



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:32 AM UTC

PDB ID : 4I7Z / pdb_00004i7z
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:

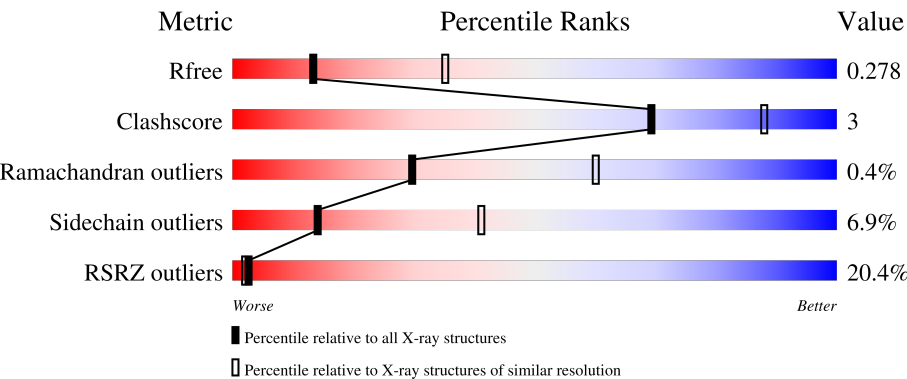
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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.



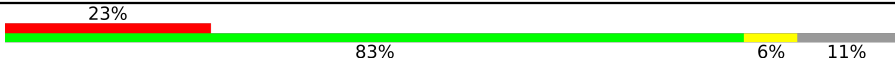
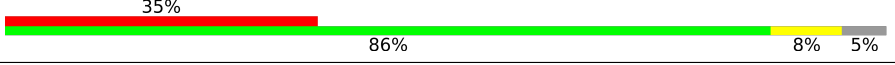
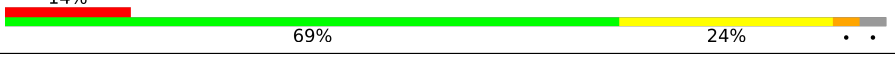
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	3% 88% 11% .
2	B	160	14% 94% 6% .
3	C	289	33% 87% 13%
4	D	179	4% 21% 79% .
5	E	32	31% 88% 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
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	-	-	-

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
1	A	213	Total	C	H	N	O	S	0	0	0
			3419	1132	1721	270	286	10			

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

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

- Molecule 3 is a protein called Apocytochrome f.

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

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
4	D	38	Total	C	H	N	O	S	0	0	0
			591	194	299	47	49	2			

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

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

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

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

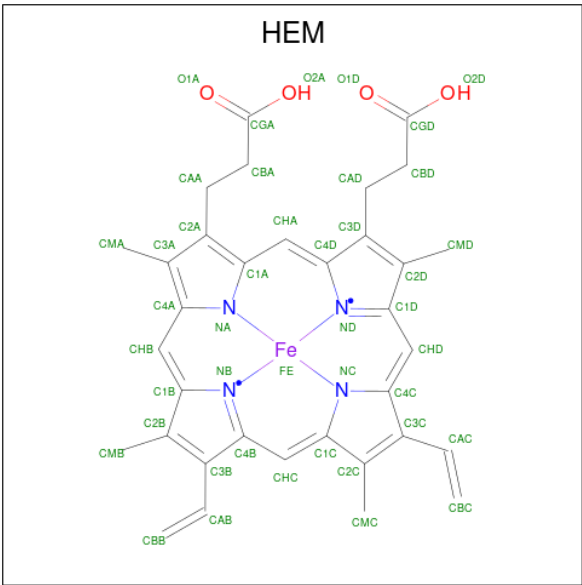
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

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

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

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

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



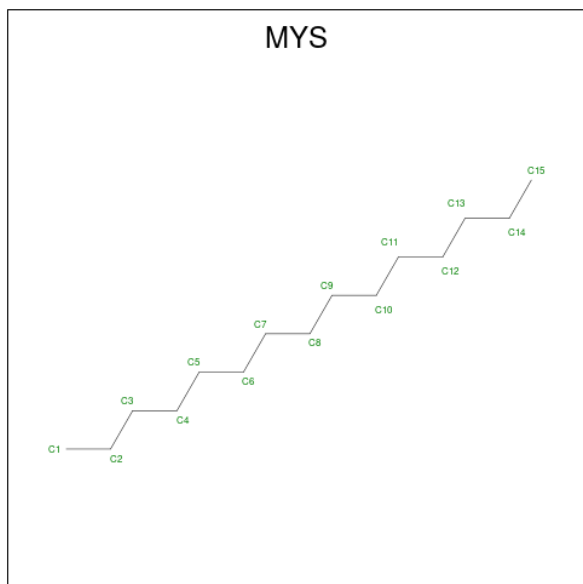
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	N	O			
9	A	1	43	34	1	4	4		0	0
9	A	1	43	34	1	4	4		0	0
9	A	1	43	34	1	4	4		0	0

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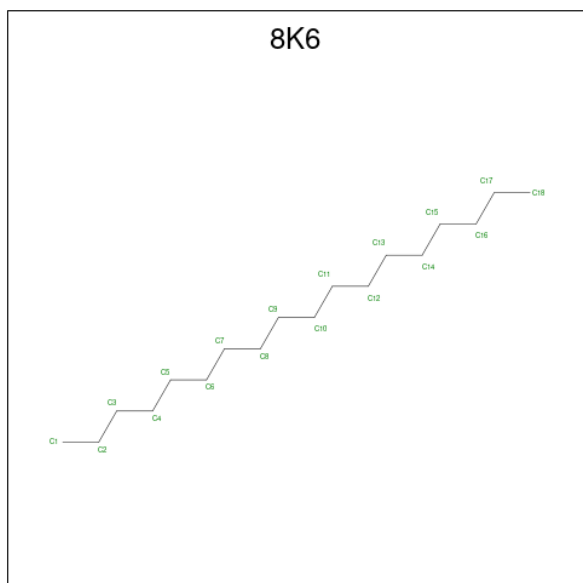
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is PENTADECANE (CCD ID: MYS) (formula: $C_{15}H_{32}$).



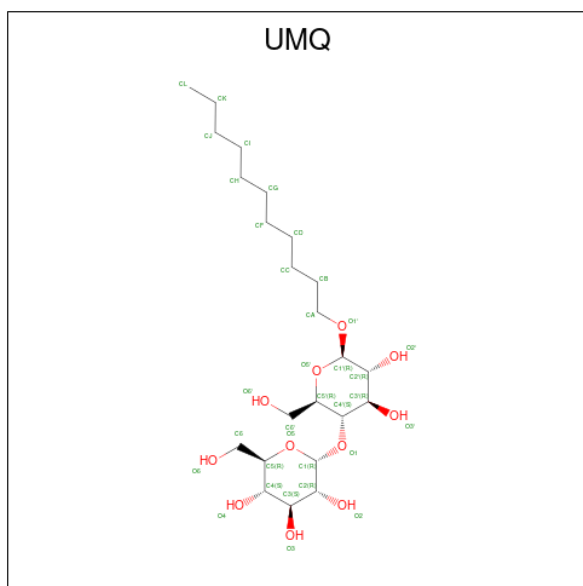
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	H	0	0
			47	15	32		

- Molecule 11 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).



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

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

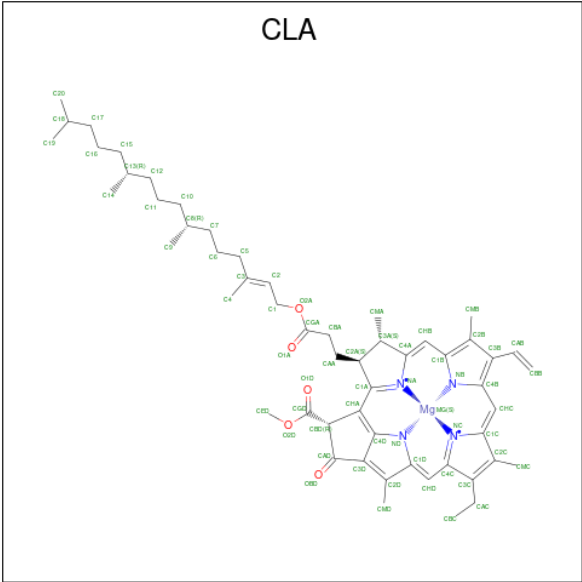


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			78	23	44	11		

- Molecule 13 is CADMIUM ION (CCD ID: CD) (formula: Cd).

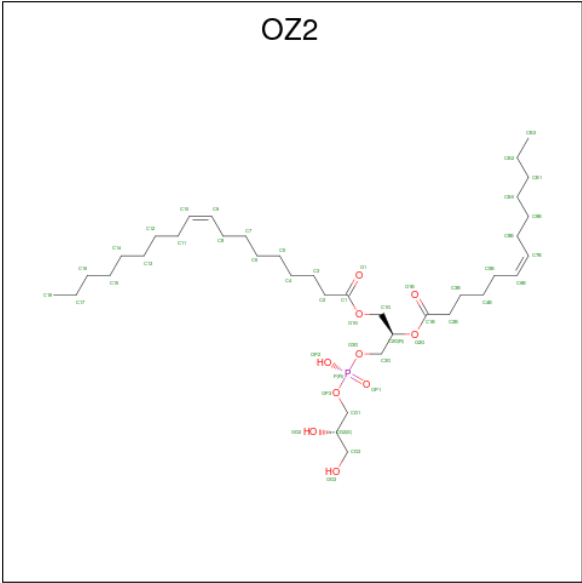
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Cd	0	0
			1	1		
13	B	1	Total	Cd	0	0
			1	1		
13	C	1	Total	Cd	0	0
			1	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
14	B	1	129	55	64	1	4	5	0	0

- Molecule 15 is (2R)-3-{[(R)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-2-[(6Z)-tridec-6-enoyloxy]propyl (9Z)-octadec-9-enoate (CCD ID: OZ2) (formula: C₃₇H₆₉O₁₀P).



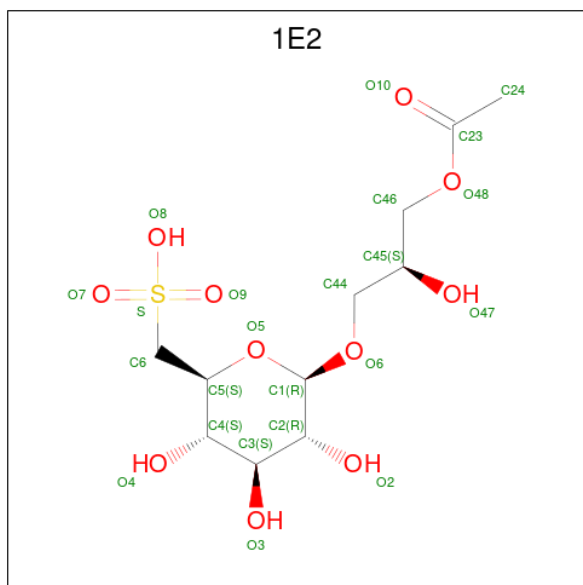
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
15	B	1	32	21	10	1	0	0
15	C	1	38	27	10	1	0	0

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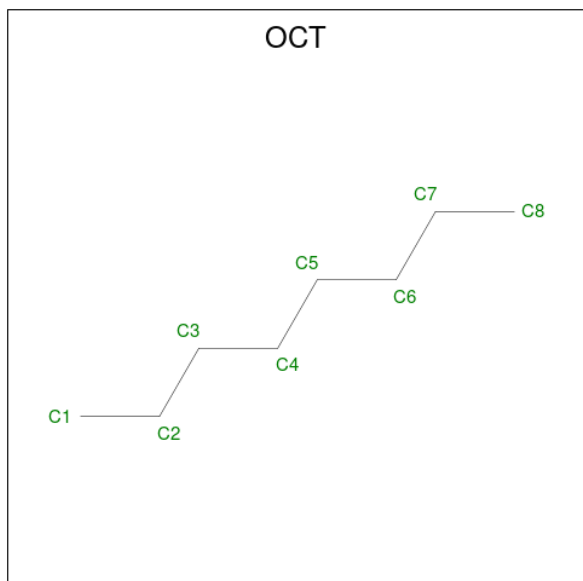
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	G	1	Total	C	O	P	0	0
			44	33	10	1		

- Molecule 16 is (2S)-3-(acetyloxy)-2-hydroxypropyl 6-deoxy-6-sulfo-beta-D-glucopyranoside (CCD ID: 1E2) (formula: C₁₁H₂₀O₁₁S).



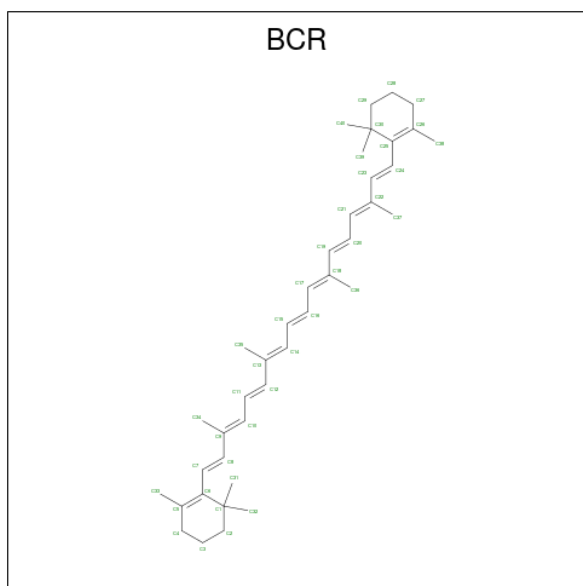
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	O	S	0	0
			23	11	11	1		

- Molecule 17 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



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

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



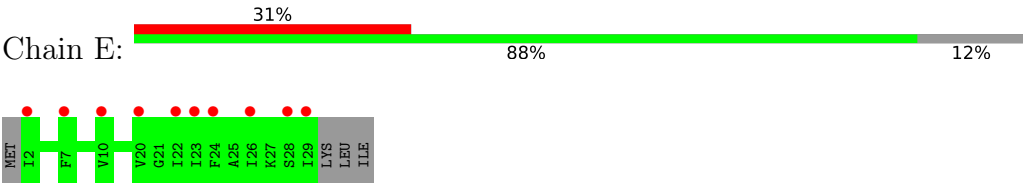
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	G	1	Total	C	H	0	0
			96	40	56		

- Molecule 19 is water.

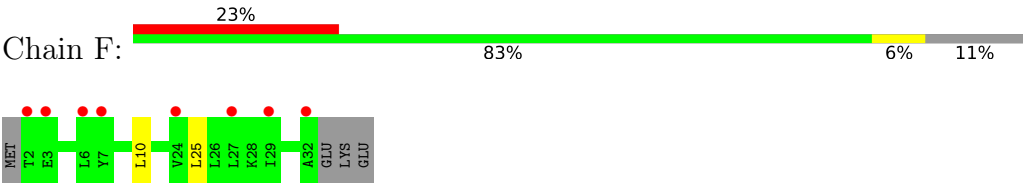
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	8	Total	O	0	0
			8	8		
19	B	4	Total	O	0	0
			4	4		
19	C	1	Total	O	0	0
			1	1		

LEU	SER	LEU	ALA	LEU	CYS	HIS	ALA	THR	VAL	GLN	ASP	ASP	ASN	ILE	VAL	LEU	THR	PRO	TRP	THR	THR	GLU	THR	ASP	PHE	ARG	THR	GLY	GLU	LYS	PRO	TRP	TRP	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

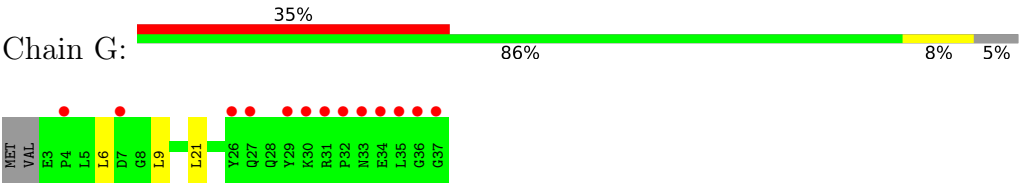
● Molecule 5: Cytochrome b6-f complex subunit 6



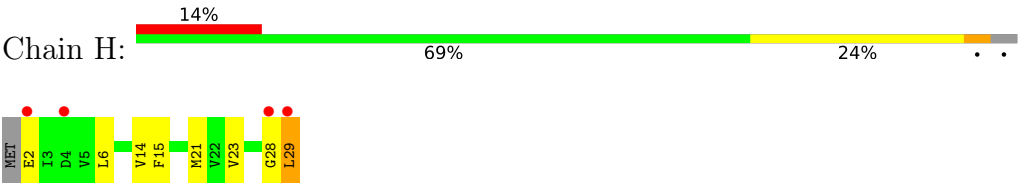
● Molecule 6: Cytochrome b6-f complex subunit 7



● Molecule 7: Cytochrome b6-f complex subunit 5



● Molecule 8: Cytochrome b6-f complex subunit 8



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309, REFMAC	Depositor
R, R_{free}	0.248 , 0.272 0.255 , 0.278	Depositor DCC
R_{free} test set	3406 reflections (5.04%)	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)	0.35 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, MYS, BCR, OCT, CD, OZ2, 1E2, 8K6, CLA, 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	0.39	0/1750	0.71	0/2388
2	B	0.35	0/1280	0.68	0/1755
3	C	0.34	0/2264	0.65	0/3082
4	D	0.36	0/300	0.67	0/408
5	E	0.39	0/220	0.76	0/297
6	F	0.30	0/238	0.67	0/321
7	G	0.32	0/274	0.65	0/371
8	H	0.38	0/228	0.77	0/313
All	All	0.36	0/6554	0.68	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 [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	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	24	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	1	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	1	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:HBC2	9:A:303:HEM:HMC2	1.51	0.91
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: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
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
3:C:226:LYS:HG3	3:C:227:ALA:H	1.85	0.41
1:A:199:MET:HE2	9:A:302:HEM:HMB3	2.03	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
9:A:303:HEM:HMC2	9:A:303:HEM:CBC	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	12	38
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%)	30	60

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

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%)	170 (93%)	13 (7%)	13	39
2	B	136/137 (99%)	132 (97%)	4 (3%)	37	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	242/243 (100%)	223 (92%)	19 (8%)	11	35
4	D	31/146 (21%)	30 (97%)	1 (3%)	34	70
5	E	21/25 (84%)	21 (100%)	0	100	100
6	F	23/27 (85%)	21 (91%)	2 (9%)	9	30
7	G	26/28 (93%)	23 (88%)	3 (12%)	5	18
8	H	23/24 (96%)	18 (78%)	5 (22%)	1	3
All	All	685/814 (84%)	638 (93%)	47 (7%)	14	41

All (47) 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	36	LEU
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	75	ILE
2	B	96	LEU
2	B	108	LEU
3	C	57	LYS
3	C	58	LEU
3	C	70	LEU
3	C	116	VAL
3	C	131	VAL
3	C	140	LYS
3	C	189	GLU
3	C	194	LYS
3	C	200	GLN
3	C	201	THR
3	C	218	ILE
3	C	232	THR

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Mol	Chain	Res	Type
3	C	233	ASN
3	C	249	LEU
3	C	254	ARG
3	C	264	LEU
3	C	267	LEU
3	C	271	MET
3	C	278	GLN
4	D	22	LEU
6	F	10	LEU
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. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
3	C	110	GLN
3	C	135	ASN
3	C	200	GLN
3	C	234	ASN
7	G	33	ASN
8	H	27	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 [i](#)

There are no oligosaccharides 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
15	OZ2	G	102	-	43,43,47	1.19	4 (9%)	46,49,53	1.16	2 (4%)
11	8K6	A	305	-	17,17,17	0.25	0	16,16,16	0.55	0
9	HEM	A	302	1	50,50,50	1.82	9 (18%)	67,82,82	1.21	3 (4%)
15	OZ2	B	203	-	31,31,47	1.27	3 (9%)	34,37,53	1.53	5 (14%)
17	OCT	F	101	-	7,7,7	0.31	0	6,6,6	0.66	0
10	MYS	A	304	-	14,14,14	0.40	0	13,13,13	0.79	0
12	UMQ	A	306	-	35,35,35	1.23	5 (14%)	46,46,46	2.34	11 (23%)
14	CLA	B	201	19	69,73,73	1.18	6 (8%)	82,113,113	1.35	7 (8%)
15	OZ2	C	303	-	37,37,47	1.27	4 (10%)	40,43,53	1.23	3 (7%)
9	HEM	A	301	1	50,50,50	1.81	10 (20%)	67,82,82	1.21	5 (7%)
16	1E2	D	201	-	21,23,23	1.79	1 (4%)	30,33,33	2.78	8 (26%)
18	BCR	G	101	-	41,41,41	2.09	18 (43%)	56,56,56	2.29	22 (39%)
9	HEM	C	301	3	50,50,50	1.86	11 (22%)	67,82,82	1.32	6 (8%)
12	UMQ	A	307	-	35,35,35	1.29	5 (14%)	46,46,46	2.48	11 (23%)
9	HEM	A	303	19	50,50,50	1.99	9 (18%)	67,82,82	1.44	8 (11%)
12	UMQ	A	308	-	35,35,35	1.29	6 (17%)	46,46,46	2.02	9 (19%)

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
15	OZ2	G	102	-	-	13/48/48/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	8K6	A	305	-	-	4/15/15/15	-
9	HEM	A	302	1	-	2/14/54/54	-
15	OZ2	B	203	-	1/1/5/9	12/35/35/52	-
17	OCT	F	101	-	-	0/5/5/5	-
10	MYS	A	304	-	-	2/12/12/12	-
12	UMQ	A	306	-	3/3/10/10	9/20/60/60	0/2/2/2
14	CLA	B	201	19	1/1/17/20	15/39/115/115	-
9	HEM	C	301	3	-	5/14/54/54	-
15	OZ2	C	303	-	-	15/42/42/52	-
9	HEM	A	301	1	-	5/14/54/54	-
9	HEM	A	303	19	-	5/14/54/54	-
18	BCR	G	101	-	-	17/29/63/63	0/2/2/2
16	1E2	D	201	-	1/1/8/8	6/15/35/35	0/1/1/1
12	UMQ	A	307	-	3/3/10/10	8/20/60/60	0/2/2/2
12	UMQ	A	308	-	2/2/10/10	5/20/60/60	0/2/2/2

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	301	HEM	C3D-C2D	7.81	1.53	1.36
9	A	301	HEM	C3D-C2D	7.77	1.53	1.36
9	A	302	HEM	C3D-C2D	7.76	1.53	1.36
9	A	303	HEM	C3D-C2D	7.54	1.53	1.36
16	D	201	1E2	O47-C45	-6.61	1.24	1.43
9	C	301	HEM	FE-NB	5.52	2.11	1.94
9	A	303	HEM	FE-ND	5.44	2.11	1.94
9	A	303	HEM	FE-NB	4.56	2.08	1.94
9	A	303	HEM	FE-NC	4.26	2.09	1.95
9	A	301	HEM	FE-NA	4.16	2.08	1.95
9	A	302	HEM	FE-ND	3.97	2.07	1.94
9	A	303	HEM	FE-NA	3.92	2.08	1.95
9	A	302	HEM	FE-NB	3.77	2.06	1.94
15	G	102	OZ2	C10-C9	3.73	1.52	1.31
15	B	203	OZ2	O2G-C2G	-3.64	1.38	1.46
15	G	102	OZ2	C7B-C6B	3.58	1.52	1.31
9	A	302	HEM	FE-NC	3.54	2.06	1.95
15	C	303	OZ2	O2G-C2G	-3.54	1.38	1.46
14	B	201	CLA	C4B-NB	3.48	1.42	1.37
18	G	101	BCR	C26-C25	3.47	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	101	BCR	C20-C21	3.46	1.53	1.43
9	A	301	HEM	FE-ND	3.45	2.05	1.94
14	B	201	CLA	C1D-ND	3.39	1.42	1.37
18	G	101	BCR	C23-C22	3.33	1.53	1.46
18	G	101	BCR	C15-C14	3.27	1.53	1.43
9	C	301	HEM	FE-NA	3.22	2.05	1.95
15	B	203	OZ2	C10-C9	3.22	1.50	1.31
18	G	101	BCR	C16-C17	3.17	1.53	1.43
15	C	303	OZ2	C10-C9	3.17	1.49	1.29
15	C	303	OZ2	C7B-C6B	3.17	1.49	1.31
9	A	301	HEM	FE-NB	3.16	2.04	1.94
18	G	101	BCR	C11-C10	3.15	1.53	1.43
15	G	102	OZ2	O2G-C2G	-3.12	1.39	1.46
18	G	101	BCR	C8-C9	3.08	1.52	1.46
9	A	303	HEM	CAB-C3B	3.04	1.55	1.47
12	A	307	UMQ	C4-C5	-3.01	1.46	1.53
9	C	301	HEM	FE-ND	2.98	2.04	1.94
9	A	301	HEM	CAC-C3C	2.94	1.55	1.47
9	A	301	HEM	CAB-C3B	2.94	1.55	1.47
9	A	302	HEM	CAC-C3C	2.92	1.55	1.47
18	G	101	BCR	C32-C1	-2.91	1.48	1.53
18	G	101	BCR	C19-C18	2.89	1.52	1.46
9	C	301	HEM	CAC-C3C	2.87	1.55	1.47
18	G	101	BCR	C12-C13	2.85	1.52	1.46
15	C	303	OZ2	O1G-C1G	-2.82	1.38	1.45
9	A	302	HEM	CAB-C3B	2.80	1.54	1.47
15	B	203	OZ2	O1G-C1G	-2.79	1.38	1.45
9	A	301	HEM	FE-NC	2.78	2.04	1.95
9	A	303	HEM	CAC-C3C	2.75	1.54	1.47
12	A	308	UMQ	O5'-C5'	-2.75	1.37	1.44
9	C	301	HEM	CAB-C3B	2.72	1.54	1.47
14	B	201	CLA	C1B-C2B	2.71	1.49	1.43
12	A	308	UMQ	C4-C5	-2.68	1.47	1.53
12	A	306	UMQ	O5'-C5'	-2.65	1.37	1.44
14	B	201	CLA	C3B-C4B	2.61	1.50	1.42
12	A	307	UMQ	O2'-C2'	-2.58	1.36	1.43
15	G	102	OZ2	O1G-C1	2.44	1.40	1.33
9	C	301	HEM	FE-NC	2.44	2.03	1.95
12	A	308	UMQ	C3-C4	-2.44	1.46	1.52
12	A	306	UMQ	O2'-C2'	-2.43	1.36	1.43
12	A	306	UMQ	C3-C4	-2.43	1.46	1.52
12	A	308	UMQ	O2'-C2'	-2.42	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	307	UMQ	C3-C4	-2.40	1.46	1.52
12	A	306	UMQ	C4-C5	-2.39	1.47	1.53
12	A	307	UMQ	O3'-C3'	-2.37	1.37	1.43
18	G	101	BCR	C24-C25	2.33	1.53	1.45
18	G	101	BCR	C24-C23	2.32	1.40	1.33
12	A	306	UMQ	O3'-C3'	-2.32	1.37	1.43
12	A	307	UMQ	O5'-C5'	-2.31	1.38	1.44
12	A	308	UMQ	O3'-C3'	-2.29	1.37	1.43
14	B	201	CLA	CHC-C1C	2.27	1.43	1.38
9	A	302	HEM	FE-NA	2.24	2.02	1.95
12	A	308	UMQ	C4'-C5'	-2.18	1.47	1.52
18	G	101	BCR	C40-C30	-2.13	1.49	1.53
14	B	201	CLA	CMD-C2D	-2.12	1.46	1.50
18	G	101	BCR	C7-C6	2.12	1.52	1.45
18	G	101	BCR	C31-C1	-2.11	1.49	1.53
9	C	301	HEM	CMD-C2D	2.11	1.55	1.50
9	A	302	HEM	CMA-C3A	2.09	1.55	1.50
9	A	303	HEM	CMC-C2C	2.08	1.55	1.50
9	C	301	HEM	CMC-C2C	2.07	1.55	1.50
9	C	301	HEM	CMB-C2B	2.07	1.55	1.50
9	A	301	HEM	CMB-C2B	2.06	1.55	1.50
9	A	301	HEM	CMA-C3A	2.06	1.55	1.50
9	A	302	HEM	C2A-C3A	-2.05	1.33	1.38
18	G	101	BCR	C5-C6	2.05	1.38	1.34
18	G	101	BCR	C29-C28	-2.04	1.47	1.52
18	G	101	BCR	C20-C19	2.03	1.40	1.34
9	A	303	HEM	CMB-C2B	2.02	1.54	1.50
9	A	301	HEM	CMC-C2C	2.01	1.54	1.50
9	C	301	HEM	CMA-C3A	2.00	1.54	1.50

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	306	UMQ	O5-C5-C4	7.98	124.07	109.70
12	A	307	UMQ	O1'-C1'-C2'	7.32	119.39	108.27
12	A	307	UMQ	O5'-C5'-C4'	7.24	124.68	109.72
16	D	201	1E2	O7-S-C6	7.21	117.53	106.76
14	B	201	CLA	C4A-NA-C1A	6.91	109.83	106.68
12	A	308	UMQ	O5-C5-C4	6.25	120.97	109.70
16	D	201	1E2	O8-S-O9	-6.10	96.14	111.40
16	D	201	1E2	O9-S-C6	-5.74	98.19	106.76
16	D	201	1E2	O8-S-C6	5.71	116.99	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	303	HEM	C4D-ND-C1D	5.67	111.92	105.21
9	C	301	HEM	C4D-ND-C1D	5.46	111.67	105.21
16	D	201	1E2	O7-S-O9	-5.42	96.20	113.82
9	A	302	HEM	C4D-ND-C1D	5.15	111.30	105.21
18	G	101	BCR	C24-C23-C22	-5.08	118.72	126.23
12	A	307	UMQ	O1-C1-C2	5.04	120.49	108.09
12	A	307	UMQ	CA-O1'-C1'	4.97	122.18	113.68
9	A	301	HEM	C4D-ND-C1D	4.90	111.01	105.21
12	A	306	UMQ	O2-C2-C1	4.87	121.67	110.08
12	A	307	UMQ	O5-C1-C2	4.86	120.35	110.37
12	A	308	UMQ	O5-C5-C6	4.80	118.34	106.44
12	A	306	UMQ	O2-C2-C3	4.80	121.68	110.38
12	A	307	UMQ	O5'-C1'-O1'	4.76	121.28	110.04
18	G	101	BCR	C7-C8-C9	-4.74	119.23	126.23
18	G	101	BCR	C15-C14-C13	-4.72	120.66	127.28
12	A	306	UMQ	O1-C1-C2	4.63	119.48	108.09
15	B	203	OZ2	O2G-C1B-C2B	4.61	119.30	111.09
18	G	101	BCR	C16-C17-C18	-4.58	120.85	127.28
12	A	306	UMQ	O5-C5-C6	4.50	117.59	106.44
18	G	101	BCR	C11-C10-C9	-4.47	121.00	127.28
18	G	101	BCR	C2-C1-C6	4.41	116.84	110.44
18	G	101	BCR	C33-C5-C6	-4.36	119.73	124.48
12	A	308	UMQ	O2-C2-C3	4.31	120.54	110.38
12	A	308	UMQ	CA-O1'-C1'	4.31	121.04	113.68
12	A	307	UMQ	O5'-C1'-C2'	4.28	119.16	110.37
12	A	307	UMQ	O5'-C5'-C6'	4.27	117.02	106.44
12	A	308	UMQ	C1-C2-C3	4.22	118.88	110.01
12	A	308	UMQ	O2-C2-C1	4.14	119.94	110.08
12	A	306	UMQ	O5-C1-C2	4.14	118.87	110.37
12	A	306	UMQ	O1-C1-O5	4.07	121.39	110.69
16	D	201	1E2	O8-S-O7	3.96	121.30	111.40
9	A	303	HEM	CAD-C3D-C4D	3.66	131.08	124.70
15	B	203	OZ2	O1G-C1G-C2G	3.63	118.86	108.40
18	G	101	BCR	C20-C21-C22	-3.61	122.22	127.28
15	G	102	OZ2	O2G-C1B-C2B	3.59	119.25	111.48
15	C	303	OZ2	O1G-C1G-C2G	3.57	118.68	108.40
15	C	303	OZ2	O2G-C1B-C2B	3.48	119.00	111.48
18	G	101	BCR	C33-C5-C4	3.40	120.85	113.60
18	G	101	BCR	C38-C26-C25	-3.39	120.78	124.48
14	B	201	CLA	CAA-CBA-CGA	-3.23	104.05	113.21
12	A	307	UMQ	O1-C1-O5	3.17	119.03	110.69
18	G	101	BCR	C23-C24-C25	-3.13	118.63	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	306	UMQ	CA-O1'-C1'	3.13	119.03	113.68
12	A	308	UMQ	C1-O1-C4'	-3.08	110.67	117.98
14	B	201	CLA	C3B-C4B-NB	-3.07	107.79	110.53
15	G	102	OZ2	O1G-C1G-C2G	2.99	117.01	108.40
15	B	203	OZ2	O1G-C1-C2	2.94	120.81	111.83
12	A	306	UMQ	C1-C2-C3	2.91	116.13	110.01
12	A	307	UMQ	C1-O1-C4'	-2.90	111.09	117.98
12	A	308	UMQ	C6-C5-C4	2.85	120.01	113.02
14	B	201	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
9	A	303	HEM	C2A-C1A-NA	-2.81	107.04	110.15
9	C	301	HEM	C3B-C4B-NB	-2.80	107.46	109.47
14	B	201	CLA	C9-C8-C10	2.79	121.23	111.27
18	G	101	BCR	C32-C1-C6	-2.72	105.98	110.24
12	A	306	UMQ	O1'-C1'-C2'	2.71	112.39	108.27
18	G	101	BCR	C38-C26-C27	2.66	119.27	113.60
12	A	307	UMQ	C3'-C4'-C5'	2.62	116.75	110.93
9	A	303	HEM	CAD-C3D-C2D	-2.60	123.00	127.87
18	G	101	BCR	C29-C30-C25	2.58	114.19	110.44
18	G	101	BCR	C16-C15-C14	-2.56	118.27	123.52
15	B	203	OZ2	O2G-C1B-O1B	-2.50	118.16	122.99
9	A	303	HEM	CHD-C1D-ND	2.47	127.09	124.42
9	A	302	HEM	C3B-C2B-C1B	2.47	108.26	106.41
18	G	101	BCR	C34-C9-C10	-2.45	118.84	122.82
18	G	101	BCR	C4-C5-C6	-2.43	119.42	122.70
16	D	201	1E2	O5-C1-C2	-2.40	105.44	110.37
18	G	101	BCR	C20-C19-C18	-2.38	119.83	126.36
18	G	101	BCR	C8-C7-C6	-2.37	120.66	127.00
12	A	308	UMQ	C3'-C4'-C5'	-2.28	105.87	110.93
15	C	303	OZ2	O1G-C1-C2	2.28	118.79	111.83
16	D	201	1E2	O5-C5-C4	-2.27	105.61	109.70
9	A	302	HEM	O2A-CGA-CBA	2.26	121.14	114.00
9	C	301	HEM	C1B-NB-C4B	2.26	107.88	105.21
18	G	101	BCR	C11-C12-C13	-2.24	120.21	126.36
18	G	101	BCR	C1-C6-C5	-2.23	119.59	122.64
9	A	303	HEM	C3B-C2B-C1B	2.22	108.08	106.41
9	C	301	HEM	CAD-CBD-CGD	-2.22	107.78	113.67
14	B	201	CLA	CHB-C4A-NA	2.21	127.59	124.40
9	A	303	HEM	C3D-C4D-ND	-2.19	107.77	110.17
14	B	201	CLA	O2D-CGD-CBD	2.17	115.03	111.23
12	A	306	UMQ	C1'-O5'-C5'	-2.17	109.47	113.72
9	A	301	HEM	C1B-NB-C4B	2.16	107.76	105.21
9	A	301	HEM	CHA-C4D-ND	2.16	127.03	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	303	HEM	O1D-CGD-CBD	-2.14	116.30	123.09
9	C	301	HEM	C3B-C2B-C1B	2.12	108.00	106.41
9	C	301	HEM	CMD-C2D-C1D	2.11	128.34	125.03
9	A	301	HEM	CHB-C1B-NB	2.10	126.97	124.37
15	B	203	OZ2	C2G-O2G-C1B	2.09	121.53	117.85
18	G	101	BCR	C27-C26-C25	-2.04	119.95	122.70
9	A	301	HEM	C3B-C4B-NB	-2.02	108.02	109.47

All (11) chirality outliers are listed below:

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

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
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	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
12	A	306	UMQ	O5-C1-O1-C4'
16	D	201	1E2	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
12	A	307	UMQ	C2-C1-O1-C4'
15	C	303	OZ2	OP3-CG1-CG2-OG2
12	A	308	UMQ	O5'-C5'-C6'-O6'
14	B	201	CLA	CBD-CGD-O2D-CED
12	A	307	UMQ	O5-C5-C6-O6
9	C	301	HEM	C2D-C3D-CAD-CBD
12	A	306	UMQ	O5-C5-C6-O6
12	A	308	UMQ	C4-C5-C6-O6
14	B	201	CLA	C11-C10-C8-C9
16	D	201	1E2	O6-C44-C45-C46
12	A	307	UMQ	C4-C5-C6-O6
16	D	201	1E2	C2-C1-O6-C44
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
14	B	201	CLA	C11-C12-C13-C15
16	D	201	1E2	O10-C23-O48-C46
12	A	308	UMQ	C4'-C5'-C6'-O6'
15	C	303	OZ2	C1-C2-C3-C4
12	A	307	UMQ	O5'-C5'-C6'-O6'
14	B	201	CLA	C8-C10-C11-C12
12	A	307	UMQ	C4'-C5'-C6'-O6'
15	B	203	OZ2	C11-C10-C9-C8
9	C	301	HEM	C4D-C3D-CAD-CBD
12	A	306	UMQ	C2'-C1'-O1'-CA
15	G	102	OZ2	C1B-C2B-C3B-C4B
9	A	302	HEM	C1A-C2A-CAA-CBA
9	A	303	HEM	C1A-C2A-CAA-CBA
18	G	101	BCR	C11-C12-C13-C35
9	A	301	HEM	C2D-C3D-CAD-CBD
18	G	101	BCR	C12-C13-C14-C15
14	B	201	CLA	O1D-CGD-O2D-CED
15	G	102	OZ2	C1-C2-C3-C4
12	A	306	UMQ	C5'-C4'-O1-C1
15	B	203	OZ2	OG2-CG2-CG3-OG3
15	B	203	OZ2	C1-C2-C3-C4
10	A	304	MYS	C5-C6-C7-C8
15	C	303	OZ2	C2B-C3B-C4B-C5B
15	B	203	OZ2	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	A	306	UMQ	C3'-C4'-O1-C1
10	A	304	MYS	C7-C8-C9-C10
12	A	307	UMQ	CD-CF-CG-CH
9	A	301	HEM	C2A-CAA-CBA-CGA
15	C	303	OZ2	C2B-C1B-O2G-C2G
15	C	303	OZ2	C5-C6-C7-C8
9	C	301	HEM	C4B-C3B-CAB-CBB
9	A	301	HEM	C4D-C3D-CAD-CBD
15	C	303	OZ2	O1-C1-O1G-C1G
15	G	102	OZ2	C3-C4-C5-C6
14	B	201	CLA	C13-C15-C16-C17
15	G	102	OZ2	O1G-C1G-C2G-C3G
15	B	203	OZ2	C2-C3-C4-C5
14	B	201	CLA	O2A-C1-C2-C3
12	A	308	UMQ	CF-CG-CH-CI
18	G	101	BCR	C16-C17-C18-C19
11	A	305	8K6	C5-C6-C7-C8
11	A	305	8K6	C4-C5-C6-C7
14	B	201	CLA	C11-C12-C13-C14
15	G	102	OZ2	C5-C6-C7-C8
12	A	306	UMQ	CI-CJ-CK-CL
14	B	201	CLA	C10-C11-C12-C13
15	C	303	OZ2	C8B-C9B-CB0-CB1
14	B	201	CLA	C15-C16-C17-C18
18	G	101	BCR	C23-C24-C25-C30
15	C	303	OZ2	CG2-CG1-OP3-P
18	G	101	BCR	C35-C13-C14-C15
15	B	203	OZ2	C10-C11-C12-C13
14	B	201	CLA	C11-C10-C8-C7
15	G	102	OZ2	CG2-CG1-OP3-P
15	B	203	OZ2	C3G-O3G-P-OP2
15	B	203	OZ2	C3G-O3G-P-OP3
15	C	303	OZ2	C3G-O3G-P-OP1
15	C	303	OZ2	CG1-OP3-P-OP1
15	G	102	OZ2	CG1-OP3-P-OP2
12	A	306	UMQ	O5'-C5'-C6'-O6'
14	B	201	CLA	C6-C7-C8-C9
15	G	102	OZ2	C4B-C5B-C6B-C7B
9	A	302	HEM	C3A-C2A-CAA-CBA
9	A	303	HEM	C3A-C2A-CAA-CBA
12	A	308	UMQ	O1'-CA-CB-CC
18	G	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
15	C	303	OZ2	C7-C8-C9-C10
18	G	101	BCR	C11-C10-C9-C8
18	G	101	BCR	C23-C24-C25-C26
15	B	203	OZ2	C9-C10-C11-C12
15	G	102	OZ2	C7-C8-C9-C10
15	C	303	OZ2	C2G-C3G-O3G-P
11	A	305	8K6	C6-C7-C8-C9
12	A	306	UMQ	CD-CF-CG-CH
9	A	301	HEM	C3D-CAD-CBD-CGD
11	A	305	8K6	C7-C8-C9-C10
12	A	307	UMQ	CC-CD-CF-CG
15	G	102	OZ2	C6B-C7B-C8B-C9B
15	C	303	OZ2	C4B-C5B-C6B-C7B
9	C	301	HEM	CAD-CBD-CGD-O2D
15	G	102	OZ2	C10-C11-C12-C13
15	G	102	OZ2	O1-C1-O1G-C1G
14	B	201	CLA	C6-C7-C8-C10
9	C	301	HEM	CAD-CBD-CGD-O1D
18	G	101	BCR	C1-C6-C7-C8
14	B	201	CLA	CAA-CBA-CGA-O2A
9	A	301	HEM	CAA-CBA-CGA-O1A
9	A	303	HEM	C2B-C3B-CAB-CBB
14	B	201	CLA	CAA-CBA-CGA-O1A

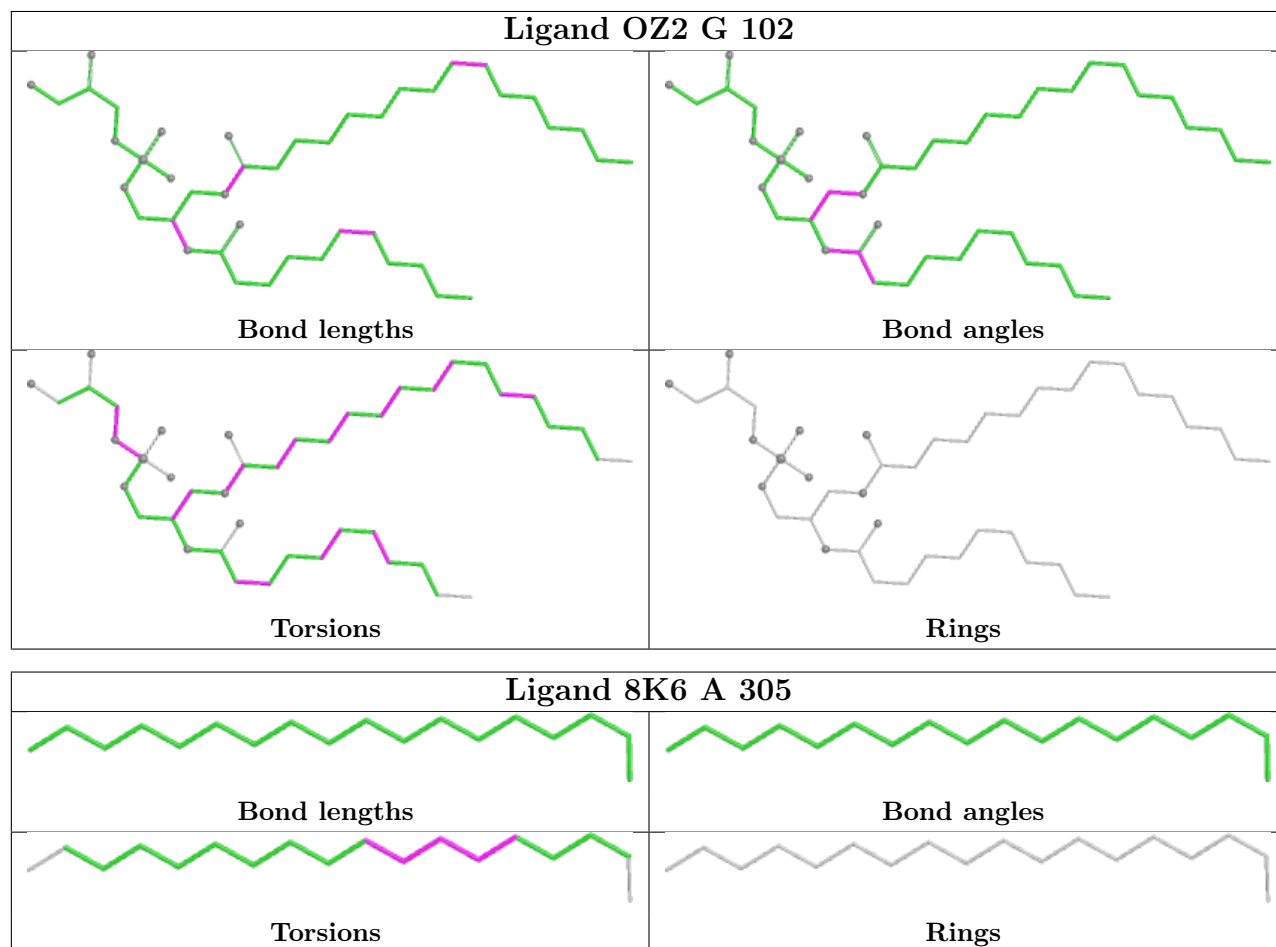
There are no ring outliers.

8 monomers are involved in 34 short contacts:

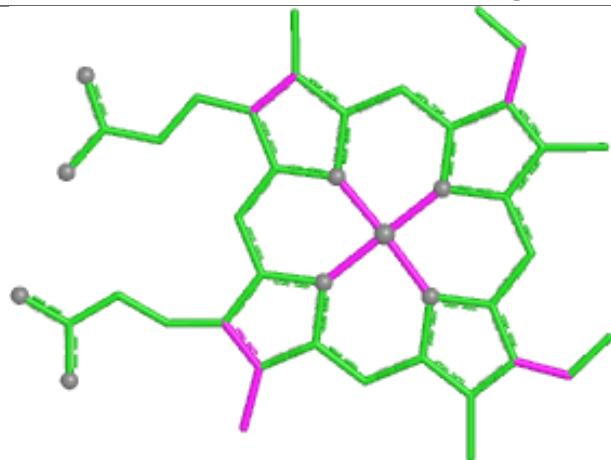
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	G	102	OZ2	1	0
9	A	302	HEM	9	0
12	A	306	UMQ	1	0
14	B	201	CLA	1	0
9	A	301	HEM	7	0
16	D	201	1E2	1	0
9	C	301	HEM	6	0
9	A	303	HEM	8	0

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 than 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.

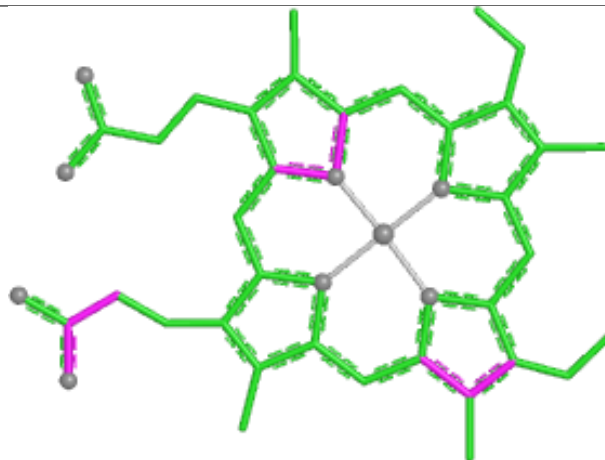
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



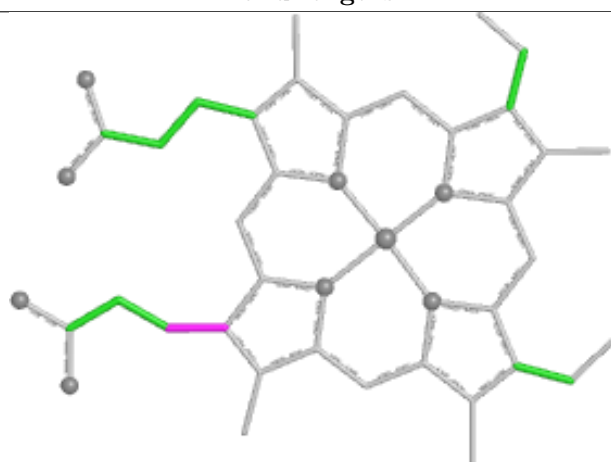
Ligand HEM A 302



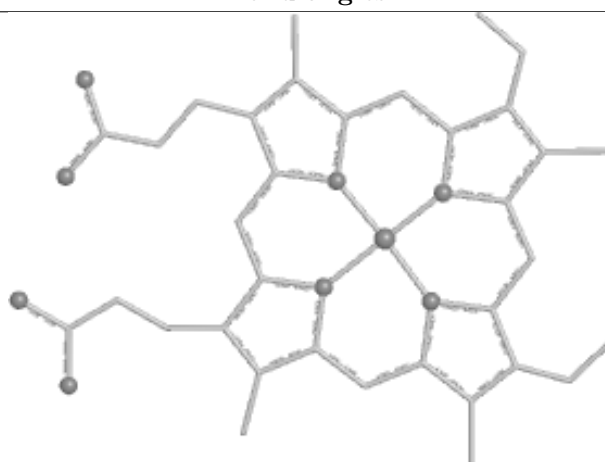
Bond lengths



Bond angles

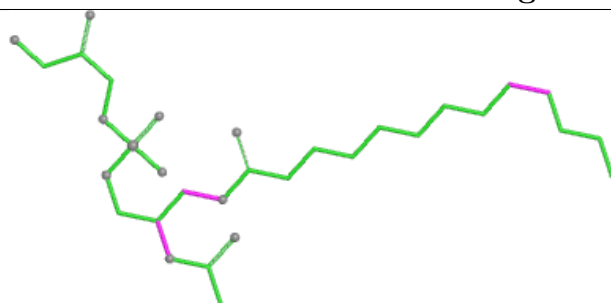


Torsions

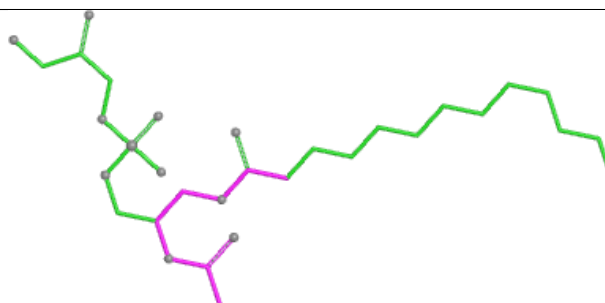


Rings

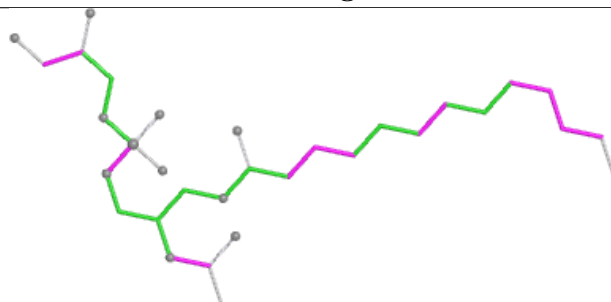
Ligand OZ2 B 203



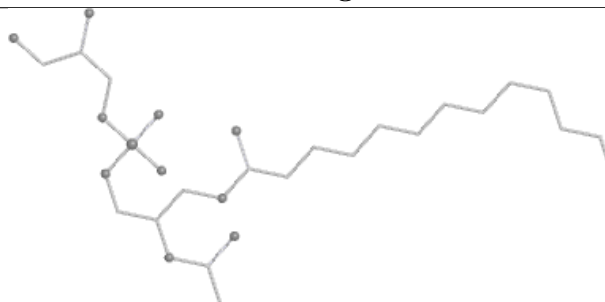
Bond lengths



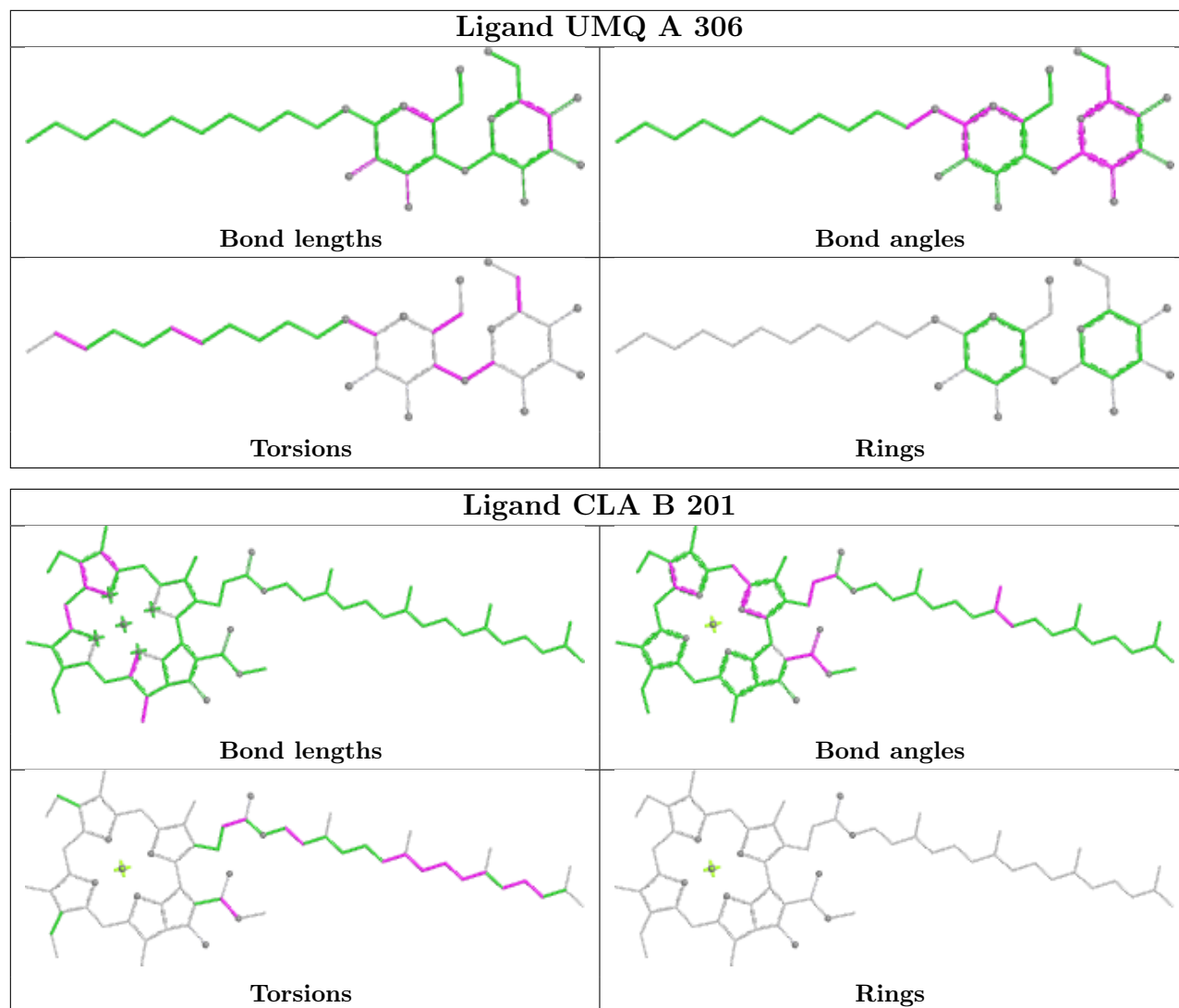
Bond angles

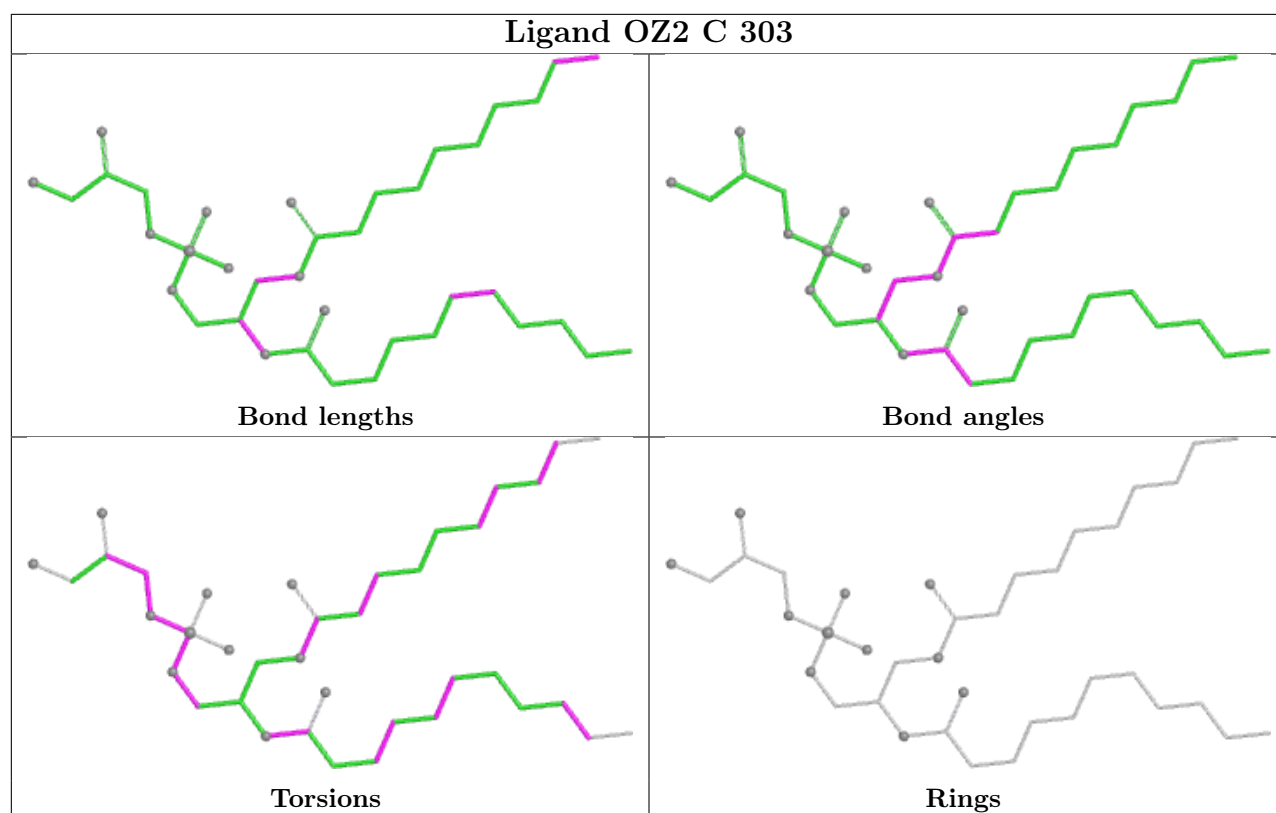


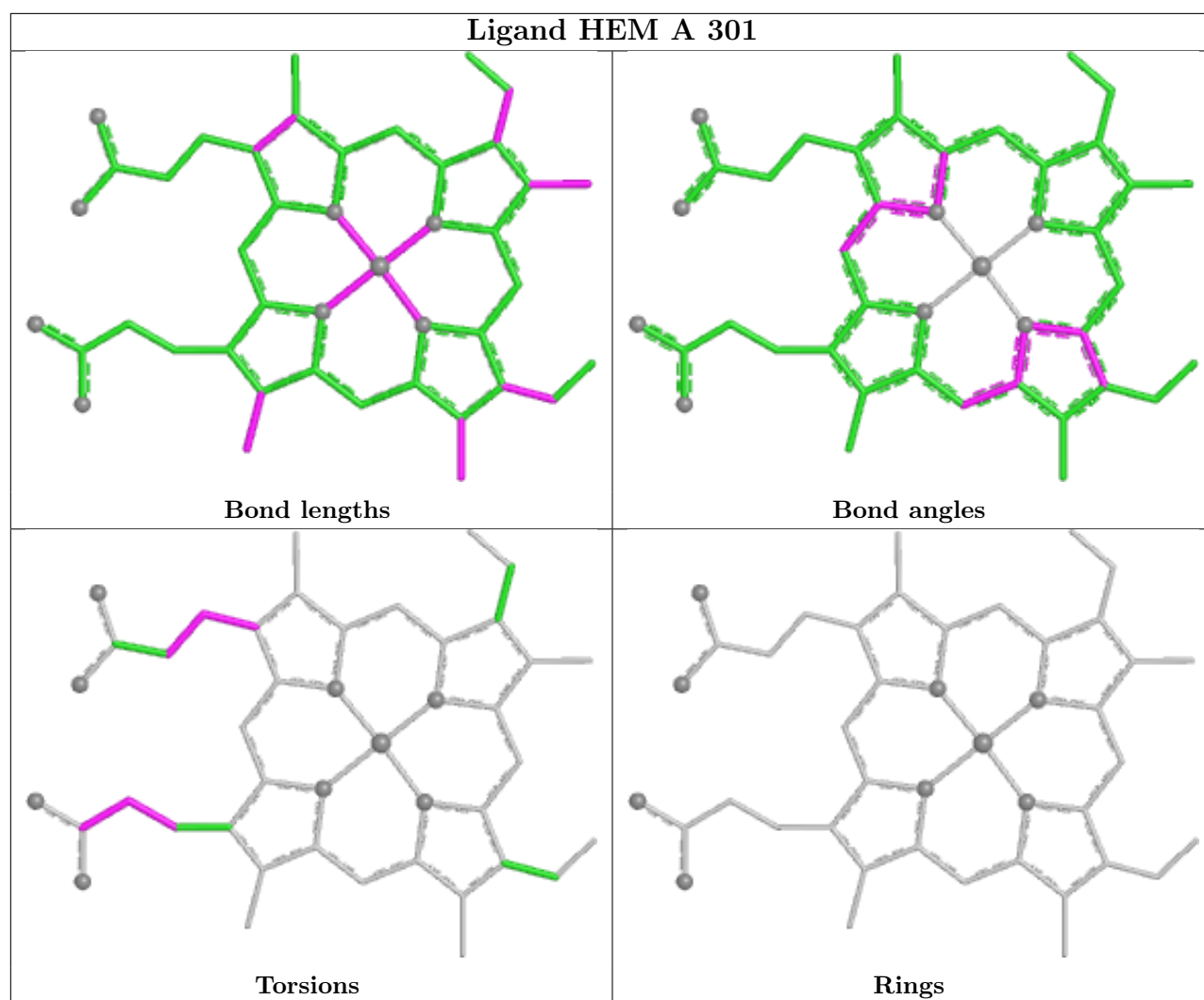
Torsions

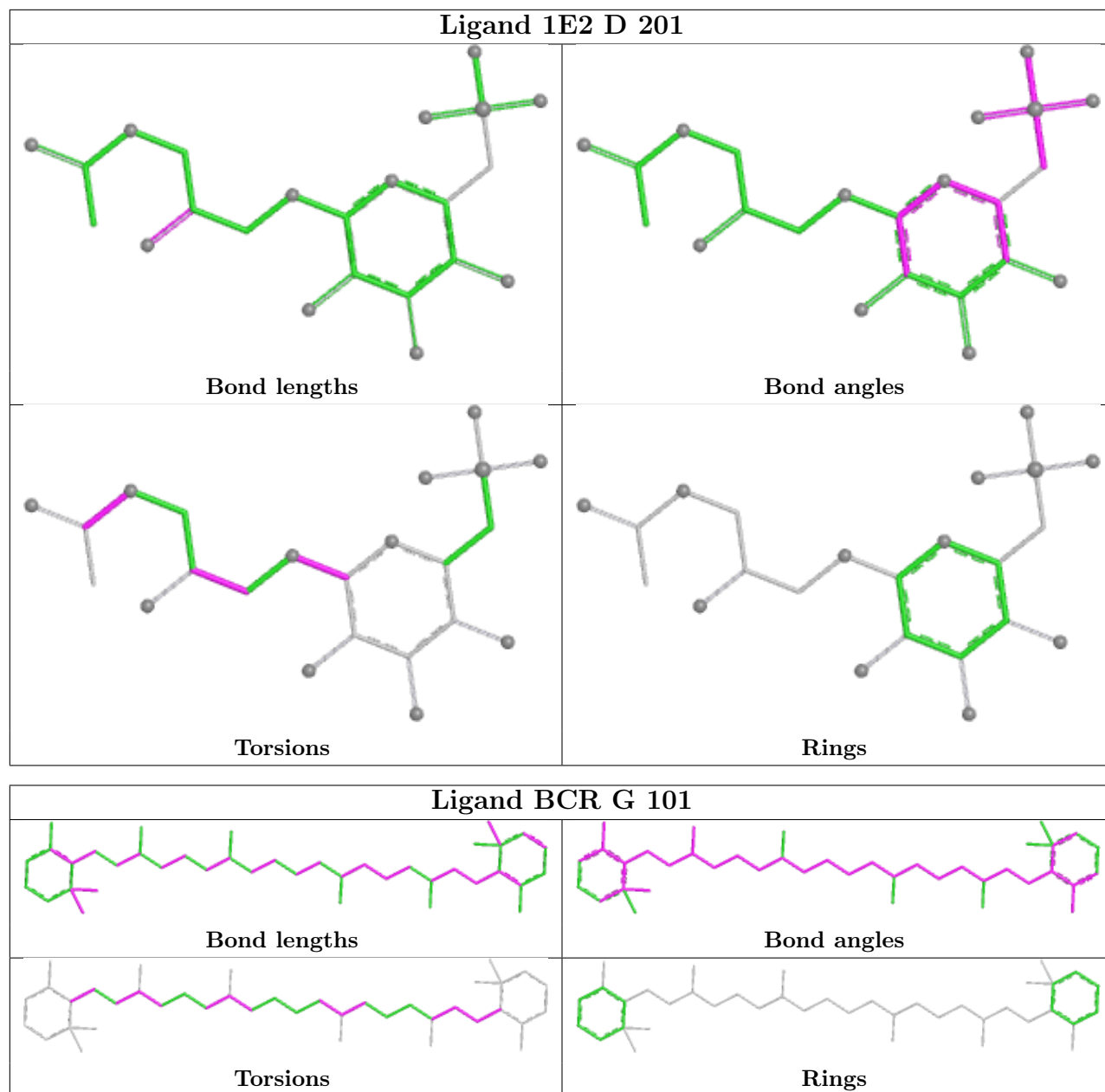


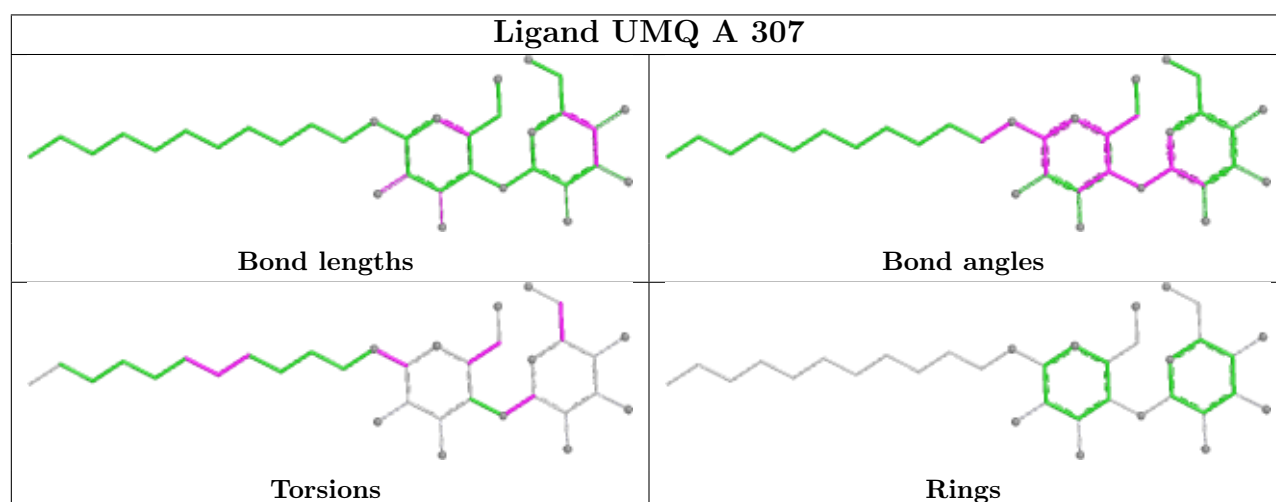
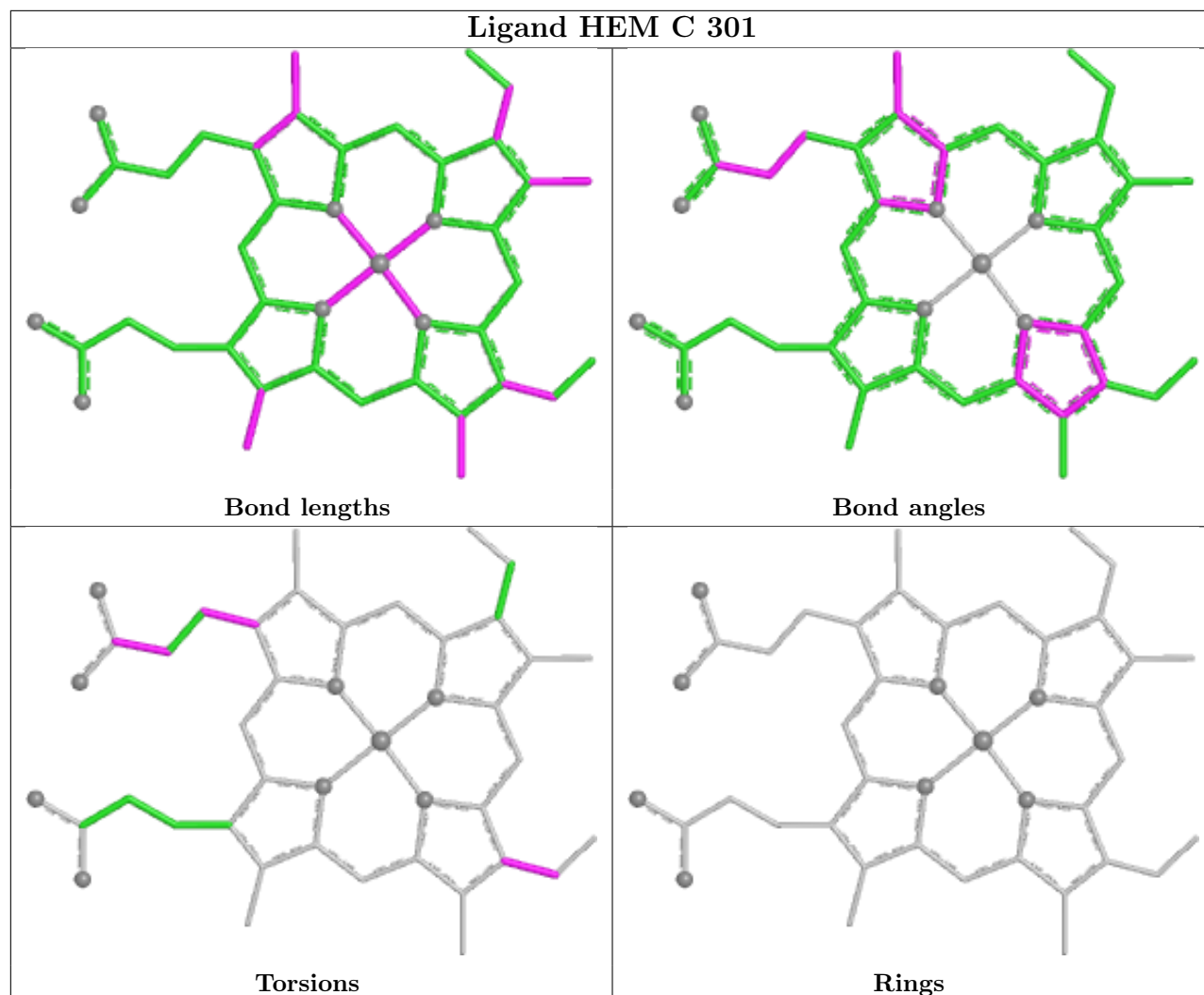
Rings

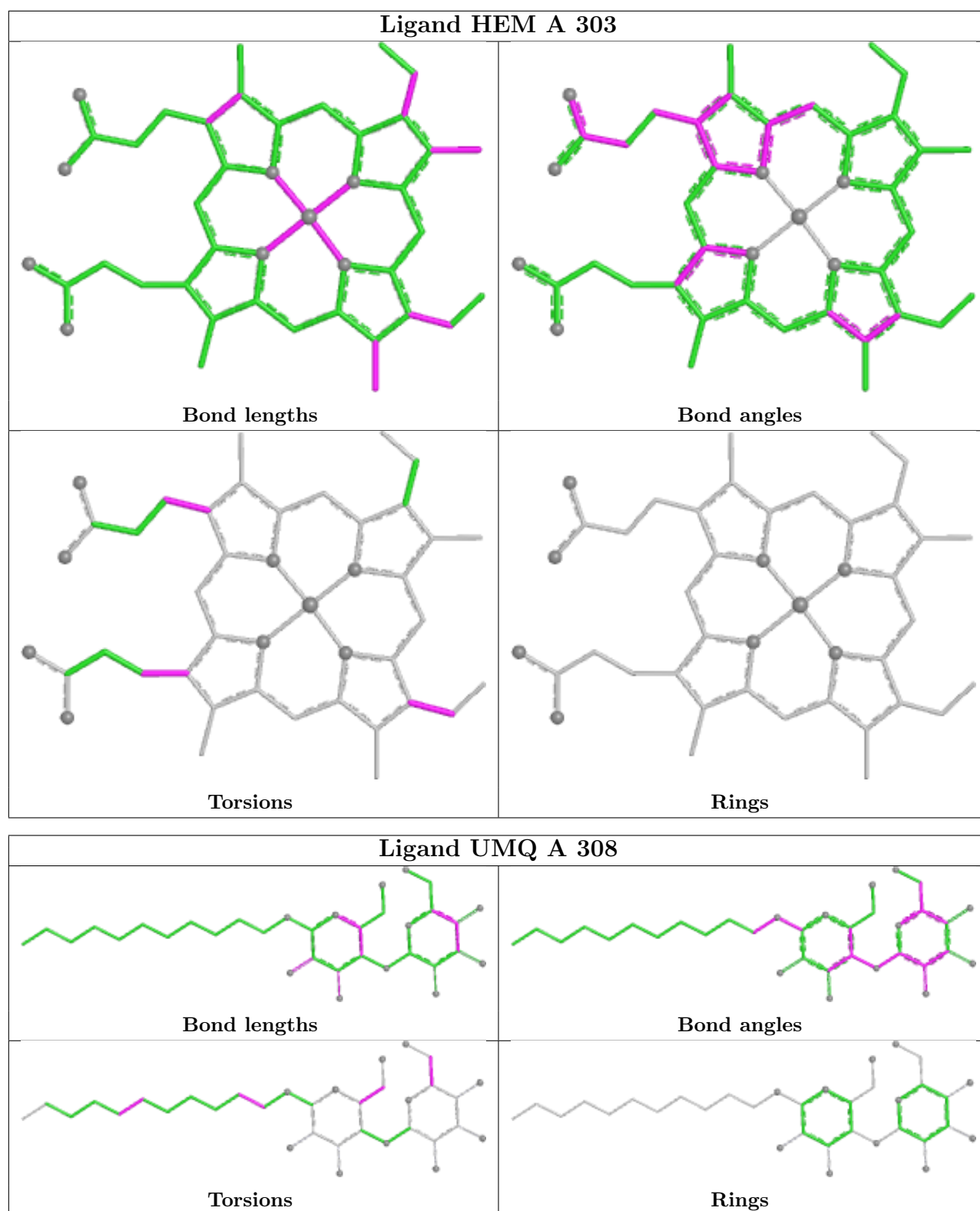












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	0.25	6 (2%) 55 45	50, 71, 106, 147	0
2	B	159/160 (99%)	0.67	22 (13%) 6 5	55, 93, 140, 198	0
3	C	288/289 (99%)	1.43	96 (33%) 1 1	60, 104, 239, 279	1 (0%)
4	D	38/179 (21%)	1.08	8 (21%) 2 2	55, 88, 182, 246	0
5	E	28/32 (87%)	1.71	10 (35%) 1 0	90, 103, 130, 152	0
6	F	31/35 (88%)	1.39	8 (25%) 1 1	78, 96, 136, 141	0
7	G	35/37 (94%)	2.31	13 (37%) 1 0	66, 91, 210, 274	0
8	H	28/29 (96%)	0.54	4 (14%) 6 5	74, 84, 106, 131	0
All	All	820/976 (84%)	0.98	167 (20%) 3 2	50, 91, 201, 279	1 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	37	GLY	19.8
2	B	2	ALA	10.7
7	G	36	GLY	10.1
7	G	33	ASN	9.5
3	C	219	VAL	8.8
2	B	74	GLU	8.3
4	D	10	VAL	7.7
7	G	34	GLU	7.1
3	C	206	THR	7.1
7	G	35	LEU	6.5
3	C	230	ALA	6.5
3	C	220	SER	6.4
3	C	207	VAL	6.2
2	B	160	PHE	6.1
8	H	29	LEU	5.9
6	F	2	THR	5.6

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Mol	Chain	Res	Type	RSRZ
5	E	28	SER	5.5
6	F	32	ALA	5.5
7	G	32	PRO	5.2
7	G	31	ARG	5.2
3	C	201	THR	5.1
5	E	29	ILE	5.0
3	C	190	TYR	5.0
3	C	196	GLN	4.9
3	C	224	ALA	4.8
4	D	9	ASP	4.8
2	B	75	ILE	4.7
2	B	119	LYS	4.7
3	C	176	ALA	4.7
3	C	92	GLU	4.6
3	C	203	SER	4.6
3	C	87	GLU	4.4
3	C	202	ASP	4.4
4	D	13	MET	4.3
3	C	256	LYS	4.3
3	C	95	LYS	4.1
2	B	3	THR	4.1
2	B	76	LEU	4.1
2	B	142	TRP	4.1
1	A	215	LEU	4.1
3	C	225	VAL	4.1
6	F	3	GLU	4.1
6	F	29	ILE	4.0
5	E	20	VAL	4.0
3	C	287	MET	4.0
3	C	96	LYS	3.9
3	C	217	LEU	3.9
1	A	13	GLU	3.9
3	C	183	ILE	3.8
3	C	181	THR	3.8
5	E	2	ILE	3.8
3	C	140	LYS	3.8
3	C	218	ILE	3.7
5	E	26	ILE	3.7
3	C	212	PRO	3.7
1	A	111	LYS	3.6
3	C	100	ASP	3.6
3	C	98	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	152	ASP	3.6
3	C	182	LYS	3.6
3	C	21	VAL	3.6
3	C	58	LEU	3.6
6	F	27	LEU	3.6
3	C	122	GLU	3.5
3	C	216	GLU	3.5
5	E	23	ILE	3.5
3	C	187	GLU	3.5
4	D	46	SER	3.5
3	C	67	LYS	3.5
3	C	123	GLN	3.5
3	C	288	ASN	3.5
7	G	27	GLN	3.4
3	C	281	LYS	3.4
3	C	240	PHE	3.4
3	C	204	GLY	3.3
4	D	15	ARG	3.3
3	C	184	ALA	3.2
3	C	223	GLN	3.2
2	B	118	ASN	3.2
3	C	99	GLY	3.2
3	C	195	TYR	3.2
8	H	28	GLY	3.2
3	C	57	LYS	3.1
6	F	7	TYR	3.1
3	C	222	GLY	3.1
3	C	170	ASN	3.0
3	C	68	VAL	3.0
3	C	284	ALA	3.0
3	C	189	GLU	3.0
7	G	29	TYR	2.9
3	C	215	PRO	2.9
3	C	226	LYS	2.9
3	C	174	ALA	2.9
8	H	2	GLU	2.9
3	C	213	ALA	2.9
2	B	88	LEU	2.9
3	C	90	ILE	2.9
3	C	59	GLN	2.8
3	C	188	ASP	2.8
3	C	186	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	207	ARG	2.8
2	B	120	PHE	2.8
7	G	4	PRO	2.8
3	C	209	ASP	2.8
2	B	29	GLU	2.7
1	A	3	ASN	2.7
3	C	214	GLY	2.7
5	E	22	ILE	2.7
3	C	192	ASN	2.7
7	G	7	ASP	2.7
3	C	173	THR	2.7
3	C	23	ALA	2.6
3	C	200	GLN	2.6
3	C	286	GLU	2.6
2	B	156	THR	2.6
3	C	171	VAL	2.6
3	C	177	THR	2.6
3	C	175	SER	2.5
3	C	64	ASP	2.5
7	G	26	TYR	2.5
3	C	56	THR	2.5
2	B	153	LYS	2.5
3	C	185	LYS	2.5
3	C	80	GLU	2.5
3	C	165	GLU	2.5
3	C	19	ARG	2.5
3	C	125	GLN	2.5
4	D	12	ASP	2.4
3	C	178	GLY	2.4
2	B	26	TYR	2.4
3	C	28	ALA	2.4
2	B	73	LEU	2.4
2	B	159	LEU	2.4
3	C	9	TYR	2.4
6	F	6	LEU	2.4
3	C	124	TYR	2.4
3	C	193	VAL	2.3
7	G	30	LYS	2.3
3	C	119	LEU	2.3
2	B	90	SER	2.3
1	A	136	TYR	2.3
3	C	179	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	180	ILE	2.3
3	C	166	LYS	2.3
3	C	221	GLU	2.3
3	C	229	GLU	2.2
2	B	151	LEU	2.2
2	B	155	LEU	2.2
3	C	199	ILE	2.2
5	E	10	VAL	2.2
3	C	163	THR	2.2
3	C	108	GLU	2.2
4	D	17	GLN	2.1
3	C	205	LYS	2.1
2	B	125	ARG	2.1
4	D	16	ARG	2.1
3	C	24	ASN	2.1
3	C	208	VAL	2.1
3	C	120	PRO	2.1
3	C	69	GLY	2.1
5	E	7	PHE	2.1
3	C	141	ASN	2.0
3	C	88	GLU	2.0
6	F	24	VAL	2.0
5	E	24	PHE	2.0
8	H	4	ASP	2.0
3	C	4	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

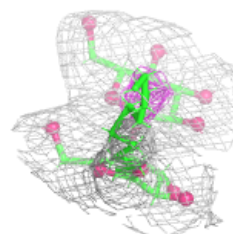
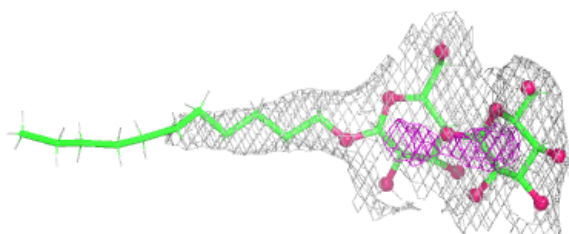
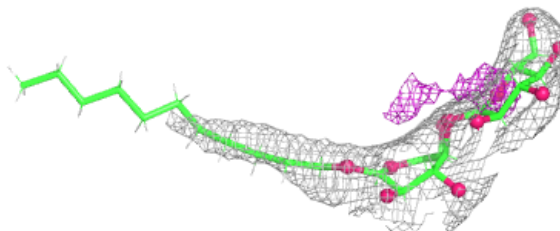
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	OCT	F	101	8/8	0.71	0.36	102,123,135,135	0
12	UMQ	A	307	34/34	0.80	0.22	115,144,174,177	0
12	UMQ	A	306	34/34	0.80	0.26	85,138,194,197	0
18	BCR	G	101	40/40	0.83	0.29	68,95,177,180	0
16	1E2	D	201	23/23	0.84	0.21	104,110,123,134	0
10	MYS	A	304	15/15	0.85	0.27	77,94,102,102	0
15	OZ2	G	102	44/48	0.86	0.28	58,102,166,169	0
12	UMQ	A	308	34/34	0.86	0.22	109,146,192,197	0
15	OZ2	C	303	38/48	0.87	0.28	54,108,185,186	0
11	8K6	A	305	18/18	0.90	0.26	96,120,123,123	0
15	OZ2	B	203	32/48	0.92	0.20	91,97,127,128	0
14	CLA	B	201	65/65	0.94	0.16	68,98,132,135	0
9	HEM	A	303	43/43	0.96	0.15	50,74,88,89	0
13	CD	C	302	1/1	0.97	0.07	142,142,142,142	0
9	HEM	C	301	43/43	0.98	0.11	76,82,98,107	0
9	HEM	A	302	43/43	0.98	0.11	51,64,74,79	0
13	CD	B	202	1/1	0.99	0.06	124,124,124,124	0
9	HEM	A	301	43/43	0.99	0.07	38,50,63,75	0
13	CD	A	309	1/1	0.99	0.07	85,85,85,85	0

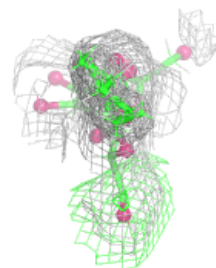
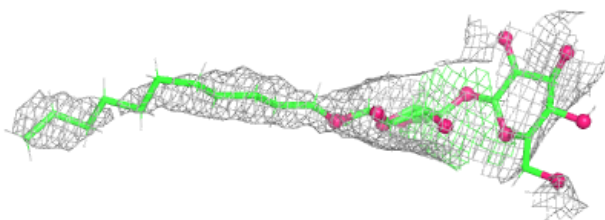
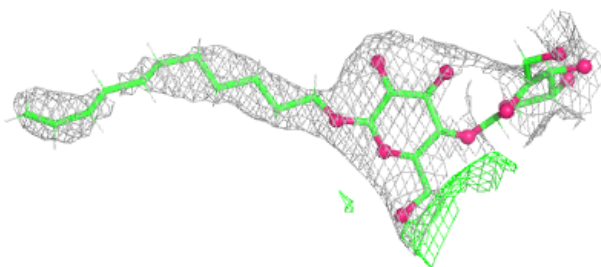
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UMQ A 307:

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

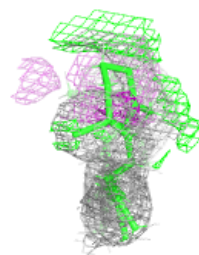
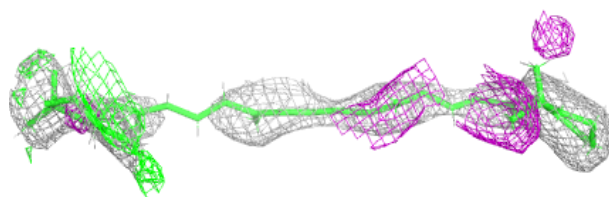
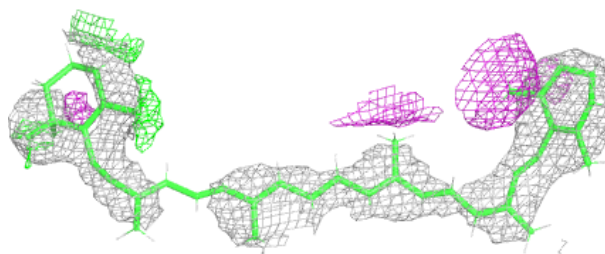
**Electron density around UMQ A 306:**

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



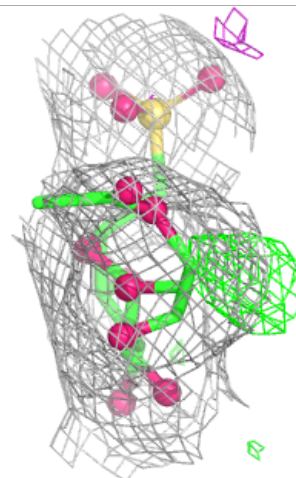
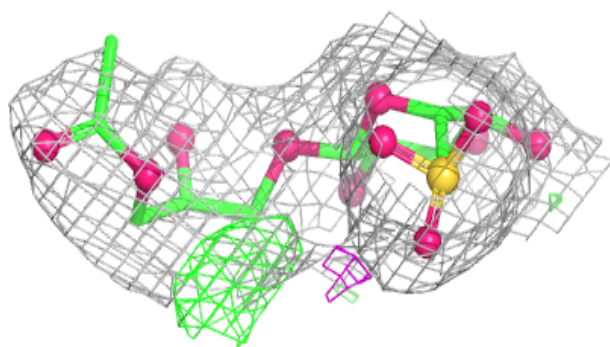
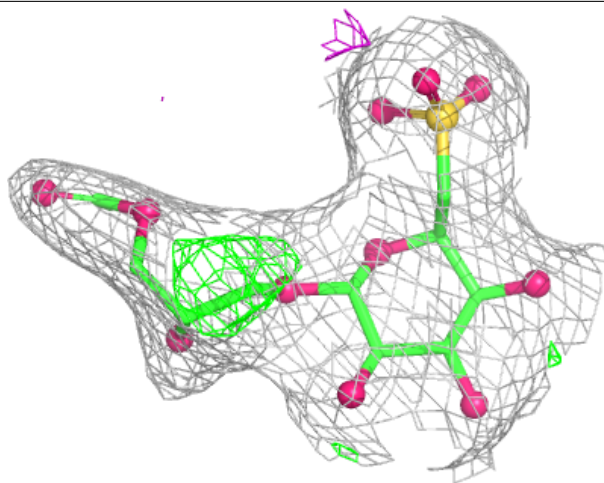
Electron density around BCR G 101:

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



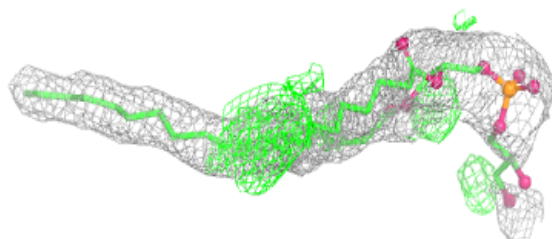
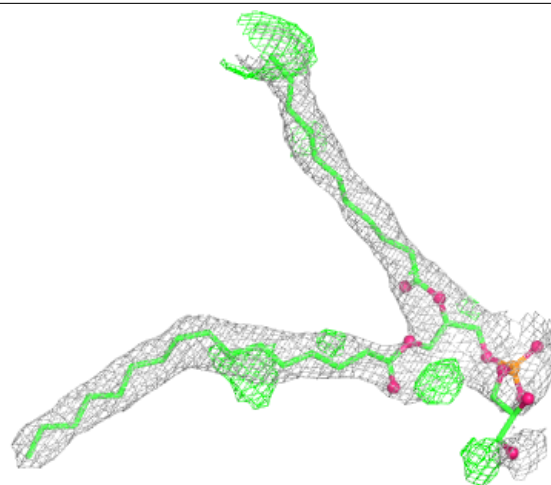
Electron density around 1E2 D 201:

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



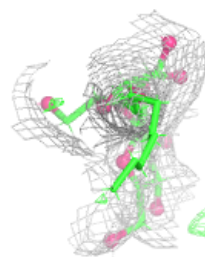
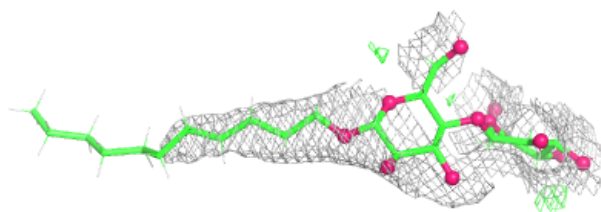
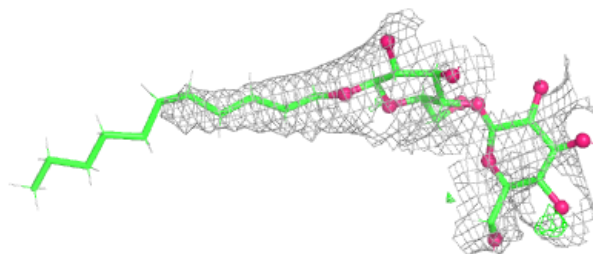
Electron density around OZ2 G 102:

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

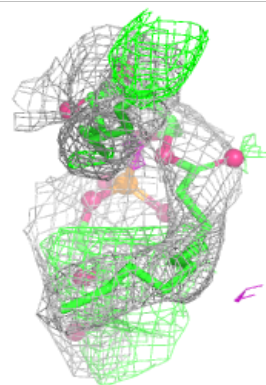
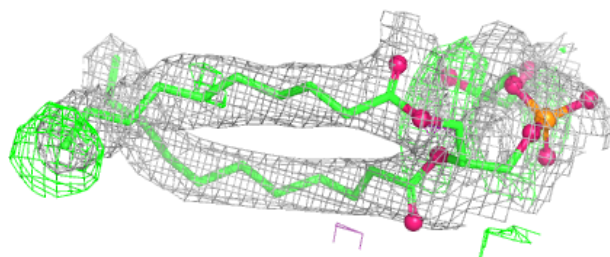
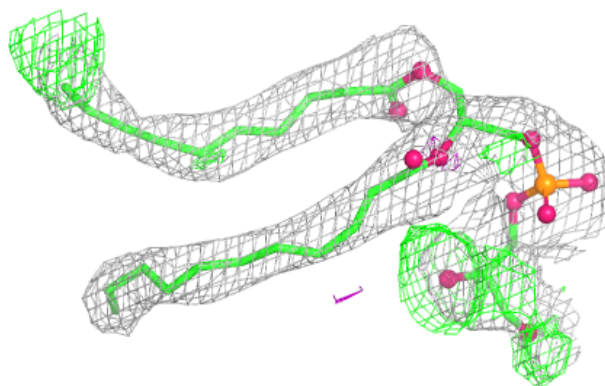


Electron density around UMQ A 308:

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

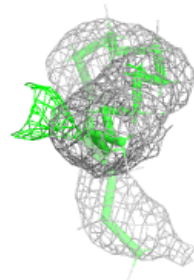
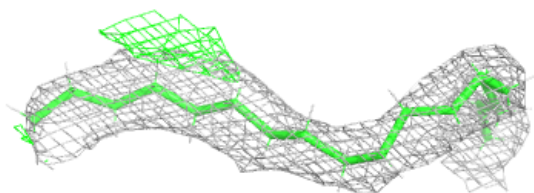
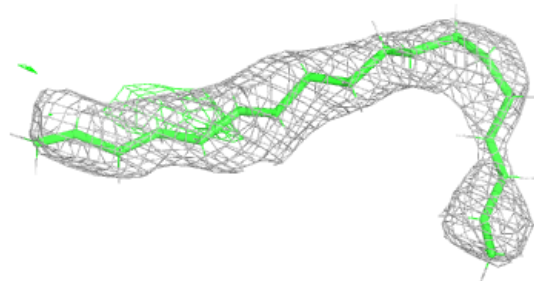
**Electron density around OZ2 C 303:**

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

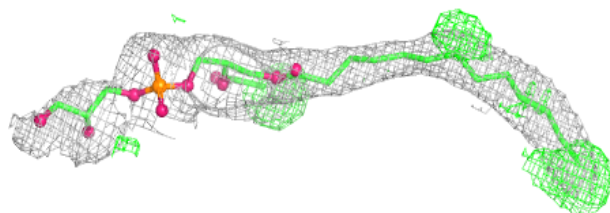
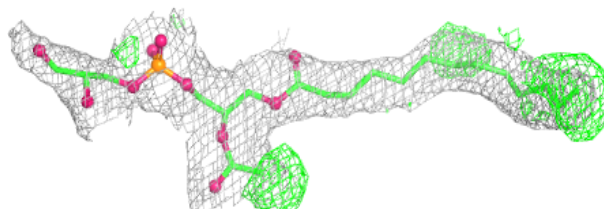


Electron density around 8K6 A 305:

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

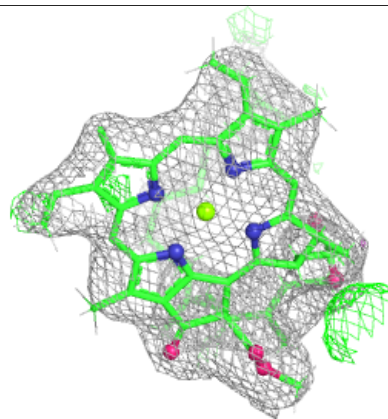
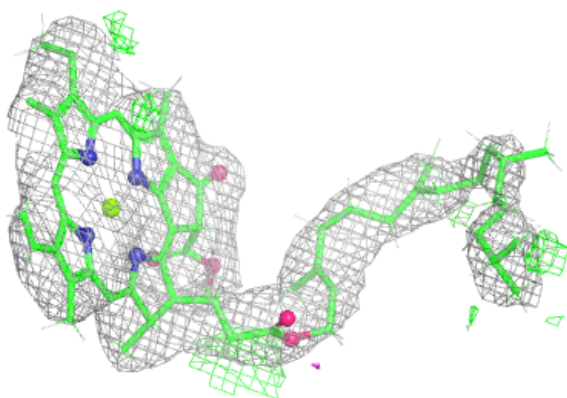
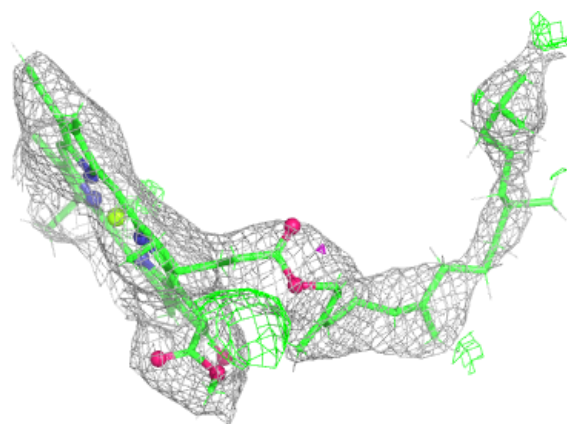
**Electron density around OZ2 B 203:**

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



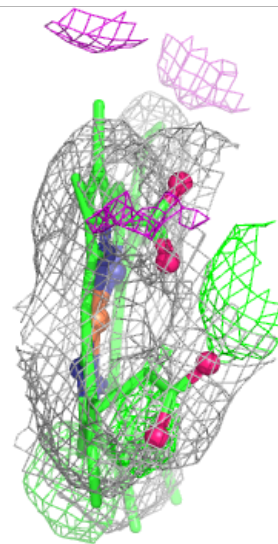
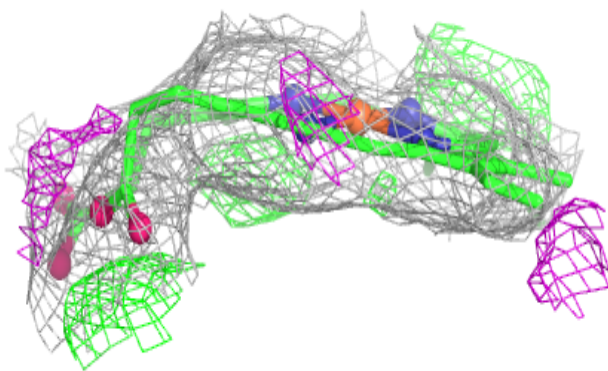
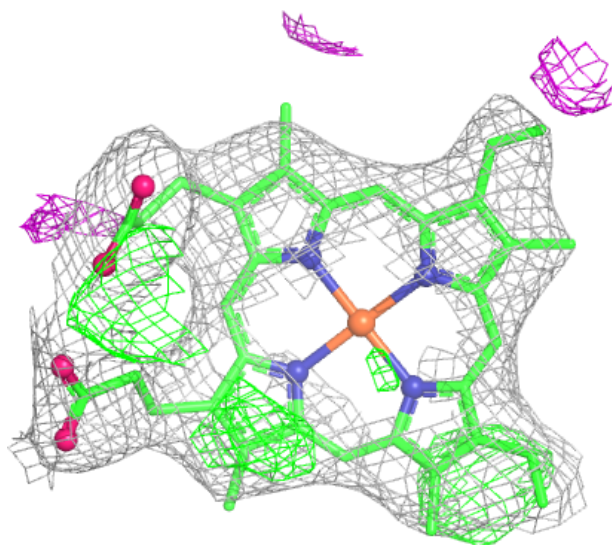
Electron density around CLA B 201:

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



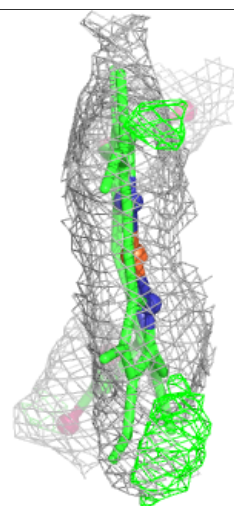
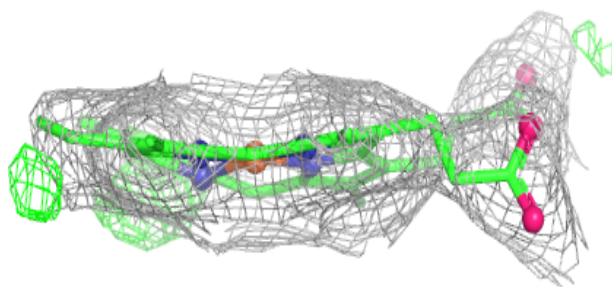
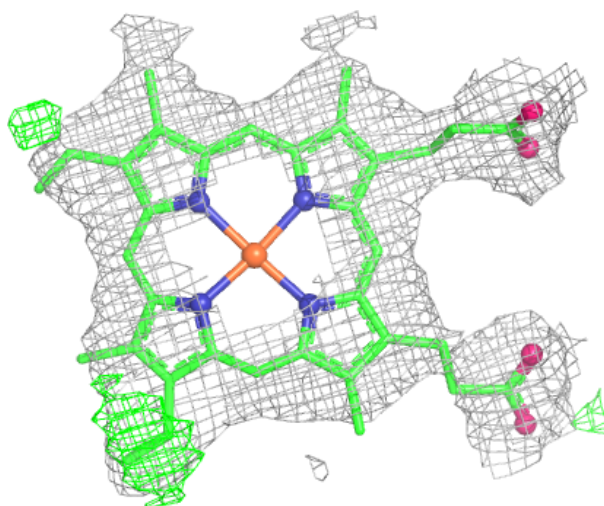
Electron density around HEM A 303:

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



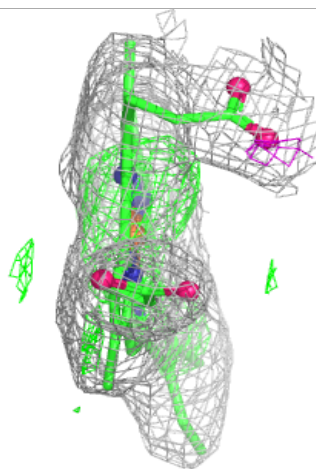
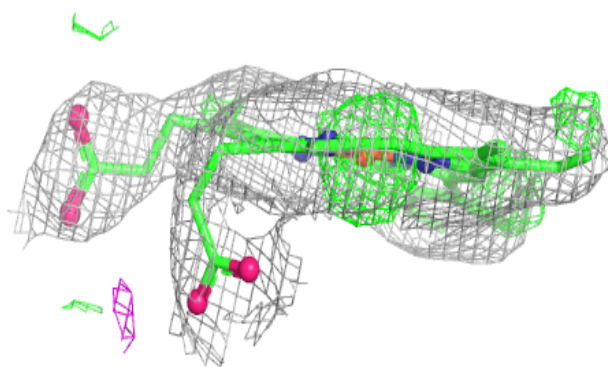
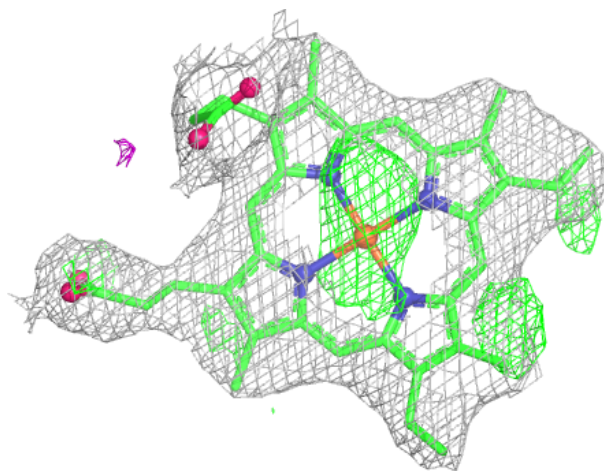
Electron density around HEM C 301:

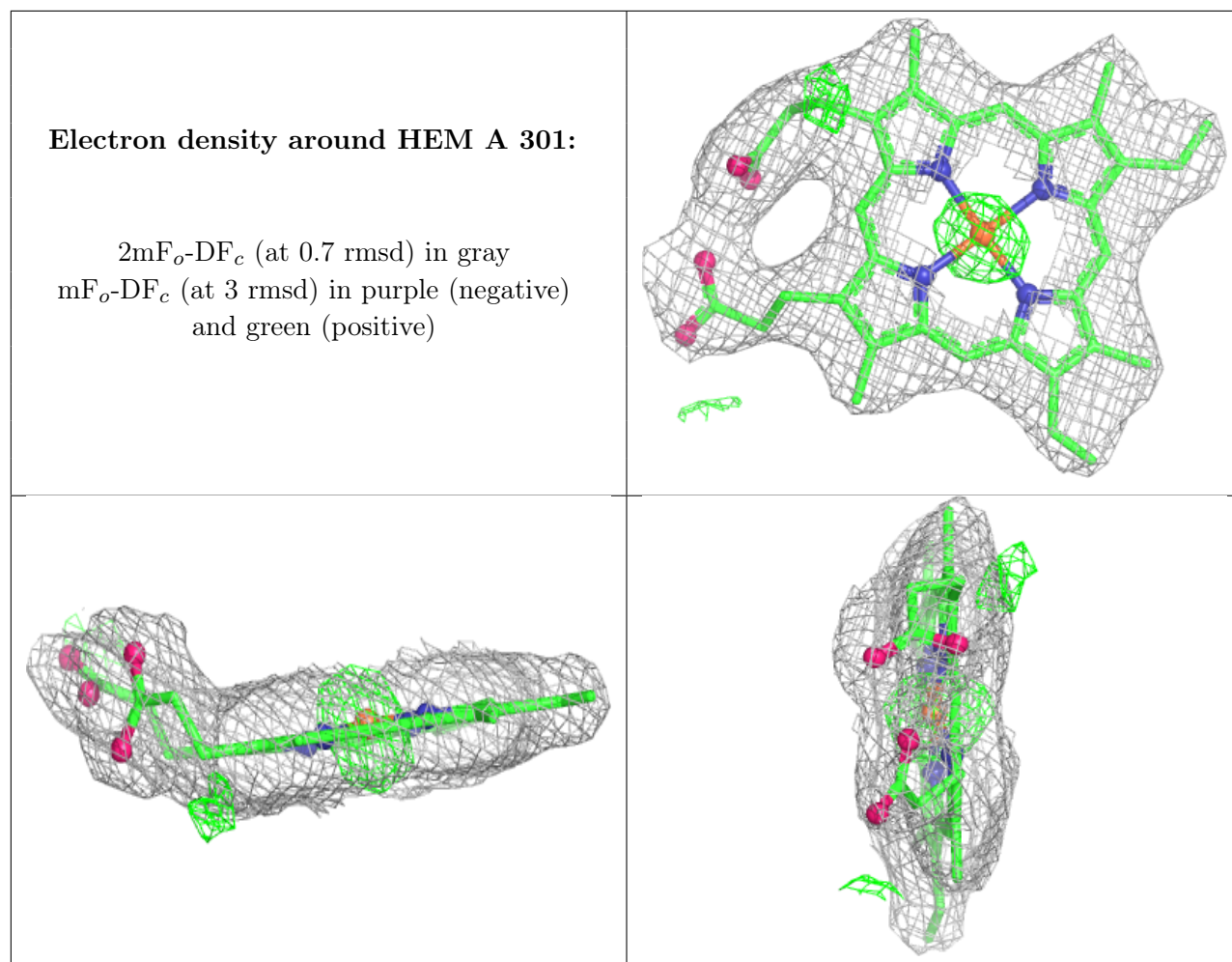
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.