Full wwPDB X-ray Structure Validation Report (i)

Mar 1, 2021 – 05:01 PM EST

PDB ID	:	4OGQ
Title	:	Internal Lipid Architecture of the Hetero-Oligomeric Cytochrome b6f Complex
Authors	:	Hasan, S.S.; Cramer, W.A.
Deposited on	:	2014-01-16
Resolution	:	2.50 Å(reported)

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

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

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

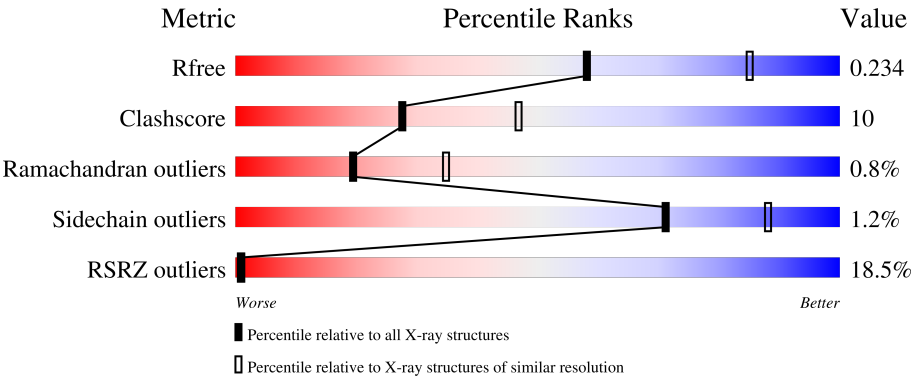
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



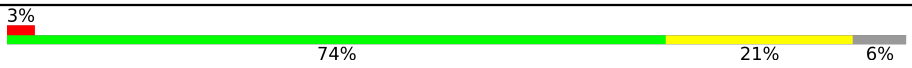
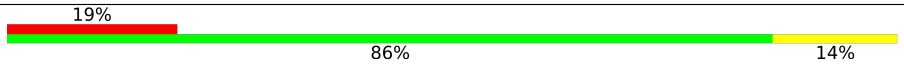
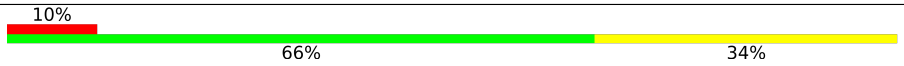
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	215	13% 93% 7%
2	B	160	14% 89% 10%
3	C	333	14% 70% 14% 16%
4	D	179	36% 74% 18% 7%
5	E	31	16% 77% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	34	
7	G	37	
8	H	29	

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
10	UMQ	A	304	-	-	-	X
10	UMQ	B	203[B]	-	-	-	X
10	UMQ	D	201	-	-	-	X
10	UMQ	G	101	-	-	-	X
11	7PH	B	206	-	-	-	X
12	8K6	B	202[A]	-	-	-	X
14	CLA	B	204	X	-	-	-
20	2WD	D	206	-	-	-	X
23	OCT	F	102	-	-	-	X
24	1O2	F	103	X	-	-	X

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 8396 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 b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1708	1139	271	288	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	S	0	0	0
			1232	825	194	208	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2137	1361	355	415	6			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1250	791	213	240	6			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	31	Total	C	N	O	S	0	0	0
			228	157	35	35	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	32	Total	C	N	O	S	0	0	0
			231	156	36	38	1			

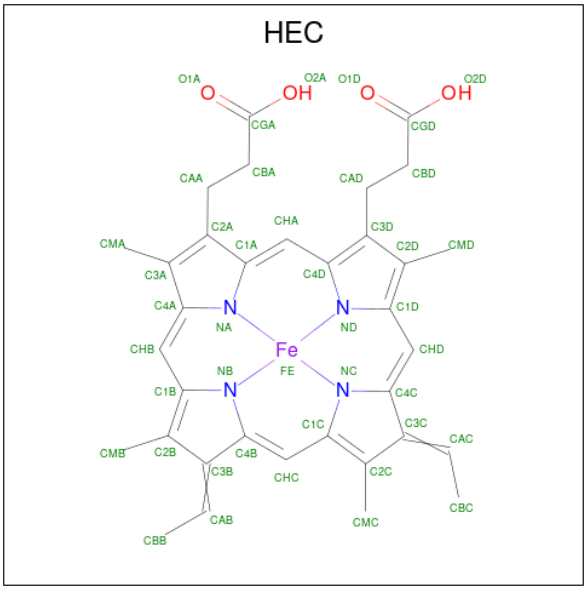
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	37	Total	C	N	O	S	0	0	0
			282	188	44	49	1			

- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

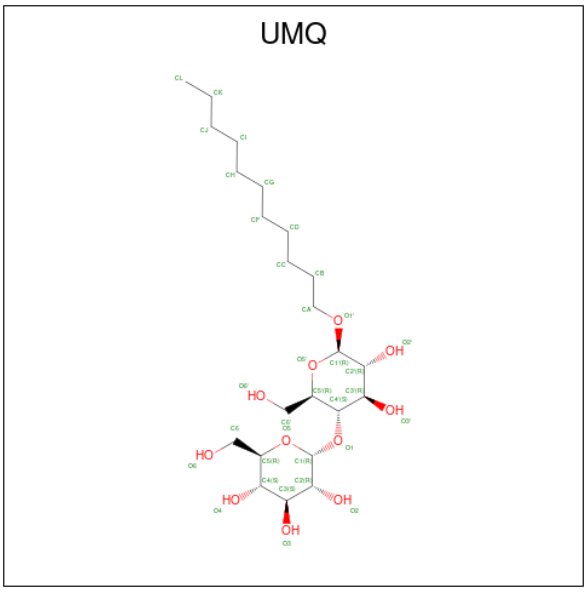
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	29	Total	C	N	O	S	0	0	0
			228	155	36	35	2			

- Molecule 9 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



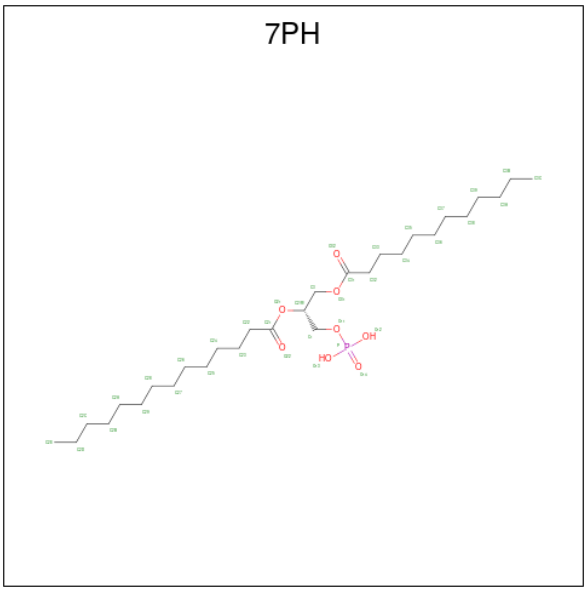
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



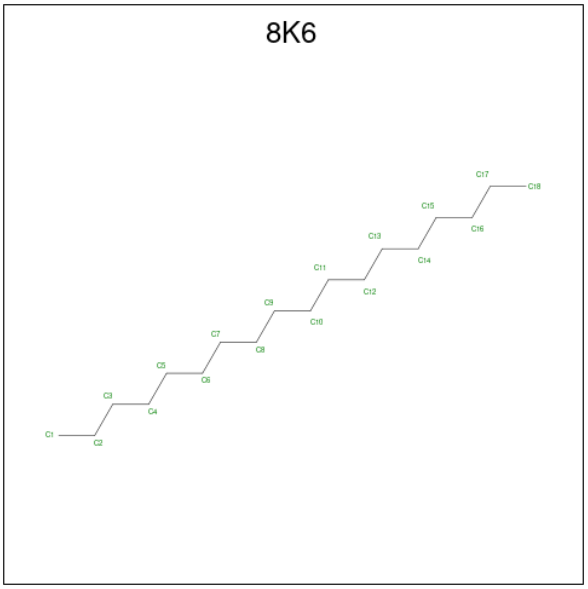
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 34 23 11	0	0
10	B	1	Total C O 34 23 11	0	0
10	B	1	Total C O 34 23 11	0	1
10	D	1	Total C O 34 23 11	0	0
10	G	1	Total C O 34 23 11	0	0

- Molecule 11 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



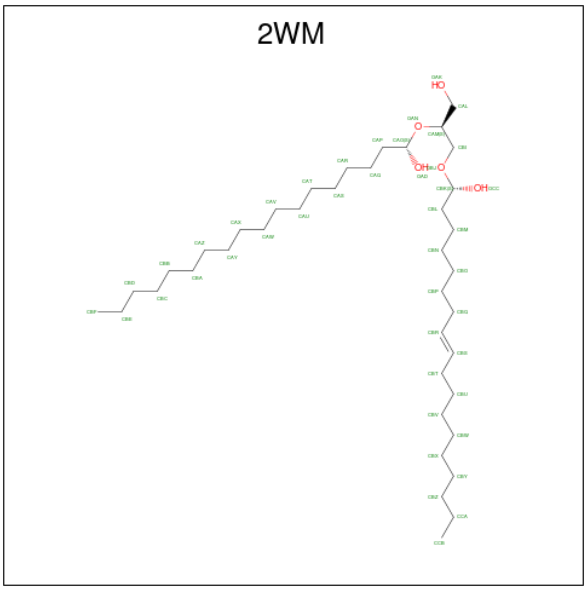
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 32 27 5	0	0
11	B	1	Total C O 32 27 5	0	0
11	C	1	Total C O 32 27 5	0	0
11	D	1	Total C O 32 27 5	0	0
11	F	1	Total C O 32 27 5	0	0

- Molecule 12 is Octadecane (three-letter code: 8K6) (formula: $C_{18}H_{38}$).



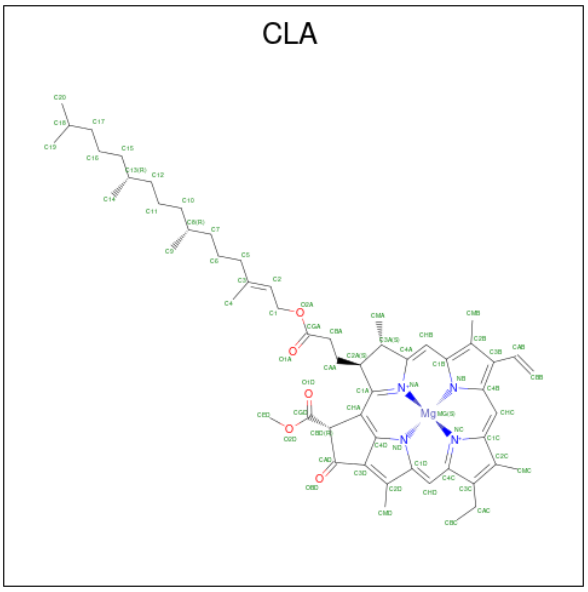
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C 18 18	0	0
12	A	1	Total C 18 18	0	0
12	A	1	Total C 14 14	0	0
12	B	1	Total C 18 18	0	1

- Molecule 13 is (1S,8E)-1-{[(2S)-3-hydroxy-2-{[(1S)-1-hydroxyoctadecyl]oxy}propyl]oxy}octadec-8-en-1-ol (three-letter code: 2WM) (formula: $C_{39}H_{78}O_5$).



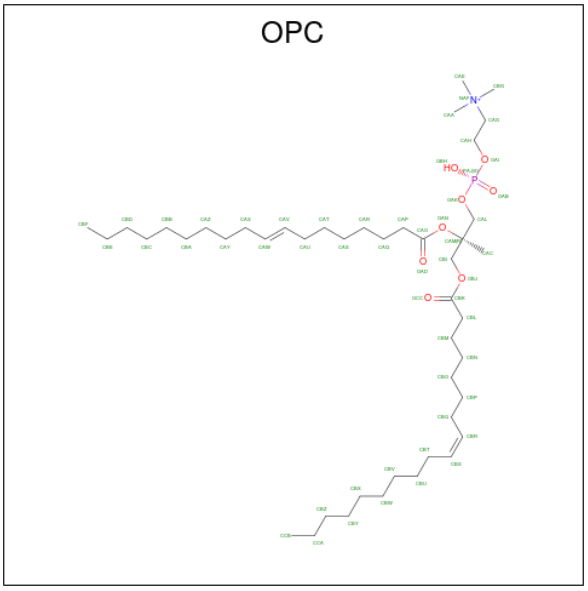
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 44 39 5	0	0

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 15 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: $C_{45}H_{87}NO_8P$).

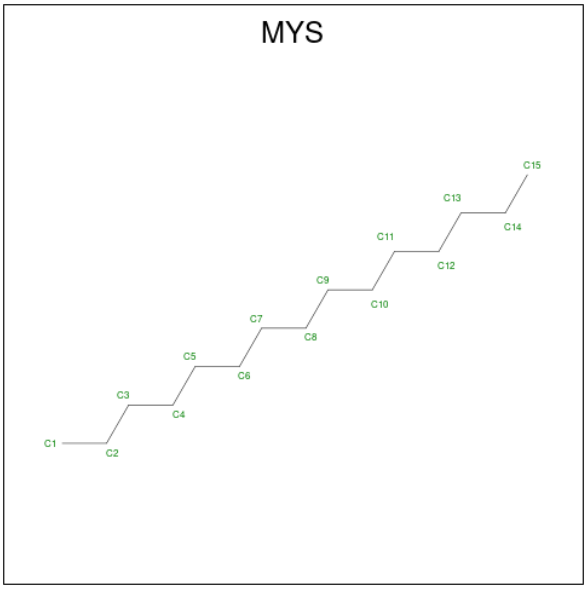


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 16 is CADMIUM ION (three-letter code: CD) (formula: Cd).

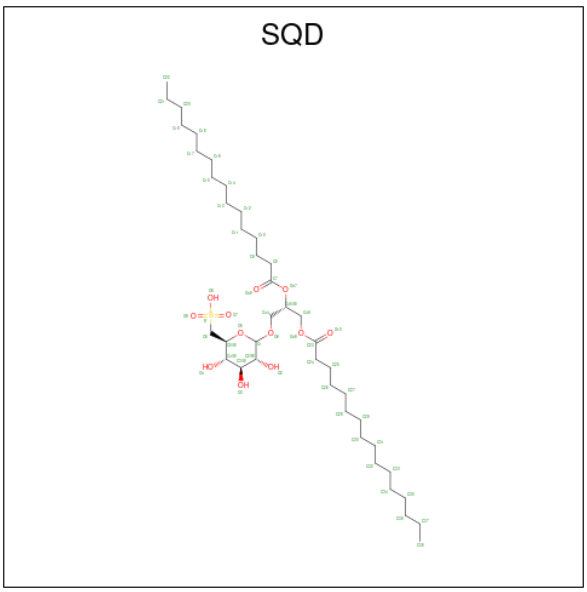
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total Cd 1 1	0	0

- Molecule 17 is PENTADECANE (three-letter code: MYS) (formula: $C_{15}H_{32}$).



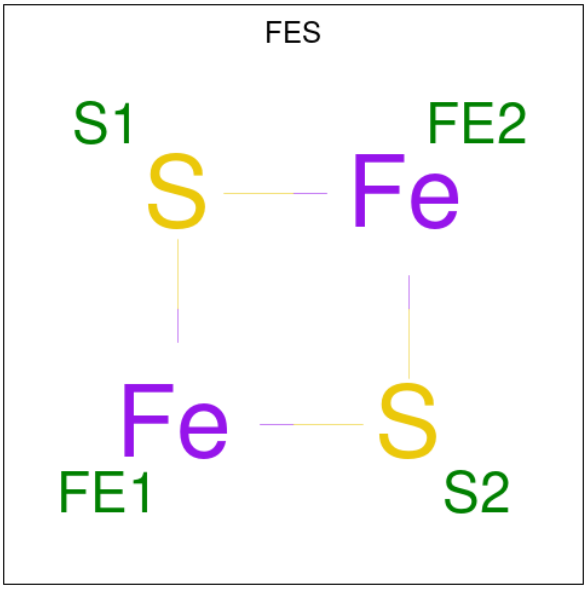
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total C 15 15	0	0

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



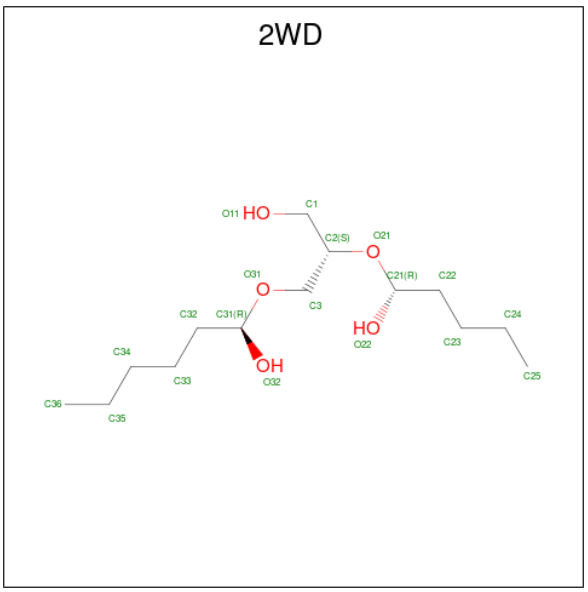
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



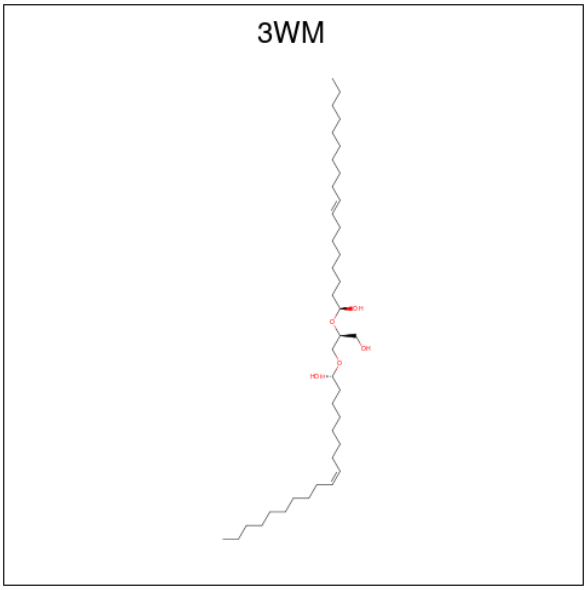
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is (1R)-1-{[(2S)-3-hydroxy-2-{[(1R)-1-hydroxypentyl]oxy}propyl]oxy}hexan-1-ol (three-letter code: 2WD) (formula: $C_{14}H_{30}O_5$).



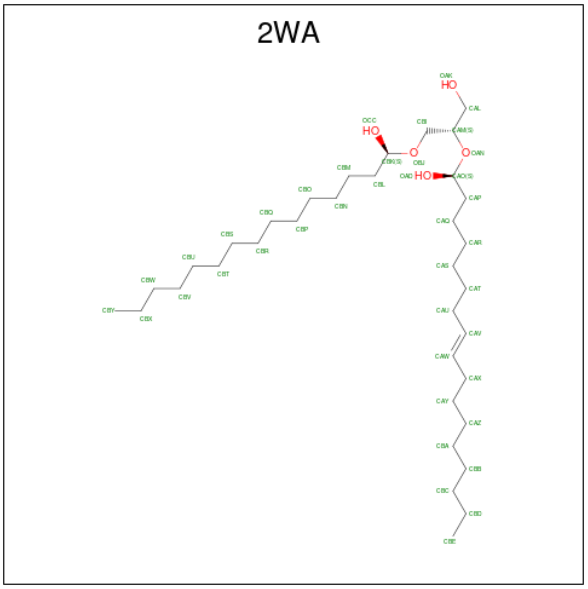
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C O 19 14 5	0	0

- Molecule 21 is (1S,8E,1'R,8'Z)-1,1'-{[(2S)-3-hydroxypropane-1,2-diyl]bis(oxy)}bisoctadec-8-en-1-ol (three-letter code: 3WM) (formula: $C_{39}H_{76}O_5$).



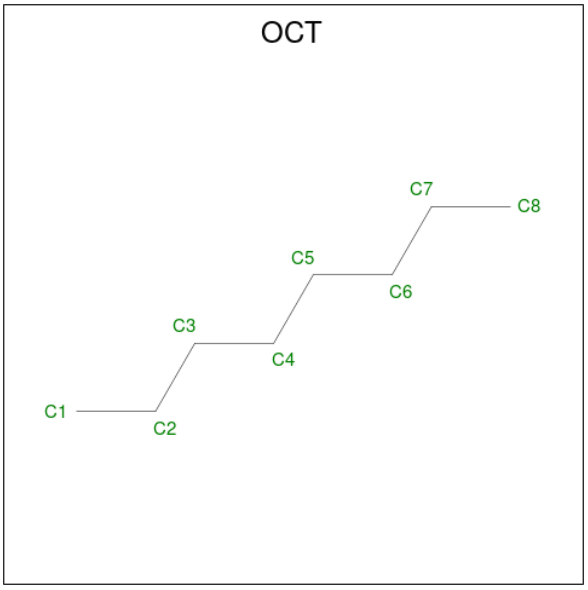
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	E	1	Total C O 44 39 5	0	0

- Molecule 22 is (1S,8E)-1-{[(2S)-1-hydroxy-3-{[(1S)-1-hydroxypentadecyl]oxy}propan-2-yl]oxy}heptadec-8-en-1-ol (three-letter code: 2WA) (formula: $C_{35}H_{70}O_5$).



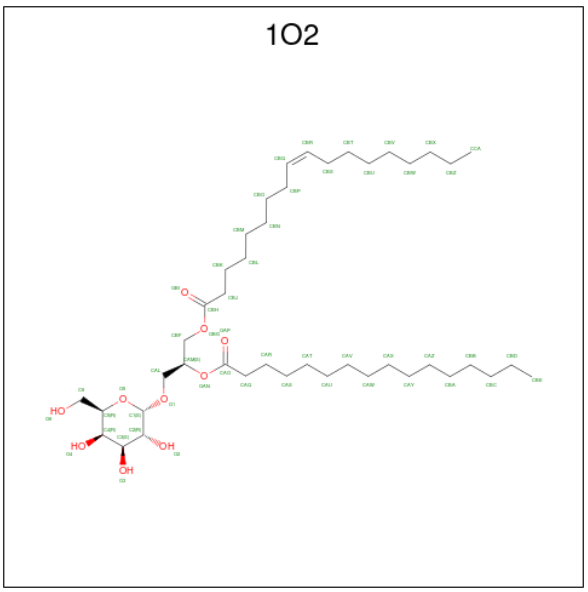
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total C O 40 35 5	0	0

- Molecule 23 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



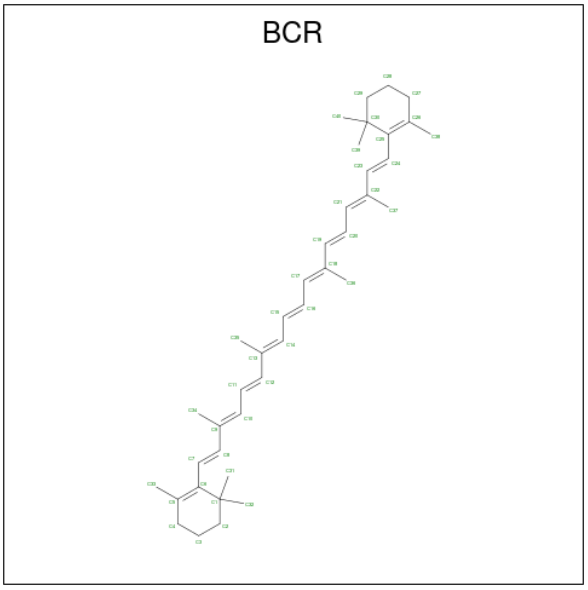
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	F	1	Total C 8 8	0	0

- Molecule 24 is (2S)-3-(alpha-D-galactopyranosyloxy)-2-(hexadecanoyloxy)propyl (9Z)-octadec-9-enoate (three-letter code: 1O2) (formula: $C_{43}H_{80}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	F	1	Total C O 49 39 10	0	0

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	G	1	Total C 40 40	0	0

- Molecule 26 is water.

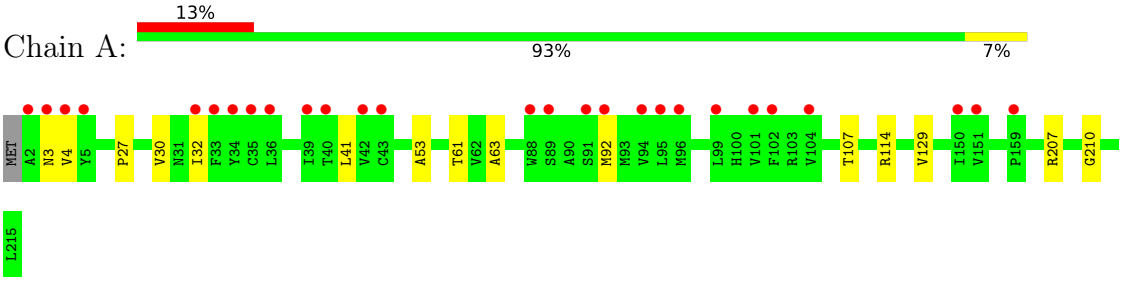
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	21	Total O 21 21	0	0
26	B	25	Total O 25 25	0	0
26	C	38	Total O 38 38	0	0
26	D	1	Total O 1 1	0	0
26	F	1	Total O 1 1	0	0
26	G	7	Total O 7 7	0	0

3 Residue-property plots (i)

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

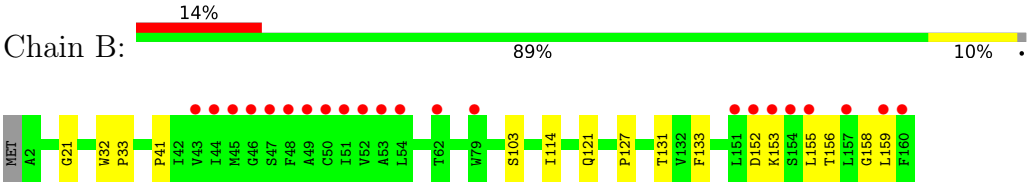
• Molecule 1: Cytochrome b6

Chain A:



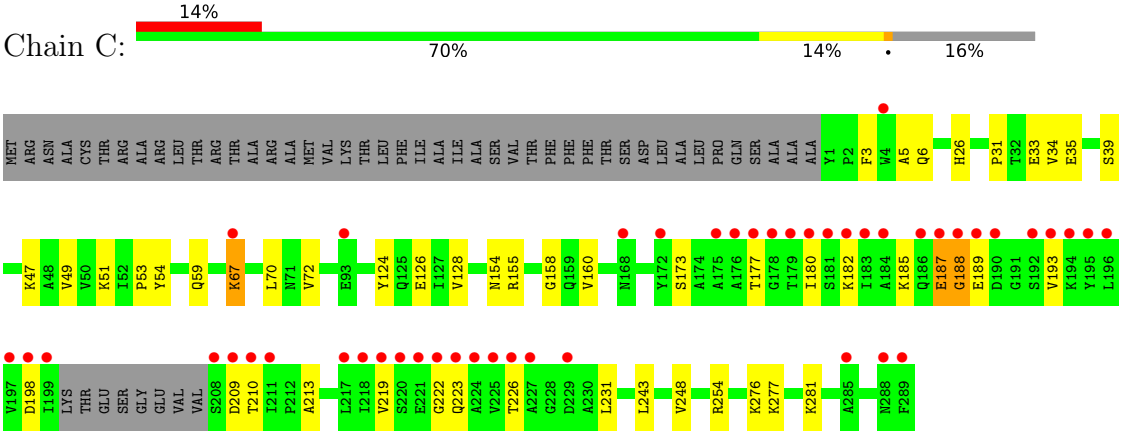
• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:



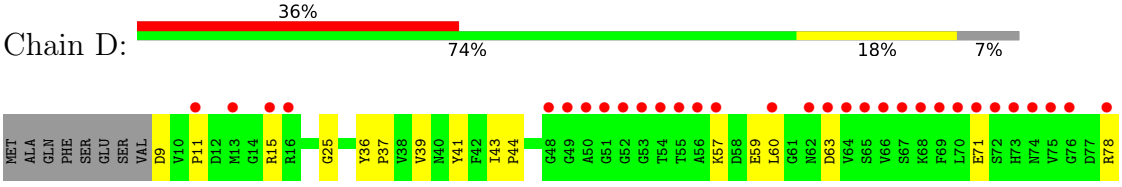
• Molecule 3: Apocytochrome f

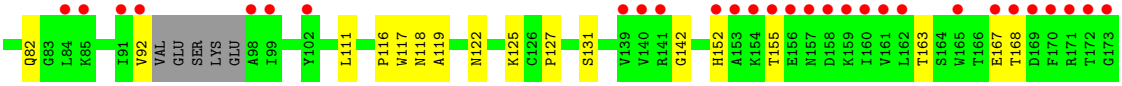
Chain C:



• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1

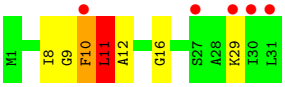
Chain D:





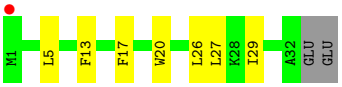
• Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:



• Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:

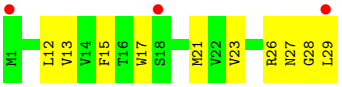


• Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:

• Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	159.23Å 159.23Å 365.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.57 – 2.50 39.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.57-2.50) 89.3 (39.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.201 , 0.232 0.206 , 0.234	Depositor DCC
R_{free} test set	4694 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 80.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: 8K6, HEC, 2WD, OCT, FES, SQD, 3WM, 2WM, 1O2, OPC, UMQ, CLA, BCR, CD, MYS, 7PH, 2WA

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	0/1761	0.41	0/2401
2	B	0.23	0/1271	0.38	0/1742
3	C	0.22	0/2182	0.38	0/2972
4	D	0.22	0/1281	0.40	0/1745
5	E	0.25	0/231	0.65	0/309
6	F	0.22	0/234	0.33	0/315
7	G	0.23	0/287	0.34	0/387
8	H	0.26	0/234	0.39	0/319
All	All	0.23	0/7481	0.40	0/10190

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1721	14	0
2	B	1232	0	1278	14	0
3	C	2137	0	2122	29	0
4	D	1250	0	1208	20	0
5	E	228	0	257	9	0
6	F	231	0	252	8	0
7	G	282	0	303	4	0
8	H	228	0	243	9	0
9	A	129	0	95	10	0
9	C	43	0	31	4	0
10	A	34	0	44	9	0
10	B	68	0	87	17	0
10	D	34	0	44	4	0
10	G	34	0	44	4	0
11	A	32	0	45	1	0
11	B	32	0	45	5	0
11	C	32	0	45	4	0
11	D	32	0	45	1	0
11	F	32	0	45	6	0
12	A	50	0	103	8	0
12	B	18	0	38	3	0
13	A	44	0	78	0	0
14	B	65	0	72	4	0
15	B	54	0	83	5	0
16	C	1	0	0	0	0
17	D	15	0	32	1	0
18	D	54	0	77	2	0
19	D	4	0	0	0	0
20	D	19	0	30	2	0
21	E	44	0	76	9	0
22	F	40	0	70	7	0
23	F	8	0	18	0	0
24	F	49	0	69	11	0
25	G	40	0	56	2	0
26	A	21	0	0	0	0
26	B	25	0	0	1	0
26	C	38	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	D	1	0	0	0	0
26	F	1	0	0	0	0
26	G	7	0	0	0	0
All	All	8396	0	8756	170	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 10.

All (170) 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)
10:G:101:UMQ:O5'	10:G:101:UMQ:C5'	1.63	1.46
10:A:304:UMQ:O5'	10:A:304:UMQ:C5'	1.63	1.45
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C5'	1.63	1.44
10:B:201:UMQ:C1'	10:B:201:UMQ:O5'	1.69	1.41
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C1'	1.69	1.38
10:D:201:UMQ:O5'	10:D:201:UMQ:C1'	1.69	1.38
10:A:304:UMQ:O5'	10:A:304:UMQ:C1'	1.69	1.38
10:G:101:UMQ:O5'	10:G:101:UMQ:C1'	1.69	1.37
10:D:201:UMQ:C1'	10:D:201:UMQ:C5'	2.46	0.93
10:G:101:UMQ:C5'	10:G:101:UMQ:C1'	2.47	0.93
10:B:203[B]:UMQ:C5'	10:B:203[B]:UMQ:C1'	2.47	0.92
10:A:304:UMQ:C5'	10:A:304:UMQ:C1'	2.48	0.92
10:B:201:UMQ:C1'	10:B:201:UMQ:C5'	2.48	0.92
10:A:304:UMQ:H6'2	10:A:304:UMQ:H11	1.59	0.83
3:C:34:VAL:HG23	3:C:243:LEU:HD23	1.70	0.73
11:C:303:7PH:H25	11:C:303:7PH:H35A	1.70	0.72
5:E:8:ILE:HD11	21:E:101:3WM:H11	1.71	0.71
2:B:41:PRO:HG3	12:B:202[A]:8K6:H92C	1.73	0.71
10:B:201:UMQ:H51	10:B:201:UMQ:H6'1	1.73	0.71
1:A:61:THR:HG22	1:A:63:ALA:H	1.56	0.70
8:H:26:ARG:HE	8:H:29:LEU:HD11	1.57	0.70
1:A:41:LEU:HD23	9:A:303:HEC:HBC3	1.74	0.70
3:C:31:PRO:O	3:C:155:ARG:NH2	2.26	0.69
1:A:4:VAL:HG13	11:A:305:7PH:H34	1.74	0.69
4:D:131:SER:HA	4:D:142:GLY:HA3	1.76	0.67
1:A:114:ARG:NH1	1:A:210:GLY:O	2.29	0.66
10:D:201:UMQ:H51	10:D:201:UMQ:H4'1	1.79	0.65
3:C:26:HIS:CG	3:C:154:ASN:HD21	2.14	0.64
3:C:33:GLU:HB2	3:C:51:LYS:HB2	1.81	0.62
10:D:201:UMQ:H4'1	10:D:201:UMQ:C5	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:103:1O2:HBSA	24:F:103:1O2:HAZA	1.82	0.60
21:E:101:3WM:H29	21:E:101:3WM:H44	1.83	0.60
24:F:103:1O2:HBQ	24:F:103:1O2:HAY	1.83	0.60
4:D:15:ARG:HH12	5:E:29:LYS:HE3	1.67	0.59
3:C:281:LYS:NZ	4:D:9:ASP:O	2.29	0.59
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C6'	2.47	0.58
24:F:103:1O2:HAY	24:F:103:1O2:CBQ	2.33	0.58
3:C:3:PHE:HA	3:C:6:GLN:HG2	1.84	0.58
2:B:32:TRP:CE2	10:B:201:UMQ:HC2	2.39	0.58
6:F:29:ILE:HG22	24:F:103:1O2:HAS	1.85	0.57
21:E:101:3WM:H53	8:H:12:LEU:HD21	1.86	0.57
10:B:203[B]:UMQ:H11	10:B:203[B]:UMQ:H6'1	1.85	0.57
11:B:206:7PH:H29A	11:B:206:7PH:H24	1.86	0.57
9:A:303:HEC:HMD3	10:B:203[B]:UMQ:H6'2	1.88	0.56
2:B:114:ILE:HD13	15:B:205:OPC:HAT2	1.88	0.56
10:A:304:UMQ:O5'	10:A:304:UMQ:C6'	2.47	0.55
6:F:13:PHE:CD2	22:F:101:2WA:H14	2.41	0.55
3:C:59:GLN:HB3	3:C:67:LYS:HG3	1.89	0.55
2:B:127:PRO:HD2	15:B:205:OPC:HAG1	1.88	0.55
10:G:101:UMQ:O5'	10:G:101:UMQ:C6'	2.48	0.54
3:C:180:ILE:HB	3:C:223:GLN:H	1.73	0.54
3:C:70:LEU:HD13	3:C:155:ARG:HB3	1.90	0.54
5:E:10:PHE:H	5:E:11:LEU:HB2	1.73	0.54
1:A:32:ILE:N	8:H:29:LEU:HD13	2.23	0.54
21:E:101:3WM:H1	24:F:103:1O2:HBEA	1.89	0.53
6:F:26:LEU:HD13	6:F:29:ILE:HD11	1.90	0.53
5:E:10:PHE:CD2	8:H:13:VAL:HG11	2.44	0.53
4:D:11:PRO:HA	4:D:15:ARG:HD2	1.91	0.53
12:A:308:8K6:H112	12:A:308:8K6:H72C	1.90	0.52
4:D:59:GLU:HG2	4:D:60:LEU:HD12	1.90	0.52
7:G:34:GLU:HG2	7:G:35:LEU:HG	1.91	0.52
10:A:304:UMQ:HL3	10:B:201:UMQ:HK2	1.91	0.51
2:B:133:PHE:HA	14:B:204:CLA:HBB1	1.93	0.51
22:F:101:2WA:H2	11:F:104:7PH:H2B	1.92	0.51
12:A:308:8K6:H72C	12:A:308:8K6:C13	2.40	0.51
3:C:5:ALA:HB2	9:C:301:HEC:HHC	1.93	0.51
2:B:33:PRO:HG3	18:D:204:SQD:H4	1.91	0.51
1:A:92:MET:HB3	21:E:101:3WM:H76	1.93	0.50
11:C:303:7PH:H25	11:C:303:7PH:C35	2.39	0.50
21:E:101:3WM:H1	24:F:103:1O2:CBE	2.41	0.50
21:E:101:3WM:H65	8:H:15:PHE:CD1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ILE:HG13	3:C:219:VAL:HG11	1.92	0.50
8:H:23:VAL:HG13	8:H:28:GLY:HA2	1.93	0.50
4:D:78:ARG:HD3	4:D:92:VAL:HG22	1.93	0.50
3:C:158:GLY:H	9:C:301:HEC:C3D	2.25	0.50
4:D:78:ARG:HG3	4:D:117:TRP:CD1	2.47	0.49
9:C:301:HEC:HMC1	9:C:301:HEC:HBC3	1.95	0.49
20:D:206:2WD:O22	20:D:206:2WD:H2	2.12	0.49
10:A:304:UMQ:HF2	10:A:304:UMQ:CJ	2.42	0.49
14:B:204:CLA:O1D	22:F:101:2WA:H66	2.13	0.48
11:B:206:7PH:H29A	11:B:206:7PH:C24	2.44	0.48
5:E:9:GLY:HA2	5:E:12:ALA:HB3	1.95	0.48
1:A:27:PRO:HG2	1:A:30:VAL:HG23	1.95	0.48
6:F:17:PHE:CE1	11:F:104:7PH:H29	2.49	0.47
12:A:306:8K6:H61C	12:A:306:8K6:H101	1.97	0.47
12:A:308:8K6:H72C	12:A:308:8K6:H131	1.97	0.47
24:F:103:1O2:HBQ	24:F:103:1O2:HAWA	1.97	0.47
1:A:129:VAL:HG21	14:B:204:CLA:H43	1.96	0.46
4:D:39:VAL:HG11	20:D:206:2WD:H19	1.97	0.46
4:D:57:LYS:NZ	4:D:63:ASP:OD1	2.49	0.46
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.96	0.46
6:F:5:LEU:HD21	7:G:11:LEU:HD12	1.98	0.46
24:F:103:1O2:HBMA	24:F:103:1O2:HBJA	1.74	0.46
4:D:57:LYS:O	4:D:82:GLN:N	2.45	0.46
2:B:41:PRO:HG3	10:B:203[B]:UMQ:HF1	1.97	0.45
2:B:153:LYS:HG3	2:B:158:GLY:H	1.81	0.45
15:B:205:OPC:HAH2	15:B:205:OPC:HAA3	1.61	0.45
4:D:118:ASN:HD22	4:D:125:LYS:HE2	1.80	0.45
22:F:101:2WA:CBL	22:F:101:2WA:H34	2.46	0.45
24:F:103:1O2:HBSA	24:F:103:1O2:CAZ	2.45	0.45
4:D:25:GLY:HA2	18:D:204:SQD:H311	1.99	0.45
5:E:10:PHE:HD2	8:H:13:VAL:HG21	1.81	0.45
11:C:303:7PH:H33A	11:C:303:7PH:H36	1.74	0.45
3:C:209:ASP:OD1	3:C:210:THR:N	2.50	0.45
5:E:11:LEU:HD22	5:E:11:LEU:HA	1.78	0.45
1:A:53:ALA:HB1	4:D:41:TYR:CE1	2.52	0.45
2:B:131:THR:HG23	11:B:206:7PH:H25	1.98	0.45
6:F:27:LEU:HD21	8:H:27:ASN:HA	1.98	0.45
1:A:129:VAL:HG21	14:B:204:CLA:H11	1.99	0.45
3:C:160:VAL:O	9:C:301:HEC:HAC	2.17	0.45
9:A:303:HEC:C1A	10:B:203[B]:UMQ:H62	2.47	0.45
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:206:7PH:H35A	11:B:206:7PH:H38	1.68	0.44
4:D:117:TRP:HE1	4:D:119:ALA:HB2	1.83	0.44
6:F:20:TRP:CD2	11:F:104:7PH:H34A	2.52	0.44
9:A:303:HEC:HBA2	10:B:203[B]:UMQ:H41	2.00	0.44
3:C:182:LYS:HB2	3:C:198:ASP:H	1.82	0.44
11:F:104:7PH:H39A	11:F:104:7PH:H36	1.72	0.44
2:B:156:THR:HG22	2:B:159:LEU:H	1.81	0.44
10:A:304:UMQ:HB1	10:A:304:UMQ:H2'1	2.01	0.43
2:B:103:SER:OG	15:B:205:OPC:HBD2	2.18	0.43
3:C:54:TYR:HB3	3:C:155:ARG:HD3	1.99	0.43
3:C:193:VAL:HB	3:C:213:ALA:HB2	2.00	0.43
12:A:308:8K6:H171	12:A:308:8K6:H142	1.68	0.43
3:C:59:GLN:CB	3:C:67:LYS:HG3	2.49	0.43
11:F:104:7PH:H27A	25:G:102:BCR:C22	2.49	0.43
12:B:202[A]:8K6:H112	12:B:202[A]:8K6:H142	1.64	0.43
22:F:101:2WA:H44	7:G:2:VAL:HG11	2.00	0.42
25:G:102:BCR:H361	25:G:102:BCR:H20C	1.80	0.42
15:B:205:OPC:HBP1	15:B:205:OPC:HBS	1.79	0.42
5:E:16:GLY:CA	24:F:103:1O2:HBUA	2.49	0.42
4:D:116:PRO:HD2	4:D:127:PRO:HD3	2.01	0.42
12:A:308:8K6:H132	12:A:308:8K6:H62C	2.01	0.42
3:C:177:THR:HG23	3:C:226:THR:HA	2.01	0.42
4:D:167:GLU:HG2	4:D:168:THR:H	1.85	0.42
1:A:92:MET:SD	21:E:101:3WM:H71	2.60	0.42
9:A:302:HEC:HMB1	9:A:302:HEC:HBB2	2.02	0.42
3:C:51:LYS:HG2	3:C:126:GLU:HG2	2.01	0.42
3:C:53:PRO:HD2	3:C:155:ARG:HH21	1.85	0.42
3:C:277:LYS:NZ	26:C:402:HOH:O	2.53	0.42
11:B:206:7PH:H35	7:G:22:PHE:CD2	2.54	0.41
4:D:152:HIS:HB2	4:D:163:THR:OG1	2.21	0.41
12:A:307:8K6:H121	12:A:307:8K6:H152	1.84	0.41
2:B:32:TRP:NE1	10:B:201:UMQ:HA2	2.35	0.41
1:A:207:ARG:NH1	10:B:203[B]:UMQ:O2	2.54	0.41
21:E:101:3WM:H58	21:E:101:3WM:H55	1.74	0.41
12:A:306:8K6:H132	12:A:307:8K6:H81C	2.03	0.41
4:D:122:ASN:O	4:D:122:ASN:ND2	2.54	0.41
6:F:5:LEU:HD22	22:F:101:2WA:H28	2.01	0.41
26:B:310:HOH:O	3:C:276:LYS:NZ	2.53	0.41
3:C:35:GLU:HB2	3:C:49:VAL:HB	2.03	0.41
3:C:39:SER:HB3	3:C:248:VAL:HB	2.02	0.41
3:C:187:GLU:HB2	3:C:188:GLY:H	1.72	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:101:2WA:H34	22:F:101:2WA:H42	2.03	0.41
1:A:114:ARG:NH2	2:B:21:GLY:O	2.54	0.41
3:C:72:VAL:HG21	3:C:124:TYR:O	2.21	0.41
3:C:254:ARG:HA	11:D:203:7PH:H25	2.03	0.41
11:C:303:7PH:O32	11:C:303:7PH:H34	2.15	0.41
10:A:304:UMQ:CL	10:B:201:UMQ:HI2	2.51	0.41
8:H:17:TRP:O	8:H:21:MET:HG2	2.21	0.41
9:A:301:HEC:HMC1	9:A:301:HEC:HBC2	2.03	0.40
9:A:303:HEC:HHD	9:A:303:HEC:CBC	2.51	0.40
1:A:107:THR:O	2:B:121:GLN:HB3	2.21	0.40
9:A:301:HEC:CBB	9:A:301:HEC:HMB1	2.52	0.40
9:A:303:HEC:HBC2	12:B:202[A]:8K6:H151	2.02	0.40
5:E:16:GLY:HA3	24:F:103:1O2:HBUA	2.03	0.40
9:A:302:HEC:HMB1	9:A:302:HEC:CBB	2.52	0.40
17:D:202:MYS:H112	17:D:202:MYS:H82	1.64	0.40
4:D:43:ILE:HA	4:D:44:PRO:HD3	1.91	0.40
11:F:104:7PH:H29A	11:F:104:7PH:H2C	1.82	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	212/215 (99%)	202 (95%)	9 (4%)	1 (0%)	29 48
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100 100
3	C	277/333 (83%)	249 (90%)	23 (8%)	5 (2%)	8 14
4	D	162/179 (90%)	147 (91%)	15 (9%)	0	100 100
5	E	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3 5
6	F	30/34 (88%)	30 (100%)	0	0	100 100
7	G	35/37 (95%)	34 (97%)	1 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	H	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
All	All	929/1018 (91%)	865 (93%)	57 (6%)	7 (1%)	19 35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	173	SER
1	A	3	ASN
3	C	185	LYS
5	E	11	LEU
3	C	189	GLU
3	C	222	GLY
3	C	188	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	183/184 (100%)	183 (100%)	0	100 100
2	B	133/134 (99%)	131 (98%)	2 (2%)	65 85
3	C	231/272 (85%)	228 (99%)	3 (1%)	69 87
4	D	133/145 (92%)	130 (98%)	3 (2%)	50 76
5	E	21/21 (100%)	20 (95%)	1 (5%)	25 48
6	F	22/24 (92%)	22 (100%)	0	100 100
7	G	29/29 (100%)	29 (100%)	0	100 100
8	H	24/24 (100%)	24 (100%)	0	100 100
All	All	776/833 (93%)	767 (99%)	9 (1%)	71 88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	152	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	155	LEU
3	C	67	LYS
3	C	187	GLU
3	C	231	LEU
4	D	71	GLU
4	D	111	LEU
4	D	155	THR
5	E	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	154	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\#\|Z\|>2$
18	SQD	D	204	-	53,54,54	0.96	5 (9%)	62,65,65	1.47	9 (14%)
12	8K6	A	306	-	17,17,17	0.09	0	16,16,16	0.85	0
11	7PH	B	206	-	31,31,37	1.28	2 (6%)	33,33,42	1.16	2 (6%)
19	FES	D	205	4	0,4,4	0.00	-	-		
11	7PH	F	104	-	31,31,37	1.28	2 (6%)	33,33,42	1.19	2 (6%)
11	7PH	D	203	-	31,31,37	1.28	2 (6%)	33,33,42	1.13	2 (6%)
14	CLA	B	204	26	59,73,73	1.45	5 (8%)	67,113,113	1.39	7 (10%)
23	OCT	F	102	-	7,7,7	0.13	0	6,6,6	0.71	0
9	HEC	C	301	3	26,50,50	2.43	5 (19%)	18,82,82	1.86	6 (33%)
22	2WA	F	101	-	39,39,39	0.89	1 (2%)	39,41,41	0.53	0
10	UMQ	G	101	-	35,35,35	3.73	17 (48%)	46,46,46	2.11	6 (13%)
17	MYS	D	202	-	14,14,14	0.09	0	13,13,13	0.84	0
25	BCR	G	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.15	4 (7%)
21	3WM	E	101	-	43,43,43	0.77	1 (2%)	43,45,45	0.52	0
12	8K6	A	308	-	13,13,17	0.10	0	12,12,16	0.79	0
24	1O2	F	103	-	49,49,53	1.45	5 (10%)	57,57,61	1.10	6 (10%)
10	UMQ	D	201	-	35,35,35	3.74	17 (48%)	46,46,46	2.12	9 (19%)
11	7PH	A	305	-	31,31,37	1.27	2 (6%)	33,33,42	1.19	2 (6%)
10	UMQ	A	304	-	35,35,35	3.73	17 (48%)	46,46,46	2.07	7 (15%)
9	HEC	A	301	1	26,50,50	2.44	5 (19%)	18,82,82	1.83	6 (33%)
10	UMQ	B	203[B]	-	35,35,35	3.73	17 (48%)	46,46,46	2.09	7 (15%)
9	HEC	A	303	1,26	26,50,50	2.61	6 (23%)	18,82,82	1.65	3 (16%)
10	UMQ	B	201	-	35,35,35	3.72	17 (48%)	46,46,46	2.10	6 (13%)
13	2WM	A	309	-	43,43,43	0.66	2 (4%)	43,45,45	0.50	0
9	HEC	A	302	1	26,50,50	2.44	5 (19%)	18,82,82	1.82	6 (33%)
20	2WD	D	206	-	18,18,18	1.14	1 (5%)	18,20,20	0.57	0
11	7PH	C	303	-	31,31,37	1.28	2 (6%)	33,33,42	1.21	2 (6%)
15	OPC	B	205	-	53,53,54	1.03	2 (3%)	59,61,64	1.00	2 (3%)
12	8K6	A	307	-	17,17,17	0.08	0	16,16,16	0.88	0
12	8K6	B	202[A]	-	17,17,17	0.09	0	16,16,16	0.86	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
18	SQD	D	204	-	-	15/49/69/69	0/1/1/1
12	8K6	A	306	-	-	2/15/15/15	-
11	7PH	B	206	-	-	16/33/33/39	-
19	FES	D	205	4	-	-	0/1/1/1
11	7PH	F	104	-	-	11/33/33/39	-
11	7PH	D	203	-	-	13/33/33/39	-
14	CLA	B	204	26	3/3/20/25	8/37/135/135	-
23	OCT	F	102	-	-	1/5/5/5	-
9	HEC	C	301	3	-	0/6/54/54	-
22	2WA	F	101	-	-	20/41/41/41	-
10	UMQ	G	101	-	-	6/20/60/60	0/2/2/2
17	MYS	D	202	-	-	3/12/12/12	-
25	BCR	G	102	-	-	9/29/63/63	0/2/2/2
21	3WM	E	101	-	-	24/45/45/45	-
12	8K6	A	308	-	-	8/11/11/15	-
24	1O2	F	103	-	1/1/8/10	25/44/64/68	0/1/1/1
10	UMQ	D	201	-	-	7/20/60/60	0/2/2/2
11	7PH	A	305	-	-	14/33/33/39	-
10	UMQ	A	304	-	-	10/20/60/60	0/2/2/2
9	HEC	A	301	1	-	1/6/54/54	-
10	UMQ	B	203[B]	-	-	9/20/60/60	0/2/2/2
9	HEC	A	303	1,26	-	0/6/54/54	-
10	UMQ	B	201	-	-	3/20/60/60	0/2/2/2
13	2WM	A	309	-	-	25/45/45/45	-
9	HEC	A	302	1	-	3/6/54/54	-
20	2WD	D	206	-	-	7/20/20/20	-
11	7PH	C	303	-	-	22/33/33/39	-
15	OPC	B	205	-	-	19/57/57/60	-
12	8K6	A	307	-	-	3/15/15/15	-
12	8K6	B	202[A]	-	-	5/15/15/15	-

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	203[B]	UMQ	O5'-C1'	10.81	1.69	1.41
10	D	201	UMQ	O5'-C1'	10.80	1.69	1.41
10	A	304	UMQ	O5'-C1'	10.80	1.69	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	101	UMQ	O5'-C1'	10.80	1.69	1.41
10	B	201	UMQ	O5'-C1'	10.77	1.69	1.41
10	B	201	UMQ	O3'-C3'	8.53	1.63	1.43
10	G	101	UMQ	O3'-C3'	8.50	1.63	1.43
10	B	203[B]	UMQ	O3'-C3'	8.47	1.62	1.43
10	A	304	UMQ	O3'-C3'	8.44	1.62	1.43
10	D	201	UMQ	O3'-C3'	8.41	1.62	1.43
10	A	304	UMQ	O5'-C5'	7.92	1.63	1.44
10	G	101	UMQ	O5'-C5'	7.90	1.63	1.44
10	B	203[B]	UMQ	O5'-C5'	7.89	1.63	1.44
10	D	201	UMQ	O5'-C5'	7.83	1.63	1.44
14	B	204	CLA	C4B-NB	7.80	1.42	1.35
10	B	201	UMQ	O5'-C5'	7.77	1.63	1.44
9	A	303	HEC	C3C-C2C	-6.73	1.33	1.40
10	D	201	UMQ	O5-C5	6.25	1.59	1.44
10	A	304	UMQ	O5-C5	6.06	1.59	1.44
10	B	203[B]	UMQ	O5-C5	6.06	1.59	1.44
10	B	201	UMQ	O5-C5	6.00	1.58	1.44
10	G	101	UMQ	O5-C5	5.99	1.58	1.44
10	B	203[B]	UMQ	C6-C5	-5.88	1.32	1.51
10	B	201	UMQ	C6-C5	-5.85	1.32	1.51
10	D	201	UMQ	C6-C5	-5.83	1.32	1.51
10	A	304	UMQ	C6-C5	-5.82	1.32	1.51
10	G	101	UMQ	C6-C5	-5.80	1.32	1.51
9	A	303	HEC	C3B-C2B	-5.50	1.35	1.40
9	C	301	HEC	C3D-C2D	5.50	1.54	1.37
9	A	303	HEC	C3D-C2D	5.47	1.53	1.37
9	A	301	HEC	C3C-C2C	-5.44	1.35	1.40
9	A	302	HEC	C3B-C2B	-5.43	1.35	1.40
9	C	301	HEC	C3C-C2C	-5.42	1.35	1.40
9	A	301	HEC	C3D-C2D	5.38	1.53	1.37
9	A	301	HEC	C3B-C2B	-5.38	1.35	1.40
9	A	302	HEC	C3D-C2D	5.38	1.53	1.37
9	C	301	HEC	C3B-C2B	-5.31	1.35	1.40
9	A	302	HEC	C3C-C2C	-5.28	1.35	1.40
10	B	201	UMQ	O1'-C1'	-4.76	1.32	1.40
10	A	304	UMQ	O1'-C1'	-4.74	1.32	1.40
10	D	201	UMQ	O1'-C1'	-4.73	1.32	1.40
10	G	101	UMQ	O1'-C1'	-4.71	1.32	1.40
10	B	203[B]	UMQ	O1'-C1'	-4.67	1.32	1.40
10	A	304	UMQ	C3'-C4'	-4.65	1.39	1.52
10	B	201	UMQ	C3'-C4'	-4.62	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	101	UMQ	C3'-C4'	-4.60	1.40	1.52
10	D	201	UMQ	C3'-C4'	-4.59	1.40	1.52
10	B	203[B]	UMQ	C3'-C4'	-4.58	1.40	1.52
10	A	304	UMQ	O2-C2	4.50	1.53	1.43
10	B	203[B]	UMQ	O2-C2	4.47	1.53	1.43
10	D	201	UMQ	O2-C2	4.46	1.53	1.43
10	B	201	UMQ	O2-C2	4.44	1.53	1.43
10	G	101	UMQ	O2-C2	4.44	1.53	1.43
24	F	103	1O2	OBG-CBH	4.38	1.46	1.33
10	D	201	UMQ	C3-C2	-4.37	1.41	1.52
24	F	103	1O2	CBR-CBQ	4.36	1.57	1.31
10	G	101	UMQ	C3-C2	-4.35	1.41	1.52
10	B	203[B]	UMQ	C3-C2	-4.33	1.41	1.52
10	A	304	UMQ	C3-C2	-4.28	1.41	1.52
11	C	303	7PH	O31-C31	4.28	1.45	1.33
11	D	203	7PH	O31-C31	4.27	1.45	1.33
10	B	201	UMQ	C3-C2	-4.27	1.41	1.52
11	F	104	7PH	O31-C31	4.25	1.45	1.33
11	B	206	7PH	O31-C31	4.24	1.45	1.33
11	A	305	7PH	O31-C31	4.19	1.45	1.33
24	F	103	1O2	OAN-CAO	4.18	1.46	1.34
11	D	203	7PH	O21-C21	4.17	1.46	1.34
11	C	303	7PH	O21-C21	4.17	1.46	1.34
11	F	104	7PH	O21-C21	4.16	1.46	1.34
11	B	206	7PH	O21-C21	4.14	1.46	1.34
9	A	302	HEC	CBC-CAC	-4.14	1.33	1.49
11	A	305	7PH	O21-C21	4.14	1.46	1.34
9	A	303	HEC	CBC-CAC	-4.12	1.34	1.49
9	A	302	HEC	CBB-CAB	-4.10	1.34	1.49
9	A	301	HEC	CBB-CAB	-4.08	1.34	1.49
9	C	301	HEC	CBB-CAB	-4.08	1.34	1.49
9	A	303	HEC	CBB-CAB	-4.07	1.34	1.49
9	A	301	HEC	CBC-CAC	-4.05	1.34	1.49
9	C	301	HEC	CBC-CAC	-4.05	1.34	1.49
15	B	205	OPC	OBJ-CBK	3.79	1.44	1.33
10	G	101	UMQ	C4-C5	3.74	1.60	1.53
10	D	201	UMQ	C4-C5	3.72	1.60	1.53
10	B	201	UMQ	C4-C5	3.68	1.60	1.53
10	B	203[B]	UMQ	C4-C5	3.66	1.60	1.53
10	A	304	UMQ	C3'-C2'	-3.66	1.43	1.52
10	A	304	UMQ	C4-C5	3.66	1.60	1.53
10	B	201	UMQ	C3'-C2'	-3.61	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	101	UMQ	C3'-C2'	-3.59	1.43	1.52
10	B	203[B]	UMQ	C3'-C2'	-3.59	1.43	1.52
20	D	206	2WD	O21-C2	-3.56	1.39	1.44
10	D	201	UMQ	C3'-C2'	-3.56	1.43	1.52
10	B	203[B]	UMQ	O3-C3	3.37	1.50	1.43
10	G	101	UMQ	O3-C3	3.36	1.50	1.43
24	F	103	1O2	O5-C1	3.36	1.50	1.41
10	B	201	UMQ	O3-C3	3.35	1.50	1.43
10	D	201	UMQ	O3-C3	3.33	1.50	1.43
25	G	102	BCR	C1-C6	-3.33	1.49	1.53
10	A	304	UMQ	O3-C3	3.31	1.50	1.43
18	D	204	SQD	O48-C23	3.22	1.42	1.33
14	B	204	CLA	CHC-C1C	3.21	1.43	1.35
10	B	203[B]	UMQ	C6'-C5'	-3.06	1.41	1.51
15	B	205	OPC	OAN-CAO	3.05	1.42	1.34
10	G	101	UMQ	C6'-C5'	-2.99	1.41	1.51
10	D	201	UMQ	C6'-C5'	-2.97	1.41	1.51
10	B	201	UMQ	C6'-C5'	-2.97	1.41	1.51
10	A	304	UMQ	C6'-C5'	-2.95	1.42	1.51
10	A	304	UMQ	O1-C4'	2.93	1.51	1.43
10	B	203[B]	UMQ	O1-C4'	2.91	1.51	1.43
13	A	309	2WM	CAV-CAW	-2.87	1.35	1.51
24	F	103	1O2	CAQ-CAO	2.85	1.59	1.50
18	D	204	SQD	O47-C7	2.84	1.42	1.34
10	G	101	UMQ	O1-C4'	2.84	1.51	1.43
10	D	201	UMQ	O1-C4'	2.83	1.51	1.43
10	B	201	UMQ	O1-C4'	2.75	1.51	1.43
25	G	102	BCR	C30-C25	-2.74	1.50	1.53
14	B	204	CLA	C1D-C2D	2.65	1.48	1.42
10	B	203[B]	UMQ	C1-C2	-2.59	1.45	1.52
10	G	101	UMQ	C1-C2	-2.57	1.45	1.52
10	D	201	UMQ	C1-C2	-2.57	1.45	1.52
10	B	201	UMQ	C1-C2	-2.55	1.45	1.52
10	G	101	UMQ	O2'-C2'	2.53	1.48	1.43
10	B	201	UMQ	O2'-C2'	2.53	1.48	1.43
10	D	201	UMQ	O2'-C2'	2.52	1.48	1.43
10	A	304	UMQ	O2'-C2'	2.47	1.48	1.43
10	A	304	UMQ	C1-C2	-2.46	1.45	1.52
10	B	203[B]	UMQ	O2'-C2'	2.44	1.48	1.43
14	B	204	CLA	CMB-C2B	-2.44	1.46	1.51
13	A	309	2WM	OAN-CAM	-2.41	1.41	1.44
21	E	101	3WM	OAN-CAM	-2.38	1.41	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	201	UMQ	O5-C1	2.24	1.47	1.41
22	F	101	2WA	CBS-CBR	-2.20	1.39	1.51
10	A	304	UMQ	O5-C1	2.18	1.47	1.41
18	D	204	SQD	O2-C2	-2.17	1.37	1.43
10	B	203[B]	UMQ	O5-C1	2.13	1.47	1.41
10	G	101	UMQ	O5-C1	2.09	1.47	1.41
14	B	204	CLA	CMD-C2D	-2.07	1.46	1.51
18	D	204	SQD	O3-C3	-2.07	1.38	1.43
10	B	201	UMQ	O5-C1	2.05	1.47	1.41
9	A	303	HEC	CAD-C3D	2.03	1.55	1.52
18	D	204	SQD	O4-C4	-2.01	1.38	1.43

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	201	UMQ	C1'-O5'-C5'	-9.30	95.44	113.69
10	G	101	UMQ	C1'-O5'-C5'	-8.96	96.10	113.69
10	B	203[B]	UMQ	C1'-O5'-C5'	-8.80	96.41	113.69
10	A	304	UMQ	C1'-O5'-C5'	-8.75	96.50	113.69
10	B	201	UMQ	C1'-O5'-C5'	-8.72	96.57	113.69
10	B	203[B]	UMQ	C2'-C3'-C4'	6.96	125.58	109.68
10	D	201	UMQ	C2'-C3'-C4'	6.92	125.47	109.68
10	B	201	UMQ	C2'-C3'-C4'	6.79	125.20	109.68
10	A	304	UMQ	C2'-C3'-C4'	6.78	125.15	109.68
10	G	101	UMQ	C2'-C3'-C4'	6.76	125.12	109.68
14	B	204	CLA	C4A-NA-C1A	5.73	109.28	106.71
10	B	201	UMQ	O5-C5-C4	-4.18	102.11	109.69
10	G	101	UMQ	O5-C5-C4	-4.04	102.35	109.69
24	F	103	1O2	OAN-CAO-CAQ	4.02	120.17	111.50
10	A	304	UMQ	O5-C5-C4	-4.02	102.40	109.69
11	C	303	7PH	O21-C21-C22	3.88	119.86	111.50
15	B	205	OPC	OAN-CAO-CAP	3.82	119.74	111.50
11	F	104	7PH	O21-C21-C22	3.77	119.62	111.50
18	D	204	SQD	O9-S-C6	3.77	111.42	106.94
10	B	201	UMQ	C1-O1-C4'	-3.77	108.65	117.96
11	A	305	7PH	O21-C21-C22	3.76	119.60	111.50
18	D	204	SQD	O9-S-O7	-3.74	101.02	113.95
10	G	101	UMQ	C1-O1-C4'	-3.71	108.79	117.96
18	D	204	SQD	O47-C7-C8	3.69	119.44	111.50
18	D	204	SQD	O7-S-C6	3.64	111.26	106.94
14	B	204	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
9	C	301	HEC	CMB-C2B-C1B	-3.53	123.04	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	206	7PH	O21-C21-C22	3.53	119.10	111.50
9	A	302	HEC	CMC-C2C-C1C	-3.50	123.08	128.46
10	B	203[B]	UMQ	C1-O1-C4'	-3.42	109.50	117.96
9	C	301	HEC	CMC-C2C-C1C	-3.41	123.23	128.46
9	A	303	HEC	CMB-C2B-C1B	-3.39	123.26	128.46
10	B	203[B]	UMQ	O5-C5-C4	-3.38	103.56	109.69
9	A	301	HEC	CMB-C2B-C1B	-3.33	123.35	128.46
9	A	301	HEC	CMC-C2C-C1C	-3.29	123.41	128.46
9	A	302	HEC	CMB-C2B-C1B	-3.18	123.57	128.46
11	D	203	7PH	O21-C21-C22	3.14	118.26	111.50
10	A	304	UMQ	C1-O1-C4'	-3.13	110.21	117.96
18	D	204	SQD	O6-C1-C2	3.07	113.10	108.30
9	A	302	HEC	CBD-CAD-C3D	-3.05	106.85	112.49
10	D	201	UMQ	O5-C5-C4	-3.03	104.19	109.69
18	D	204	SQD	O8-S-C6	2.96	110.45	105.74
14	B	204	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
14	B	204	CLA	CMB-C2B-C3B	2.85	130.01	124.68
9	A	302	HEC	CMC-C2C-C3C	2.81	129.12	125.82
9	C	301	HEC	CMB-C2B-C3B	2.81	129.12	125.82
18	D	204	SQD	C44-O6-C1	2.67	118.95	113.74
10	D	201	UMQ	O5-C1-C2	2.65	115.97	110.35
24	F	103	1O2	OBG-CBH-CBJ	2.64	120.20	111.91
9	A	303	HEC	CMB-C2B-C3B	2.61	128.89	125.82
11	C	303	7PH	O31-C31-C32	2.59	120.05	111.91
25	G	102	BCR	C33-C5-C6	-2.59	121.62	124.53
15	B	205	OPC	OBJ-CBK-CBL	2.59	120.03	111.91
9	A	301	HEC	CBD-CAD-C3D	-2.58	107.72	112.49
18	D	204	SQD	O48-C23-C24	2.57	119.99	111.91
11	B	206	7PH	O31-C31-C32	2.57	119.97	111.91
11	F	104	7PH	O31-C31-C32	2.56	119.95	111.91
9	A	301	HEC	C1D-C2D-C3D	-2.56	105.22	107.00
25	G	102	BCR	C27-C26-C25	2.51	126.38	122.73
11	A	305	7PH	O31-C31-C32	2.51	119.78	111.91
10	A	304	UMQ	C1-C2-C3	2.50	115.20	110.00
14	B	204	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
9	A	301	HEC	CMC-C2C-C3C	2.46	128.71	125.82
10	G	101	UMQ	C1-C2-C3	2.44	115.07	110.00
10	D	201	UMQ	C1-C2-C3	2.42	115.04	110.00
9	C	301	HEC	CMC-C2C-C3C	2.42	128.66	125.82
9	A	303	HEC	CAD-CBD-CGD	-2.40	108.65	112.67
14	B	204	CLA	CMD-C2D-C3D	2.40	129.16	124.68
9	A	302	HEC	C1D-C2D-C3D	-2.39	105.33	107.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	301	HEC	CMB-C2B-C3B	2.38	128.62	125.82
9	A	302	HEC	CMB-C2B-C3B	2.38	128.61	125.82
9	C	301	HEC	C1D-C2D-C3D	-2.37	105.35	107.00
10	D	201	UMQ	C1-O1-C4'	-2.27	112.34	117.96
18	D	204	SQD	O5-C5-C4	2.27	113.81	109.69
10	B	203[B]	UMQ	C1-C2-C3	2.27	114.72	110.00
10	D	201	UMQ	C1-O5-C5	2.27	118.14	113.69
25	G	102	BCR	C7-C8-C9	-2.27	122.81	126.23
10	B	203[B]	UMQ	O5-C5-C6	2.26	112.06	106.44
11	D	203	7PH	O31-C31-C32	2.26	118.99	111.91
10	G	101	UMQ	C3-C4-C5	2.23	114.21	110.24
14	B	204	CLA	CHB-C4A-NA	2.22	127.58	124.51
25	G	102	BCR	C24-C23-C22	-2.17	122.95	126.23
10	B	203[B]	UMQ	O5'-C5'-C4'	2.16	114.31	109.75
24	F	103	1O2	C1-C2-C3	2.14	114.46	110.00
24	F	103	1O2	C4-C3-C2	2.12	114.52	110.82
10	D	201	UMQ	O3'-C3'-C2'	-2.11	105.47	110.35
24	F	103	1O2	O5-C1-C2	2.08	114.75	110.35
10	B	201	UMQ	C1-C2-C3	2.08	114.32	110.00
9	C	301	HEC	CBA-CAA-C2A	-2.06	108.68	112.48
10	D	201	UMQ	C3-C4-C5	2.05	113.89	110.24
10	B	201	UMQ	O3'-C3'-C2'	-2.04	105.63	110.35
10	A	304	UMQ	O5-C1-C2	2.04	114.66	110.35
24	F	103	1O2	C3-C4-C5	2.02	113.85	110.24
10	A	304	UMQ	O5-C5-C6	2.01	111.43	106.44

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	B	204	CLA	NA
14	B	204	CLA	NC
14	B	204	CLA	ND
24	F	103	1O2	C1

All (289) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	304	UMQ	O5'-C1'-O1'-CA
10	A	304	UMQ	CB-CA-O1'-C1'
10	B	203[B]	UMQ	O5'-C1'-O1'-CA
11	A	305	7PH	O11-C1-C2-C3
11	A	305	7PH	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	206	7PH	O11-C1-C2-C3
11	B	206	7PH	O11-C1-C2-O21
11	C	303	7PH	O11-C1-C2-C3
11	C	303	7PH	O11-C1-C2-O21
11	C	303	7PH	O32-C31-O31-C3
11	C	303	7PH	C32-C31-O31-C3
11	D	203	7PH	O11-C1-C2-O21
11	D	203	7PH	C22-C21-O21-C2
11	F	104	7PH	O11-C1-C2-C3
11	F	104	7PH	O11-C1-C2-O21
13	A	309	2WM	OAD-CAO-OAN-CAM
13	A	309	2WM	OAK-CAL-CAM-OAN
13	A	309	2WM	OCC-CBK-CBL-CBM
18	D	204	SQD	C2-C1-O6-C44
18	D	204	SQD	O6-C44-C45-O47
18	D	204	SQD	O47-C45-C46-O48
20	D	206	2WD	O11-C1-C2-C3
20	D	206	2WD	O11-C1-C2-O21
20	D	206	2WD	C1-C2-O21-C21
21	E	101	3WM	OAD-CAO-OAN-CAM
21	E	101	3WM	OAK-CAL-CAM-OAN
21	E	101	3WM	OAK-CAL-CAM-CBI
21	E	101	3WM	OCC-CBK-OBJ-CBI
21	E	101	3WM	OCC-CBK-CBL-CBM
22	F	101	2WA	OAD-CAO-OAN-CAM
22	F	101	2WA	OAK-CAL-CAM-OAN
24	F	103	1O2	C2-C1-O1-CAL
25	G	102	BCR	C7-C8-C9-C34
25	G	102	BCR	C22-C23-C24-C25
10	D	201	UMQ	O5-C1-O1-C4'
11	F	104	7PH	O22-C21-O21-C2
11	A	305	7PH	C32-C31-O31-C3
11	D	203	7PH	C32-C31-O31-C3
24	F	103	1O2	CBP-CBQ-CBR-CBS
22	F	101	2WA	CBP-CBQ-CBR-CBS
11	D	203	7PH	O22-C21-O21-C2
24	F	103	1O2	CBJ-CBK-CBL-CBM
24	F	103	1O2	CBL-CBM-CBN-CBO
11	A	305	7PH	O32-C31-O31-C3
24	F	103	1O2	OBI-CBH-OBG-CBF
24	F	103	1O2	O5-C5-C6-O6
11	A	305	7PH	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	206	7PH	C22-C21-O21-C2
11	F	104	7PH	C22-C21-O21-C2
15	B	205	OPC	CAP-CAO-OAN-CAM
11	A	305	7PH	C22-C23-C24-C25
22	F	101	2WA	CBR-CBS-CBT-CBU
18	D	204	SQD	O5-C1-O6-C44
13	A	309	2WM	CAU-CAV-CAW-CAX
11	C	303	7PH	C31-C32-C33-C34
11	D	203	7PH	O32-C31-O31-C3
11	B	206	7PH	C32-C31-O31-C3
11	F	104	7PH	C32-C31-O31-C3
24	F	103	1O2	CBJ-CBH-OBG-CBF
10	D	201	UMQ	C2'-C1'-O1'-CA
11	B	206	7PH	O32-C31-O31-C3
14	B	204	CLA	C10-C11-C12-C13
15	B	205	OPC	CBK-CBL-CBM-CBN
24	F	103	1O2	C4-C5-C6-O6
24	F	103	1O2	O5-C1-O1-CAL
11	F	104	7PH	O32-C31-O31-C3
13	A	309	2WM	CBN-CBO-CBP-CBQ
11	A	305	7PH	C32-C33-C34-C35
11	A	305	7PH	C31-C32-C33-C34
11	D	203	7PH	C22-C23-C24-C25
13	A	309	2WM	OAN-CAO-CAP-CAQ
21	E	101	3WM	CBL-CBM-CBN-CBO
11	A	305	7PH	O22-C21-O21-C2
11	B	206	7PH	O22-C21-O21-C2
15	B	205	OPC	OAD-CAO-OAN-CAM
11	A	305	7PH	C33-C34-C35-C36
12	A	307	8K6	C5-C6-C7-C8
24	F	103	1O2	CAS-CAT-CAU-CAV
25	G	102	BCR	C11-C10-C9-C8
13	A	309	2WM	CBM-CBN-CBO-CBP
18	D	204	SQD	C9-C10-C11-C12
10	D	201	UMQ	O5-C5-C6-O6
24	F	103	1O2	CBH-CBJ-CBK-CBL
17	D	202	MYS	C7-C8-C9-C10
10	B	203[B]	UMQ	O5-C5-C6-O6
24	F	103	1O2	CAT-CAU-CAV-CAW
10	G	101	UMQ	O5-C5-C6-O6
12	A	308	8K6	C12-C13-C14-C15
15	B	205	OPC	CAS-CAT-CAU-CAV

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	309	2WM	CBT-CBU-CBV-CBW
22	F	101	2WA	CBN-CBO-CBP-CBQ
11	B	206	7PH	C24-C25-C26-C27
13	A	309	2WM	CAY-CAZ-CBA-CBB
15	B	205	OPC	CAR-CAS-CAT-CAU
24	F	103	1O2	CAY-CAZ-CBA-CBB
11	B	206	7PH	C33-C34-C35-C36
22	F	101	2WA	CAQ-CAR-CAS-CAT
14	B	204	CLA	C3A-C2A-CAA-CBA
21	E	101	3WM	CBM-CBN-CBO-CBP
13	A	309	2WM	CAS-CAT-CAU-CAV
10	B	201	UMQ	O5-C1-O1-C4'
13	A	309	2WM	OAD-CAO-CAP-CAQ
20	D	206	2WD	O22-C21-C22-C23
22	F	101	2WA	CBT-CBU-CBV-CBW
21	E	101	3WM	CBS-CBT-CBU-CBV
18	D	204	SQD	C31-C32-C33-C34
24	F	103	1O2	CAW-CAX-CAY-CAZ
15	B	205	OPC	CBL-CBM-CBN-CBO
10	A	304	UMQ	CG-CH-CI-CJ
12	A	308	8K6	C13-C14-C15-C16
21	E	101	3WM	CAP-CAQ-CAR-CAS
11	C	303	7PH	C21-C22-C23-C24
21	E	101	3WM	CBB-CBC-CBD-CBE
11	B	206	7PH	C25-C26-C27-C28
10	B	203[B]	UMQ	CA-CB-CC-CD
12	A	308	8K6	C9-C10-C11-C12
11	C	303	7PH	C22-C21-O21-C2
18	D	204	SQD	C8-C7-O47-C45
12	A	308	8K6	C11-C10-C9-C8
10	A	304	UMQ	C2'-C1'-O1'-CA
10	B	203[B]	UMQ	C2'-C1'-O1'-CA
20	D	206	2WD	O21-C2-C3-O31
10	B	203[B]	UMQ	O1'-CA-CB-CC
21	E	101	3WM	CAW-CAX-CAY-CAZ
21	E	101	3WM	CBO-CBP-CBQ-CBR
22	F	101	2WA	CAW-CAX-CAY-CAZ
10	G	101	UMQ	O5'-C5'-C6'-O6'
14	B	204	CLA	C1A-C2A-CAA-CBA
11	C	303	7PH	O22-C21-O21-C2
24	F	103	1O2	CBQ-CBR-CBS-CBT
12	A	306	8K6	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	F	101	2WA	CBA-CBB-CBC-CBD
24	F	103	1O2	CAV-CAW-CAX-CAY
11	B	206	7PH	C32-C33-C34-C35
12	B	202[A]	8K6	C9-C10-C11-C12
22	F	101	2WA	CAY-CAZ-CBA-CBB
12	B	202[A]	8K6	C10-C11-C12-C13
17	D	202	MYS	C11-C10-C9-C8
10	G	101	UMQ	CA-CB-CC-CD
10	D	201	UMQ	O1'-CA-CB-CC
15	B	205	OPC	CBT-CBU-CBV-CBW
18	D	204	SQD	O6-C44-C45-C46
20	D	206	2WD	C1-C2-C3-O31
24	F	103	1O2	O1-CAL-CAM-CBF
10	G	101	UMQ	C4-C5-C6-O6
12	A	308	8K6	C10-C11-C12-C13
10	A	304	UMQ	C2-C1-O1-C4'
15	B	205	OPC	CBC-CBD-CBE-CBF
13	A	309	2WM	OBJ-CBK-CBL-CBM
20	D	206	2WD	O21-C21-C22-C23
10	D	201	UMQ	O5'-C1'-O1'-CA
21	E	101	3WM	CAS-CAT-CAU-CAV
24	F	103	1O2	CBR-CBS-CBT-CBU
15	B	205	OPC	CBU-CBV-CBW-CBX
11	D	203	7PH	C2A-C2B-C2C-C2D
10	A	304	UMQ	C5'-C4'-O1-C1
11	C	303	7PH	C27-C28-C29-C2A
13	A	309	2WM	OAN-CAM-CBI-OBJ
14	B	204	CLA	C16-C17-C18-C20
10	A	304	UMQ	C3'-C4'-O1-C1
10	A	304	UMQ	CC-CD-CF-CG
10	B	201	UMQ	CB-CA-O1'-C1'
22	F	101	2WA	CAP-CAQ-CAR-CAS
15	B	205	OPC	CAX-CAY-CAZ-CBA
11	C	303	7PH	C1-C2-C3-O31
11	F	104	7PH	C1-C2-C3-O31
18	D	204	SQD	C44-C45-C46-O48
22	F	101	2WA	CAL-CAM-CBI-OBJ
10	D	201	UMQ	CA-CB-CC-CD
18	D	204	SQD	C11-C12-C13-C14
10	D	201	UMQ	C4-C5-C6-O6
18	D	204	SQD	C10-C11-C12-C13
21	E	101	3WM	CAX-CAY-CAZ-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	205	OPC	CAP-CAQ-CAR-CAS
11	D	203	7PH	O11-C1-C2-C3
22	F	101	2WA	OAK-CAL-CAM-CBI
10	A	304	UMQ	CH-CI-CJ-CK
12	A	306	8K6	C10-C11-C12-C13
25	G	102	BCR	C23-C24-C25-C26
25	G	102	BCR	C23-C24-C25-C30
10	B	203[B]	UMQ	C4-C5-C6-O6
11	D	203	7PH	C38-C39-C3A-C3B
21	E	101	3WM	OBJ-CBK-CBL-CBM
11	F	104	7PH	C31-C32-C33-C34
14	B	204	CLA	C16-C17-C18-C19
12	B	202[A]	8K6	C3-C4-C5-C6
13	A	309	2WM	CBV-CBW-CBX-CBY
11	B	206	7PH	C3-C2-O21-C21
11	C	303	7PH	C3-C2-O21-C21
11	D	203	7PH	C1-C2-O21-C21
11	F	104	7PH	C3-C2-O21-C21
13	A	309	2WM	CAL-CAM-CBI-OBJ
11	B	206	7PH	C35-C36-C37-C38
11	C	303	7PH	O21-C2-C3-O31
11	F	104	7PH	O21-C21-C22-C23
21	E	101	3WM	CBQ-CBR-CBS-CBT
15	B	205	OPC	CAW-CAX-CAY-CAZ
9	A	302	HEC	C2A-CAA-CBA-CGA
11	B	206	7PH	C34-C35-C36-C37
11	A	305	7PH	C34-C35-C36-C37
11	B	206	7PH	C23-C24-C25-C26
10	G	101	UMQ	CI-CJ-CK-CL
13	A	309	2WM	CBL-CBK-OBJ-CBI
22	F	101	2WA	CBL-CBK-OBJ-CBI
15	B	205	OPC	CBS-CBT-CBU-CBV
11	C	303	7PH	C26-C27-C28-C29
18	D	204	SQD	C7-C8-C9-C10
24	F	103	1O2	CAR-CAS-CAT-CAU
9	A	302	HEC	C1A-C2A-CAA-CBA
9	A	302	HEC	C3A-C2A-CAA-CBA
22	F	101	2WA	OAN-CAM-CBI-OBJ
24	F	103	1O2	O1-CAL-CAM-OAN
22	F	101	2WA	CAM-CBI-OBJ-CBK
12	B	202[A]	8K6	C11-C12-C13-C14
21	E	101	3WM	OAN-CAO-CAP-CAQ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	304	UMQ	O5-C1-O1-C4'
13	A	309	2WM	CBY-CBZ-CCA-CCB
13	A	309	2WM	CBR-CBS-CBT-CBU
21	E	101	3WM	OAD-CAO-CAP-CAQ
11	F	104	7PH	C29-C2A-C2B-C2C
13	A	309	2WM	CAZ-CBA-CBB-CBC
25	G	102	BCR	C7-C8-C9-C10
14	B	204	CLA	C4-C3-C5-C6
15	B	205	OPC	CBV-CBW-CBX-CBY
11	A	305	7PH	C3-C2-O21-C21
12	A	307	8K6	C13-C14-C15-C16
21	E	101	3WM	CAQ-CAR-CAS-CAT
10	B	203[B]	UMQ	C5'-C4'-O1-C1
12	A	307	8K6	C15-C16-C17-C18
12	B	202[A]	8K6	C6-C7-C8-C9
24	F	103	1O2	CBA-CBB-CBC-CBD
11	D	203	7PH	O21-C21-C22-C23
15	B	205	OPC	CBN-CBO-CBP-CBQ
9	A	301	HEC	C2A-CAA-CBA-CGA
11	D	203	7PH	C28-C29-C2A-C2B
22	F	101	2WA	CAO-CAP-CAQ-CAR
21	E	101	3WM	CBT-CBU-CBV-CBW
10	G	101	UMQ	O1'-CA-CB-CC
12	A	308	8K6	C6-C7-C8-C9
18	D	204	SQD	C15-C16-C17-C18
24	F	103	1O2	OAN-CAM-CBF-OBG
11	C	303	7PH	C23-C24-C25-C26
13	A	309	2WM	CBL-CBM-CBN-CBO
14	B	204	CLA	O2A-C1-C2-C3
13	A	309	2WM	CBK-CBL-CBM-CBN
21	E	101	3WM	CAO-CAP-CAQ-CAR
22	F	101	2WA	CBV-CBW-CBX-CBY
24	F	103	1O2	OBG-CBH-CBJ-CBK
12	A	308	8K6	C14-C15-C16-C17
14	B	204	CLA	C2-C3-C5-C6
11	A	305	7PH	O21-C21-C22-C23
10	B	201	UMQ	C2-C1-O1-C4'
25	G	102	BCR	C1-C6-C7-C8
18	D	204	SQD	C12-C13-C14-C15
23	F	102	OCT	C1-C2-C3-C4
11	C	303	7PH	C25-C26-C27-C28
10	B	203[B]	UMQ	C3'-C4'-O1-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	A	308	8K6	C7-C8-C9-C10
22	F	101	2WA	OBJ-CBK-CBL-CBM
21	E	101	3WM	CAV-CAW-CAX-CAY
25	G	102	BCR	C11-C10-C9-C34
15	B	205	OPC	CAT-CAU-CAV-CAW
11	C	303	7PH	C24-C25-C26-C27
11	D	203	7PH	C33-C34-C35-C36
13	A	309	2WM	CAW-CAX-CAY-CAZ
17	D	202	MYS	C11-C12-C13-C14
11	C	303	7PH	C33-C34-C35-C36
15	B	205	OPC	CBR-CBS-CBT-CBU
21	E	101	3WM	CAT-CAU-CAV-CAW
11	C	303	7PH	O21-C21-C22-C23
24	F	103	1O2	OAN-CAO-CAQ-CAR
11	A	305	7PH	C21-C22-C23-C24
22	F	101	2WA	CAT-CAU-CAV-CAW
11	C	303	7PH	C2A-C2B-C2C-C2D
24	F	103	1O2	OAP-CAO-CAQ-CAR
13	A	309	2WM	CBA-CBB-CBC-CBD
13	A	309	2WM	CBX-CBY-CBZ-CCA
21	E	101	3WM	CAZ-CBA-CBB-CBC
25	G	102	BCR	C5-C6-C7-C8
11	C	303	7PH	O22-C21-C22-C23
18	D	204	SQD	O47-C7-C8-C9
11	C	303	7PH	C28-C29-C2A-C2B
11	B	206	7PH	O31-C31-C32-C33
13	A	309	2WM	CBW-CBX-CBY-CBZ
15	B	205	OPC	OAK-CAL-CAM-OAN
10	B	203[B]	UMQ	CB-CA-O1'-C1'
11	B	206	7PH	O32-C31-C32-C33
15	B	205	OPC	CBA-CBB-CBC-CBD
11	C	303	7PH	O32-C31-C32-C33

There are no ring outliers.

27 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	D	204	SQD	2	0
12	A	306	8K6	2	0
11	B	206	7PH	5	0
11	F	104	7PH	6	0
11	D	203	7PH	1	0

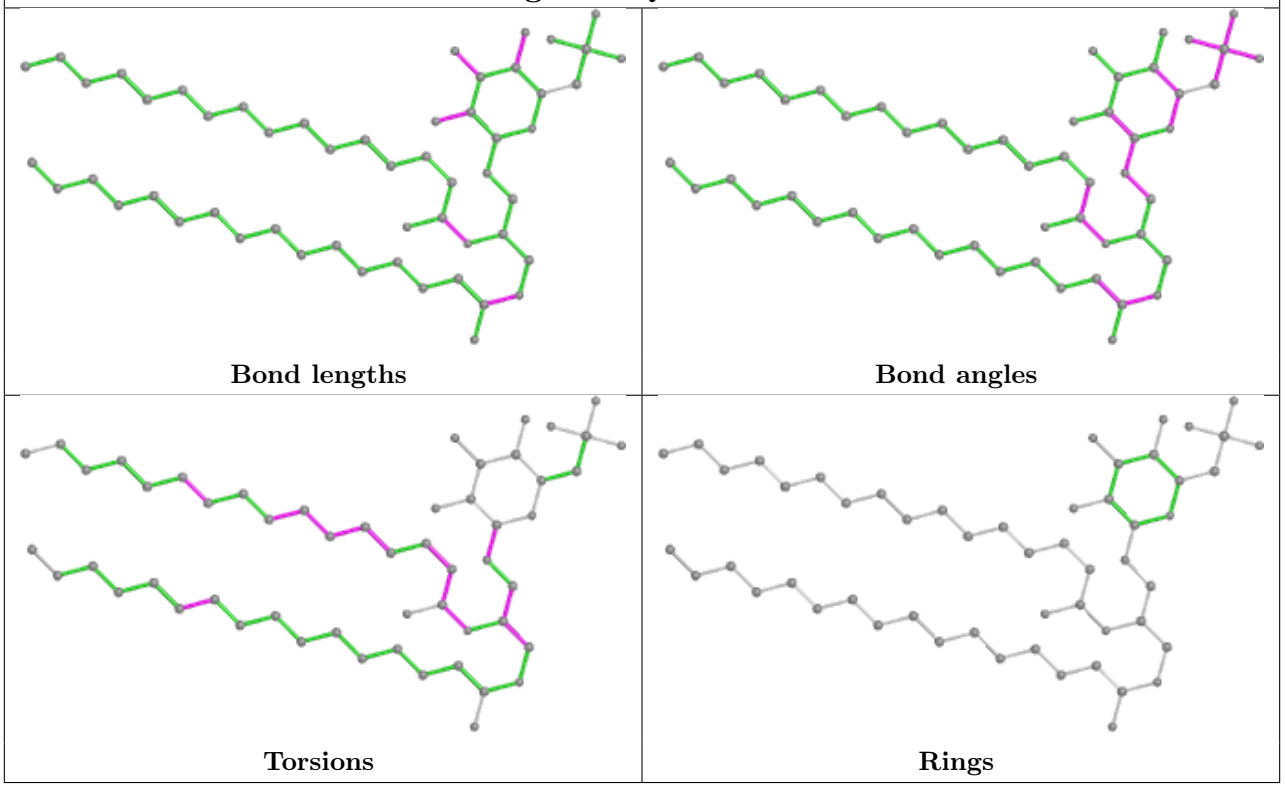
Continued on next page...

Continued from previous page...

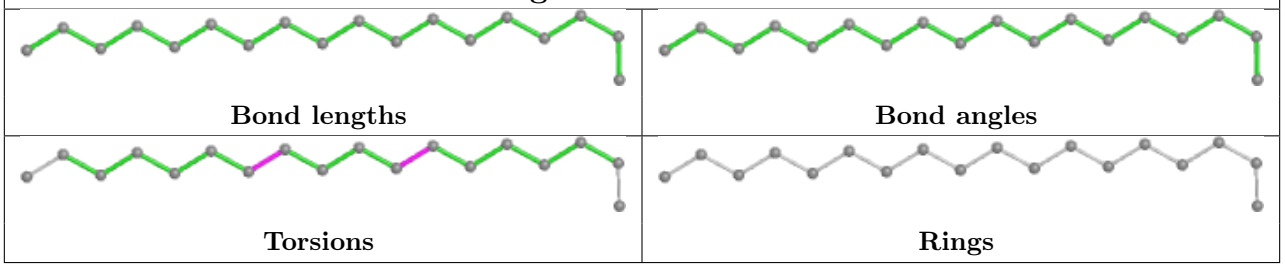
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	204	CLA	4	0
9	C	301	HEC	4	0
22	F	101	2WA	7	0
10	G	101	UMQ	4	0
17	D	202	MYS	1	0
25	G	102	BCR	2	0
21	E	101	3WM	9	0
12	A	308	8K6	5	0
24	F	103	1O2	11	0
10	D	201	UMQ	4	0
11	A	305	7PH	1	0
10	A	304	UMQ	9	0
9	A	301	HEC	2	0
10	B	203[B]	UMQ	10	0
9	A	303	HEC	6	0
10	B	201	UMQ	7	0
9	A	302	HEC	2	0
20	D	206	2WD	2	0
11	C	303	7PH	4	0
15	B	205	OPC	5	0
12	A	307	8K6	2	0
12	B	202[A]	8K6	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

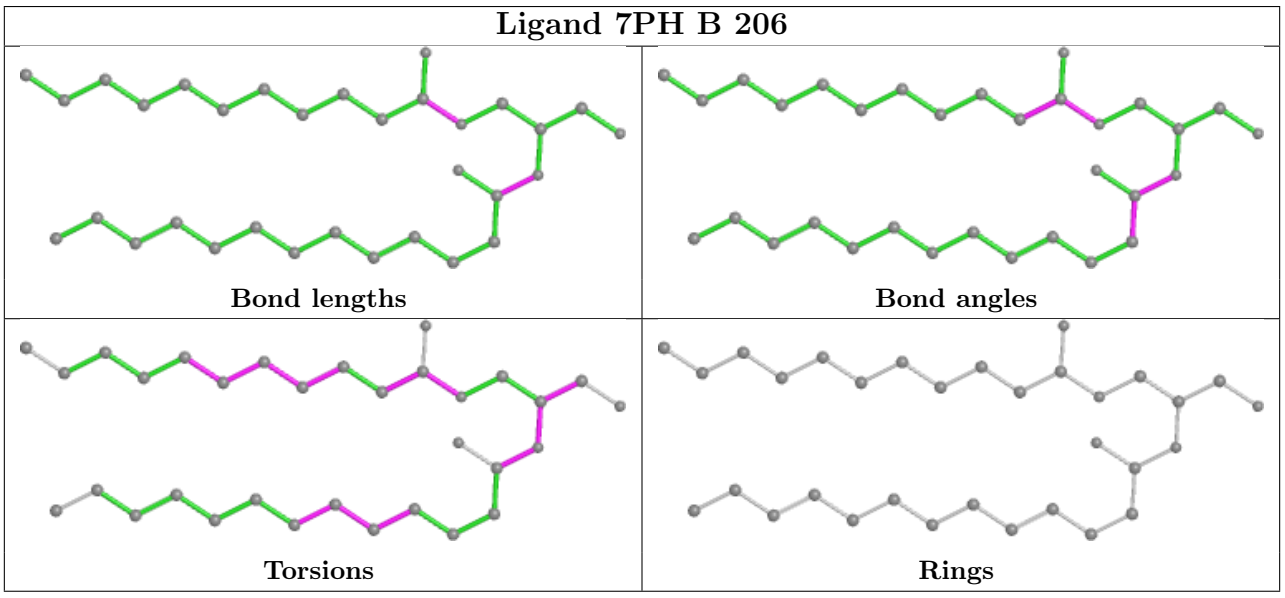
Ligand SQD D 204



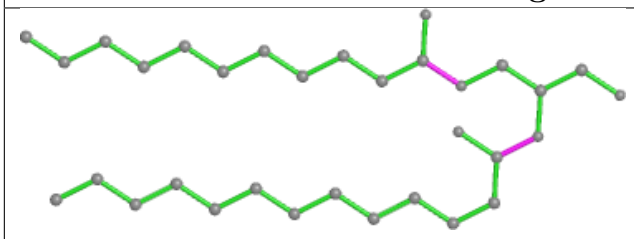
Ligand 8K6 A 306



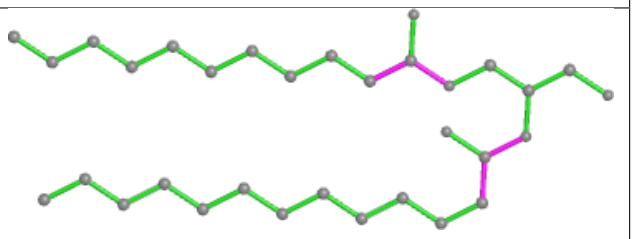
Ligand 7PH B 206



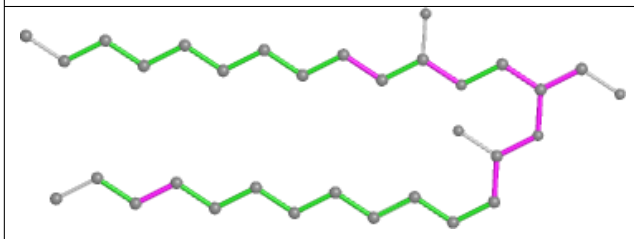
Ligand 7PH F 104



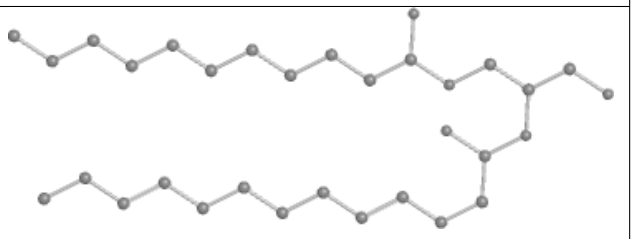
Bond lengths



Bond angles

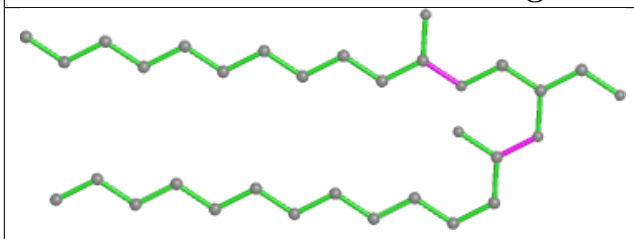


Torsions

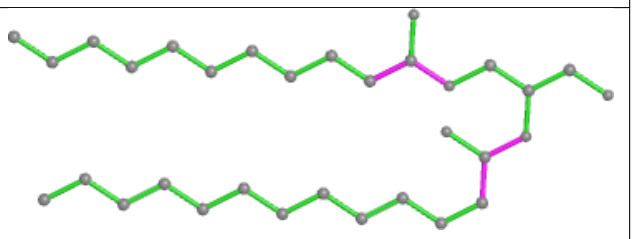


Rings

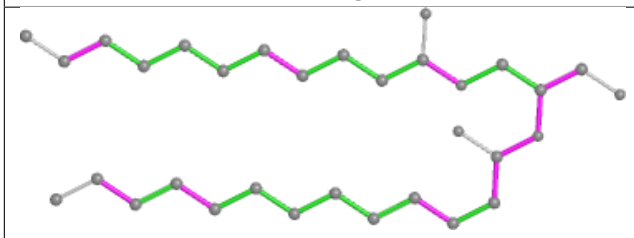
Ligand 7PH D 203



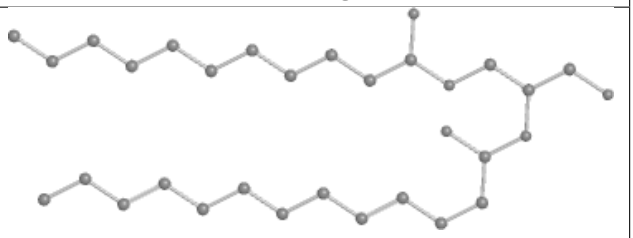
Bond lengths



Bond angles

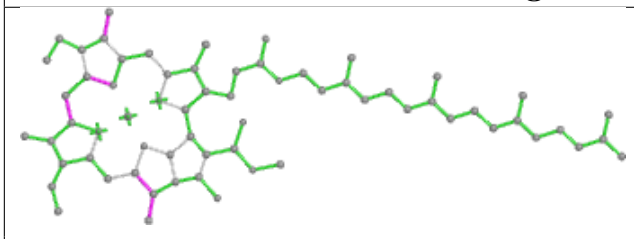


Torsions

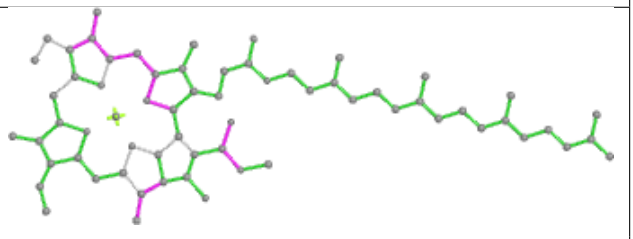


Rings

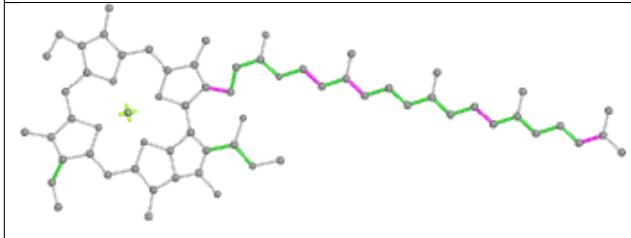
Ligand CLA B 204



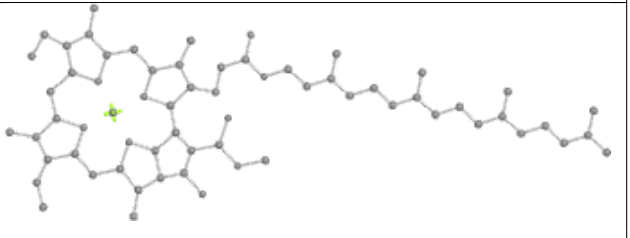
Bond lengths



Bond angles

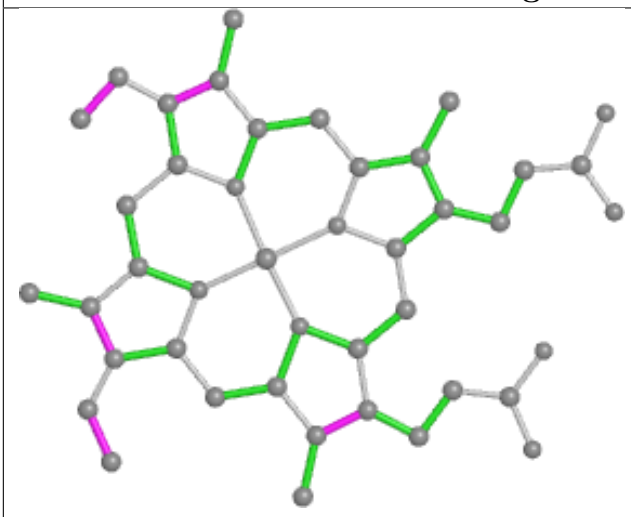


Torsions

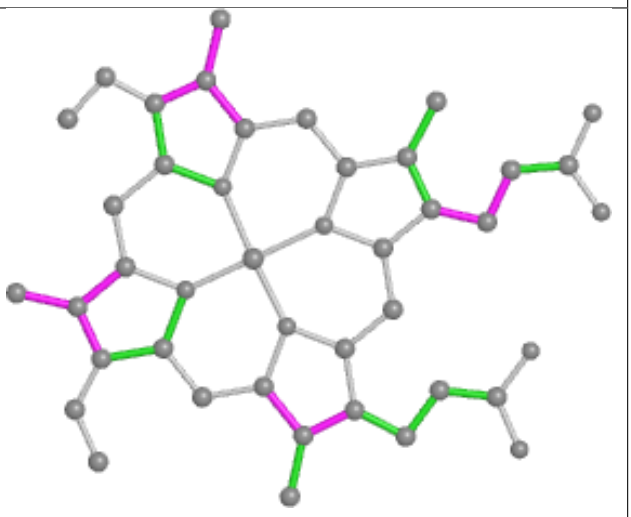


Rings

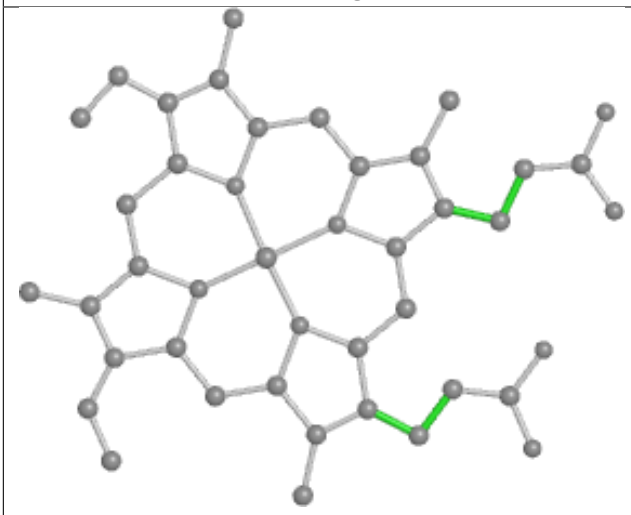
Ligand HEC C 301



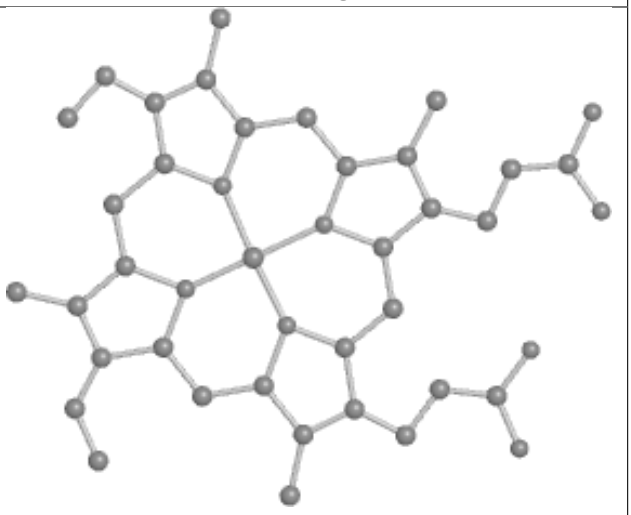
Bond lengths



Bond angles

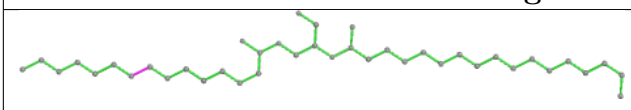


Torsions

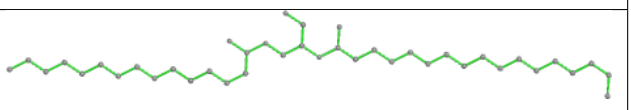


Rings

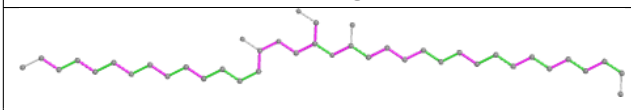
Ligand 2WA F 101



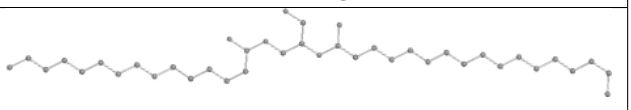
Bond lengths



Bond angles

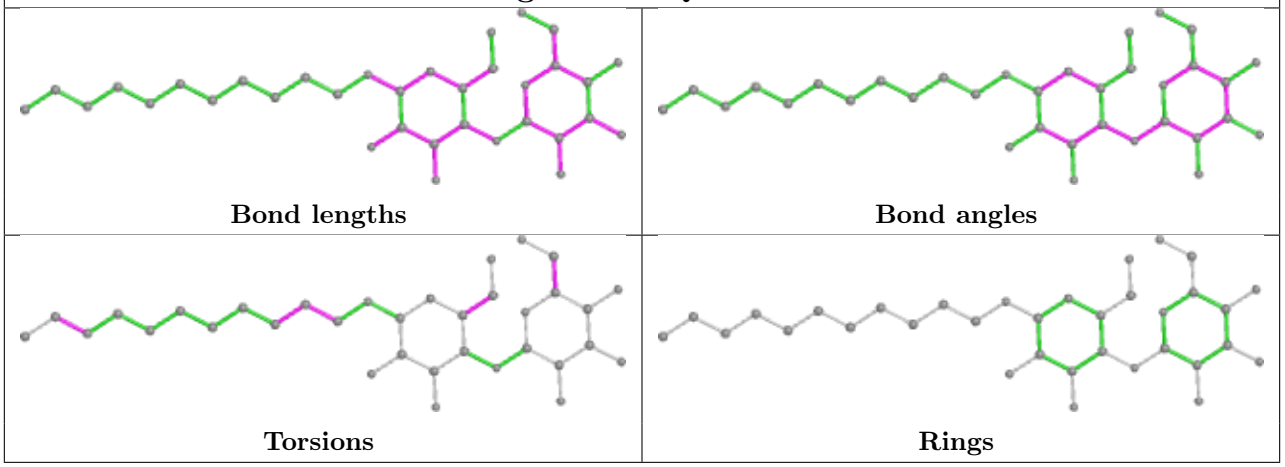


Torsions

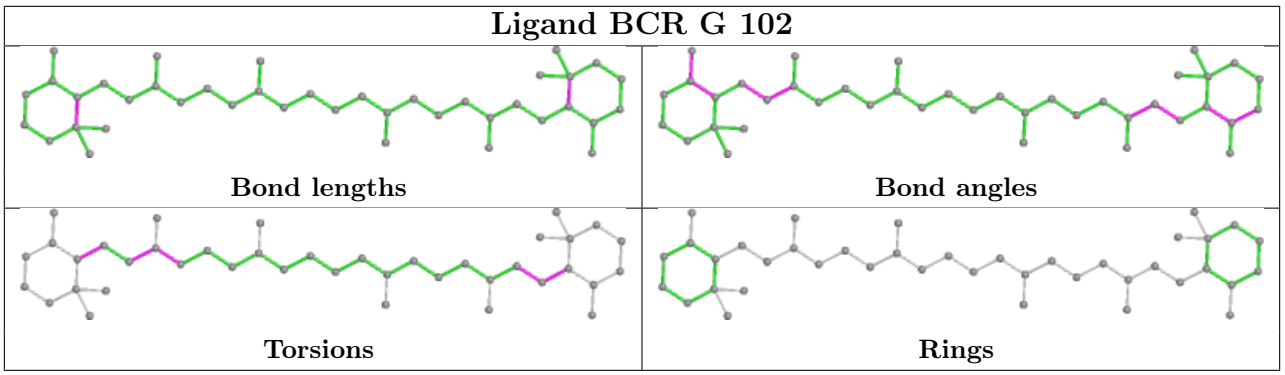


Rings

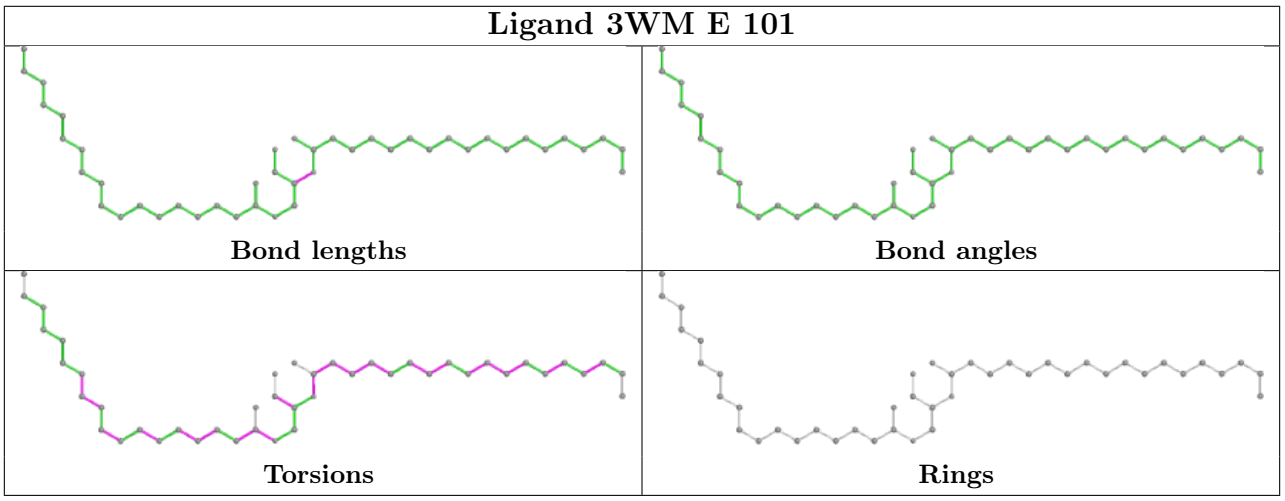
Ligand UMQ G 101



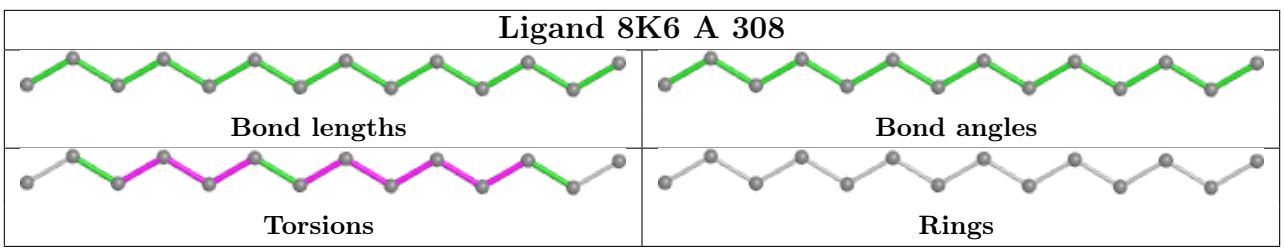
Ligand BCR G 102



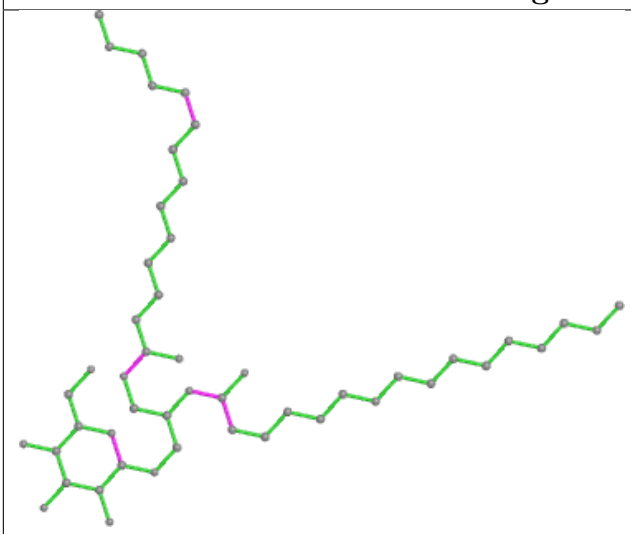
Ligand 3WM E 101



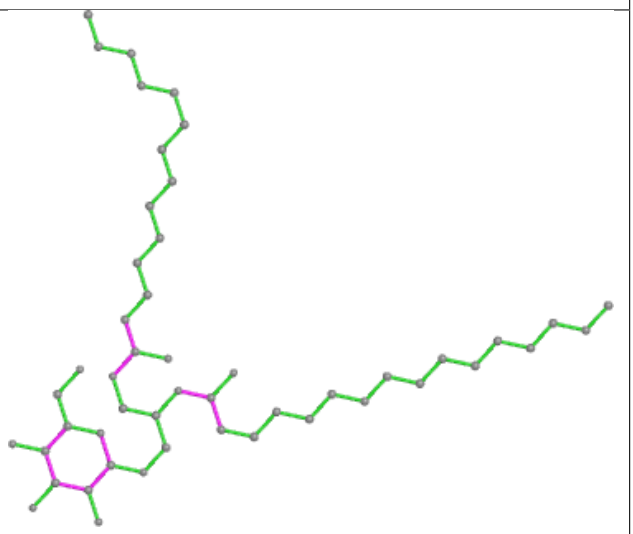
Ligand 8K6 A 308



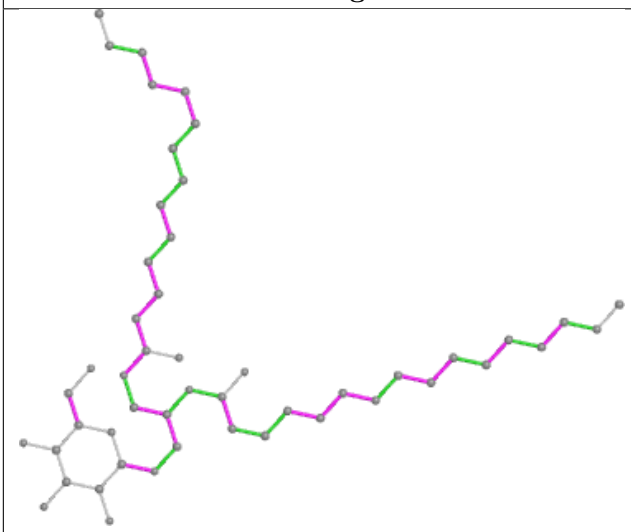
Ligand 1O2 F 103



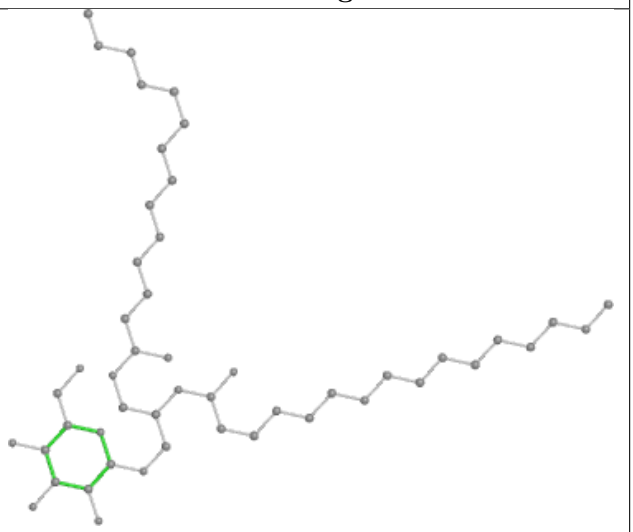
Bond lengths



Bond angles

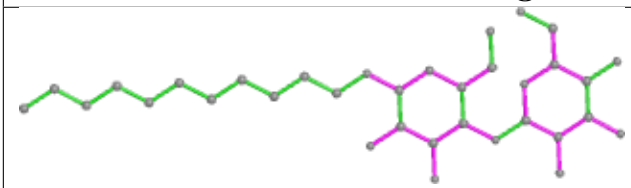


Torsions

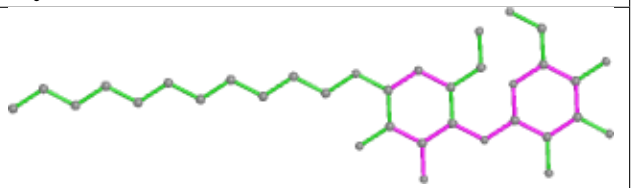


Rings

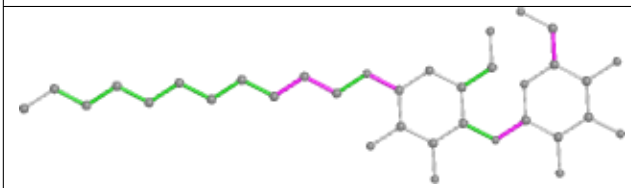
Ligand UMQ D 201



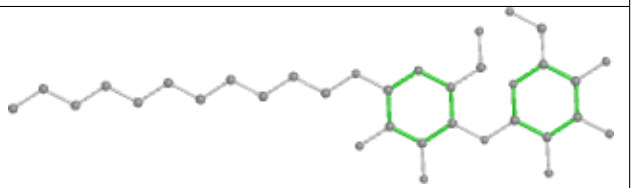
Bond lengths



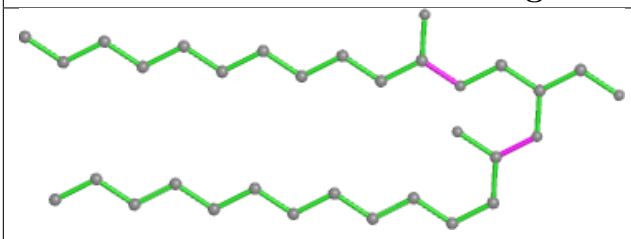
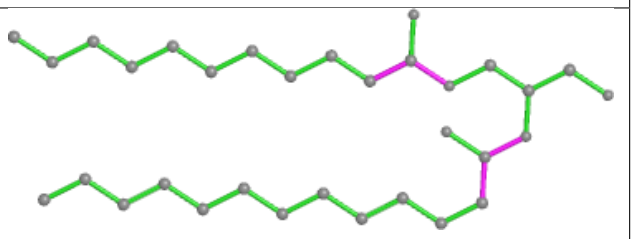
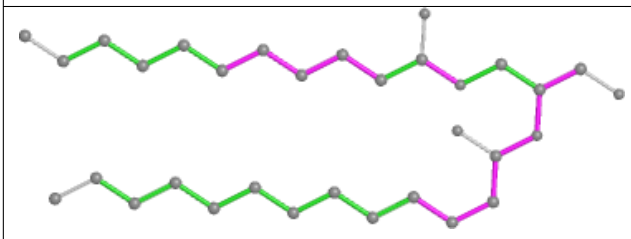
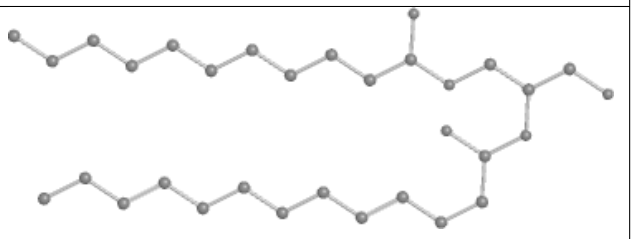
Bond angles

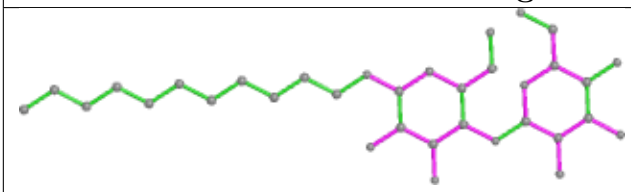
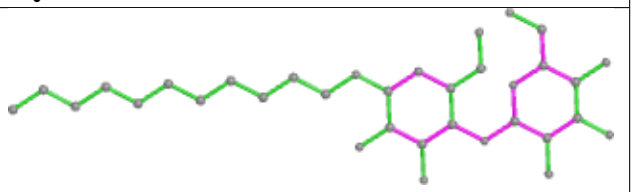
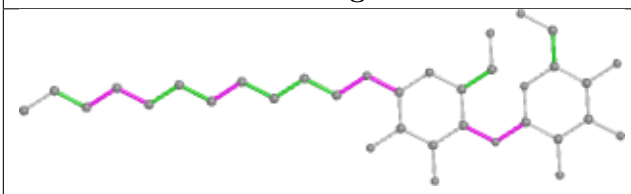
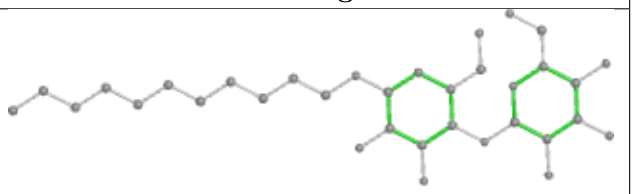


Torsions

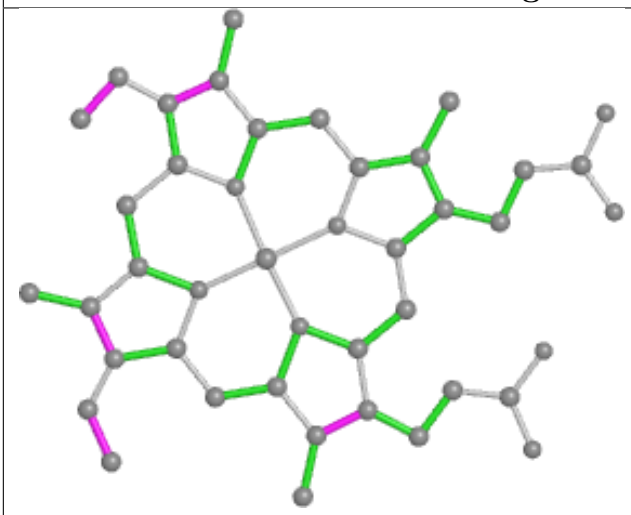


Rings

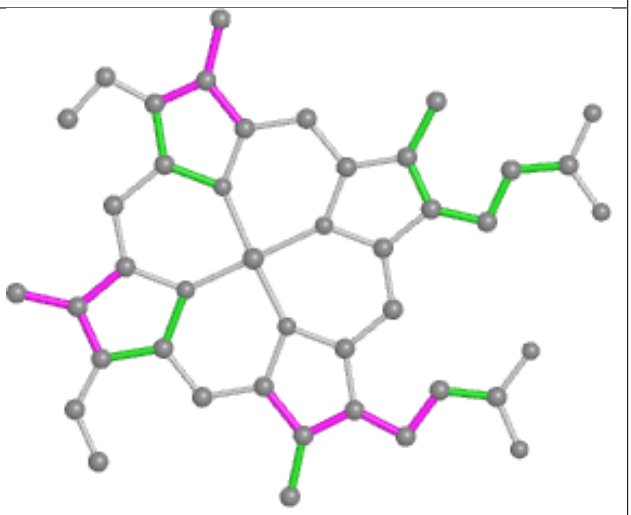
Ligand 7PH A 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UMQ A 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

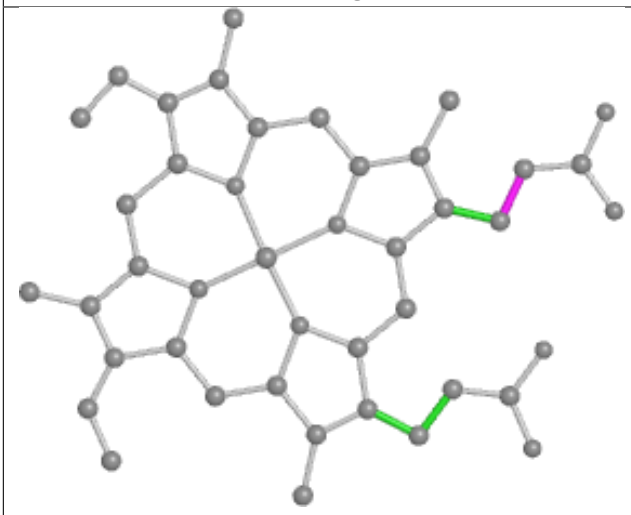
Ligand HEC A 301



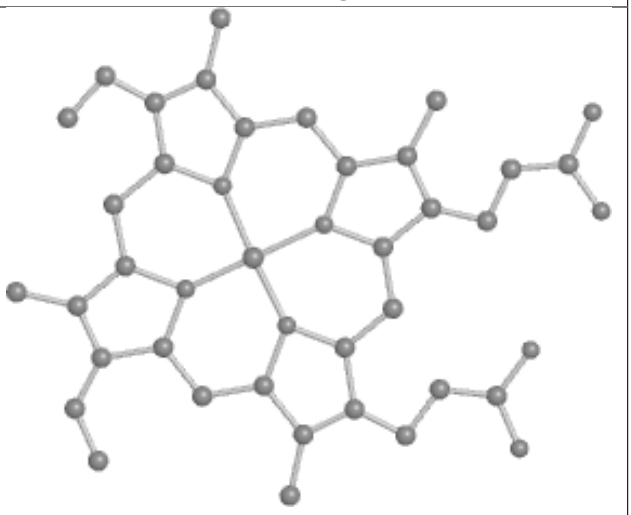
Bond lengths



Bond angles

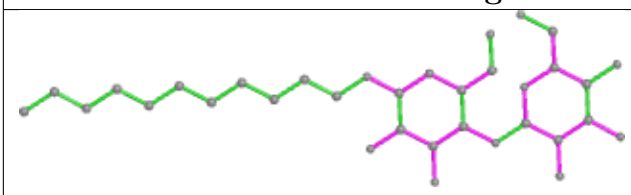


Torsions

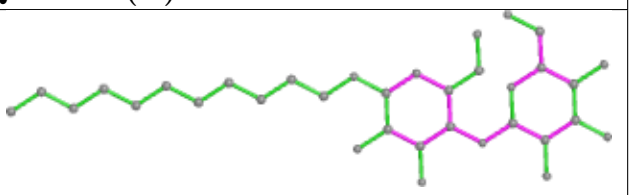


Rings

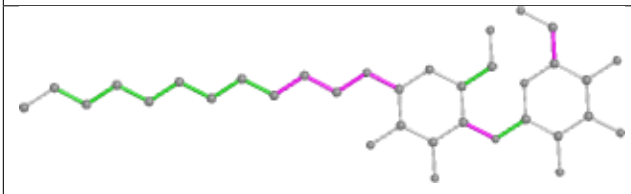
Ligand UMQ B 203 (B)



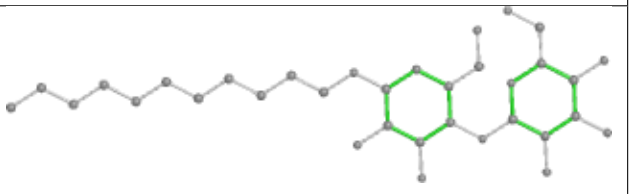
Bond lengths



Bond angles

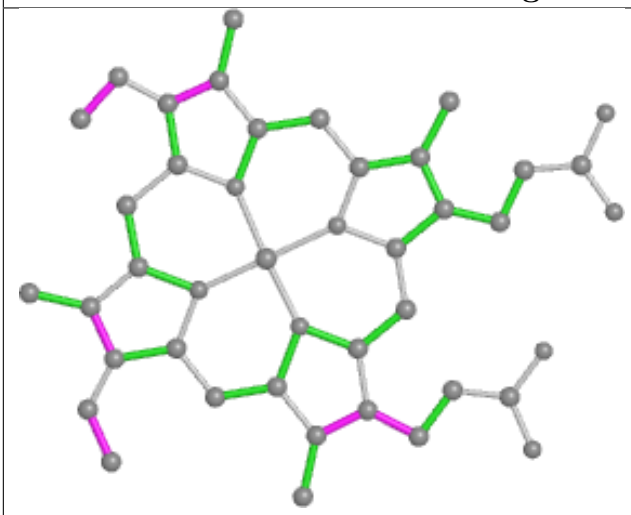


Torsions

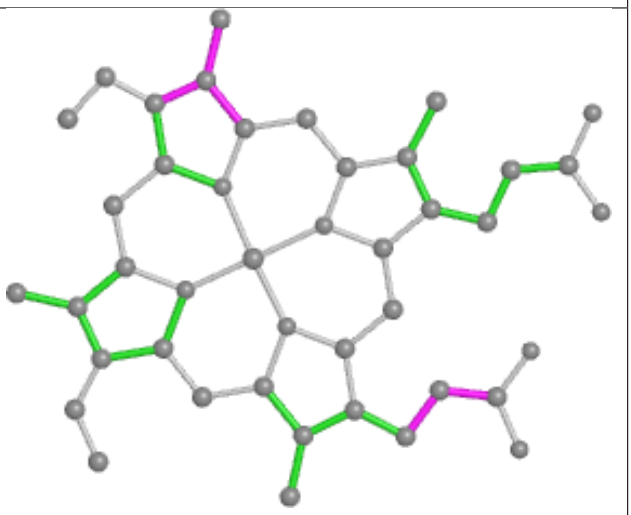


Rings

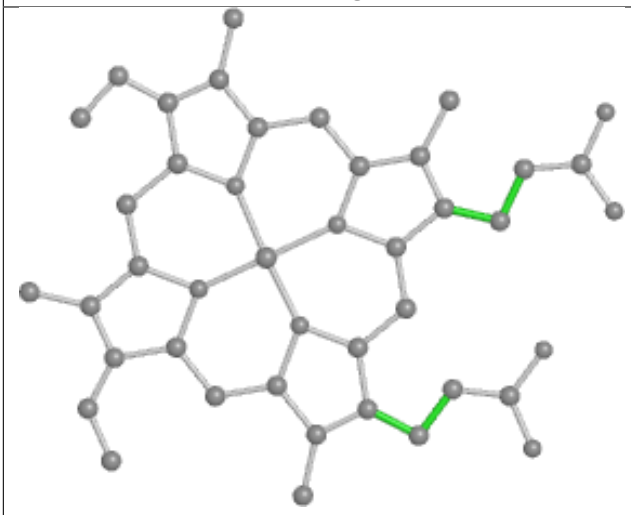
Ligand HEC A 303



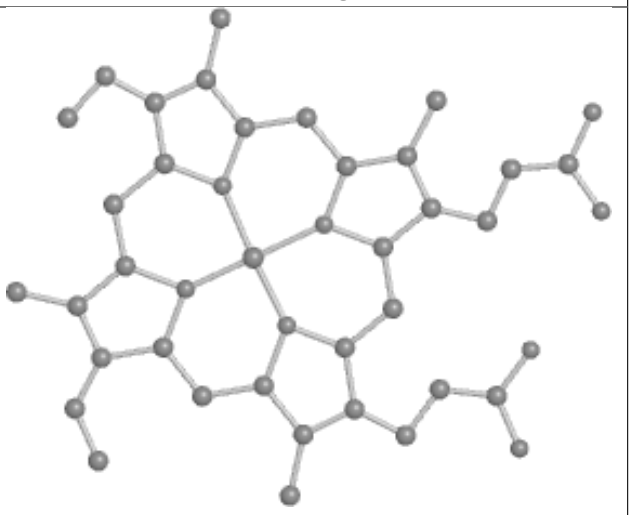
Bond lengths



Bond angles

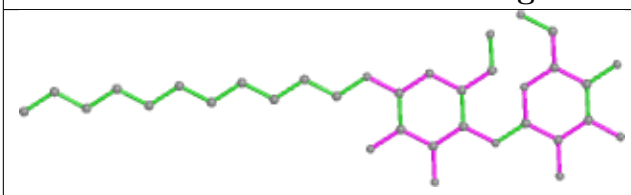


Torsions

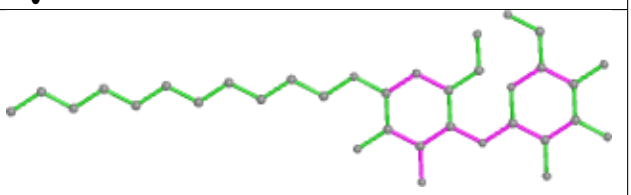


Rings

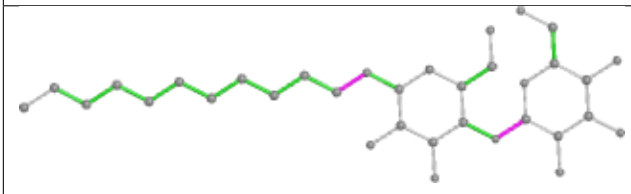
Ligand UMQ B 201



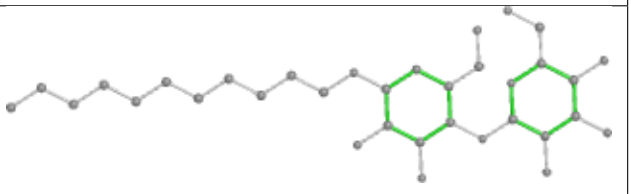
Bond lengths



Bond angles

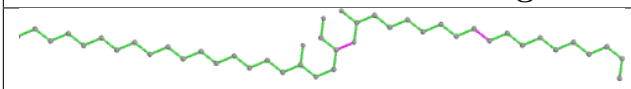


Torsions

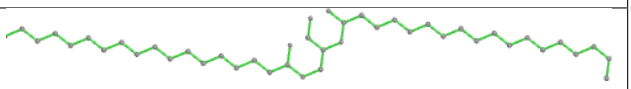


Rings

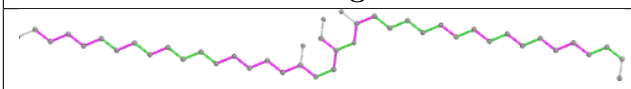
Ligand 2WM A 309



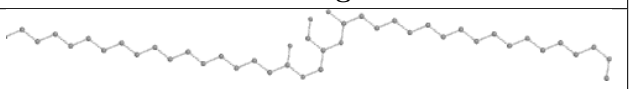
Bond lengths



Bond angles

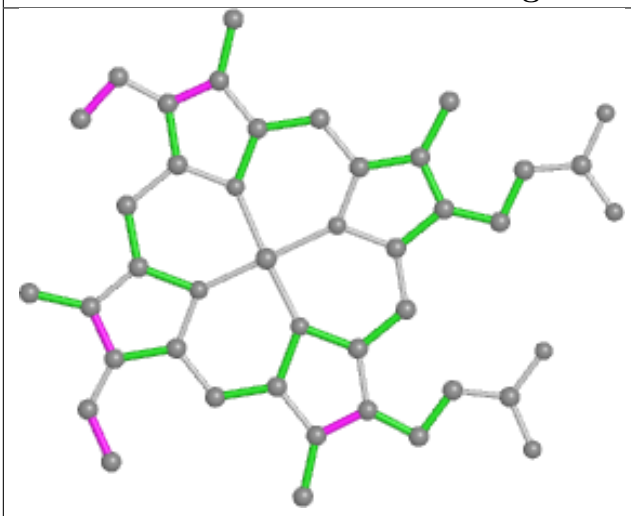


Torsions

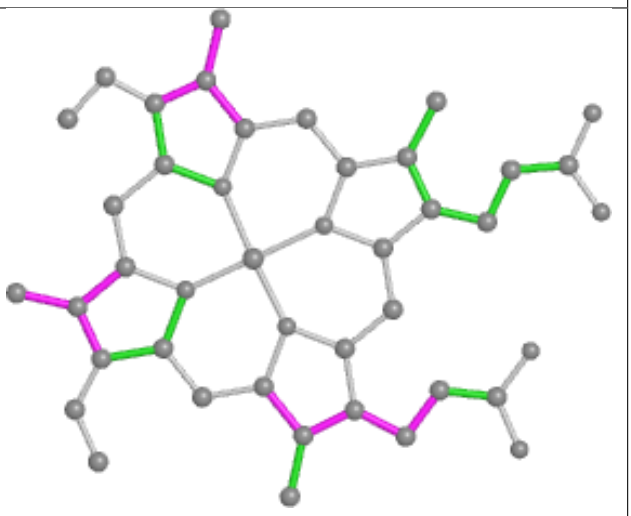


Rings

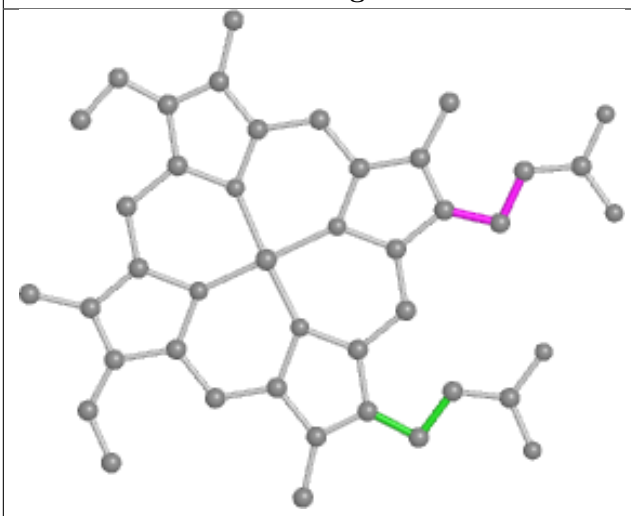
Ligand HEC A 302



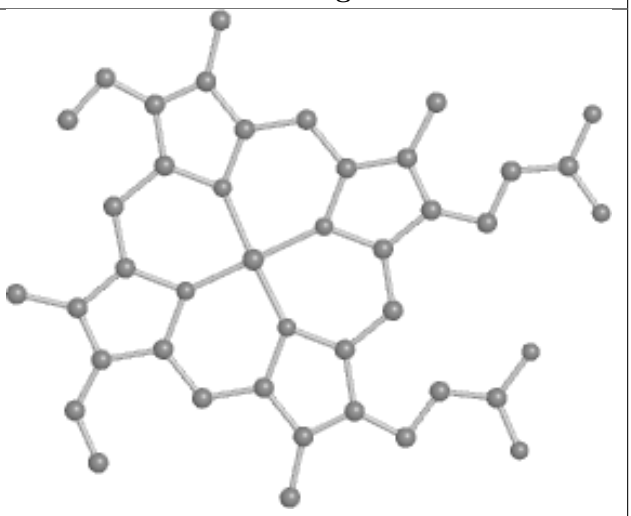
Bond lengths



Bond angles

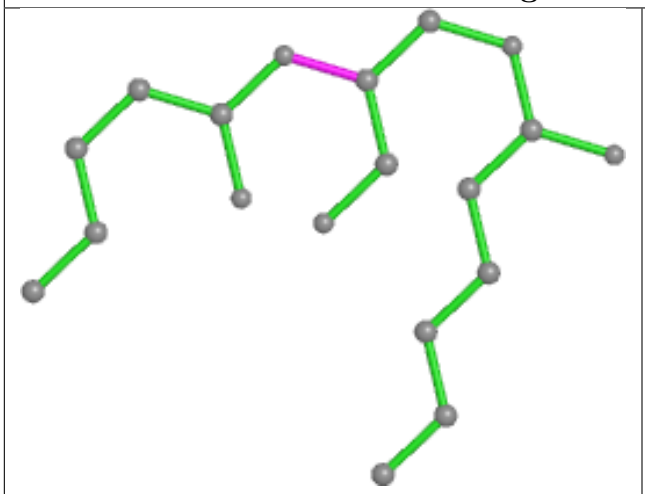


Torsions

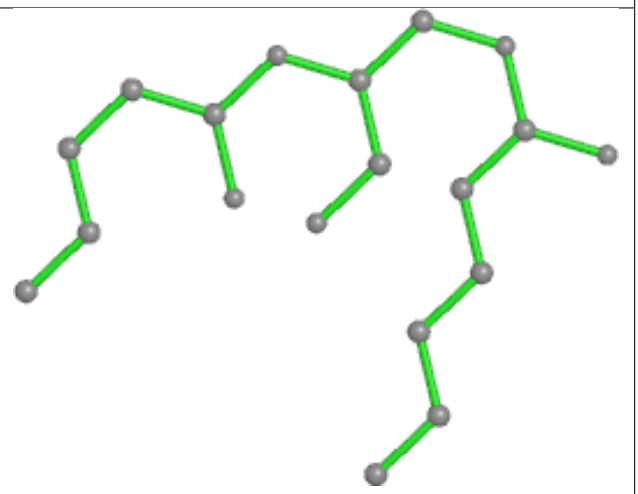


Rings

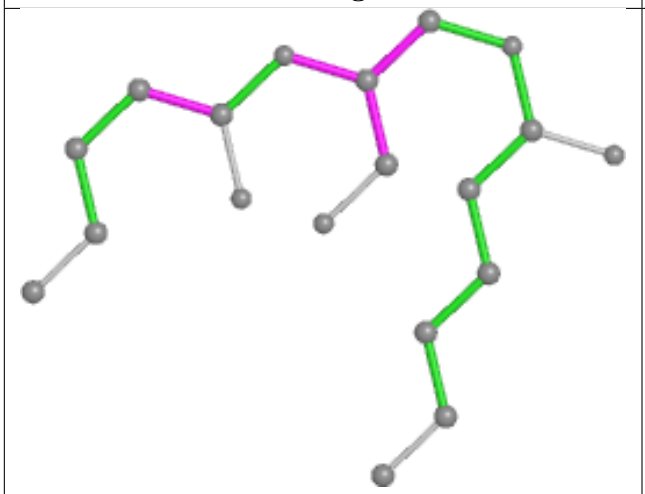
Ligand 2WD D 206



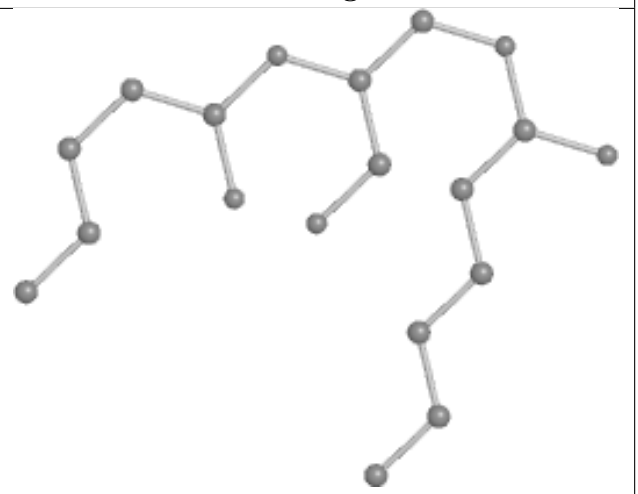
Bond lengths



Bond angles

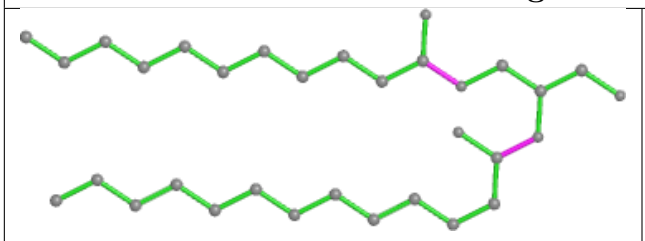


Torsions

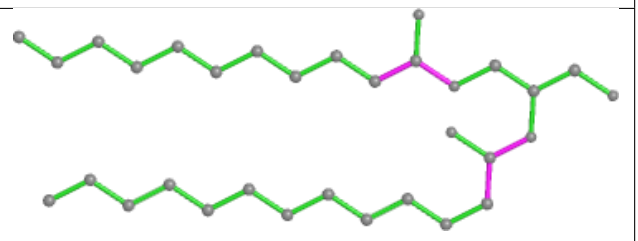


Rings

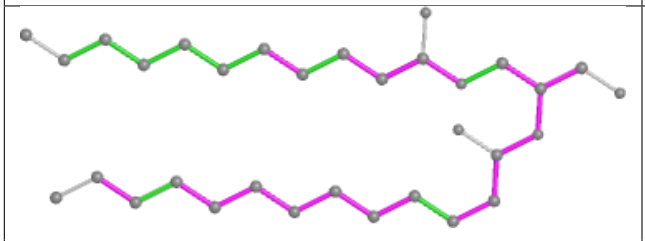
Ligand 7PH C 303



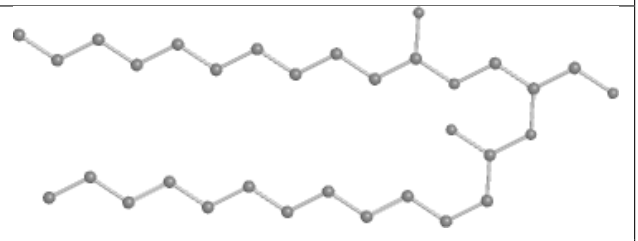
Bond lengths



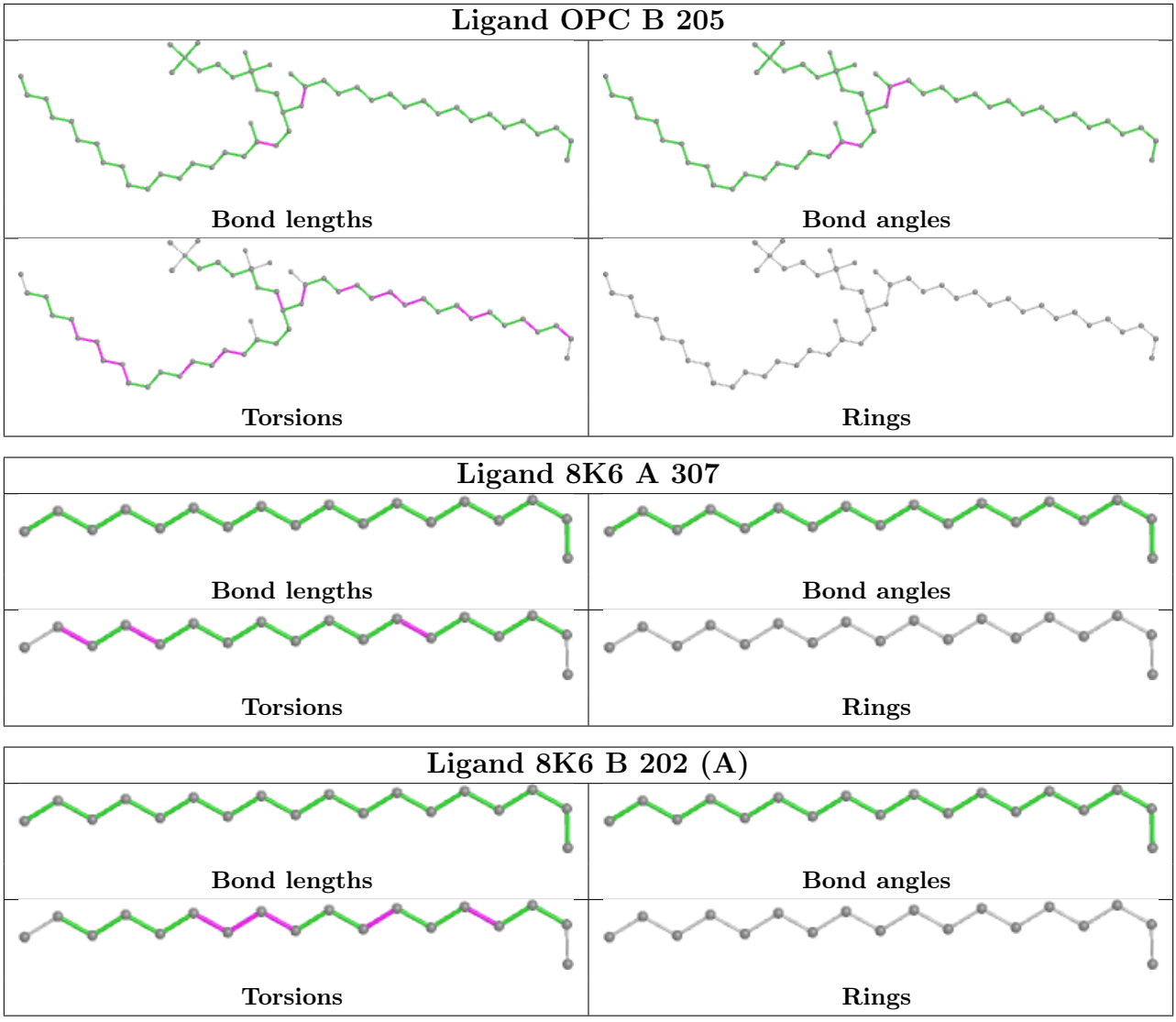
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	214/215 (99%)	0.47	27 (12%)	3	3	43, 59, 97, 186	0
2	B	159/160 (99%)	0.54	22 (13%)	2	2	52, 77, 124, 195	0
3	C	281/333 (84%)	0.89	47 (16%)	1	1	57, 85, 191, 249	0
4	D	166/179 (92%)	2.12	64 (38%)	0	0	50, 145, 205, 239	0
5	E	31/31 (100%)	0.42	5 (16%)	1	1	81, 98, 123, 153	0
6	F	32/34 (94%)	0.13	1 (3%)	49	52	69, 87, 131, 169	0
7	G	37/37 (100%)	1.08	7 (18%)	1	1	57, 74, 144, 155	0
8	H	29/29 (100%)	1.10	3 (10%)	6	6	59, 71, 100, 144	0
All	All	949/1018 (93%)	0.93	176 (18%)	1	1	43, 81, 185, 249	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	199	ILE	12.1
2	B	160	PHE	11.6
4	D	69	PHE	9.7
3	C	183	ILE	9.2
3	C	196	LEU	9.2
4	D	70	LEU	8.6
4	D	56	ALA	8.2
3	C	176	ALA	8.0
4	D	75	VAL	7.6
4	D	67	SER	7.6
4	D	160	ILE	7.3
3	C	188	GLY	7.3
4	D	64	VAL	7.2
3	C	189	GLU	7.2
3	C	192	SER	7.1
2	B	159	LEU	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	197	VAL	6.8
3	C	225	VAL	6.7
4	D	66	VAL	6.4
4	D	161	VAL	6.4
4	D	49	GLY	6.4
3	C	193	VAL	6.4
4	D	92	VAL	6.3
4	D	159	LYS	6.2
4	D	172	THR	6.2
4	D	50	ALA	6.1
4	D	102	TYR	6.0
1	A	2	ALA	5.9
4	D	55	THR	5.9
3	C	186	GLN	5.9
3	C	190	ASP	5.8
7	G	37	GLY	5.6
3	C	198	ASP	5.6
4	D	173	GLY	5.5
4	D	156	GLU	5.5
3	C	220	SER	5.5
4	D	85	LYS	5.4
3	C	224	ALA	5.3
3	C	180	ILE	5.3
4	D	51	GLY	5.3
4	D	62	ASN	5.3
4	D	157	ASN	5.2
3	C	184	ALA	5.1
4	D	171	ARG	5.1
3	C	219	VAL	5.0
4	D	72	SER	5.0
4	D	174	GLU	4.9
4	D	168	THR	4.9
3	C	218	ILE	4.9
4	D	48	GLY	4.8
4	D	76	GLY	4.8
4	D	57	LYS	4.8
4	D	60	LEU	4.7
4	D	71	GLU	4.7
3	C	177	THR	4.7
4	D	63	ASP	4.7
4	D	53	GLY	4.7
2	B	153	LYS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	182	LYS	4.6
3	C	289	PHE	4.6
4	D	179	SER	4.5
2	B	47	SER	4.5
2	B	157	LEU	4.5
5	E	31	LEU	4.5
3	C	221	GLU	4.5
4	D	162	LEU	4.4
3	C	288	ASN	4.4
4	D	158	ASP	4.4
4	D	98	ALA	4.4
4	D	73	HIS	4.3
2	B	50	CYS	4.3
3	C	179	THR	4.2
4	D	140	VAL	4.1
3	C	195	TYR	4.1
4	D	52	GLY	4.1
4	D	175	GLU	4.0
4	D	99	ILE	3.9
4	D	154	LYS	3.9
3	C	285	ALA	3.9
3	C	208	SER	3.8
4	D	65	SER	3.8
1	A	92	MET	3.8
4	D	141	ARG	3.8
2	B	46	GLY	3.7
4	D	165	TRP	3.6
3	C	209	ASP	3.6
3	C	181	SER	3.5
4	D	170	PHE	3.5
3	C	211	ILE	3.5
1	A	95	LEU	3.5
3	C	226	THR	3.5
4	D	155	THR	3.4
1	A	35	CYS	3.4
1	A	99	LEU	3.4
4	D	169	ASP	3.4
6	F	1	MET	3.4
1	A	96	MET	3.4
8	H	1	MET	3.3
2	B	151	LEU	3.3
4	D	54	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	151	VAL	3.2
4	D	13	MET	3.2
2	B	154	SER	3.2
2	B	152	ASP	3.1
5	E	27	SER	3.1
4	D	91	ILE	3.1
3	C	223	GLN	3.1
3	C	194	LYS	3.1
1	A	43	CYS	3.1
1	A	36	LEU	3.1
2	B	155	LEU	3.0
1	A	39	ILE	3.0
2	B	51	ILE	3.0
4	D	74	ASN	3.0
3	C	210	THR	3.0
4	D	15	ARG	3.0
4	D	176	PRO	2.9
2	B	44	ILE	2.9
3	C	4	TRP	2.9
4	D	16	ARG	2.9
1	A	150	ILE	2.8
4	D	68	LYS	2.8
5	E	29	LYS	2.8
2	B	54	LEU	2.8
3	C	187	GLU	2.7
2	B	62	THR	2.7
3	C	222	GLY	2.7
1	A	33	PHE	2.7
5	E	10	PHE	2.7
3	C	178	GLY	2.7
7	G	1	MET	2.7
1	A	4	VAL	2.6
2	B	49	ALA	2.6
3	C	175	ALA	2.6
1	A	32	ILE	2.6
3	C	172	TYR	2.6
1	A	88	TRP	2.6
2	B	79	TRP	2.6
3	C	229	ASP	2.6
3	C	217	LEU	2.6
4	D	167	GLU	2.5
1	A	101	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	34	TYR	2.5
4	D	78	ARG	2.4
4	D	153	ALA	2.4
1	A	94	VAL	2.4
2	B	43	VAL	2.4
7	G	26	TYR	2.4
4	D	84	LEU	2.4
4	D	152	HIS	2.3
4	D	11	PRO	2.3
1	A	89	SER	2.3
8	H	29	LEU	2.3
2	B	48	PHE	2.3
3	C	227	ALA	2.3
3	C	93	GLU	2.3
7	G	10	VAL	2.3
3	C	168	ASN	2.2
1	A	91	SER	2.2
1	A	40	THR	2.2
1	A	102	PHE	2.2
4	D	139	VAL	2.2
2	B	45	MET	2.1
2	B	53	ALA	2.1
1	A	5	TYR	2.1
7	G	17	THR	2.1
5	E	30	ILE	2.1
7	G	13	LEU	2.1
3	C	67	LYS	2.1
1	A	42	VAL	2.1
8	H	18	SER	2.1
2	B	52	VAL	2.0
1	A	3	ASN	2.0
7	G	30	LYS	2.0
1	A	159	PRO	2.0
1	A	104	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

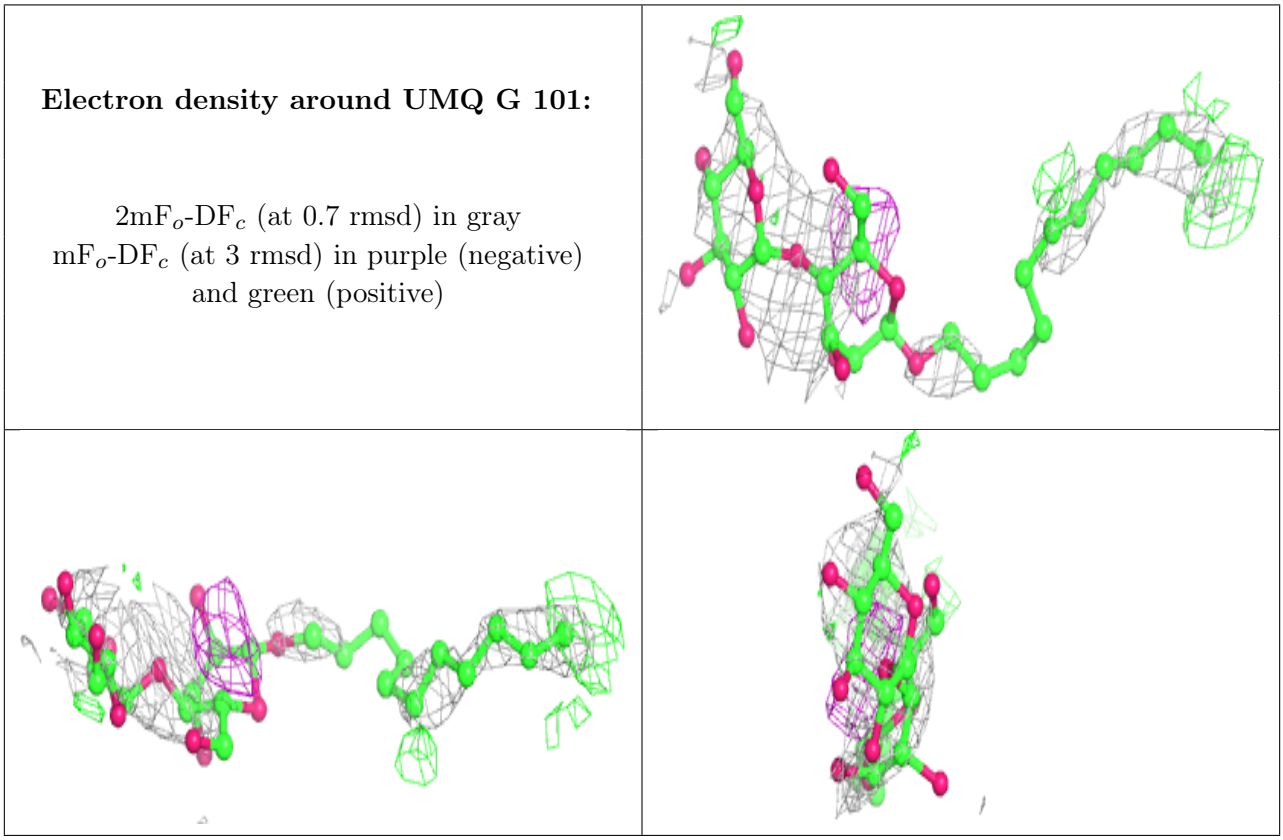
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
10	UMQ	G	101	34/34	0.51	0.69	81,173,199,284	0
11	7PH	B	206	32/38	0.55	0.70	77,132,182,184	0
17	MYS	D	202	15/15	0.56	0.39	93,107,121,126	0
10	UMQ	D	201	34/34	0.59	0.65	102,210,248,264	0
21	3WM	E	101	44/44	0.62	0.35	60,97,122,125	0
12	8K6	A	306	18/18	0.63	0.30	93,113,147,148	0
22	2WA	F	101	40/40	0.63	0.38	70,111,169,182	0
12	8K6	B	202[A]	18/18	0.64	0.46	47,102,122,122	18
20	2WD	D	206	19/19	0.64	0.67	75,123,142,145	0
11	7PH	D	203	32/38	0.65	0.25	54,81,153,157	0
24	1O2	F	103	49/53	0.65	0.63	80,127,216,220	0
25	BCR	G	102	40/40	0.66	0.35	49,74,116,122	0
10	UMQ	A	304	34/34	0.67	0.46	127,146,201,254	0
16	CD	C	302	1/1	0.67	0.11	136,136,136,136	1
11	7PH	C	303	32/38	0.67	0.40	73,117,149,150	0
12	8K6	A	307	18/18	0.67	0.36	76,108,124,127	0
11	7PH	A	305	32/38	0.71	0.37	93,126,189,190	0
23	OCT	F	102	8/8	0.75	0.48	101,106,110,116	0
10	UMQ	B	203[B]	34/34	0.77	0.41	80,103,132,144	34
13	2WM	A	309	44/44	0.77	0.29	70,96,152,158	0
12	8K6	A	308	14/18	0.78	0.30	62,82,95,99	0
11	7PH	F	104	32/38	0.81	0.28	81,101,172,175	0
10	UMQ	B	201	34/34	0.86	0.30	64,114,151,224	0
18	SQD	D	204	54/54	0.92	0.27	73,116,159,177	0
14	CLA	B	204	65/65	0.93	0.21	59,79,107,117	0
15	OPC	B	205	54/55	0.95	0.23	55,92,121,137	0
9	HEC	A	303	43/43	0.97	0.21	47,66,85,95	0
9	HEC	A	301	43/43	0.98	0.18	31,50,65,78	0
9	HEC	C	301	43/43	0.98	0.17	46,69,96,113	0
9	HEC	A	302	43/43	0.99	0.23	34,57,71,76	0
19	FES	D	205	4/4	0.99	0.06	96,97,100,102	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.

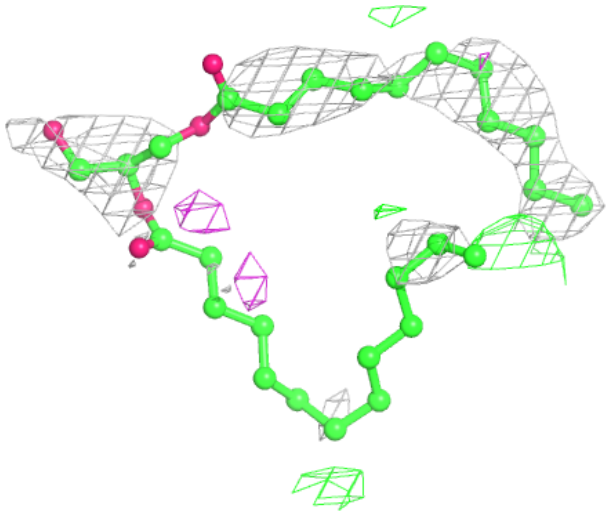
Electron density around UMQ G 101:

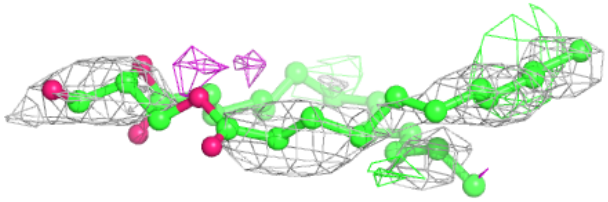
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

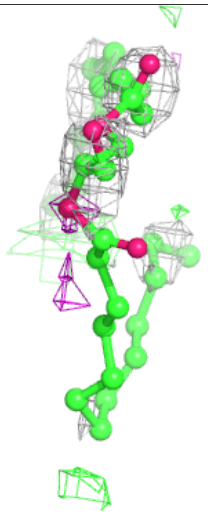


Electron density around 7PH B 206:

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

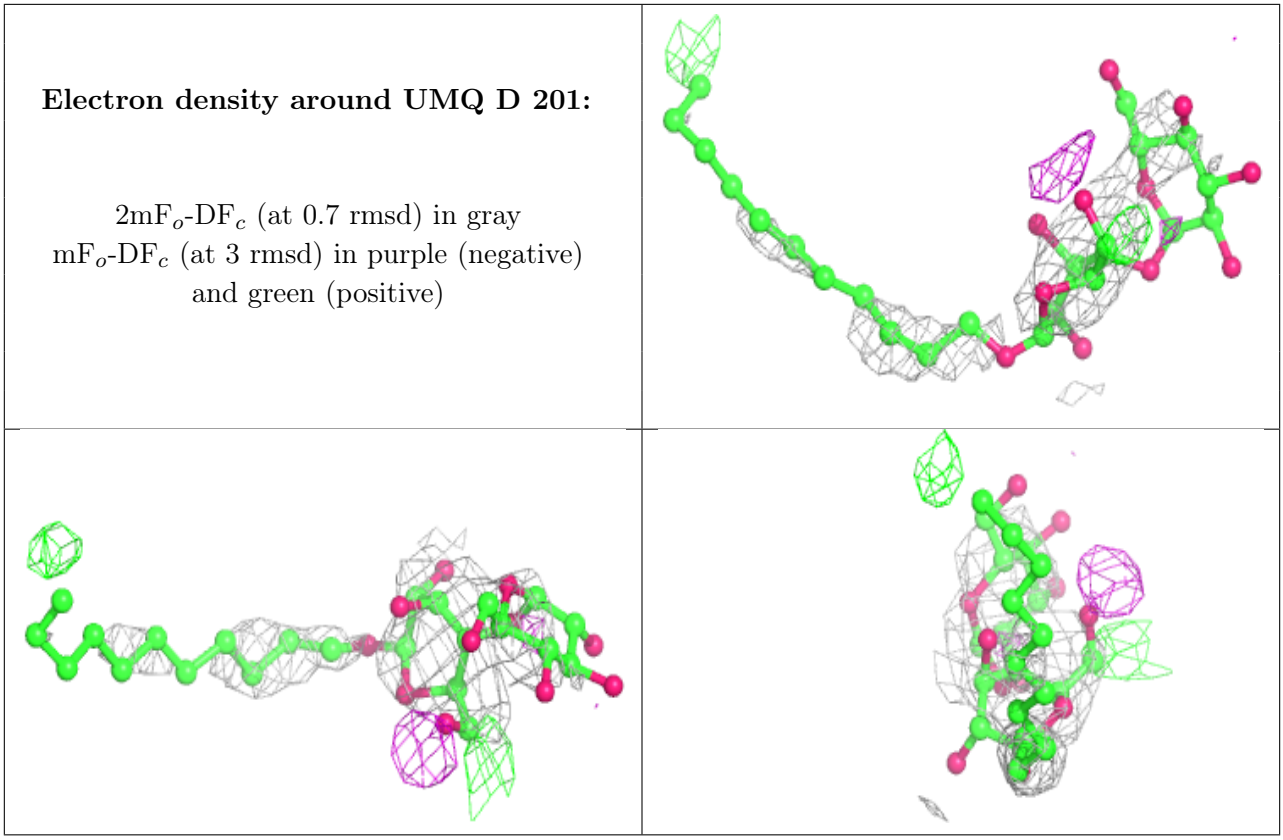






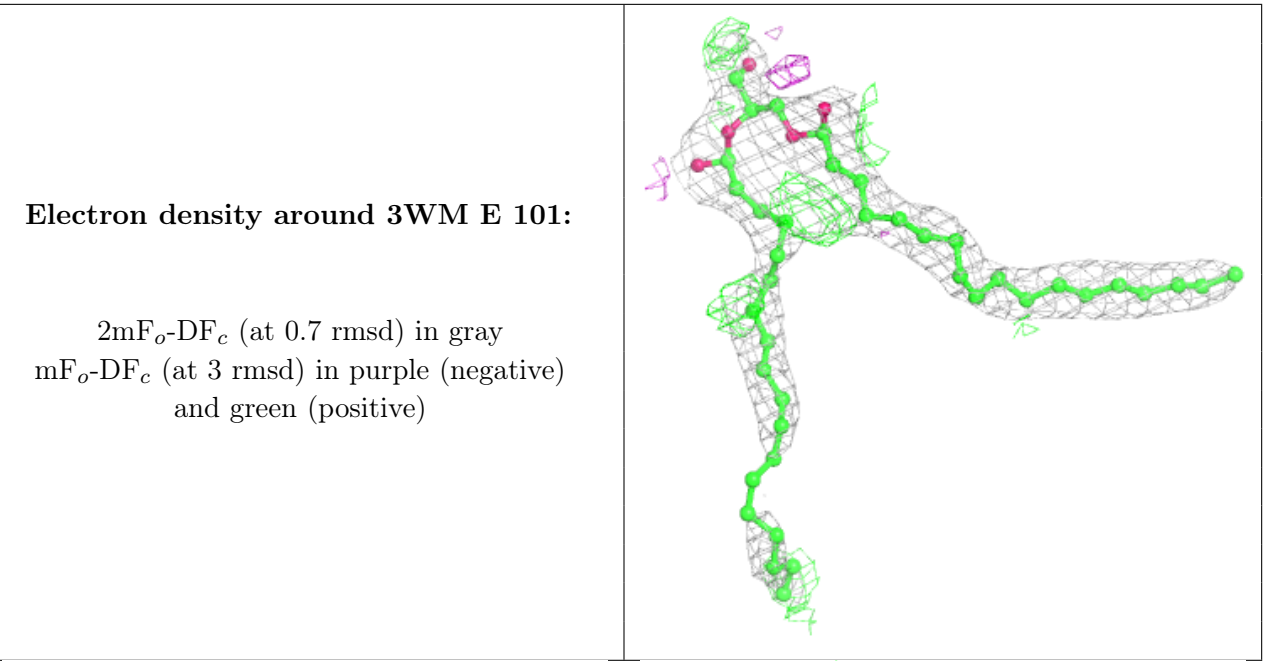
Electron density around UMQ D 201:

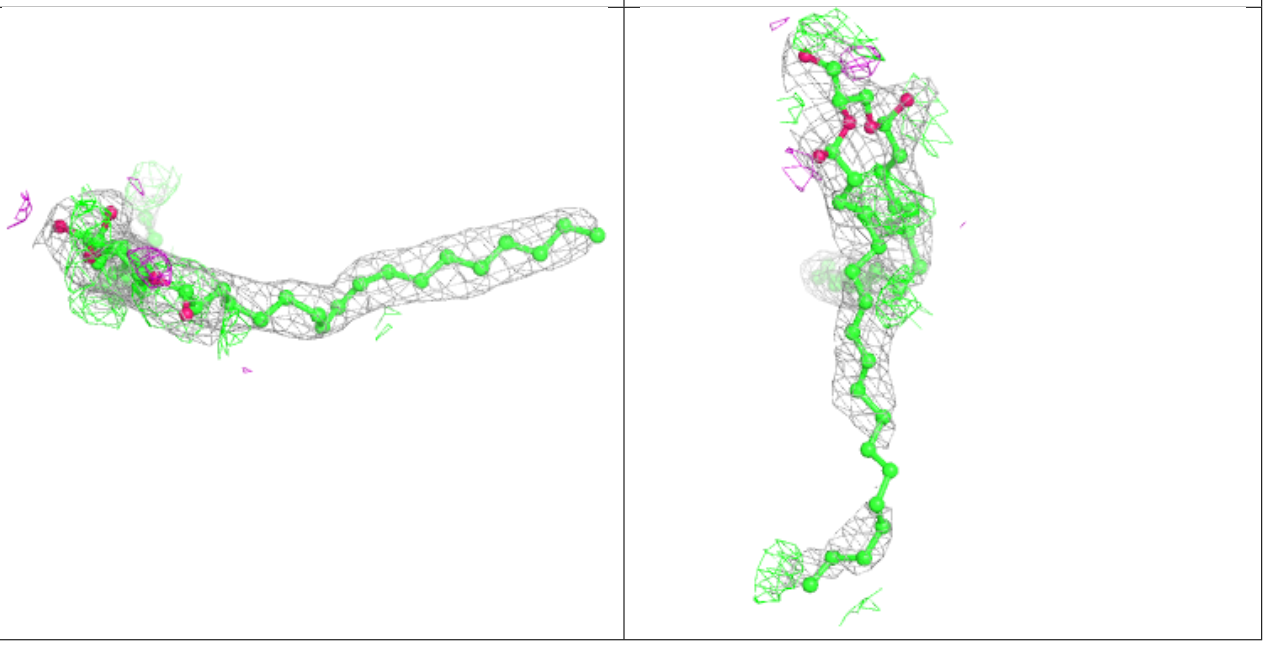
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 3WM E 101:

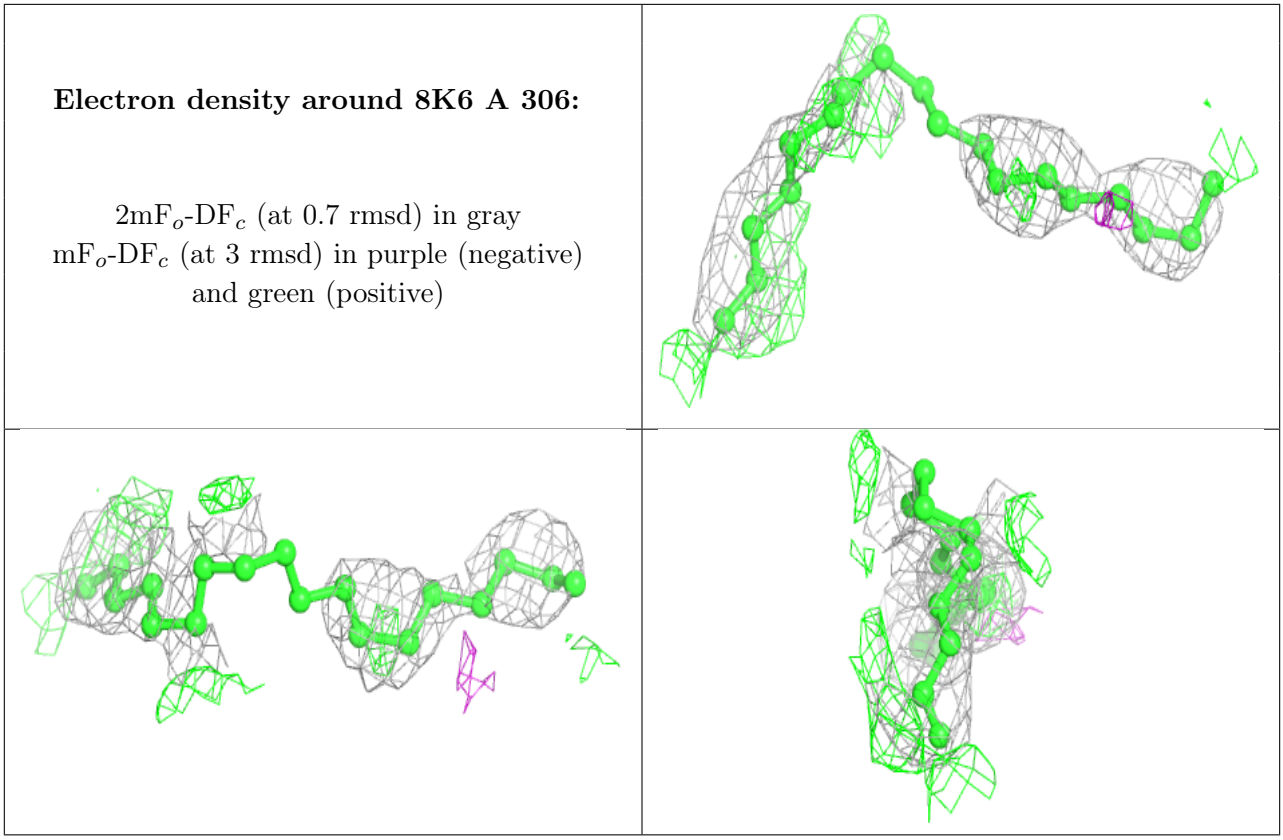
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





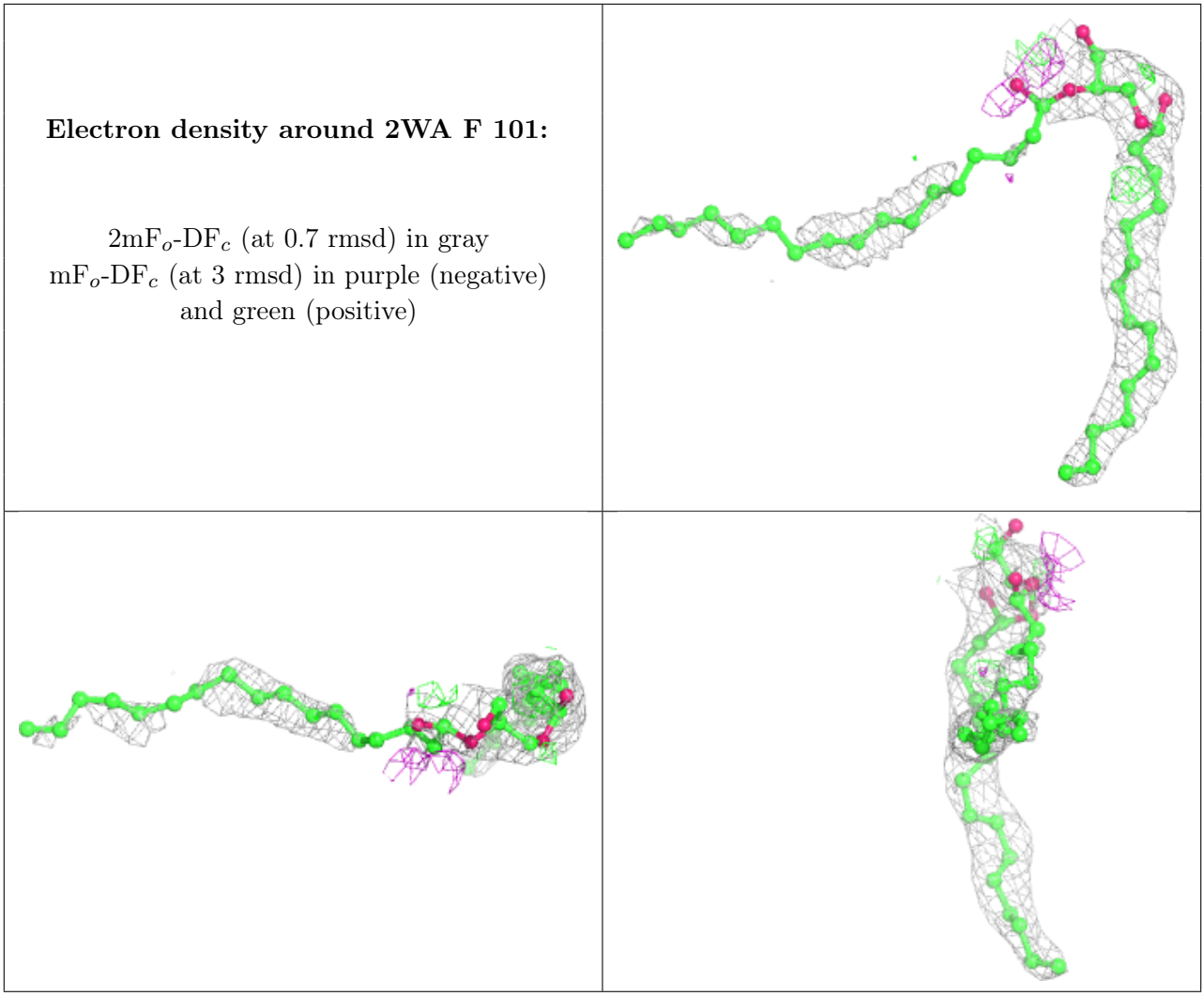
Electron density around 8K6 A 306:

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



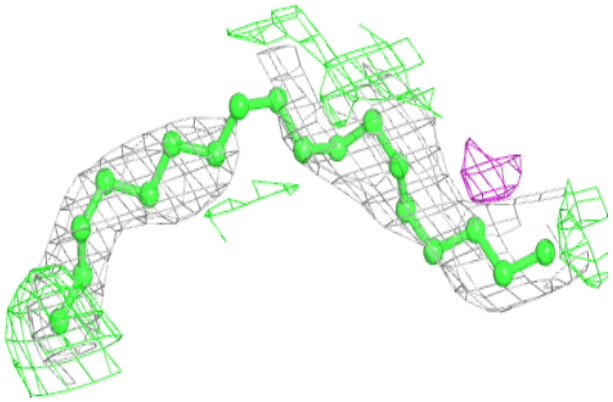
Electron density around 2WA F 101:

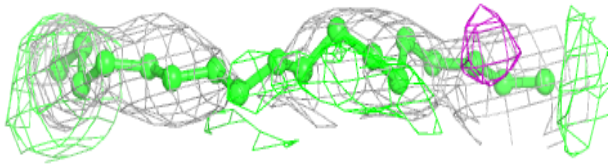
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

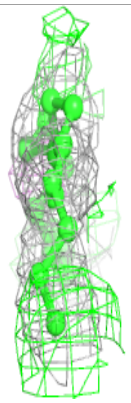


Electron density around 8K6 B 202 (A):

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

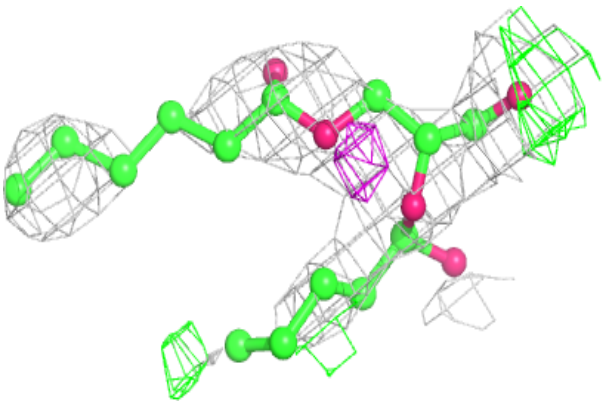


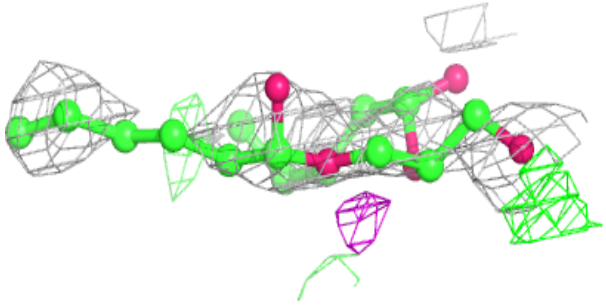




Electron density around 2WD D 206:

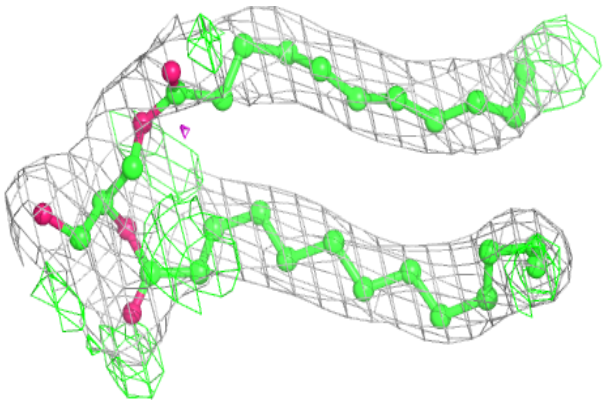
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

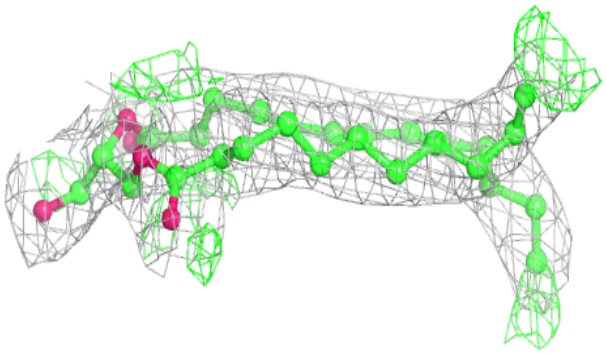




Electron density around 7PH D 203:

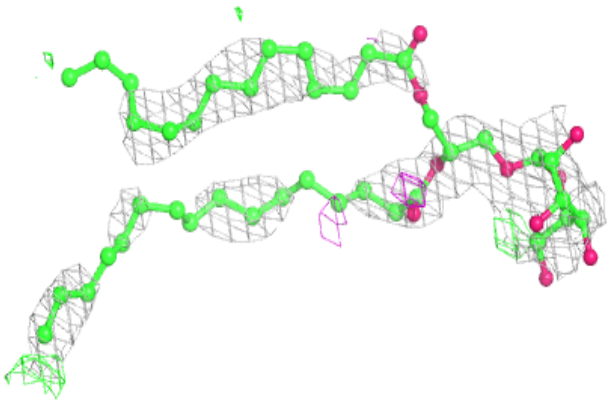
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

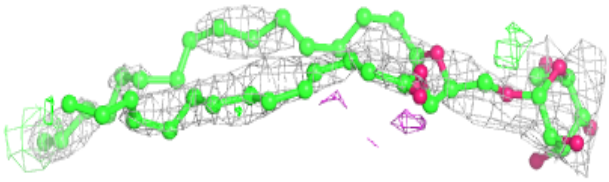




Electron density around 1O2 F 103:

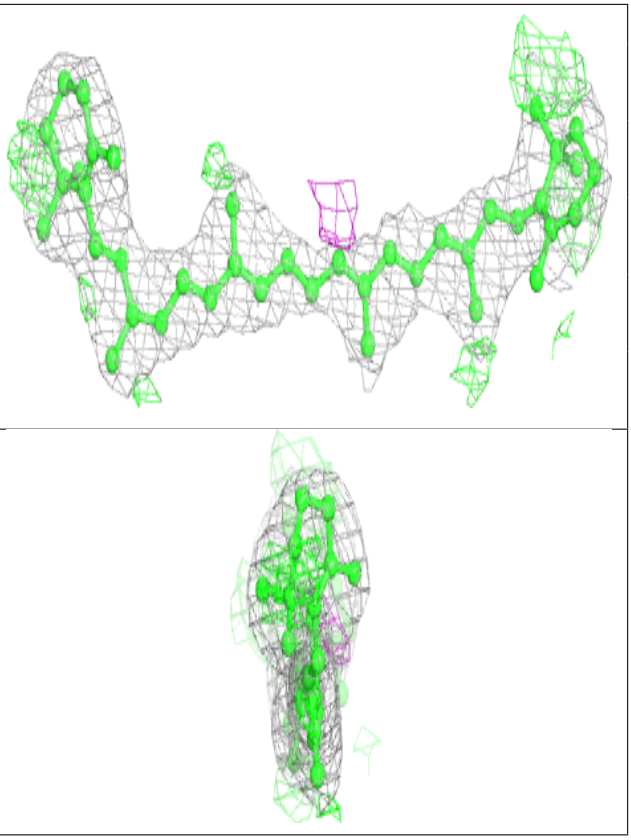
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





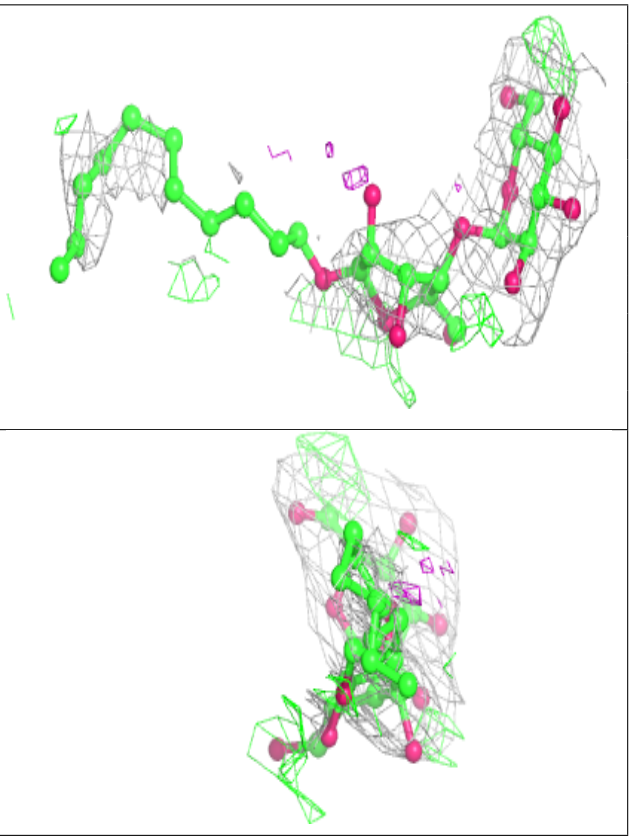
Electron density around BCR G 102:

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



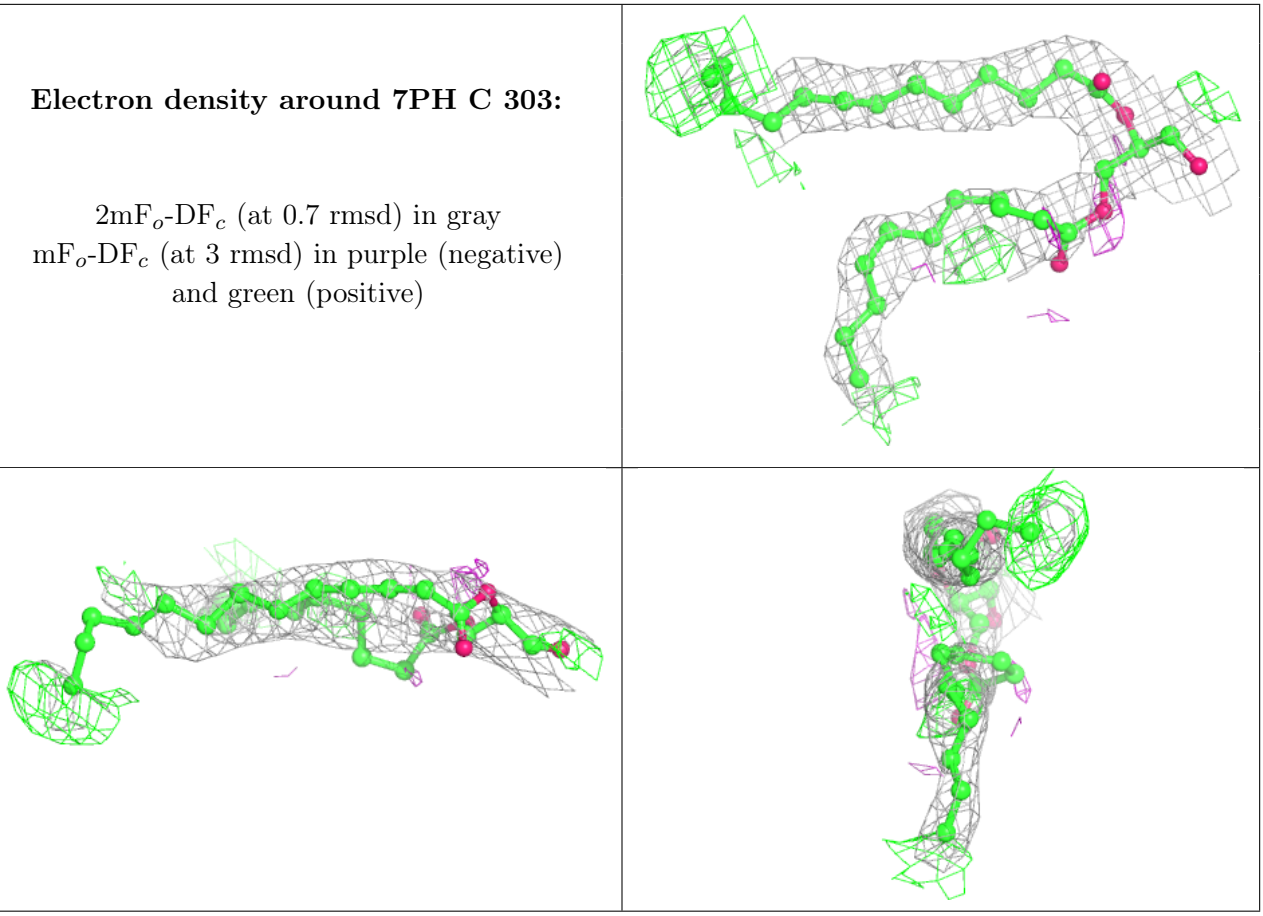
Electron density around UMQ A 304:

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



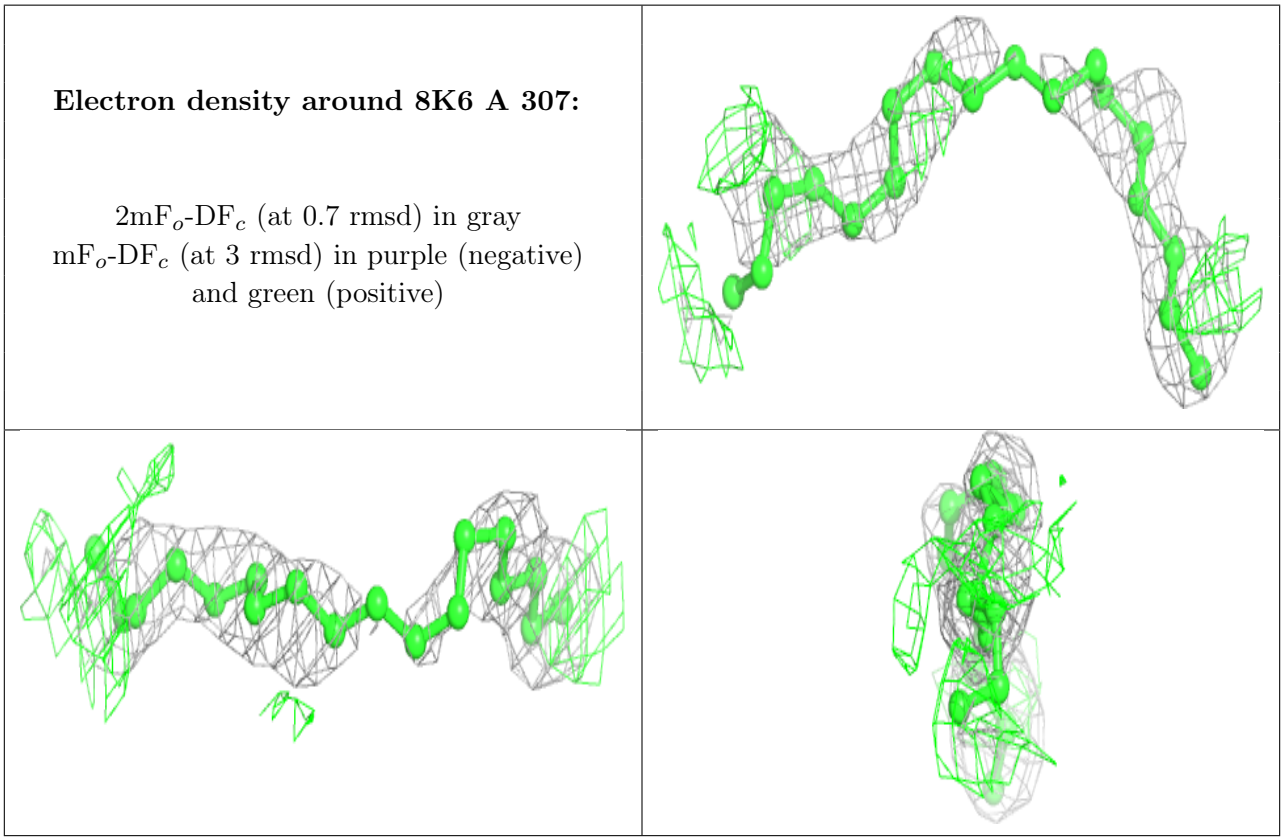
Electron density around 7PH C 303:

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



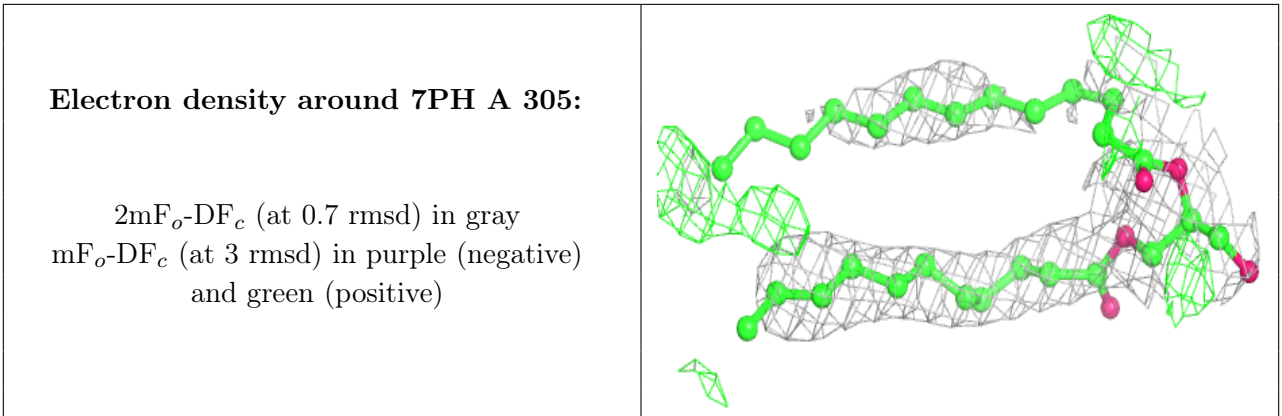
Electron density around 8K6 A 307:

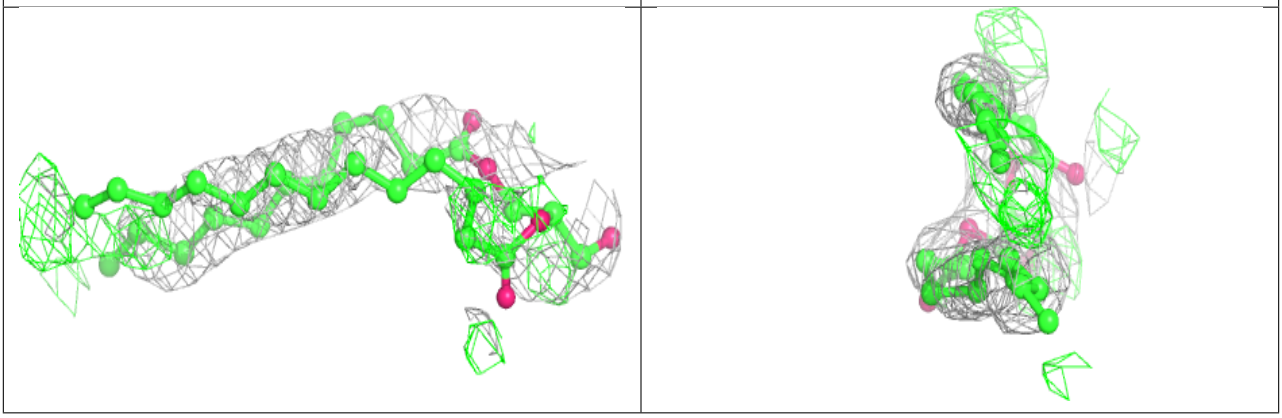
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 7PH A 305:

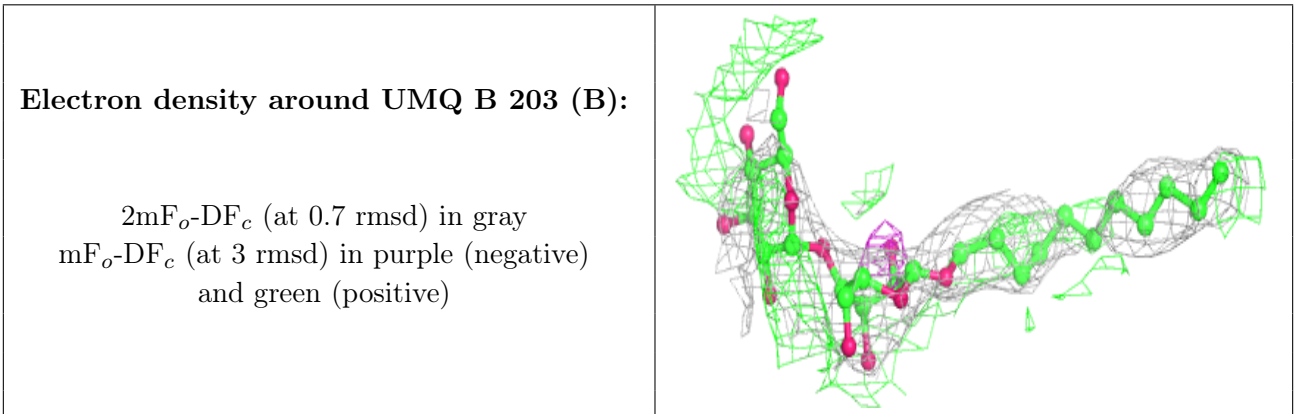
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

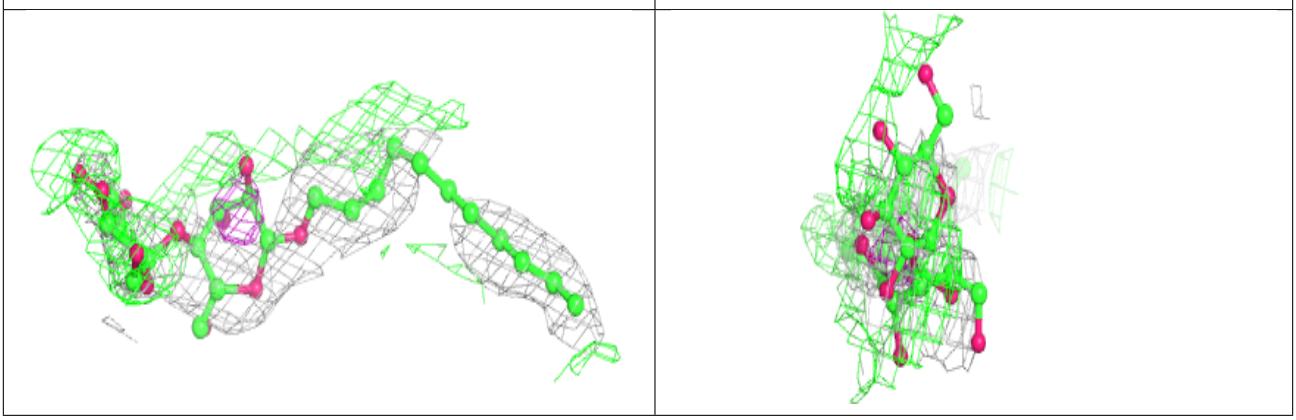




Electron density around UMQ B 203 (B):

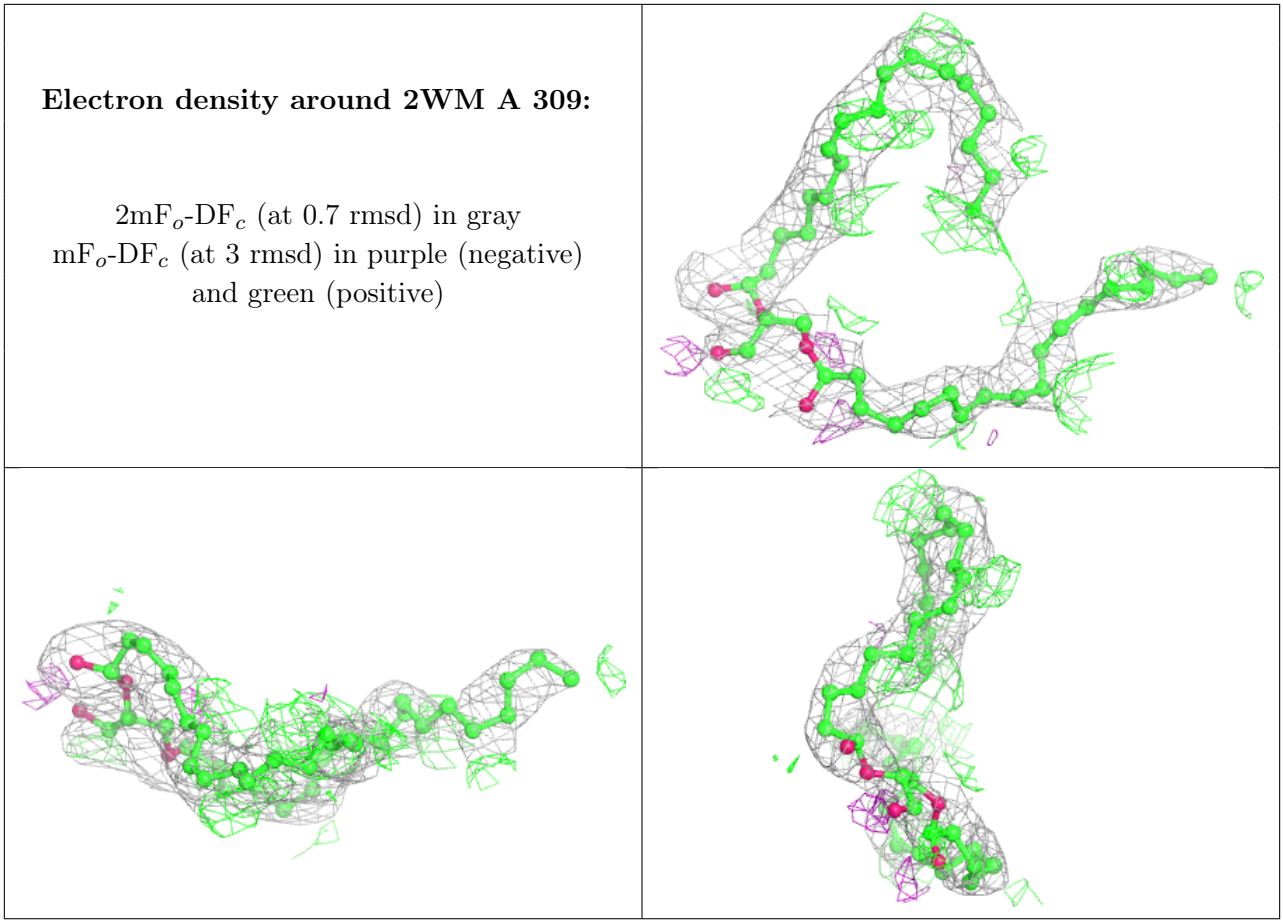
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





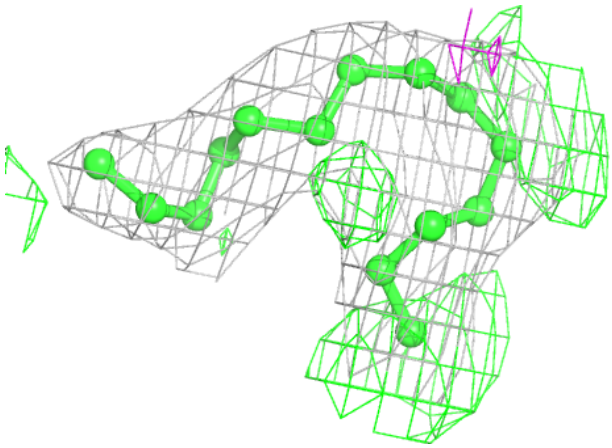
Electron density around 2WM A 309:

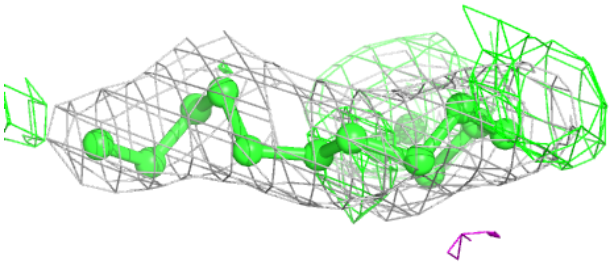
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

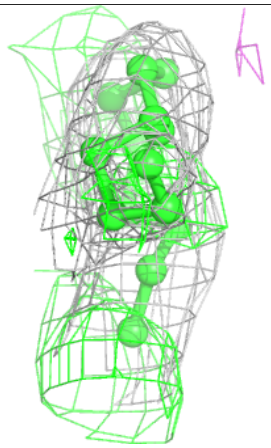


Electron density around 8K6 A 308:

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

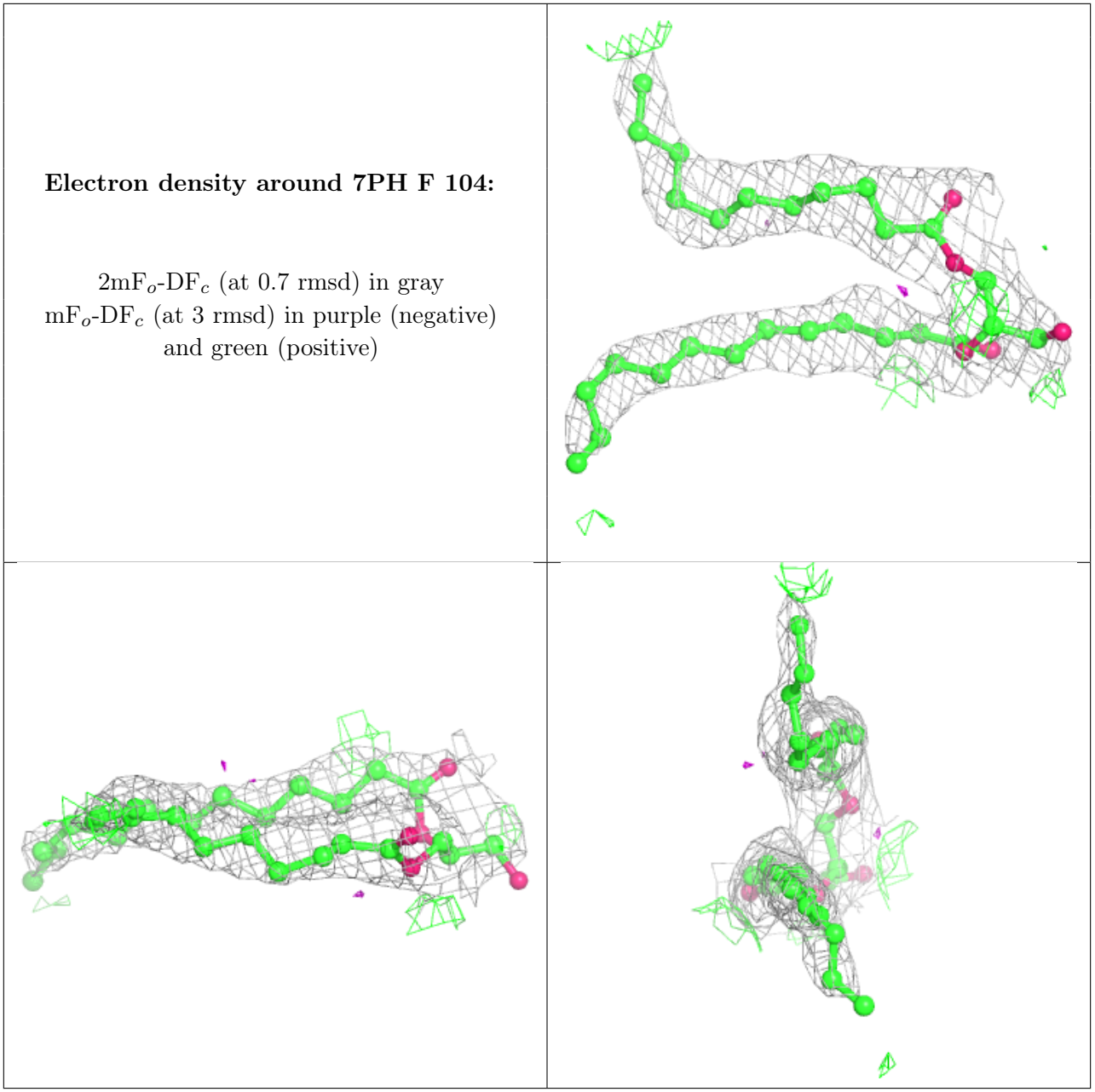






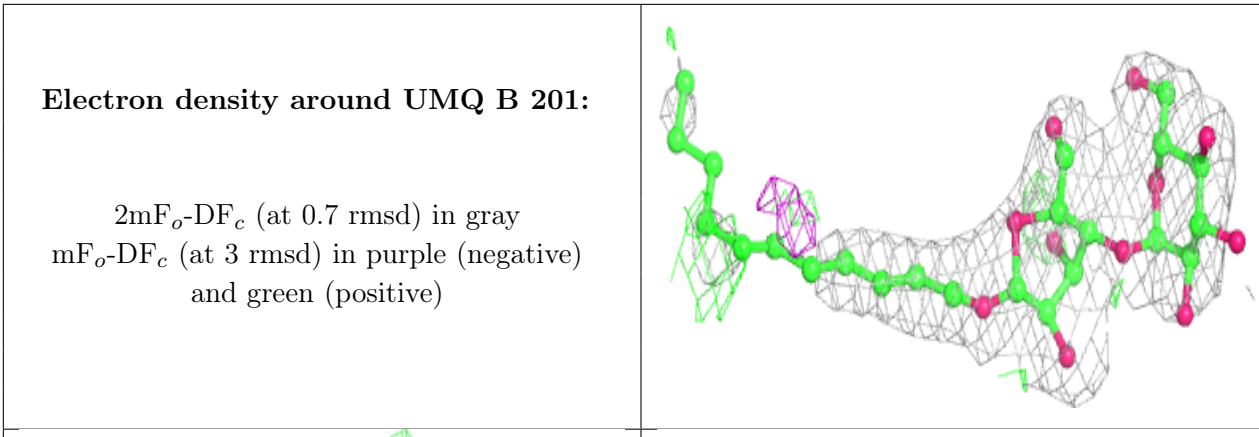
Electron density around 7PH F 104:

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



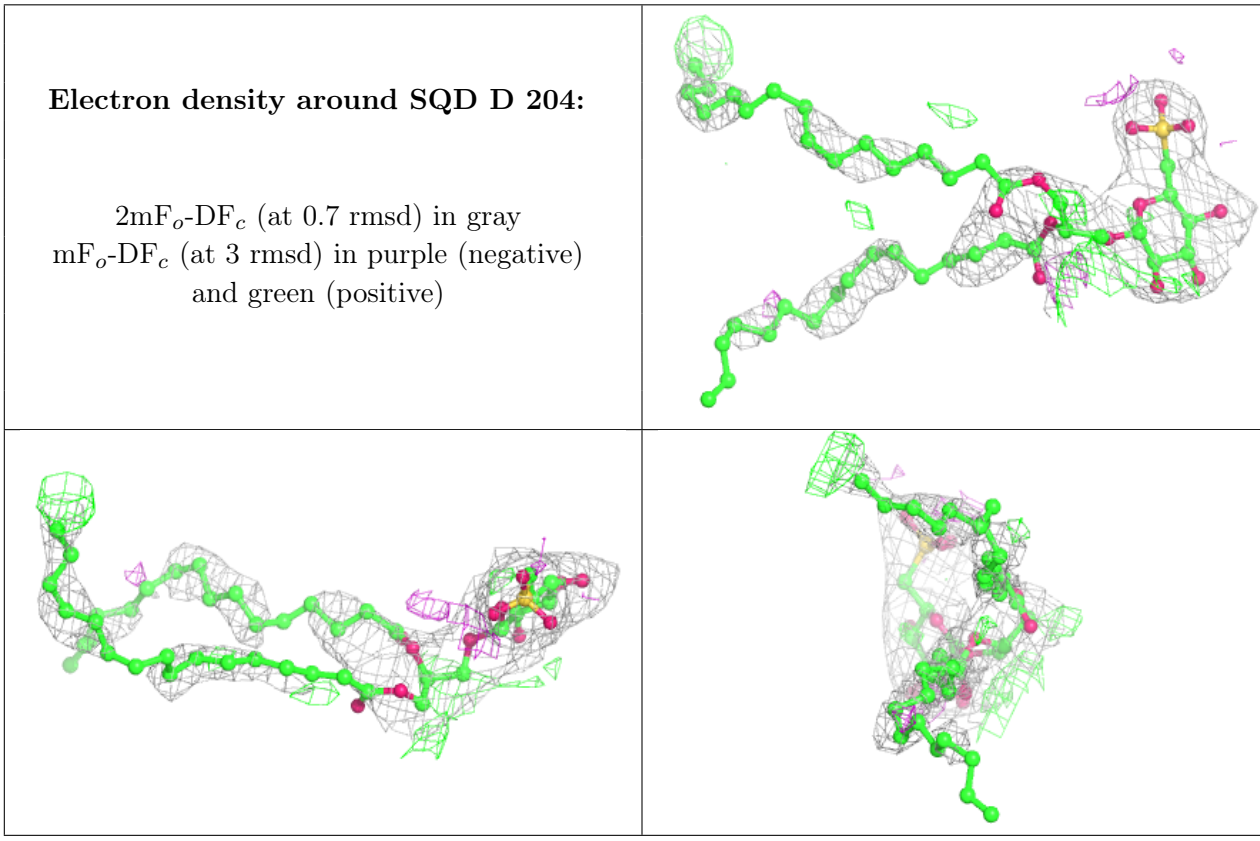
Electron density around UMQ B 201:

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



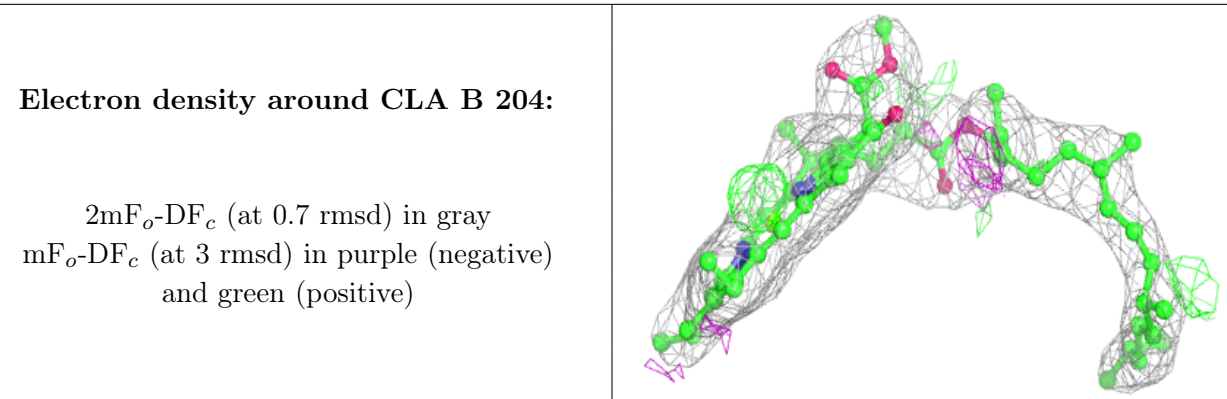
Electron density around SQD D 204:

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



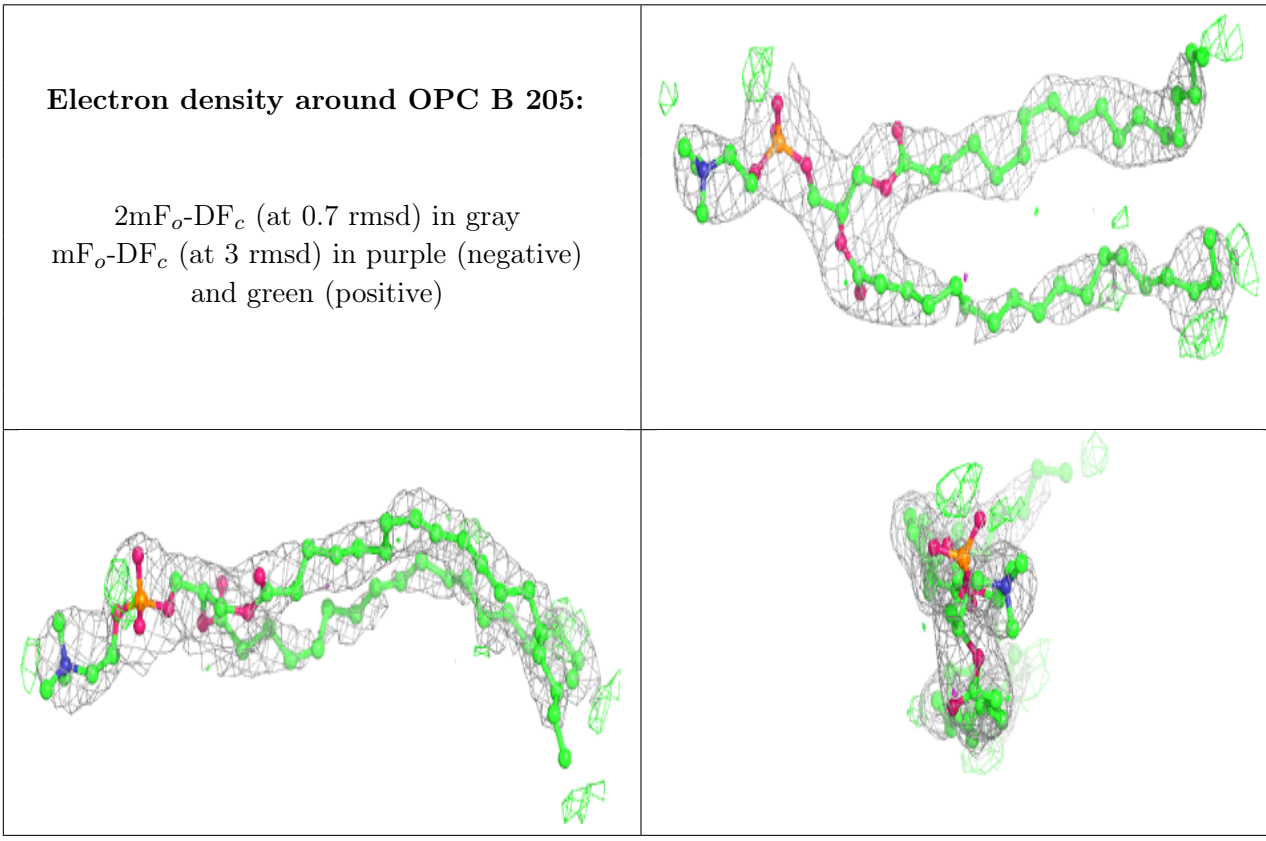
Electron density around CLA B 204:

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



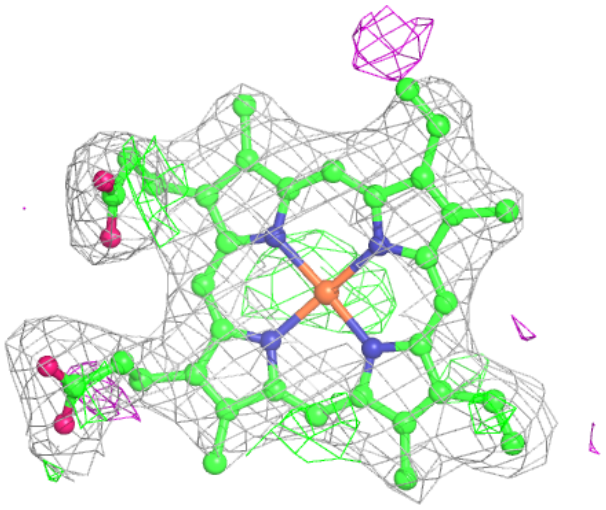
Electron density around OPC B 205:

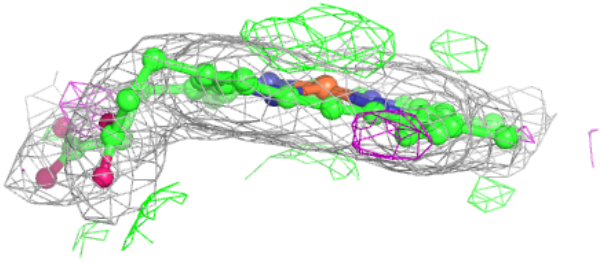
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

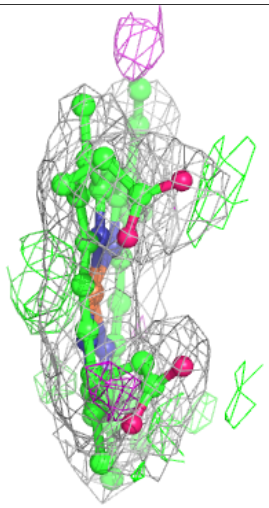


Electron density around HEC A 303:

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

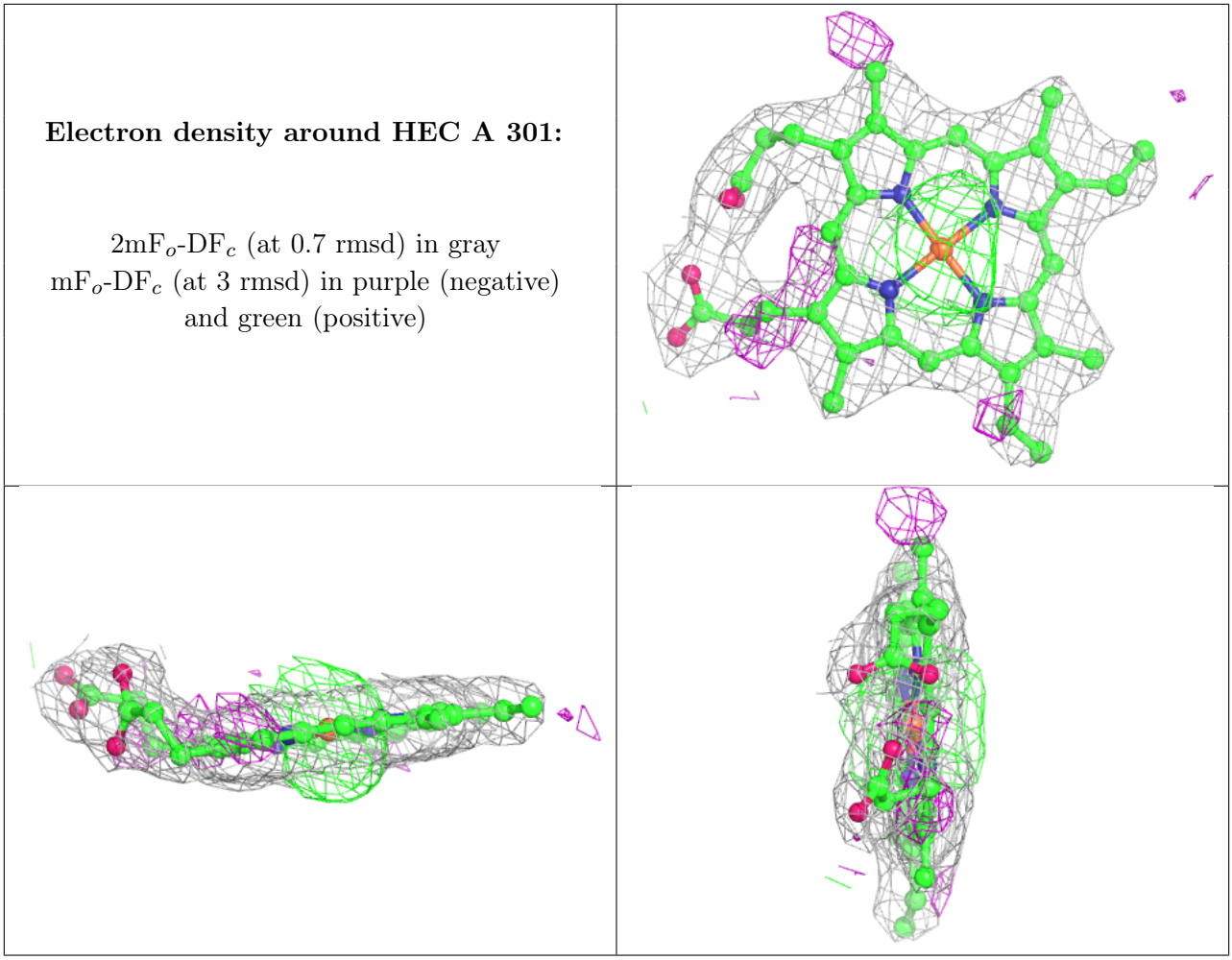






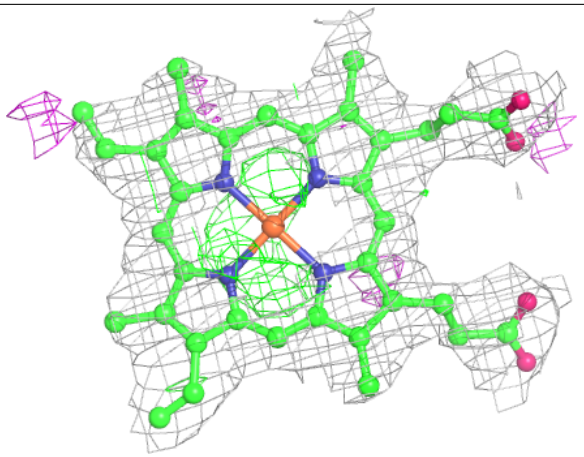
Electron density around HEC A 301:

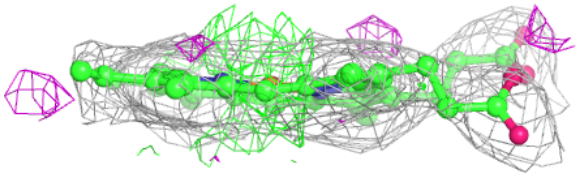
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

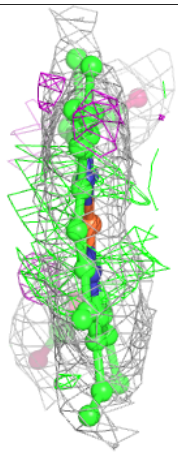


Electron density around HEC C 301:

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

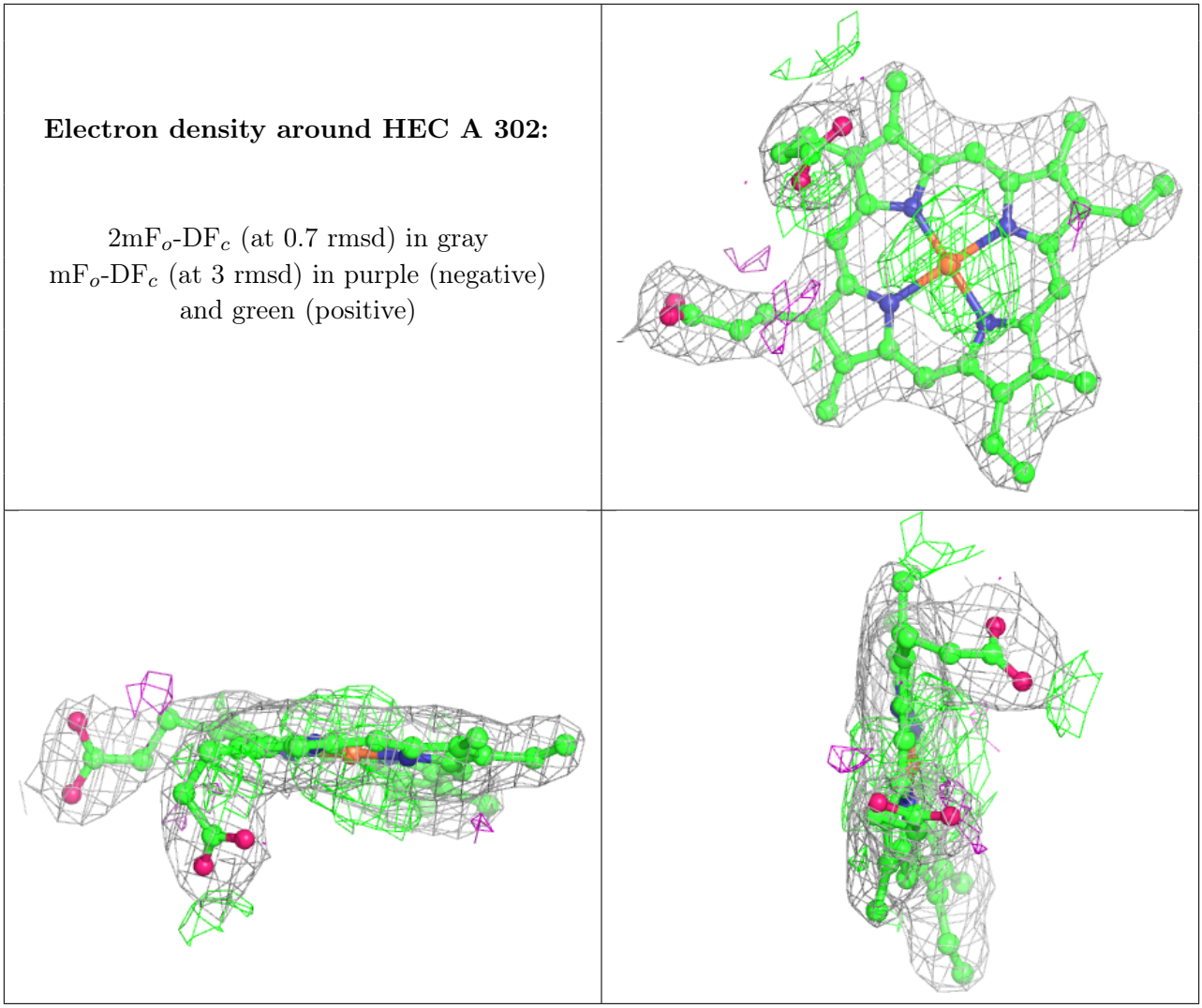






Electron density around HEC A 302:

$2mF_o$-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

There are no such residues in this entry.