Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 03:18 PM JST

PDB ID	:	7XMB
Title	:	Crystal structure of Bovine heart cytochrome c oxidase, the structure complexed with an allosteric inhibitor T113
Authors	:	Nishida, Y.; Shinzawa-Itoh, K.; Mizuno, N.; Kumasaka, T.; Yoshikawa, S.; Tsukihara, T.; Shintani, Y.; Takashima, S.
Deposited on	:	2022-04-25
Resolution	:	2.20 Å(reported)

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

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

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

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

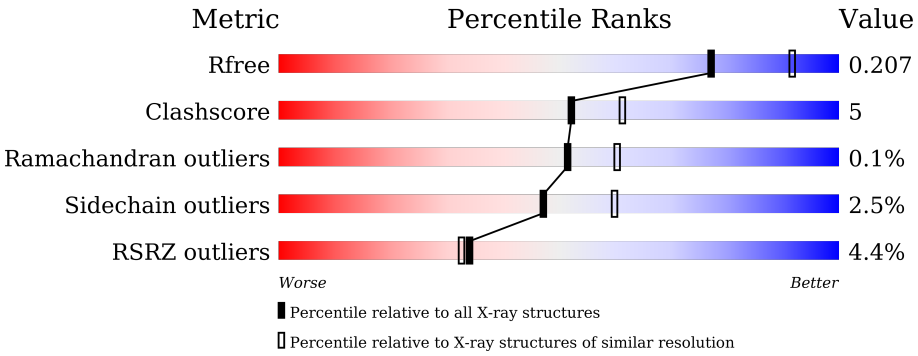
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	88% 12%
1	N	514	% 87% 12%
2	B	581	% 32% 7% 61%
2	O	581	2% 32% 6% 61%
3	C	261	% 89% 10%

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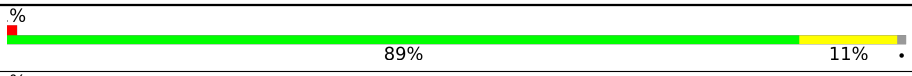
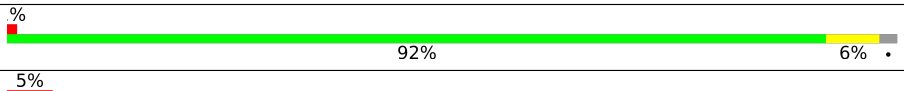
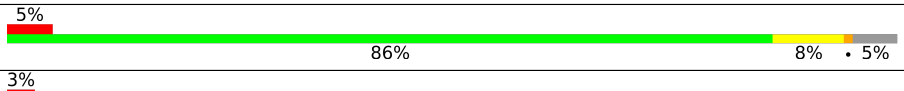
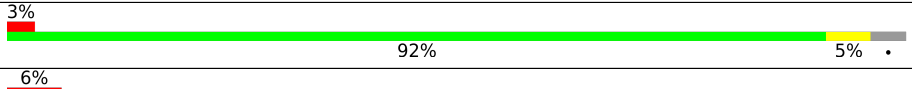
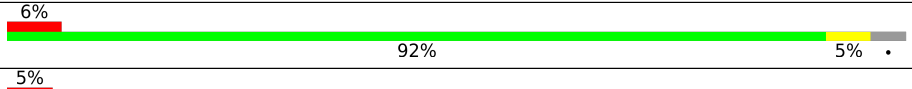
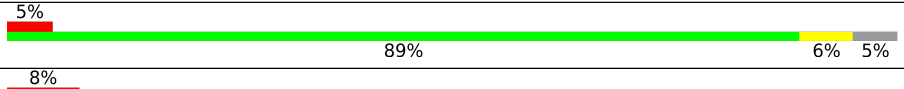
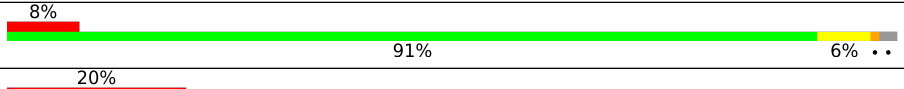
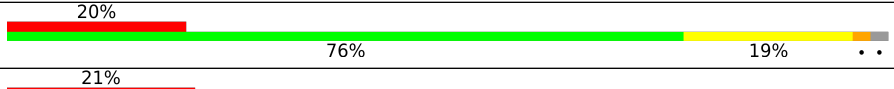
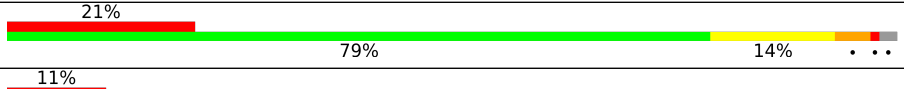
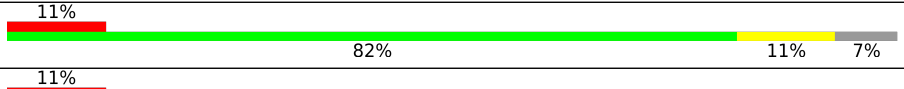
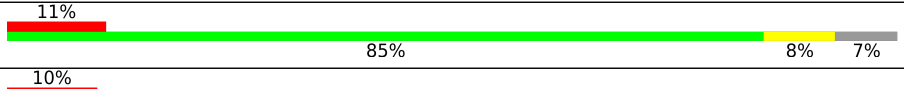
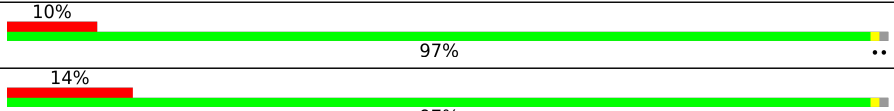
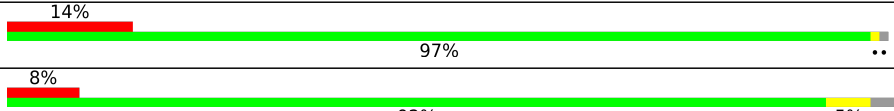
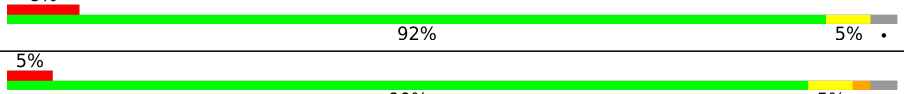
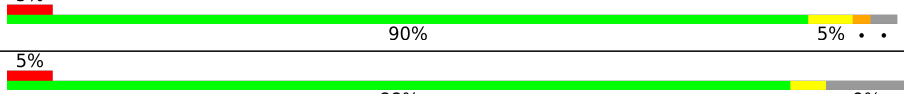
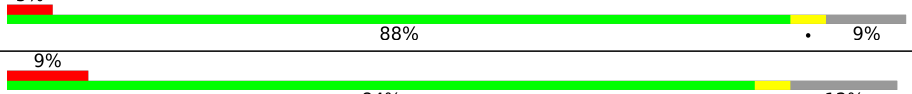
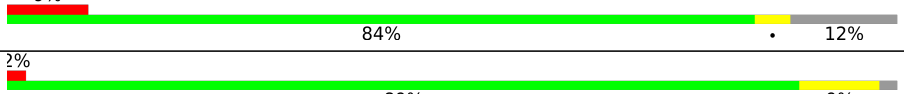
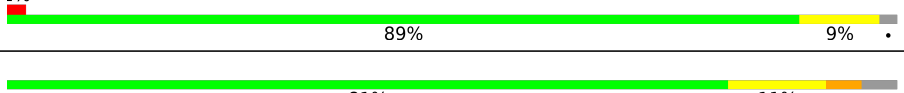
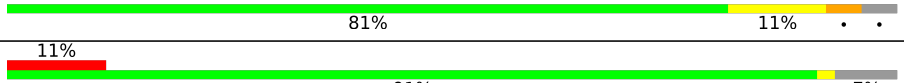
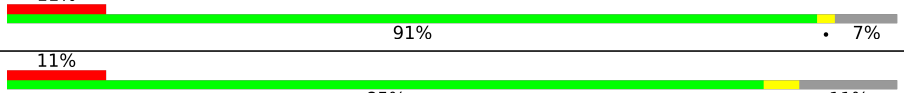
Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	J6X	A	608	-	-	-	X
22	CHD	C	304	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	PEK	C	309	-	-	-	X
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 33764 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	21	0
			4194	2797	649	710	38			
1	N	514	Total	C	N	O	S	0	23	0
			4208	2805	651	713	39			

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	4	0
			1861	1210	287	345	19			
2	O	227	Total	C	N	O	S	0	6	0
			1878	1220	289	349	20			

- 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	7	0
			2166	1445	344	361	16			
3	P	259	Total	C	N	O	S	0	6	0
			2157	1440	342	359	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	2	0
			1213	791	198	220	4			
4	Q	139	Total	C	N	O	S	0	2	0
			1178	769	192	213	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	2	0
			729	452	130	141	6			
6	S	96	Total	C	N	O	S	0	1	0
			740	460	131	143	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	82	Total	C	N	O	P	S	0	1	0
			678	436	129	111	1	1			
7	T	82	Total	C	N	O	P	S	0	1	0
			678	436	129	111	1	1			

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	1	0
			460	296	77	84	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	51	Total	C	N	O	S	0	0	0
			402	260	68	72	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

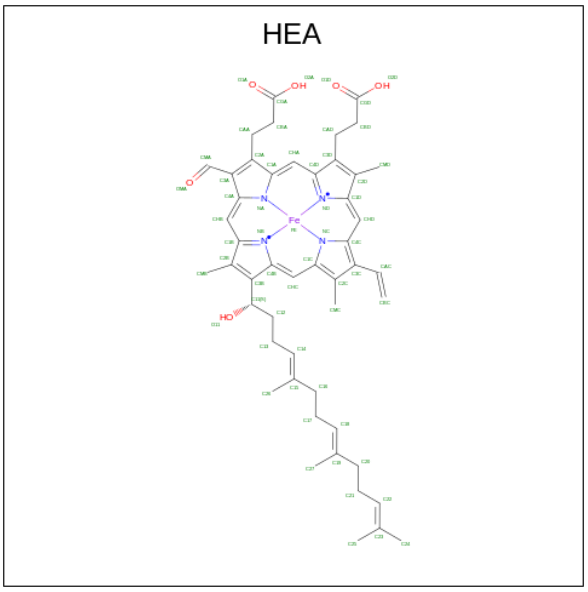
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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	45	Total	C	N	O	S	0	1	0
			378	253	63	59	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	41	Total	C	N	O	0	0	0
			320	214	50	56			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	1
			78	66	1	4	7		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	1
			78	66	1	4	7		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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

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

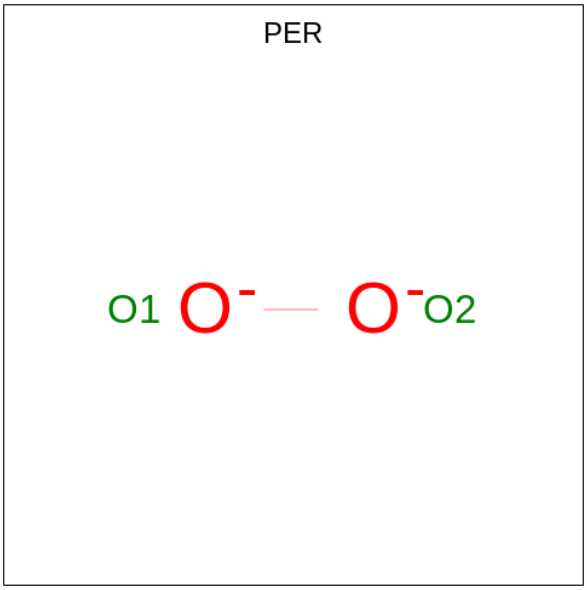
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

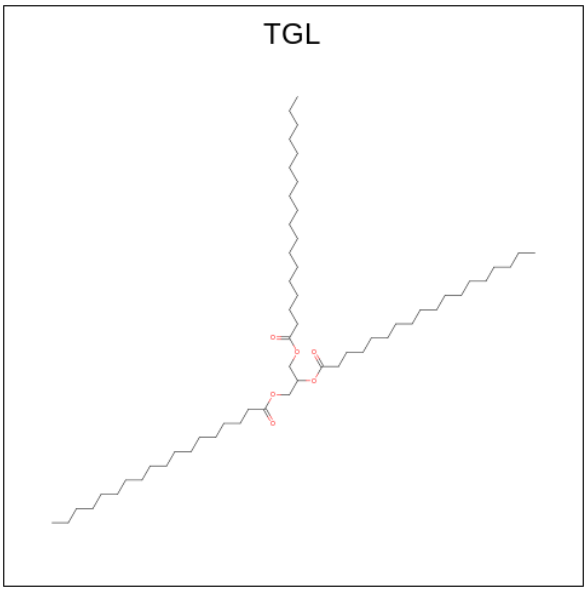
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



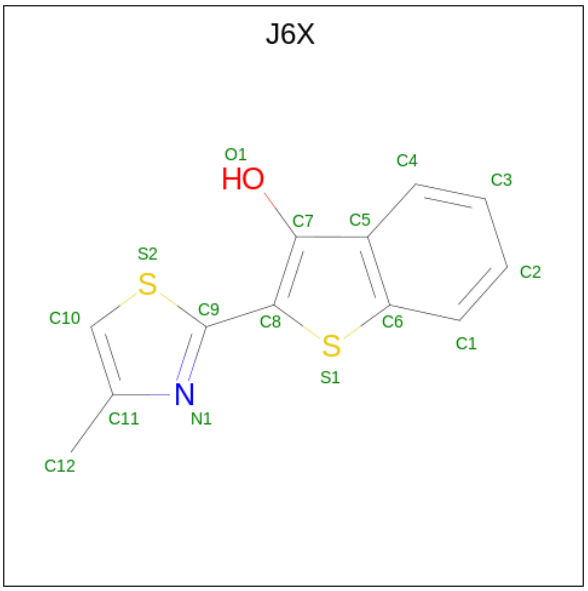
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

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



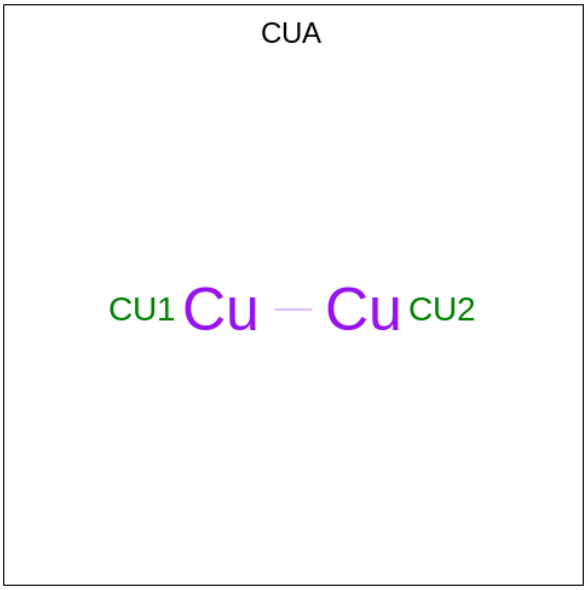
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	Q	1	Total C O 63 57 6	0	0
19	Y	1	Total C O 63 57 6	0	0

- Molecule 20 is 2-(4-methyl-1,3-thiazol-2-yl)-1-benzothiophen-3-ol (three-letter code: J6X) (formula: $C_{12}H_9NOS_2$) (labeled as "Ligand of Interest" by depositor).



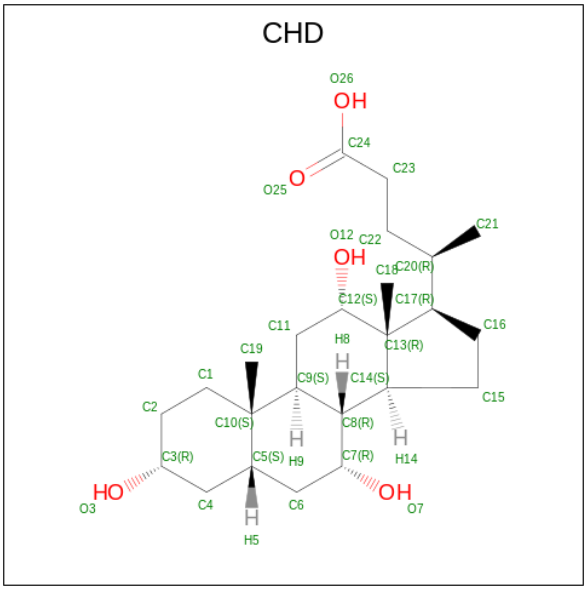
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C N O S 16 12 1 1 2	0	0
20	N	1	Total C N O S 16 12 1 1 2	0	0

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



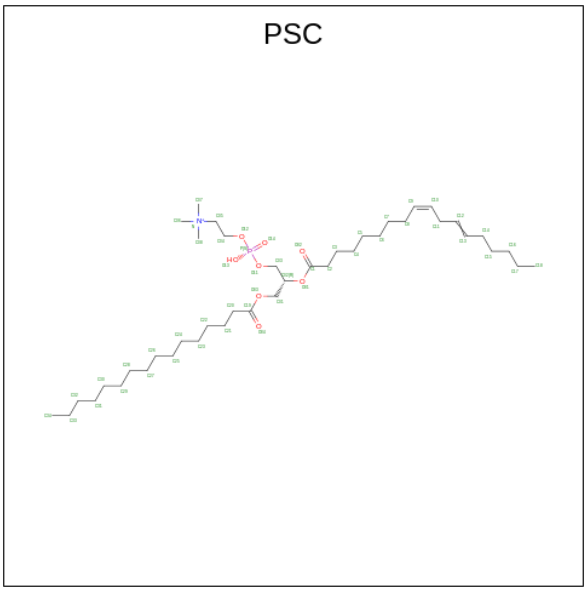
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

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



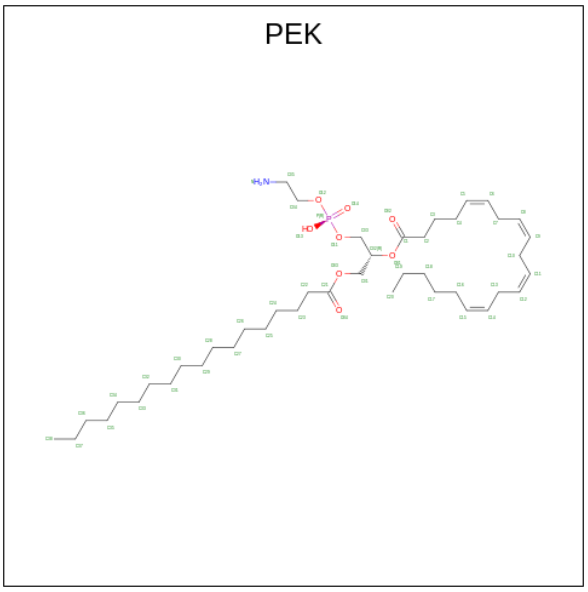
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	N	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

- Molecule 24 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
24	B	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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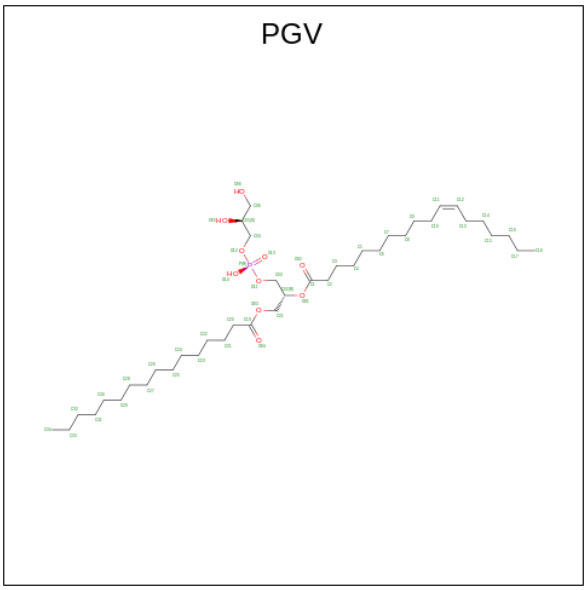
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 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
25	C	1	Total	C	O	P	0	0
			51	40	10	1		
25	C	1	Total	C	O	P	0	0
			51	40	10	1		
25	C	1	Total	C	O	P	0	0
			51	40	10	1		
25	D	1	Total	C	O	P	0	0
			51	40	10	1		
25	N	1	Total	C	O	P	0	0
			51	40	10	1		

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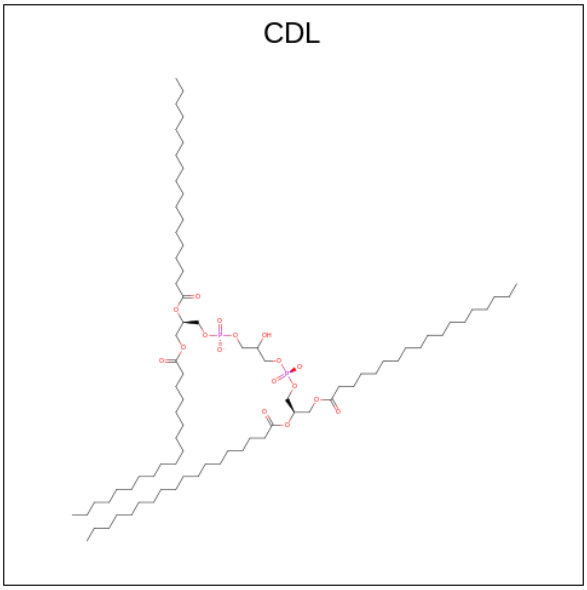
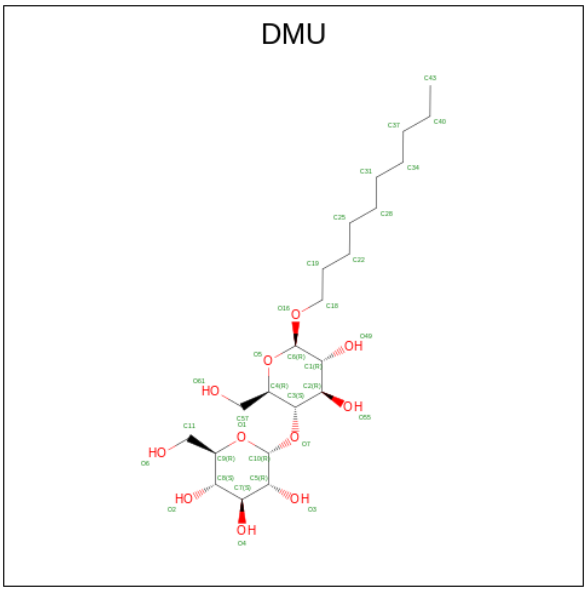
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	N	1	Total	C	O	P	0	0
			51	40	10	1		
25	P	1	Total	C	O	P	0	0
			51	40	10	1		
25	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	274	Total O 274 274	0	0
29	B	193	Total O 193 193	0	1
29	C	152	Total O 152 152	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	179	Total O 179 179	0	0
29	E	126	Total O 126 126	0	0
29	F	119	Total O 119 119	0	0
29	G	60	Total O 60 60	0	0
29	H	74	Total O 74 74	0	0
29	I	48	Total O 48 48	0	0
29	J	38	Total O 38 38	0	0
29	K	38	Total O 38 38	0	0
29	L	39	Total O 39 39	0	0
29	M	35	Total O 35 35	0	0
29	N	288	Total O 288 288	0	0
29	O	148	Total O 148 148	0	1
29	P	143	Total O 143 143	0	0
29	Q	71	Total O 71 71	0	0
29	R	84	Total O 84 84	0	0
29	S	115	Total O 115 115	0	0
29	T	59	Total O 59 59	0	0
29	U	63	Total O 63 63	0	0
29	V	28	Total O 28 28	0	0
29	W	35	Total O 35 35	0	0
29	X	25	Total O 25 25	0	0

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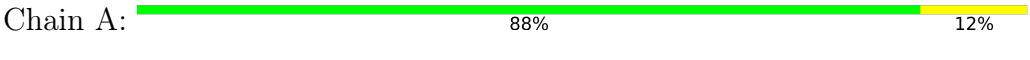
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Y	39	Total O 39 39	0	0
29	Z	22	Total O 22 22	0	0

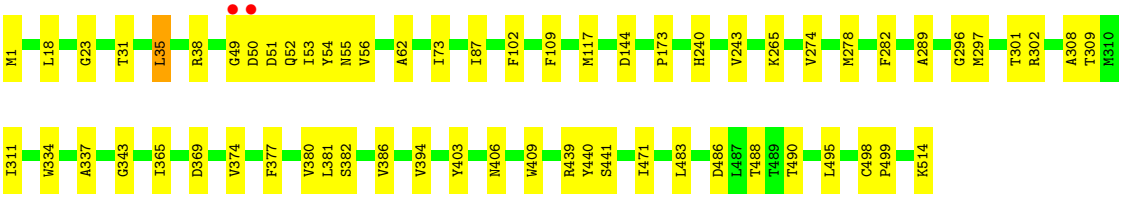
3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c oxidase subunit 1

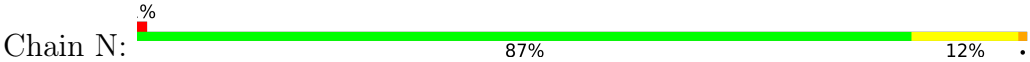
Chain A:

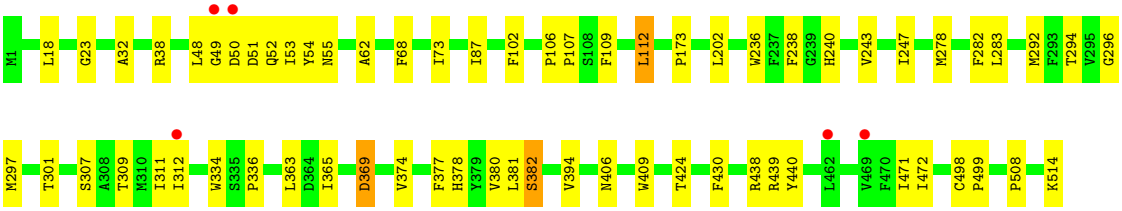




• Molecule 1: Cytochrome c oxidase subunit 1

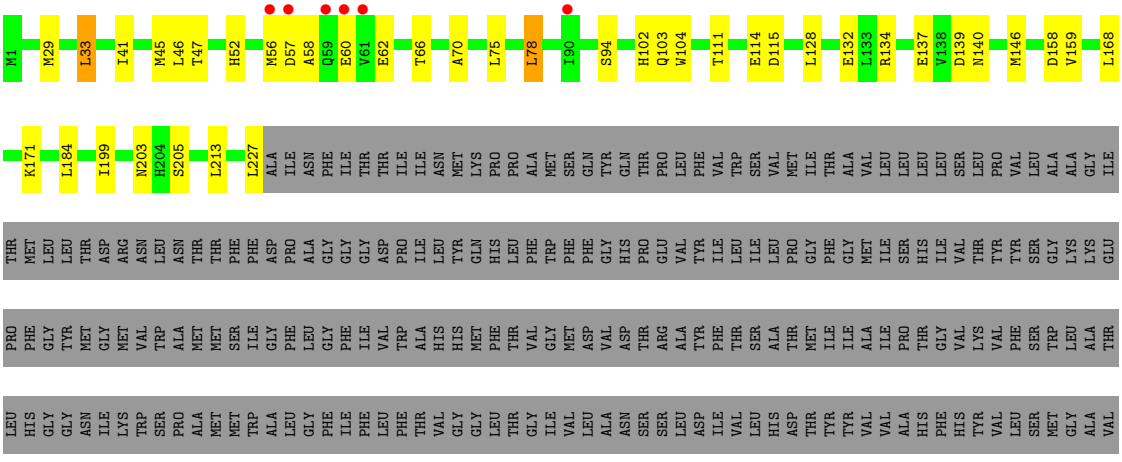
Chain N:

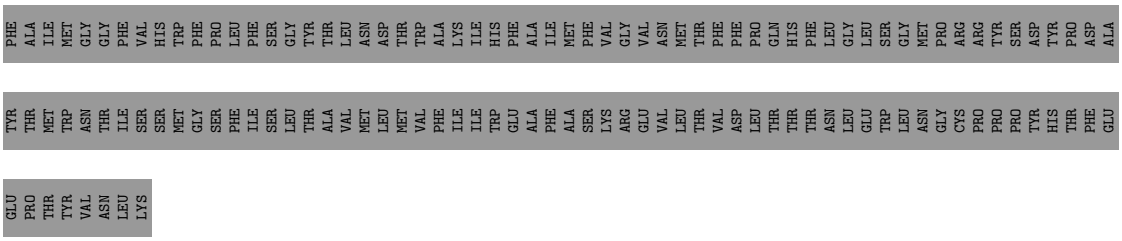




• Molecule 2: CYTOCHROME C OXIDASE

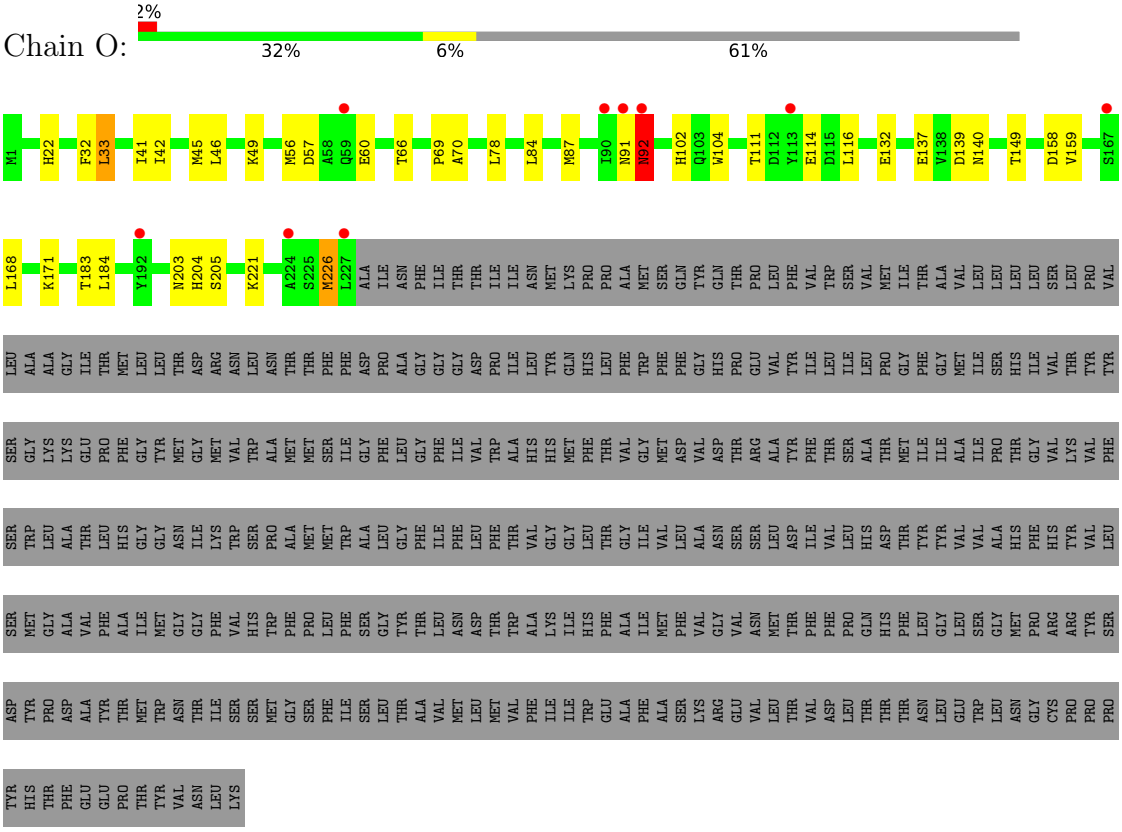
Chain B:





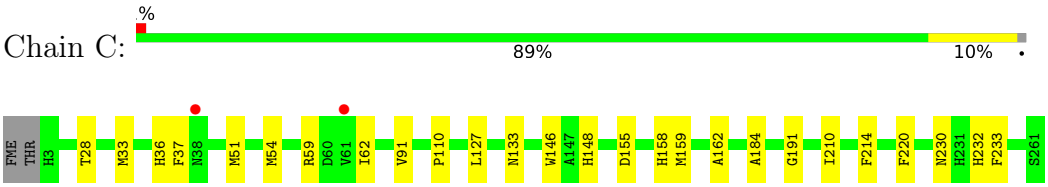
• Molecule 2: CYTOCHROME C OXIDASE

Chain O:



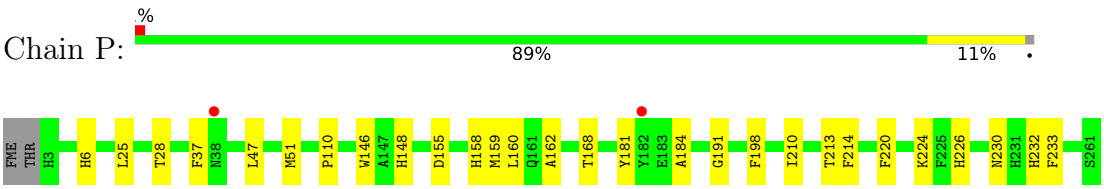
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



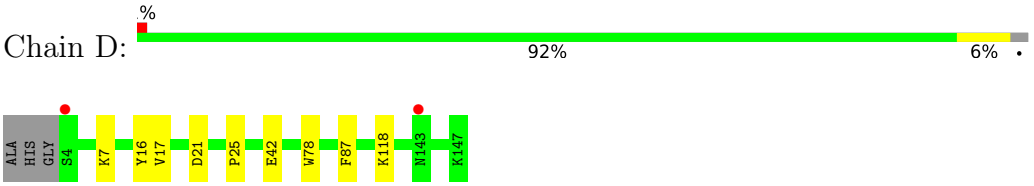
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



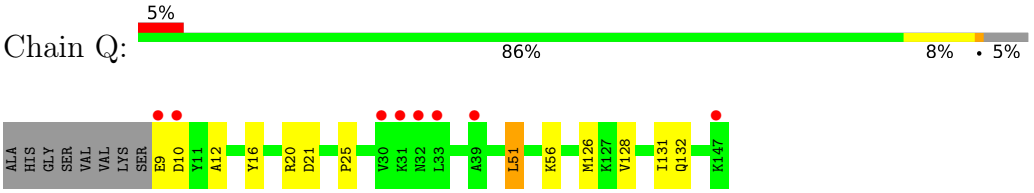
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



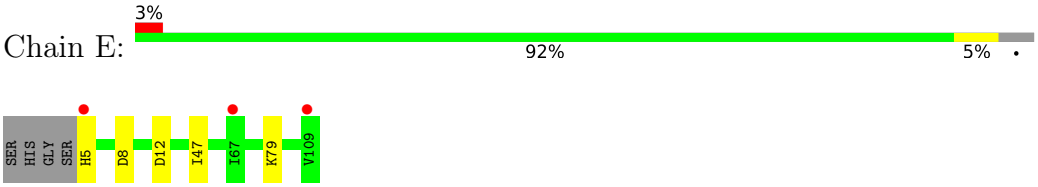
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



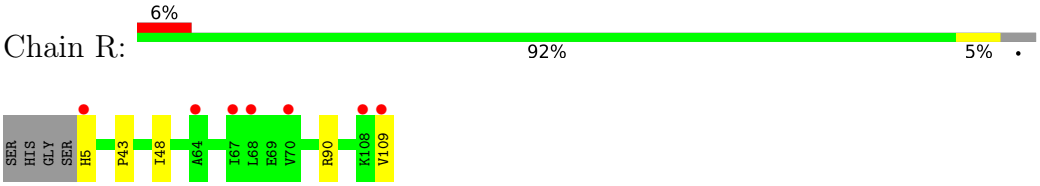
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:



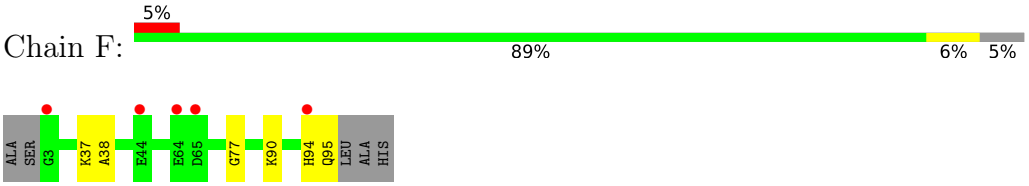
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:



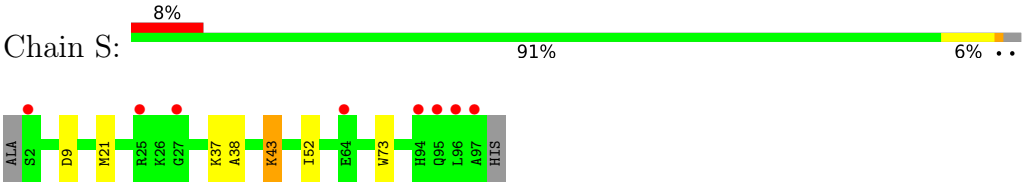
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



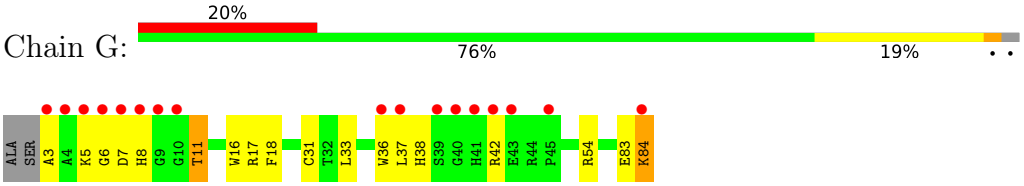
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



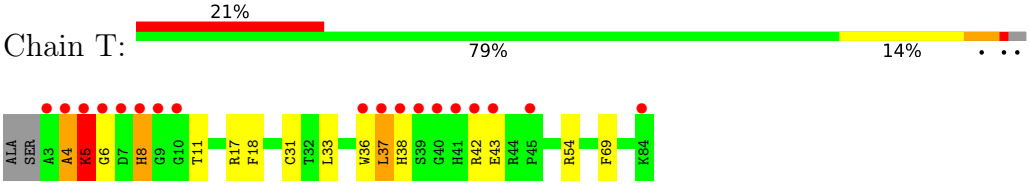
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



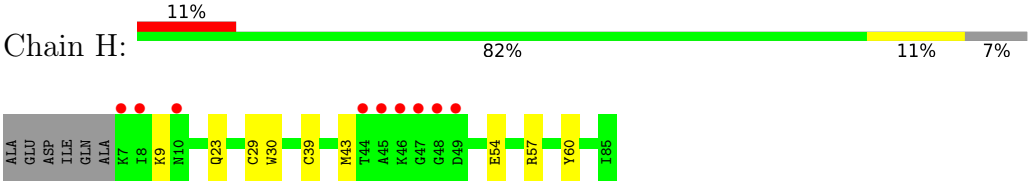
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



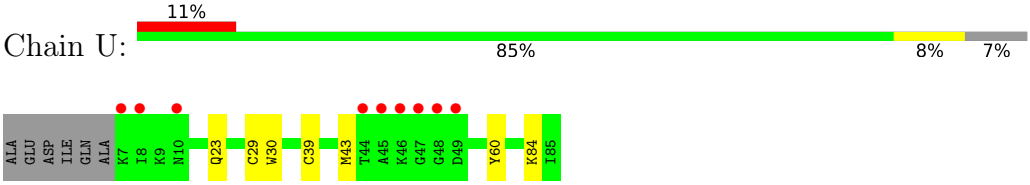
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



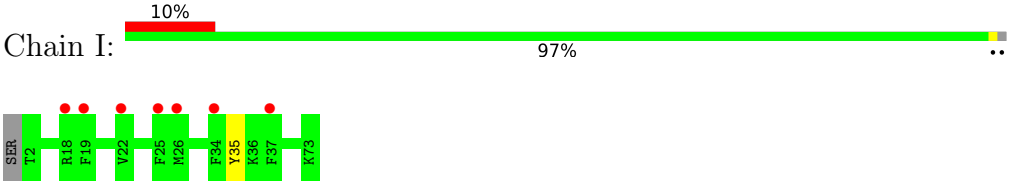
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



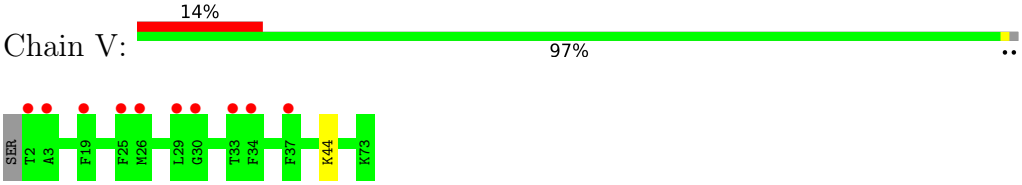
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



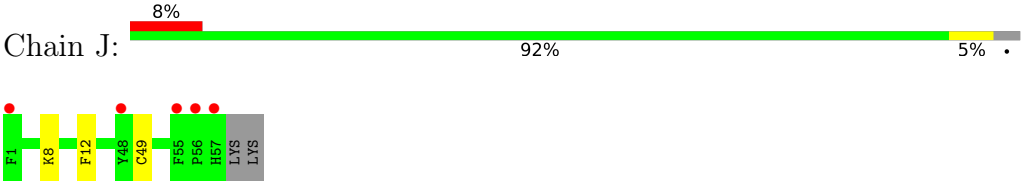
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



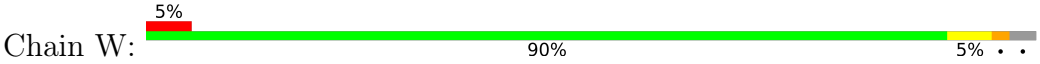
• Molecule 10: Cytochrome c oxidase subunit 7A1

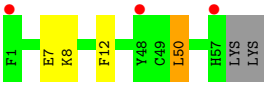
Chain J:



• Molecule 10: Cytochrome c oxidase subunit 7A1

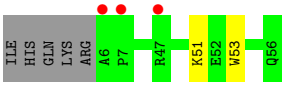
Chain W:





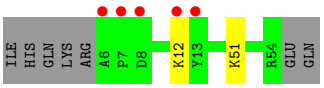
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:



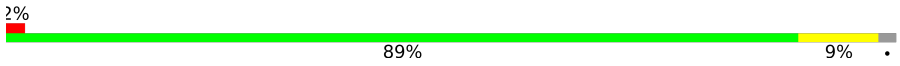
• Molecule 11: Cytochrome c oxidase subunit 7B

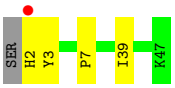
Chain X:



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

Chain L:



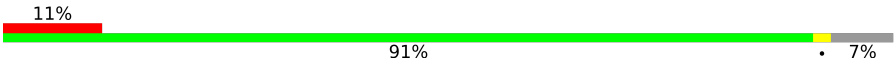


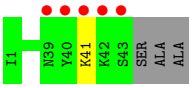
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:

• Molecule 13: Cytochrome c oxidase subunit 8B

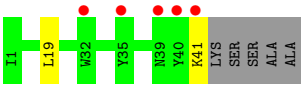
Chain M:





• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.10Å 204.34Å 177.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.20 29.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.98-2.20) 99.9 (29.98-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.204 0.181 , 0.207	Depositor DCC
R_{free} test set	16655 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33764	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CDL, PER, DMU, CUA, PEK, CHD, TPO, HEA, FME, PGV, J6X, ZN, TGL, CU, NA, PSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/4324	0.43	0/5905
1	N	0.26	0/4338	0.44	0/5923
2	B	0.25	0/1899	0.47	0/2587
2	O	0.25	0/1916	0.46	0/2609
3	C	0.25	0/2253	0.40	0/3077
3	P	0.25	0/2244	0.40	0/3065
4	D	0.24	0/1248	0.41	0/1684
4	Q	0.24	0/1213	0.42	0/1637
5	E	0.24	0/882	0.47	0/1196
5	R	0.26	0/882	0.48	0/1196
6	F	0.25	0/745	0.50	0/1011
6	S	0.24	0/756	0.50	0/1026
7	G	0.30	0/695	0.52	0/945
7	T	0.29	0/695	0.58	0/945
8	H	0.25	0/682	0.51	0/921
8	U	0.26	0/682	0.52	0/921
9	I	0.28	0/605	0.51	0/802
9	V	0.27	0/605	0.50	0/802
10	J	0.25	0/462	0.43	0/625
10	W	0.26	0/471	0.44	0/637
11	K	0.27	0/416	0.48	0/570
11	X	0.24	0/405	0.46	0/556
12	L	0.26	0/393	0.43	0/526
12	Y	0.27	0/391	0.43	0/525
13	M	0.24	0/345	0.40	0/470
13	Z	0.24	0/330	0.39	0/451
All	All	0.26	0/29877	0.45	0/40612

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4194	0	4168	52	0
1	N	4208	0	4180	59	0
2	B	1861	0	1860	27	0
2	O	1878	0	1873	31	0
3	C	2166	0	2075	27	0
3	P	2157	0	2068	25	0
4	D	1213	0	1199	15	0
4	Q	1178	0	1158	9	0
5	E	863	0	857	3	0
5	R	863	0	857	2	0
6	F	729	0	705	3	0
6	S	740	0	721	6	0
7	G	678	0	639	8	0
7	T	678	0	639	11	0
8	H	662	0	623	4	0
8	U	662	0	623	3	0
9	I	592	0	604	1	0
9	V	592	0	604	1	0
10	J	451	0	446	5	0
10	W	460	0	451	4	0
11	K	402	0	380	1	0
11	X	391	0	374	0	0
12	L	380	0	380	3	0
12	Y	378	0	375	6	0
13	M	335	0	352	1	0
13	Z	320	0	334	1	0
14	A	138	0	112	6	0
14	N	138	0	112	12	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	N	1	0	0	0	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	A	63	0	110	0	0
19	D	63	0	110	5	0
19	L	63	0	110	1	0
19	N	63	0	110	4	0
19	Q	63	0	110	2	0
19	Y	63	0	110	7	0
20	A	16	0	0	2	0
20	N	16	0	0	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	1	0
22	N	29	0	39	1	0
22	O	29	0	39	1	0
22	P	29	0	39	1	0
23	B	52	0	80	5	0
23	O	52	0	80	10	0
24	B	53	0	77	4	0
24	C	106	0	154	10	0
24	G	53	0	77	2	0
24	P	106	0	154	6	0
25	C	153	0	228	8	0
25	D	51	0	76	12	0
25	N	102	0	152	4	0
25	P	102	0	152	8	0
26	C	100	0	156	13	0
26	G	100	0	156	11	0
26	P	100	0	156	12	0
26	T	100	0	156	17	0
27	C	33	0	42	7	0
27	M	33	0	42	0	0
27	W	33	0	42	2	0
27	Z	33	0	42	0	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	274	0	0	8	0
29	B	193	0	0	3	0
29	C	152	0	0	4	0
29	D	179	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	E	126	0	0	1	0
29	F	119	0	0	1	0
29	G	60	0	0	1	0
29	H	74	0	0	0	0
29	I	48	0	0	0	0
29	J	38	0	0	0	0
29	K	38	0	0	0	0
29	L	39	0	0	0	0
29	M	35	0	0	0	0
29	N	288	0	0	12	0
29	O	148	0	0	3	0
29	P	143	0	0	2	0
29	Q	71	0	0	0	0
29	R	84	0	0	1	0
29	S	115	0	0	1	0
29	T	59	0	0	1	0
29	U	63	0	0	0	0
29	V	28	0	0	0	0
29	W	35	0	0	0	0
29	X	25	0	0	0	0
29	Y	39	0	0	1	0
29	Z	22	0	0	0	0
All	All	33764	0	31685	344	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (344) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:304:CDL:H1O1	10:W:12:PHE:HE2	1.13	0.94
4:D:87[A]:PHE:CD2	25:D:201:PGV:H141	2.04	0.93
19:D:202:TGL:HC32	19:D:202:TGL:HG12	1.60	0.81
1:A:50[D]:ASP:OD1	29:A:701:HOH:O	2.01	0.79
1:N:439:ARG:O	29:N:701:HOH:O	2.02	0.77
1:N:50[D]:ASP:OD1	29:N:702:HOH:O	2.05	0.75
3:C:220:PHE:HB2	26:C:303:CDL:H711	1.69	0.74
12:Y:25:MET:HG2	19:Y:101:TGL:HA62	1.71	0.73
1:N:50[C]:ASP:OD1	29:N:702:HOH:O	2.08	0.72
1:A:50[C]:ASP:OD1	29:A:701:HOH:O	2.09	0.71
24:B:604:PEK:H051	7:T:17:ARG:HH12	1.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:102:CDL:H471	2:O:70:ALA:HB1	1.75	0.69
4:D:87[A]:PHE:CD2	25:D:201:PGV:C14	2.76	0.68
7:G:38:HIS:CE1	26:G:102:CDL:H111	2.27	0.68
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.58	0.68
26:T:101:CDL:H382	26:T:101:CDL:H161	1.76	0.68
3:C:233:PHE:N	25:C:302:PGV:O14	2.26	0.68
26:T:101:CDL:H511	26:T:101:CDL:H202	1.74	0.67
3:C:148:HIS:NE2	29:C:401:HOH:O	2.27	0.67
2:B:205:SER:OG	29:B:701:HOH:O	2.11	0.67
3:P:148:HIS:NE2	29:P:401:HOH:O	2.27	0.67
2:O:91:ASN:ND2	2:O:183:THR:OG1	2.28	0.67
4:D:87[A]:PHE:CE2	25:D:201:PGV:C14	2.78	0.66
1:A:377:PHE:HA	1:A:380[D]:VAL:HG12	1.78	0.66
2:B:203:ASN:OD1	29:B:702:HOH:O	2.14	0.65
2:O:91:ASN:O	2:O:92:ASN:ND2	2.29	0.65
6:S:9:ASP:HB3	6:S:21[B]:MET:HE1	1.77	0.64
1:N:49[C]:GLY:O	29:N:703:HOH:O	2.14	0.64
3:P:233:PHE:N	25:P:303:PGV:O14	2.28	0.64
4:D:87[A]:PHE:CE1	25:D:201:PGV:H151	2.32	0.64
3:C:91:VAL:HG13	24:C:309:PEK:H14	1.80	0.63
1:A:56:VAL:HG12	20:A:608:J6X:C10	2.28	0.63
1:N:68:PHE:HE2	1:N:112:LEU:HD12	1.64	0.63
1:N:377:PHE:HA	1:N:380[D]:VAL:HG12	1.80	0.62
2:B:57:ASP:H	23:B:603:PSC:H201	1.63	0.62
1:A:56:VAL:HG12	20:A:608:J6X:S2	2.40	0.62
1:N:377:PHE:HA	1:N:380[C]:VAL:HG22	1.81	0.62
25:C:302:PGV:H162	26:C:303:CDL:H622	1.81	0.61
24:C:309:PEK:H362	26:T:101:CDL:H871	1.83	0.61
3:P:210:ILE:HG12	25:P:303:PGV:H132	1.82	0.61
1:N:514:LYS:N	29:N:707:HOH:O	2.34	0.61
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.83	0.60
2:B:70:ALA:HB1	26:T:101:CDL:H451	1.83	0.60
24:P:306:PEK:H011	7:T:69:PHE:HB3	1.83	0.60
7:T:37:LEU:HD23	26:T:101:CDL:H361	1.83	0.60
4:D:87[A]:PHE:CZ	25:D:201:PGV:C15	2.84	0.60
3:P:226:HIS:CE1	26:P:304:CDL:HB32	2.37	0.60
24:B:604:PEK:H041	7:T:17:ARG:HH22	1.67	0.58
4:D:87[A]:PHE:CZ	25:D:201:PGV:H151	2.38	0.58
1:N:508:PRO:HG3	3:P:6:HIS:HB3	1.85	0.58
1:N:55[D]:ASN:ND2	29:O:703:HOH:O	2.36	0.58
3:C:54[B]:MET:HG2	25:C:301:PGV:H61	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:20:ARG:HH22	19:Y:101:TGL:HC42	1.69	0.57
1:A:377:PHE:HA	1:A:380[C]:VAL:HG22	1.86	0.57
26:T:101:CDL:H781	26:T:101:CDL:H562	1.86	0.57
1:A:302[B]:ARG:HH12	1:A:365:ILE:HD11	1.69	0.57
3:P:51[A]:MET:SD	26:P:304:CDL:H621	2.44	0.57
3:C:54[A]:MET:HG2	25:C:301:PGV:H61	1.87	0.57
7:T:31:CYS:SG	26:T:101:CDL:H551	2.44	0.56
3:P:232:HIS:NE2	29:P:401:HOH:O	2.32	0.56
12:Y:13:PHE:HA	19:Y:101:TGL:HC41	1.87	0.56
1:A:49[D]:GLY:HA3	13:M:41:LYS:HE3	1.88	0.56
25:C:302:PGV:H183	26:C:303:CDL:H642	1.87	0.56
3:P:220:PHE:HB2	26:P:304:CDL:H711	1.88	0.56
1:A:439:ARG:O	29:A:702:HOH:O	2.18	0.56
7:G:84:LYS:NZ	7:G:84:LYS:H	2.04	0.56
26:P:304:CDL:HB22	10:W:8:LYS:HE3	1.88	0.56
3:P:213:THR:HG23	26:P:304:CDL:H771	1.88	0.55
2:O:91:ASN:C	2:O:92:ASN:HD22	2.10	0.55
1:A:55[D]:ASN:ND2	29:B:709:HOH:O	2.38	0.55
1:N:472:ILE:HD13	19:Y:101:TGL:H202	1.89	0.55
3:P:181:TYR:O	24:P:306:PEK:N	2.39	0.55
2:O:84:LEU:HA	2:O:87:MET:HE2	1.89	0.55
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.89	0.54
7:G:84:LYS:H	7:G:84:LYS:HZ2	1.53	0.54
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.90	0.54
24:C:306:PEK:H242	22:O:602:CHD:H12A	1.90	0.54
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.43	0.54
20:N:611:J6X:S2	20:N:611:J6X:O1	2.66	0.54
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.34	0.54
1:A:49[C]:GLY:O	29:A:703:HOH:O	2.18	0.54
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.90	0.54
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.90	0.53
2:O:91:ASN:HB2	2:O:149:THR:HG21	1.91	0.53
1:N:430:PHE:HE1	19:N:608:TGL:HB22	1.74	0.53
4:Q:9:GLU:HG2	4:Q:10:ASP:N	2.24	0.53
1:N:309:THR:O	1:N:312[B]:ILE:HD13	2.09	0.52
2:O:56:MET:HA	23:O:603:PSC:H202	1.90	0.52
2:O:41:ILE:HG21	23:O:603:PSC:H321	1.91	0.52
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.45	0.52
26:T:101:CDL:H311	26:T:101:CDL:OA7	2.10	0.51
12:Y:21:LEU:HA	12:Y:24[B]:MET:HE2	1.92	0.51
1:N:430:PHE:CE1	19:N:608:TGL:HB22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ARG:HB2	26:C:303:CDL:H512	1.92	0.51
7:G:3:ALA:HA	1:N:282:PHE:HD1	1.75	0.51
26:P:304:CDL:O1	10:W:8:LYS:HD2	2.10	0.51
2:B:41:ILE:HG21	23:B:603:PSC:H332	1.91	0.51
3:C:232:HIS:NE2	29:C:401:HOH:O	2.34	0.51
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.93	0.51
7:T:4:ALA:O	7:T:6:GLY:N	2.44	0.51
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
4:Q:9:GLU:N	4:Q:9:GLU:OE1	2.44	0.51
3:C:28:THR:HG22	25:C:301:PGV:H182	1.93	0.50
26:G:102:CDL:H241	26:G:102:CDL:H541	1.93	0.50
25:N:610:PGV:H321	25:N:610:PGV:H142	1.92	0.50
10:W:50:LEU:HG	27:W:101:DMU:H23	1.94	0.50
26:C:303:CDL:HB22	10:J:8:LYS:HE3	1.93	0.50
3:P:210:ILE:HG23	25:P:303:PGV:H91	1.93	0.50
4:D:87[A]:PHE:CG	25:D:201:PGV:H141	2.46	0.50
7:G:31:CYS:SG	26:G:102:CDL:H551	2.51	0.49
26:G:102:CDL:H112	26:G:102:CDL:H1	1.93	0.49
3:C:33[A]:MET:HG3	27:C:308:DMU:H8	1.95	0.49
27:C:308:DMU:H11	10:J:49:CYS:HB3	1.95	0.49
1:A:297[A]:MET:HE2	1:A:301:THR:HG21	1.95	0.49
3:C:210:ILE:HG12	25:C:302:PGV:H132	1.94	0.49
1:A:308:ALA:O	1:A:311[B]:ILE:HG22	2.13	0.49
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.48	0.49
1:A:52[D]:GLN:O	1:A:56:VAL:HG23	2.12	0.49
3:C:184:ALA:HB3	24:G:101:PEK:H051	1.94	0.49
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.94	0.49
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.48	0.49
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.95	0.49
1:A:31:THR:O	1:A:35:LEU:HD22	2.13	0.48
1:A:52[D]:GLN:HB3	29:A:701:HOH:O	2.13	0.48
1:N:240:HIS:O	1:N:243:VAL:HG22	2.13	0.48
26:T:101:CDL:H1	26:T:101:CDL:H111	1.94	0.48
1:N:18:LEU:HB3	1:N:102:PHE:CZ	2.48	0.48
1:N:440:TYR:CZ	2:O:205:SER:HA	2.49	0.48
23:O:603:PSC:H311	23:O:603:PSC:H282	1.56	0.48
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.14	0.48
3:P:210:ILE:HG23	25:P:303:PGV:H11	1.96	0.48
1:A:282:PHE:HZ	26:T:101:CDL:H761	1.79	0.48
4:D:87[A]:PHE:CE2	25:D:201:PGV:C15	2.96	0.48
26:G:102:CDL:H511	26:G:102:CDL:H201	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HB3	1:A:102:PHE:CZ	2.49	0.48
1:A:374:VAL:HA	1:A:377:PHE:CE2	2.48	0.48
24:B:604:PEK:C05	7:T:17:ARG:HH12	2.23	0.48
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.96	0.48
2:B:139:ASP:OD1	2:B:140:ASN:N	2.46	0.47
25:P:303:PGV:H161	26:P:304:CDL:H671	1.95	0.47
26:C:303:CDL:O1	10:J:12:PHE:HE2	1.97	0.47
5:E:79:LYS:NZ	29:E:204:HOH:O	2.45	0.47
1:N:51[C]:ASP:OD2	29:N:704:HOH:O	2.20	0.47
1:N:292:MET:HB2	1:N:297[A]:MET:HE1	1.96	0.47
1:A:240:HIS:O	1:A:243:VAL:HG22	2.13	0.47
1:N:50[D]:ASP:HB3	1:N:53[D]:ILE:HB	1.96	0.47
2:O:41:ILE:O	2:O:45:MET:HG2	2.15	0.47
3:C:133:ASN:ND2	29:C:402:HOH:O	2.35	0.47
7:G:7:ASP:HB2	1:N:278[A]:MET:SD	2.55	0.47
22:N:609:CHD:H222	25:P:302:PGV:H202	1.95	0.47
2:B:41:ILE:O	2:B:45:MET:HG2	2.14	0.47
6:S:43:LYS:NZ	29:S:204:HOH:O	2.47	0.47
1:A:274:VAL:O	1:A:278:MET:HG3	2.15	0.47
12:Y:2:HIS:N	29:Y:201:HOH:O	2.48	0.47
26:P:304:CDL:H402	26:P:304:CDL:H372	1.52	0.46
1:N:48[C]:LEU:HB2	29:N:811:HOH:O	2.15	0.46
6:F:77:GLY:O	6:F:90:LYS:NZ	2.48	0.46
1:A:51[D]:ASP:OD2	1:A:441:SER:OG	2.27	0.46
26:C:303:CDL:H361	26:C:303:CDL:H182	1.98	0.46
29:N:707:HOH:O	6:S:37:LYS:HA	2.16	0.46
1:A:406:ASN:HD21	25:D:201:PGV:H31	1.80	0.46
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.98	0.46
24:P:301:PEK:H011	24:P:301:PEK:H221	1.37	0.46
1:A:55[C]:ASN:ND2	29:A:702:HOH:O	2.44	0.46
26:T:101:CDL:H531	26:T:101:CDL:H222	1.98	0.46
1:A:289:ALA:HB1	1:A:297[B]:MET:HE1	1.98	0.46
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.52	0.46
24:C:309:PEK:H231	7:T:8:HIS:CE1	2.51	0.46
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.51	0.46
2:B:47:THR:HB	19:D:202:TGL:H181	1.96	0.45
2:B:56:MET:HA	23:B:603:PSC:C20	2.46	0.45
3:C:191:GLY:HA3	29:G:203:HOH:O	2.16	0.45
1:N:309:THR:HG22	14:N:602:HEA:HMB2	1.97	0.45
14:N:602:HEA:H243	2:O:69:PRO:HB3	1.98	0.45
26:C:303:CDL:HB22	10:J:8:LYS:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:139:ASP:OD1	2:O:140:ASN:N	2.49	0.45
1:N:52[D]:GLN:N	29:N:702:HOH:O	2.42	0.45
1:A:52[C]:GLN:HB3	29:A:701:HOH:O	2.16	0.45
25:D:201:PGV:H202	25:D:201:PGV:H011	1.34	0.45
2:B:111:THR:HA	2:B:114:GLU:O	2.17	0.45
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.99	0.45
1:N:52[C]:GLN:HB3	29:N:702:HOH:O	2.16	0.45
8:U:39:CYS:O	8:U:43:MET:HG2	2.15	0.45
19:Y:101:TGL:HC92	19:Y:101:TGL:HC61	1.53	0.45
1:A:73:ILE:HD13	14:A:601[D]:HEA:H22	1.99	0.45
26:T:101:CDL:H541	26:T:101:CDL:H712	1.98	0.45
2:B:158:ASP:OD1	2:B:159:VAL:N	2.49	0.45
1:N:73:ILE:HD13	14:N:601[C]:HEA:H242	1.99	0.45
26:C:303:CDL:H421	26:C:303:CDL:H452	1.75	0.45
1:N:87:ILE:O	1:N:173:PRO:HD3	2.16	0.45
1:N:377:PHE:O	1:N:381[D]:LEU:HB3	2.16	0.45
26:P:304:CDL:HB21	26:P:304:CDL:HA32	1.99	0.45
3:C:155:ASP:OD2	3:C:158:HIS:ND1	2.37	0.44
24:C:306:PEK:H041	7:G:17:ARG:HH12	1.82	0.44
24:G:101:PEK:H42	24:G:101:PEK:H72	1.43	0.44
1:N:498:CYS:HA	1:N:499:PRO:HA	1.88	0.44
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.52	0.44
1:A:54[D]:TYR:HB2	29:A:708:HOH:O	2.17	0.44
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.52	0.44
1:A:144:ASP:OD2	3:C:36:HIS:NE2	2.37	0.44
2:B:56:MET:HG2	23:B:603:PSC:H221	1.99	0.44
26:G:102:CDL:H322	26:G:102:CDL:HA62	1.99	0.44
25:D:201:PGV:H161	25:D:201:PGV:H132	1.67	0.44
1:N:297[B]:MET:HE2	1:N:301:THR:HG21	1.99	0.44
1:N:378:HIS:O	1:N:382[D]:SER:HB2	2.17	0.44
1:N:406:ASN:HD21	25:N:610:PGV:H21	1.81	0.44
4:D:87[A]:PHE:CE2	25:D:201:PGV:H142	2.52	0.44
24:P:306:PEK:H132	24:P:306:PEK:H102	1.67	0.44
19:Y:101:TGL:H291	19:Y:101:TGL:H122	1.84	0.44
1:A:486:ASP:OD1	4:D:17[B]:VAL:HG21	2.17	0.44
1:A:488:THR:HB	1:A:495:LEU:HD13	2.00	0.44
2:B:103:GLN:HA	2:B:104:TRP:HA	1.76	0.44
26:G:102:CDL:H171	1:N:307:SER:CB	2.47	0.44
25:N:607:PGV:H182	3:P:28:THR:HG22	2.00	0.44
19:N:608:TGL:H232	19:N:608:TGL:H262	1.67	0.44
2:O:158:ASP:OD1	2:O:159:VAL:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:PHE:CD2	27:C:308:DMU:H13	2.53	0.44
4:Q:51:LEU:HB3	4:Q:56:LYS:HG3	1.99	0.44
26:T:101:CDL:H571	26:T:101:CDL:H782	1.98	0.44
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	2.00	0.43
2:O:22[B]:HIS:CD2	9:V:44:LYS:HE3	2.53	0.43
1:A:377:PHE:O	1:A:381[D]:LEU:HB3	2.18	0.43
3:C:37:PHE:CE2	27:C:308:DMU:H13	2.53	0.43
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.53	0.43
1:A:87:ILE:O	1:A:173:PRO:HD3	2.19	0.43
3:C:37:PHE:CG	27:C:308:DMU:H9	2.53	0.43
1:A:117[A]:MET:SD	12:L:39:ILE:HG12	2.58	0.43
1:A:409:TRP:HB3	1:A:471:ILE:HG12	2.00	0.43
2:B:146:MET:HA	2:B:213:LEU:HD12	2.00	0.43
1:N:283:LEU:HD13	1:N:312[B]:ILE:HG22	2.01	0.43
14:N:602:HEA:HMD1	14:N:602:HEA:HBD2	2.00	0.43
1:A:343:GLY:HA2	19:D:202:TGL:H212	2.00	0.43
3:C:62:ILE:HD12	26:C:303:CDL:H511	2.00	0.43
24:C:306:PEK:H5	24:C:306:PEK:O04	2.19	0.43
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.43
2:O:56:MET:CA	23:O:603:PSC:H202	2.49	0.43
3:P:191:GLY:HA3	29:T:205:HOH:O	2.17	0.43
3:P:224:LYS:HE3	26:P:304:CDL:H131	1.99	0.43
2:B:128:LEU:HD11	2:B:134:ARG:HA	2.01	0.43
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.00	0.43
1:A:386:VAL:HG21	14:A:601[C]:HEA:H261	2.00	0.43
2:B:58:ALA:O	2:B:62:GLU:HG3	2.18	0.43
3:C:220:PHE:CB	26:C:303:CDL:H711	2.43	0.43
1:N:54[D]:TYR:HB2	29:N:811:HOH:O	2.19	0.43
25:N:610:PGV:H322	13:Z:19:LEU:HD23	2.01	0.43
3:P:184:ALA:HB3	24:P:306:PEK:H051	2.00	0.43
6:S:52:ILE:H	6:S:52:ILE:HG13	1.74	0.43
1:A:498:CYS:HA	1:A:499:PRO:HA	1.90	0.43
5:R:43:PRO:HB2	5:R:48:ILE:HD11	2.01	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.00	0.43
22:C:304:CHD:H222	22:C:304:CHD:H162	1.57	0.43
4:D:42:GLU:OE1	29:D:301:HOH:O	2.21	0.43
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.54	0.43
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.89	0.43
2:O:57:ASP:H	23:O:603:PSC:H202	1.84	0.42
19:Y:101:TGL:H352	19:Y:101:TGL:H191	1.87	0.42
1:A:334:TRP:HZ3	19:D:202:TGL:HA72	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:102:CDL:H252	26:G:102:CDL:H221	1.64	0.42
3:P:198:PHE:CZ	24:P:306:PEK:H042	2.54	0.42
4:D:21:ASP:OD1	4:D:21:ASP:N	2.50	0.42
6:F:94:HIS:ND1	29:F:202:HOH:O	2.37	0.42
24:C:306:PEK:H051	29:C:492:HOH:O	2.18	0.42
1:N:409:TRP:HB3	1:N:471:ILE:HG12	2.01	0.42
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.01	0.42
24:C:309:PEK:H352	7:T:5:LYS:HD3	2.01	0.42
26:G:102:CDL:H792	26:G:102:CDL:H571	2.01	0.42
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.41	0.42
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.20	0.42
2:O:168:LEU:HD13	2:O:184:LEU:HG	2.01	0.42
25:P:302:PGV:O02	25:P:302:PGV:H61	2.20	0.42
1:N:51[C]:ASP:OD2	2:O:204:HIS:N	2.52	0.42
2:B:33:LEU:HD12	2:B:33:LEU:HA	1.86	0.42
19:Q:201:TGL:H121	19:Q:201:TGL:HB92	1.83	0.42
2:B:102:HIS:O	2:B:104:TRP:HA	2.19	0.42
24:B:604:PEK:H14	3:P:168:THR:HG22	2.01	0.42
3:C:91:VAL:HG22	24:C:309:PEK:H12	2.01	0.42
1:N:236:TRP:HH2	14:N:602:HEA:HBD1	1.84	0.42
2:O:102:HIS:O	2:O:104:TRP:HA	2.19	0.42
23:O:603:PSC:H21	23:O:603:PSC:H231	2.02	0.42
3:P:155:ASP:OD2	3:P:158:HIS:ND1	2.35	0.42
4:D:118:LYS:HB3	11:K:53:TRP:HB3	2.00	0.42
19:N:608:TGL:HB82	2:O:32[A]:PHE:CE1	2.55	0.42
12:L:2:HIS:CG	12:L:3:TYR:H	2.38	0.41
1:N:68:PHE:CE2	1:N:112:LEU:HD12	2.50	0.41
1:A:403:TYR:CZ	12:L:7:PRO:HB2	2.56	0.41
3:C:37:PHE:CD2	27:C:308:DMU:H9	2.55	0.41
2:O:203:ASN:OD1	29:O:701:HOH:O	2.22	0.41
26:T:101:CDL:OA7	26:T:101:CDL:H342	2.20	0.41
26:T:101:CDL:H651	26:T:101:CDL:H622	1.79	0.41
4:D:78:TRP:N	19:D:202:TGL:HB22	2.35	0.41
3:P:37:PHE:CD2	27:W:101:DMU:H13	2.54	0.41
14:A:601[C]:HEA:H271	14:A:601[C]:HEA:H212	1.84	0.41
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.89	0.41
3:C:210:ILE:HG21	25:C:302:PGV:H281	2.02	0.41
26:G:102:CDL:H761	1:N:282:PHE:HZ	1.85	0.41
8:H:39:CYS:O	8:H:43:MET:HG2	2.20	0.41
3:C:51[A]:MET:SD	26:C:303:CDL:H612	2.61	0.41
26:T:101:CDL:H151	26:T:101:CDL:H182	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50[D]:ASP:HB3	1:A:53[D]:ILE:HG22	2.01	0.41
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.56	0.41
3:P:160:LEU:HD13	22:P:305:CHD:H181	2.02	0.41
26:C:303:CDL:H171	26:C:303:CDL:H201	1.70	0.41
2:O:33:LEU:HD12	2:O:33:LEU:HA	1.85	0.41
1:A:439:ARG:HD3	2:B:199:ILE:HB	2.03	0.41
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.55	0.41
2:O:111:THR:HA	2:O:114:GLU:O	2.20	0.41
7:T:5:LYS:HG2	7:T:6:GLY:H	1.85	0.41
2:B:29:MET:HB2	9:I:35:TYR:CE1	2.56	0.41
1:N:202:LEU:HD22	1:N:238:PHE:CE2	2.56	0.41
1:N:236:TRP:CH2	14:N:602:HEA:HBD1	2.56	0.41
1:N:369:ASP:HA	1:N:438:ARG:HD3	2.02	0.41
14:N:602:HEA:HMB1	14:N:602:HEA:H11	1.96	0.41
25:P:303:PGV:H152	26:P:304:CDL:H632	2.01	0.41
4:Q:16:TYR:CE1	4:Q:25:PRO:HG2	2.56	0.41
4:Q:131:ILE:HG22	4:Q:132:GLN:HG3	2.03	0.41
1:A:440:TYR:CZ	2:B:205:SER:HA	2.55	0.41
27:C:308:DMU:C22	10:J:49:CYS:HB3	2.51	0.41
2:O:41:ILE:HD13	23:O:603:PSC:H342	2.03	0.41
23:O:603:PSC:H232	23:O:603:PSC:H201	1.95	0.41
4:Q:21:ASP:OD1	4:Q:21:ASP:N	2.47	0.41
23:O:603:PSC:H221	23:O:603:PSC:H252	1.81	0.40
5:R:90:ARG:NH2	29:R:201:HOH:O	2.33	0.40
23:B:603:PSC:H081	5:E:8:ASP:OD1	2.22	0.40
1:N:247:ILE:HD12	1:N:247:ILE:HA	1.93	0.40
2:O:42:ILE:HG21	19:Q:201:TGL:H232	2.03	0.40
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.21	0.40
24:C:309:PEK:H221	24:C:309:PEK:H012	1.87	0.40
5:E:12:ASP:HA	5:E:47:ILE:HD11	2.03	0.40
19:L:101:TGL:H231	19:L:101:TGL:H202	1.41	0.40
1:N:112:LEU:HG	29:N:944:HOH:O	2.21	0.40
1:N:294:THR:HG22	1:N:365:ILE:HD13	2.03	0.40
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.03	0.40
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	2.03	0.40
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.97	0.40
1:N:381[D]:LEU:HB2	14:N:602:HEA:CAC	2.52	0.40
23:O:603:PSC:H22	29:O:835:HOH:O	2.21	0.40
26:T:101:CDL:H832	26:T:101:CDL:H802	1.94	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	533/514 (104%)	518 (97%)	15 (3%)	0	100	100
1	N	535/514 (104%)	520 (97%)	15 (3%)	0	100	100
2	B	229/581 (39%)	225 (98%)	4 (2%)	0	100	100
2	O	231/581 (40%)	225 (97%)	5 (2%)	1 (0%)	34	37
3	C	264/261 (101%)	260 (98%)	4 (2%)	0	100	100
3	P	263/261 (101%)	259 (98%)	4 (2%)	0	100	100
4	D	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
4	Q	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	93/98 (95%)	92 (99%)	1 (1%)	0	100	100
6	S	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
7	G	80/84 (95%)	75 (94%)	4 (5%)	1 (1%)	12	9
7	T	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	2	0
8	H	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
8	U	77/85 (91%)	75 (97%)	2 (3%)	0	100	100
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	Z	39/46 (85%)	39 (100%)	0	0	100 100
All	All	3564/4320 (82%)	3481 (98%)	77 (2%)	6 (0%)	51 55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	T	5	LYS
7	G	6	GLY
7	T	4	ALA
7	T	36[A]	TRP
7	T	36[B]	TRP
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	446/426 (105%)	440 (99%)	6 (1%)	69 81
1	N	448/426 (105%)	439 (98%)	9 (2%)	55 69
2	B	214/511 (42%)	205 (96%)	9 (4%)	30 38
2	O	216/511 (42%)	207 (96%)	9 (4%)	30 38
3	C	231/225 (103%)	227 (98%)	4 (2%)	60 74
3	P	230/225 (102%)	227 (99%)	3 (1%)	69 81
4	D	130/129 (101%)	129 (99%)	1 (1%)	81 90
4	Q	125/129 (97%)	124 (99%)	1 (1%)	81 90
5	E	93/95 (98%)	92 (99%)	1 (1%)	73 85
5	R	93/95 (98%)	91 (98%)	2 (2%)	52 65
6	F	80/81 (99%)	78 (98%)	2 (2%)	47 60
6	S	81/81 (100%)	80 (99%)	1 (1%)	71 83
7	G	67/67 (100%)	56 (84%)	11 (16%)	2 2
7	T	67/67 (100%)	58 (87%)	9 (13%)	4 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	71/75 (95%)	68 (96%)	3 (4%)	30 38
8	U	71/75 (95%)	68 (96%)	3 (4%)	30 38
9	I	57/58 (98%)	57 (100%)	0	100 100
9	V	57/58 (98%)	57 (100%)	0	100 100
10	J	48/50 (96%)	48 (100%)	0	100 100
10	W	49/50 (98%)	47 (96%)	2 (4%)	30 39
11	K	41/46 (89%)	40 (98%)	1 (2%)	49 62
11	X	40/46 (87%)	38 (95%)	2 (5%)	24 30
12	L	39/40 (98%)	39 (100%)	0	100 100
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24 29
13	M	37/38 (97%)	37 (100%)	0	100 100
13	Z	35/38 (92%)	34 (97%)	1 (3%)	42 54
All	All	3105/3682 (84%)	3023 (97%)	82 (3%)	47 58

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	109	PHE
1	A	369	ASP
1	A	382[C]	SER
1	A	382[D]	SER
2	B	33	LEU
2	B	52	HIS
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	94	SER
2	B	115	ASP
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	7	LYS
5	E	5	HIS

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Mol	Chain	Res	Type
6	F	37	LYS
6	F	95	GLN
7	G	5	LYS
7	G	8	HIS
7	G	18	PHE
7	G	33	LEU
7	G	36[A]	TRP
7	G	36[B]	TRP
7	G	37	LEU
7	G	42	ARG
7	G	54	ARG
7	G	83	GLU
7	G	84	LYS
8	H	9	LYS
8	H	29	CYS
8	H	60	TYR
11	K	51	LYS
1	N	38	ARG
1	N	109	PHE
1	N	112	LEU
1	N	311[A]	ILE
1	N	311[B]	ILE
1	N	363	LEU
1	N	369	ASP
1	N	382[C]	SER
1	N	382[D]	SER
2	O	33	LEU
2	O	60[A]	GLU
2	O	60[B]	GLU
2	O	66	THR
2	O	78	LEU
2	O	92	ASN
2	O	171	LYS
2	O	221	LYS
2	O	226	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	51	LEU
5	R	5	HIS
5	R	109	VAL
6	S	43	LYS

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Mol	Chain	Res	Type
7	T	5	LYS
7	T	8	HIS
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG
7	T	43	GLU
7	T	54	ARG
8	U	29	CYS
8	U	60	TYR
8	U	84	LYS
10	W	7	GLU
10	W	50	LEU
11	X	12	LYS
11	X	51	LYS
12	Y	2	HIS
12	Y	20	ARG
13	Z	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
7	G	34	ASN
7	G	38	HIS
2	O	91	ASN
2	O	92	ASN
5	R	78	HIS
8	U	37	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.48	0	7,9,11	1.37	1 (14%)
7	TPO	G	11	7	8,10,11	1.28	1 (12%)	10,14,16	1.10	1 (10%)
2	FME	O	1	2	8,9,10	0.49	0	7,9,11	1.29	0
2	FME	B	1	2	8,9,10	0.49	0	7,9,11	1.32	0
7	TPO	T	11	7	8,10,11	1.31	1 (12%)	10,14,16	0.83	0
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	1.17	0

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
1	FME	A	1	1	-	6/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
1	FME	N	1	1	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.76	1.59	1.50
7	T	11	TPO	P-O1P	2.74	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	11	TPO	CG2-CB-CA	3.12	119.32	113.16
1	A	1	FME	O1-CN-N	-2.26	119.31	125.27

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	CA-CB-OG1-P
1	A	1	FME	CA-CB-CG-SD
1	N	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
1	N	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
1	N	1	FME	CB-CG-SD-CE
1	N	1	FME	O1-CN-N-CA
7	T	11	TPO	CB-OG1-P-O3P
1	A	1	FME	CB-CA-N-CN
7	T	11	TPO	CB-OG1-P-O2P
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CUA	B	601	2	0,1,1	-	-	-		
19	TGL	Q	201	-	62,62,62	0.98	3 (4%)	65,65,65	1.10	5 (7%)
20	J6X	N	611	-	11,18,18	3.54	5 (45%)	6,26,26	1.37	1 (16%)
25	PGV	C	301	-	50,50,50	0.35	0	53,56,56	0.37	0
25	PGV	N	610	-	50,50,50	0.92	2 (4%)	53,56,56	1.16	7 (13%)
22	CHD	O	602	-	32,32,32	0.81	1 (3%)	51,51,51	1.04	2 (3%)
25	PGV	C	302	-	50,50,50	0.97	2 (4%)	53,56,56	1.11	4 (7%)
19	TGL	L	101	-	62,62,62	1.00	3 (4%)	65,65,65	0.99	4 (6%)
26	CDL	P	304	-	99,99,99	1.31	12 (12%)	105,111,111	1.56	13 (12%)
18	PER	A	606	14,15	0,1,1	-	-	-		
21	CUA	O	601	2	0,1,1	-	-	-		
22	CHD	N	609	-	32,32,32	0.80	0	51,51,51	0.97	0
19	TGL	Y	101	-	62,62,62	1.01	3 (4%)	65,65,65	1.15	4 (6%)
14	HEA	N	601[C]	-	57,67,67	1.49	9 (15%)	61,103,103	1.56	12 (19%)
26	CDL	T	101	-	99,99,99	1.32	12 (12%)	105,111,111	1.34	9 (8%)
24	PEK	C	306	-	52,52,52	0.86	2 (3%)	55,57,57	1.34	9 (16%)
14	HEA	A	602	18,1	57,67,67	1.49	9 (15%)	61,103,103	1.67	18 (29%)
27	DMU	C	308	-	34,34,34	0.45	1 (2%)	45,45,45	0.99	2 (4%)
24	PEK	P	306	-	52,52,52	0.94	2 (3%)	55,57,57	1.28	6 (10%)
19	TGL	D	202	-	62,62,62	0.97	3 (4%)	65,65,65	0.99	4 (6%)
23	PSC	O	603	-	51,51,51	1.10	3 (5%)	57,59,59	1.55	5 (8%)
24	PEK	C	309	-	52,52,52	0.92	2 (3%)	55,57,57	1.14	5 (9%)
24	PEK	G	101	-	52,52,52	0.93	2 (3%)	55,57,57	1.18	5 (9%)
25	PGV	D	201	-	50,50,50	0.35	0	53,56,56	0.31	0
27	DMU	Z	101	-	34,34,34	0.38	0	45,45,45	0.87	1 (2%)
24	PEK	B	604	-	52,52,52	0.91	2 (3%)	55,57,57	1.45	8 (14%)
14	HEA	A	601[C]	-	57,67,67	1.50	9 (15%)	61,103,103	1.57	9 (14%)
26	CDL	G	102	-	99,99,99	1.32	12 (12%)	105,111,111	1.38	10 (9%)
14	HEA	N	602	18,1	57,67,67	1.50	9 (15%)	61,103,103	1.66	15 (24%)
25	PGV	P	302	-	50,50,50	0.96	2 (4%)	53,56,56	1.55	10 (18%)
19	TGL	A	607	-	62,62,62	0.98	3 (4%)	65,65,65	1.11	5 (7%)
25	PGV	N	607	-	50,50,50	0.36	0	53,56,56	0.40	0
24	PEK	P	301	-	52,52,52	0.27	0	55,57,57	0.42	0
22	CHD	C	304	-	32,32,32	0.84	1 (3%)	51,51,51	1.30	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	DMU	M	101	-	34,34,34	0.35	0	45,45,45	0.83	1 (2%)
25	PGV	C	307	-	50,50,50	0.98	2 (4%)	53,56,56	1.38	6 (11%)
14	HEA	N	601[D]	-	57,67,67	1.49	9 (15%)	61,103,103	1.57	11 (18%)
23	PSC	B	603	-	51,51,51	1.09	3 (5%)	57,59,59	1.25	5 (8%)
22	CHD	B	602	-	32,32,32	0.81	1 (3%)	51,51,51	1.07	4 (7%)
27	DMU	W	101	-	34,34,34	0.35	0	45,45,45	0.83	1 (2%)
22	CHD	P	305	-	32,32,32	0.82	1 (3%)	51,51,51	1.25	6 (11%)
19	TGL	N	608	-	62,62,62	0.99	3 (4%)	65,65,65	1.06	5 (7%)
18	PER	N	606	14,15	0,1,1	-	-	-		
22	CHD	C	305	-	32,32,32	0.81	1 (3%)	51,51,51	1.00	0
26	CDL	C	303	-	99,99,99	1.33	12 (12%)	105,111,111	1.51	14 (13%)
25	PGV	P	303	-	50,50,50	0.99	2 (4%)	53,56,56	1.23	5 (9%)
20	J6X	A	608	-	11,18,18	4.02	5 (45%)	6,26,26	1.44	1 (16%)
14	HEA	A	601[D]	-	57,67,67	1.50	9 (15%)	61,103,103	1.57	11 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	Q	201	-	-	28/65/65/65	-
20	J6X	N	611	-	-	0/0/4/4	0/3/3/3
25	PGV	C	301	-	-	15/55/55/55	-
25	PGV	N	610	-	-	18/55/55/55	-
22	CHD	O	602	-	-	2/9/74/74	0/4/4/4
25	PGV	C	302	-	-	14/55/55/55	-
19	TGL	L	101	-	-	31/65/65/65	-
26	CDL	P	304	-	-	35/110/110/110	-
22	CHD	N	609	-	-	3/9/74/74	0/4/4/4
19	TGL	Y	101	-	-	38/65/65/65	-
14	HEA	N	601[C]	-	-	6/32/76/76	-
26	CDL	T	101	-	-	40/110/110/110	-
24	PEK	C	306	-	-	17/56/56/56	-
14	HEA	A	602	18,1	-	7/32/76/76	-
27	DMU	C	308	-	-	4/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	P	306	-	-	20/56/56/56	-
19	TGL	D	202	-	-	29/65/65/65	-
23	PSC	O	603	-	-	28/55/55/55	-
24	PEK	C	309	-	-	21/56/56/56	-
24	PEK	G	101	-	-	16/56/56/56	-
25	PGV	D	201	-	-	34/55/55/55	-
27	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
24	PEK	B	604	-	-	24/56/56/56	-
14	HEA	A	601[C]	-	-	6/32/76/76	-
26	CDL	G	102	-	-	41/110/110/110	-
14	HEA	N	602	18,1	-	6/32/76/76	-
25	PGV	P	302	-	-	19/55/55/55	-
19	TGL	A	607	-	-	20/65/65/65	-
25	PGV	N	607	-	-	14/55/55/55	-
24	PEK	P	301	-	-	28/56/56/56	-
22	CHD	C	304	-	-	8/9/74/74	0/4/4/4
27	DMU	M	101	-	-	4/19/59/59	0/2/2/2
25	PGV	C	307	-	-	22/55/55/55	-
14	HEA	N	601[D]	-	-	6/32/76/76	-
23	PSC	B	603	-	-	28/55/55/55	-
22	CHD	B	602	-	-	2/9/74/74	0/4/4/4
27	DMU	W	101	-	-	4/19/59/59	0/2/2/2
22	CHD	P	305	-	-	4/9/74/74	0/4/4/4
19	TGL	N	608	-	-	26/65/65/65	-
22	CHD	C	305	-	-	1/9/74/74	0/4/4/4
26	CDL	C	303	-	-	52/110/110/110	-
25	PGV	P	303	-	-	17/55/55/55	-
20	J6X	A	608	-	-	0/0/4/4	0/3/3/3
14	HEA	A	601[D]	-	-	5/32/76/76	-

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	608	J6X	C9-S2	-11.16	1.58	1.73
20	N	611	J6X	C9-S2	-9.31	1.60	1.73
25	C	307	PGV	O03-C19	4.77	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	306	PEK	O03-C21	4.64	1.46	1.33
26	C	303	CDL	OA6-CA5	4.58	1.47	1.34
25	P	303	PGV	O03-C19	4.54	1.46	1.33
23	O	603	PSC	O01-C1	4.53	1.47	1.34
26	C	303	CDL	OA8-CA7	4.50	1.46	1.33
24	G	101	PEK	O03-C21	4.48	1.46	1.33
25	P	302	PGV	O01-C1	4.43	1.46	1.34
25	C	302	PGV	O01-C1	4.43	1.46	1.34
25	P	302	PGV	O03-C19	4.42	1.46	1.33
23	B	603	PSC	O01-C1	4.42	1.46	1.34
19	L	101	TGL	OG1-CA1	4.40	1.46	1.33
19	Y	101	TGL	OG2-CB1	4.40	1.46	1.34
26	T	101	CDL	OA8-CA7	4.40	1.46	1.33
19	N	608	TGL	OG1-CA1	4.40	1.46	1.33
24	B	604	PEK	O03-C21	4.39	1.46	1.33
24	C	309	PEK	O03-C21	4.39	1.46	1.33
26	G	102	CDL	OA8-CA7	4.39	1.46	1.33
25	N	610	PGV	O03-C19	4.38	1.46	1.33
26	G	102	CDL	OB8-CB7	4.36	1.46	1.33
20	A	608	J6X	C4-C5	-4.35	1.33	1.42
19	Y	101	TGL	OG3-CC1	4.34	1.46	1.33
26	P	304	CDL	OA6-CA5	4.33	1.46	1.34
19	A	607	TGL	OG1-CA1	4.32	1.46	1.33
25	C	302	PGV	O03-C19	4.32	1.46	1.33
26	T	101	CDL	OB8-CB7	4.30	1.45	1.33
19	Q	201	TGL	OG1-CA1	4.28	1.45	1.33
20	N	611	J6X	C4-C5	-4.28	1.33	1.42
19	Y	101	TGL	OG1-CA1	4.28	1.45	1.33
25	P	303	PGV	O01-C1	4.28	1.46	1.34
19	D	202	TGL	OG1-CA1	4.27	1.45	1.33
19	L	101	TGL	OG2-CB1	4.24	1.46	1.34
26	T	101	CDL	OA6-CA5	4.23	1.46	1.34
19	Q	201	TGL	OG3-CC1	4.22	1.45	1.33
26	P	304	CDL	OB6-CB5	4.22	1.46	1.34
26	G	102	CDL	OB6-CB5	4.21	1.46	1.34
19	N	608	TGL	OG3-CC1	4.20	1.45	1.33
19	L	101	TGL	OG3-CC1	4.18	1.45	1.33
26	G	102	CDL	OA6-CA5	4.17	1.46	1.34
19	A	607	TGL	OG3-CC1	4.16	1.45	1.33
19	D	202	TGL	OG3-CC1	4.16	1.45	1.33
26	P	304	CDL	OA8-CA7	4.14	1.45	1.33
24	C	309	PEK	O01-C1	4.13	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	CDL	OB6-CB5	4.12	1.45	1.34
24	B	604	PEK	O01-C1	4.08	1.45	1.34
26	C	303	CDL	OB6-CB5	4.07	1.45	1.34
25	C	307	PGV	O01-C1	4.06	1.45	1.34
19	A	607	TGL	OG2-CB1	4.04	1.45	1.34
24	C	306	PEK	O03-C21	4.01	1.45	1.33
19	N	608	TGL	OG2-CB1	4.00	1.45	1.34
24	G	101	PEK	O01-C1	3.97	1.45	1.34
24	C	306	PEK	O01-C1	3.97	1.45	1.34
26	P	304	CDL	OB8-CB7	3.96	1.44	1.33
19	Q	201	TGL	OG2-CB1	3.94	1.45	1.34
20	A	608	J6X	C7-C5	-3.92	1.34	1.40
25	N	610	PGV	O01-C1	3.92	1.45	1.34
26	C	303	CDL	OB8-CB7	3.88	1.44	1.33
24	P	306	PEK	O01-C1	3.87	1.45	1.34
23	O	603	PSC	O03-C19	3.87	1.44	1.33
23	B	603	PSC	O03-C19	3.83	1.44	1.33
20	N	611	J6X	C7-C5	-3.78	1.35	1.40
19	D	202	TGL	OG2-CB1	3.77	1.44	1.34
14	N	602	HEA	CHD-C1D	3.69	1.44	1.35
23	O	603	PSC	C13-C12	3.69	1.53	1.31
14	A	602	HEA	CHD-C1D	3.67	1.44	1.35
23	B	603	PSC	C13-C12	3.67	1.53	1.31
14	A	602	HEA	C4D-C3D	-3.66	1.38	1.45
14	A	601[C]	HEA	CHD-C1D	3.66	1.44	1.35
14	A	601[D]	HEA	CHD-C1D	3.66	1.44	1.35
14	N	601[C]	HEA	CHD-C1D	3.62	1.44	1.35
14	N	601[D]	HEA	CHD-C1D	3.62	1.44	1.35
14	A	601[C]	HEA	CHC-C4B	3.60	1.44	1.35
14	A	601[D]	HEA	CHC-C4B	3.60	1.44	1.35
14	N	601[C]	HEA	CHC-C4B	3.59	1.44	1.35
14	N	601[D]	HEA	CHC-C4B	3.59	1.44	1.35
14	N	602	HEA	C4D-C3D	-3.55	1.38	1.45
14	A	602	HEA	CHC-C4B	3.54	1.44	1.35
14	A	601[C]	HEA	C4D-C3D	-3.53	1.39	1.45
14	A	601[D]	HEA	C4D-C3D	-3.53	1.39	1.45
14	N	602	HEA	CHC-C4B	3.47	1.43	1.35
26	C	303	CDL	C19-C18	-3.45	1.32	1.51
26	C	303	CDL	C22-C21	-3.45	1.32	1.51
14	N	602	HEA	C4B-C3B	-3.44	1.38	1.44
14	N	601[C]	HEA	C4D-C3D	-3.44	1.39	1.45
14	N	601[D]	HEA	C4D-C3D	-3.44	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	304	CDL	C62-C61	-3.43	1.32	1.51
14	N	601[C]	HEA	C4B-C3B	-3.38	1.38	1.44
14	N	601[D]	HEA	C4B-C3B	-3.38	1.38	1.44
26	T	101	CDL	C59-C58	-3.38	1.32	1.51
26	G	102	CDL	C62-C61	-3.38	1.32	1.51
14	A	602	HEA	C4B-C3B	-3.38	1.38	1.44
26	P	304	CDL	C59-C58	-3.37	1.32	1.51
26	T	101	CDL	C62-C61	-3.36	1.32	1.51
14	A	601[C]	HEA	C4B-C3B	-3.35	1.39	1.44
14	A	601[D]	HEA	C4B-C3B	-3.35	1.39	1.44
26	P	304	CDL	C79-C78	-3.33	1.32	1.51
26	C	303	CDL	C62-C61	-3.33	1.32	1.51
26	G	102	CDL	C59-C58	-3.32	1.32	1.51
26	G	102	CDL	C39-C38	-3.32	1.33	1.51
26	C	303	CDL	C59-C58	-3.32	1.33	1.51
26	P	304	CDL	C22-C21	-3.31	1.33	1.51
26	P	304	CDL	C19-C18	-3.31	1.33	1.51
26	G	102	CDL	C82-C81	-3.30	1.33	1.51
26	G	102	CDL	C19-C18	-3.30	1.33	1.51
26	T	101	CDL	C42-C41	-3.30	1.33	1.51
26	C	303	CDL	C82-C81	-3.29	1.33	1.51
26	C	303	CDL	C79-C78	-3.29	1.33	1.51
26	C	303	CDL	C39-C38	-3.29	1.33	1.51
26	G	102	CDL	C42-C41	-3.28	1.33	1.51
14	A	601[C]	HEA	C1D-ND	-3.28	1.34	1.40
14	A	601[D]	HEA	C1D-ND	-3.28	1.34	1.40
26	P	304	CDL	C82-C81	-3.28	1.33	1.51
26	G	102	CDL	C79-C78	-3.28	1.33	1.51
26	G	102	CDL	C22-C21	-3.27	1.33	1.51
26	T	101	CDL	C22-C21	-3.26	1.33	1.51
26	T	101	CDL	C79-C78	-3.26	1.33	1.51
26	T	101	CDL	C39-C38	-3.24	1.33	1.51
26	T	101	CDL	C19-C18	-3.24	1.33	1.51
14	N	601[C]	HEA	C1D-ND	-3.24	1.34	1.40
14	N	601[D]	HEA	C1D-ND	-3.24	1.34	1.40
14	N	602	HEA	C1D-ND	-3.23	1.34	1.40
26	T	101	CDL	C82-C81	-3.22	1.33	1.51
26	C	303	CDL	C42-C41	-3.22	1.33	1.51
26	P	304	CDL	C39-C38	-3.21	1.33	1.51
26	P	304	CDL	C42-C41	-3.20	1.33	1.51
14	N	602	HEA	C4B-NB	-3.17	1.34	1.40
14	A	602	HEA	C1D-ND	-3.16	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[C]	HEA	C4B-NB	-3.10	1.35	1.40
14	A	601[D]	HEA	C4B-NB	-3.10	1.35	1.40
14	N	601[C]	HEA	C4B-NB	-3.08	1.35	1.40
14	N	601[D]	HEA	C4B-NB	-3.08	1.35	1.40
14	A	602	HEA	C4B-NB	-3.08	1.35	1.40
20	N	611	J6X	C10-S2	-3.01	1.65	1.70
20	A	608	J6X	C10-S2	-2.96	1.66	1.70
14	N	601[C]	HEA	C1D-C2D	-2.93	1.38	1.44
14	N	601[D]	HEA	C1D-C2D	-2.93	1.38	1.44
14	A	601[C]	HEA	C1D-C2D	-2.90	1.39	1.44
14	A	601[D]	HEA	C1D-C2D	-2.90	1.39	1.44
14	A	602	HEA	C1B-C2B	-2.87	1.39	1.44
14	N	602	HEA	C1B-C2B	-2.81	1.39	1.44
14	A	601[C]	HEA	C1B-C2B	-2.78	1.39	1.44
14	A	601[D]	HEA	C1B-C2B	-2.78	1.39	1.44
14	N	602	HEA	C1D-C2D	-2.78	1.39	1.44
14	N	601[C]	HEA	C1B-C2B	-2.77	1.39	1.44
14	N	601[D]	HEA	C1B-C2B	-2.77	1.39	1.44
14	A	602	HEA	C1D-C2D	-2.74	1.39	1.44
20	A	608	J6X	C1-C6	-2.32	1.33	1.40
20	N	611	J6X	C1-C6	-2.27	1.33	1.40
22	C	304	CHD	C13-C14	-2.19	1.51	1.55
22	P	305	CHD	C13-C14	-2.15	1.51	1.55
14	A	602	HEA	C4D-ND	-2.11	1.34	1.38
22	O	602	CHD	C13-C14	-2.10	1.51	1.55
22	B	602	CHD	C13-C14	-2.08	1.52	1.55
14	N	601[C]	HEA	C1B-NB	-2.06	1.34	1.38
14	N	601[D]	HEA	C1B-NB	-2.06	1.34	1.38
14	N	602	HEA	C4D-ND	-2.05	1.34	1.38
27	C	308	DMU	O16-C6	2.05	1.43	1.40
22	C	305	CHD	C13-C14	-2.05	1.52	1.55
14	A	601[C]	HEA	C1B-NB	-2.04	1.34	1.38
14	A	601[D]	HEA	C1B-NB	-2.04	1.34	1.38

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	603	PSC	O01-C1-C2	7.81	128.34	111.50
26	P	304	CDL	CA6-CA4-CA3	-6.43	96.58	111.79
26	C	303	CDL	CB4-OB6-CB5	-6.13	102.70	117.79
26	T	101	CDL	OA6-CA5-C11	5.63	123.63	111.50
19	Y	101	TGL	OG2-CB1-CB2	5.42	123.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	102	CDL	OB6-CB5-C51	5.35	123.03	111.50
26	G	102	CDL	OA6-CA5-C11	5.25	122.81	111.50
25	P	302	PGV	O03-C19-C20	4.88	127.21	111.91
26	T	101	CDL	OB6-CB5-C51	4.86	121.97	111.50
23	B	603	PSC	O01-C1-C2	4.79	121.83	111.50
26	C	303	CDL	OB6-CB5-C51	4.74	121.71	111.50
25	C	307	PGV	O03-C19-C20	4.71	126.70	111.91
26	C	303	CDL	OA6-CA5-C11	4.64	121.51	111.50
24	B	604	PEK	O01-C1-C2	4.64	121.50	111.50
26	P	304	CDL	OB6-CB5-C51	4.59	121.40	111.50
19	Q	201	TGL	OG2-CB1-CB2	4.34	120.86	111.50
19	A	607	TGL	OG2-CB1-CB2	4.33	120.83	111.50
25	P	303	PGV	O03-C19-C20	4.32	125.47	111.91
24	P	306	PEK	C2-C3-C4	-4.25	105.66	113.23
24	B	604	PEK	C02-O01-C1	-4.21	107.41	117.79
26	G	102	CDL	CB4-OB6-CB5	-4.18	107.49	117.79
14	A	601[C]	HEA	C13-C12-C11	-4.15	108.12	114.35
26	T	101	CDL	CB4-OB6-CB5	-4.07	107.77	117.79
25	P	302	PGV	C02-O01-C1	3.92	127.44	117.79
26	P	304	CDL	OA8-CA7-C31	3.87	124.06	111.91
19	N	608	TGL	OG2-CB1-CB2	3.86	119.81	111.50
26	P	304	CDL	CB4-OB6-CB5	-3.85	108.31	117.79
14	N	601[C]	HEA	CBA-CAA-C2A	3.79	119.00	112.60
14	N	601[D]	HEA	CBA-CAA-C2A	3.79	119.00	112.60
24	B	604	PEK	O03-C21-C22	3.76	123.72	111.91
26	G	102	CDL	CA4-OA6-CA5	-3.65	108.81	117.79
23	O	603	PSC	O01-C1-O02	-3.62	114.95	123.70
19	L	101	TGL	OG2-CB1-CB2	3.61	119.28	111.50
24	P	306	PEK	O03-C21-C22	3.61	123.23	111.91
24	G	101	PEK	O03-C21-C22	3.55	123.06	111.91
25	C	302	PGV	O01-C1-C2	3.53	119.11	111.50
22	C	304	CHD	C13-C17-C20	-3.48	115.34	119.50
24	C	309	PEK	O01-C1-C2	3.47	118.97	111.50
25	P	303	PGV	O01-C1-C2	3.45	118.93	111.50
14	A	601[C]	HEA	CBA-CAA-C2A	3.42	118.36	112.60
14	A	601[D]	HEA	CBA-CAA-C2A	3.42	118.36	112.60
25	C	307	PGV	O01-C1-C2	3.41	118.85	111.50
25	P	302	PGV	O03-C19-O04	-3.40	115.00	123.59
24	C	306	PEK	O01-C1-C2	3.38	118.80	111.50
26	P	304	CDL	OA6-CA5-C11	3.34	118.70	111.50
25	P	303	PGV	O03-C19-O04	-3.30	115.27	123.59
26	C	303	CDL	CB6-CB4-CB3	-3.29	104.01	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	303	CDL	CA6-CA4-CA3	-3.28	104.03	111.79
26	P	304	CDL	OB8-CB7-C71	3.26	122.13	111.91
19	Q	201	TGL	CG2-OG2-CB1	-3.24	109.82	117.79
24	C	306	PEK	O03-C21-C22	3.23	122.04	111.91
25	C	302	PGV	O03-C19-C20	3.21	121.99	111.91
14	N	601[D]	HEA	C13-C12-C11	-3.20	109.53	114.35
14	N	601[C]	HEA	CAA-CBA-CGA	-3.20	104.79	113.76
14	N	601[D]	HEA	CAA-CBA-CGA	-3.20	104.79	113.76
25	P	302	PGV	C21-C20-C19	-3.19	102.01	113.62
26	P	304	CDL	C32-C31-CA7	-3.17	102.11	113.62
14	A	601[C]	HEA	CAA-CBA-CGA	-3.15	104.92	113.76
14	A	601[D]	HEA	CAA-CBA-CGA	-3.15	104.92	113.76
25	C	307	PGV	C01-O03-C19	3.15	128.77	117.12
14	A	601[D]	HEA	C13-C12-C11	-3.11	109.67	114.35
25	P	302	PGV	C01-O03-C19	3.10	128.59	117.12
23	B	603	PSC	O01-C02-C03	3.09	119.59	108.40
26	C	303	CDL	OA8-CA7-C31	3.03	121.41	111.91
25	N	610	PGV	O03-C19-C20	3.02	121.40	111.91
25	N	610	PGV	C4-C3-C2	-3.01	102.37	113.19
26	P	304	CDL	CA4-OA6-CA5	-3.01	110.38	117.79
25	C	307	PGV	O03-C19-O04	-2.96	116.11	123.59
23	O	603	PSC	C21-C20-C19	-2.93	102.98	113.62
19	N	608	TGL	OG1-CA1-CA2	2.92	121.07	111.91
26	T	101	CDL	OA8-CA7-C31	2.92	121.06	111.91
19	D	202	TGL	CG2-OG2-CB1	-2.92	110.61	117.79
23	O	603	PSC	C03-C02-C01	-2.91	104.91	111.79
14	A	602	HEA	CMB-C2B-C3B	-2.89	124.83	130.34
14	N	602	HEA	CMC-C2C-C3C	2.89	130.08	124.68
14	A	602	HEA	CMC-C2C-C1C	-2.88	124.03	128.46
14	N	602	HEA	C27-C19-C20	2.86	120.09	115.27
14	A	601[D]	HEA	C17-C18-C19	-2.84	120.81	127.66
19	D	202	TGL	OG2-CB1-CB2	2.84	117.63	111.50
22	P	305	CHD	C14-C8-C9	-2.82	105.85	109.71
19	A	607	TGL	CG2-OG2-CB1	-2.81	110.87	117.79
19	Q	201	TGL	OG1-CA1-CA2	2.80	120.71	111.91
14	A	602	HEA	CHA-C4D-C3D	-2.80	120.73	124.84
24	P	306	PEK	O12-P-O14	-2.79	98.17	109.07
14	A	602	HEA	C27-C19-C20	2.78	119.95	115.27
24	G	101	PEK	O01-C1-C2	2.78	117.48	111.50
14	N	602	HEA	CMC-C2C-C1C	-2.76	124.22	128.46
25	N	610	PGV	C03-C02-C01	-2.76	105.26	111.79
19	A	607	TGL	OG1-CA1-CA2	2.75	120.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601[C]	HEA	C27-C19-C20	2.71	119.83	115.27
22	C	304	CHD	C14-C13-C12	2.71	109.92	107.40
24	B	604	PEK	C01-O03-C21	2.71	127.14	117.12
14	N	602	HEA	C26-C15-C16	2.70	119.81	115.27
23	O	603	PSC	C3-C2-C1	-2.70	103.82	113.62
14	A	602	HEA	CMC-C2C-C3C	2.69	129.72	124.68
24	C	306	PEK	C01-O03-C21	2.69	127.09	117.12
22	P	305	CHD	C11-C9-C10	-2.69	110.96	113.73
14	N	602	HEA	CHA-C4D-C3D	-2.68	120.89	124.84
14	A	602	HEA	C13-C14-C15	-2.68	121.20	127.66
14	N	602	HEA	CAA-CBA-CGA	-2.68	106.25	113.76
14	N	602	HEA	C13-C14-C15	-2.67	121.24	127.66
14	A	601[C]	HEA	C3C-C4C-NC	2.66	112.66	109.21
14	A	601[D]	HEA	C3C-C4C-NC	2.66	112.66	109.21
14	A	602	HEA	C26-C15-C16	2.66	119.75	115.27
22	P	305	CHD	C1-C2-C3	2.66	113.88	110.47
14	N	602	HEA	CMB-C2B-C3B	-2.66	125.28	130.34
14	A	601[D]	HEA	C13-C14-C15	-2.65	121.27	127.66
20	A	608	J6X	C12-C11-C10	-2.65	122.06	129.06
14	A	602	HEA	CAA-CBA-CGA	-2.63	106.38	113.76
24	G	101	PEK	C02-O01-C1	-2.63	111.31	117.79
14	A	602	HEA	CAD-CBD-CGD	-2.63	107.95	113.60
25	C	302	PGV	C01-O03-C19	2.62	126.83	117.12
25	P	302	PGV	O01-C02-C01	2.62	117.88	108.40
19	N	608	TGL	CG2-OG2-CB1	-2.62	111.35	117.79
14	N	601[C]	HEA	C3C-C4C-NC	2.62	112.59	109.21
14	N	601[D]	HEA	C3C-C4C-NC	2.62	112.59	109.21
24	B	604	PEK	O11-P-O14	-2.61	98.88	109.07
14	N	601[D]	HEA	C13-C14-C15	-2.60	121.40	127.66
14	N	601[C]	HEA	C13-C12-C11	-2.60	110.44	114.35
24	P	306	PEK	O01-C1-C2	2.59	117.08	111.50
27	Z	101	DMU	O1-C9-C8	2.59	114.39	109.69
26	G	102	CDL	CB6-CB4-CB3	-2.59	105.67	111.79
14	N	602	HEA	C3B-C4B-NB	2.58	112.90	109.84
14	N	601[D]	HEA	C17-C18-C19	-2.58	121.45	127.66
22	C	304	CHD	C21-C20-C17	-2.55	109.02	112.92
26	C	303	CDL	OB8-CB7-C71	2.55	119.89	111.91
25	C	302	PGV	O03-C19-O04	-2.54	117.18	123.59
27	W	101	DMU	C18-O16-C6	-2.54	109.63	113.84
22	C	304	CHD	C13-C14-C8	-2.54	111.50	114.74
14	N	601[C]	HEA	C27-C19-C20	2.54	119.54	115.27
22	P	305	CHD	C13-C14-C8	-2.53	111.50	114.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	PEK	O03-C21-O04	-2.52	117.23	123.59
19	D	202	TGL	OG1-CA1-CA2	2.52	119.82	111.91
26	P	304	CDL	OA8-CA7-OA9	-2.52	117.23	123.59
14	N	601[C]	HEA	C17-C18-C19	-2.51	121.61	127.66
26	P	304	CDL	C72-C71-CB7	-2.50	104.53	113.62
19	N	608	TGL	OG3-CC1-CC2	2.50	119.75	111.91
14	N	601[D]	HEA	C26-C15-C16	2.47	119.43	115.27
14	A	601[D]	HEA	C26-C15-C16	2.47	119.42	115.27
27	C	308	DMU	O5-C6-C1	-2.47	105.12	110.35
14	A	601[D]	HEA	C27-C19-C20	2.47	119.42	115.27
27	C	308	DMU	O16-C6-C1	2.47	112.15	108.30
26	T	101	CDL	CB6-CB4-CB3	-2.47	105.96	111.79
19	L	101	TGL	OG1-CA1-CA2	2.46	119.64	111.91
24	C	309	PEK	C2-C3-C4	-2.46	108.83	113.23
14	N	601[C]	HEA	C13-C14-C15	-2.46	121.75	127.66
22	C	304	CHD	C14-C8-C9	-2.45	106.35	109.71
26	P	304	CDL	OB8-CB6-CB4	2.44	115.54	108.43
14	N	602	HEA	C13-C12-C11	-2.42	110.71	114.35
23	B	603	PSC	C21-C20-C19	-2.42	104.83	113.62
19	Y	101	TGL	OG1-CA1-CA2	2.41	119.48	111.91
24	B	604	PEK	O01-C1-O02	-2.41	117.88	123.70
14	A	601[C]	HEA	CMC-C2C-C1C	-2.41	124.76	128.46
14	A	601[D]	HEA	CMC-C2C-C1C	-2.41	124.76	128.46
14	A	601[C]	HEA	C25-C23-C24	2.41	119.92	114.60
22	B	602	CHD	C13-C17-C20	-2.41	116.62	119.50
24	G	101	PEK	O03-C21-O04	-2.40	117.53	123.59
26	C	303	CDL	OA8-CA6-CA4	2.40	115.42	108.43
24	C	309	PEK	O03-C21-C22	2.39	119.42	111.91
19	A	607	TGL	OG3-CC1-CC2	2.38	119.37	111.91
24	P	306	PEK	O03-C21-O04	-2.37	117.60	123.59
19	Q	201	TGL	OG3-CC1-CC2	2.37	119.35	111.91
20	N	611	J6X	C12-C11-C10	-2.37	122.78	129.06
14	A	602	HEA	CBA-CAA-C2A	2.37	116.60	112.60
24	C	309	PEK	O03-C01-C02	2.37	115.33	108.43
24	C	306	PEK	O11-P-O14	-2.37	99.82	109.07
14	N	602	HEA	C3D-C4D-ND	2.37	112.65	110.36
26	G	102	CDL	OA8-CA7-C31	2.37	119.33	111.91
24	P	306	PEK	C02-O01-C1	-2.36	111.97	117.79
14	N	602	HEA	CAD-CBD-CGD	-2.36	108.52	113.60
14	A	602	HEA	C3C-C4C-NC	2.36	112.26	109.21
24	C	306	PEK	O13-P-O14	2.35	123.87	112.24
25	N	610	PGV	O14-P-O13	2.35	123.86	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	602	CHD	C13-C17-C20	-2.35	116.69	119.50
14	A	602	HEA	C25-C23-C24	2.35	119.79	114.60
14	N	602	HEA	C25-C23-C24	2.34	119.78	114.60
24	C	306	PEK	O03-C21-O04	-2.34	117.69	123.59
14	N	601[D]	HEA	C27-C19-C20	2.34	119.21	115.27
25	P	302	PGV	O01-C1-C2	2.33	116.52	111.50
22	C	304	CHD	C23-C22-C20	-2.33	110.27	114.52
14	N	601[C]	HEA	C25-C23-C24	2.31	119.72	114.60
26	G	102	CDL	OB6-CB5-OB7	-2.31	118.11	123.70
26	C	303	CDL	C21-C20-C19	-2.31	102.69	114.42
26	T	101	CDL	OB8-CB7-C71	2.31	119.16	111.91
26	P	304	CDL	OB8-CB7-OB9	-2.31	117.77	123.59
19	Y	101	TGL	OG2-CB1-OB1	-2.30	118.14	123.70
14	N	601[C]	HEA	CMC-C2C-C1C	-2.30	124.92	128.46
14	N	601[D]	HEA	CMC-C2C-C1C	-2.30	124.92	128.46
26	C	303	CDL	OB6-CB5-OB7	-2.30	118.14	123.70
14	A	601[C]	HEA	C17-C18-C19	-2.30	122.12	127.66
14	A	602	HEA	CMB-C2B-C1B	2.30	128.53	125.04
14	A	602	HEA	C3B-C4B-NB	2.30	112.56	109.84
14	N	601[D]	HEA	C25-C23-C24	2.29	119.67	114.60
26	C	303	CDL	OA8-CA7-OA9	-2.29	117.81	123.59
26	G	102	CDL	OB8-CB7-C71	2.29	119.09	111.91
26	C	303	CDL	OA6-CA4-CA3	2.29	116.69	108.40
14	A	602	HEA	C3D-C4D-ND	2.29	112.57	110.36
26	G	102	CDL	OA6-CA5-OA7	-2.29	118.18	123.70
25	N	610	PGV	O03-C19-O04	-2.28	117.83	123.59
26	C	303	CDL	OB6-CB4-CB3	2.27	116.63	108.40
14	A	601[D]	HEA	C25-C23-C24	2.26	119.61	114.60
25	P	302	PGV	O14-P-O13	2.26	123.42	112.24
25	C	307	PGV	C21-C20-C19	-2.25	105.43	113.62
19	Q	201	TGL	OG2-CB1-OB1	-2.25	118.27	123.70
19	Y	101	TGL	OG3-CC1-CC2	2.24	118.93	111.91
22	P	305	CHD	C10-C9-C8	2.23	114.21	111.82
14	N	601[C]	HEA	C16-C17-C18	-2.21	104.60	111.88
26	T	101	CDL	OB6-CB5-OB7	-2.21	118.36	123.70
27	M	101	DMU	C18-O16-C6	-2.21	110.18	113.84
25	P	303	PGV	C01-O03-C19	2.19	125.24	117.12
25	C	307	PGV	O14-P-O13	2.18	123.03	112.24
19	D	202	TGL	CC3-CC2-CC1	-2.18	105.69	113.62
14	N	602	HEA	C3C-C4C-NC	2.17	112.02	109.21
22	C	304	CHD	C11-C9-C10	-2.17	111.49	113.73
14	A	602	HEA	C13-C12-C11	-2.16	111.10	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CHD	C17-C13-C14	2.16	102.27	100.09
24	C	306	PEK	C02-O01-C1	-2.14	112.52	117.79
23	B	603	PSC	O13-P-O14	2.14	122.81	112.24
24	G	101	PEK	O12-P-O14	-2.13	100.74	109.07
26	C	303	CDL	OB8-CB7-OB9	-2.13	118.22	123.59
25	P	302	PGV	O01-C02-C03	-2.12	100.72	108.40
24	B	604	PEK	P-O11-C03	2.10	133.99	121.68
19	L	101	TGL	CC3-CC2-CC1	-2.10	105.99	113.62
14	A	602	HEA	CHA-C4D-ND	2.09	126.70	124.43
22	B	602	CHD	C13-C14-C8	-2.09	112.07	114.74
26	P	304	CDL	OB6-CB5-OB7	-2.09	118.65	123.70
26	G	102	CDL	C42-C41-C40	2.09	125.02	114.42
25	N	610	PGV	O03-C01-C02	2.09	114.50	108.43
26	T	101	CDL	OA4-PA1-OA3	2.08	122.52	112.24
22	C	304	CHD	C4-C3-C2	-2.08	108.07	110.55
26	T	101	CDL	OA6-CA5-OA7	-2.07	118.70	123.70
25	P	302	PGV	O03-C01-C02	-2.06	102.44	108.43
19	A	607	TGL	OG2-CB1-OB1	-2.06	118.73	123.70
23	B	603	PSC	O01-C1-O02	-2.06	118.73	123.70
25	N	610	PGV	C21-C20-C19	-2.05	106.16	113.62
24	C	309	PEK	C03-C02-C01	-2.05	106.95	111.79
24	C	306	PEK	C2-C3-C4	-2.04	109.60	113.23
19	N	608	TGL	OG2-CB1-OB1	-2.03	118.79	123.70
24	C	306	PEK	C23-C22-C21	-2.03	106.23	113.62
14	N	601[C]	HEA	CHB-C1B-C2B	-2.03	121.81	124.98
14	N	601[D]	HEA	CHB-C1B-C2B	-2.03	121.81	124.98
14	A	601[C]	HEA	CHA-C4D-C3D	-2.03	121.86	124.84
14	A	601[D]	HEA	CHA-C4D-C3D	-2.03	121.86	124.84
22	P	305	CHD	C9-C10-C5	2.03	111.43	108.58
25	P	303	PGV	C02-O01-C1	-2.02	112.81	117.79
22	O	602	CHD	C17-C13-C14	2.02	102.13	100.09
14	N	601[C]	HEA	C27-C19-C18	-2.01	118.53	123.68
19	L	101	TGL	OG3-CC1-CC2	2.00	118.19	111.91
14	N	602	HEA	CMB-C2B-C1B	2.00	128.09	125.04
14	A	602	HEA	C2D-C1D-ND	2.00	112.21	109.84
22	B	602	CHD	C23-C22-C20	-2.00	110.86	114.52

There are no chirality outliers.

All (747) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	601[C]	HEA	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
14	N	602	HEA	C2D-C3D-CAD-CBD
14	N	602	HEA	C4D-C3D-CAD-CBD
19	L	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	CB2-CB1-OG2-CG2
23	B	603	PSC	C03-O11-P-O13
23	B	603	PSC	C04-O12-P-O11
23	B	603	PSC	O12-C04-C05-N
23	B	603	PSC	O02-C1-O01-C02
23	B	603	PSC	C2-C1-O01-C02
23	O	603	PSC	C04-O12-P-O13
23	O	603	PSC	O02-C1-O01-C02
24	B	604	PEK	C04-O12-P-O13
24	B	604	PEK	C04-O12-P-O14
24	B	604	PEK	O12-C04-C05-N
24	B	604	PEK	C2-C1-O01-C02
24	B	604	PEK	O04-C21-O03-C01
24	B	604	PEK	C22-C21-O03-C01
24	B	604	PEK	C13-C14-C15-C16
24	C	306	PEK	C04-O12-P-O14
24	C	306	PEK	O04-C21-O03-C01
24	C	306	PEK	C22-C21-O03-C01
24	C	309	PEK	O04-C21-O03-C01
24	C	309	PEK	C22-C21-O03-C01
24	P	301	PEK	C03-O11-P-O12
24	P	301	PEK	C03-O11-P-O13
24	P	301	PEK	O12-C04-C05-N
24	P	301	PEK	O04-C21-O03-C01
24	P	301	PEK	C22-C21-O03-C01
24	P	306	PEK	C03-O11-P-O13
24	P	306	PEK	C04-O12-P-O13
24	P	306	PEK	C04-O12-P-O14
24	P	306	PEK	O12-C04-C05-N
24	P	306	PEK	O04-C21-O03-C01
24	P	306	PEK	C22-C21-O03-C01
25	C	302	PGV	C04-O12-P-O13
25	C	302	PGV	C04-O12-P-O14
25	C	302	PGV	C10-C11-C12-C13
25	C	307	PGV	C03-O11-P-O13
25	C	307	PGV	C04-O12-P-O11
25	C	307	PGV	C04-O12-P-O13
25	C	307	PGV	C04-O12-P-O14
25	C	307	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
25	C	307	PGV	O04-C19-O03-C01
25	C	307	PGV	C20-C19-O03-C01
25	D	201	PGV	C04-C05-C06-O06
25	D	201	PGV	C2-C1-O01-C02
25	D	201	PGV	O04-C19-O03-C01
25	D	201	PGV	C20-C19-O03-C01
25	N	610	PGV	C04-O12-P-O13
25	N	610	PGV	O03-C01-C02-O01
25	P	302	PGV	C04-O12-P-O14
25	P	303	PGV	C04-O12-P-O14
26	C	303	CDL	OA6-CA4-CA6-OA8
26	C	303	CDL	C11-CA5-OA6-CA4
26	C	303	CDL	CB2-OB2-PB2-OB3
26	C	303	CDL	CB2-OB2-PB2-OB4
26	C	303	CDL	CB3-OB5-PB2-OB3
26	C	303	CDL	CB3-OB5-PB2-OB4
26	G	102	CDL	CA2-OA2-PA1-OA3
26	G	102	CDL	CA2-OA2-PA1-OA4
26	G	102	CDL	CA2-OA2-PA1-OA5
26	G	102	CDL	CB2-OB2-PB2-OB4
26	G	102	CDL	CB3-OB5-PB2-OB4
26	P	304	CDL	CA2-OA2-PA1-OA3
26	P	304	CDL	CB2-OB2-PB2-OB3
26	P	304	CDL	CB2-OB2-PB2-OB5
26	P	304	CDL	CB3-OB5-PB2-OB3
26	P	304	CDL	C51-CB5-OB6-CB4
26	T	101	CDL	CA2-OA2-PA1-OA3
26	T	101	CDL	CA3-OA5-PA1-OA3
26	T	101	CDL	OA9-CA7-OA8-CA6
26	T	101	CDL	C31-CA7-OA8-CA6
26	T	101	CDL	CB2-OB2-PB2-OB4
26	T	101	CDL	CB3-OB5-PB2-OB4
26	T	101	CDL	OB6-CB4-CB6-OB8
25	P	302	PGV	O04-C19-O03-C01
26	G	102	CDL	OA9-CA7-OA8-CA6
25	P	302	PGV	C20-C19-O03-C01
26	C	303	CDL	C31-CA7-OA8-CA6
26	G	102	CDL	C31-CA7-OA8-CA6
25	P	303	PGV	O04-C19-O03-C01
26	C	303	CDL	OA9-CA7-OA8-CA6
19	L	101	TGL	OB1-CB1-OG2-CG2
19	Y	101	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
24	B	604	PEK	O02-C1-O01-C02
25	D	201	PGV	O02-C1-O01-C02
26	C	303	CDL	OA7-CA5-OA6-CA4
26	P	304	CDL	OB7-CB5-OB6-CB4
26	T	101	CDL	OA7-CA5-OA6-CA4
23	O	603	PSC	C2-C1-O01-C02
26	P	304	CDL	OA9-CA7-OA8-CA6
22	C	304	CHD	C16-C17-C20-C21
22	C	304	CHD	C13-C17-C20-C21
22	C	304	CHD	C16-C17-C20-C22
22	C	304	CHD	C13-C17-C20-C22
22	C	304	CHD	C20-C22-C23-C24
25	D	201	PGV	C13-C14-C15-C16
26	T	101	CDL	C60-C61-C62-C63
19	Q	201	TGL	CC2-CC1-OG3-CG3
24	G	101	PEK	C22-C21-O03-C01
24	P	306	PEK	C13-C14-C15-C16
24	P	301	PEK	C27-C28-C29-C30
19	Q	201	TGL	OC1-CC1-OG3-CG3
24	G	101	PEK	O04-C21-O03-C01
23	O	603	PSC	C04-C05-N-C06
24	P	301	PEK	C30-C31-C32-C33
25	P	303	PGV	C20-C19-O03-C01
26	P	304	CDL	C71-CB7-OB8-CB6
26	P	304	CDL	OB9-CB7-OB8-CB6
27	W	101	DMU	O6-C11-C9-O1
24	P	301	PEK	C2-C1-O01-C02
26	P	304	CDL	C11-CA5-OA6-CA4
26	T	101	CDL	C11-CA5-OA6-CA4
19	N	608	TGL	C23-C24-C25-C26
24	P	301	PEK	C34-C35-C36-C37
26	P	304	CDL	C37-C38-C39-C40
26	P	304	CDL	C40-C41-C42-C43
26	T	101	CDL	C80-C81-C82-C83
24	P	301	PEK	C23-C24-C25-C26
26	P	304	CDL	C80-C81-C82-C83
26	P	304	CDL	C31-CA7-OA8-CA6
24	P	301	PEK	O02-C1-O01-C02
26	P	304	CDL	OA7-CA5-OA6-CA4
14	N	601[D]	HEA	C26-C15-C16-C17
23	O	603	PSC	O04-C19-O03-C01
26	C	303	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	O	603	PSC	C20-C19-O03-C01
24	B	604	PEK	C10-C11-C12-C13
25	C	301	PGV	C26-C27-C28-C29
19	Q	201	TGL	CB9-C10-C11-C12
25	C	302	PGV	O12-C04-C05-C06
25	P	303	PGV	O12-C04-C05-C06
26	C	303	CDL	CB2-C1-CA2-OA2
25	D	201	PGV	C24-C25-C26-C27
19	D	202	TGL	CC2-CC1-OG3-CG3
19	L	101	TGL	C20-C21-C22-C23
26	C	303	CDL	O1-C1-CA2-OA2
24	P	301	PEK	C1-C2-C3-C4
27	C	308	DMU	C1-C6-O16-C18
26	G	102	CDL	OB6-CB4-CB6-OB8
23	O	603	PSC	C24-C25-C26-C27
19	A	607	TGL	CB1-CB2-CB3-CB4
25	C	302	PGV	C20-C19-O03-C01
23	B	603	PSC	C11-C10-C9-C8
23	B	603	PSC	C20-C21-C22-C23
26	T	101	CDL	C40-C41-C42-C43
25	D	201	PGV	O05-C05-C06-O06
25	C	302	PGV	O04-C19-O03-C01
19	Y	101	TGL	CC1-CC2-CC3-CC4
25	D	201	PGV	C19-C20-C21-C22
19	D	202	TGL	CB1-CB2-CB3-CB4
19	Q	201	TGL	CB1-CB2-CB3-CB4
25	N	607	PGV	C26-C27-C28-C29
19	D	202	TGL	OC1-CC1-OG3-CG3
26	P	304	CDL	CB7-C71-C72-C73
25	N	610	PGV	O12-C04-C05-O05
26	G	102	CDL	C80-C81-C82-C83
25	N	607	PGV	C19-C20-C21-C22
22	P	305	CHD	C17-C20-C22-C23
25	C	301	PGV	C4-C5-C6-C7
25	N	610	PGV	O04-C19-O03-C01
23	B	603	PSC	C03-O11-P-O12
23	O	603	PSC	C04-O12-P-O11
24	B	604	PEK	C04-O12-P-O11
24	P	301	PEK	C04-O12-P-O11
24	P	306	PEK	C03-O11-P-O12
24	P	306	PEK	C04-O12-P-O11
25	C	302	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
25	N	610	PGV	C04-O12-P-O11
25	P	302	PGV	C04-O12-P-O11
25	P	303	PGV	C04-O12-P-O11
26	C	303	CDL	CA2-OA2-PA1-OA5
26	C	303	CDL	CA3-OA5-PA1-OA2
26	C	303	CDL	CB2-OB2-PB2-OB5
26	C	303	CDL	CB3-OB5-PB2-OB2
26	G	102	CDL	CB2-OB2-PB2-OB5
26	G	102	CDL	CB3-OB5-PB2-OB2
26	P	304	CDL	CA2-OA2-PA1-OA5
26	T	101	CDL	CB2-OB2-PB2-OB5
26	T	101	CDL	CB3-OB5-PB2-OB2
19	A	607	TGL	CC2-CC1-OG3-CG3
27	W	101	DMU	O16-C18-C19-C22
25	D	201	PGV	C1-C2-C3-C4
24	C	309	PEK	O02-C1-O01-C02
25	N	610	PGV	C20-C19-O03-C01
27	W	101	DMU	O6-C11-C9-C8
24	C	309	PEK	C28-C29-C30-C31
26	P	304	CDL	C77-C78-C79-C80
19	N	608	TGL	CB2-CB1-OG2-CG2
24	C	309	PEK	C2-C1-O01-C02
26	C	303	CDL	C51-CB5-OB6-CB4
19	D	202	TGL	CA3-CA4-CA5-CA6
19	L	101	TGL	C21-C22-C23-C24
19	N	608	TGL	CA6-CA7-CA8-CA9
19	Q	201	TGL	CA4-CA5-CA6-CA7
19	Q	201	TGL	C11-C10-CB9-CB8
19	Y	101	TGL	CB9-C10-C11-C12
25	N	607	PGV	C29-C30-C31-C32
26	G	102	CDL	C13-C14-C15-C16
26	G	102	CDL	C20-C21-C22-C23
19	Q	201	TGL	C23-C24-C25-C26
19	Y	101	TGL	CG1-CG2-OG2-CB1
25	P	302	PGV	C01-C02-O01-C1
19	N	608	TGL	OB1-CB1-OG2-CG2
26	C	303	CDL	OB7-CB5-OB6-CB4
19	N	608	TGL	CC7-CC8-CC9-C15
19	N	608	TGL	C21-C22-C23-C24
19	Y	101	TGL	CC2-CC3-CC4-CC5
19	Y	101	TGL	C15-C16-C17-C18
24	C	309	PEK	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	C	309	PEK	C10-C11-C12-C13
24	P	301	PEK	C7-C8-C9-C10
19	A	607	TGL	C10-C11-C12-C13
19	L	101	TGL	CC2-CC3-CC4-CC5
19	N	608	TGL	CA4-CA5-CA6-CA7
19	Q	201	TGL	CA7-CA8-CA9-C20
19	Q	201	TGL	CA9-C20-C21-C22
25	C	301	PGV	C29-C30-C31-C32
25	C	302	PGV	O12-C04-C05-O05
19	L	101	TGL	CC6-CC7-CC8-CC9
26	G	102	CDL	C60-C61-C62-C63
22	P	305	CHD	C21-C20-C22-C23
25	C	301	PGV	C19-C20-C21-C22
19	L	101	TGL	CB5-CB6-CB7-CB8
24	P	301	PEK	C32-C33-C34-C35
26	G	102	CDL	C37-C38-C39-C40
26	T	101	CDL	C37-C38-C39-C40
14	A	601[C]	HEA	C26-C15-C16-C17
19	D	202	TGL	CC2-CC3-CC4-CC5
19	D	202	TGL	CA9-C20-C21-C22
24	C	309	PEK	C23-C24-C25-C26
26	C	303	CDL	C21-C22-C23-C24
19	D	202	TGL	CA7-CA8-CA9-C20
19	D	202	TGL	C15-C16-C17-C18
19	L	101	TGL	C16-C17-C18-C19
19	Q	201	TGL	C15-C16-C17-C18
23	O	603	PSC	C26-C27-C28-C29
26	C	303	CDL	C18-C19-C20-C21
26	C	303	CDL	C62-C63-C64-C65
26	G	102	CDL	C14-C15-C16-C17
19	A	607	TGL	CC7-CC8-CC9-C15
19	D	202	TGL	C16-C15-CC9-CC8
25	D	201	PGV	C22-C23-C24-C25
26	P	304	CDL	C60-C61-C62-C63
19	L	101	TGL	C14-C29-C30-C31
19	Q	201	TGL	CC3-CC4-CC5-CC6
26	C	303	CDL	C20-C21-C22-C23
26	C	303	CDL	C80-C81-C82-C83
19	Q	201	TGL	C16-C15-CC9-CC8
19	Q	201	TGL	C14-C29-C30-C31
19	Q	201	TGL	C19-C33-C34-C35
19	Y	101	TGL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	P	301	PEK	C28-C29-C30-C31
26	C	303	CDL	C16-C17-C18-C19
26	G	102	CDL	C42-C43-C44-C45
23	O	603	PSC	C04-C05-N-C07
23	O	603	PSC	C04-C05-N-C08
19	A	607	TGL	CA9-C20-C21-C22
19	Y	101	TGL	CC4-CC5-CC6-CC7
25	C	307	PGV	C21-C22-C23-C24
25	D	201	PGV	C7-C8-C9-C10
25	D	201	PGV	C27-C28-C29-C30
26	G	102	CDL	C11-C12-C13-C14
24	C	309	PEK	O12-C04-C05-N
23	B	603	PSC	C26-C27-C28-C29
23	O	603	PSC	C3-C4-C5-C6
26	P	304	CDL	C17-C18-C19-C20
23	B	603	PSC	C19-C20-C21-C22
19	N	608	TGL	C12-C13-C14-C29
19	Y	101	TGL	C21-C20-CA9-CA8
27	C	308	DMU	C19-C18-O16-C6
26	P	304	CDL	C20-C21-C22-C23
26	C	303	CDL	C57-C58-C59-C60
19	A	607	TGL	OC1-CC1-OG3-CG3
14	A	601[C]	HEA	C14-C15-C16-C17
14	N	601[D]	HEA	C14-C15-C16-C17
19	Q	201	TGL	CC2-CC3-CC4-CC5
25	P	302	PGV	C28-C29-C30-C31
19	L	101	TGL	CA5-CA6-CA7-CA8
19	Y	101	TGL	C17-C18-C19-C33
26	G	102	CDL	C17-C18-C19-C20
19	A	607	TGL	C21-C22-C23-C24
19	D	202	TGL	C20-C21-C22-C23
25	P	303	PGV	O12-C04-C05-O05
19	A	607	TGL	CA7-CA8-CA9-C20
19	D	202	TGL	CB4-CB5-CB6-CB7
25	N	610	PGV	O12-C04-C05-C06
19	D	202	TGL	C22-C23-C24-C25
25	C	302	PGV	C28-C29-C30-C31
26	T	101	CDL	C77-C78-C79-C80
27	W	101	DMU	C18-C19-C22-C25
19	D	202	TGL	CB9-C10-C11-C12
26	C	303	CDL	C37-C38-C39-C40
26	G	102	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
27	M	101	DMU	C19-C22-C25-C28
19	A	607	TGL	CB9-C10-C11-C12
25	D	201	PGV	C26-C27-C28-C29
26	P	304	CDL	C71-C72-C73-C74
19	Y	101	TGL	CA2-CA1-OG1-CG1
19	L	101	TGL	CC1-CC2-CC3-CC4
19	Y	101	TGL	CB7-CB8-CB9-C10
25	D	201	PGV	C15-C16-C17-C18
26	G	102	CDL	C41-C42-C43-C44
19	L	101	TGL	C10-C11-C12-C13
26	C	303	CDL	C40-C41-C42-C43
24	C	306	PEK	C4-C5-C6-C7
25	C	301	PGV	C11-C10-C9-C8
25	C	301	PGV	C12-C13-C14-C15
25	D	201	PGV	C12-C13-C14-C15
19	N	608	TGL	CC2-CC1-OG3-CG3
19	A	607	TGL	CA4-CA5-CA6-CA7
19	L	101	TGL	CA9-C20-C21-C22
23	O	603	PSC	C4-C5-C6-C7
25	D	201	PGV	C30-C31-C32-C33
26	P	304	CDL	C43-C44-C45-C46
26	T	101	CDL	C56-C57-C58-C59
25	C	301	PGV	C14-C15-C16-C17
23	B	603	PSC	C1-C2-C3-C4
24	C	306	PEK	C2-C1-O01-C02
25	N	610	PGV	C2-C1-O01-C02
26	G	102	CDL	OA5-CA3-CA4-OA6
26	T	101	CDL	OA5-CA3-CA4-OA6
25	N	610	PGV	O02-C1-O01-C02
19	N	608	TGL	OG1-CG1-CG2-OG2
25	P	303	PGV	O03-C01-C02-O01
19	Q	201	TGL	CB2-CB3-CB4-CB5
25	N	607	PGV	C12-C13-C14-C15
19	A	607	TGL	CC5-CC6-CC7-CC8
24	P	306	PEK	C7-C8-C9-C10
25	C	307	PGV	C10-C11-C12-C13
19	Y	101	TGL	OA1-CA1-OG1-CG1
24	C	306	PEK	O02-C1-O01-C02
19	A	607	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	CA4-CA5-CA6-CA7
19	Y	101	TGL	CA5-CA6-CA7-CA8
25	C	307	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
26	T	101	CDL	CA2-OA2-PA1-OA5
19	Q	201	TGL	CA5-CA6-CA7-CA8
19	N	608	TGL	CB7-CB8-CB9-C10
24	B	604	PEK	C01-C02-C03-O11
26	T	101	CDL	OA5-CA3-CA4-CA6
19	L	101	TGL	C12-C13-C14-C29
19	D	202	TGL	C10-C11-C12-C13
24	P	306	PEK	C2-C3-C4-C5
19	Y	101	TGL	CC2-CC1-OG3-CG3
19	Q	201	TGL	CC5-CC6-CC7-CC8
25	D	201	PGV	C21-C22-C23-C24
19	N	608	TGL	OG1-CG1-CG2-CG3
25	P	303	PGV	O03-C01-C02-C03
26	C	303	CDL	CA3-CA4-CA6-OA8
26	C	303	CDL	CB3-CB4-CB6-OB8
24	C	306	PEK	C13-C14-C15-C16
25	C	301	PGV	C10-C11-C12-C13
25	D	201	PGV	C10-C11-C12-C13
14	A	602	HEA	C4D-C3D-CAD-CBD
24	G	101	PEK	C31-C32-C33-C34
26	P	304	CDL	C62-C63-C64-C65
25	D	201	PGV	C31-C32-C33-C34
25	C	302	PGV	C12-C13-C14-C15
25	N	607	PGV	C11-C10-C9-C8
24	G	101	PEK	C1-C2-C3-C4
19	D	202	TGL	C19-C33-C34-C35
19	Y	101	TGL	CC7-CC8-CC9-C15
19	Y	101	TGL	C18-C19-C33-C34
25	P	302	PGV	C30-C31-C32-C33
19	Y	101	TGL	CB2-CB3-CB4-CB5
26	T	101	CDL	C24-C25-C26-C27
24	P	301	PEK	C24-C25-C26-C27
19	A	607	TGL	C23-C24-C25-C26
19	Y	101	TGL	CA2-CA3-CA4-CA5
23	B	603	PSC	C21-C22-C23-C24
19	N	608	TGL	CB5-CB6-CB7-CB8
25	D	201	PGV	O01-C02-C03-O11
24	P	301	PEK	C13-C14-C15-C16
23	B	603	PSC	C25-C26-C27-C28
19	D	202	TGL	CB5-CB6-CB7-CB8
19	A	607	TGL	CC6-CC7-CC8-CC9
26	C	303	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
24	P	301	PEK	O03-C01-C02-O01
26	T	101	CDL	OA6-CA4-CA6-OA8
19	A	607	TGL	OB1-CB1-OG2-CG2
19	N	608	TGL	OC1-CC1-OG3-CG3
19	N	608	TGL	CB4-CB5-CB6-CB7
25	C	301	PGV	O03-C19-C20-C21
19	Y	101	TGL	CB6-CB7-CB8-CB9
25	P	302	PGV	C2-C3-C4-C5
25	P	302	PGV	C6-C7-C8-C9
26	P	304	CDL	C22-C23-C24-C25
25	D	201	PGV	C29-C30-C31-C32
25	C	307	PGV	C04-C05-C06-O06
19	L	101	TGL	CA2-CA1-OG1-CG1
24	C	309	PEK	C13-C14-C15-C16
26	T	101	CDL	C58-C59-C60-C61
25	C	307	PGV	C01-C02-C03-O11
25	D	201	PGV	C01-C02-C03-O11
26	G	102	CDL	OA5-CA3-CA4-CA6
14	A	602	HEA	C2D-C3D-CAD-CBD
19	L	101	TGL	CA3-CA4-CA5-CA6
27	Z	101	DMU	C19-C22-C25-C28
25	N	607	PGV	O03-C19-C20-C21
19	D	202	TGL	C11-C12-C13-C14
19	Q	201	TGL	CB5-CB6-CB7-CB8
19	Q	201	TGL	CC7-CC8-CC9-C15
24	P	301	PEK	C25-C26-C27-C28
25	P	302	PGV	C14-C15-C16-C17
19	L	101	TGL	OG1-CG1-CG2-CG3
19	Y	101	TGL	OG1-CG1-CG2-CG3
23	B	603	PSC	O03-C01-C02-C03
24	G	101	PEK	O03-C01-C02-C03
25	C	307	PGV	O03-C01-C02-C03
25	P	302	PGV	O03-C01-C02-C03
26	G	102	CDL	CB3-CB4-CB6-OB8
26	T	101	CDL	CA3-CA4-CA6-OA8
24	G	101	PEK	C7-C8-C9-C10
24	P	306	PEK	C4-C5-C6-C7
25	P	303	PGV	C10-C11-C12-C13
19	Y	101	TGL	OC1-CC1-OG3-CG3
19	Y	101	TGL	C19-C33-C34-C35
19	D	202	TGL	CA2-CA3-CA4-CA5
27	M	101	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
26	P	304	CDL	C57-C58-C59-C60
23	B	603	PSC	C9-C10-C11-C12
23	B	603	PSC	C10-C11-C12-C13
23	O	603	PSC	C9-C10-C11-C12
23	O	603	PSC	C10-C11-C12-C13
24	B	604	PEK	C5-C6-C7-C8
24	B	604	PEK	C6-C7-C8-C9
24	B	604	PEK	C11-C10-C9-C8
24	B	604	PEK	C9-C10-C11-C12
24	B	604	PEK	C11-C12-C13-C14
24	B	604	PEK	C12-C13-C14-C15
24	C	306	PEK	C5-C6-C7-C8
24	C	306	PEK	C6-C7-C8-C9
24	C	306	PEK	C11-C10-C9-C8
24	C	306	PEK	C9-C10-C11-C12
24	C	306	PEK	C11-C12-C13-C14
24	C	306	PEK	C12-C13-C14-C15
24	C	309	PEK	C6-C7-C8-C9
24	C	309	PEK	C11-C10-C9-C8
24	C	309	PEK	C9-C10-C11-C12
24	C	309	PEK	C11-C12-C13-C14
24	C	309	PEK	C12-C13-C14-C15
24	G	101	PEK	C6-C7-C8-C9
24	G	101	PEK	C11-C10-C9-C8
24	P	301	PEK	C11-C10-C9-C8
24	P	301	PEK	C11-C12-C13-C14
24	P	301	PEK	C12-C13-C14-C15
24	P	306	PEK	C9-C10-C11-C12
26	C	303	CDL	OA5-CA3-CA4-OA6
26	G	102	CDL	C19-C20-C21-C22
26	T	101	CDL	C32-C33-C34-C35
25	P	303	PGV	C22-C23-C24-C25
19	Q	201	TGL	OG2-CG2-CG3-OG3
19	Y	101	TGL	OG2-CG2-CG3-OG3
25	C	307	PGV	O03-C01-C02-O01
19	D	202	TGL	C16-C17-C18-C19
27	C	308	DMU	O5-C6-O16-C18
25	N	607	PGV	C13-C14-C15-C16
26	G	102	CDL	OA7-CA5-OA6-CA4
25	C	307	PGV	C20-C21-C22-C23
19	L	101	TGL	OA1-CA1-OG1-CG1
24	P	306	PEK	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
25	D	201	PGV	C02-C03-O11-P
25	P	302	PGV	C02-C03-O11-P
26	G	102	CDL	CB4-CB3-OB5-PB2
26	P	304	CDL	C1-CA2-OA2-PA1
26	T	101	CDL	CB4-CB3-OB5-PB2
26	T	101	CDL	C20-C21-C22-C23
19	D	202	TGL	CC5-CC6-CC7-CC8
25	P	302	PGV	C3-C4-C5-C6
23	B	603	PSC	C01-C02-C03-O11
26	C	303	CDL	OA5-CA3-CA4-CA6
26	G	102	CDL	C40-C41-C42-C43
19	D	202	TGL	CC4-CC5-CC6-CC7
23	O	603	PSC	C29-C30-C31-C32
26	C	303	CDL	C52-C53-C54-C55
19	N	608	TGL	C24-C25-C26-C27
19	Y	101	TGL	CC6-CC7-CC8-CC9
19	N	608	TGL	C13-C14-C29-C30
25	D	201	PGV	C2-C3-C4-C5
26	G	102	CDL	C77-C78-C79-C80
19	A	607	TGL	C21-C20-CA9-CA8
23	O	603	PSC	C01-C02-O01-C1
14	A	601[C]	HEA	C27-C19-C20-C21
25	P	302	PGV	C1-C2-C3-C4
19	Q	201	TGL	CG1-CG2-CG3-OG3
24	B	604	PEK	O03-C01-C02-C03
24	P	301	PEK	O03-C01-C02-C03
25	C	302	PGV	C02-C03-O11-P
25	N	610	PGV	O03-C01-C02-C03
25	P	303	PGV	C02-C03-O11-P
26	T	101	CDL	CB3-CB4-CB6-OB8
19	Q	201	TGL	CB2-CB1-OG2-CG2
26	G	102	CDL	C11-CA5-OA6-CA4
23	O	603	PSC	O01-C02-C03-O11
19	Q	201	TGL	OG1-CA1-CA2-CA3
26	C	303	CDL	C36-C37-C38-C39
26	C	303	CDL	C41-C42-C43-C44
25	D	201	PGV	C25-C26-C27-C28
19	Y	101	TGL	OG1-CG1-CG2-OG2
26	C	303	CDL	OB6-CB4-CB6-OB8
23	O	603	PSC	C28-C29-C30-C31
25	P	303	PGV	C11-C10-C9-C8
14	A	601[D]	HEA	C26-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	Q	201	TGL	OB1-CB1-OG2-CG2
26	T	101	CDL	OB7-CB5-OB6-CB4
19	N	608	TGL	CB1-CB2-CB3-CB4
24	B	604	PEK	C4-C5-C6-C7
27	Z	101	DMU	C22-C25-C28-C31
19	L	101	TGL	CC5-CC6-CC7-CC8
19	N	608	TGL	CC3-CC4-CC5-CC6
26	P	304	CDL	CB3-OB5-PB2-OB2
19	A	607	TGL	CC1-CC2-CC3-CC4
26	C	303	CDL	C31-C32-C33-C34
23	B	603	PSC	C03-O11-P-O14
23	B	603	PSC	C04-O12-P-O13
24	P	301	PEK	C03-O11-P-O14
24	P	301	PEK	C04-O12-P-O13
24	P	306	PEK	C03-O11-P-O14
25	N	610	PGV	C04-O12-P-O14
25	P	303	PGV	C04-O12-P-O13
26	C	303	CDL	CA2-OA2-PA1-OA3
26	C	303	CDL	CA3-OA5-PA1-OA3
26	P	304	CDL	CA3-OA5-PA1-OA4
24	C	309	PEK	C01-C02-C03-O11
19	D	202	TGL	C18-C19-C33-C34
25	C	301	PGV	C7-C8-C9-C10
25	N	607	PGV	C14-C15-C16-C17
26	T	101	CDL	C79-C80-C81-C82
19	N	608	TGL	CA2-CA3-CA4-CA5
24	G	101	PEK	C4-C5-C6-C7
25	C	302	PGV	C19-C20-C21-C22
19	Y	101	TGL	C21-C22-C23-C24
23	O	603	PSC	C19-C20-C21-C22
27	Z	101	DMU	C28-C31-C34-C37
23	B	603	PSC	O01-C02-C03-O11
24	B	604	PEK	O01-C02-C03-O11
19	A	607	TGL	C20-C21-C22-C23
23	O	603	PSC	C20-C21-C22-C23
26	C	303	CDL	C73-C74-C75-C76
26	T	101	CDL	C51-CB5-OB6-CB4
19	Q	201	TGL	C21-C22-C23-C24
19	L	101	TGL	C24-C25-C26-C27
19	Y	101	TGL	CG1-CG2-CG3-OG3
23	O	603	PSC	O12-C04-C05-N
19	D	202	TGL	OG2-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	OG1-CG1-CG2-OG2
24	G	101	PEK	O03-C01-C02-O01
25	P	302	PGV	O03-C01-C02-O01
24	P	301	PEK	C10-C11-C12-C13
25	P	302	PGV	C10-C11-C12-C13
25	D	201	PGV	C05-C04-O12-P
19	Y	101	TGL	C11-C10-CB9-CB8
19	L	101	TGL	C11-C12-C13-C14
26	G	102	CDL	C62-C63-C64-C65
24	C	309	PEK	C1-C2-C3-C4
26	P	304	CDL	C52-C51-CB5-OB6
25	C	301	PGV	C15-C16-C17-C18
19	L	101	TGL	C21-C20-CA9-CA8
26	C	303	CDL	C38-C39-C40-C41
19	D	202	TGL	CC3-CC4-CC5-CC6
25	C	301	PGV	C31-C32-C33-C34
25	N	607	PGV	C15-C16-C17-C18
23	B	603	PSC	O03-C19-C20-C21
26	C	303	CDL	C1-CA2-OA2-PA1
26	T	101	CDL	C13-C14-C15-C16
25	C	307	PGV	C22-C23-C24-C25
26	C	303	CDL	C56-C57-C58-C59
23	O	603	PSC	C12-C13-C14-C15
25	C	307	PGV	C9-C10-C11-C12
24	C	309	PEK	C33-C34-C35-C36
24	C	306	PEK	C04-O12-P-O11
25	D	201	PGV	C04-O12-P-O11
25	N	610	PGV	C03-O11-P-O12
26	G	102	CDL	CA3-OA5-PA1-OA2
26	T	101	CDL	CA3-OA5-PA1-OA2
25	N	610	PGV	C11-C12-C13-C14
26	G	102	CDL	OB7-CB5-OB6-CB4
19	L	101	TGL	C23-C24-C25-C26
19	Y	101	TGL	CB3-CB4-CB5-CB6
26	T	101	CDL	C1-CB2-OB2-PB2
23	B	603	PSC	C12-C13-C14-C15
24	B	604	PEK	C14-C15-C16-C17
26	P	304	CDL	C38-C39-C40-C41
26	G	102	CDL	C31-C32-C33-C34
25	N	610	PGV	C10-C11-C12-C13
14	N	602	HEA	CAA-CBA-CGA-O1A
19	A	607	TGL	C11-C10-CB9-CB8

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Mol	Chain	Res	Type	Atoms
27	M	101	DMU	C28-C31-C34-C37
26	C	303	CDL	C83-C84-C85-C86
25	N	607	PGV	C30-C31-C32-C33
22	B	602	CHD	C22-C23-C24-O26
26	T	101	CDL	C75-C76-C77-C78
26	C	303	CDL	C58-C59-C60-C61
27	M	101	DMU	C34-C37-C40-C43
23	O	603	PSC	C22-C23-C24-C25
22	O	602	CHD	C22-C23-C24-O26
25	D	201	PGV	O03-C01-C02-O01
25	C	301	PGV	C11-C12-C13-C14
19	Y	101	TGL	C22-C23-C24-C25
22	B	602	CHD	C22-C23-C24-O25
25	N	610	PGV	C31-C32-C33-C34
26	G	102	CDL	C43-C44-C45-C46
19	Q	201	TGL	C29-C30-C31-C32
14	N	601[C]	HEA	CAA-CBA-CGA-O1A
14	N	601[D]	HEA	CAA-CBA-CGA-O1A
24	G	101	PEK	C13-C14-C15-C16
24	G	101	PEK	C16-C17-C18-C19
19	L	101	TGL	CG1-CG2-OG2-CB1
23	B	603	PSC	C03-C02-O01-C1
26	C	303	CDL	CA3-CA4-OA6-CA5
22	O	602	CHD	C22-C23-C24-O25
24	C	309	PEK	C5-C6-C7-C8
24	G	101	PEK	C03-O11-P-O12
24	G	101	PEK	C9-C10-C11-C12
24	P	306	PEK	C5-C6-C7-C8
24	P	306	PEK	C11-C10-C9-C8
24	P	306	PEK	C23-C24-C25-C26
19	D	202	TGL	OG3-CC1-CC2-CC3
14	A	602	HEA	CAA-CBA-CGA-O1A
14	A	602	HEA	CAD-CBD-CGD-O2D
19	L	101	TGL	CB6-CB7-CB8-CB9
14	A	602	HEA	CAD-CBD-CGD-O1D
25	C	307	PGV	C2-C3-C4-C5
14	N	602	HEA	CAA-CBA-CGA-O2A
19	Y	101	TGL	C11-C12-C13-C14
19	D	202	TGL	C21-C22-C23-C24
24	C	306	PEK	C29-C30-C31-C32
26	T	101	CDL	CA5-C11-C12-C13
24	G	101	PEK	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	N	607	PGV	C10-C11-C12-C13
19	N	608	TGL	C21-C20-CA9-CA8
14	A	602	HEA	CAA-CBA-CGA-O2A
19	Y	101	TGL	CA1-CA2-CA3-CA4
24	P	306	PEK	C26-C27-C28-C29
26	T	101	CDL	C72-C73-C74-C75
19	L	101	TGL	OG3-CC1-CC2-CC3
22	N	609	CHD	C22-C23-C24-O26
25	C	301	PGV	O04-C19-C20-C21
14	N	601[C]	HEA	CAD-CBD-CGD-O1D
14	N	601[D]	HEA	CAD-CBD-CGD-O1D
26	C	303	CDL	C60-C61-C62-C63
19	N	608	TGL	CC5-CC6-CC7-CC8
26	P	304	CDL	C41-C42-C43-C44
25	C	302	PGV	C9-C10-C11-C12
25	C	302	PGV	C11-C12-C13-C14
25	N	610	PGV	C9-C10-C11-C12
22	P	305	CHD	C22-C23-C24-O26
19	Y	101	TGL	CC5-CC6-CC7-CC8
26	C	303	CDL	C39-C40-C41-C42
25	P	302	PGV	C15-C16-C17-C18
25	N	607	PGV	O04-C19-C20-C21
14	A	601[C]	HEA	C18-C19-C20-C21
14	A	601[D]	HEA	C14-C15-C16-C17
23	O	603	PSC	O03-C19-C20-C21
19	D	202	TGL	C29-C30-C31-C32
23	O	603	PSC	C7-C8-C9-C10
24	C	306	PEK	C14-C15-C16-C17
22	C	304	CHD	C21-C20-C22-C23
24	G	101	PEK	O02-C1-O01-C02
23	B	603	PSC	C7-C8-C9-C10
25	P	303	PGV	C9-C10-C11-C12
19	D	202	TGL	CC7-CC8-CC9-C15
14	A	601[C]	HEA	CAD-CBD-CGD-O1D
14	A	601[D]	HEA	CAD-CBD-CGD-O1D
22	N	609	CHD	C22-C23-C24-O25
25	N	607	PGV	C23-C24-C25-C26
25	P	303	PGV	O03-C19-C20-C21
26	T	101	CDL	C32-C31-CA7-OA8
14	N	601[C]	HEA	C27-C19-C20-C21
14	N	602	HEA	CAD-CBD-CGD-O2D
24	B	604	PEK	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	G	102	CDL	C32-C31-CA7-OA8
23	B	603	PSC	O04-C19-O03-C01
24	P	301	PEK	C3-C4-C5-C6
24	P	306	PEK	C15-C16-C17-C18
23	O	603	PSC	O03-C01-C02-C03
25	D	201	PGV	O03-C01-C02-C03
22	N	609	CHD	C21-C20-C22-C23
26	P	304	CDL	OB5-CB3-CB4-OB6
19	N	608	TGL	OG1-CA1-CA2-CA3
25	D	201	PGV	O03-C19-C20-C21
14	N	602	HEA	CAD-CBD-CGD-O1D
26	G	102	CDL	C12-C13-C14-C15
26	C	303	CDL	C32-C31-CA7-OA8
24	C	306	PEK	C3-C4-C5-C6
25	N	607	PGV	C11-C12-C13-C14
19	L	101	TGL	C22-C23-C24-C25
27	Z	101	DMU	O16-C18-C19-C22
14	N	601[C]	HEA	CAA-CBA-CGA-O2A
14	N	601[D]	HEA	CAA-CBA-CGA-O2A
19	L	101	TGL	CA7-CA8-CA9-C20
26	T	101	CDL	C14-C15-C16-C17
19	A	607	TGL	OG1-CG1-CG2-OG2
14	A	601[C]	HEA	CAD-CBD-CGD-O2D
14	A	601[D]	HEA	CAD-CBD-CGD-O2D
22	C	305	CHD	C22-C23-C24-O25
19	N	608	TGL	C11-C12-C13-C14
14	N	601[C]	HEA	CAD-CBD-CGD-O2D
14	N	601[D]	HEA	CAD-CBD-CGD-O2D
22	P	305	CHD	C22-C23-C24-O25
19	Y	101	TGL	C16-C17-C18-C19
26	G	102	CDL	C1-CB2-OB2-PB2
25	N	610	PGV	C7-C8-C9-C10
26	P	304	CDL	C36-C37-C38-C39
24	B	604	PEK	C3-C4-C5-C6
24	C	309	PEK	C14-C15-C16-C17
26	G	102	CDL	C16-C17-C18-C19
23	B	603	PSC	C20-C19-O03-C01
26	G	102	CDL	C51-CB5-OB6-CB4
23	O	603	PSC	C5-C6-C7-C8
25	C	307	PGV	C11-C12-C13-C14
26	G	102	CDL	C32-C31-CA7-OA9
25	C	307	PGV	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
19	N	608	TGL	OA1-CA1-CA2-CA3
26	C	303	CDL	C32-C31-CA7-OA9
26	C	303	CDL	C72-C73-C74-C75
19	D	202	TGL	CG1-CG2-CG3-OG3
27	C	308	DMU	C22-C25-C28-C31
19	N	608	TGL	C19-C33-C34-C35
25	D	201	PGV	C04-O12-P-O13
25	N	610	PGV	C03-O11-P-O14
25	P	303	PGV	C1-C2-C3-C4
24	B	604	PEK	O02-C1-C2-C3
25	D	201	PGV	O04-C19-C20-C21
19	Q	201	TGL	OA1-CA1-CA2-CA3
22	C	304	CHD	C22-C23-C24-O25
26	P	304	CDL	C59-C60-C61-C62
19	Y	101	TGL	C12-C13-C14-C29
19	L	101	TGL	CG3-CG2-OG2-CB1
26	C	303	CDL	CA6-CA4-OA6-CA5
25	P	303	PGV	O04-C19-C20-C21
26	T	101	CDL	C32-C31-CA7-OA9
25	C	307	PGV	O05-C05-C06-O06
25	P	302	PGV	C23-C24-C25-C26
25	P	302	PGV	C9-C10-C11-C12
25	D	201	PGV	C6-C7-C8-C9
14	A	601[D]	HEA	C27-C19-C20-C21
14	A	602	HEA	C26-C15-C16-C17
19	L	101	TGL	CC7-CC8-CC9-C15
22	C	304	CHD	C22-C23-C24-O26
23	B	603	PSC	C04-C05-N-C08
25	C	301	PGV	C13-C14-C15-C16
23	B	603	PSC	C29-C30-C31-C32
24	C	309	PEK	C17-C18-C19-C20
25	C	307	PGV	C23-C24-C25-C26

There are no ring outliers.

38 monomers are involved in 168 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Q	201	TGL	2	0
20	N	611	J6X	1	0
25	C	301	PGV	3	0
25	N	610	PGV	3	0
22	O	602	CHD	1	0

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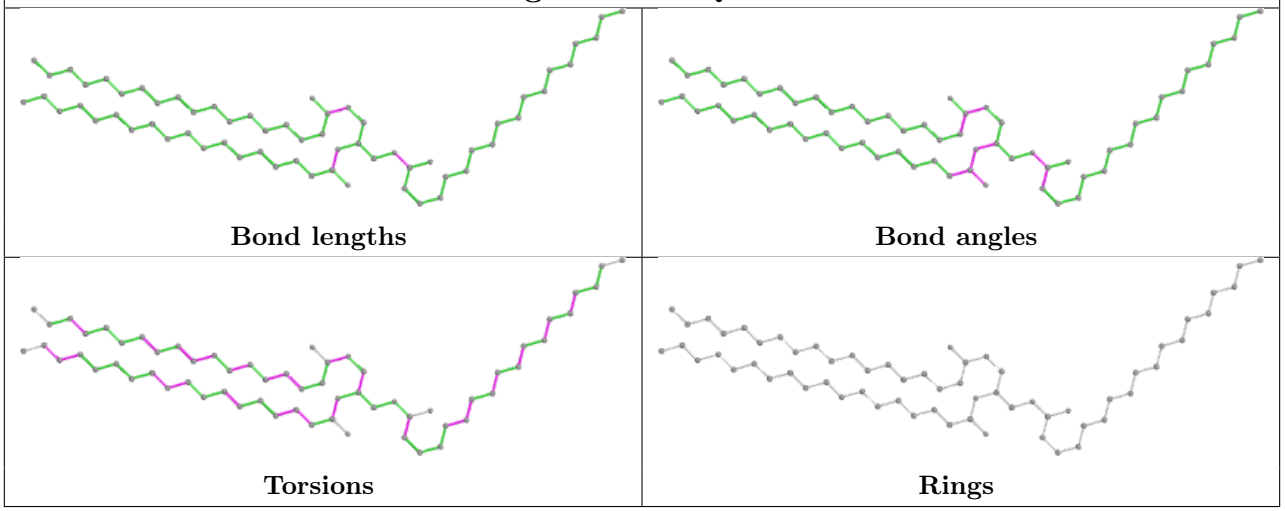
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	302	PGV	5	0
19	L	101	TGL	1	0
26	P	304	CDL	12	0
22	N	609	CHD	1	0
19	Y	101	TGL	7	0
14	N	601[C]	HEA	3	0
26	T	101	CDL	17	0
24	C	306	PEK	4	0
14	A	602	HEA	2	0
27	C	308	DMU	7	0
24	P	306	PEK	5	0
19	D	202	TGL	5	0
23	O	603	PSC	10	0
24	C	309	PEK	6	0
24	G	101	PEK	2	0
25	D	201	PGV	12	0
24	B	604	PEK	4	0
14	A	601[C]	HEA	3	0
26	G	102	CDL	11	0
14	N	602	HEA	8	0
25	P	302	PGV	2	0
25	N	607	PGV	1	0
24	P	301	PEK	1	0
22	C	304	CHD	1	0
14	N	601[D]	HEA	1	0
23	B	603	PSC	5	0
27	W	101	DMU	2	0
22	P	305	CHD	1	0
19	N	608	TGL	4	0
26	C	303	CDL	13	0
25	P	303	PGV	6	0
20	A	608	J6X	2	0
14	A	601[D]	HEA	1	0

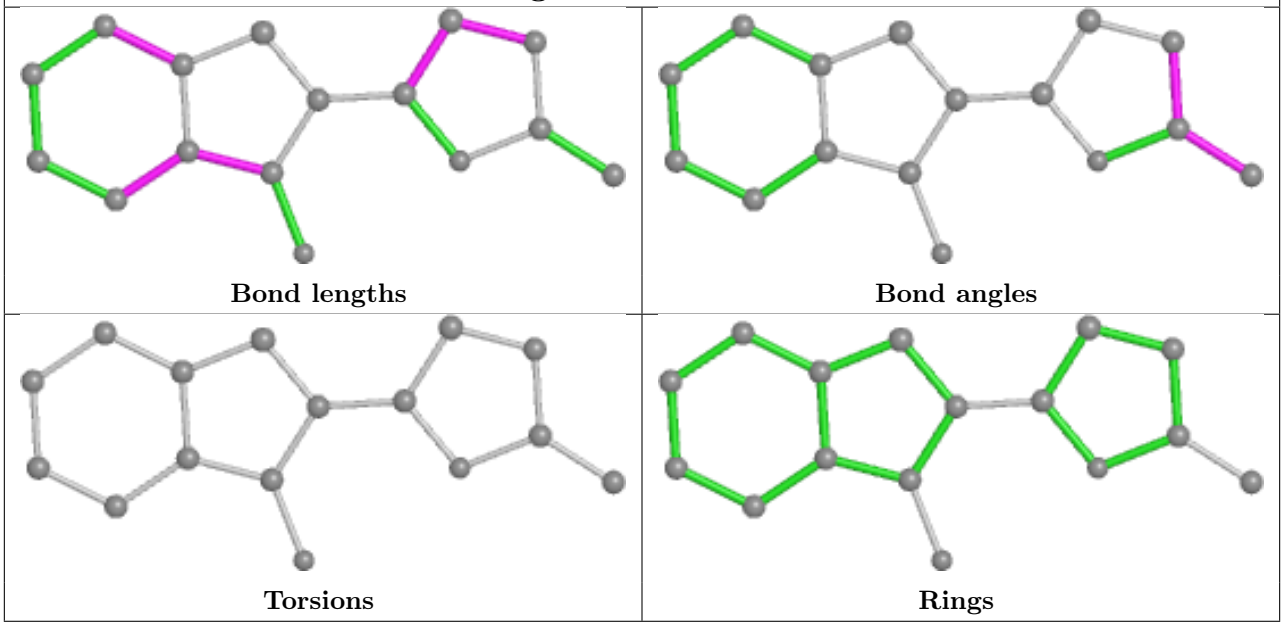
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

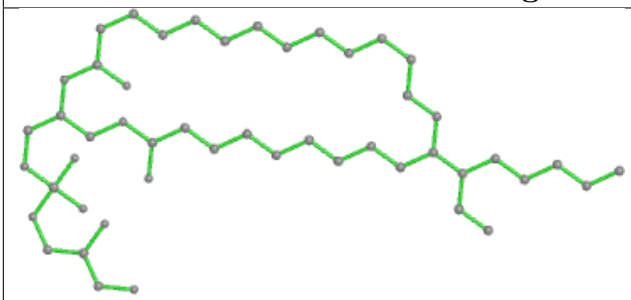
Ligand TGL Q 201



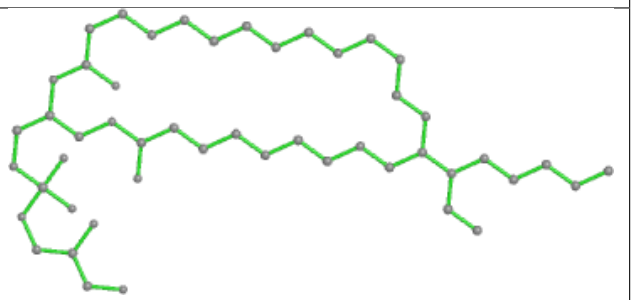
Ligand J6X N 611



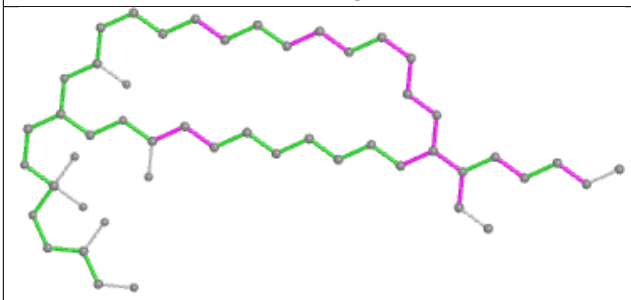
Ligand PGV C 301



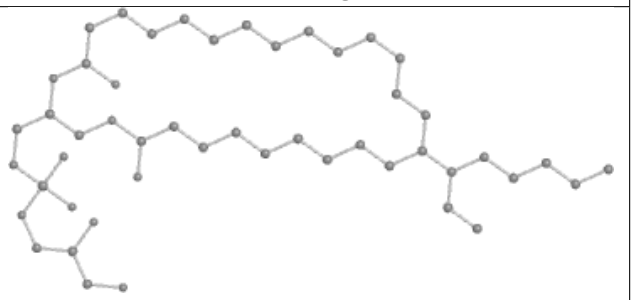
Bond lengths



Bond angles

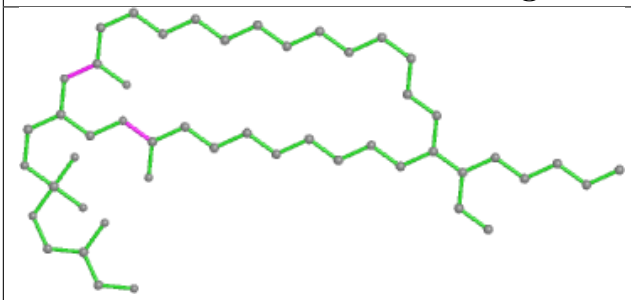


Torsions

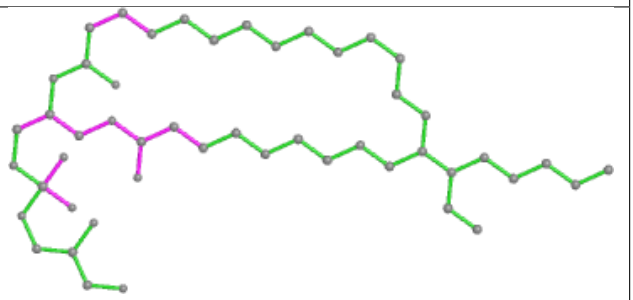


Rings

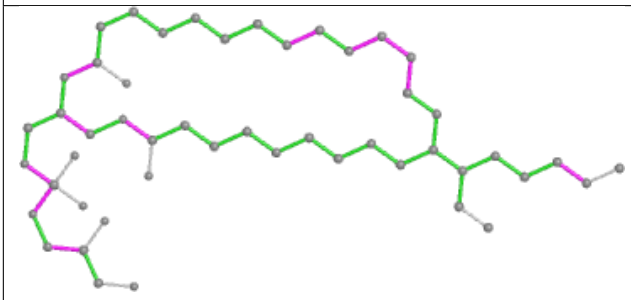
Ligand PGV N 610



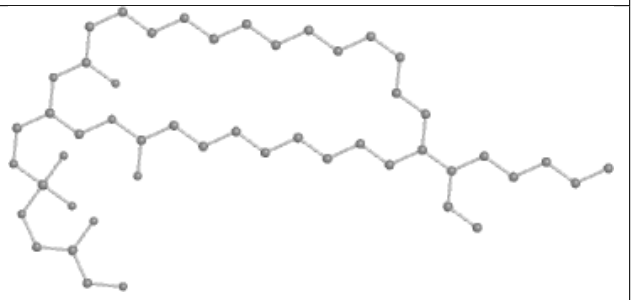
Bond lengths



Bond angles

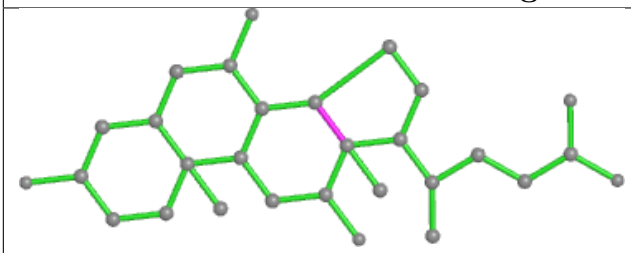


Torsions

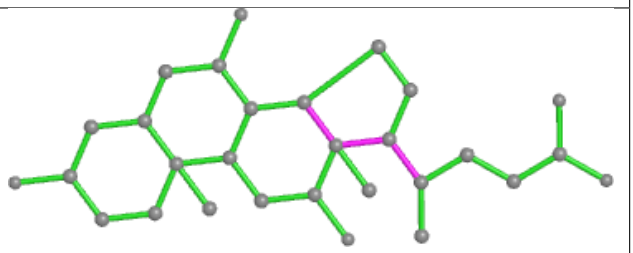


Rings

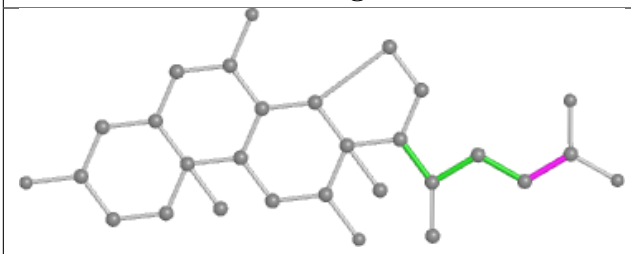
Ligand CHD O 602



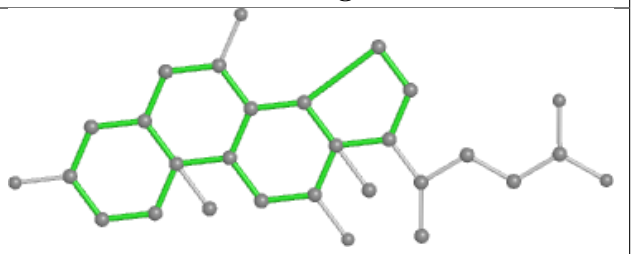
Bond lengths



Bond angles

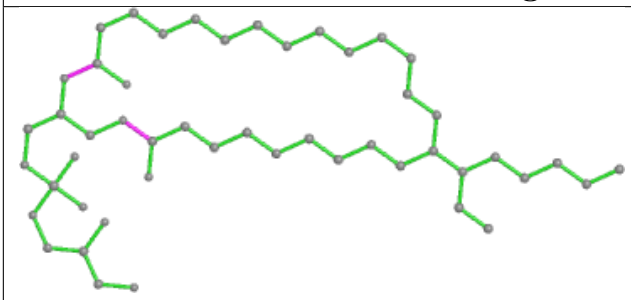


Torsions

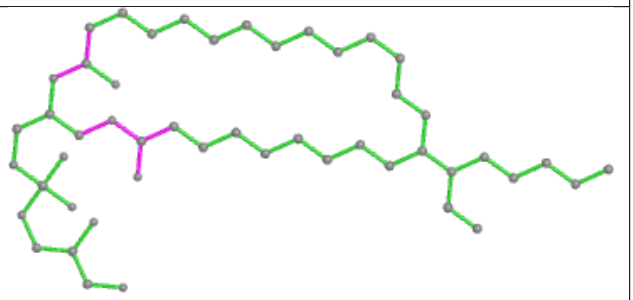


Rings

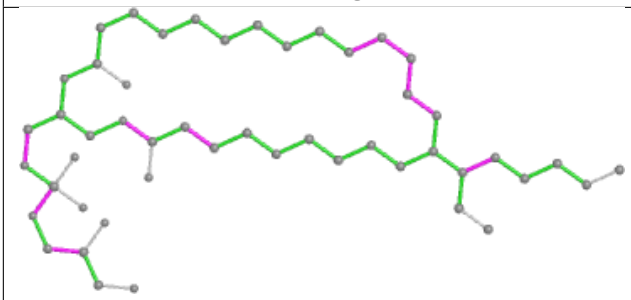
Ligand PGV C 302



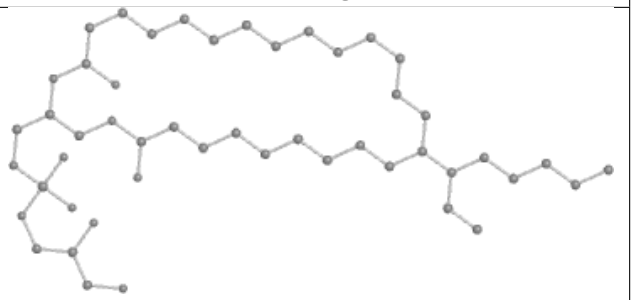
Bond lengths



Bond angles

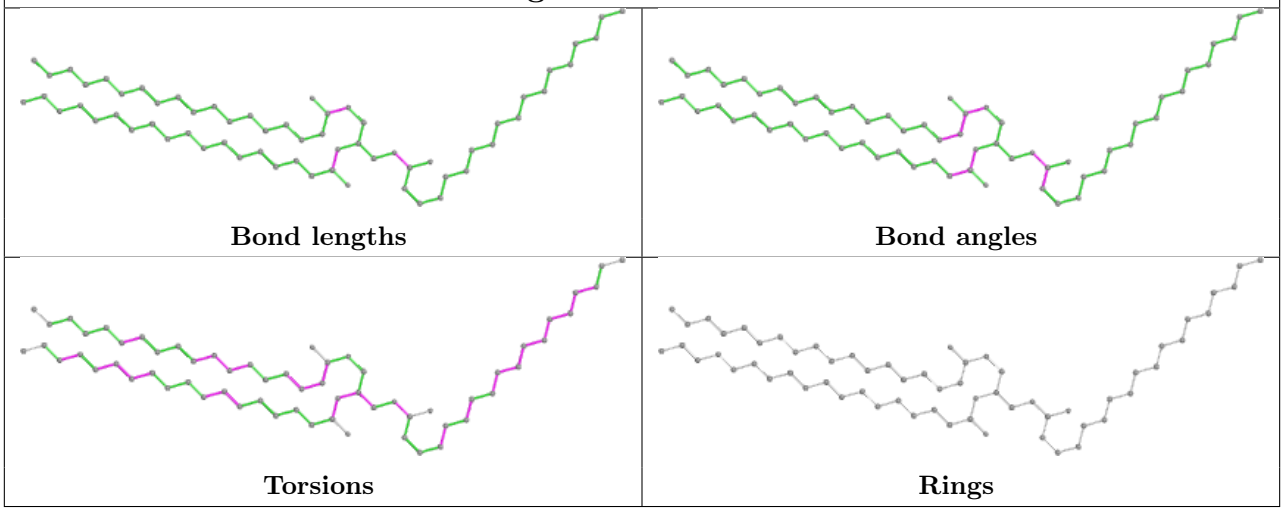


Torsions

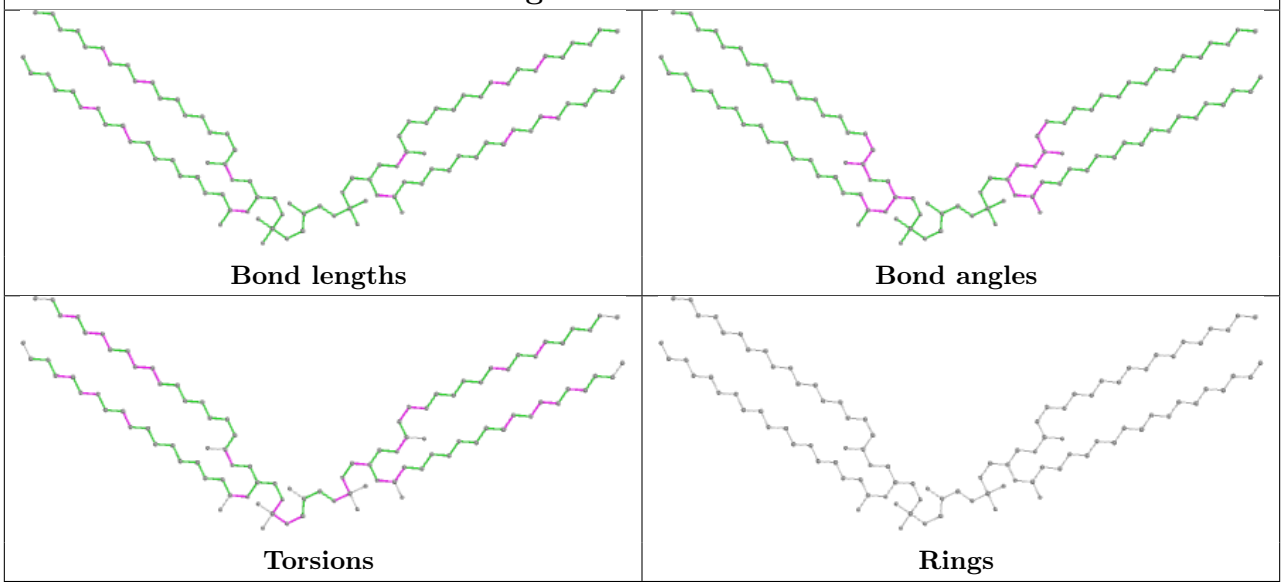


Rings

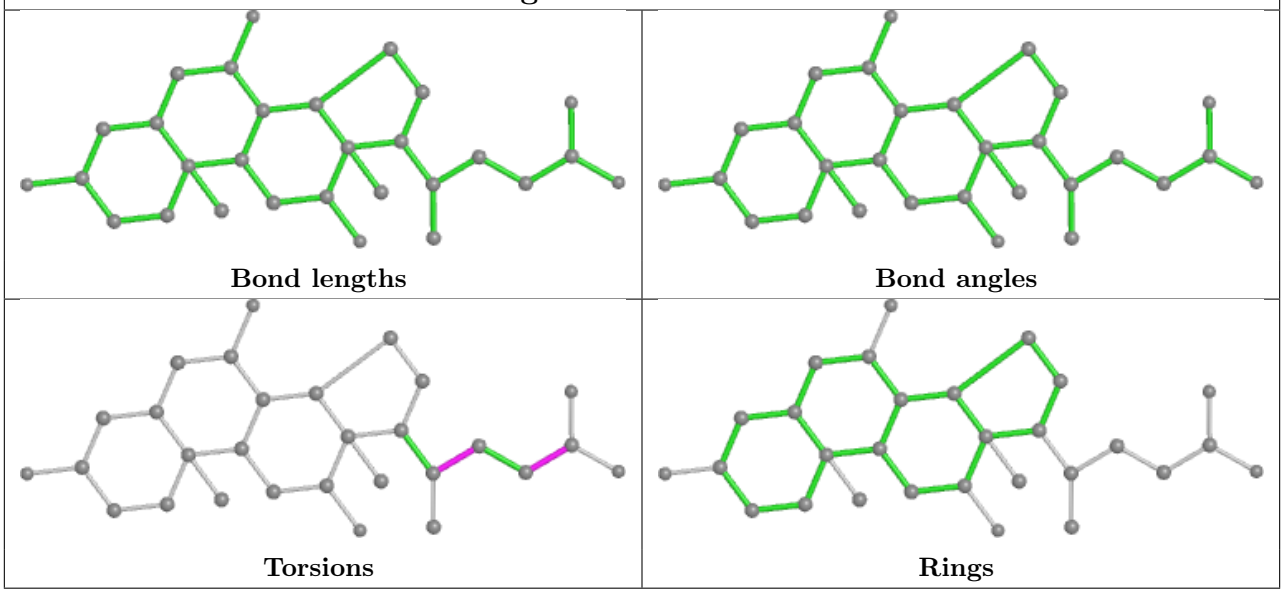
Ligand TGL L 101



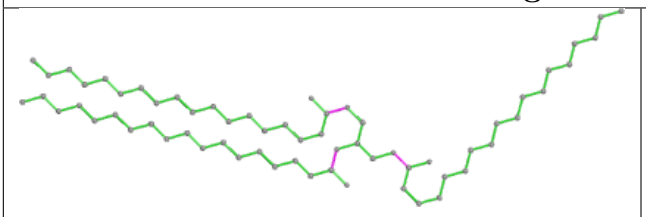
Ligand CDL P 304



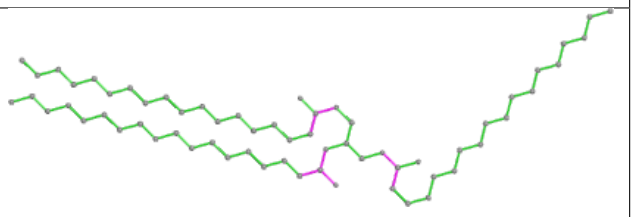
Ligand CHD N 609



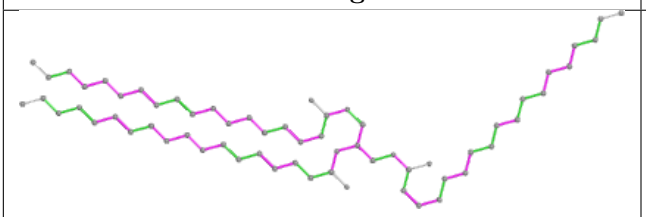
Ligand TGL Y 101



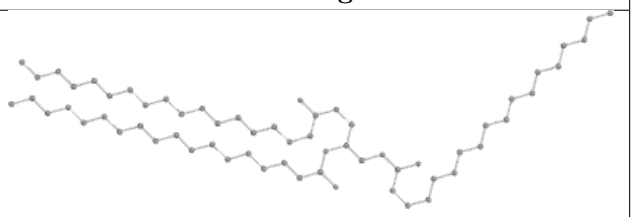
Bond lengths



Bond angles

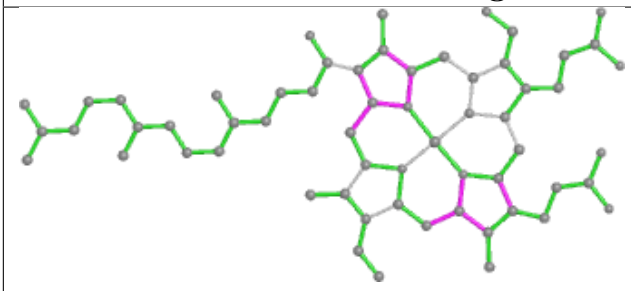


Torsions

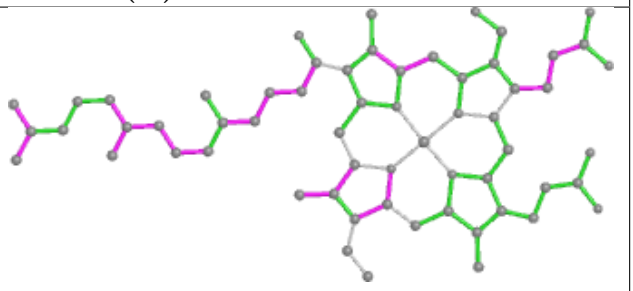


Rings

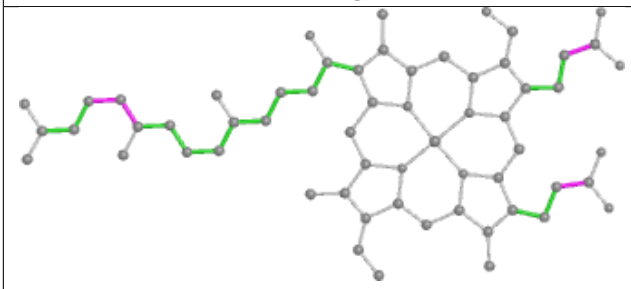
Ligand HEA N 601 (C)



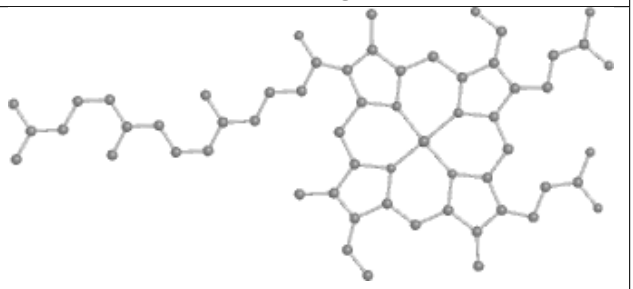
Bond lengths



Bond angles

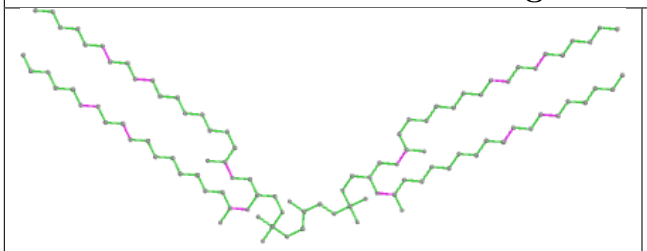


Torsions

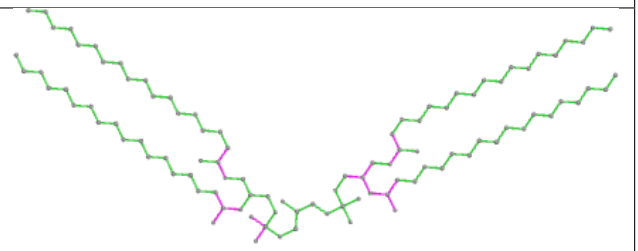


Rings

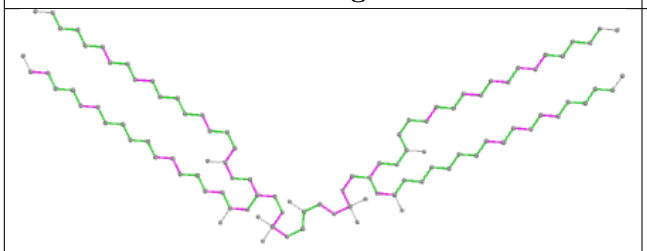
Ligand CDL T 101



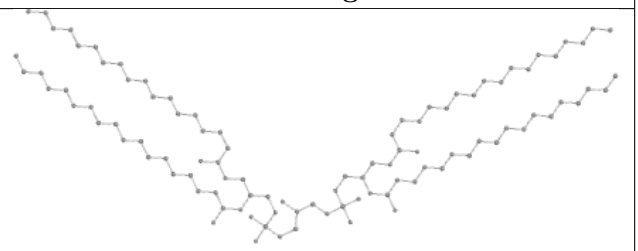
Bond lengths



Bond angles

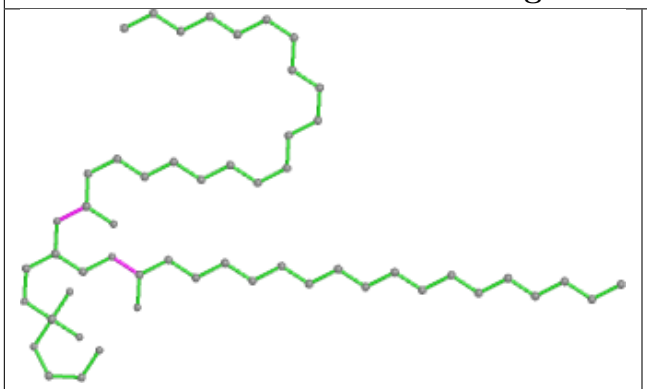


Torsions

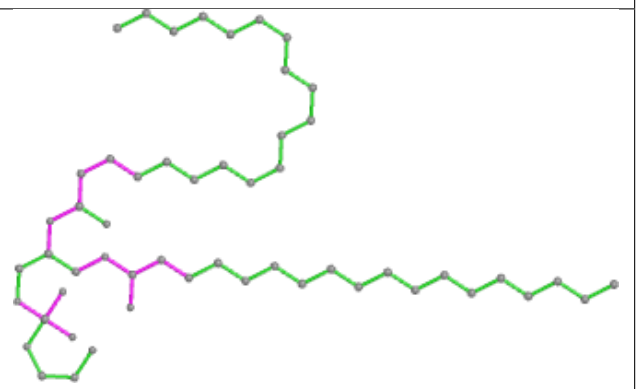


Rings

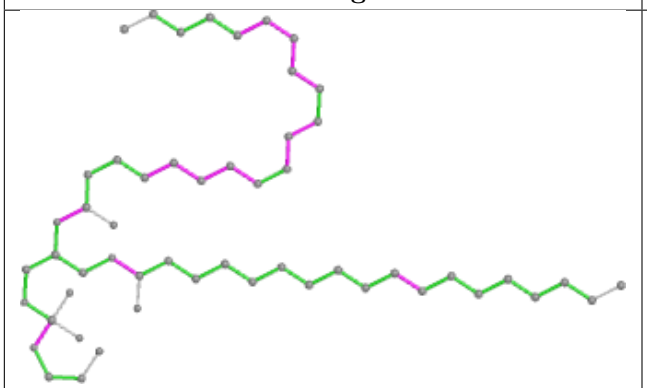
Ligand PEK C 306



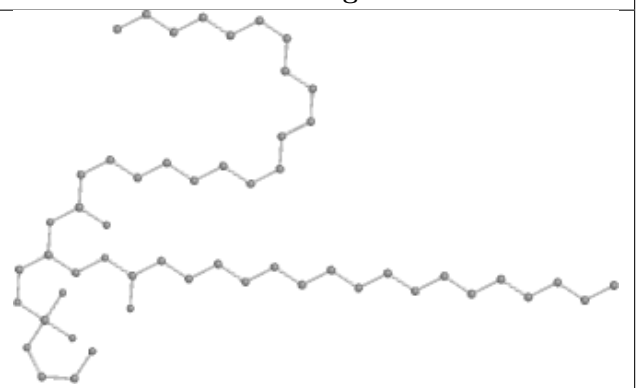
Bond lengths



Bond angles

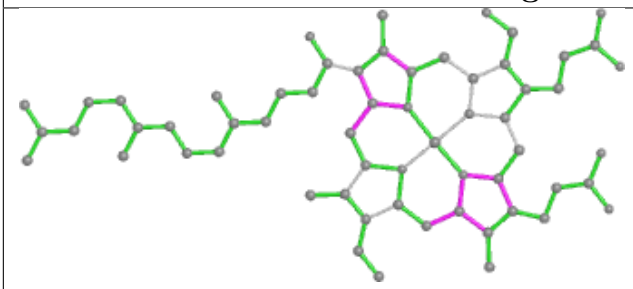


Torsions

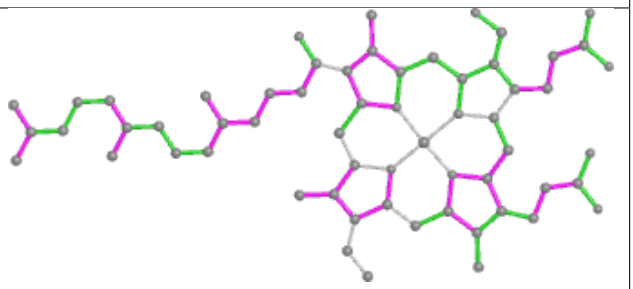


Rings

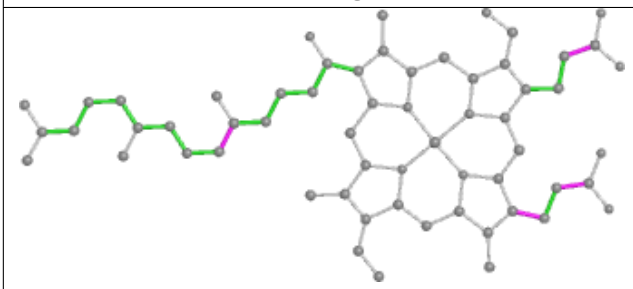
Ligand HEA A 602



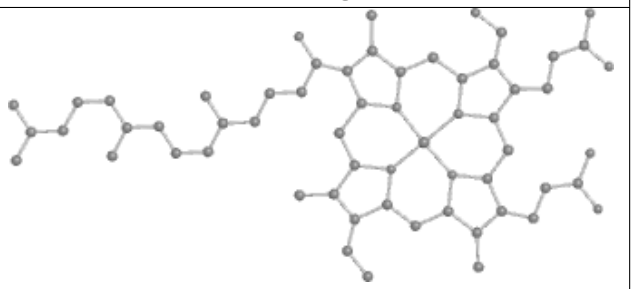
Bond lengths



Bond angles

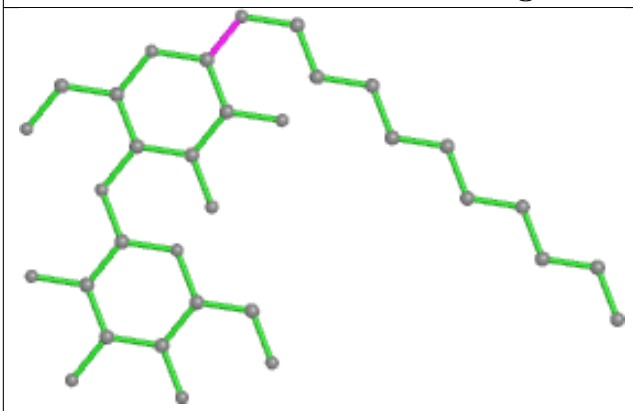


Torsions

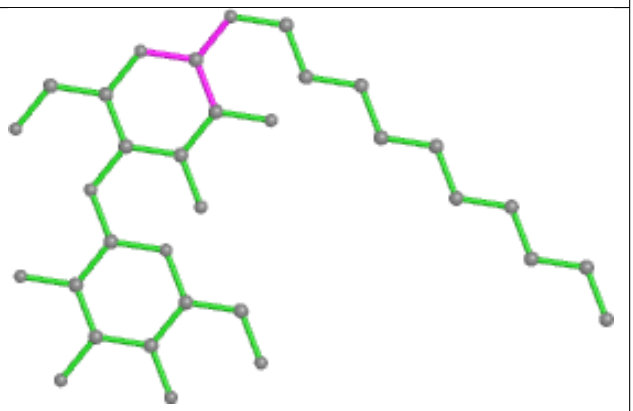


Rings

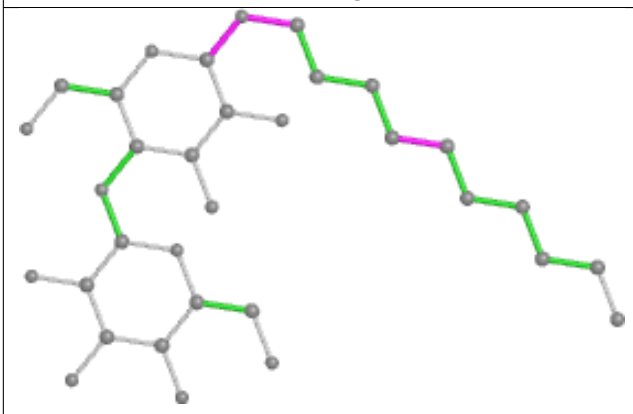
Ligand DMU C 308



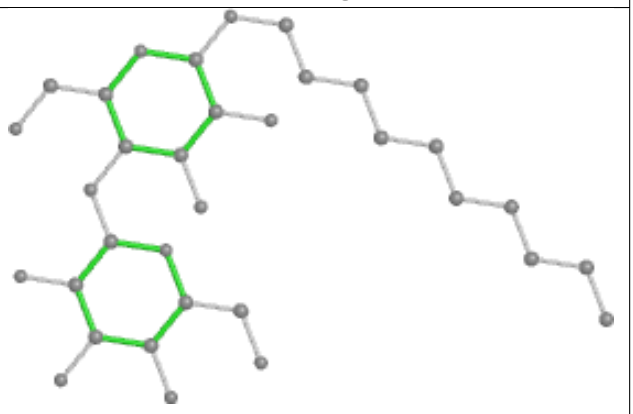
Bond lengths



Bond angles

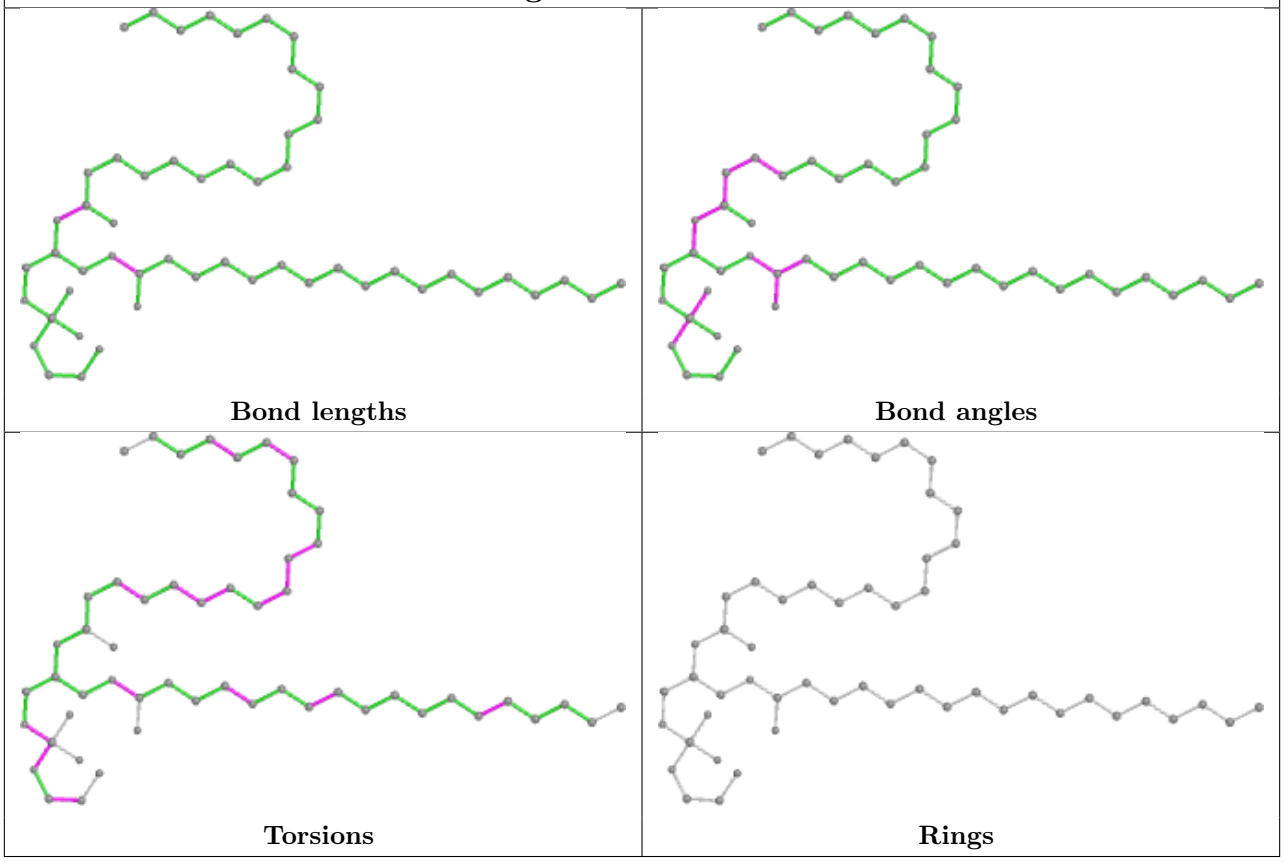


Torsions

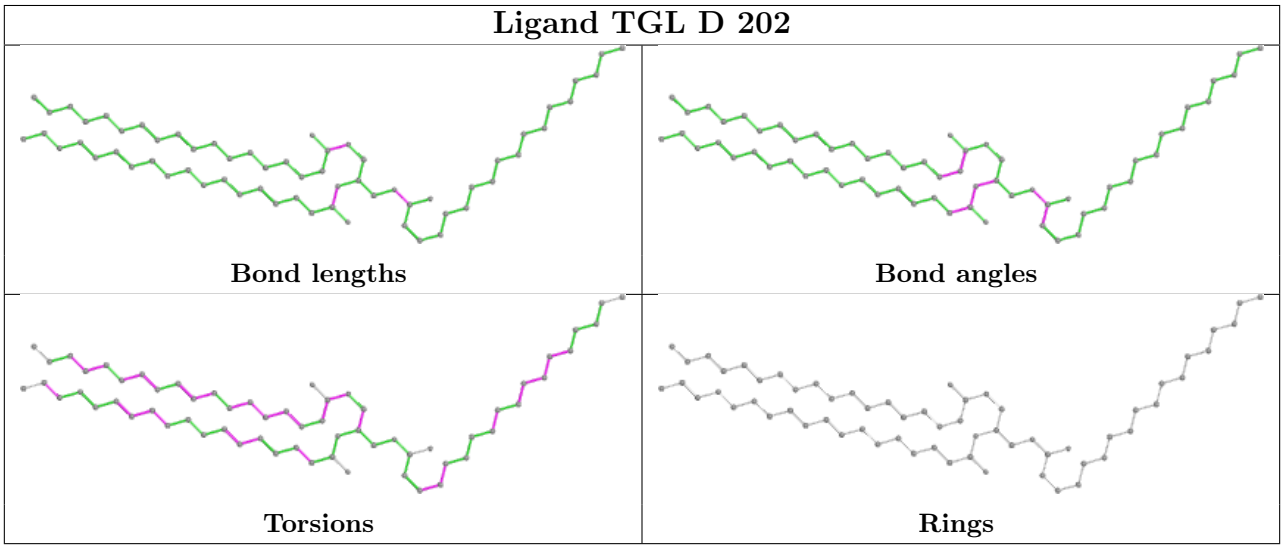


Rings

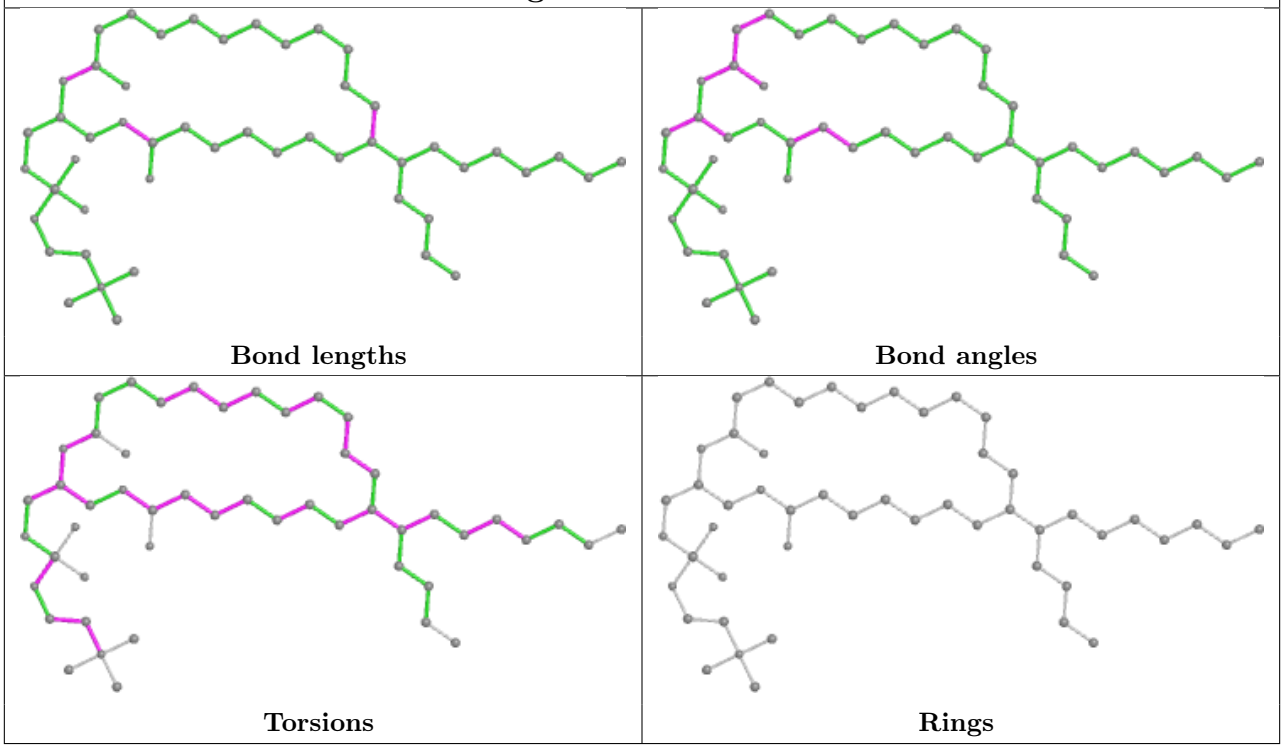
Ligand PEK P 306



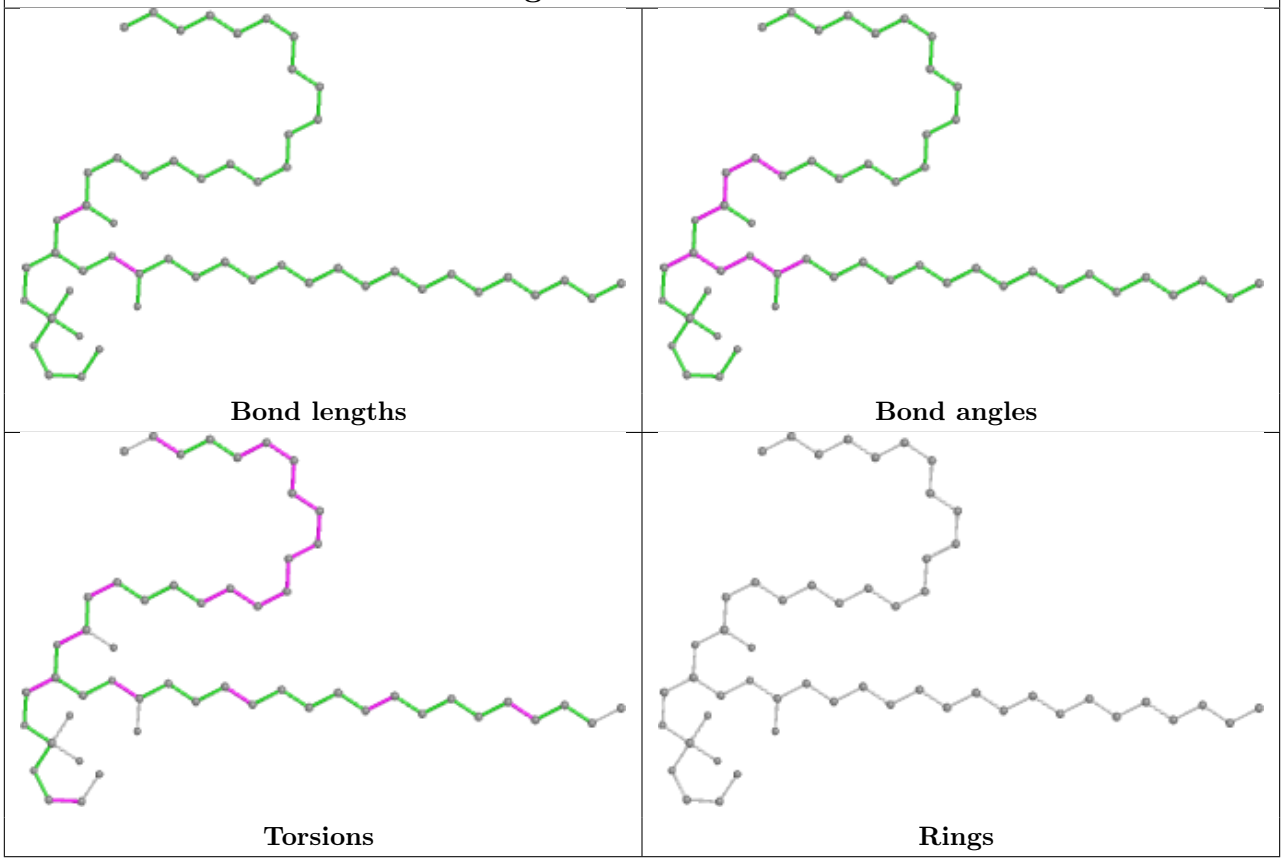
Ligand TGL D 202



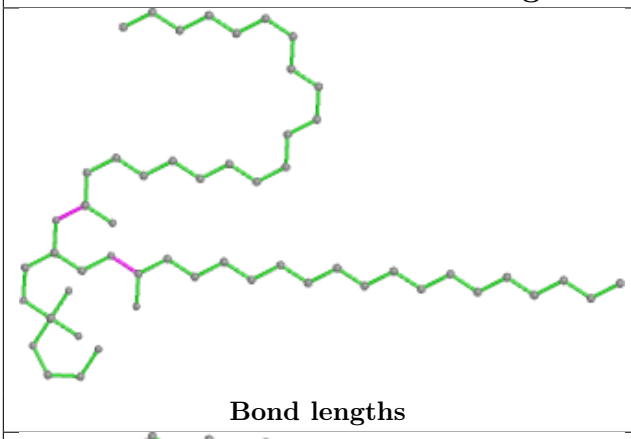
Ligand PSC O 603



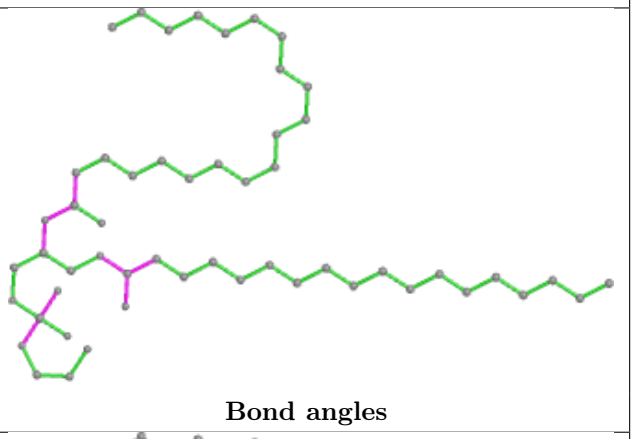
Ligand PEK C 309



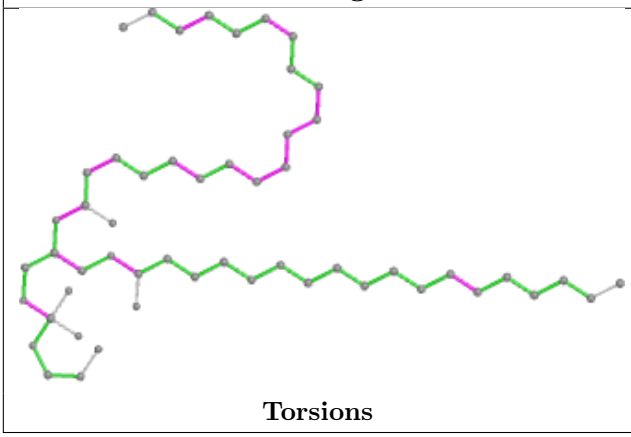
Ligand PEK G 101



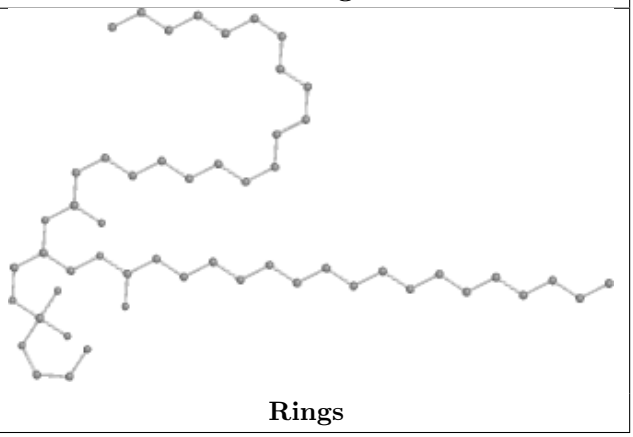
Bond lengths



Bond angles

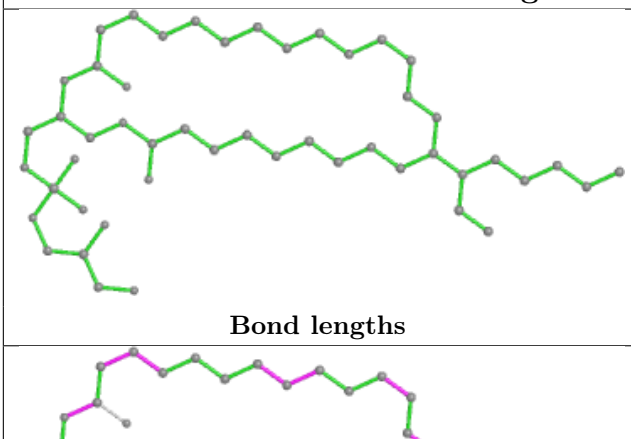


Torsions

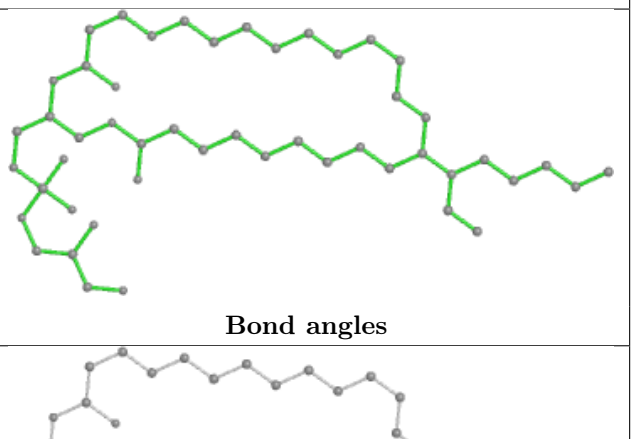


Rings

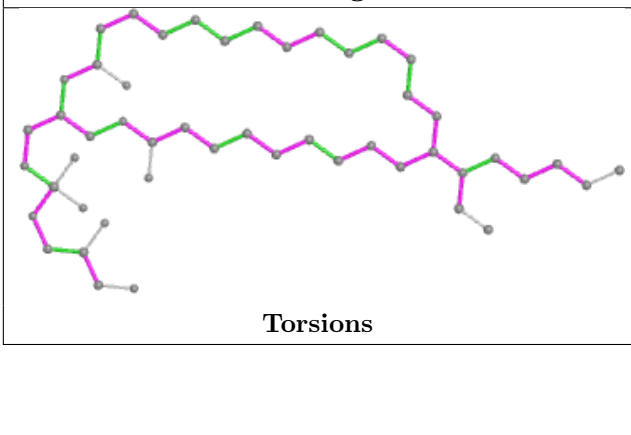
Ligand PGV D 201



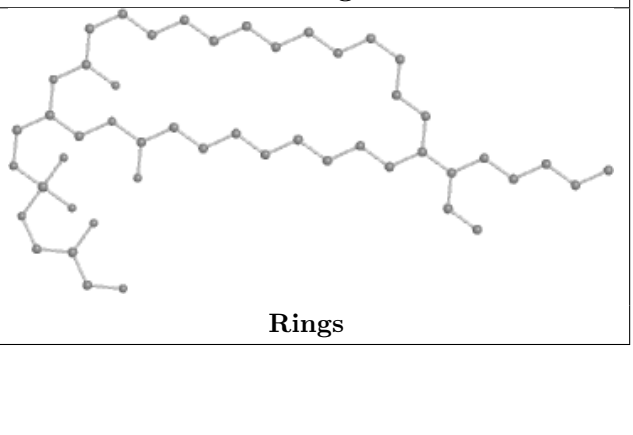
Bond lengths



Bond angles

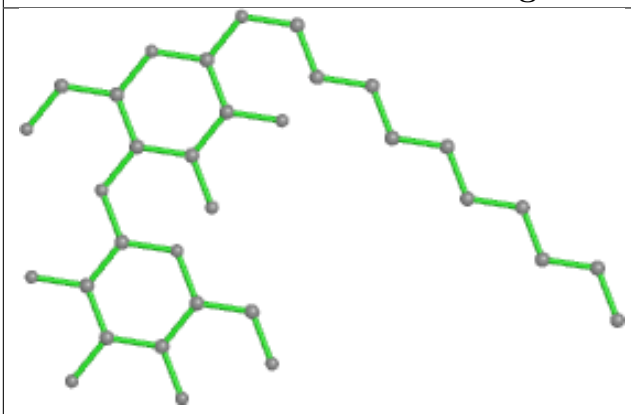


Torsions

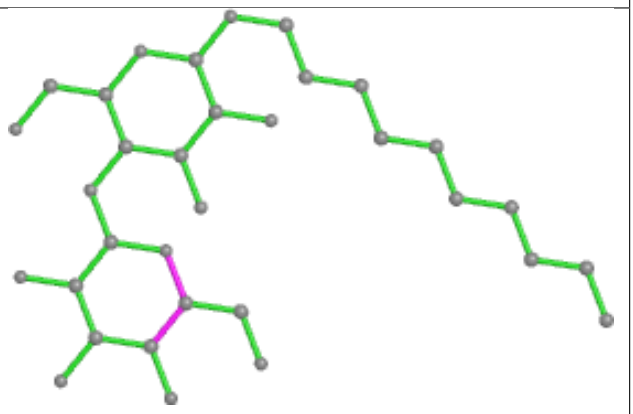


Rings

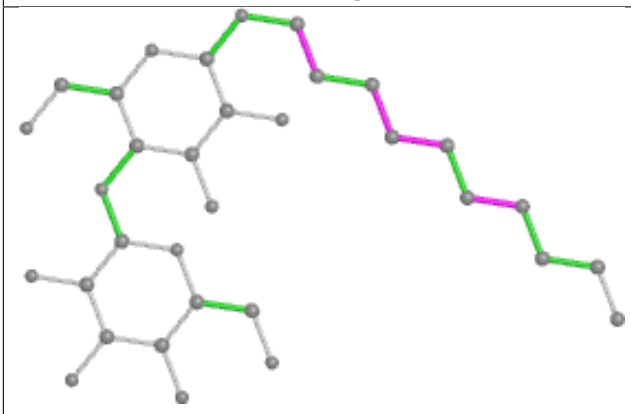
Ligand DMU Z 101



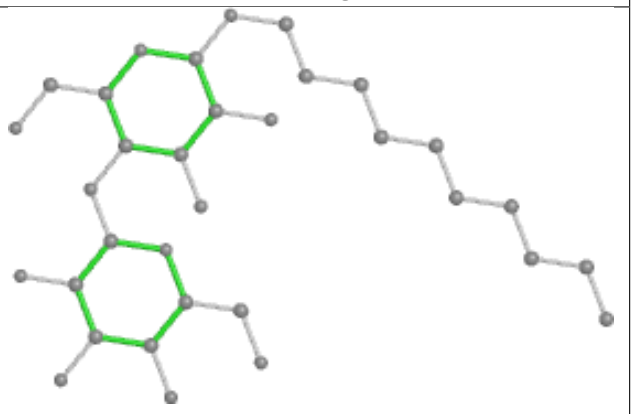
Bond lengths



Bond angles

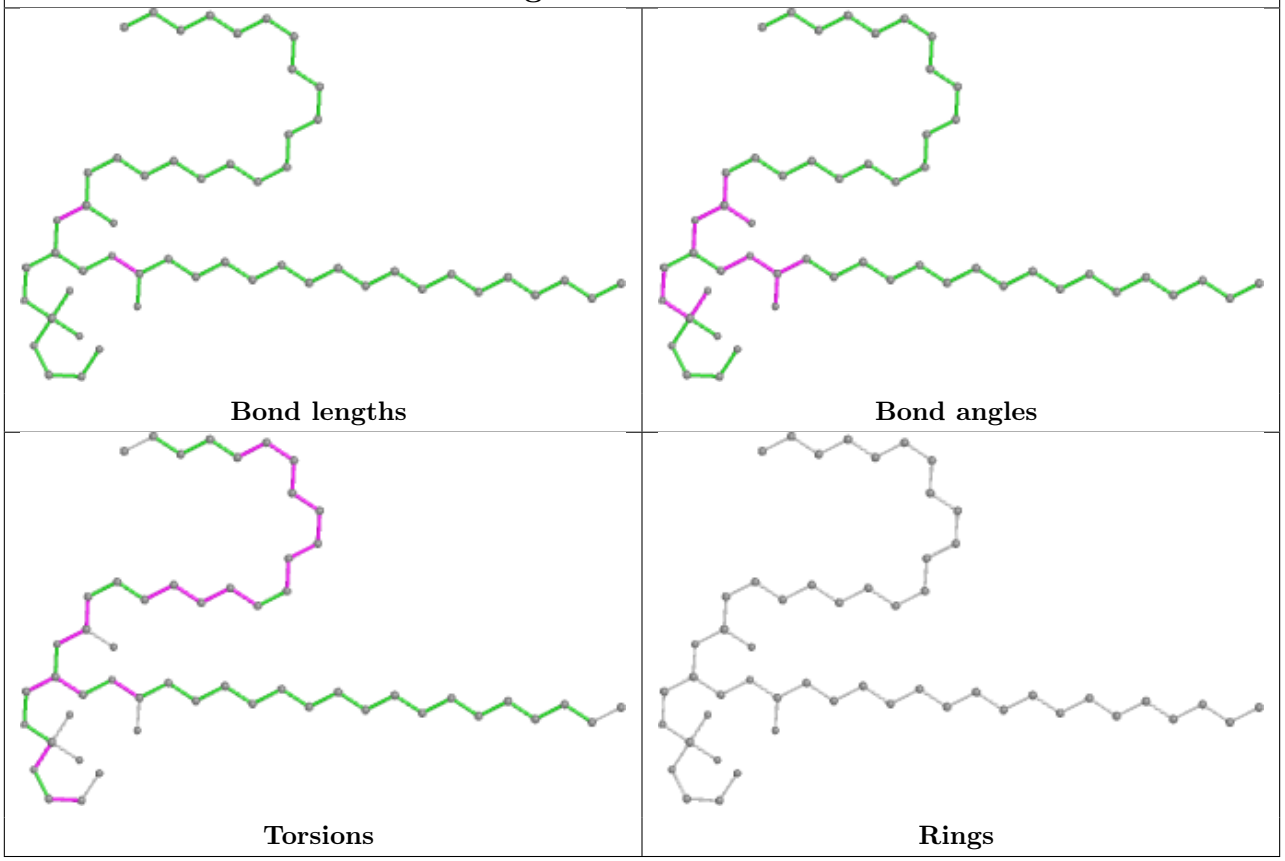


Torsions

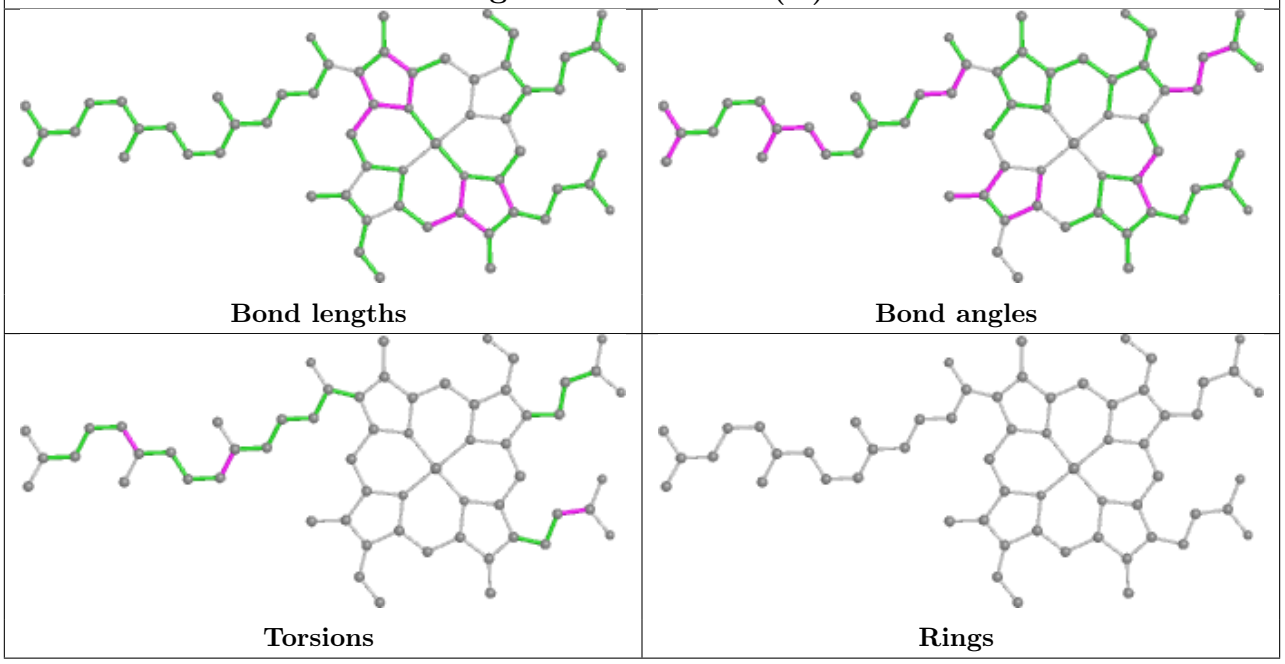


Rings

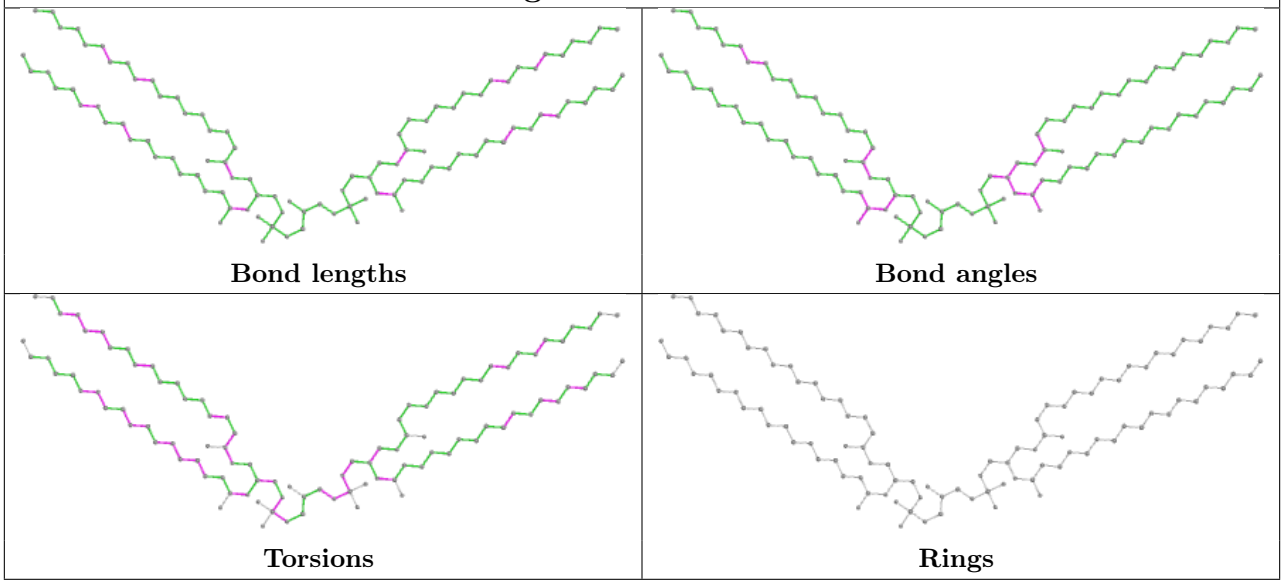
Ligand PEK B 604



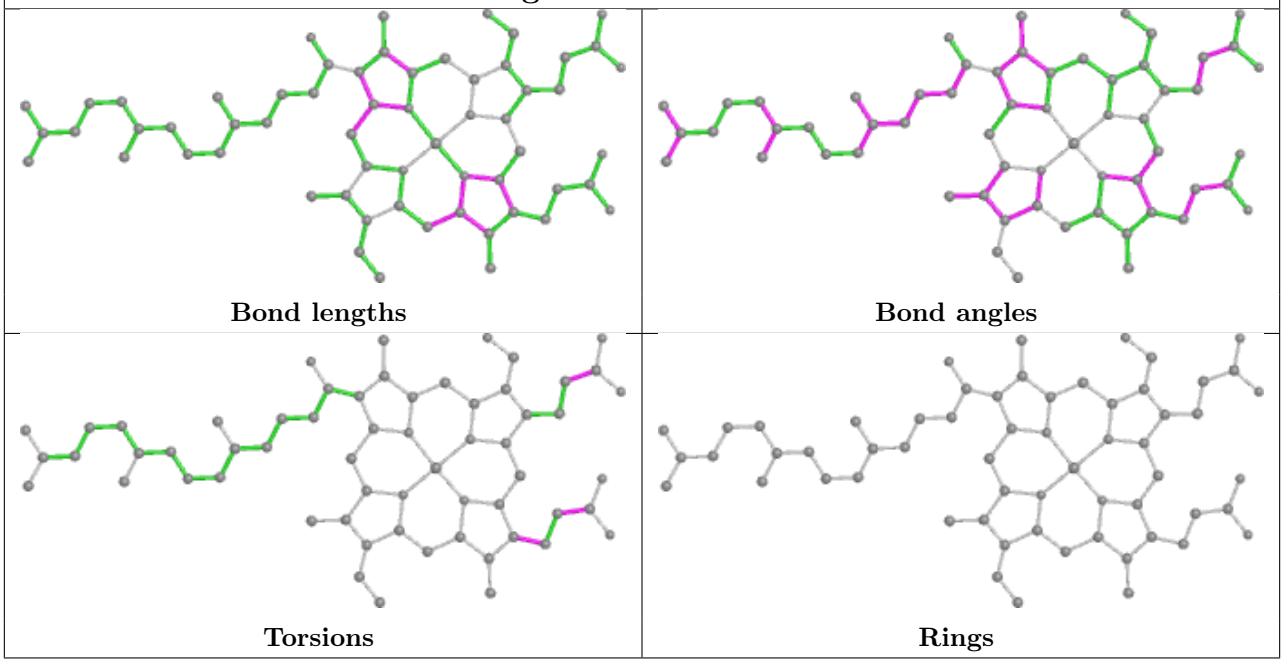
Ligand HEA A 601 (C)



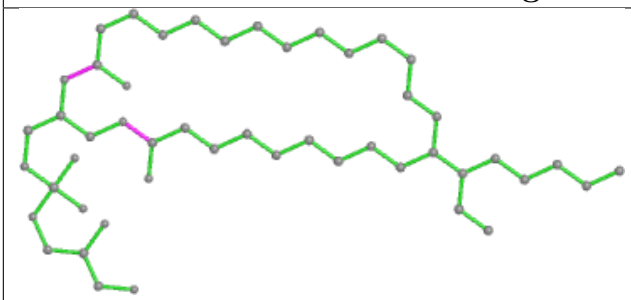
Ligand CDL G 102



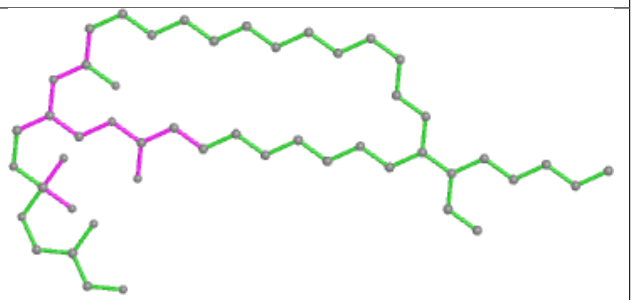
Ligand HEA N 602



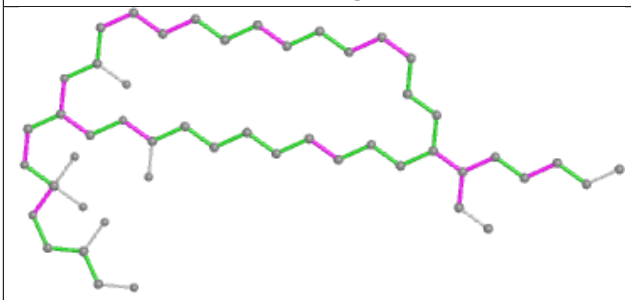
Ligand PGV P 302



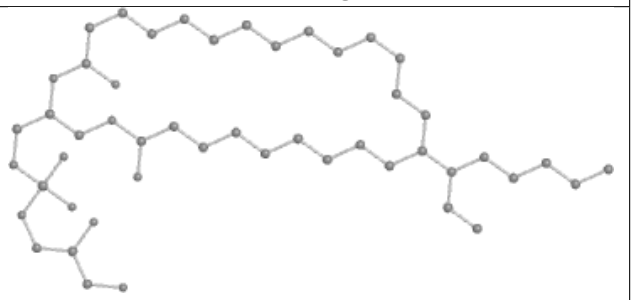
Bond lengths



Bond angles

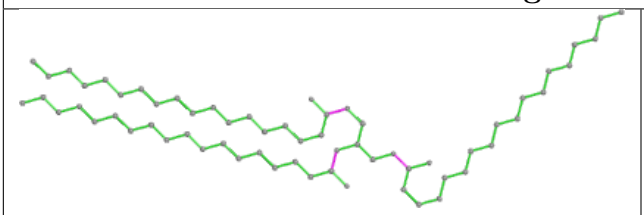


Torsions

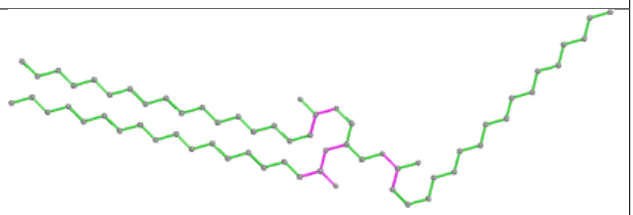


Rings

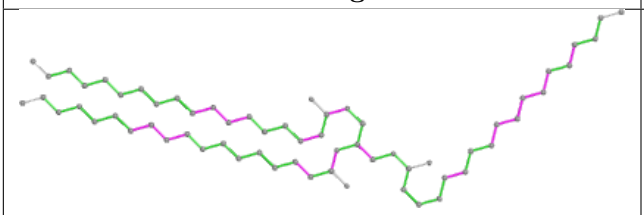
Ligand TGL A 607



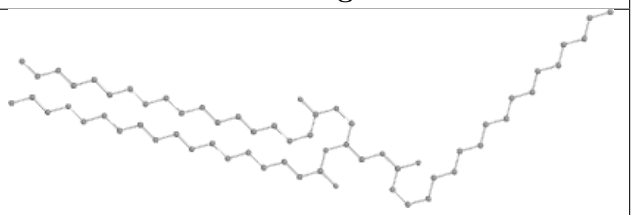
Bond lengths



Bond angles

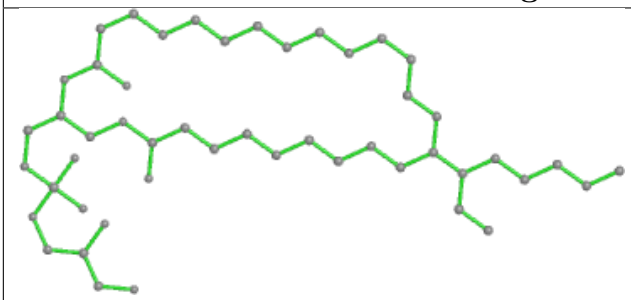


Torsions

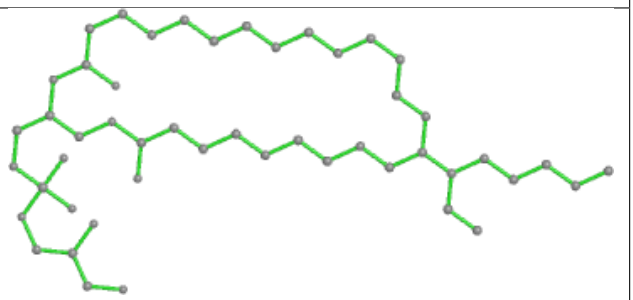


Rings

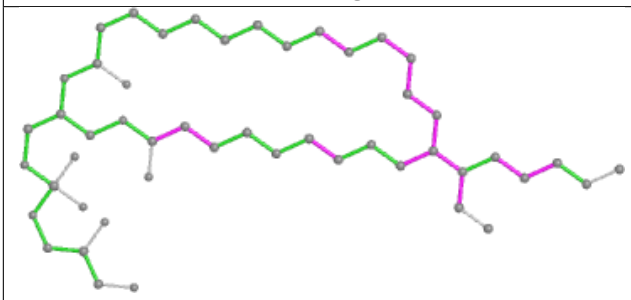
Ligand PGV N 607



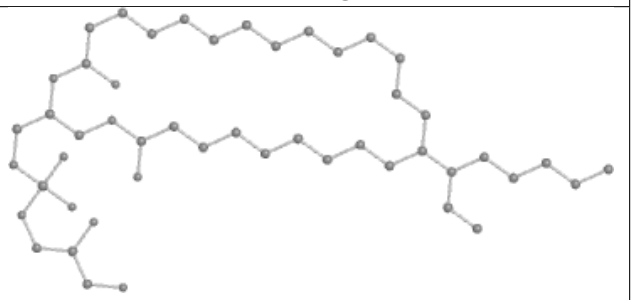
Bond lengths



Bond angles

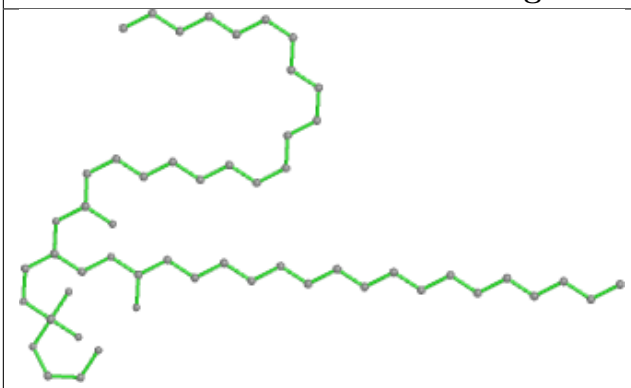


Torsions

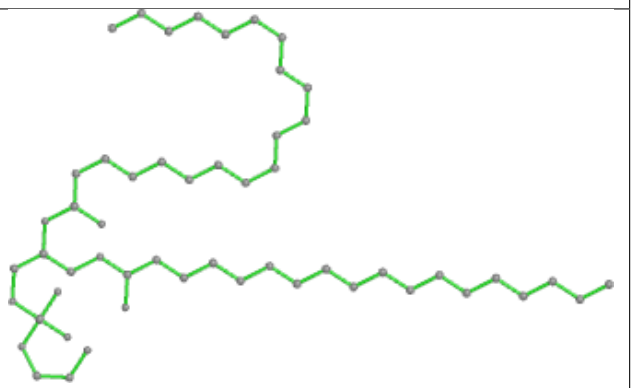


Rings

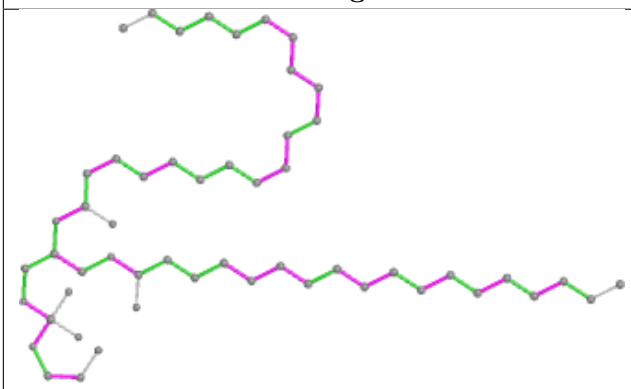
Ligand PEK P 301



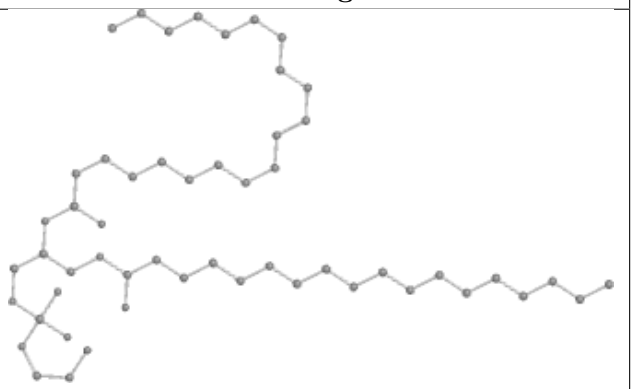
Bond lengths



Bond angles

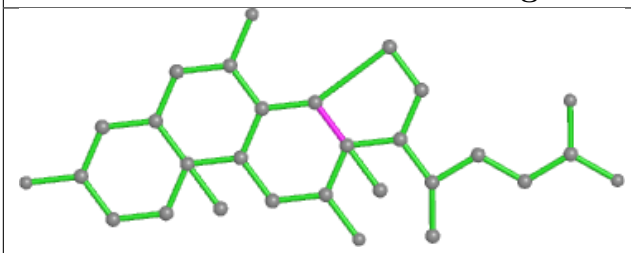


Torsions

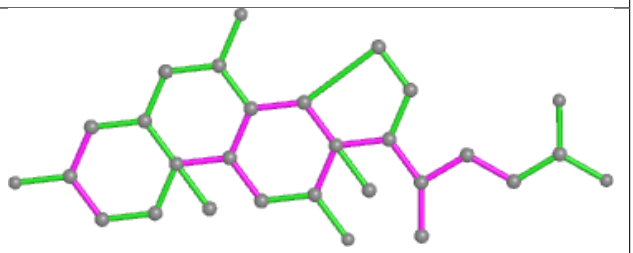


Rings

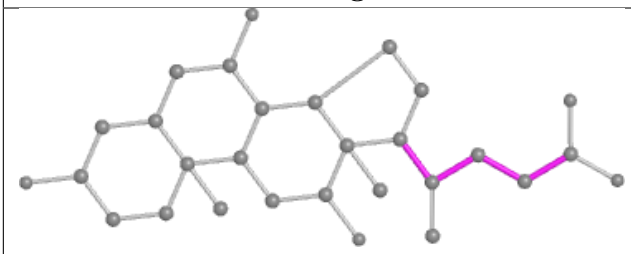
Ligand CHD C 304



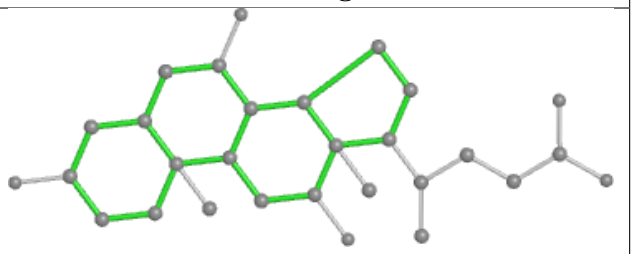
Bond lengths



Bond angles

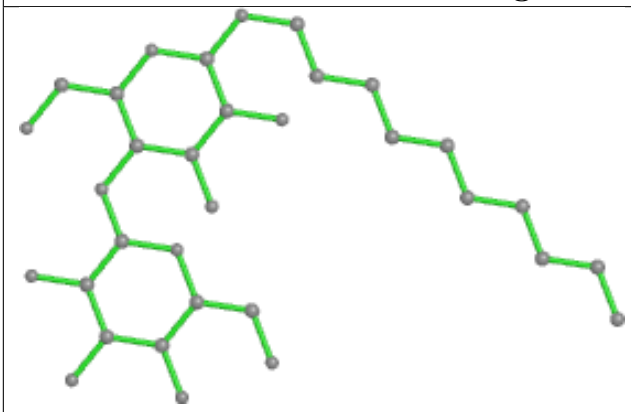


Torsions

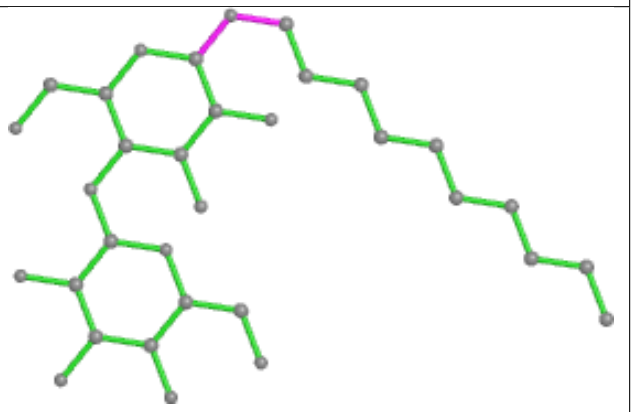


Rings

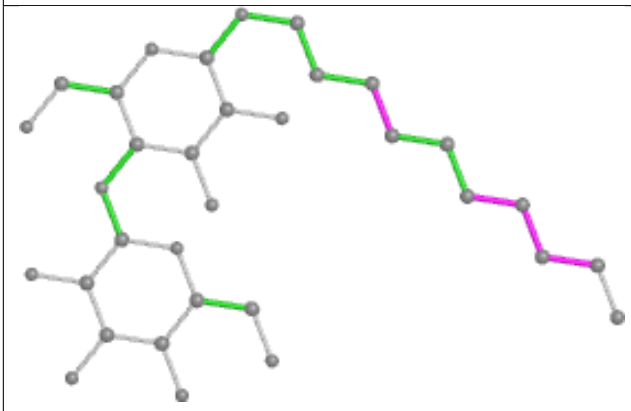
Ligand DMU M 101



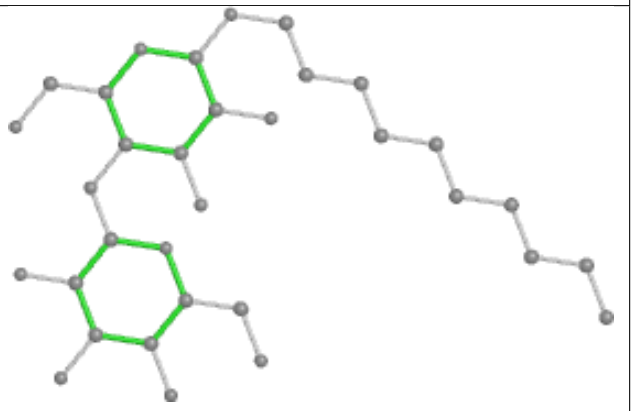
Bond lengths



Bond angles

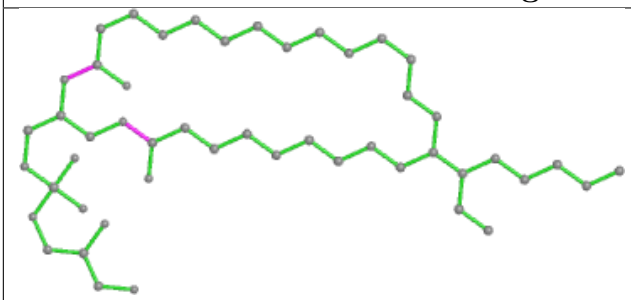


Torsions

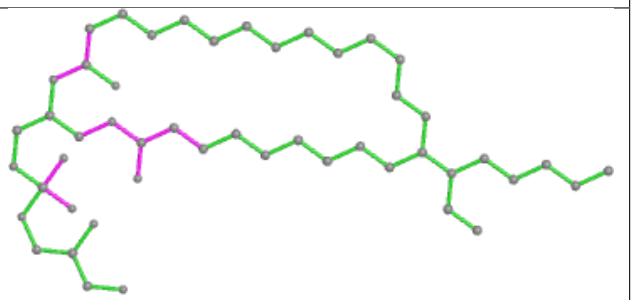


Rings

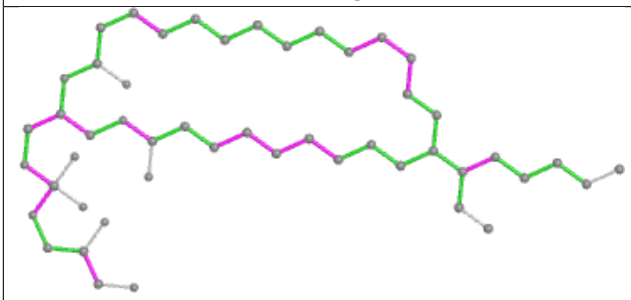
Ligand PGV C 307



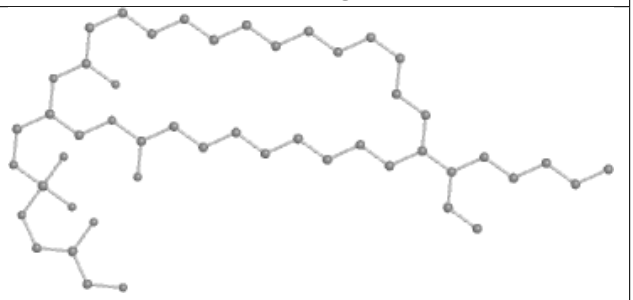
Bond lengths



Bond angles

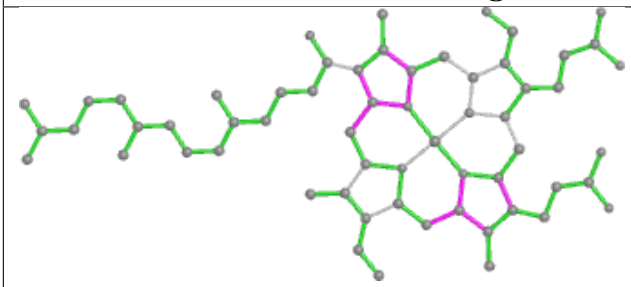


Torsions

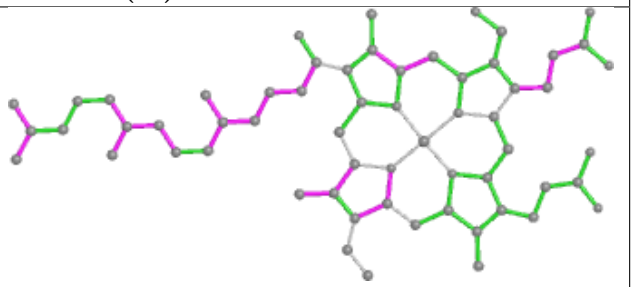


Rings

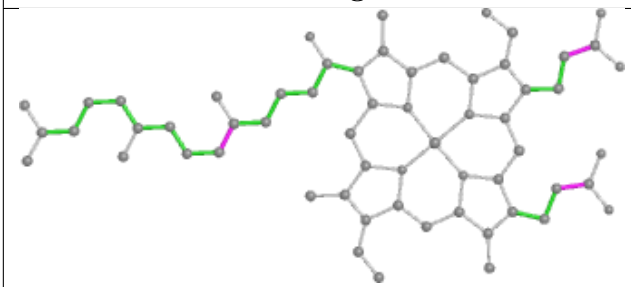
Ligand HEA N 601 (D)



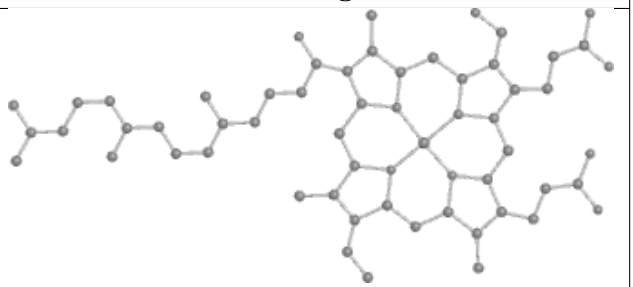
Bond lengths



Bond angles

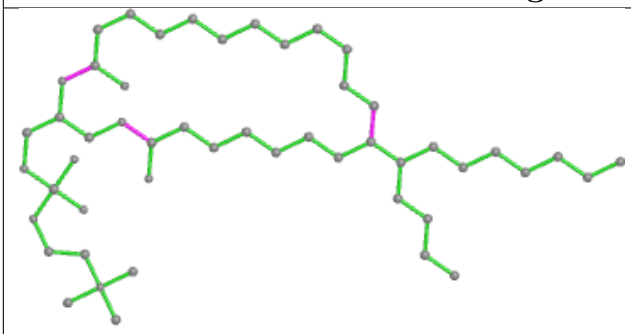


Torsions

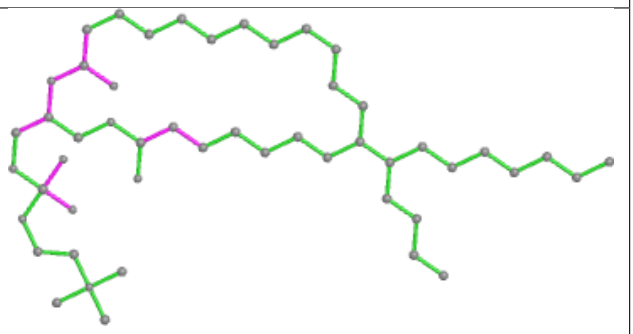


Rings

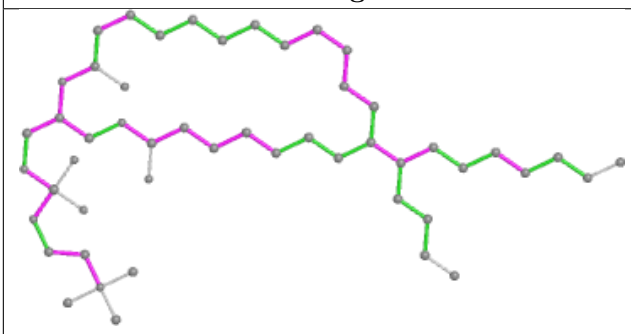
Ligand PSC B 603



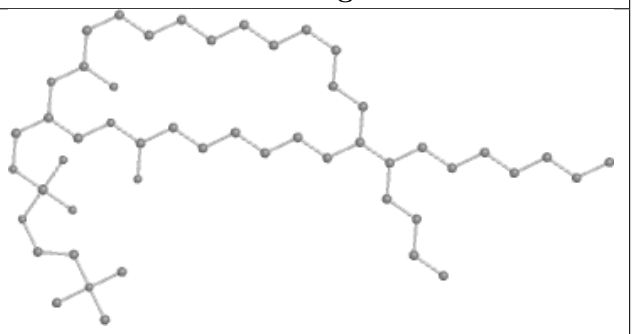
Bond lengths



Bond angles

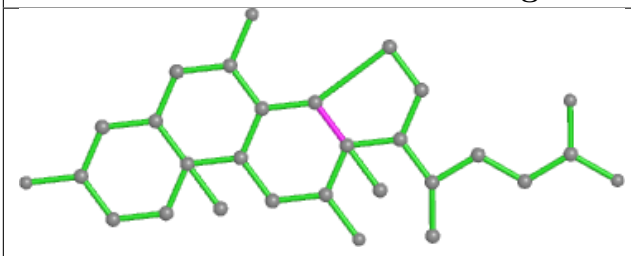


Torsions

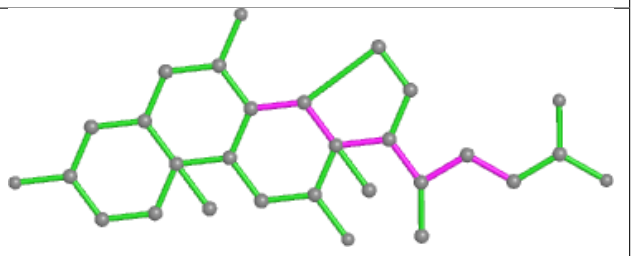


Rings

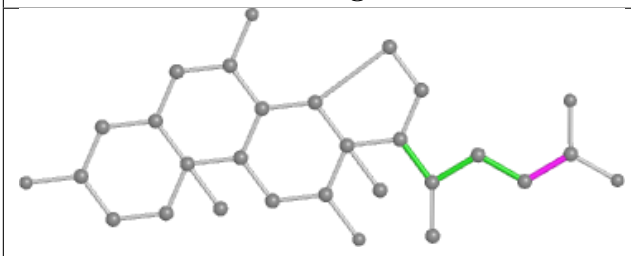
Ligand CHD B 602



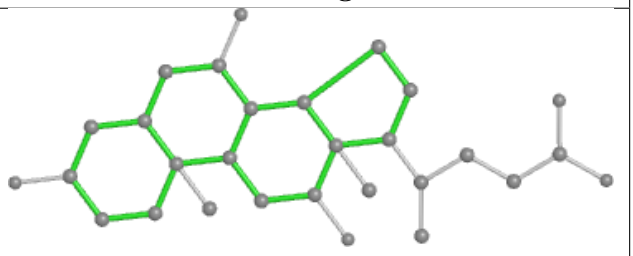
Bond lengths



Bond angles

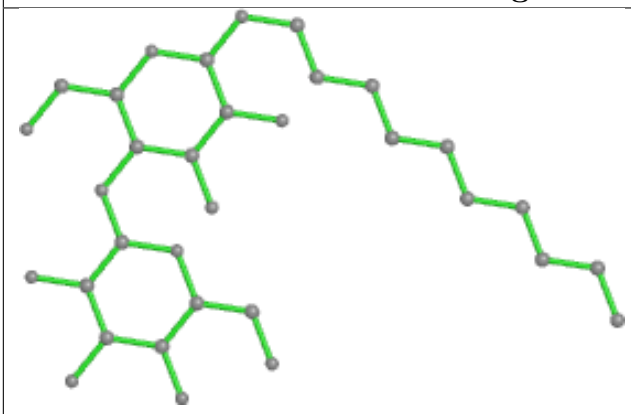


Torsions

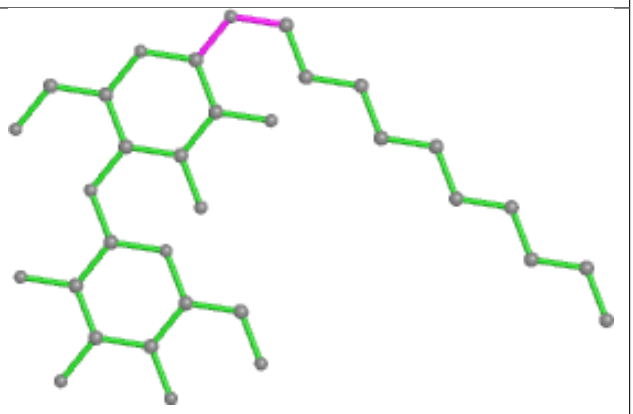


Rings

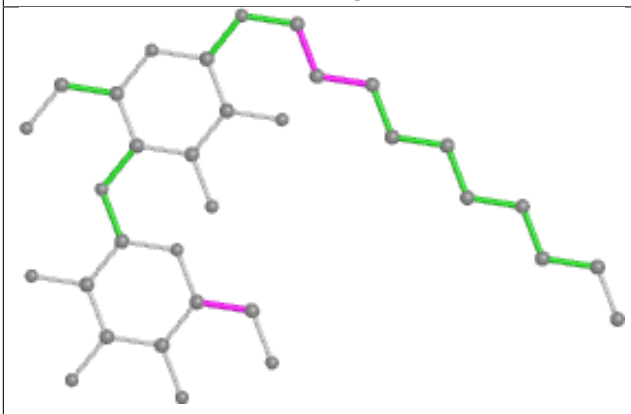
Ligand DMU W 101



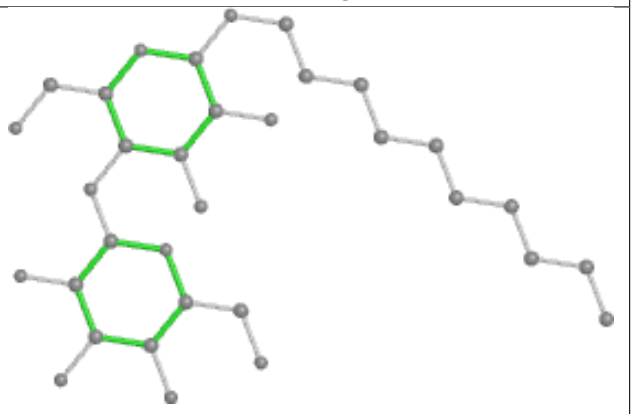
Bond lengths



Bond angles

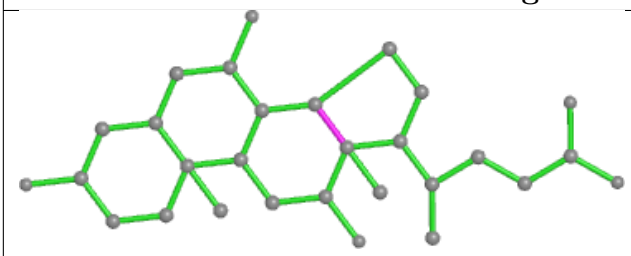


Torsions

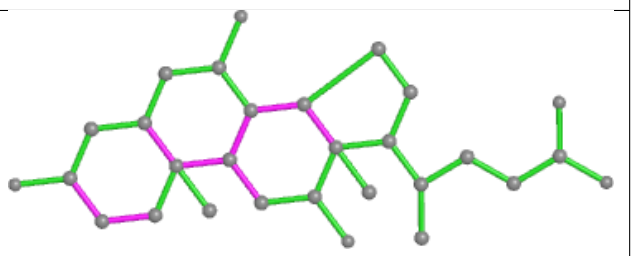


Rings

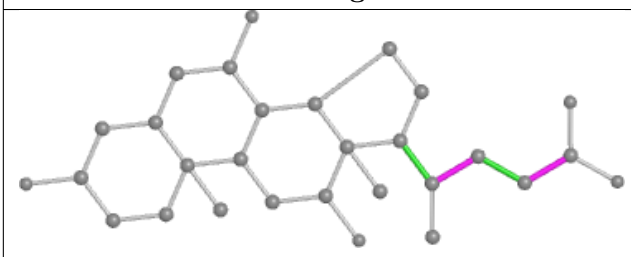
Ligand CHD P 305



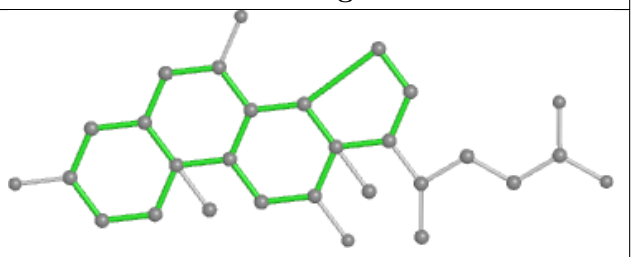
Bond lengths



Bond angles

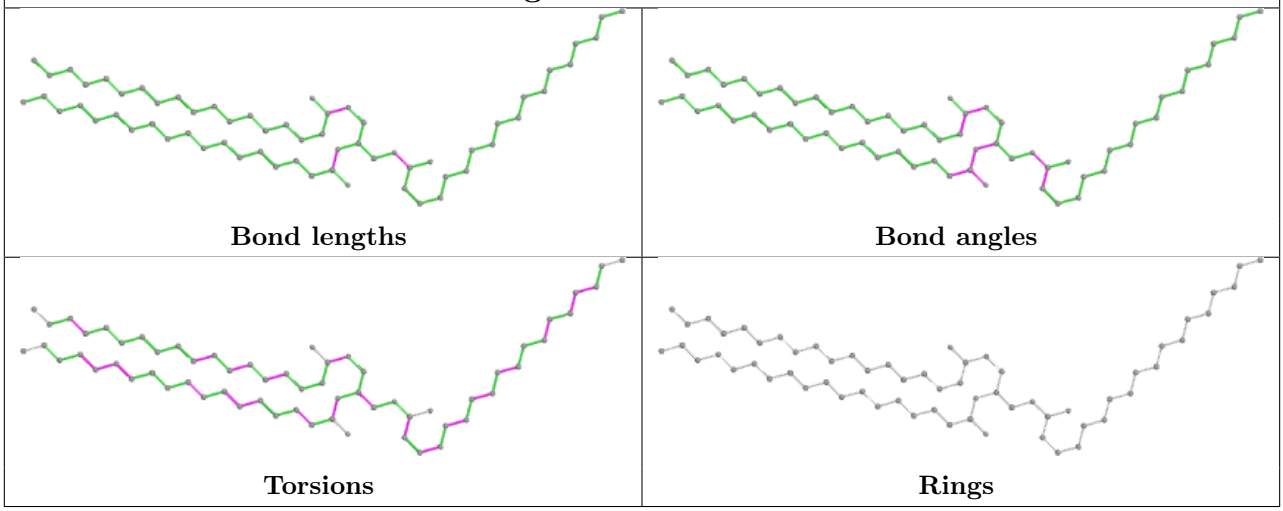


Torsions

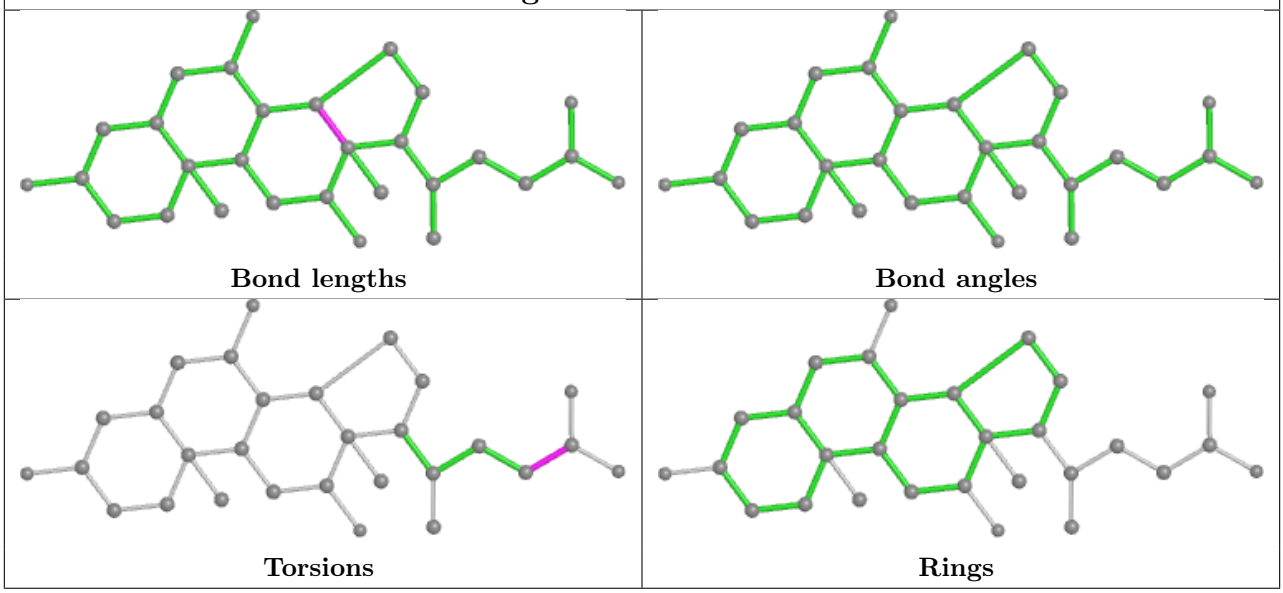


Rings

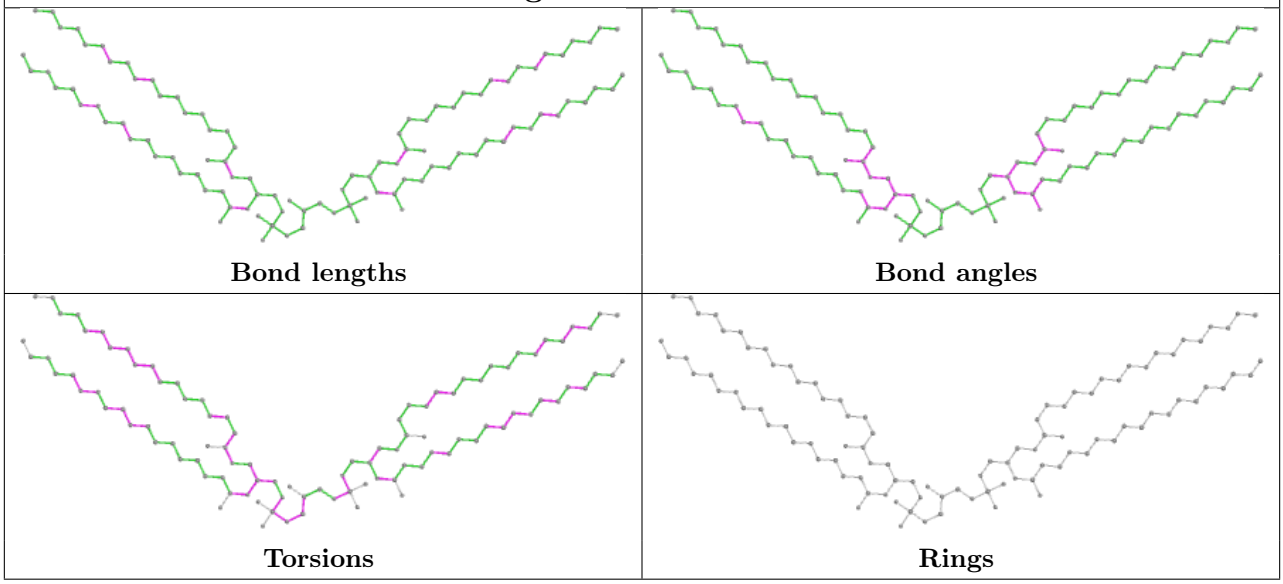
Ligand TGL N 608



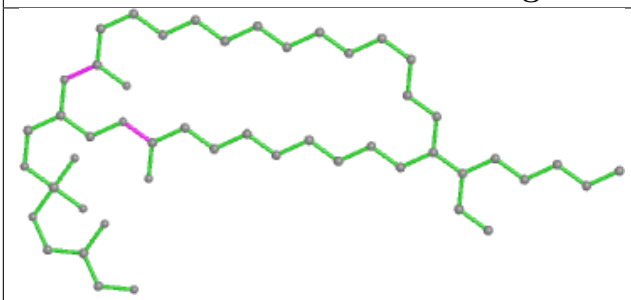
Ligand CHD C 305



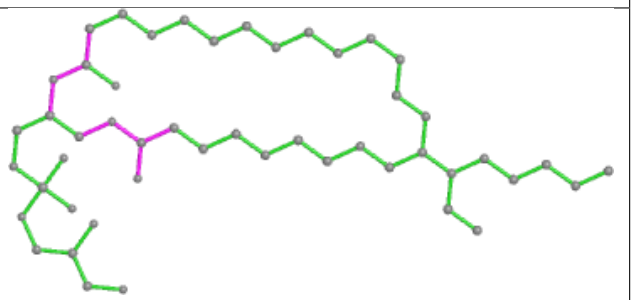
Ligand CDL C 303



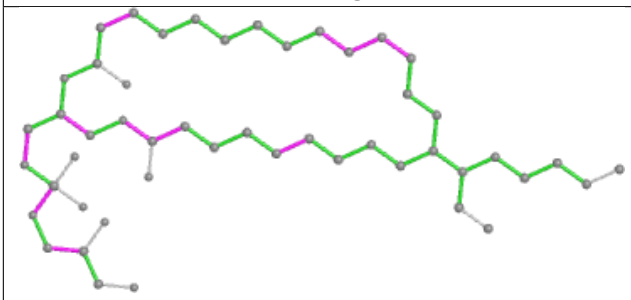
Ligand PGV P 303



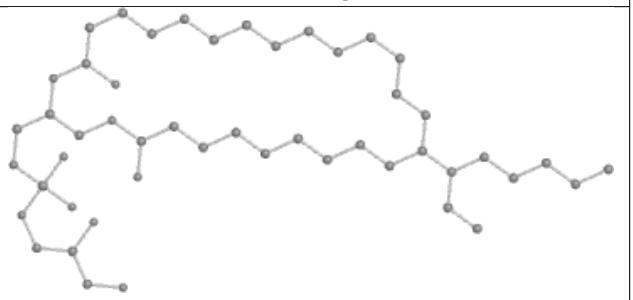
Bond lengths



Bond angles

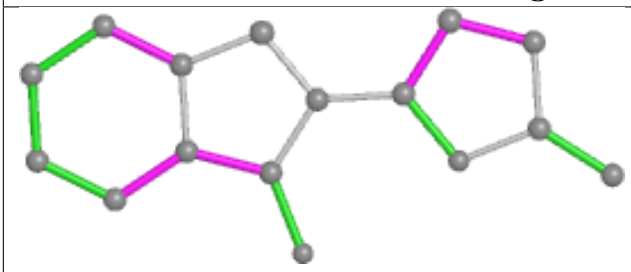


Torsions

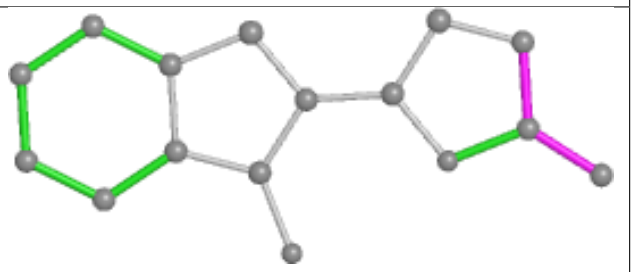


Rings

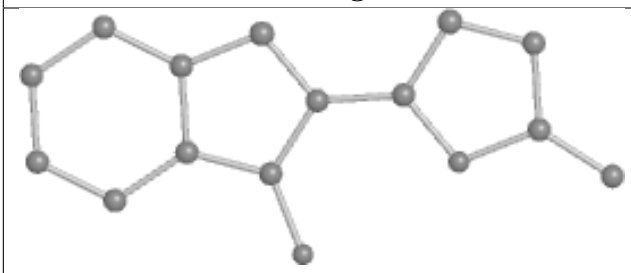
Ligand J6X A 608



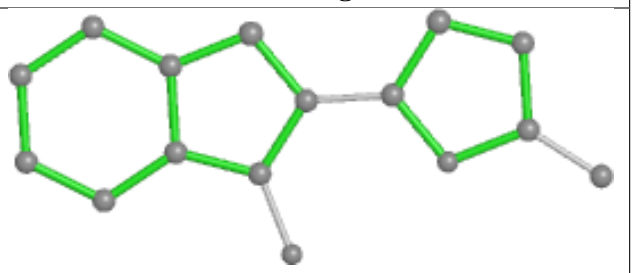
Bond lengths



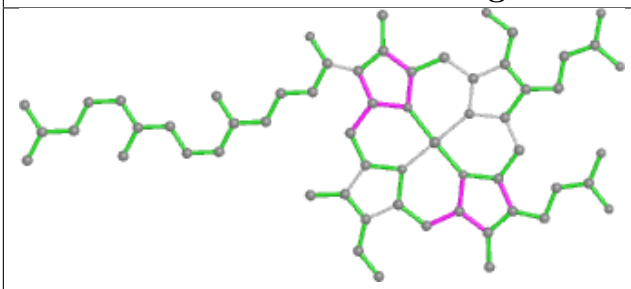
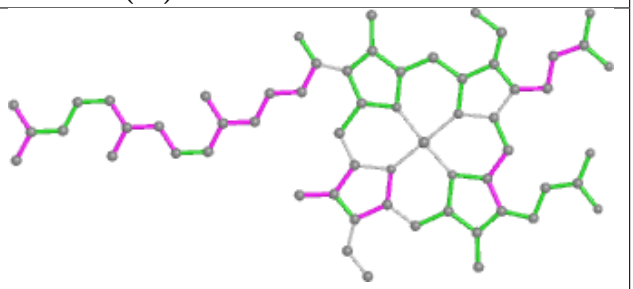
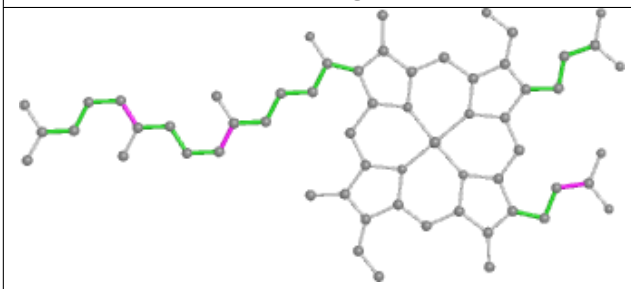
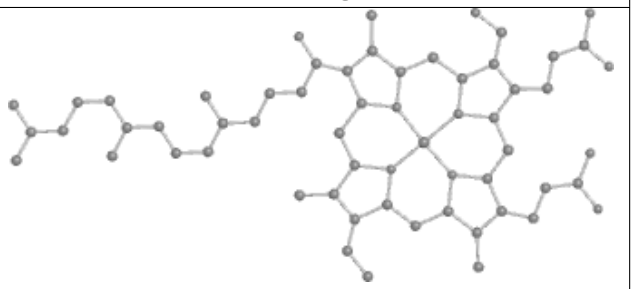
Bond angles



Torsions



Rings

Ligand HEA A 601 (D)	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.50	2 (0%) 92 91	20, 27, 37, 94	0
1	N	513/514 (99%)	-0.44	5 (0%) 82 81	20, 29, 40, 81	0
2	B	226/581 (38%)	-0.22	6 (2%) 54 52	22, 35, 63, 118	0
2	O	226/581 (38%)	-0.12	9 (3%) 38 36	28, 40, 68, 122	0
3	C	259/261 (99%)	-0.52	2 (0%) 86 85	22, 30, 46, 95	0
3	P	259/261 (99%)	-0.45	2 (0%) 86 85	23, 31, 48, 91	0
4	D	144/147 (97%)	-0.42	2 (1%) 75 73	27, 37, 60, 96	0
4	Q	139/147 (94%)	0.12	8 (5%) 23 22	34, 49, 78, 126	0
5	E	105/109 (96%)	-0.23	3 (2%) 51 49	28, 37, 65, 125	0
5	R	105/109 (96%)	0.13	7 (6%) 17 16	32, 45, 75, 139	0
6	F	93/98 (94%)	-0.12	5 (5%) 25 24	25, 38, 65, 120	0
6	S	96/98 (97%)	-0.04	8 (8%) 11 10	24, 37, 74, 105	0
7	G	81/84 (96%)	0.59	17 (20%) 1 1	26, 39, 121, 185	0
7	T	81/84 (96%)	0.68	18 (22%) 0 0	26, 42, 118, 163	0
8	H	79/85 (92%)	0.05	9 (11%) 5 4	29, 39, 113, 130	0
8	U	79/85 (92%)	0.31	9 (11%) 5 4	33, 44, 123, 153	0
9	I	72/73 (98%)	0.38	7 (9%) 7 6	34, 48, 74, 94	0
9	V	72/73 (98%)	0.62	10 (13%) 2 2	33, 54, 84, 112	0
10	J	57/59 (96%)	0.05	5 (8%) 10 8	30, 42, 79, 90	0
10	W	57/59 (96%)	0.03	3 (5%) 26 25	30, 43, 78, 116	0
11	K	51/56 (91%)	0.32	3 (5%) 22 21	33, 41, 63, 87	0
11	X	49/56 (87%)	0.60	5 (10%) 6 6	41, 50, 75, 83	0
12	L	46/47 (97%)	-0.50	1 (2%) 62 59	26, 33, 54, 112	0
12	Y	45/47 (95%)	-0.41	0 100 100	30, 40, 66, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.09	5 (11%) 4 4	28, 33, 81, 127	0
13	Z	41/46 (89%)	-0.02	5 (12%) 4 3	36, 42, 76, 89	0
All	All	3531/4320 (81%)	-0.19	156 (4%) 34 32	20, 35, 70, 185	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	8	HIS	9.8
8	H	45	ALA	8.2
5	R	5	HIS	8.0
11	X	6	ALA	7.1
5	R	109	VAL	6.9
7	G	7	ASP	6.4
9	I	37	PHE	6.4
8	U	45	ALA	6.3
7	T	6	GLY	6.1
9	V	37	PHE	5.8
7	T	4	ALA	5.7
8	U	8	ILE	5.6
2	O	90	ILE	5.2
7	G	8	HIS	5.2
9	V	2	THR	5.1
10	W	57	HIS	5.1
5	E	5	HIS	5.1
7	T	5	LYS	5.0
7	G	36[A]	TRP	4.8
13	M	42	LYS	4.8
10	J	57	HIS	4.8
11	X	7	PRO	4.7
7	G	40	GLY	4.7
10	J	56	PRO	4.7
1	N	49[C]	GLY	4.7
10	J	1	PHE	4.7
8	U	10	ASN	4.7
7	G	5	LYS	4.6
7	T	3	ALA	4.4
11	K	7	PRO	4.3
6	S	95	GLN	4.3
7	T	36[A]	TRP	4.3
8	U	48	GLY	4.3
11	K	6	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
8	H	46	LYS	4.0
13	M	43	SER	4.0
8	U	44	THR	3.9
7	G	42	ARG	3.9
6	S	97	ALA	3.9
9	V	26	MET	3.9
7	G	41	HIS	3.8
2	B	90	ILE	3.8
4	Q	39	ALA	3.8
9	V	34	PHE	3.8
7	G	9	GLY	3.8
5	E	109	VAL	3.7
7	T	39	SER	3.7
11	X	13	TYR	3.7
7	G	3	ALA	3.7
12	L	2	HIS	3.7
7	T	40	GLY	3.7
13	Z	39	ASN	3.7
7	G	4	ALA	3.6
8	U	47	GLY	3.6
8	H	44	THR	3.6
8	H	49	ASP	3.6
2	O	91	ASN	3.5
6	S	96	LEU	3.5
13	Z	40	TYR	3.5
7	G	39	SER	3.5
7	G	84	LYS	3.5
4	Q	147	LYS	3.5
8	U	49	ASP	3.4
6	S	2	SER	3.4
1	A	49[C]	GLY	3.3
2	O	227	LEU	3.3
2	B	60	GLU	3.3
2	B	57	ASP	3.3
8	U	7	LYS	3.3
9	V	19	PHE	3.3
7	T	84	LYS	3.3
2	B	59	GLN	3.3
1	A	50[C]	ASP	3.2
11	X	12	LYS	3.2
7	T	10	GLY	3.2
7	T	42	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
13	M	40	TYR	3.2
7	G	43	GLU	3.1
8	H	48	GLY	3.1
9	I	19	PHE	3.1
8	H	10	ASN	3.1
7	T	7	ASP	3.0
9	I	26	MET	3.0
8	H	8	ILE	3.0
4	Q	10	ASP	3.0
8	U	46	LYS	3.0
7	T	41	HIS	2.9
10	J	55	PHE	2.9
9	V	33	THR	2.9
9	V	25	PHE	2.9
4	Q	32	ASN	2.8
2	O	113	TYR	2.8
7	T	9	GLY	2.8
4	Q	33	LEU	2.8
7	G	37	LEU	2.8
2	O	224	ALA	2.8
8	H	7	LYS	2.7
7	G	6	GLY	2.7
9	I	34	PHE	2.7
4	Q	9	GLU	2.7
8	H	47	GLY	2.7
9	I	25	PHE	2.7
4	Q	31	LYS	2.7
13	Z	41	LYS	2.6
2	O	167	SER	2.6
2	O	192	TYR	2.6
9	I	22	VAL	2.6
10	W	1	PHE	2.5
6	F	65	ASP	2.5
7	T	45	PRO	2.5
6	S	94	HIS	2.5
9	V	29	LEU	2.5
13	M	39	ASN	2.5
7	G	45	PRO	2.5
5	R	68	LEU	2.5
5	R	108	LYS	2.5
9	I	18	ARG	2.5
1	N	312[A]	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	44	GLU	2.4
1	N	469	VAL	2.4
4	D	4	SER	2.4
7	T	43	GLU	2.4
7	T	37	LEU	2.4
5	R	67	ILE	2.3
6	F	94	HIS	2.3
6	F	64	GLU	2.3
10	W	48	TYR	2.3
4	D	143	ASN	2.3
11	X	8	ASP	2.3
4	Q	30	VAL	2.3
6	F	3	GLY	2.3
7	T	38	HIS	2.3
5	R	64	ALA	2.3
2	B	61	VAL	2.3
6	S	25	ARG	2.3
2	O	92	ASN	2.3
5	R	70	VAL	2.3
13	Z	35	TYR	2.2
1	N	50[C]	ASP	2.2
11	K	47	ARG	2.2
3	P	182	TYR	2.2
2	O	59	GLN	2.2
10	J	48	TYR	2.1
3	P	38	ASN	2.1
2	B	56	MET	2.1
13	Z	32	TRP	2.1
13	M	41	LYS	2.1
7	G	10	GLY	2.1
9	V	30	GLY	2.1
3	C	38	ASN	2.1
1	N	462	LEU	2.1
6	S	27	GLY	2.1
6	S	64	GLU	2.1
5	E	67	ILE	2.0
9	V	3	ALA	2.0
3	C	61	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.63	0.44	81,125,214,234	0
7	TPO	T	11	11/12	0.71	0.42	106,148,176,206	0
1	FME	N	1	10/11	0.90	0.25	42,45,80,87	0
1	FME	A	1	10/11	0.95	0.30	40,50,64,117	0
2	FME	B	1	10/11	0.97	0.18	29,33,43,90	0
2	FME	O	1	10/11	0.97	0.14	32,40,48,69	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
24	PEK	C	309	53/53	0.49	0.49	38,93,179,194	0
24	PEK	C	306	53/53	0.51	0.34	42,80,164,192	0
24	PEK	B	604	53/53	0.51	0.38	45,88,160,182	0
22	CHD	P	305	29/29	0.53	0.39	67,107,138,141	0
22	CHD	C	304	29/29	0.59	0.45	77,111,137,141	0
23	PSC	B	603	52/52	0.60	0.37	42,121,226,245	0
24	PEK	P	301	53/53	0.61	0.30	46,91,158,171	0
26	CDL	T	101	100/100	0.63	0.33	47,91,167,201	0
19	TGL	Y	101	63/63	0.64	0.28	35,66,126,160	0
26	CDL	G	102	100/100	0.65	0.37	53,101,153,190	0
27	DMU	C	308	33/33	0.65	0.35	43,87,112,117	0
23	PSC	O	603	52/52	0.66	0.37	39,92,202,217	0
26	CDL	P	304	100/100	0.66	0.31	35,86,132,143	0
25	PGV	P	302	51/51	0.68	0.31	53,88,141,169	0
25	PGV	N	610	51/51	0.70	0.37	36,86,170,185	0
27	DMU	W	101	33/33	0.70	0.38	42,80,102,106	0

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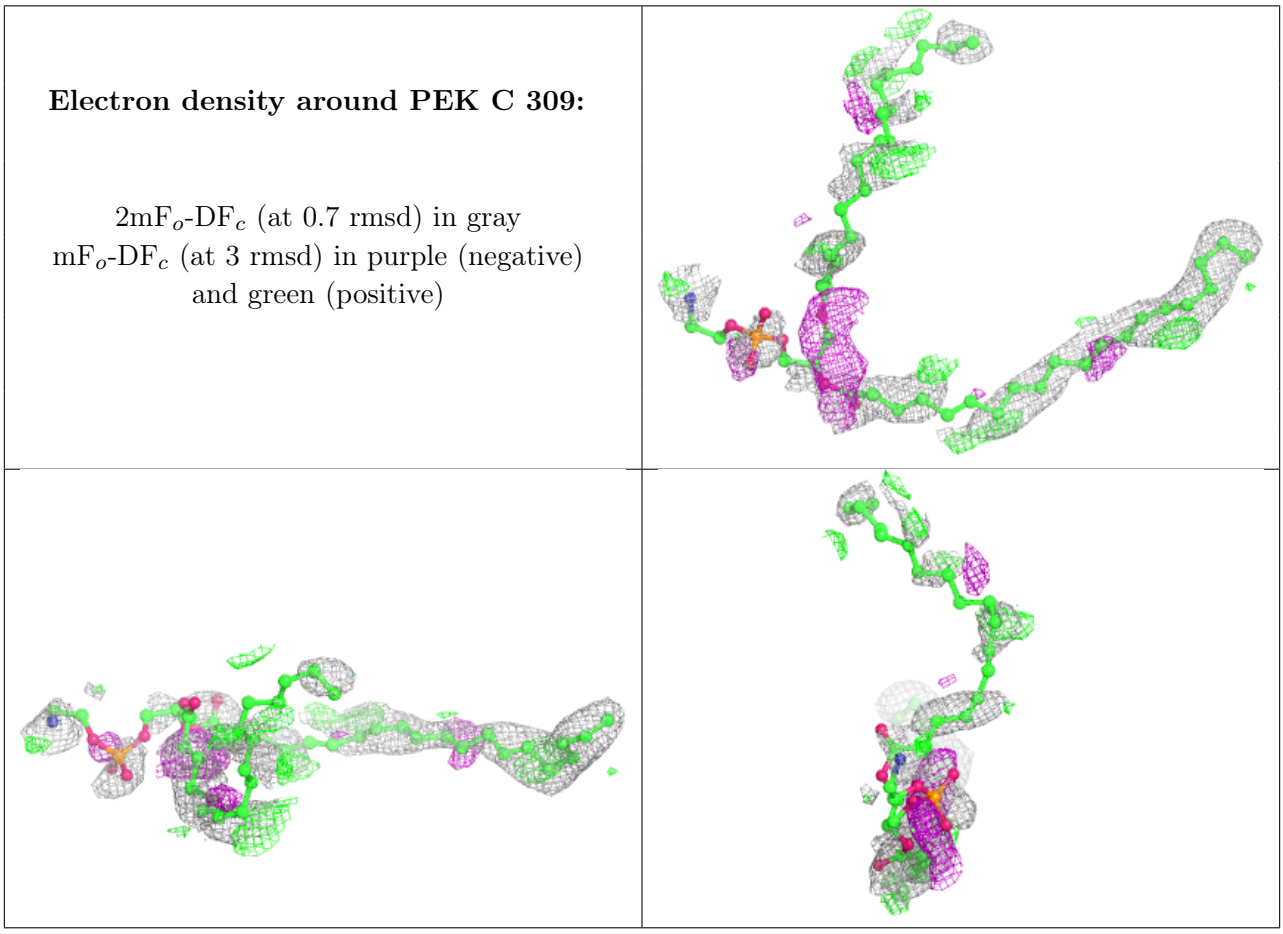
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	CDL	C	303	100/100	0.71	0.33	39,84,145,168	0
19	TGL	Q	201	63/63	0.71	0.23	40,80,119,139	0
19	TGL	L	101	63/63	0.75	0.22	39,58,106,124	0
27	DMU	Z	101	33/33	0.76	0.31	40,56,78,86	0
25	PGV	C	307	51/51	0.77	0.32	39,89,133,173	0
19	TGL	A	607	63/63	0.78	0.22	39,77,104,126	0
27	DMU	M	101	33/33	0.78	0.26	30,46,66,80	0
20	J6X	A	608	16/16	0.78	0.43	38,55,103,128	16
20	J6X	N	611	16/16	0.78	0.33	31,52,82,113	16
19	TGL	N	608	63/63	0.79	0.22	39,77,118,138	0
19	TGL	D	202	63/63	0.81	0.20	41,71,106,123	0
25	PGV	D	201	51/51	0.81	0.29	29,78,125,170	0
24	PEK	P	306	53/53	0.89	0.23	30,49,100,115	0
25	PGV	P	303	51/51	0.90	0.26	23,40,95,105	0
22	CHD	C	305	29/29	0.90	0.11	20,32,40,51	0
25	PGV	C	302	51/51	0.90	0.29	21,41,85,88	0
22	CHD	N	609	29/29	0.91	0.11	22,35,45,47	0
24	PEK	G	101	53/53	0.91	0.23	28,52,111,133	0
22	CHD	O	602	29/29	0.94	0.09	17,26,37,46	0
14	HEA	A	601[C]	60/60	0.95	0.14	10,28,49,53	18
14	HEA	A	601[D]	60/60	0.95	0.14	6,28,44,55	18
14	HEA	N	601[C]	60/60	0.95	0.17	17,33,60,66	18
25	PGV	C	301	51/51	0.95	0.23	18,41,60,72	0
14	HEA	N	601[D]	60/60	0.95	0.17	7,28,41,43	18
22	CHD	B	602	29/29	0.95	0.08	16,27,39,50	0
28	ZN	S	101	1/1	0.95	0.14	25,25,25,25	0
14	HEA	A	602	60/60	0.96	0.12	15,24,39,44	0
14	HEA	N	602	60/60	0.96	0.12	17,26,38,41	0
25	PGV	N	607	51/51	0.96	0.18	18,43,66,75	0
28	ZN	F	101	1/1	0.97	0.17	25,25,25,25	0
18	PER	N	606	2/2	0.97	0.25	50,50,50,61	0
16	MG	A	604	1/1	0.98	0.10	14,14,14,14	0
17	NA	N	605	1/1	0.98	0.08	19,19,19,19	0
18	PER	A	606	2/2	0.98	0.13	45,45,45,54	0
15	CU	N	603	1/1	0.98	0.03	20,20,20,20	0
16	MG	N	604	1/1	0.99	0.10	16,16,16,16	0
21	CUA	B	601	2/2	0.99	0.02	19,19,19,21	0
21	CUA	O	601	2/2	0.99	0.03	22,22,22,23	0
17	NA	A	605	1/1	0.99	0.07	16,16,16,16	0
15	CU	A	603	1/1	0.99	0.03	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

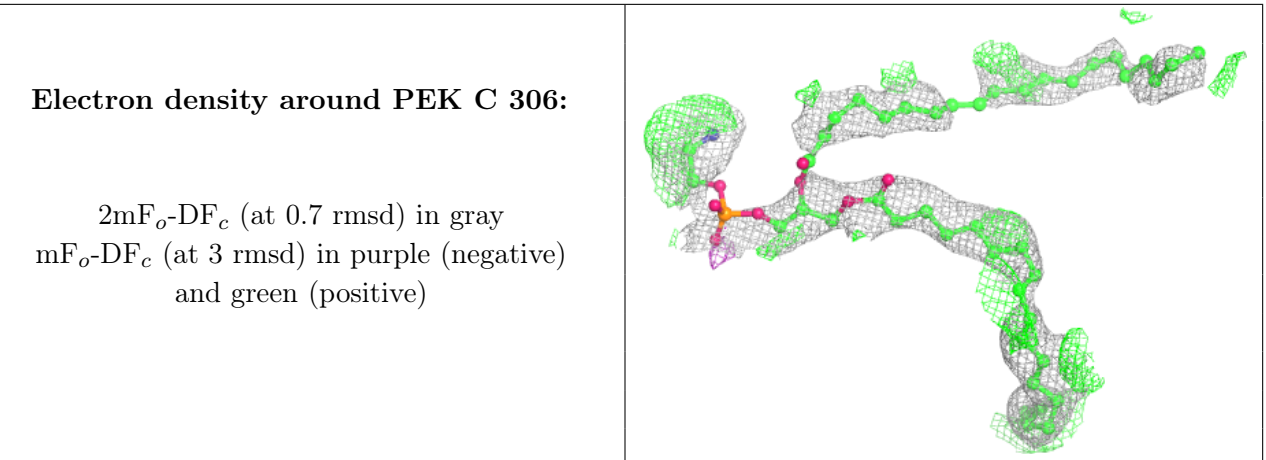
Electron density around PEK C 309:

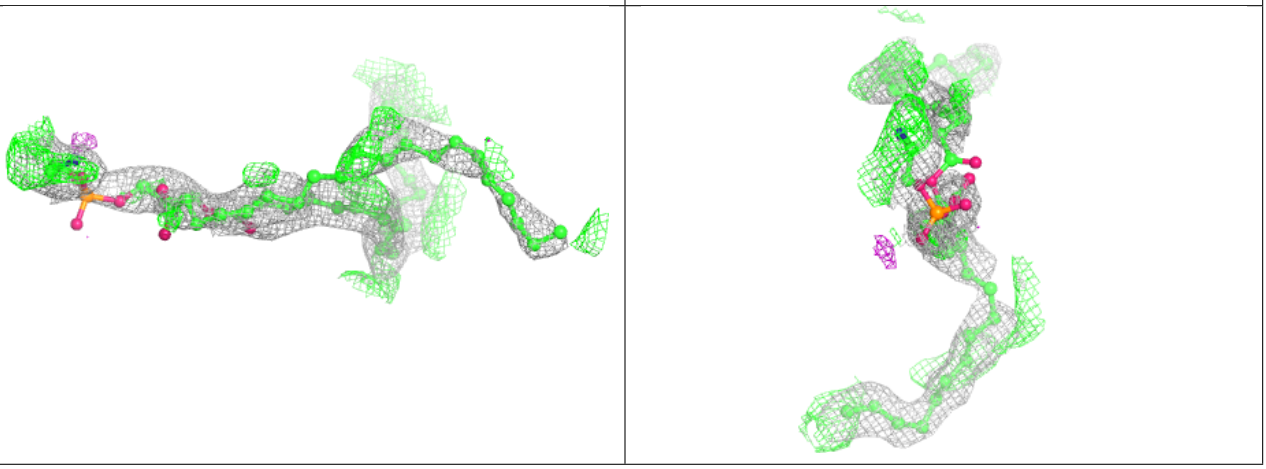
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PEK C 306:

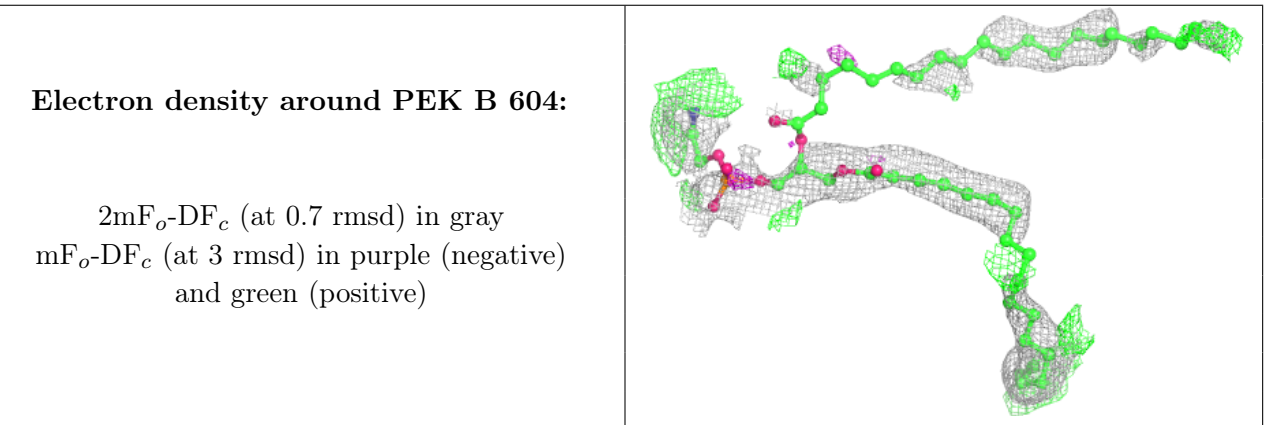
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

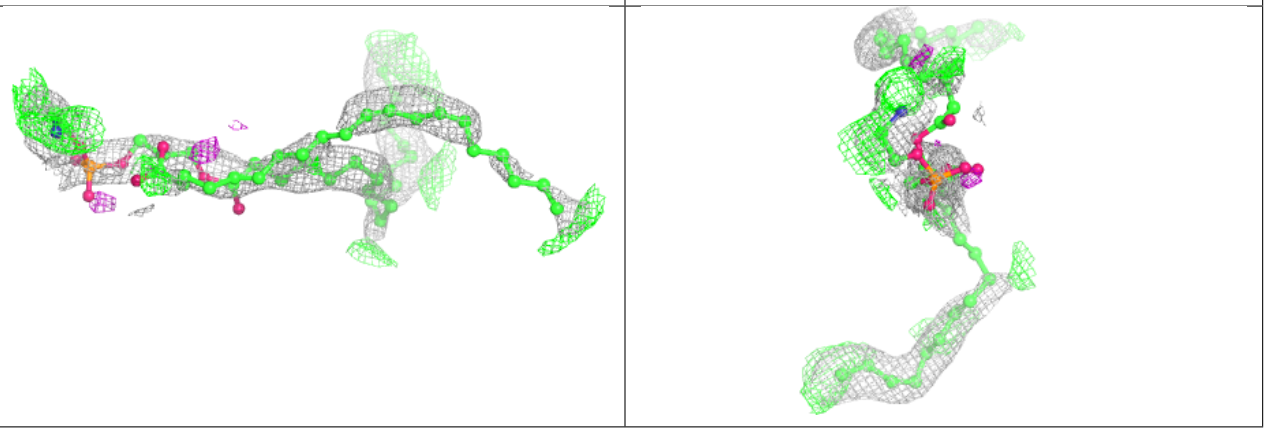




Electron density around PEK B 604:

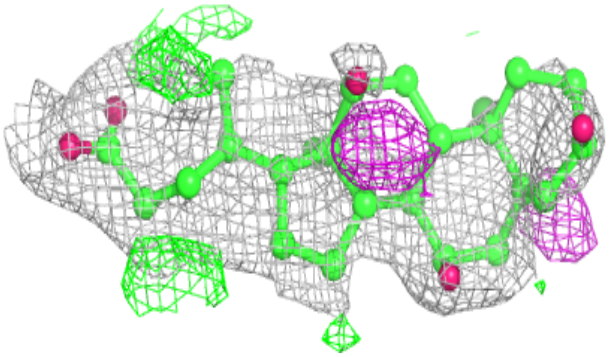
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

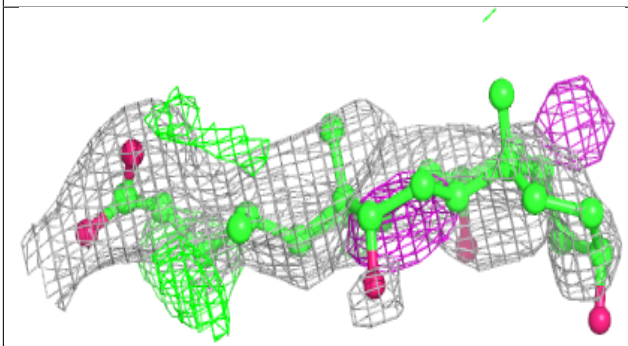


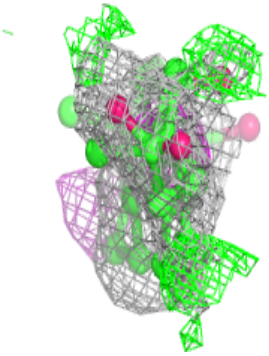


Electron density around CHD P 305:

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

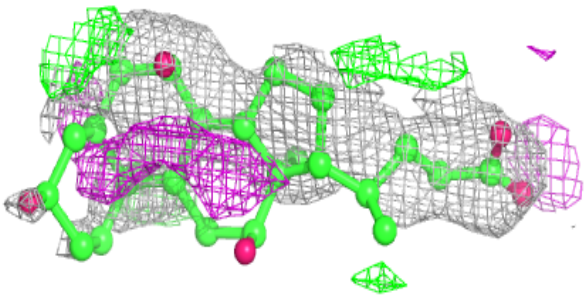


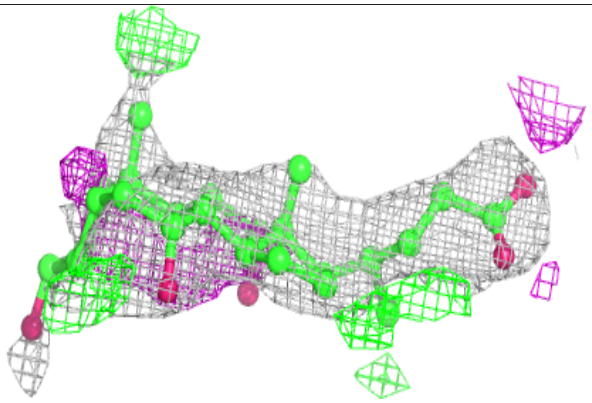


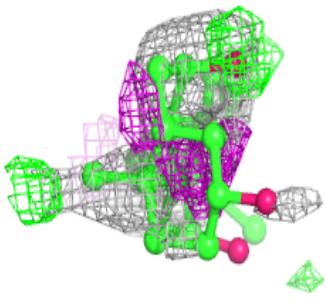


Electron density around CHD C 304:

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

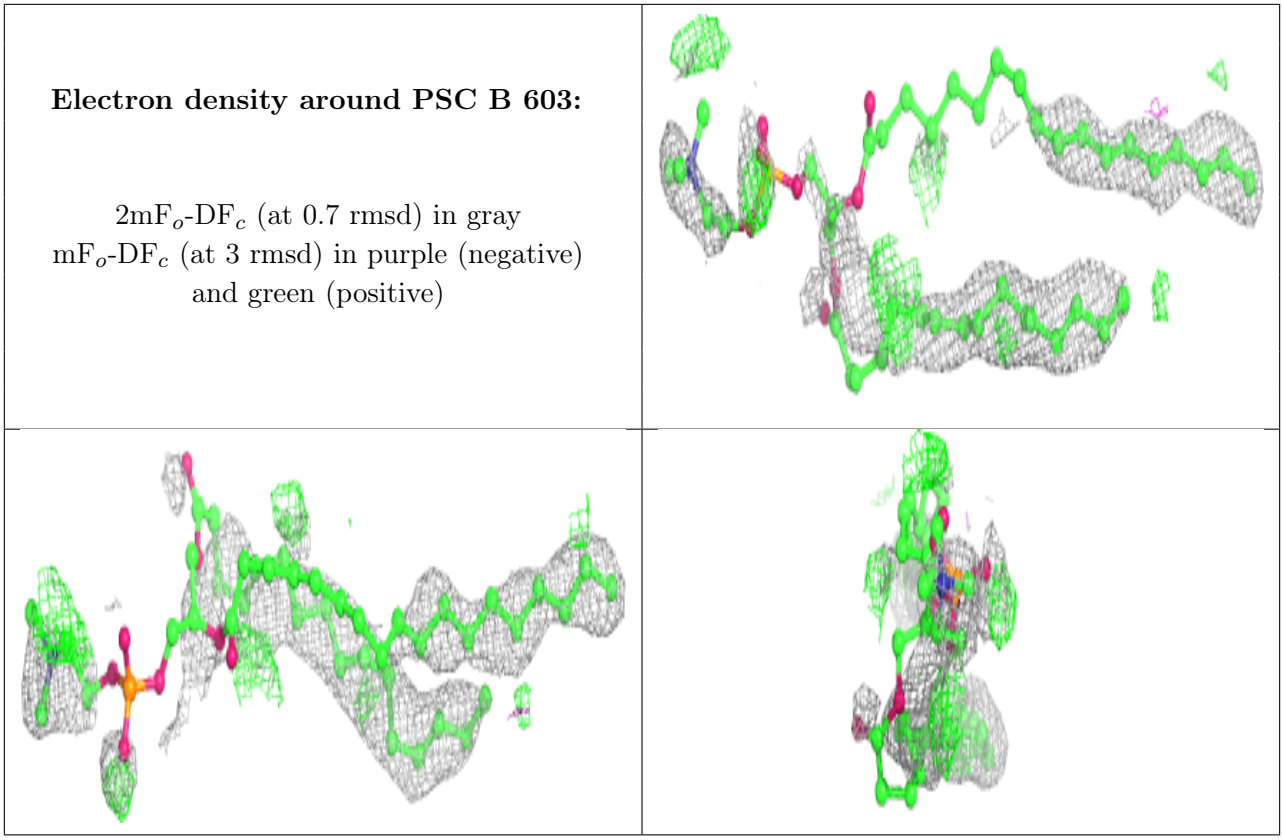






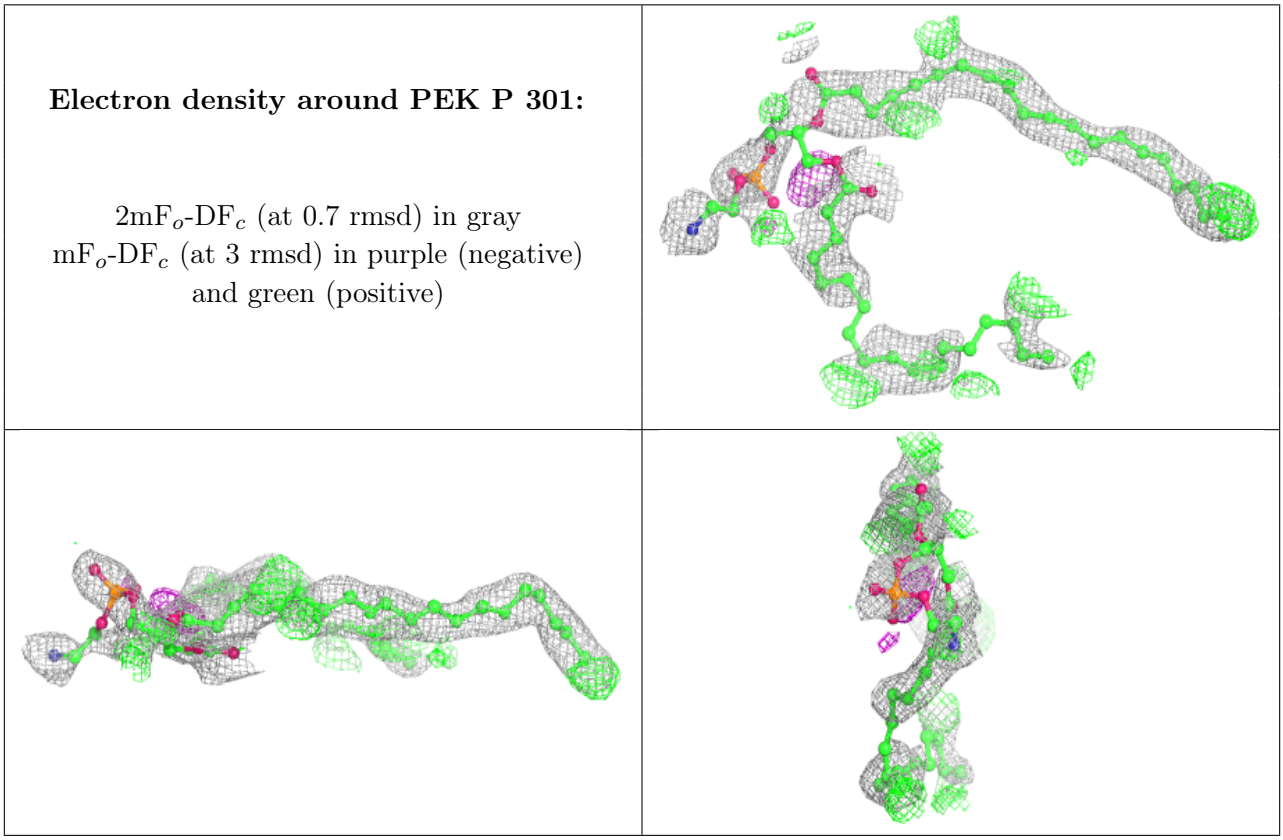
Electron density around PSC B 603:

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



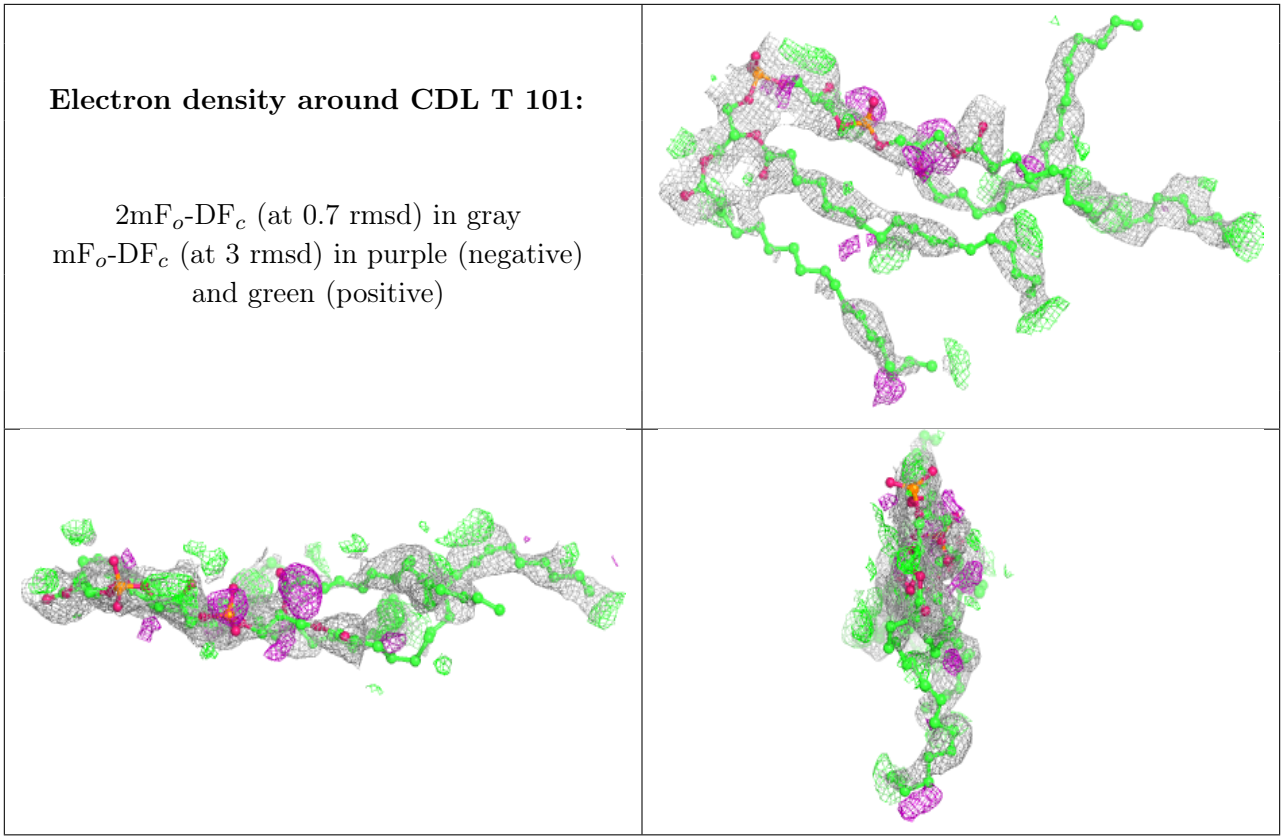
Electron density around PEK P 301:

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



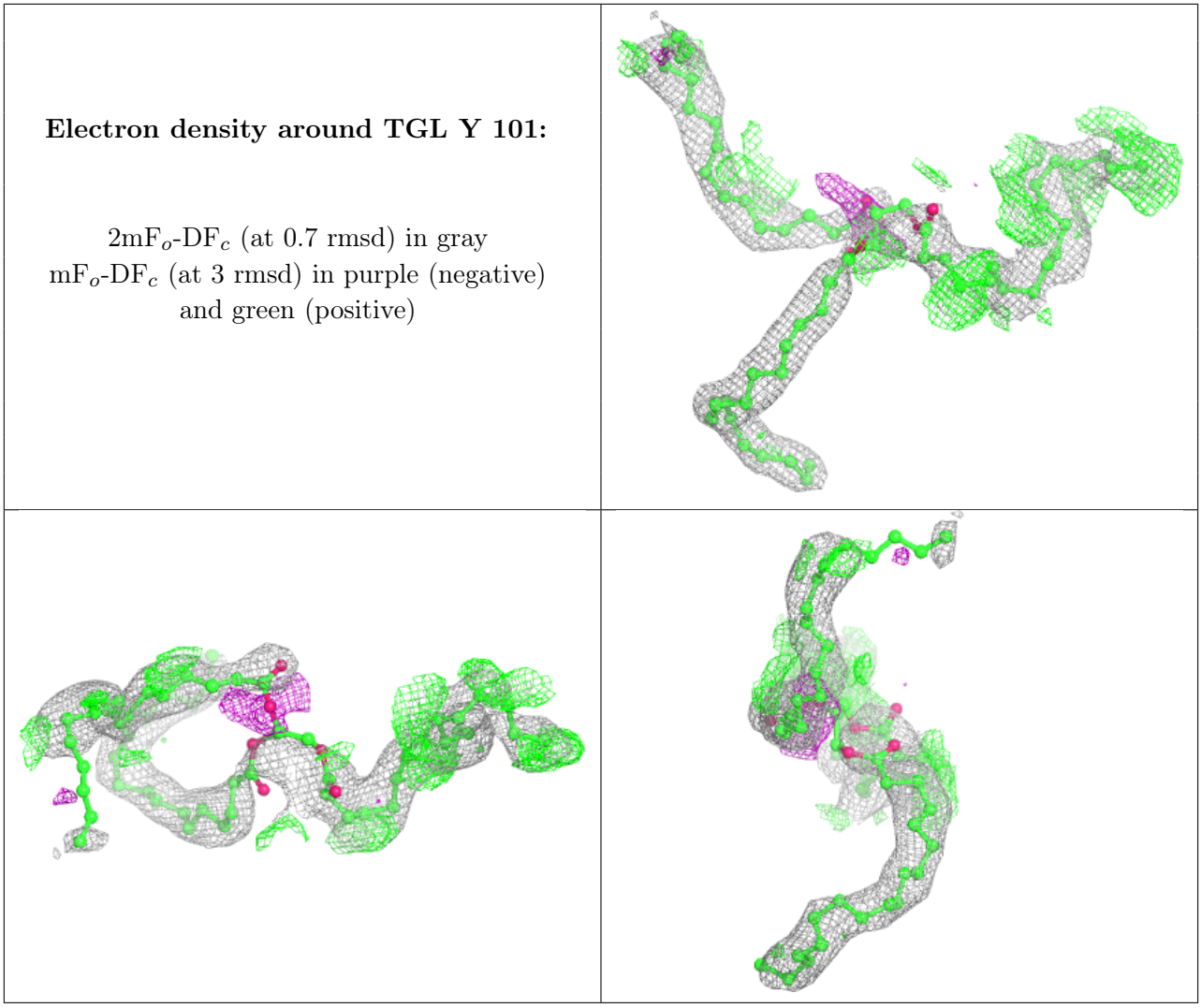
Electron density around CDL T 101:

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



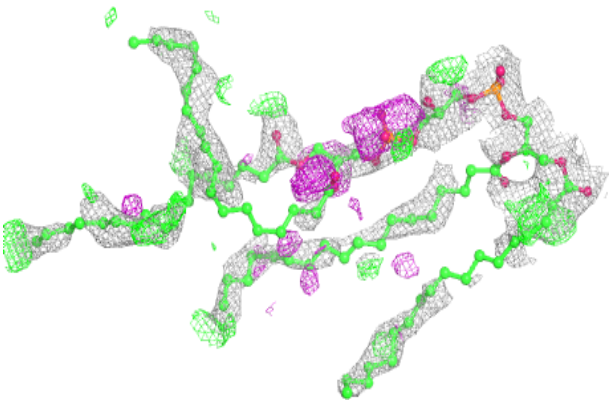
Electron density around TGL Y 101:

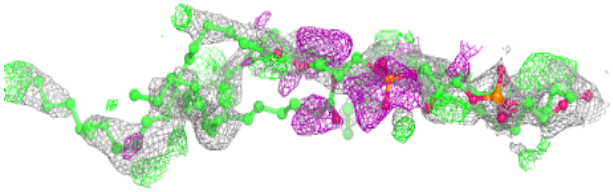
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

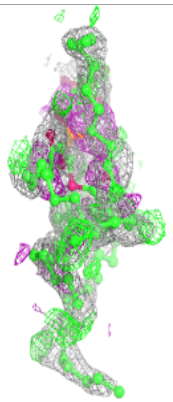


Electron density around CDL G 102:

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

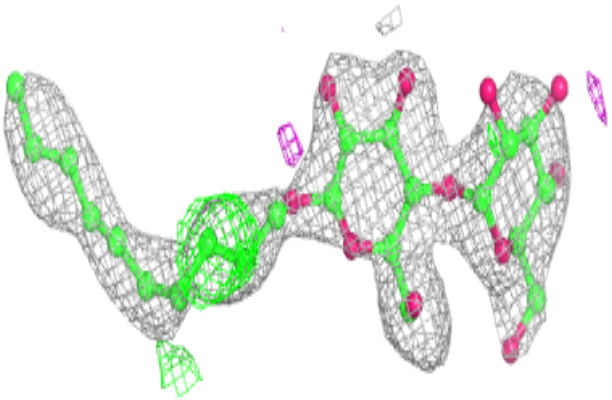


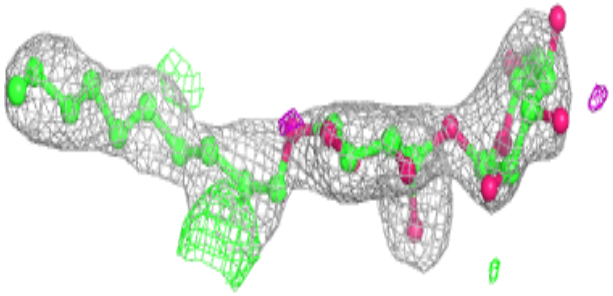


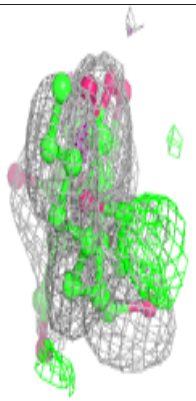


Electron density around DMU C 308:

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

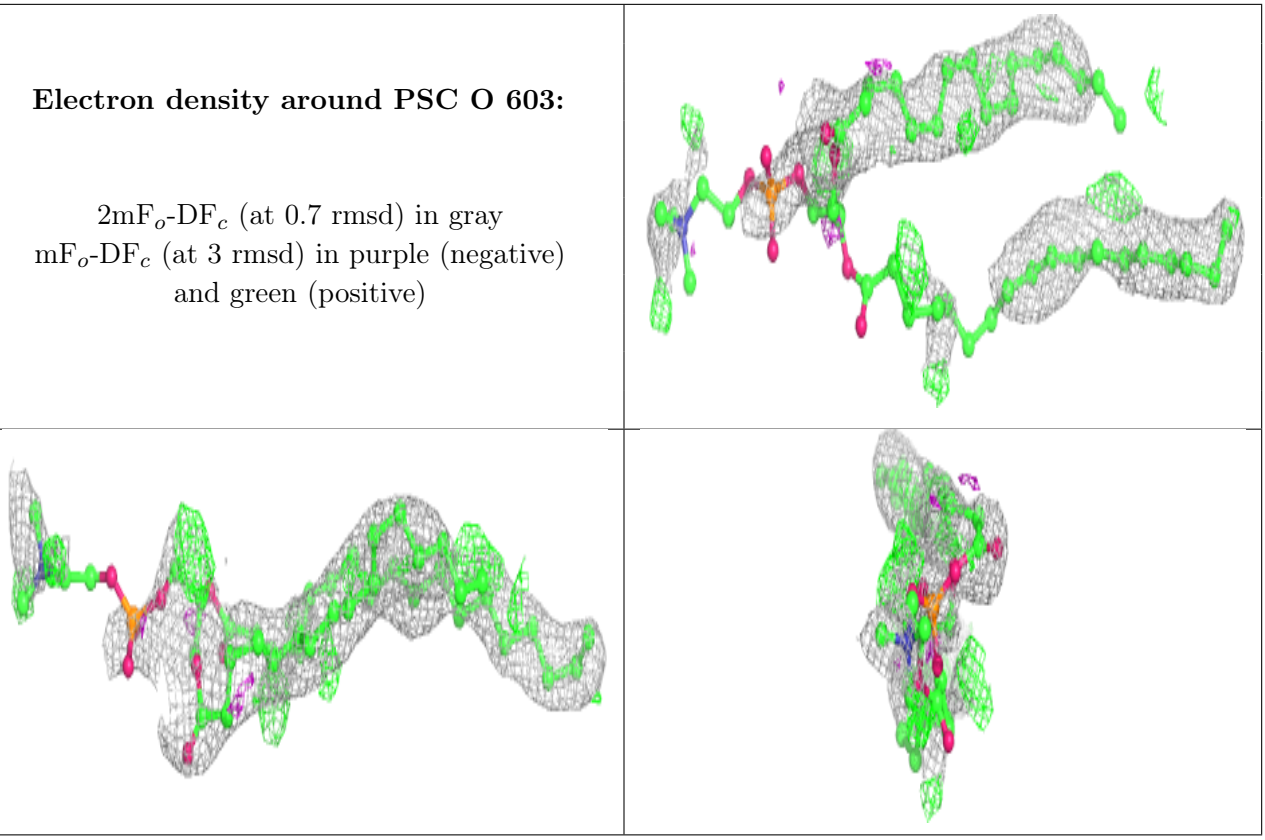






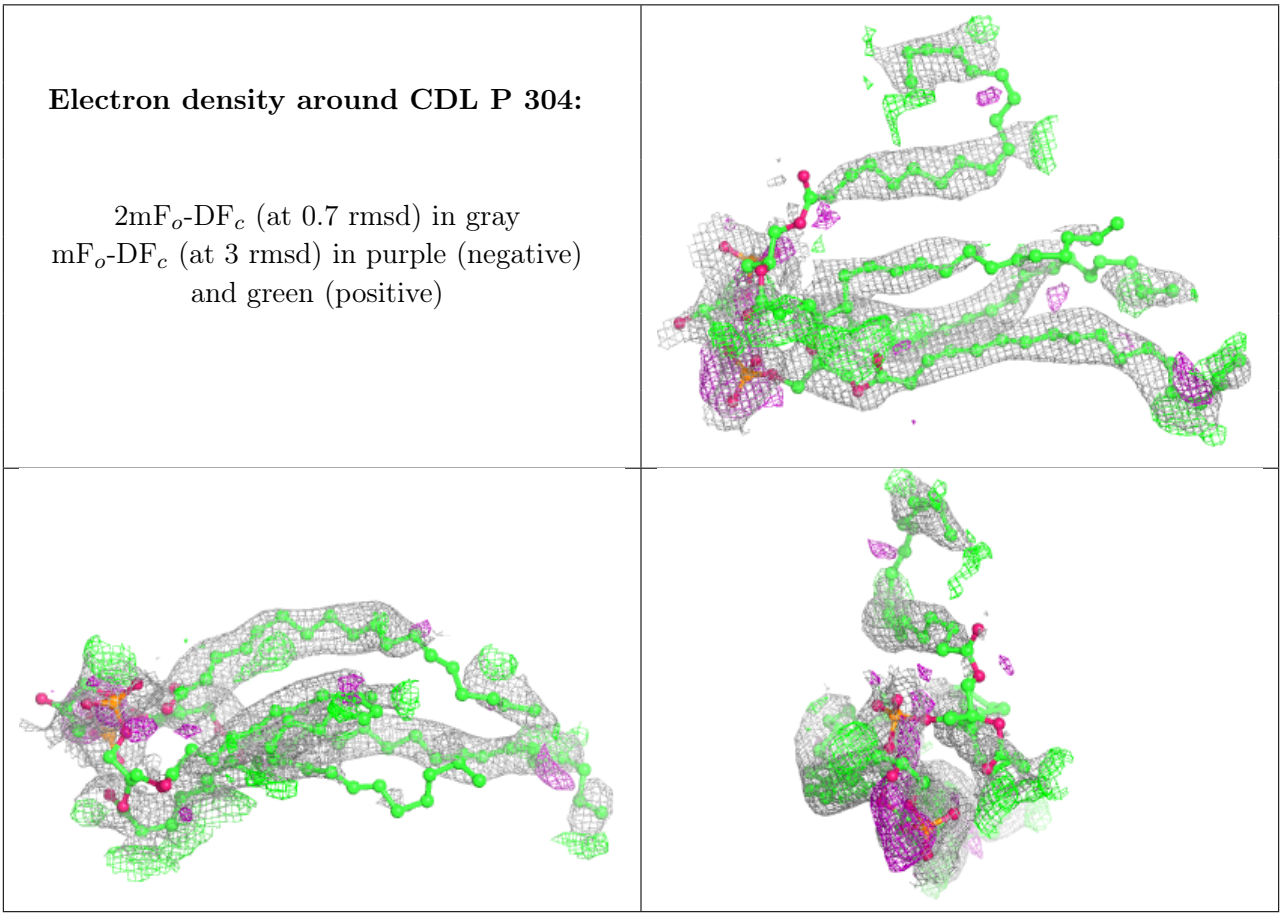
Electron density around PSC O 603:

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



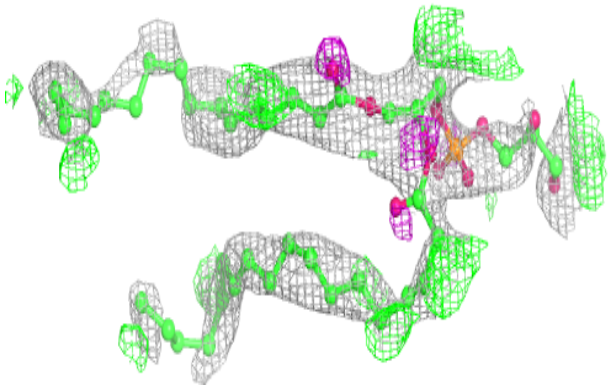
Electron density around CDL P 304:

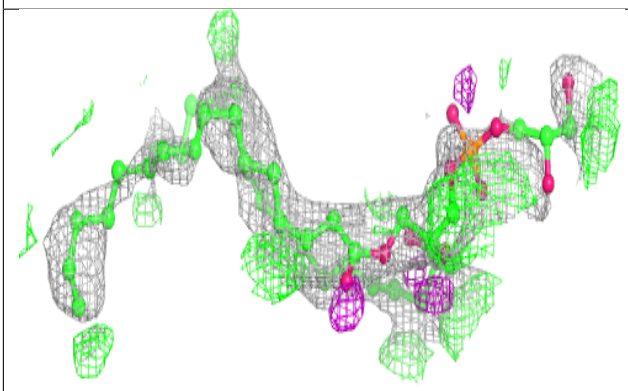
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

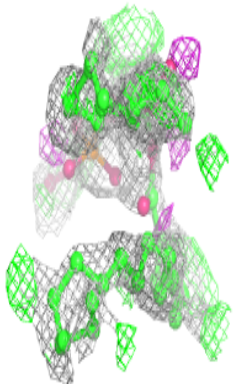


Electron density around PGV P 302:

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

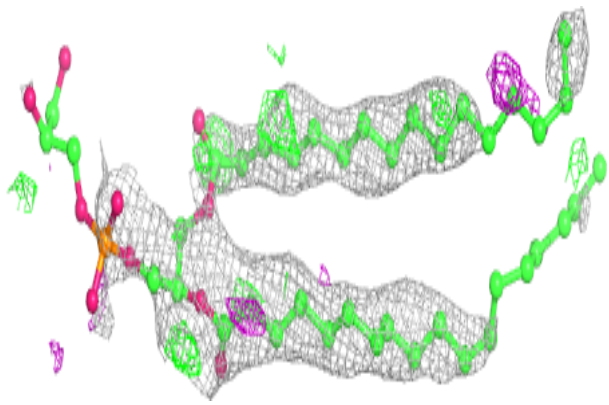


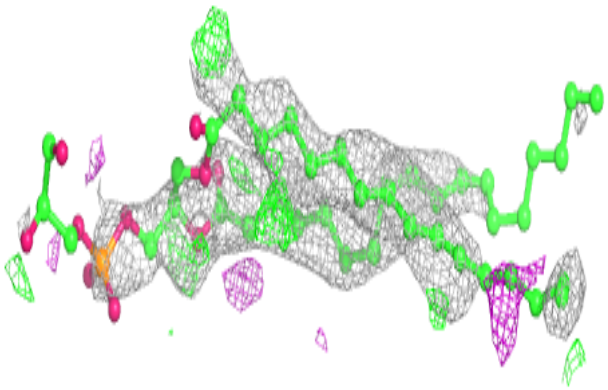


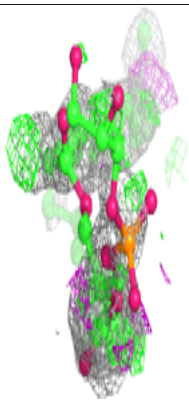


Electron density around PGV N 610:

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

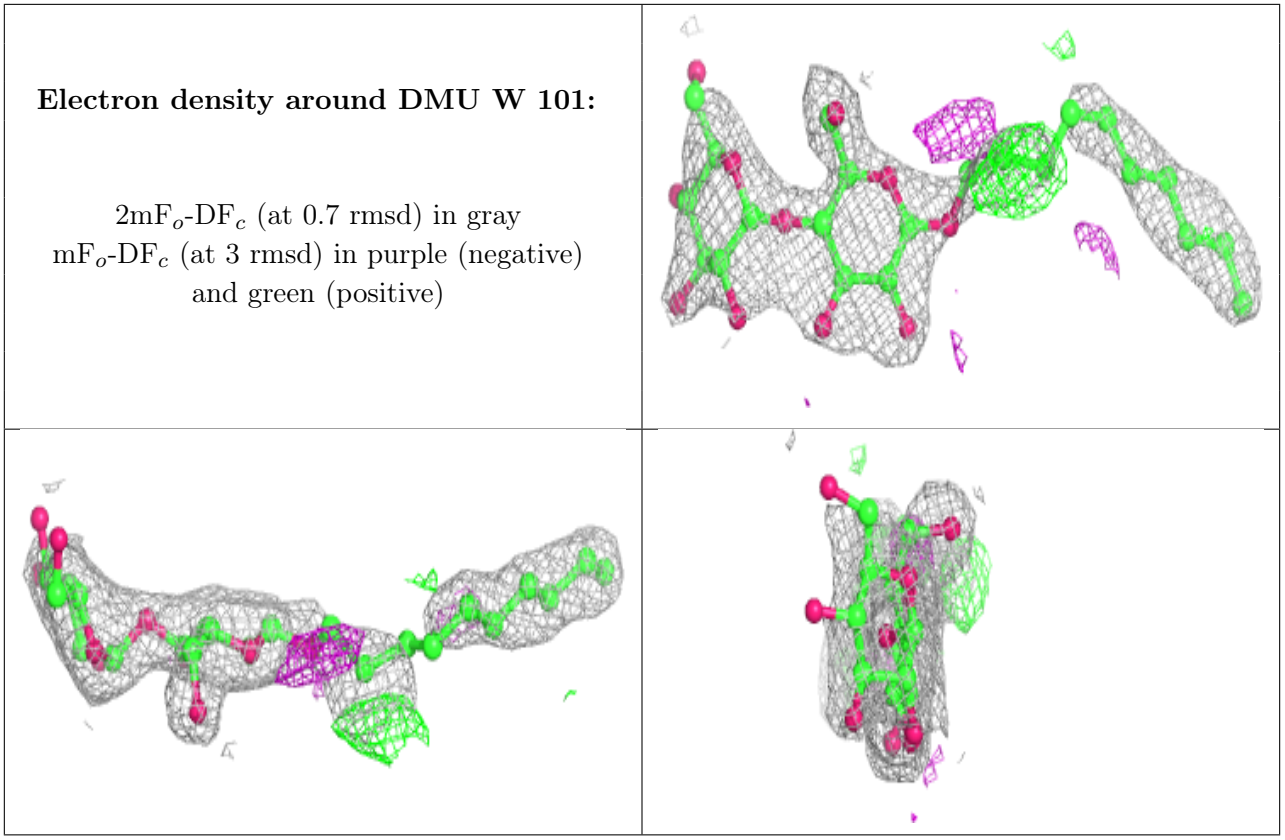






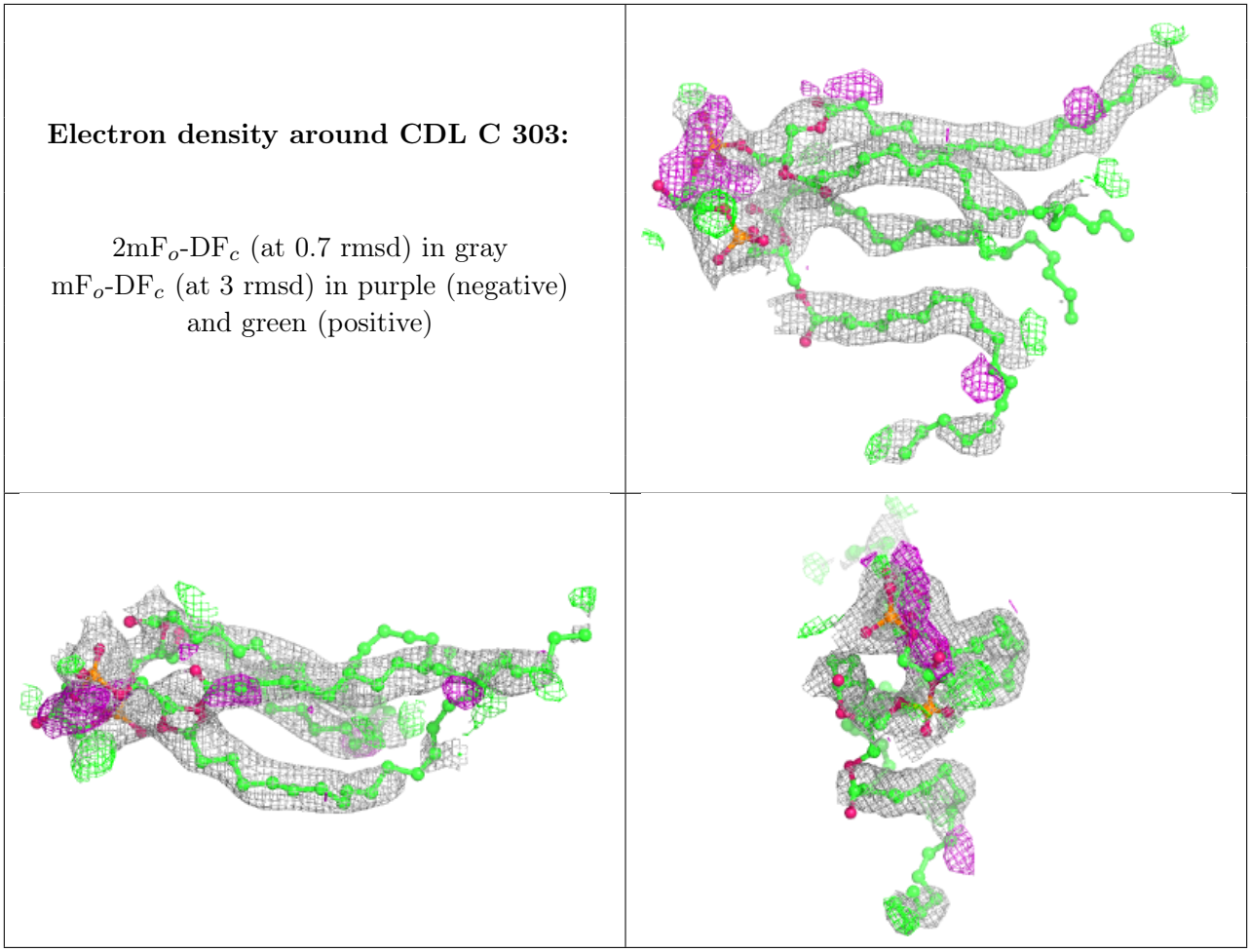
Electron density around DMU W 101:

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



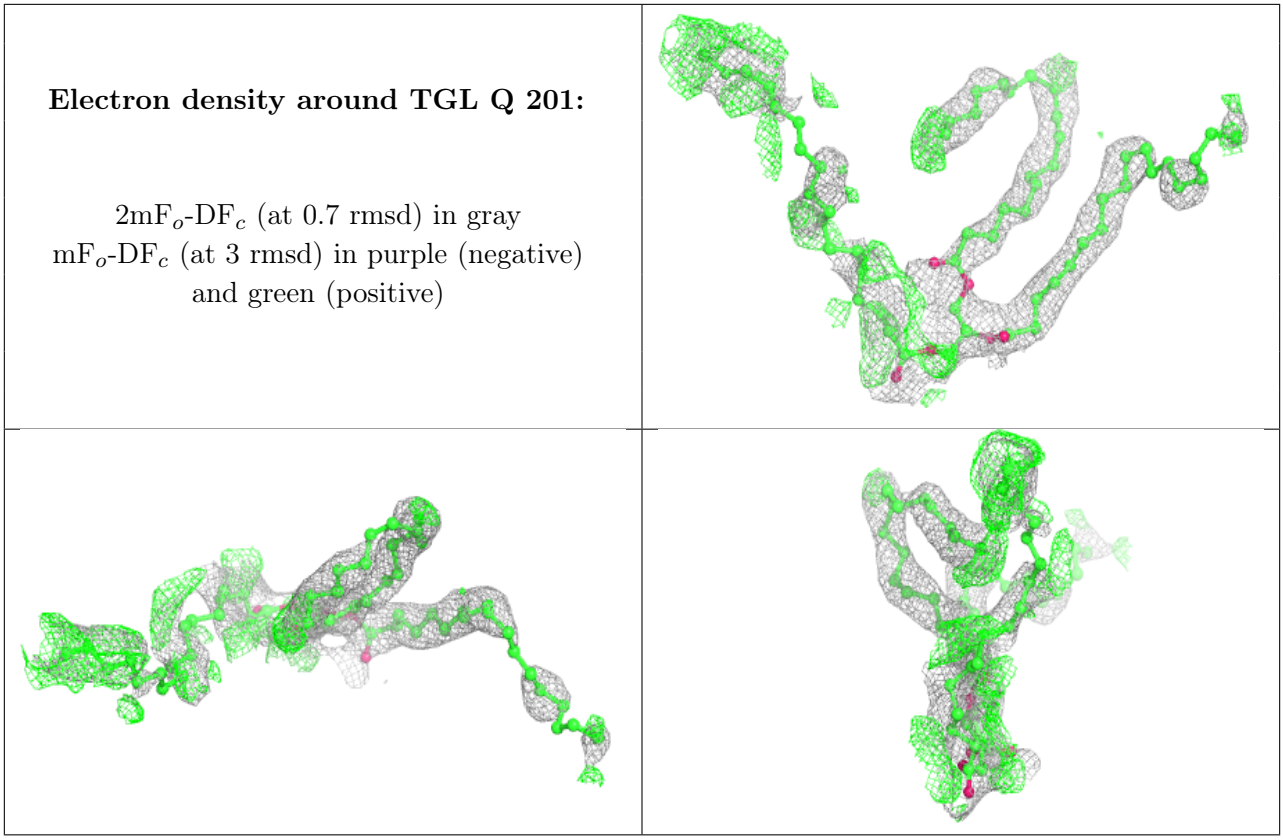
Electron density around CDL C 303:

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



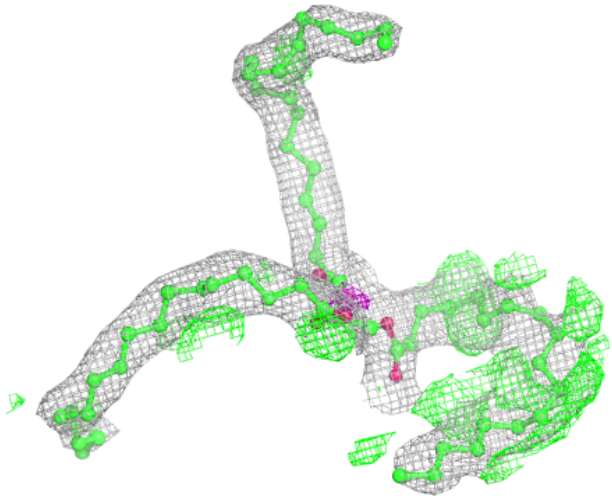
Electron density around TGL Q 201:

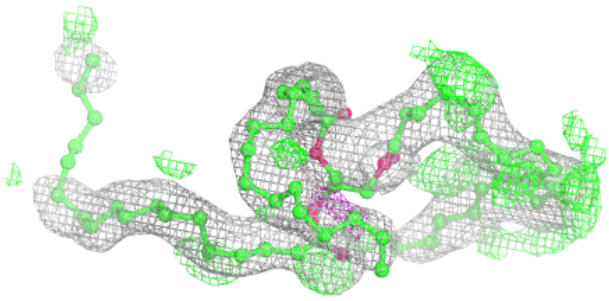
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

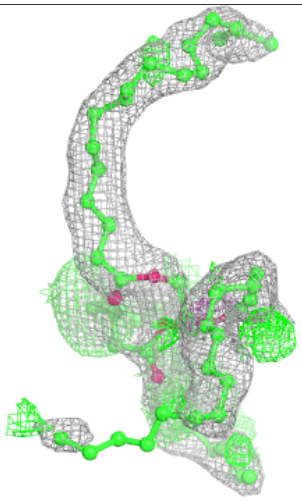


Electron density around TGL L 101:

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

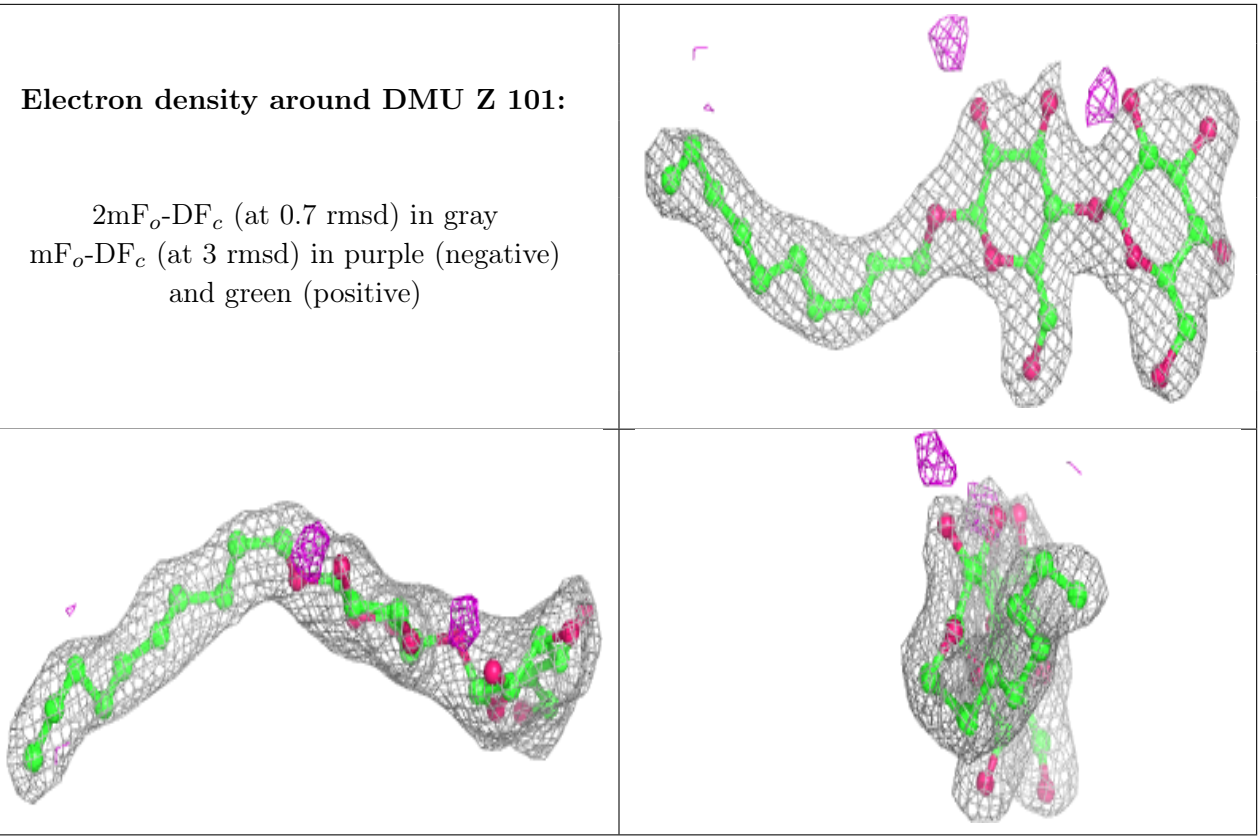






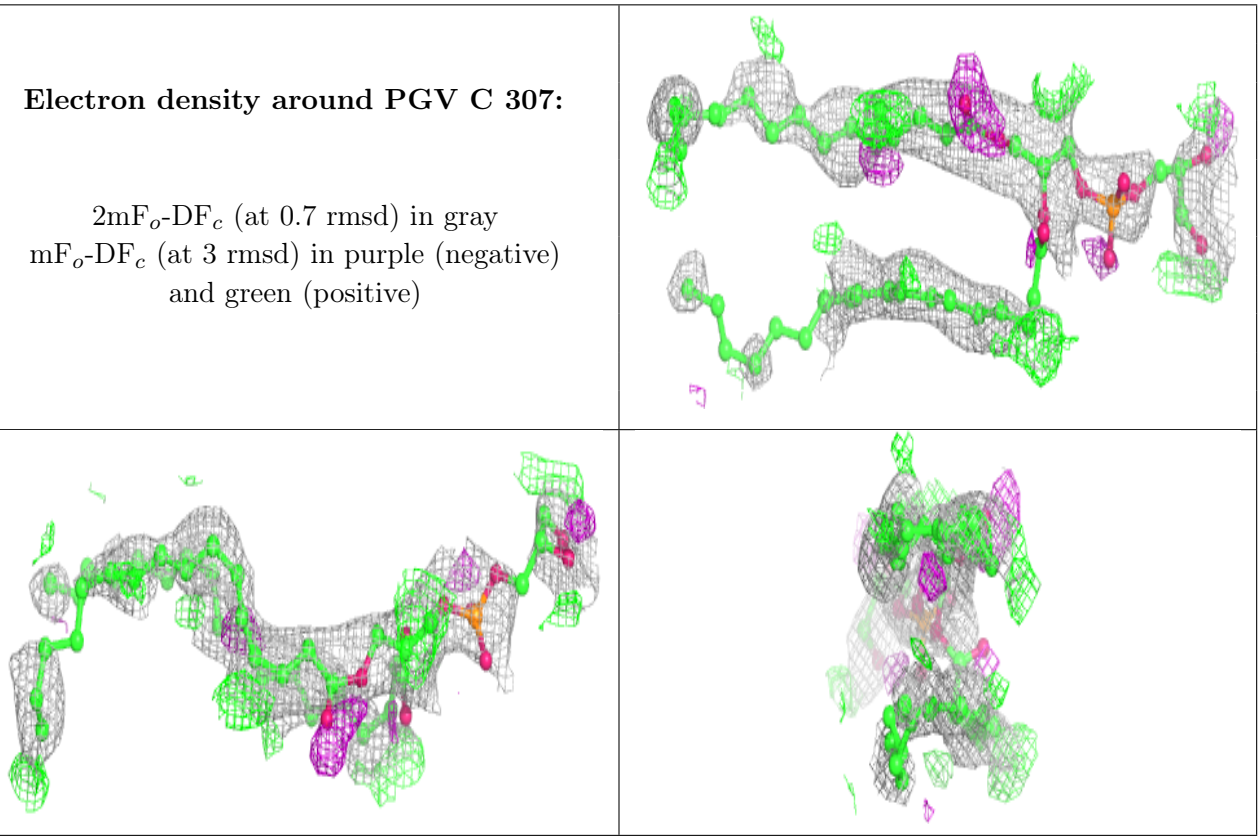
Electron density around DMU Z 101:

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



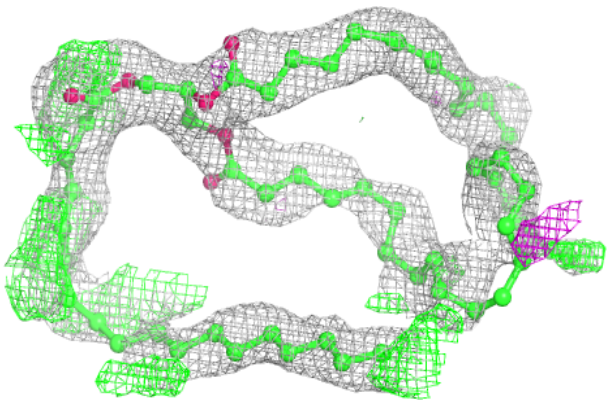
Electron density around PGV C 307:

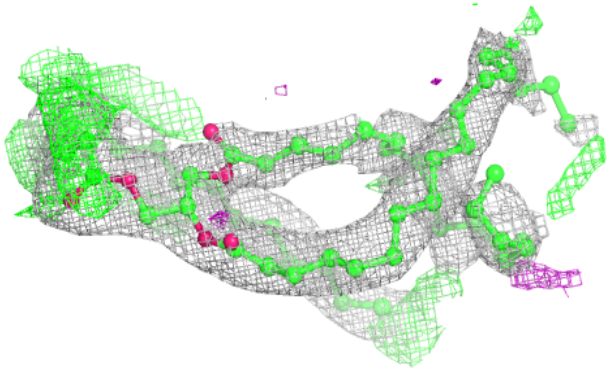
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

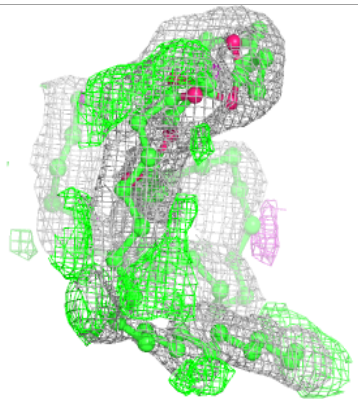


Electron density around TGL A 607:

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

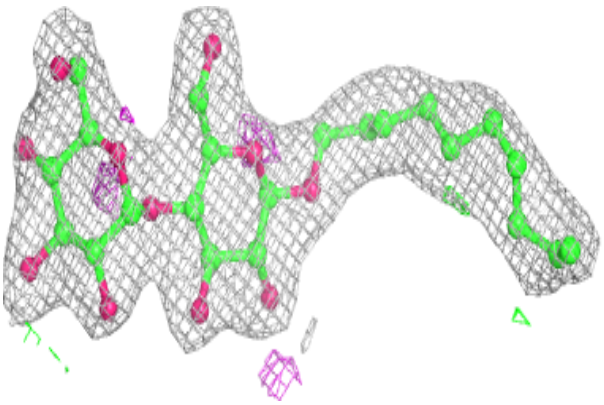


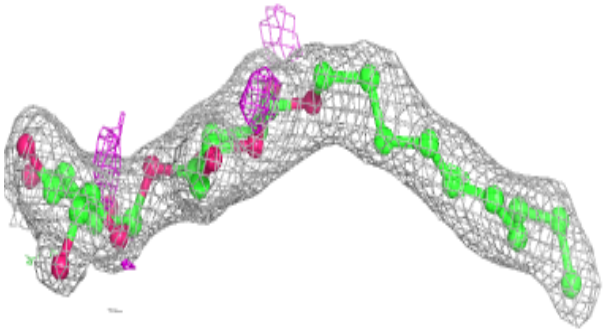


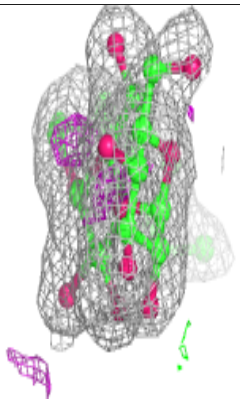


Electron density around DMU M 101:

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

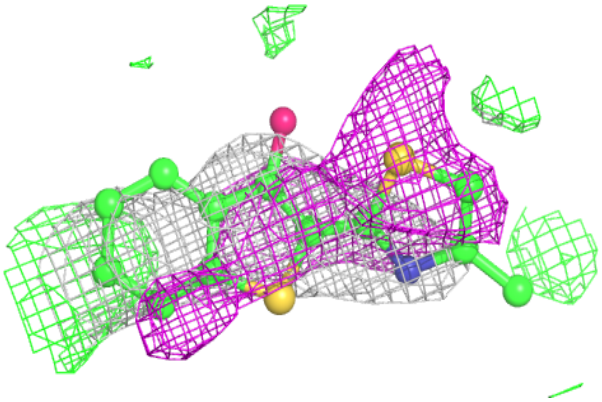


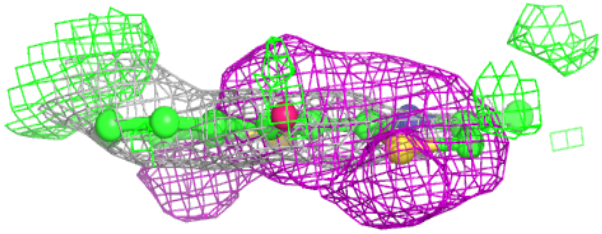


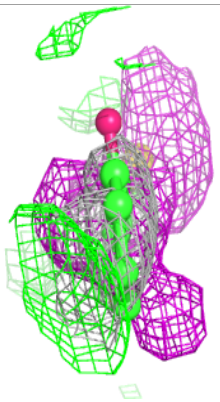


Electron density around J6X A 608:

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

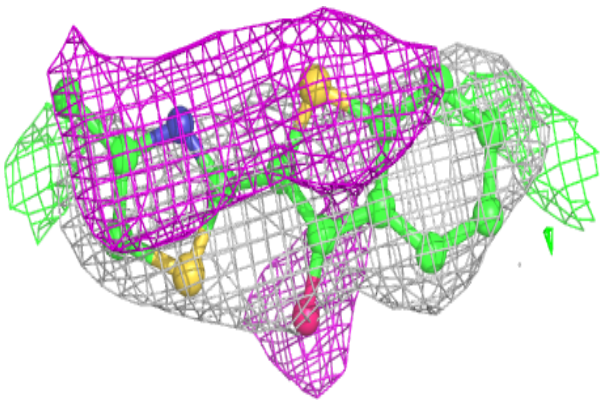


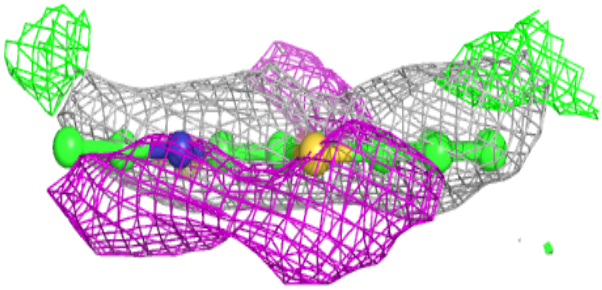


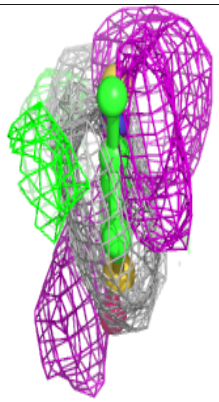


Electron density around J6X N 611:

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

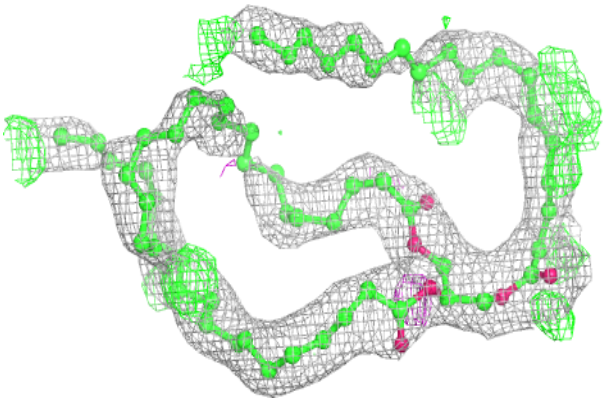


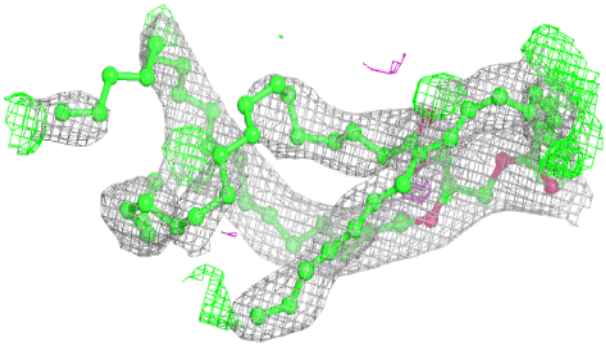


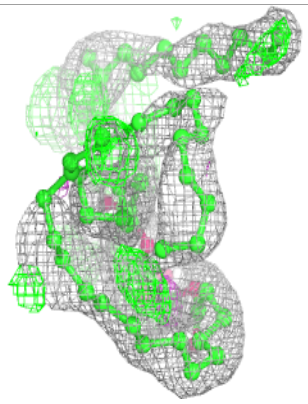


Electron density around TGL N 608:

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

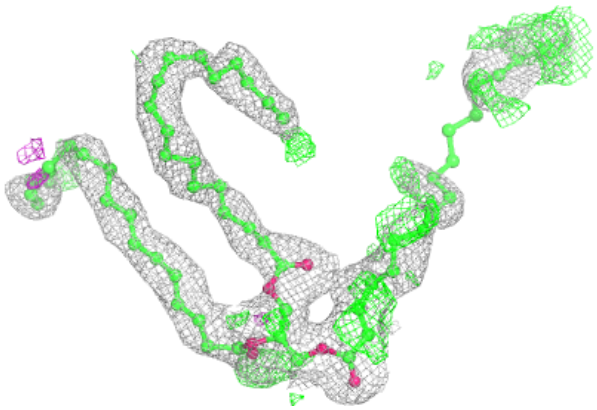


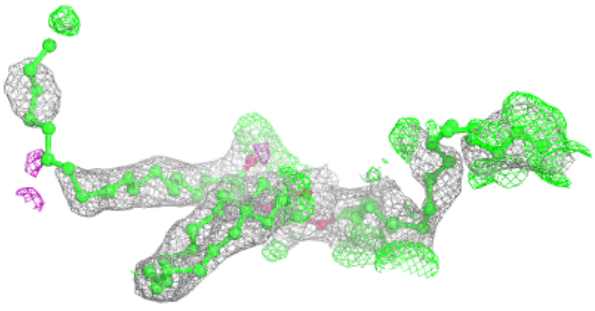


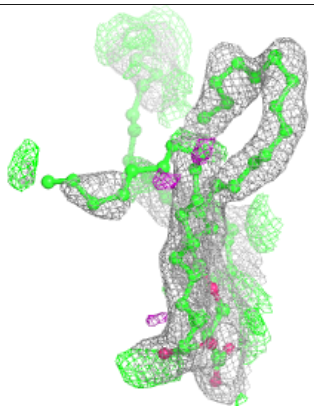


Electron density around TGL D 202:

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

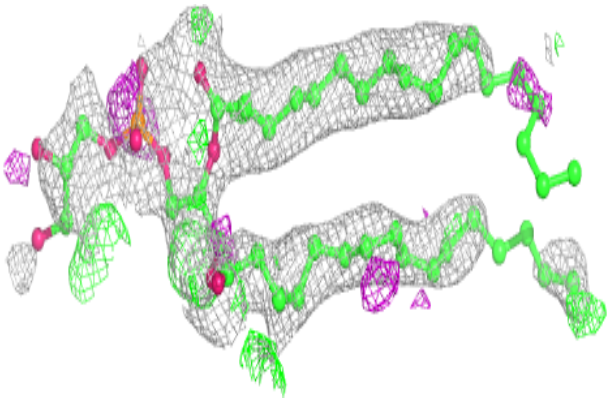


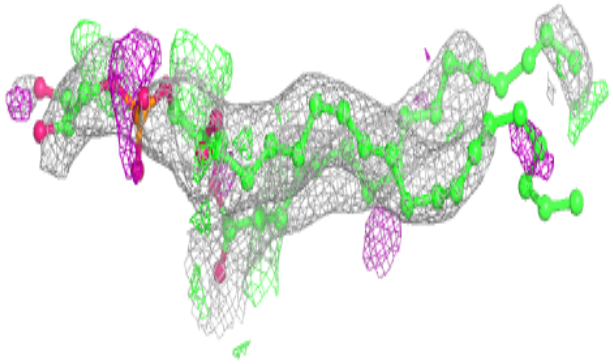


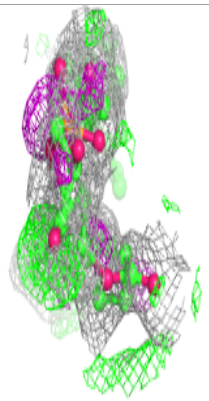


Electron density around PGV D 201:

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

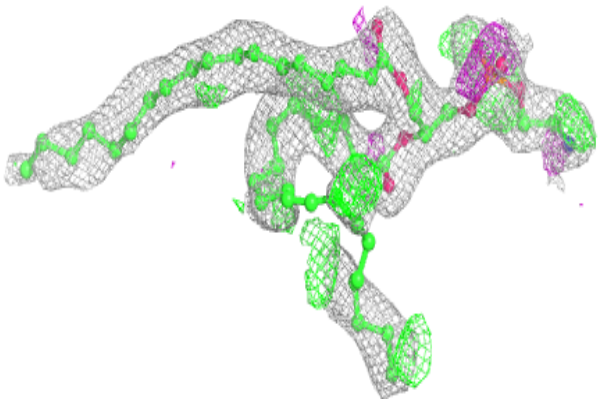


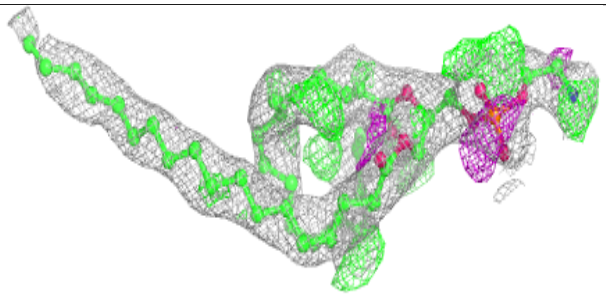


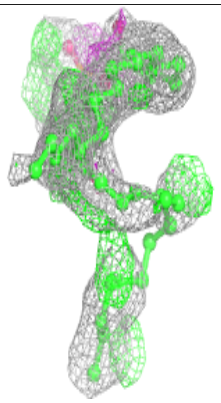


Electron density around PEK P 306:

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

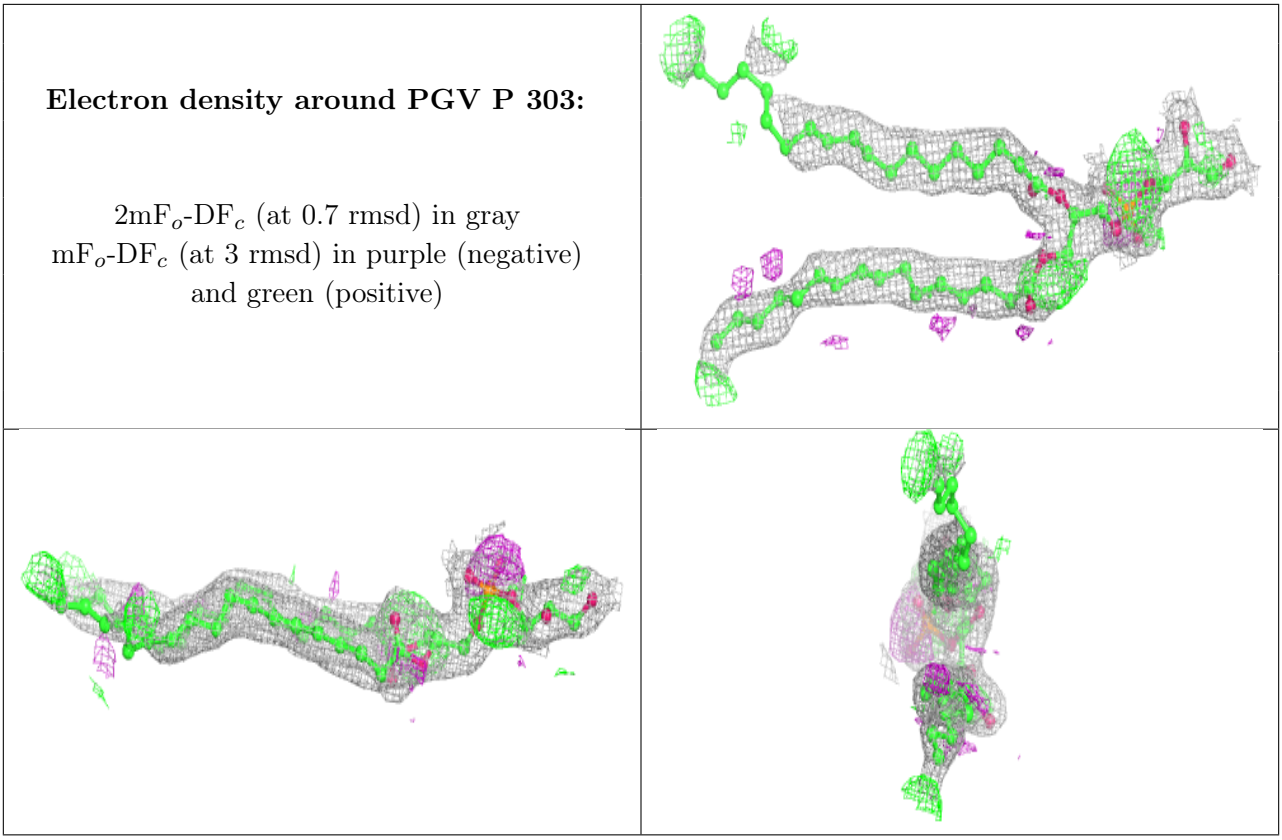






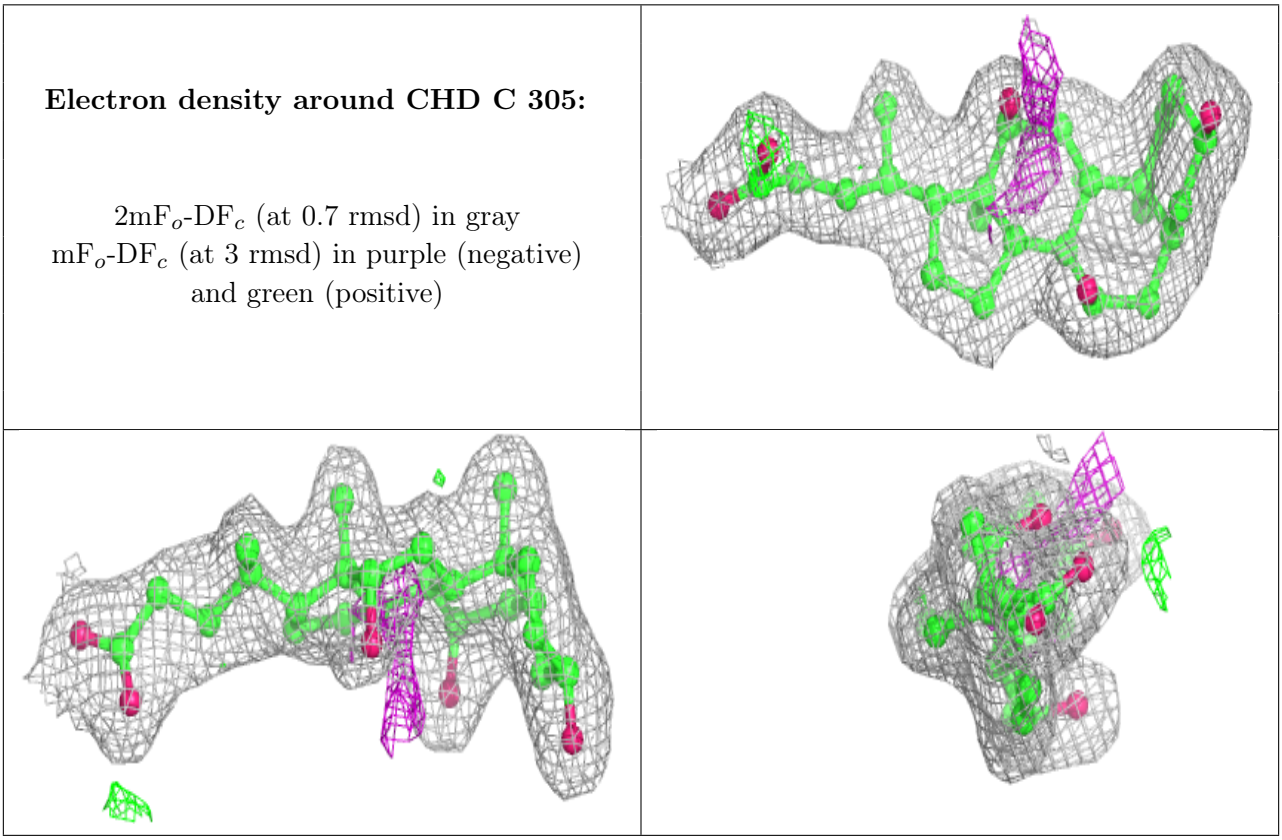
Electron density around PGV P 303:

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



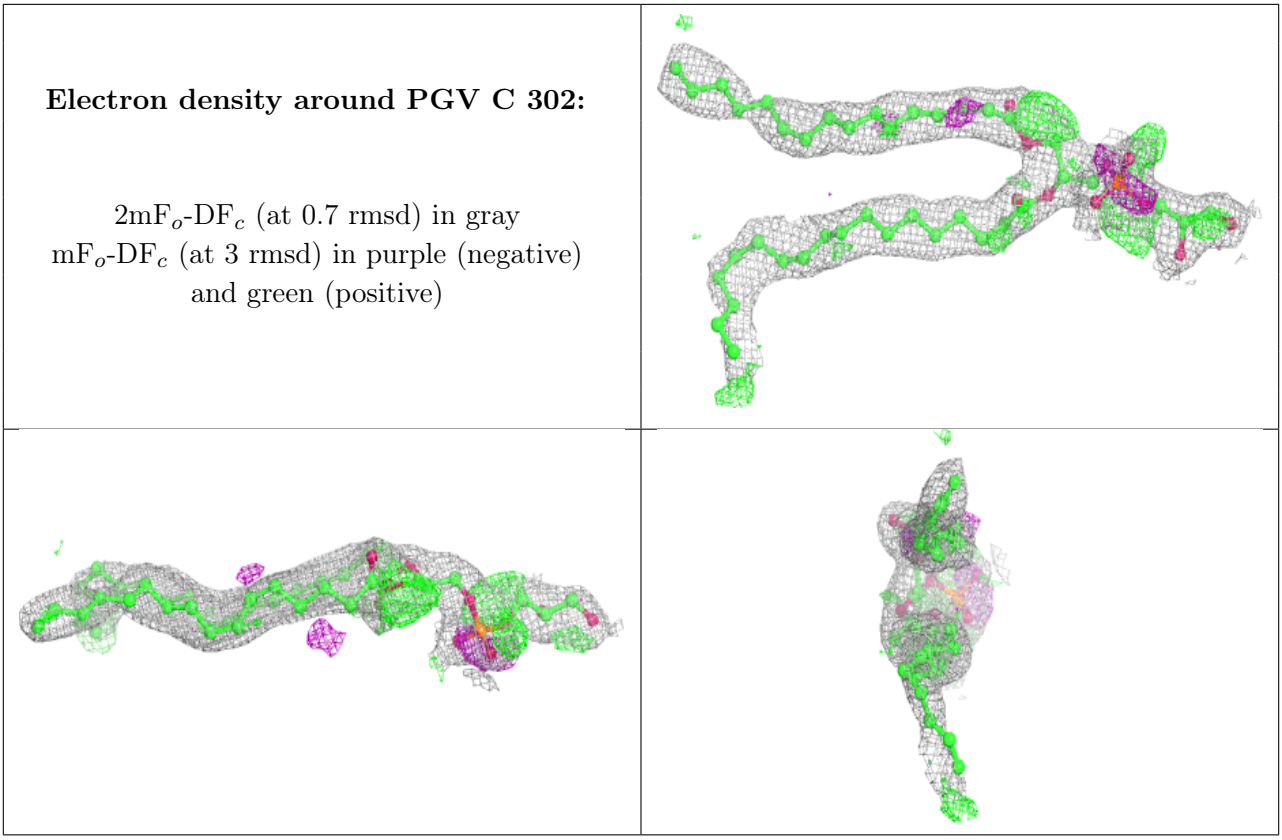
Electron density around CHD C 305:

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



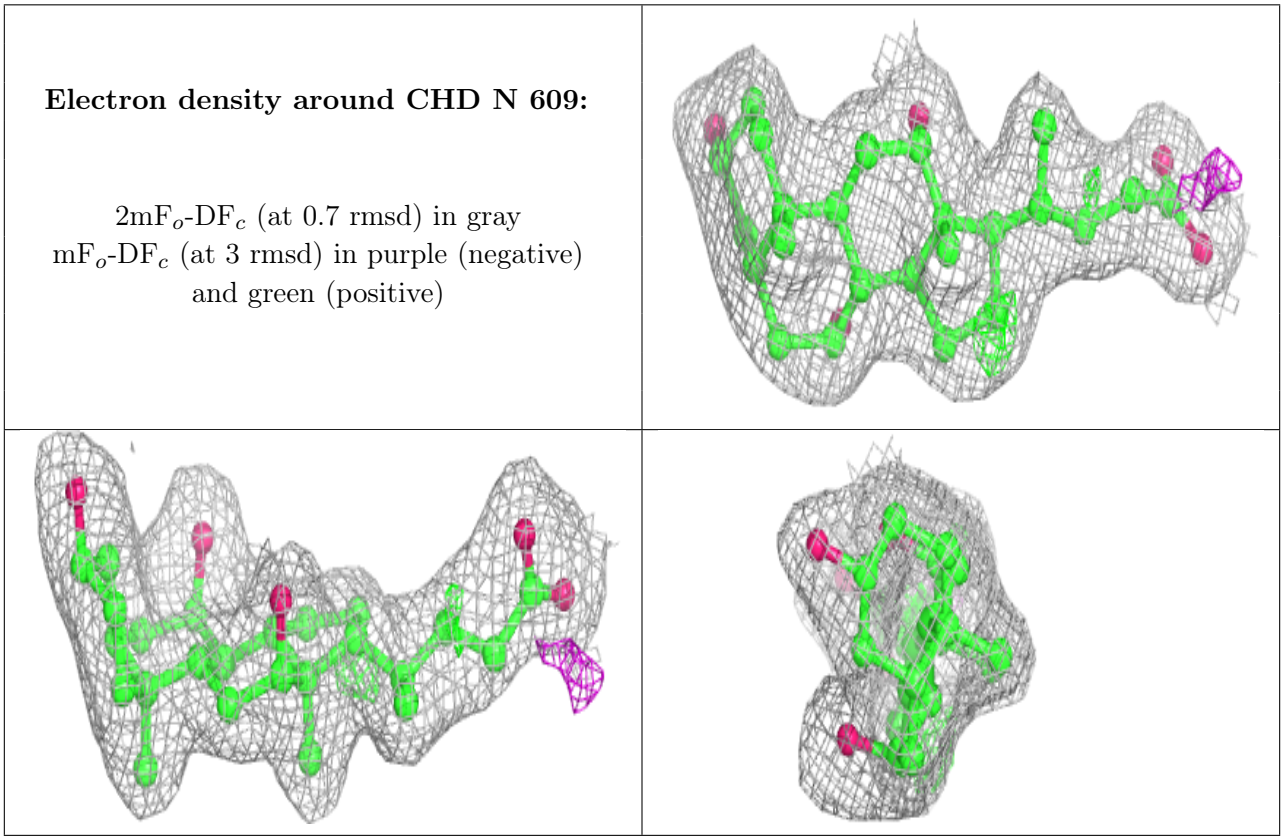
Electron density around PGV C 302:

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



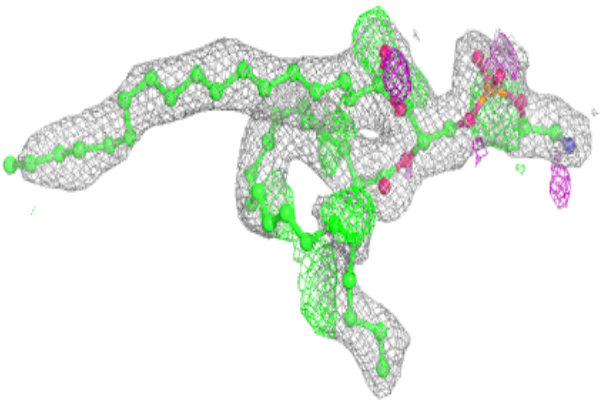
Electron density around CHD N 609:

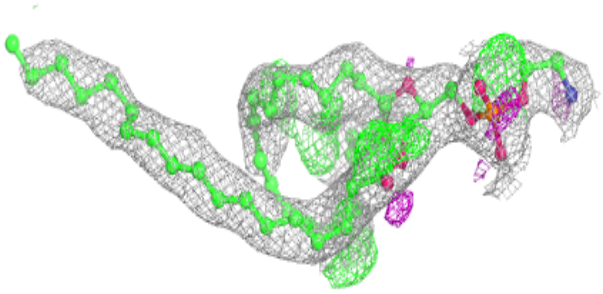
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

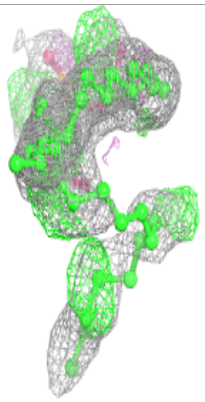


Electron density around PEK G 101:

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

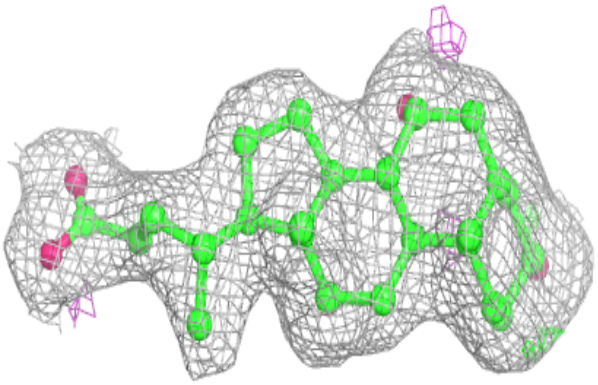


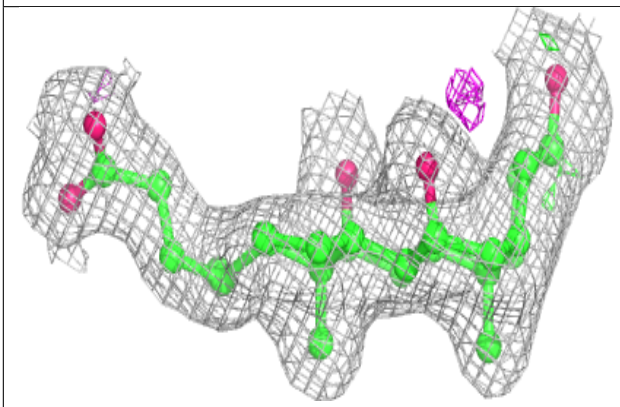


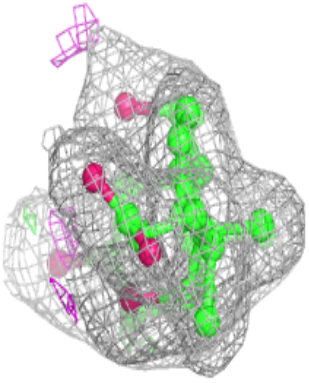


Electron density around CHD O 602:

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

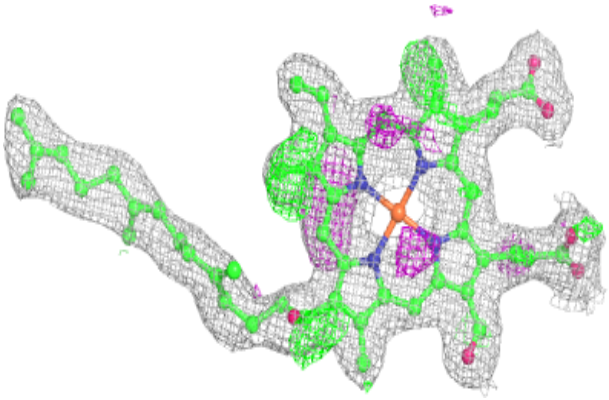


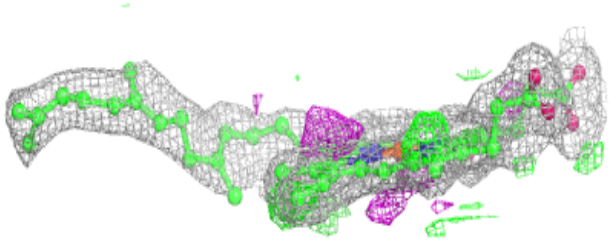


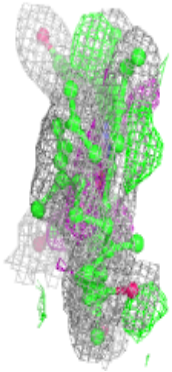


Electron density around HEA A 601 (C):

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

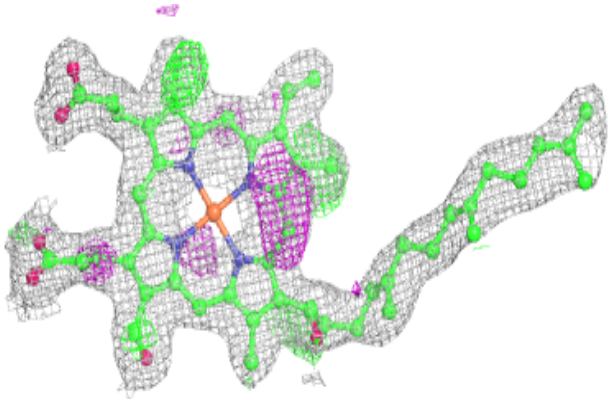


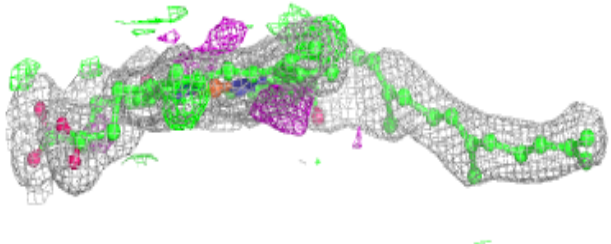


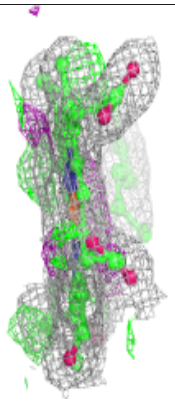


Electron density around HEA A 601 (D):

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

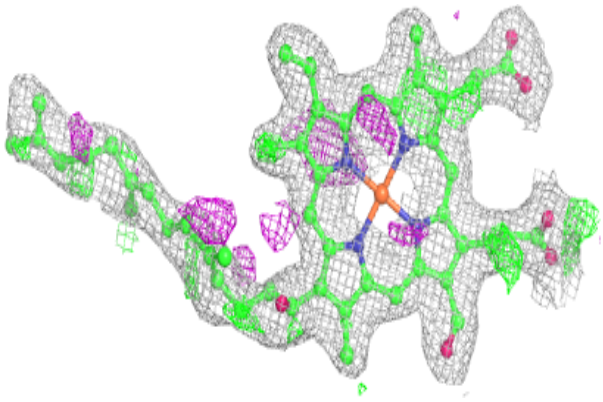


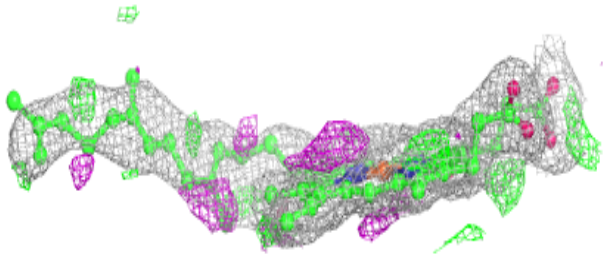


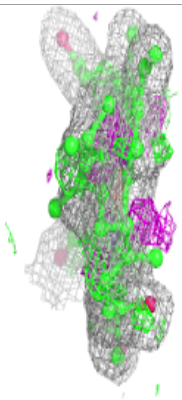


Electron density around HEA N 601 (C):

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

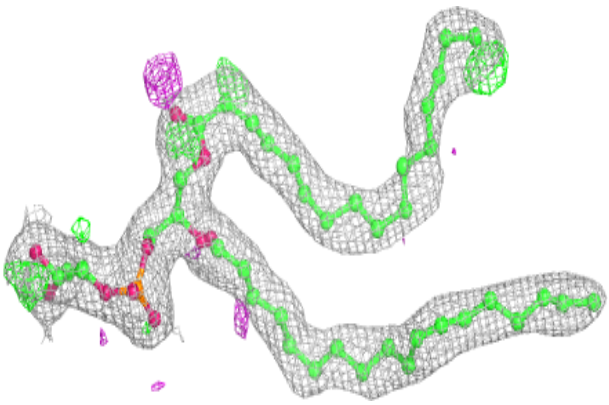


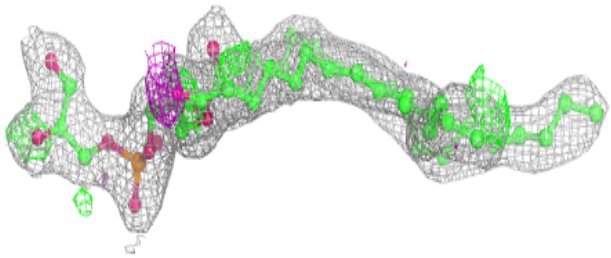


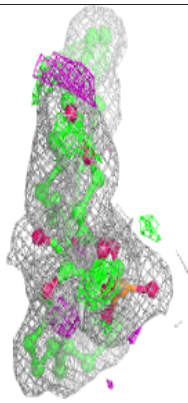


Electron density around PGV C 301:

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

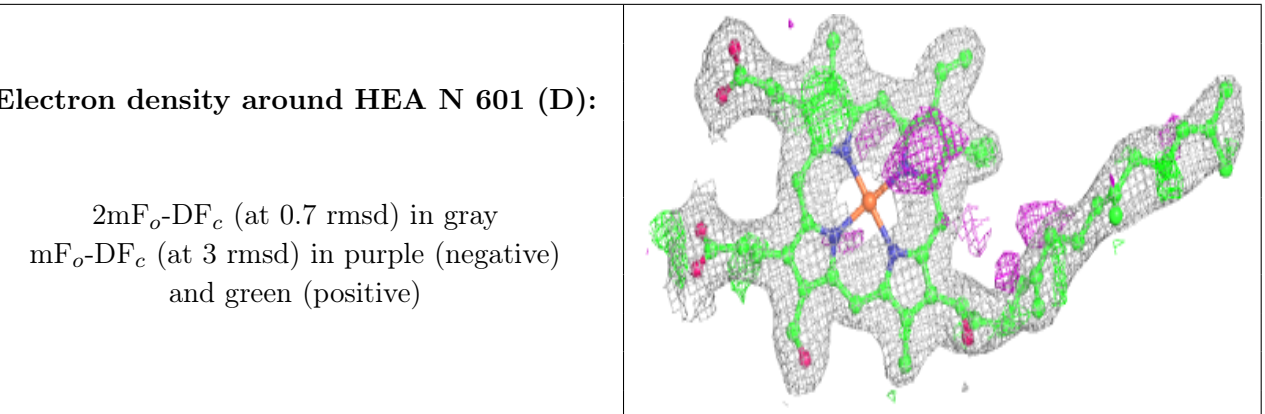


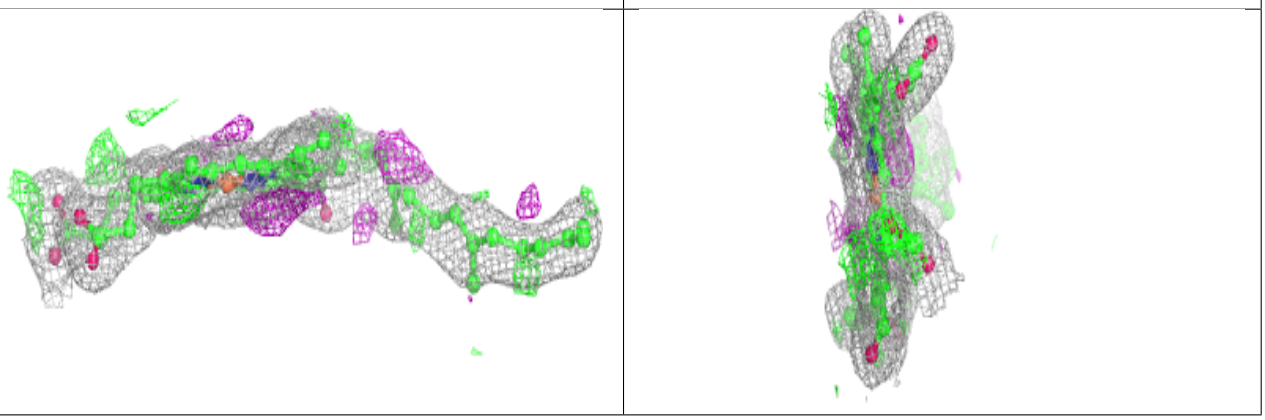




Electron density around HEA N 601 (D):

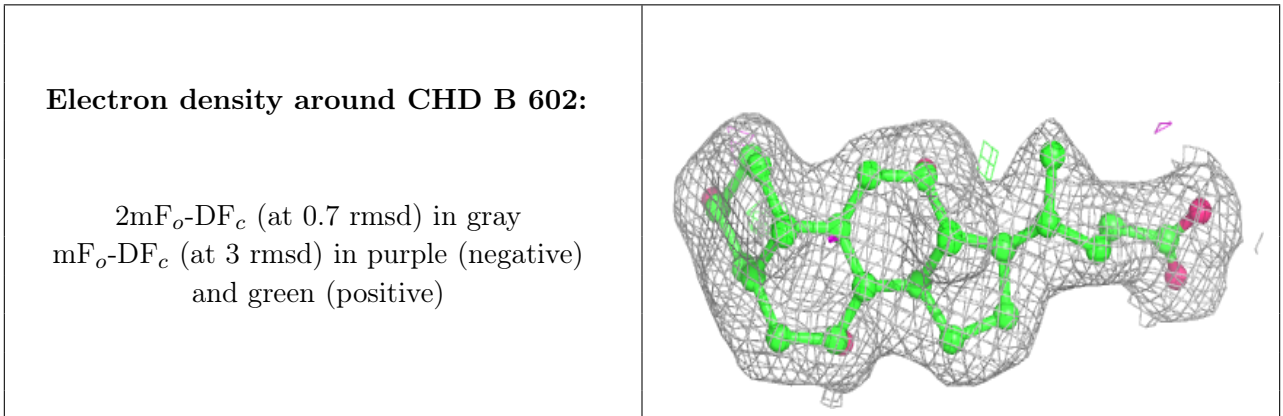
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

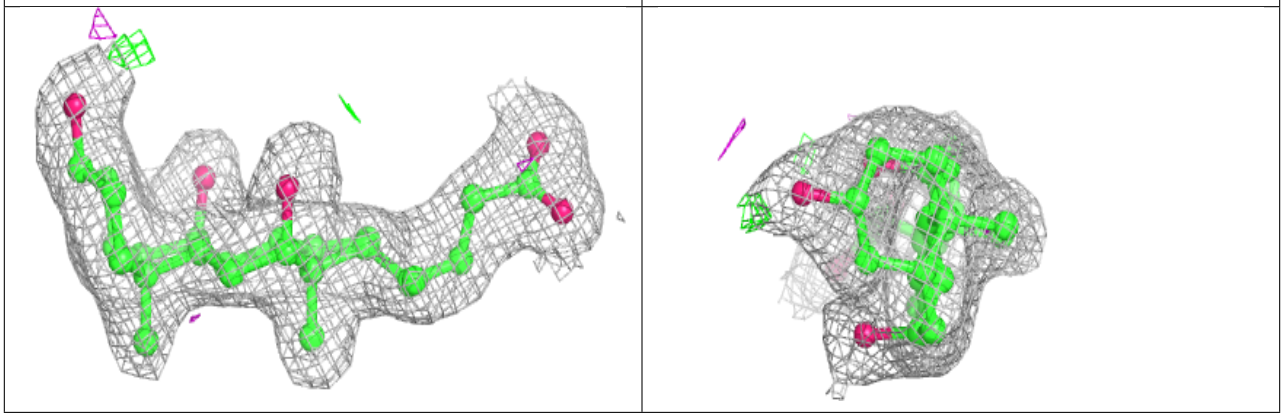




Electron density around CHD B 602:

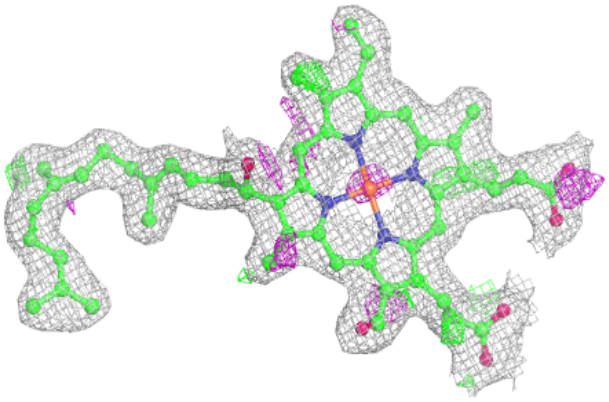
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

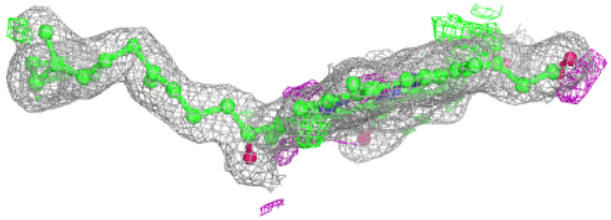


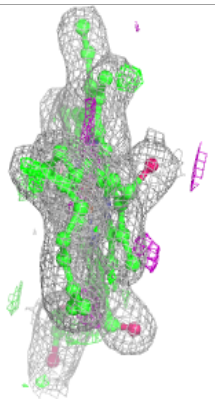


Electron density around HEA A 602:

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

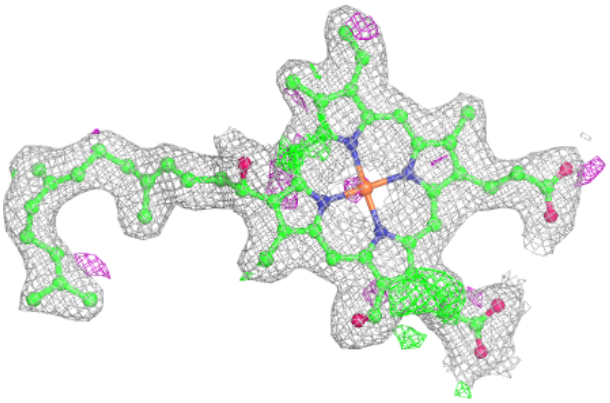


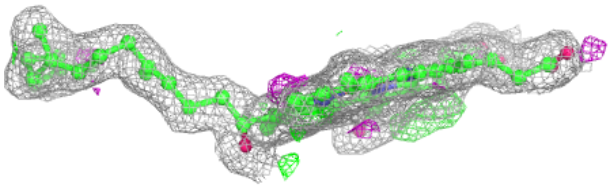


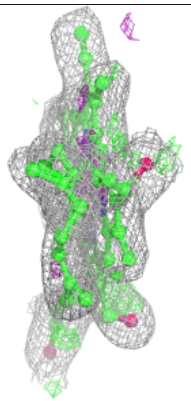


Electron density around HEA N 602:

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

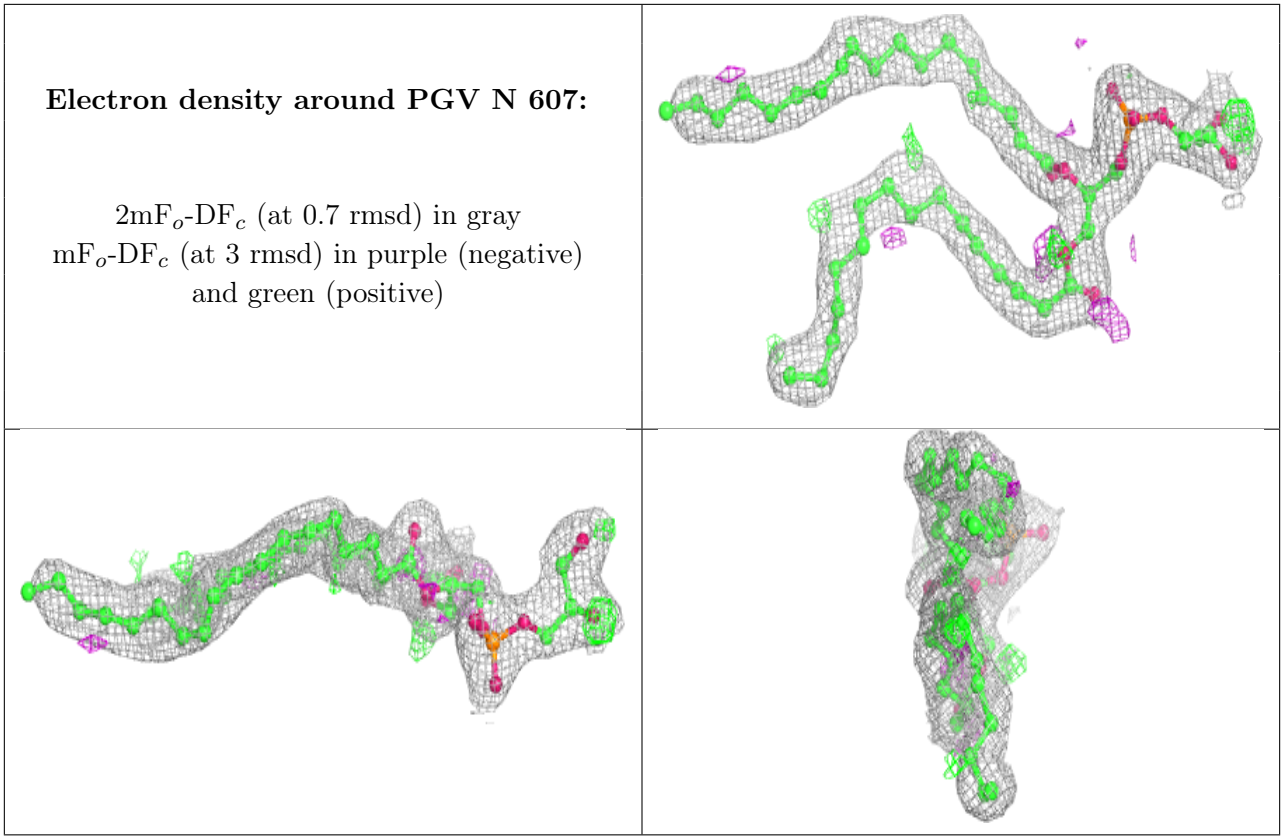






Electron density around PGV N 607:

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



6.5 Other polymers (i)

There are no such residues in this entry.