



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 9, 2019 – 03:24 AM EDT

PDB ID : 4PV1
Title : Cytochrome B6F structure from *M. lamosus* with the quinone analog inhibitor stigmatellin
Authors : Hasan, S.S.; Yamashita, E.; Cramer, W.A.
Deposited on : 2014-03-14
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

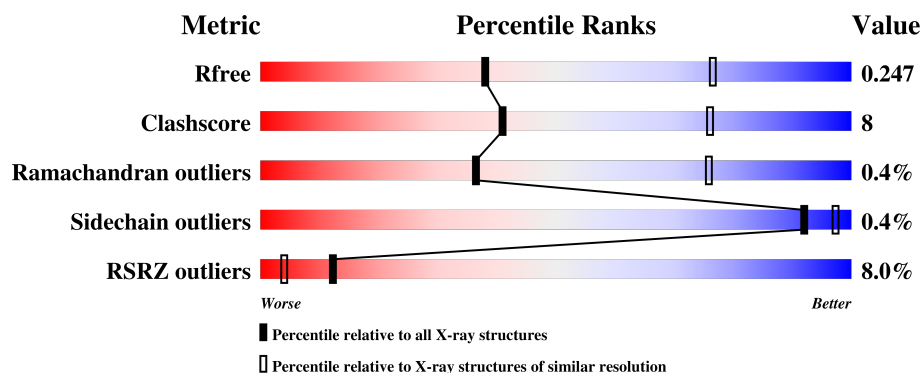
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	B	160	<div> <div>2%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
3	C	289	<div> <div>12%</div> <div>86%</div> <div>14%</div> </div>
4	D	179	<div> <div>20%</div> <div>72%</div> <div>17%</div> <div>12%</div> </div>
5	E	32	<div> <div>75%</div> <div>13%</div> <div>13%</div> </div>

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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
13	SMA	A	308	X	-	-	-
15	8K6	B	201	-	-	-	X
16	CLA	B	204	X	-	-	-
17	OPC	D	203	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 8049 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	5	0	0
			1698	1132	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	N	O	S	2	0	0
			1241	836	192	208	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2216	1415	369	424	8			

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	158	Total	C	N	O	S	0	0	0
			1221	783	210	221	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	28	Total	C	N	O	0	0	0
			215	156	29	30			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	31	Total	C	N	O	S	0	0	0
			234	160	34	39	1			

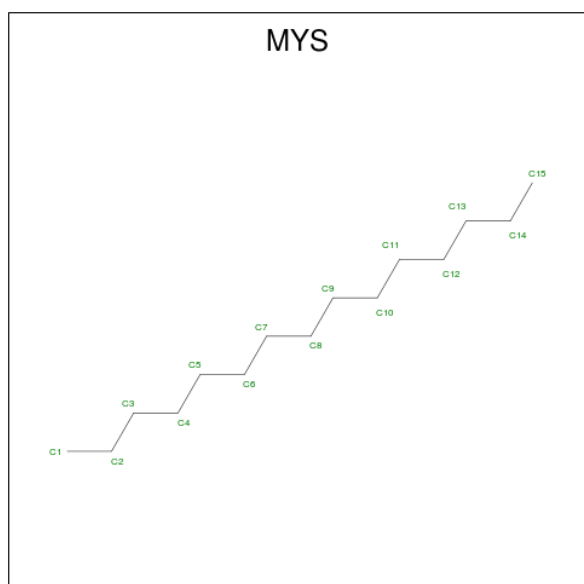
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	37	Total	C	N	O	S	4	0	0
			283	188	44	50	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	28	Total	C	N	O	S	0	0	0
			222	151	35	35	1			

- Molecule 9 is PENTADECANE (three-letter code: MYS) (formula: C₁₅H₃₂).

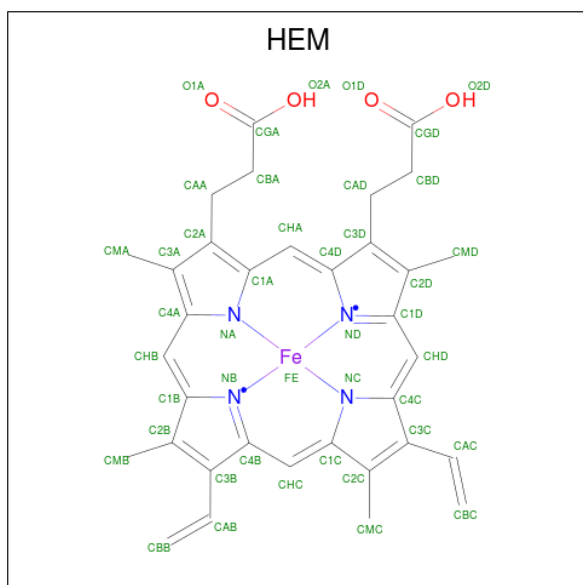


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C	0	0
			15	15		

- Molecule 10 is CADMIUM ION (three-letter code: CD) (formula: Cd).

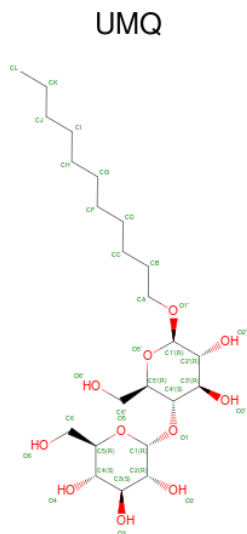
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cd 1 1	0	0
10	A	1	Total Cd 1 1	0	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



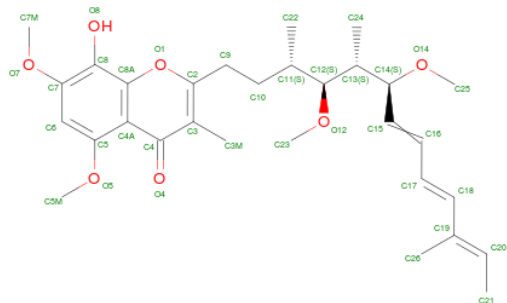
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C Fe N O 43 34 1 4 4	0	0
11	A	1	Total C Fe N O 43 34 1 4 4	0	0
11	A	1	Total C Fe N O 43 34 1 4 4	0	0
11	C	1	Total C Fe N O 43 34 1 4 4	0	0

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



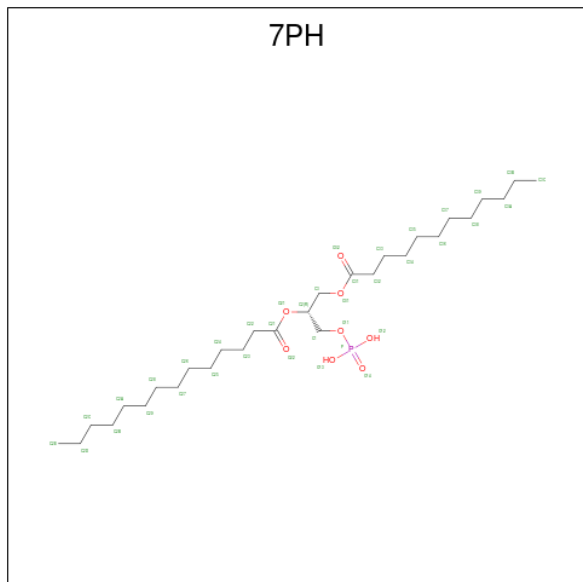
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total 34	C 23	O 11	6	0
12	A	1	Total 34	C 23	O 11	2	0
12	B	1	Total 34	C 23	O 11	0	0

- Molecule 13 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇).



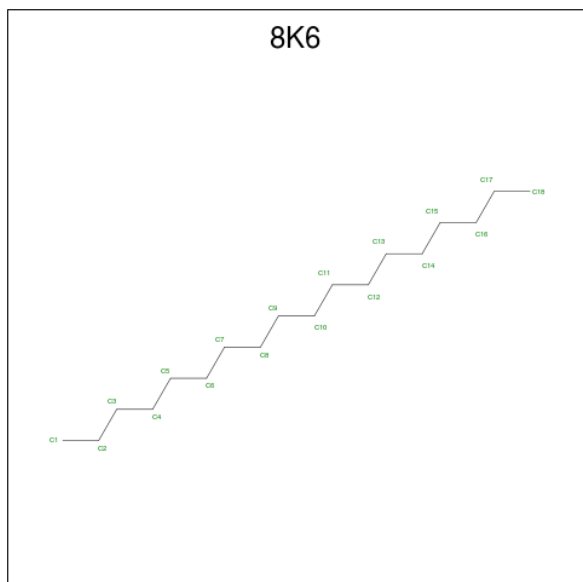
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	3	0
			37	30	7		

- Molecule 14 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



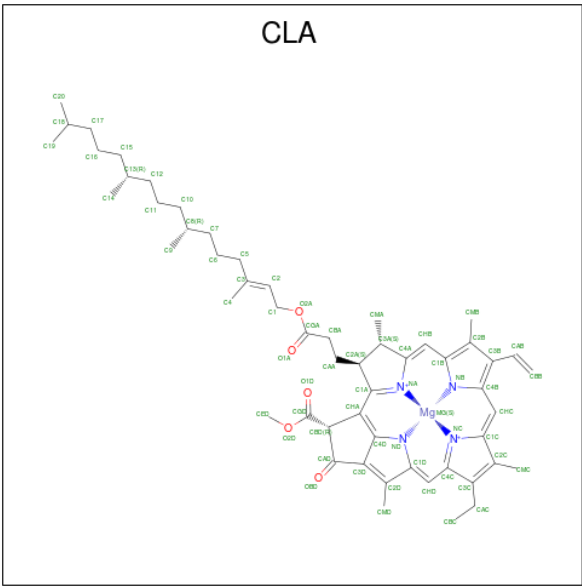
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	3	0
			32	27	5		

- Molecule 15 is Octadecane (three-letter code: 8K6) (formula: $C_{18}H_{38}$).



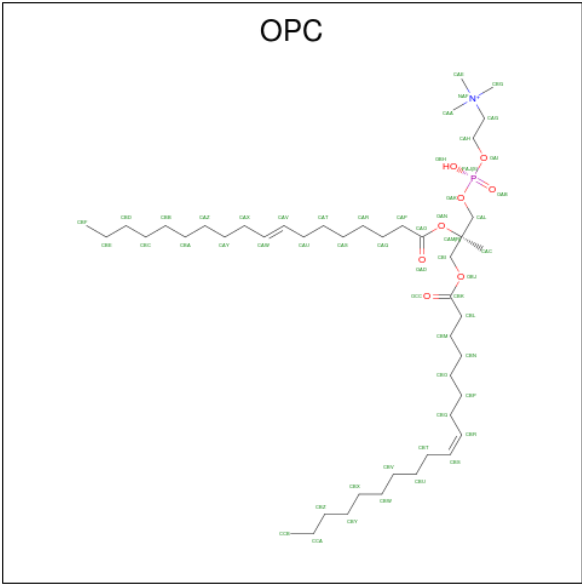
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	1	Total	C	0	0
			18	18		

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 17 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: C₄₅H₈₇NO₈P).



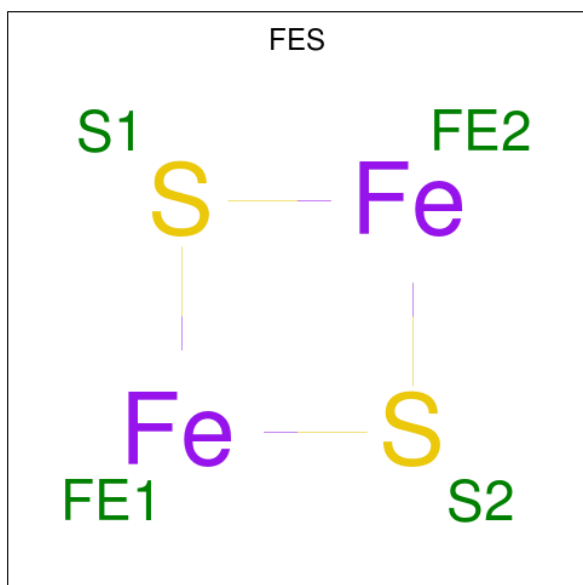
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
17	B	1	54	44	1	8	1	0	0

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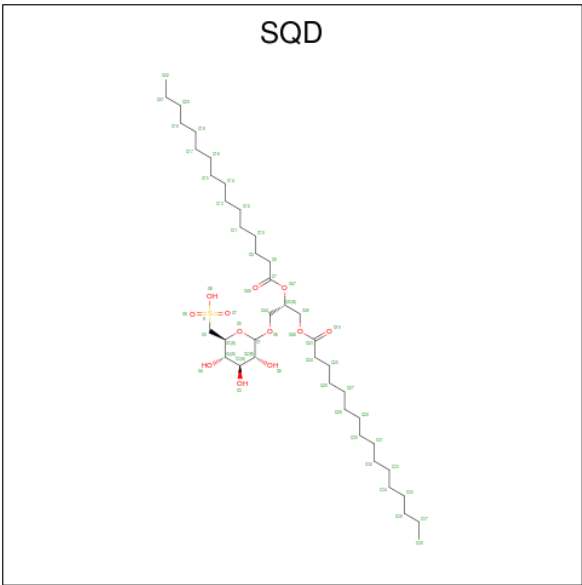
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	N	O	P	1	0
			54	44	1	8	1		
17	E	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



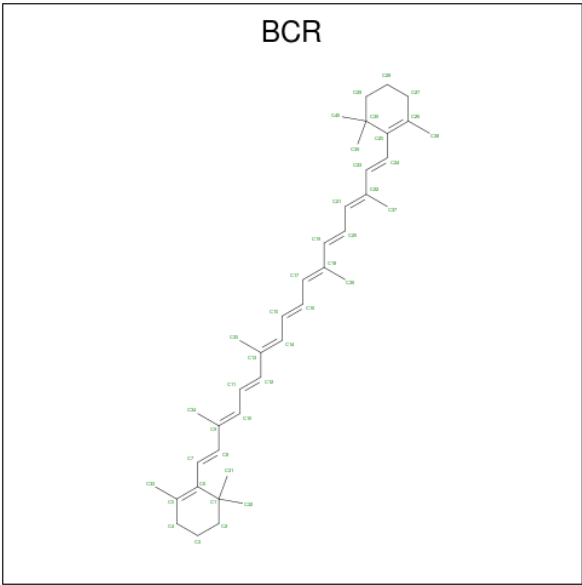
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	S	30	0
			54	41	12	1		

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	G	1	Total	C	14	0
			40	40		

- Molecule 21 is water.

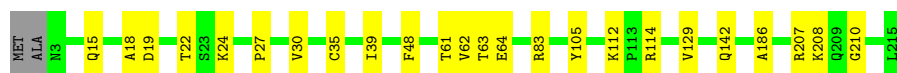
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	8	Total 8	O 8	0	0
21	B	5	Total 5	O 5	0	0
21	C	2	Total 2	O 2	0	0
21	G	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)


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

• Molecule 1: Cytochrome b6

Chain A: 




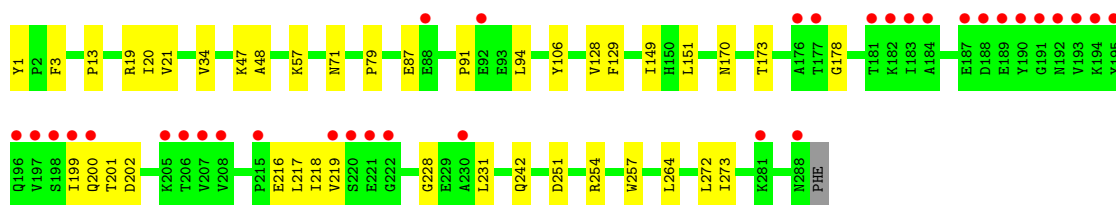
• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B: 



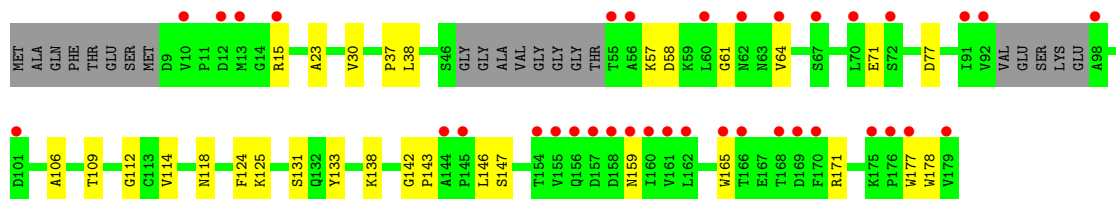
• Molecule 3: Apocytochrome f

Chain C: 



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

Chain D: 

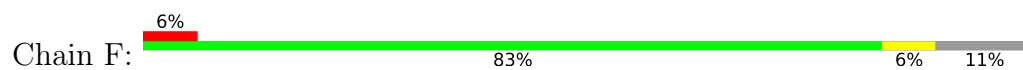


• Molecule 5: Cytochrome b6-f complex subunit 6

Chain E: 



- Molecule 6: Cytochrome b6-f complex subunit 7



- 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	159.09Å 159.09Å 361.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.34 – 3.00 48.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.2 (48.34-3.00) 83.4 (48.34-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496), REFMAC	Depositor
R, R_{free}	0.216 , 0.247 0.220 , 0.247	Depositor DCC
R_{free} test set	2560 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	85.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8049	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, CLA, CD, 7PH, BCR, FES, OPC, HEM, 8K6, SMA, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/1750	0.37	0/2388
2	B	0.21	0/1280	0.37	0/1755
3	C	0.21	0/2264	0.39	0/3082
4	D	0.20	0/1252	0.37	0/1705
5	E	0.22	0/220	0.35	0/297
6	F	0.21	0/238	0.32	0/321
7	G	0.21	0/289	0.37	0/391
8	H	0.20	0/228	0.32	0/313
All	All	0.21	0/7521	0.37	0/10252

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	0	1719	25	1
2	B	1241	0	1296	17	0
3	C	2216	0	2232	24	1
4	D	1221	0	1206	19	0
5	E	215	0	237	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	234	0	248	2	0
7	G	283	0	289	1	0
8	H	222	0	227	2	0
9	A	15	0	32	3	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	129	0	90	11	0
11	C	43	0	30	3	0
12	A	68	0	87	10	0
12	B	34	0	44	10	0
13	A	37	0	41	7	0
14	A	32	0	45	3	0
15	B	18	0	38	0	0
16	B	65	0	72	5	0
17	B	54	0	83	5	0
17	D	54	0	83	4	0
17	E	54	0	83	12	0
18	D	4	0	0	0	0
19	D	54	0	78	1	0
20	G	40	0	56	1	0
21	A	8	0	0	0	0
21	B	5	0	0	1	0
21	C	2	0	0	0	0
21	G	1	0	0	0	0
All	All	8049	0	8316	124	1

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 8.

The worst 5 of 124 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)
12:B:203:UMQ:O5'	12:B:203:UMQ:C5'	1.63	1.46
1:A:35:CYS:SG	11:A:305:HEM:CAB	2.04	1.44
12:B:203:UMQ:O5'	12:B:203:UMQ:C1'	1.69	1.41
12:A:307:UMQ:O5'	12:A:307:UMQ:C1'	1.69	1.40
1:A:35:CYS:SG	11:A:305:HEM:CBB	2.18	1.31

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:NZ	3:C:87:GLU:OE1[8_665]	2.19	0.01

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%)	201 (95%)	10 (5%)	0	100	100
2	B	157/160 (98%)	150 (96%)	7 (4%)	0	100	100
3	C	286/289 (99%)	256 (90%)	28 (10%)	2 (1%)	24	64
4	D	152/179 (85%)	127 (84%)	23 (15%)	2 (1%)	13	49
5	E	26/32 (81%)	26 (100%)	0	0	100	100
6	F	29/35 (83%)	27 (93%)	2 (7%)	0	100	100
7	G	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
8	H	26/29 (90%)	26 (100%)	0	0	100	100
All	All	922/976 (94%)	846 (92%)	72 (8%)	4 (0%)	36	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	71	GLU
4	D	112	GLY
3	C	20	ILE
3	C	21	VAL

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/184 (100%)	183 (100%)	0	100	100
2	B	136/137 (99%)	136 (100%)	0	100	100
3	C	242/243 (100%)	241 (100%)	1 (0%)	92	97
4	D	132/146 (90%)	132 (100%)	0	100	100
5	E	21/25 (84%)	20 (95%)	1 (5%)	28	66
6	F	23/27 (85%)	23 (100%)	0	100	100
7	G	28/28 (100%)	27 (96%)	1 (4%)	38	75
8	H	23/24 (96%)	23 (100%)	0	100	100
All	All	788/814 (97%)	785 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	264	LEU
5	E	11	PHE
7	G	35	LEU

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	MYS	A	301	-	14,14,14	0.10	0	13,13,13	0.79	0
11	HEM	A	303	1	27,50,50	2.14	5 (18%)	17,82,82	1.33	2 (11%)
11	HEM	A	304	1	27,50,50	2.08	6 (22%)	17,82,82	1.47	5 (29%)
11	HEM	A	305	13,21	27,50,50	2.11	5 (18%)	17,82,82	1.35	2 (11%)
12	UMQ	A	306	-	35,35,35	3.70	17 (48%)	46,46,46	2.13	6 (13%)
12	UMQ	A	307	-	35,35,35	3.71	17 (48%)	46,46,46	2.09	5 (10%)
13	SMA	A	308	11	35,38,38	2.75	10 (28%)	44,52,52	2.17	10 (22%)
14	7PH	A	309	-	31,31,37	1.26	2 (6%)	33,33,42	1.18	2 (6%)
15	8K6	B	201	-	17,17,17	0.09	0	16,16,16	0.85	0
12	UMQ	B	203	-	35,35,35	3.72	17 (48%)	46,46,46	2.05	5 (10%)
16	CLA	B	204	21	57,73,73	1.02	4 (7%)	66,113,113	1.45	7 (10%)
17	OPC	B	205	-	53,53,54	1.04	2 (3%)	59,61,64	0.98	2 (3%)
11	HEM	C	301	3	27,50,50	2.16	5 (18%)	17,82,82	1.46	3 (17%)
18	FES	D	201	4	0,4,4	0.00	-	-	-	-
19	SQD	D	202	-	53,54,54	0.95	5 (9%)	62,65,65	1.46	9 (14%)
17	OPC	D	203	-	53,53,54	1.03	2 (3%)	59,61,64	0.98	2 (3%)
17	OPC	E	101	-	53,53,54	1.03	2 (3%)	59,61,64	1.00	2 (3%)
20	BCR	G	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	4 (7%)

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	MYS	A	301	-	-	3/12/12/12	-
11	HEM	A	303	1	-	1/6/54/54	-
11	HEM	A	304	1	-	2/6/54/54	-
11	HEM	A	305	13,21	-	2/6/54/54	-
12	UMQ	A	306	-	-	9/20/60/60	0/2/2/2
12	UMQ	A	307	-	-	1/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SMA	A	308	11	1/1/5/10	18/33/34/34	0/2/2/2
14	7PH	A	309	-	-	7/33/33/39	-
15	8K6	B	201	-	-	5/15/15/15	-
12	UMQ	B	203	-	-	8/20/60/60	0/2/2/2
16	CLA	B	204	21	3/3/20/25	12/37/135/135	-
17	OPC	B	205	-	-	23/57/57/60	-
11	HEM	C	301	3	-	0/6/54/54	-
18	FES	D	201	4	-	-	0/1/1/1
19	SQD	D	202	-	-	18/49/69/69	0/1/1/1
17	OPC	D	203	-	-	29/57/57/60	-
17	OPC	E	101	-	-	31/57/57/60	-
20	BCR	G	101	-	-	12/29/63/63	0/2/2/2

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	203	UMQ	O5'-C1'	10.78	1.69	1.41
12	A	307	UMQ	O5'-C1'	10.77	1.69	1.41
12	A	306	UMQ	O5'-C1'	10.76	1.69	1.41
12	B	203	UMQ	O3'-C3'	8.47	1.63	1.43
12	A	307	UMQ	O3'-C3'	8.47	1.63	1.43

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	307	UMQ	C1'-O5'-C5'	-8.72	96.52	113.70
12	A	306	UMQ	C1'-O5'-C5'	-8.68	96.59	113.70
12	B	203	UMQ	C1'-O5'-C5'	-8.61	96.73	113.70
13	A	308	SMA	O7-C7-C8	-7.19	107.34	114.54
13	A	308	SMA	O1-C2-C9	7.06	120.28	111.91

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	308	SMA	C12
16	B	204	CLA	NC
16	B	204	CLA	ND
16	B	204	CLA	NA

5 of 181 torsion outliers are listed below:

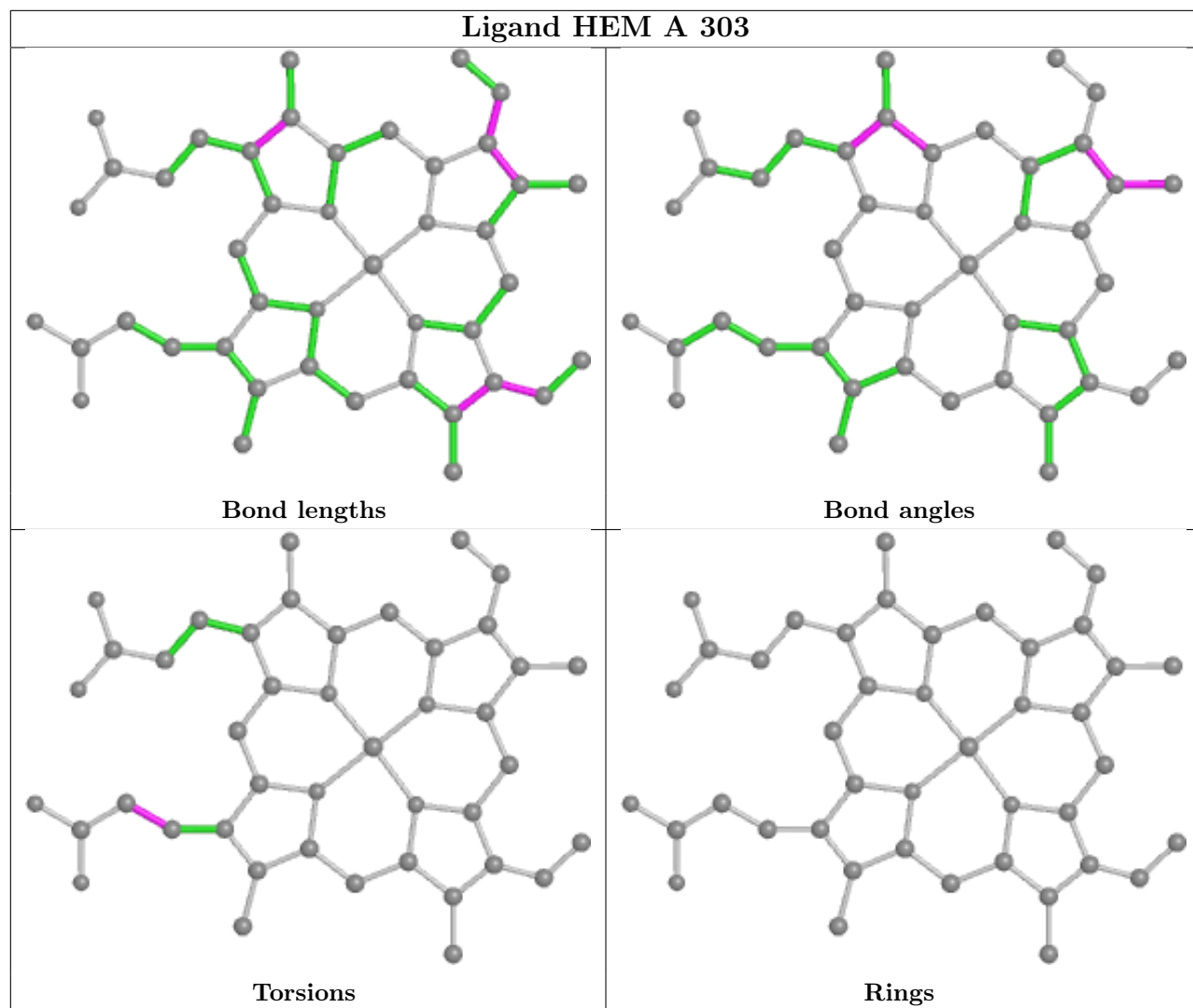
Mol	Chain	Res	Type	Atoms
20	G	101	BCR	C6-C7-C8-C9
20	G	101	BCR	C7-C8-C9-C10
20	G	101	BCR	C7-C8-C9-C34
20	G	101	BCR	C19-C20-C21-C22
12	A	307	UMQ	CB-CA-O1'-C1'

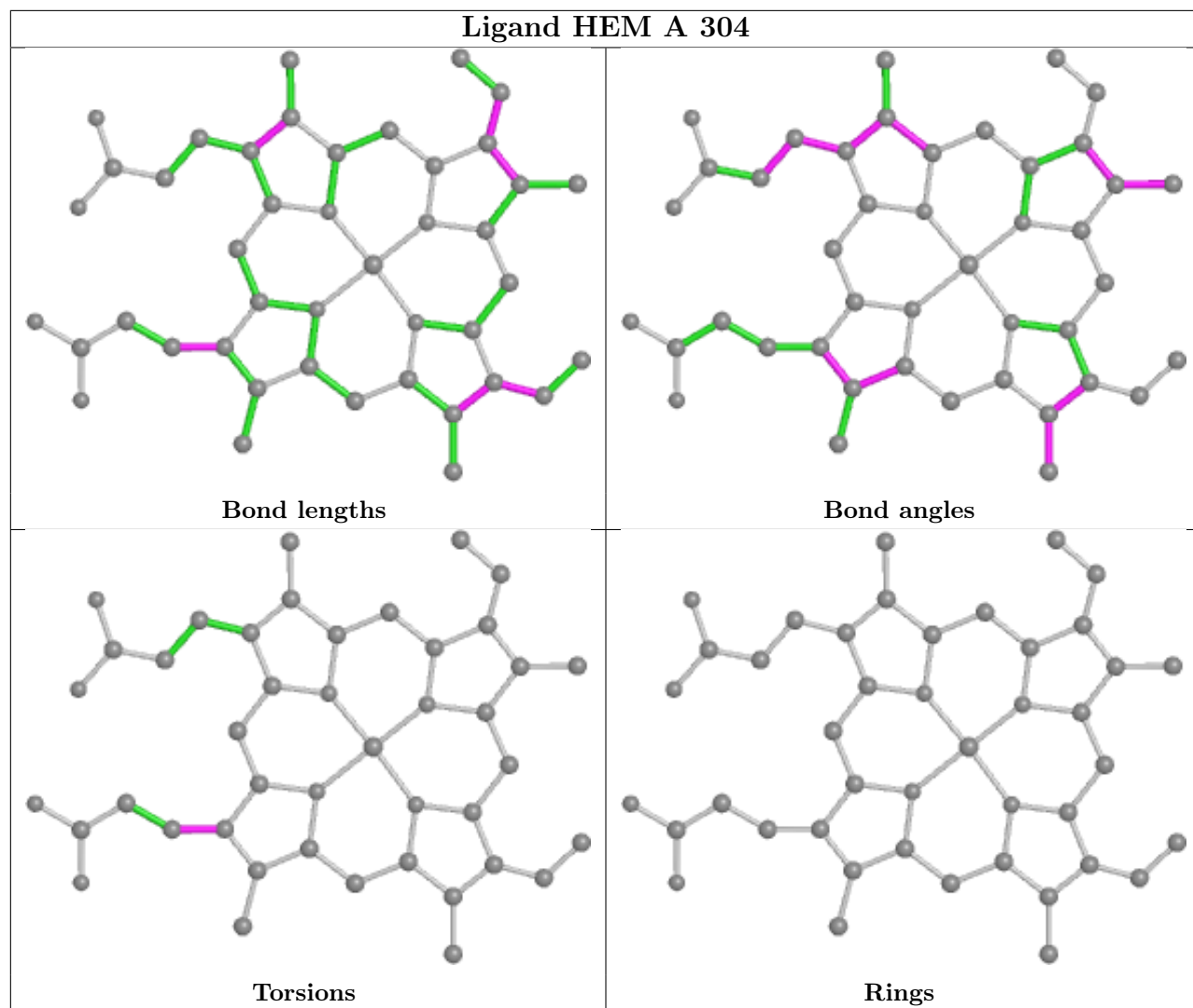
There are no ring outliers.

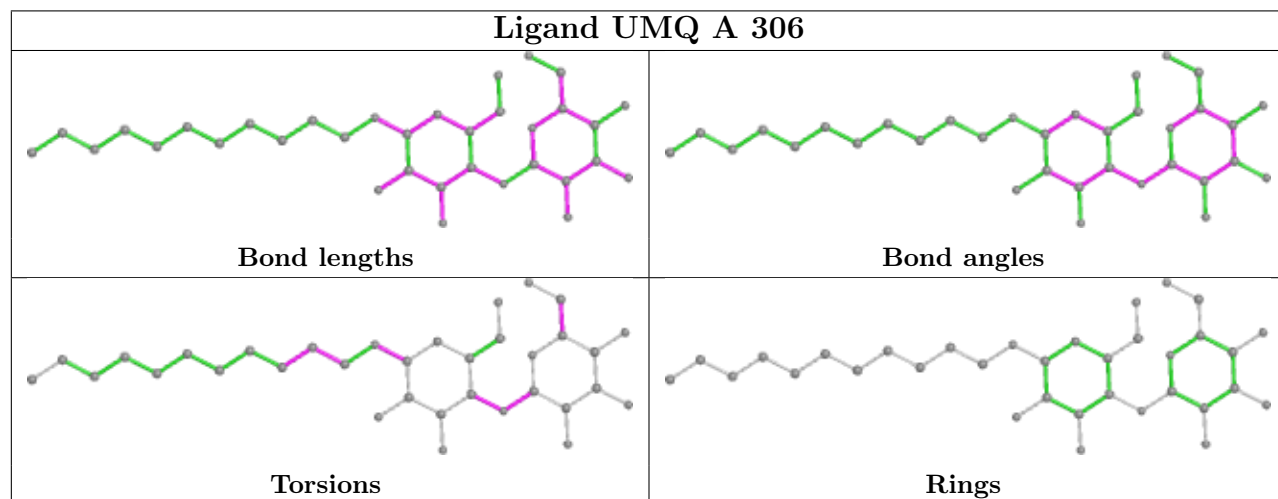
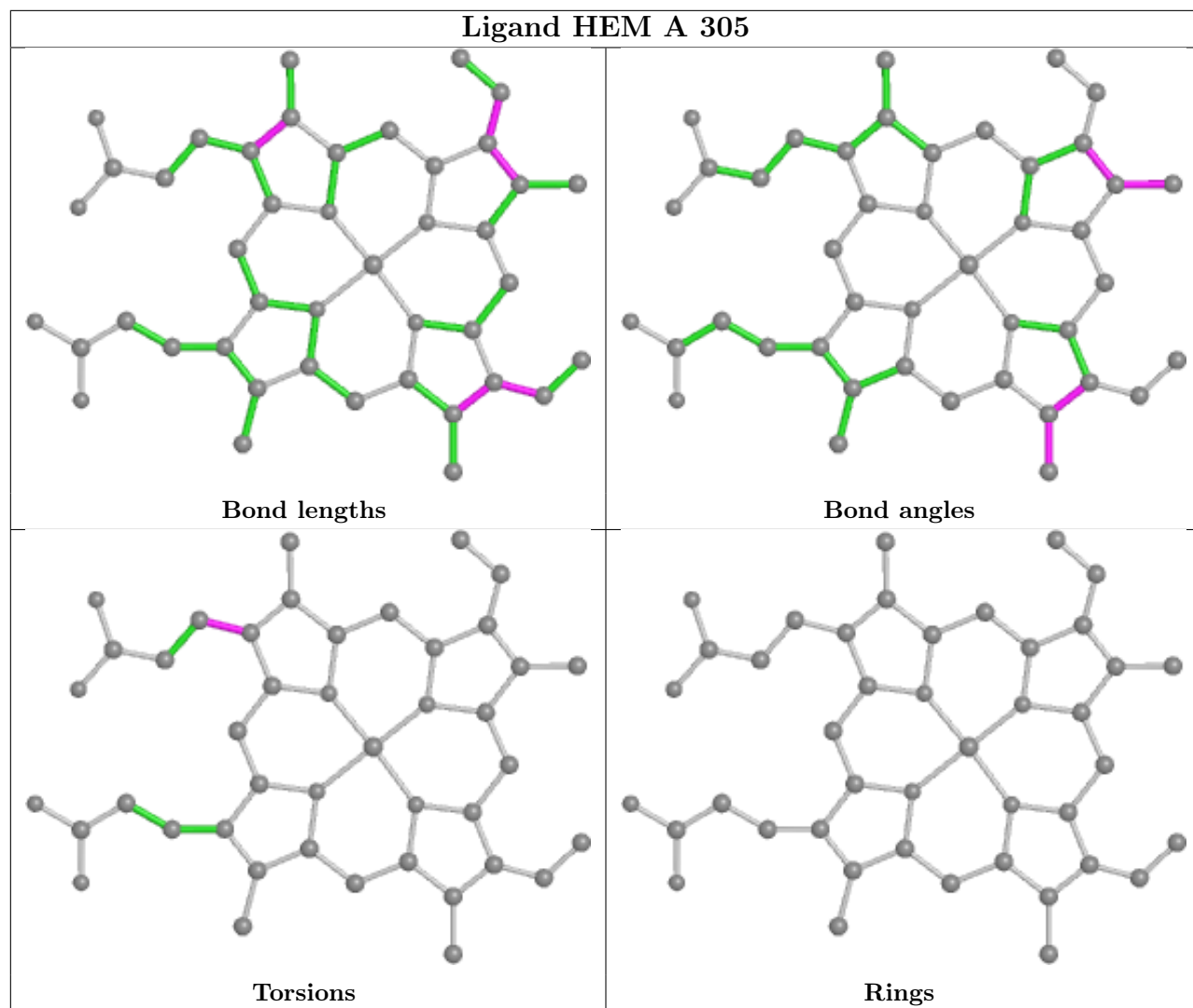
16 monomers are involved in 68 short contacts:

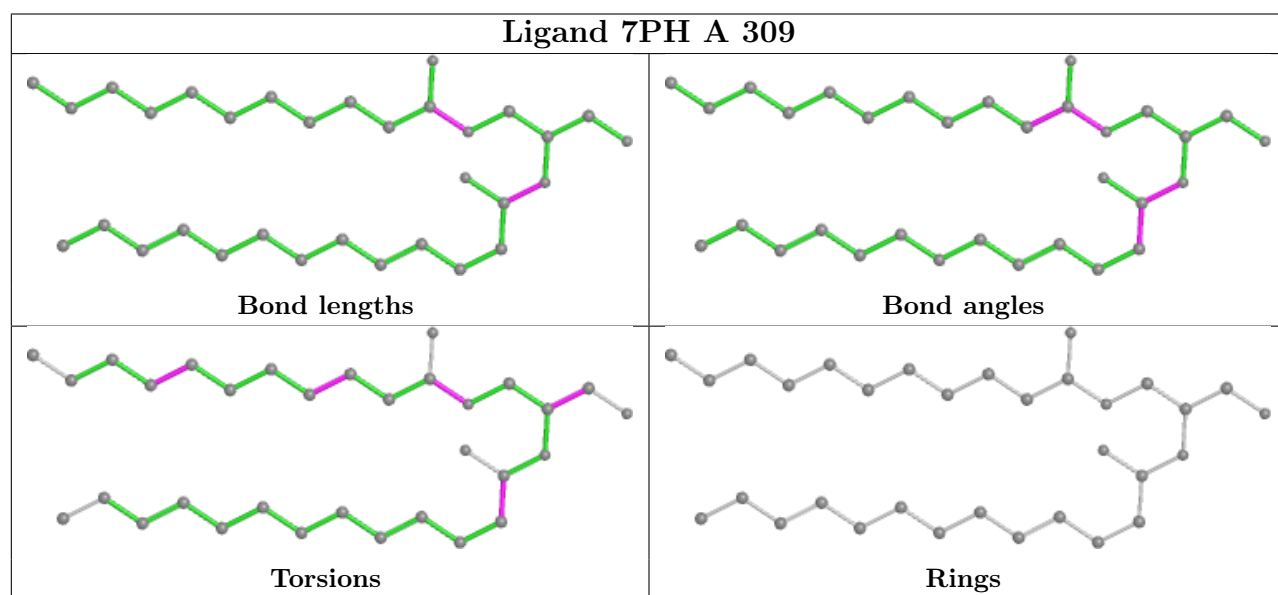
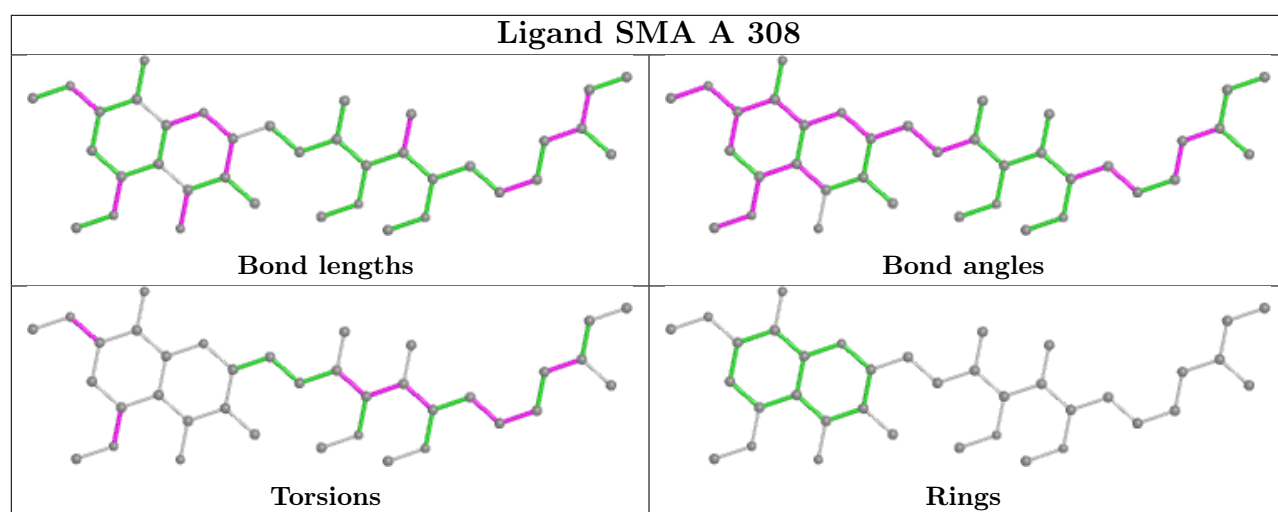
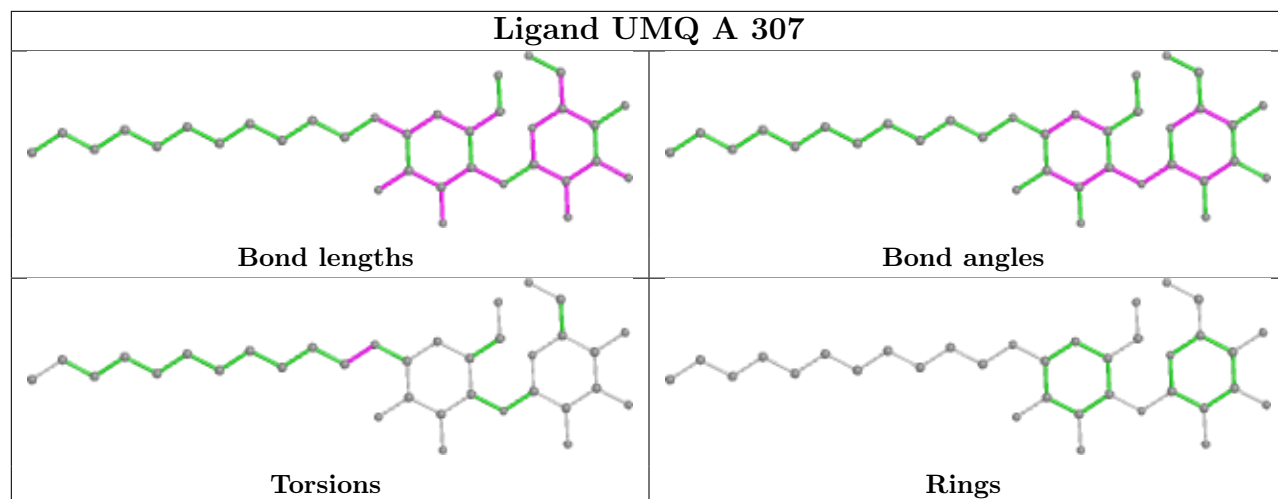
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	MYS	3	0
11	A	303	HEM	3	0
11	A	304	HEM	2	0
11	A	305	HEM	6	0
12	A	306	UMQ	7	0
12	A	307	UMQ	3	0
13	A	308	SMA	7	0
14	A	309	7PH	3	0
12	B	203	UMQ	10	0
16	B	204	CLA	5	0
17	B	205	OPC	5	0
11	C	301	HEM	3	0
19	D	202	SQD	1	0
17	D	203	OPC	4	0
17	E	101	OPC	12	0
20	G	101	BCR	1	0

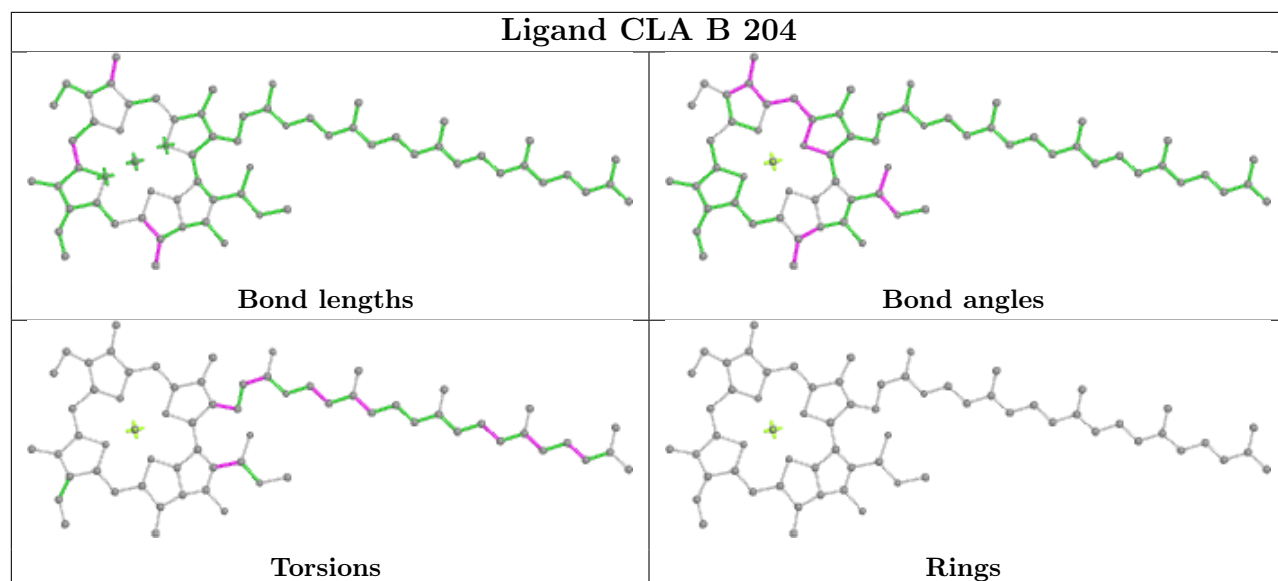
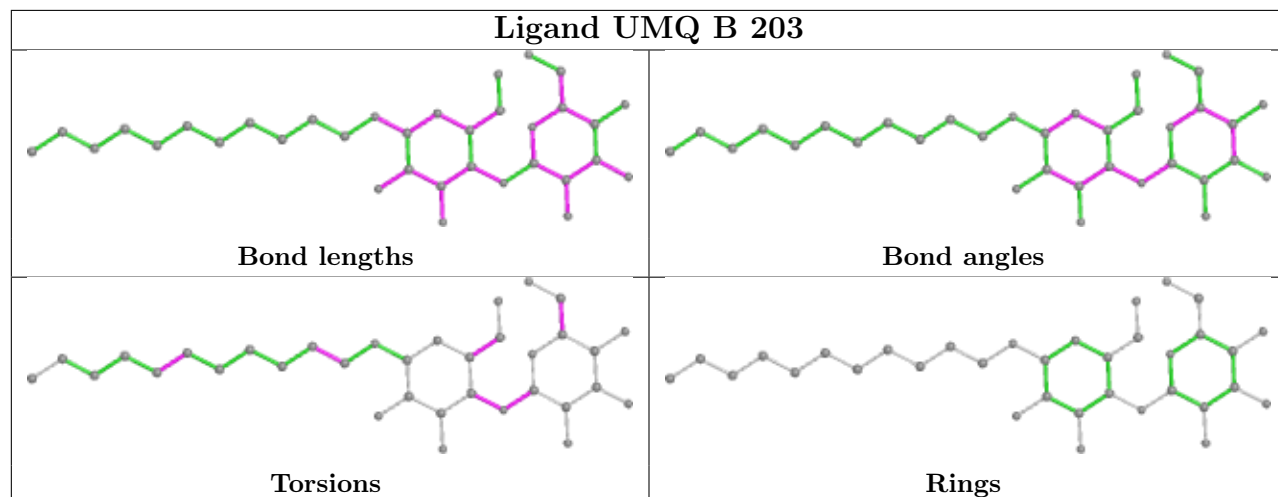
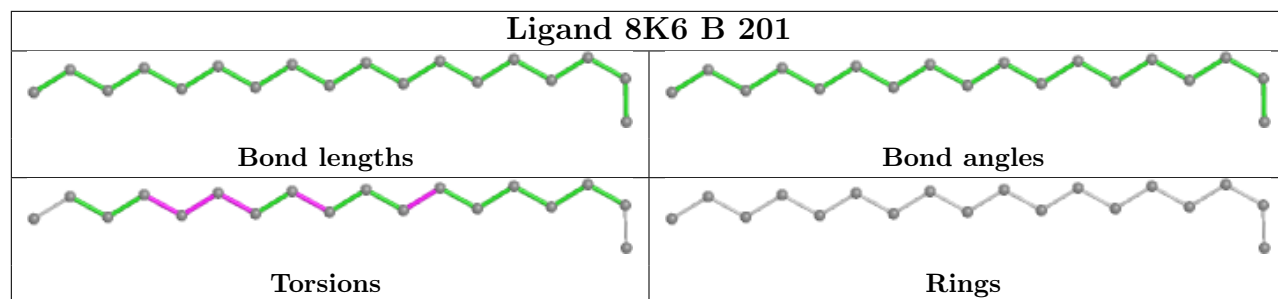
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

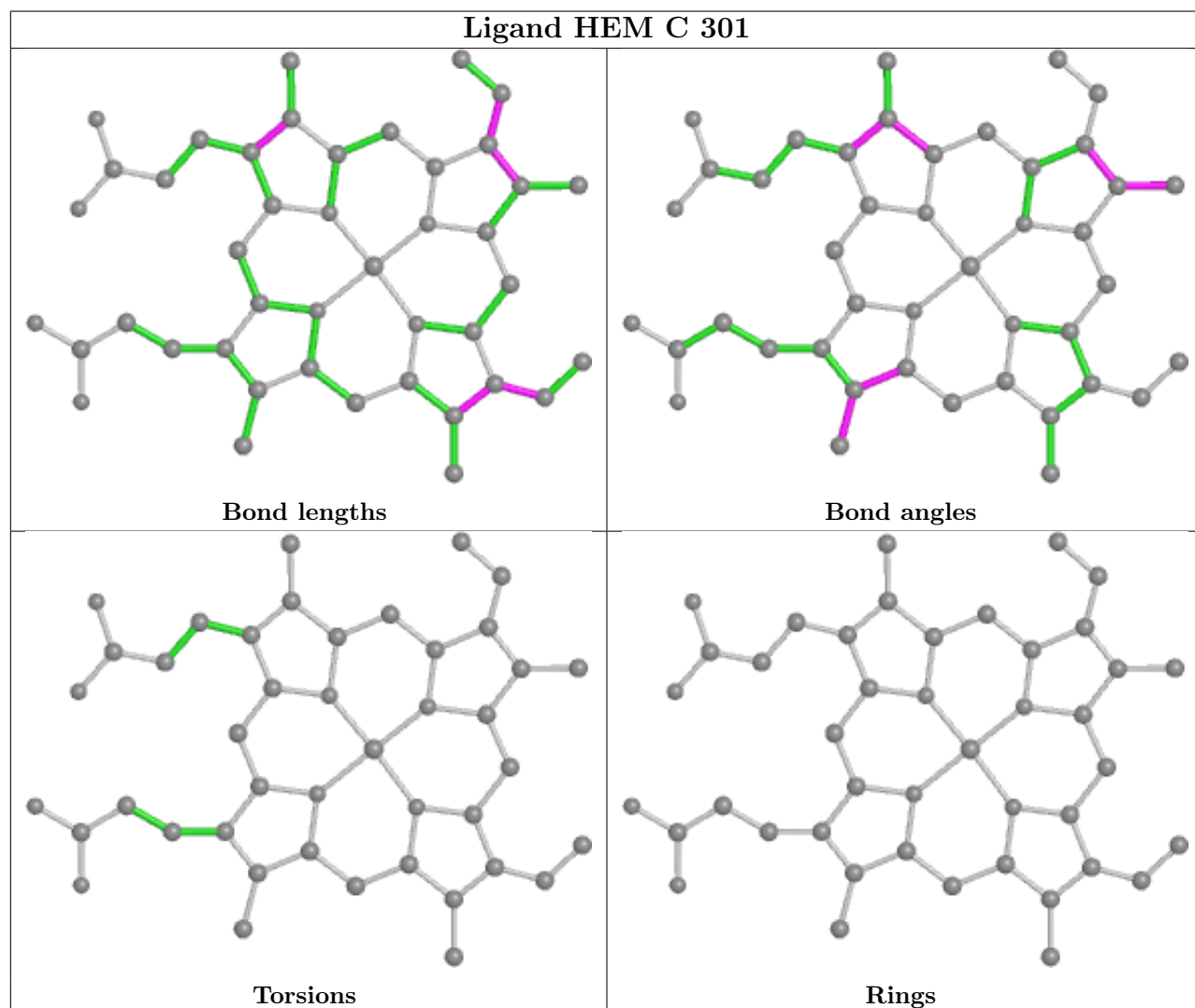
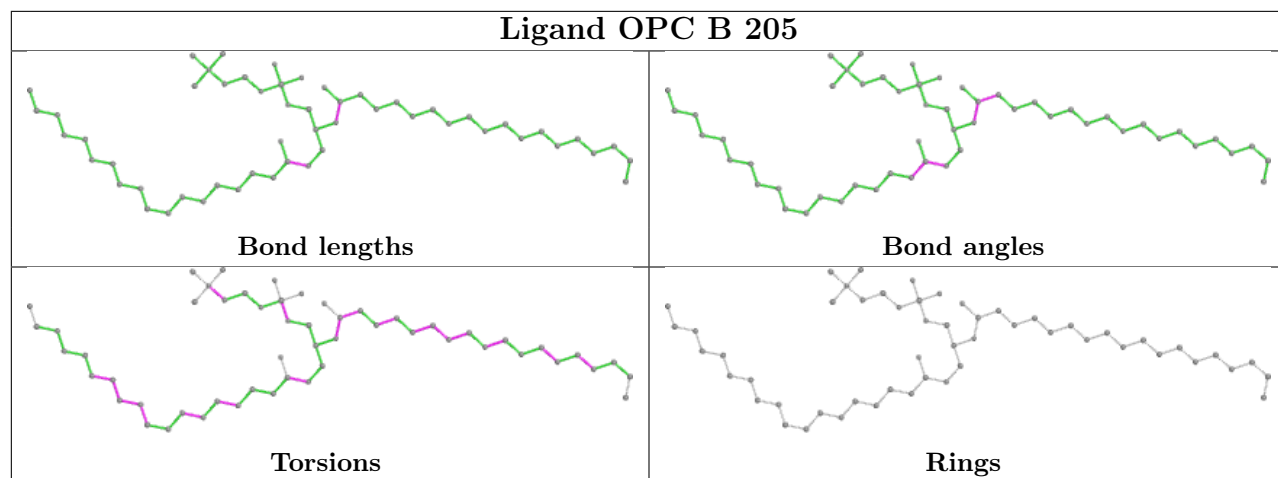


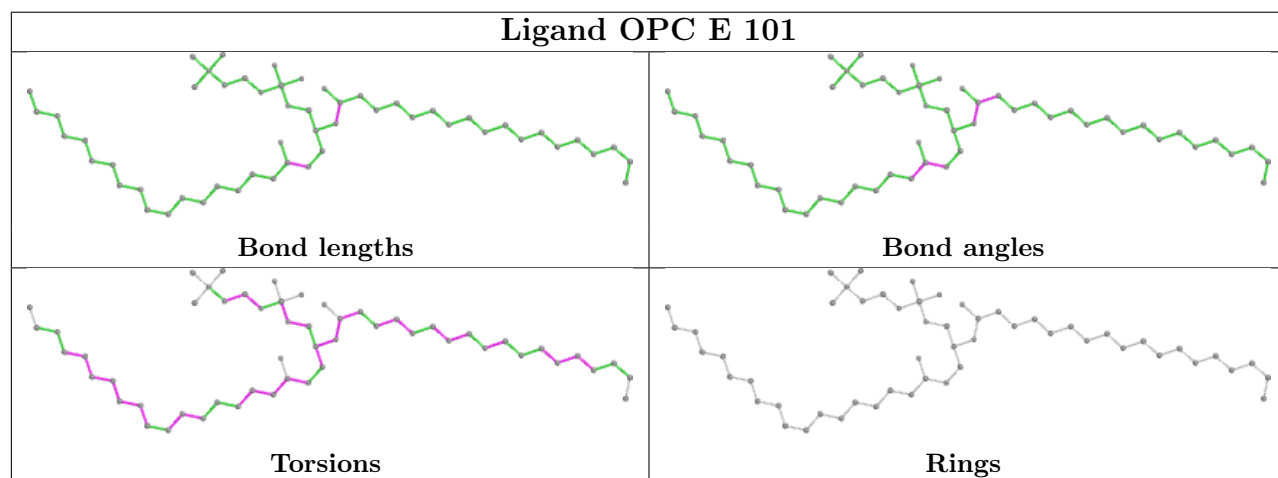
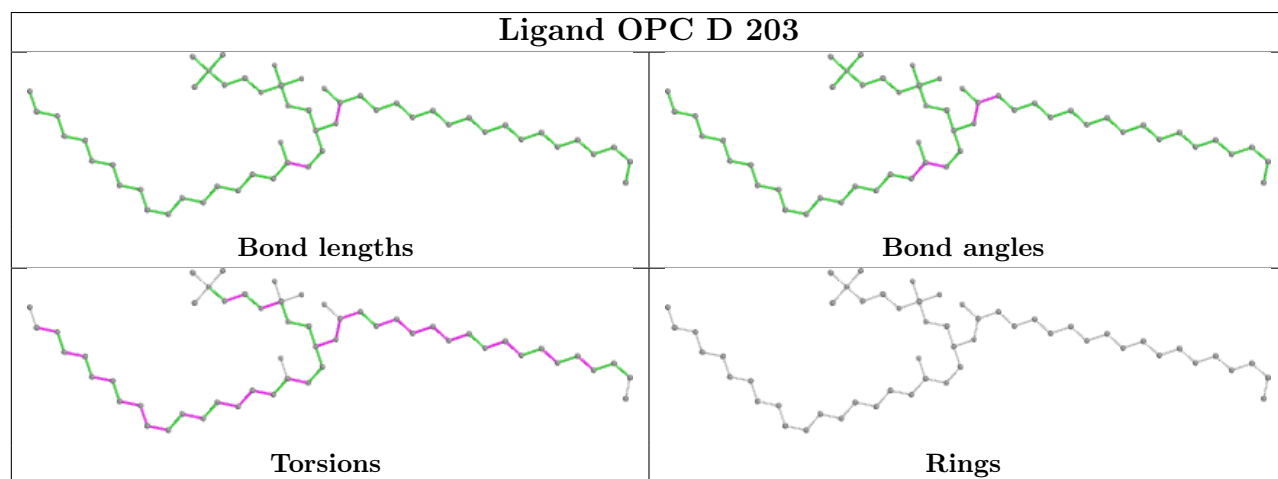
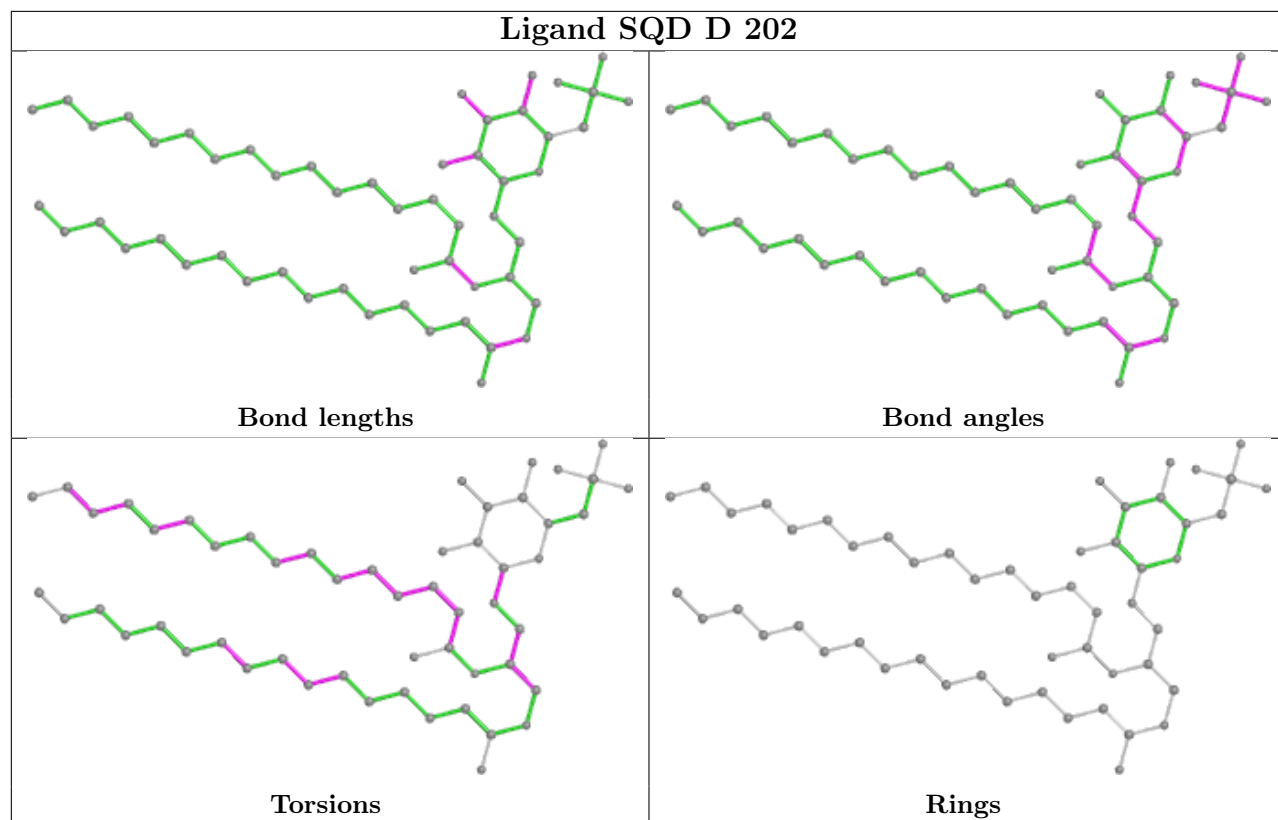


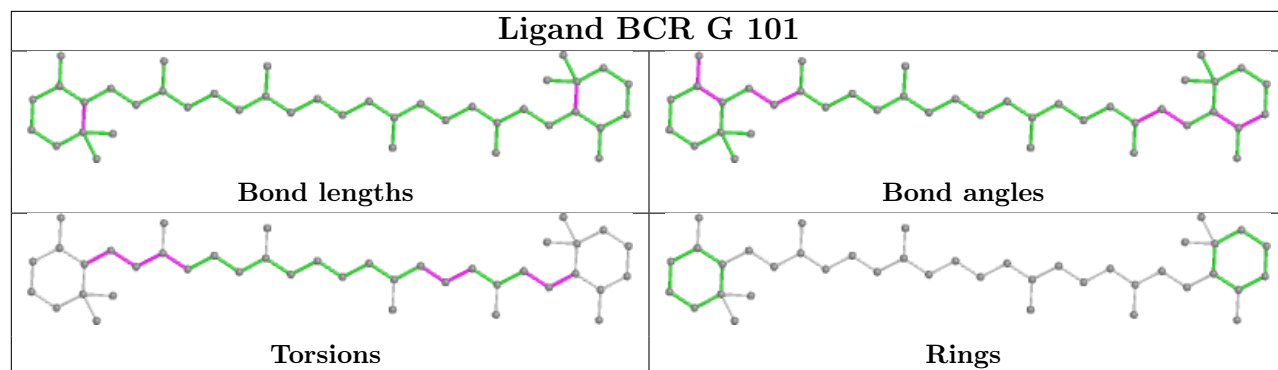












5.7 Other polymers [i](#)

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, 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%)	-0.27	0 100 100	49, 74, 114, 157	5 (2%)
2	B	159/160 (99%)	-0.25	3 (1%) 66 37	60, 96, 139, 208	2 (1%)
3	C	288/289 (99%)	0.28	34 (11%) 4 1	67, 110, 237, 280	0
4	D	158/179 (88%)	0.98	36 (22%) 0 0	65, 170, 227, 287	0
5	E	28/32 (87%)	-0.55	0 100 100	92, 108, 131, 153	0
6	F	31/35 (88%)	0.19	2 (6%) 19 6	83, 100, 159, 177	0
7	G	37/37 (100%)	-0.02	0 100 100	74, 93, 202, 239	4 (10%)
8	H	28/29 (96%)	-0.22	0 100 100	77, 90, 128, 148	0
All	All	942/976 (96%)	0.13	75 (7%) 12 4	49, 100, 212, 287	11 (1%)

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	220	SER	6.9
3	C	192	ASN	6.1
6	F	32	ALA	5.9
4	D	56	ALA	5.7
4	D	159	ASN	5.6

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 carbohydrates in this entry.

6.4 Ligands ⓘ

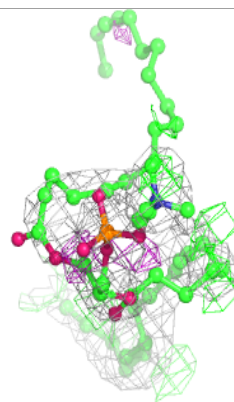
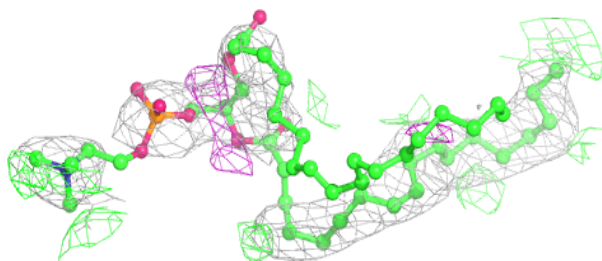
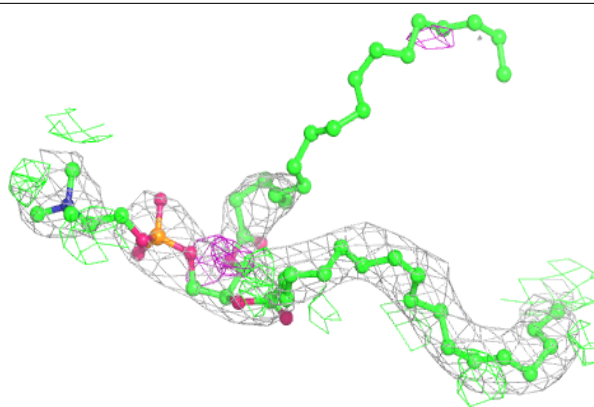
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	OPC	D	203	54/55	0.71	0.41	67,125,194,215	1
12	UMQ	A	306	34/34	0.73	0.41	72,128,148,161	7
15	8K6	B	201	18/18	0.77	0.43	74,93,107,115	0
14	7PH	A	309	32/38	0.81	0.39	53,85,112,116	4
10	CD	B	202	1/1	0.81	0.20	231,231,231,231	0
12	UMQ	B	203	34/34	0.83	0.30	107,167,218,223	0
17	OPC	E	101	54/55	0.86	0.34	67,112,195,227	0
13	SMA	A	308	37/37	0.87	0.35	77,110,157,166	12
9	MYS	A	301	15/15	0.89	0.34	50,68,85,86	0
12	UMQ	A	307	34/34	0.89	0.36	100,139,156,232	3
20	BCR	G	101	40/40	0.89	0.36	57,80,98,107	14
19	SQD	D	202	54/54	0.90	0.19	104,125,149,154	30
17	OPC	B	205	54/55	0.90	0.34	80,118,150,151	0
16	CLA	B	204	65/65	0.94	0.23	69,97,126,131	0
18	FES	D	201	4/4	0.94	0.13	151,161,163,260	0
11	HEM	C	301	43/43	0.97	0.23	60,87,128,141	0
11	HEM	A	305	43/43	0.98	0.21	71,96,110,126	0
10	CD	A	302	1/1	0.99	0.20	100,100,100,100	0
11	HEM	A	303	43/43	0.99	0.23	47,67,82,100	0
11	HEM	A	304	43/43	0.99	0.21	46,68,82,91	0

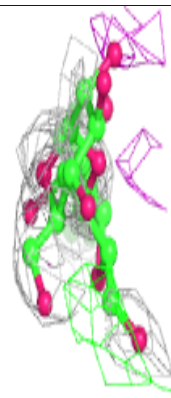
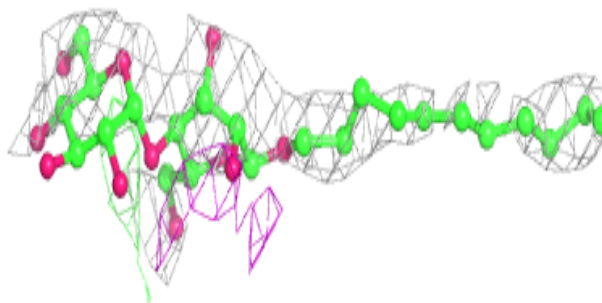
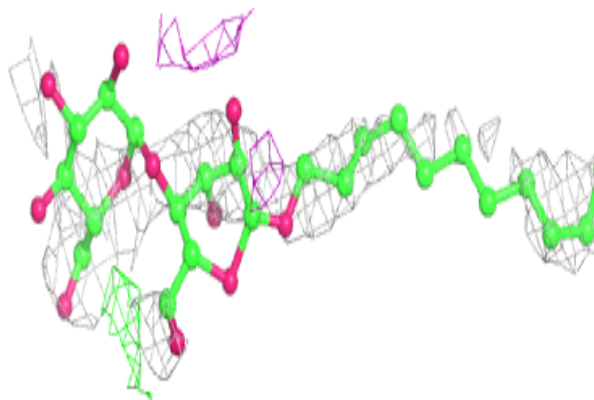
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OPC D 203:

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

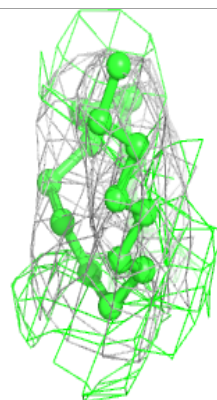
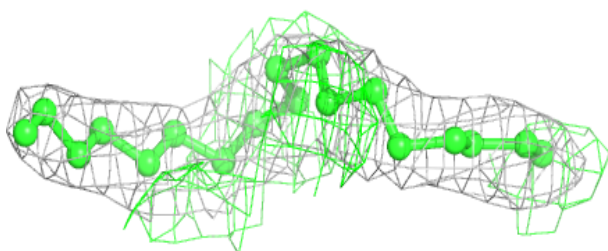
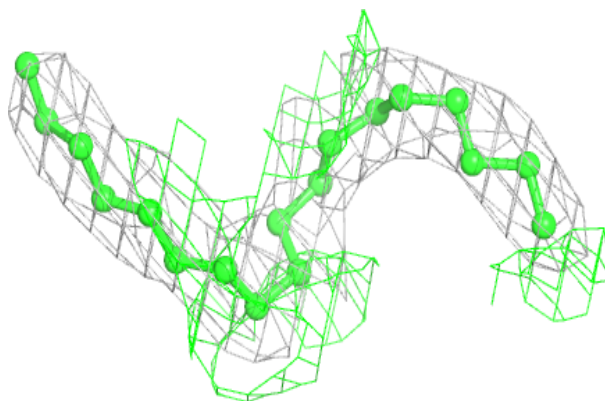
**Electron density around UMQ A 306:**

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

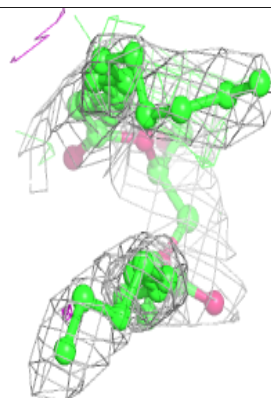
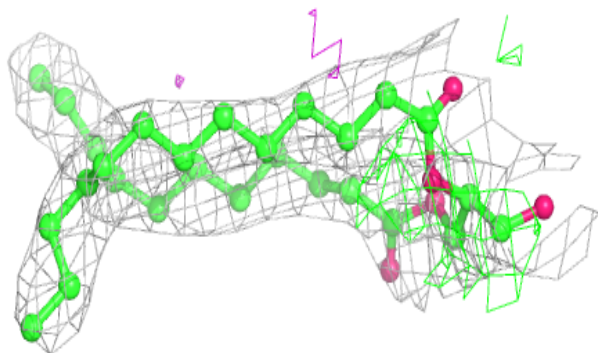
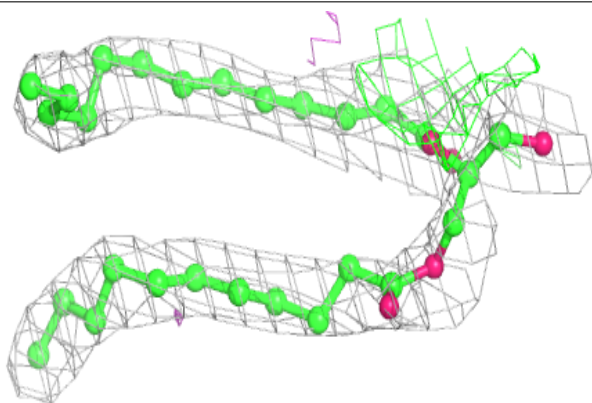


Electron density around 8K6 B 201:

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

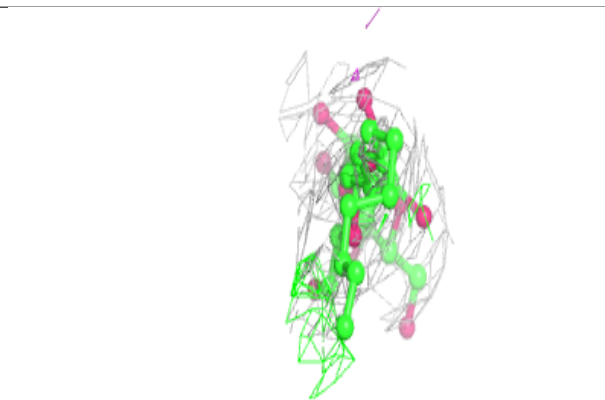
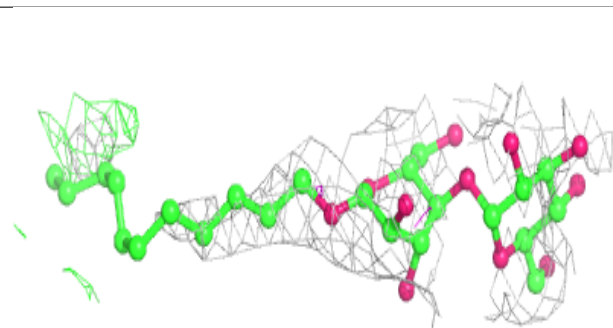
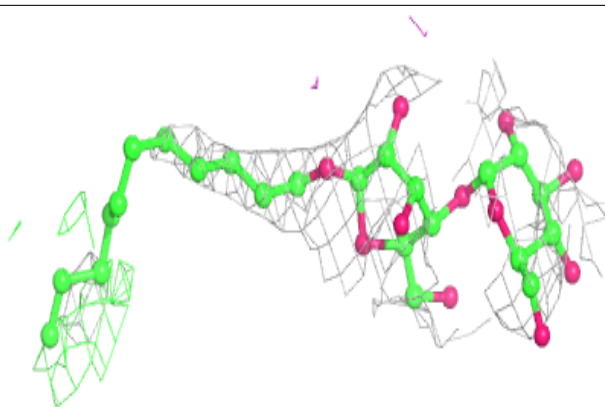
**Electron density around 7PH A 309:**

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

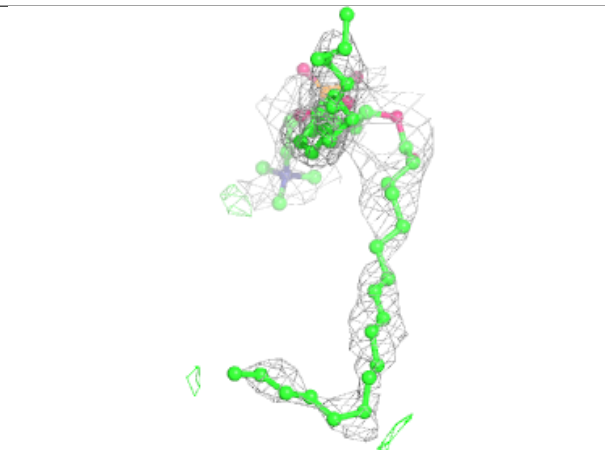
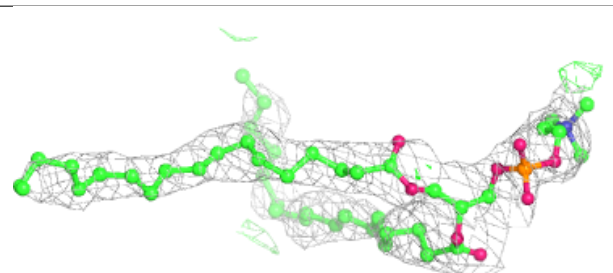
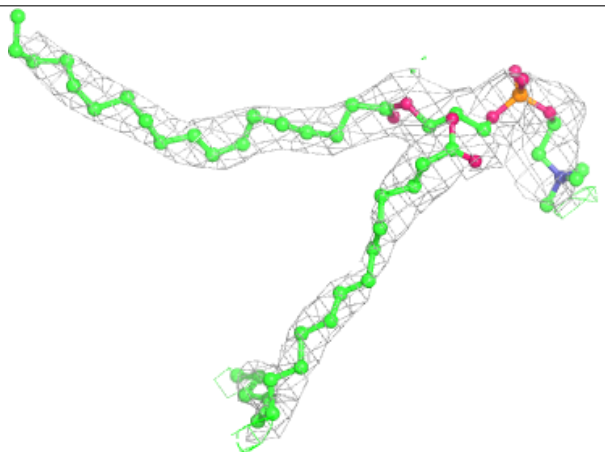


Electron density around UMQ B 203:

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

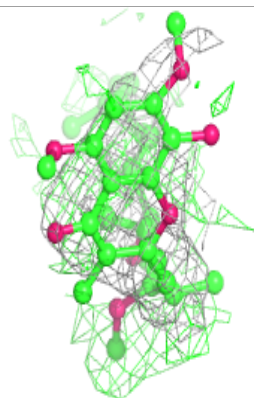
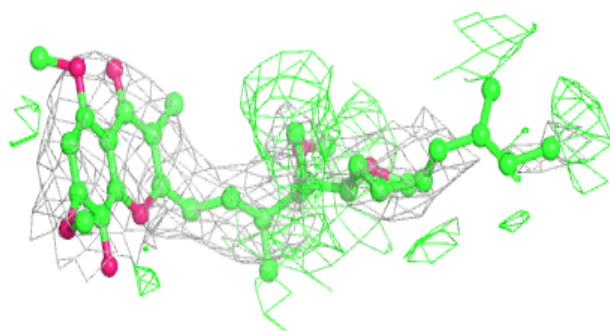
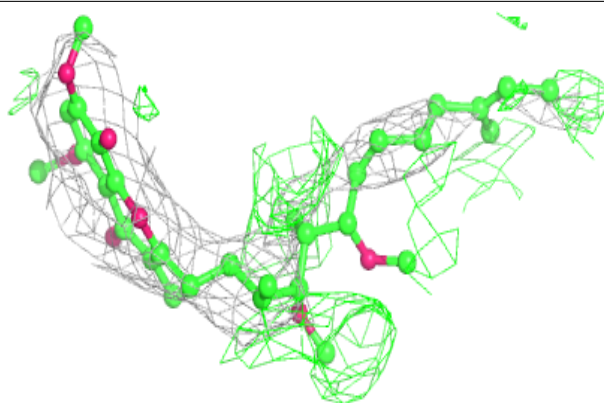
**Electron density around OPC E 101:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

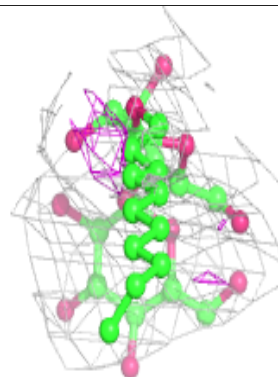
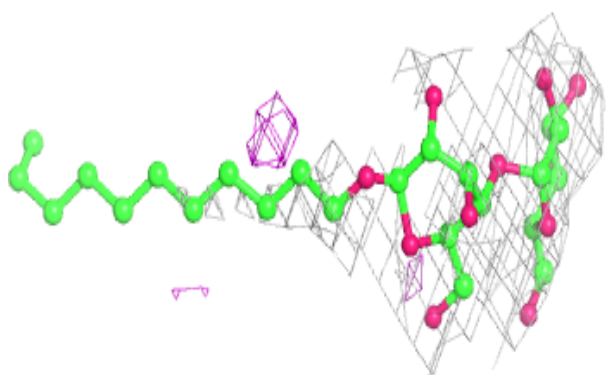
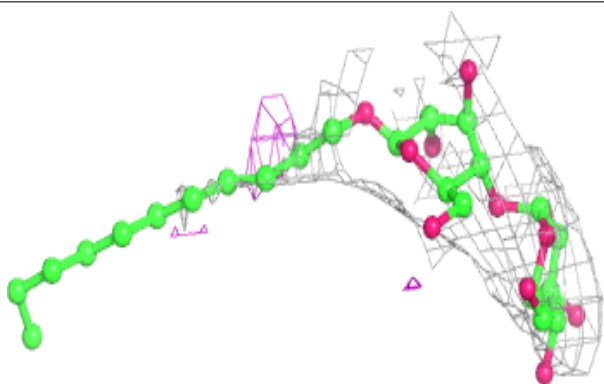


Electron density around SMA A 308:

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

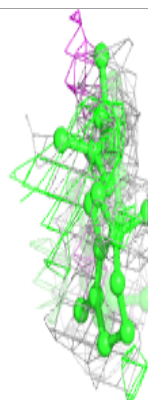
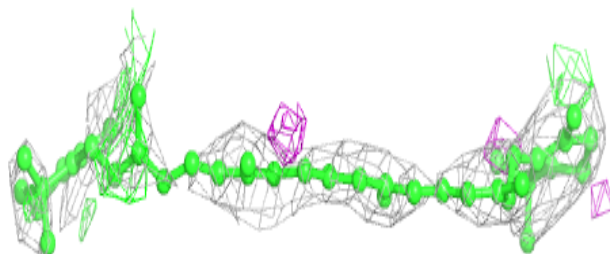
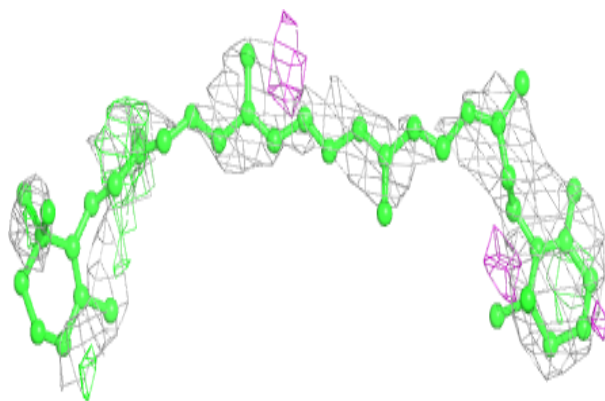
**Electron density around UMQ A 307:**

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and green (positive)

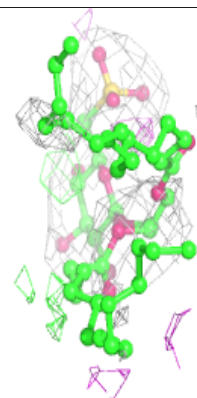
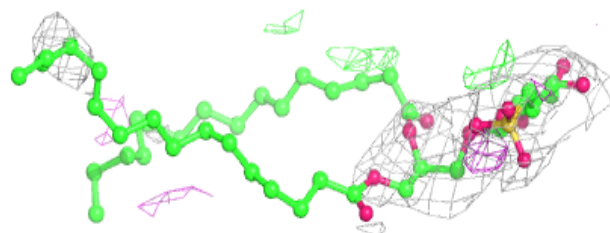
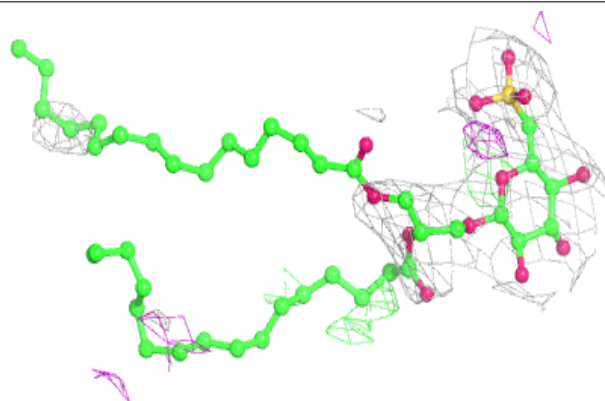


Electron density around BCR G 101:

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

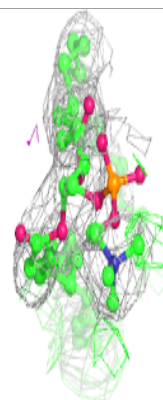
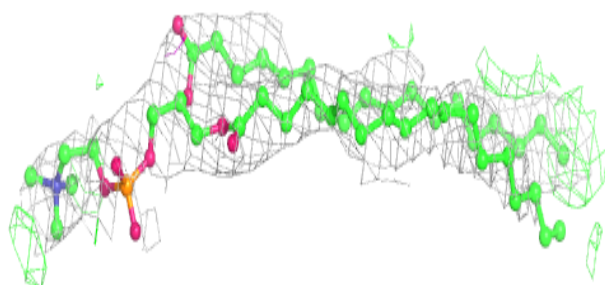
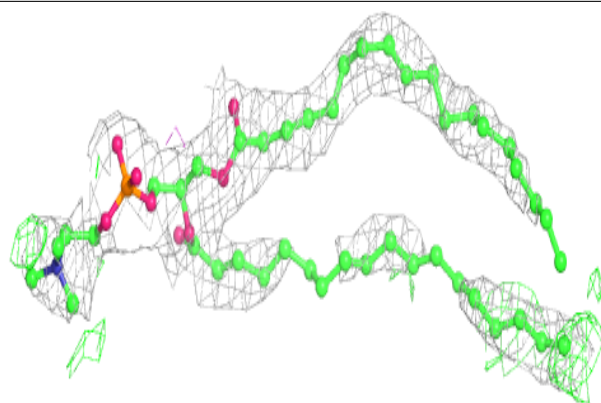
**Electron density around SQD D 202:**

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

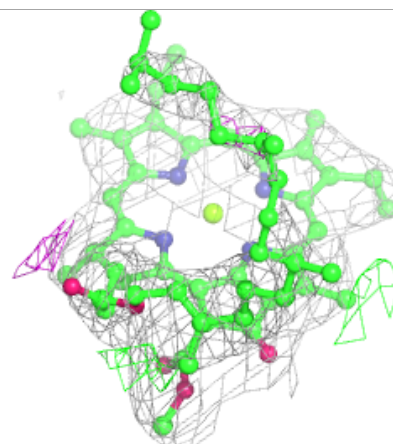
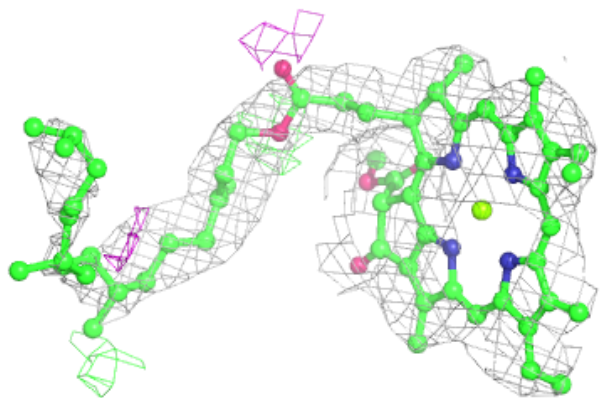
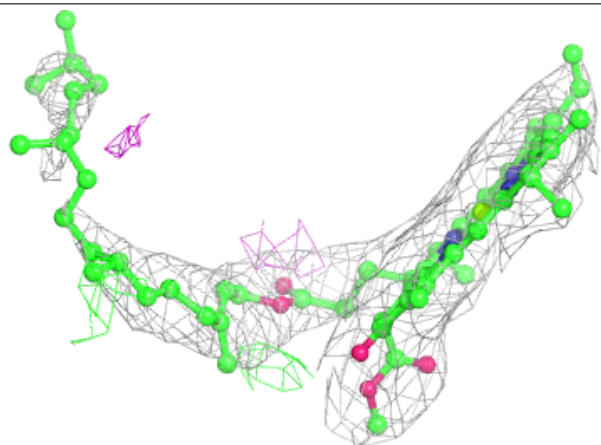


Electron density around OPC B 205:

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

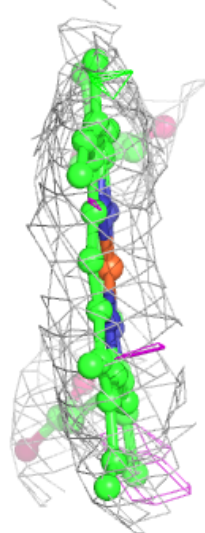
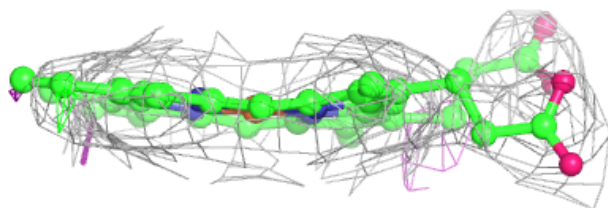
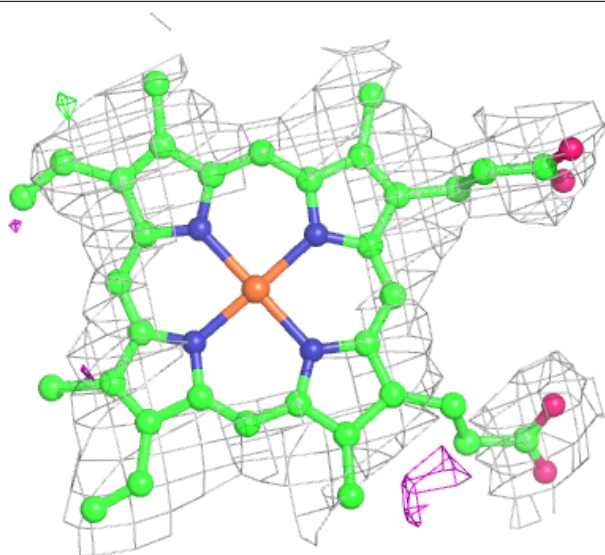
**Electron density around CLA B 204:**

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



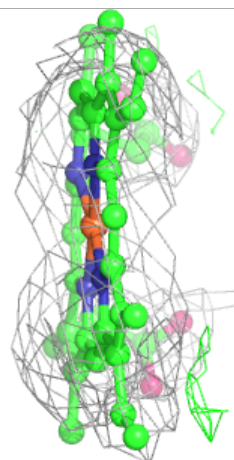
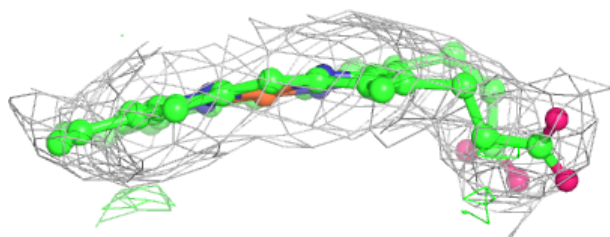
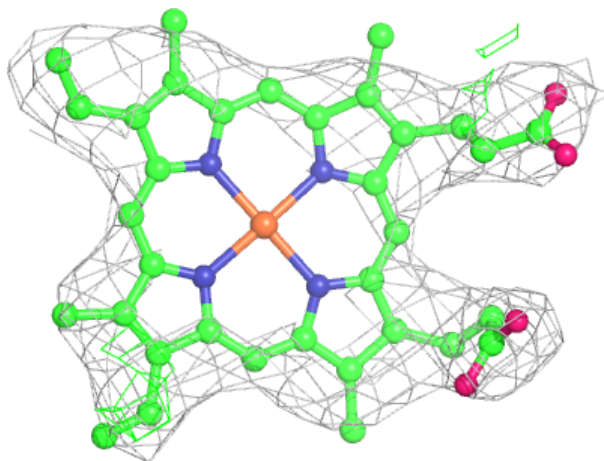
Electron density around HEM C 301:

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



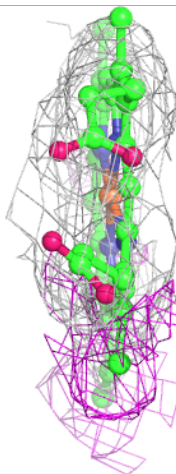
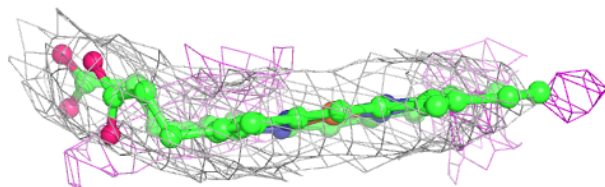
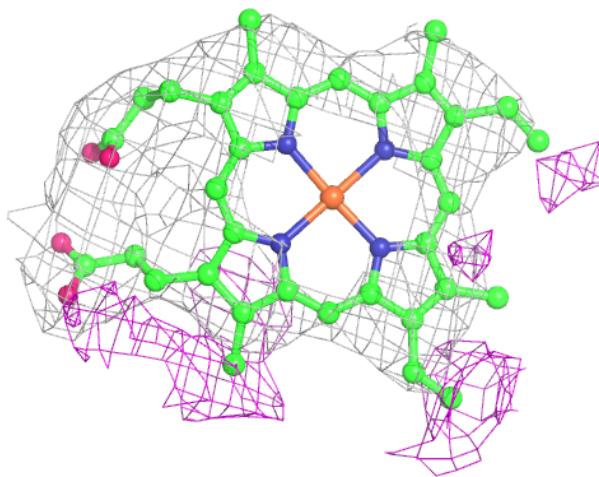
Electron density around HEM A 305:

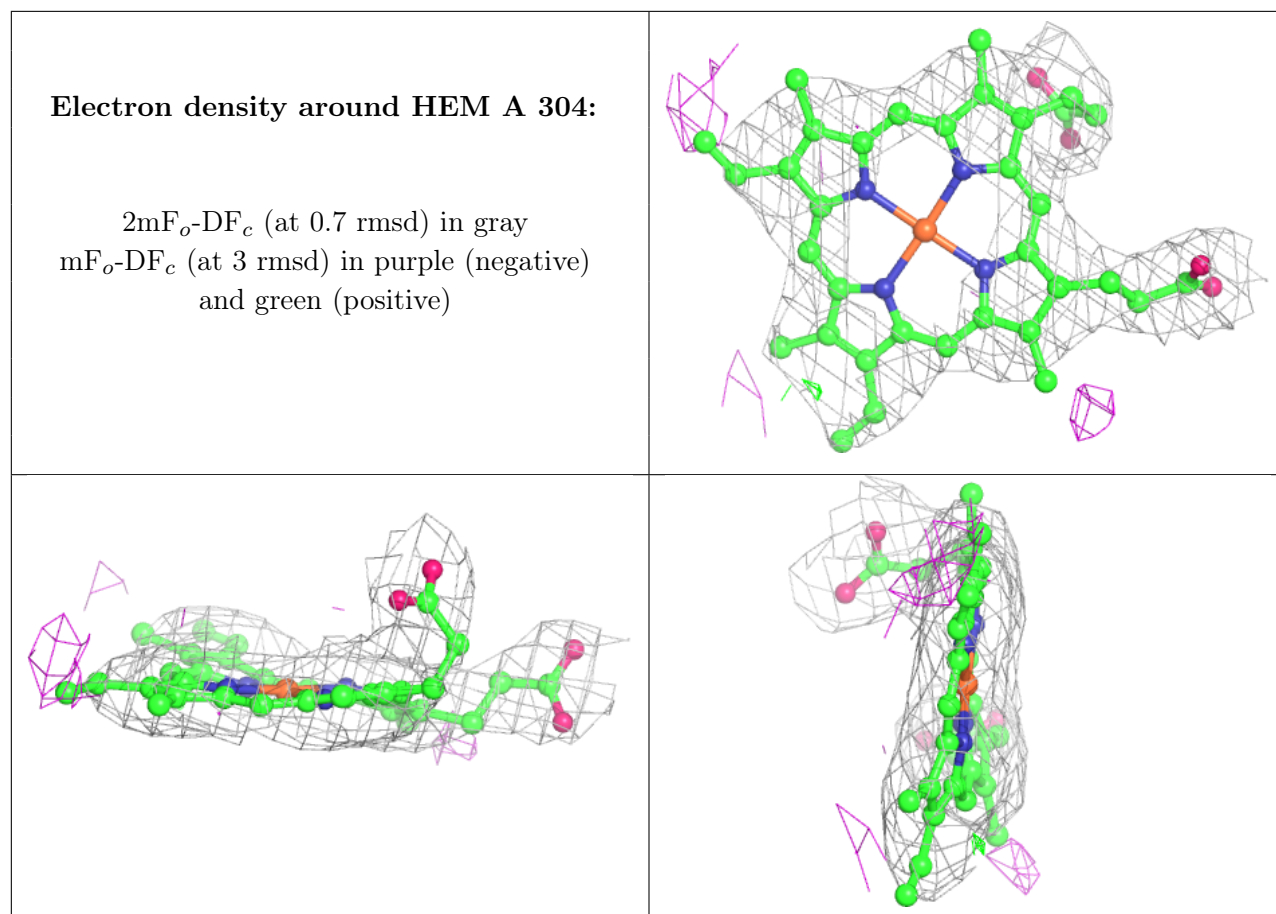
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.