Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:49 am BST

PDB ID	:	4H0L
Title	:	Cytochrome b6f Complex Crystal Structure from Mastigocladus laminosus with n-Side Inhibitor NQNO
Authors	:	Hasan, S.S.; Yamashita, E.; Baniulis, D.; Cramer, W.A.
Deposited on	:	2012-09-08
Resolution	:	3.25 Å(reported)

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

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

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

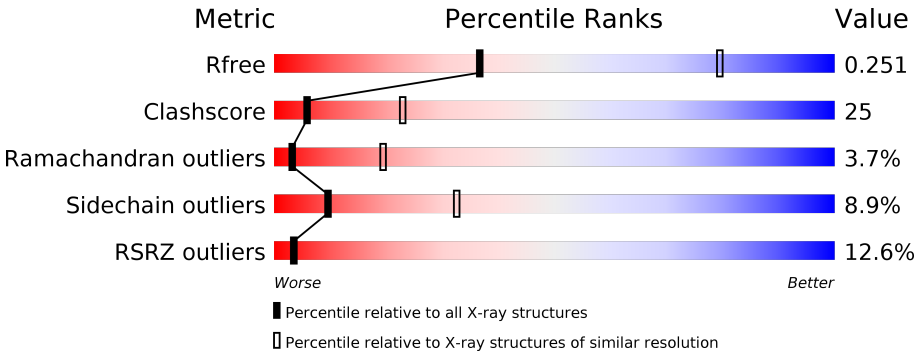
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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	68% 28% • •
2	B	160	54% 41% • •
3	C	289	17% 51% 40% 7% ••
4	D	179	37% 50% 33% 6% • 10%
5	E	32	9% 25% 53% 22%
6	F	35	3% 54% 34% • 9%

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Mol	Chain	Length	Quality of chain
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
12	UMQ	A	306	X	-	-	X
12	UMQ	A	307	X	-	-	-
12	UMQ	A	309	X	-	-	-
12	UMQ	C	301	X	-	-	X
13	QNO	A	308	X	-	-	-
14	CLA	B	202	X	-	-	-
16	SQD	D	201	X	-	-	X
17	BCR	G	101	-	X	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 16219 atoms, of which 8226 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	213	Total	C	H	N	O	S	0	0	0
			3420	1132	1722	270	286	10			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	160	Total	C	H	N	O	S	0	0	0
			2558	841	1309	193	209	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	286	Total	C	H	N	O	S	0	0	0
			4419	1406	2219	366	421	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	PRO	GLU	SEE REMARK 999	UNP P83793

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	161	Total	C	H	N	O	S	0	0	0
			2460	791	1224	213	225	7			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	32	Total	C	H	N	O	S	0	0	0
			532	179	284	34	34	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	H	N	O	S	0	0	0
			502	165	260	35	40	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	37	Total	C	H	N	O	S	0	0	0
			572	188	289	44	50	1			

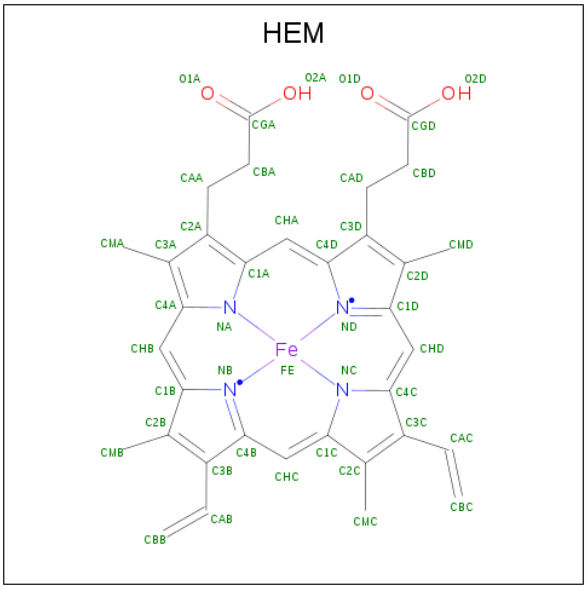
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	29	Total	C	H	N	O	S	0	0	0
			469	156	239	36	36	2			

- Molecule 9 is CADMIUM ION (three-letter code: CD) (formula: Cd).

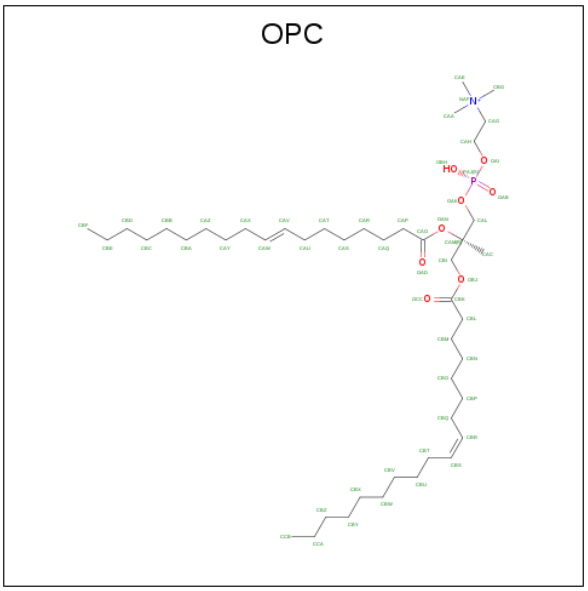
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cd	0	0
			1	1		
9	A	1	Total	Cd	0	0
			1	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



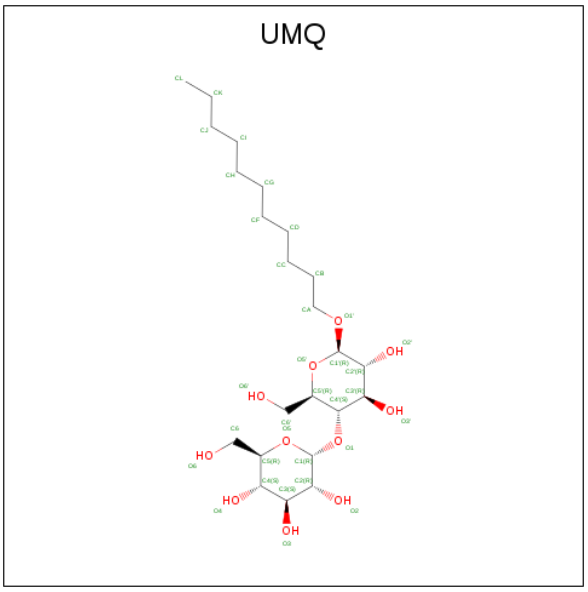
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 11 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: $C_{45}H_{87}NO_8P$).



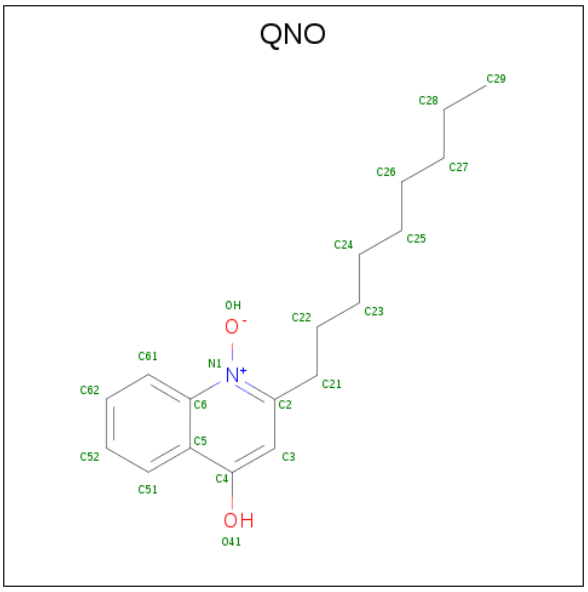
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	A	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		
11	B	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



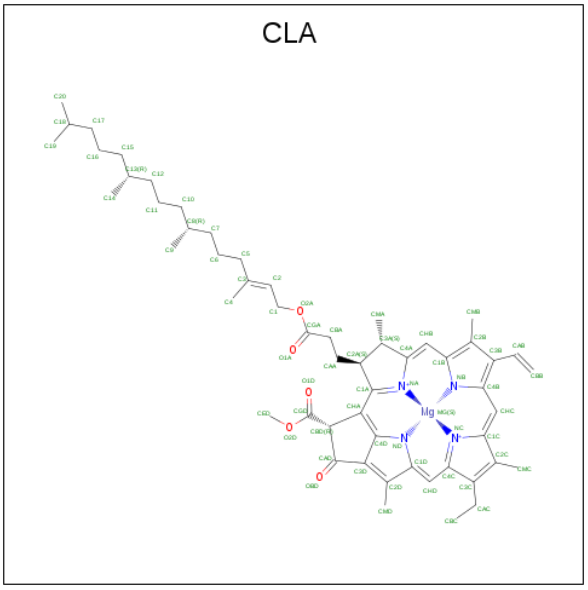
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	C	1	Total	C	H	O	0	0
			78	23	44	11		

- Molecule 13 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (three-letter code: QNO) (formula: $C_{18}H_{25}NO_2$).



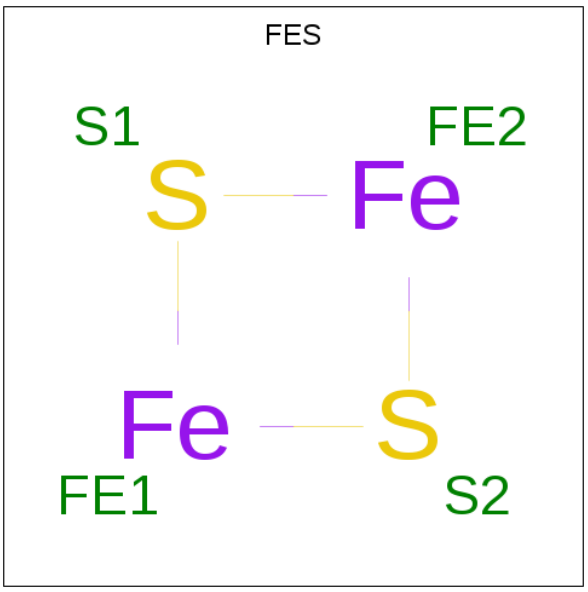
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	N	O	0	0
			46	18	25	1	2		

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



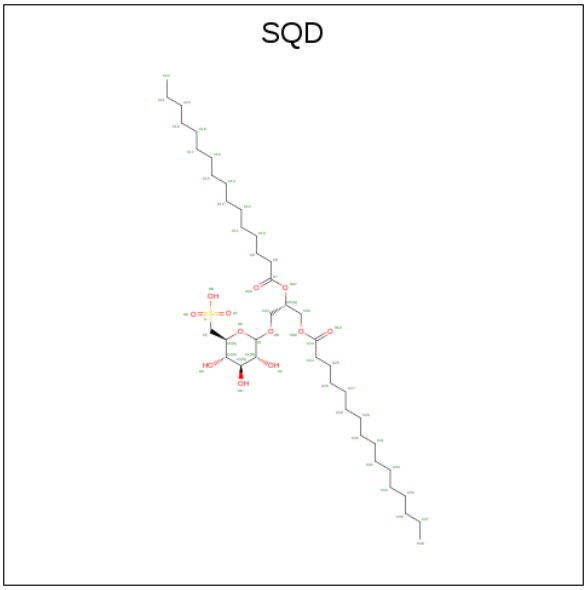
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			127	55	62	1	4	5		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



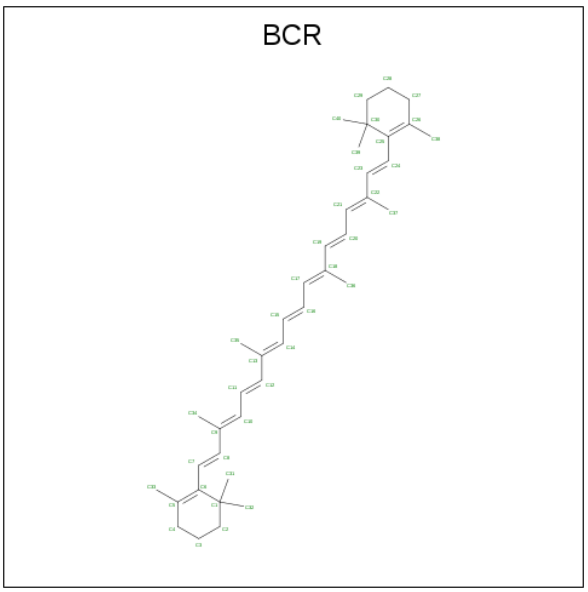
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total Fe S 4 2 2	0	0

- Molecule 16 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
16	D	1	Total C H O S 131 41 78 11 1	1	0

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total C H 96 40 56	0	0

- Molecule 18 is water.

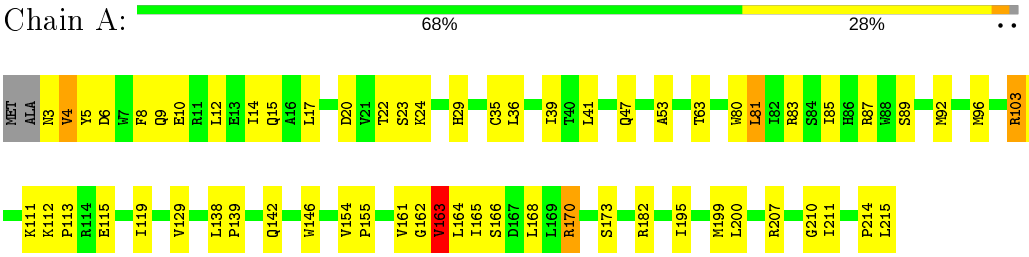
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	2	Total O 2 2	0	0
18	B	3	Total O 3 3	0	0
18	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

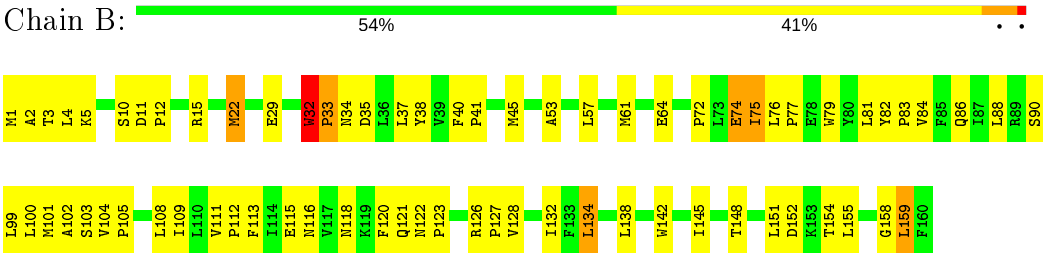
- Molecule 1: Cytochrome b6

Chain A:



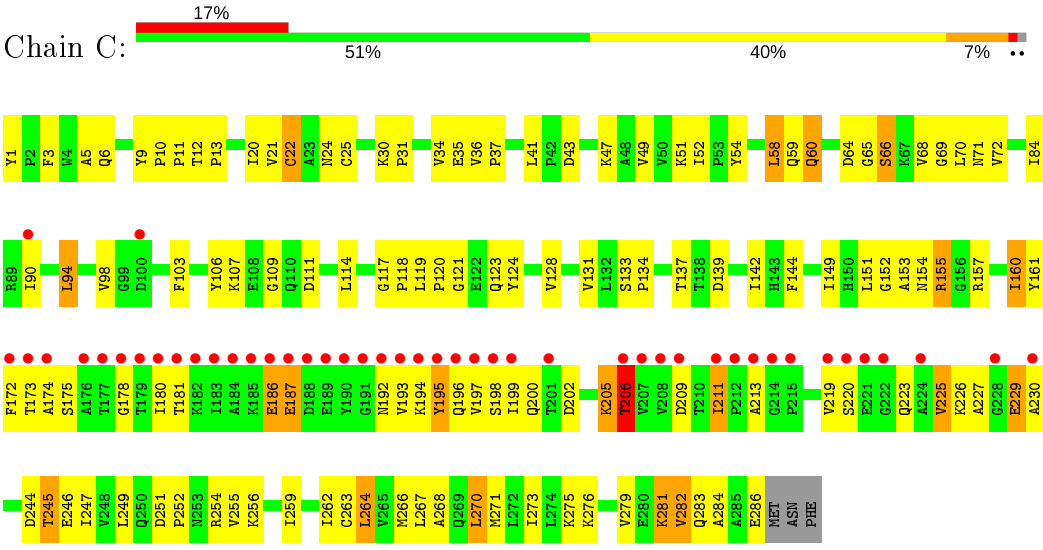
- Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:



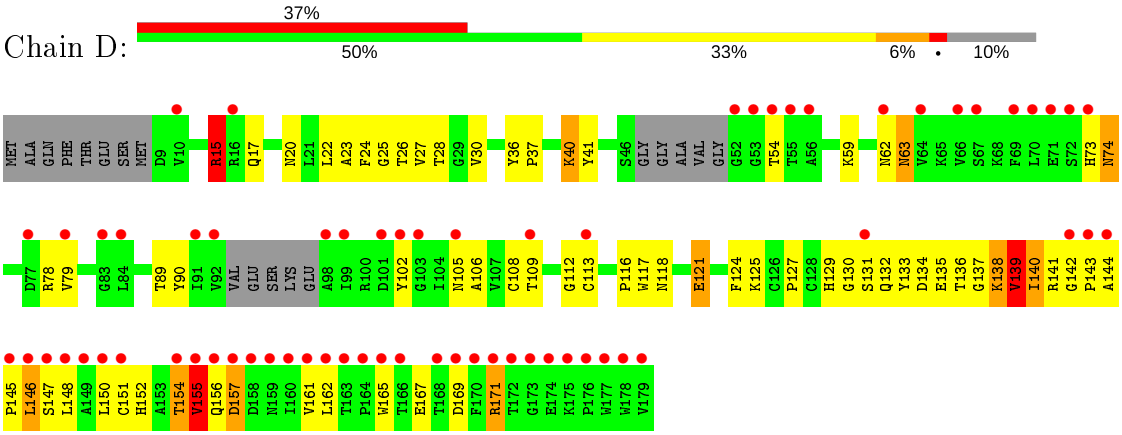
- Molecule 3: Apocytochrome f

Chain C:



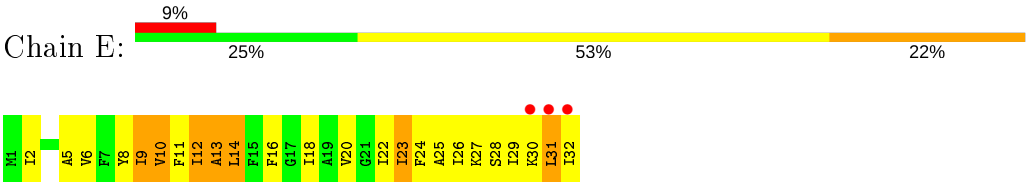
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit

Chain D:



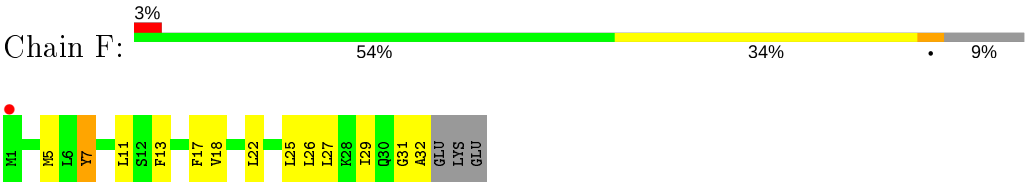
- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:



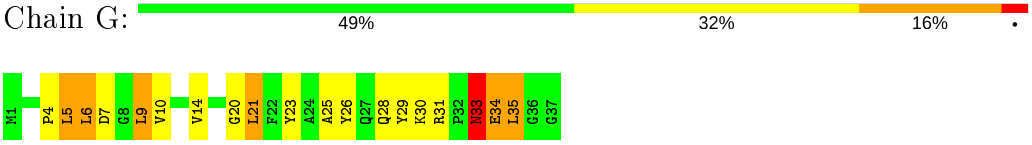
- Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:



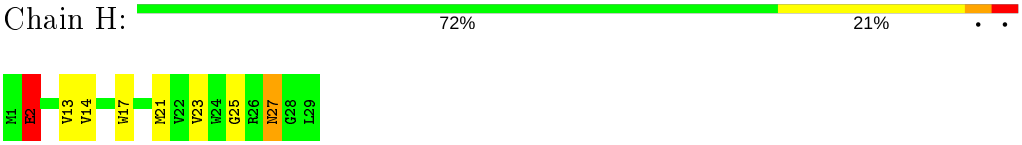
- Molecule 7: Cytochrome b6-f complex subunit 5

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	159.13Å 159.13Å 362.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.25 48.45 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.45-3.25) 99.6 (48.45-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029, PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.218 , 0.247 0.225 , 0.251	Depositor DCC
R_{free} test set	2186 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	96.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 86.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16219	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, CLA, CD, FES, OPC, HEM, QNO, BCR, SQD

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	0.40	0/1750	0.55	0/2388
2	B	0.34	0/1288	0.63	1/1765 (0.1%)
3	C	0.37	0/2248	0.60	0/3061
4	D	0.29	0/1267	0.58	1/1725 (0.1%)
5	E	0.47	0/253	0.94	0/340
6	F	0.40	0/246	0.52	0/331
7	G	0.42	0/289	0.75	1/391 (0.3%)
8	H	0.40	0/236	0.55	0/323
All	All	0.37	0/7577	0.61	3/10324 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
5	E	0	1
7	G	0	1
8	H	0	2
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	32	TRP	C-N-CD	-8.06	102.87	120.60
7	G	35	LEU	CA-CB-CG	5.34	127.58	115.30
4	D	15	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2	ALA	Peptide
2	B	32	TRP	Peptide
5	E	28	SER	Peptide
7	G	33	ASN	Peptide
8	H	2	GLU	Peptide
8	H	27	ASN	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	1698	1722	1720	64	2
2	B	1249	1309	1308	59	0
3	C	2200	2219	2218	119	2
4	D	1236	1224	1219	92	0
5	E	248	284	284	47	0
6	F	242	260	260	15	0
7	G	283	289	289	25	0
8	H	230	239	239	10	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	129	90	90	13	0
10	C	43	30	30	11	0
11	A	54	83	83	9	0
11	B	54	83	83	4	0
12	A	102	129	128	8	0
12	C	34	44	42	4	0
13	A	21	25	25	2	0
14	B	65	62	71	5	0
15	D	4	0	0	1	0
16	D	53	78	74	18	0
17	G	40	56	56	9	0
18	A	2	0	0	0	0
18	B	3	0	0	0	0
18	C	1	0	0	0	0
All	All	7993	8226	8219	406	2

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 25.

All (406) 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)
4:D:15:ARG:NH1	5:E:30:LYS:O	1.87	1.07
3:C:22:CYS:SG	10:C:302:HEM:C3B	2.51	1.04
3:C:271:MET:HE1	4:D:22:LEU:HD23	1.44	0.99
3:C:25:CYS:SG	10:C:302:HEM:CAC	2.51	0.99
4:D:25:GLY:HA3	16:D:201:SQD:H341	1.42	0.99
4:D:25:GLY:HA2	16:D:201:SQD:H311	1.52	0.92
4:D:25:GLY:O	16:D:201:SQD:H332	1.72	0.89
5:E:6:VAL:O	5:E:9:ILE:O	1.92	0.88
5:E:20:VAL:HG22	6:F:29:ILE:HD11	1.55	0.87
4:D:25:GLY:HA3	16:D:201:SQD:C34	2.06	0.85
5:E:20:VAL:HG22	6:F:29:ILE:CD1	2.04	0.85
14:B:202:CLA:HBB1	14:B:202:CLA:HHC	1.58	0.85
1:A:163:VAL:HG12	1:A:164:LEU:N	1.92	0.84
3:C:22:CYS:SG	10:C:302:HEM:CAB	2.68	0.81
3:C:35:GLU:OE1	3:C:51:LYS:NZ	2.13	0.80
4:D:134:ASP:OD2	4:D:171:ARG:NH2	2.15	0.79
1:A:35:CYS:SG	10:A:304:HEM:CAB	2.71	0.79
4:D:138:LYS:HD3	4:D:171:ARG:CZ	2.11	0.79
2:B:109:ILE:O	2:B:112:PRO:HD2	1.84	0.77
3:C:117:GLY:HA2	3:C:119:LEU:HG	1.66	0.76
3:C:25:CYS:SG	10:C:302:HEM:CBC	2.73	0.76
1:A:35:CYS:SG	10:A:304:HEM:CBB	2.74	0.76
1:A:113:PRO:HG3	2:B:22:MET:HE3	1.69	0.75
3:C:41:LEU:HD22	3:C:252:PRO:HG3	1.67	0.75
6:F:22:LEU:O	6:F:26:LEU:HD23	1.86	0.75
7:G:4:PRO:O	7:G:7:ASP:N	2.20	0.74
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.23	0.74
5:E:26:ILE:HG23	5:E:31:LEU:HB3	1.71	0.73
4:D:15:ARG:NH2	5:E:29:ILE:O	2.22	0.72
4:D:25:GLY:HA2	16:D:201:SQD:C31	2.19	0.72
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.72	0.71
4:D:136:THR:OG1	4:D:171:ARG:NE	2.18	0.71
10:A:302:HEM:HMB2	10:A:302:HEM:HBB2	1.73	0.70
1:A:8:PHE:HB3	1:A:14:ILE:HG13	1.73	0.70
4:D:25:GLY:CA	16:D:201:SQD:H341	2.21	0.70
4:D:118:ASN:OD1	4:D:121:GLU:HB2	1.91	0.70
8:H:17:TRP:O	8:H:21:MET:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:GLY:CA	16:D:201:SQD:H311	2.22	0.70
3:C:65:GLY:O	3:C:66:SER:O	2.10	0.69
1:A:111:LYS:NZ	2:B:120:PHE:O	2.25	0.69
4:D:15:ARG:CZ	5:E:30:LYS:O	2.39	0.69
1:A:41:LEU:HD23	10:A:304:HEM:HBC2	1.74	0.69
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.75	0.69
3:C:283:GLN:O	3:C:286:GLU:HG2	1.92	0.69
4:D:102:TYR:OH	4:D:136:THR:HA	1.93	0.68
4:D:15:ARG:HH12	5:E:31:LEU:HA	1.58	0.68
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.29	0.68
10:A:303:HEM:HMC2	10:A:303:HEM:HBC2	1.75	0.68
4:D:25:GLY:C	16:D:201:SQD:H332	2.13	0.68
3:C:232:THR:O	3:C:233:ASN:OD1	2.11	0.67
5:E:22:ILE:O	5:E:23:ILE:O	2.12	0.67
1:A:113:PRO:HG3	2:B:22:MET:CE	2.24	0.67
3:C:225:VAL:CG1	3:C:229:GLU:HG2	2.24	0.67
3:C:21:VAL:O	3:C:24:ASN:HB2	1.95	0.67
4:D:62:ASN:O	4:D:63:ASN:ND2	2.28	0.67
1:A:83:ARG:NH2	2:B:61:MET:O	2.28	0.67
1:A:24:LYS:NZ	12:A:306:UMQ:O3	2.27	0.67
4:D:131:SER:HA	4:D:142:GLY:HA3	1.76	0.67
1:A:142:GLN:HG3	2:B:72:PRO:HG3	1.76	0.66
3:C:268:ALA:HB2	4:D:26:THR:HG22	1.78	0.66
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.77	0.66
4:D:73:HIS:CE1	4:D:79:VAL:HG13	2.31	0.66
3:C:276:LYS:HE2	8:H:25:GLY:O	1.95	0.66
4:D:138:LYS:HD3	4:D:171:ARG:NH1	2.11	0.65
1:A:3:ASN:ND2	1:A:6:ASP:OD2	2.30	0.65
17:G:101:BCR:C21	17:G:101:BCR:H382	2.26	0.65
4:D:109:THR:HG22	4:D:144:ALA:HB1	1.77	0.65
3:C:219:VAL:HG21	3:C:231:LEU:HB2	1.79	0.65
7:G:33:ASN:O	7:G:34:GLU:O	2.14	0.65
1:A:161:VAL:HG12	1:A:165:ILE:HG13	1.79	0.65
3:C:211:ILE:O	3:C:211:ILE:HG13	1.96	0.65
3:C:22:CYS:SG	10:C:302:HEM:C4B	2.89	0.65
4:D:139:VAL:O	4:D:140:ILE:HB	1.97	0.64
4:D:136:THR:HG1	4:D:171:ARG:HE	1.43	0.64
4:D:25:GLY:CA	16:D:201:SQD:C34	2.75	0.64
4:D:129:HIS:HB2	15:D:200:FES:S1	2.38	0.64
3:C:64:ASP:OD1	3:C:65:GLY:N	2.31	0.64
3:C:175:SER:HB2	3:C:209:ASP:OD1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ALA:HB2	3:C:231:LEU:HD23	1.80	0.63
6:F:31:GLY:O	6:F:32:ALA:CB	2.47	0.63
6:F:27:LEU:HD11	8:H:27:ASN:HA	1.81	0.63
2:B:128:VAL:O	2:B:132:ILE:HD12	1.99	0.63
4:D:137:GLY:O	4:D:138:LYS:O	2.17	0.63
4:D:145:PRO:O	4:D:146:LEU:HD13	1.99	0.63
2:B:154:THR:HG23	2:B:155:LEU:N	2.14	0.62
4:D:25:GLY:CA	16:D:201:SQD:C33	2.78	0.62
5:E:9:ILE:O	5:E:10:VAL:HG23	1.98	0.62
3:C:25:CYS:SG	10:C:302:HEM:HAC	2.40	0.62
5:E:14:LEU:O	5:E:18:ILE:HG13	1.98	0.62
4:D:165:TRP:CD1	4:D:167:GLU:O	2.52	0.62
3:C:271:MET:CE	4:D:22:LEU:HD23	2.26	0.62
4:D:25:GLY:HA2	16:D:201:SQD:C32	2.30	0.62
11:A:305:OPC:HBZ2	17:G:101:BCR:H333	1.80	0.62
3:C:193:VAL:HB	3:C:213:ALA:HB2	1.82	0.61
2:B:142:TRP:CZ2	2:B:155:LEU:O	2.54	0.61
1:A:39:ILE:HD11	17:G:101:BCR:H313	1.83	0.61
5:E:16:PHE:HZ	6:F:25:LEU:HD22	1.65	0.61
3:C:279:VAL:O	3:C:283:GLN:HG3	1.99	0.61
2:B:151:LEU:O	2:B:154:THR:HG22	2.01	0.61
2:B:37:LEU:HD23	2:B:38:TYR:CE2	2.36	0.61
3:C:144:PHE:CZ	3:C:251:ASP:HB2	2.36	0.61
2:B:74:GLU:OE2	2:B:75:ILE:N	2.34	0.60
1:A:161:VAL:CG1	1:A:165:ILE:HG13	2.30	0.60
3:C:262:ILE:HG23	8:H:14:VAL:HG13	1.83	0.60
1:A:35:CYS:HG	10:A:304:HEM:CAB	2.10	0.60
3:C:3:PHE:HB2	3:C:6:GLN:NE2	2.16	0.60
3:C:144:PHE:CE1	3:C:251:ASP:HB2	2.37	0.60
3:C:34:VAL:HG22	3:C:151:LEU:HD22	1.84	0.60
1:A:103:ARG:O	1:A:107:THR:HB	2.02	0.59
4:D:73:HIS:O	4:D:74:ASN:HB2	2.01	0.59
2:B:32:TRP:CD1	2:B:33:PRO:CD	2.86	0.59
4:D:152:HIS:CE1	4:D:165:TRP:CE3	2.90	0.59
3:C:5:ALA:HB2	10:C:302:HEM:HBB2	1.83	0.59
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.84	0.59
5:E:5:ALA:O	5:E:9:ILE:HG12	2.03	0.58
1:A:92:MET:CE	11:A:305:OPC:HBY2	2.34	0.58
5:E:12:ILE:O	5:E:13:ALA:CB	2.52	0.58
3:C:58:LEU:HD12	3:C:59:GLN:N	2.18	0.58
5:E:12:ILE:O	5:E:13:ALA:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:ASP:HB3	3:C:254:ARG:CD	2.33	0.58
4:D:165:TRP:NE1	4:D:167:GLU:O	2.37	0.58
3:C:173:THR:OG1	3:C:174:ALA:N	2.37	0.57
10:A:304:HEM:O2D	13:A:308:QNO:H3	2.04	0.57
2:B:84:VAL:HG13	2:B:101:MET:CG	2.34	0.57
3:C:172:PHE:HB2	3:C:232:THR:HG21	1.86	0.57
3:C:273:ILE:HD12	8:H:25:GLY:HA3	1.85	0.57
3:C:171:VAL:HG12	3:C:234:ASN:HA	1.87	0.57
2:B:79:TRP:CD1	7:G:6:LEU:CD1	2.87	0.57
4:D:118:ASN:OD1	4:D:121:GLU:CB	2.53	0.56
6:F:13:PHE:CE2	6:F:17:PHE:HE1	2.23	0.56
3:C:173:THR:O	3:C:231:LEU:HG	2.05	0.56
4:D:124:PHE:HB2	4:D:133:TYR:HB2	1.87	0.56
1:A:92:MET:HE2	11:A:305:OPC:HBY2	1.86	0.56
4:D:15:ARG:NH1	5:E:31:LEU:HA	2.21	0.56
5:E:27:LYS:O	5:E:30:LYS:N	2.39	0.56
1:A:142:GLN:HA	1:A:142:GLN:OE1	2.05	0.56
3:C:84:ILE:HD12	3:C:103:PHE:CD1	2.41	0.56
3:C:197:VAL:O	3:C:209:ASP:N	2.38	0.56
2:B:95:LEU:O	2:B:95:LEU:HD23	2.06	0.55
6:F:31:GLY:O	6:F:32:ALA:HB2	2.06	0.55
4:D:143:PRO:O	4:D:145:PRO:HD3	2.07	0.55
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.88	0.55
6:F:7:TYR:O	6:F:11:LEU:HD12	2.07	0.55
3:C:194:LYS:O	3:C:196:GLN:N	2.40	0.55
3:C:71:ASN:HB2	10:C:302:HEM:O2A	2.06	0.55
12:C:301:UMQ:O5	12:C:301:UMQ:H6'2	2.06	0.55
3:C:187:GLU:HG3	3:C:187:GLU:O	2.07	0.55
3:C:225:VAL:HG11	3:C:229:GLU:HG2	1.89	0.55
3:C:52:ILE:HG12	3:C:153:ALA:HB1	1.88	0.54
12:A:309:UMQ:HJ1	16:D:201:SQD:H121	1.88	0.54
4:D:15:ARG:NH2	5:E:30:LYS:O	2.39	0.54
5:E:9:ILE:O	5:E:10:VAL:CB	2.54	0.54
1:A:8:PHE:HB3	1:A:14:ILE:CG1	2.36	0.54
7:G:20:GLY:N	17:G:101:BCR:H363	2.23	0.54
3:C:225:VAL:HG12	3:C:229:GLU:HG2	1.89	0.54
11:A:305:OPC:CBP	7:G:5:LEU:HD11	2.37	0.54
1:A:106:LEU:HD12	7:G:21:LEU:HD23	1.89	0.54
1:A:111:LYS:O	1:A:112:LYS:C	2.45	0.54
10:A:304:HEM:HMB1	10:A:304:HEM:HBB2	1.90	0.54
4:D:138:LYS:HA	4:D:147:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:24:PHE:O	5:E:25:ALA:C	2.46	0.53
1:A:168:LEU:O	1:A:182:ARG:NH1	2.41	0.53
5:E:23:ILE:O	5:E:26:ILE:N	2.42	0.53
1:A:103:ARG:NH1	1:A:104:VAL:HA	2.24	0.53
3:C:160:ILE:O	10:C:302:HEM:HMD1	2.08	0.53
3:C:90:ILE:HG23	3:C:94:LEU:HD13	1.90	0.53
4:D:25:GLY:CA	16:D:201:SQD:H332	2.39	0.53
2:B:122:ASN:OD1	2:B:123:PRO:HD2	2.09	0.53
4:D:78:ARG:HG3	4:D:117:TRP:CD1	2.44	0.53
3:C:271:MET:HE2	4:D:22:LEU:HB3	1.91	0.52
3:C:30:LYS:HB3	3:C:31:PRO:HD2	1.90	0.52
7:G:4:PRO:O	7:G:5:LEU:C	2.46	0.52
11:A:305:OPC:CBW	7:G:9:LEU:HD21	2.39	0.52
1:A:35:CYS:SG	10:A:304:HEM:C3B	3.02	0.52
11:A:305:OPC:HAX1	11:A:305:OPC:HBC1	1.90	0.52
1:A:163:VAL:O	1:A:166:SER:N	2.42	0.52
1:A:35:CYS:O	1:A:39:ILE:HD12	2.10	0.52
2:B:154:THR:CG2	2:B:155:LEU:N	2.73	0.52
2:B:37:LEU:CD2	2:B:38:TYR:CE2	2.93	0.52
4:D:116:PRO:HD2	4:D:125:LYS:O	2.09	0.52
4:D:138:LYS:HA	4:D:147:SER:CB	2.40	0.52
7:G:29:TYR:CD2	7:G:29:TYR:O	2.63	0.52
2:B:158:GLY:O	2:B:159:LEU:HD23	2.10	0.52
3:C:30:LYS:HB2	3:C:155:ARG:NH1	2.25	0.51
7:G:26:TYR:O	7:G:30:LYS:HG3	2.11	0.51
1:A:146:TRP:CD1	2:B:72:PRO:HD3	2.44	0.51
3:C:84:ILE:HD12	3:C:103:PHE:CG	2.46	0.51
3:C:194:LYS:O	3:C:195:TYR:C	2.48	0.51
3:C:231:LEU:HD12	3:C:232:THR:HG23	1.93	0.51
7:G:29:TYR:HD2	7:G:30:LYS:HG2	1.76	0.51
7:G:28:GLN:C	7:G:30:LYS:H	2.14	0.51
5:E:26:ILE:O	5:E:31:LEU:HB2	2.11	0.51
1:A:138:LEU:N	1:A:139:PRO:CD	2.74	0.51
3:C:34:VAL:HG22	3:C:151:LEU:CD2	2.41	0.50
10:C:302:HEM:HBC2	10:C:302:HEM:HMC2	1.93	0.50
4:D:138:LYS:HD2	4:D:171:ARG:HG3	1.92	0.50
1:A:39:ILE:HG22	1:A:96:MET:HG3	1.93	0.50
3:C:199:ILE:C	3:C:200:GLN:HG3	2.32	0.50
1:A:195:ILE:O	1:A:199:MET:HG3	2.12	0.50
1:A:215:LEU:HB2	7:G:28:GLN:OE1	2.12	0.50
1:A:103:ARG:HH11	1:A:104:VAL:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ASP:O	2:B:15:ARG:HG3	2.12	0.50
3:C:200:GLN:HA	3:C:205:LYS:HG2	1.94	0.50
5:E:16:PHE:CE2	6:F:26:LEU:HD22	2.47	0.50
3:C:154:ASN:CG	3:C:155:ARG:N	2.65	0.49
4:D:28:THR:HB	16:D:201:SQD:H322	1.93	0.49
3:C:84:ILE:HD11	3:C:114:LEU:HD13	1.94	0.49
10:A:304:HEM:HBC2	10:A:304:HEM:HHD	1.95	0.49
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.28	0.49
5:E:22:ILE:HG22	5:E:22:ILE:O	2.11	0.49
6:F:25:LEU:O	6:F:29:ILE:HG23	2.13	0.49
1:A:210:GLY:HA2	10:A:304:HEM:O1A	2.13	0.49
4:D:36:TYR:HB3	4:D:37:PRO:CD	2.42	0.49
1:A:115:GLU:O	1:A:119:ILE:HG13	2.13	0.49
1:A:22:THR:HG21	12:A:309:UMQ:H2'1	1.95	0.49
2:B:102:ALA:O	2:B:105:PRO:HD2	2.12	0.49
2:B:113:PHE:O	2:B:116:ASN:HB2	2.13	0.49
3:C:71:ASN:OD1	3:C:120:PRO:HA	2.11	0.49
3:C:151:LEU:HD12	3:C:152:GLY:H	1.77	0.49
6:F:13:PHE:CE2	6:F:17:PHE:CE1	3.00	0.49
1:A:103:ARG:HA	7:G:21:LEU:HD21	1.94	0.48
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.28	0.48
3:C:180:ILE:HG13	3:C:198:SER:O	2.13	0.48
10:C:302:HEM:HHC	10:C:302:HEM:HBB2	1.95	0.48
1:A:20:ASP:OD1	12:A:306:UMQ:O3	2.15	0.48
3:C:226:LYS:HG2	3:C:227:ALA:H	1.79	0.48
3:C:180:ILE:HD11	3:C:197:VAL:HG13	1.94	0.48
2:B:84:VAL:HG13	2:B:101:MET:HG2	1.94	0.48
3:C:275:LYS:HE2	4:D:20:ASN:OD1	2.13	0.48
4:D:156:GLN:HB2	4:D:161:VAL:CG2	2.44	0.48
2:B:142:TRP:HZ2	2:B:155:LEU:O	1.96	0.48
3:C:180:ILE:CD1	3:C:197:VAL:CG1	2.92	0.48
14:B:202:CLA:C3C	11:B:203:OPC:HBT1	2.43	0.48
2:B:100:LEU:CD2	11:B:203:OPC:HBX2	2.43	0.48
2:B:37:LEU:HD23	2:B:38:TYR:CD2	2.49	0.48
7:G:10:VAL:O	7:G:14:VAL:HG23	2.13	0.48
7:G:5:LEU:O	7:G:9:LEU:HB2	2.14	0.48
2:B:142:TRP:CH2	2:B:155:LEU:HD23	2.48	0.47
3:C:281:LYS:O	3:C:282:VAL:C	2.52	0.47
5:E:22:ILE:O	5:E:22:ILE:CG2	2.62	0.47
2:B:99:LEU:O	2:B:103:SER:OG	2.30	0.47
5:E:9:ILE:O	5:E:10:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:ARG:HG2	7:G:31:ARG:HH11	1.79	0.47
3:C:94:LEU:O	3:C:98:VAL:HG23	2.14	0.47
4:D:25:GLY:HA2	16:D:201:SQD:C33	2.42	0.47
3:C:281:LYS:HG2	3:C:282:VAL:N	2.29	0.47
4:D:73:HIS:CE1	4:D:79:VAL:CG1	2.98	0.47
3:C:36:VAL:HG21	3:C:247:ILE:HB	1.97	0.47
2:B:104:VAL:O	2:B:108:LEU:HB2	2.15	0.47
4:D:154:THR:C	4:D:155:VAL:HG22	2.35	0.47
4:D:156:GLN:HB2	4:D:161:VAL:HG23	1.95	0.47
16:D:201:SQD:H161	16:D:201:SQD:H131	1.55	0.47
3:C:36:VAL:HG11	3:C:149:ILE:HD13	1.96	0.47
12:C:301:UMQ:HL3	4:D:37:PRO:CG	2.45	0.47
5:E:16:PHE:CZ	6:F:25:LEU:HD22	2.48	0.46
5:E:26:ILE:CG2	5:E:31:LEU:HB3	2.44	0.46
5:E:9:ILE:O	5:E:10:VAL:CG2	2.61	0.46
3:C:139:ASP:CG	3:C:142:ILE:HG12	2.36	0.46
4:D:15:ARG:NH1	5:E:31:LEU:HG	2.30	0.46
2:B:32:TRP:HE1	16:D:201:SQD:HO3	1.62	0.46
5:E:24:PHE:O	5:E:27:LYS:N	2.48	0.46
4:D:125:LYS:O	4:D:127:PRO:HD3	2.14	0.46
3:C:271:MET:HB3	4:D:23:ALA:HA	1.97	0.46
17:G:101:BCR:H21C	17:G:101:BCR:H382	1.97	0.46
2:B:118:ASN:ND2	11:B:203:OPC:HAH1	2.30	0.46
3:C:60:GLN:OE1	3:C:157:ARG:HG3	2.16	0.46
4:D:141:ARG:HG2	4:D:142:GLY:H	1.80	0.46
3:C:3:PHE:O	3:C:6:GLN:HG2	2.16	0.46
4:D:169:ASP:OD2	4:D:171:ARG:HB3	2.15	0.46
5:E:2:ILE:O	5:E:6:VAL:HG23	2.14	0.46
2:B:10:SER:O	2:B:12:PRO:HD3	2.15	0.46
3:C:59:GLN:HB3	3:C:68:VAL:O	2.16	0.46
2:B:79:TRP:CD1	7:G:6:LEU:HD11	2.51	0.46
1:A:154:VAL:HB	1:A:155:PRO:HD3	1.98	0.46
3:C:88:GLU:HG2	3:C:88:GLU:O	2.16	0.46
4:D:108:CYS:HB2	4:D:113:CYS:O	2.15	0.46
4:D:124:PHE:O	4:D:132:GLN:HA	2.15	0.46
11:B:203:OPC:HAE2	11:B:203:OPC:OAI	2.15	0.46
3:C:229:GLU:OE2	3:C:230:ALA:N	2.48	0.46
4:D:152:HIS:ND1	4:D:165:TRP:CE3	2.84	0.46
2:B:45:MET:HE3	4:D:27:VAL:HG22	1.99	0.46
5:E:9:ILE:HG12	5:E:9:ILE:H	1.59	0.45
12:C:301:UMQ:C5	12:C:301:UMQ:H6'2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:TYR:HA	4:D:151:CYS:O	2.17	0.45
5:E:16:PHE:CE2	6:F:26:LEU:CD2	3.00	0.45
1:A:29:HIS:CG	1:A:214:PRO:HA	2.51	0.45
2:B:145:ILE:O	2:B:148:THR:HB	2.17	0.45
4:D:130:GLY:C	4:D:141:ARG:HH21	2.19	0.45
4:D:73:HIS:CE1	4:D:79:VAL:HG22	2.52	0.45
11:A:305:OPC:HBW2	7:G:9:LEU:HD21	1.97	0.45
14:B:202:CLA:O2A	14:B:202:CLA:C4	2.65	0.45
4:D:152:HIS:O	4:D:162:LEU:HD23	2.16	0.45
2:B:111:VAL:N	2:B:112:PRO:HD2	2.32	0.45
2:B:86:GLN:O	2:B:90:SER:OG	2.27	0.45
3:C:54:TYR:OH	3:C:121:GLY:HA3	2.16	0.45
1:A:111:LYS:HE2	2:B:115:GLU:O	2.16	0.45
3:C:12:THR:OG1	3:C:13:PRO:HD2	2.17	0.45
2:B:37:LEU:CD2	2:B:38:TYR:CZ	3.00	0.45
5:E:22:ILE:O	5:E:26:ILE:HB	2.17	0.45
1:A:39:ILE:CD1	17:G:101:BCR:C31	2.95	0.45
3:C:180:ILE:HD12	3:C:197:VAL:CG1	2.47	0.45
3:C:271:MET:CE	4:D:22:LEU:HB3	2.47	0.45
4:D:130:GLY:C	4:D:141:ARG:NH2	2.71	0.45
2:B:33:PRO:HA	2:B:37:LEU:HB3	1.99	0.44
4:D:73:HIS:ND1	4:D:79:VAL:CG2	2.80	0.44
7:G:29:TYR:CG	7:G:29:TYR:O	2.69	0.44
1:A:207:ARG:NH1	13:A:308:QNO:H3	2.32	0.44
4:D:40:LYS:HA	4:D:40:LYS:HD2	1.83	0.44
1:A:35:CYS:C	1:A:39:ILE:HD12	2.38	0.44
1:A:4:VAL:O	1:A:5:TYR:C	2.55	0.44
2:B:77:PRO:HB2	2:B:81:LEU:HD12	1.99	0.44
3:C:266:MET:SD	8:H:13:VAL:HG12	2.58	0.44
4:D:154:THR:C	4:D:155:VAL:CG2	2.85	0.44
3:C:1:TYR:HD2	3:C:118:PRO:HG3	1.83	0.44
4:D:73:HIS:ND1	4:D:79:VAL:HG22	2.32	0.44
1:A:92:MET:CE	11:A:305:OPC:HCB2	2.48	0.44
3:C:151:LEU:HD12	3:C:152:GLY:N	2.33	0.44
3:C:255:VAL:O	3:C:259:ILE:HG13	2.17	0.44
3:C:270:LEU:HA	8:H:21:MET:CE	2.48	0.44
7:G:34:GLU:O	7:G:35:LEU:HD12	2.17	0.44
11:A:305:OPC:HBG3	11:A:305:OPC:OAI	2.17	0.44
3:C:262:ILE:HG23	8:H:14:VAL:CG1	2.47	0.43
3:C:47:LYS:HG3	3:C:128:VAL:HG13	2.00	0.43
8:H:23:VAL:O	8:H:27:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HG	2:B:5:LYS:N	2.33	0.43
4:D:145:PRO:O	4:D:146:LEU:CD1	2.65	0.43
4:D:133:TYR:CD2	4:D:148:LEU:HG	2.53	0.43
1:A:166:SER:O	1:A:170:ARG:HG2	2.18	0.43
2:B:53:ALA:O	2:B:57:LEU:HG	2.18	0.43
3:C:20:ILE:HD13	3:C:152:GLY:HA3	2.01	0.43
3:C:211:ILE:O	3:C:211:ILE:CG1	2.65	0.43
2:B:3:THR:O	2:B:29:GLU:HA	2.19	0.43
3:C:219:VAL:HG12	3:C:220:SER:N	2.34	0.43
2:B:32:TRP:NE1	16:D:201:SQD:O3	2.50	0.43
7:G:21:LEU:HA	7:G:21:LEU:HD12	1.89	0.43
2:B:134:LEU:HA	2:B:134:LEU:HD12	1.79	0.43
3:C:109:GLY:O	3:C:111:ASP:N	2.50	0.43
3:C:10:PRO:N	3:C:11:PRO:HD3	2.33	0.43
3:C:206:THR:O	3:C:206:THR:CG2	2.65	0.43
4:D:78:ARG:HG3	4:D:117:TRP:NE1	2.34	0.43
4:D:90:TYR:CD1	4:D:106:ALA:HB2	2.53	0.43
5:E:26:ILE:HG21	5:E:32:ILE:CD1	2.49	0.43
3:C:161:TYR:O	3:C:163:THR:N	2.52	0.42
3:C:262:ILE:HG22	3:C:263:CYS:N	2.34	0.42
3:C:58:LEU:C	3:C:58:LEU:HD12	2.38	0.42
14:B:202:CLA:H42	14:B:202:CLA:O2A	2.19	0.42
3:C:178:GLY:HA3	3:C:202:ASP:OD2	2.19	0.42
3:C:251:ASP:OD2	3:C:252:PRO:HD2	2.19	0.42
3:C:281:LYS:O	3:C:284:ALA:N	2.47	0.42
4:D:89:THR:HG22	4:D:105:ASN:HA	2.01	0.42
12:A:306:UMQ:HB2	12:A:306:UMQ:O2'	2.18	0.42
4:D:156:GLN:O	4:D:157:ASP:C	2.57	0.42
3:C:245:THR:OG1	3:C:246:GLU:N	2.51	0.42
3:C:68:VAL:HG22	3:C:69:GLY:N	2.33	0.42
4:D:138:LYS:HA	4:D:147:SER:HB3	2.01	0.42
5:E:23:ILE:HD13	5:E:23:ILE:HG21	1.85	0.42
5:E:26:ILE:HG23	5:E:31:LEU:CB	2.47	0.42
1:A:6:ASP:O	1:A:10:GLU:HG3	2.20	0.42
3:C:199:ILE:C	3:C:200:GLN:CG	2.88	0.42
5:E:16:PHE:HE1	5:E:20:VAL:HG21	1.85	0.42
1:A:161:VAL:HG13	1:A:164:LEU:HD12	2.02	0.42
1:A:83:ARG:HD2	10:A:302:HEM:O1D	2.20	0.42
1:A:108:GLY:HA3	2:B:121:GLN:HA	2.01	0.42
1:A:154:VAL:HG22	2:B:88:LEU:HD21	2.02	0.42
12:A:306:UMQ:CA	12:A:306:UMQ:O2'	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:306:UMQ:O5	12:A:306:UMQ:C3'	2.67	0.42
3:C:43:ASP:HA	3:C:133:SER:O	2.19	0.42
3:C:36:VAL:HG23	3:C:37:PRO:O	2.18	0.42
4:D:15:ARG:HH12	5:E:31:LEU:CA	2.31	0.42
5:E:22:ILE:O	5:E:23:ILE:C	2.53	0.42
2:B:37:LEU:HD21	4:D:24:PHE:HZ	1.84	0.42
3:C:10:PRO:N	3:C:11:PRO:CD	2.83	0.41
3:C:35:GLU:HB2	3:C:49:VAL:HB	2.01	0.41
17:G:101:BCR:H351	17:G:101:BCR:H15C	1.89	0.41
1:A:9:GLN:OE1	1:A:15:GLN:HB2	2.20	0.41
1:A:39:ILE:HD11	17:G:101:BCR:C31	2.49	0.41
3:C:264:LEU:HD13	4:D:30:VAL:CG2	2.49	0.41
3:C:9:TYR:O	3:C:106:TYR:OH	2.32	0.41
2:B:40:PHE:HB2	2:B:41:PRO:HD3	2.02	0.41
12:C:301:UMQ:HL3	4:D:37:PRO:HG3	2.02	0.41
4:D:15:ARG:HH12	5:E:30:LYS:C	2.12	0.41
5:E:10:VAL:O	5:E:14:LEU:HD12	2.19	0.41
3:C:273:ILE:HD12	8:H:25:GLY:CA	2.50	0.41
5:E:18:ILE:O	5:E:22:ILE:HG13	2.21	0.41
1:A:80:TRP:CH2	3:C:254:ARG:HG2	2.55	0.41
1:A:53:ALA:HB1	4:D:41:TYR:CE2	2.56	0.41
5:E:29:ILE:O	5:E:29:ILE:HG22	2.21	0.41
5:E:23:ILE:O	5:E:26:ILE:HB	2.20	0.41
7:G:29:TYR:HD2	7:G:30:LYS:CG	2.33	0.41
1:A:211:ILE:N	10:A:304:HEM:O1A	2.54	0.41
3:C:72:VAL:HG21	3:C:124:TYR:O	2.20	0.41
1:A:103:ARG:HD2	1:A:103:ARG:O	2.21	0.41
1:A:14:ILE:HG22	12:A:307:UMQ:HD1	2.03	0.41
2:B:32:TRP:CG	2:B:33:PRO:N	2.89	0.41
3:C:223:GLN:HB3	3:C:225:VAL:CG2	2.51	0.41
3:C:281:LYS:O	3:C:283:GLN:N	2.54	0.41
2:B:126:ARG:N	2:B:127:PRO:HD3	2.35	0.40
3:C:171:VAL:HG12	3:C:233:ASN:O	2.21	0.40
1:A:129:VAL:HG21	14:B:202:CLA:H43	2.02	0.40
2:B:75:ILE:O	2:B:75:ILE:HG12	2.20	0.40
6:F:18:VAL:O	6:F:22:LEU:HG	2.21	0.40
1:A:81:LEU:HD22	1:A:85:ILE:HG13	2.04	0.40
3:C:70:LEU:HD23	3:C:70:LEU:H	1.86	0.40
4:D:140:ILE:O	4:D:140:ILE:HG13	2.21	0.40
3:C:134:PRO:HB2	3:C:142:ILE:HG21	2.04	0.40
7:G:23:TYR:CD1	17:G:101:BCR:H21C	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:NZ	3:C:87:GLU:OE1[8_665]	1.82	0.38
1:A:112:LYS:HZ2	3:C:87:GLU:OE1[8_665]	1.41	0.19

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	211/215 (98%)	187 (89%)	19 (9%)	5 (2%)	6 28
2	B	158/160 (99%)	143 (90%)	11 (7%)	4 (2%)	5 28
3	C	284/289 (98%)	235 (83%)	41 (14%)	8 (3%)	5 25
4	D	155/179 (87%)	123 (79%)	22 (14%)	10 (6%)	1 9
5	E	30/32 (94%)	16 (53%)	11 (37%)	3 (10%)	0 3
6	F	30/35 (86%)	29 (97%)	1 (3%)	0	100 100
7	G	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1 5
8	H	27/29 (93%)	26 (96%)	0	1 (4%)	3 19
All	All	930/976 (95%)	785 (84%)	111 (12%)	34 (4%)	3 19

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
2	B	33	PRO
2	B	34	ASN
2	B	75	ILE
3	C	66	SER
3	C	186	GLU
3	C	192	ASN
3	C	195	TYR

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Mol	Chain	Res	Type
4	D	138	LYS
4	D	139	VAL
4	D	140	ILE
5	E	10	VAL
5	E	13	ALA
5	E	23	ILE
7	G	34	GLU
1	A	23	SER
2	B	22	MET
3	C	233	ASN
4	D	63	ASN
4	D	121	GLU
4	D	171	ARG
1	A	4	VAL
3	C	187	GLU
3	C	282	VAL
4	D	74	ASN
4	D	112	GLY
4	D	155	VAL
1	A	170	ARG
3	C	206	THR
4	D	157	ASP
7	G	5	LEU
7	G	33	ASN
8	H	2	GLU
1	A	163	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	183/184 (100%)	172 (94%)	11 (6%)	19 49
2	B	137/137 (100%)	127 (93%)	10 (7%)	14 40
3	C	240/243 (99%)	212 (88%)	28 (12%)	5 21
4	D	133/146 (91%)	122 (92%)	11 (8%)	11 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	25/25 (100%)	20 (80%)	5 (20%)	1 5
6	F	24/27 (89%)	22 (92%)	2 (8%)	11 36
7	G	28/28 (100%)	25 (89%)	3 (11%)	6 25
8	H	24/24 (100%)	23 (96%)	1 (4%)	30 59
All	All	794/814 (98%)	723 (91%)	71 (9%)	9 32

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	LEU
1	A	36	LEU
1	A	63	THR
1	A	81	LEU
1	A	87	ARG
1	A	103	ARG
1	A	107	THR
1	A	163	VAL
1	A	173	SER
1	A	200	LEU
2	B	1	MET
2	B	35	ASP
2	B	64	GLU
2	B	74	GLU
2	B	76	LEU
2	B	96	LEU
2	B	134	LEU
2	B	138	LEU
2	B	152	ASP
2	B	159	LEU
3	C	22	CYS
3	C	58	LEU
3	C	60	GLN
3	C	88	GLU
3	C	94	LEU
3	C	107	LYS
3	C	123	GLN
3	C	131	VAL
3	C	137	THR
3	C	155	ARG
3	C	160	ILE

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Mol	Chain	Res	Type
3	C	171	VAL
3	C	181	THR
3	C	186	GLU
3	C	205	LYS
3	C	206	THR
3	C	211	ILE
3	C	225	VAL
3	C	229	GLU
3	C	233	ASN
3	C	244	ASP
3	C	245	THR
3	C	249	LEU
3	C	256	LYS
3	C	264	LEU
3	C	267	LEU
3	C	270	LEU
3	C	281	LYS
4	D	15	ARG
4	D	17	GLN
4	D	40	LYS
4	D	54	THR
4	D	59	LYS
4	D	135	GLU
4	D	139	VAL
4	D	146	LEU
4	D	150	LEU
4	D	154	THR
4	D	155	VAL
5	E	9	ILE
5	E	11	PHE
5	E	12	ILE
5	E	14	LEU
5	E	31	LEU
6	F	5	MET
6	F	7	TYR
7	G	6	LEU
7	G	9	LEU
7	G	21	LEU
8	H	2	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
3	C	154	ASN
3	C	233	ASN
4	D	63	ASN
4	D	159	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
10	HEM	A	303	1	27,50,50	2.15	5 (18%)	17,82,82	1.50	4 (23%)
12	UMQ	A	307	-	35,35,35	1.28	5 (14%)	46,46,46	2.03	13 (28%)
12	UMQ	A	309	-	35,35,35	1.25	5 (14%)	46,46,46	2.62	17 (36%)
11	OPC	A	305	-	53,53,54	1.01	4 (7%)	59,61,64	1.13	4 (6%)
10	HEM	C	302	3	27,50,50	2.16	5 (18%)	17,82,82	1.57	3 (17%)
17	BCR	G	101	-	41,41,41	2.32	24 (58%)	56,56,56	2.43	23 (41%)
12	UMQ	C	301	-	35,35,35	1.31	5 (14%)	46,46,46	1.96	11 (23%)
16	SQD	D	201	-	52,53,54	3.27	16 (30%)	60,63,65	2.52	18 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	QNO	A	308	10	22,22,22	2.66	6 (27%)	20,28,28	2.26	2 (10%)
12	UMQ	A	306	-	35,35,35	1.18	5 (14%)	46,46,46	1.77	8 (17%)
10	HEM	A	304	18,13	27,50,50	2.27	6 (22%)	17,82,82	1.51	4 (23%)
11	OPC	B	203	-	53,53,54	1.04	3 (5%)	59,61,64	0.94	3 (5%)
14	CLA	B	202	18	59,73,73	1.50	6 (10%)	67,113,113	1.63	12 (17%)
15	FES	D	200	4	0,4,4	0.00	-	-		
10	HEM	A	302	1	27,50,50	2.07	5 (18%)	17,82,82	1.88	5 (29%)

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
16	SQD	D	201	-	3/3/9/9	27/49/65/69	0/1/1/1
12	UMQ	A	307	-	2/2/10/10	8/20/60/60	0/2/2/2
12	UMQ	A	309	-	4/4/10/10	15/20/60/60	0/2/2/2
10	HEM	A	303	1	-	0/6/54/54	-
11	OPC	A	305	-	-	24/57/57/60	-
10	HEM	C	302	3	-	0/6/54/54	-
17	BCR	G	101	-	-	24/29/63/63	0/2/2/2
12	UMQ	C	301	-	1/1/10/10	7/20/60/60	0/2/2/2
13	QNO	A	308	10	1/1/0/0	4/9/9/9	0/2/2/2
12	UMQ	A	306	-	1/1/10/10	10/20/60/60	0/2/2/2
10	HEM	A	304	18,13	-	0/6/54/54	-
11	OPC	B	203	-	-	24/57/57/60	-
14	CLA	B	202	18	4/4/22/25	18/37/135/135	-
15	FES	D	200	4	-	-	0/1/1/1
10	HEM	A	302	1	-	1/6/54/54	-

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C2-C3	-11.53	1.32	1.52
16	D	201	SQD	O6-C44	9.11	1.60	1.43
14	B	202	CLA	C4B-NB	8.03	1.42	1.35
16	D	201	SQD	C8-C7	7.72	1.73	1.50
16	D	201	SQD	C4-C5	-6.32	1.39	1.53
13	A	308	QNO	OH-N1	-5.98	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	O5-C1	5.98	1.57	1.42
16	D	201	SQD	O47-C7	5.97	1.51	1.34
13	A	308	QNO	C5-C6	-5.79	1.33	1.42
10	A	304	HEM	C3D-C2D	5.69	1.54	1.37
13	A	308	QNO	C4-C5	-5.35	1.31	1.42
10	C	302	HEM	C3D-C2D	5.28	1.53	1.37
10	A	302	HEM	C3D-C2D	5.28	1.53	1.37
10	A	304	HEM	C3C-C2C	-5.21	1.33	1.40
10	A	303	HEM	C3D-C2D	5.17	1.53	1.37
13	A	308	QNO	C3-C2	5.12	1.47	1.38
10	C	302	HEM	C3B-C2B	-4.73	1.33	1.40
10	A	303	HEM	C3C-C2C	-4.65	1.33	1.40
16	D	201	SQD	O47-C45	4.59	1.58	1.46
16	D	201	SQD	C3-C4	4.53	1.59	1.52
16	D	201	SQD	C46-C45	-4.46	1.37	1.50
16	D	201	SQD	C2-C1	-4.46	1.41	1.51
10	A	303	HEM	C3B-C2B	-4.20	1.34	1.40
10	A	302	HEM	C3C-C2C	-4.11	1.34	1.40
10	A	304	HEM	C3B-C2B	-4.09	1.34	1.40
10	C	302	HEM	C3C-C2C	-4.09	1.34	1.40
10	A	304	HEM	C3B-CAB	4.00	1.56	1.47
10	A	302	HEM	C3B-C2B	-3.91	1.34	1.40
13	A	308	QNO	C2-N1	3.90	1.43	1.36
16	D	201	SQD	C6-S	3.82	1.91	1.77
10	C	302	HEM	C3B-CAB	3.78	1.55	1.47
10	A	303	HEM	C3B-CAB	3.73	1.55	1.47
11	A	305	OPC	OAN-CAO	3.68	1.44	1.34
10	A	304	HEM	C3C-CAC	3.62	1.55	1.47
13	A	308	QNO	C6-N1	-3.55	1.32	1.39
10	C	302	HEM	C3C-CAC	3.52	1.55	1.47
11	B	203	OPC	OAN-CAO	3.51	1.44	1.34
17	G	101	BCR	C23-C22	3.49	1.53	1.45
17	G	101	BCR	C17-C18	3.47	1.40	1.35
17	G	101	BCR	C14-C13	3.40	1.40	1.35
10	A	302	HEM	C3C-CAC	3.39	1.54	1.47
17	G	101	BCR	C20-C21	3.38	1.53	1.43
17	G	101	BCR	C21-C22	3.36	1.40	1.35
17	G	101	BCR	C15-C14	3.35	1.53	1.43
17	G	101	BCR	C26-C25	3.32	1.40	1.34
17	G	101	BCR	C11-C10	3.27	1.53	1.43
10	A	302	HEM	C3B-CAB	3.27	1.54	1.47
17	G	101	BCR	C12-C13	3.24	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	202	CLA	CHC-C1C	3.24	1.43	1.35
10	A	303	HEM	C3C-CAC	3.22	1.54	1.47
16	D	201	SQD	O5-C5	3.21	1.52	1.44
17	G	101	BCR	C19-C18	3.21	1.52	1.45
17	G	101	BCR	C16-C17	3.18	1.53	1.43
12	A	307	UMQ	C4-C5	-3.00	1.46	1.53
12	A	306	UMQ	C4-C5	-2.92	1.46	1.53
12	C	301	UMQ	C4-C5	-2.84	1.47	1.53
14	B	202	CLA	C1D-C2D	2.84	1.49	1.42
12	C	301	UMQ	O2'-C2'	-2.82	1.36	1.43
17	G	101	BCR	C8-C9	2.82	1.52	1.45
11	B	203	OPC	OBJ-CBK	2.81	1.41	1.33
17	G	101	BCR	C31-C1	-2.81	1.48	1.53
12	C	301	UMQ	O5'-C5'	-2.75	1.37	1.44
12	A	309	UMQ	C4-C5	-2.73	1.47	1.53
16	D	201	SQD	O48-C46	-2.68	1.39	1.45
17	G	101	BCR	C32-C1	-2.61	1.48	1.53
17	G	101	BCR	C10-C9	2.58	1.39	1.35
16	D	201	SQD	C9-C8	2.58	1.61	1.52
12	A	309	UMQ	O5'-C5'	-2.53	1.38	1.44
12	A	306	UMQ	O2'-C2'	-2.52	1.37	1.43
12	A	309	UMQ	O2'-C2'	-2.52	1.37	1.43
14	B	202	CLA	CMB-C2B	-2.49	1.46	1.51
12	A	307	UMQ	O3'-C3'	-2.48	1.37	1.43
17	G	101	BCR	C24-C23	2.46	1.40	1.33
12	A	307	UMQ	O5'-C5'	-2.46	1.38	1.44
12	A	309	UMQ	C3-C4	-2.46	1.46	1.52
12	A	307	UMQ	O2'-C2'	-2.42	1.37	1.43
11	A	305	OPC	OBJ-CBI	-2.41	1.39	1.45
11	A	305	OPC	OBJ-CBK	2.39	1.40	1.33
16	D	201	SQD	C10-C9	2.36	1.64	1.51
17	G	101	BCR	C40-C30	-2.36	1.49	1.53
17	G	101	BCR	C20-C19	2.35	1.40	1.34
12	A	306	UMQ	O5'-C5'	-2.34	1.38	1.44
12	A	307	UMQ	C3-C4	-2.34	1.46	1.52
12	C	301	UMQ	C3-C4	-2.31	1.46	1.52
12	A	306	UMQ	O3'-C3'	-2.30	1.37	1.43
17	G	101	BCR	C24-C25	2.29	1.53	1.45
17	G	101	BCR	C11-C12	2.27	1.40	1.34
12	C	301	UMQ	O3'-C3'	-2.26	1.37	1.43
14	B	202	CLA	C3B-C2B	-2.21	1.37	1.40
10	A	304	HEM	CAD-C3D	2.19	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	309	UMQ	O3'-C3'	-2.16	1.37	1.43
11	A	305	OPC	CAV-CAW	2.16	1.44	1.31
11	B	203	OPC	CAV-CAW	2.16	1.44	1.31
17	G	101	BCR	C1-C6	-2.14	1.50	1.53
16	D	201	SQD	C18-C17	2.09	1.63	1.51
17	G	101	BCR	C39-C30	-2.08	1.49	1.53
17	G	101	BCR	C7-C6	2.03	1.52	1.45
17	G	101	BCR	C29-C28	-2.03	1.47	1.52
12	A	306	UMQ	O5-C5	-2.02	1.39	1.44
14	B	202	CLA	CMC-C2C	-2.00	1.46	1.50

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	201	SQD	C3-C4-C5	9.70	119.63	109.97
13	A	308	QNO	C3-C2-N1	-9.08	108.97	118.94
14	B	202	CLA	C4A-NA-C1A	6.99	109.85	106.71
12	A	309	UMQ	O5'-C1'-C2'	6.37	123.84	110.35
12	A	309	UMQ	O1'-C1'-C2'	6.31	118.15	108.30
12	C	301	UMQ	O1'-C1'-C2'	6.27	118.10	108.30
16	D	201	SQD	C2-C3-C4	6.07	119.50	110.69
17	G	101	BCR	C7-C8-C9	-6.00	117.17	126.23
12	A	306	UMQ	CA-O1'-C1'	5.50	122.96	113.84
16	D	201	SQD	C1-O5-C5	5.40	121.42	113.03
11	A	305	OPC	OAN-CAO-CAP	5.16	122.62	111.50
17	G	101	BCR	C16-C17-C18	-4.94	120.27	127.31
16	D	201	SQD	O4-C4-C5	4.89	121.45	109.30
12	C	301	UMQ	O1-C1-O5	4.87	124.27	110.67
12	A	307	UMQ	O2'-C2'-C1'	4.86	121.85	110.05
17	G	101	BCR	C20-C21-C22	-4.82	120.43	127.31
12	A	307	UMQ	O2'-C2'-C3'	4.79	121.42	110.35
16	D	201	SQD	O9-S-C6	4.79	112.63	106.94
12	A	309	UMQ	CA-O1'-C1'	4.77	121.75	113.84
17	G	101	BCR	C15-C14-C13	-4.76	120.51	127.31
16	D	201	SQD	O3-C3-C4	4.71	119.57	110.14
12	A	307	UMQ	CA-O1'-C1'	4.66	121.57	113.84
12	A	309	UMQ	C2'-C3'-C4'	4.61	120.22	109.68
12	A	309	UMQ	O3-C3-C4	4.58	120.94	110.35
12	A	306	UMQ	O1-C4'-C5'	4.51	121.81	109.45
12	C	301	UMQ	C1'-C2'-C3'	-4.51	100.61	110.00
17	G	101	BCR	C24-C23-C22	-4.41	119.57	126.23
16	D	201	SQD	O3-C3-C2	4.40	120.86	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	302	HEM	CBA-CAA-C2A	-4.39	104.39	112.49
17	G	101	BCR	C1-C6-C5	-4.37	116.46	122.61
16	D	201	SQD	O7-S-C6	4.35	112.11	106.94
12	A	309	UMQ	O3-C3-C2	4.34	120.39	110.35
16	D	201	SQD	O4-C4-C3	4.33	118.29	109.99
17	G	101	BCR	C33-C5-C6	-4.32	119.68	124.53
12	A	307	UMQ	O2-C2-C1	4.32	120.54	110.05
12	A	309	UMQ	O2-C2-C3	4.30	120.30	110.35
12	A	309	UMQ	C4-C3-C2	4.27	118.28	110.82
12	A	309	UMQ	O2-C2-C1	4.19	120.22	110.05
12	A	307	UMQ	C1-C2-C3	4.17	118.67	110.00
12	A	307	UMQ	O2-C2-C3	4.16	119.96	110.35
12	C	301	UMQ	O1-C1-C2	4.11	118.75	108.10
12	A	306	UMQ	C3'-C4'-C5'	4.05	120.22	110.93
12	A	309	UMQ	C1-C2-C3	3.93	118.17	110.00
12	A	309	UMQ	O3'-C3'-C4'	3.86	120.18	109.94
16	D	201	SQD	O47-C7-C8	3.73	119.55	111.50
16	D	201	SQD	O9-S-O7	-3.72	101.09	113.95
12	A	309	UMQ	O3'-C3'-C2'	3.71	118.92	110.35
10	A	304	HEM	CBA-CAA-C2A	-3.70	105.67	112.49
14	B	202	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
12	A	306	UMQ	O1-C4'-C3'	3.58	116.81	107.28
17	G	101	BCR	C23-C24-C25	-3.57	117.18	127.20
17	G	101	BCR	C33-C5-C4	3.55	120.44	113.62
16	D	201	SQD	C44-O6-C1	3.48	120.53	113.80
11	B	203	OPC	OAN-CAO-CAP	3.41	118.85	111.50
17	G	101	BCR	C38-C26-C25	-3.25	120.88	124.53
12	C	301	UMQ	C1'-O5'-C5'	-3.24	107.34	113.69
12	C	301	UMQ	C1-C2-C3	-3.21	103.32	110.00
17	G	101	BCR	C20-C19-C18	-3.15	117.56	126.42
12	A	306	UMQ	C1-O1-C4'	-3.14	110.19	117.96
17	G	101	BCR	C37-C22-C21	-3.13	118.54	122.92
12	C	301	UMQ	C1-O5-C5	-3.08	107.64	113.69
10	C	302	HEM	C1D-C2D-C3D	-3.07	104.86	107.00
12	A	309	UMQ	O5'-C1'-O1'	3.06	117.22	109.97
12	A	307	UMQ	C1'-O5'-C5'	-3.06	107.69	113.69
14	B	202	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
14	B	202	CLA	CAA-CBA-CGA	-2.99	104.52	113.25
17	G	101	BCR	C31-C1-C6	-2.99	105.45	110.30
12	A	307	UMQ	O5'-C1'-C2'	-2.97	104.06	110.35
12	A	307	UMQ	C1'-C2'-C3'	2.96	116.15	110.00
17	G	101	BCR	C29-C30-C25	2.86	114.89	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	101	BCR	C38-C26-C27	2.85	119.10	113.62
10	C	302	HEM	CBD-CAD-C3D	-2.80	107.32	112.48
17	G	101	BCR	C34-C9-C10	-2.80	119.00	122.92
17	G	101	BCR	C8-C9-C10	2.75	123.16	118.94
11	B	203	OPC	OBJ-CBK-CBL	2.74	120.52	111.91
10	A	303	HEM	C1D-C2D-C3D	-2.73	105.09	107.00
12	A	306	UMQ	C1-C2-C3	2.70	115.61	110.00
12	A	306	UMQ	O1-C1-C2	2.69	115.08	108.10
12	A	307	UMQ	O1'-C1'-C2'	2.67	112.47	108.30
14	B	202	CLA	CHB-C4A-NA	2.64	128.17	124.51
10	A	303	HEM	CBD-CAD-C3D	-2.63	107.63	112.48
14	B	202	CLA	C9-C8-C10	2.61	120.74	111.29
14	B	202	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
16	D	201	SQD	O6-C1-C2	-2.56	106.38	109.04
12	A	309	UMQ	O5-C5-C4	2.50	114.23	109.69
12	C	301	UMQ	C4-C3-C2	-2.48	106.50	110.82
10	A	303	HEM	C4A-C3A-C2A	2.47	108.71	107.00
12	A	309	UMQ	C1-O5-C5	2.39	118.39	113.69
10	A	302	HEM	CMB-C2B-C3B	2.39	129.15	124.68
11	A	305	OPC	CBI-CAM-CAL	-2.39	106.14	111.79
17	G	101	BCR	C35-C13-C14	-2.37	119.61	122.92
17	G	101	BCR	C3-C4-C5	2.36	118.29	114.08
10	A	303	HEM	CMC-C2C-C3C	2.36	129.10	124.68
12	C	301	UMQ	O5-C1-C2	2.36	115.33	110.35
14	B	202	CLA	CAA-C2A-C1A	-2.35	104.27	111.97
17	G	101	BCR	C11-C10-C9	-2.35	123.96	127.31
16	D	201	SQD	O5-C1-C2	2.34	114.41	110.87
11	A	305	OPC	OAN-CAO-OAD	-2.30	118.15	123.70
10	A	302	HEM	C1D-C2D-C3D	-2.29	105.40	107.00
16	D	201	SQD	C13-C12-C11	2.29	126.04	114.42
17	G	101	BCR	C1-C6-C7	2.29	122.25	115.78
12	A	307	UMQ	O5'-C5'-C4'	2.29	114.57	109.75
11	A	305	OPC	OBJ-CBK-CBL	2.29	119.08	111.91
11	B	203	OPC	OAN-CAO-OAD	-2.27	118.21	123.70
16	D	201	SQD	C45-O47-C7	2.26	123.36	117.79
10	A	302	HEM	CAA-CBA-CGA	-2.26	108.88	112.67
14	B	202	CLA	CMB-C2B-C3B	2.26	128.90	124.68
12	C	301	UMQ	O5'-C1'-C2'	-2.25	105.58	110.35
12	A	307	UMQ	C1-O5-C5	-2.24	109.30	113.69
12	A	309	UMQ	O5'-C5'-C4'	2.24	114.47	109.75
12	A	306	UMQ	O1'-C1'-C2'	2.23	111.78	108.30
16	D	201	SQD	O48-C23-C24	2.18	118.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	304	HEM	C3C-C4C-NC	-2.17	106.85	110.94
12	A	309	UMQ	O5-C5-C6	2.16	111.81	106.44
10	A	304	HEM	CMB-C2B-C3B	2.15	128.69	124.68
12	A	307	UMQ	C6-C5-C4	-2.12	108.03	113.00
10	A	302	HEM	C4C-C3C-C2C	2.11	108.37	106.90
16	D	201	SQD	O8-S-C6	2.10	109.09	105.74
17	G	101	BCR	C8-C7-C6	-2.08	121.37	127.20
12	C	301	UMQ	CA-O1'-C1'	-2.08	110.40	113.84
10	C	302	HEM	CBA-CAA-C2A	-2.04	108.72	112.49
17	G	101	BCR	C40-C30-C25	-2.03	107.01	110.30
10	A	304	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
13	A	308	QNO	O41-C4-C5	2.02	118.83	116.31
14	B	202	CLA	C3A-C2A-C1A	2.01	104.35	101.34
14	B	202	CLA	CMD-C2D-C3D	2.01	128.44	124.68
14	B	202	CLA	CAA-C2A-C3A	-2.01	107.29	112.78

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	307	UMQ	C2'
12	A	307	UMQ	C2
12	A	309	UMQ	C3
12	A	309	UMQ	C1'
12	A	309	UMQ	C2
12	A	309	UMQ	C3'
12	C	301	UMQ	C1
16	D	201	SQD	C4
16	D	201	SQD	C3
16	D	201	SQD	C5
13	A	308	QNO	C2
12	A	306	UMQ	C4'
14	B	202	CLA	C8
14	B	202	CLA	NC
14	B	202	CLA	ND
14	B	202	CLA	NA

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	305	OPC	NAF-CAG-CAH-OAI
17	G	101	BCR	C1-C6-C7-C8
17	G	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	G	101	BCR	C6-C7-C8-C9
17	G	101	BCR	C7-C8-C9-C10
17	G	101	BCR	C7-C8-C9-C34
17	G	101	BCR	C11-C12-C13-C14
17	G	101	BCR	C11-C12-C13-C35
17	G	101	BCR	C36-C18-C19-C20
17	G	101	BCR	C20-C21-C22-C37
17	G	101	BCR	C21-C22-C23-C24
17	G	101	BCR	C37-C22-C23-C24
17	G	101	BCR	C22-C23-C24-C25
16	D	201	SQD	C2-C1-O6-C44
16	D	201	SQD	O5-C1-O6-C44
16	D	201	SQD	O47-C45-C46-O48
16	D	201	SQD	C5-C6-S-O7
16	D	201	SQD	C5-C6-S-O8
16	D	201	SQD	C5-C6-S-O9
12	A	306	UMQ	C2'-C1'-O1'-CA
14	B	202	CLA	C1A-C2A-CAA-CBA
14	B	202	CLA	C3A-C2A-CAA-CBA
14	B	202	CLA	CBD-CGD-O2D-CED
14	B	202	CLA	O2A-C1-C2-C3
11	B	203	OPC	CAH-OAI-PAJ-OAB
11	B	203	OPC	NAF-CAG-CAH-OAI
12	A	306	UMQ	C3'-C4'-O1-C1
14	B	202	CLA	O1D-CGD-O2D-CED
12	C	301	UMQ	O5-C1-O1-C4'
16	D	201	SQD	O49-C7-O47-C45
12	A	307	UMQ	O5-C5-C6-O6
12	A	309	UMQ	O5-C5-C6-O6
16	D	201	SQD	C13-C14-C15-C16
12	A	306	UMQ	O5'-C5'-C6'-O6'
11	B	203	OPC	OAD-CAO-OAN-CAM
12	A	307	UMQ	C4-C5-C6-O6
16	D	201	SQD	C8-C7-O47-C45
11	B	203	OPC	CAP-CAO-OAN-CAM
12	C	301	UMQ	O5'-C5'-C6'-O6'
16	D	201	SQD	C31-C32-C33-C34
12	C	301	UMQ	C4'-C5'-C6'-O6'
12	A	309	UMQ	O5'-C5'-C6'-O6'
16	D	201	SQD	C33-C34-C35-C36
12	A	306	UMQ	O5'-C1'-O1'-CA
12	A	309	UMQ	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	A	309	UMQ	C4'-C5'-C6'-O6'
12	A	306	UMQ	C4'-C5'-C6'-O6'
14	B	202	CLA	C13-C15-C16-C17
12	A	309	UMQ	C2'-C1'-O1'-CA
11	B	203	OPC	CBK-CBL-CBM-CBN
11	A	305	OPC	CAO-CAP-CAQ-CAR
11	B	203	OPC	CAO-CAP-CAQ-CAR
16	D	201	SQD	C23-C24-C25-C26
17	G	101	BCR	C10-C11-C12-C13
17	G	101	BCR	C18-C19-C20-C21
11	B	203	OPC	CBQ-CBR-CBS-CBT
11	B	203	OPC	CAH-OAI-PAJ-OAK
13	A	308	QNO	C2-C21-C22-C23
14	B	202	CLA	C10-C11-C12-C13
12	A	309	UMQ	O1'-CA-CB-CC
12	A	309	UMQ	O5-C1-O1-C4'
11	A	305	OPC	CAP-CAQ-CAR-CAS
12	C	301	UMQ	CH-CI-CJ-CK
16	D	201	SQD	C29-C30-C31-C32
12	A	309	UMQ	CC-CD-CF-CG
12	A	307	UMQ	CH-CI-CJ-CK
11	B	203	OPC	CAR-CAS-CAT-CAU
16	D	201	SQD	C9-C10-C11-C12
17	G	101	BCR	C12-C13-C14-C15
17	G	101	BCR	C16-C17-C18-C19
12	A	307	UMQ	C4'-C5'-C6'-O6'
12	A	306	UMQ	CB-CC-CD-CF
11	A	305	OPC	CBV-CBW-CBX-CBY
12	A	307	UMQ	CF-CG-CH-CI
11	A	305	OPC	CAX-CAY-CAZ-CBA
16	D	201	SQD	C14-C15-C16-C17
14	B	202	CLA	C16-C17-C18-C20
12	A	309	UMQ	O5'-C1'-O1'-CA
12	C	301	UMQ	CD-CF-CG-CH
16	D	201	SQD	C18-C19-C20-C21
11	A	305	OPC	CBN-CBO-CBP-CBQ
17	G	101	BCR	C23-C24-C25-C26
17	G	101	BCR	C23-C24-C25-C30
14	B	202	CLA	C3-C5-C6-C7
11	A	305	OPC	CAY-CAZ-CBA-CBB
11	A	305	OPC	OCC-CBK-OBJ-CBI
11	A	305	OPC	CBK-CBL-CBM-CBN

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Mol	Chain	Res	Type	Atoms
12	A	309	UMQ	CF-CG-CH-CI
11	B	203	OPC	CBM-CBN-CBO-CBP
11	A	305	OPC	CAW-CAX-CAY-CAZ
16	D	201	SQD	C24-C25-C26-C27
11	A	305	OPC	CBS-CBT-CBU-CBV
12	A	309	UMQ	CB-CC-CD-CF
16	D	201	SQD	C44-C45-C46-O48
16	D	201	SQD	C28-C29-C30-C31
13	A	308	QNO	C22-C23-C24-C25
11	B	203	OPC	CBL-CBM-CBN-CBO
12	A	306	UMQ	O5-C5-C6-O6
11	A	305	OPC	OAN-CAM-CBI-OBJ
12	C	301	UMQ	CI-CJ-CK-CL
14	B	202	CLA	C6-C7-C8-C10
11	A	305	OPC	CAQ-CAR-CAS-CAT
17	G	101	BCR	C17-C18-C19-C20
11	A	305	OPC	CBL-CBK-OBJ-CBI
13	A	308	QNO	C21-C22-C23-C24
10	A	302	HEM	C3D-CAD-CBD-CGD
16	D	201	SQD	C11-C10-C9-C8
12	A	307	UMQ	CB-CA-O1'-C1'
12	A	309	UMQ	CB-CA-O1'-C1'
12	A	306	UMQ	CB-CA-O1'-C1'
11	A	305	OPC	CAL-CAM-CBI-OBJ
11	B	203	OPC	CBS-CBT-CBU-CBV
14	B	202	CLA	C11-C10-C8-C9
14	B	202	CLA	C16-C17-C18-C19
12	A	306	UMQ	CI-CJ-CK-CL
16	D	201	SQD	O10-C23-O48-C46
17	G	101	BCR	C16-C17-C18-C36
14	B	202	CLA	CAD-CBD-CGD-O2D
11	B	203	OPC	CBO-CBP-CBQ-CBR
17	G	101	BCR	C14-C15-C16-C17
11	A	305	OPC	CBO-CBP-CBQ-CBR
11	B	203	OPC	CAS-CAT-CAU-CAV
16	D	201	SQD	C27-C28-C29-C30
11	A	305	OPC	CAH-OAI-PAJ-OAK
11	A	305	OPC	CBY-CBZ-CCA-CCB
11	A	305	OPC	CAH-OAI-PAJ-OBH
11	A	305	OPC	CAH-OAI-PAJ-OAB
14	B	202	CLA	C11-C10-C8-C7
12	A	309	UMQ	CG-CH-CI-CJ

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Mol	Chain	Res	Type	Atoms
16	D	201	SQD	C44-C45-O47-C7
11	B	203	OPC	CBU-CBV-CBW-CBX
12	A	309	UMQ	CH-CI-CJ-CK
12	A	307	UMQ	O5'-C5'-C6'-O6'
12	A	307	UMQ	CA-CB-CC-CD
16	D	201	SQD	C12-C13-C14-C15
11	B	203	OPC	CBN-CBO-CBP-CBQ
17	G	101	BCR	C9-C10-C11-C12
17	G	101	BCR	C11-C10-C9-C34
11	A	305	OPC	CAZ-CBA-CBB-CBC
11	A	305	OPC	CAT-CAU-CAV-CAW
17	G	101	BCR	C11-C10-C9-C8
16	D	201	SQD	O6-C44-C45-O47
12	C	301	UMQ	O1'-CA-CB-CC
13	A	308	QNO	C26-C27-C28-C29
11	B	203	OPC	CBP-CBQ-CBR-CBS
12	A	309	UMQ	CD-CF-CG-CH
11	B	203	OPC	CAV-CAW-CAX-CAY
11	B	203	OPC	CBC-CBD-CBE-CBF
14	B	202	CLA	C2-C3-C5-C6
11	A	305	OPC	CBM-CBN-CBO-CBP
14	B	202	CLA	C8-C10-C11-C12
12	A	306	UMQ	CA-CB-CC-CD
11	B	203	OPC	CBT-CBU-CBV-CBW
14	B	202	CLA	C6-C7-C8-C9
16	D	201	SQD	C7-C8-C9-C10
11	B	203	OPC	CAQ-CAR-CAS-CAT
14	B	202	CLA	C4-C3-C5-C6
16	D	201	SQD	O49-C7-C8-C9
11	B	203	OPC	CAH-CAG-NAF-CAE
11	B	203	OPC	CAT-CAU-CAV-CAW
11	A	305	OPC	OAN-CAO-CAP-CAQ
11	B	203	OPC	CAH-CAG-NAF-CBG

There are no ring outliers.

15 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	303	HEM	1	0
12	A	307	UMQ	1	0
12	A	309	UMQ	2	0
11	A	305	OPC	9	0

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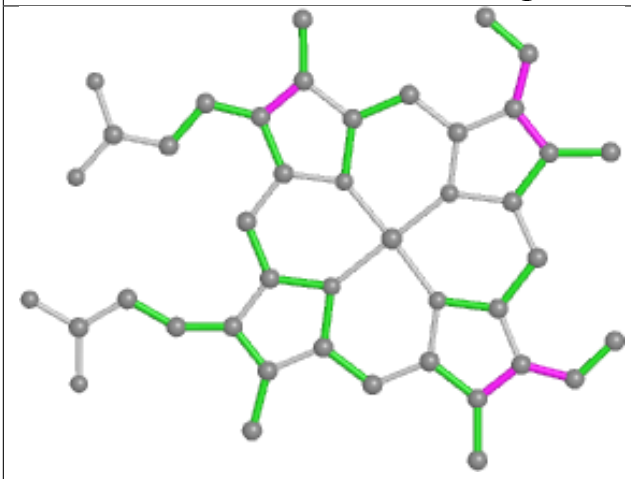
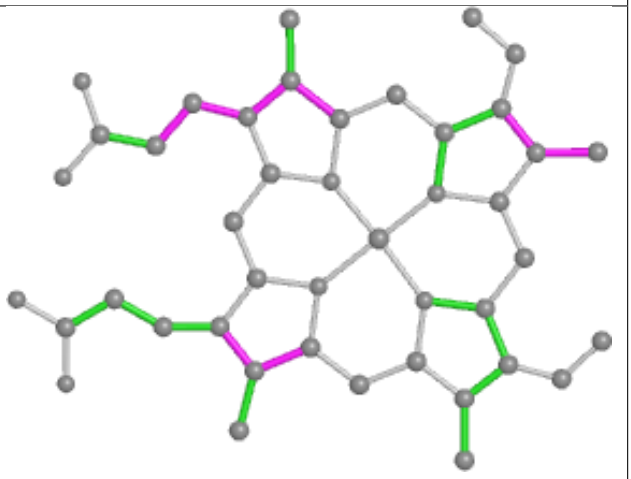
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	302	HEM	11	0
17	G	101	BCR	9	0
12	C	301	UMQ	4	0
16	D	201	SQD	18	0
13	A	308	QNO	2	0
12	A	306	UMQ	5	0
10	A	304	HEM	10	0
11	B	203	OPC	4	0
14	B	202	CLA	5	0
15	D	200	FES	1	0
10	A	302	HEM	2	0

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

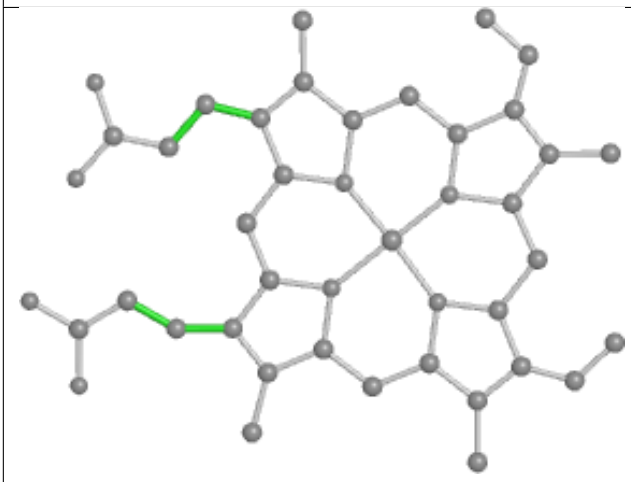
Ligand HEM A 303



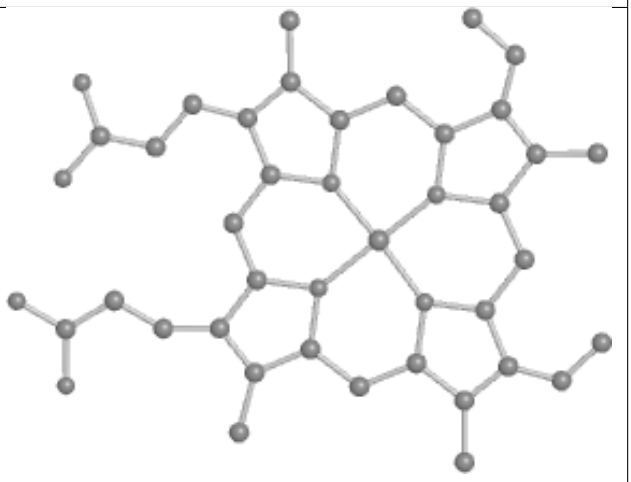
Bond lengths



Bond angles

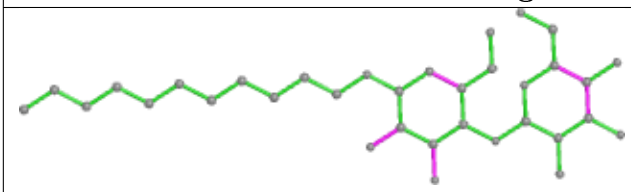


Torsions

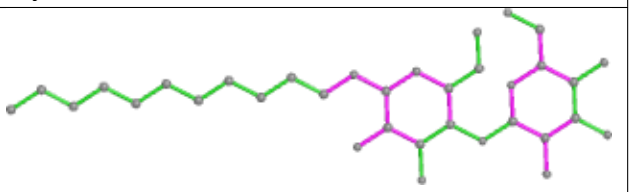


Rings

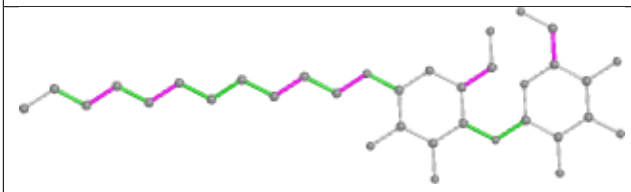
Ligand UMQ A 307



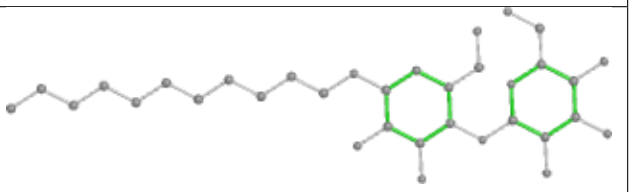
Bond lengths



Bond angles

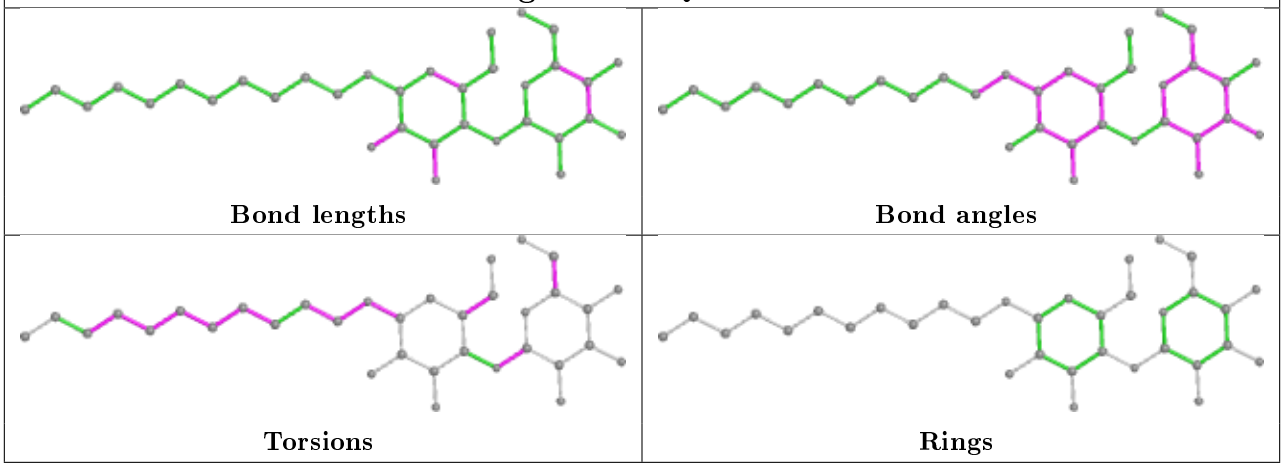


Torsions

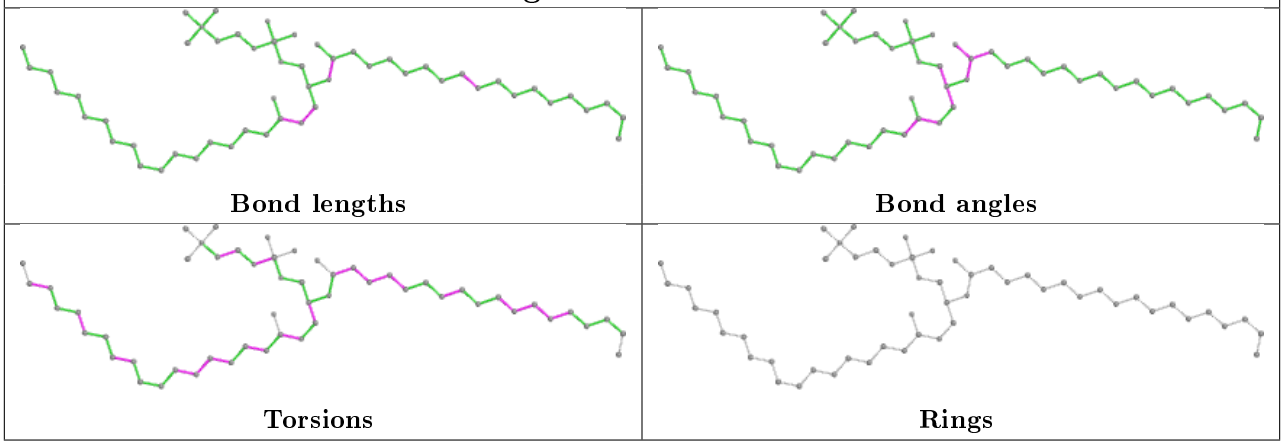


Rings

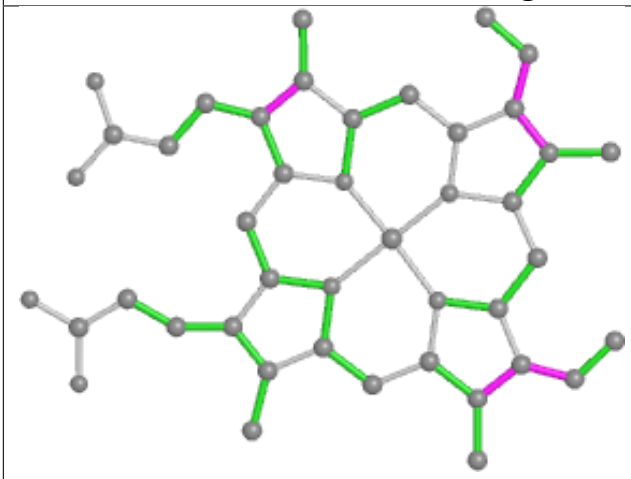
Ligand UMQ A 309



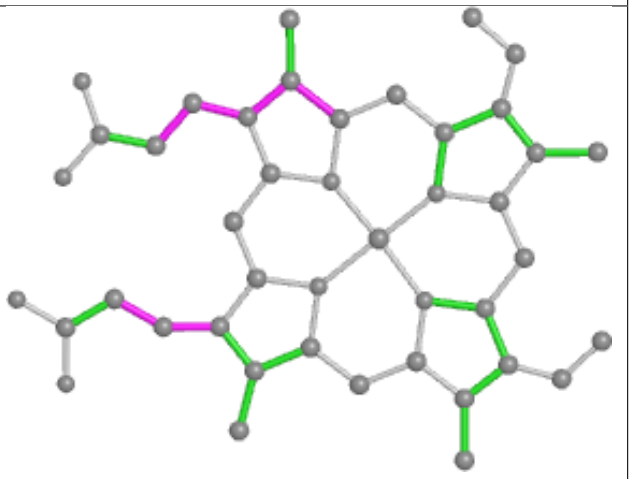
Ligand OPC A 305



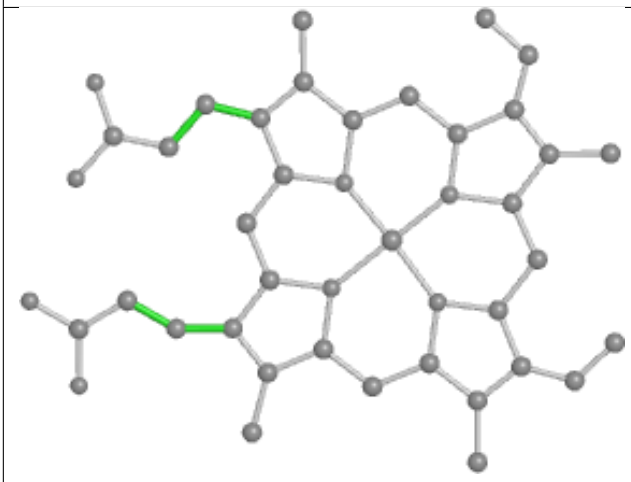
Ligand HEM C 302



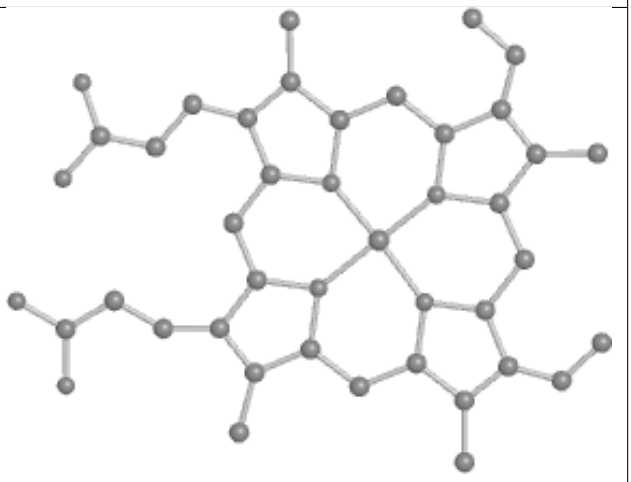
Bond lengths



Bond angles

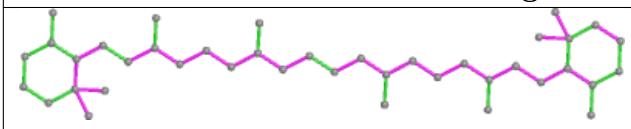


Torsions

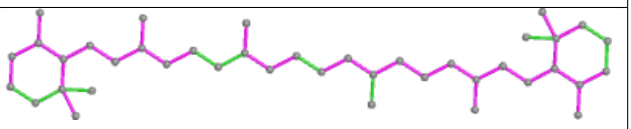


Rings

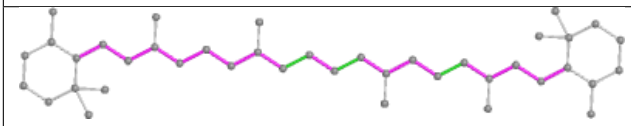
Ligand BCR G 101



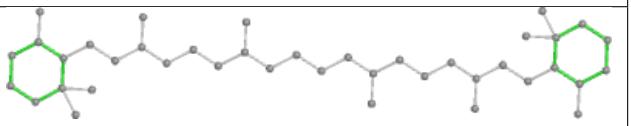
Bond lengths



Bond angles

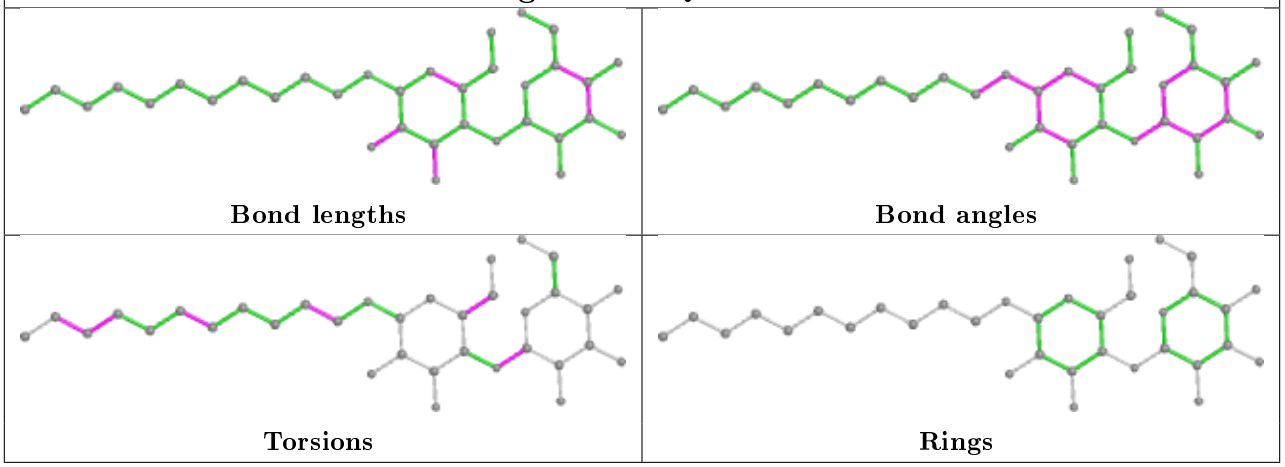


Torsions

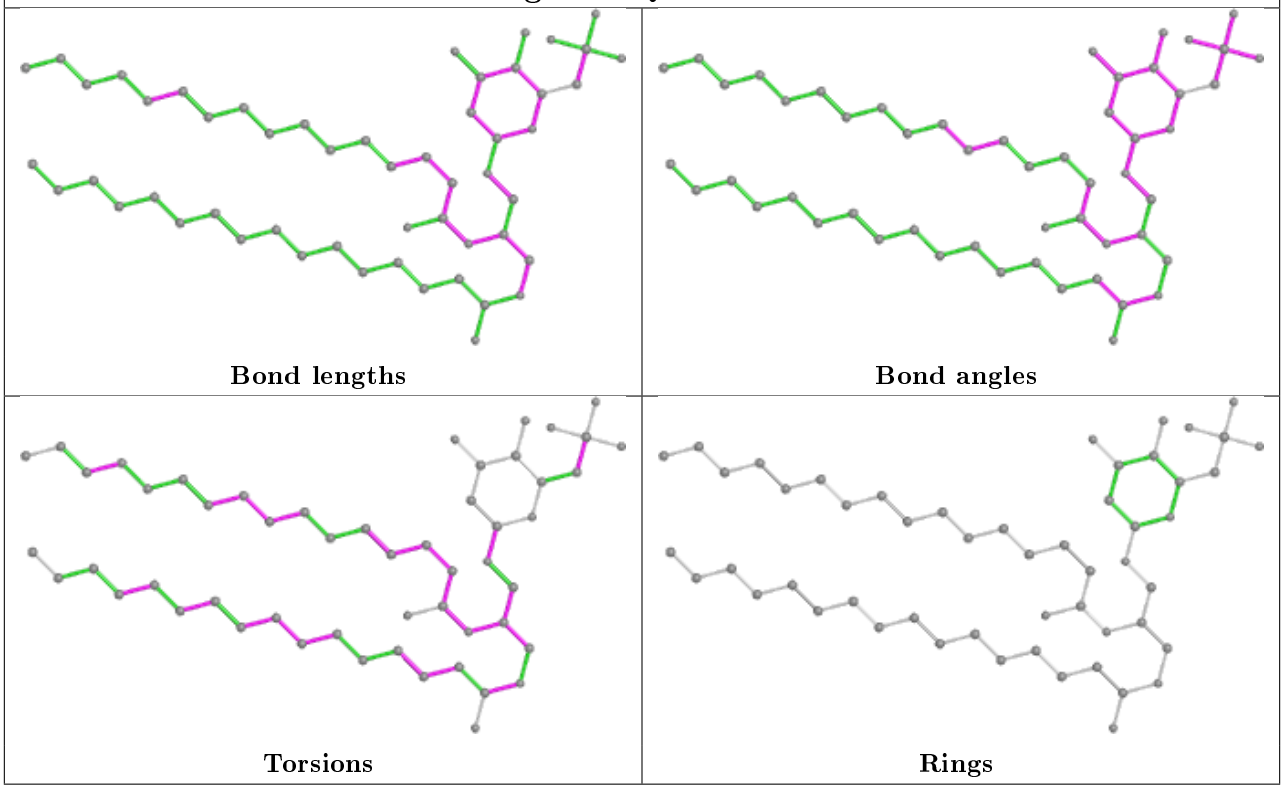


Rings

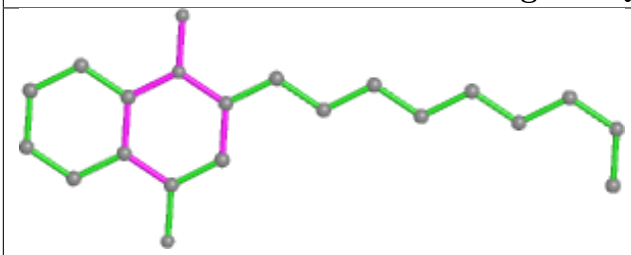
Ligand UMQ C 301



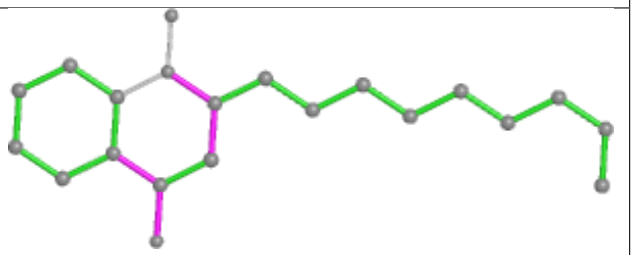
Ligand SQD D 201



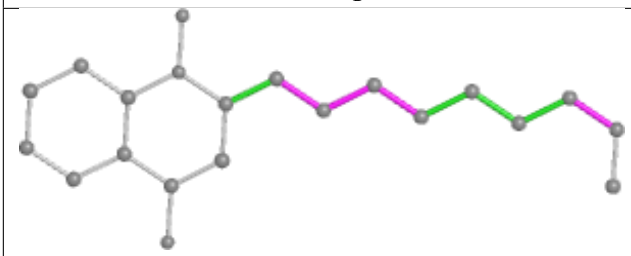
Ligand QNO A 308



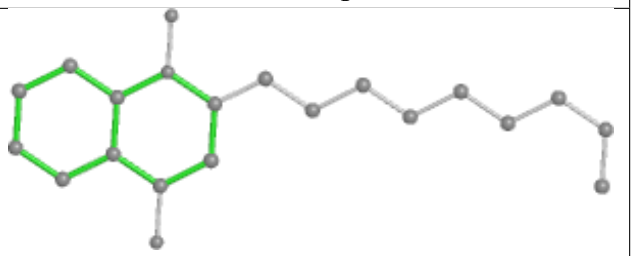
Bond lengths



Bond angles

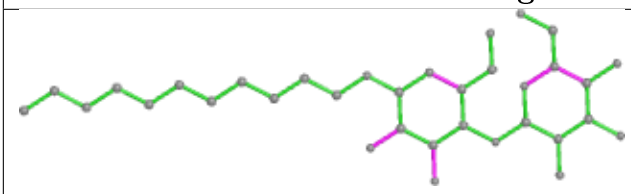


Torsions

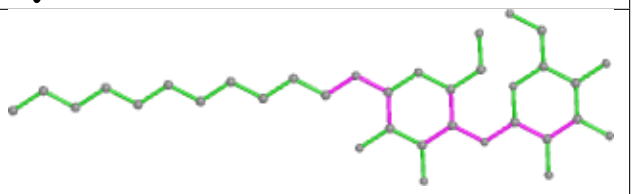


Rings

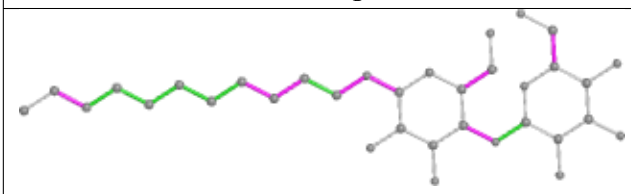
Ligand UMQ A 306



Bond lengths



Bond angles



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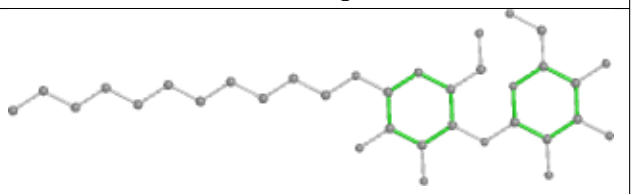
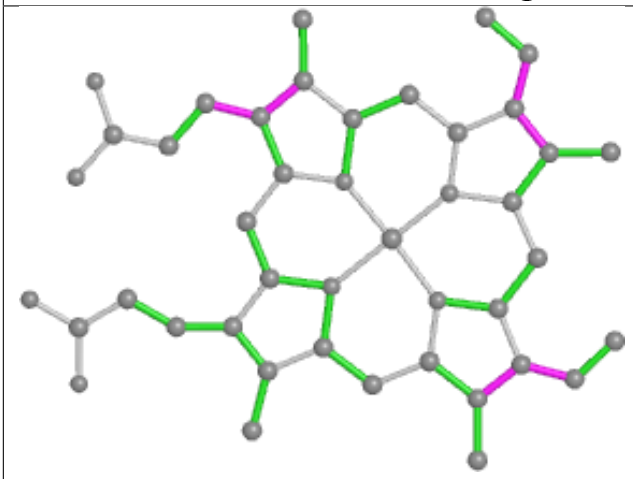
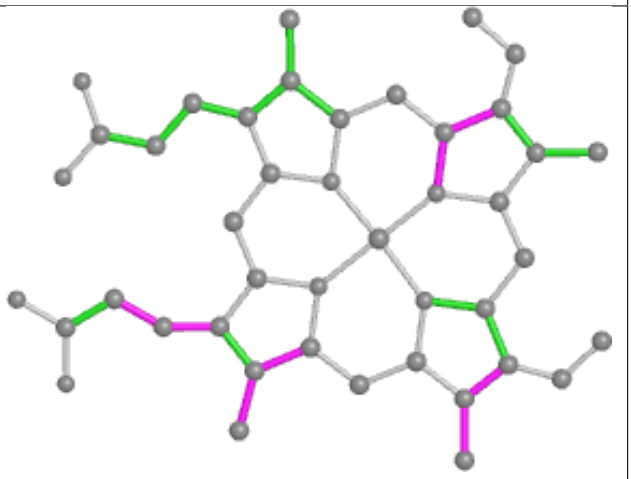


Rings

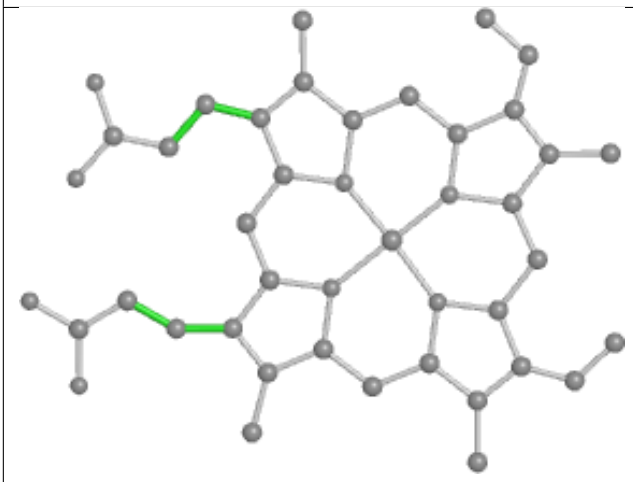
Ligand HEM A 304



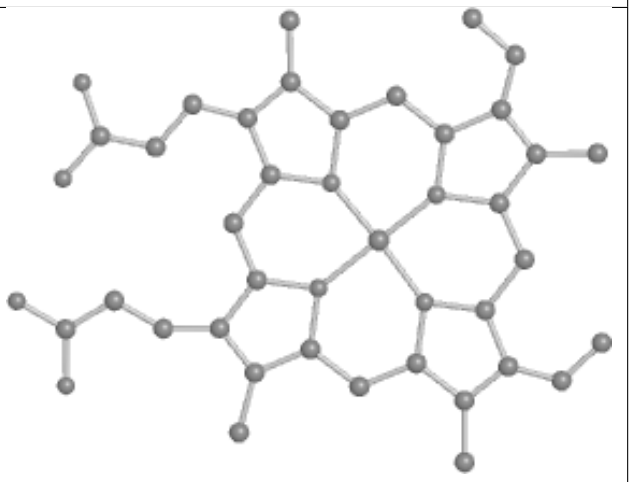
Bond lengths



Bond angles

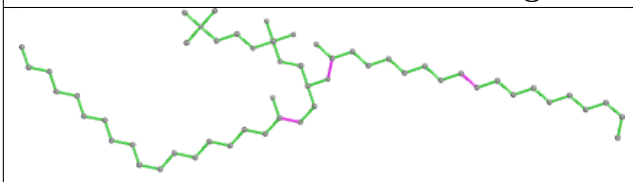


Torsions

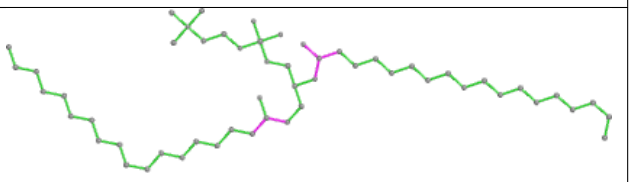


Rings

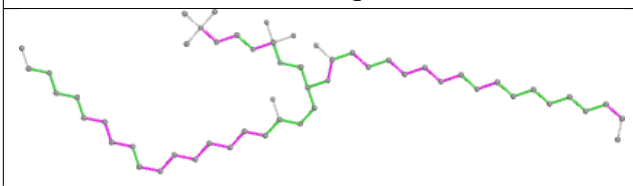
Ligand OPC B 203



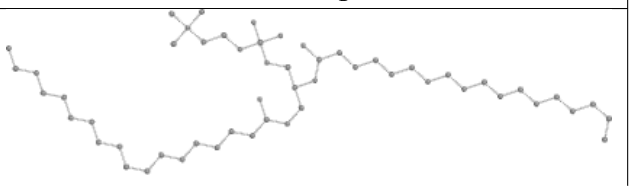
Bond lengths



Bond angles

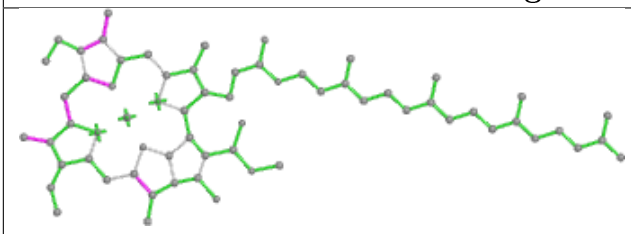


Torsions

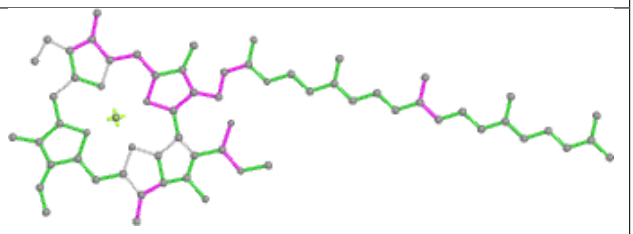


Rings

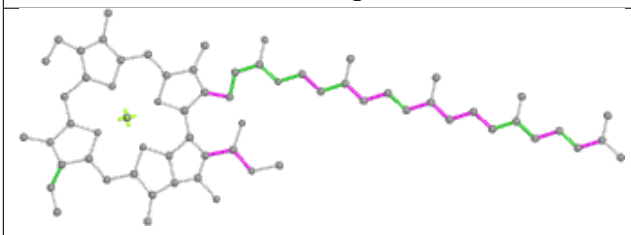
Ligand CLA B 202



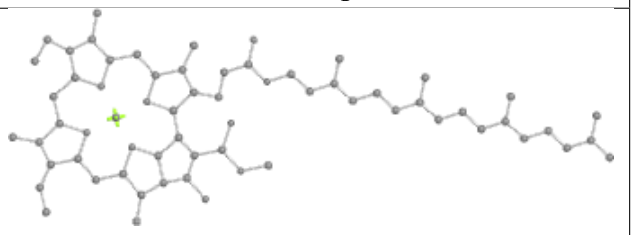
Bond lengths



Bond angles

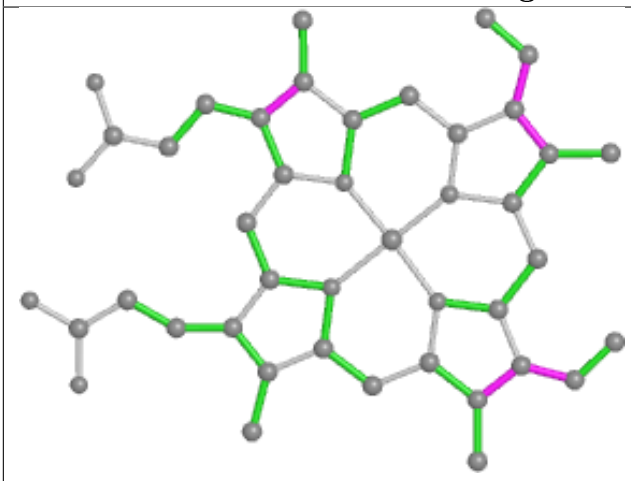


Torsions

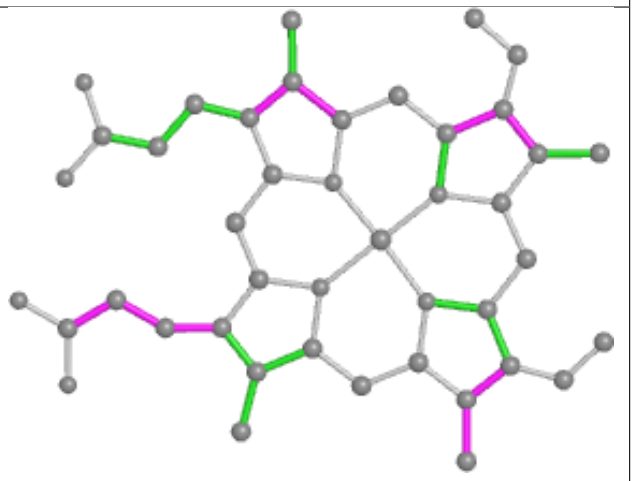


Rings

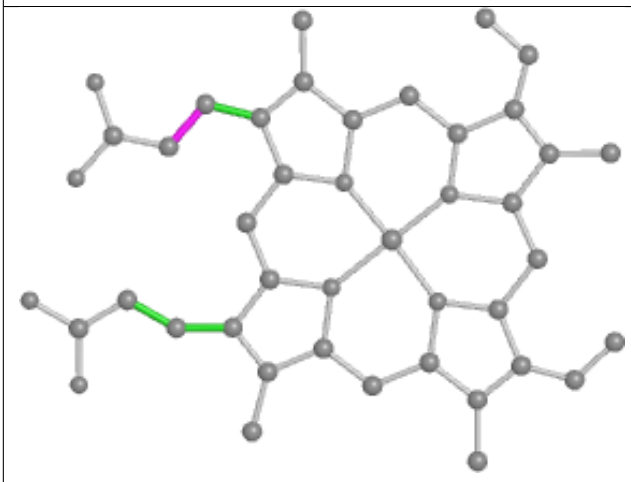
Ligand HEM A 302



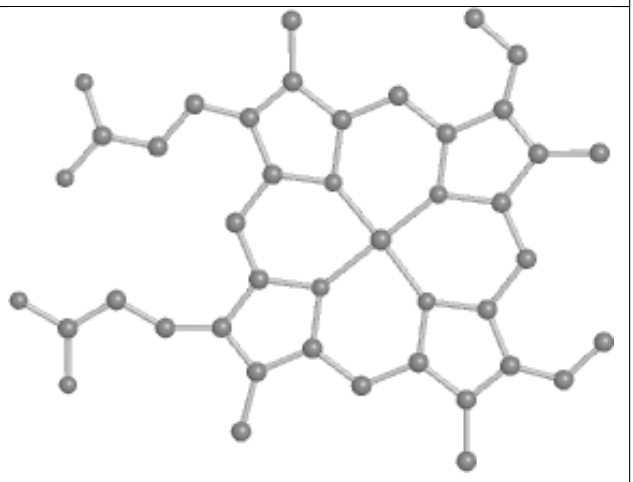
Bond lengths



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	213/215 (99%)	0.04	0 100 100	43, 62, 92, 143	0
2	B	160/160 (100%)	0.06	0 100 100	53, 79, 125, 155	0
3	C	286/289 (98%)	0.86	50 (17%) 1 1	57, 91, 188, 215	1 (0%)
4	D	161/179 (89%)	1.66	66 (40%) 0 0	56, 141, 182, 199	0
5	E	32/32 (100%)	0.18	3 (9%) 8 9	72, 94, 125, 148	0
6	F	32/35 (91%)	0.28	1 (3%) 49 47	67, 86, 141, 149	0
7	G	37/37 (100%)	0.24	0 100 100	61, 80, 151, 154	0
8	H	29/29 (100%)	0.40	0 100 100	65, 77, 101, 130	0
All	All	950/976 (97%)	0.60	120 (12%) 3 3	43, 84, 174, 215	1 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	220	SER	7.8
3	C	199	ILE	6.8
4	D	70	LEU	6.6
3	C	184	ALA	6.4
4	D	160	ILE	6.4
4	D	144	ALA	6.1
3	C	193	VAL	6.0
4	D	175	LYS	5.9
4	D	56	ALA	5.8
3	C	195	TYR	5.7
3	C	192	ASN	5.6
3	C	194	LYS	5.5
4	D	179	VAL	5.3
3	C	182	LYS	5.1
4	D	161	VAL	5.0
3	C	181	THR	4.9

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Mol	Chain	Res	Type	RSRZ
4	D	162	LEU	4.7
4	D	73	HIS	4.7
4	D	145	PRO	4.7
3	C	198	SER	4.6
4	D	158	ASP	4.5
4	D	170	PHE	4.5
4	D	159	ASN	4.4
3	C	206	THR	4.4
3	C	183	ILE	4.4
4	D	98	ALA	4.4
3	C	190	TYR	4.3
3	C	191	GLY	4.3
4	D	151	CYS	4.3
4	D	156	GLN	4.2
3	C	176	ALA	4.1
4	D	148	LEU	4.1
3	C	211	ILE	4.0
3	C	179	THR	4.0
4	D	177	TRP	3.9
3	C	197	VAL	3.9
4	D	54	THR	3.9
5	E	32	ILE	3.9
3	C	212	PRO	3.9
3	C	207	VAL	3.8
4	D	67	SER	3.8
4	D	157	ASP	3.8
3	C	188	ASP	3.7
3	C	213	ALA	3.7
3	C	196	GLN	3.6
4	D	169	ASP	3.6
4	D	62	ASN	3.6
4	D	99	ILE	3.6
4	D	149	ALA	3.6
4	D	176	PRO	3.6
4	D	55	THR	3.6
4	D	64	VAL	3.6
3	C	189	GLU	3.5
4	D	143	PRO	3.5
4	D	72	SER	3.4
4	D	53	GLY	3.4
4	D	165	TRP	3.3
4	D	92	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
4	D	147	SER	3.3
4	D	77	ASP	3.2
3	C	219	VAL	3.2
4	D	146	LEU	3.2
3	C	172	PHE	3.2
4	D	171	ARG	3.2
4	D	154	THR	3.2
4	D	101	ASP	3.2
3	C	186	GLU	3.1
4	D	163	THR	3.0
4	D	166	THR	3.0
3	C	224	ALA	3.0
4	D	71	GLU	3.0
3	C	214	GLY	3.0
4	D	91	ILE	3.0
3	C	178	GLY	2.9
4	D	172	THR	2.9
3	C	88	GLU	2.9
4	D	174	GLU	2.9
3	C	222	GLY	2.9
4	D	69	PHE	2.8
4	D	142	GLY	2.8
4	D	102	TYR	2.7
4	D	66	VAL	2.7
3	C	174	ALA	2.6
3	C	177	THR	2.6
4	D	168	THR	2.6
3	C	86	PRO	2.6
3	C	231	LEU	2.6
5	E	30	LYS	2.6
6	F	1	MET	2.6
3	C	180	ILE	2.6
3	C	185	LYS	2.5
3	C	85	ALA	2.5
4	D	84	LEU	2.5
4	D	178	TRP	2.5
3	C	90	ILE	2.5
3	C	173	THR	2.4
3	C	228	GLY	2.4
3	C	221	GLU	2.4
4	D	150	LEU	2.4
3	C	208	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	187	GLU	2.3
4	D	109	THR	2.3
4	D	79	VAL	2.3
4	D	173	GLY	2.3
4	D	52	GLY	2.3
4	D	164	PRO	2.3
4	D	10	VAL	2.3
3	C	215	PRO	2.2
5	E	31	LEU	2.2
4	D	16	ARG	2.2
4	D	113	CYS	2.2
3	C	230	ALA	2.1
3	C	201	THR	2.1
3	C	209	ASP	2.1
3	C	100	ASP	2.1
4	D	83	GLY	2.1
4	D	155	VAL	2.1
4	D	103	GLY	2.1
4	D	131	SER	2.0
4	D	105	ASN	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 carbohydrates 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
12	UMQ	A	306	34/34	0.71	0.46	61,148,192,198	0
16	SQD	D	201	53/54	0.74	0.55	83,150,191,196	1
12	UMQ	C	301	34/34	0.76	0.52	51,119,203,224	0

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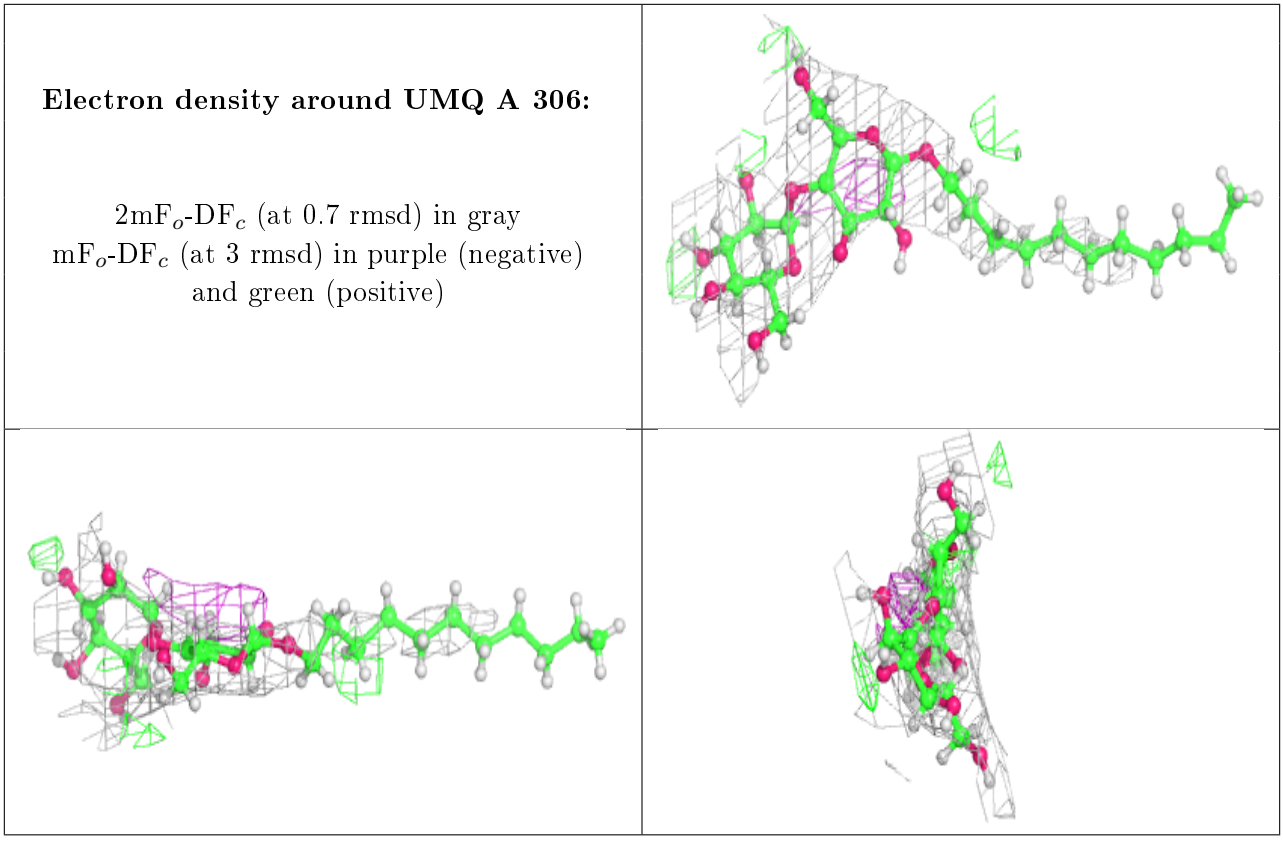
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	UMQ	A	309	34/34	0.79	0.33	87,162,229,238	0
17	BCR	G	101	40/40	0.82	0.48	51,97,180,199	0
11	OPC	A	305	54/55	0.82	0.46	62,118,206,229	0
12	UMQ	A	307	34/34	0.86	0.34	81,138,182,186	0
13	QNO	A	308	21/21	0.87	0.34	83,113,154,167	0
11	OPC	B	203	54/55	0.90	0.52	66,126,180,198	0
14	CLA	B	202	65/65	0.95	0.30	59,90,133,153	0
10	HEM	C	302	43/43	0.96	0.29	52,81,118,122	0
15	FES	D	200	4/4	0.96	0.08	108,129,130,138	0
10	HEM	A	304	43/43	0.97	0.29	54,80,107,112	0
9	CD	B	201	1/1	0.97	0.25	186,186,186,186	0
10	HEM	A	303	43/43	0.98	0.29	39,58,82,83	0
9	CD	A	301	1/1	0.98	0.23	83,83,83,83	0
10	HEM	A	302	43/43	0.99	0.29	35,58,79,112	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.

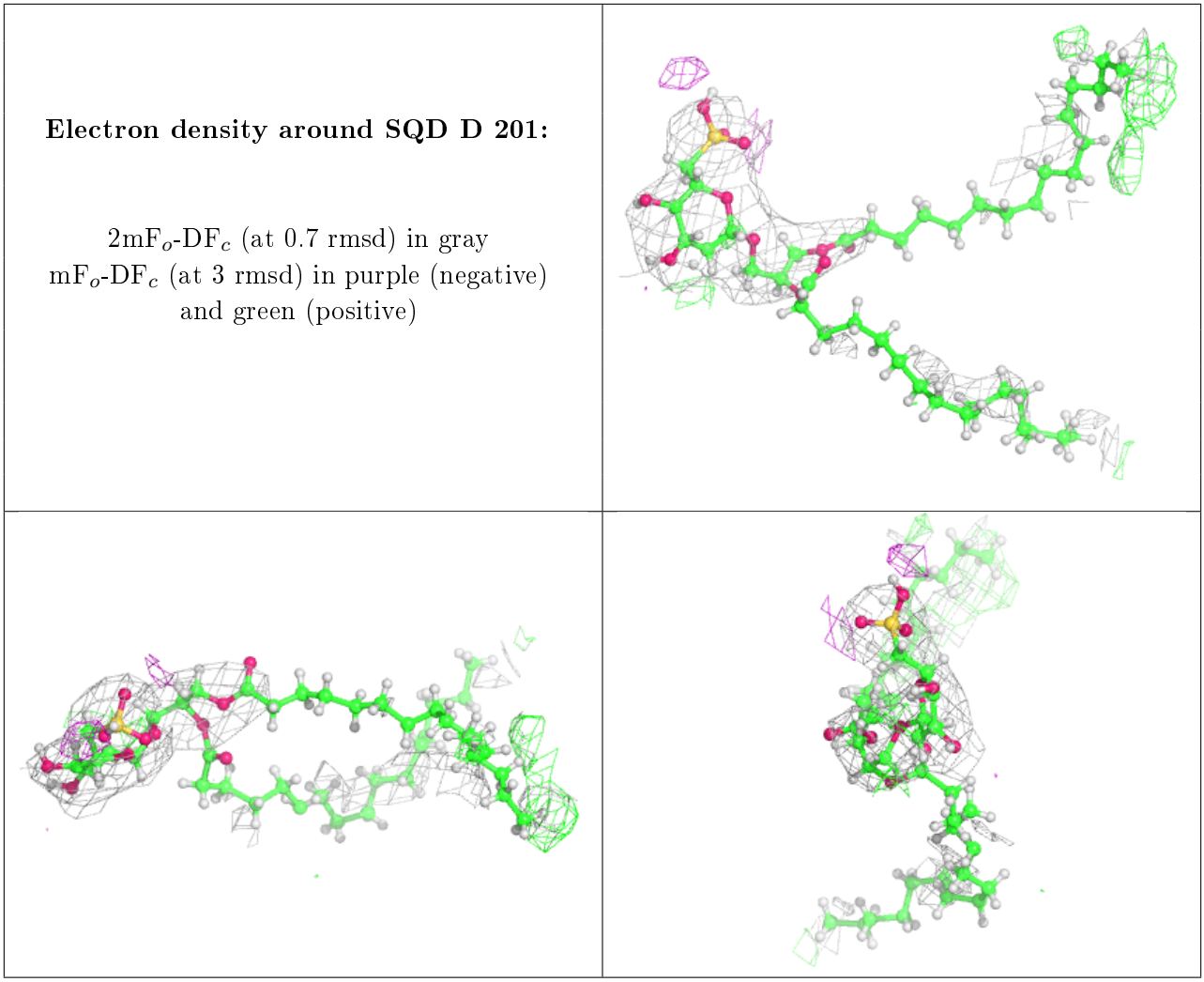
Electron density around UMQ A 306:

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



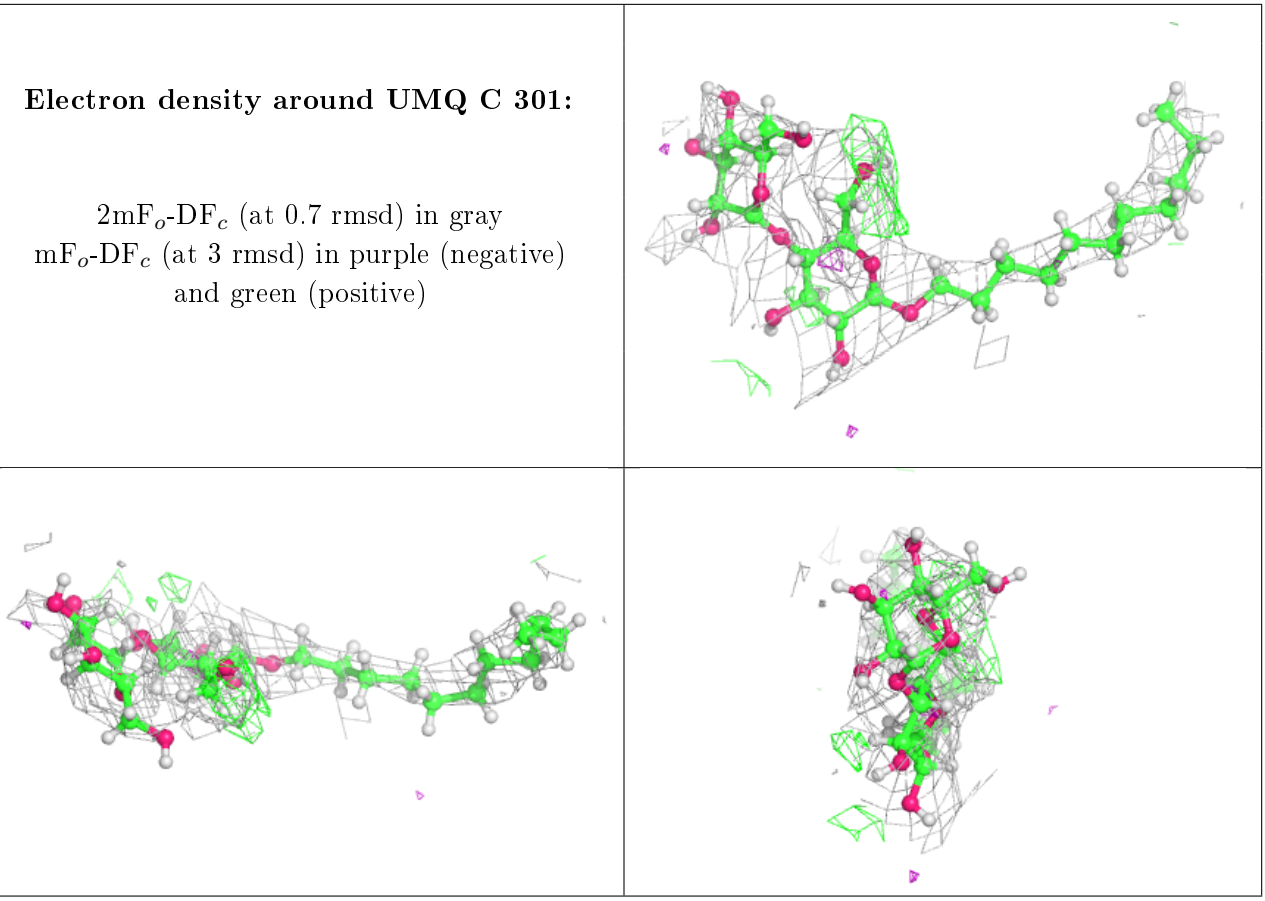
Electron density around SQD D 201:

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



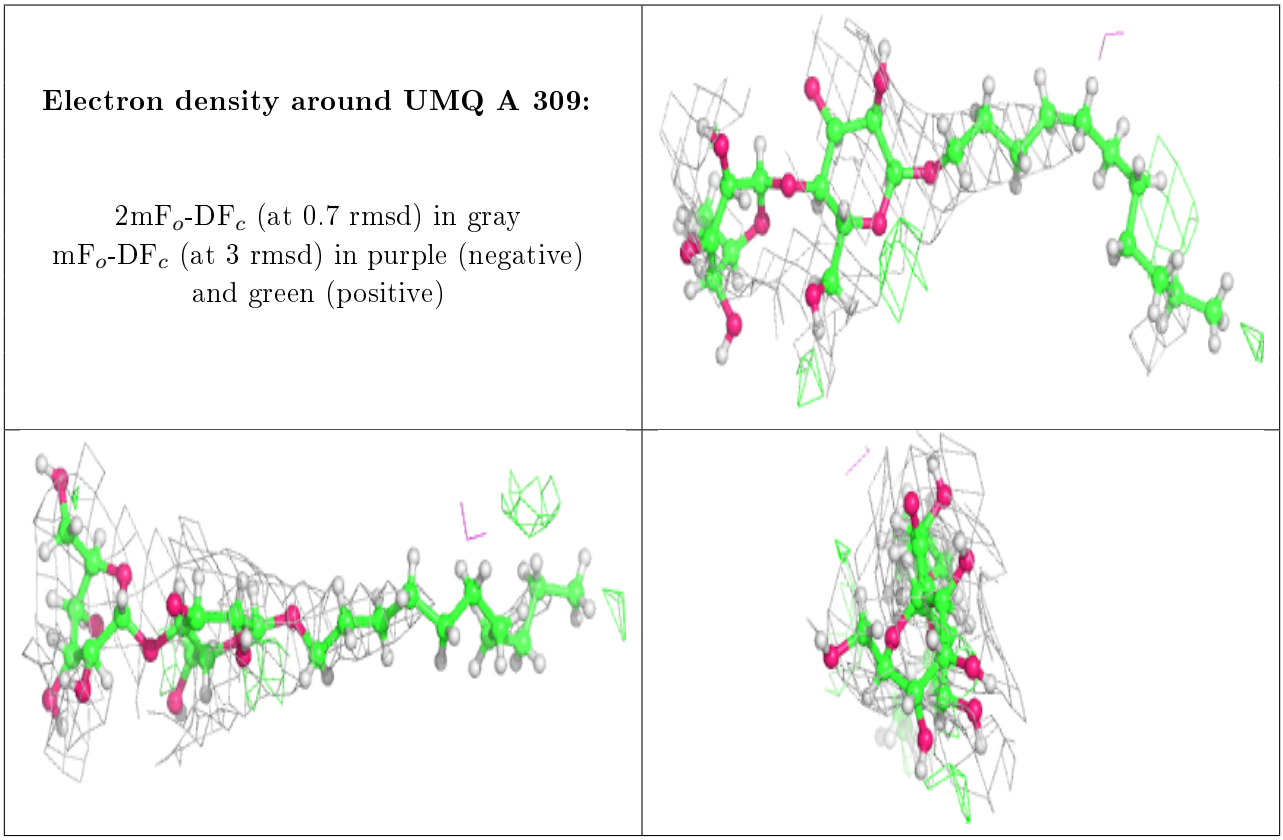
Electron density around UMQ C 301:

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



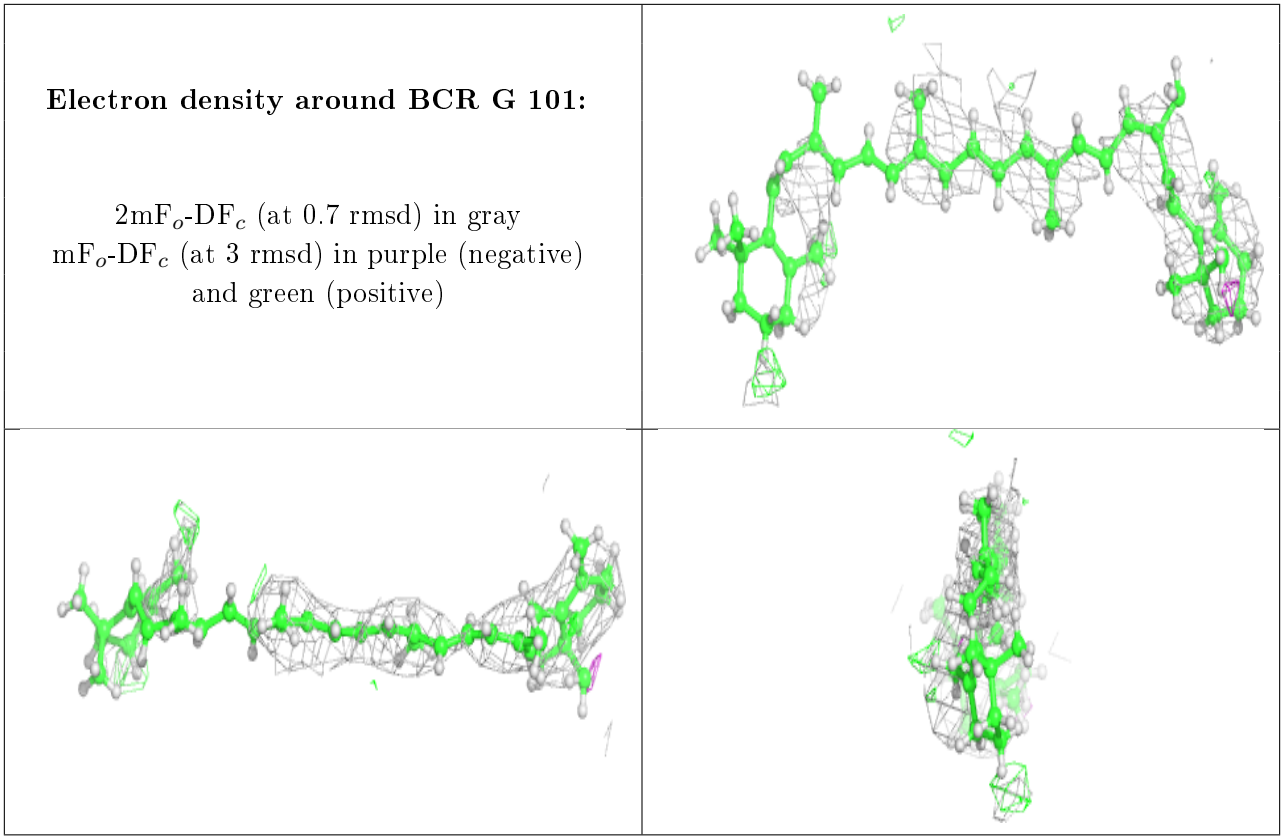
Electron density around UMQ A 309:

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



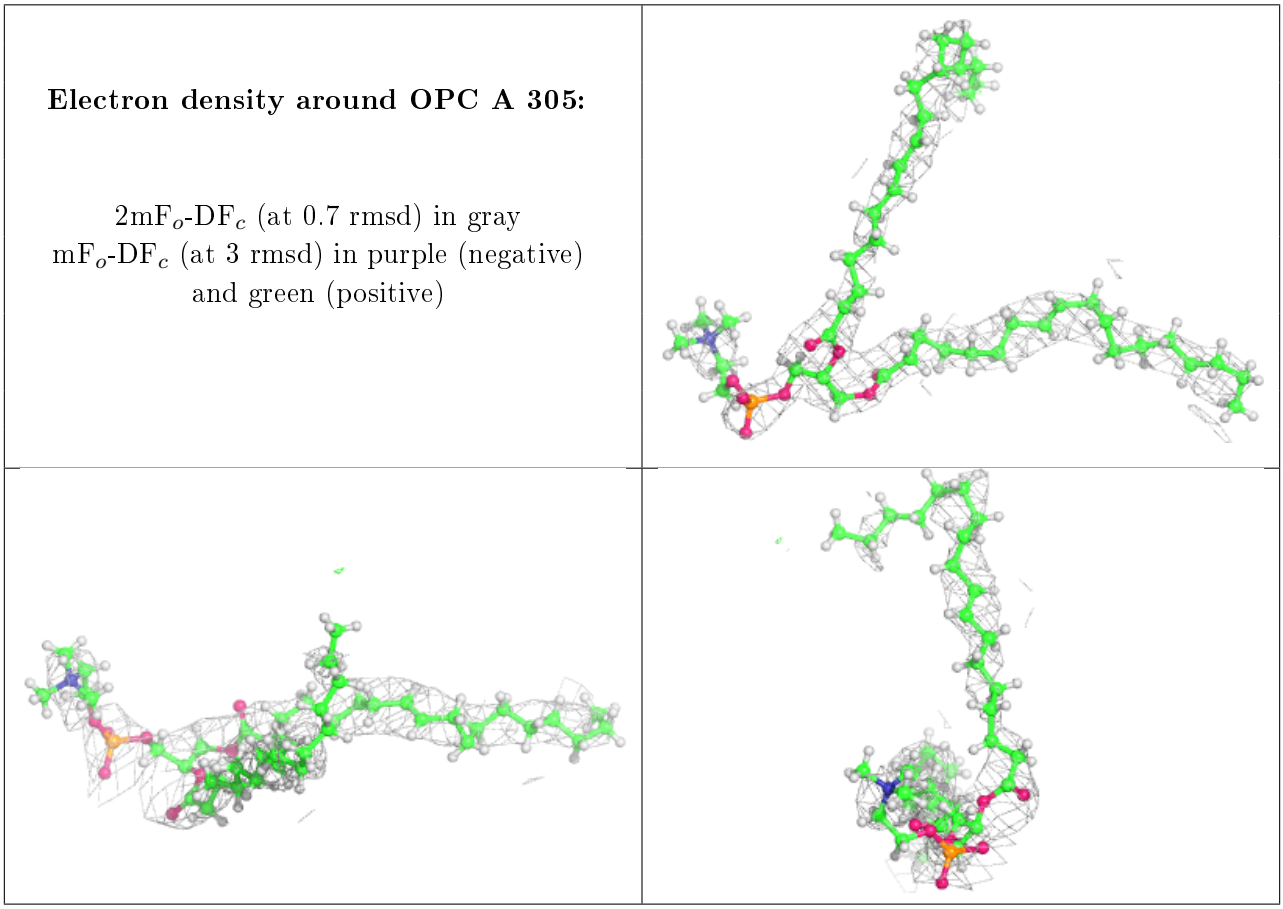
Electron density around BCR G 101:

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



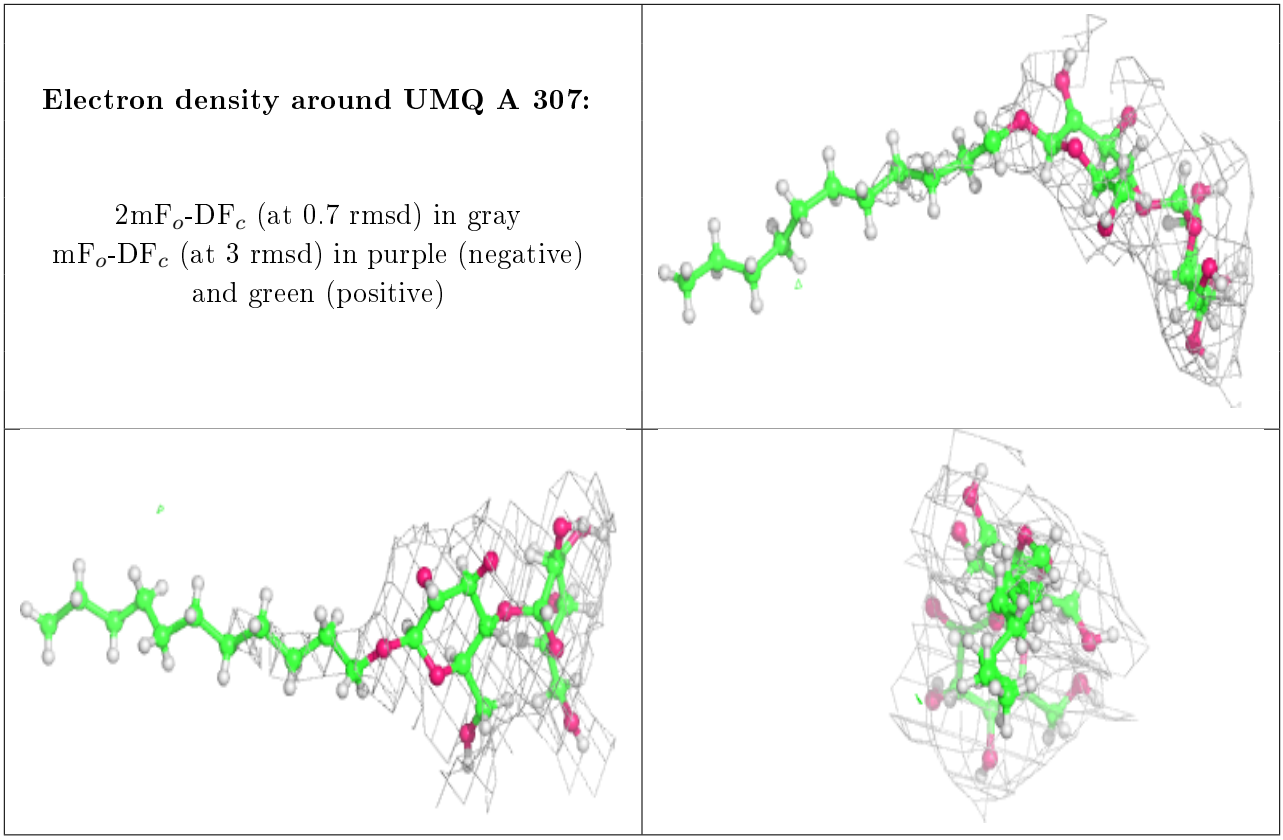
Electron density around OPC A 305:

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



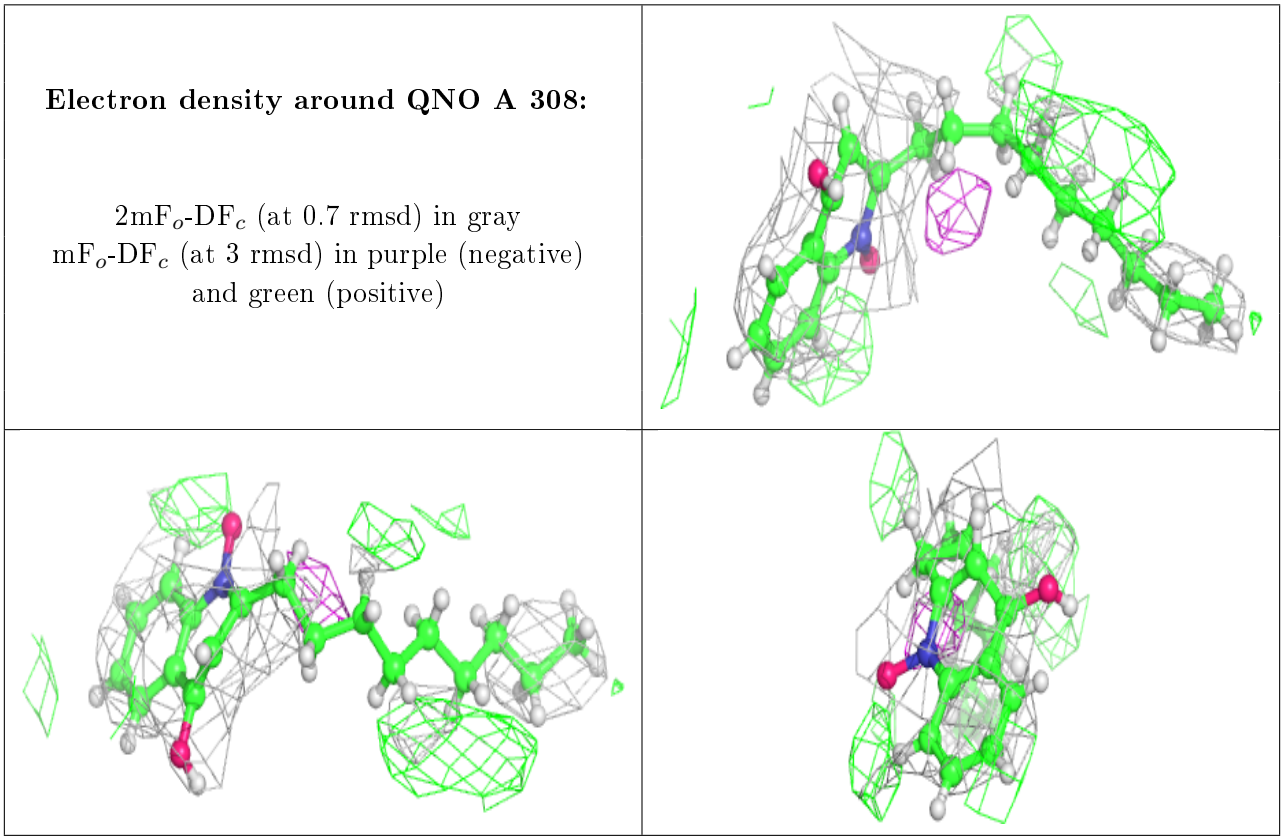
Electron density around UMQ A 307:

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



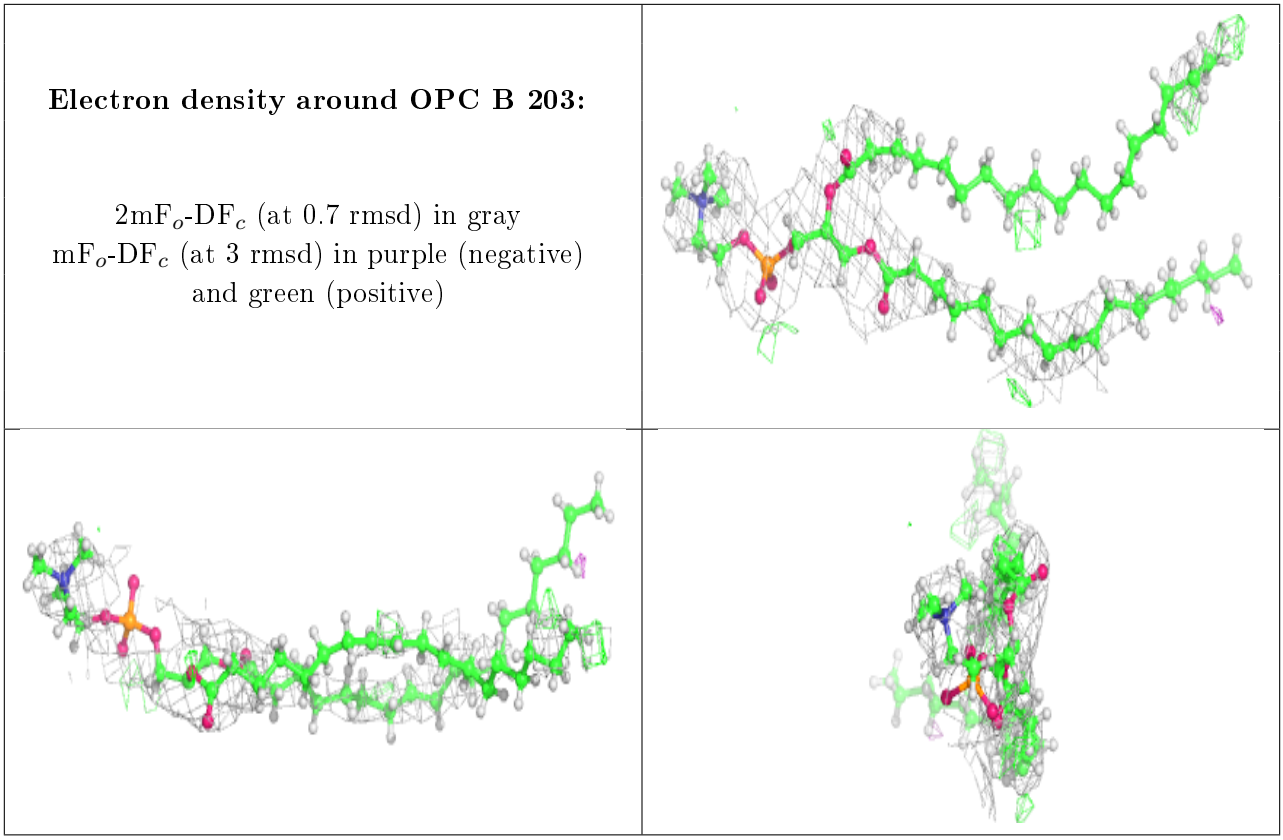
Electron density around QNO A 308:

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



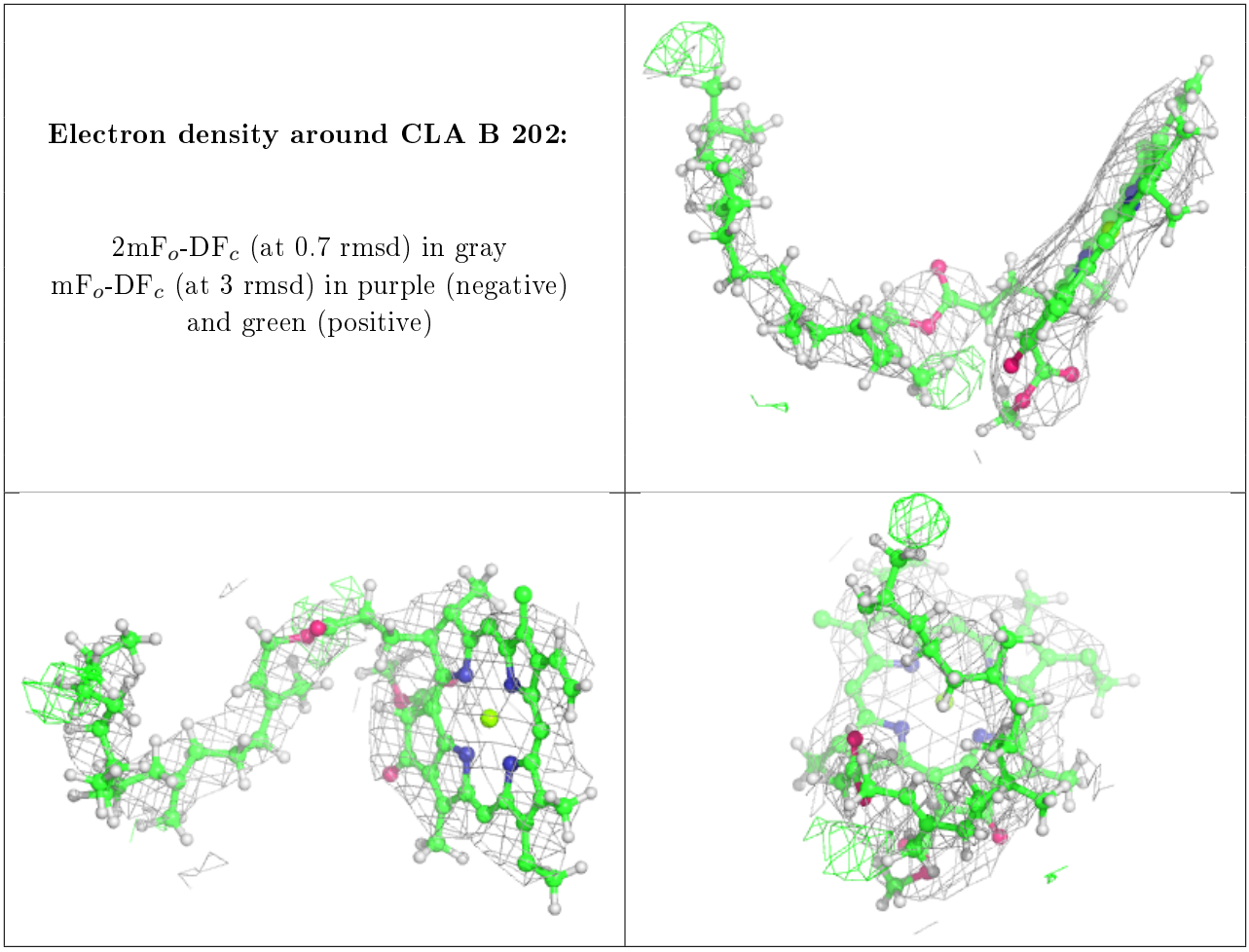
Electron density around OPC B 203:

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



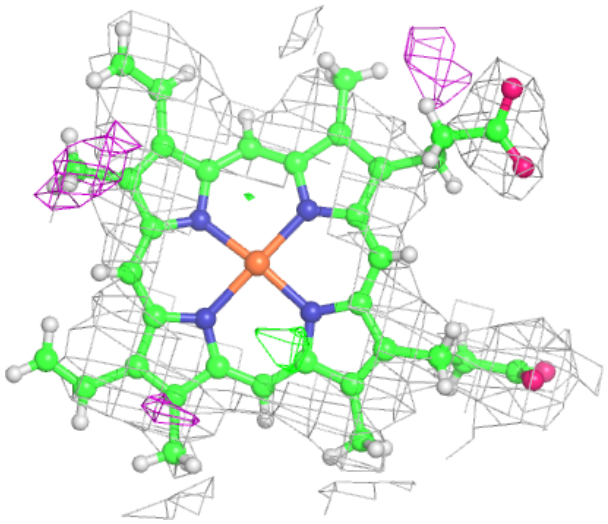
Electron density around CLA B 202:

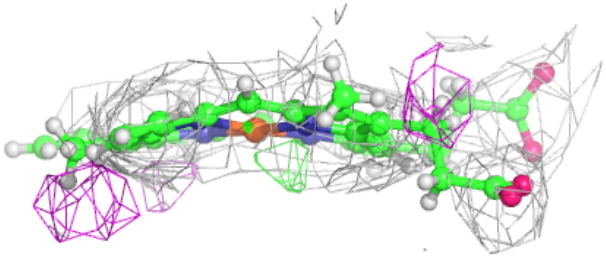
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

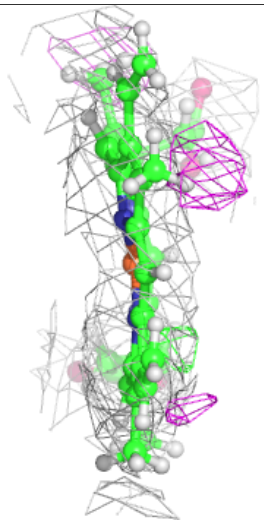


Electron density around HEM C 302:

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

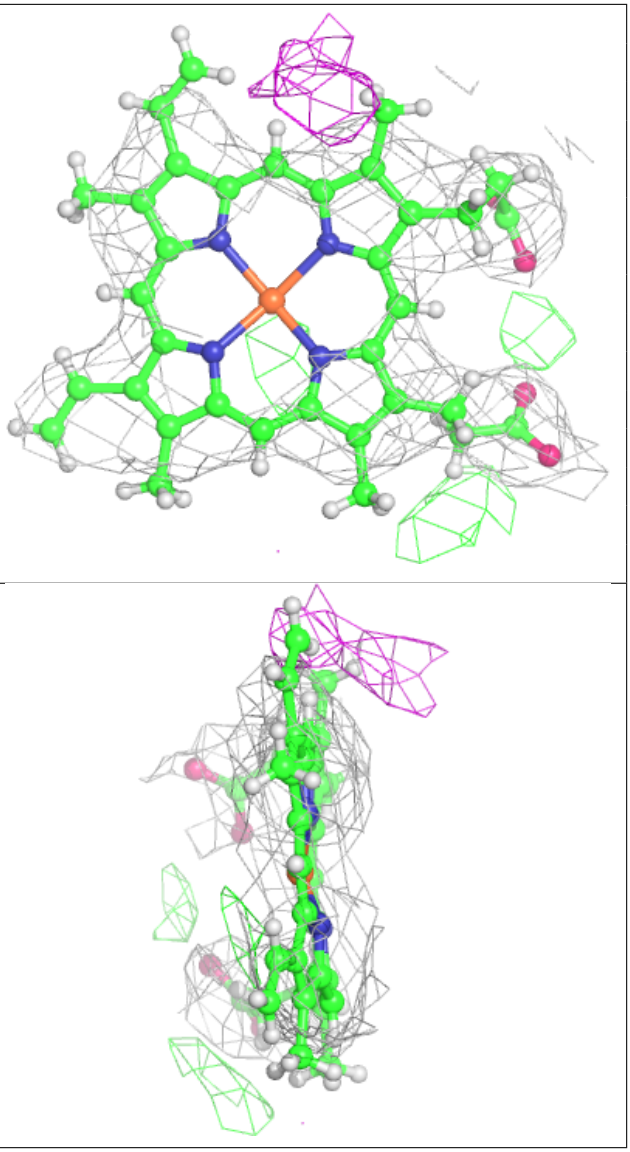






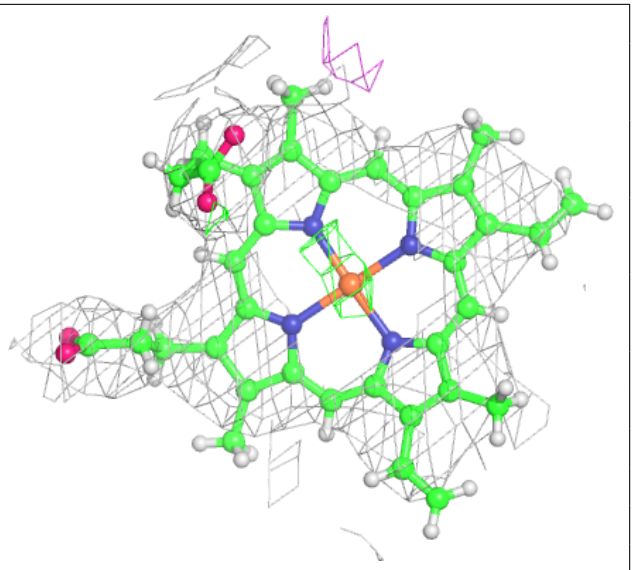
Electron density around HEM A 304:

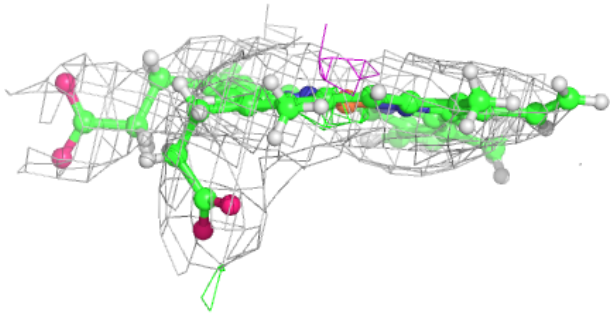
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

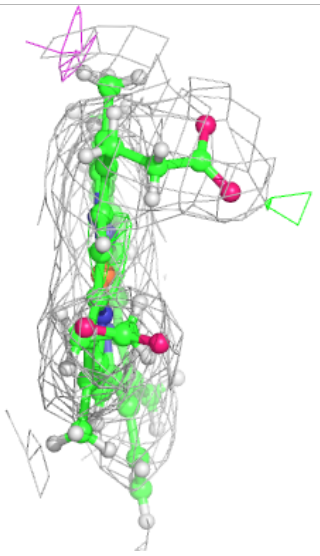


Electron density around HEM A 303:

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

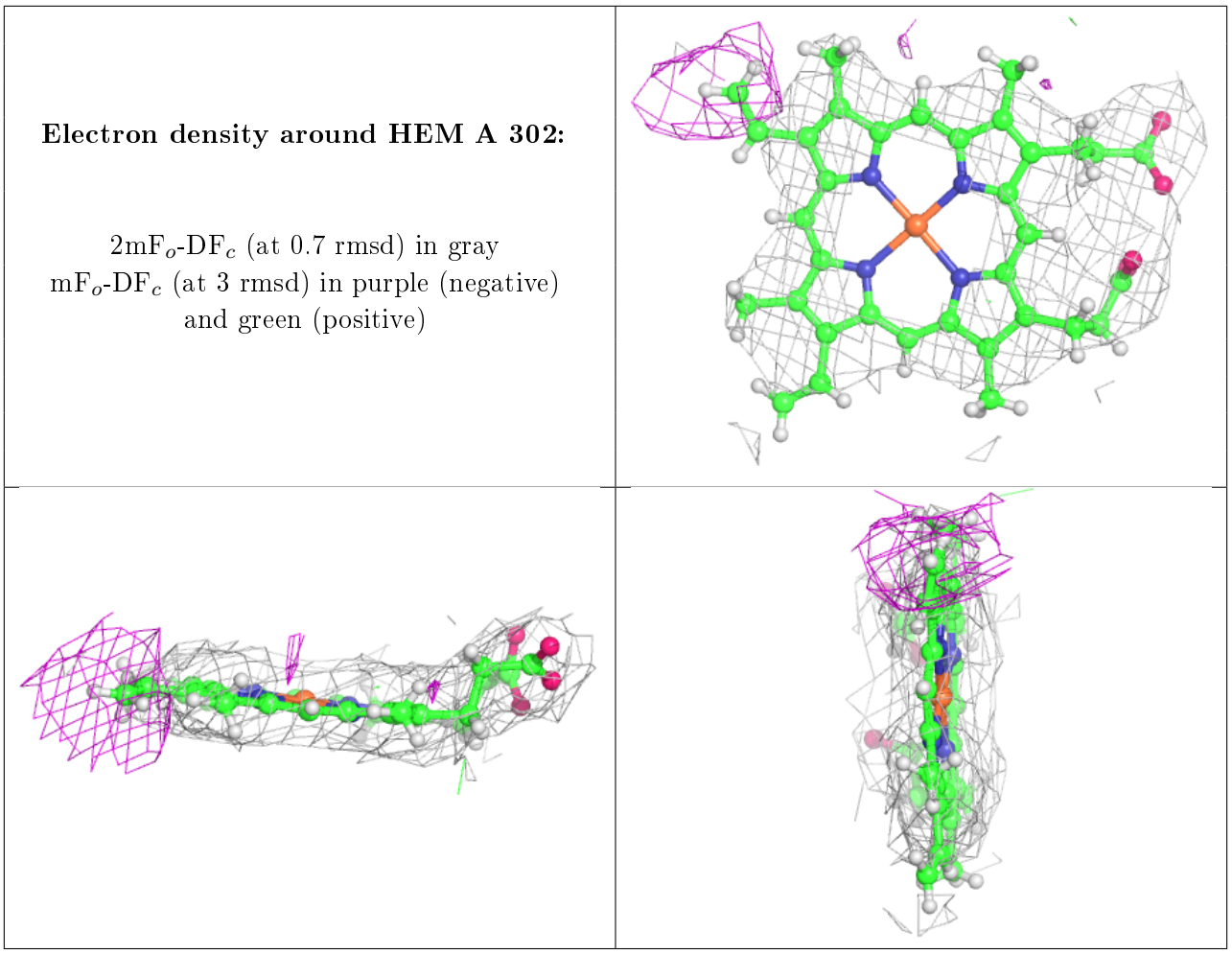






Electron density around HEM A 302:

$2mF_o$-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.