78	2.13	125.25	114.42
24	G	103	CDL	OA8-CA7-OA9	-2.13	118.22	123.59
28	G	101	DMU	C10-O7-C3	-2.13	112.69	117.96
26	O	303	PSC	O03-C19-O04	-2.13	118.22	123.59
24	C	303	CDL	OA8-CA6-CA4	2.12	114.61	108.43
15	N	602	HEA	C13-C12-C11	-2.12	111.17	114.35
25	C	306	PEK	O03-C21-O04	-2.12	118.25	123.59
19	L	101	TGL	OC1-CC1-CC2	-2.12	115.48	123.73
20	C	307	PGV	O04-C19-C20	-2.11	115.50	123.73
20	P	305	PGV	O03-C19-O04	-2.11	118.27	123.59
26	O	303	PSC	C29-C28-C27	-2.11	103.73	114.42
28	G	101	DMU	O3-C5-C10	2.11	115.16	110.05
19	N	609	TGL	C15-CC9-CC8	2.10	125.09	114.42
24	T	102	CDL	C80-C79-C78	2.10	125.09	114.42
22	B	302	CHD	C11-C12-C13	2.09	113.39	111.24
24	P	306	CDL	CA6-OA8-CA7	2.09	124.84	117.12
20	P	305	PGV	O06-C06-C05	-2.08	100.23	110.20
19	A	607	TGL	C16-C15-CC9	2.08	124.97	114.42
19	N	609	TGL	C16-C15-CC9	2.07	124.92	114.42
24	G	103	CDL	C39-C38-C37	2.07	124.91	114.42
20	A	609	PGV	C6-C5-C4	-2.04	104.05	114.42
24	C	303	CDL	C61-C60-C59	-2.04	104.05	114.42
19	D	201	TGL	CC3-CC2-CC1	-2.04	106.21	113.62
22	P	308	CHD	C9-C8-C7	2.04	114.31	111.88
20	C	307	PGV	O03-C19-O04	-2.04	118.45	123.59
15	N	603	HEA	CMB-C2B-C3B	2.03	128.67	124.69
19	N	610	TGL	OG2-CG2-CG3	2.03	115.76	108.40
25	G	102	PEK	C28-C27-C26	-2.03	104.11	114.42
15	N	603	HEA	CMC-C2C-C1C	-2.03	125.35	128.46
19	D	201	TGL	C20-CA9-CA8	2.03	124.71	114.42
20	C	307	PGV	C01-O03-C19	2.03	124.62	117.12
19	N	610	TGL	CB4-CB3-CB2	-2.02	105.92	113.19
19	Q	201	TGL	C16-C15-CC9	2.02	124.67	114.42
28	M	101	DMU	O1-C10-C5	-2.02	106.08	110.35
24	G	103	CDL	C23-C22-C21	2.01	124.64	114.42
19	D	201	TGL	C16-C15-CC9	2.01	124.63	114.42
28	M	101	DMU	C22-C19-C18	-2.01	104.58	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	607	TGL	CG1-OG1-CA1	2.00	124.54	117.12
15	A	603	HEA	C12-C13-C14	-2.00	106.95	112.23

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	602	HEA	ND
15	A	602	HEA	NB
15	A	603	HEA	ND
15	A	603	HEA	NB
15	N	602	HEA	ND
15	N	602	HEA	NA
15	N	602	HEA	NB
15	N	603	HEA	ND
15	N	603	HEA	NB

All (950) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	602	HEA	C16-C17-C18-C19
19	A	607	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	CC2-CC1-OG3-CG3
20	A	609	PGV	C03-O11-P-O12
20	A	609	PGV	C03-O11-P-O13
20	A	609	PGV	C03-O11-P-O14
20	A	609	PGV	C04-O12-P-O13
20	A	609	PGV	C02-C03-O11-P
20	A	609	PGV	C04-C05-C06-O06
20	A	609	PGV	O02-C1-O01-C02
20	A	609	PGV	C2-C1-O01-C02
20	C	307	PGV	C2-C1-O01-C02
20	N	607	PGV	C02-C03-O11-P
20	N	607	PGV	C04-C05-C06-O06
20	N	607	PGV	O02-C1-O01-C02
20	N	607	PGV	C2-C1-O01-C02
20	P	302	PGV	C03-O11-P-O13
20	P	302	PGV	C2-C1-O01-C02
20	P	302	PGV	C10-C11-C12-C13
24	C	303	CDL	CA2-C1-CB2-OB2
24	C	303	CDL	CA2-OA2-PA1-OA3
24	C	303	CDL	CA2-OA2-PA1-OA4
24	C	303	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
24	C	303	CDL	OA7-CA5-OA6-CA4
24	C	303	CDL	C11-CA5-OA6-CA4
24	C	303	CDL	CB2-OB2-PB2-OB3
24	C	303	CDL	CB2-OB2-PB2-OB4
24	C	303	CDL	CB2-OB2-PB2-OB5
24	G	103	CDL	C11-CA5-OA6-CA4
24	G	103	CDL	C1-CB2-OB2-PB2
24	G	103	CDL	CB3-OB5-PB2-OB2
24	G	103	CDL	CB3-OB5-PB2-OB3
24	G	103	CDL	CB3-OB5-PB2-OB4
24	P	306	CDL	CA2-OA2-PA1-OA3
24	P	306	CDL	CA2-OA2-PA1-OA4
24	P	306	CDL	CA2-OA2-PA1-OA5
24	P	306	CDL	CA3-OA5-PA1-OA2
24	P	306	CDL	CA3-OA5-PA1-OA3
24	P	306	CDL	CA3-OA5-PA1-OA4
24	P	306	CDL	OA7-CA5-OA6-CA4
24	P	306	CDL	C11-CA5-OA6-CA4
24	P	306	CDL	CB2-OB2-PB2-OB4
24	P	306	CDL	CB2-OB2-PB2-OB5
24	T	102	CDL	CA2-C1-CB2-OB2
24	T	102	CDL	C1-CB2-OB2-PB2
24	T	102	CDL	CB3-OB5-PB2-OB2
24	T	102	CDL	CB3-OB5-PB2-OB3
24	T	102	CDL	CB3-OB5-PB2-OB4
25	C	306	PEK	C03-O11-P-O12
25	C	306	PEK	C03-O11-P-O14
25	C	306	PEK	C04-O12-P-O13
25	C	306	PEK	C04-O12-P-O14
25	G	102	PEK	C11-C12-C13-C14
25	G	104	PEK	O03-C01-C02-O01
25	G	104	PEK	O12-C04-C05-N
25	G	104	PEK	C7-C8-C9-C10
25	P	309	PEK	C04-O12-P-O13
25	P	309	PEK	O12-C04-C05-N
25	T	101	PEK	C03-O11-P-O13
25	T	101	PEK	C03-O11-P-O14
25	T	101	PEK	C04-O12-P-O13
25	T	101	PEK	C04-O12-P-O14
25	T	101	PEK	O03-C01-C02-O01
25	T	101	PEK	O12-C04-C05-N
25	T	101	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	E	201	PSC	C03-O11-P-O14
26	E	201	PSC	C03-C02-O01-C1
26	E	201	PSC	C11-C10-C9-C8
26	O	303	PSC	C04-O12-P-O13
26	O	303	PSC	O12-C04-C05-N
28	G	101	DMU	O5-C6-O16-C18
28	G	101	DMU	C19-C18-O16-C6
28	P	301	DMU	C1-C6-O16-C18
28	P	301	DMU	O5-C6-O16-C18
19	D	201	TGL	OC1-CC1-OG3-CG3
20	A	609	PGV	O04-C19-O03-C01
20	N	607	PGV	O04-C19-O03-C01
20	A	609	PGV	C20-C19-O03-C01
20	N	607	PGV	C20-C19-O03-C01
19	Q	201	TGL	OC1-CC1-OG3-CG3
26	O	303	PSC	O04-C19-O03-C01
19	A	607	TGL	OB1-CB1-OG2-CG2
20	C	307	PGV	O02-C1-O01-C02
24	G	103	CDL	OA7-CA5-OA6-CA4
26	E	201	PSC	C02-C01-O03-C19
19	Q	201	TGL	CA2-CA1-OG1-CG1
19	Q	201	TGL	CC2-CC1-OG3-CG3
26	O	303	PSC	C20-C19-O03-C01
20	C	302	PGV	C10-C11-C12-C13
20	C	307	PGV	C10-C11-C12-C13
20	P	305	PGV	C10-C11-C12-C13
25	C	306	PEK	C4-C5-C6-C7
25	G	102	PEK	C10-C11-C12-C13
25	G	102	PEK	C13-C14-C15-C16
25	G	104	PEK	C4-C5-C6-C7
25	G	104	PEK	C13-C14-C15-C16
25	P	304	PEK	C13-C14-C15-C16
25	T	101	PEK	C13-C14-C15-C16
26	O	303	PSC	C11-C10-C9-C8
24	C	303	CDL	C62-C63-C64-C65
20	P	302	PGV	O02-C1-O01-C02
26	E	201	PSC	C04-C05-N-C06
28	G	101	DMU	O6-C11-C9-O1
24	T	102	CDL	C79-C80-C81-C82
24	C	303	CDL	O1-C1-CB2-OB2
24	G	103	CDL	O1-C1-CB2-OB2
24	P	306	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
24	P	306	CDL	O1-C1-CB2-OB2
24	T	102	CDL	O1-C1-CB2-OB2
19	N	610	TGL	CA2-CA1-OG1-CG1
19	Q	201	TGL	OA1-CA1-OG1-CG1
24	P	306	CDL	C51-CB5-OB6-CB4
24	T	102	CDL	C11-CA5-OA6-CA4
19	D	201	TGL	C13-C14-C29-C30
19	L	101	TGL	C20-C21-C22-C23
19	Q	201	TGL	CB9-C10-C11-C12
19	Q	201	TGL	C16-C15-CC9-CC8
24	T	102	CDL	C56-C57-C58-C59
20	C	307	PGV	C20-C21-C22-C23
26	E	201	PSC	C20-C21-C22-C23
28	P	301	DMU	O5-C4-C57-O61
19	N	609	TGL	C12-C13-C14-C29
24	G	103	CDL	C56-C57-C58-C59
28	Z	101	DMU	O6-C11-C9-O1
24	P	306	CDL	OB7-CB5-OB6-CB4
24	G	103	CDL	C15-C16-C17-C18
20	N	607	PGV	C05-C04-O12-P
28	M	101	DMU	O6-C11-C9-C8
19	L	101	TGL	CC3-CC4-CC5-CC6
24	T	102	CDL	C15-C16-C17-C18
22	P	307	CHD	C21-C20-C22-C23
19	N	610	TGL	OA1-CA1-OG1-CG1
15	N	602	HEA	C15-C16-C17-C18
28	Z	101	DMU	O6-C11-C9-C8
22	C	304	CHD	C17-C20-C22-C23
22	P	307	CHD	C17-C20-C22-C23
25	G	102	PEK	C7-C8-C9-C10
26	O	303	PSC	C11-C12-C13-C14
19	D	201	TGL	C21-C22-C23-C24
19	Q	201	TGL	C21-C22-C23-C24
24	G	103	CDL	C63-C64-C65-C66
24	T	102	CDL	C73-C74-C75-C76
24	P	306	CDL	C82-C83-C84-C85
24	C	303	CDL	CB2-C1-CA2-OA2
24	G	103	CDL	CA2-C1-CB2-OB2
24	P	306	CDL	CB2-C1-CA2-OA2
24	T	102	CDL	OA7-CA5-OA6-CA4
26	O	303	PSC	O02-C1-O01-C02
19	A	607	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
25	T	101	PEK	C28-C29-C30-C31
19	A	607	TGL	CC2-CC1-OG3-CG3
19	L	101	TGL	CA2-CA1-OG1-CG1
19	N	609	TGL	CC2-CC1-OG3-CG3
24	G	103	CDL	C31-CA7-OA8-CA6
24	T	102	CDL	C31-CA7-OA8-CA6
25	T	101	PEK	C22-C21-O03-C01
26	E	201	PSC	C20-C19-O03-C01
24	T	102	CDL	C22-C23-C24-C25
24	G	103	CDL	C41-C42-C43-C44
24	G	103	CDL	C22-C23-C24-C25
19	N	609	TGL	CA9-C20-C21-C22
20	P	302	PGV	O12-C04-C05-O05
28	G	101	DMU	C1-C6-O16-C18
20	A	608	PGV	C26-C27-C28-C29
28	M	101	DMU	O6-C11-C9-O1
28	G	101	DMU	C3-C4-C57-O61
26	O	303	PSC	C2-C1-O01-C02
28	G	101	DMU	O6-C11-C9-C8
28	P	301	DMU	O6-C11-C9-C8
26	E	201	PSC	C1-C2-C3-C4
19	N	609	TGL	OC1-CC1-OG3-CG3
24	G	103	CDL	OA9-CA7-OA8-CA6
26	E	201	PSC	O04-C19-O03-C01
28	P	301	DMU	C3-C4-C57-O61
26	E	201	PSC	C28-C29-C30-C31
19	D	201	TGL	CB1-CB2-CB3-CB4
20	A	609	PGV	C1-C2-C3-C4
20	C	307	PGV	C1-C2-C3-C4
24	G	103	CDL	CA7-C31-C32-C33
25	G	102	PEK	C4-C5-C6-C7
25	P	309	PEK	C7-C8-C9-C10
25	T	101	PEK	C7-C8-C9-C10
25	T	101	PEK	C10-C11-C12-C13
19	A	607	TGL	CA1-CA2-CA3-CA4
19	A	607	TGL	CB1-CB2-CB3-CB4
19	N	609	TGL	CA1-CA2-CA3-CA4
20	C	307	PGV	C19-C20-C21-C22
20	P	302	PGV	C1-C2-C3-C4
24	G	103	CDL	CA5-C11-C12-C13
24	P	306	CDL	CB7-C71-C72-C73
24	T	102	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
26	O	303	PSC	C19-C20-C21-C22
20	C	307	PGV	C2-C3-C4-C5
22	C	304	CHD	C21-C20-C22-C23
24	T	102	CDL	CA7-C31-C32-C33
19	A	607	TGL	OC1-CC1-OG3-CG3
24	T	102	CDL	OA9-CA7-OA8-CA6
19	L	101	TGL	CC1-CC2-CC3-CC4
20	C	307	PGV	O12-C04-C05-O05
24	C	303	CDL	O1-C1-CA2-OA2
19	N	609	TGL	OB1-CB1-OG2-CG2
25	G	104	PEK	C22-C21-O03-C01
25	T	101	PEK	O04-C21-O03-C01
20	N	607	PGV	C19-C20-C21-C22
26	E	201	PSC	C11-C12-C13-C14
19	L	101	TGL	OA1-CA1-OG1-CG1
19	N	609	TGL	CB2-CB1-OG2-CG2
19	A	607	TGL	C16-C15-CC9-CC8
19	N	609	TGL	C22-C23-C24-C25
20	N	607	PGV	C04-O12-P-O11
24	C	303	CDL	CA3-OA5-PA1-OA2
25	C	306	PEK	C04-O12-P-O11
25	P	309	PEK	C04-O12-P-O11
25	T	101	PEK	C03-O11-P-O12
25	T	101	PEK	C04-O12-P-O11
26	O	303	PSC	C04-O12-P-O11
24	T	102	CDL	C63-C64-C65-C66
25	G	102	PEK	C1-C2-C3-C4
20	C	307	PGV	O12-C04-C05-C06
24	P	306	CDL	CA2-C1-CB2-OB2
26	E	201	PSC	C04-C05-N-C07
26	O	303	PSC	C04-C05-N-C06
26	O	303	PSC	C04-C05-N-C07
26	O	303	PSC	C04-C05-N-C08
25	G	104	PEK	C2-C3-C4-C5
26	O	303	PSC	C22-C23-C24-C25
19	D	201	TGL	C17-C18-C19-C33
19	L	101	TGL	CC6-CC7-CC8-CC9
19	N	609	TGL	CA5-CA6-CA7-CA8
19	N	610	TGL	CA3-CA4-CA5-CA6
19	N	610	TGL	CC3-CC4-CC5-CC6
20	P	302	PGV	C29-C30-C31-C32
24	G	103	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
24	P	306	CDL	C37-C38-C39-C40
24	P	306	CDL	C51-C52-C53-C54
24	T	102	CDL	C18-C19-C20-C21
25	C	306	PEK	C29-C30-C31-C32
25	G	104	PEK	C27-C28-C29-C30
19	A	607	TGL	CB3-CB4-CB5-CB6
19	A	607	TGL	CB4-CB5-CB6-CB7
19	D	201	TGL	CA6-CA7-CA8-CA9
19	L	101	TGL	C16-C15-CC9-CC8
20	A	609	PGV	C14-C15-C16-C17
20	C	302	PGV	C7-C8-C9-C10
20	C	307	PGV	C6-C7-C8-C9
20	N	608	PGV	C26-C27-C28-C29
24	G	103	CDL	C61-C62-C63-C64
24	T	102	CDL	C59-C60-C61-C62
19	A	607	TGL	CG1-CG2-OG2-CB1
19	D	201	TGL	CG3-CG2-OG2-CB1
19	A	607	TGL	C14-C29-C30-C31
19	L	101	TGL	CB6-CB7-CB8-CB9
19	N	610	TGL	CC6-CC7-CC8-CC9
24	P	306	CDL	C58-C59-C60-C61
25	T	101	PEK	C32-C33-C34-C35
28	G	101	DMU	O5-C4-C57-O61
20	N	607	PGV	C10-C11-C12-C13
25	P	304	PEK	C4-C5-C6-C7
19	L	101	TGL	C21-C20-CA9-CA8
19	Q	201	TGL	CA2-CA3-CA4-CA5
19	Q	201	TGL	C17-C18-C19-C33
20	A	608	PGV	C29-C30-C31-C32
24	C	303	CDL	C17-C18-C19-C20
24	C	303	CDL	C19-C20-C21-C22
24	T	102	CDL	C82-C83-C84-C85
20	N	607	PGV	O12-C04-C05-O05
24	G	103	CDL	O1-C1-CA2-OA2
19	D	201	TGL	CC2-CC3-CC4-CC5
19	N	610	TGL	CB4-CB5-CB6-CB7
24	C	303	CDL	CB7-C71-C72-C73
24	P	306	CDL	CA5-C11-C12-C13
19	N	609	TGL	C16-C17-C18-C19
19	N	610	TGL	CB9-C10-C11-C12
20	C	307	PGV	C3-C4-C5-C6
26	E	201	PSC	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
25	G	104	PEK	O04-C21-O03-C01
19	D	201	TGL	C21-C20-CA9-CA8
19	N	610	TGL	C23-C24-C25-C26
19	Q	201	TGL	CC6-CC7-CC8-CC9
20	C	302	PGV	C14-C15-C16-C17
19	Q	201	TGL	CB1-CB2-CB3-CB4
19	N	609	TGL	CC7-CC8-CC9-C15
19	N	610	TGL	CB5-CB6-CB7-CB8
19	N	610	TGL	C16-C15-CC9-CC8
20	N	608	PGV	C23-C24-C25-C26
20	P	302	PGV	C3-C4-C5-C6
24	T	102	CDL	C55-C56-C57-C58
25	P	309	PEK	C33-C34-C35-C36
25	T	101	PEK	C34-C35-C36-C37
19	N	610	TGL	C11-C10-CB9-CB8
24	C	303	CDL	C60-C61-C62-C63
24	C	303	CDL	C81-C82-C83-C84
26	O	303	PSC	C29-C30-C31-C32
20	C	307	PGV	C04-C05-C06-O06
19	D	201	TGL	CA2-CA3-CA4-CA5
19	N	609	TGL	C17-C18-C19-C33
20	N	607	PGV	C22-C23-C24-C25
24	C	303	CDL	C71-C72-C73-C74
24	P	306	CDL	C14-C15-C16-C17
24	P	306	CDL	C83-C84-C85-C86
25	G	102	PEK	C25-C26-C27-C28
26	E	201	PSC	C13-C14-C15-C16
24	T	102	CDL	CA5-C11-C12-C13
19	A	607	TGL	CA9-C20-C21-C22
19	D	201	TGL	C12-C13-C14-C29
19	L	101	TGL	CC4-CC5-CC6-CC7
19	N	609	TGL	CC4-CC5-CC6-CC7
19	N	610	TGL	C22-C23-C24-C25
20	C	307	PGV	C30-C31-C32-C33
20	P	302	PGV	C23-C24-C25-C26
24	C	303	CDL	C58-C59-C60-C61
24	G	103	CDL	C38-C39-C40-C41
24	G	103	CDL	C54-C55-C56-C57
24	P	306	CDL	C72-C73-C74-C75
24	T	102	CDL	C11-C12-C13-C14
25	G	102	PEK	C24-C25-C26-C27
25	G	104	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	G	104	PEK	C33-C34-C35-C36
25	G	104	PEK	C34-C35-C36-C37
25	P	304	PEK	C31-C32-C33-C34
25	T	101	PEK	C33-C34-C35-C36
28	M	101	DMU	C19-C22-C25-C28
28	Z	101	DMU	C25-C28-C31-C34
26	E	201	PSC	C04-C05-N-C08
19	A	607	TGL	C11-C10-CB9-CB8
19	N	609	TGL	C14-C29-C30-C31
24	C	303	CDL	C16-C17-C18-C19
24	C	303	CDL	C76-C77-C78-C79
24	T	102	CDL	C54-C55-C56-C57
25	G	104	PEK	C25-C26-C27-C28
25	G	104	PEK	C32-C33-C34-C35
19	N	609	TGL	C15-C16-C17-C18
19	A	607	TGL	CB9-C10-C11-C12
19	N	609	TGL	CA2-CA3-CA4-CA5
19	Q	201	TGL	CB5-CB6-CB7-CB8
20	C	307	PGV	C22-C23-C24-C25
22	C	304	CHD	C20-C22-C23-C24
24	P	306	CDL	C61-C62-C63-C64
20	C	307	PGV	C26-C27-C28-C29
24	C	303	CDL	C41-C42-C43-C44
25	P	309	PEK	C34-C35-C36-C37
26	E	201	PSC	C29-C30-C31-C32
19	A	607	TGL	CB6-CB7-CB8-CB9
19	N	610	TGL	CA9-C20-C21-C22
19	N	610	TGL	C14-C29-C30-C31
20	P	305	PGV	C22-C23-C24-C25
24	P	306	CDL	C73-C74-C75-C76
19	A	607	TGL	C17-C18-C19-C33
20	A	609	PGV	C21-C22-C23-C24
20	C	302	PGV	C27-C28-C29-C30
20	P	302	PGV	C13-C14-C15-C16
24	P	306	CDL	C42-C43-C44-C45
25	G	104	PEK	C10-C11-C12-C13
19	Q	201	TGL	C19-C33-C34-C35
20	A	609	PGV	C7-C8-C9-C10
25	P	304	PEK	C26-C27-C28-C29
19	Q	201	TGL	CC4-CC5-CC6-CC7
26	E	201	PSC	C26-C27-C28-C29
24	C	303	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CC6-CC7-CC8-CC9
19	N	609	TGL	C20-C21-C22-C23
20	P	305	PGV	C14-C15-C16-C17
24	P	306	CDL	C12-C13-C14-C15
24	P	306	CDL	C15-C16-C17-C18
25	T	101	PEK	C27-C28-C29-C30
20	A	609	PGV	O05-C05-C06-O06
20	C	307	PGV	O05-C05-C06-O06
20	N	607	PGV	O05-C05-C06-O06
19	A	607	TGL	CA5-CA6-CA7-CA8
19	L	101	TGL	C21-C22-C23-C24
24	C	303	CDL	C72-C73-C74-C75
24	G	103	CDL	C18-C19-C20-C21
24	T	102	CDL	C36-C37-C38-C39
25	G	104	PEK	C30-C31-C32-C33
20	N	608	PGV	C11-C10-C9-C8
25	P	304	PEK	C15-C16-C17-C18
25	P	309	PEK	C2-C3-C4-C5
20	P	302	PGV	C19-C20-C21-C22
28	Z	101	DMU	C19-C22-C25-C28
19	Q	201	TGL	CB2-CB3-CB4-CB5
24	P	306	CDL	C71-C72-C73-C74
26	O	303	PSC	C20-C21-C22-C23
20	P	302	PGV	C6-C7-C8-C9
24	C	303	CDL	C12-C13-C14-C15
19	N	610	TGL	CC1-CC2-CC3-CC4
20	P	302	PGV	O12-C04-C05-C06
19	N	609	TGL	CB4-CB5-CB6-CB7
20	P	302	PGV	C14-C15-C16-C17
19	L	101	TGL	OB1-CB1-OG2-CG2
24	C	303	CDL	OB7-CB5-OB6-CB4
19	D	201	TGL	C18-C19-C33-C34
19	L	101	TGL	C18-C19-C33-C34
19	N	610	TGL	CA2-CA3-CA4-CA5
19	N	610	TGL	C17-C18-C19-C33
24	C	303	CDL	C36-C37-C38-C39
24	C	303	CDL	C53-C54-C55-C56
24	G	103	CDL	C62-C63-C64-C65
24	G	103	CDL	C78-C79-C80-C81
24	P	306	CDL	C60-C61-C62-C63
20	C	302	PGV	C25-C26-C27-C28
20	P	305	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	C	303	CDL	C73-C74-C75-C76
25	P	309	PEK	C28-C29-C30-C31
19	L	101	TGL	C22-C23-C24-C25
24	P	306	CDL	C16-C17-C18-C19
25	G	102	PEK	C23-C24-C25-C26
25	C	306	PEK	C25-C26-C27-C28
20	N	607	PGV	C2-C3-C4-C5
19	N	609	TGL	CA3-CA4-CA5-CA6
20	C	302	PGV	C22-C23-C24-C25
20	P	302	PGV	C24-C25-C26-C27
28	P	301	DMU	C28-C31-C34-C37
20	A	609	PGV	C10-C11-C12-C13
25	C	306	PEK	C10-C11-C12-C13
25	T	101	PEK	C4-C5-C6-C7
24	P	306	CDL	C78-C79-C80-C81
25	P	304	PEK	C25-C26-C27-C28
25	G	102	PEK	C2-C3-C4-C5
25	G	104	PEK	C15-C16-C17-C18
25	P	304	PEK	C1-C2-C3-C4
24	P	306	CDL	C36-C37-C38-C39
24	P	306	CDL	C80-C81-C82-C83
25	G	102	PEK	C16-C17-C18-C19
19	L	101	TGL	C12-C13-C14-C29
26	O	303	PSC	C2-C3-C4-C5
24	G	103	CDL	CB5-C51-C52-C53
19	D	201	TGL	C11-C10-CB9-CB8
19	Q	201	TGL	C12-C13-C14-C29
28	M	101	DMU	C22-C25-C28-C31
24	T	102	CDL	C71-C72-C73-C74
25	G	104	PEK	C16-C17-C18-C19
24	C	303	CDL	C11-C12-C13-C14
24	C	303	CDL	C13-C14-C15-C16
24	C	303	CDL	C83-C84-C85-C86
24	G	103	CDL	C57-C58-C59-C60
20	P	305	PGV	C1-C2-C3-C4
19	L	101	TGL	CB2-CB1-OG2-CG2
19	N	610	TGL	CB2-CB1-OG2-CG2
25	G	104	PEK	C2-C1-O01-C02
20	C	307	PGV	O01-C02-C03-O11
19	D	201	TGL	C10-C11-C12-C13
20	P	302	PGV	C25-C26-C27-C28
20	P	302	PGV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
24	G	103	CDL	C36-C37-C38-C39
24	T	102	CDL	C80-C81-C82-C83
19	N	610	TGL	OB1-CB1-OG2-CG2
19	N	609	TGL	CB9-C10-C11-C12
24	T	102	CDL	C75-C76-C77-C78
19	L	101	TGL	C19-C33-C34-C35
24	C	303	CDL	C42-C43-C44-C45
19	N	609	TGL	C21-C20-CA9-CA8
19	Q	201	TGL	CA6-CA7-CA8-CA9
25	P	309	PEK	C25-C26-C27-C28
24	T	102	CDL	C39-C40-C41-C42
19	A	607	TGL	C16-C17-C18-C19
20	C	302	PGV	C28-C29-C30-C31
24	T	102	CDL	C31-C32-C33-C34
25	G	104	PEK	O02-C1-O01-C02
19	N	610	TGL	CC9-C15-C16-C17
25	P	304	PEK	C32-C33-C34-C35
25	P	309	PEK	C22-C23-C24-C25
26	E	201	PSC	C03-O11-P-O12
20	C	307	PGV	C13-C14-C15-C16
20	A	608	PGV	C19-C20-C21-C22
20	A	608	PGV	C14-C15-C16-C17
19	D	201	TGL	CA2-CA1-OG1-CG1
20	C	307	PGV	C01-C02-C03-O11
24	C	303	CDL	OA5-CA3-CA4-CA6
24	G	103	CDL	OA5-CA3-CA4-CA6
19	L	101	TGL	CA5-CA6-CA7-CA8
20	N	607	PGV	C24-C25-C26-C27
24	P	306	CDL	C77-C78-C79-C80
24	T	102	CDL	C41-C42-C43-C44
28	G	101	DMU	O16-C18-C19-C22
20	P	305	PGV	C12-C13-C14-C15
25	C	306	PEK	C24-C25-C26-C27
19	D	201	TGL	C22-C23-C24-C25
19	D	201	TGL	C24-C25-C26-C27
19	N	610	TGL	C21-C22-C23-C24
19	N	610	TGL	CC4-CC5-CC6-CC7
20	A	609	PGV	C24-C25-C26-C27
25	C	306	PEK	C33-C34-C35-C36
25	G	104	PEK	C22-C23-C24-C25
19	A	607	TGL	CC4-CC5-CC6-CC7
28	Z	101	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
19	N	610	TGL	C25-C26-C27-C28
20	A	609	PGV	O03-C01-C02-C03
24	C	303	CDL	CB3-CB4-CB6-OB8
20	N	608	PGV	C10-C11-C12-C13
19	D	201	TGL	C15-C16-C17-C18
24	C	303	CDL	C61-C62-C63-C64
24	P	306	CDL	C74-C75-C76-C77
19	L	101	TGL	C29-C30-C31-C32
19	Q	201	TGL	C33-C34-C35-C36
25	C	306	PEK	C26-C27-C28-C29
19	L	101	TGL	CC7-CC8-CC9-C15
20	A	608	PGV	C30-C31-C32-C33
20	N	608	PGV	C24-C25-C26-C27
24	T	102	CDL	C61-C62-C63-C64
26	E	201	PSC	C19-C20-C21-C22
24	P	306	CDL	C24-C25-C26-C27
26	O	303	PSC	C24-C25-C26-C27
19	N	609	TGL	C21-C22-C23-C24
24	C	303	CDL	C24-C25-C26-C27
20	A	609	PGV	C11-C10-C9-C8
20	C	307	PGV	C11-C10-C9-C8
25	G	102	PEK	C15-C16-C17-C18
25	P	304	PEK	C2-C3-C4-C5
19	A	607	TGL	C21-C22-C23-C24
24	T	102	CDL	C81-C82-C83-C84
25	T	101	PEK	C26-C27-C28-C29
20	N	608	PGV	C31-C32-C33-C34
20	P	302	PGV	C7-C8-C9-C10
19	D	201	TGL	C11-C12-C13-C14
20	A	609	PGV	C26-C27-C28-C29
20	N	607	PGV	C03-C02-O01-C1
19	N	610	TGL	CC2-CC3-CC4-CC5
20	N	607	PGV	C23-C24-C25-C26
20	P	302	PGV	C15-C16-C17-C18
24	P	306	CDL	C21-C22-C23-C24
19	N	610	TGL	C29-C30-C31-C32
20	P	302	PGV	C31-C32-C33-C34
25	C	306	PEK	O01-C02-C03-O11
24	C	303	CDL	CA5-C11-C12-C13
26	O	303	PSC	C1-C2-C3-C4
28	G	101	DMU	C2-C3-O7-C10
24	G	103	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	C20-C21-C22-C23
19	D	201	TGL	C19-C33-C34-C35
19	D	201	TGL	OA1-CA1-OG1-CG1
24	G	103	CDL	C14-C15-C16-C17
24	G	103	CDL	C31-C32-C33-C34
24	G	103	CDL	C74-C75-C76-C77
24	T	102	CDL	C44-C45-C46-C47
20	P	302	PGV	C22-C23-C24-C25
20	P	302	PGV	C30-C31-C32-C33
24	C	303	CDL	C59-C60-C61-C62
24	P	306	CDL	C13-C14-C15-C16
24	T	102	CDL	C16-C17-C18-C19
25	G	102	PEK	C17-C18-C19-C20
24	C	303	CDL	C84-C85-C86-C87
24	P	306	CDL	C79-C80-C81-C82
24	T	102	CDL	C24-C25-C26-C27
25	T	101	PEK	C25-C26-C27-C28
25	P	304	PEK	C16-C17-C18-C19
26	O	303	PSC	C28-C29-C30-C31
20	N	607	PGV	O12-C04-C05-C06
19	L	101	TGL	C10-C11-C12-C13
19	Q	201	TGL	C21-C20-CA9-CA8
19	Q	201	TGL	C16-C17-C18-C19
20	A	608	PGV	C31-C32-C33-C34
25	T	101	PEK	C29-C30-C31-C32
28	Z	101	DMU	C34-C37-C40-C43
25	P	304	PEK	C10-C11-C12-C13
19	L	101	TGL	C11-C12-C13-C14
20	N	607	PGV	C01-C02-C03-O11
24	P	306	CDL	OA5-CA3-CA4-CA6
24	P	306	CDL	OB5-CB3-CB4-CB6
24	T	102	CDL	OA5-CA3-CA4-CA6
19	D	201	TGL	CB9-C10-C11-C12
19	N	610	TGL	C11-C12-C13-C14
24	T	102	CDL	C62-C63-C64-C65
24	T	102	CDL	C71-CB7-OB8-CB6
22	P	307	CHD	C16-C17-C20-C22
19	D	201	TGL	CC1-CC2-CC3-CC4
28	G	101	DMU	C4-C3-O7-C10
22	P	307	CHD	C20-C22-C23-C24
26	E	201	PSC	C23-C24-C25-C26
19	A	607	TGL	CC5-CC6-CC7-CC8

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Mol	Chain	Res	Type	Atoms
24	G	103	CDL	CB7-C71-C72-C73
20	C	307	PGV	C02-C03-O11-P
20	P	302	PGV	C02-C03-O11-P
20	P	302	PGV	C05-C04-O12-P
19	A	607	TGL	C22-C23-C24-C25
20	P	305	PGV	C26-C27-C28-C29
19	D	201	TGL	CA5-CA6-CA7-CA8
19	Q	201	TGL	CA9-C20-C21-C22
24	P	306	CDL	C59-C60-C61-C62
25	G	102	PEK	C27-C28-C29-C30
28	M	101	DMU	O5-C4-C57-O61
19	Q	201	TGL	OG1-CG1-CG2-CG3
19	Q	201	TGL	CG1-CG2-CG3-OG3
25	G	104	PEK	O03-C01-C02-C03
26	O	303	PSC	O03-C01-C02-C03
20	N	607	PGV	C7-C8-C9-C10
25	P	304	PEK	C7-C8-C9-C10
24	C	303	CDL	C32-C33-C34-C35
25	P	309	PEK	C32-C33-C34-C35
26	O	303	PSC	C5-C6-C7-C8
25	G	102	PEK	C3-C4-C5-C6
25	P	304	PEK	C3-C4-C5-C6
25	C	306	PEK	C11-C10-C9-C8
25	C	306	PEK	C9-C10-C11-C12
25	G	102	PEK	C9-C10-C11-C12
25	G	104	PEK	C03-O11-P-O12
25	G	104	PEK	C9-C10-C11-C12
25	G	104	PEK	C11-C12-C13-C14
25	G	104	PEK	C12-C13-C14-C15
25	P	304	PEK	C5-C6-C7-C8
25	P	304	PEK	C9-C10-C11-C12
25	P	309	PEK	C9-C10-C11-C12
25	T	101	PEK	C5-C6-C7-C8
25	T	101	PEK	C9-C10-C11-C12
25	T	101	PEK	C12-C13-C14-C15
26	E	201	PSC	C04-O12-P-O11
26	E	201	PSC	C9-C10-C11-C12
26	E	201	PSC	C10-C11-C12-C13
26	O	303	PSC	C9-C10-C11-C12
19	N	609	TGL	CA4-CA5-CA6-CA7
20	A	609	PGV	O01-C02-C03-O11
20	P	302	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
24	P	306	CDL	OA5-CA3-CA4-OA6
24	T	102	CDL	OA5-CA3-CA4-OA6
25	T	101	PEK	O01-C02-C03-O11
25	C	306	PEK	C30-C31-C32-C33
19	N	610	TGL	CC5-CC6-CC7-CC8
19	Q	201	TGL	C10-C11-C12-C13
19	A	607	TGL	OG1-CG1-CG2-OG2
19	D	201	TGL	OG1-CG1-CG2-OG2
19	Q	201	TGL	OG2-CG2-CG3-OG3
24	G	103	CDL	OB6-CB4-CB6-OB8
24	P	306	CDL	OB6-CB4-CB6-OB8
24	T	102	CDL	OB6-CB4-CB6-OB8
26	O	303	PSC	O03-C01-C02-O01
26	O	303	PSC	C31-C32-C33-C34
25	C	306	PEK	C1-C2-C3-C4
15	A	602	HEA	C19-C20-C21-C22
26	O	303	PSC	C4-C5-C6-C7
19	Q	201	TGL	CA5-CA6-CA7-CA8
26	O	303	PSC	C23-C24-C25-C26
19	N	609	TGL	CC5-CC6-CC7-CC8
20	P	305	PGV	C02-C03-O11-P
24	C	303	CDL	C1-CA2-OA2-PA1
24	P	306	CDL	C1-CA2-OA2-PA1
24	T	102	CDL	CA4-CA3-OA5-PA1
20	P	302	PGV	C12-C13-C14-C15
20	C	307	PGV	C24-C25-C26-C27
26	O	303	PSC	C21-C22-C23-C24
24	C	303	CDL	C75-C76-C77-C78
25	P	304	PEK	C17-C18-C19-C20
25	P	304	PEK	C2-C1-O01-C02
19	Q	201	TGL	CA4-CA5-CA6-CA7
25	C	306	PEK	C34-C35-C36-C37
19	L	101	TGL	C11-C10-CB9-CB8
28	G	101	DMU	C25-C28-C31-C34
24	C	303	CDL	OB5-CB3-CB4-CB6
25	G	104	PEK	C01-C02-C03-O11
25	T	101	PEK	C01-C02-C03-O11
20	A	609	PGV	C25-C26-C27-C28
25	T	101	PEK	C16-C17-C18-C19
24	T	102	CDL	C37-C38-C39-C40
24	C	303	CDL	C34-C35-C36-C37
19	Q	201	TGL	C18-C19-C33-C34

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Mol	Chain	Res	Type	Atoms
20	C	307	PGV	C31-C32-C33-C34
24	C	303	CDL	C74-C75-C76-C77
24	C	303	CDL	C40-C41-C42-C43
19	D	201	TGL	CC5-CC6-CC7-CC8
25	P	309	PEK	C29-C30-C31-C32
26	O	303	PSC	C03-C02-O01-C1
19	D	201	TGL	CA9-C20-C21-C22
24	P	306	CDL	C76-C77-C78-C79
19	D	201	TGL	C14-C29-C30-C31
24	G	103	CDL	C40-C41-C42-C43
20	A	609	PGV	C31-C32-C33-C34
25	G	102	PEK	C35-C36-C37-C38
24	C	303	CDL	CA3-CA4-CA6-OA8
24	P	306	CDL	CA3-CA4-CA6-OA8
24	P	306	CDL	CB3-CB4-CB6-OB8
25	T	101	PEK	O03-C01-C02-C03
20	N	607	PGV	O01-C02-C03-O11
24	C	303	CDL	OA5-CA3-CA4-OA6
24	G	103	CDL	OA5-CA3-CA4-OA6
26	E	201	PSC	O01-C02-C03-O11
19	A	607	TGL	CA4-CA5-CA6-CA7
19	D	201	TGL	C16-C15-CC9-CC8
24	T	102	CDL	OB9-CB7-OB8-CB6
19	L	101	TGL	OG2-CG2-CG3-OG3
19	N	610	TGL	OG2-CG2-CG3-OG3
24	C	303	CDL	OA6-CA4-CA6-OA8
19	N	609	TGL	C18-C19-C33-C34
24	T	102	CDL	C14-C15-C16-C17
20	C	302	PGV	C13-C14-C15-C16
20	A	609	PGV	C12-C13-C14-C15
20	N	608	PGV	C12-C13-C14-C15
24	G	103	CDL	C44-C45-C46-C47
20	P	302	PGV	C9-C10-C11-C12
28	P	301	DMU	C25-C28-C31-C34
25	P	309	PEK	O04-C21-O03-C01
19	A	607	TGL	C13-C14-C29-C30
20	A	609	PGV	C28-C29-C30-C31
24	G	103	CDL	C13-C14-C15-C16
25	P	309	PEK	C22-C21-O03-C01
19	N	609	TGL	CB6-CB7-CB8-CB9
24	C	303	CDL	C35-C36-C37-C38
25	P	304	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CC3-CC4-CC5-CC6
19	N	609	TGL	C24-C25-C26-C27
20	A	609	PGV	C04-O12-P-O11
20	P	302	PGV	C03-O11-P-O12
24	G	103	CDL	CB2-OB2-PB2-OB5
24	T	102	CDL	CB2-OB2-PB2-OB5
19	A	607	TGL	CC7-CC8-CC9-C15
20	A	609	PGV	C05-C04-O12-P
20	C	302	PGV	C02-C03-O11-P
24	C	303	CDL	CA4-CA3-OA5-PA1
20	C	302	PGV	C26-C27-C28-C29
20	N	607	PGV	C04-O12-P-O13
24	C	303	CDL	CA3-OA5-PA1-OA3
24	P	306	CDL	CB2-OB2-PB2-OB3
26	E	201	PSC	C03-O11-P-O13
26	E	201	PSC	C04-O12-P-O13
24	C	303	CDL	CB5-C51-C52-C53
25	C	306	PEK	C01-C02-C03-O11
26	E	201	PSC	C01-C02-C03-O11
25	C	306	PEK	C28-C29-C30-C31
19	L	101	TGL	OG2-CB1-CB2-CB3
26	E	201	PSC	C31-C32-C33-C34
19	N	609	TGL	C23-C24-C25-C26
20	C	302	PGV	C15-C16-C17-C18
25	P	304	PEK	C24-C25-C26-C27
25	P	304	PEK	C05-C04-O12-P
26	O	303	PSC	C05-C04-O12-P
20	C	307	PGV	C27-C28-C29-C30
19	Q	201	TGL	C11-C10-CB9-CB8
25	C	306	PEK	C15-C16-C17-C18
24	P	306	CDL	CA7-C31-C32-C33
19	L	101	TGL	C24-C25-C26-C27
20	N	607	PGV	C14-C15-C16-C17
24	C	303	CDL	OB5-CB3-CB4-OB6
25	G	104	PEK	O01-C02-C03-O11
25	G	102	PEK	C28-C29-C30-C31
19	L	101	TGL	CA6-CA7-CA8-CA9
20	C	302	PGV	C20-C21-C22-C23
24	T	102	CDL	C64-C65-C66-C67
20	N	607	PGV	C21-C22-C23-C24
19	L	101	TGL	CG1-CG2-CG3-OG3
19	N	610	TGL	CG1-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
20	N	608	PGV	C25-C26-C27-C28
24	C	303	CDL	C57-C58-C59-C60
26	E	201	PSC	O12-C04-C05-N
19	Q	201	TGL	OG1-CG1-CG2-OG2
20	A	609	PGV	O03-C01-C02-O01
24	P	306	CDL	OA6-CA4-CA6-OA8
25	P	304	PEK	O03-C01-C02-O01
25	C	306	PEK	C7-C8-C9-C10
19	Q	201	TGL	CC3-CC4-CC5-CC6
24	G	103	CDL	C73-C74-C75-C76
20	P	305	PGV	C28-C29-C30-C31
20	P	305	PGV	C21-C22-C23-C24
19	L	101	TGL	OG1-CA1-CA2-CA3
24	P	306	CDL	C44-C45-C46-C47
19	L	101	TGL	CA3-CA4-CA5-CA6
19	D	201	TGL	C16-C17-C18-C19
28	M	101	DMU	C28-C31-C34-C37
26	O	303	PSC	O03-C19-C20-C21
24	T	102	CDL	C40-C41-C42-C43
25	C	306	PEK	O04-C21-O03-C01
20	N	608	PGV	C29-C30-C31-C32
20	P	302	PGV	C4-C5-C6-C7
24	C	303	CDL	C38-C39-C40-C41
24	P	306	CDL	C43-C44-C45-C46
19	N	609	TGL	CG1-CG2-OG2-CB1
20	A	609	PGV	C03-C02-O01-C1
20	P	302	PGV	C01-C02-C03-O11
22	P	307	CHD	C13-C17-C20-C22
19	A	607	TGL	CA6-CA7-CA8-CA9
20	A	609	PGV	O03-C19-C20-C21
19	Q	201	TGL	CC7-CC8-CC9-C15
24	G	103	CDL	C17-C18-C19-C20
20	N	607	PGV	C5-C6-C7-C8
25	C	306	PEK	C22-C21-O03-C01
25	T	101	PEK	C3-C4-C5-C6
24	C	303	CDL	OB6-CB4-CB6-OB8
19	N	610	TGL	C12-C13-C14-C29
20	C	307	PGV	C04-O12-P-O11
20	N	607	PGV	C03-O11-P-O12
20	P	302	PGV	C04-O12-P-O11
24	T	102	CDL	CA3-OA5-PA1-OA2
25	C	306	PEK	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	OG1-CG1-CG2-CG3
24	G	103	CDL	CB3-CB4-CB6-OB8
24	T	102	CDL	CB3-CB4-CB6-OB8
19	A	607	TGL	C24-C25-C26-C27
19	N	610	TGL	CC7-CC8-CC9-C15
24	G	103	CDL	C55-C56-C57-C58
19	N	610	TGL	CA7-CA8-CA9-C20
24	G	103	CDL	C34-C35-C36-C37
24	P	306	CDL	C35-C36-C37-C38
22	P	307	CHD	C16-C17-C20-C21
20	C	302	PGV	C23-C24-C25-C26
20	N	607	PGV	C20-C21-C22-C23
24	G	103	CDL	C16-C17-C18-C19
25	P	309	PEK	C23-C24-C25-C26
24	T	102	CDL	CB7-C71-C72-C73
20	P	305	PGV	C05-C04-O12-P
24	G	103	CDL	CB4-CB3-OB5-PB2
24	P	306	CDL	CA4-CA3-OA5-PA1
24	G	103	CDL	C35-C36-C37-C38
24	P	306	CDL	C19-C20-C21-C22
25	G	104	PEK	C29-C30-C31-C32
25	P	309	PEK	C15-C16-C17-C18
20	A	608	PGV	C10-C11-C12-C13
24	G	103	CDL	C75-C76-C77-C78
20	A	608	PGV	C23-C24-C25-C26
24	P	306	CDL	C41-C42-C43-C44
26	E	201	PSC	O02-C1-O01-C02
19	D	201	TGL	OG2-CB1-CB2-CB3
20	A	608	PGV	C11-C10-C9-C8
25	T	101	PEK	C2-C3-C4-C5
20	A	609	PGV	C11-C12-C13-C14
20	P	305	PGV	C30-C31-C32-C33
19	L	101	TGL	CC9-C15-C16-C17
24	G	103	CDL	C79-C80-C81-C82
19	D	201	TGL	OG1-CA1-CA2-CA3
20	C	302	PGV	C05-C04-O12-P
24	C	303	CDL	C20-C21-C22-C23
19	N	610	TGL	OG2-CB1-CB2-CB3
19	A	607	TGL	C18-C19-C33-C34
24	G	103	CDL	C71-CB7-OB8-CB6
28	M	101	DMU	C18-C19-C22-C25
19	D	201	TGL	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
20	C	307	PGV	C14-C15-C16-C17
24	T	102	CDL	CA3-CA4-CA6-OA8
19	A	607	TGL	C15-C16-C17-C18
24	C	303	CDL	C23-C24-C25-C26
19	Q	201	TGL	CG3-CG2-OG2-CB1
25	G	104	PEK	C14-C15-C16-C17
19	N	609	TGL	CA6-CA7-CA8-CA9
25	C	306	PEK	C5-C6-C7-C8
25	C	306	PEK	C6-C7-C8-C9
25	G	104	PEK	C5-C6-C7-C8
25	P	304	PEK	C11-C12-C13-C14
25	P	309	PEK	C5-C6-C7-C8
24	P	306	CDL	C18-C19-C20-C21
19	A	607	TGL	C25-C26-C27-C28
24	G	103	CDL	C80-C81-C82-C83
20	C	307	PGV	C29-C30-C31-C32
25	C	306	PEK	C13-C14-C15-C16
19	N	610	TGL	C21-C20-CA9-CA8
26	O	303	PSC	C27-C28-C29-C30
24	G	103	CDL	OB9-CB7-OB8-CB6
19	L	101	TGL	C23-C24-C25-C26
26	E	201	PSC	O01-C1-C2-C3
25	G	104	PEK	C21-C22-C23-C24
20	A	608	PGV	O03-C19-C20-C21
24	G	103	CDL	C37-C38-C39-C40
24	C	303	CDL	C43-C44-C45-C46
20	N	608	PGV	O03-C19-C20-C21
25	P	309	PEK	C26-C27-C28-C29
25	P	304	PEK	C34-C35-C36-C37
25	G	102	PEK	C34-C35-C36-C37
25	P	304	PEK	C14-C15-C16-C17
24	P	306	CDL	OB5-CB3-CB4-OB6
20	P	305	PGV	C7-C8-C9-C10
24	G	103	CDL	C84-C85-C86-C87
20	C	307	PGV	C11-C12-C13-C14
24	P	306	CDL	C11-C12-C13-C14
25	P	304	PEK	C35-C36-C37-C38
25	C	306	PEK	O03-C01-C02-O01
19	L	101	TGL	CB7-CB8-CB9-C10
19	N	609	TGL	OG1-CA1-CA2-CA3
26	E	201	PSC	C30-C31-C32-C33
24	P	306	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	E	201	PSC	C7-C8-C9-C10
15	N	602	HEA	C27-C19-C20-C21
20	C	302	PGV	C12-C13-C14-C15
19	L	101	TGL	CB3-CB4-CB5-CB6
20	A	609	PGV	C22-C23-C24-C25
20	C	307	PGV	O04-C19-O03-C01
20	A	609	PGV	C9-C10-C11-C12
25	G	102	PEK	C14-C15-C16-C17
26	O	303	PSC	C7-C8-C9-C10
19	Q	201	TGL	C20-C21-C22-C23
25	T	101	PEK	O01-C1-C2-C3
20	P	302	PGV	O01-C1-C2-C3
26	E	201	PSC	O03-C19-C20-C21
25	G	104	PEK	C28-C29-C30-C31
20	C	302	PGV	C9-C10-C11-C12
19	N	609	TGL	CB3-CB4-CB5-CB6
20	N	607	PGV	C15-C16-C17-C18
25	P	309	PEK	C13-C14-C15-C16
24	P	306	CDL	C52-C51-CB5-OB6
25	G	102	PEK	O01-C1-C2-C3
19	L	101	TGL	OB1-CB1-CB2-CB3
24	P	306	CDL	C57-C58-C59-C60
24	C	303	CDL	C80-C81-C82-C83
28	G	101	DMU	C5-C10-O7-C3
20	P	305	PGV	C23-C24-C25-C26
24	P	306	CDL	C12-C11-CA5-OA6
20	N	607	PGV	O03-C01-C02-O01
20	C	307	PGV	C23-C24-C25-C26
20	N	608	PGV	C7-C8-C9-C10
19	Q	201	TGL	OG3-CC1-CC2-CC3
26	O	303	PSC	O01-C1-C2-C3
20	C	307	PGV	C20-C19-O03-C01
25	C	306	PEK	O01-C1-C2-C3
15	N	602	HEA	C26-C15-C16-C17
24	P	306	CDL	C32-C33-C34-C35
19	A	607	TGL	OA1-CA1-OG1-CG1
26	E	201	PSC	C2-C1-O01-C02
19	A	607	TGL	CC1-CC2-CC3-CC4
20	N	608	PGV	C11-C12-C13-C14
25	P	309	PEK	C14-C15-C16-C17
22	P	307	CHD	C13-C17-C20-C21
25	T	101	PEK	O02-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	OG3-CC1-CC2-CC3
19	A	607	TGL	CB2-CB3-CB4-CB5
24	P	306	CDL	C52-C51-CB5-OB7
24	G	103	CDL	C82-C83-C84-C85
19	N	609	TGL	OA1-CA1-CA2-CA3
26	E	201	PSC	O04-C19-C20-C21
20	P	305	PGV	C13-C14-C15-C16
25	G	102	PEK	C30-C31-C32-C33
24	P	306	CDL	C52-C53-C54-C55
24	P	306	CDL	C12-C11-CA5-OA7
24	C	303	CDL	C51-C52-C53-C54
25	T	101	PEK	C24-C25-C26-C27
20	P	302	PGV	O02-C1-C2-C3
19	N	610	TGL	CB7-CB8-CB9-C10
20	N	607	PGV	C03-O11-P-O13
20	P	302	PGV	C03-O11-P-O14
24	T	102	CDL	C52-C53-C54-C55
25	G	102	PEK	O02-C1-C2-C3
24	T	102	CDL	C78-C79-C80-C81
25	G	102	PEK	O12-C04-C05-N
26	O	303	PSC	O02-C1-C2-C3
25	P	304	PEK	O01-C1-C2-C3
20	P	302	PGV	C2-C3-C4-C5
20	P	305	PGV	C25-C26-C27-C28
26	E	201	PSC	C05-C04-O12-P
19	Q	201	TGL	OG1-CA1-CA2-CA3
20	N	607	PGV	C9-C10-C11-C12
24	T	102	CDL	C20-C21-C22-C23
24	P	306	CDL	C55-C56-C57-C58
24	C	303	CDL	C12-C11-CA5-OA6
25	G	104	PEK	O01-C1-C2-C3
19	D	201	TGL	CB2-CB3-CB4-CB5
15	A	603	HEA	C26-C15-C16-C17
19	D	201	TGL	OC1-CC1-CC2-CC3
24	C	303	CDL	C12-C11-CA5-OA7
24	P	306	CDL	C32-C31-CA7-OA9
25	C	306	PEK	O02-C1-C2-C3
19	Q	201	TGL	OC1-CC1-CC2-CC3
25	T	101	PEK	O03-C21-C22-C23
25	T	101	PEK	C35-C36-C37-C38
25	T	101	PEK	O04-C21-C22-C23
24	C	303	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
24	P	306	CDL	C32-C31-CA7-OA8
25	P	309	PEK	C17-C18-C19-C20
24	C	303	CDL	C32-C31-CA7-OA8

There are no ring outliers.

37 monomers are involved in 286 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	305	CHD	1	0
15	A	602	HEA	7	0
26	O	303	PSC	17	0
19	N	610	TGL	14	0
28	G	101	DMU	4	0
22	B	302	CHD	2	0
25	T	101	PEK	22	0
19	A	607	TGL	6	0
20	P	305	PGV	3	0
15	N	603	HEA	2	0
25	G	102	PEK	2	0
20	N	608	PGV	1	0
15	N	602	HEA	6	0
24	G	103	CDL	26	0
20	N	607	PGV	9	0
28	P	301	DMU	3	0
19	L	101	TGL	14	0
15	A	603	HEA	2	0
24	C	303	CDL	17	0
20	C	307	PGV	3	0
20	A	609	PGV	8	0
20	P	302	PGV	2	0
19	D	201	TGL	12	0
22	O	302	CHD	1	0
25	P	304	PEK	5	0
22	C	304	CHD	5	0
25	G	104	PEK	11	0
20	C	302	PGV	2	0
22	P	308	CHD	1	0
24	T	102	CDL	27	0
19	Q	201	TGL	2	0
26	E	201	PSC	16	0
22	P	307	CHD	7	0
25	P	309	PEK	8	0

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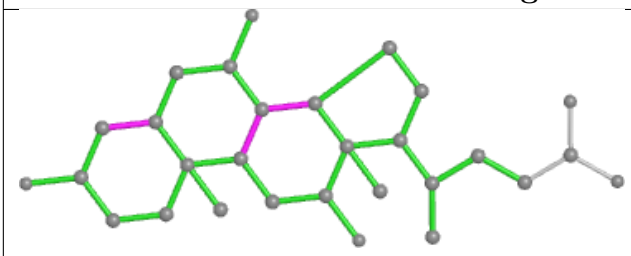
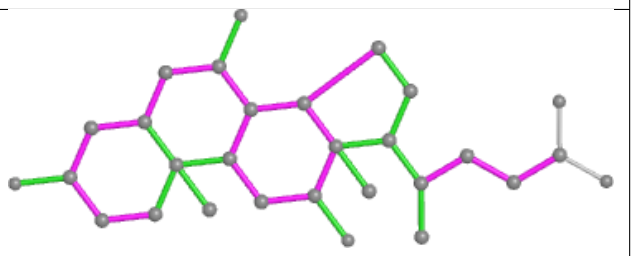
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	P	306	CDL	20	0
25	C	306	PEK	6	0
19	N	609	TGL	8	0

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.

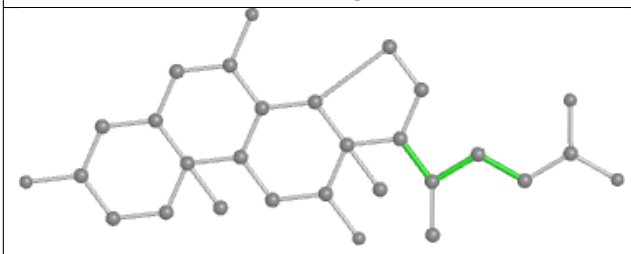
Ligand CHD C 305



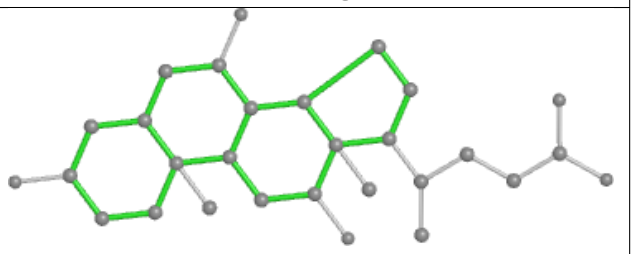
Bond lengths



Bond angles

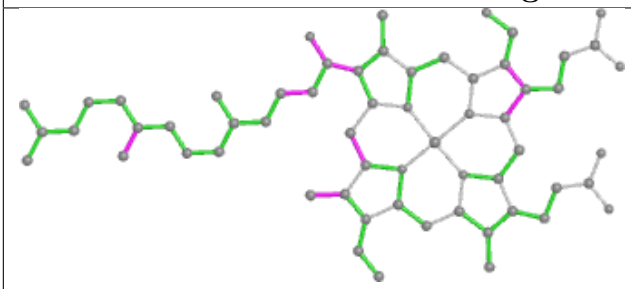


Torsions

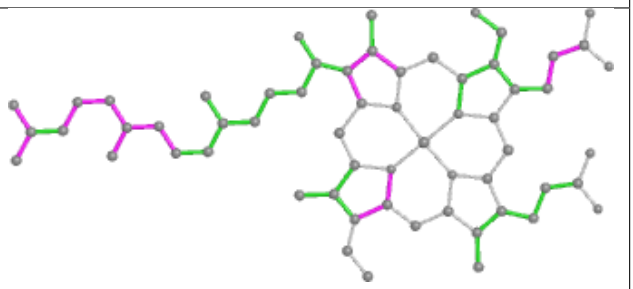


Rings

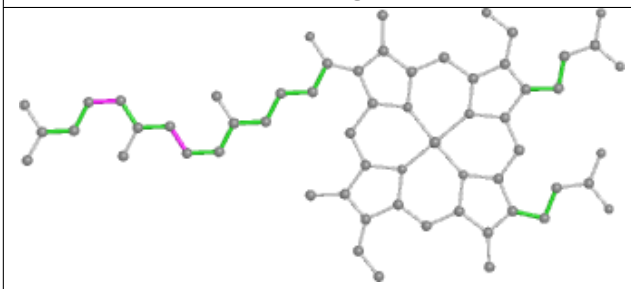
Ligand HEA A 602



Bond lengths



Bond angles



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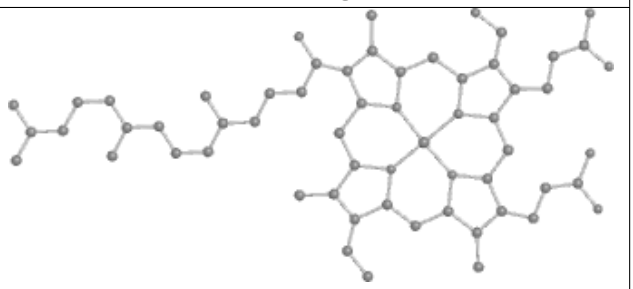
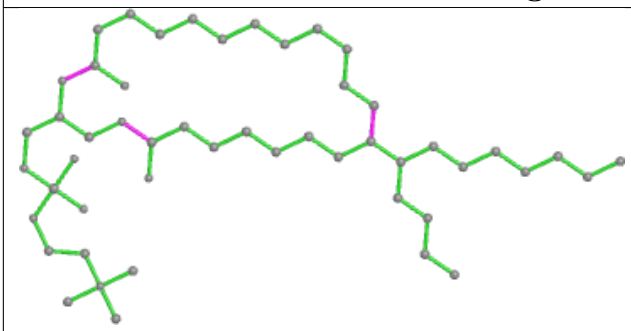
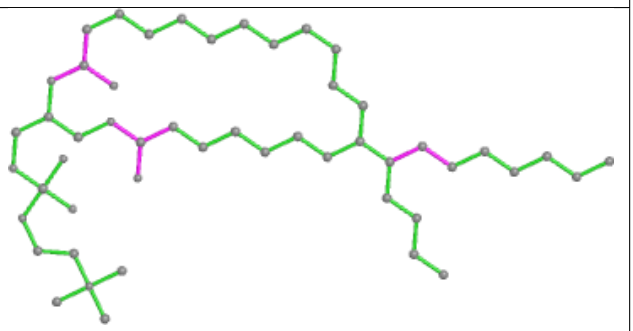


Rings

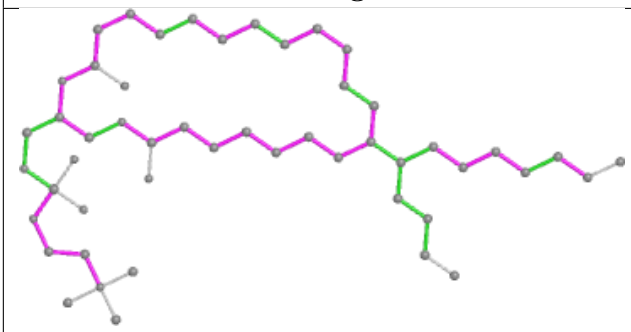
Ligand PSC O 303



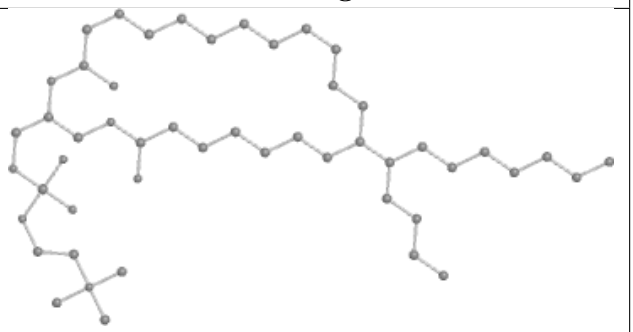
Bond lengths



Bond angles

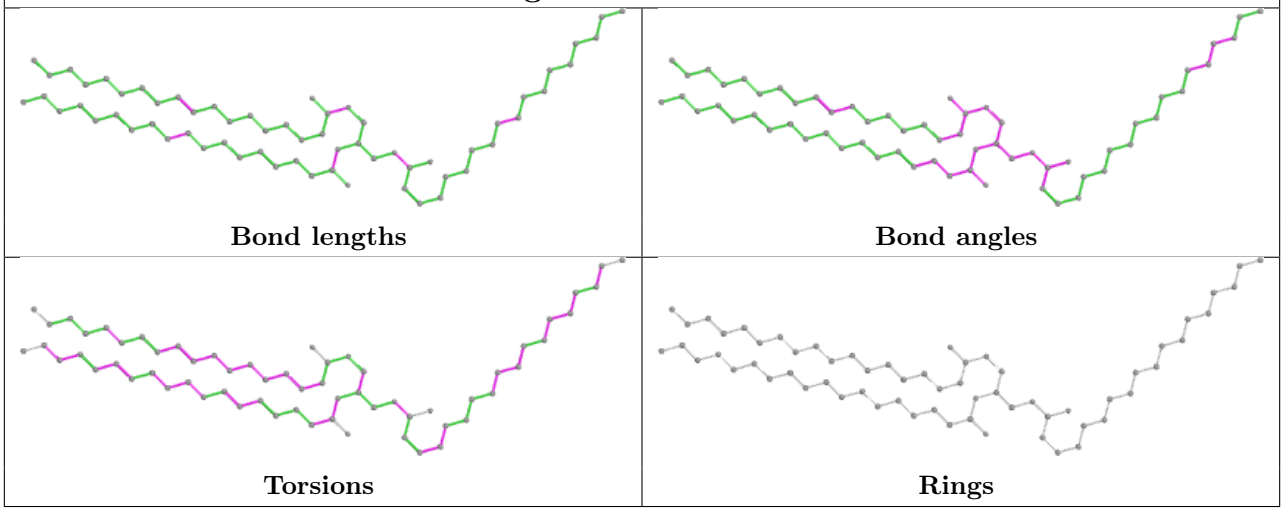


Torsions

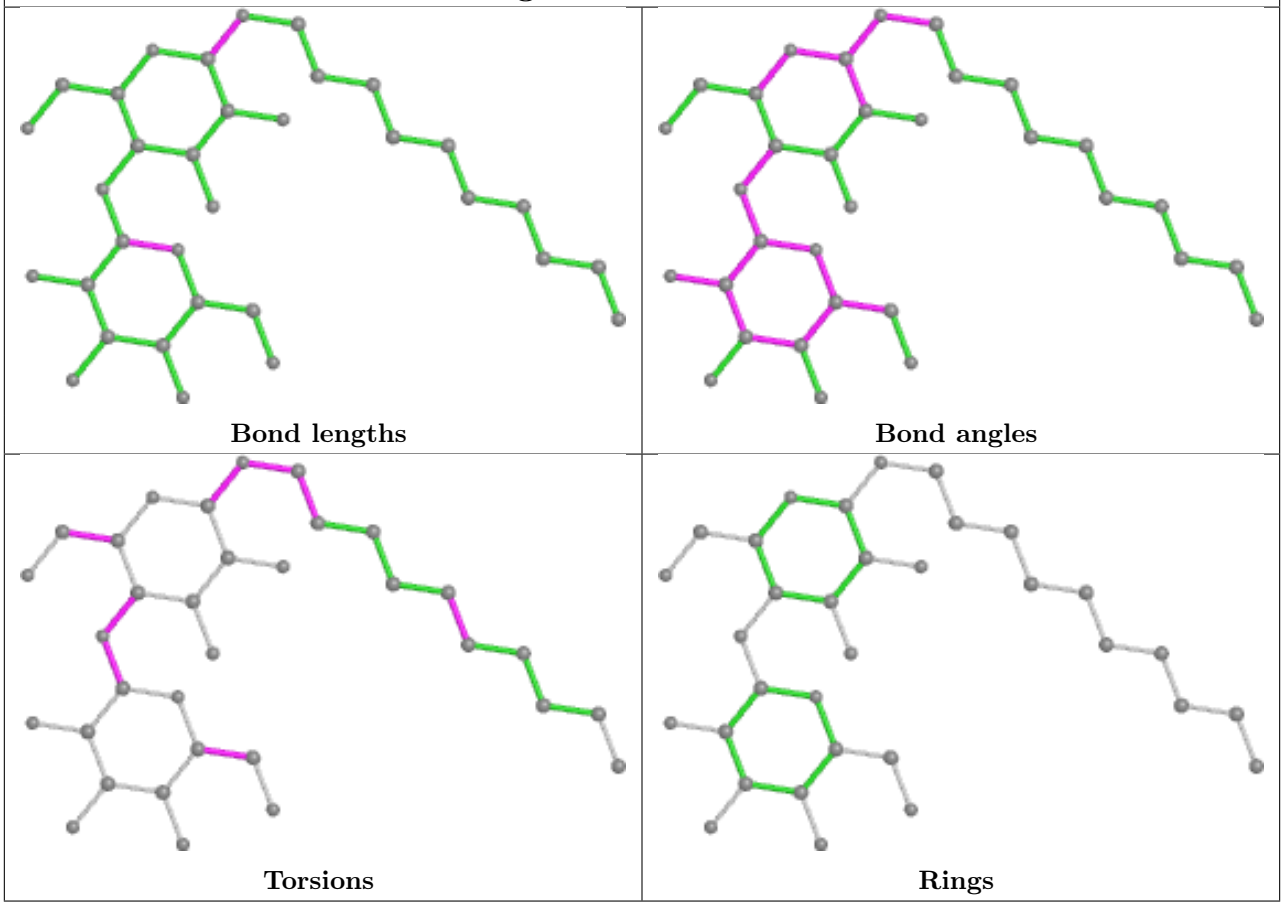


Rings

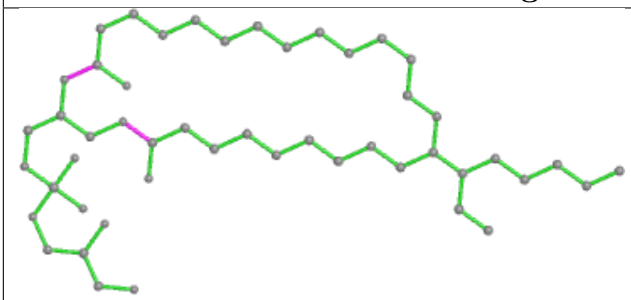
Ligand TGL N 610



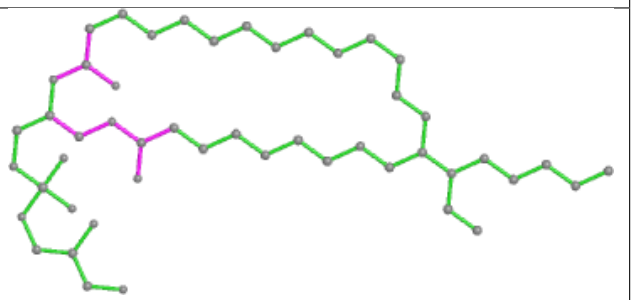
Ligand DMU G 101



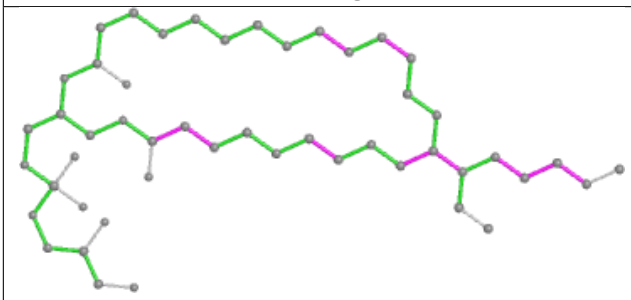
Ligand PGV A 608



Bond lengths



Bond angles



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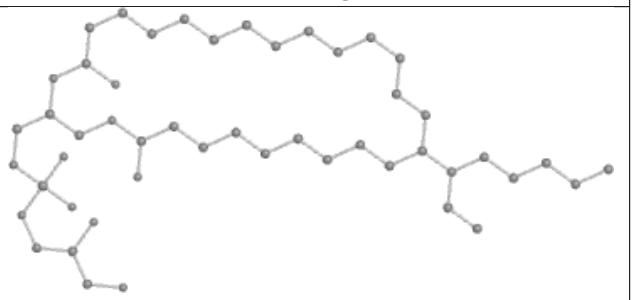
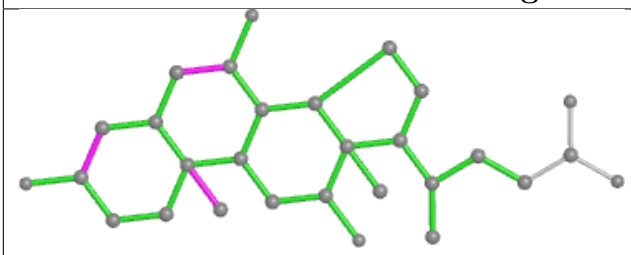


Rings

Ligand CHD B 302



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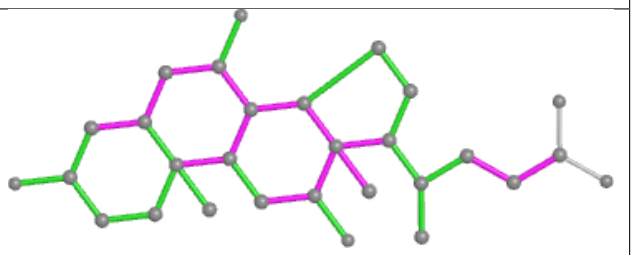
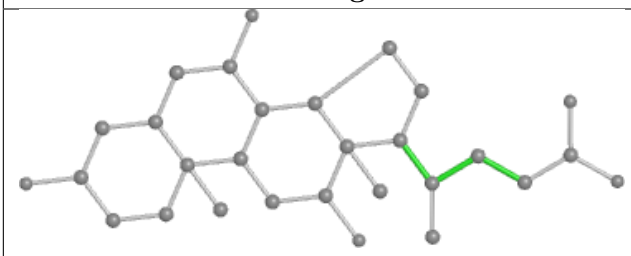


Bond angles



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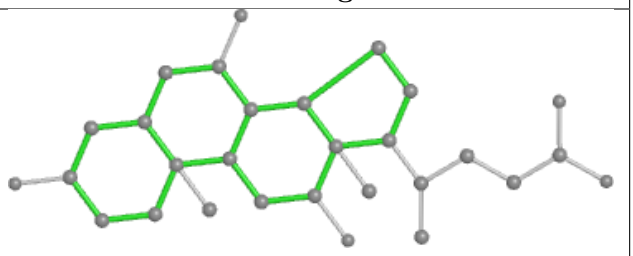
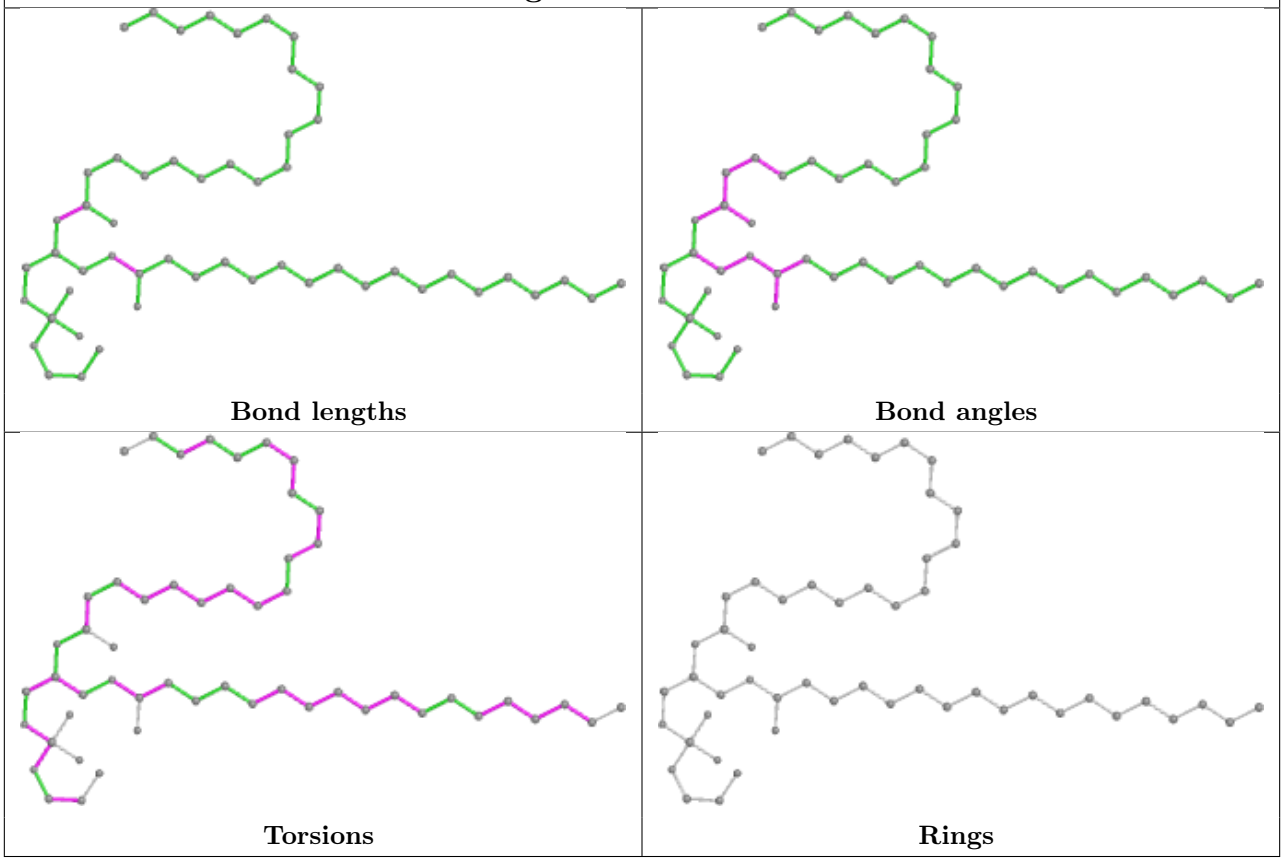
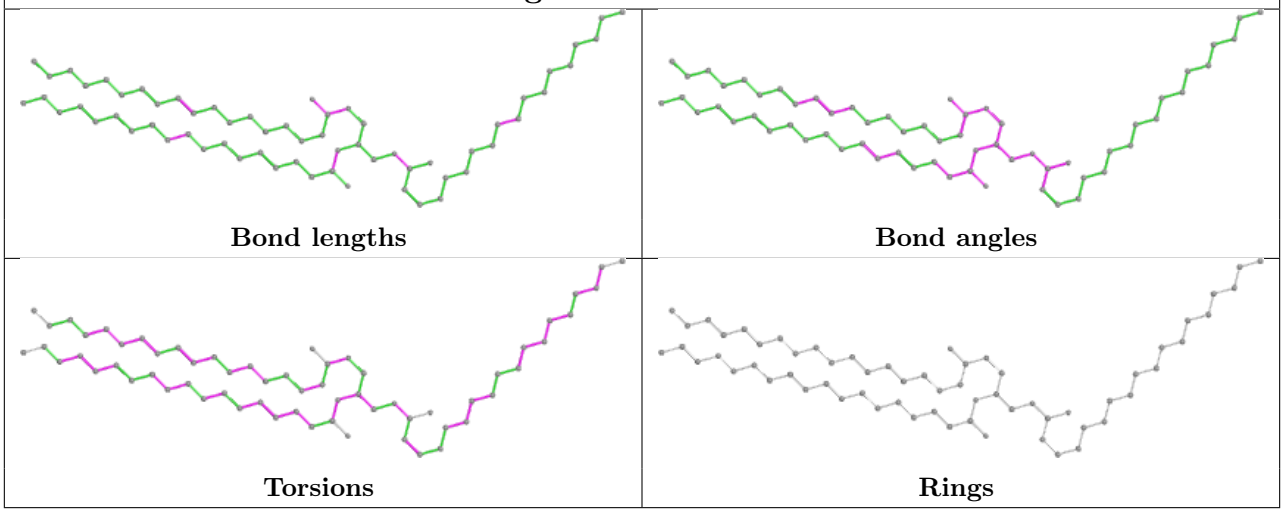


Rings

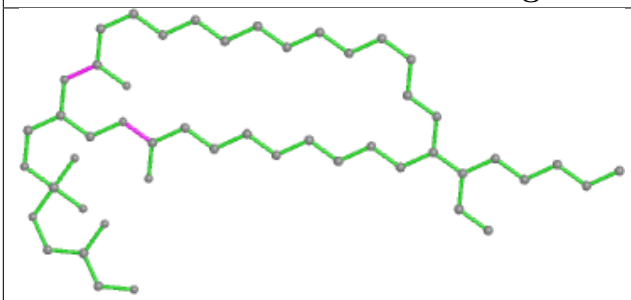
Ligand PEK T 101



Ligand TGL A 607



Ligand PGV P 305



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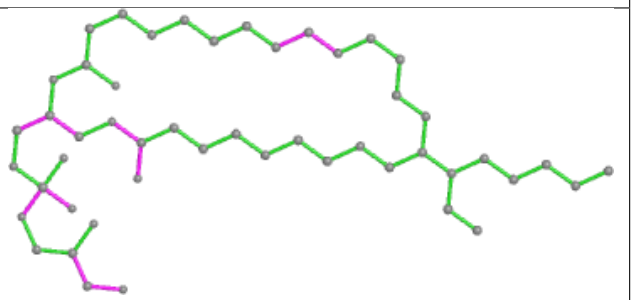
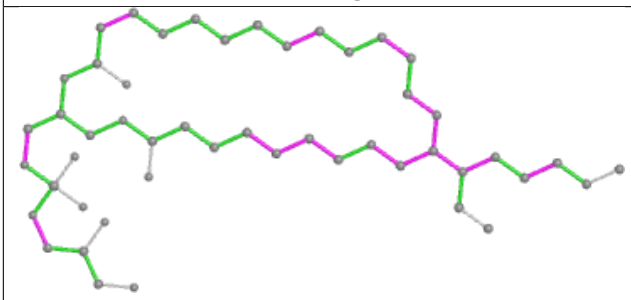


Bond angles



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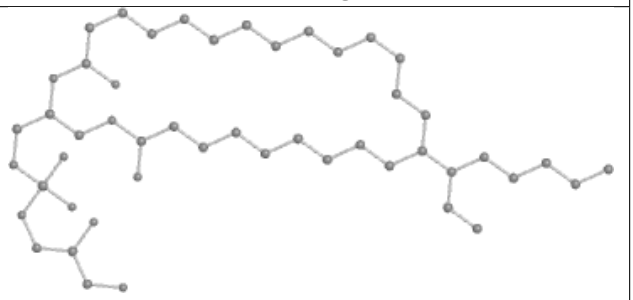
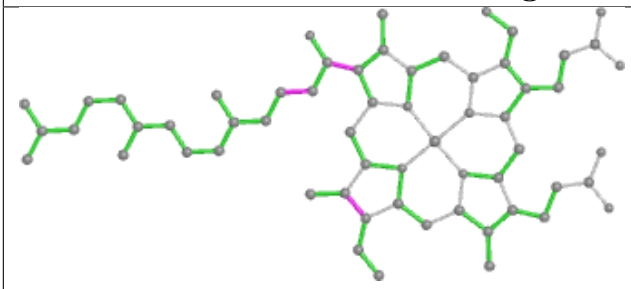
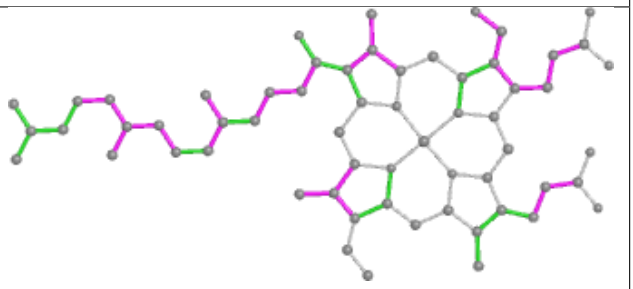


Rings

Ligand HEA N 603



Bond lengths



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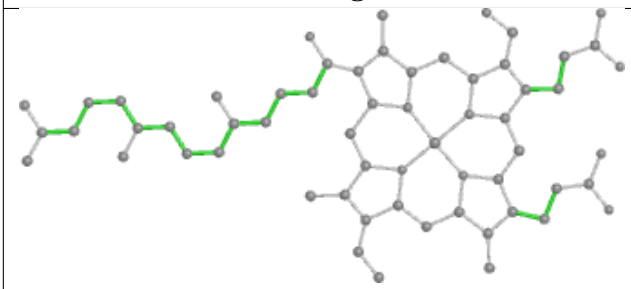
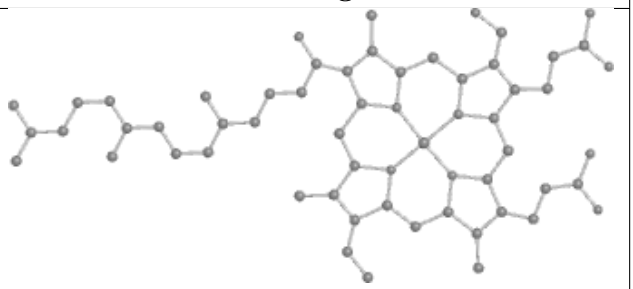
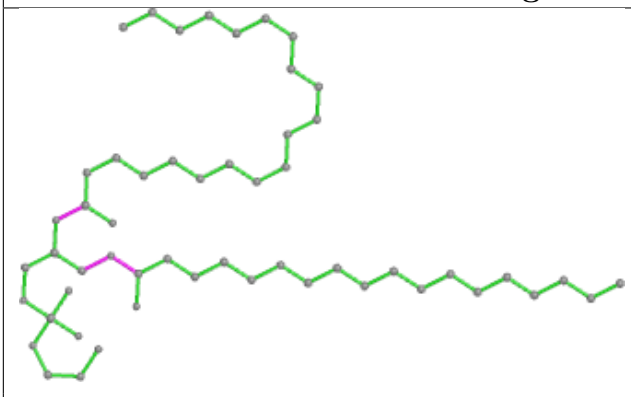


Torsions

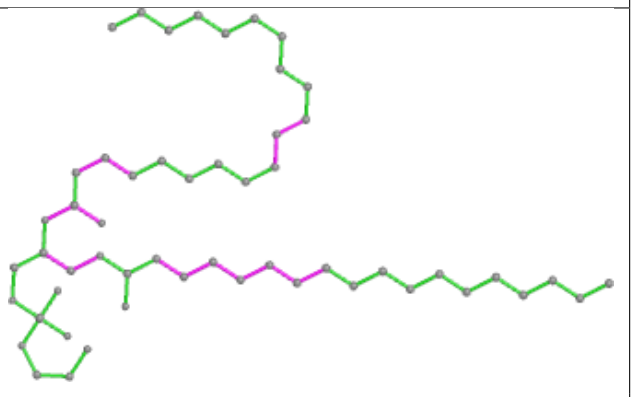


Rings

Ligand PEK G 102



Bond lengths



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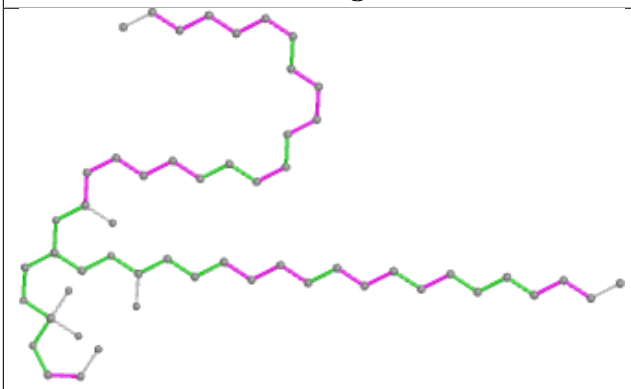

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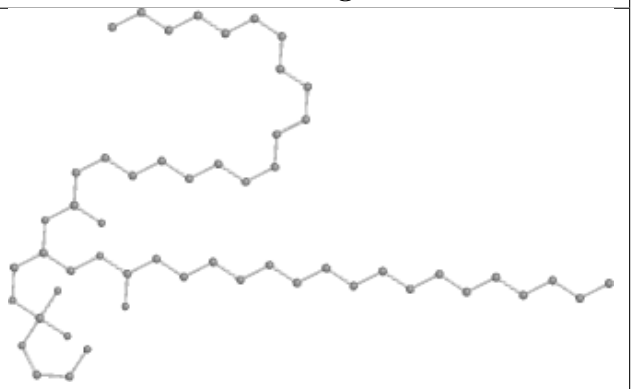
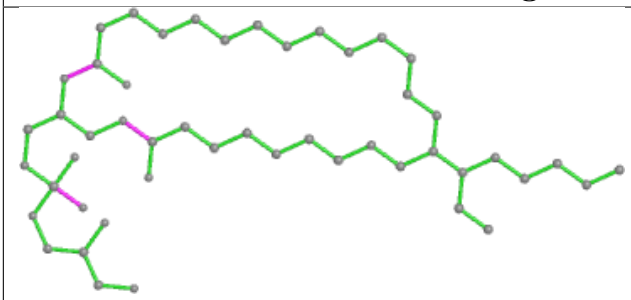


Rings

Ligand PGV N 608



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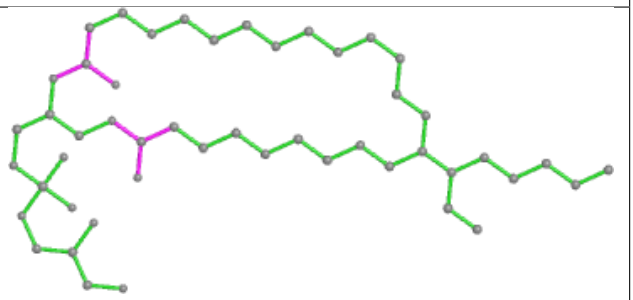
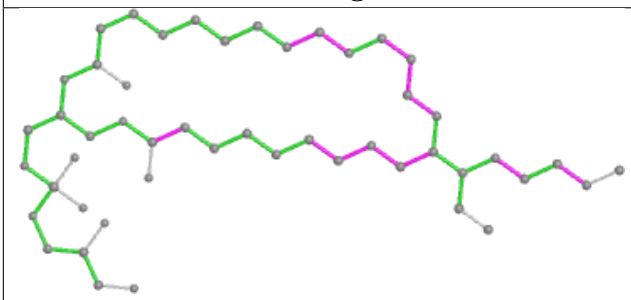


Bond angles



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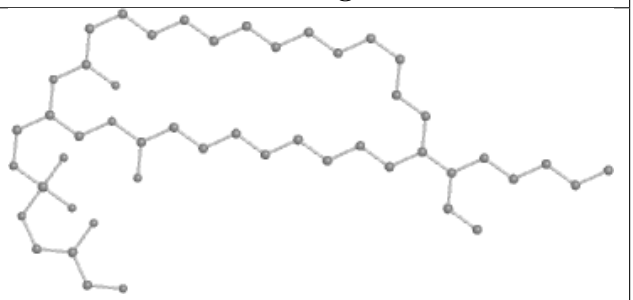
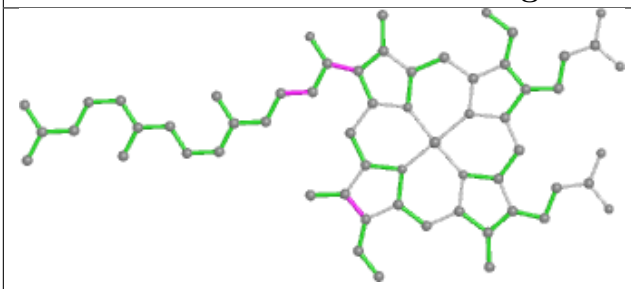


Rings

Ligand HEA N 602



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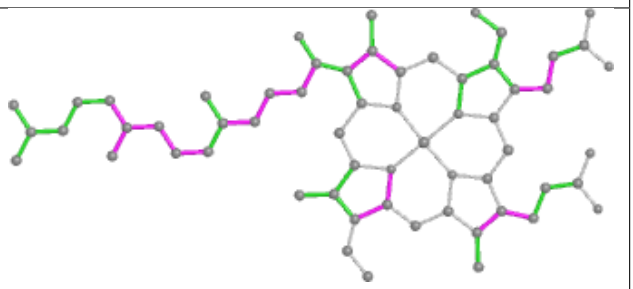
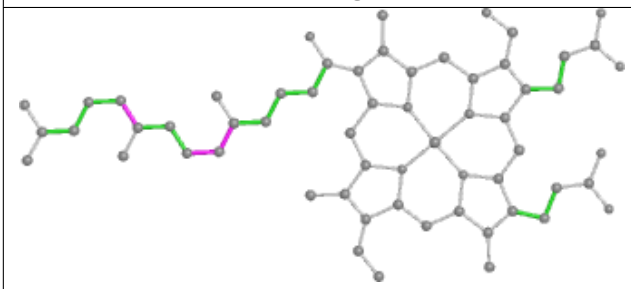


Bond angles



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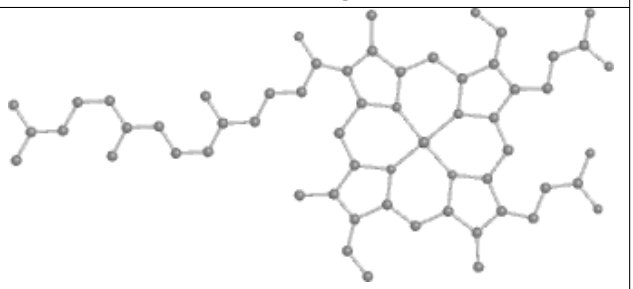
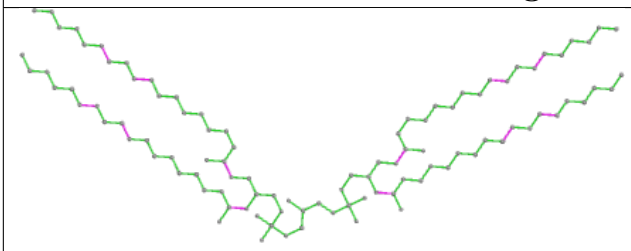
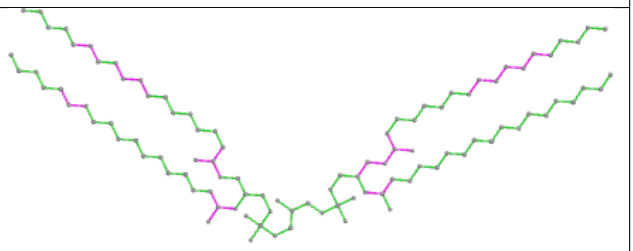


Rings

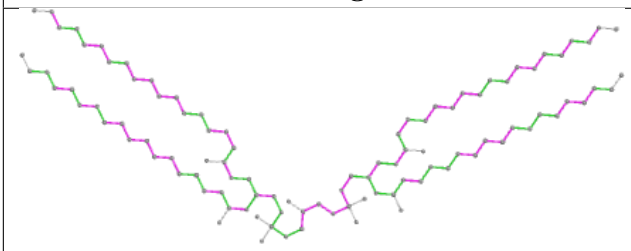
Ligand CDL G 103



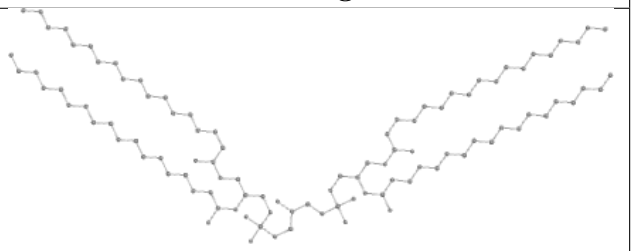
Bond lengths



Bond angles

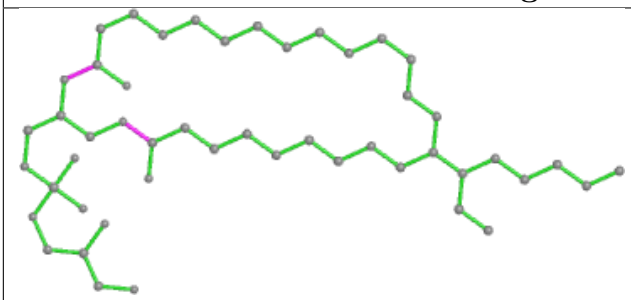


Torsions

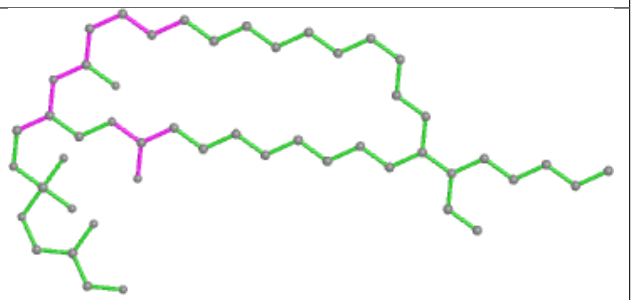


Rings

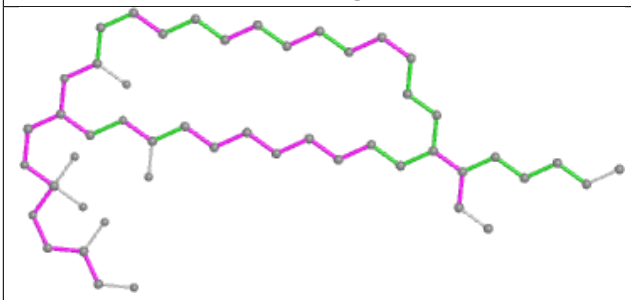
Ligand PGV N 607



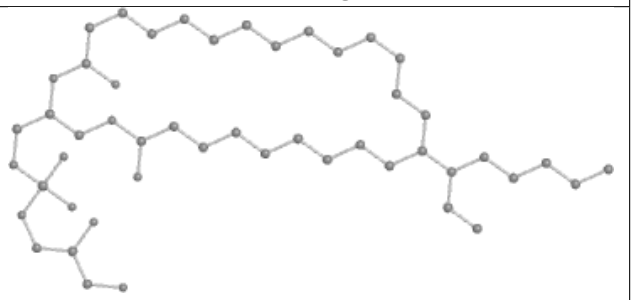
Bond lengths



Bond angles

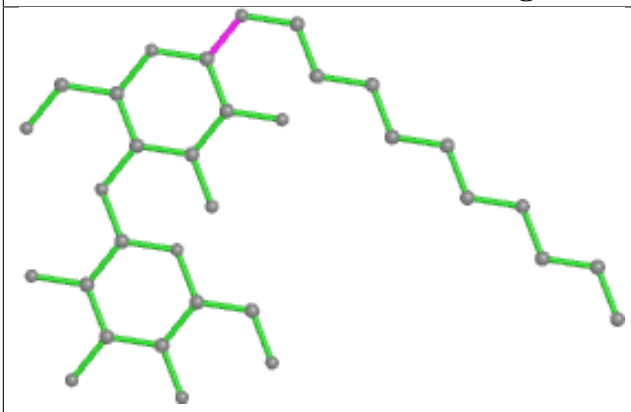


Torsions

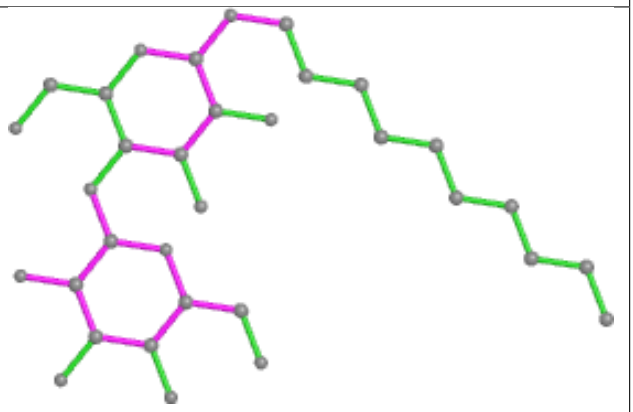


Rings

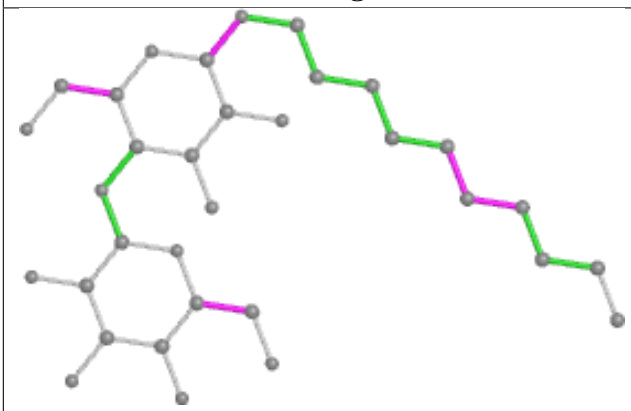
Ligand DMU P 301



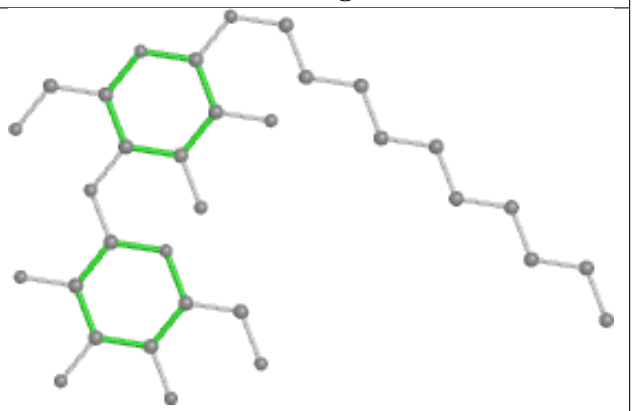
Bond lengths



Bond angles

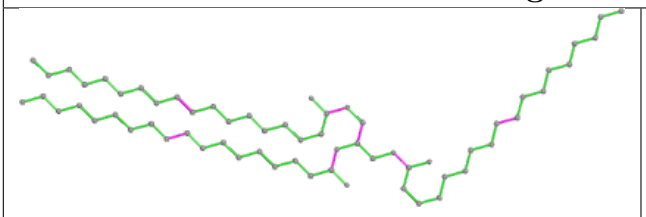


Torsions

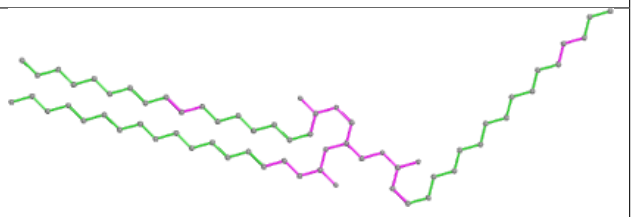


Rings

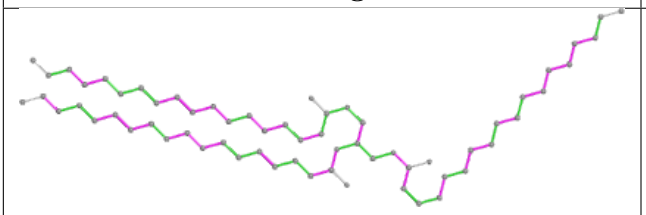
Ligand TGL L 101



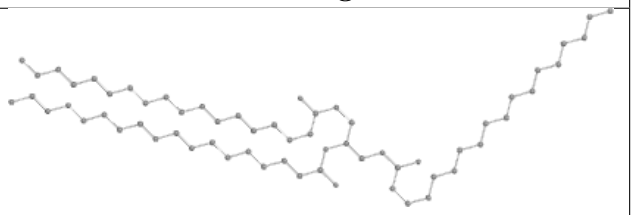
Bond lengths



Bond angles

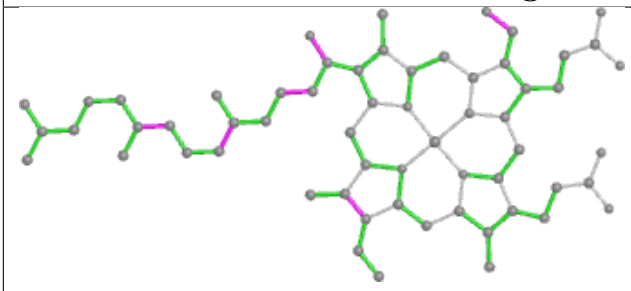


Torsions

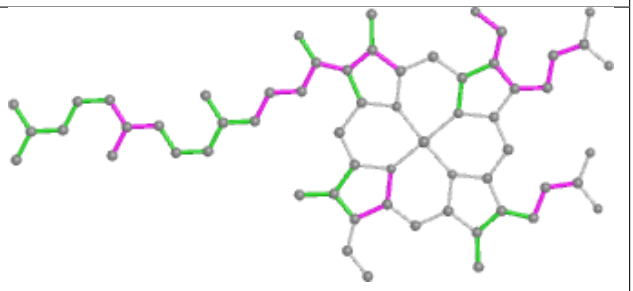


Rings

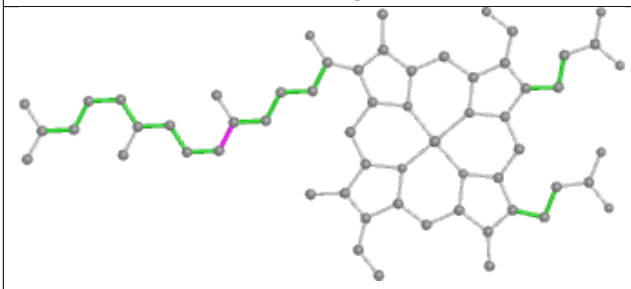
Ligand HEA A 603



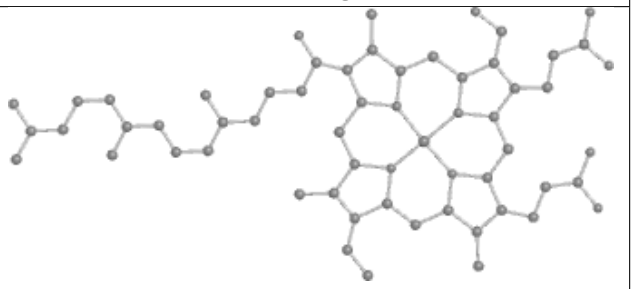
Bond lengths



Bond angles

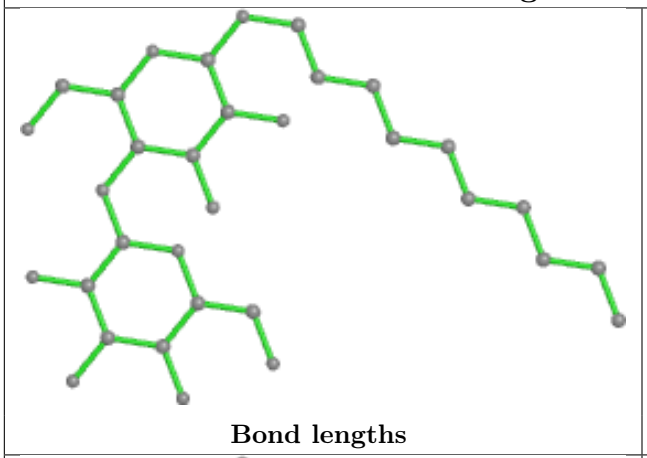


Torsions

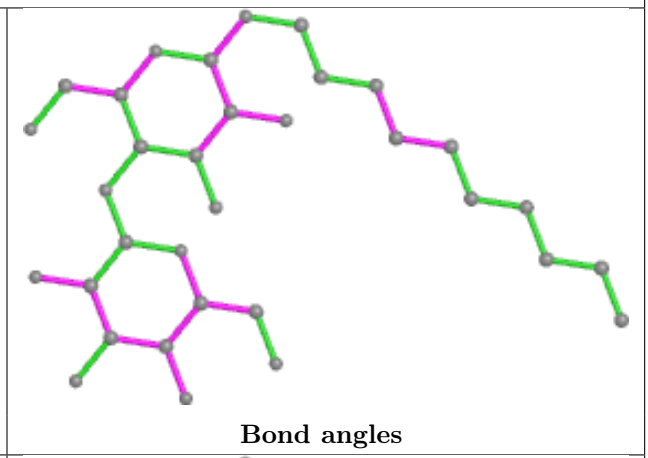


Rings

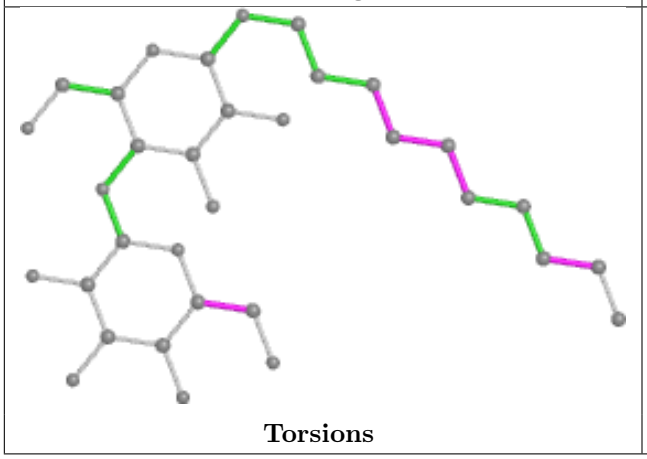
Ligand DMU Z 101



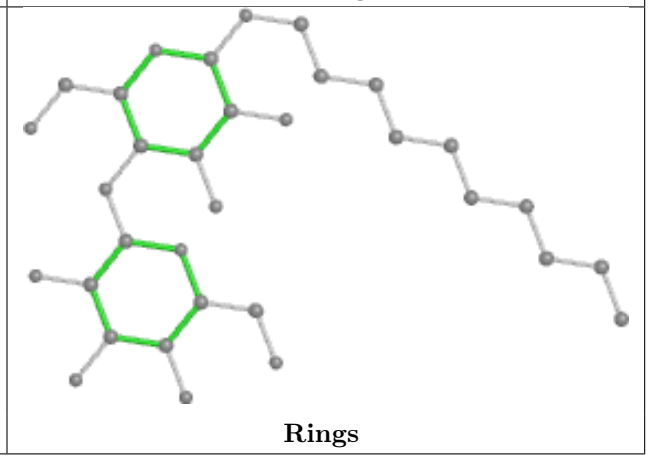
Bond lengths



Bond angles

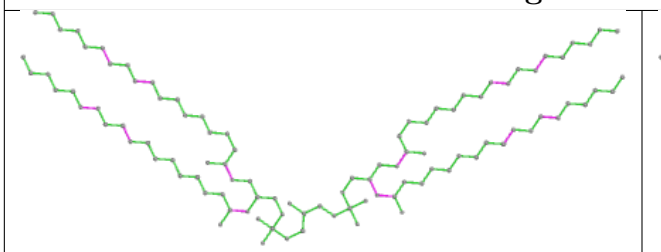


Torsions

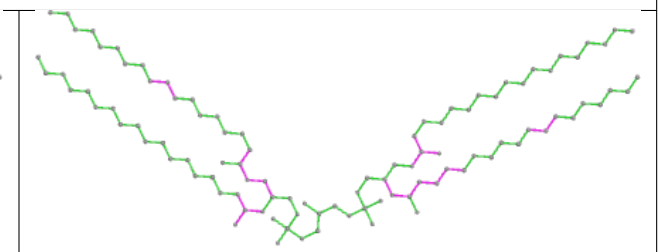


Rings

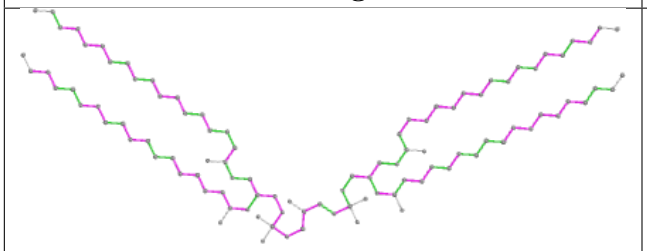
Ligand CDL C 303



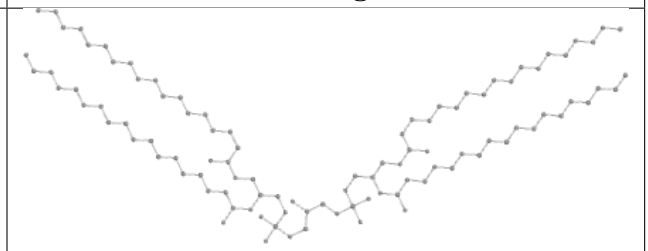
Bond lengths



Bond angles

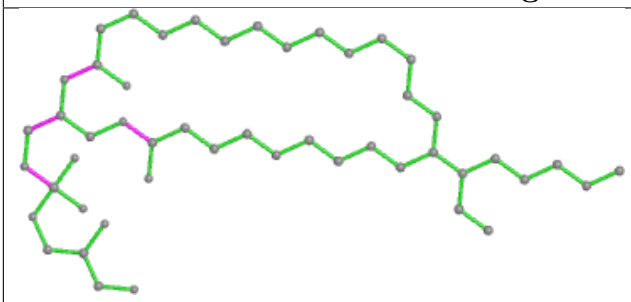


Torsions

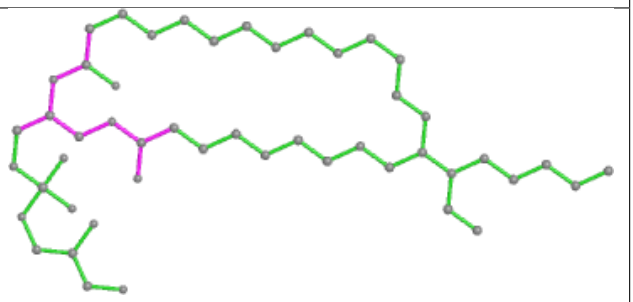


Rings

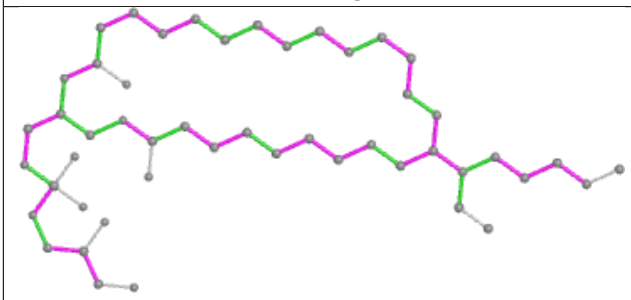
Ligand PGV C 307



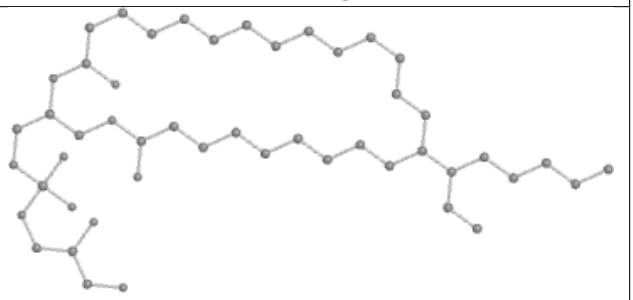
Bond lengths



Bond angles

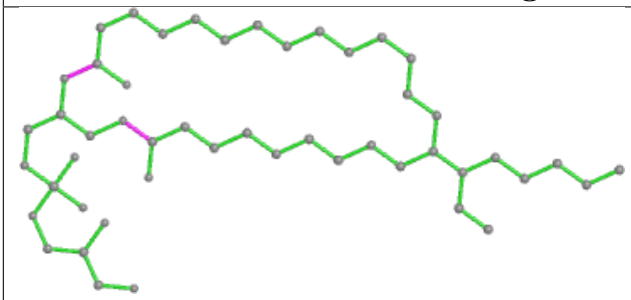


Torsions

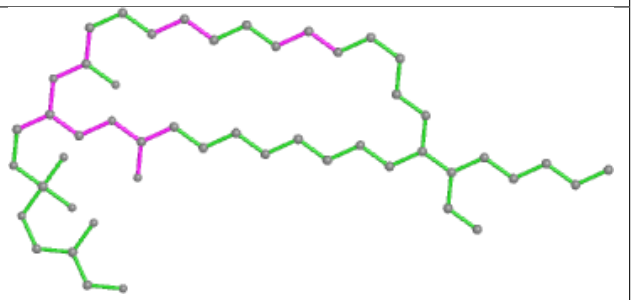


Rings

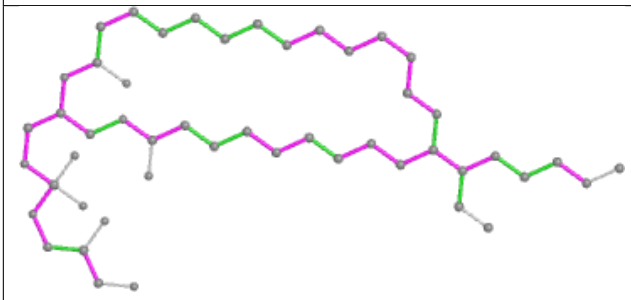
Ligand PGV A 609



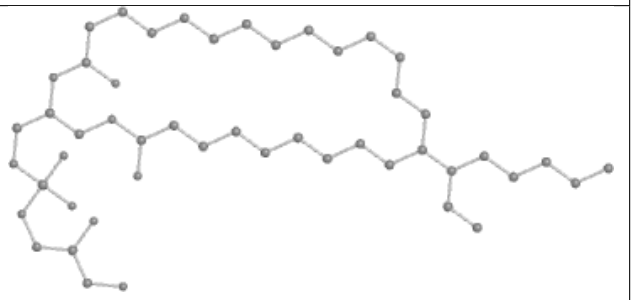
Bond lengths



Bond angles

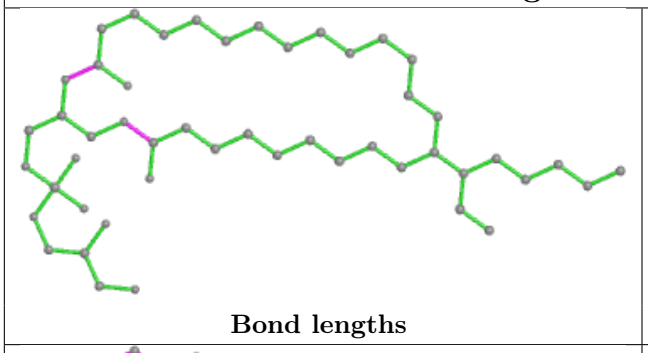


Torsions

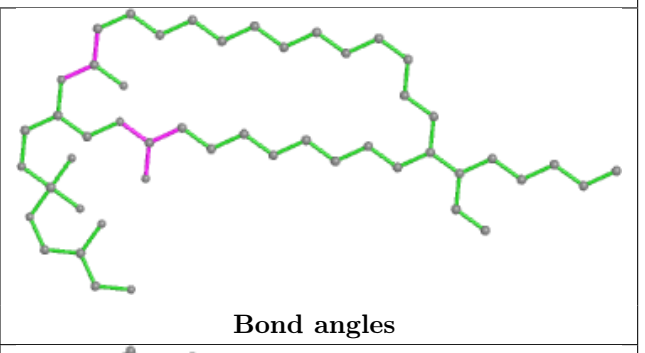


Rings

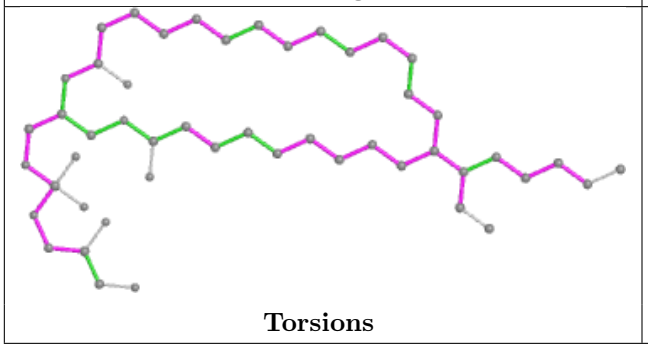
Ligand PGV P 302



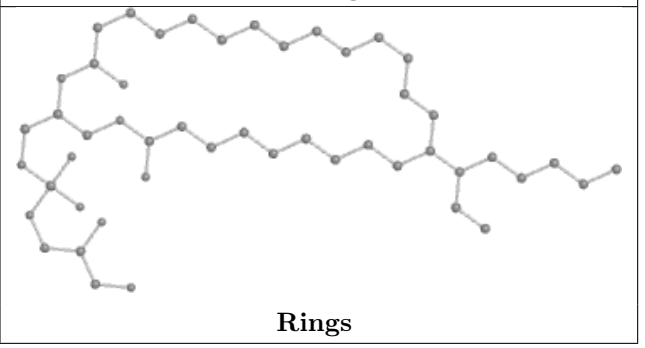
Bond lengths



Bond angles

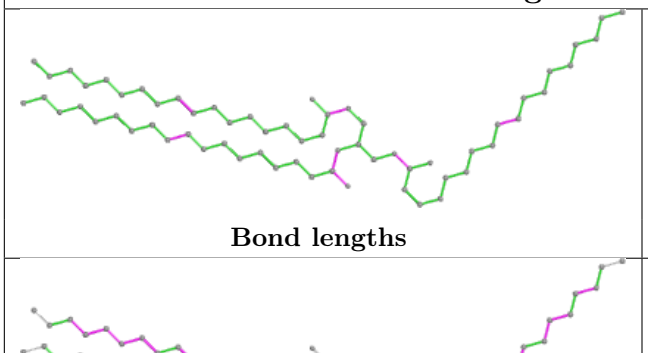


Torsions

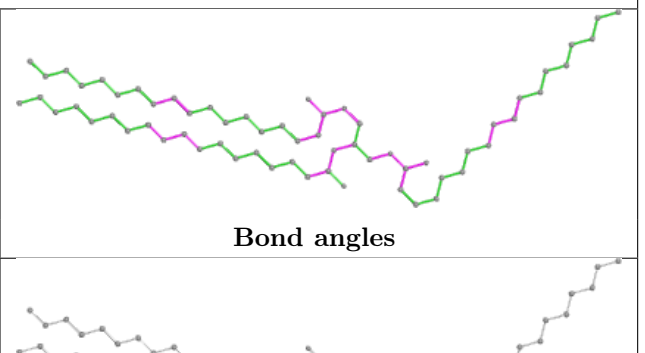


Rings

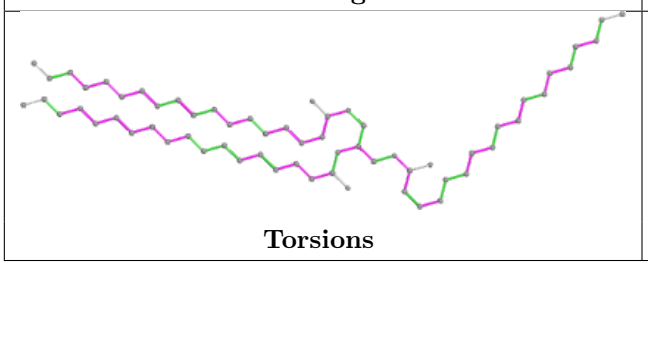
Ligand TGL D 201



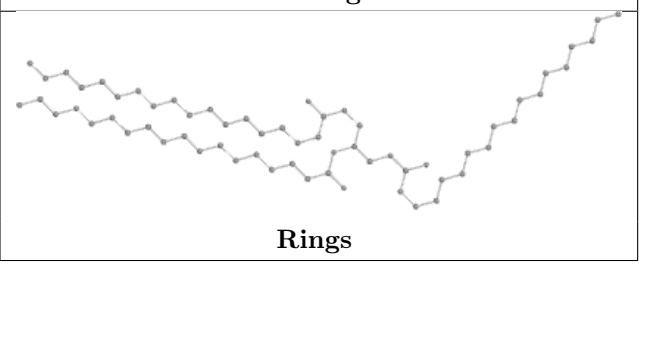
Bond lengths



Bond angles

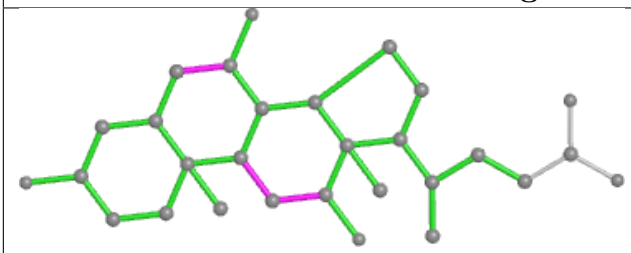


Torsions

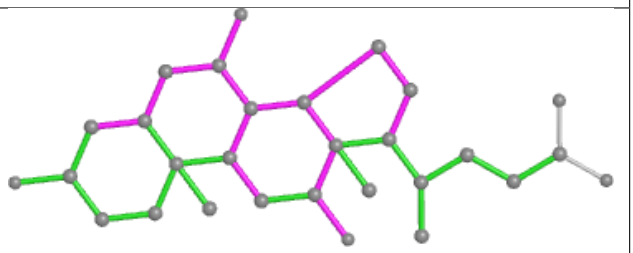


Rings

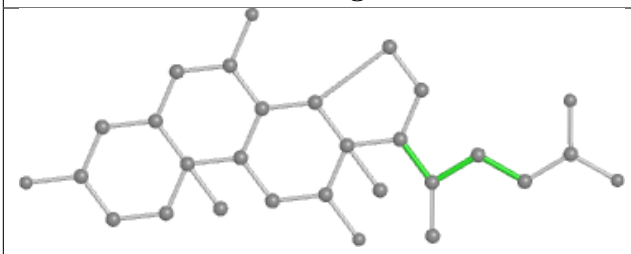
Ligand CHD O 302



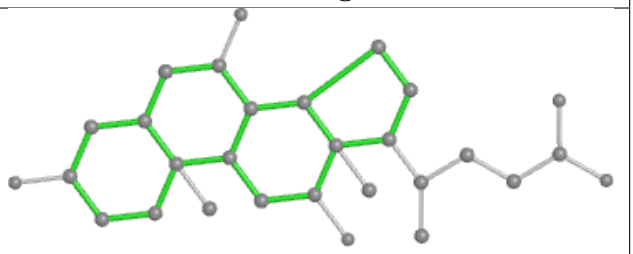
Bond lengths



Bond angles

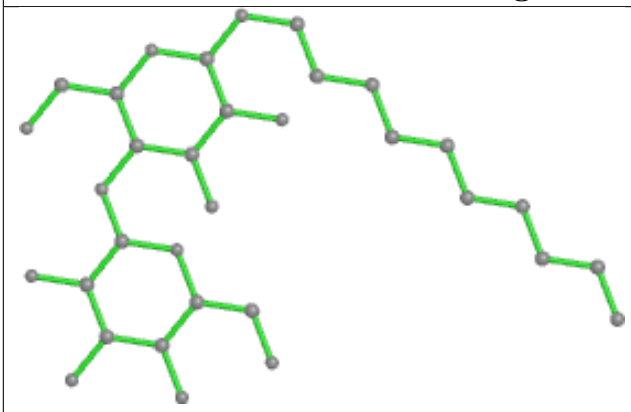


Torsions

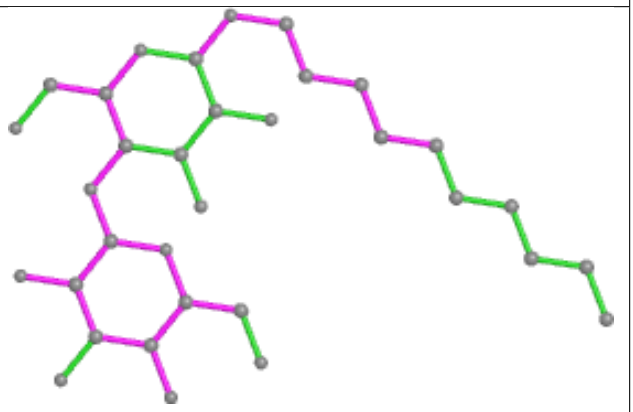


Rings

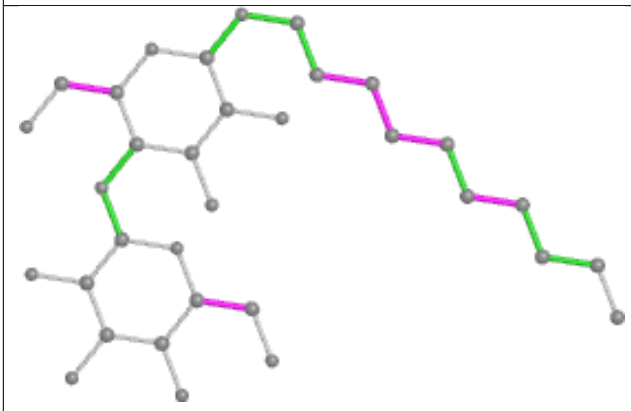
Ligand DMU M 101



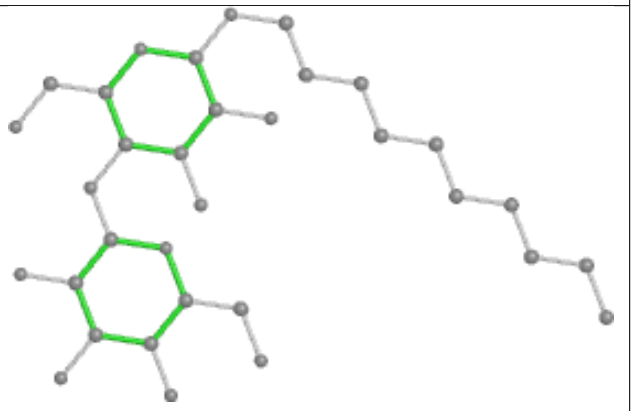
Bond lengths



Bond angles

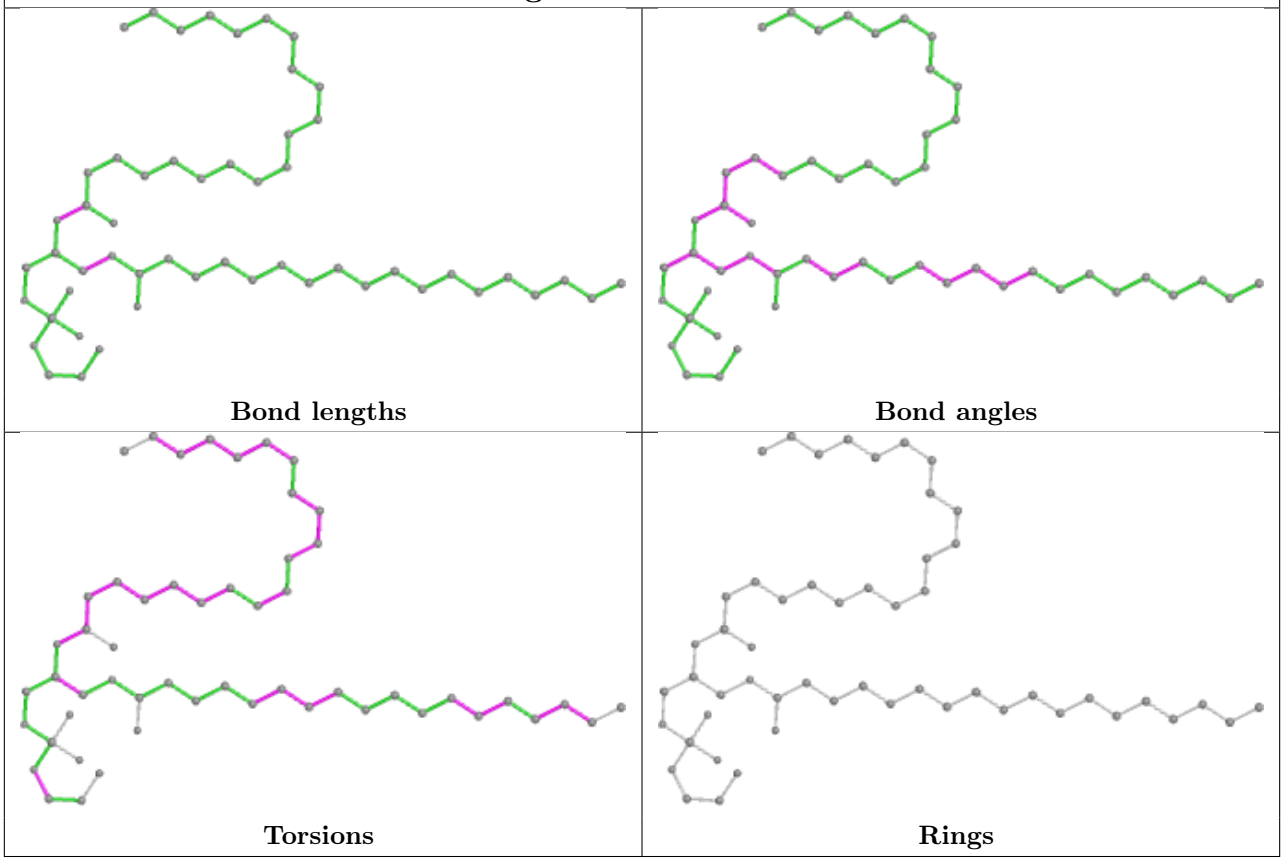


Torsions

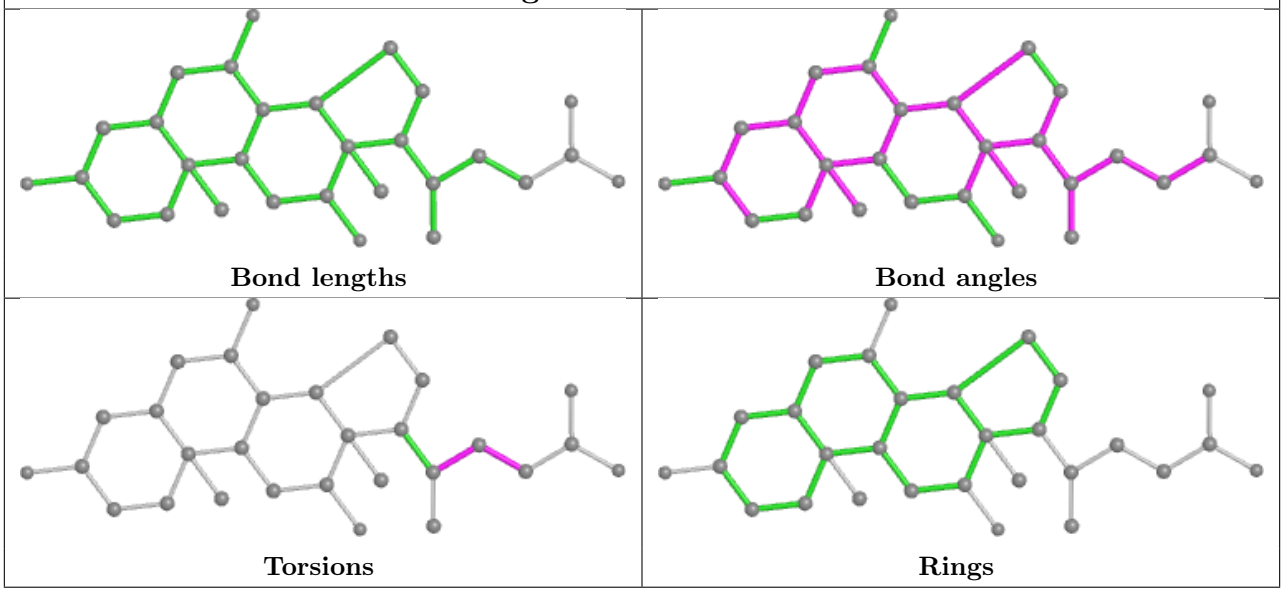


Rings

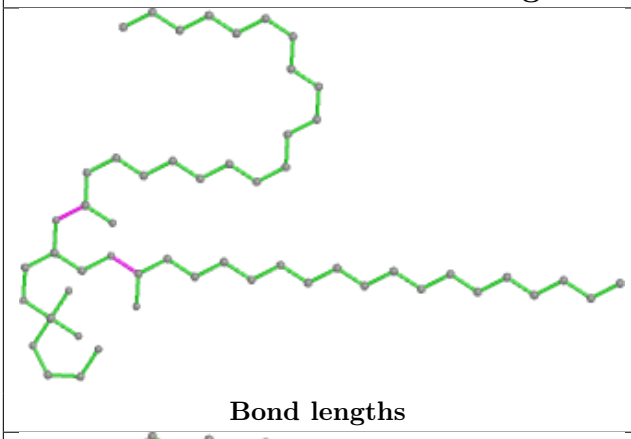
Ligand PEK P 304



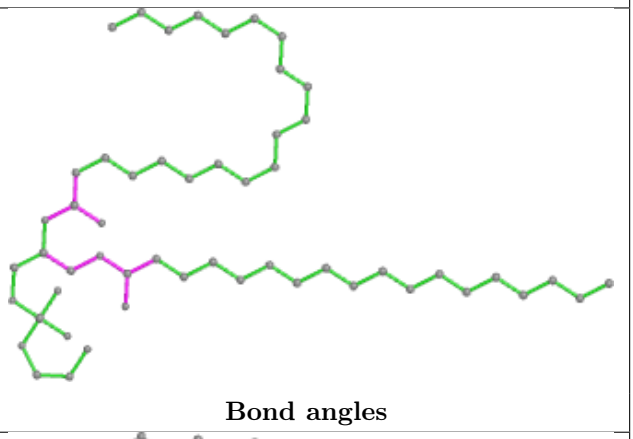
Ligand CHD C 304



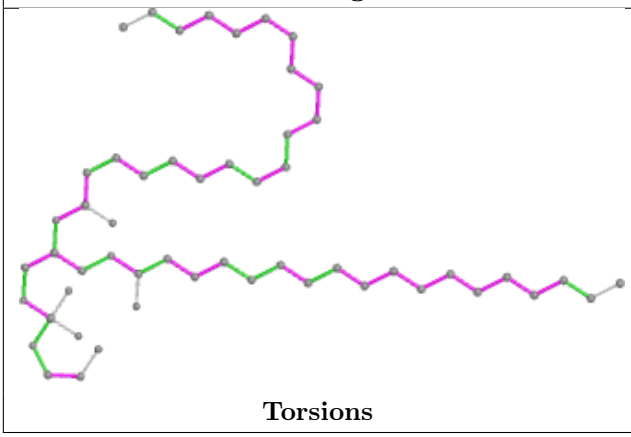
Ligand PEK G 104



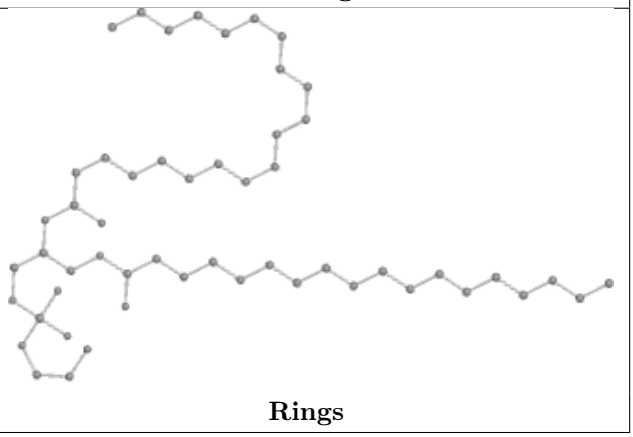
Bond lengths



Bond angles

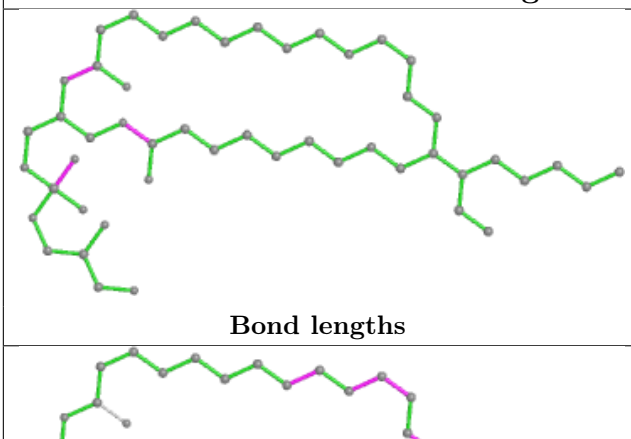


Torsions

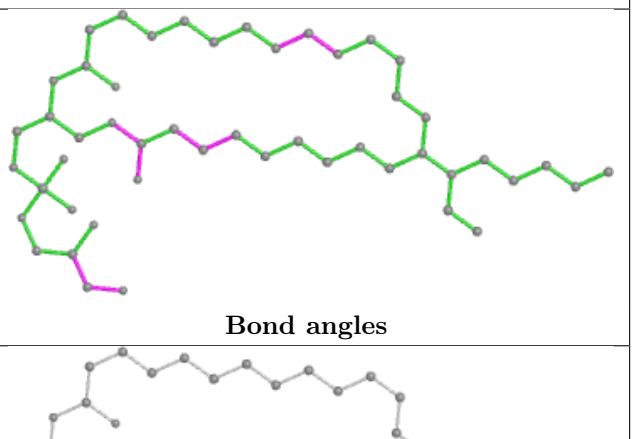


Rings

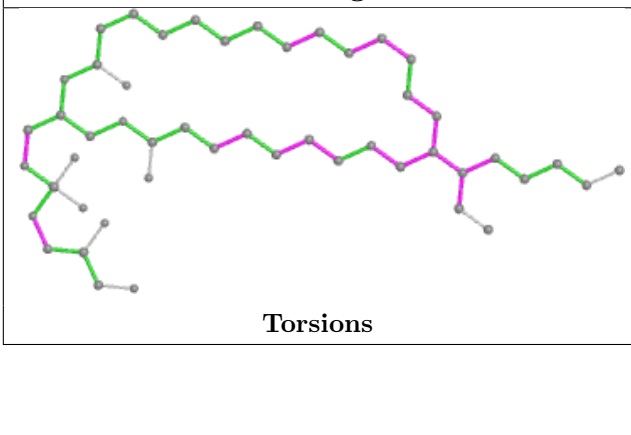
Ligand PGV C 302



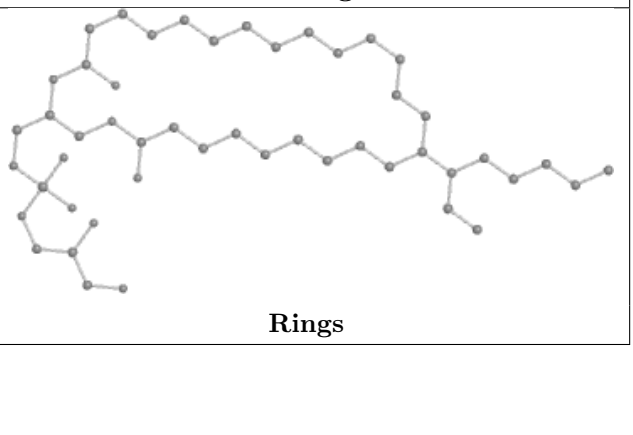
Bond lengths



Bond angles

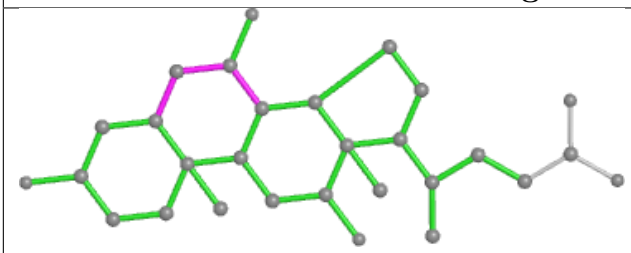


Torsions

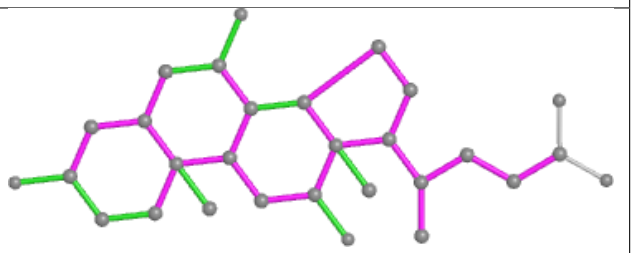


Rings

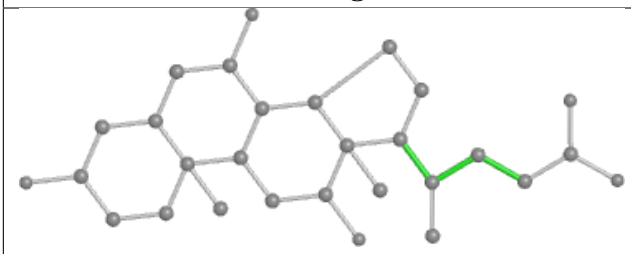
Ligand CHD P 308



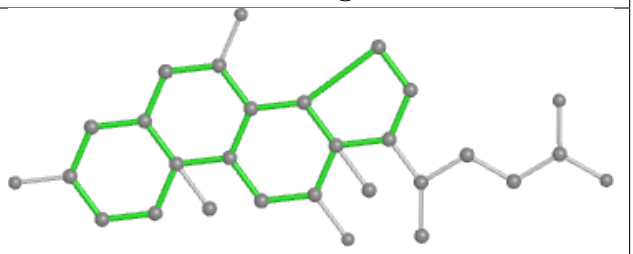
Bond lengths



Bond angles

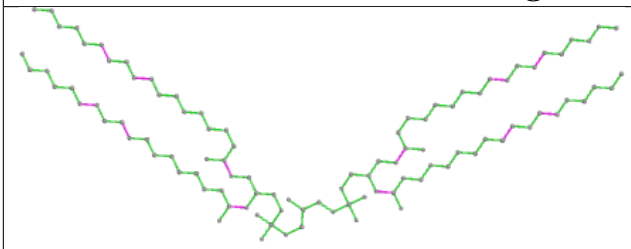


Torsions

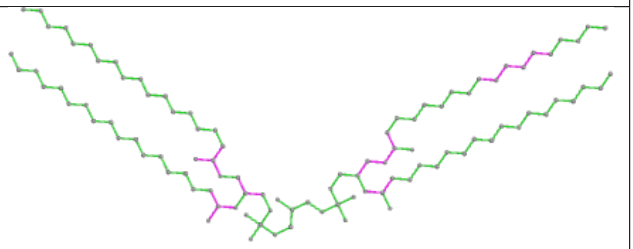


Rings

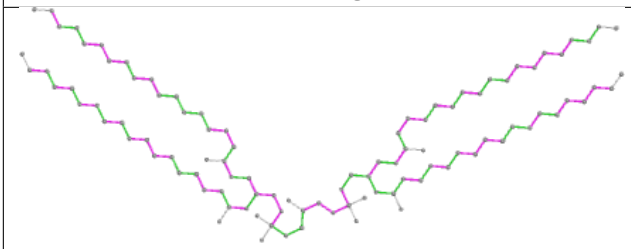
Ligand CDL T 102



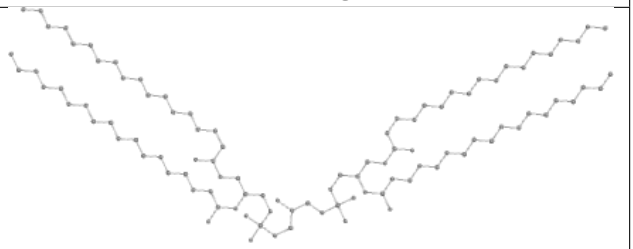
Bond lengths



Bond angles

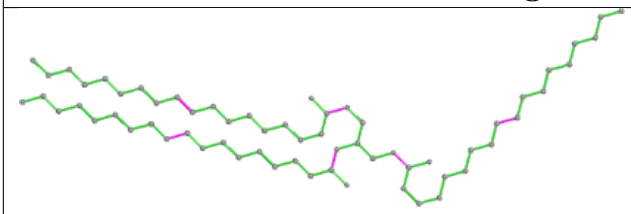


Torsions

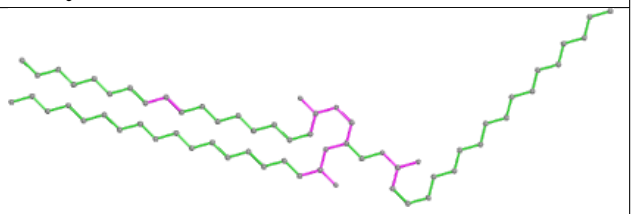


Rings

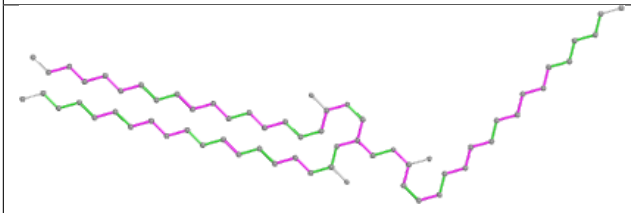
Ligand TGL Q 201



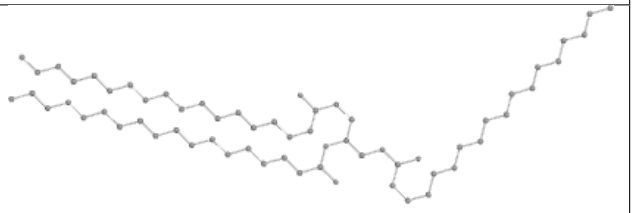
Bond lengths



Bond angles

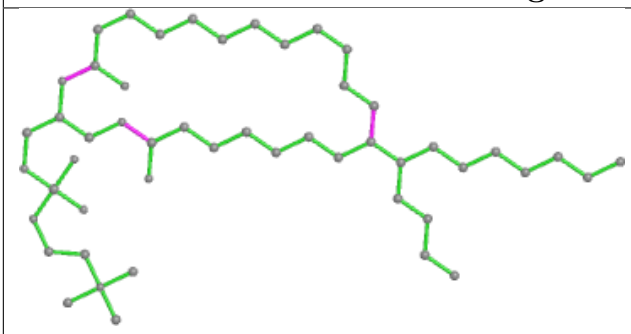


Torsions

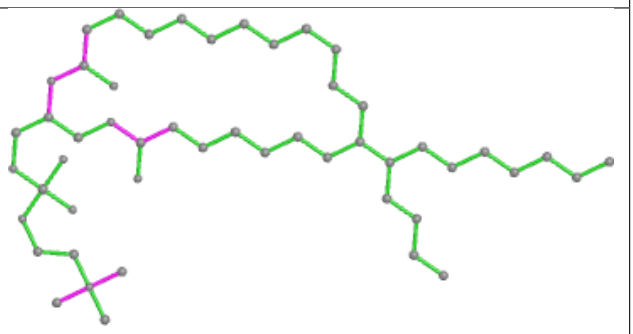


Rings

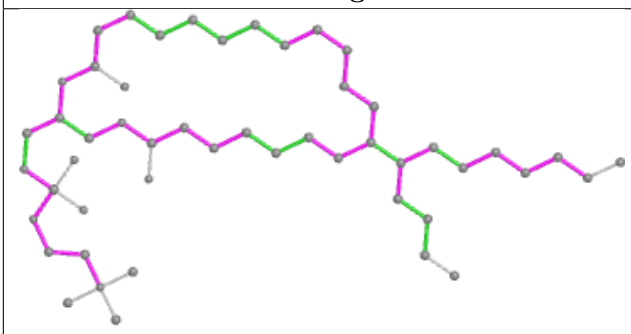
Ligand PSC E 201



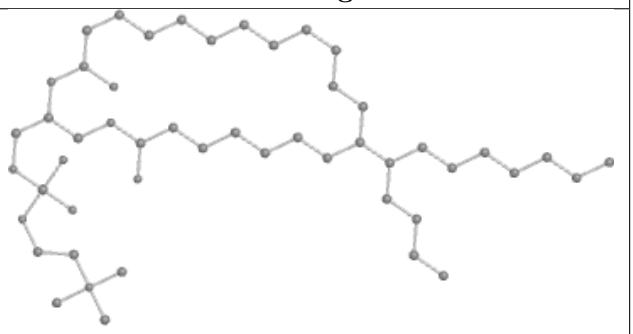
Bond lengths



Bond angles

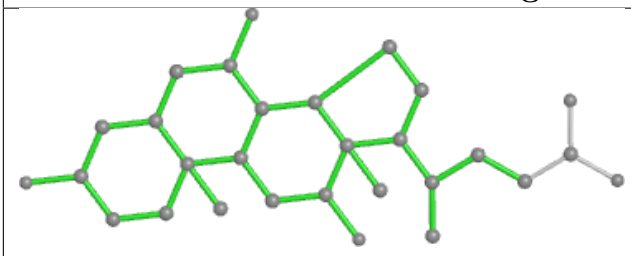


Torsions

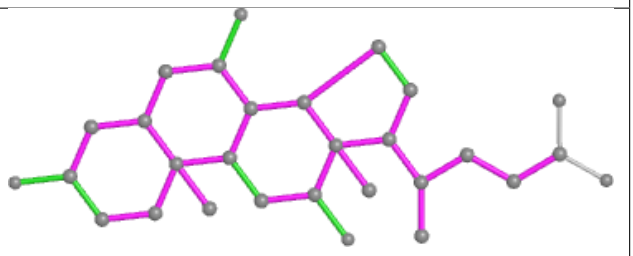


Rings

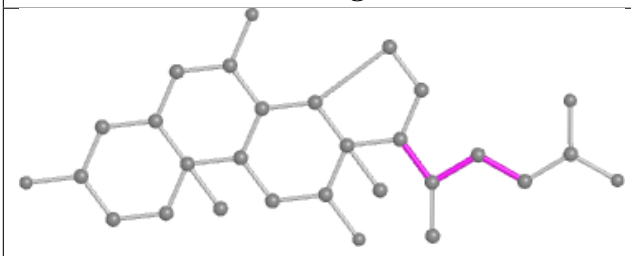
Ligand CHD P 307



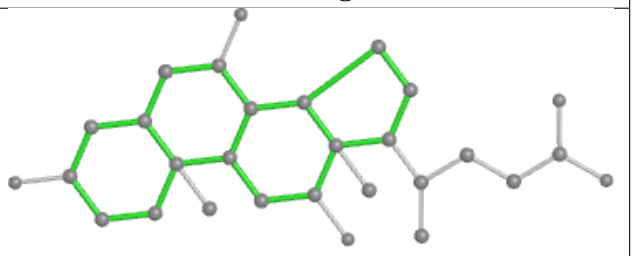
Bond lengths



Bond angles

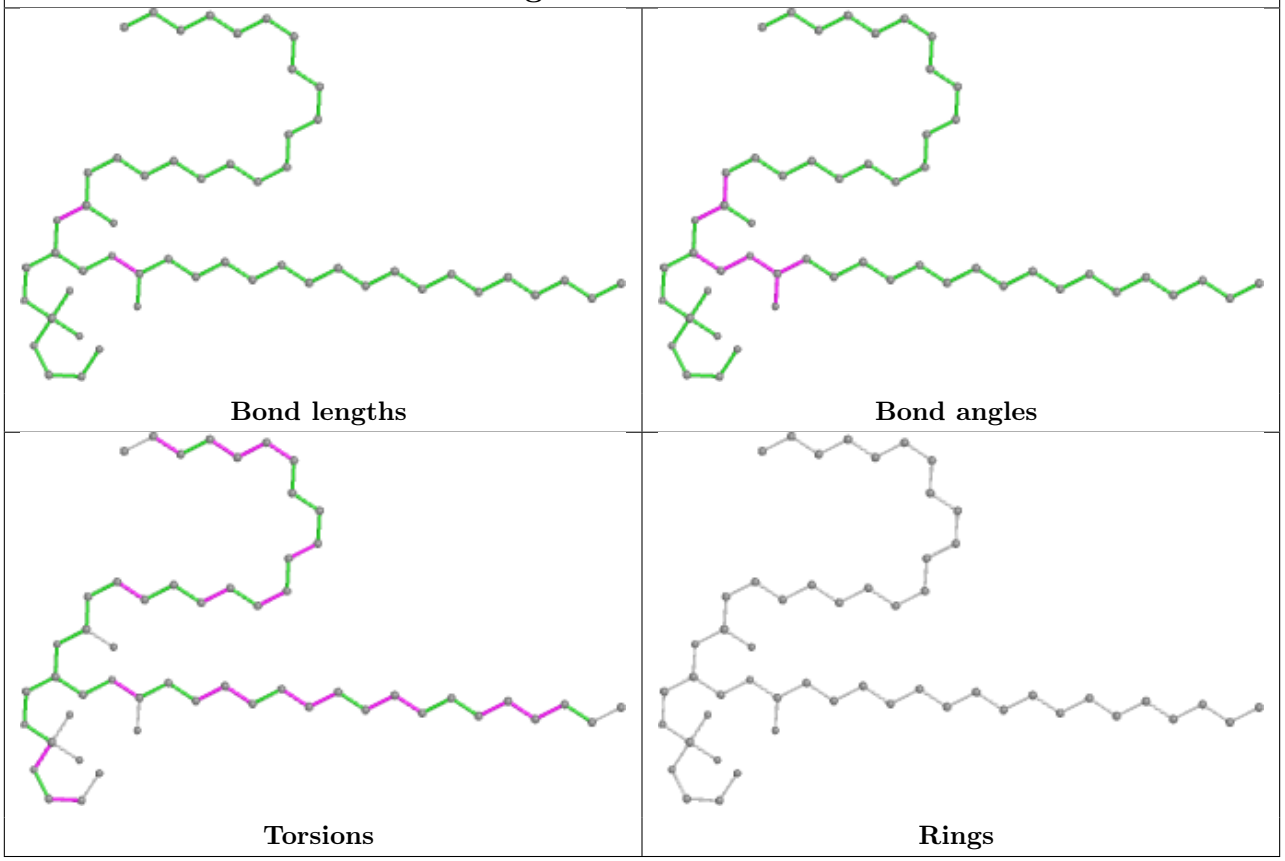


Torsions

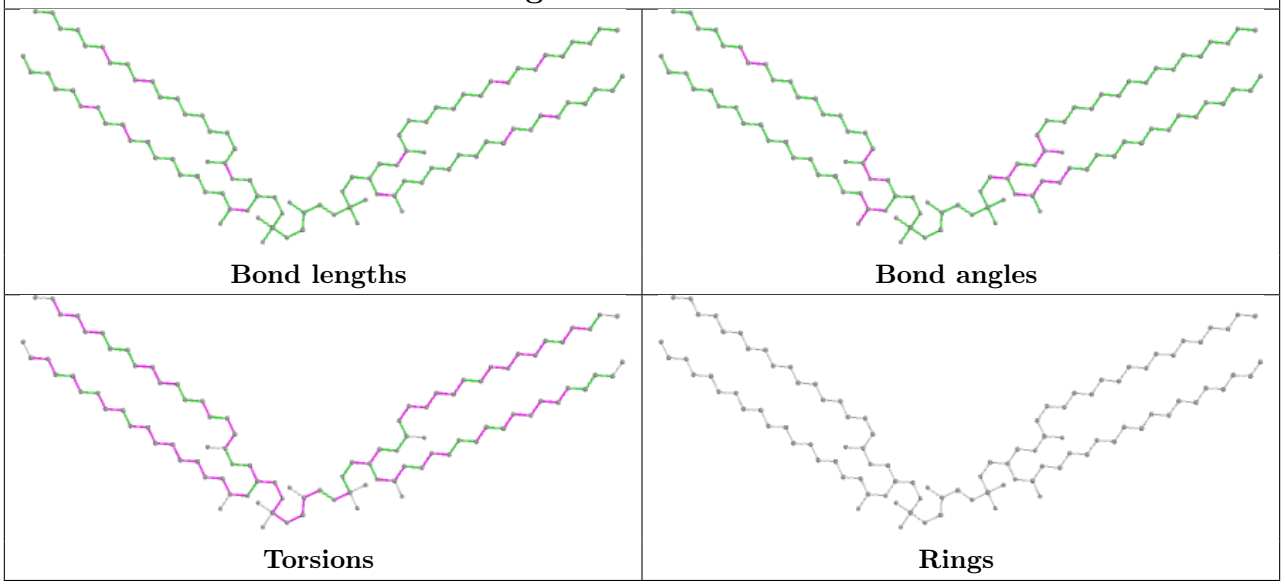


Rings

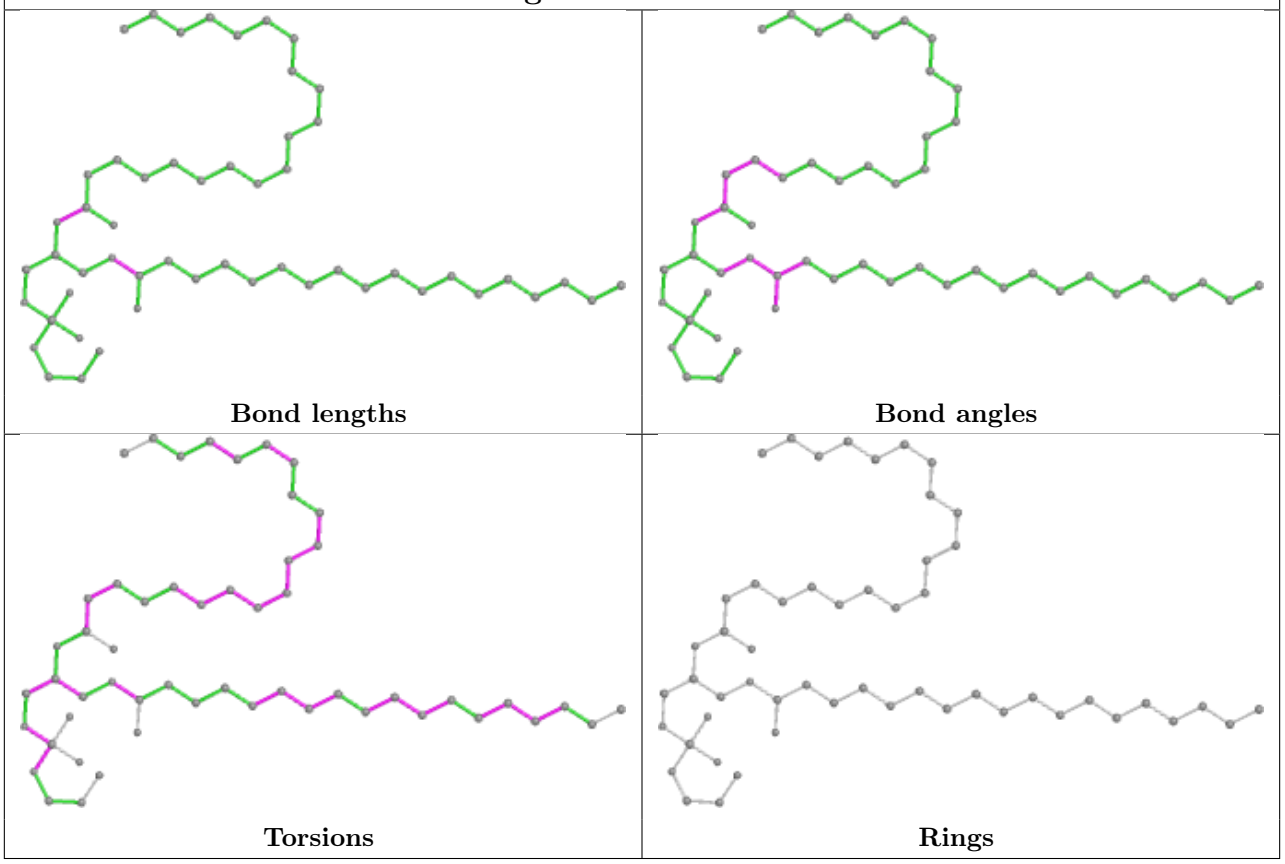
Ligand PEK P 309



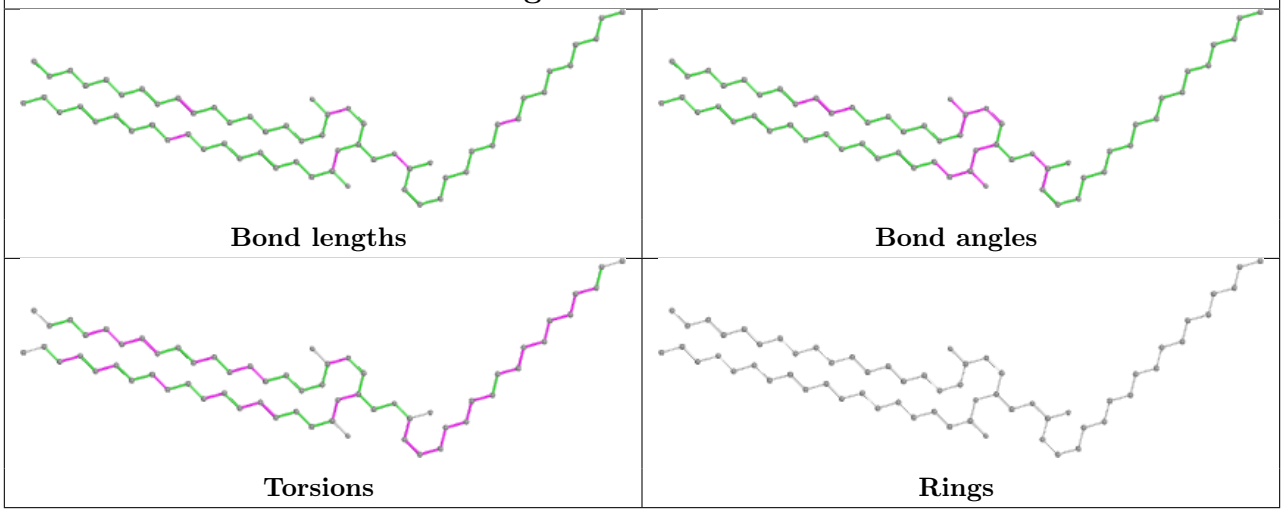
Ligand CDL P 306



Ligand PEK C 306



Ligand TGL N 609



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%)	-0.06	3 (0%) 89 88	21, 27, 35, 67	0
1	N	513/514 (99%)	-0.06	4 (0%) 86 85	26, 35, 47, 76	0
2	B	226/227 (99%)	-0.39	5 (2%) 62 60	24, 33, 55, 80	0
2	O	226/227 (99%)	-0.17	4 (1%) 68 66	34, 45, 69, 94	0
3	C	259/261 (99%)	-0.27	3 (1%) 79 78	25, 33, 44, 64	0
3	P	259/261 (99%)	-0.21	4 (1%) 73 72	29, 37, 49, 69	0
4	D	144/147 (97%)	-0.44	1 (0%) 87 87	28, 36, 52, 69	0
4	Q	144/147 (97%)	1.08	20 (13%) 2 2	41, 58, 83, 130	0
5	E	105/109 (96%)	-0.20	2 (1%) 66 65	28, 36, 59, 99	0
5	R	105/109 (96%)	0.23	4 (3%) 40 39	36, 47, 66, 104	0
6	F	98/98 (100%)	0.71	8 (8%) 11 11	29, 39, 97, 134	0
6	S	98/98 (100%)	0.71	10 (10%) 6 6	31, 45, 103, 128	0
7	G	83/85 (97%)	1.02	16 (19%) 1 0	31, 39, 110, 123	0
7	T	83/85 (97%)	0.98	17 (20%) 1 0	32, 47, 104, 119	0
8	H	79/85 (92%)	0.14	8 (10%) 7 6	30, 40, 88, 113	0
8	U	79/85 (92%)	0.45	9 (11%) 5 4	39, 50, 97, 125	0
9	I	72/73 (98%)	0.16	3 (4%) 36 35	34, 44, 65, 71	0
9	V	72/73 (98%)	0.70	8 (11%) 5 4	35, 60, 75, 102	0
10	J	58/59 (98%)	0.62	8 (13%) 2 2	33, 43, 72, 103	0
10	W	58/59 (98%)	0.70	8 (13%) 2 2	41, 52, 85, 125	0
11	K	49/56 (87%)	-0.29	0 100 100	34, 40, 52, 57	0
11	X	49/56 (87%)	1.52	18 (36%) 0 0	47, 59, 76, 84	0
12	L	46/47 (97%)	-0.32	0 100 100	28, 33, 55, 83	0
12	Y	46/47 (97%)	-0.05	1 (2%) 62 60	38, 50, 74, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.18	5 (11%) 4 4	29, 34, 90, 114	0
13	Z	43/46 (93%)	0.53	8 (18%) 1 1	46, 54, 122, 136	0
All	All	3550/3614 (98%)	0.10	177 (4%) 28 28	21, 38, 72, 136	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	25.4
4	Q	6	VAL	23.8
6	S	97	ALA	17.3
6	F	97	ALA	14.6
6	S	96	LEU	13.8
6	S	1	ALA	12.8
6	F	1	ALA	12.8
6	F	98	HIS	12.7
6	F	96	LEU	12.2
7	G	2	SER	11.0
6	S	2	SER	10.8
10	J	1	PHE	10.7
6	F	95	GLN	10.5
6	F	2	SER	10.4
7	G	3	ALA	9.6
7	G	1	ALA	9.4
4	Q	7	LYS	8.8
10	W	58	LYS	8.6
10	W	1	PHE	8.2
6	S	94	HIS	8.1
7	T	1	ALA	8.1
7	T	3	ALA	7.7
10	J	58	LYS	7.6
6	S	98	HIS	7.6
4	Q	4	SER	7.6
5	R	5	HIS	7.1
8	U	7	LYS	7.0
4	Q	8	SER	7.0
8	H	7	LYS	6.9
7	G	5	LYS	6.6
8	U	8	ILE	6.2
7	G	42	ARG	6.0
7	T	2	SER	6.0
8	H	8	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
6	F	94	HIS	5.9
13	M	43	SER	5.8
6	S	95	GLN	5.5
8	U	10	ASN	5.5
9	V	2	THR	5.5
13	Z	43	SER	5.5
7	T	42	ARG	5.5
4	Q	147	LYS	5.3
7	T	36	TRP	5.3
7	T	41	HIS	5.3
7	G	40	GLY	5.1
7	G	4	ALA	5.1
13	Z	42	LYS	5.1
5	R	109	VAL	5.1
6	F	3	GLY	5.0
9	I	37	PHE	5.0
7	T	4	ALA	5.0
7	T	5	LYS	4.9
7	T	40	GLY	4.8
13	Z	35	TYR	4.7
8	H	45	ALA	4.6
11	X	13	TYR	4.6
7	G	9	GLY	4.5
7	G	41	HIS	4.5
13	M	40	TYR	4.4
7	T	8	HIS	4.4
13	Z	40	TYR	4.3
7	G	8	HIS	4.3
11	X	23	THR	4.3
6	S	93	PRO	4.3
13	Z	39	ASN	4.2
7	T	84	LYS	4.2
7	T	39	SER	4.2
8	H	44	THR	4.1
2	O	113	TYR	4.0
7	G	6	GLY	4.0
9	V	37	PHE	3.9
7	G	36	TRP	3.8
8	H	46	LYS	3.8
13	Z	37	LEU	3.8
11	X	27	ALA	3.8
10	J	2	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
12	Y	47	LYS	3.8
6	S	3	GLY	3.7
8	U	9	LYS	3.7
2	O	91	ASN	3.7
2	B	59	GLN	3.6
13	M	42	LYS	3.6
4	Q	102	TYR	3.6
5	E	109	VAL	3.6
4	Q	53	ILE	3.5
7	G	43	GLU	3.5
4	Q	51	LEU	3.5
11	X	6	ALA	3.4
11	X	7	PRO	3.4
8	H	47	GLY	3.2
10	W	52	TRP	3.2
2	B	60	GLU	3.2
7	G	7	ASP	3.2
3	P	91	VAL	3.2
5	E	5	HIS	3.2
8	H	43	MET	3.2
8	U	45	ALA	3.2
10	J	57	HIS	3.1
10	W	57	HIS	3.0
10	W	26	ALA	3.0
11	X	19	ALA	3.0
7	G	84	LYS	3.0
4	Q	107	ILE	3.0
13	M	39	ASN	3.0
10	J	48	TYR	2.9
10	W	4	ARG	2.9
11	X	16	ALA	2.9
4	Q	101	HIS	2.9
10	W	48	TYR	2.9
2	O	226	MET	2.9
7	T	10	GLY	2.9
10	J	52	TRP	2.9
1	N	201	VAL	2.8
2	O	90	ILE	2.8
7	T	43	GLU	2.8
8	U	44	THR	2.8
11	X	34	THR	2.8
4	Q	33	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
7	T	6	GLY	2.8
9	V	25	PHE	2.8
11	X	24	PHE	2.8
4	Q	58	GLU	2.7
3	P	3	HIS	2.7
5	R	52	LEU	2.7
3	C	92	LEU	2.7
13	Z	41	LYS	2.7
13	Z	32	TRP	2.7
4	Q	138	TRP	2.6
10	W	2	GLU	2.6
8	U	50	VAL	2.6
5	R	96	LEU	2.6
4	D	147	LYS	2.5
11	X	35	GLN	2.5
10	J	4	ARG	2.5
1	A	197	LEU	2.5
11	X	52	GLU	2.4
11	X	47	ARG	2.4
1	N	197	LEU	2.4
11	X	18	LEU	2.4
10	J	30	ILE	2.4
2	B	57	ASP	2.4
9	V	34	PHE	2.4
9	V	53	ASN	2.4
7	T	9	GLY	2.4
4	Q	140	TYR	2.3
4	Q	106	PRO	2.3
4	Q	35	ALA	2.3
9	I	52	ARG	2.3
1	N	193	VAL	2.3
11	X	15	ASN	2.3
3	P	88	ILE	2.3
4	Q	10	ASP	2.3
4	Q	111	PHE	2.3
8	U	49	ASP	2.3
13	M	35	TYR	2.2
3	P	85	LEU	2.2
11	X	21	GLY	2.2
9	V	26	MET	2.2
11	X	12	LYS	2.2
2	B	55	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	58	ALA	2.2
1	A	201	VAL	2.1
9	V	48	ALA	2.1
3	C	91	VAL	2.1
4	Q	145	TRP	2.1
9	V	29	LEU	2.1
6	S	44	GLU	2.1
9	I	18	ARG	2.1
3	C	88	ILE	2.1
7	T	7	ASP	2.1
8	U	47	GLY	2.1
1	N	196	LEU	2.0
1	A	237	PHE	2.0
7	G	12	GLY	2.0
11	X	31	TYR	2.0
8	H	48	GLY	2.0
11	X	46	GLY	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
9	SAC	V	1	9/10	0.24	0.59	113,117,118,119	0
7	TPO	G	11	11/12	0.53	0.39	83,91,111,114	0
7	TPO	T	11	11/12	0.55	0.36	87,95,113,113	0
9	SAC	I	1	9/10	0.80	0.18	68,71,73,74	0
1	FME	A	1	10/11	0.93	0.14	44,53,74,81	0
1	FME	N	1	10/11	0.95	0.17	52,58,75,76	0
2	FME	B	1	10/11	0.97	0.12	32,34,43,59	0
2	FME	O	1	10/11	0.98	0.14	45,47,58,65	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	P	301	33/33	0.32	0.44	132,165,171,171	0
25	PEK	C	306	53/53	0.48	0.30	53,92,130,133	0
25	PEK	T	101	53/53	0.52	0.49	62,105,129,130	0
28	DMU	G	101	33/33	0.53	0.29	103,146,153,154	0
25	PEK	P	309	53/53	0.55	0.36	47,97,125,127	0
24	CDL	G	103	100/100	0.57	0.37	73,101,133,138	0
25	PEK	G	104	53/53	0.58	0.50	60,112,135,137	0
26	PSC	O	303	52/52	0.58	0.34	57,105,133,136	0
24	CDL	T	102	100/100	0.61	0.35	68,101,133,137	0
20	PGV	P	302	51/51	0.64	0.43	74,105,119,121	0
20	PGV	C	307	51/51	0.65	0.41	62,90,111,112	0
19	TGL	N	610	63/63	0.66	0.32	57,80,98,100	0
24	CDL	P	306	100/100	0.67	0.37	57,103,125,132	0
22	CHD	C	304	29/29	0.70	0.48	92,125,126,127	0
19	TGL	Q	201	63/63	0.71	0.25	64,87,97,100	0
22	CHD	P	307	29/29	0.71	0.37	91,121,122,124	0
20	PGV	N	607	51/51	0.72	0.32	54,92,119,123	0
23	UNX	C	301	1/1	0.73	0.24	38,38,38,38	0
20	PGV	A	609	51/51	0.73	0.28	34,78,100,106	0
26	PSC	E	201	52/52	0.73	0.34	53,106,127,129	0
24	CDL	C	303	100/100	0.74	0.39	44,96,128,130	0
19	TGL	D	201	63/63	0.75	0.22	46,69,82,83	0
19	TGL	L	101	63/63	0.77	0.27	38,61,82,85	0
28	DMU	Z	101	33/33	0.81	0.30	57,70,87,91	0
19	TGL	N	609	63/63	0.83	0.22	57,84,100,103	0
19	TGL	A	607	63/63	0.84	0.21	49,77,97,100	0
17	MG	N	605	1/1	0.85	0.15	39,39,39,39	0
18	NA	N	606	1/1	0.85	0.33	53,53,53,53	0
18	NA	A	606	1/1	0.87	0.29	45,45,45,45	0
22	CHD	C	305	29/29	0.90	0.15	37,44,47,48	0
28	DMU	M	101	33/33	0.91	0.16	43,49,68,70	0
22	CHD	P	308	29/29	0.92	0.13	41,47,50,50	0
23	UNX	P	303	1/1	0.92	0.30	35,35,35,35	0
25	PEK	P	304	53/53	0.93	0.17	38,60,93,95	0
20	PGV	P	305	51/51	0.95	0.14	31,47,86,89	0
25	PEK	G	102	53/53	0.95	0.14	29,50,79,81	0
20	PGV	A	608	51/51	0.96	0.13	24,41,65,70	0

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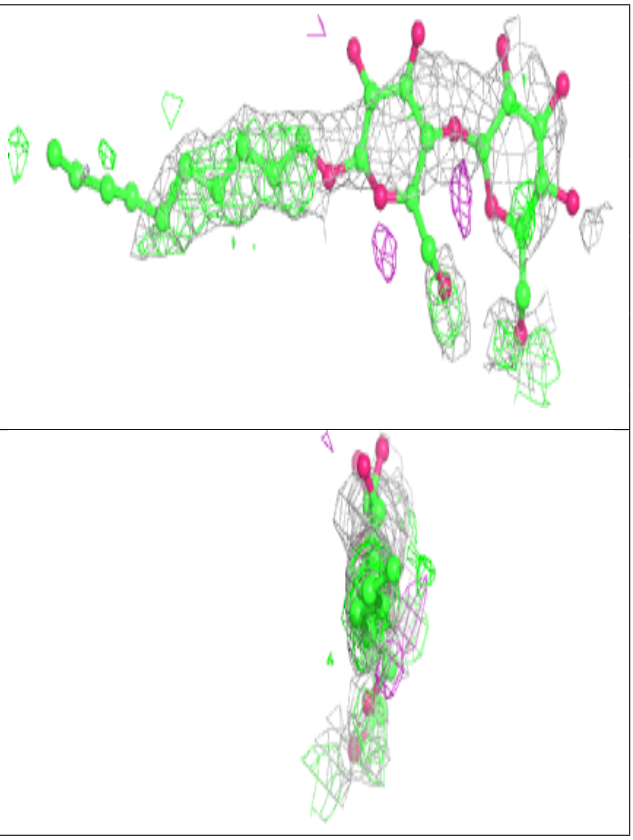
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	PGV	C	302	51/51	0.96	0.12	26,37,79,82	0
20	PGV	N	608	51/51	0.96	0.14	30,49,74,76	0
22	CHD	B	302	29/29	0.97	0.09	33,37,42,53	0
17	MG	A	605	1/1	0.97	0.13	27,27,27,27	0
15	HEA	N	602	60/60	0.97	0.10	15,31,57,63	0
22	CHD	O	302	29/29	0.97	0.10	33,37,43,45	0
15	HEA	A	602	60/60	0.98	0.13	17,23,51,55	0
14	CYN	N	601	2/2	0.99	0.15	30,30,30,31	0
15	HEA	N	603	60/60	0.99	0.13	25,30,39,42	0
14	CYN	A	601	2/2	0.99	0.15	20,20,20,24	0
15	HEA	A	603	60/60	0.99	0.12	18,23,33,35	0
21	CUA	B	301	2/2	0.99	0.13	26,26,26,27	0
21	CUA	O	301	2/2	0.99	0.10	38,38,38,38	0
16	CU	A	604	1/1	1.00	0.13	25,25,25,25	0
16	CU	N	604	1/1	1.00	0.13	30,30,30,30	0
27	ZN	F	101	1/1	1.00	0.09	35,35,35,35	0
27	ZN	S	101	1/1	1.00	0.08	40,40,40,40	0

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

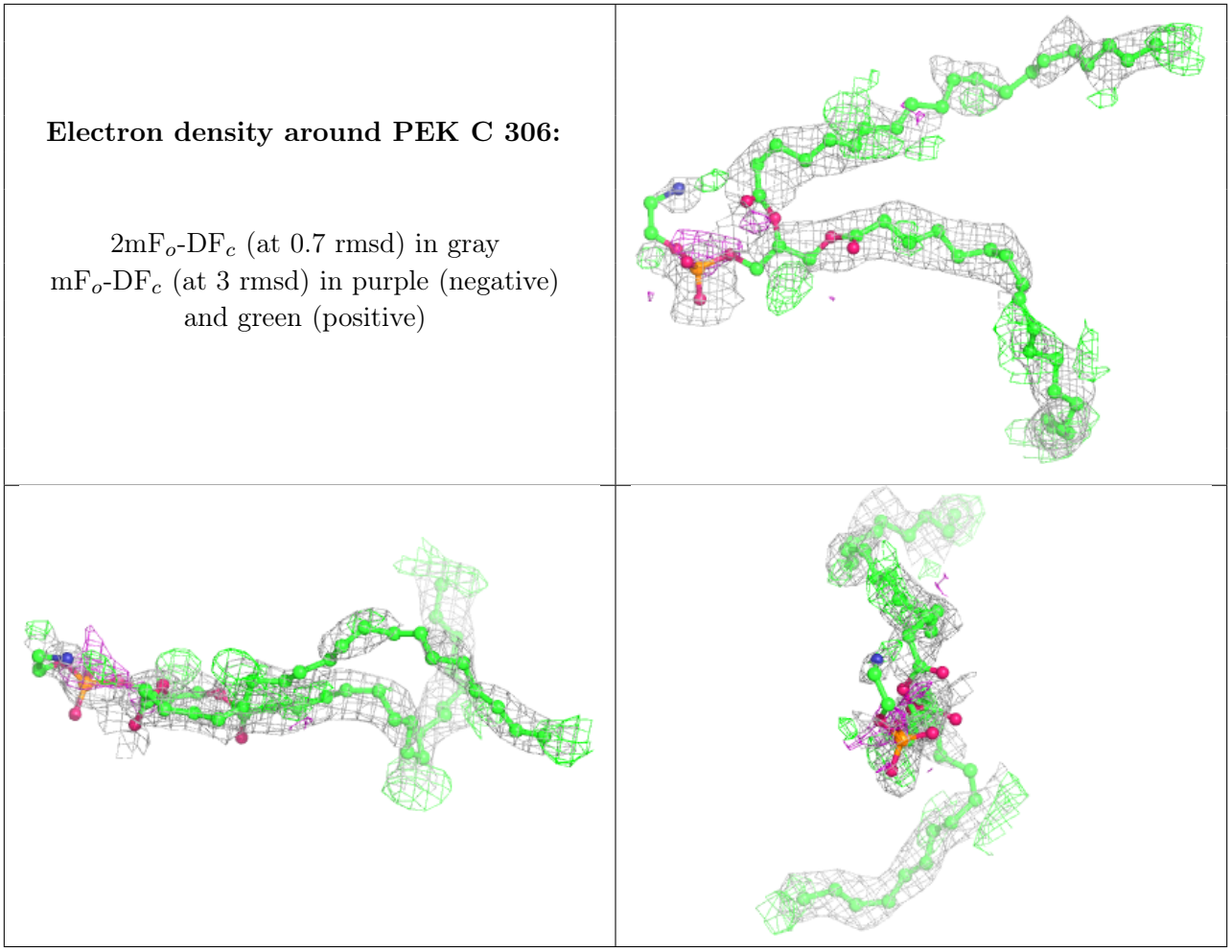
Electron density around DMU P 301:

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



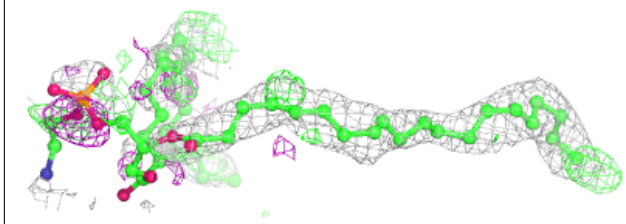
Electron density around PEK C 306:

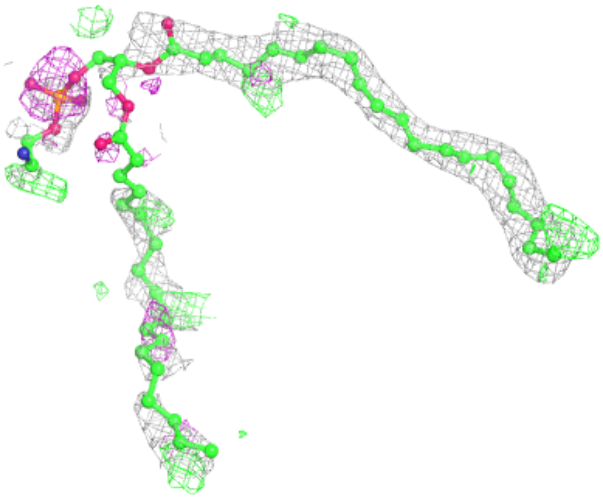
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PEK T 101:

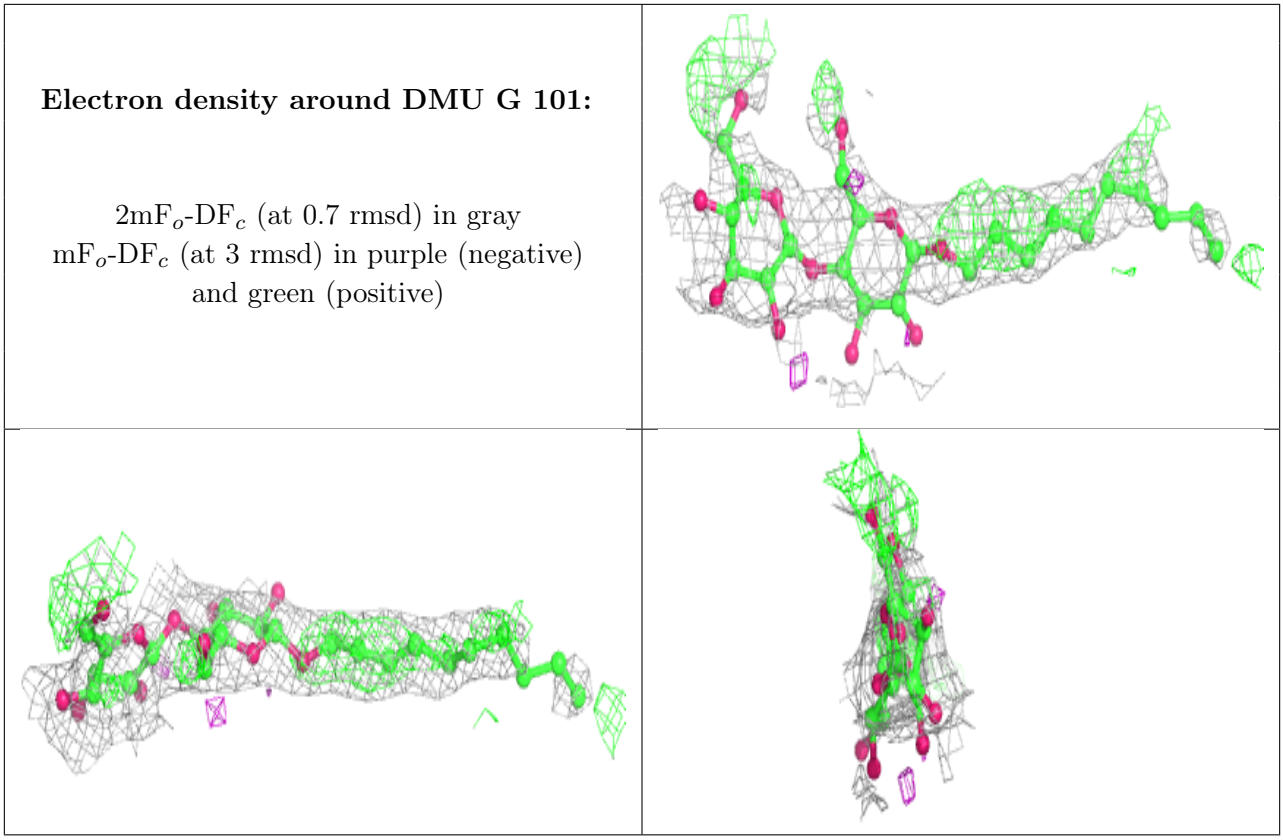
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





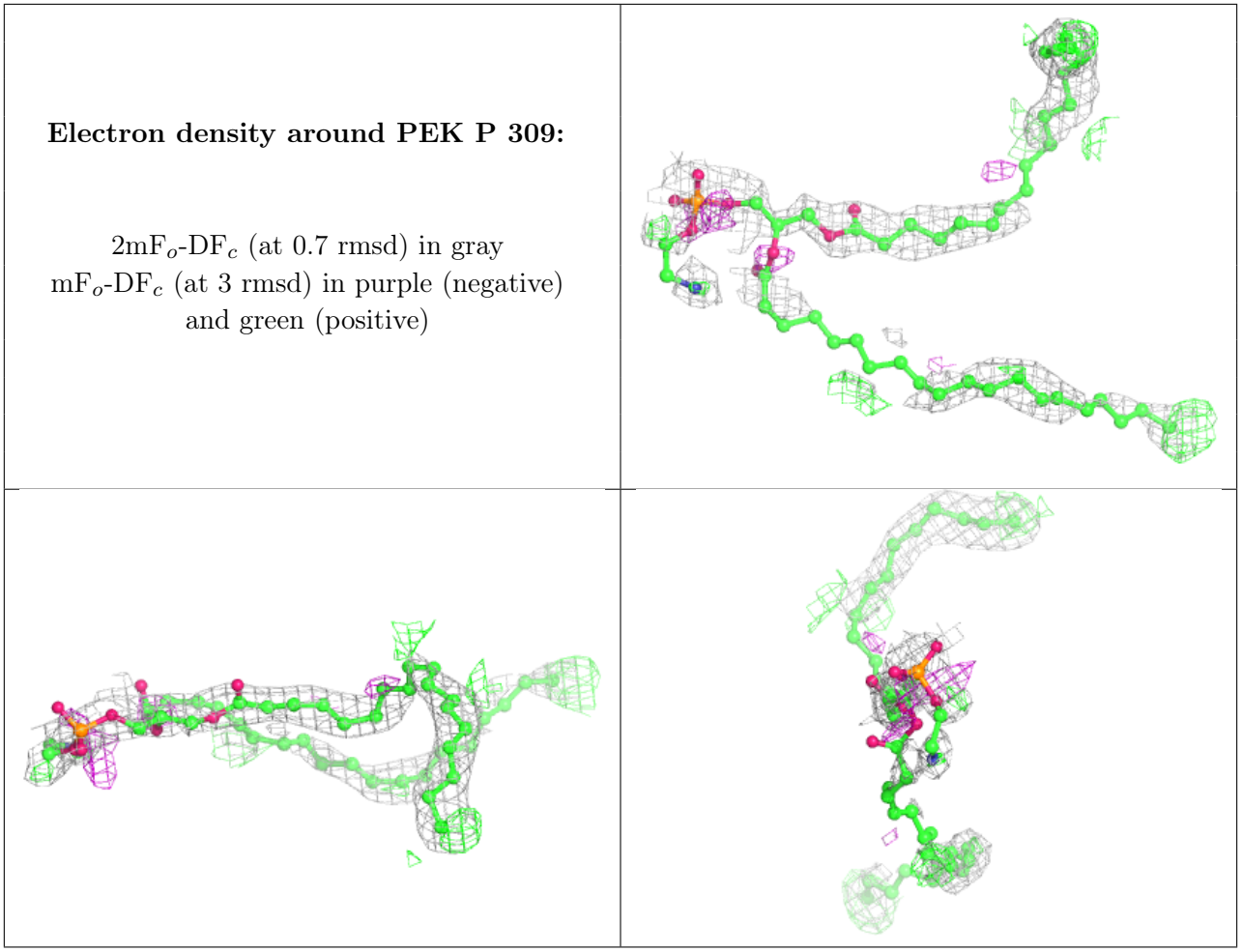
Electron density around DMU G 101:

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



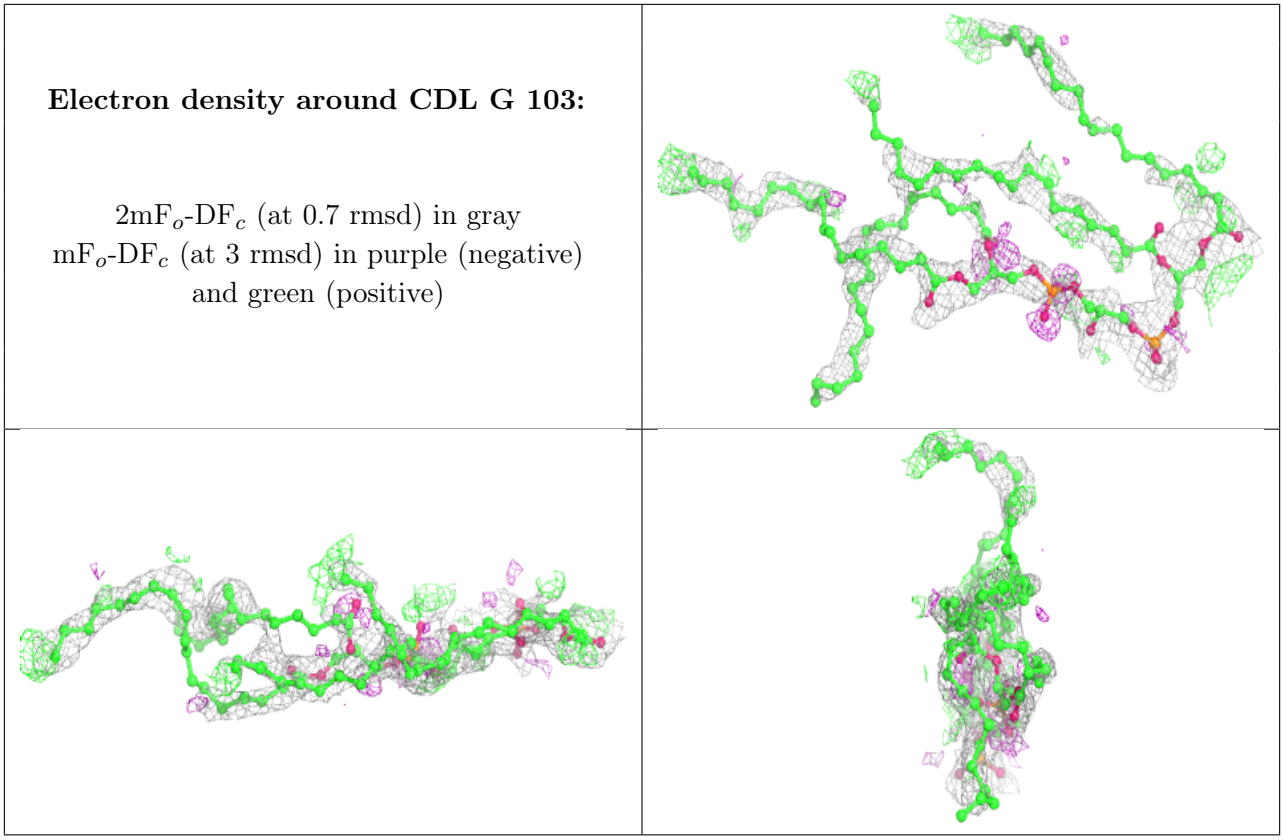
Electron density around PEK P 309:

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



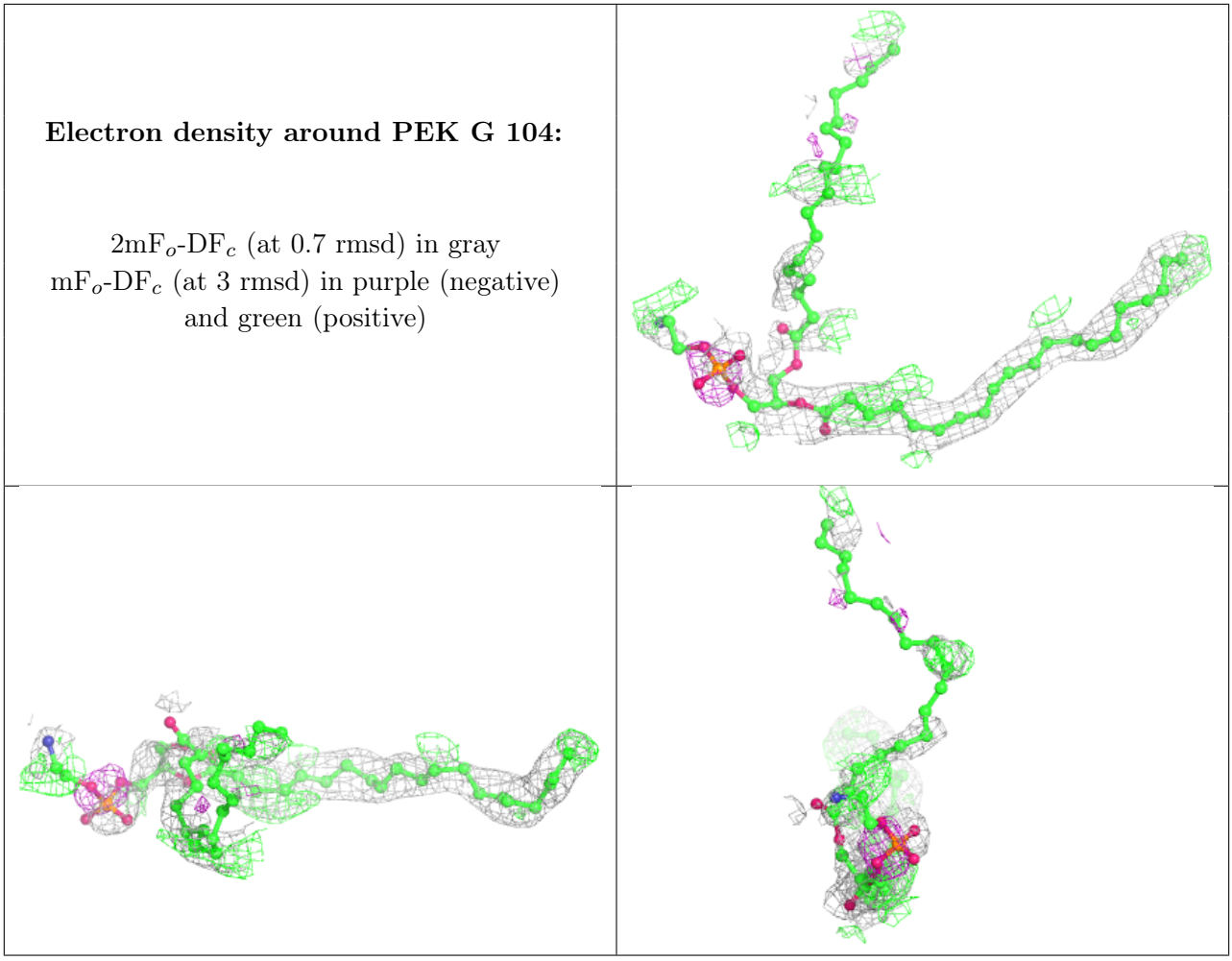
Electron density around CDL G 103:

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



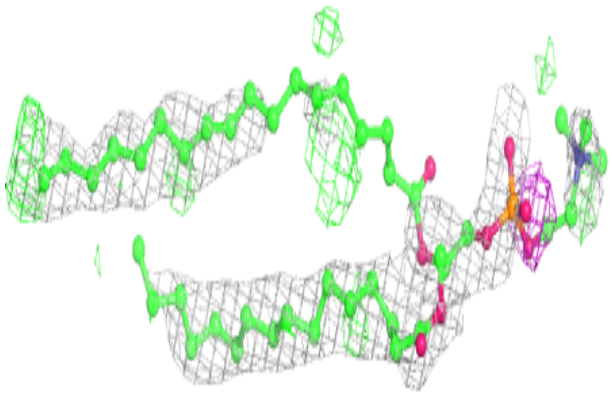
Electron density around PEK G 104:

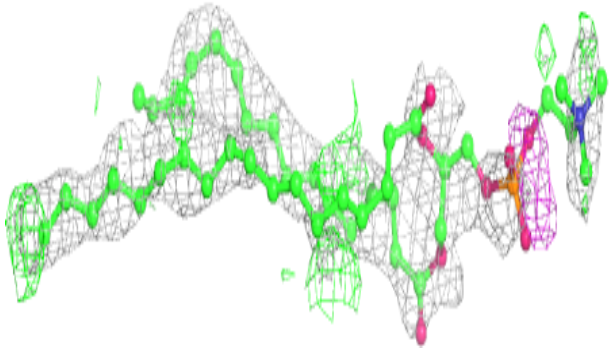
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

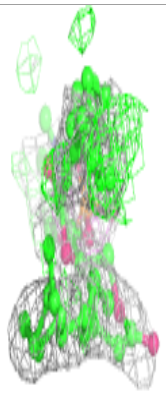


Electron density around PSC O 303:

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

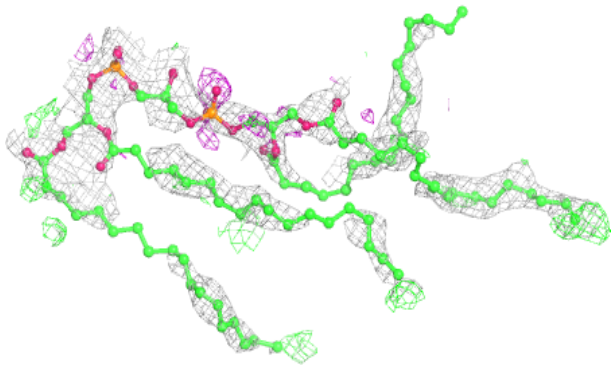


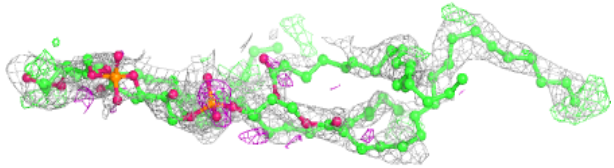


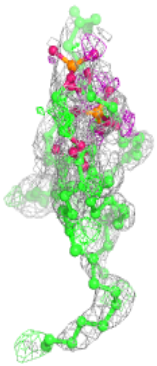


Electron density around CDL T 102:

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

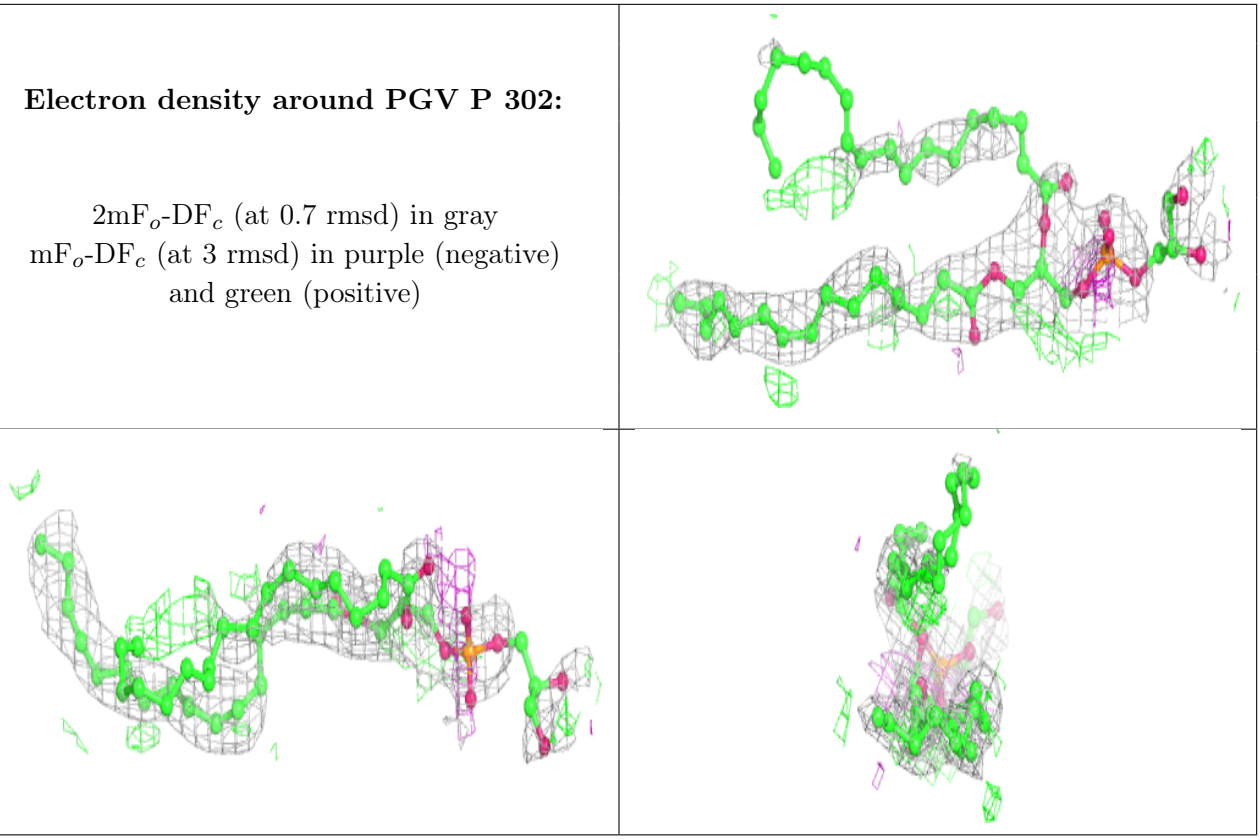






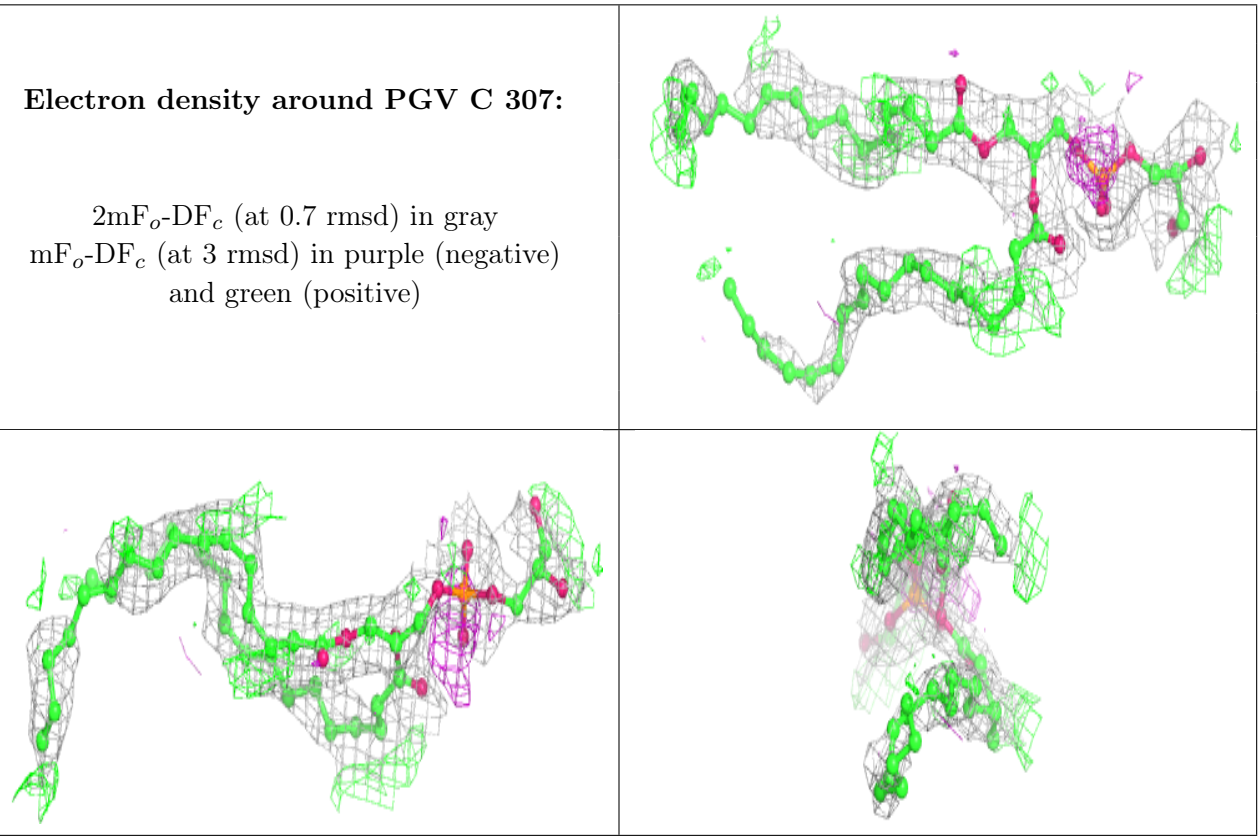
Electron density around PGV P 302:

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



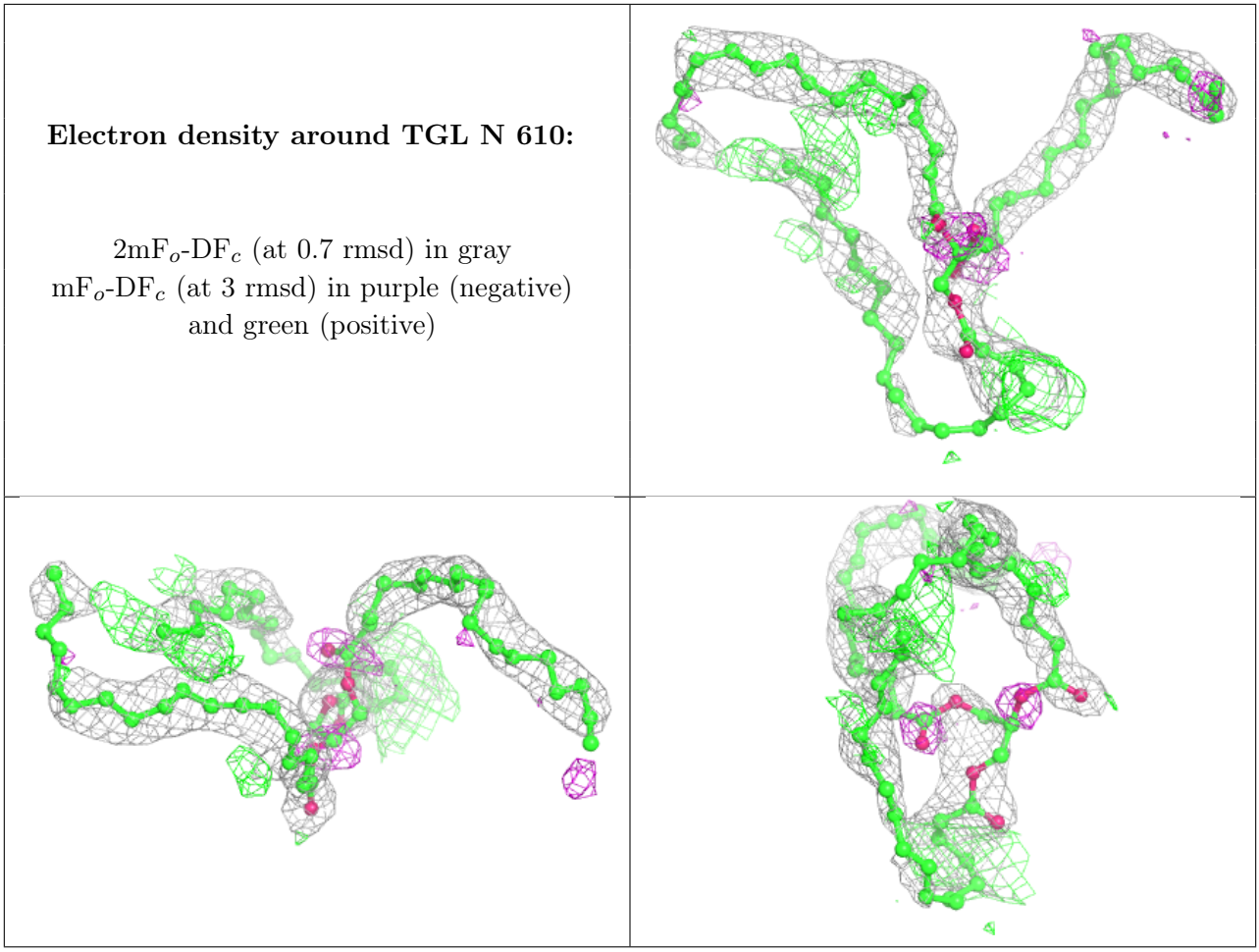
Electron density around PGV C 307:

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



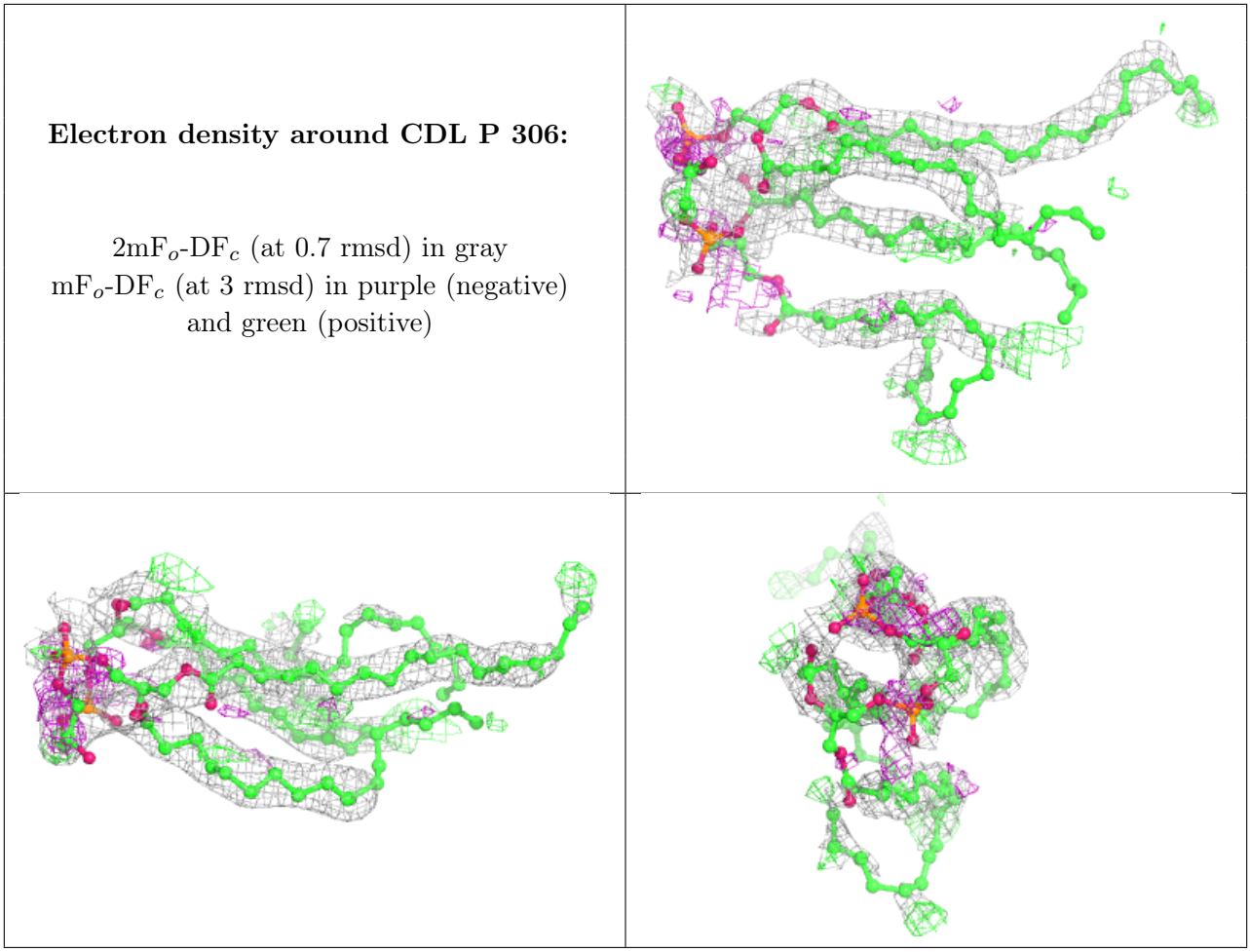
Electron density around TGL N 610:

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



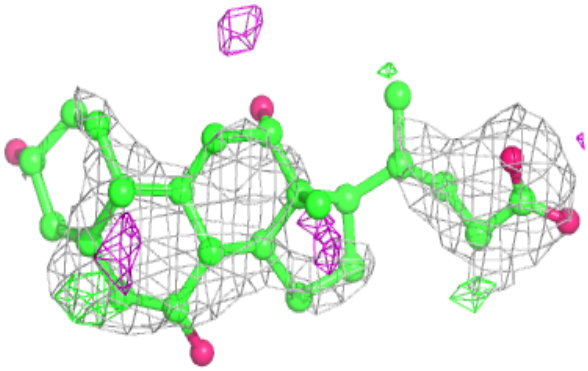
Electron density around CDL P 306:

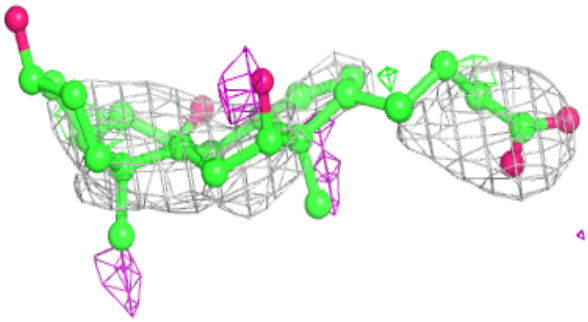
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

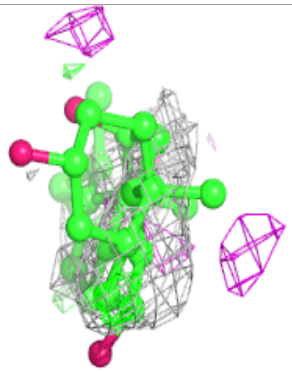


Electron density around CHD C 304:

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

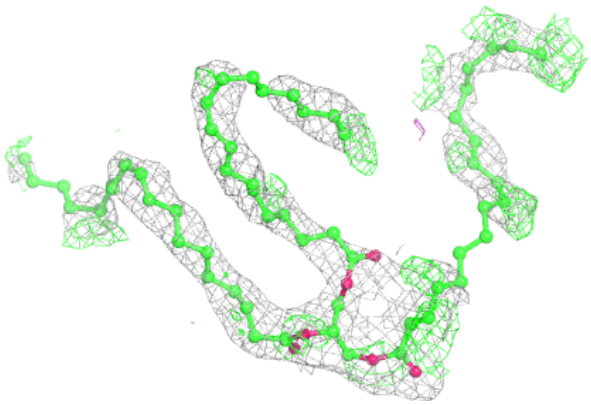


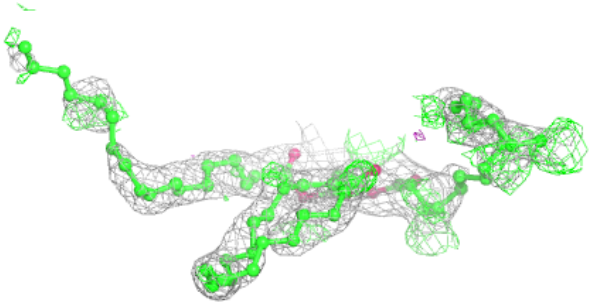


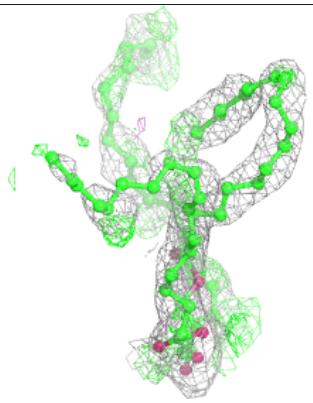


Electron density around TGL Q 201:

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

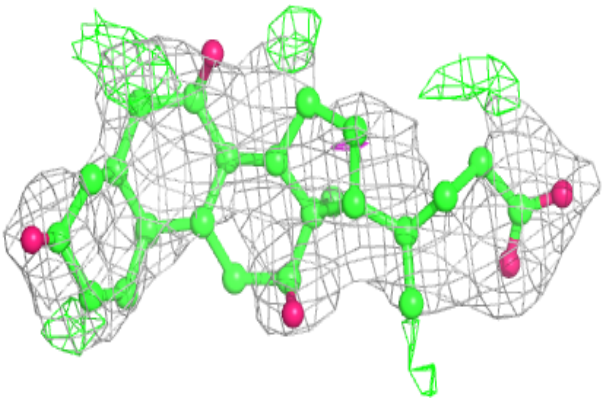


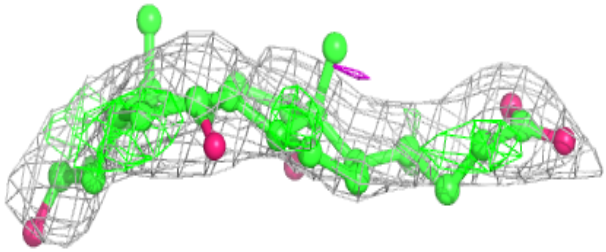


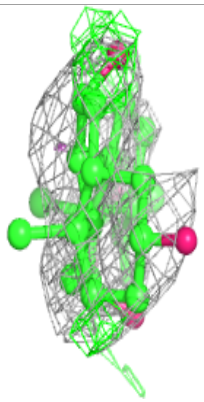


Electron density around CHD P 307:

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

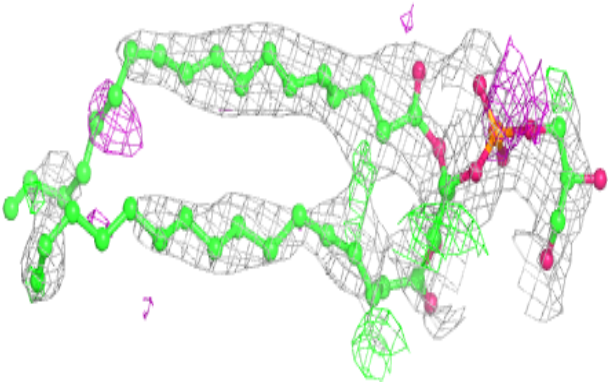


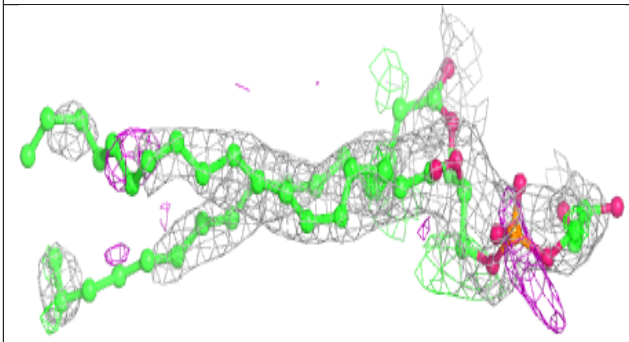


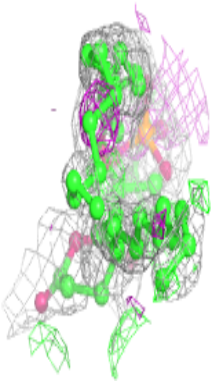


Electron density around PGV N 607:

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

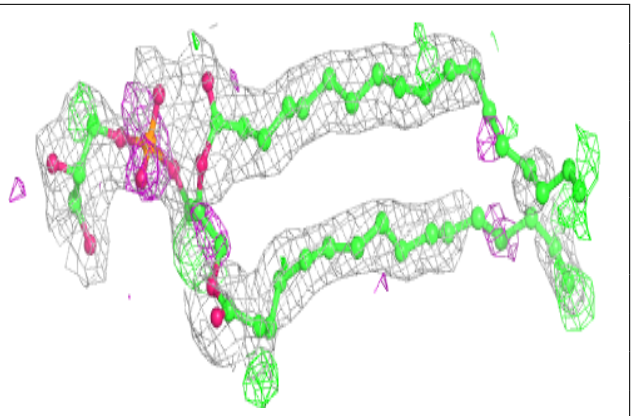


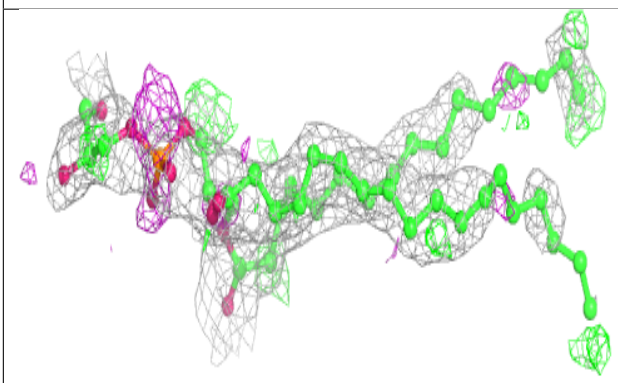




Electron density around PGV A 609:

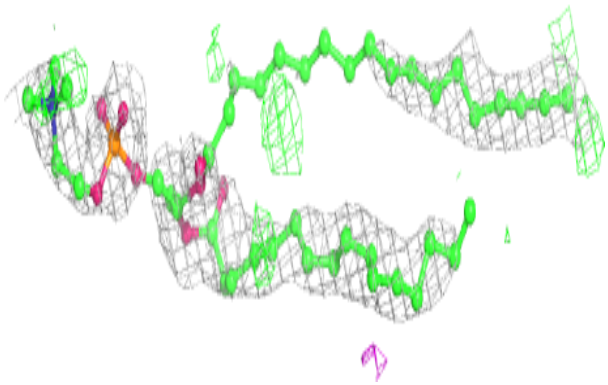
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

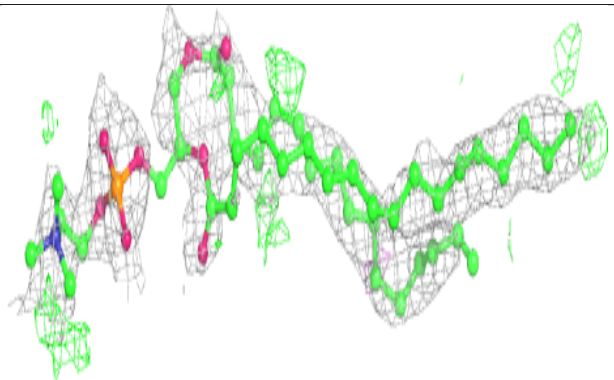


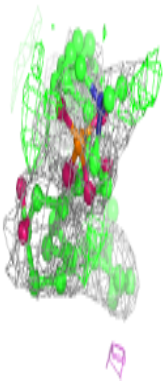


Electron density around PSC E 201:

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

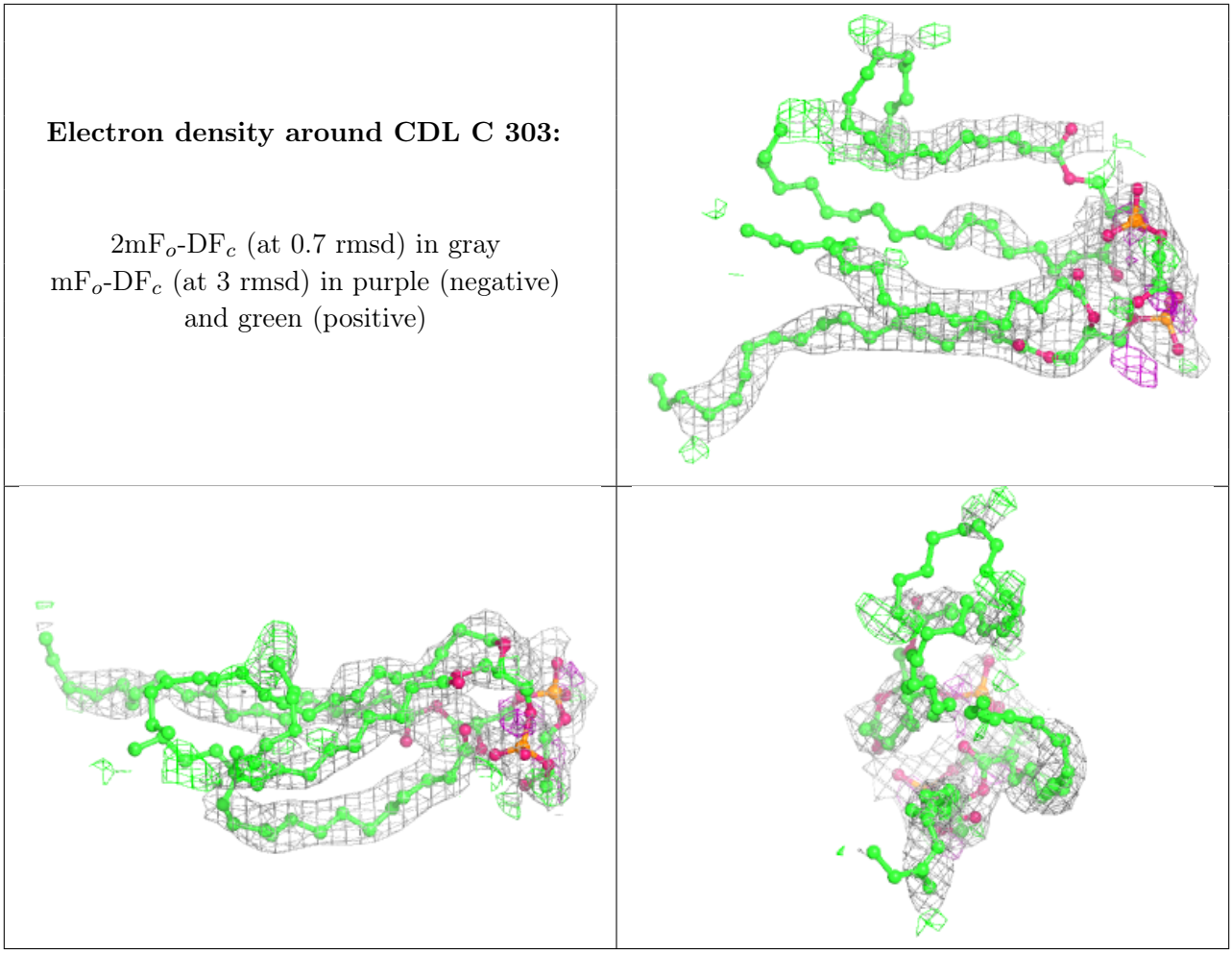






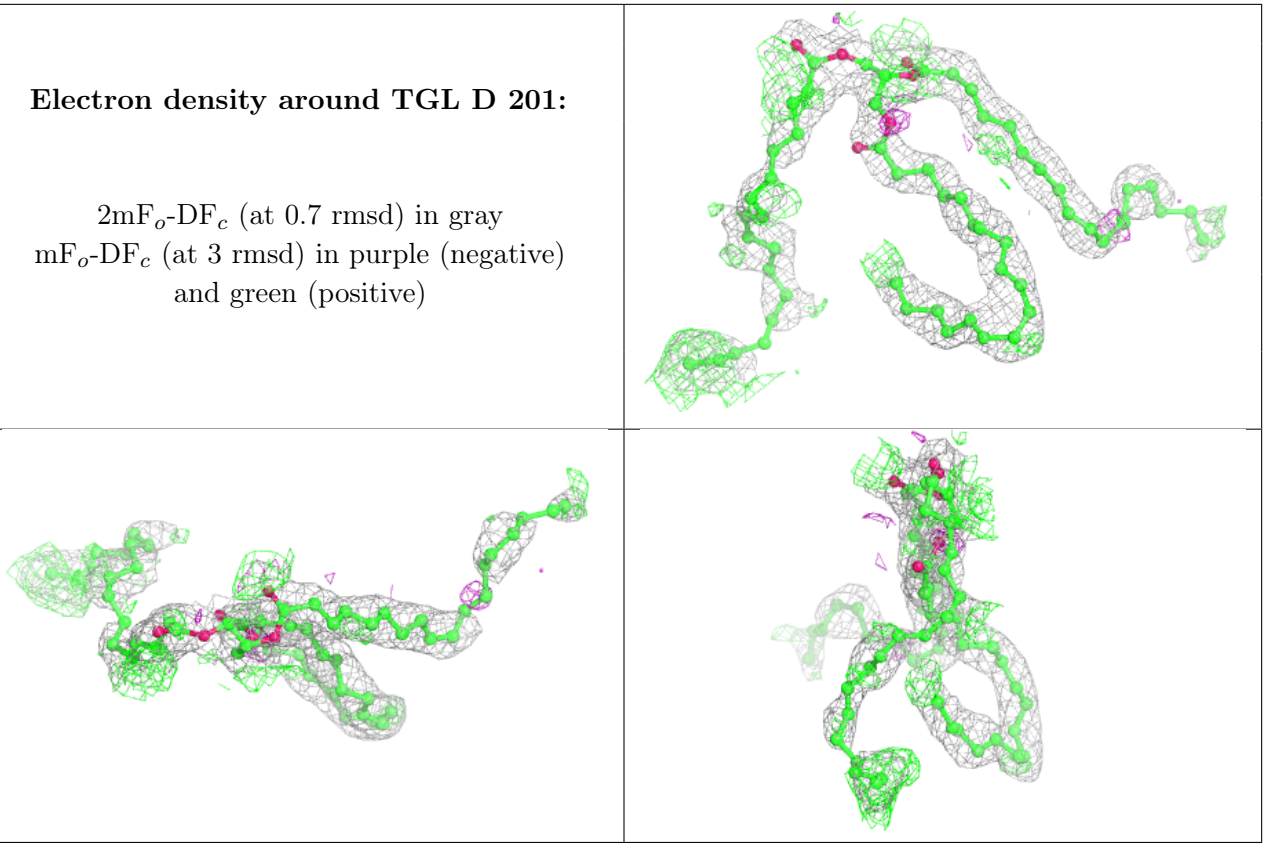
Electron density around CDL C 303:

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



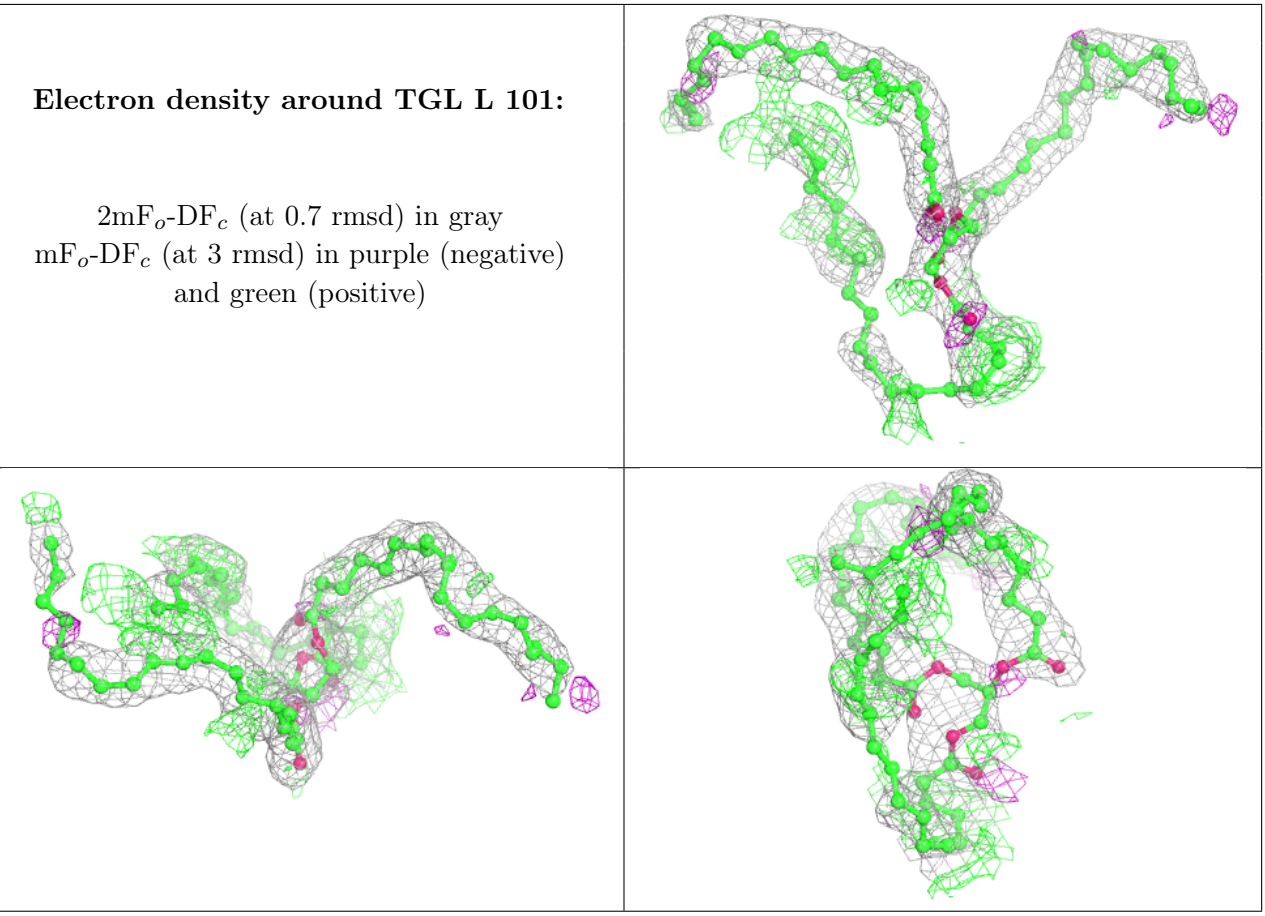
Electron density around TGL D 201:

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



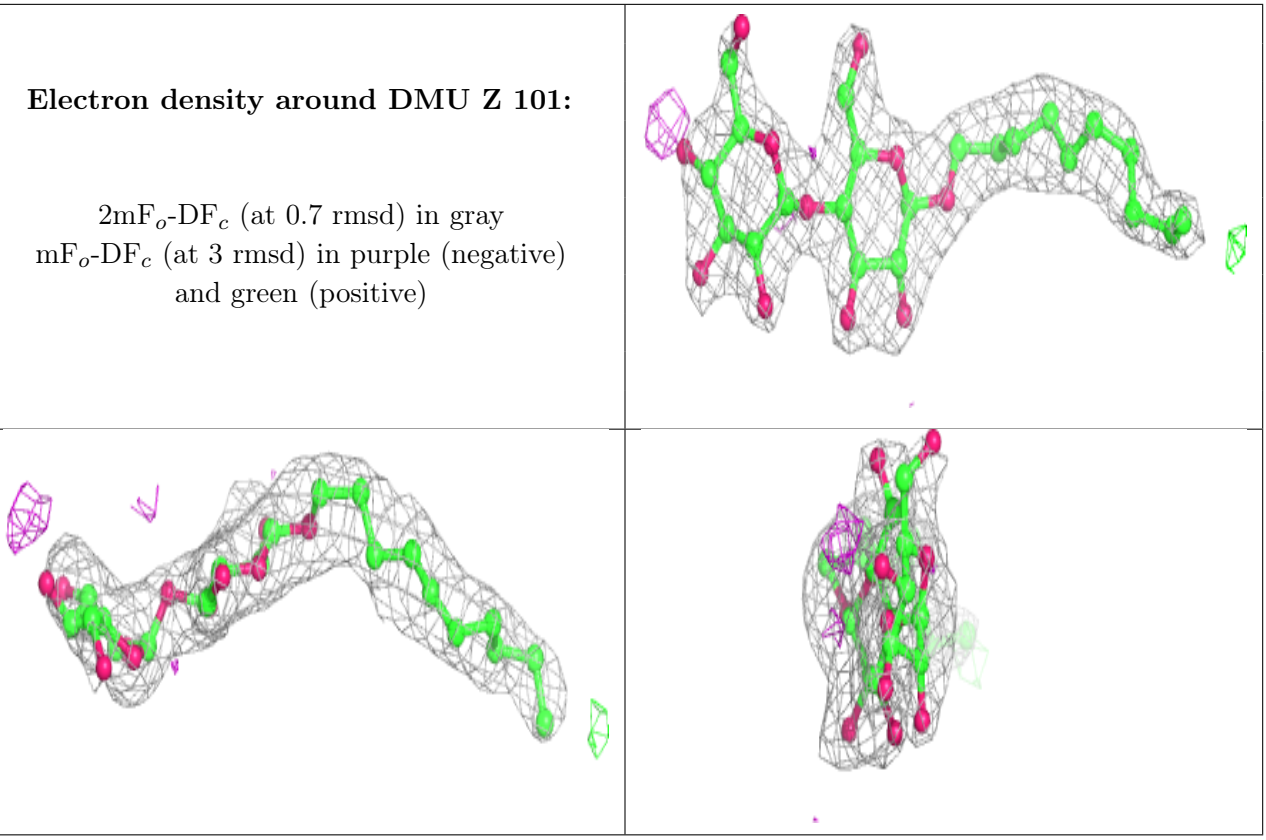
Electron density around TGL L 101:

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



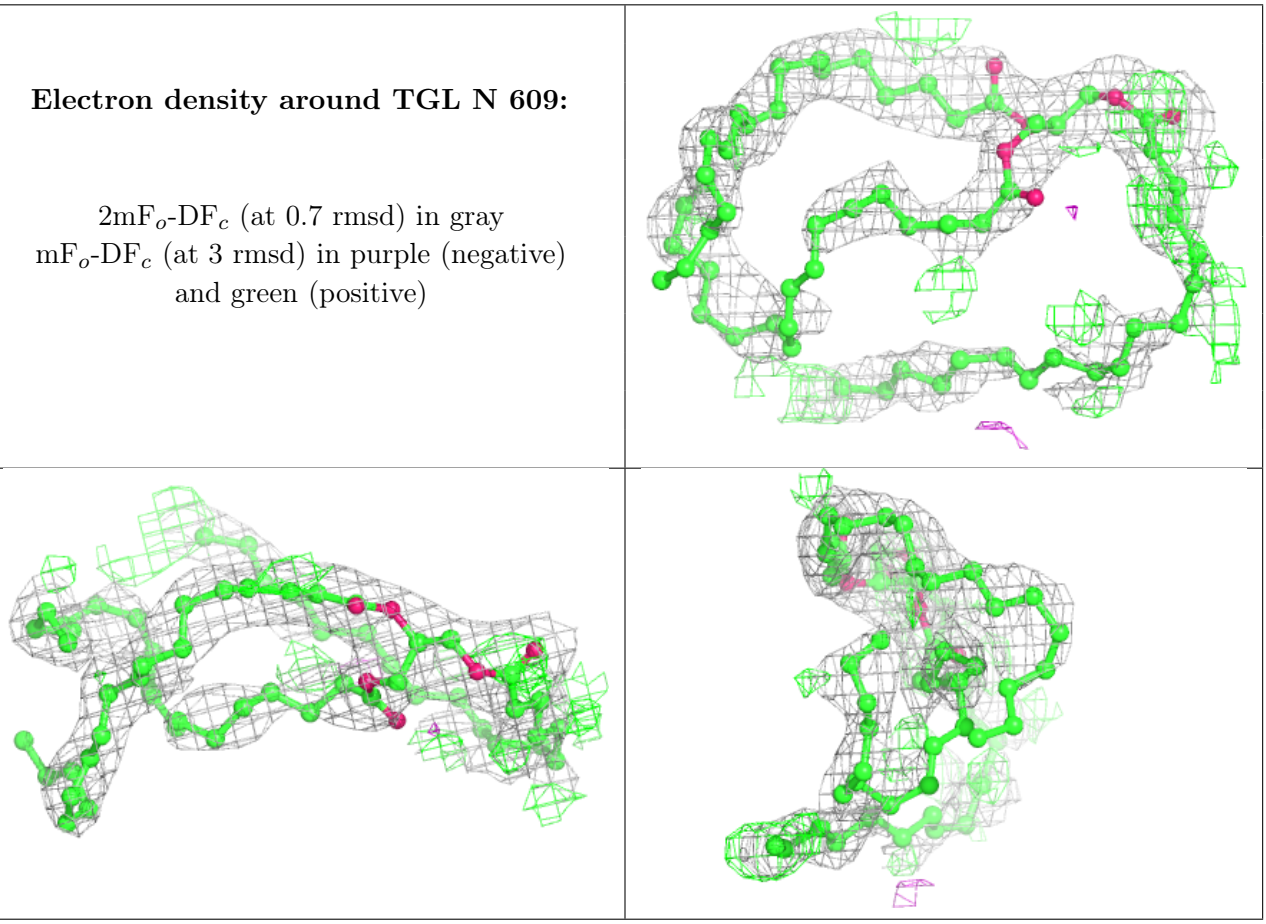
Electron density around DMU Z 101:

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



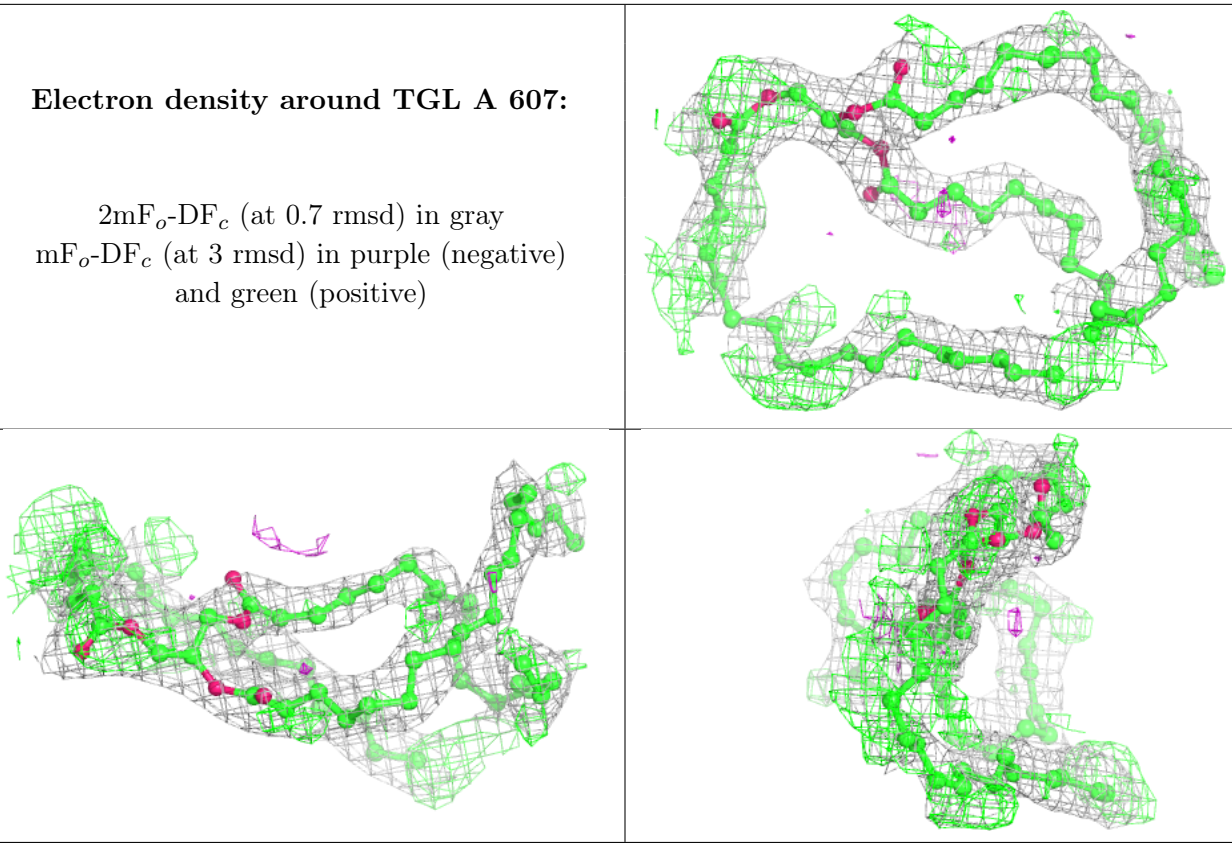
Electron density around TGL N 609:

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



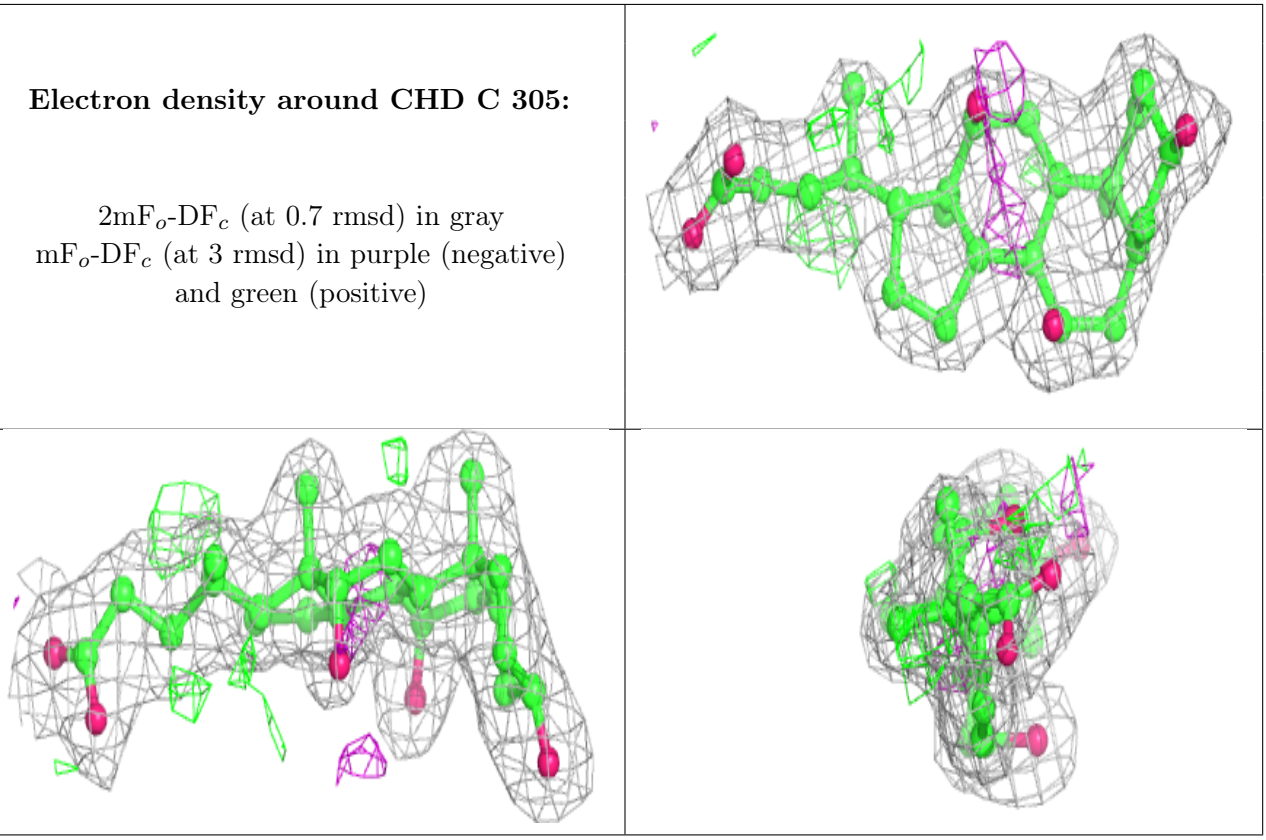
Electron density around TGL A 607:

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



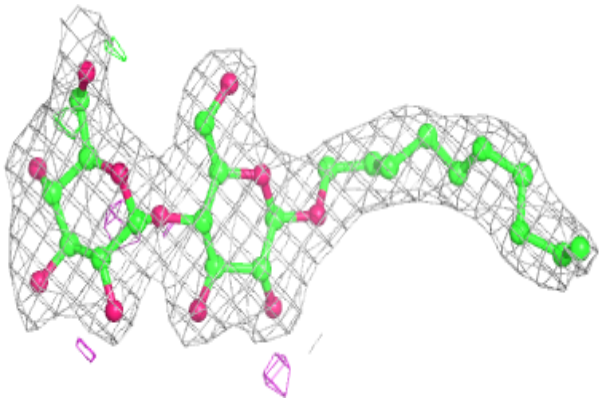
Electron density around CHD C 305:

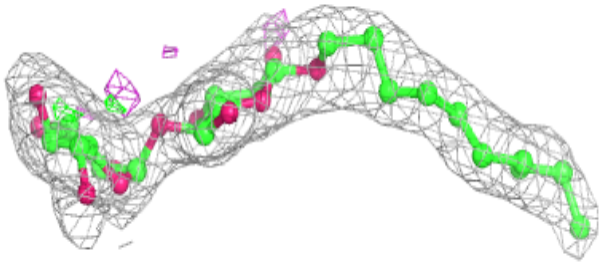
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

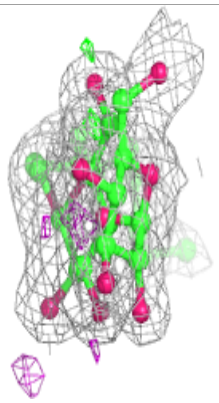


Electron density around DMU M 101:

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

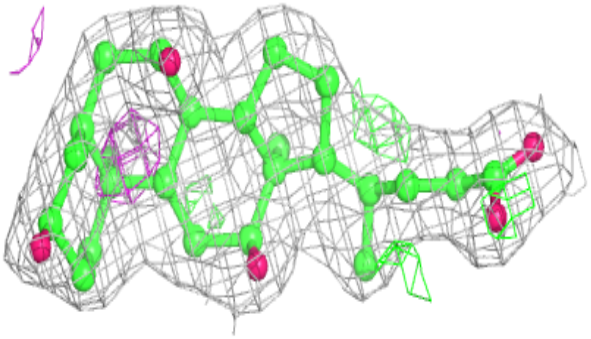


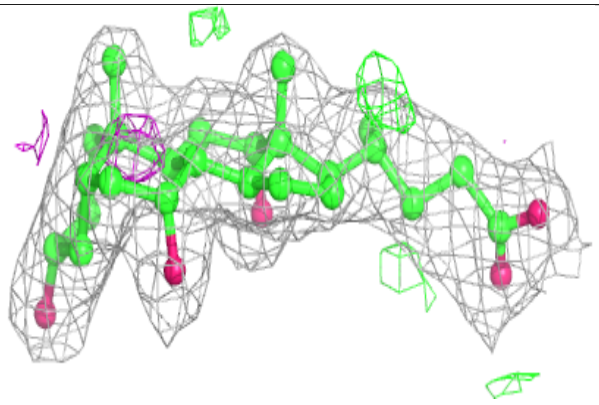


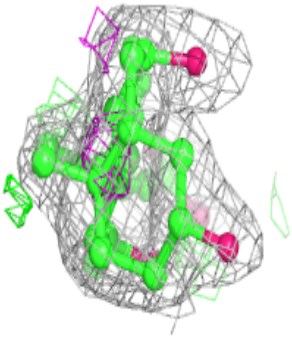


Electron density around CHD P 308:

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

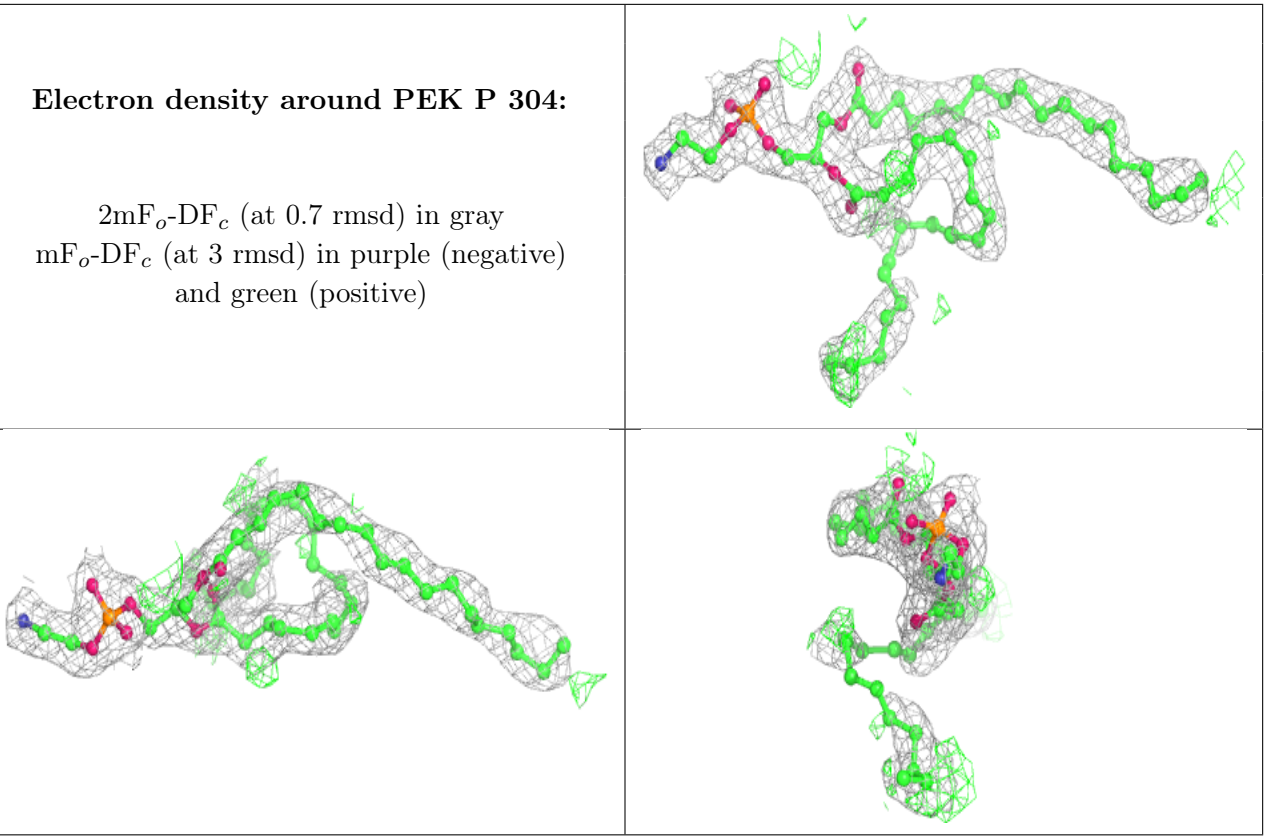






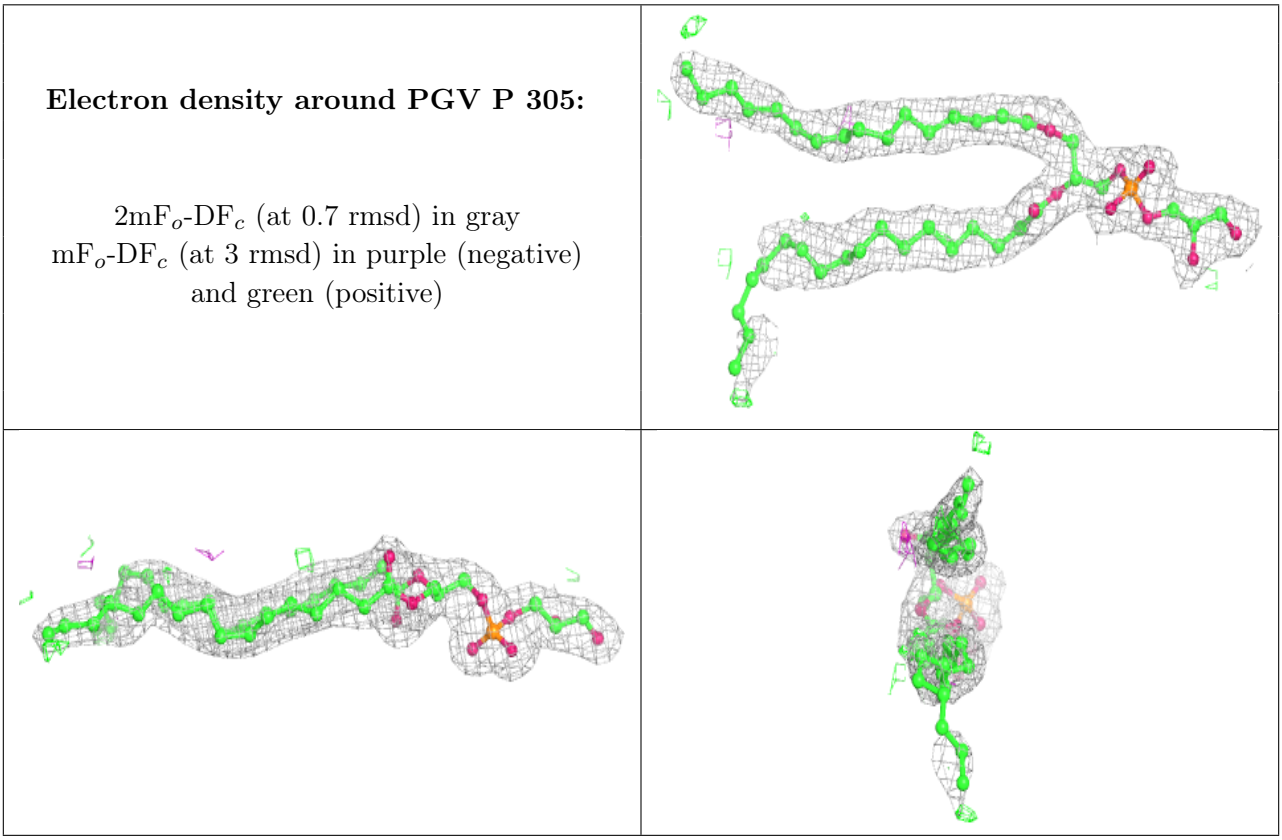
Electron density around PEK P 304:

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



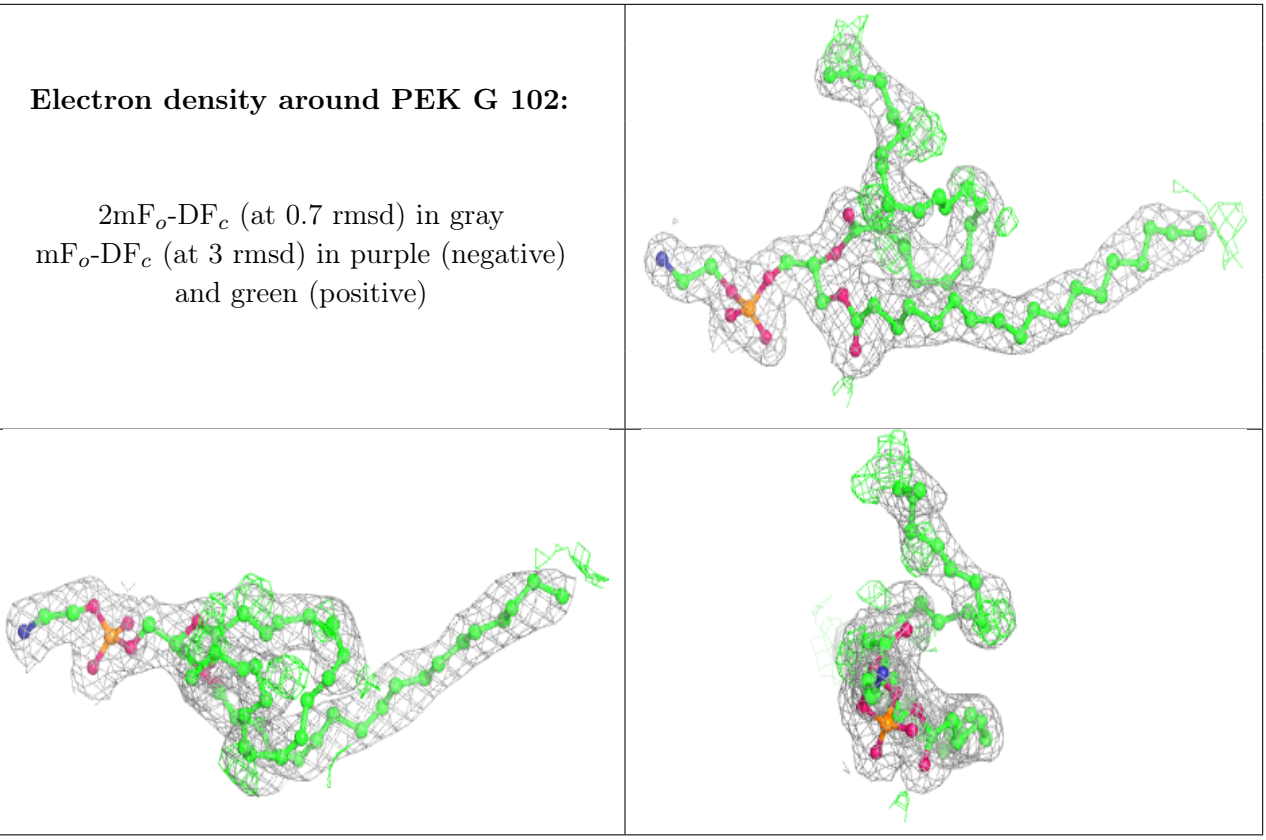
Electron density around PGV P 305:

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



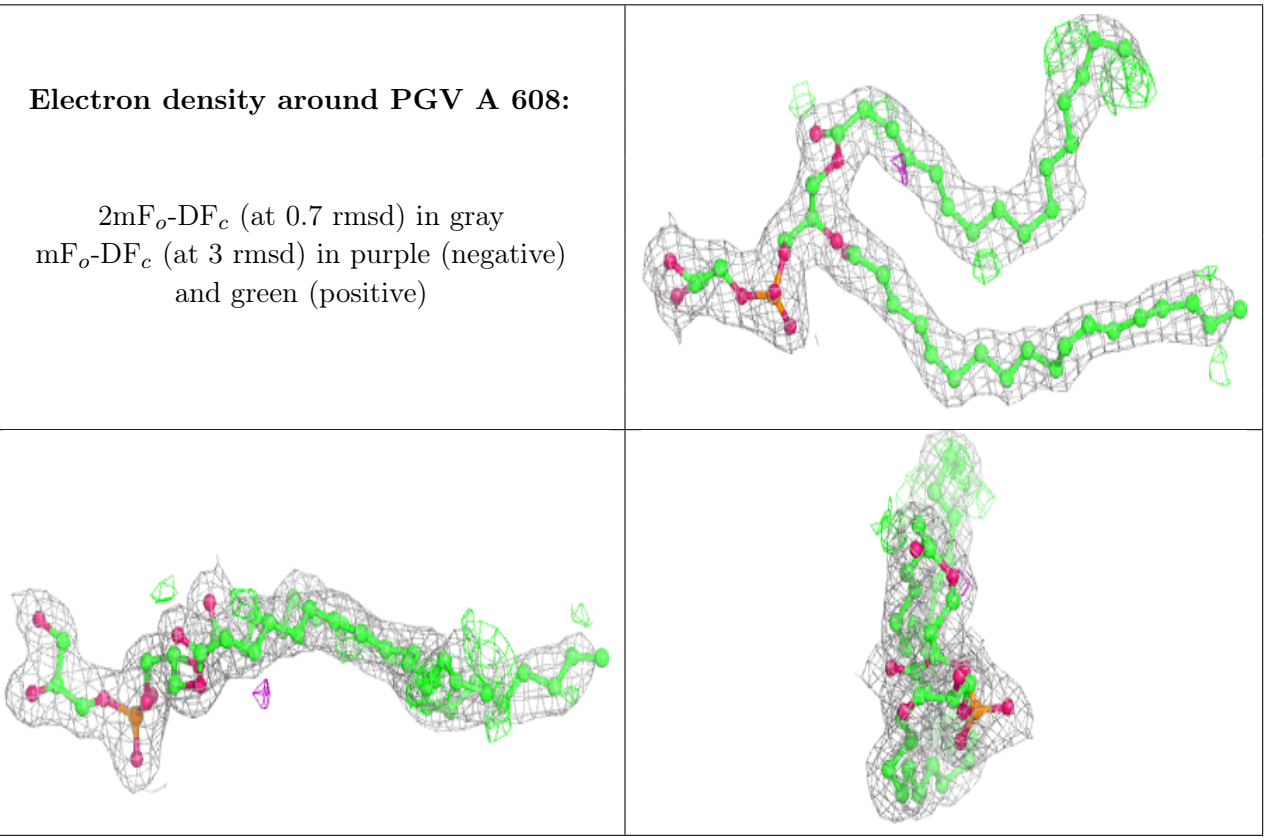
Electron density around PEK G 102:

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



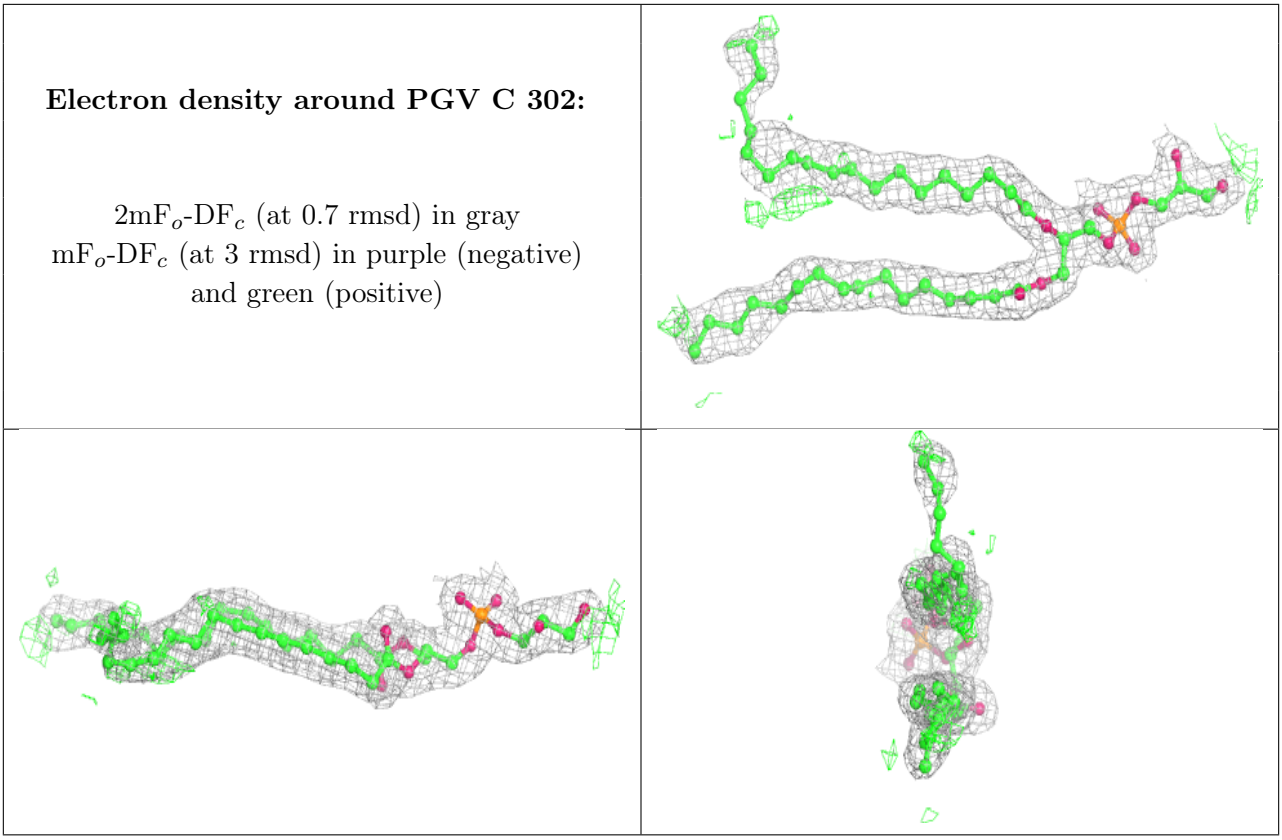
Electron density around PGV A 608:

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



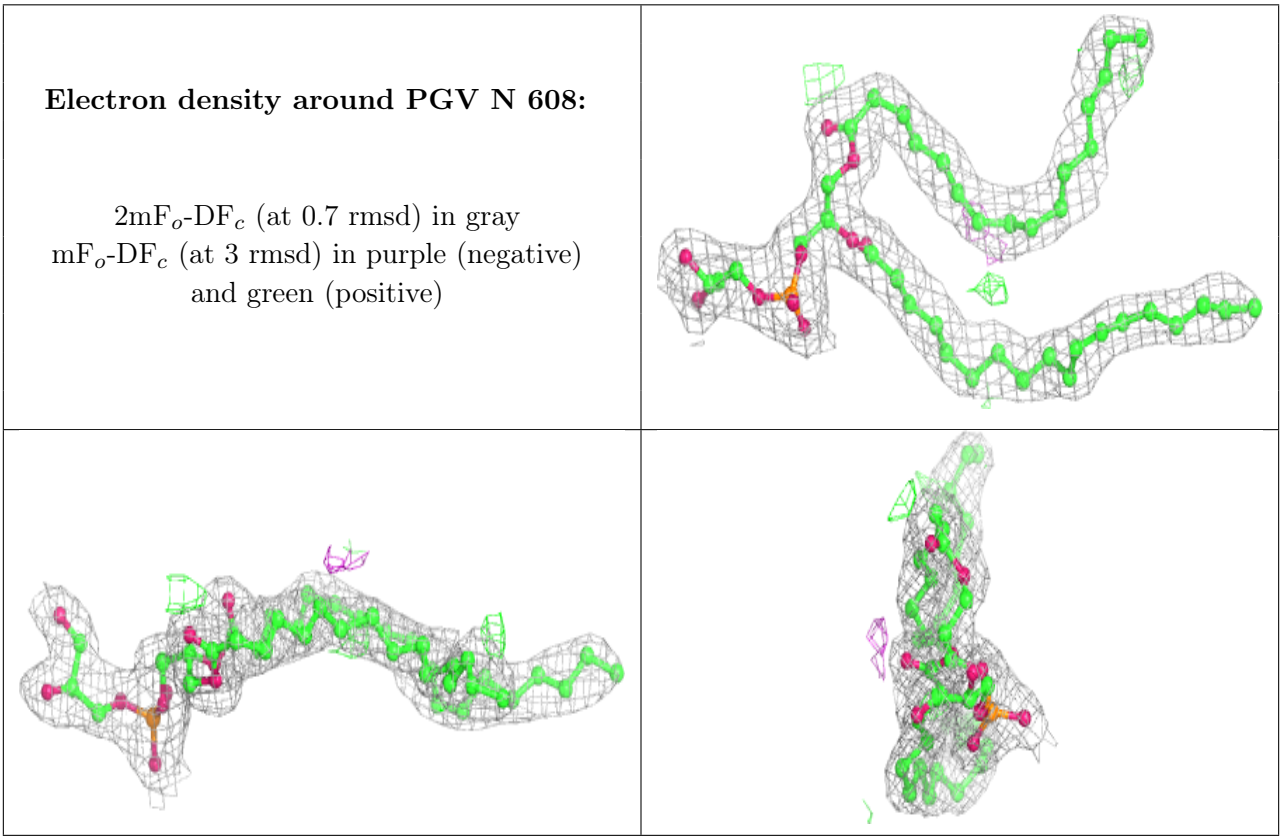
Electron density around PGV C 302:

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



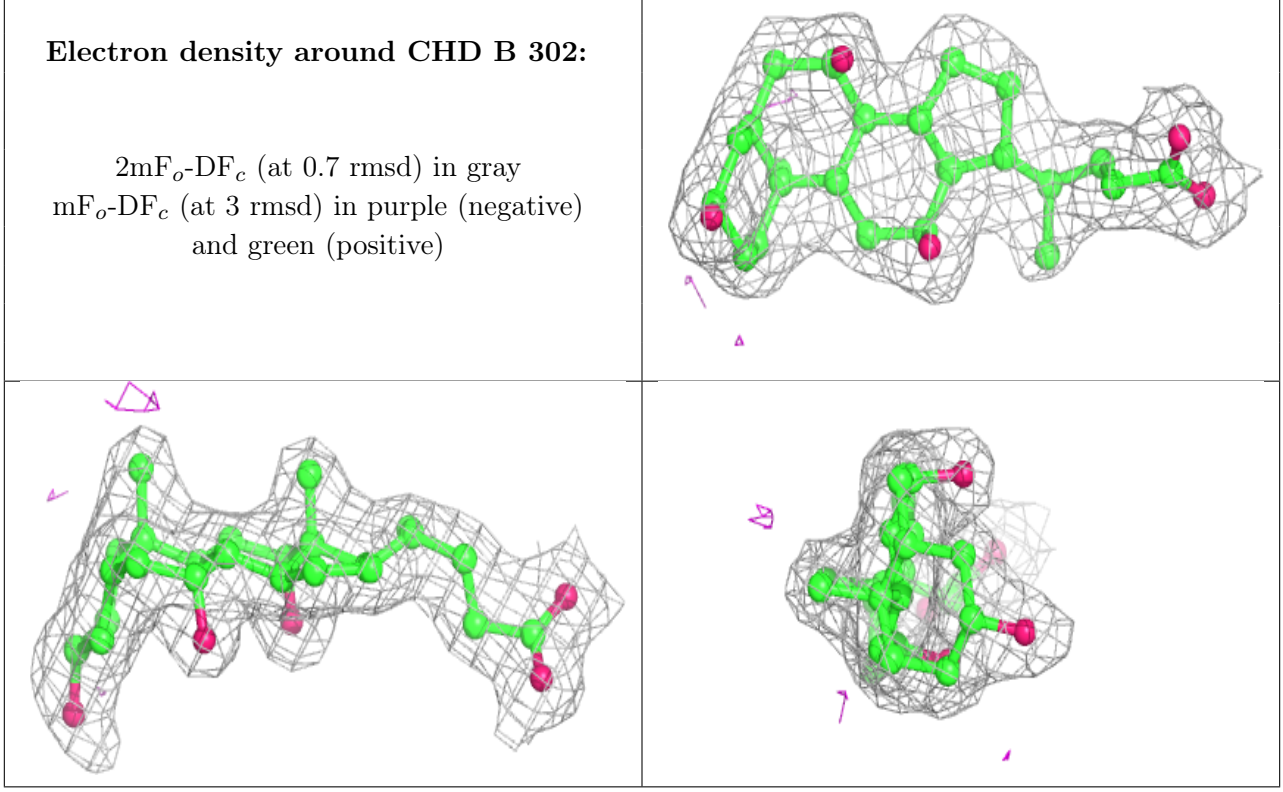
Electron density around PGV N 608:

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



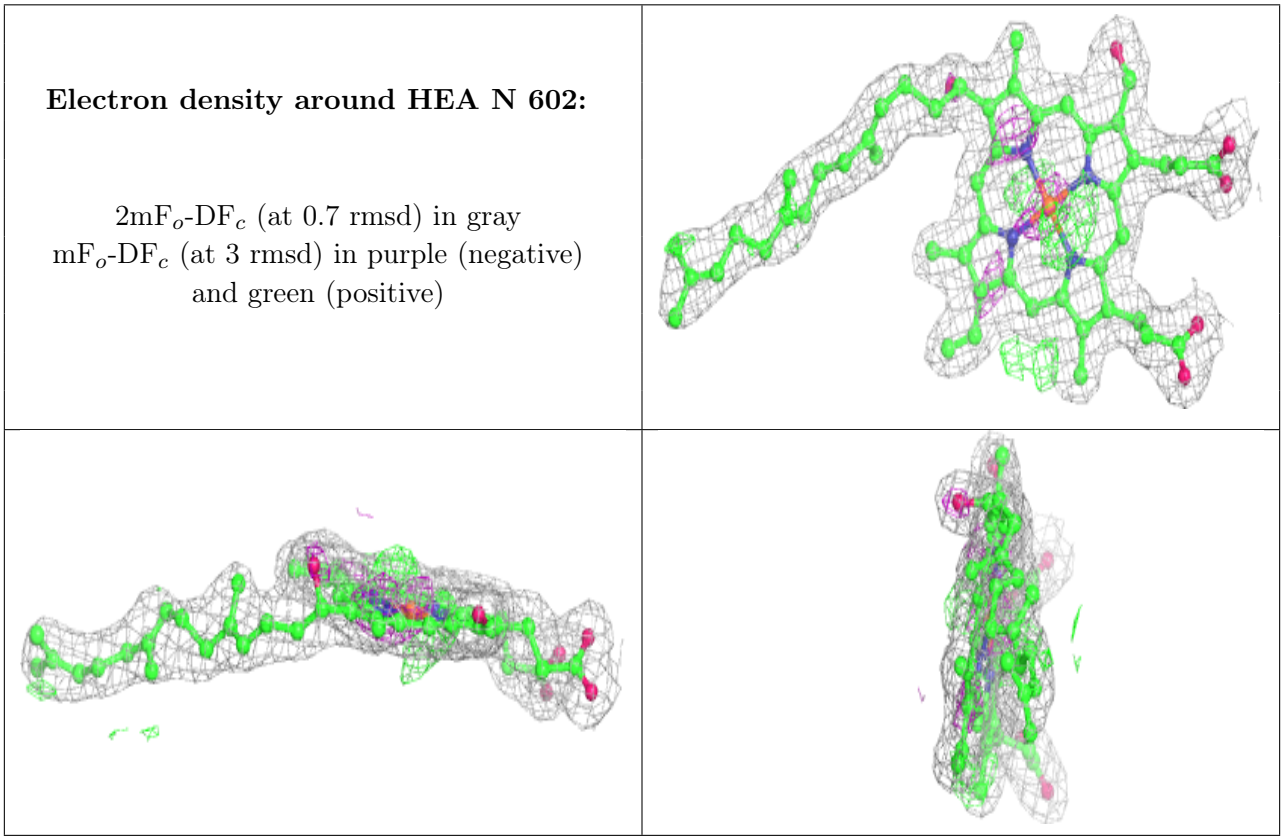
Electron density around CHD B 302:

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



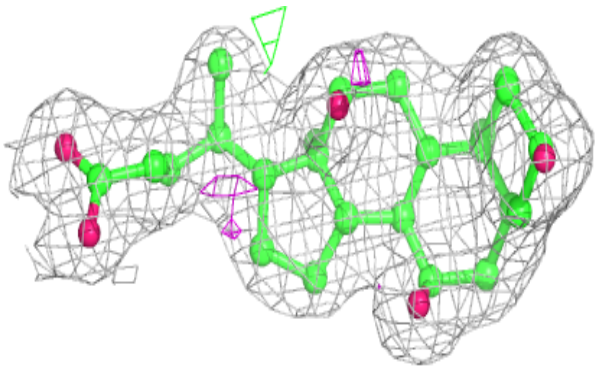
Electron density around HEA N 602:

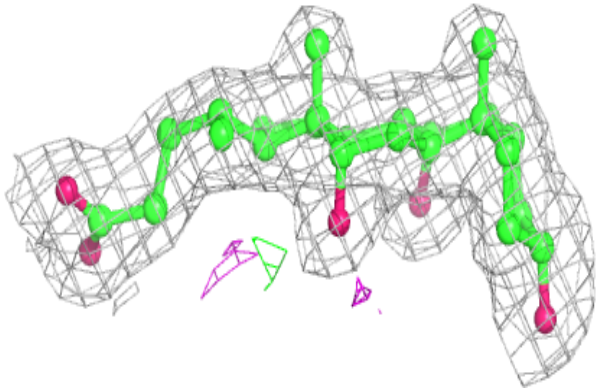
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

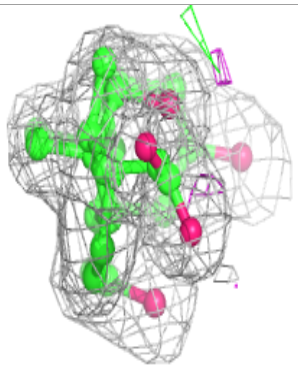


Electron density around CHD O 302:

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

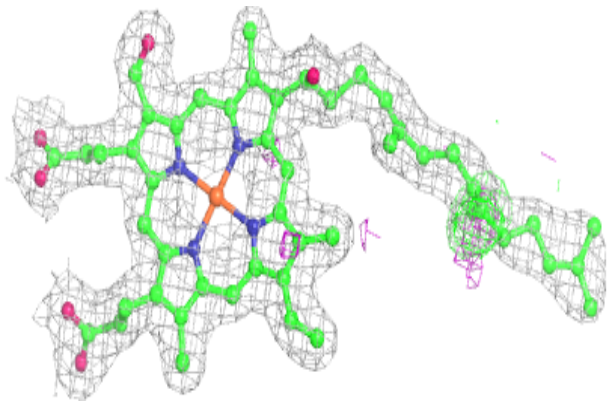


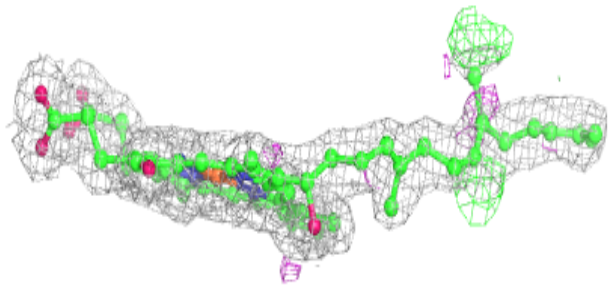


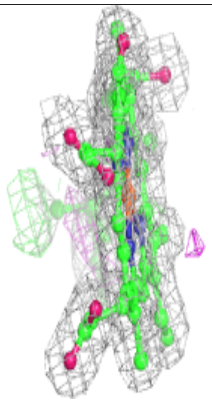


Electron density around HEA A 602:

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

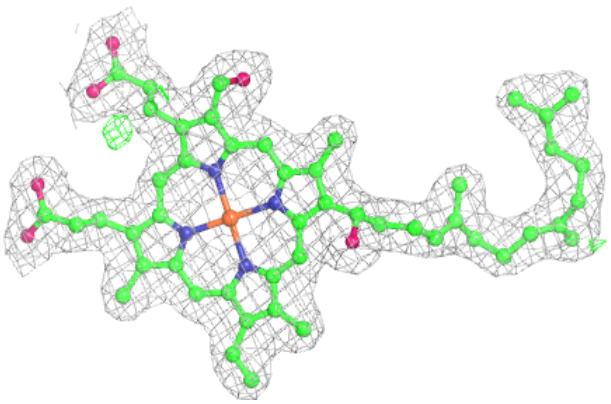


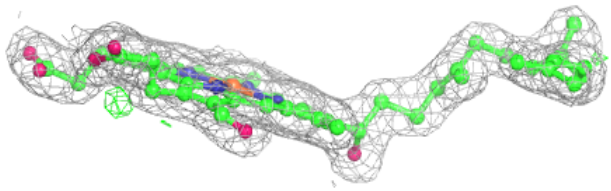


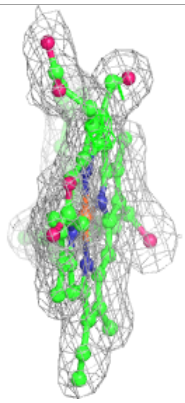


Electron density around HEA N 603:

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

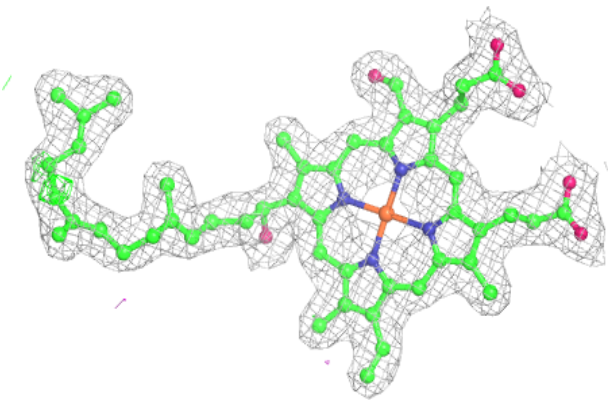


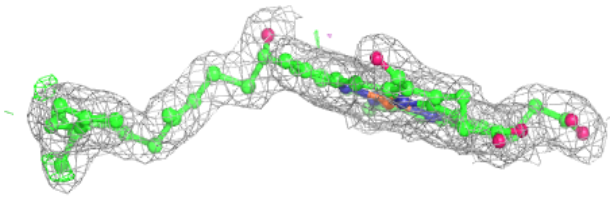


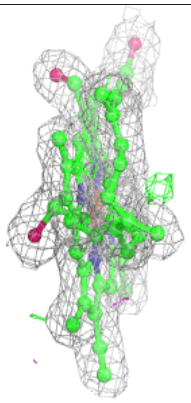


Electron density around HEA A 603:

$2mF_o$-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.