



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 01:25 AM BST

PDB ID : 2E76  
Title : Crystal Structure of the Cytochrome b6f Complex with tridecyl-stigmatellin (TDS) from *M.laminosus*  
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.  
Deposited on : 2007-01-05  
Resolution : 3.41 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

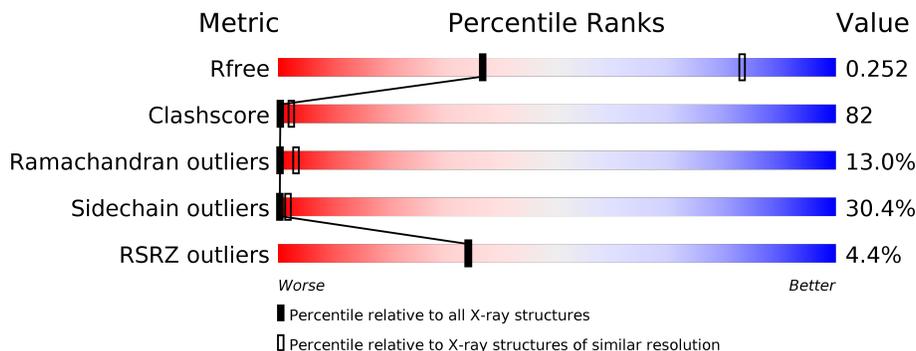
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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  $\geq 3$ , 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	
2	B	160	
3	C	289	
4	D	179	
5	E	32	
6	F	35	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HEM	A	302	-	-	X	-
10	HEM	A	303	-	-	X	-
10	HEM	C	301	-	-	X	-
12	UMQ	A	1101	X	-	-	-
12	UMQ	A	1102	X	-	-	-
12	UMQ	A	1103	X	-	-	-
12	UMQ	A	1104	X	-	-	-
13	CLA	B	201	X	-	-	-
14	TDS	B	1201	-	X	X	-
14	TDS	B	1202	-	X	-	-
16	SQD	D	201	X	X	-	-

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 8112 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
			Total	C	N	O	S			
1	A	215	1711	1140	272	288	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	160	1249	841	193	209	6	0	0	0

- Molecule 3 is a protein called Apocytochrome f.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	168	1288	823	221	237	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	32	248	179	34	34	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	32	242	165	35	40	2	0	0	0

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

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

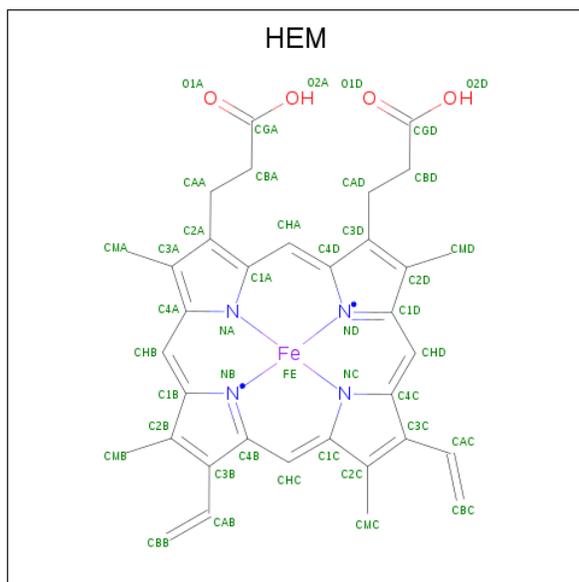
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	29	230	156	36	36	2	0	0	0

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

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

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



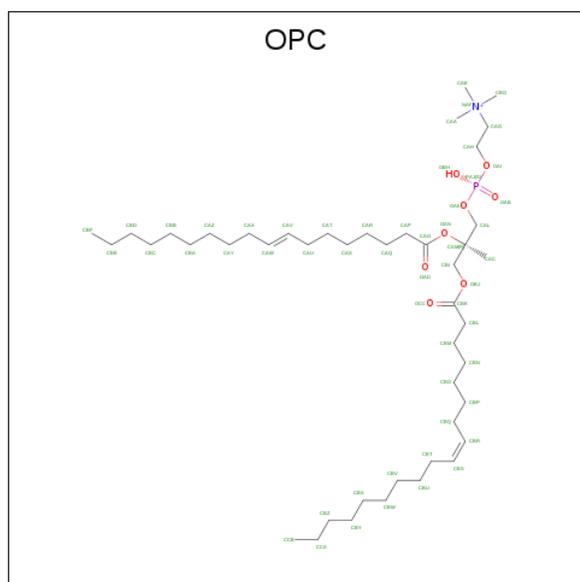
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
10	A	1	43	34	1	4	4	0	0
10	A	1	43	34	1	4	4	0	0
10	A	1	43	34	1	4	4	0	0

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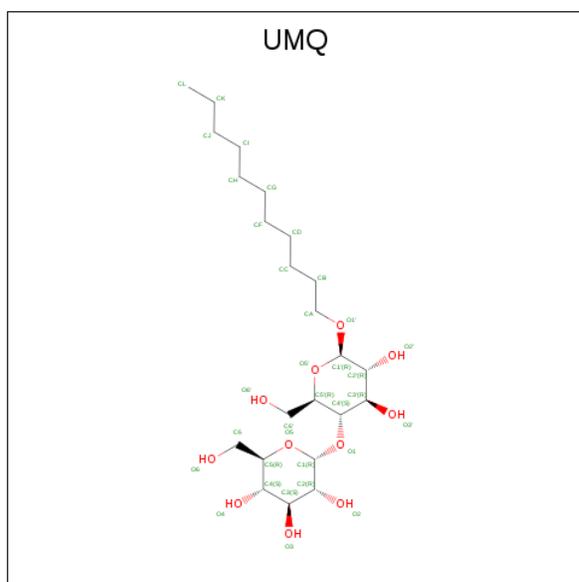
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
10	C	1	43	34	1	4	4	0	0

- Molecule 11 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: C<sub>45</sub>H<sub>87</sub>NO<sub>8</sub>P).



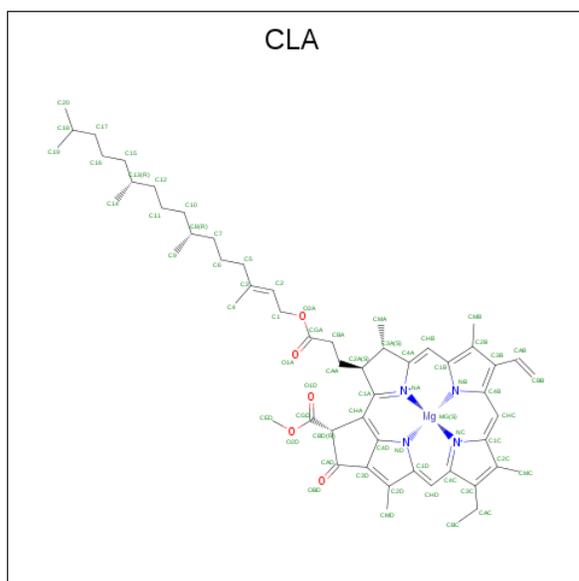
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	A	1	54	44	1	8	1	0	0
11	B	1	54	44	1	8	1	0	0

- Molecule 12 is UNDECYL-MALTOSE (three-letter code: UMQ) (formula: C<sub>23</sub>H<sub>44</sub>O<sub>11</sub>).



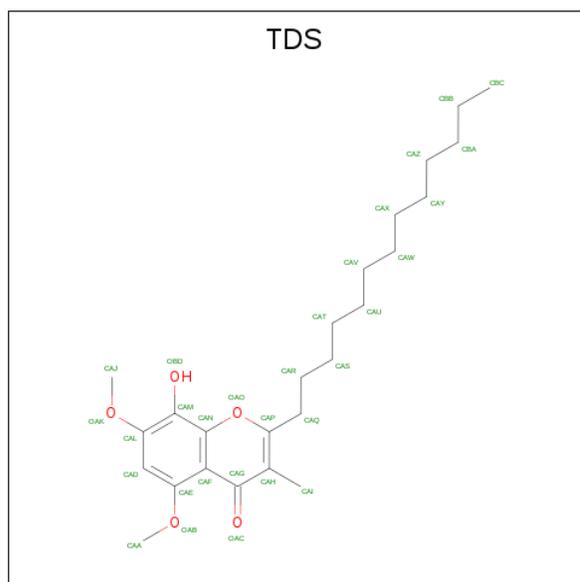
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



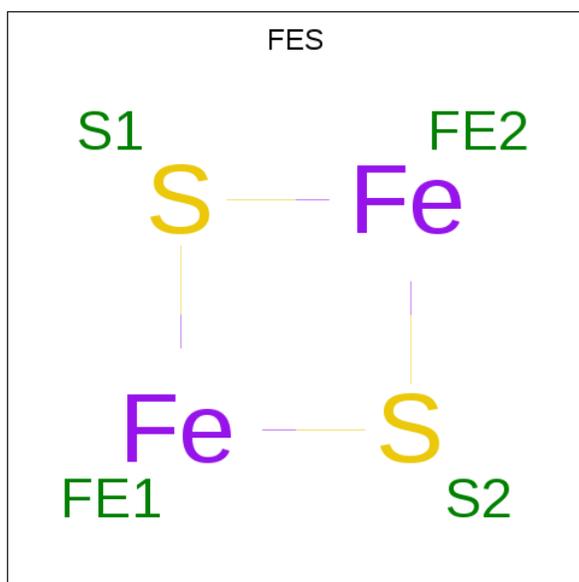
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	B	1	65	55	1	4	5	0	0

- Molecule 14 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (three-letter code: TDS) (formula: C<sub>25</sub>H<sub>38</sub>O<sub>5</sub>).



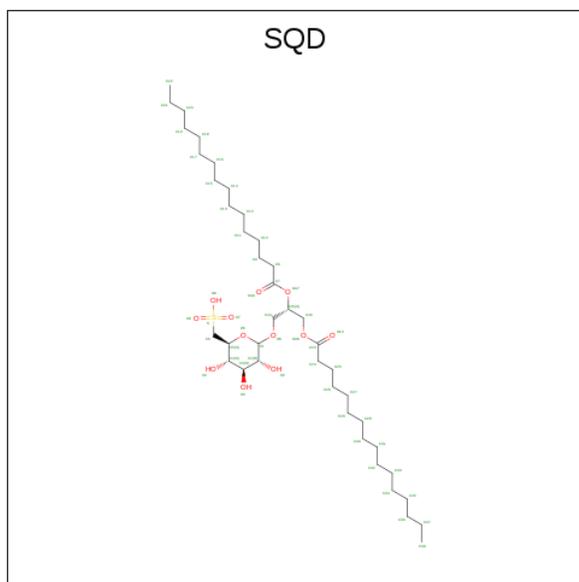
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	B	1	30	25	5	0	0
14	B	1	30	25	5	0	0

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



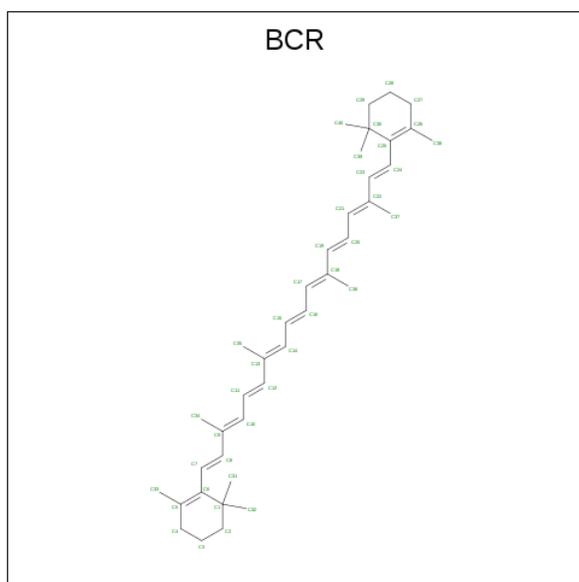
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



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

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



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

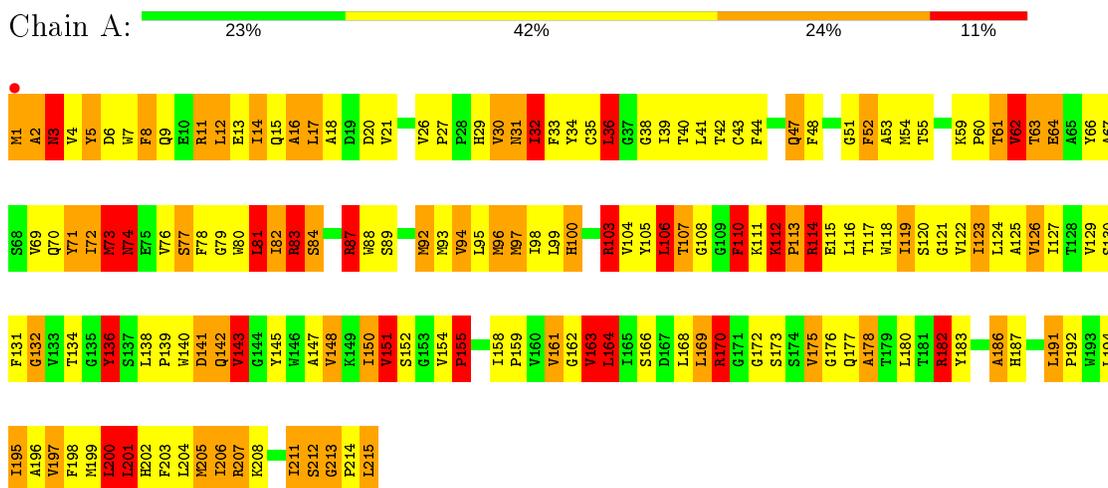
- Molecule 18 is water.

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

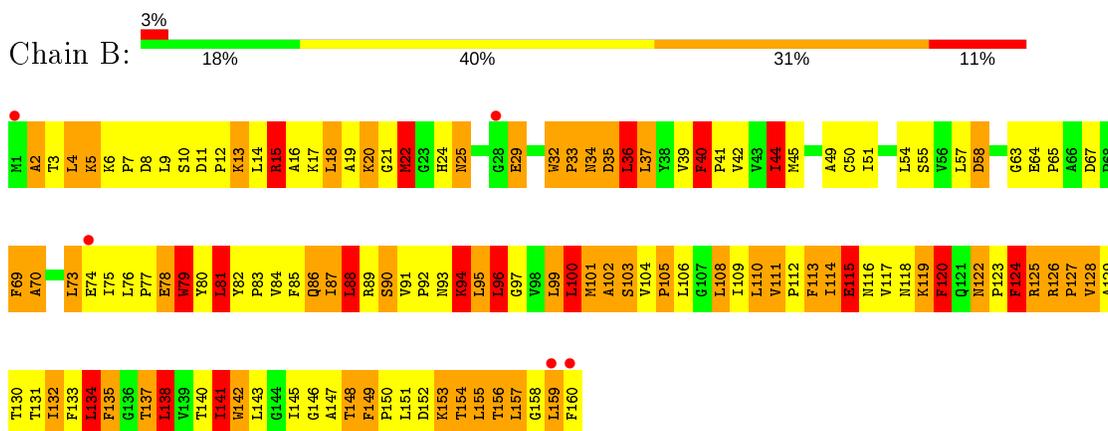
### 3 Residue-property plots

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

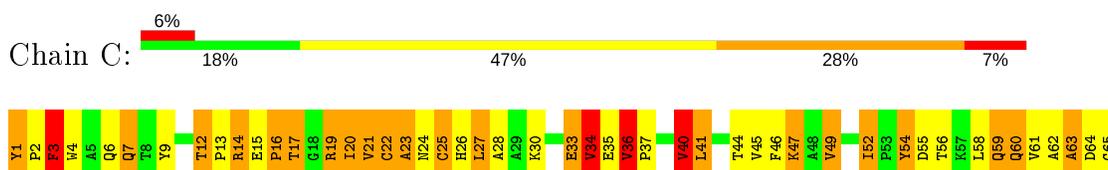
- Molecule 1: Cytochrome b6

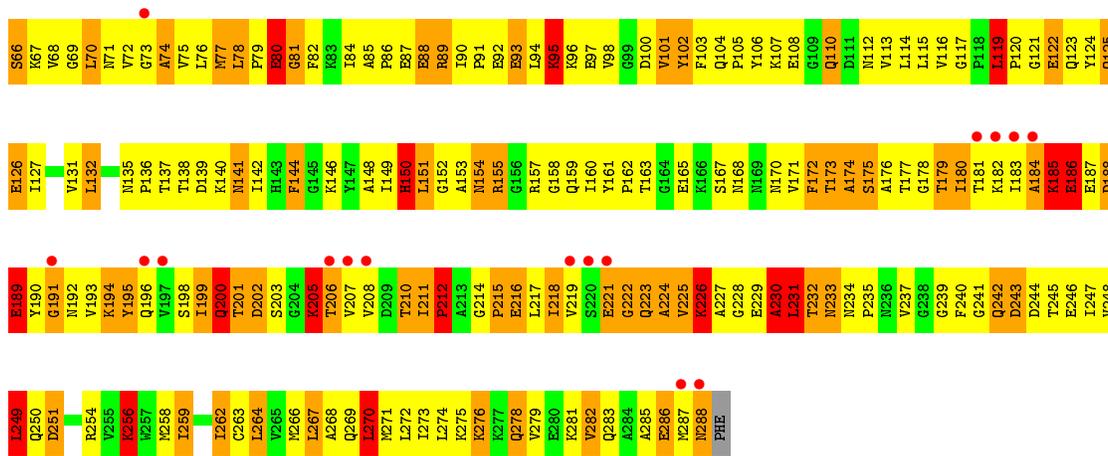


- Molecule 2: Cytochrome b6-f complex subunit 4

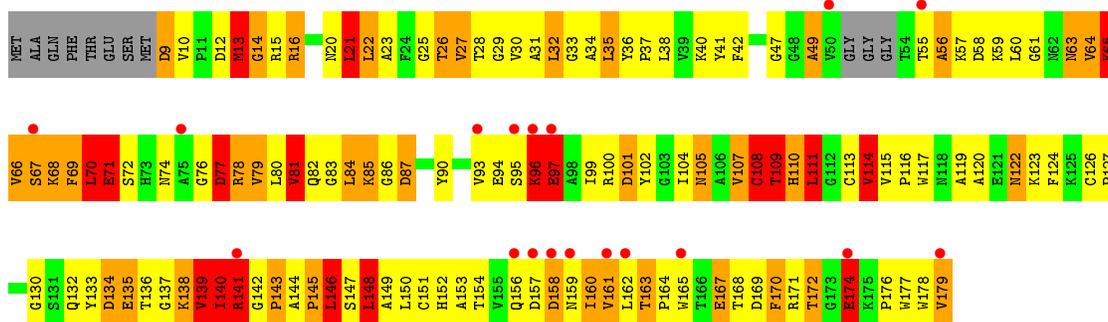
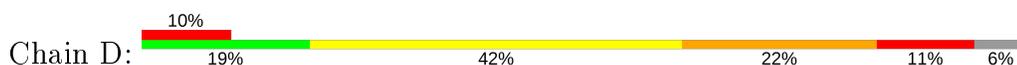


- Molecule 3: Apocytochrome f





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



• 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

Chain H:  14% 38% 34% 14%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.23Å 157.23Å 363.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.27 – 3.41 39.21 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.27-3.41) 99.7 (39.21-3.41)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.84 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.256 0.182 , 0.252	Depositor DCC
$R_{free}$ test set	1852 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.6	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 103.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CLA, CD, FES, OPC, TDS, 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	1.81	32/1763 (1.8%)	1.85	50/2405 (2.1%)
2	B	1.89	26/1288 (2.0%)	1.96	34/1765 (1.9%)
3	C	1.47	21/2264 (0.9%)	1.51	30/3082 (1.0%)
4	D	1.29	6/1320 (0.5%)	1.49	27/1798 (1.5%)
5	E	1.82	5/253 (2.0%)	1.88	8/340 (2.4%)
6	F	2.11	7/246 (2.8%)	2.03	9/331 (2.7%)
7	G	2.14	7/289 (2.4%)	2.25	13/391 (3.3%)
8	H	2.01	5/236 (2.1%)	1.86	8/323 (2.5%)
All	All	1.68	109/7659 (1.4%)	1.74	179/10435 (1.7%)

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
1	A	0	4
2	B	0	3
3	C	0	7
4	D	0	5
5	E	0	1
6	F	0	3
7	G	0	2
8	H	0	2
All	All	0	27

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	3	GLU	CG-CD	16.26	1.76	1.51
3	C	246	GLU	CD-OE2	12.18	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246	GLU	CG-CD	11.96	1.69	1.51
6	F	3	GLU	CB-CG	11.17	1.73	1.52
2	B	115	GLU	CG-CD	11.11	1.68	1.51

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	ARG	NE-CZ-NH2	-14.05	113.27	120.30
7	G	7	ASP	CB-CG-OD1	12.97	129.97	118.30
7	G	9	LEU	CA-CB-CG	-12.37	86.84	115.30
2	B	15	ARG	NE-CZ-NH1	11.62	126.11	120.30
5	E	23	ILE	CB-CA-C	-10.85	89.90	111.60

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LYS	Peptide
1	A	161	VAL	Peptide
1	A	2	ALA	Peptide
1	A	73	MET	Peptide
2	B	2	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1711	0	1736	303	0
2	B	1249	0	1308	254	0
3	C	2216	0	2233	404	1
4	D	1288	0	1273	229	0
5	E	248	0	284	39	0
6	F	242	0	260	61	0
7	G	283	0	289	75	1
8	H	230	0	239	51	0
9	A	1	0	0	0	0
10	A	129	0	90	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	43	0	30	29	0
11	A	54	0	79	18	0
11	B	54	0	83	2	0
12	A	136	0	165	6	0
13	B	65	0	72	5	0
14	B	60	0	70	41	0
15	D	4	0	0	1	0
16	D	54	0	53	9	0
17	G	40	0	52	9	0
18	A	2	0	0	0	0
18	B	2	0	0	0	0
18	C	1	0	0	0	0
All	All	8112	0	8316	1350	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 82.

The worst 5 of 1350 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)
6:F:25:LEU:CG	6:F:25:LEU:CD1	1.77	1.62
3:C:256:LYS:CD	3:C:256:LYS:CG	1.80	1.59
2:B:138:LEU:CD1	2:B:138:LEU:CG	1.74	1.59
7:G:3:GLU:CD	7:G:3:GLU:CG	1.76	1.52
3:C:256:LYS:NZ	3:C:256:LYS:CE	1.74	1.50

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)
3:C:108:GLU:OE2	7:G:33:ASN:CB[8_565]	2.09	0.11

## 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%)	154 (72%)	41 (19%)	18 (8%)	1	8
2	B	158/160 (99%)	89 (56%)	43 (27%)	26 (16%)	0	1
3	C	286/289 (99%)	204 (71%)	51 (18%)	31 (11%)	0	5
4	D	164/179 (92%)	114 (70%)	28 (17%)	22 (13%)	0	3
5	E	30/32 (94%)	15 (50%)	11 (37%)	4 (13%)	0	3
6	F	30/35 (86%)	15 (50%)	8 (27%)	7 (23%)	0	0
7	G	35/37 (95%)	11 (31%)	15 (43%)	9 (26%)	0	0
8	H	27/29 (93%)	15 (56%)	6 (22%)	6 (22%)	0	1
All	All	943/976 (97%)	617 (65%)	203 (22%)	123 (13%)	0	3

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ALA
1	A	36	LEU
1	A	73	MET
1	A	74	ASN
1	A	112	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%)	135 (73%)	49 (27%)	0	2
2	B	137/137 (100%)	95 (69%)	42 (31%)	0	2
3	C	242/243 (100%)	164 (68%)	78 (32%)	0	1
4	D	139/146 (95%)	100 (72%)	39 (28%)	0	2
5	E	25/25 (100%)	18 (72%)	7 (28%)	0	2
6	F	24/27 (89%)	14 (58%)	10 (42%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	28/28 (100%)	15 (54%)	13 (46%)	0	0
8	H	24/24 (100%)	18 (75%)	6 (25%)	0	2
All	All	803/814 (99%)	559 (70%)	244 (30%)	0	2

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	80	GLU
3	C	186	GLU
7	G	1	MET
3	C	93	GLU
3	C	125	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	110	GLN
3	C	154	ASN
3	C	250	GLN
3	C	60	GLN
3	C	288	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is 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
10	HEM	A	303	1,18,14	27,50,50	3.02	8 (29%)	17,82,82	2.58	4 (23%)
11	OPC	B	1001	-	53,53,54	2.19	19 (35%)	59,61,64	2.69	25 (42%)
13	CLA	B	201	18	59,73,73	2.19	17 (28%)	67,113,113	2.84	28 (41%)
14	TDS	B	1201	-	28,31,31	3.44	9 (32%)	35,40,40	5.85	20 (57%)
15	FES	D	200	4	0,4,4	0.00	-	-	-	-
12	UMQ	A	1101	-	35,35,35	1.76	5 (14%)	46,46,46	3.03	24 (52%)
10	HEM	A	302	1	27,50,50	2.92	13 (48%)	17,82,82	3.26	8 (47%)
14	TDS	B	1202	10	28,31,31	3.21	11 (39%)	35,40,40	6.46	21 (60%)
10	HEM	A	301	1	27,50,50	2.51	13 (48%)	17,82,82	2.51	6 (35%)
12	UMQ	A	1102	-	35,35,35	2.17	9 (25%)	46,46,46	3.01	18 (39%)
10	HEM	C	301	3	27,50,50	2.42	13 (48%)	17,82,82	2.82	5 (29%)
16	SQD	D	201	-	53,54,54	2.77	26 (49%)	62,65,65	5.05	31 (50%)
12	UMQ	A	1103	-	35,35,35	1.98	5 (14%)	46,46,46	2.59	14 (30%)
11	OPC	A	1002	-	53,53,54	1.98	14 (26%)	59,61,64	2.87	21 (35%)
17	BCR	G	101	-	41,41,41	3.53	24 (58%)	56,56,56	6.65	25 (44%)
12	UMQ	A	1104	-	35,35,35	1.58	3 (8%)	46,46,46	3.01	19 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SQD	D	201	-	3/3/9/9	27/49/69/69	0/1/1/1
10	HEM	A	303	1,18,14	-	2/6/54/54	-
13	CLA	B	201	18	4/4/20/25	13/37/135/135	-
14	TDS	B	1201	-	-	11/16/17/17	0/2/2/2
15	FES	D	200	4	-	-	0/1/1/1
12	UMQ	A	1101	-	2/2/10/10	10/20/60/60	0/2/2/2
10	HEM	A	302	1	-	4/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	TDS	B	1202	10	-	11/16/17/17	0/2/2/2
11	OPC	B	1001	-	-	23/57/57/60	-
10	HEM	A	301	1	-	2/6/54/54	-
12	UMQ	A	1102	-	2/2/10/10	12/20/60/60	0/2/2/2
10	HEM	C	301	3	-	0/6/54/54	-
12	UMQ	A	1103	-	2/2/10/10	11/20/60/60	0/2/2/2
11	OPC	A	1002	-	-	33/57/57/60	-
17	BCR	G	101	-	-	12/29/63/63	0/2/2/2
12	UMQ	A	1104	-	2/2/10/10	13/20/60/60	0/2/2/2

The worst 5 of 189 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	101	BCR	C8-C9	-10.31	1.23	1.45
10	A	303	HEM	C3B-C2B	-9.80	1.26	1.40
14	B	1201	TDS	CAL-CAM	9.68	1.53	1.40
14	B	1202	TDS	CAD-CAL	-9.32	1.21	1.38
10	A	302	HEM	C3C-C2C	-8.61	1.28	1.40

The worst 5 of 269 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C24-C23-C22	27.50	167.78	126.23
17	G	101	BCR	C7-C8-C9	25.85	165.30	126.23
14	B	1202	TDS	CAE-CAD-CAL	21.93	155.92	119.89
14	B	1201	TDS	CAE-CAD-CAL	20.47	153.53	119.89
17	G	101	BCR	C8-C7-C6	17.67	176.84	127.20

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	201	CLA	C8
13	B	201	CLA	NC
13	B	201	CLA	ND
13	B	201	CLA	NA
12	A	1101	UMQ	C2'

5 of 184 torsion outliers are listed below:

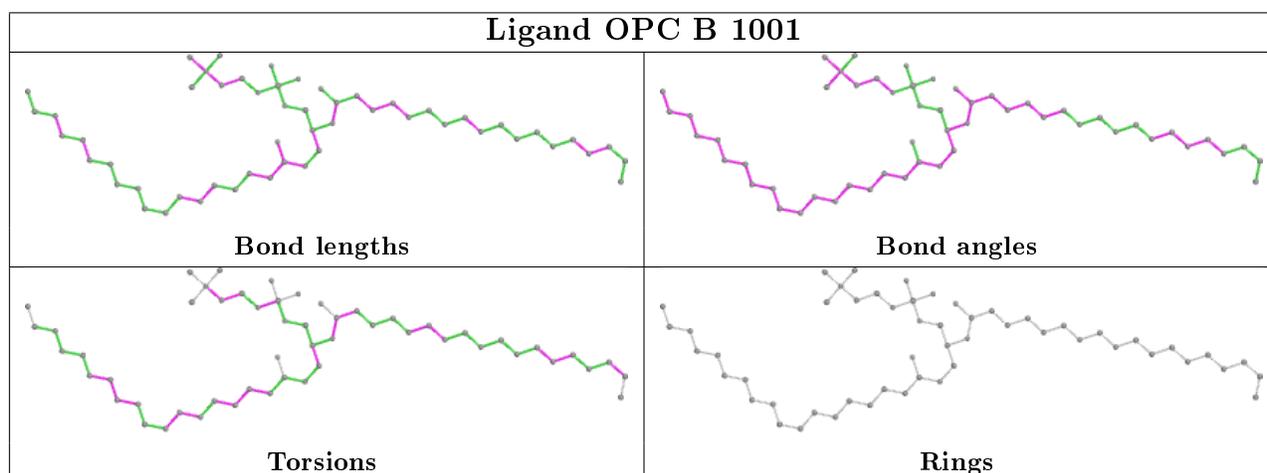
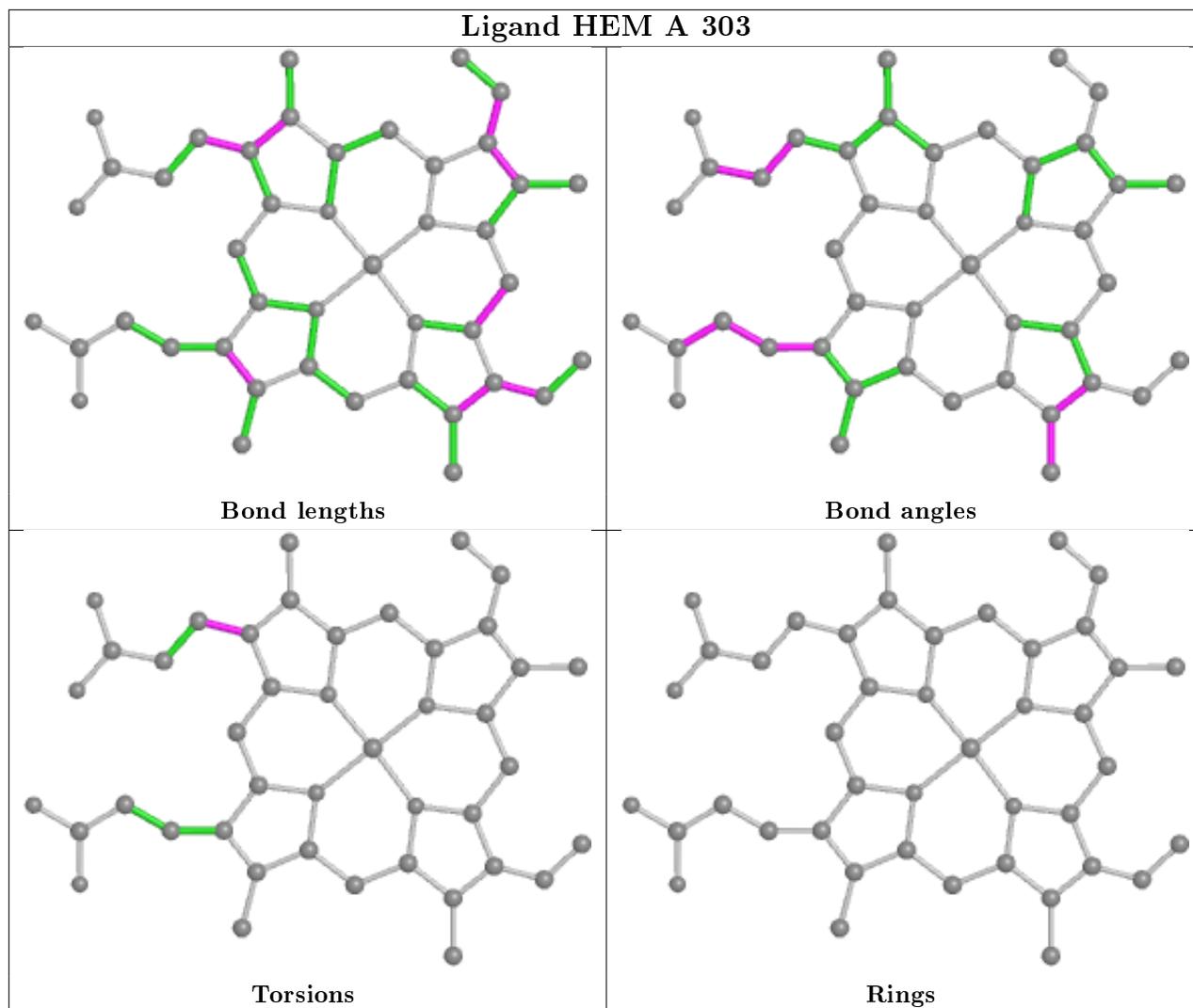
Mol	Chain	Res	Type	Atoms
10	A	303	HEM	C2D-C3D-CAD-CBD
10	A	303	HEM	C4D-C3D-CAD-CBD
11	B	1001	OPC	CAH-OAI-PAJ-OBH
11	B	1001	OPC	NAF-CAG-CAH-OAI
11	B	1001	OPC	CBO-CBP-CBQ-CBR

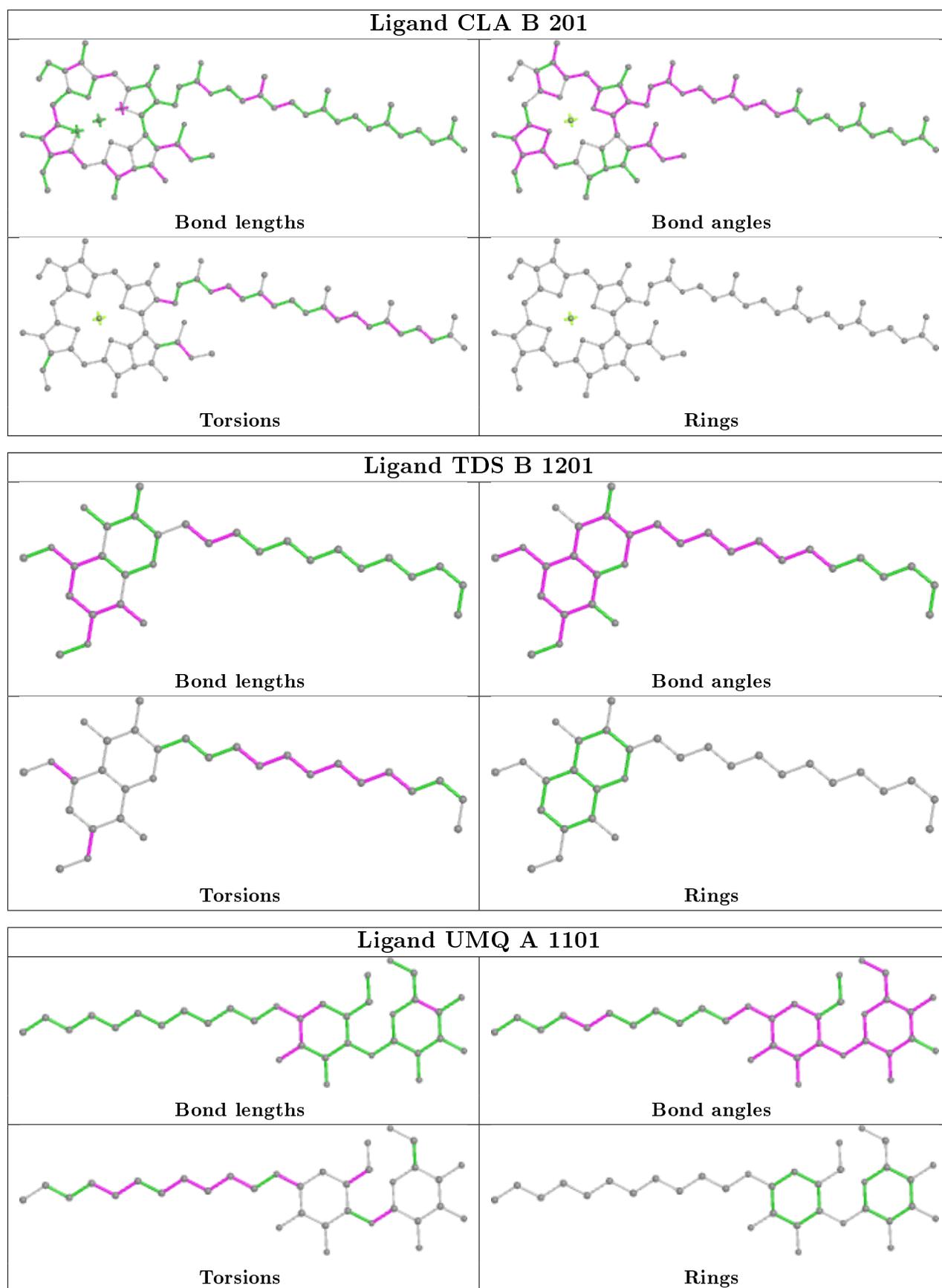
There are no ring outliers.

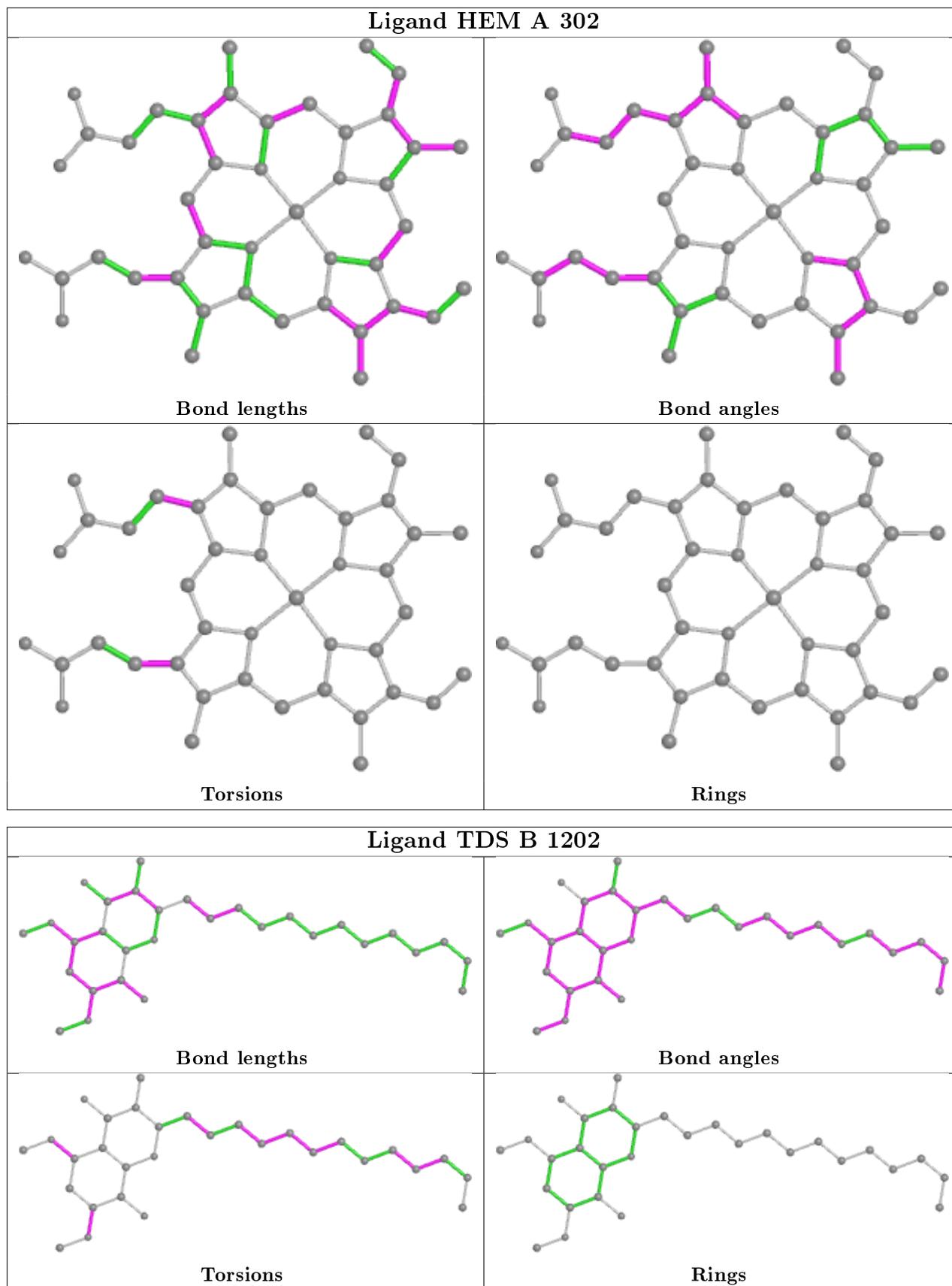
15 monomers are involved in 175 short contacts:

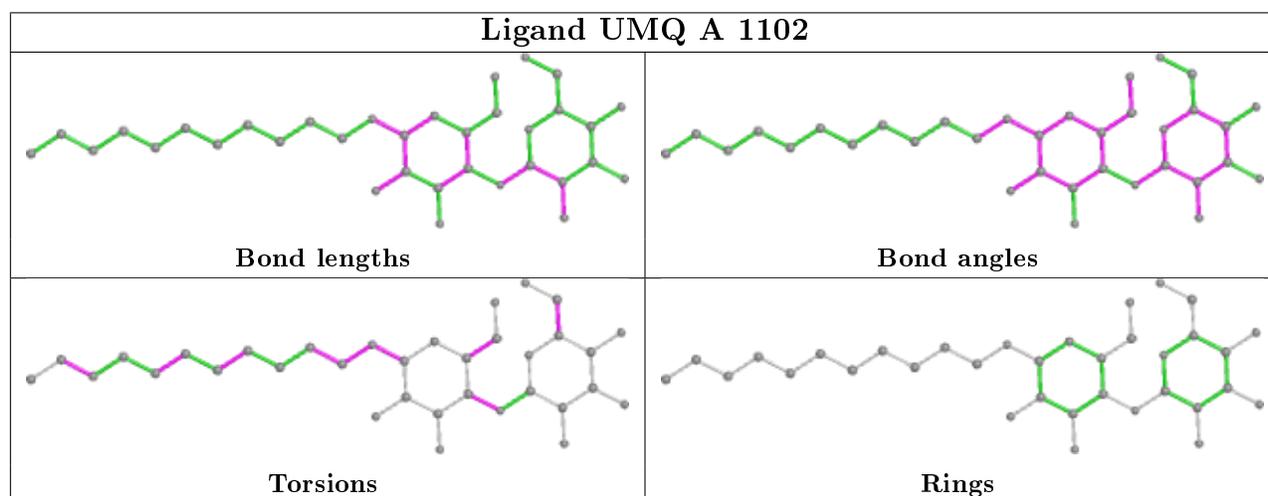
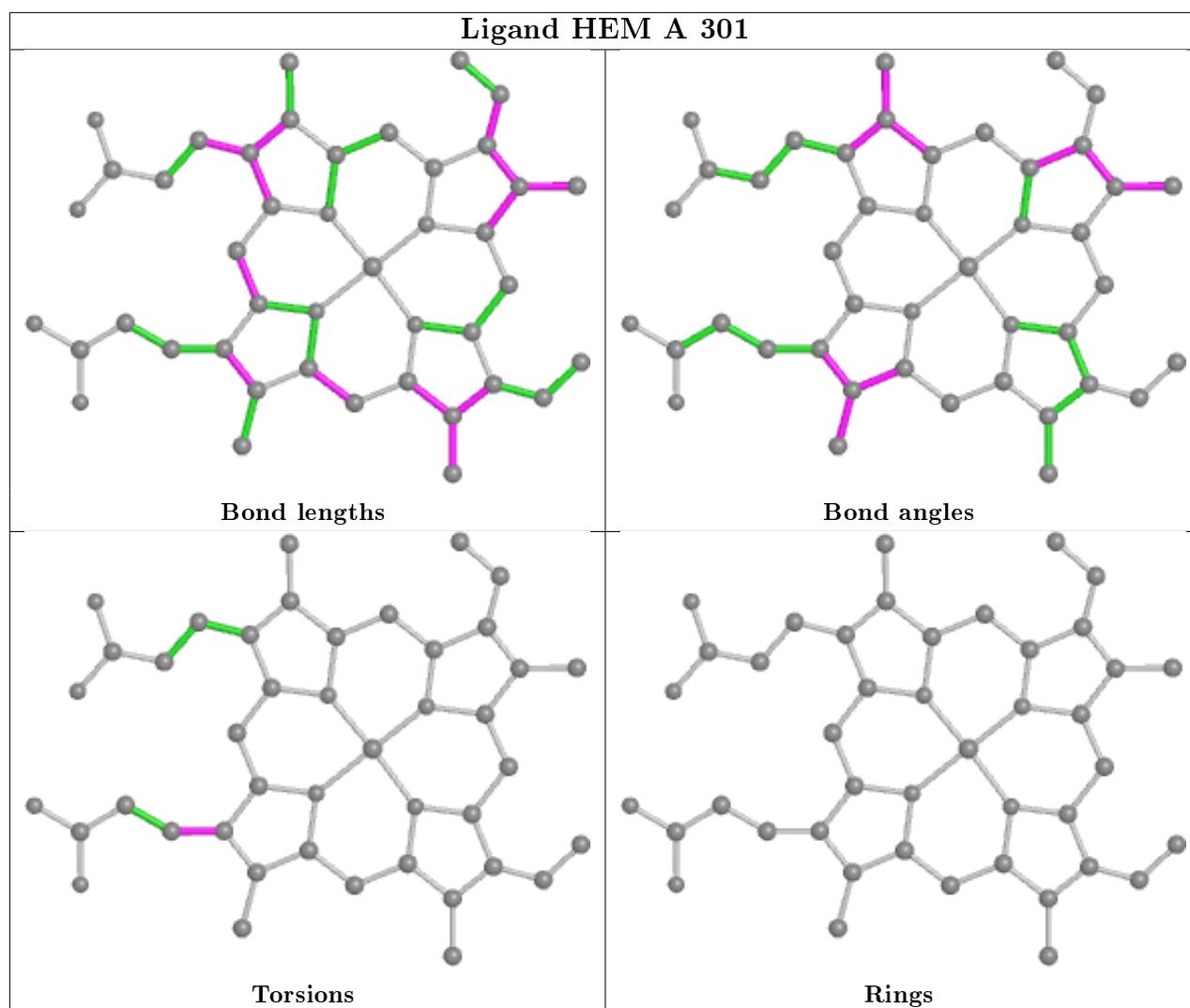
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	303	HEM	25	0
11	B	1001	OPC	2	0
13	B	201	CLA	5	0
14	B	1201	TDS	21	0
15	D	200	FES	1	0
12	A	1101	UMQ	2	0
10	A	302	HEM	22	0
14	B	1202	TDS	20	0
10	A	301	HEM	17	0
12	A	1102	UMQ	1	0
10	C	301	HEM	29	0
16	D	201	SQD	9	0
11	A	1002	OPC	18	0
17	G	101	BCR	9	0
12	A	1104	UMQ	3	0

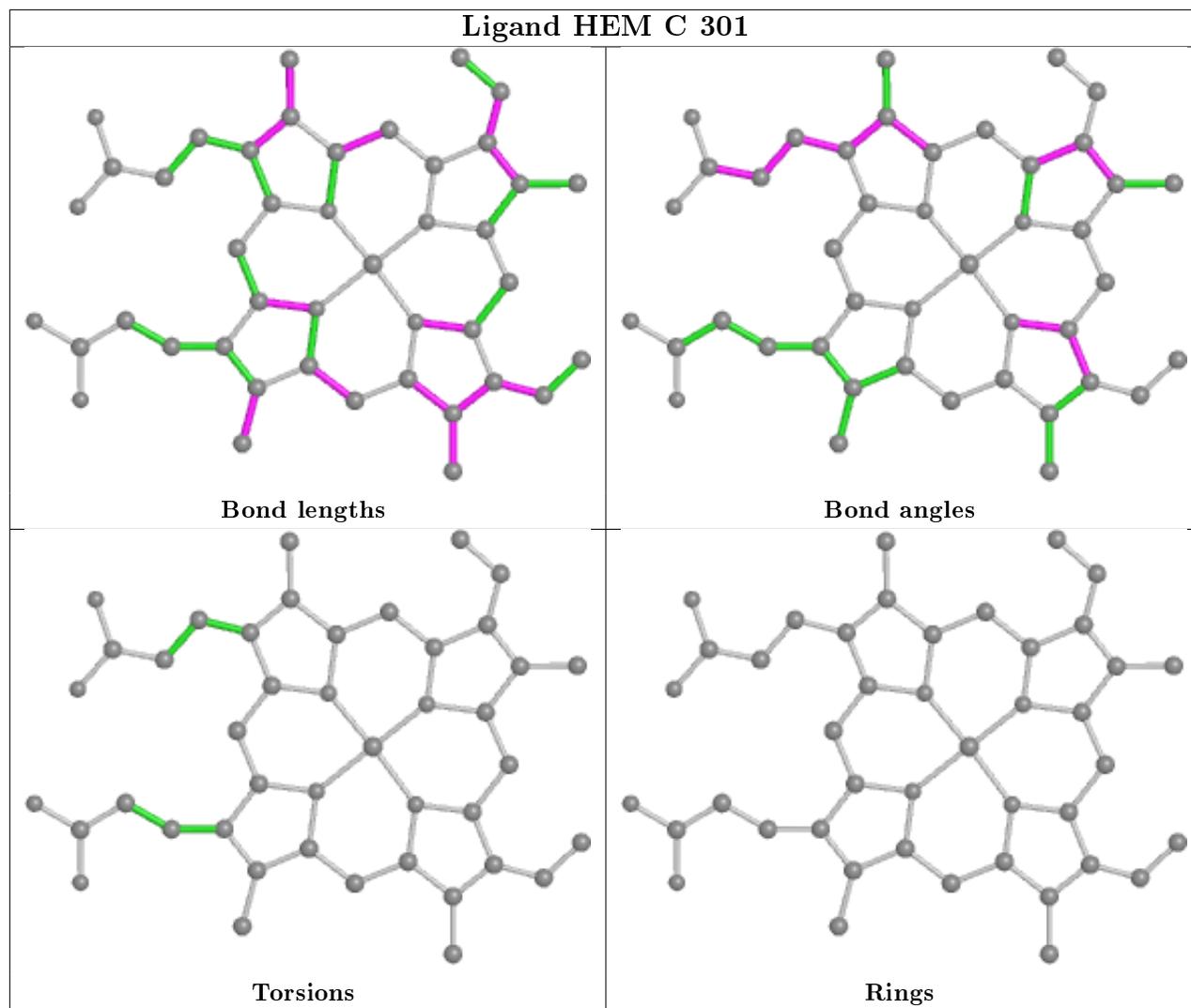
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

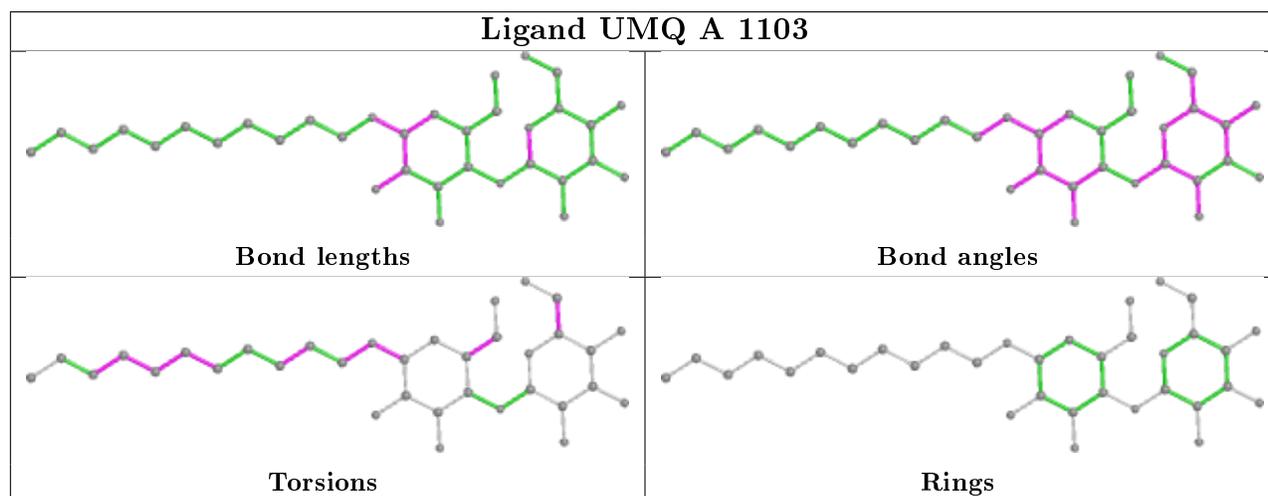
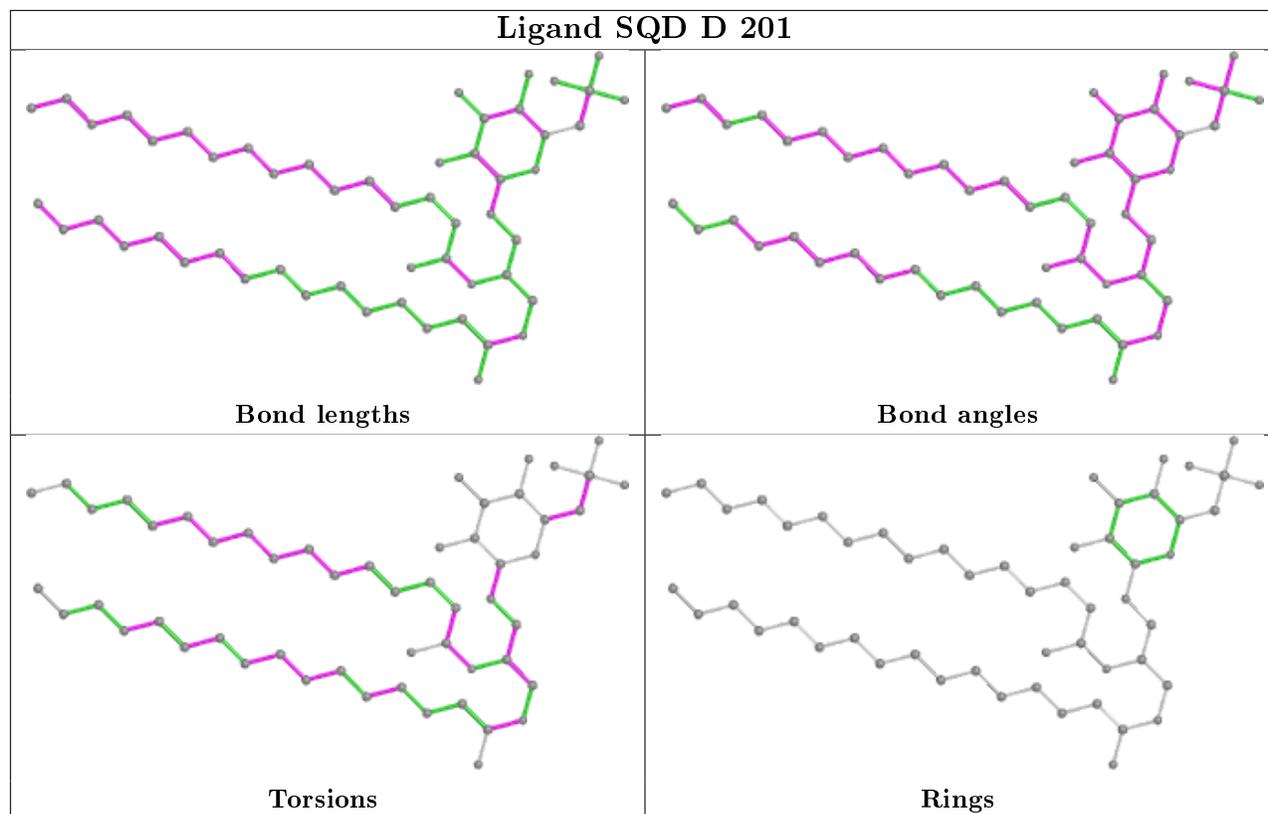


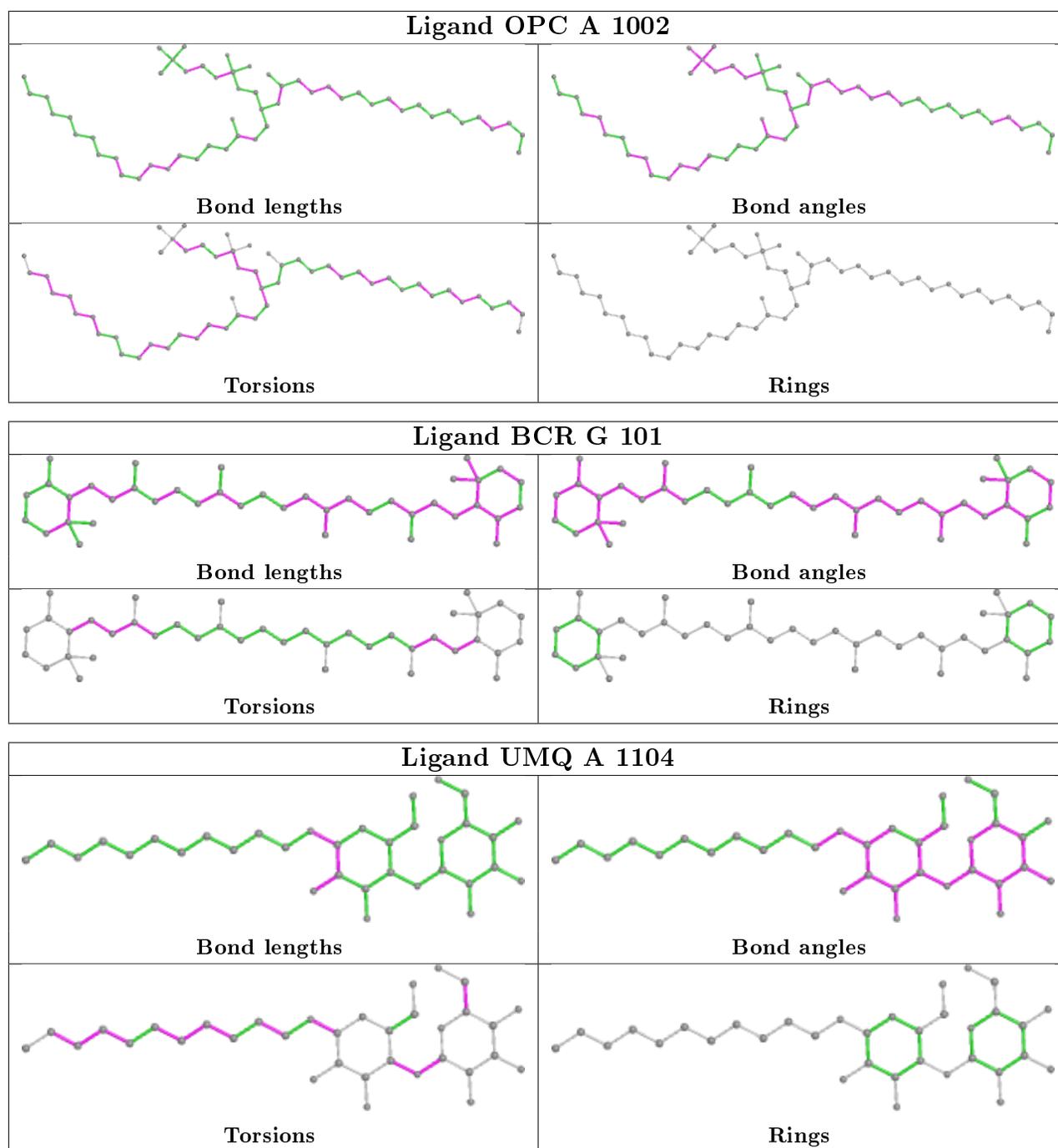












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	215/215 (100%)	-0.60	1 (0%) 91 90	5, 31, 72, 170	0
2	B	160/160 (100%)	-0.44	5 (3%) 49 48	22, 50, 97, 146	0
3	C	288/289 (99%)	0.10	16 (5%) 24 25	7, 55, 142, 159	1 (0%)
4	D	168/179 (93%)	0.73	18 (10%) 6 8	24, 90, 140, 156	0
5	E	32/32 (100%)	-0.17	2 (6%) 20 21	39, 63, 93, 110	0
6	F	32/35 (91%)	-0.59	0 100 100	35, 50, 112, 121	0
7	G	37/37 (100%)	-0.42	0 100 100	29, 44, 119, 138	0
8	H	29/29 (100%)	-0.62	0 100 100	31, 42, 72, 95	0
All	All	961/976 (98%)	-0.11	42 (4%) 34 34	5, 52, 132, 170	1 (0%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	95	SER	13.5
4	D	96	LYS	12.6
3	C	220	SER	4.9
4	D	75	ALA	4.9
4	D	179	VAL	4.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

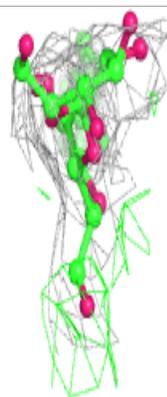
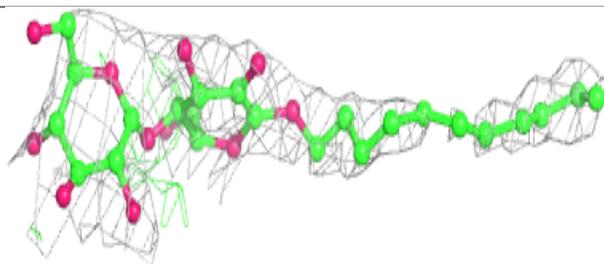
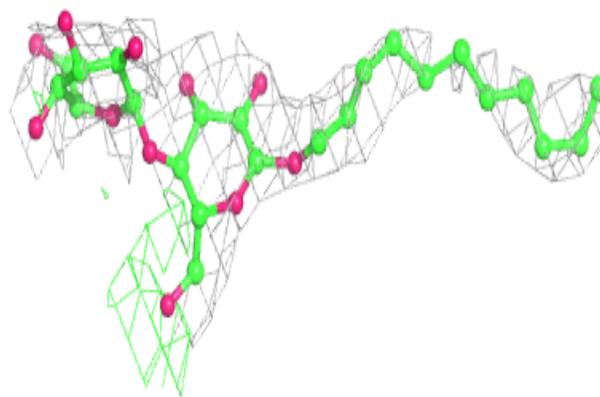
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
12	UMQ	A	1102	34/34	0.78	0.39	47,118,166,176	0
12	UMQ	A	1103	34/34	0.84	0.47	58,109,133,141	0
17	BCR	G	101	40/40	0.84	0.35	24,63,149,159	0
12	UMQ	A	1104	34/34	0.84	0.35	61,129,164,178	0
16	SQD	D	201	54/54	0.85	0.58	44,147,189,215	0
11	OPC	A	1002	54/55	0.88	0.39	19,84,180,191	0
14	TDS	B	1201	30/30	0.91	0.26	46,83,113,127	0
12	UMQ	A	1101	34/34	0.91	0.31	18,110,147,150	0
11	OPC	B	1001	54/55	0.94	0.39	28,80,117,123	0
13	CLA	B	201	65/65	0.95	0.20	23,51,105,119	0
14	TDS	B	1202	30/30	0.97	0.18	32,78,98,120	0
10	HEM	C	301	43/43	0.98	0.25	3,35,79,104	0
10	HEM	A	302	43/43	0.99	0.17	6,26,45,63	0
9	CD	A	216	1/1	0.99	0.08	63,63,63,63	0
15	FES	D	200	4/4	0.99	0.06	59,69,70,72	0
10	HEM	A	301	43/43	0.99	0.16	2,21,41,74	0
10	HEM	A	303	43/43	0.99	0.16	21,48,67,87	0

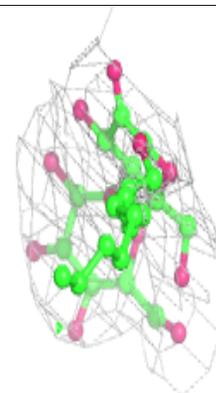
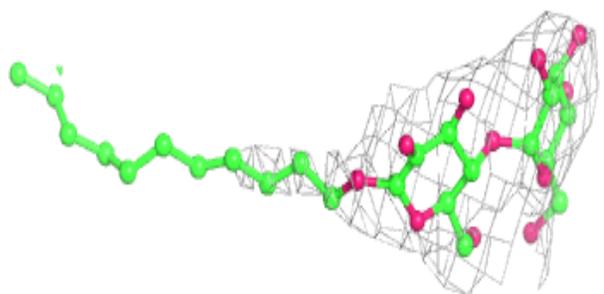
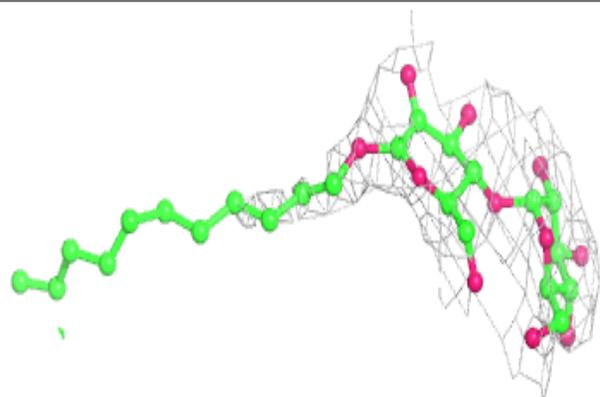
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UMQ A 1102:**

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

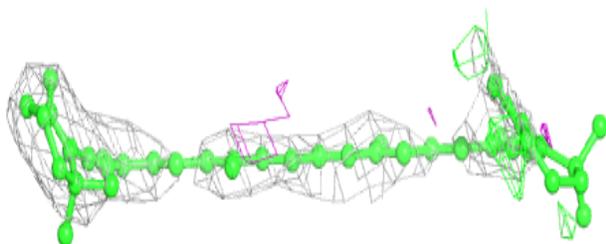
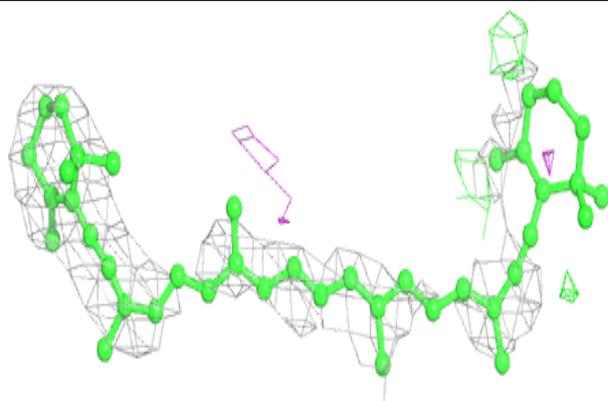
**Electron density around UMQ A 1103:**

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

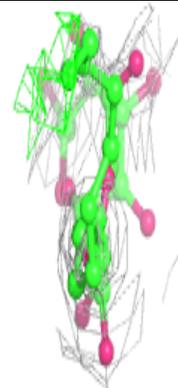
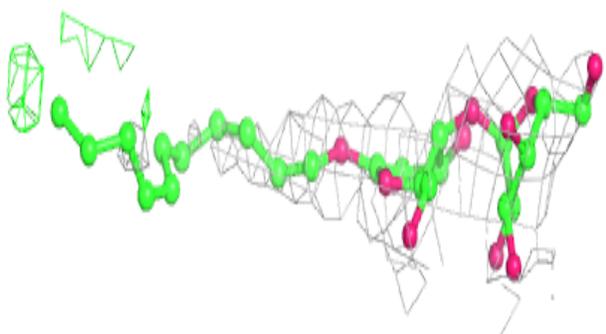
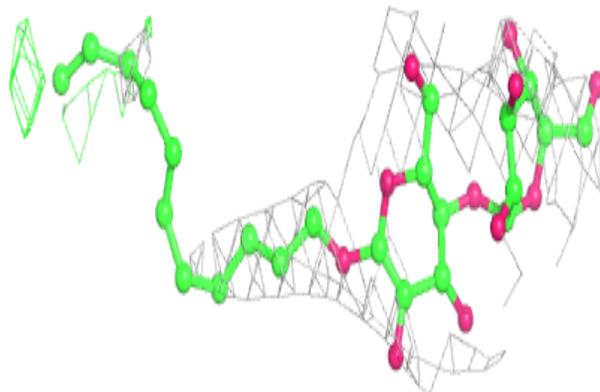


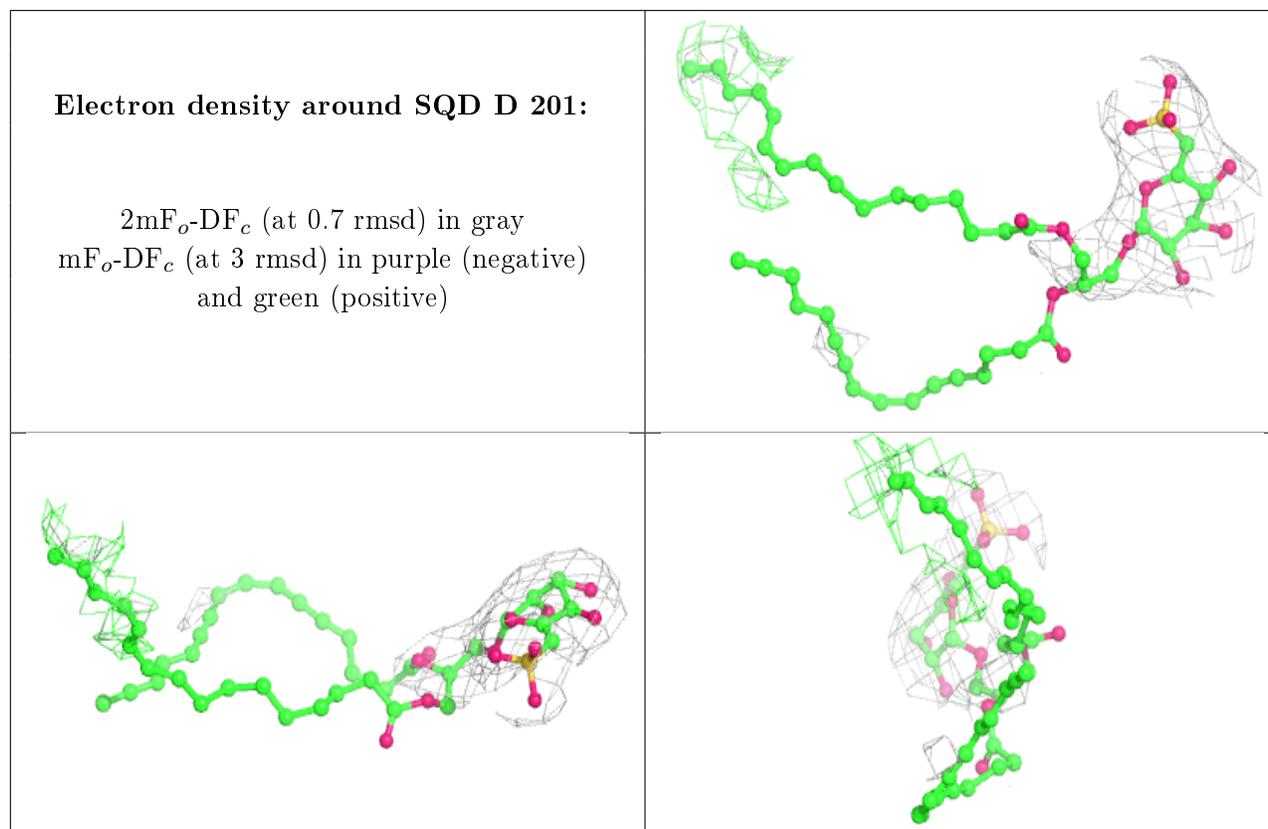
**Electron density around BCR G 101:**

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

**Electron density around UMQ A 1104:**

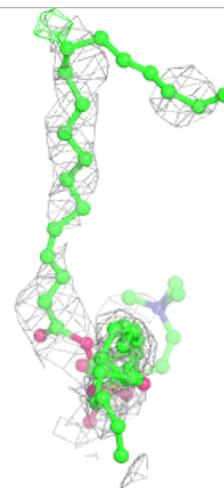
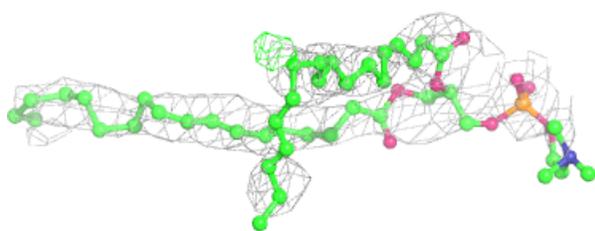
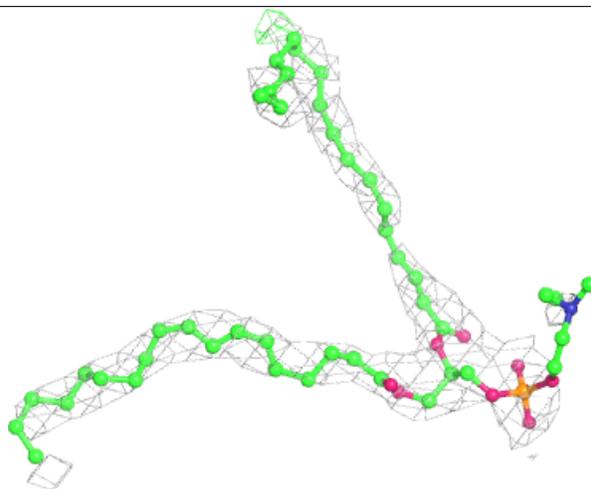
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





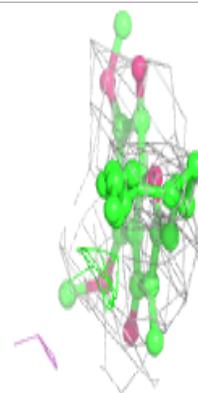
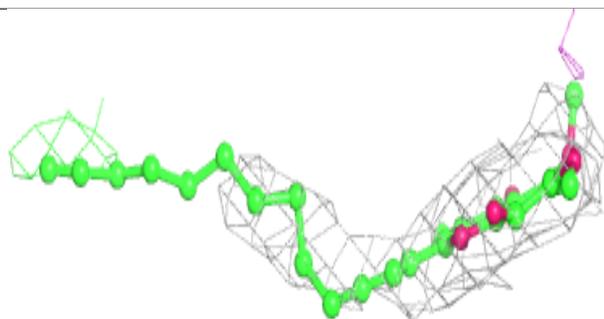
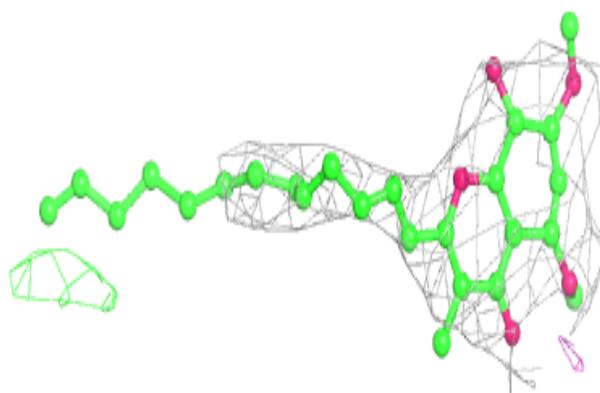
**Electron density around OPC A 1002:**

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

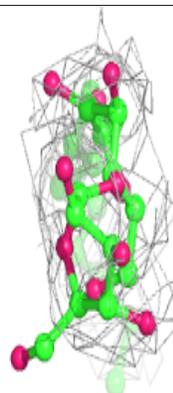
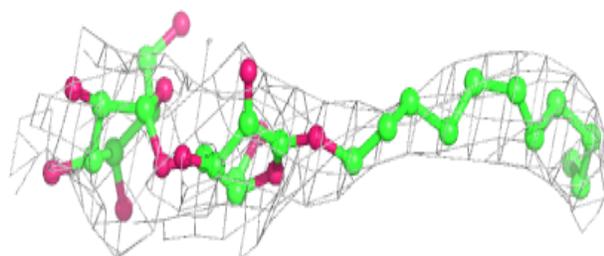
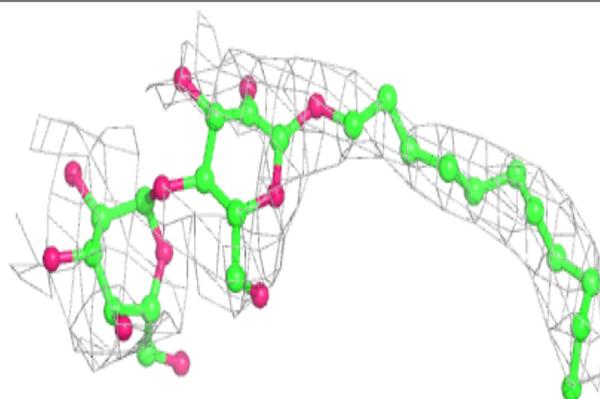


**Electron density around TDS B 1201:**

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

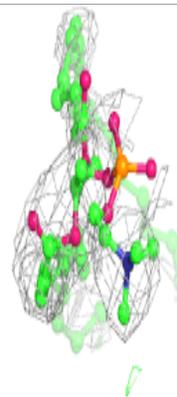
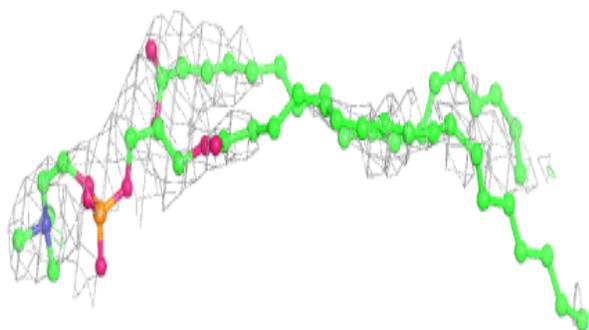
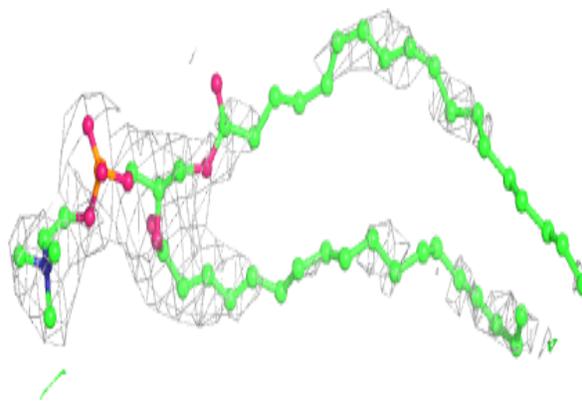
**Electron density around UMQ A 1101:**

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

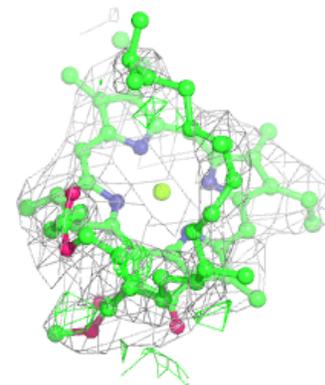
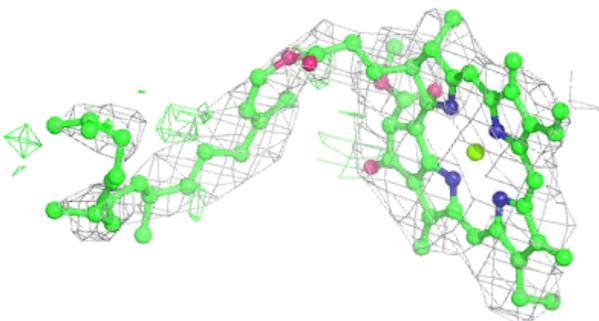
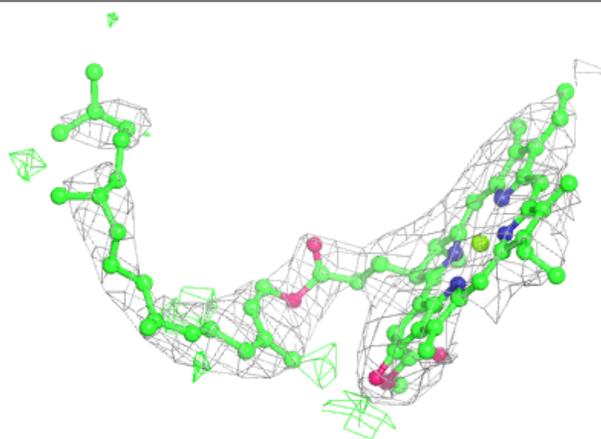


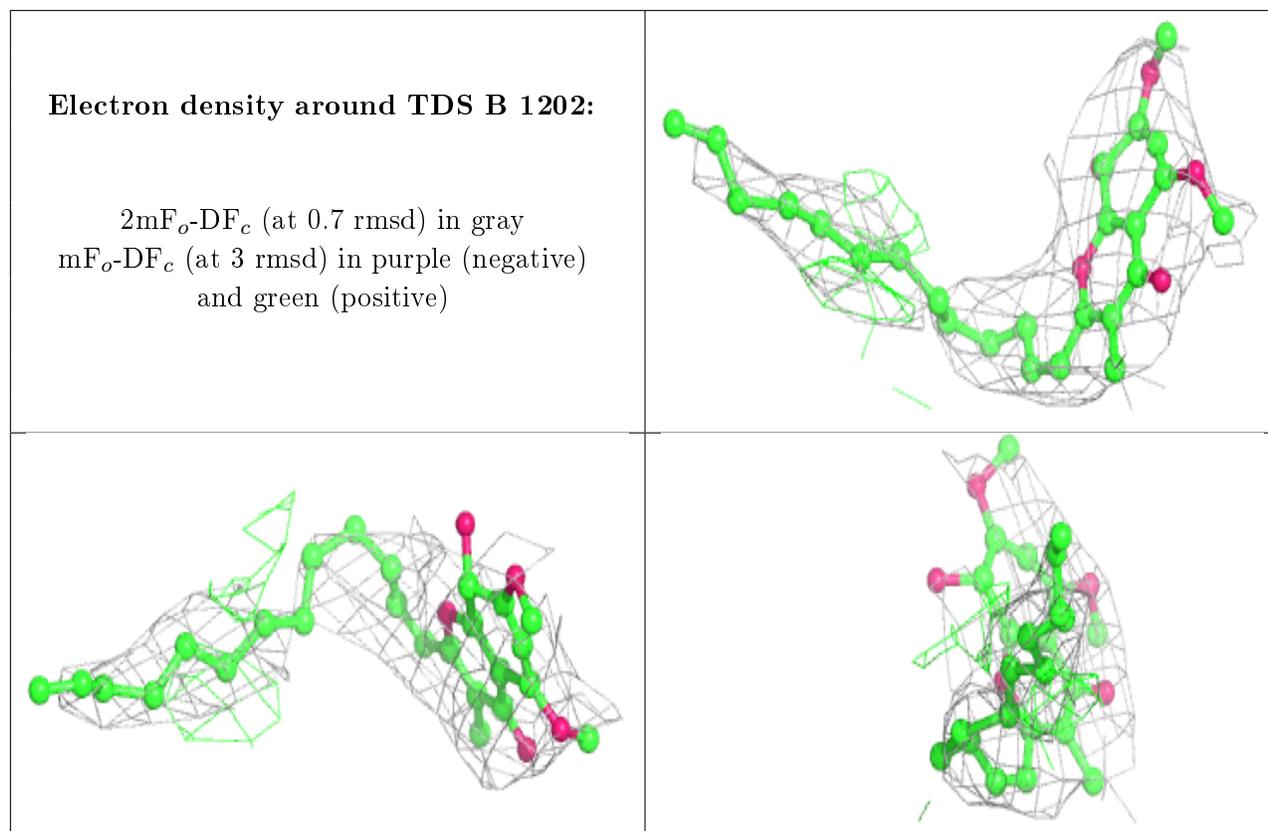
**Electron density around OPC B 1001:**

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

**Electron density around CLA B 201:**

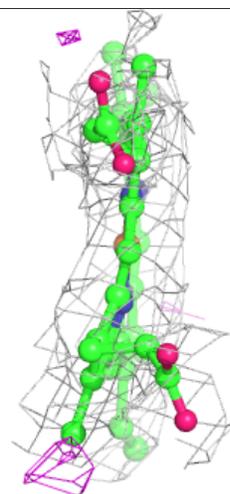
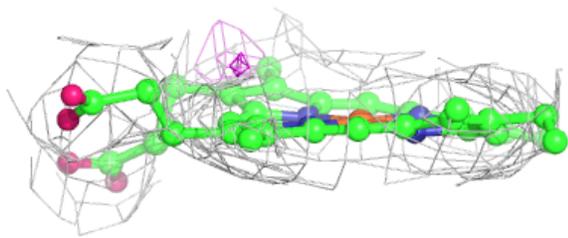
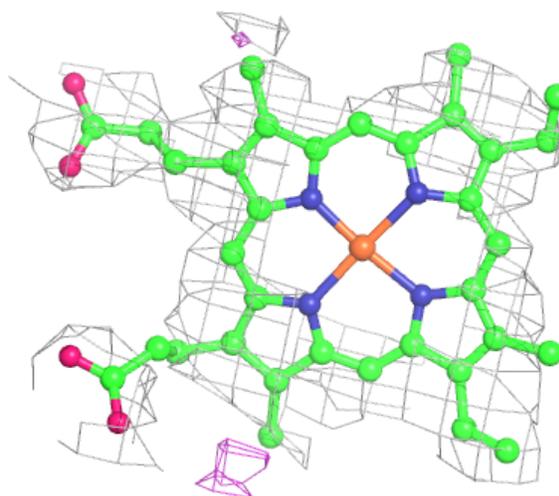
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





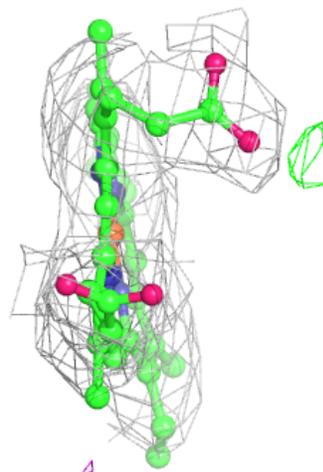
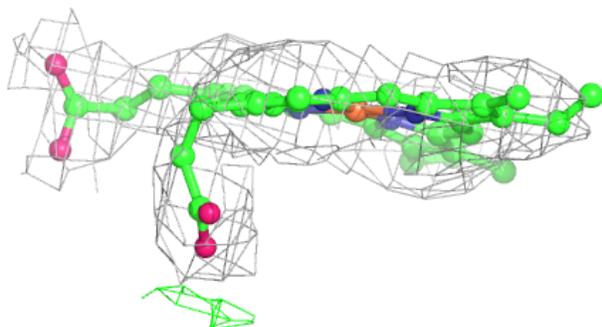
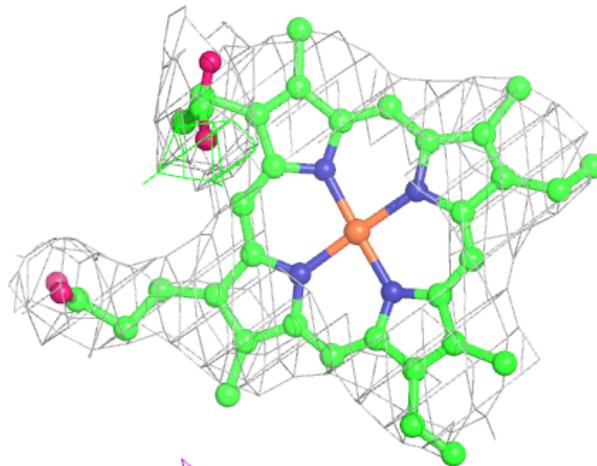
**Electron density around HEM C 301:**

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



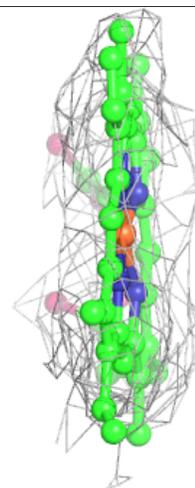
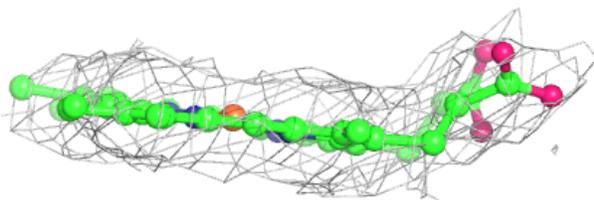
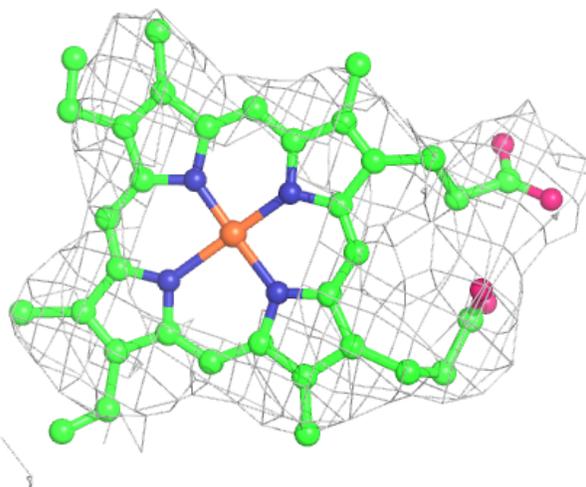
**Electron density around HEM A 302:**

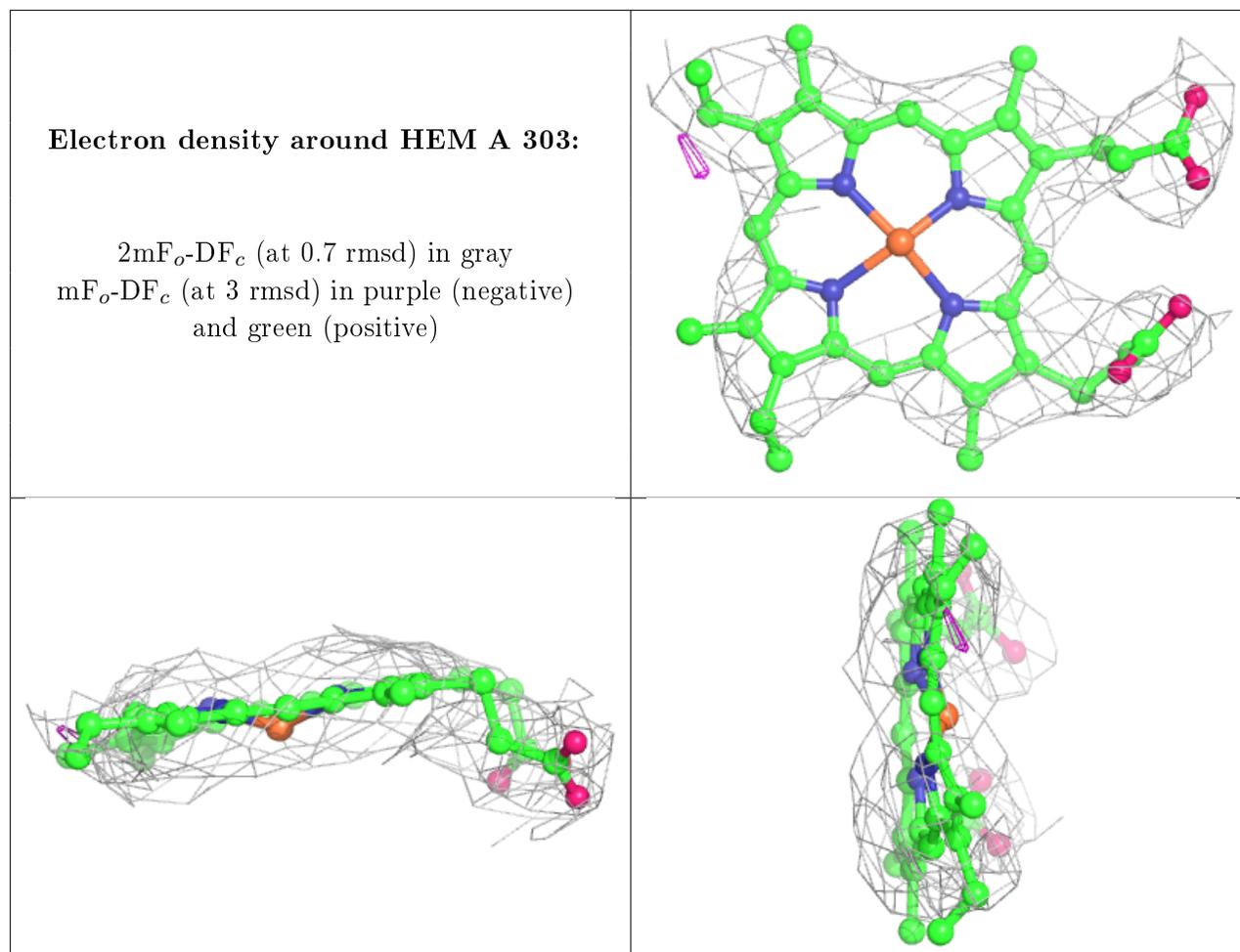
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.