Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 07:27 PM EST

PDB ID	:	4I7Z
Title	:	Crystal structure of cytochrome b6f in DOPG, with disordered Rieske Iron-Sulfur Protein soluble domain
Authors	:	Hasan, S.S.; Stofleth, J.T.; Yamashita, E.; Cramer, W.A.
Deposited on	:	2012-12-01
Resolution	:	2.80 Å(reported)

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

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

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

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

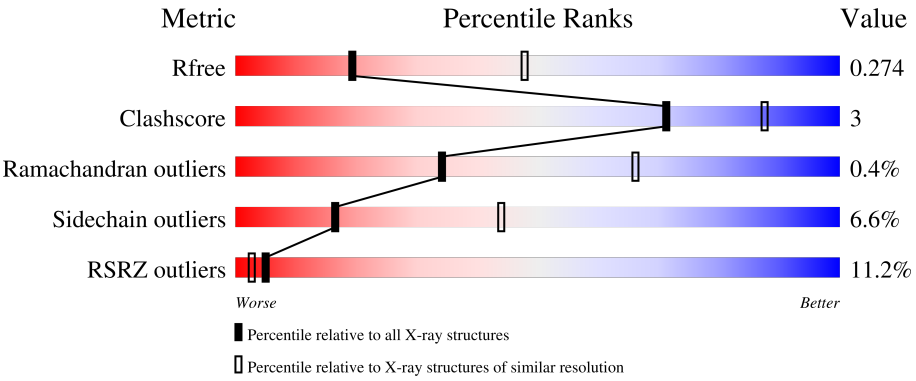
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	215	89% 10%
2	B	160	5% 94% 6%
3	C	289	23% 88% 11%
4	D	179	3% 21% 79%
5	E	32	9% 84% 12%

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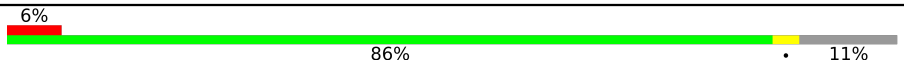
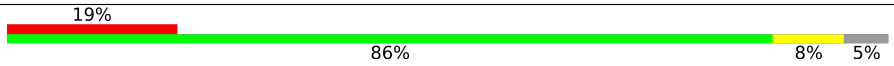
Mol	Chain	Length	Quality of chain
6	F	35	
7	G	37	
8	H	29	

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
11	8K6	A	305	-	-	-	X
12	UMQ	A	306	X	-	-	-
12	UMQ	A	307	X	-	-	-
12	UMQ	A	308	X	-	-	-
14	CLA	B	201	X	-	-	-
15	OZ2	B	203	X	-	-	-
16	1E2	D	201	X	-	-	-
17	OCT	F	101	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 13828 atoms, of which 6869 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
			Total	C	H	N	O	S			
1	A	213	3419	1132	1721	270	286	10	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	159	2538	836	1297	192	208	5	0	0	0

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	288	4450	1415	2234	369	424	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	PRO	GLU	engineered mutation	UNP P83793

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	38	591	194	299	47	49	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	E	28	452	156	237	29	30	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	31	Total	C	H	N	O	S	0	0	0
			482	160	248	34	39	1			

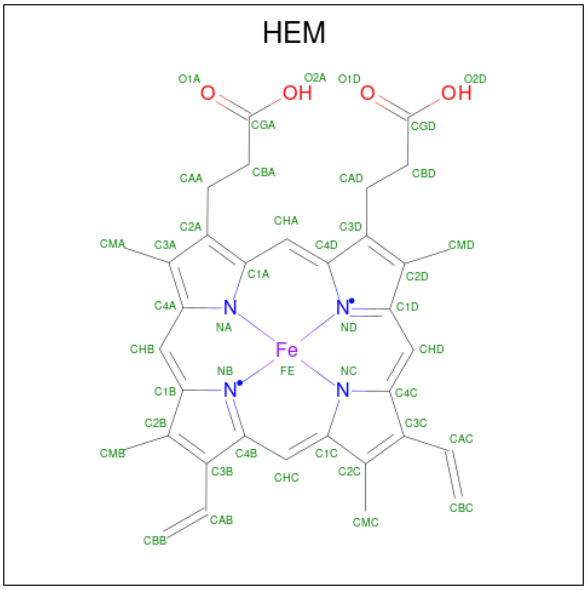
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	35	Total	C	H	N	O	0	0	0
			536	178	268	42	48			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	28	Total	C	H	N	O	S	0	0	0
			449	151	227	35	35	1			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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		

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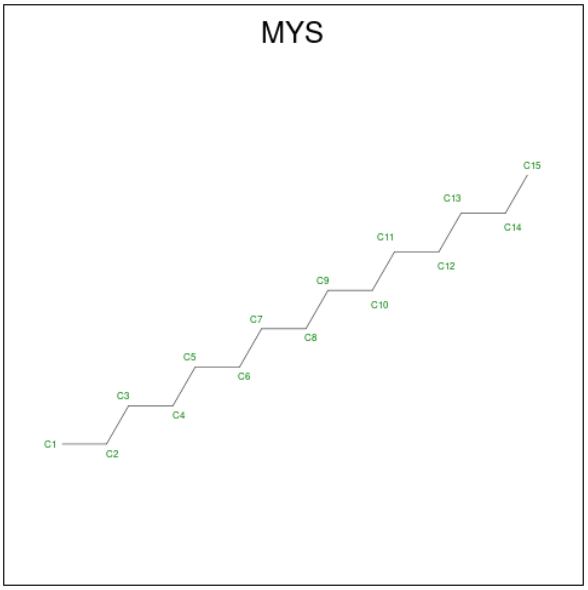
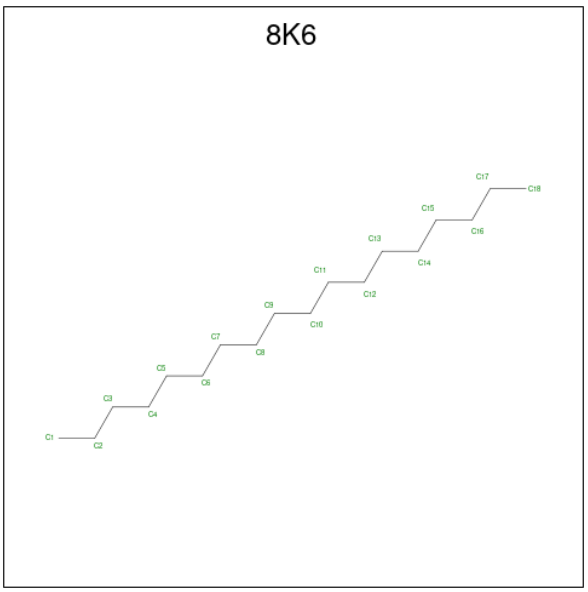
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is PENTADECANE (three-letter code: MYS) (formula: $C_{15}H_{32}$).



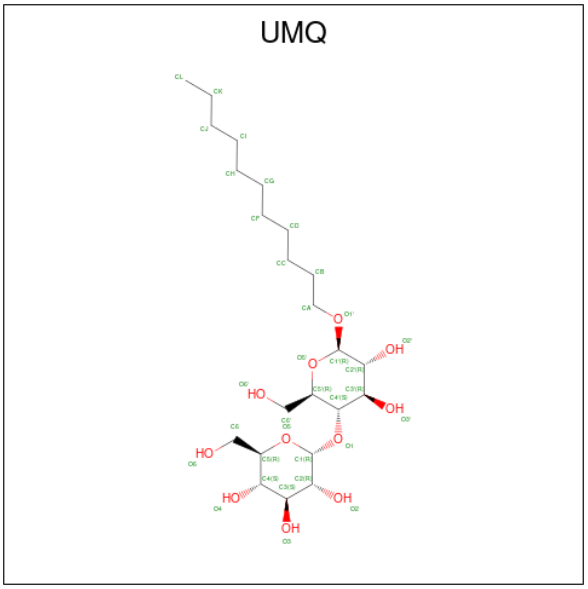
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	H	0	0
			47	15	32		

- Molecule 11 is Octadecane (three-letter code: 8K6) (formula: $C_{18}H_{38}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C H 56 18 38	0	0

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

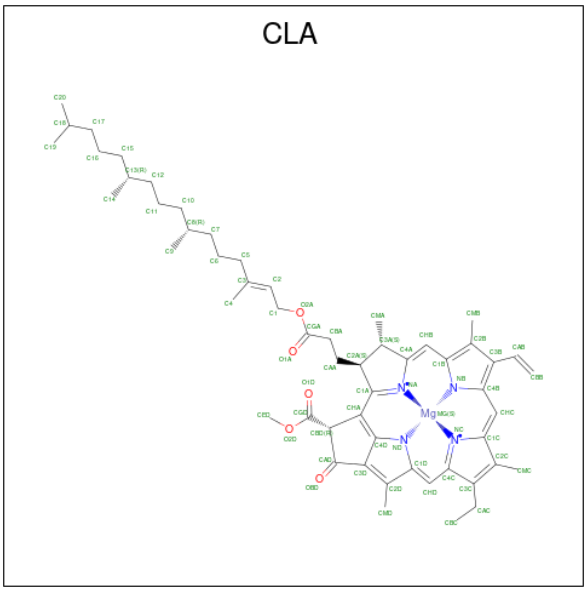


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C H O 77 23 43 11	0	0
12	A	1	Total C H O 77 23 43 11	0	0
12	A	1	Total C H O 78 23 44 11	0	0

- Molecule 13 is CADMIUM ION (three-letter code: CD) (formula: Cd).

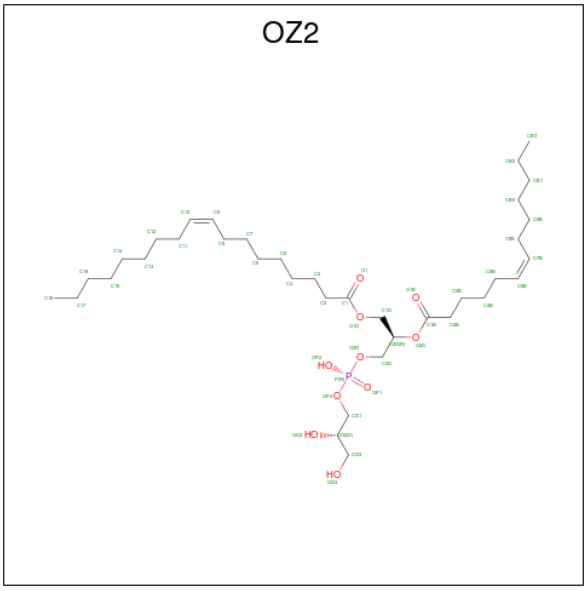
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total Cd 1 1	0	0
13	B	1	Total Cd 1 1	0	0
13	C	1	Total Cd 1 1	0	0

- 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	H	Mg	N	O	0	0
			129	55	64	1	4	5		

- Molecule 15 is (2R)-3-{[(R)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-2-[(6Z)-tridec-6-enoyloxy]propyl (9Z)-octadec-9-enoate (three-letter code: OZ2) (formula: $C_{37}H_{69}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	O	P	0	0
			32	21	10	1		
15	C	1	Total	C	O	P	0	0
			38	27	10	1		

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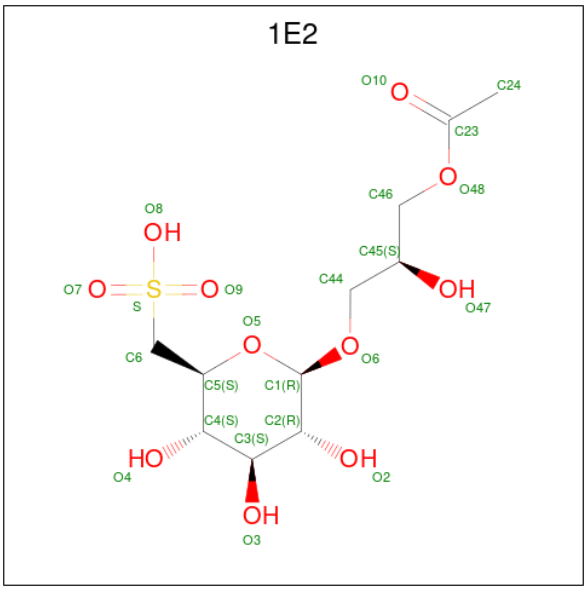
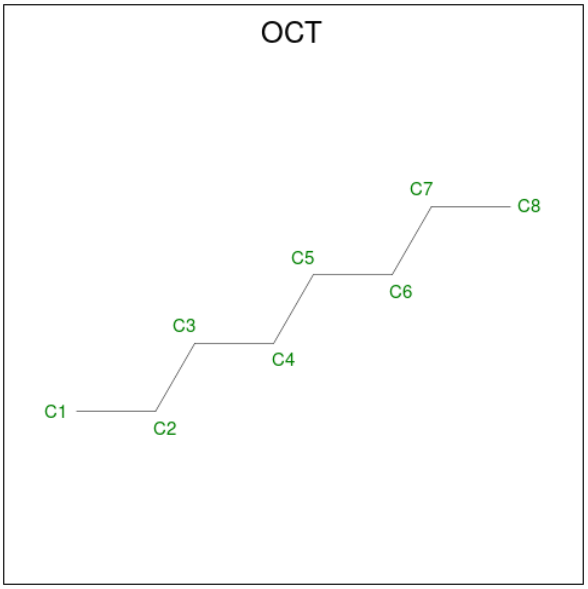
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	G	1	Total	C	O	P	0	0
			44	33	10	1		

- Molecule 16 is (2S)-3-(acetyloxy)-2-hydroxypropyl 6-deoxy-6-sulfo-beta-D-glucopyranoside (three-letter code: 1E2) (formula: $C_{11}H_{20}O_{11}S$).



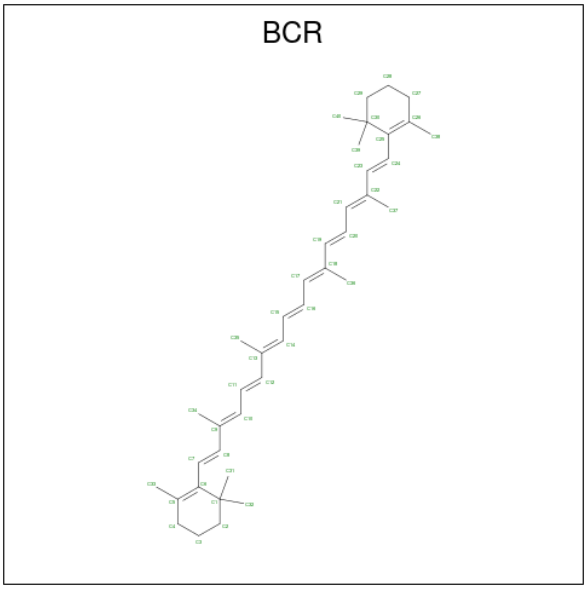
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	O	S	0	0
			23	11	11	1		

- Molecule 17 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	F	1	Total C H 26 8 18	0	0

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 19 is water.

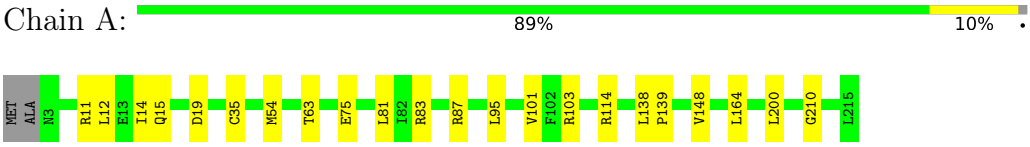
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	8	Total O 8 8	0	0
19	B	4	Total O 4 4	0	0
19	C	1	Total O 1 1	0	0

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.

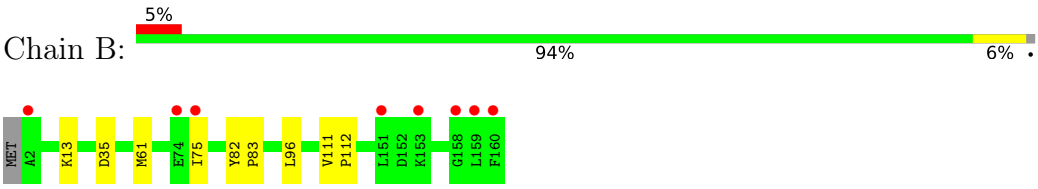
• Molecule 1: Cytochrome b6

Chain A:



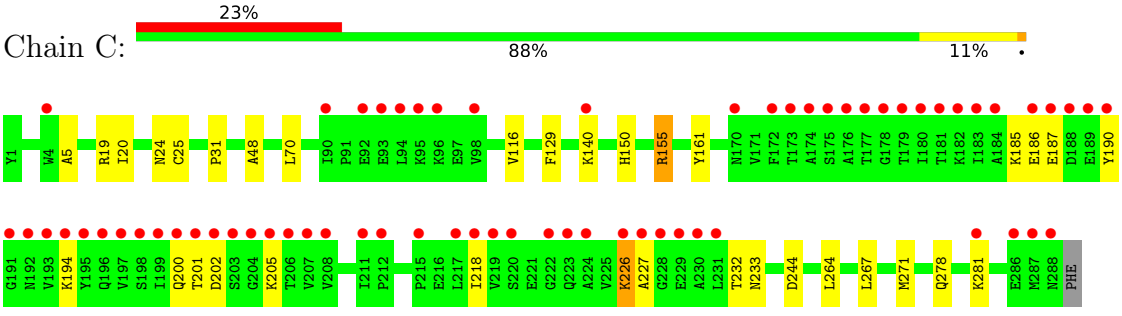
• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:



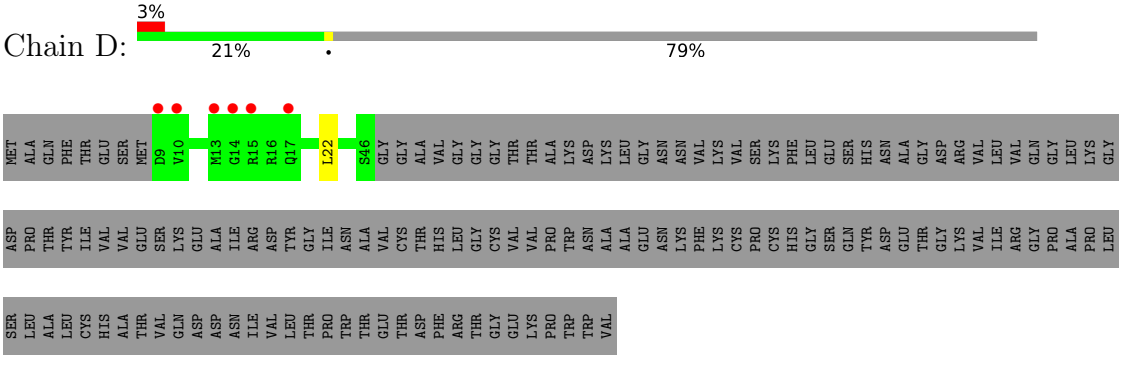
• Molecule 3: Apocytochrome f

Chain C:



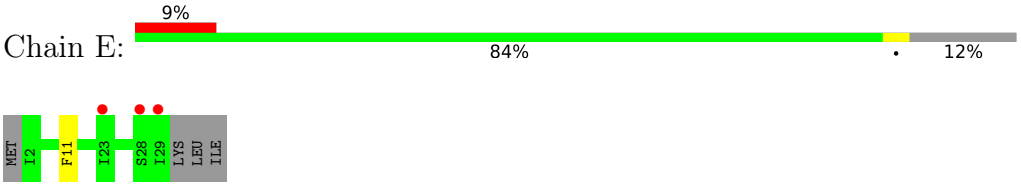
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit

Chain D:



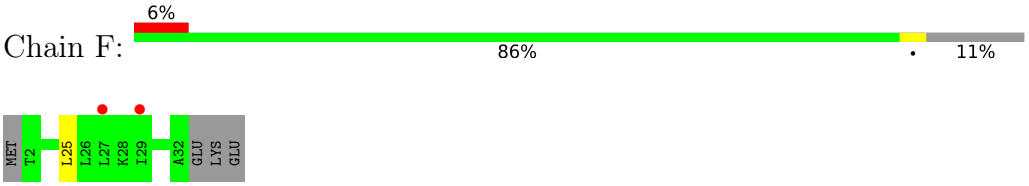
• Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:



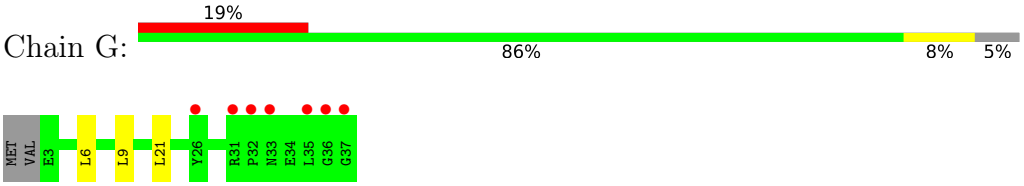
• Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:



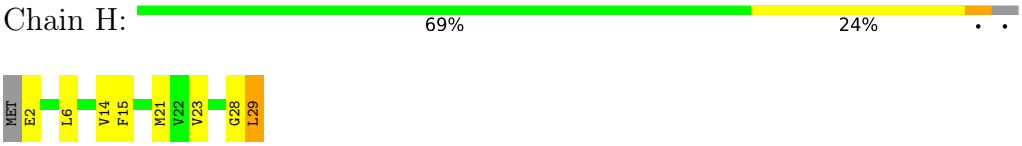
• Molecule 7: Cytochrome b6-f complex subunit 5

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	159.45Å 159.45Å 362.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 2.80 48.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.52-2.80) 99.2 (48.52-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309, REFMAC	Depositor
R, R_{free}	0.248 , 0.272 0.251 , 0.274	Depositor DCC
R_{free} test set	3406 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13828	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, BCR, 1E2, MYS, OZ2, UMQ, CLA, CD, OCT, HEM

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	0.30	0/1750	0.45	0/2388
2	B	0.26	0/1280	0.41	0/1755
3	C	0.26	0/2264	0.44	0/3082
4	D	0.28	0/300	0.40	0/408
5	E	0.28	0/220	0.42	0/297
6	F	0.28	0/238	0.40	0/321
7	G	0.29	0/274	0.39	0/371
8	H	0.29	0/228	0.47	0/313
All	All	0.28	0/6554	0.43	0/8935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1721	1720	9	0
2	B	1241	1297	1296	3	0
3	C	2216	2234	2233	9	0
4	D	292	299	299	0	0
5	E	215	237	237	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	234	248	248	0	0
7	G	268	268	268	0	0
8	H	222	227	227	4	0
9	A	129	0	90	23	0
9	C	43	0	30	6	0
10	A	15	32	32	0	0
11	A	18	38	38	0	0
12	A	102	130	126	2	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
14	B	65	64	71	1	0
15	B	32	0	32	0	0
15	C	38	0	43	0	0
15	G	44	0	54	1	0
16	D	23	0	18	2	0
17	F	8	18	18	0	0
18	G	40	56	56	0	0
19	A	8	0	0	1	0
19	B	4	0	0	0	0
19	C	1	0	0	0	0
All	All	6959	6869	7136	49	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 3.

All (49) 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)
9:A:303:HEM:HHA	9:A:303:HEM:HBD1	1.52	0.90
9:A:302:HEM:HBC2	9:A:302:HEM:HMC2	1.58	0.83
9:A:303:HEM:HMC1	9:A:303:HEM:HBC2	1.60	0.83
9:A:303:HEM:HBB2	9:A:303:HEM:HMB1	1.65	0.79
9:C:301:HEM:HMC1	9:C:301:HEM:HBC2	1.65	0.77
9:A:302:HEM:HMB1	9:A:302:HEM:HBB2	1.66	0.77
9:C:301:HEM:HBB2	9:C:301:HEM:HHC	1.68	0.76
9:A:301:HEM:HMC1	9:A:301:HEM:HBC2	1.67	0.76
12:A:306:UMQ:H11	12:A:306:UMQ:O3'	1.89	0.73
9:A:303:HEM:HBC2	9:A:303:HEM:CMC	2.25	0.66
9:A:301:HEM:HMB1	9:A:301:HEM:HBB2	1.77	0.66
14:B:201:CLA:HBB1	14:B:201:CLA:HHC	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:302:HEM:HBB2	9:A:302:HEM:CMB	2.27	0.64
9:A:301:HEM:HBC2	9:A:301:HEM:CMC	2.28	0.63
3:C:185:LYS:O	3:C:187:GLU:N	2.32	0.62
1:A:114:ARG:NH1	1:A:210:GLY:O	2.32	0.61
1:A:83:ARG:NH2	2:B:61:MET:O	2.34	0.61
3:C:25:CYS:SG	9:C:301:HEM:CAC	2.90	0.59
3:C:5:ALA:HB2	9:C:301:HEM:HBB2	1.85	0.59
1:A:83:ARG:NH1	9:A:301:HEM:O1D	2.35	0.59
9:C:301:HEM:HBC2	9:C:301:HEM:CMC	2.33	0.59
1:A:35:CYS:SG	9:A:303:HEM:CAB	2.91	0.59
9:A:302:HEM:HBC2	9:A:302:HEM:CMC	2.32	0.58
9:A:303:HEM:HBB2	9:A:303:HEM:CMB	2.34	0.58
1:A:35:CYS:HG	9:A:303:HEM:CAB	2.20	0.55
9:A:302:HEM:HBA1	9:A:302:HEM:HHA	1.89	0.54
15:G:102:OZ2:H11	8:H:15:PHE:CD1	2.42	0.54
9:A:302:HEM:HMA2	19:A:401:HOH:O	2.09	0.53
9:A:301:HEM:HBB2	9:A:301:HEM:CMB	2.40	0.51
3:C:150:HIS:ND1	3:C:244:ASP:OD1	2.43	0.48
8:H:23:VAL:HA	8:H:28:GLY:HA3	1.96	0.47
9:A:303:HEM:HBA1	9:A:303:HEM:O1D	2.14	0.47
3:C:31:PRO:O	3:C:155:ARG:NH2	2.44	0.46
1:A:15:GLN:NE2	1:A:19:ASP:OD1	2.49	0.45
1:A:54:MET:CE	9:A:301:HEM:HBA1	2.47	0.45
9:A:302:HEM:HMB1	9:A:302:HEM:CBB	2.43	0.44
8:H:29:LEU:HD12	8:H:29:LEU:N	2.33	0.44
3:C:19:ARG:NH1	3:C:24:ASN:OD1	2.48	0.43
9:A:301:HEM:HMC1	9:A:301:HEM:CBC	2.43	0.43
8:H:23:VAL:O	8:H:28:GLY:N	2.47	0.43
3:C:161:TYR:CE2	9:C:301:HEM:HBD2	2.54	0.42
16:D:201:1E2:H15	16:D:201:1E2:H4	1.75	0.42
2:B:82:TYR:HB2	2:B:83:PRO:HD3	2.01	0.42
1:A:138:LEU:N	1:A:139:PRO:CD	2.83	0.41
12:A:308:UMQ:HO61	16:D:201:1E2:H19	1.61	0.41
3:C:226:LYS:HG3	3:C:227:ALA:H	1.85	0.41
2:B:111:VAL:N	2:B:112:PRO:HD2	2.36	0.40
3:C:48:ALA:HB3	3:C:129:PHE:HB2	2.04	0.40
1:A:101:VAL:CG2	9:A:302:HEM:HMC3	2.51	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	211/215 (98%)	205 (97%)	6 (3%)	0	100 100
2	B	157/160 (98%)	152 (97%)	5 (3%)	0	100 100
3	C	286/289 (99%)	244 (85%)	39 (14%)	3 (1%)	15 44
4	D	36/179 (20%)	35 (97%)	1 (3%)	0	100 100
5	E	26/32 (81%)	25 (96%)	1 (4%)	0	100 100
6	F	29/35 (83%)	28 (97%)	1 (3%)	0	100 100
7	G	33/37 (89%)	30 (91%)	3 (9%)	0	100 100
8	H	26/29 (90%)	26 (100%)	0	0	100 100
All	All	804/976 (82%)	745 (93%)	56 (7%)	3 (0%)	34 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	186	GLU
3	C	205	LYS
3	C	20	ILE

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%)	171 (93%)	12 (7%)	16 44
2	B	136/137 (99%)	132 (97%)	4 (3%)	42 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	242/243 (100%)	224 (93%)	18 (7%)	13 37
4	D	31/146 (21%)	30 (97%)	1 (3%)	39 73
5	E	21/25 (84%)	20 (95%)	1 (5%)	25 58
6	F	23/27 (85%)	22 (96%)	1 (4%)	29 62
7	G	26/28 (93%)	23 (88%)	3 (12%)	5 17
8	H	23/24 (96%)	18 (78%)	5 (22%)	1 3
All	All	685/814 (84%)	640 (93%)	45 (7%)	16 44

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	12	LEU
1	A	14	ILE
1	A	63	THR
1	A	75	GLU
1	A	81	LEU
1	A	87	ARG
1	A	95	LEU
1	A	103	ARG
1	A	148	VAL
1	A	164	LEU
1	A	200	LEU
2	B	13	LYS
2	B	35	ASP
2	B	75	ILE
2	B	96	LEU
3	C	70	LEU
3	C	116	VAL
3	C	140	LYS
3	C	155	ARG
3	C	190	TYR
3	C	194	LYS
3	C	200	GLN
3	C	201	THR
3	C	202	ASP
3	C	218	ILE
3	C	226	LYS
3	C	232	THR
3	C	233	ASN

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Mol	Chain	Res	Type
3	C	264	LEU
3	C	267	LEU
3	C	271	MET
3	C	278	GLN
3	C	281	LYS
4	D	22	LEU
5	E	11	PHE
6	F	25	LEU
7	G	6	LEU
7	G	9	LEU
7	G	21	LEU
8	H	2	GLU
8	H	6	LEU
8	H	14	VAL
8	H	21	MET
8	H	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
9	HEM	C	301	3	41,50,50	1.93	6 (14%)	45,82,82	1.70	8 (17%)
18	BCR	G	101	-	41,41,41	2.19	21 (51%)	56,56,56	2.27	21 (37%)
9	HEM	A	301	1	41,50,50	1.90	5 (12%)	45,82,82	1.63	7 (15%)
15	OZ2	G	102	-	43,43,47	1.16	4 (9%)	46,49,53	1.15	2 (4%)
11	8K6	A	305	-	17,17,17	0.20	0	16,16,16	0.53	0
10	MYS	A	304	-	14,14,14	0.32	0	13,13,13	0.79	0
16	1E2	D	201	-	22,23,23	1.77	2 (9%)	30,33,33	3.14	9 (30%)
12	UMQ	A	306	-	35,35,35	1.25	5 (14%)	46,46,46	2.31	12 (26%)
15	OZ2	B	203	-	31,31,47	1.23	3 (9%)	34,37,53	1.49	4 (11%)
12	UMQ	A	308	-	35,35,35	1.31	6 (17%)	46,46,46	2.01	9 (19%)
12	UMQ	A	307	-	35,35,35	1.31	5 (14%)	46,46,46	2.43	11 (23%)
17	OCT	F	101	-	7,7,7	0.25	0	6,6,6	0.65	0
9	HEM	A	302	1	41,50,50	1.92	5 (12%)	45,82,82	1.55	5 (11%)
14	CLA	B	201	19	65,73,73	1.53	6 (9%)	76,113,113	1.42	10 (13%)
15	OZ2	C	303	-	37,37,47	1.24	4 (10%)	40,43,53	1.22	3 (7%)
9	HEM	A	303	19	41,50,50	1.95	7 (17%)	45,82,82	1.82	10 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	C	301	3	-	5/12/54/54	-
18	BCR	G	101	-	-	18/29/63/63	0/2/2/2
9	HEM	A	301	1	-	5/12/54/54	-
15	OZ2	G	102	-	-	13/48/48/52	-
9	HEM	A	302	1	-	2/12/54/54	-
11	8K6	A	305	-	-	4/15/15/15	-
10	MYS	A	304	-	-	2/12/12/12	-
16	1E2	D	201	-	1/1/8/8	6/15/35/35	0/1/1/1
12	UMQ	A	306	-	3/3/10/10	9/20/60/60	0/2/2/2
17	OCT	F	101	-	-	0/5/5/5	-
12	UMQ	A	308	-	2/2/10/10	5/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	UMQ	A	307	-	3/3/10/10	8/20/60/60	0/2/2/2
15	OZ2	B	203	-	1/1/5/9	13/35/35/52	-
14	CLA	B	201	19	1/1/17/20	17/37/115/115	-
15	OZ2	C	303	-	-	16/42/42/52	-
9	HEM	A	303	19	-	5/12/54/54	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	201	CLA	C4B-NB	8.09	1.42	1.35
9	C	301	HEM	C3D-C2D	7.93	1.53	1.36
9	A	301	HEM	C3D-C2D	7.89	1.53	1.36
9	A	302	HEM	C3D-C2D	7.88	1.53	1.36
9	A	303	HEM	C3D-C2D	7.66	1.53	1.36
16	D	201	1E2	O47-C45	-6.44	1.24	1.43
9	A	302	HEM	C3C-C2C	-4.42	1.34	1.40
9	A	303	HEM	C3C-C2C	-4.42	1.34	1.40
9	A	301	HEM	C3C-C2C	-4.32	1.34	1.40
9	C	301	HEM	C3C-C2C	-4.04	1.34	1.40
14	B	201	CLA	C1D-ND	3.68	1.42	1.37
15	G	102	OZ2	C10-C9	3.65	1.52	1.31
9	A	301	HEM	C3C-CAC	3.62	1.55	1.47
9	A	302	HEM	C3C-CAC	3.60	1.55	1.47
9	C	301	HEM	C3C-CAC	3.53	1.55	1.47
15	G	102	OZ2	C7B-C6B	3.49	1.52	1.31
15	B	203	OZ2	O2G-C2G	-3.42	1.38	1.46
18	G	101	BCR	C26-C25	3.41	1.40	1.34
18	G	101	BCR	C20-C21	3.38	1.53	1.43
9	A	303	HEM	C3C-CAC	3.38	1.54	1.47
18	G	101	BCR	C17-C18	3.35	1.40	1.35
18	G	101	BCR	C23-C22	3.32	1.53	1.45
15	C	303	OZ2	O2G-C2G	-3.32	1.38	1.46
18	G	101	BCR	C21-C22	3.30	1.40	1.35
18	G	101	BCR	C15-C14	3.18	1.53	1.43
14	B	201	CLA	CHC-C1C	3.15	1.43	1.35
15	B	203	OZ2	C10-C9	3.14	1.50	1.31
14	B	201	CLA	C4D-ND	-3.11	1.33	1.37
15	C	303	OZ2	C10-C9	3.11	1.49	1.28
15	C	303	OZ2	C7B-C6B	3.09	1.49	1.31
18	G	101	BCR	C16-C17	3.09	1.53	1.43
18	G	101	BCR	C8-C9	3.07	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	101	BCR	C11-C10	3.07	1.53	1.43
12	A	307	UMQ	C4-C5	-3.06	1.46	1.53
9	C	301	HEM	FE-NB	3.04	2.11	1.96
9	A	303	HEM	FE-ND	2.99	2.11	1.96
9	A	303	HEM	CAB-C3B	2.96	1.55	1.47
15	G	102	OZ2	O2G-C2G	-2.93	1.39	1.46
18	G	101	BCR	C19-C18	2.88	1.52	1.45
9	A	301	HEM	CAB-C3B	2.86	1.55	1.47
18	G	101	BCR	C12-C13	2.84	1.52	1.45
18	G	101	BCR	C32-C1	-2.80	1.48	1.53
12	A	308	UMQ	O5'-C5'	-2.75	1.37	1.44
15	C	303	OZ2	O1G-C1G	-2.75	1.38	1.45
15	B	203	OZ2	O1G-C1G	-2.73	1.38	1.45
12	A	308	UMQ	C4-C5	-2.73	1.47	1.53
9	A	302	HEM	CAB-C3B	2.72	1.54	1.47
12	A	307	UMQ	O2'-C2'	-2.72	1.36	1.43
18	G	101	BCR	C14-C13	2.66	1.39	1.35
12	A	306	UMQ	O5'-C5'	-2.66	1.37	1.44
9	C	301	HEM	CAB-C3B	2.65	1.54	1.47
12	A	306	UMQ	O2'-C2'	-2.57	1.36	1.43
12	A	308	UMQ	O2'-C2'	-2.55	1.37	1.43
12	A	307	UMQ	O3'-C3'	-2.50	1.37	1.43
12	A	308	UMQ	C3-C4	-2.48	1.46	1.52
12	A	306	UMQ	C3-C4	-2.47	1.46	1.52
12	A	306	UMQ	O3'-C3'	-2.45	1.37	1.43
9	A	303	HEM	FE-NB	2.44	2.08	1.96
15	G	102	OZ2	O1G-C1	2.44	1.40	1.33
12	A	307	UMQ	C3-C4	-2.44	1.46	1.52
12	A	306	UMQ	C4-C5	-2.43	1.47	1.53
12	A	308	UMQ	O3'-C3'	-2.41	1.37	1.43
12	A	307	UMQ	O5'-C5'	-2.32	1.38	1.44
14	B	201	CLA	CMB-C2B	-2.30	1.46	1.51
18	G	101	BCR	C24-C23	2.30	1.40	1.33
9	A	301	HEM	CAA-C2A	2.29	1.55	1.52
18	G	101	BCR	C24-C25	2.24	1.53	1.45
12	A	308	UMQ	C4'-C5'	-2.22	1.47	1.52
18	G	101	BCR	C10-C9	2.18	1.38	1.35
18	G	101	BCR	C20-C19	2.10	1.40	1.34
9	A	302	HEM	FE-ND	2.07	2.07	1.96
14	B	201	CLA	CMD-C2D	-2.07	1.46	1.50
18	G	101	BCR	C40-C30	-2.05	1.49	1.53
18	G	101	BCR	C31-C1	-2.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	101	BCR	C7-C6	2.03	1.52	1.45
18	G	101	BCR	C5-C6	2.03	1.38	1.34
9	C	301	HEM	CMD-C2D	2.03	1.55	1.50
9	A	303	HEM	CAA-C2A	2.01	1.55	1.52
16	D	201	1E2	C6-S	-2.00	1.70	1.77

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	201	1E2	O7-S-C6	8.91	117.53	106.94
12	A	306	UMQ	O5-C5-C4	7.92	124.07	109.69
16	D	201	1E2	O9-S-C6	-7.36	98.19	106.94
12	A	307	UMQ	O1'-C1'-C2'	7.10	119.39	108.30
12	A	307	UMQ	O5'-C5'-C4'	7.08	124.68	109.75
16	D	201	1E2	O8-S-C6	7.06	116.99	105.74
14	B	201	CLA	C4A-NA-C1A	6.95	109.83	106.71
9	A	303	HEM	C4D-ND-C1D	6.63	111.92	105.07
9	C	301	HEM	C4D-ND-C1D	6.39	111.67	105.07
12	A	308	UMQ	O5-C5-C4	6.21	120.97	109.69
16	D	201	1E2	O8-S-O9	-6.19	96.14	111.27
9	A	302	HEM	C4D-ND-C1D	6.03	111.30	105.07
9	A	301	HEM	C4D-ND-C1D	5.74	111.01	105.07
16	D	201	1E2	O7-S-O9	-5.13	96.20	113.95
12	A	307	UMQ	CA-O1'-C1'	5.03	122.18	113.84
18	G	101	BCR	C24-C23-C22	-4.97	118.72	126.23
12	A	306	UMQ	O2-C2-C3	4.90	121.68	110.35
12	A	308	UMQ	O5-C5-C6	4.79	118.34	106.44
12	A	306	UMQ	O2-C2-C1	4.79	121.67	110.05
12	A	307	UMQ	O1-C1-C2	4.78	120.49	108.10
12	A	307	UMQ	O5'-C1'-O1'	4.77	121.28	109.97
12	A	307	UMQ	O5-C1-C2	4.72	120.35	110.35
18	G	101	BCR	C15-C14-C13	-4.66	120.66	127.31
18	G	101	BCR	C7-C8-C9	-4.64	119.23	126.23
18	G	101	BCR	C16-C17-C18	-4.53	120.85	127.31
12	A	306	UMQ	O5-C5-C6	4.49	117.59	106.44
15	B	203	OZ2	O2G-C1B-C2B	4.46	119.30	111.09
18	G	101	BCR	C11-C10-C9	-4.42	121.00	127.31
12	A	308	UMQ	O2-C2-C3	4.41	120.54	110.35
12	A	306	UMQ	O1-C1-C2	4.39	119.48	108.10
12	A	308	UMQ	CA-O1'-C1'	4.34	121.04	113.84
18	G	101	BCR	C33-C5-C6	-4.27	119.73	124.53
12	A	308	UMQ	C1-C2-C3	4.26	118.88	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	307	UMQ	O5'-C5'-C6'	4.26	117.02	106.44
12	A	307	UMQ	O5'-C1'-C2'	4.16	119.16	110.35
18	G	101	BCR	C2-C1-C6	4.13	116.84	110.48
16	D	201	1E2	O8-S-O7	4.10	121.30	111.27
12	A	308	UMQ	O2-C2-C1	4.07	119.94	110.05
12	A	306	UMQ	O5-C1-C2	4.02	118.87	110.35
9	A	303	HEM	C4C-CHD-C1D	3.90	127.70	122.56
12	A	306	UMQ	O1-C1-O5	3.84	121.39	110.67
18	G	101	BCR	C33-C5-C4	3.76	120.85	113.62
9	A	303	HEM	CAD-C3D-C4D	3.68	131.08	124.66
15	G	102	OZ2	O2G-C1B-C2B	3.59	119.25	111.50
15	B	203	OZ2	O1G-C1G-C2G	3.58	118.86	108.43
18	G	101	BCR	C20-C21-C22	-3.57	122.22	127.31
15	C	303	OZ2	O1G-C1G-C2G	3.52	118.68	108.43
15	C	303	OZ2	O2G-C1B-C2B	3.48	119.00	111.50
9	A	301	HEM	C4C-CHD-C1D	3.39	127.04	122.56
18	G	101	BCR	C38-C26-C25	-3.34	120.78	124.53
14	B	201	CLA	CAA-CBA-CGA	-3.15	104.05	113.25
12	A	306	UMQ	CA-O1'-C1'	3.13	119.03	113.84
18	G	101	BCR	C23-C24-C25	-3.05	118.63	127.20
12	A	307	UMQ	O1-C1-O5	2.99	119.03	110.67
12	A	308	UMQ	C6-C5-C4	2.99	120.01	113.00
14	B	201	CLA	CMB-C2B-C1B	-2.97	123.91	128.46
12	A	306	UMQ	C1-C2-C3	2.95	116.13	110.00
12	A	308	UMQ	C1-O1-C4'	-2.95	110.67	117.96
15	G	102	OZ2	O1G-C1G-C2G	2.95	117.01	108.43
18	G	101	BCR	C38-C26-C27	2.94	119.27	113.62
18	G	101	BCR	C34-C9-C10	-2.91	118.84	122.92
9	A	302	HEM	C4C-CHD-C1D	2.89	126.37	122.56
15	B	203	OZ2	O1G-C1-C2	2.84	120.81	111.91
14	B	201	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
12	A	307	UMQ	C1-O1-C4'	-2.78	111.09	117.96
14	B	201	CLA	C9-C8-C10	2.74	121.23	111.29
9	C	301	HEM	C1B-NB-C4B	2.72	107.88	105.07
9	C	301	HEM	CAD-CBD-CGD	-2.70	107.78	113.60
18	G	101	BCR	C32-C1-C6	-2.66	105.98	110.30
9	A	303	HEM	CAD-C3D-C2D	-2.62	123.00	127.88
12	A	306	UMQ	O1'-C1'-C2'	2.62	112.39	108.30
9	A	301	HEM	C1B-NB-C4B	2.60	107.76	105.07
18	G	101	BCR	C16-C15-C14	-2.54	118.27	123.47
12	A	307	UMQ	C3'-C4'-C5'	2.54	116.75	110.93
9	C	301	HEM	C4C-CHD-C1D	2.50	125.86	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	303	HEM	CHD-C1D-ND	2.44	127.09	124.43
9	A	303	HEM	CBA-CAA-C2A	-2.43	108.47	112.62
15	B	203	OZ2	O2G-C1B-O1B	-2.42	118.16	122.96
18	G	101	BCR	C29-C30-C25	2.41	114.19	110.48
9	A	302	HEM	C3B-C2B-C1B	2.40	108.26	106.49
9	A	303	HEM	C1B-NB-C4B	2.39	107.54	105.07
9	C	301	HEM	CMA-C3A-C4A	-2.37	124.82	128.46
18	G	101	BCR	C20-C19-C18	-2.35	119.83	126.42
18	G	101	BCR	C8-C7-C6	-2.33	120.66	127.20
16	D	201	1E2	O5-C1-C2	-2.32	105.44	110.35
9	A	301	HEM	C4B-CHC-C1C	2.28	125.57	122.56
18	G	101	BCR	C4-C5-C6	-2.28	119.42	122.73
16	D	201	1E2	O5-C5-C4	-2.25	105.61	109.69
14	B	201	CLA	CHB-C4A-NA	2.23	127.59	124.51
9	A	302	HEM	O2A-CGA-CBA	2.21	121.14	114.03
18	G	101	BCR	C11-C12-C13	-2.21	120.21	126.42
12	A	308	UMQ	C3'-C4'-C5'	-2.21	105.87	110.93
15	C	303	OZ2	O1G-C1-C2	2.19	118.79	111.91
14	B	201	CLA	CHD-C1D-ND	-2.17	122.46	124.45
9	C	301	HEM	CMD-C2D-C1D	2.16	128.34	125.04
9	A	303	HEM	C3D-C4D-ND	-2.15	107.77	110.17
9	A	301	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
18	G	101	BCR	C1-C6-C5	-2.15	119.59	122.61
9	A	301	HEM	CHA-C4D-ND	2.15	127.03	124.38
12	A	306	UMQ	C1'-O5'-C5'	-2.15	109.47	113.69
9	A	303	HEM	C3B-C2B-C1B	2.14	108.08	106.49
14	B	201	CLA	O2D-CGD-CBD	2.12	115.03	111.27
9	A	303	HEM	O1D-CGD-CBD	-2.11	116.30	123.08
14	B	201	CLA	CMB-C2B-C3B	2.10	128.61	124.68
9	A	301	HEM	CHB-C1B-NB	2.09	126.97	124.38
9	A	302	HEM	C1B-NB-C4B	2.05	107.19	105.07
9	C	301	HEM	C3B-C2B-C1B	2.04	108.00	106.49
14	B	201	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
12	A	306	UMQ	C6-C5-C4	2.02	117.74	113.00
9	C	301	HEM	CHC-C4B-C3B	2.02	127.66	124.57
16	D	201	1E2	C3-C4-C5	2.02	113.83	110.24

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	306	UMQ	C5
12	A	306	UMQ	C1

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Mol	Chain	Res	Type	Atom
12	A	306	UMQ	C2
12	A	307	UMQ	C1
12	A	307	UMQ	C1'
12	A	307	UMQ	C5'
12	A	308	UMQ	C5
12	A	308	UMQ	C2
14	B	201	CLA	ND
15	B	203	OZ2	CG2
16	D	201	1E2	C5

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	302	HEM	C1A-C2A-CAA-CBA
9	A	303	HEM	C1A-C2A-CAA-CBA
9	A	303	HEM	C3A-C2A-CAA-CBA
9	A	303	HEM	C2D-C3D-CAD-CBD
9	A	303	HEM	C4D-C3D-CAD-CBD
12	A	306	UMQ	O5'-C1'-O1'-CA
12	A	307	UMQ	O5'-C1'-O1'-CA
14	B	201	CLA	O2A-C1-C2-C3
15	B	203	OZ2	O1B-C1B-O2G-C2G
15	B	203	OZ2	C2B-C1B-O2G-C2G
15	B	203	OZ2	CG1-CG2-CG3-OG3
15	C	303	OZ2	OP3-CG1-CG2-CG3
15	G	102	OZ2	O1G-C1G-C2G-O2G
16	D	201	1E2	O6-C44-C45-O47
16	D	201	1E2	C2-C1-O6-C44
16	D	201	1E2	O5-C1-O6-C44
18	G	101	BCR	C17-C18-C19-C20
18	G	101	BCR	C36-C18-C19-C20
18	G	101	BCR	C22-C23-C24-C25
16	D	201	1E2	C24-C23-O48-C46
12	A	306	UMQ	O5-C1-O1-C4'
14	B	201	CLA	CBD-CGD-O2D-CED
12	A	307	UMQ	C2-C1-O1-C4'
15	C	303	OZ2	OP3-CG1-CG2-OG2
12	A	307	UMQ	O5-C5-C6-O6
12	A	308	UMQ	O5'-C5'-C6'-O6'
9	C	301	HEM	C2D-C3D-CAD-CBD
12	A	306	UMQ	O5-C5-C6-O6
12	A	307	UMQ	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	A	308	UMQ	C4-C5-C6-O6
16	D	201	1E2	O6-C44-C45-C46
12	A	306	UMQ	C2'-C1'-O1'-CA
14	B	201	CLA	C11-C10-C8-C9
18	G	101	BCR	C7-C8-C9-C34
18	G	101	BCR	C37-C22-C23-C24
18	G	101	BCR	C7-C8-C9-C10
18	G	101	BCR	C11-C12-C13-C14
18	G	101	BCR	C21-C22-C23-C24
15	C	303	OZ2	C2-C1-O1G-C1G
9	A	301	HEM	C2A-CAA-CBA-CGA
15	C	303	OZ2	C1-C2-C3-C4
16	D	201	1E2	O10-C23-O48-C46
14	B	201	CLA	C8-C10-C11-C12
14	B	201	CLA	C11-C12-C13-C15
12	A	307	UMQ	O5'-C5'-C6'-O6'
12	A	308	UMQ	C4'-C5'-C6'-O6'
15	B	203	OZ2	C11-C10-C9-C8
9	C	301	HEM	C4D-C3D-CAD-CBD
12	A	307	UMQ	C4'-C5'-C6'-O6'
15	G	102	OZ2	C1B-C2B-C3B-C4B
15	G	102	OZ2	C1-C2-C3-C4
9	A	301	HEM	C2D-C3D-CAD-CBD
14	B	201	CLA	O1D-CGD-O2D-CED
15	B	203	OZ2	C5-C6-C7-C8
18	G	101	BCR	C12-C13-C14-C15
10	A	304	MYS	C5-C6-C7-C8
15	B	203	OZ2	C1-C2-C3-C4
18	G	101	BCR	C11-C12-C13-C35
15	C	303	OZ2	C2B-C3B-C4B-C5B
12	A	307	UMQ	CD-CF-CG-CH
15	C	303	OZ2	C5-C6-C7-C8
10	A	304	MYS	C7-C8-C9-C10
12	A	306	UMQ	C5'-C4'-O1-C1
15	B	203	OZ2	OG2-CG2-CG3-OG3
18	G	101	BCR	C23-C24-C25-C26
18	G	101	BCR	C23-C24-C25-C30
12	A	306	UMQ	C3'-C4'-O1-C1
14	B	201	CLA	C6-C7-C8-C10
15	G	102	OZ2	C3-C4-C5-C6
15	C	303	OZ2	C2B-C1B-O2G-C2G
9	C	301	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	B	203	OZ2	C2-C3-C4-C5
9	A	301	HEM	C4D-C3D-CAD-CBD
12	A	308	UMQ	CF-CG-CH-CI
14	B	201	CLA	C13-C15-C16-C17
15	G	102	OZ2	O1G-C1G-C2G-C3G
15	C	303	OZ2	O1-C1-O1G-C1G
15	G	102	OZ2	C5-C6-C7-C8
11	A	305	8K6	C5-C6-C7-C8
12	A	306	UMQ	CI-CJ-CK-CL
11	A	305	8K6	C4-C5-C6-C7
18	G	101	BCR	C16-C17-C18-C19
14	B	201	CLA	C15-C16-C17-C18
15	C	303	OZ2	C8B-C9B-CB0-CB1
14	B	201	CLA	C10-C11-C12-C13
15	B	203	OZ2	C10-C11-C12-C13
15	B	203	OZ2	CG1-OP3-P-O3G
14	B	201	CLA	C11-C12-C13-C14
15	C	303	OZ2	CG2-CG1-OP3-P
18	G	101	BCR	C35-C13-C14-C15
15	G	102	OZ2	CG2-CG1-OP3-P
15	C	303	OZ2	CG1-OP3-P-O3G
15	B	203	OZ2	C3G-O3G-P-OP2
15	C	303	OZ2	C3G-O3G-P-OP1
15	G	102	OZ2	CG1-OP3-P-OP2
14	B	201	CLA	C11-C10-C8-C7
9	A	302	HEM	C3A-C2A-CAA-CBA
12	A	306	UMQ	O5'-C5'-C6'-O6'
15	C	303	OZ2	C2G-C3G-O3G-P
18	G	101	BCR	C1-C6-C7-C8
15	B	203	OZ2	C3G-O3G-P-OP3
14	B	201	CLA	C6-C7-C8-C9
12	A	308	UMQ	O1'-CA-CB-CC
15	G	102	OZ2	C4B-C5B-C6B-C7B
15	C	303	OZ2	C7-C8-C9-C10
15	G	102	OZ2	C7-C8-C9-C10
18	G	101	BCR	C11-C10-C9-C34
11	A	305	8K6	C6-C7-C8-C9
18	G	101	BCR	C11-C10-C9-C8
11	A	305	8K6	C7-C8-C9-C10
12	A	307	UMQ	CC-CD-CF-CG
12	A	306	UMQ	CD-CF-CG-CH
9	C	301	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	G	101	BCR	C5-C6-C7-C8
15	B	203	OZ2	C9-C10-C11-C12
14	B	201	CLA	C2-C3-C5-C6
9	A	301	HEM	C3D-CAD-CBD-CGD
15	C	303	OZ2	C4B-C5B-C6B-C7B
15	G	102	OZ2	O1-C1-O1G-C1G
15	G	102	OZ2	C6B-C7B-C8B-C9B
15	G	102	OZ2	C10-C11-C12-C13
9	C	301	HEM	CAD-CBD-CGD-O1D
14	B	201	CLA	CAA-CBA-CGA-O2A
9	A	301	HEM	CAA-CBA-CGA-O1A
15	C	303	OZ2	CG1-OP3-P-OP1
14	B	201	CLA	C4-C3-C5-C6
9	A	303	HEM	C2A-CAA-CBA-CGA
14	B	201	CLA	CAA-CBA-CGA-O1A

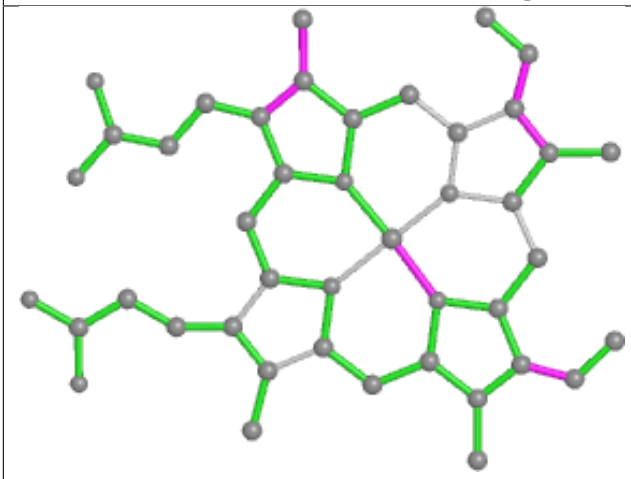
There are no ring outliers.

9 monomers are involved in 34 short contacts:

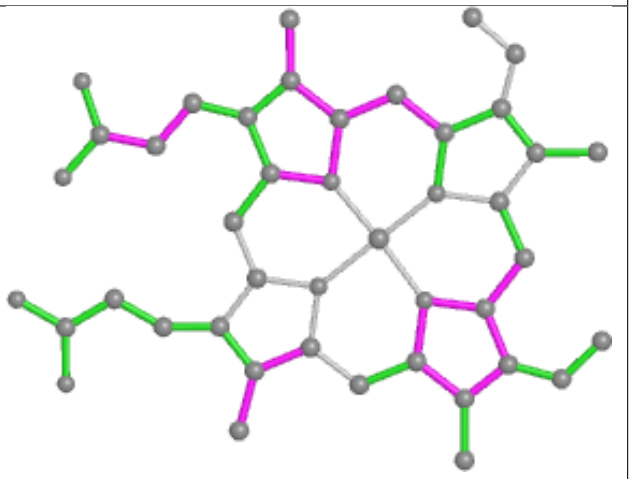
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	301	HEM	6	0
9	A	301	HEM	7	0
15	G	102	OZ2	1	0
16	D	201	1E2	2	0
12	A	306	UMQ	1	0
12	A	308	UMQ	1	0
9	A	302	HEM	8	0
14	B	201	CLA	1	0
9	A	303	HEM	8	0

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

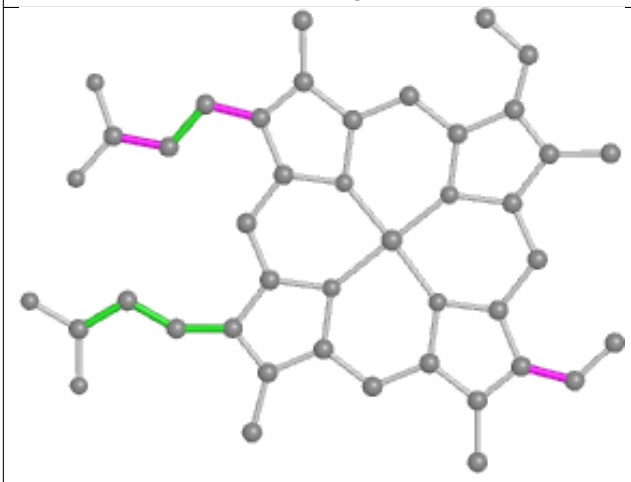
Ligand HEM C 301



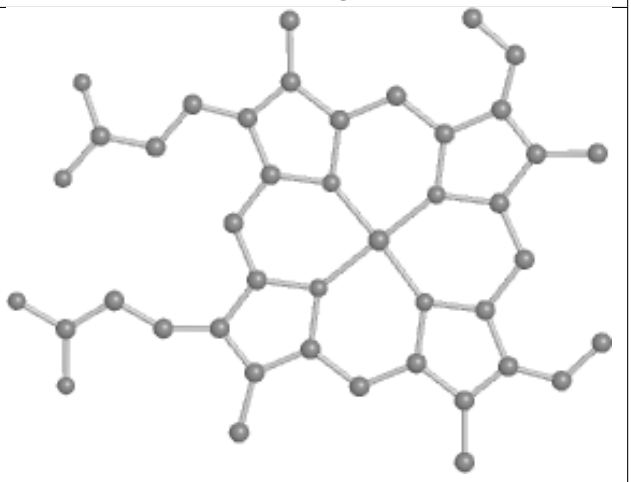
Bond lengths



Bond angles

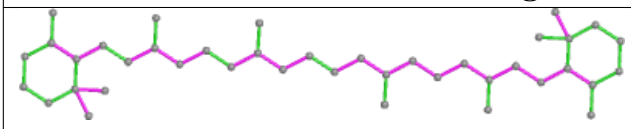


Torsions

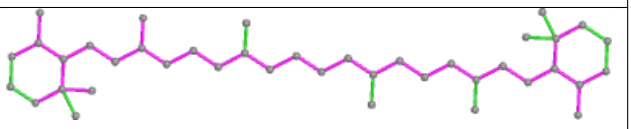


Rings

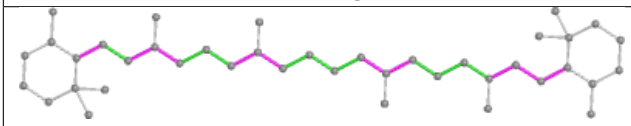
Ligand BCR G 101



Bond lengths



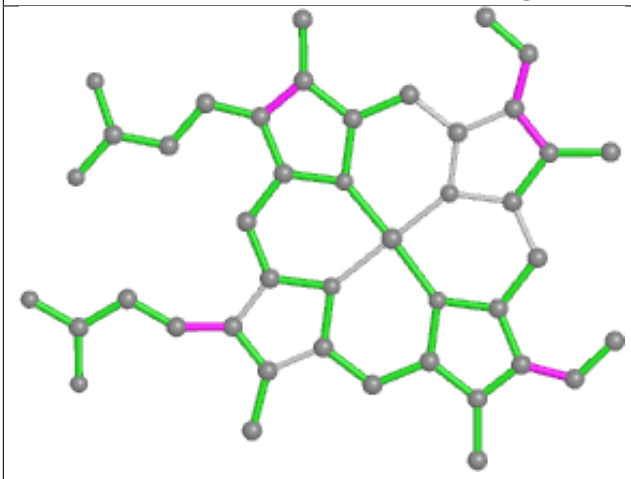
Bond angles



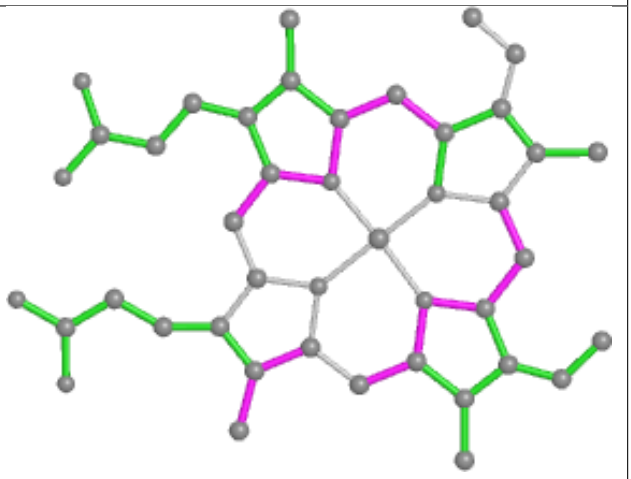
Torsions

Rings

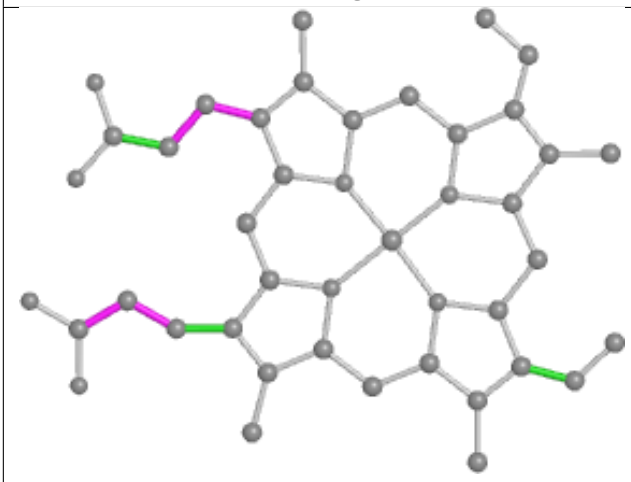
Ligand HEM A 301



Bond lengths



Bond angles



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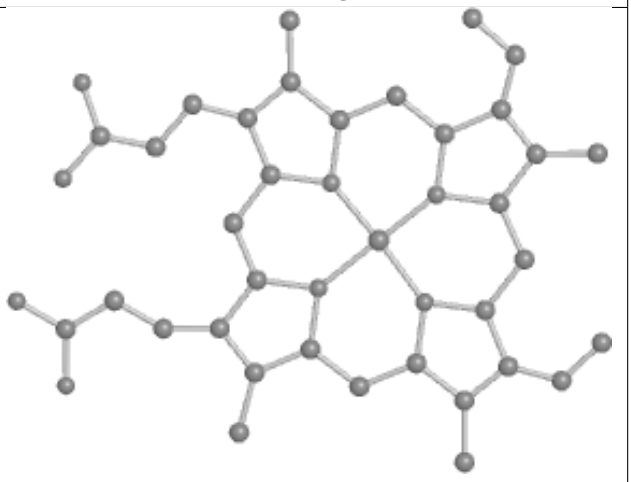
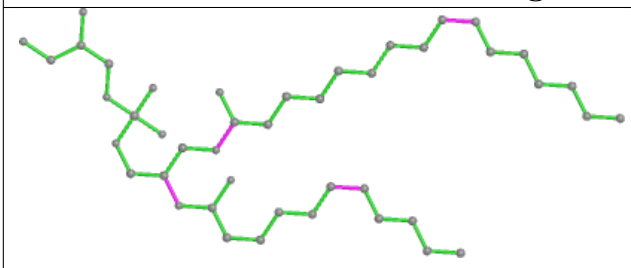
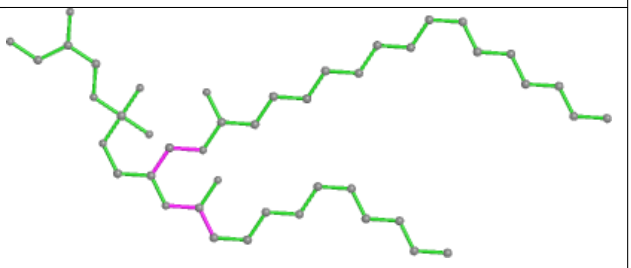


Rings

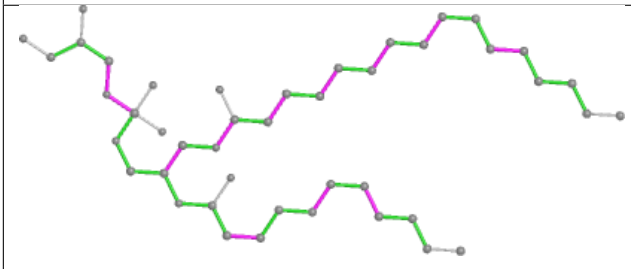
Ligand OZ2 G 102



Bond lengths



Bond angles



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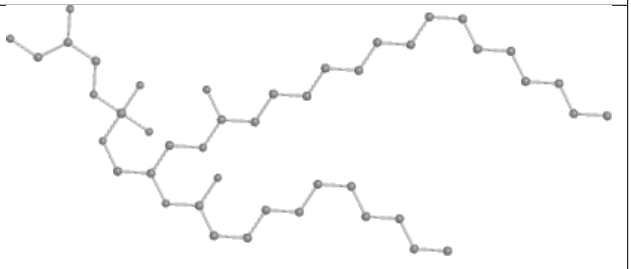
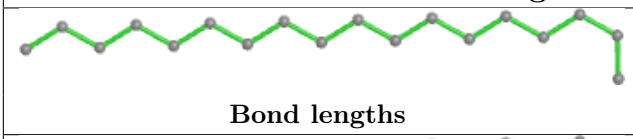
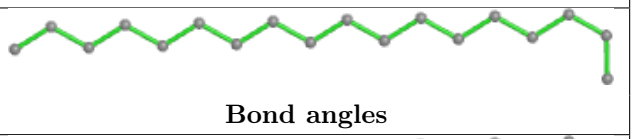


Rings

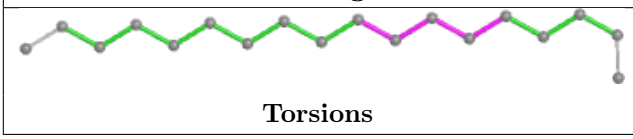
Ligand 8K6 A 305



Bond lengths



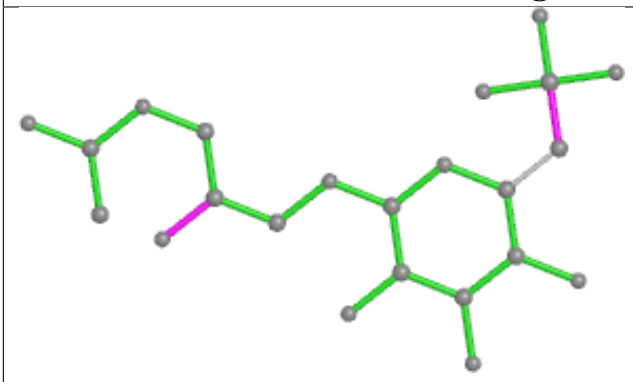
Bond angles



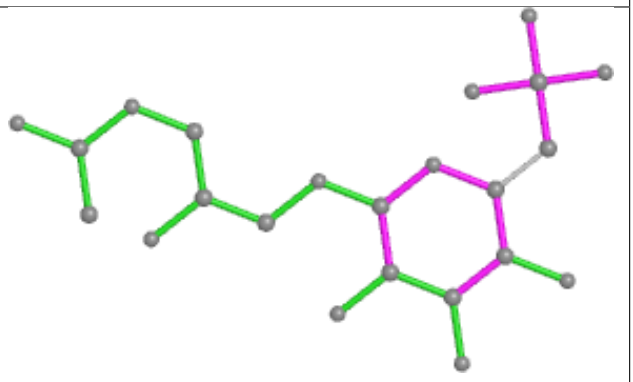
Torsions

Rings

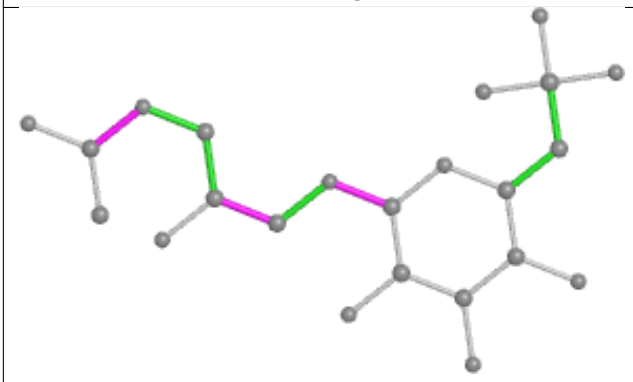
Ligand 1E2 D 201



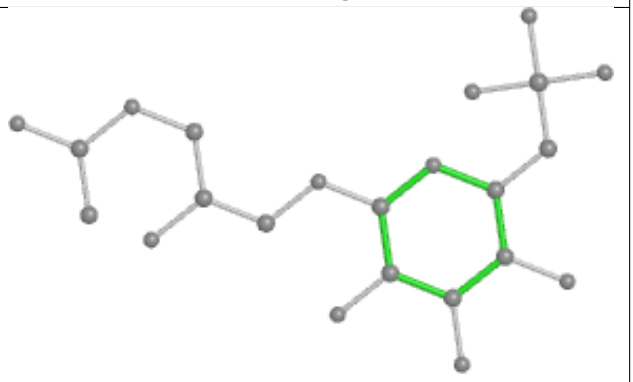
Bond lengths



Bond angles

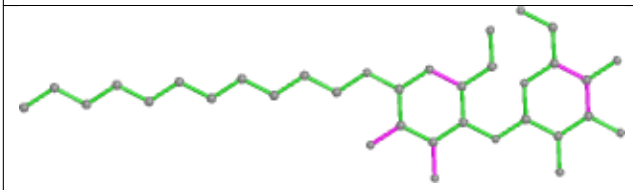


Torsions

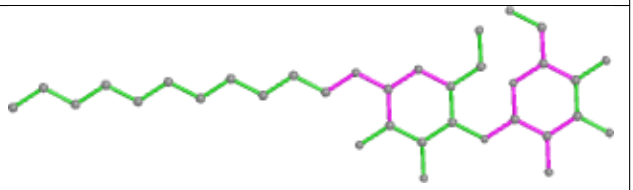


Rings

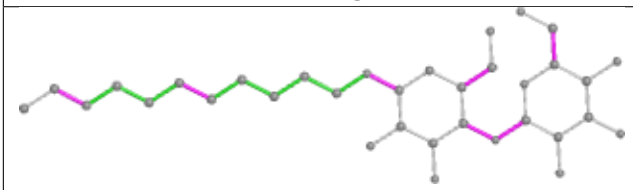
Ligand UMQ A 306



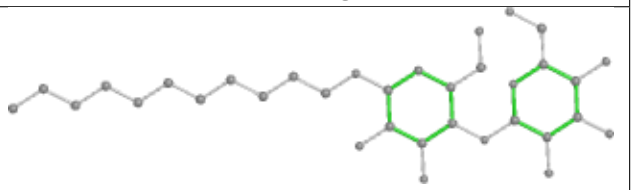
Bond lengths



Bond angles

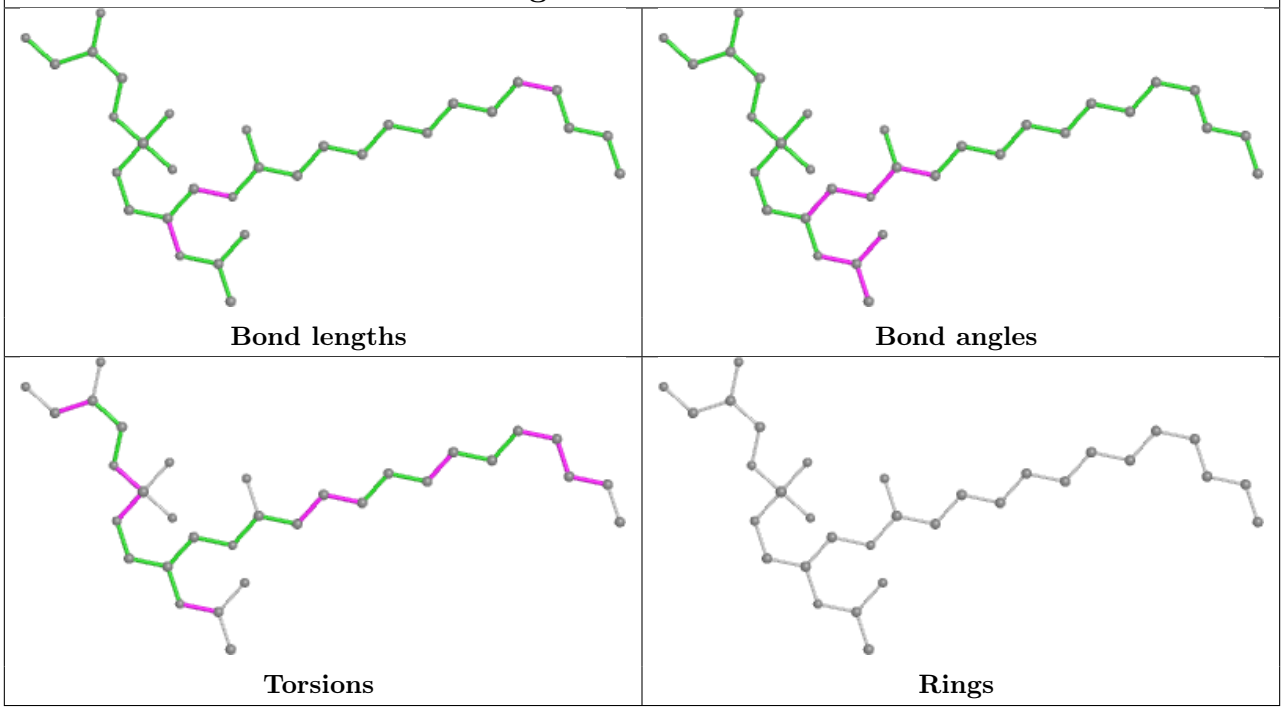


Torsions

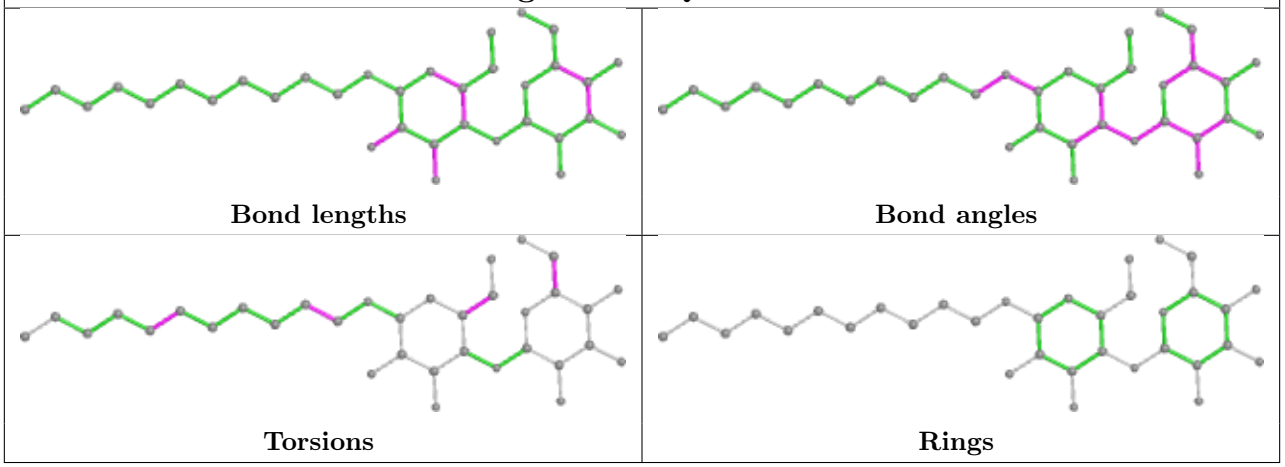


Rings

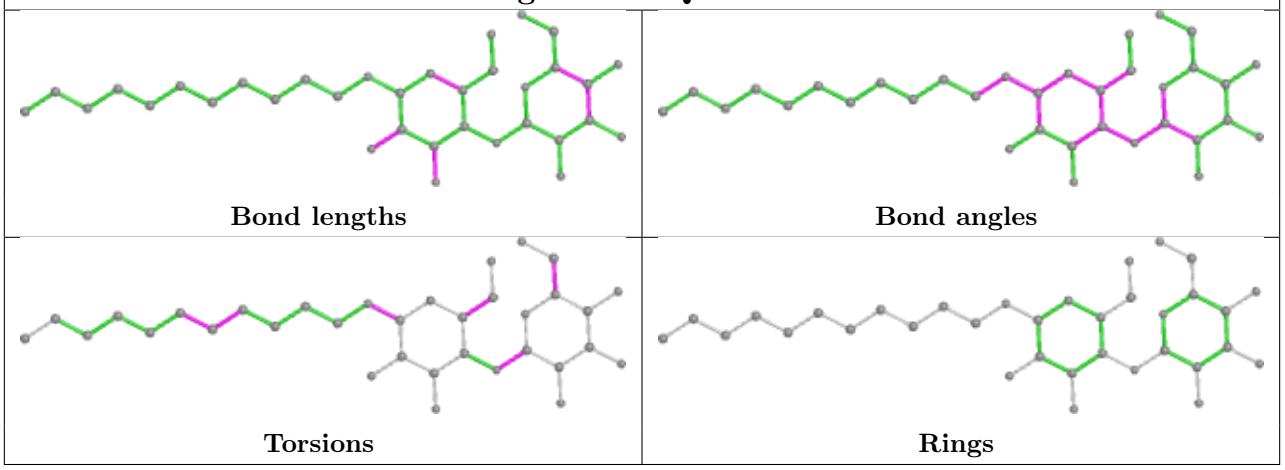
Ligand OZ2 B 203



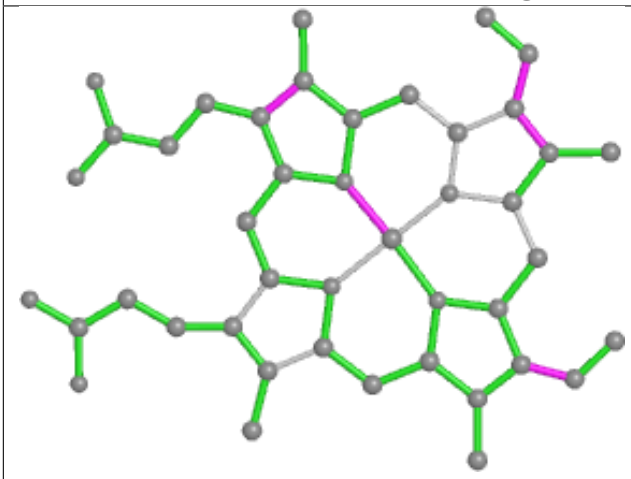
Ligand UMQ A 308



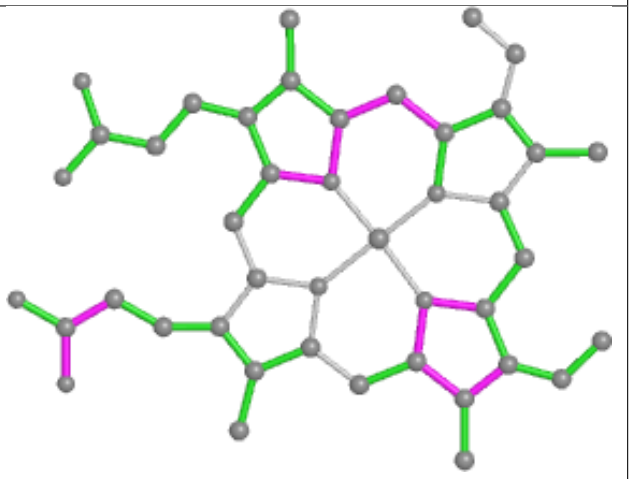
Ligand UMQ A 307



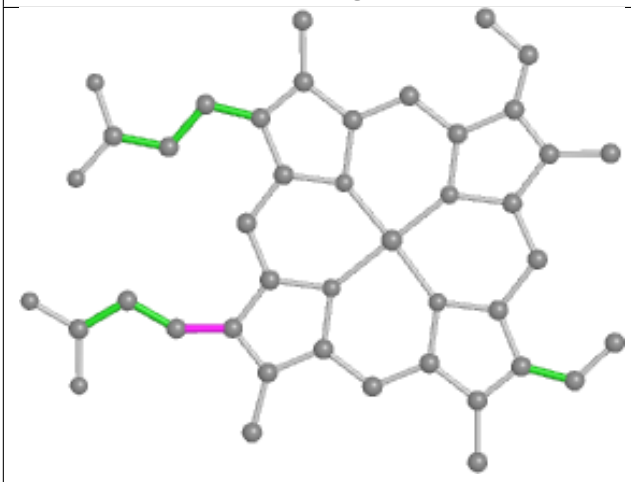
Ligand HEM A 302



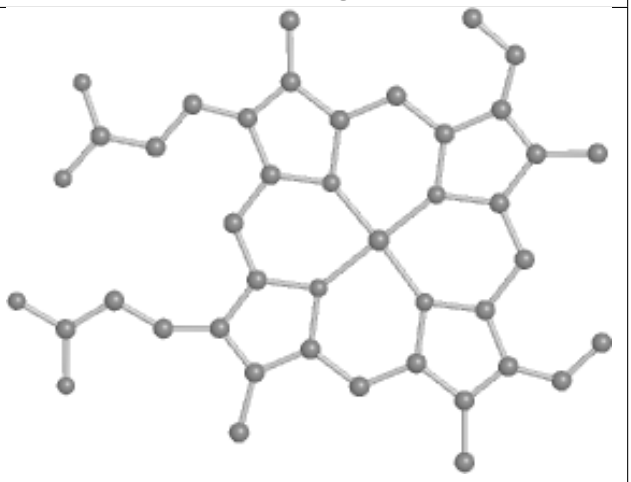
Bond lengths



Bond angles

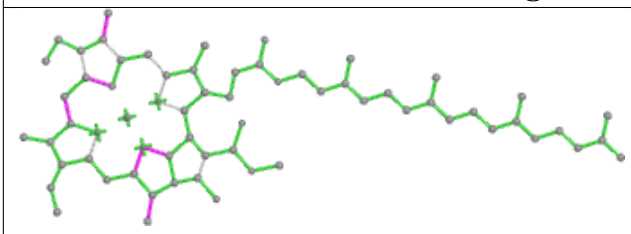


Torsions

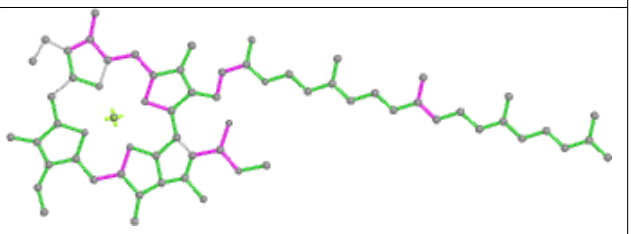


Rings

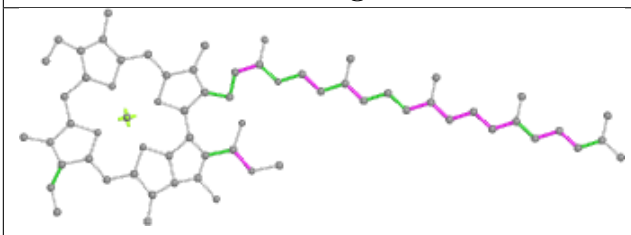
Ligand CLA B 201



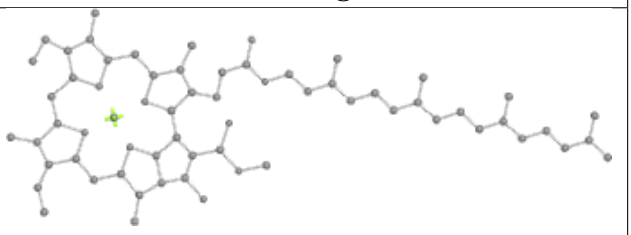
Bond lengths



Bond angles

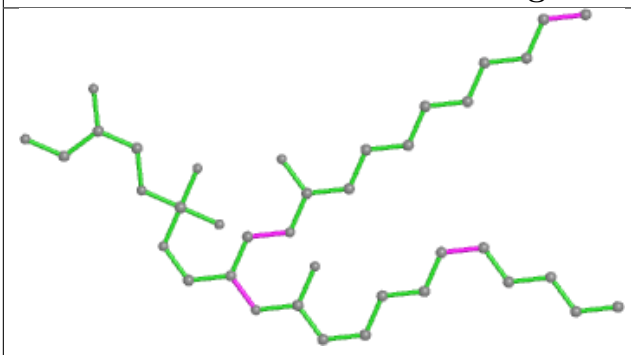


Torsions

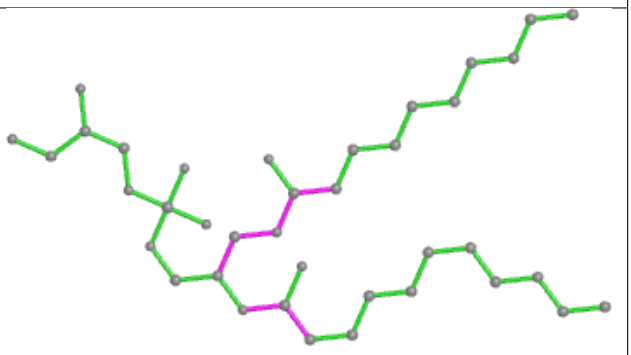


Rings

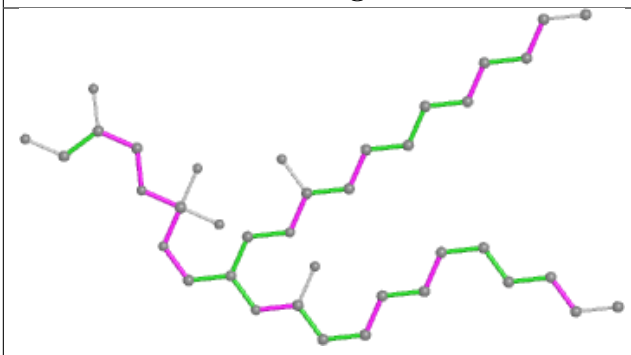
Ligand OZ2 C 303



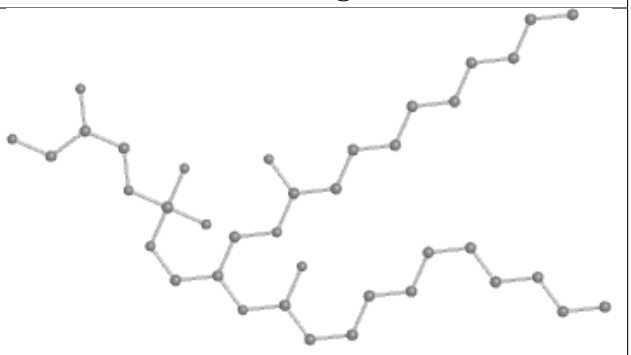
Bond lengths



Bond angles

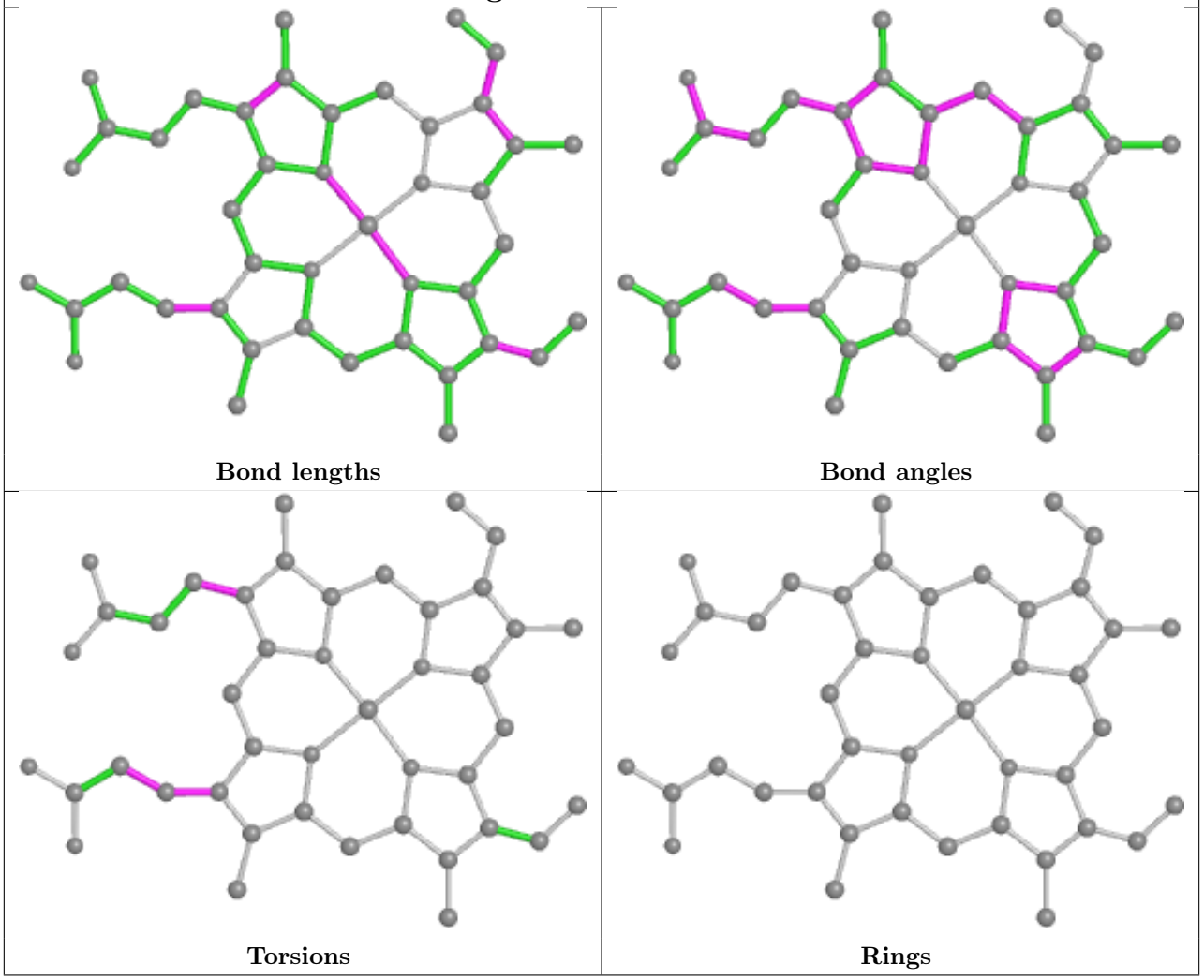


Torsions



Rings

Ligand HEM A 303



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%)	0.08	0 100 100	47, 65, 96, 135	0
2	B	159/160 (99%)	0.21	8 (5%) 28 19	51, 85, 126, 184	0
3	C	288/289 (99%)	0.93	66 (22%) 0 0	58, 95, 219, 257	1 (0%)
4	D	38/179 (21%)	0.53	6 (15%) 2 1	51, 76, 168, 214	0
5	E	28/32 (87%)	0.25	3 (10%) 6 3	83, 95, 118, 139	0
6	F	31/35 (88%)	0.32	2 (6%) 18 11	72, 87, 125, 131	0
7	G	35/37 (94%)	1.08	7 (20%) 1 0	62, 84, 193, 242	0
8	H	28/29 (96%)	0.12	0 100 100	67, 76, 99, 122	0
All	All	820/976 (84%)	0.49	92 (11%) 5 3	47, 84, 185, 257	1 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	206	THR	11.1
3	C	220	SER	9.7
3	C	219	VAL	9.3
7	G	35	LEU	7.2
7	G	36	GLY	7.2
3	C	207	VAL	7.0
3	C	176	ALA	6.9
3	C	190	TYR	6.9
3	C	287	MET	6.7
7	G	33	ASN	6.4
3	C	179	THR	5.7
4	D	10	VAL	5.6
3	C	208	VAL	5.5
3	C	224	ALA	5.1
3	C	191	GLY	5.1
3	C	199	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
3	C	288	ASN	4.9
4	D	9	ASP	4.6
3	C	203	SER	4.4
3	C	195	TYR	4.2
3	C	92	GLU	4.1
3	C	192	ASN	4.1
2	B	160	PHE	4.0
3	C	201	THR	4.0
3	C	204	GLY	3.9
3	C	177	THR	3.9
3	C	181	THR	3.8
3	C	180	ILE	3.8
3	C	200	GLN	3.8
3	C	188	ASP	3.7
3	C	205	LYS	3.7
3	C	211	ILE	3.6
3	C	218	ILE	3.6
3	C	140	LYS	3.6
3	C	230	ALA	3.6
3	C	172	PHE	3.6
3	C	96	LYS	3.5
3	C	217	LEU	3.5
7	G	37	GLY	3.3
3	C	95	LYS	3.3
2	B	151	LEU	3.3
3	C	197	VAL	3.2
3	C	189	GLU	3.2
3	C	193	VAL	3.1
4	D	13	MET	3.0
3	C	187	GLU	3.0
3	C	222	GLY	3.0
3	C	173	THR	2.9
3	C	202	ASP	2.9
3	C	215	PRO	2.9
2	B	2	ALA	2.8
3	C	196	GLN	2.8
2	B	158	GLY	2.8
3	C	186	GLU	2.8
3	C	226	LYS	2.7
3	C	98	VAL	2.7
3	C	170	ASN	2.7
3	C	184	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	174	ALA	2.7
7	G	31	ARG	2.7
3	C	194	LYS	2.6
5	E	29	ILE	2.6
3	C	182	LYS	2.6
3	C	4	TRP	2.6
4	D	15	ARG	2.5
3	C	227	ALA	2.5
2	B	159	LEU	2.4
6	F	29	ILE	2.4
3	C	198	SER	2.4
3	C	286	GLU	2.4
3	C	178	GLY	2.3
2	B	75	ILE	2.3
3	C	175	SER	2.3
6	F	27	LEU	2.3
2	B	153	LYS	2.3
7	G	26	TYR	2.2
3	C	231	LEU	2.2
3	C	90	ILE	2.2
7	G	32	PRO	2.2
2	B	74	GLU	2.2
3	C	93	GLU	2.2
5	E	23	ILE	2.2
4	D	17	GLN	2.1
3	C	281	LYS	2.1
3	C	228	GLY	2.1
5	E	28	SER	2.1
3	C	223	GLN	2.1
3	C	212	PRO	2.1
4	D	14	GLY	2.0
3	C	229	GLU	2.0
3	C	183	ILE	2.0
3	C	94	LEU	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)

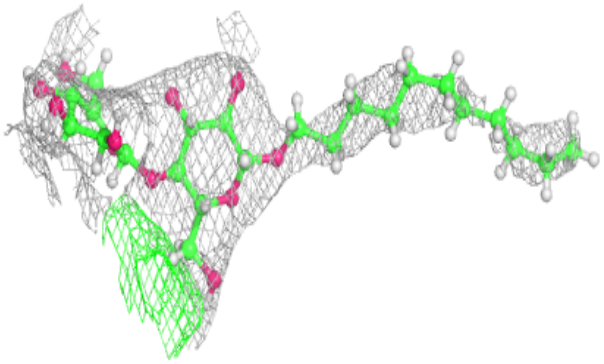
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

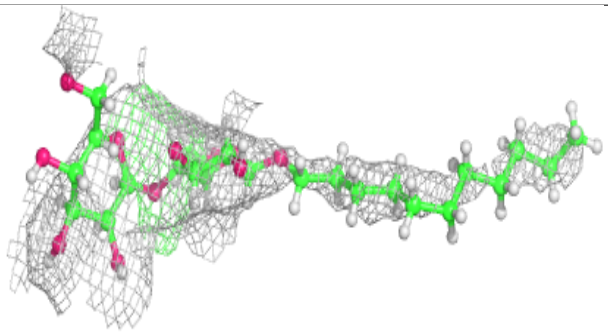
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	UMQ	A	306	34/34	0.68	0.39	85,138,194,197	0
11	8K6	A	305	18/18	0.71	0.45	96,120,123,123	0
15	OZ2	C	303	38/48	0.75	0.34	54,108,185,186	0
17	OCT	F	101	8/8	0.78	0.47	102,123,135,135	0
15	OZ2	G	102	44/48	0.81	0.27	58,102,166,169	0
12	UMQ	A	307	34/34	0.81	0.47	115,144,174,177	0
12	UMQ	A	308	34/34	0.83	0.38	109,146,192,197	0
10	MYS	A	304	15/15	0.85	0.26	77,94,102,102	0
18	BCR	G	101	40/40	0.86	0.33	68,95,177,180	0
16	1E2	D	201	23/23	0.91	0.17	104,110,123,134	0
15	OZ2	B	203	32/48	0.93	0.17	91,97,127,128	0
14	CLA	B	201	65/65	0.93	0.23	68,98,132,135	0
13	CD	C	302	1/1	0.94	0.17	142,142,142,142	0
9	HEM	A	303	43/43	0.96	0.26	50,74,88,89	0
9	HEM	C	301	43/43	0.97	0.20	76,82,98,107	0
13	CD	B	202	1/1	0.98	0.22	124,124,124,124	0
9	HEM	A	302	43/43	0.98	0.27	51,64,74,79	0
9	HEM	A	301	43/43	0.98	0.25	38,50,63,75	0
13	CD	A	309	1/1	0.99	0.20	85,85,85,85	0

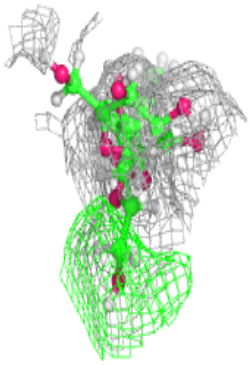
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

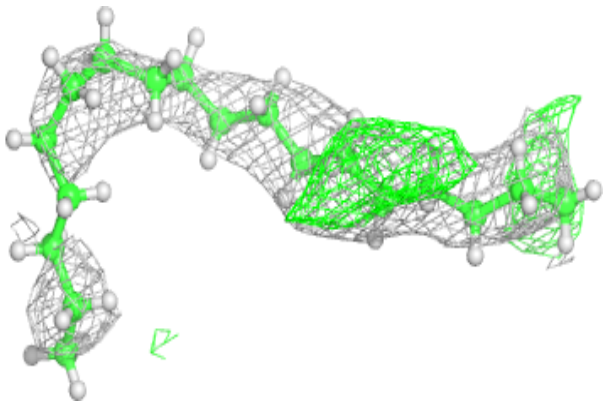


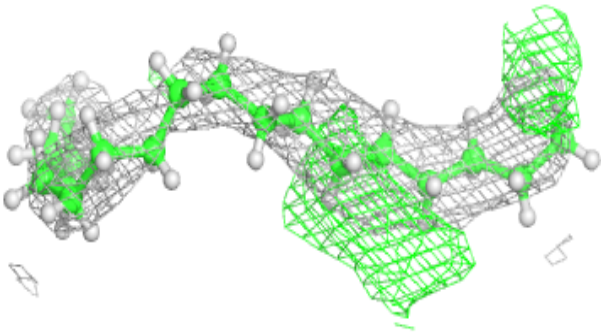


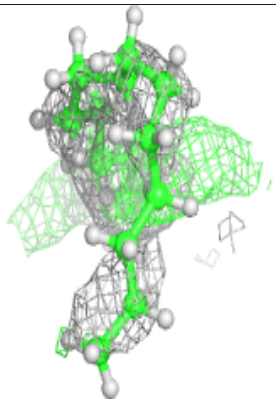


Electron density around 8K6 A 305:

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

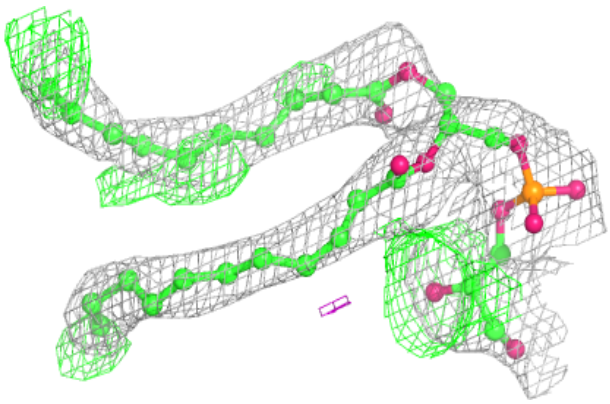


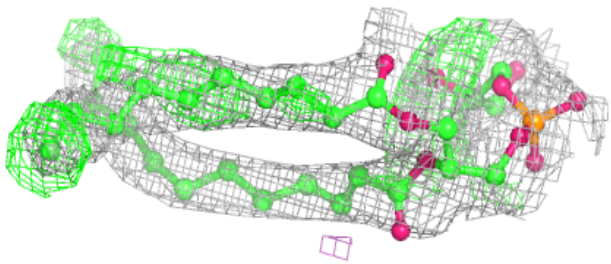


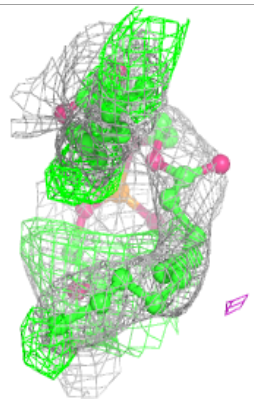


Electron density around OZ2 C 303:

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

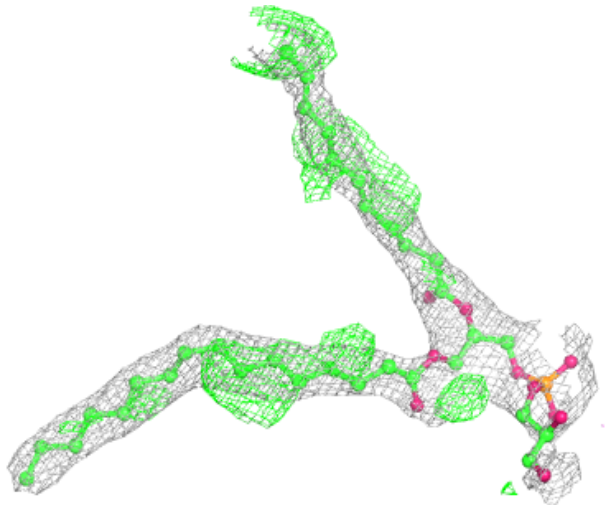


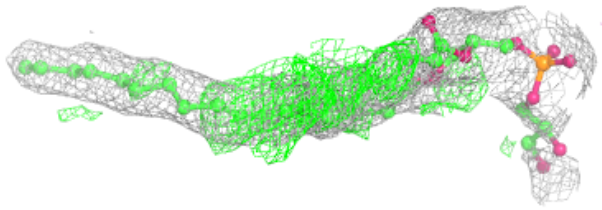


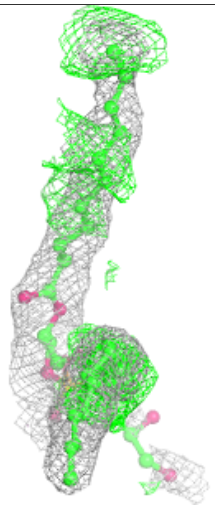


Electron density around OZ2 G 102:

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

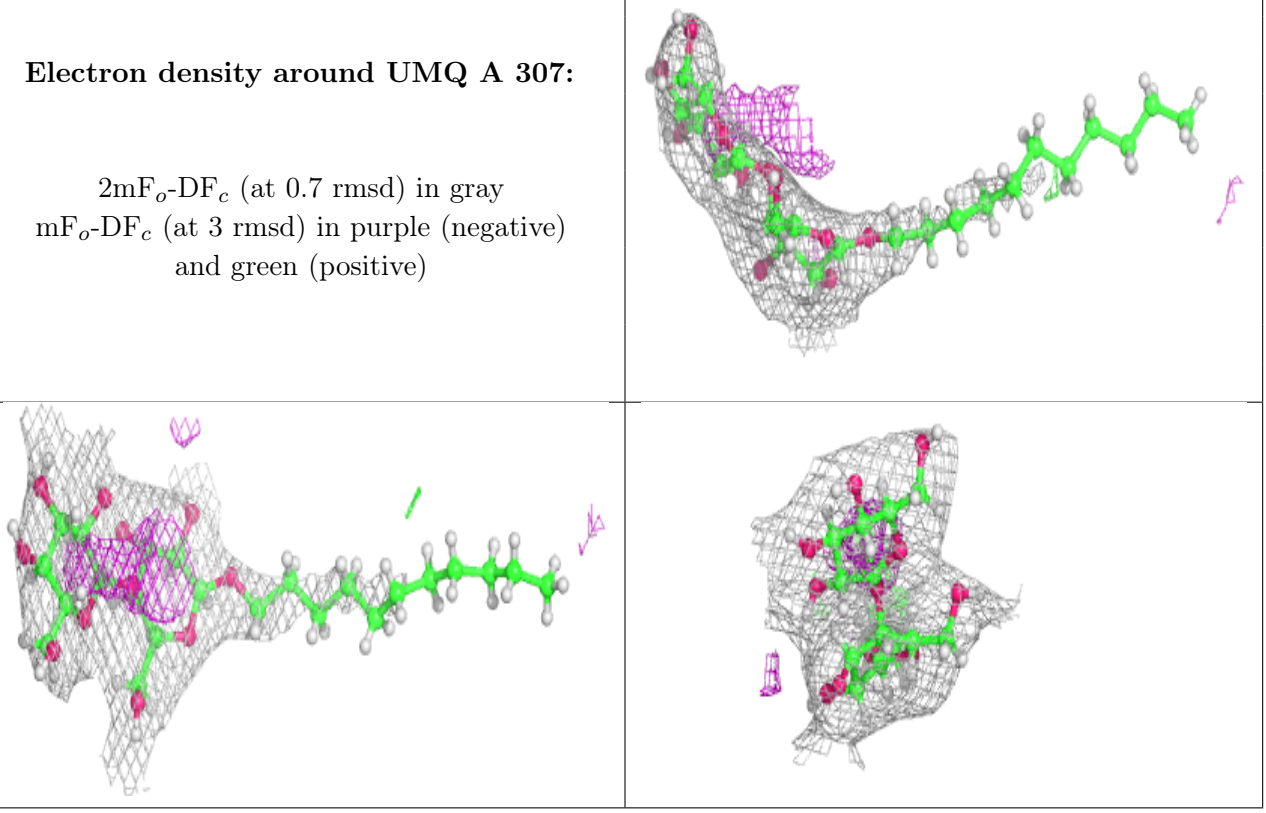






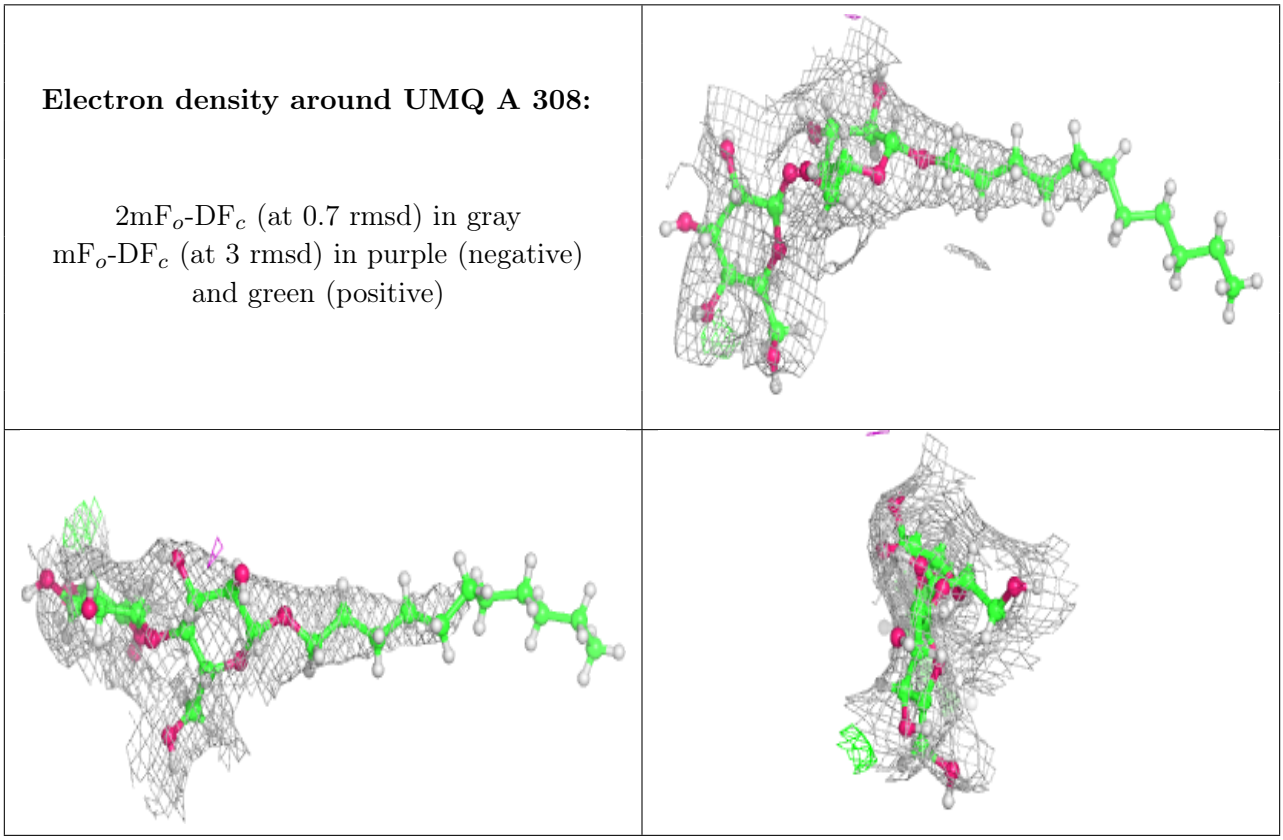
Electron density around UMQ A 307:

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



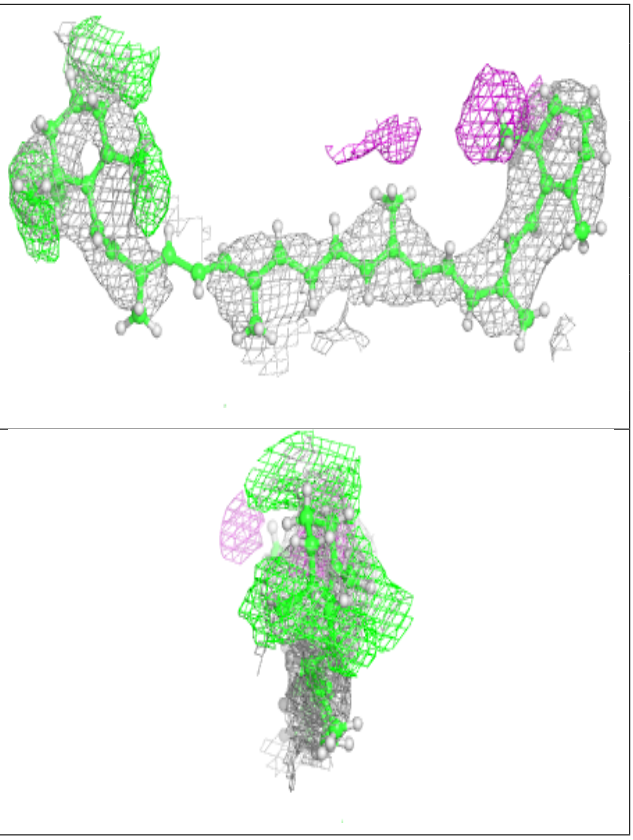
Electron density around UMQ A 308:

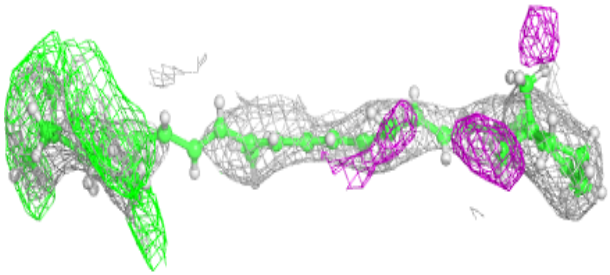
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCR G 101:

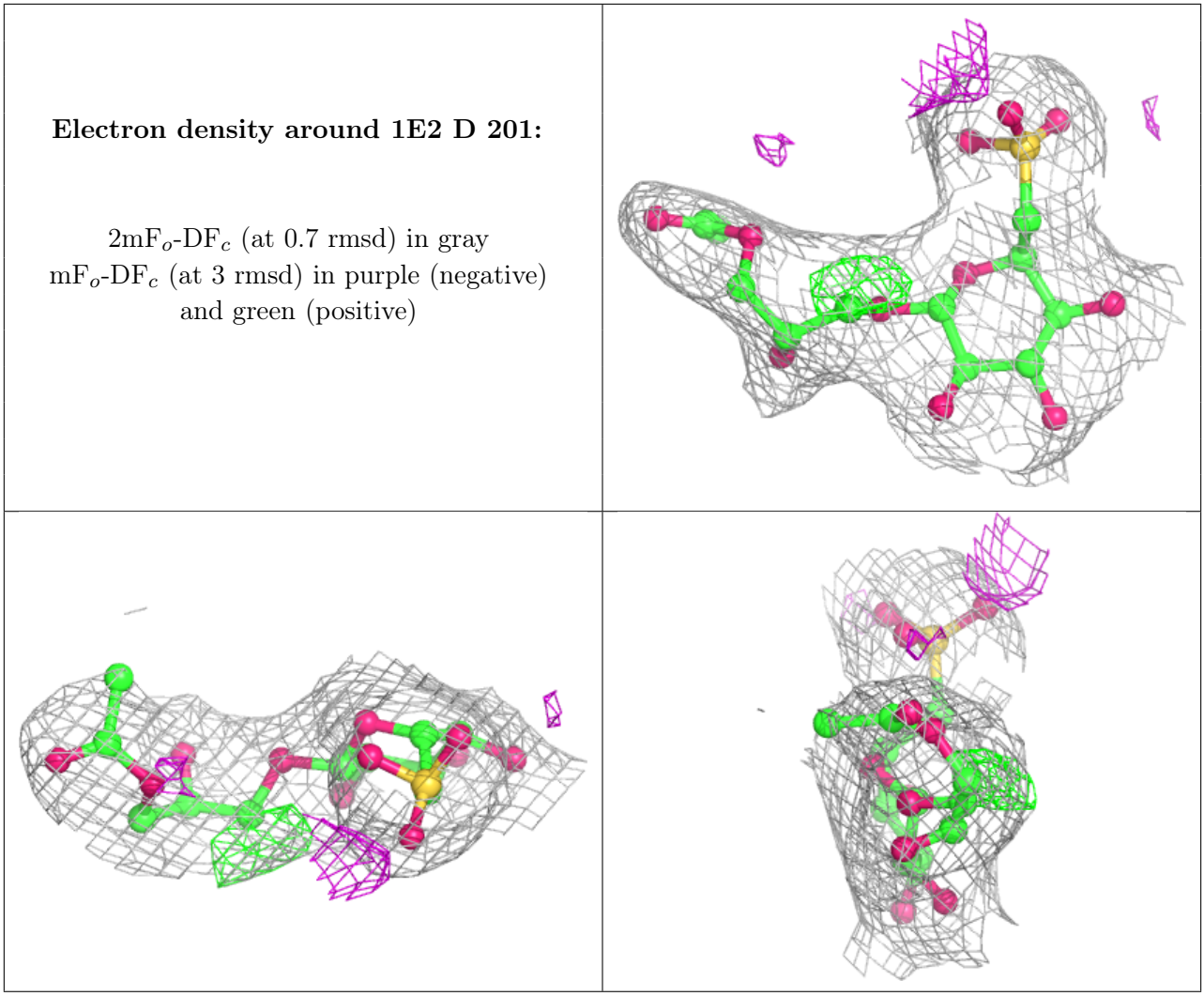
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





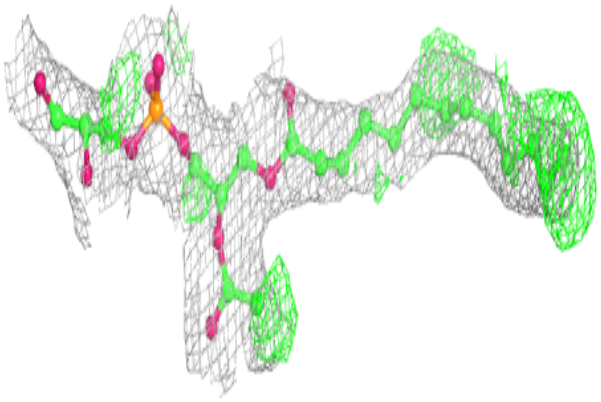
Electron density around 1E2 D 201:

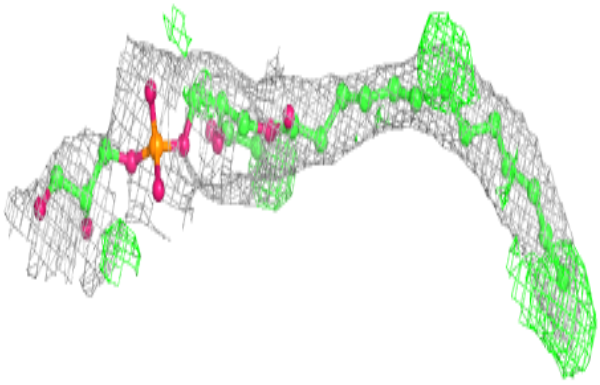
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

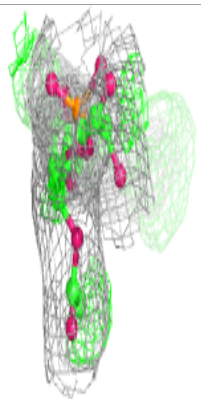


Electron density around OZ2 B 203:

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

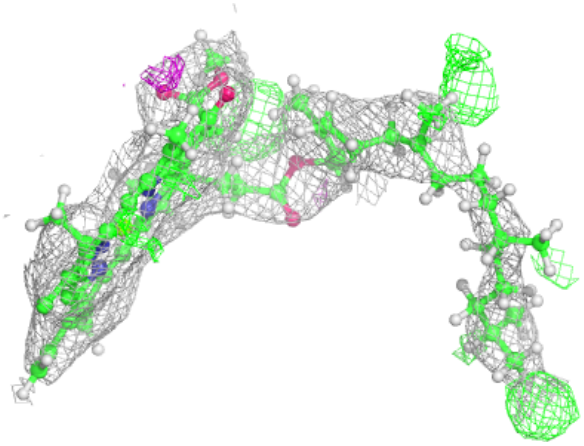


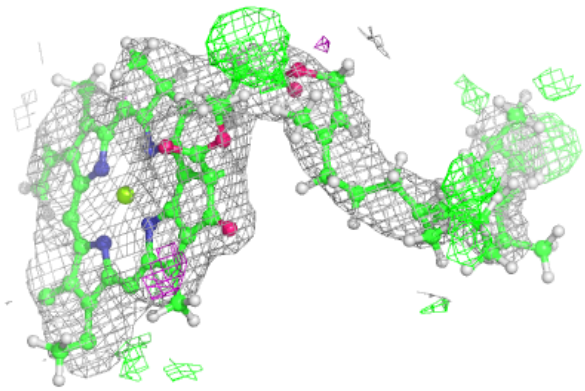


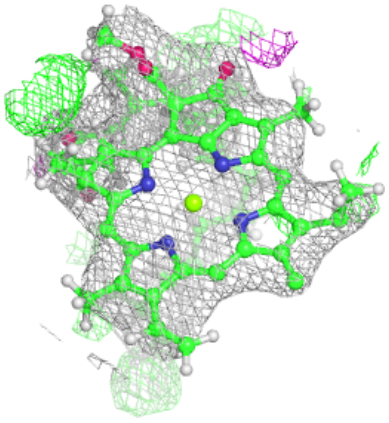


Electron density around CLA B 201:

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

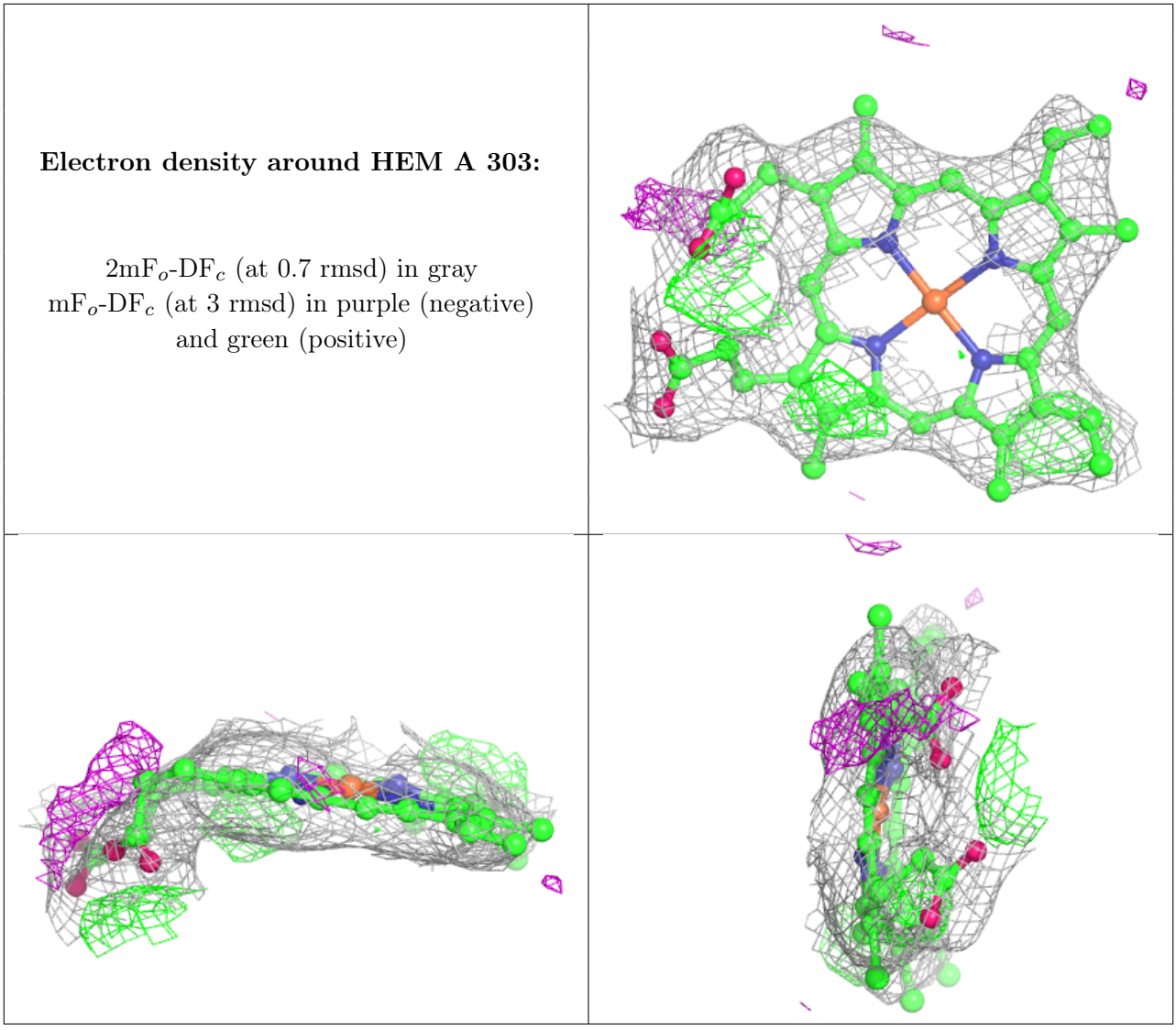






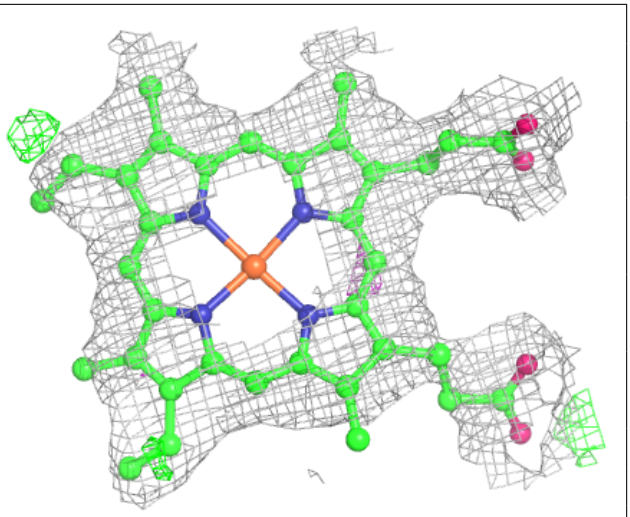
Electron density around HEM A 303:

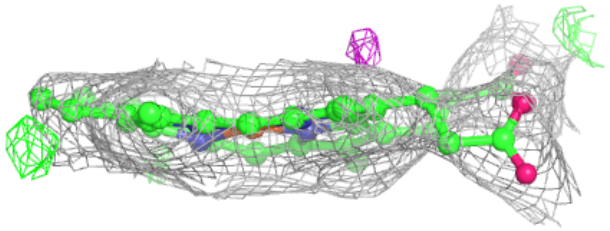
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

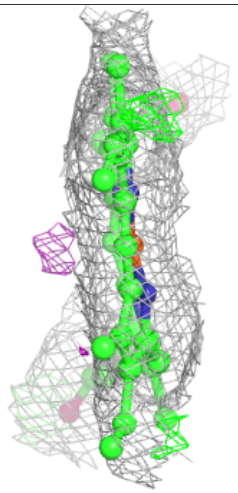


Electron density around HEM C 301:

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

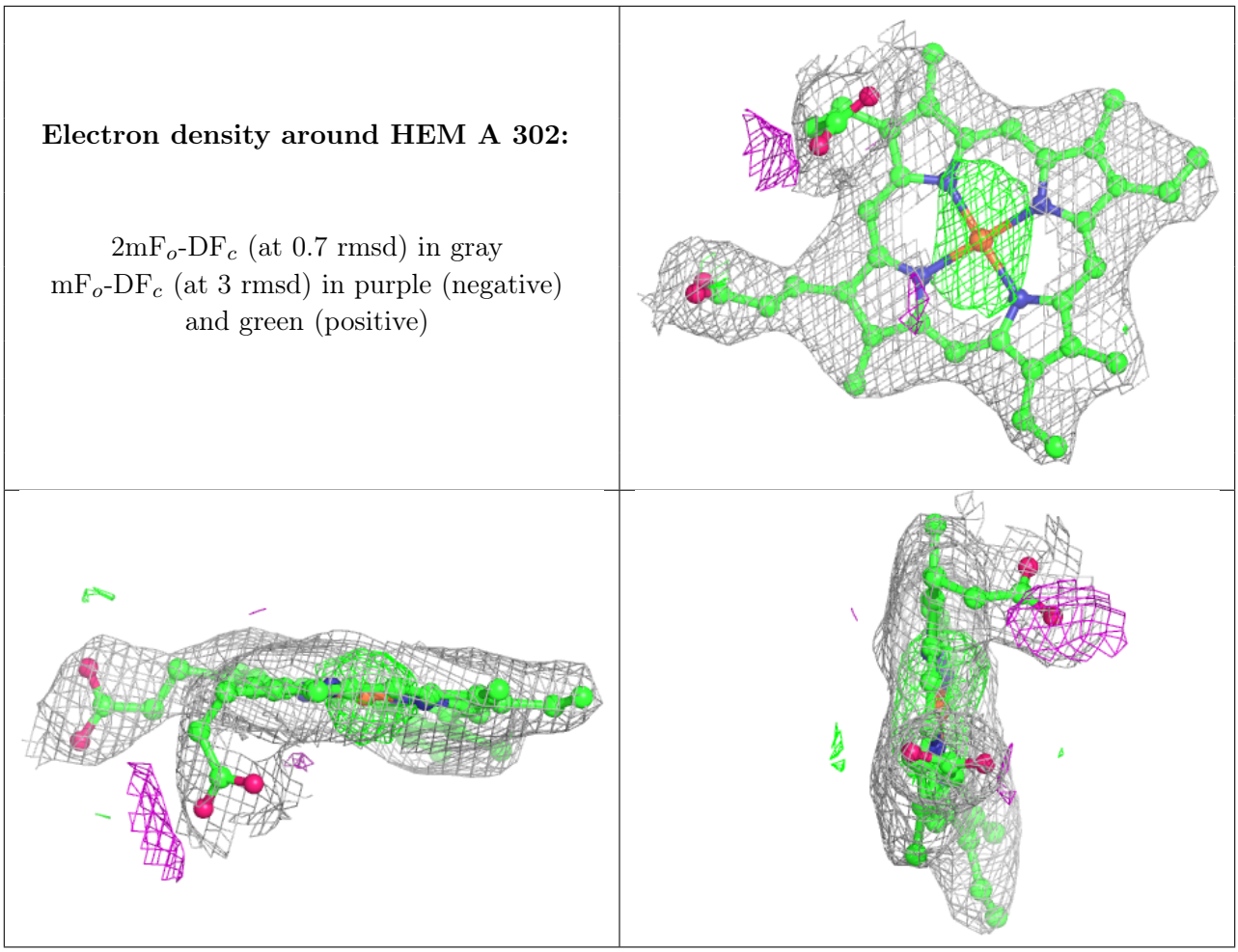






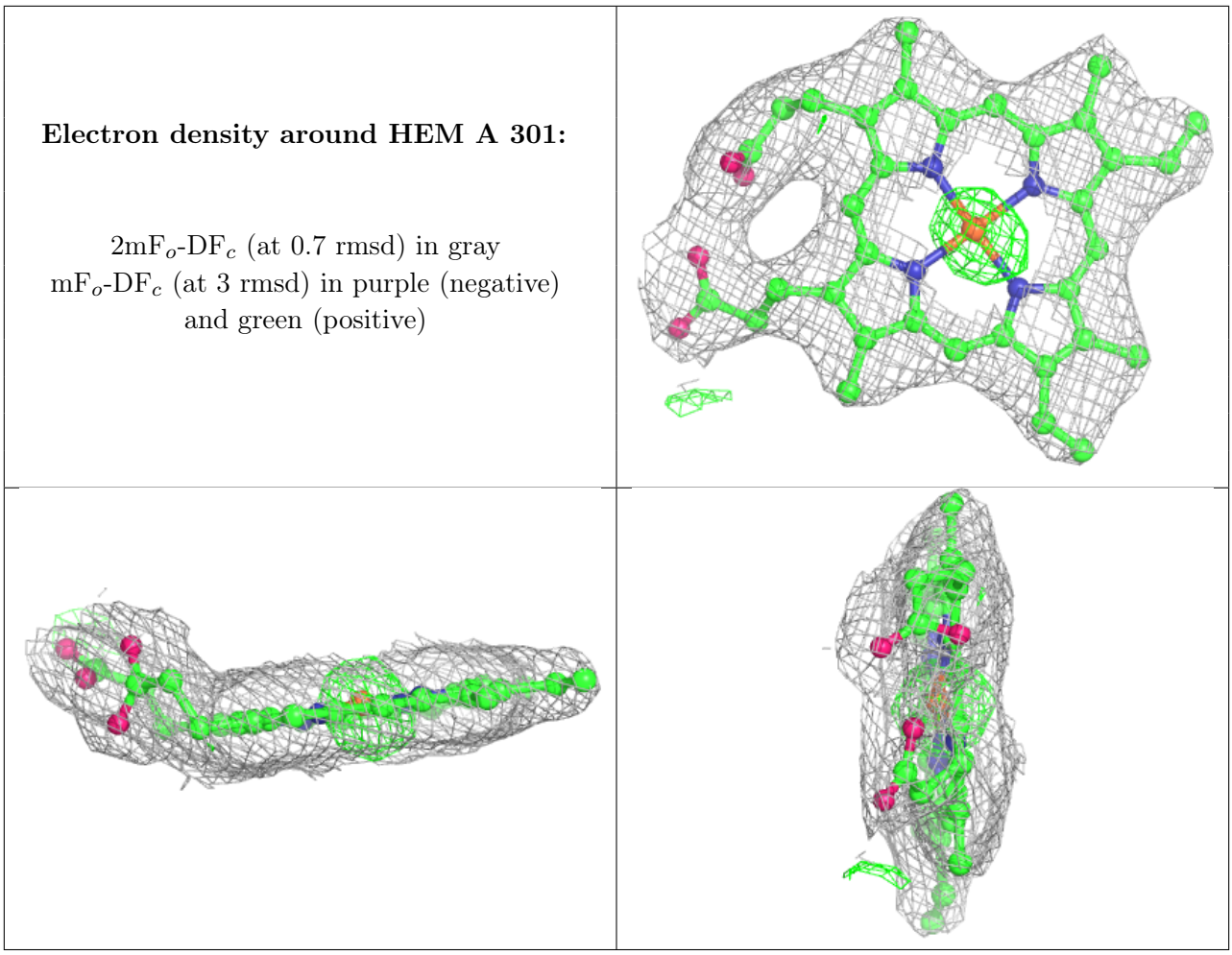
Electron density around HEM A 302:

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



Electron density around HEM 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)



6.5 Other polymers

There are no such residues in this entry.