



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 08:19 pm BST

PDB ID : 2ZT9
Title : Crystal Structure of the Cytochrome b6f Complex from Nostoc sp. PCC 7120
Authors : Craner, W.A.; Baniulis, D.; Yamashita, E.
Deposited on : 2008-09-27
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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

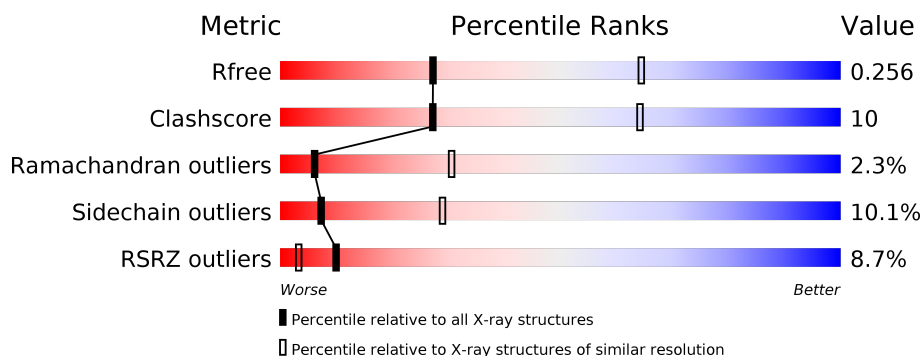
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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	<div> <div>0%</div> <div> <div>76%</div> <div>21%</div> <div>•</div> </div> </div>
2	B	160	<div> <div>2%</div> <div> <div>73%</div> <div>21%</div> <div>6%</div> <div>•</div> </div> </div>
3	C	289	<div> <div>12%</div> <div> <div>73%</div> <div>22%</div> <div>5%</div> </div> </div>
4	D	179	<div> <div>24%</div> <div> <div>76%</div> <div>16%</div> <div>•</div> <div>7%</div> </div> </div>
5	E	31	<div> <div>3%</div> <div> <div>81%</div> <div>16%</div> <div>•</div> </div> </div>
6	F	34	<div> <div>62%</div> <div> <div>24%</div> <div>9%</div> <div>6%</div> </div> </div>

Continued on next page...

Continued from previous page...

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	UMQ	A	304	X	-	-	-
10	UMQ	A	305	X	-	-	-
10	UMQ	A	306	X	-	-	-
11	CLA	B	201	X	-	-	-
12	OPC	H	30	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7912 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	215	Total	C	N	O	S	0	0	0
			1715	1144	272	288	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1239	830	195	208	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	289	Total	C	N	O	S	0	0	0
			2195	1396	364	429	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1249	791	213	239	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	31	Total	C	N	O	S	0	0	0
			227	157	35	34	1			

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

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

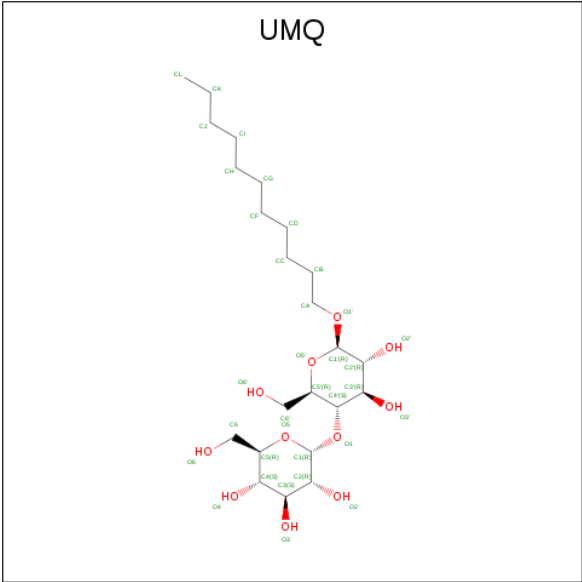
- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | G | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 281 | 188 | 44 | 48 | 1 | | | |

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | H | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 227 | 155 | 36 | 34 | 2 | | | |

- # HEM

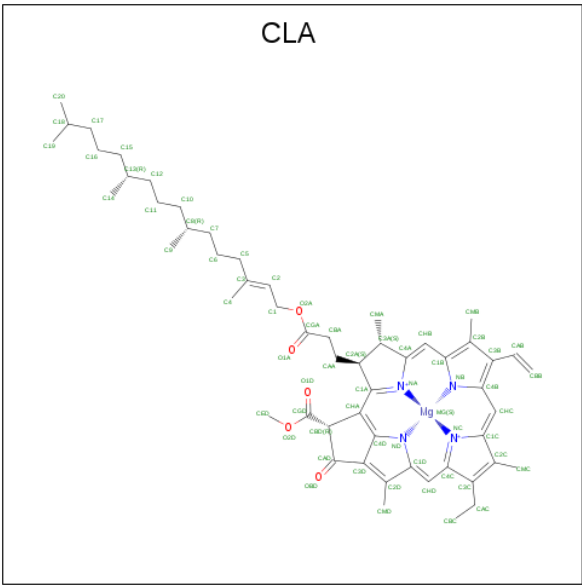
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



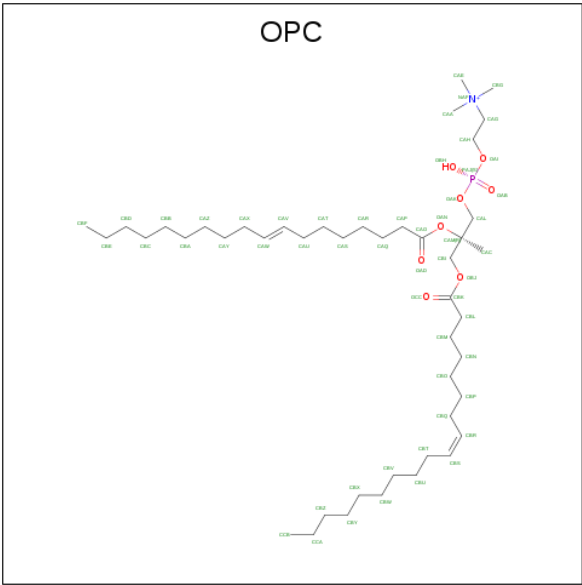
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	O			0	0
			34	23	11				
10	A	1	Total	C	O			0	0
			34	23	11				
10	A	1	Total	C	O			0	0
			34	23	11				

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



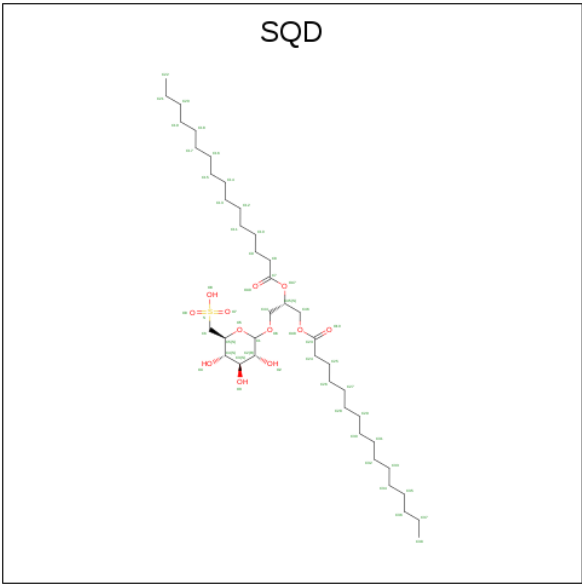
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 12 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).



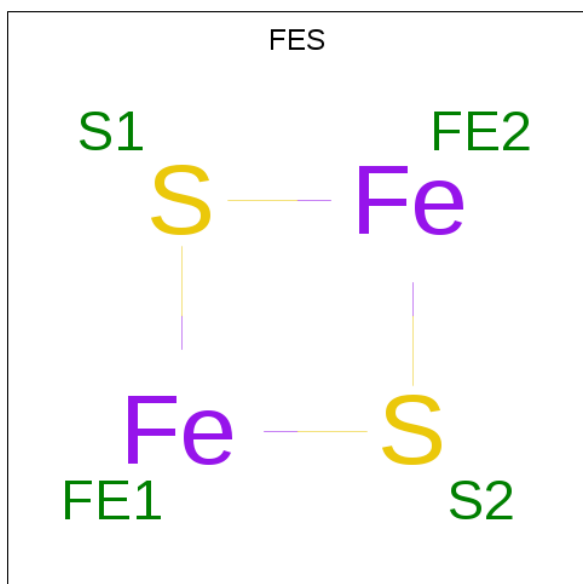
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 13 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



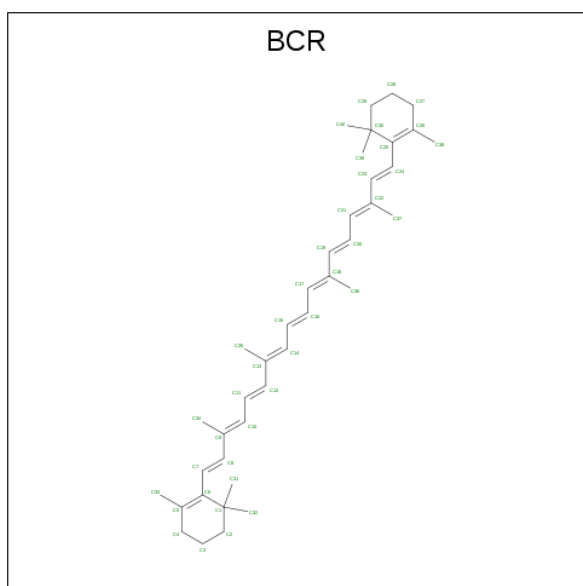
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



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

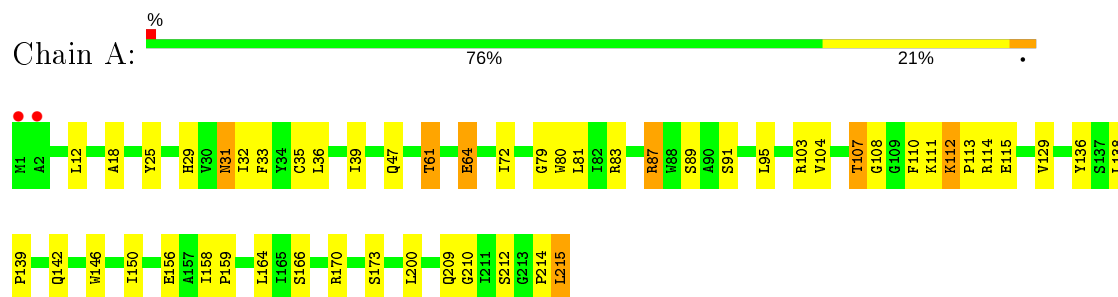
- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total O 1 1	0	0
16	B	2	Total O 2 2	0	0

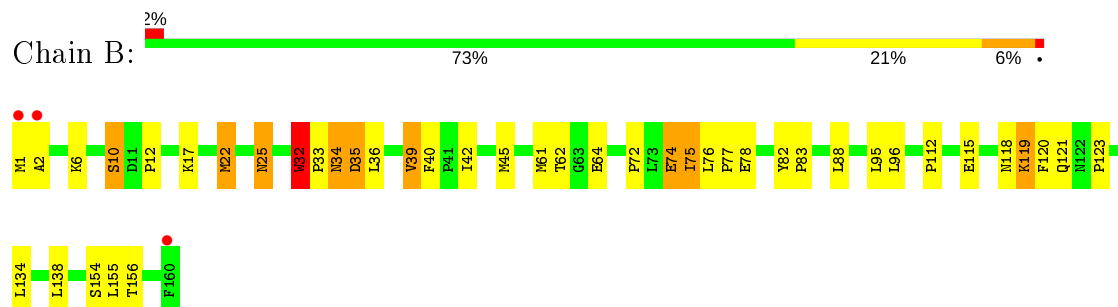
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

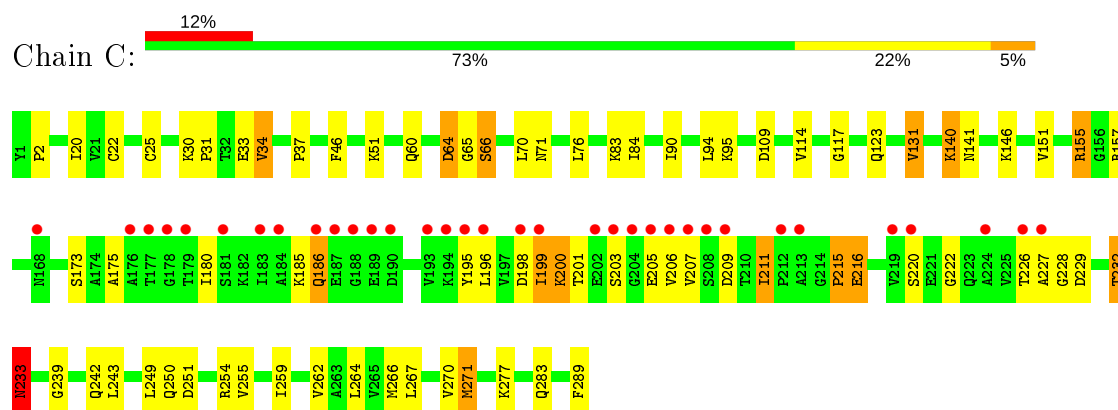
• Molecule 1: Cytochrome b6



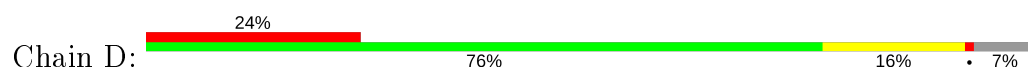
• Molecule 2: Cytochrome b6-f complex subunit 4

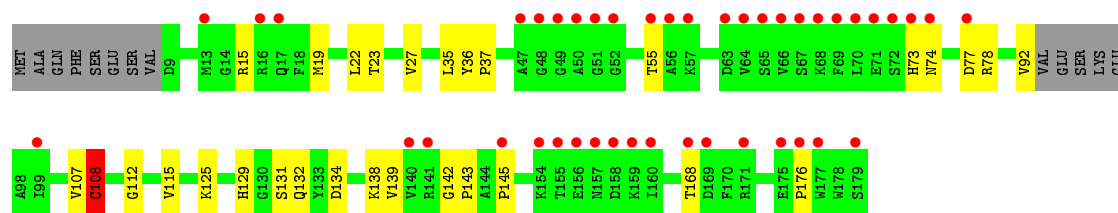


• Molecule 3: Apocytochrome f

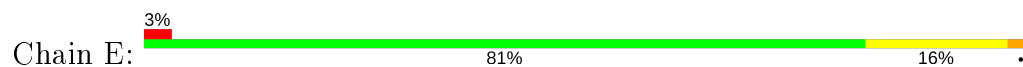


• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1





• 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	159.22Å 159.22Å 365.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.69 – 3.00 45.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.69-3.00) 98.5 (45.68-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.259 0.228 , 0.256	Depositor DCC
R_{free} test set	2770 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.2	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	0.90	EDS
Total number of atoms	7912	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/1768	0.62	0/2411
2	B	0.50	0/1278	0.66	0/1752
3	C	0.44	0/2241	0.58	0/3053
4	D	0.40	0/1280	0.55	1/1745 (0.1%)
5	E	0.45	0/230	0.52	0/309
6	F	0.45	0/234	0.56	0/315
7	G	0.48	0/286	0.65	0/387
8	H	0.51	0/233	0.66	0/319
All	All	0.46	0/7550	0.60	1/10291 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	108	CYS	CA-CB-SG	5.66	124.18	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TRP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1715	0	1734	46	0
2	B	1239	0	1290	39	0
3	C	2195	0	2183	54	0
4	D	1249	0	1208	17	0
5	E	227	0	257	3	0
6	F	231	0	252	6	0
7	G	281	0	303	12	0
8	H	227	0	243	13	0
9	A	129	0	90	8	0
9	C	43	0	30	6	0
10	A	102	0	123	4	0
11	B	65	0	72	1	0
12	B	54	0	83	0	0
12	H	54	0	83	4	0
13	B	54	0	78	1	0
14	D	4	0	0	1	0
15	G	40	0	53	7	0
16	A	1	0	0	0	0
16	B	2	0	0	0	0
All	All	7912	0	8082	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 161 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)
1:A:35:CYS:SG	9:A:303:HEM:CAB	2.17	1.32
1:A:35:CYS:SG	9:A:303:HEM:HAB	1.79	1.22
1:A:35:CYS:HG	9:A:303:HEM:CAB	1.52	1.14
3:C:25:CYS:SG	9:C:301:HEM:CAC	2.37	1.13
3:C:25:CYS:SG	9:C:301:HEM:HAC	1.93	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/215 (99%)	200 (94%)	12 (6%)	1 (0%)	29	68
2	B	158/160 (99%)	143 (90%)	10 (6%)	5 (3%)	4	22
3	C	287/289 (99%)	245 (85%)	31 (11%)	11 (4%)	3	18
4	D	162/179 (90%)	144 (89%)	16 (10%)	2 (1%)	13	48
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	F	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	4	21
7	G	35/37 (95%)	32 (91%)	1 (3%)	2 (6%)	1	10
8	H	27/29 (93%)	27 (100%)	0	0	100	100
All	All	941/974 (97%)	847 (90%)	72 (8%)	22 (2%)	6	30

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
2	B	32	TRP
3	C	64	ASP
3	C	66	SER
3	C	200	LYS

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	184/184 (100%)	169 (92%)	15 (8%)	11	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	134/134 (100%)	118 (88%)	16 (12%)	5	22
3	C	238/238 (100%)	216 (91%)	22 (9%)	9	34
4	D	133/145 (92%)	124 (93%)	9 (7%)	16	48
5	E	21/21 (100%)	18 (86%)	3 (14%)	3	15
6	F	22/24 (92%)	16 (73%)	6 (27%)	0	2
7	G	29/29 (100%)	25 (86%)	4 (14%)	3	17
8	H	24/24 (100%)	20 (83%)	4 (17%)	2	11
All	All	785/799 (98%)	706 (90%)	79 (10%)	7	29

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	94	LEU
3	C	211	ILE
7	G	21	LEU
3	C	109	ASP
3	C	141	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	122	ASN
3	C	60	GLN
6	F	30	GLN
2	B	118	ASN
4	D	132	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HEM	A	302	1	27,50,50	2.19	5 (18%)	17,82,82	1.51	3 (17%)
10	UMQ	A	306	-	35,35,35	1.52	3 (8%)	46,46,46	2.23	11 (23%)
13	SQD	B	203	-	53,54,54	1.06	3 (5%)	62,65,65	3.43	15 (24%)
14	FES	D	200	4	0,4,4	0.00	-	-	-	-
10	UMQ	A	305	-	35,35,35	1.49	3 (8%)	46,46,46	2.16	7 (15%)
12	OPC	H	30	-	53,53,54	1.99	14 (26%)	59,61,64	2.31	16 (27%)
9	HEM	A	303	-	27,50,50	2.14	5 (18%)	17,82,82	1.43	3 (17%)
12	OPC	B	202	-	53,53,54	2.01	14 (26%)	59,61,64	2.32	14 (23%)
10	UMQ	A	304	-	35,35,35	1.43	3 (8%)	46,46,46	2.11	8 (17%)
11	CLA	B	201	16	59,73,73	1.90	13 (22%)	67,113,113	2.08	18 (26%)
9	HEM	A	301	1	27,50,50	2.10	7 (25%)	17,82,82	2.37	5 (29%)
9	HEM	C	301	3	27,50,50	2.18	5 (18%)	17,82,82	1.66	4 (23%)
15	BCR	G	101	-	41,41,41	2.48	11 (26%)	56,56,56	5.43	15 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	A	302	1	-	0/6/54/54	-
10	UMQ	A	306	-	2/2/10/10	7/20/60/60	0/2/2/2
13	SQD	B	203	-	-	30/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FES	D	200	4	-	-	0/1/1/1
10	UMQ	A	305	-	2/2/10/10	13/20/60/60	0/2/2/2
12	OPC	H	30	-	-	35/57/57/60	-
9	HEM	A	303	-	-	2/6/54/54	-
12	OPC	B	202	-	-	22/57/57/60	-
10	UMQ	A	304	-	2/2/10/10	13/20/60/60	0/2/2/2
11	CLA	B	201	16	4/4/20/25	13/37/135/135	-
9	HEM	A	301	1	-	1/6/54/54	-
9	HEM	C	301	3	-	0/6/54/54	-
15	BCR	G	101	-	-	10/29/63/63	0/2/2/2

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	101	BCR	C8-C9	-8.26	1.28	1.45
15	G	101	BCR	C23-C22	-8.13	1.28	1.45
10	A	306	UMQ	C1'-C2'	-6.54	1.33	1.52
10	A	305	UMQ	C1'-C2'	-6.37	1.34	1.52
10	A	304	UMQ	C1'-C2'	-6.09	1.34	1.52

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	101	BCR	C24-C23-C22	29.62	170.99	126.23
15	G	101	BCR	C7-C8-C9	18.81	154.66	126.23
13	B	203	SQD	O9-S-C6	-15.11	88.99	106.94
15	G	101	BCR	C23-C24-C25	14.91	169.08	127.20
13	B	203	SQD	O8-S-O9	-11.58	82.97	111.27

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	306	UMQ	C2'
10	A	306	UMQ	C1'
10	A	305	UMQ	C2'
10	A	305	UMQ	C1'
10	A	304	UMQ	C2'

5 of 146 torsion outliers are listed below:

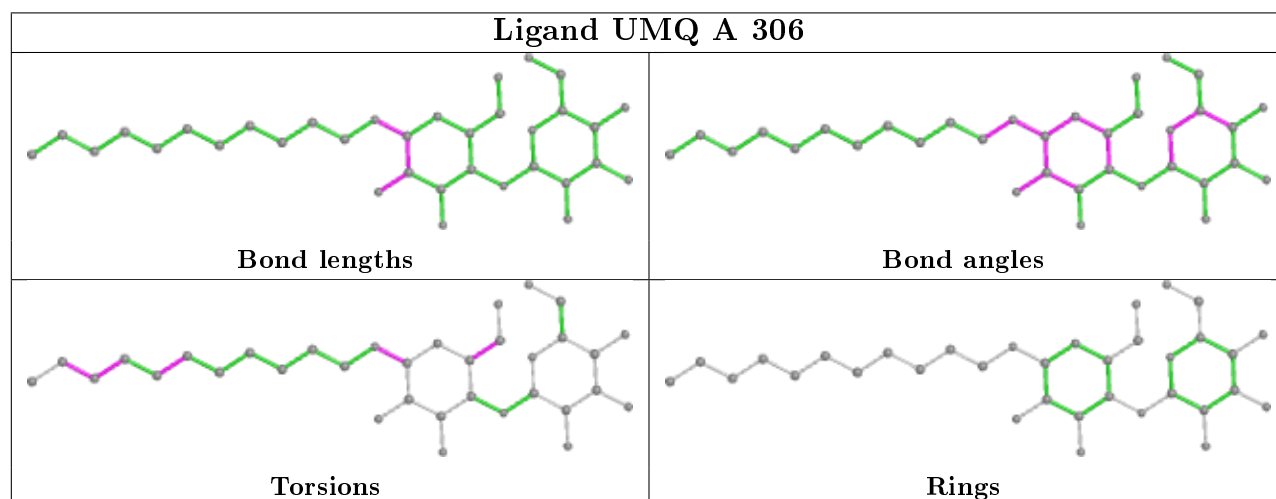
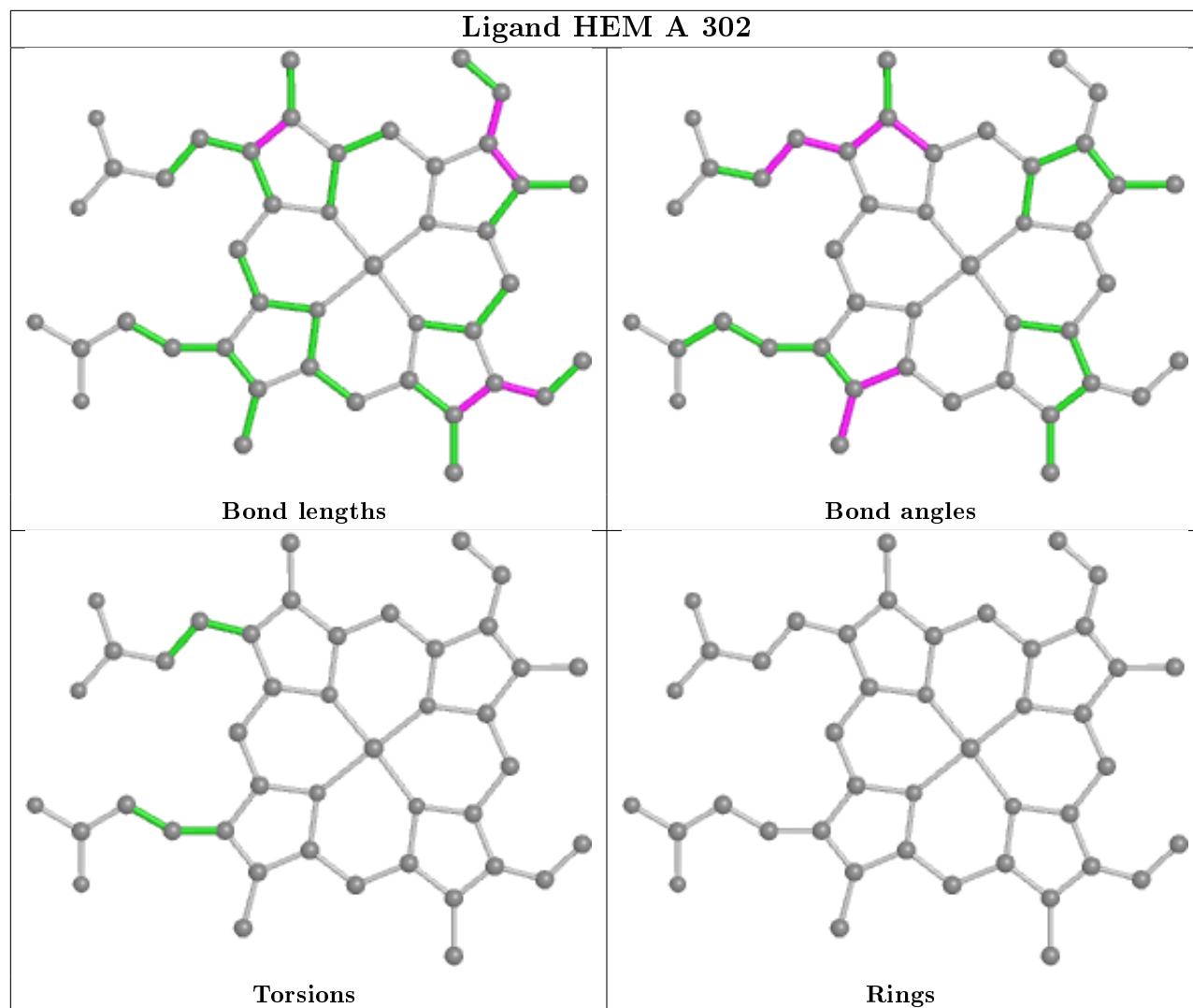
Mol	Chain	Res	Type	Atoms
13	B	203	SQD	C2-C1-O6-C44
13	B	203	SQD	O5-C1-O6-C44
13	B	203	SQD	O49-C7-O47-C45
13	B	203	SQD	C8-C7-O47-C45
13	B	203	SQD	C5-C6-S-O8

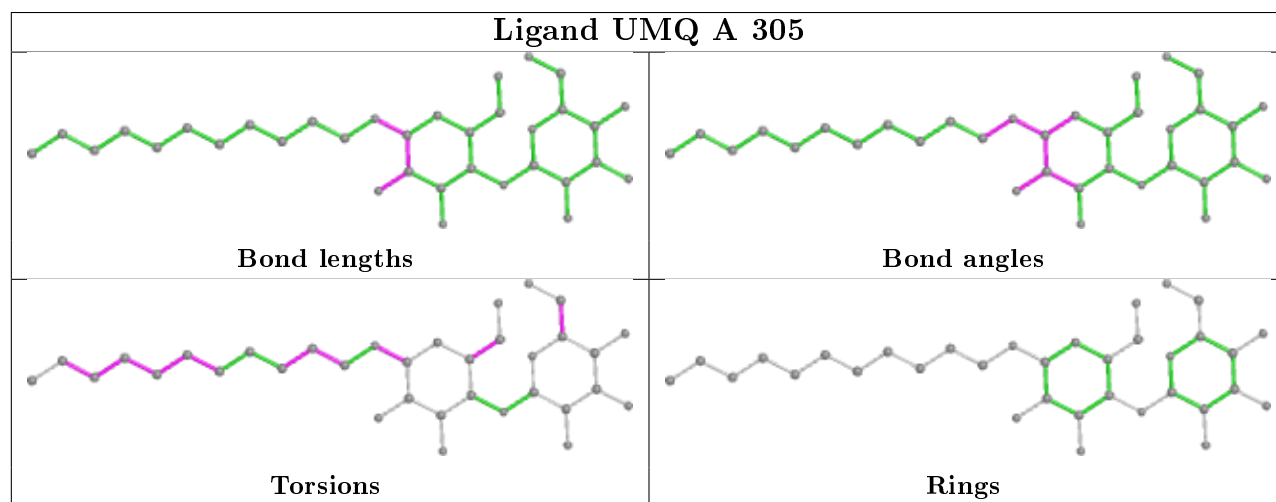
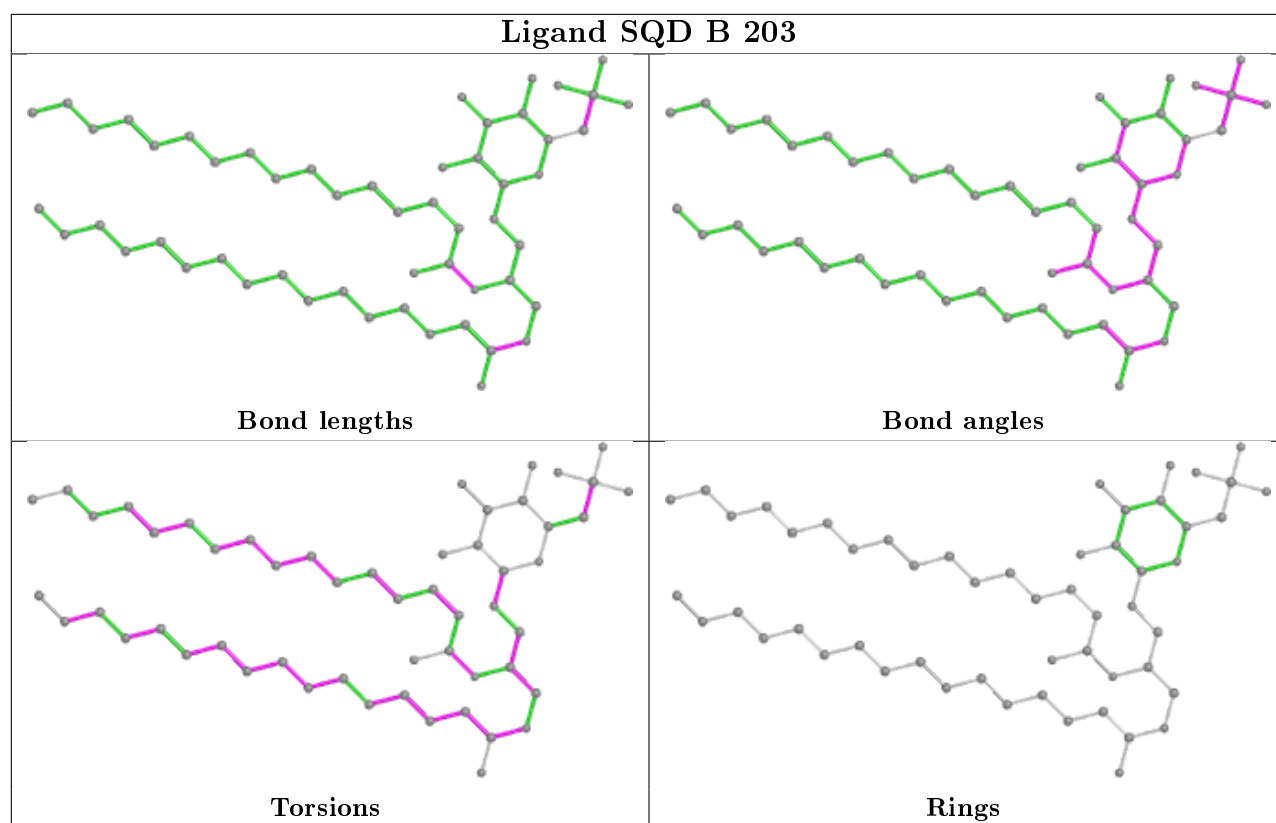
There are no ring outliers.

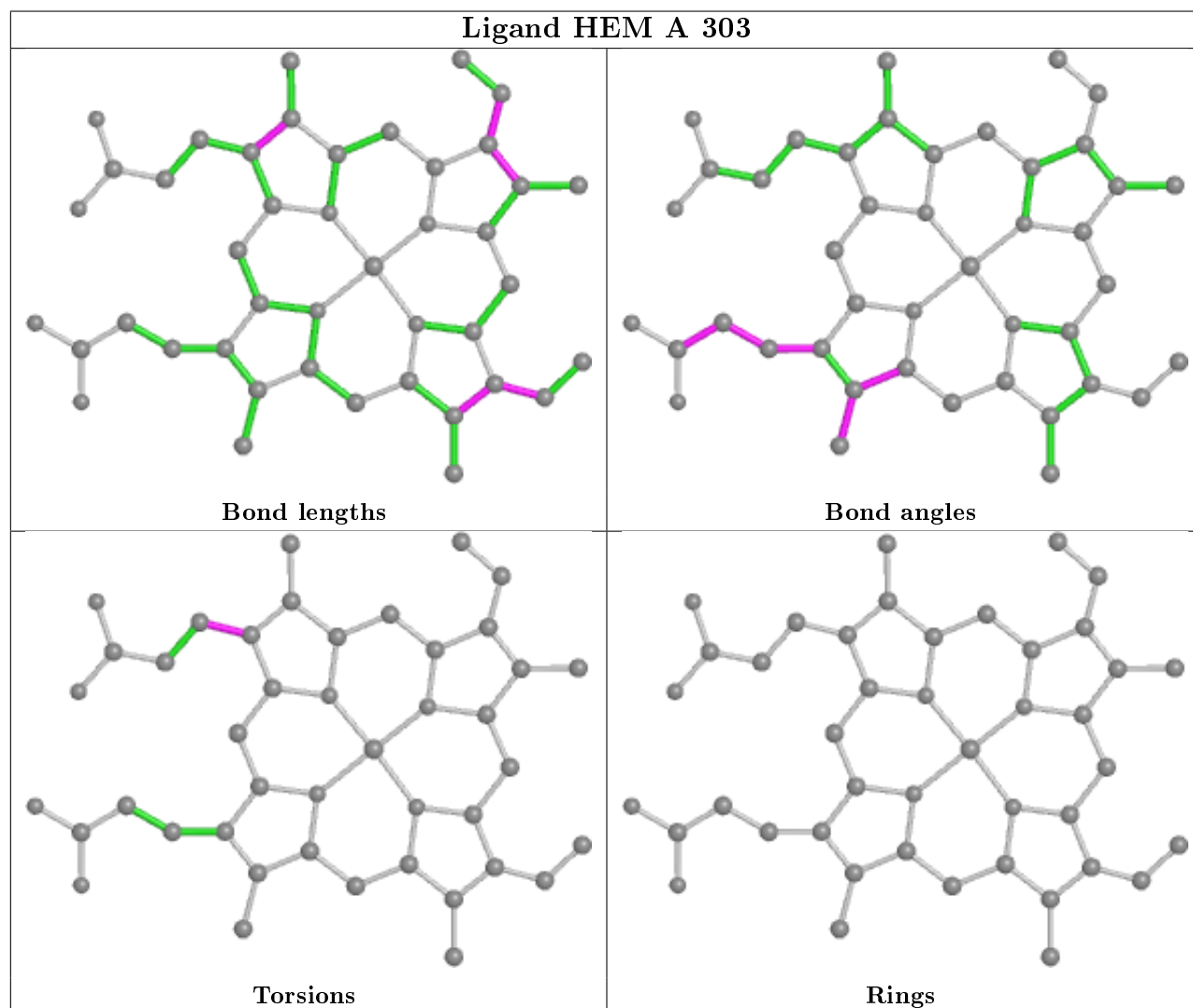
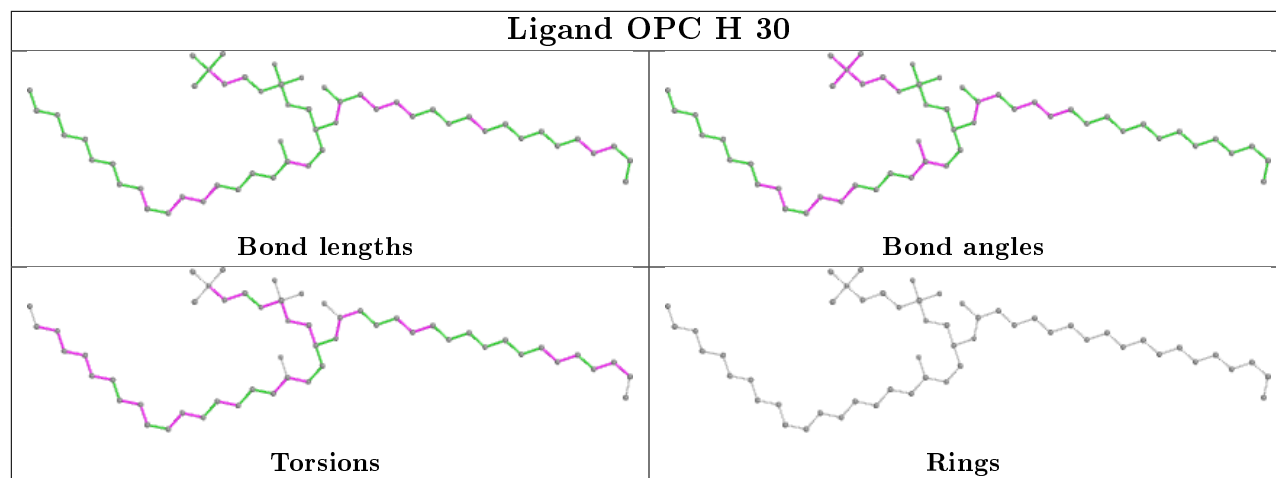
11 monomers are involved in 31 short contacts:

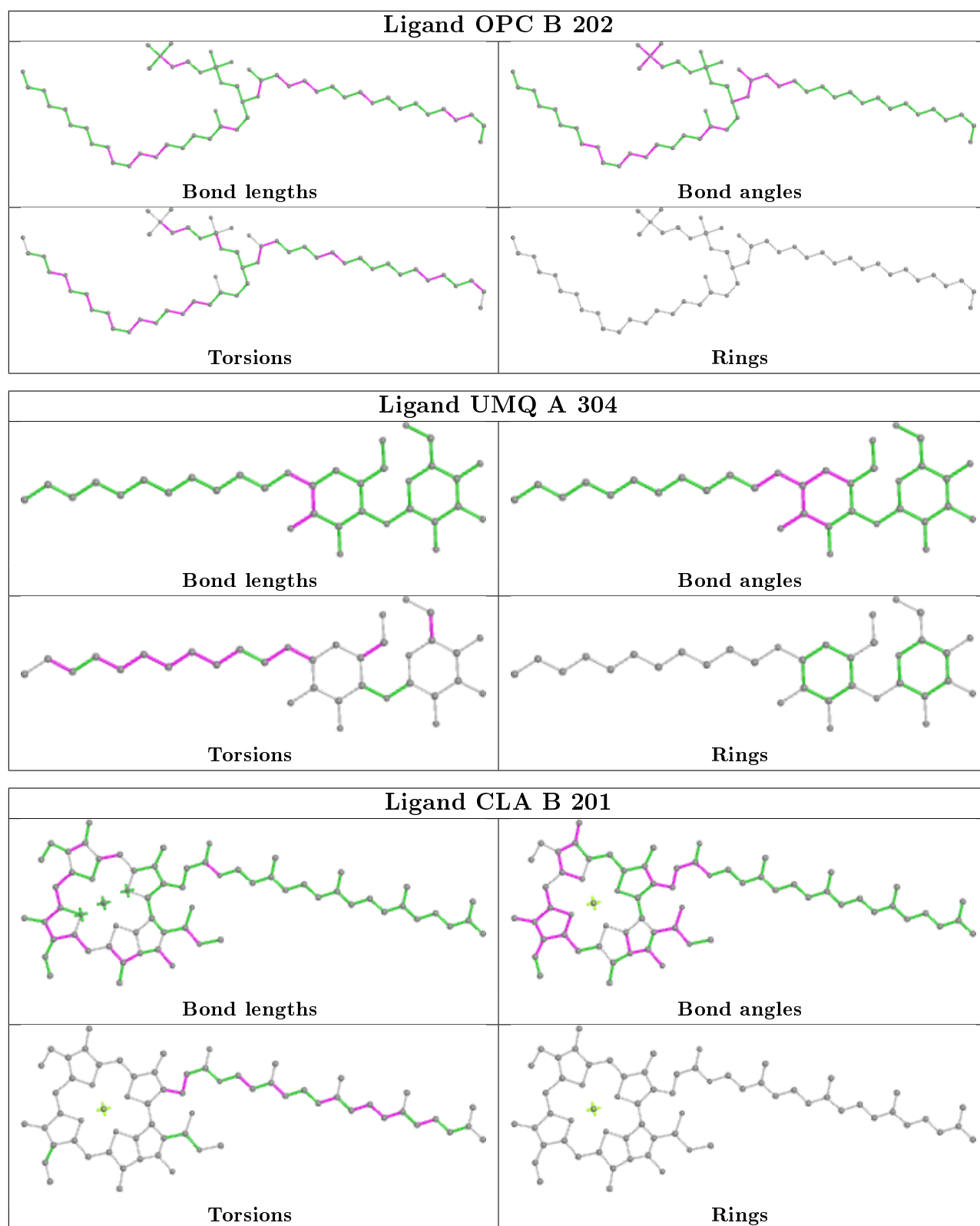
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	306	UMQ	2	0
13	B	203	SQD	1	0
14	D	200	FES	1	0
10	A	305	UMQ	1	0
12	H	30	OPC	4	0
9	A	303	HEM	6	0
10	A	304	UMQ	1	0
11	B	201	CLA	1	0
9	A	301	HEM	2	0
9	C	301	HEM	6	0
15	G	101	BCR	7	0

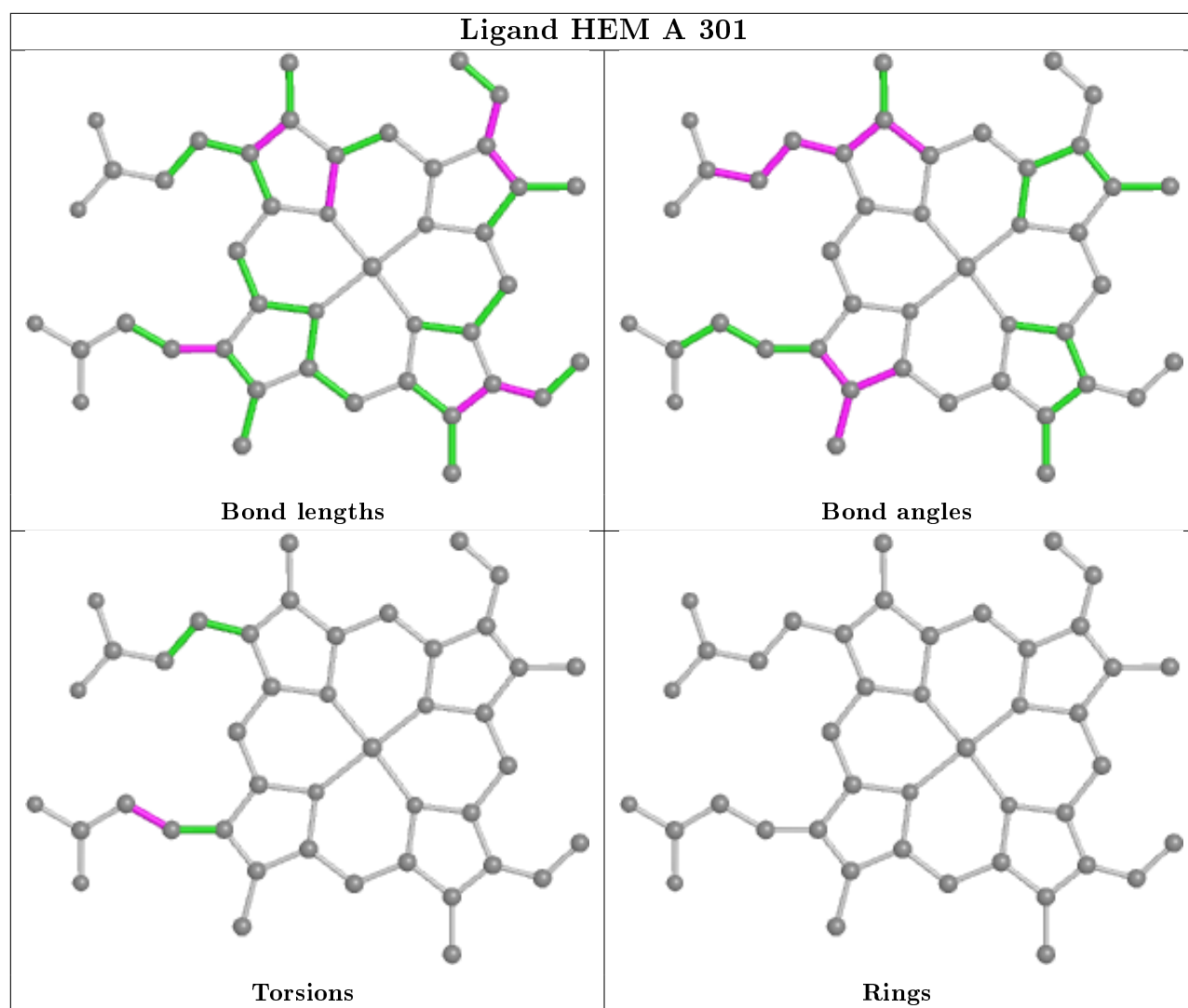
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

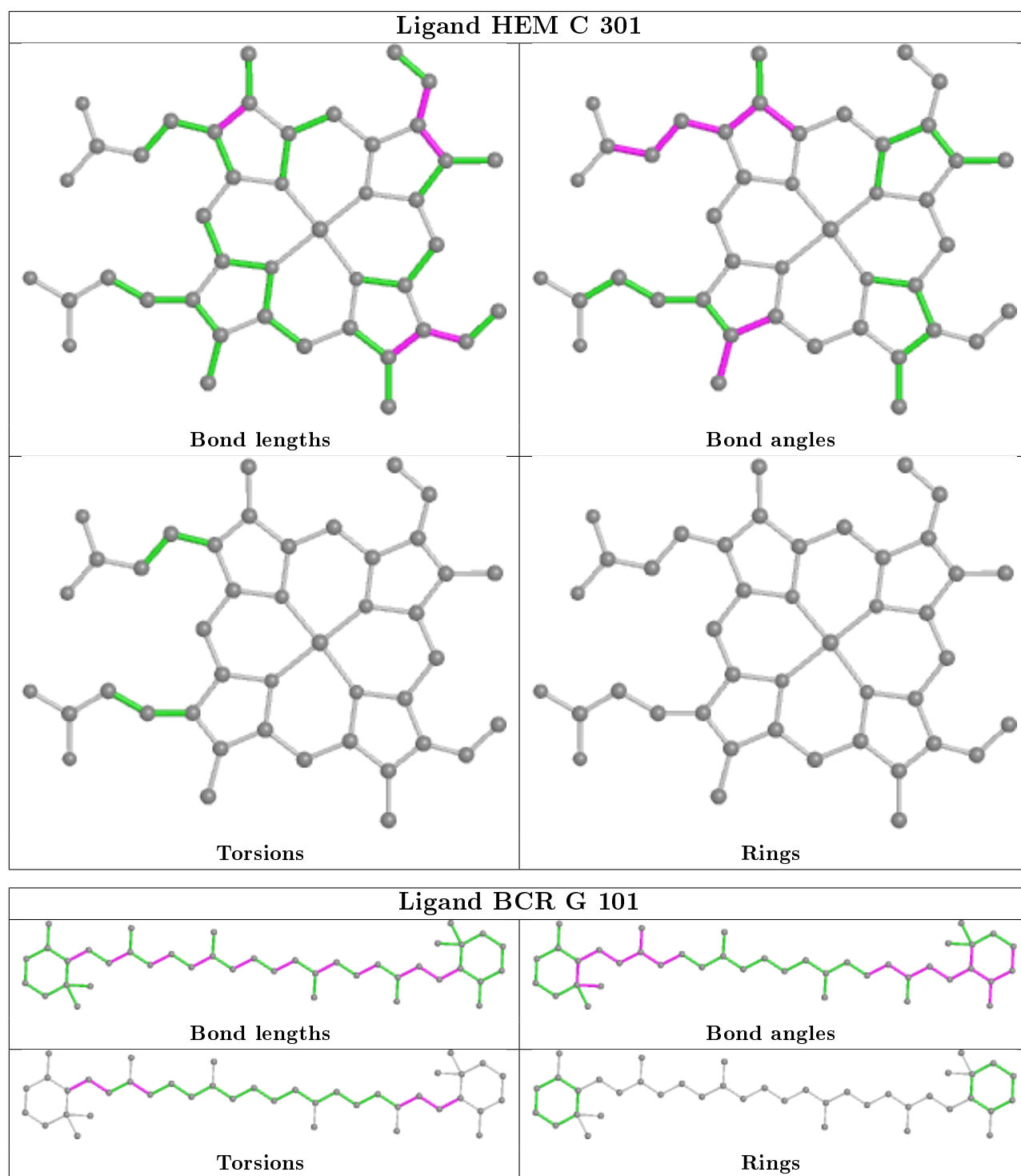












5.7 Other polymers ⓘ

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	215/215 (100%)	-0.39	2 (0%) 84 63	34, 47, 75, 102	0
2	B	160/160 (100%)	-0.19	3 (1%) 66 37	46, 63, 96, 108	0
3	C	289/289 (100%)	0.49	34 (11%) 4 1	48, 64, 136, 139	0
4	D	166/179 (92%)	1.18	43 (25%) 0 0	48, 111, 140, 143	0
5	E	31/31 (100%)	-0.28	1 (3%) 47 20	72, 78, 94, 95	0
6	F	32/34 (94%)	-0.44	0 100 100	60, 71, 88, 95	0
7	G	37/37 (100%)	-0.17	0 100 100	52, 63, 98, 99	0
8	H	29/29 (100%)	-0.35	0 100 100	57, 60, 69, 77	0
All	All	959/974 (98%)	0.19	83 (8%) 10 3	34, 64, 135, 143	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	179	SER	9.3
2	B	1	MET	6.9
3	C	203	SER	6.9
3	C	204	GLY	6.5
4	D	156	GLU	6.4

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

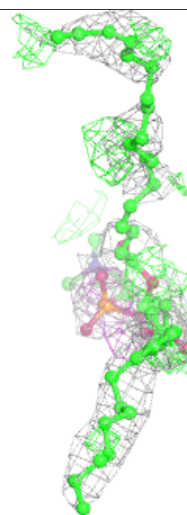
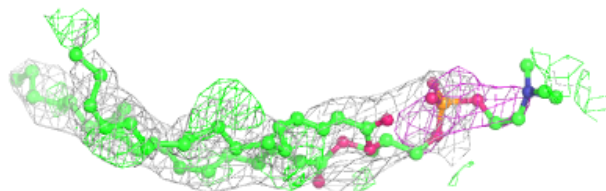
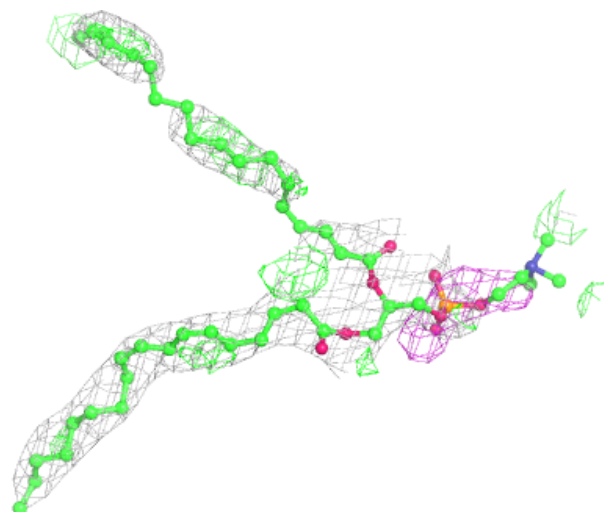
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	OPC	H	30	54/55	0.70	0.40	81,109,134,134	0
10	UMQ	A	305	34/34	0.80	0.35	135,137,140,141	0
10	UMQ	A	304	34/34	0.80	0.36	72,103,110,111	0
15	BCR	G	101	40/40	0.83	0.30	57,66,76,77	0
13	SQD	B	203	54/54	0.85	0.33	79,105,121,121	0
10	UMQ	A	306	34/34	0.87	0.28	95,100,104,104	0
12	OPC	B	202	54/55	0.90	0.41	75,82,110,111	0
11	CLA	B	201	65/65	0.94	0.23	59,64,88,89	0
9	HEM	C	301	43/43	0.97	0.23	52,55,63,64	0
14	FES	D	200	4/4	0.97	0.08	105,106,106,107	0
9	HEM	A	303	43/43	0.98	0.18	54,56,60,64	0
9	HEM	A	302	43/43	0.98	0.21	40,43,52,54	0
9	HEM	A	301	43/43	0.99	0.20	38,40,44,45	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.

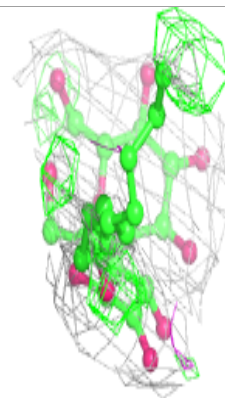
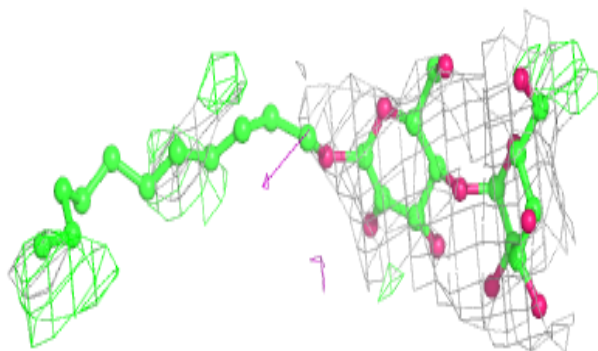
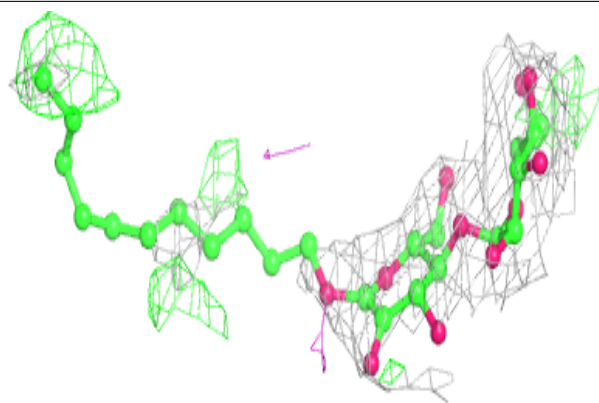
Electron density around OPC H 30:

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

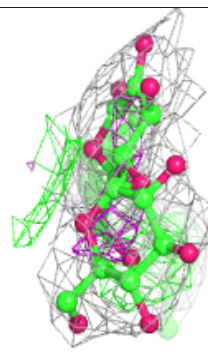
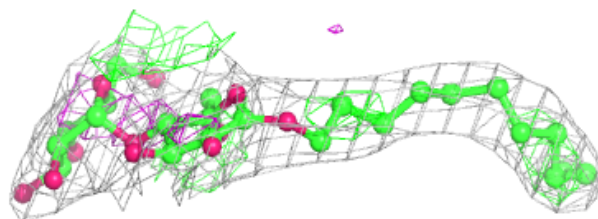
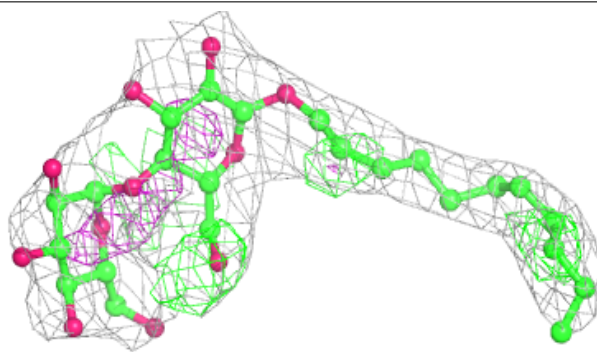


Electron density around UMQ A 305:

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

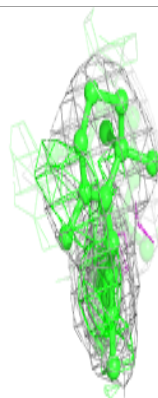
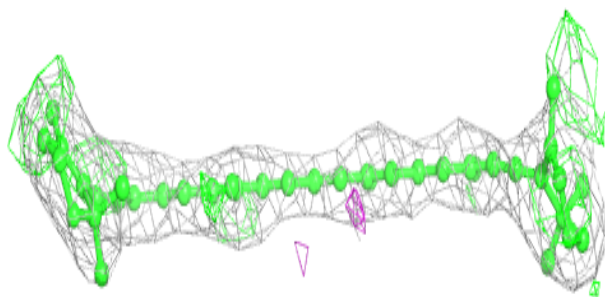
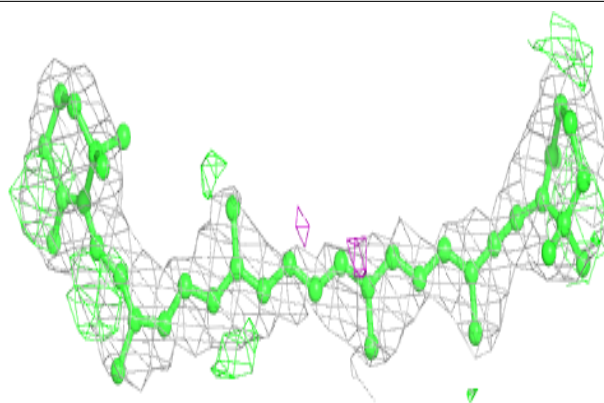
**Electron density around UMQ A 304:**

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

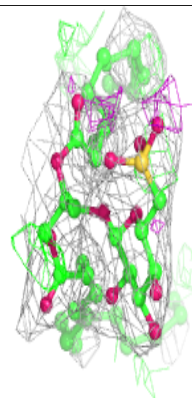
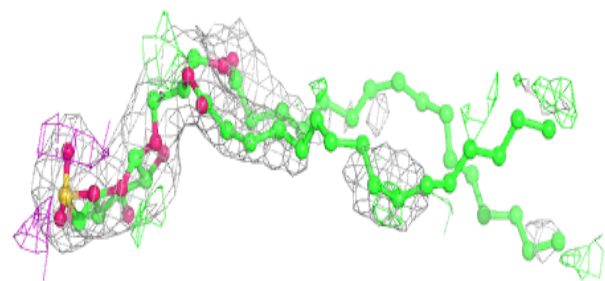
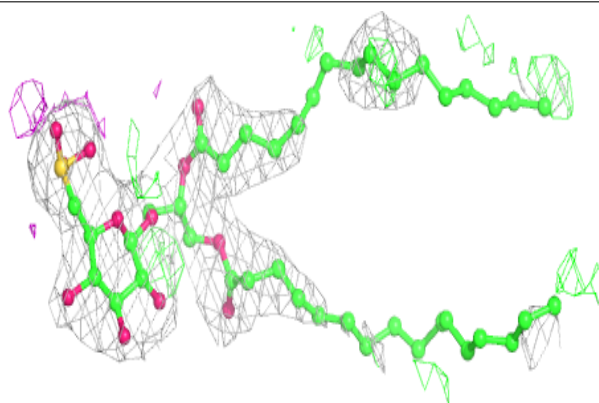


Electron density around BCR G 101:

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

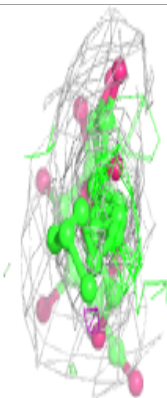
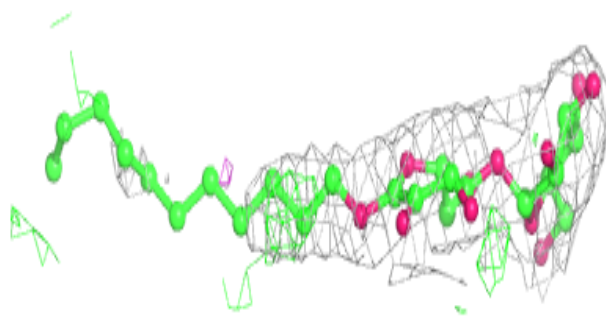
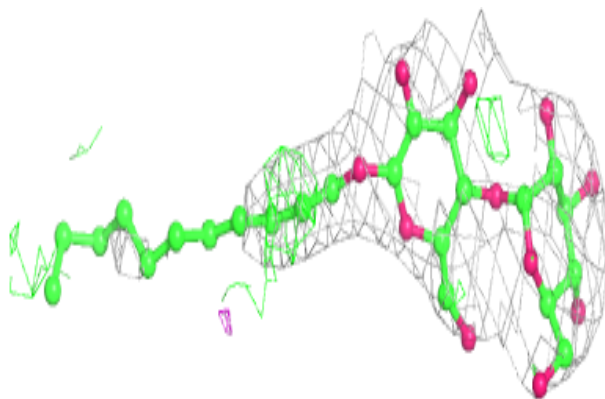
**Electron density around SQD B 203:**

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

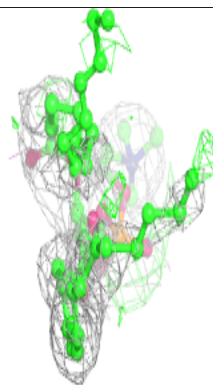
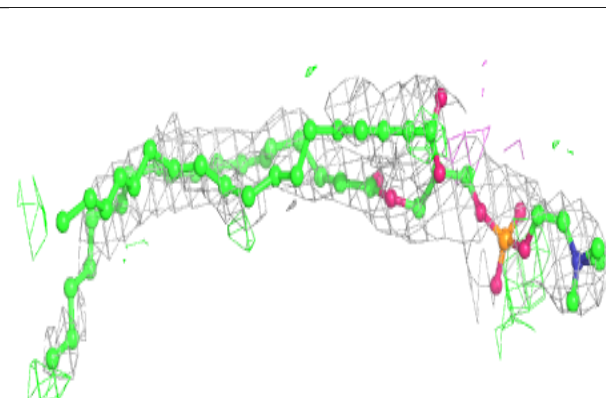
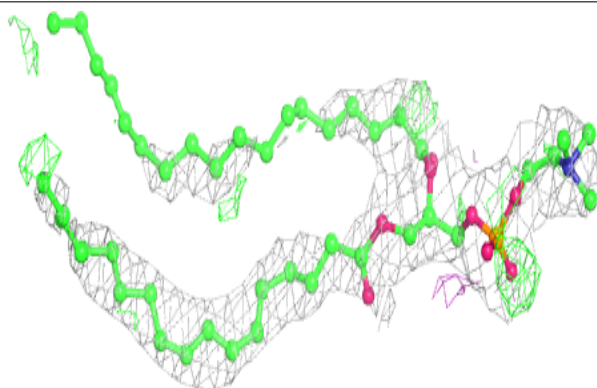


Electron density around UMQ A 306:

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

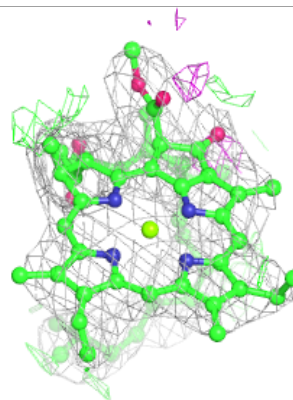
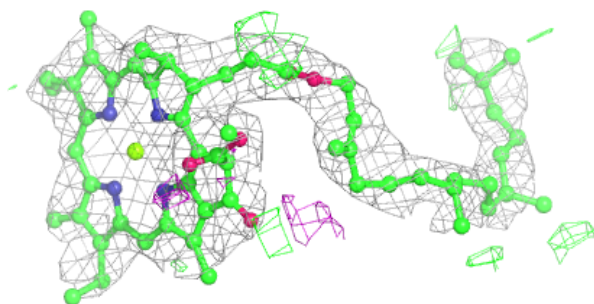
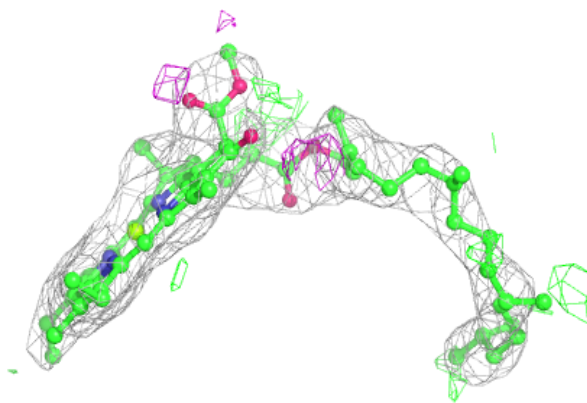
**Electron density around OPC B 202:**

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



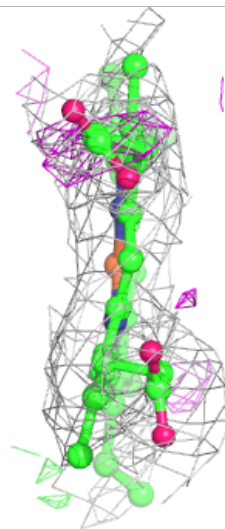
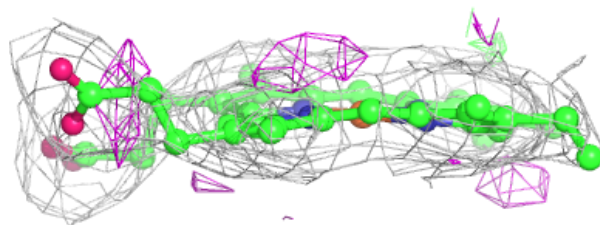
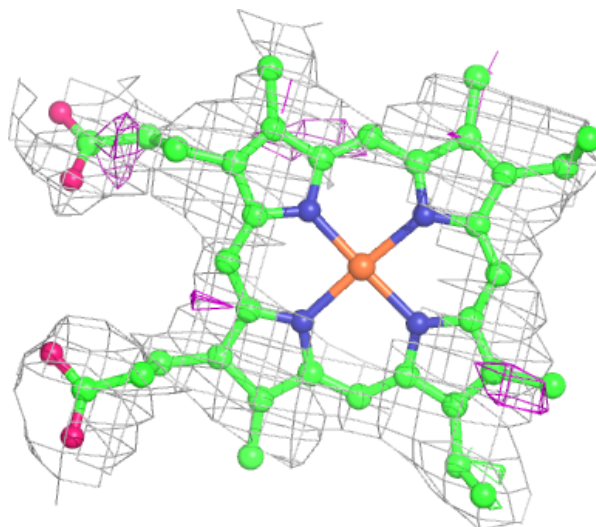
Electron density around CLA B 201:

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



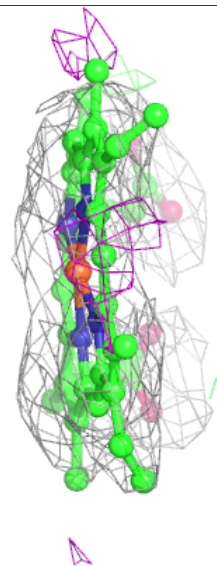
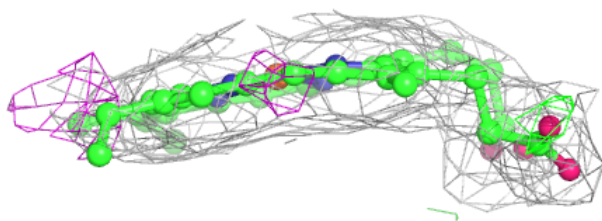
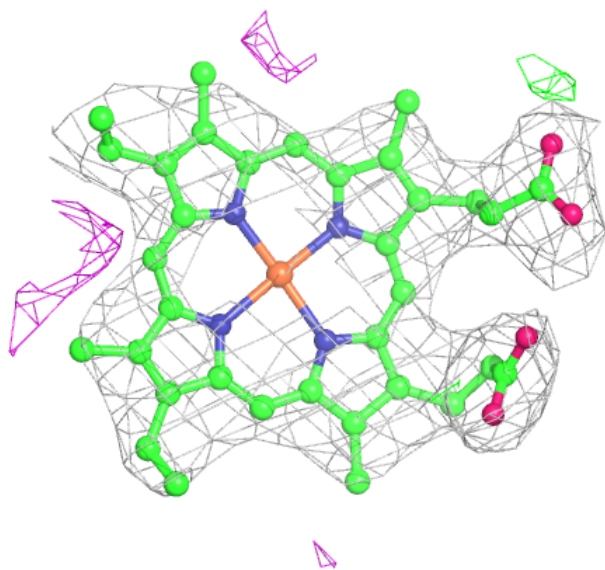
Electron density around HEM C 301:

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



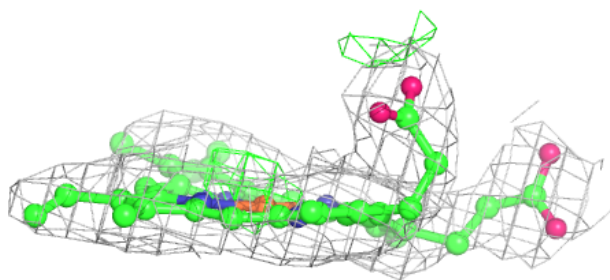
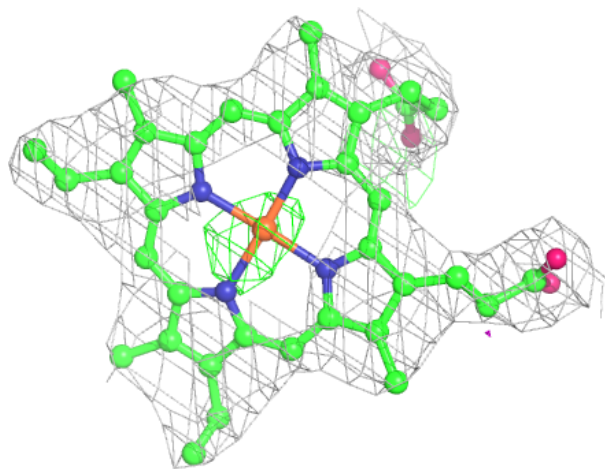
Electron density around HEM A 303:

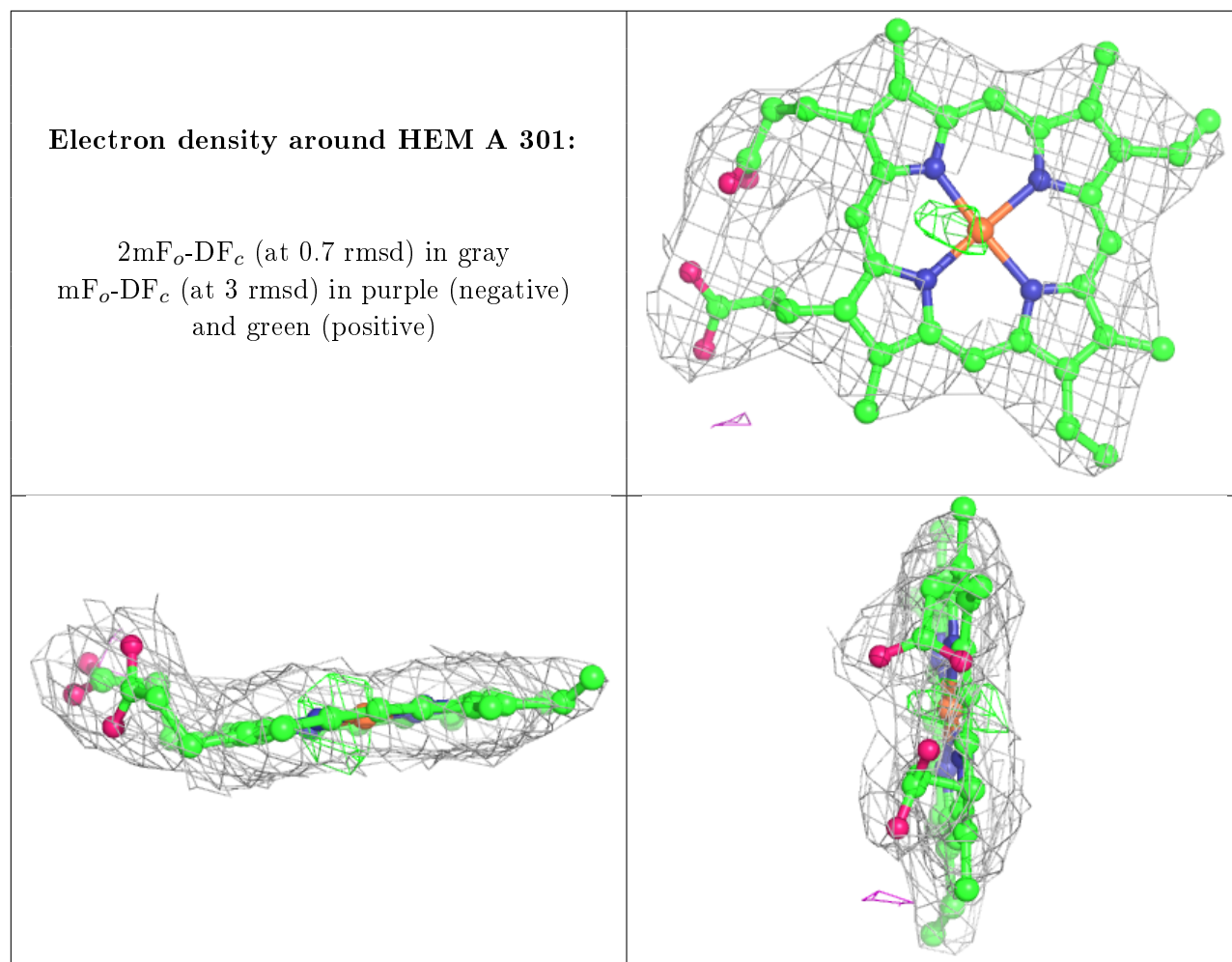
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 302:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.