



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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 : 2.11  
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

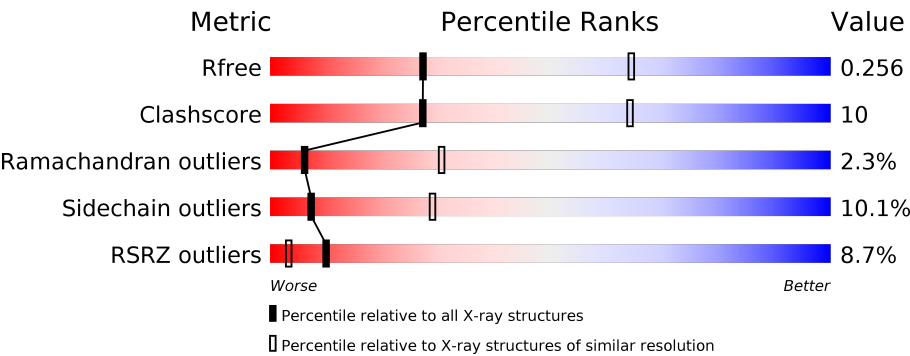
# 1 Overall quality at a glance i

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  $\geq 3$ , 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	<div><div>%</div><div><div></div><div>76%</div><div>21%</div><div></div></div><div></div></div>
2	B	160	<div><div>2%</div><div><div></div><div>73%</div><div>21%</div><div>6%</div></div><div></div></div>
3	C	289	<div><div>12%</div><div><div></div><div>73%</div><div>22%</div><div>5%</div></div><div></div></div>
4	D	179	<div><div>24%</div><div><div></div><div>76%</div><div>16%</div><div></div><div>7%</div></div><div></div></div>
5	E	31	<div><div>3%</div><div><div></div><div>81%</div><div>16%</div><div></div></div><div></div></div>
6	F	34	<div><div></div><div><div></div><div>62%</div><div>24%</div><div>9%</div><div>6%</div></div><div></div></div>

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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	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			

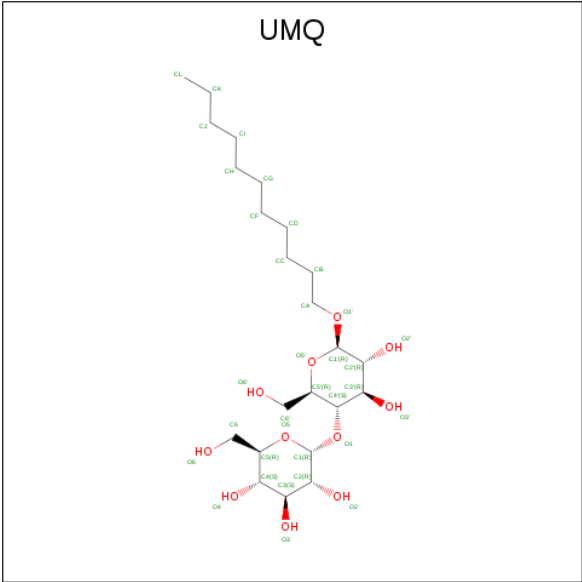
- | Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | G     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 281   | 188 | 44 | 48 |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

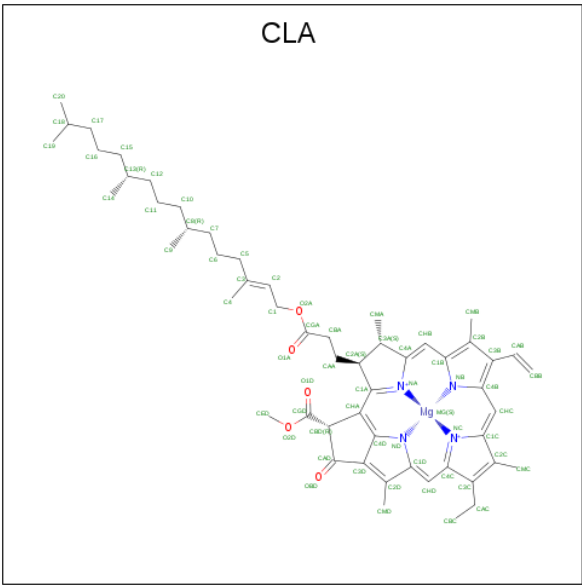
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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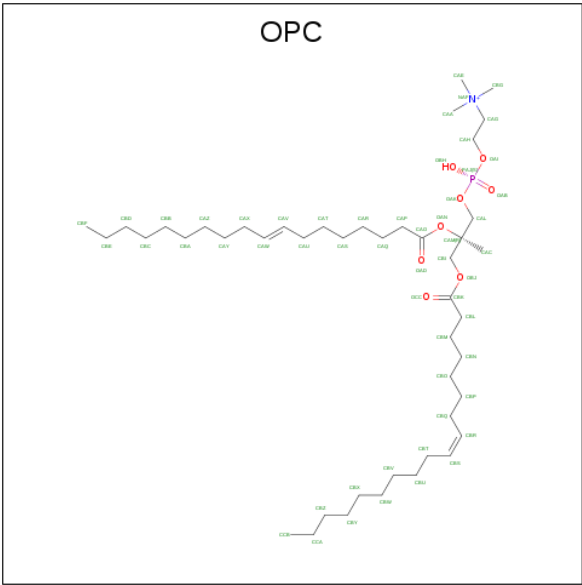
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O		0	0
			34	23	11			
10	A	1	Total	C	O		0	0
			34	23	11			
10	A	1	Total	C	O		0	0
			34	23	11			

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



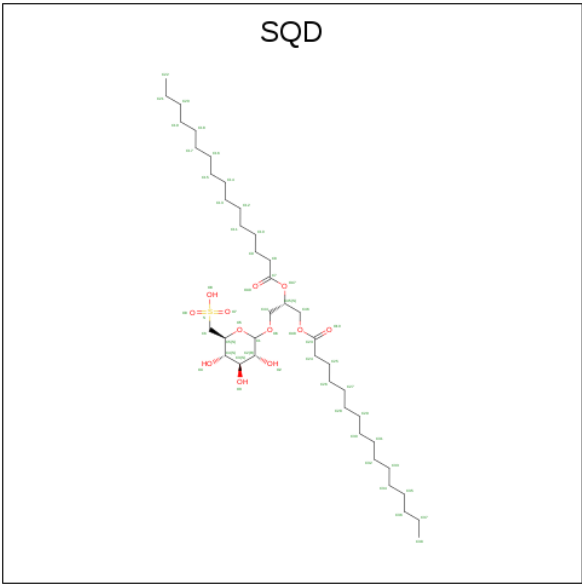
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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: C<sub>45</sub>H<sub>87</sub>NO<sub>8</sub>P).



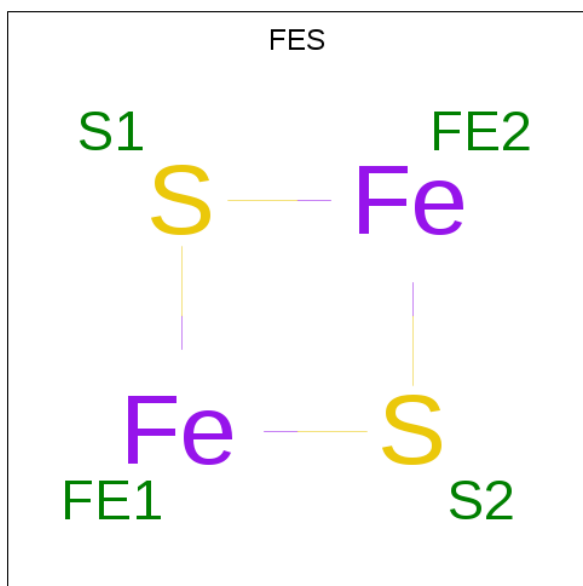
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 13 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



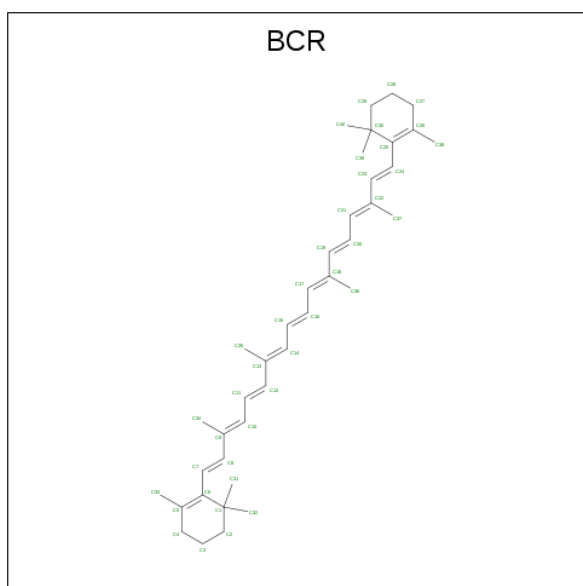
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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: C<sub>40</sub>H<sub>56</sub>).





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

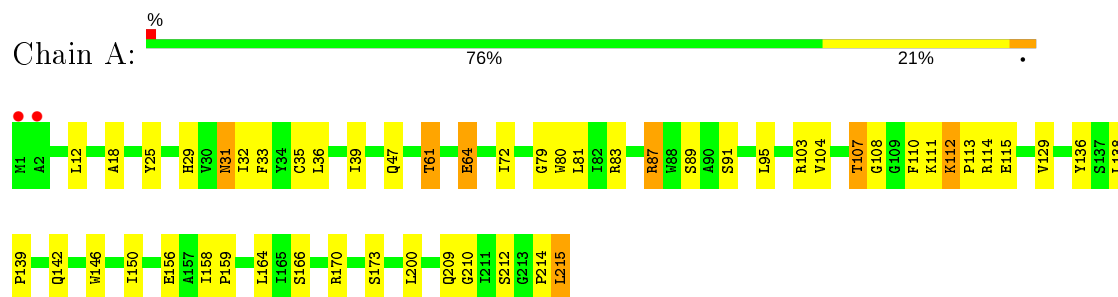
- Molecule 16 is water.

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

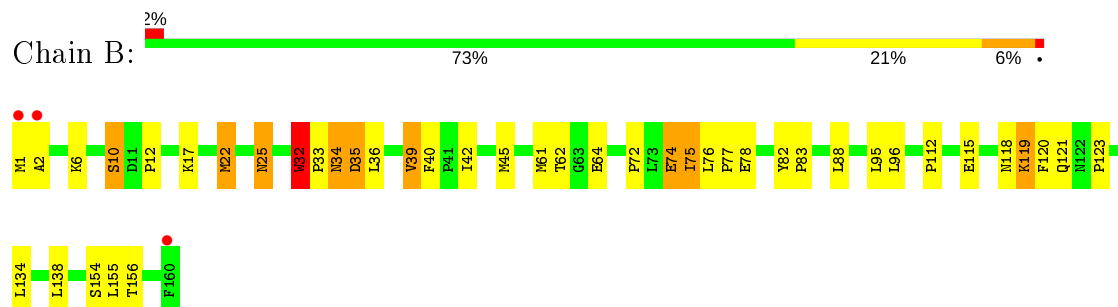
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

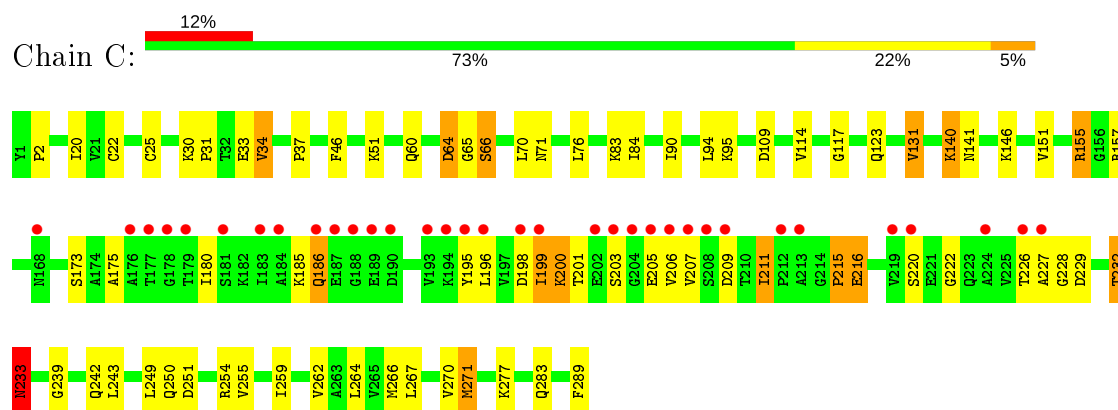
#### • Molecule 1: Cytochrome b6



#### • Molecule 2: Cytochrome b6-f complex subunit 4

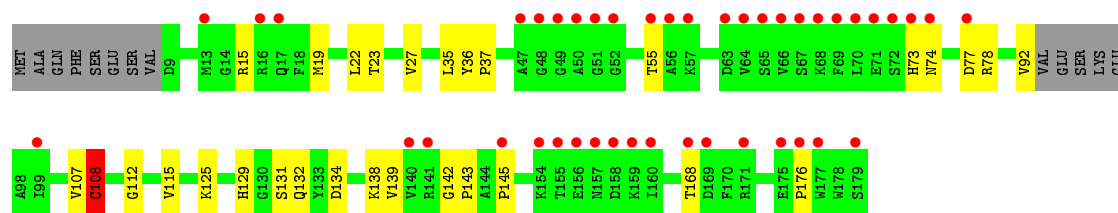


#### • Molecule 3: Apocytochrome f

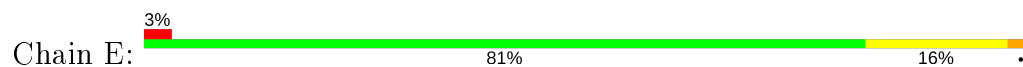


#### • Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1





• Molecule 5: Cytochrome b6-f complex subunit 6



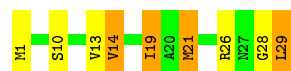
• Molecule 6: Cytochrome b6-f complex subunit 7



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<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

### 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(°)	Ideal(°)
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.

All (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
2:B:34:ASN:HD22	2:B:34:ASN:H	1.13	0.96
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.45	0.96
3:C:22:CYS:HB2	9:C:301:HEM:HAB	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:GLN:HE21	3:C:251:ASP:H	0.99	0.92
9:A:303:HEM:HHA	9:A:303:HEM:HBD1	1.55	0.87
3:C:232:THR:O	3:C:233:ASN:HB3	1.75	0.87
1:A:32:ILE:HD11	15:G:101:BCR:H322	1.60	0.82
1:A:103:ARG:NH1	1:A:104:VAL:HA	1.95	0.81
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.64	0.80
1:A:146:TRP:HB3	2:B:75:ILE:HD11	1.67	0.75
1:A:39:ILE:HD11	15:G:101:BCR:H312	1.70	0.74
3:C:250:GLN:HE21	3:C:251:ASP:N	1.81	0.73
2:B:22:MET:O	2:B:22:MET:HG2	1.88	0.73
4:D:131:SER:HA	4:D:142:GLY:HA3	1.71	0.73
1:A:83:ARG:NH1	9:A:301:HEM:O1D	2.21	0.72
2:B:34:ASN:ND2	2:B:34:ASN:H	1.84	0.70
3:C:60:GLN:HE22	3:C:157:ARG:H	1.38	0.70
1:A:112:LYS:O	1:A:115:GLU:OE1	2.10	0.70
8:H:28:GLY:C	8:H:29:LEU:HG	2.12	0.69
2:B:118:ASN:HD22	2:B:120:PHE:H	1.39	0.68
2:B:17:LYS:HB3	2:B:22:MET:O	1.93	0.68
1:A:103:ARG:O	1:A:107:THR:HB	1.94	0.67
3:C:226:THR:HG22	3:C:227:ALA:H	1.60	0.67
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.09	0.67
2:B:32:TRP:O	2:B:33:PRO:C	2.32	0.66
1:A:103:ARG:HH11	1:A:104:VAL:HA	1.58	0.66
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.32	0.64
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.80	0.64
5:E:17:ILE:O	5:E:21:LEU:HB2	1.98	0.64
1:A:32:ILE:N	8:H:29:LEU:HD13	2.14	0.62
3:C:84:ILE:HD11	3:C:114:VAL:HG11	1.82	0.62
3:C:20:ILE:HD12	3:C:242:GLN:HG2	1.83	0.60
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.31	0.60
2:B:119:LYS:O	2:B:119:LYS:HG2	2.02	0.59
1:A:39:ILE:CD1	15:G:101:BCR:H312	2.33	0.59
10:A:304:UMQ:HB1	3:C:254:ARG:HA	1.85	0.58
4:D:108:CYS:HB3	4:D:115:VAL:HG22	1.86	0.57
4:D:15:ARG:NH1	5:E:28:ALA:O	2.37	0.56
2:B:34:ASN:HD21	3:C:283:GLN:HE22	1.51	0.56
3:C:262:VAL:HG13	8:H:14:VAL:HG13	1.86	0.56
3:C:175:ALA:HB2	3:C:209:ASP:OD2	2.06	0.56
3:C:200:LYS:HG3	3:C:206:VAL:HG22	1.86	0.56
3:C:30:LYS:HG2	3:C:239:GLY:HA3	1.87	0.56
3:C:155:ARG:HD2	3:C:155:ARG:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:20:TRP:CZ3	15:G:101:BCR:H19C	2.41	0.55
3:C:31:PRO:O	3:C:155:ARG:NH2	2.41	0.54
2:B:22:MET:CG	2:B:22:MET:O	2.54	0.54
1:A:29:HIS:HB2	7:G:28:GLN:HE22	1.72	0.54
1:A:114:ARG:NH1	1:A:210:GLY:O	2.41	0.54
2:B:45:MET:CE	4:D:27:VAL:HG13	2.37	0.54
4:D:131:SER:CA	4:D:142:GLY:HA3	2.37	0.53
1:A:209:GLN:HB3	2:B:22:MET:HE2	1.91	0.53
1:A:87:ARG:NH1	2:B:78:GLU:OE1	2.40	0.53
12:H:30:OPC:HAP2	12:H:30:OPC:HBL1	1.91	0.53
4:D:107:VAL:HG12	4:D:112:GLY:HA2	1.91	0.52
3:C:173:SER:HB2	3:C:228:GLY:HA2	1.90	0.52
3:C:34:VAL:HG23	3:C:243:LEU:HD12	1.92	0.52
3:C:255:VAL:O	3:C:259:ILE:HG12	2.09	0.52
1:A:83:ARG:HD2	9:A:301:HEM:O1A	2.09	0.52
1:A:32:ILE:H	8:H:29:LEU:HD13	1.72	0.52
1:A:111:LYS:O	1:A:113:PRO:HD2	2.09	0.52
1:A:146:TRP:HB3	2:B:75:ILE:CD1	2.38	0.52
3:C:270:VAL:HA	8:H:21:MET:HE2	1.90	0.52
3:C:22:CYS:HB2	9:C:301:HEM:CAB	2.31	0.51
8:H:10:SER:O	8:H:14:VAL:HG22	2.10	0.51
2:B:61:MET:HG3	3:C:146:LYS:HD3	1.93	0.50
3:C:140:LYS:N	3:C:140:LYS:HD3	2.25	0.50
4:D:131:SER:CB	4:D:142:GLY:HA3	2.41	0.50
1:A:31:ASN:HD22	1:A:33:PHE:H	1.58	0.50
2:B:25:ASN:ND2	2:B:25:ASN:H	2.08	0.50
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.94	0.50
10:A:305:UMQ:HB2	13:B:203:SQD:O10	2.12	0.49
3:C:266:MET:O	3:C:270:VAL:HG23	2.12	0.49
7:G:20:GLY:N	15:G:101:BCR:H363	2.26	0.49
1:A:215:LEU:HG	7:G:28:GLN:OE1	2.12	0.49
8:H:1:MET:HB3	12:H:30:OPC:HAE1	1.95	0.49
8:H:28:GLY:O	8:H:29:LEU:HG	2.13	0.49
3:C:199:ILE:O	3:C:200:LYS:CB	2.61	0.49
8:H:26:ARG:HH11	8:H:29:LEU:HD11	1.77	0.49
1:A:80:TRP:CH2	3:C:254:ARG:HG2	2.48	0.48
3:C:270:VAL:HG22	8:H:21:MET:HE2	1.96	0.48
7:G:26:TYR:CE2	7:G:30:LYS:HE2	2.49	0.48
1:A:142:GLN:HG3	2:B:72:PRO:HG3	1.95	0.48
3:C:250:GLN:NE2	3:C:251:ASP:H	1.85	0.48
4:D:77:ASP:N	4:D:77:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:11:LEU:HD21	12:H:30:OPC:HAV	1.96	0.48
2:B:10:SER:O	2:B:12:PRO:HD3	2.14	0.47
1:A:25:TYR:OH	3:C:289:PHE:O	2.24	0.47
4:D:129:HIS:HB2	14:D:200:FES:S1	2.54	0.47
1:A:129:VAL:HG21	11:B:201:CLA:H43	1.96	0.47
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.49	0.47
7:G:23:TYR:OH	7:G:27:LYS:HE3	2.15	0.47
3:C:22:CYS:CB	9:C:301:HEM:HAB	2.32	0.47
1:A:150:ILE:HD11	2:B:75:ILE:HG12	1.97	0.46
1:A:72:ILE:O	1:A:79:GLY:HA3	2.16	0.46
9:A:303:HEM:HBD1	9:A:303:HEM:CHA	2.32	0.46
1:A:115:GLU:N	1:A:115:GLU:OE1	2.45	0.46
15:G:101:BCR:H20C	15:G:101:BCR:H361	1.65	0.46
3:C:64:ASP:CG	3:C:65:GLY:H	2.19	0.46
4:D:168:THR:HA	4:D:176:PRO:HD3	1.98	0.46
3:C:271:MET:HG3	4:D:23:THR:HA	1.96	0.46
2:B:32:TRP:O	2:B:34:ASN:N	2.49	0.46
1:A:29:HIS:CB	7:G:28:GLN:HE22	2.30	0.45
4:D:134:ASP:HB2	4:D:138:LYS:H	1.81	0.45
3:C:155:ARG:HD2	3:C:155:ARG:N	2.31	0.45
3:C:270:VAL:HA	8:H:21:MET:CE	2.46	0.45
6:F:26:LEU:HA	6:F:29:ILE:HG23	1.97	0.45
3:C:33:GLU:HB2	3:C:51:LYS:HB2	1.97	0.45
1:A:138:LEU:N	1:A:139:PRO:CD	2.79	0.45
2:B:36:LEU:O	2:B:40:PHE:HB2	2.16	0.45
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.98	0.45
3:C:186:GLN:HE21	3:C:196:LEU:HG	1.82	0.45
2:B:1:MET:HB3	2:B:2:ALA:H	1.61	0.45
3:C:76:LEU:HD12	3:C:151:VAL:HG22	1.99	0.45
3:C:37:PRO:HB3	12:H:30:OPC:HAH1	1.97	0.45
2:B:74:GLU:OE1	7:G:1:MET:HA	2.17	0.45
3:C:199:ILE:O	3:C:200:LYS:HB2	2.16	0.45
1:A:61:THR:HG22	1:A:64:GLU:H	1.82	0.44
3:C:30:LYS:HB3	3:C:31:PRO:HD2	1.98	0.44
3:C:232:THR:O	3:C:233:ASN:CB	2.57	0.44
1:A:35:CYS:SG	9:A:303:HEM:C3B	2.91	0.44
15:G:101:BCR:H323	8:H:19:ILE:HG12	1.98	0.44
7:G:34:GLU:HG2	7:G:35:LEU:HG	1.99	0.44
3:C:71:ASN:N	9:C:301:HEM:O2A	2.45	0.44
2:B:39:VAL:HA	2:B:42:ILE:HD12	1.99	0.44
2:B:35:ASP:HA	2:B:39:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:13:LEU:HA	7:G:16:VAL:HG23	2.00	0.43
1:A:108:GLY:HA3	2:B:121:GLN:HA	2.00	0.43
1:A:110:PHE:HD1	2:B:112:PRO:HB3	1.83	0.43
3:C:266:MET:SD	8:H:13:VAL:HG12	2.59	0.43
3:C:215:PRO:HB2	3:C:216:GLU:H	1.70	0.42
1:A:114:ARG:NH2	1:A:212:SER:HA	2.35	0.42
3:C:195:TYR:HB2	3:C:211:ILE:HG13	2.01	0.42
2:B:154:SER:C	2:B:156:THR:H	2.23	0.42
7:G:21:LEU:HA	7:G:21:LEU:HD12	1.91	0.42
6:F:5:LEU:HD21	7:G:11:LEU:HD12	2.00	0.42
4:D:78:ARG:HG2	4:D:92:VAL:HG22	2.02	0.42
3:C:90:ILE:O	3:C:95:LYS:NZ	2.53	0.42
4:D:131:SER:HB3	4:D:143:PRO:HD2	2.00	0.42
3:C:180:ILE:HA	3:C:198:ASP:O	2.20	0.42
1:A:209:GLN:O	2:B:22:MET:HB2	2.19	0.42
2:B:25:ASN:ND2	2:B:25:ASN:N	2.68	0.42
1:A:113:PRO:HB2	2:B:22:MET:CE	2.50	0.41
2:B:118:ASN:ND2	2:B:120:PHE:HD1	2.17	0.41
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.35	0.41
1:A:29:HIS:CD2	1:A:214:PRO:HA	2.55	0.41
1:A:136:TYR:CE1	2:B:78:GLU:HG3	2.55	0.41
3:C:199:ILE:HD12	3:C:207:VAL:HG23	2.02	0.41
1:A:158:ILE:HA	1:A:159:PRO:HD3	1.81	0.41
3:C:2:PRO:HG2	3:C:117:GLY:HA2	2.01	0.41
6:F:30:GLN:HE21	6:F:30:GLN:HB2	1.61	0.41
1:A:111:LYS:HE2	2:B:115:GLU:O	2.22	0.40
10:A:306:UMQ:HA2	2:B:32:TRP:NE1	2.36	0.40
5:E:15:THR:OG1	6:F:22:LEU:HD21	2.21	0.40
1:A:18:ALA:CB	10:A:306:UMQ:H6'1	2.52	0.40
3:C:180:ILE:O	3:C:222:GLY:HA2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (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
3	C	215	PRO
3	C	233	ASN
4	D	145	PRO
3	C	220	SER
6	F	2	SER
2	B	74	GLU
2	B	155	LEU
3	C	199	ILE
3	C	216	GLU
3	C	201	THR
3	C	205	GLU
7	G	27	LYS
3	C	203	SER
4	D	74	ASN
2	B	75	ILE
7	G	36	GLY
2	B	77	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/184 (100%)	169 (92%)	15 (8%)	11	39
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

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	31	ASN
1	A	36	LEU
1	A	61	THR
1	A	64	GLU
1	A	81	LEU
1	A	87	ARG
1	A	91	SER
1	A	95	LEU
1	A	107	THR
1	A	156	GLU
1	A	164	LEU
1	A	173	SER
1	A	200	LEU
1	A	215	LEU
2	B	6	LYS
2	B	10	SER
2	B	22	MET
2	B	25	ASN

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Mol	Chain	Res	Type
2	B	34	ASN
2	B	35	ASP
2	B	39	VAL
2	B	62	THR
2	B	64	GLU
2	B	76	LEU
2	B	88	LEU
2	B	95	LEU
2	B	96	LEU
2	B	119	LYS
2	B	134	LEU
2	B	138	LEU
3	C	34	VAL
3	C	66	SER
3	C	70	LEU
3	C	83	LYS
3	C	94	LEU
3	C	109	ASP
3	C	123	GLN
3	C	131	VAL
3	C	140	LYS
3	C	141	ASN
3	C	155	ARG
3	C	185	LYS
3	C	186	GLN
3	C	211	ILE
3	C	229	ASP
3	C	232	THR
3	C	233	ASN
3	C	249	LEU
3	C	264	LEU
3	C	267	LEU
3	C	271	MET
3	C	277	LYS
4	D	19	MET
4	D	22	LEU
4	D	35	LEU
4	D	55	THR
4	D	73	HIS
4	D	108	CYS
4	D	125	LYS
4	D	132	GLN

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Mol	Chain	Res	Type
4	D	139	VAL
5	E	8	ILE
5	E	10	PHE
5	E	21	LEU
6	F	6	LEU
6	F	10	LEU
6	F	22	LEU
6	F	25	LEU
6	F	29	ILE
6	F	30	GLN
7	G	6	LEU
7	G	16	VAL
7	G	21	LEU
7	G	30	LYS
8	H	14	VAL
8	H	19	ILE
8	H	21	MET
8	H	29	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
2	B	25	ASN
2	B	34	ASN
2	B	93	ASN
2	B	118	ASN
2	B	122	ASN
3	C	60	GLN
3	C	250	GLN
3	C	288	ASN
4	D	132	GLN
6	F	30	GLN
7	G	28	GLN
7	G	33	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
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

All (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
12	B	202	OPC	CAG-CAH	-5.53	1.33	1.51
9	C	301	HEM	C3D-C2D	5.45	1.53	1.37
9	A	302	HEM	C3D-C2D	5.40	1.53	1.37
11	B	201	CLA	C3B-C2B	5.19	1.47	1.40
9	A	303	HEM	C3D-C2D	5.16	1.53	1.37
12	H	30	OPC	CAG-CAH	-5.15	1.35	1.51
12	B	202	OPC	CAQ-CAP	-5.12	1.33	1.52
12	H	30	OPC	CAQ-CAP	-5.12	1.33	1.52
9	A	301	HEM	C3D-C2D	5.05	1.52	1.37
12	B	202	OPC	OBJ-CBK	5.04	1.48	1.33
11	B	201	CLA	CHC-C1C	4.96	1.47	1.35
11	B	201	CLA	C3C-C2C	4.91	1.47	1.36
12	H	30	OPC	CBP-CBQ	-4.76	1.33	1.52
11	B	201	CLA	O2D-CGD	4.68	1.44	1.33
9	A	302	HEM	C3C-C2C	-4.67	1.33	1.40
13	B	203	SQD	O47-C7	4.63	1.47	1.34
9	C	301	HEM	C3C-C2C	-4.55	1.34	1.40
15	G	101	BCR	C24-C25	-4.53	1.29	1.45
11	B	201	CLA	OBD-CAD	4.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	302	HEM	C3B-C2B	-4.47	1.34	1.40
9	A	303	HEM	C3C-C2C	-4.47	1.34	1.40
13	B	203	SQD	O48-C23	4.45	1.46	1.33
11	B	201	CLA	O2A-CGA	4.44	1.46	1.33
9	C	301	HEM	C3B-C2B	-4.40	1.34	1.40
12	H	30	OPC	OBJ-CBK	4.40	1.46	1.33
15	G	101	BCR	C12-C13	-4.38	1.36	1.45
12	H	30	OPC	OAN-CAO	4.33	1.46	1.34
12	B	202	OPC	CBP-CBQ	-4.29	1.35	1.52
15	G	101	BCR	C19-C18	-4.21	1.36	1.45
9	A	303	HEM	C3B-C2B	-4.16	1.34	1.40
9	A	301	HEM	C3C-CAC	4.13	1.56	1.47
11	B	201	CLA	C3D-C2D	4.12	1.46	1.39
10	A	306	UMQ	O2'-C2'	-4.11	1.33	1.43
12	B	202	OPC	OAN-CAO	4.10	1.45	1.34
10	A	305	UMQ	O2'-C2'	-3.99	1.33	1.43
9	A	303	HEM	C3C-CAC	3.99	1.56	1.47
9	A	301	HEM	C3B-C2B	-3.90	1.35	1.40
10	A	304	UMQ	O2'-C2'	-3.90	1.33	1.43
9	C	301	HEM	C3B-CAB	3.82	1.55	1.47
12	B	202	OPC	CAV-CAW	3.78	1.53	1.31
12	H	30	OPC	CAV-CAW	3.70	1.53	1.31
15	G	101	BCR	C7-C6	-3.66	1.32	1.45
10	A	305	UMQ	O1'-C1'	3.65	1.46	1.40
9	A	301	HEM	C3B-CAB	3.60	1.55	1.47
9	A	302	HEM	C3B-CAB	3.53	1.55	1.47
9	A	301	HEM	C3C-C2C	-3.53	1.35	1.40
10	A	306	UMQ	O1'-C1'	3.53	1.46	1.40
9	A	303	HEM	C3B-CAB	3.52	1.55	1.47
9	C	301	HEM	C3C-CAC	3.47	1.54	1.47
12	H	30	OPC	CBP-CBO	-3.36	1.32	1.51
9	A	302	HEM	C3C-CAC	3.32	1.54	1.47
10	A	304	UMQ	O1'-C1'	3.30	1.45	1.40
11	B	201	CLA	C1D-C2D	3.29	1.50	1.42
12	H	30	OPC	CAQ-CAR	-3.23	1.33	1.51
15	G	101	BCR	C24-C23	-3.21	1.23	1.33
12	B	202	OPC	CAQ-CAR	-3.15	1.33	1.51
12	H	30	OPC	CAR-CAS	-3.11	1.34	1.51
12	B	202	OPC	CAR-CAS	-3.11	1.34	1.51
12	H	30	OPC	CBB-CBC	-3.10	1.34	1.51
12	B	202	OPC	CBC-CBD	-3.09	1.34	1.51
12	B	202	OPC	CBB-CBC	-3.07	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	202	OPC	CBP-CBO	-3.05	1.34	1.51
12	H	30	OPC	CBC-CBD	-3.03	1.34	1.51
12	H	30	OPC	CBQ-CBR	-2.93	1.33	1.50
12	H	30	OPC	CBT-CBS	-2.89	1.33	1.50
9	A	301	HEM	CAA-C2A	2.85	1.56	1.52
12	B	202	OPC	CBT-CBS	-2.79	1.34	1.50
12	B	202	OPC	CBQ-CBR	-2.78	1.34	1.50
11	B	201	CLA	C1C-C2C	2.62	1.49	1.44
11	B	201	CLA	C4C-C3C	2.53	1.49	1.45
12	B	202	OPC	CAG-NAF	-2.51	1.43	1.51
15	G	101	BCR	C11-C10	-2.49	1.35	1.43
11	B	201	CLA	CHD-C4C	2.47	1.48	1.41
15	G	101	BCR	C20-C21	-2.38	1.36	1.43
15	G	101	BCR	C15-C14	-2.29	1.36	1.43
15	G	101	BCR	C16-C17	-2.29	1.36	1.43
13	B	203	SQD	C6-S	-2.27	1.69	1.77
11	B	201	CLA	C4B-CHC	2.23	1.47	1.41
12	H	30	OPC	CAG-NAF	-2.19	1.44	1.51
9	A	301	HEM	C1D-ND	2.13	1.40	1.36
11	B	201	CLA	C1B-CHB	2.06	1.46	1.41

All (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
13	B	203	SQD	O8-S-C6	9.74	121.27	105.74
13	B	203	SQD	O9-S-O7	-9.57	80.82	113.95
12	H	30	OPC	CAA-NAF-CAE	-8.77	86.43	108.97
12	H	30	OPC	CAA-NAF-CBG	-8.74	86.49	108.97
12	B	202	OPC	CAA-NAF-CBG	-8.56	86.96	108.97
12	B	202	OPC	CAA-NAF-CAE	-8.45	87.26	108.97
10	A	305	UMQ	O1'-C1'-C2'	8.37	121.38	108.30
10	A	304	UMQ	O1'-C1'-C2'	8.26	121.20	108.30
13	B	203	SQD	O7-S-C6	7.95	116.39	106.94
10	A	306	UMQ	O1'-C1'-C2'	7.44	119.91	108.30
11	B	201	CLA	C2C-C1C-NC	7.23	116.75	109.97
15	G	101	BCR	C8-C7-C6	6.77	146.21	127.20
9	A	301	HEM	CBD-CAD-C3D	-6.38	100.73	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	201	CLA	O2D-CGD-CBD	5.90	121.75	111.27
12	B	202	OPC	CAA-NAF-CAG	-5.49	87.46	109.92
10	A	305	UMQ	CA-O1'-C1'	5.27	122.58	113.84
12	H	30	OPC	CAA-NAF-CAG	-5.19	88.70	109.92
11	B	201	CLA	C3C-C4C-NC	5.03	116.22	110.57
10	A	306	UMQ	C1'-C2'-C3'	4.84	120.08	110.00
10	A	304	UMQ	C1'-C2'-C3'	4.78	119.95	110.00
10	A	306	UMQ	CA-O1'-C1'	4.78	121.76	113.84
15	G	101	BCR	C8-C9-C10	4.77	126.27	118.94
10	A	306	UMQ	O5'-C1'-C2'	4.75	120.41	110.35
13	B	203	SQD	O47-C7-C8	4.66	121.54	111.50
15	G	101	BCR	C30-C25-C26	-4.60	116.14	122.61
10	A	305	UMQ	C1'-C2'-C3'	4.58	119.54	110.00
10	A	304	UMQ	O5'-C1'-C2'	4.55	119.98	110.35
11	B	201	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
15	G	101	BCR	C34-C9-C10	-4.45	116.68	122.92
9	A	301	HEM	C1D-C2D-C3D	-4.41	103.93	107.00
10	A	305	UMQ	O2'-C2'-C1'	4.41	120.76	110.05
10	A	305	UMQ	O5'-C1'-O1'	4.31	120.19	109.97
10	A	304	UMQ	O2'-C2'-C1'	4.28	120.43	110.05
12	B	202	OPC	OAN-CAO-CAP	4.27	120.71	111.50
12	B	202	OPC	CBG-NAF-CAE	4.19	119.75	108.97
10	A	306	UMQ	O2'-C2'-C1'	4.18	120.20	110.05
10	A	306	UMQ	O5'-C1'-O1'	4.10	119.68	109.97
10	A	306	UMQ	O2'-C2'-C3'	4.05	119.72	110.35
11	B	201	CLA	C3B-C4B-NB	4.05	114.45	109.21
10	A	305	UMQ	O2'-C2'-C3'	4.05	119.70	110.35
10	A	304	UMQ	O2'-C2'-C3'	4.01	119.61	110.35
11	B	201	CLA	CHD-C4C-C3C	-3.94	119.04	124.84
12	H	30	OPC	CBG-NAF-CAE	3.92	119.05	108.97
13	B	203	SQD	O6-C44-C45	-3.91	101.46	110.90
9	A	301	HEM	CAD-CBD-CGD	-3.88	106.16	112.67
10	A	305	UMQ	O5'-C1'-C2'	3.82	118.44	110.35
10	A	304	UMQ	CA-O1'-C1'	3.80	120.14	113.84
10	A	304	UMQ	O5'-C1'-O1'	3.73	118.81	109.97
13	B	203	SQD	O6-C1-C2	3.67	114.04	108.30
12	B	202	OPC	CAR-CAQ-CAP	3.46	125.62	113.19
10	A	306	UMQ	C1-O5-C5	3.33	120.23	113.69
12	H	30	OPC	OAN-CAO-CAP	3.33	118.68	111.50
13	B	203	SQD	O8-S-O7	3.31	119.37	111.27
9	A	302	HEM	C1D-C2D-C3D	-3.26	104.73	107.00
12	H	30	OPC	CAH-CAG-NAF	3.24	126.61	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	101	BCR	C38-C26-C27	3.19	119.74	113.62
11	B	201	CLA	CMB-C2B-C3B	3.13	130.54	124.68
9	C	301	HEM	C1D-C2D-C3D	-3.08	104.85	107.00
10	A	306	UMQ	O5-C5-C4	3.08	115.28	109.69
15	G	101	BCR	C27-C26-C25	-3.06	118.29	122.73
11	B	201	CLA	CAA-CBA-CGA	-3.03	104.39	113.25
11	B	201	CLA	CAC-C3C-C4C	2.96	128.65	124.81
9	C	301	HEM	CBD-CAD-C3D	-2.94	107.06	112.48
11	B	201	CLA	O2A-CGA-CBA	2.94	121.14	111.91
12	H	30	OPC	CAE-NAF-CAG	2.92	121.88	109.92
12	B	202	OPC	CBO-CBP-CBQ	2.88	126.35	113.79
11	B	201	CLA	CMC-C2C-C1C	2.88	129.42	125.04
9	A	302	HEM	CBD-CAD-C3D	-2.87	107.20	112.48
12	B	202	OPC	OBJ-CBK-CBL	2.82	120.76	111.91
9	C	301	HEM	CAD-CBD-CGD	-2.80	107.97	112.67
9	A	303	HEM	CBA-CAA-C2A	-2.80	107.32	112.49
11	B	201	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
12	H	30	OPC	OAI-CAH-CAG	2.78	123.78	109.16
12	H	30	OPC	OBJ-CBK-CBL	2.77	120.61	111.91
13	B	203	SQD	O48-C23-C24	2.72	120.43	111.91
10	A	306	UMQ	O5'-C5'-C4'	2.71	115.47	109.75
12	H	30	OPC	CBP-CBQ-CBR	2.69	127.83	112.43
12	H	30	OPC	CBO-CBP-CBQ	2.67	125.44	113.79
11	B	201	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
11	B	201	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
13	B	203	SQD	O5-C1-C2	-2.60	104.86	110.35
12	B	202	OPC	CBP-CBQ-CBR	2.54	126.98	112.43
12	B	202	OPC	CBU-CBT-CBS	2.51	126.83	112.43
15	G	101	BCR	C30-C25-C24	2.49	122.83	115.78
9	A	301	HEM	CMA-C3A-C4A	-2.47	124.66	128.46
9	A	302	HEM	CMA-C3A-C4A	-2.45	124.69	128.46
15	G	101	BCR	C32-C1-C6	-2.44	106.35	110.30
12	B	202	OPC	CAE-NAF-CAG	2.42	119.82	109.92
12	H	30	OPC	CAR-CAS-CAT	2.41	126.66	114.42
9	A	303	HEM	CAA-CBA-CGA	-2.41	108.63	112.67
11	B	201	CLA	O1D-CGD-CBD	-2.40	119.56	124.48
12	B	202	OPC	CBG-NAF-CAG	2.40	119.73	109.92
15	G	101	BCR	C20-C21-C22	-2.36	123.95	127.31
13	B	203	SQD	C1-O5-C5	-2.36	109.06	113.69
15	G	101	BCR	C28-C27-C26	-2.33	109.92	114.08
10	A	306	UMQ	C1'-O5'-C5'	2.32	118.25	113.69
15	G	101	BCR	C38-C26-C25	-2.31	121.94	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	202	OPC	CAM-OAN-CAO	-2.31	112.11	117.79
11	B	201	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
12	H	30	OPC	OBJ-CBK-OCC	-2.25	117.91	123.59
11	B	201	CLA	C4D-C3D-CAD	2.23	109.71	108.47
13	B	203	SQD	O47-C7-O49	-2.23	118.32	123.70
9	A	301	HEM	C4A-C3A-C2A	2.22	108.54	107.00
12	H	30	OPC	CAQ-CAR-CAS	2.22	125.70	114.42
9	C	301	HEM	CMA-C3A-C4A	-2.19	125.10	128.46
12	B	202	OPC	OAN-CAO-OAD	-2.17	118.45	123.70
9	A	303	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
15	G	101	BCR	C11-C10-C9	2.10	130.30	127.31
12	H	30	OPC	CBU-CBT-CBS	2.09	124.42	112.43
10	A	304	UMQ	C1'-O5'-C5'	-2.09	109.59	113.69
12	H	30	OPC	CBG-NAF-CAG	2.06	118.36	109.92
11	B	201	CLA	OBD-CAD-C3D	-2.05	124.57	127.98
13	B	203	SQD	C1-C2-C3	-2.05	105.72	110.00
13	B	203	SQD	C45-O47-C7	-2.01	112.83	117.79

All (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'
10	A	304	UMQ	C1'
11	B	201	CLA	C8
11	B	201	CLA	NC
11	B	201	CLA	ND
11	B	201	CLA	NA

All (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
12	H	30	OPC	CAM-CAL-OAK-PAJ
12	H	30	OPC	NAF-CAG-CAH-OAI

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Mol	Chain	Res	Type	Atoms
12	H	30	OPC	CBO-CBP-CBQ-CBR
9	A	303	HEM	C2D-C3D-CAD-CBD
9	A	303	HEM	C4D-C3D-CAD-CBD
12	B	202	OPC	NAF-CAG-CAH-OAI
12	B	202	OPC	CBO-CBP-CBQ-CBR
10	A	304	UMQ	C2'-C1'-O1'-CA
11	B	201	CLA	C1A-C2A-CAA-CBA
11	B	201	CLA	C3A-C2A-CAA-CBA
11	B	201	CLA	O2A-C1-C2-C3
15	G	101	BCR	C1-C6-C7-C8
15	G	101	BCR	C5-C6-C7-C8
15	G	101	BCR	C22-C23-C24-C25
12	H	30	OPC	OAD-CAO-OAN-CAM
12	H	30	OPC	CAP-CAO-OAN-CAM
12	H	30	OPC	CBB-CBC-CBD-CBE
12	H	30	OPC	CAQ-CAR-CAS-CAT
10	A	304	UMQ	O5-C5-C6-O6
10	A	305	UMQ	O5-C5-C6-O6
10	A	306	UMQ	O5'-C5'-C6'-O6'
10	A	304	UMQ	O5'-C5'-C6'-O6'
10	A	305	UMQ	O5'-C5'-C6'-O6'
10	A	305	UMQ	C4'-C5'-C6'-O6'
13	B	203	SQD	C24-C23-O48-C46
12	H	30	OPC	CBL-CBK-OBJ-CBI
10	A	306	UMQ	C4'-C5'-C6'-O6'
10	A	305	UMQ	C4-C5-C6-O6
10	A	304	UMQ	C4-C5-C6-O6
13	B	203	SQD	C7-C8-C9-C10
15	G	101	BCR	C37-C22-C23-C24
15	G	101	BCR	C21-C22-C23-C24
12	B	202	OPC	CAP-CAO-OAN-CAM
13	B	203	SQD	O10-C23-O48-C46
12	H	30	OPC	OCC-CBK-OBJ-CBI
10	A	304	UMQ	C4'-C5'-C6'-O6'
13	B	203	SQD	C23-C24-C25-C26
12	B	202	OPC	CBK-CBL-CBM-CBN
11	B	201	CLA	C8-C10-C11-C12
11	B	201	CLA	C10-C11-C12-C13
12	H	30	OPC	CAL-OAK-PAJ-OAI
12	B	202	OPC	CAL-OAK-PAJ-OAI
12	B	202	OPC	OAD-CAO-OAN-CAM
12	B	202	OPC	CAH-CAG-NAF-CBG

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Mol	Chain	Res	Type	Atoms
10	A	304	UMQ	CF-CG-CH-CI
13	B	203	SQD	C30-C31-C32-C33
13	B	203	SQD	C28-C29-C30-C31
10	A	306	UMQ	CH-CI-CJ-CK
13	B	203	SQD	C9-C10-C11-C12
12	B	202	OPC	CAR-CAS-CAT-CAU
12	H	30	OPC	CBX-CBY-CBZ-CCA
12	B	202	OPC	CBV-CBW-CBX-CBY
10	A	306	UMQ	C2'-C1'-O1'-CA
10	A	305	UMQ	CH-CI-CJ-CK
12	H	30	OPC	CBV-CBW-CBX-CBY
12	H	30	OPC	CAZ-CBA-CBB-CBC
10	A	305	UMQ	CG-CH-CI-CJ
13	B	203	SQD	C24-C25-C26-C27
12	H	30	OPC	CAH-CAG-NAF-CAA
10	A	305	UMQ	O5'-C1'-O1'-CA
11	B	201	CLA	C13-C15-C16-C17
13	B	203	SQD	C11-C12-C13-C14
12	H	30	OPC	CAY-CAZ-CBA-CBB
10	A	306	UMQ	CF-CG-CH-CI
10	A	304	UMQ	CD-CF-CG-CH
13	B	203	SQD	C27-C28-C29-C30
10	A	304	UMQ	CA-CB-CC-CD
12	B	202	OPC	CBW-CBX-CBY-CBZ
15	G	101	BCR	C23-C24-C25-C30
10	A	305	UMQ	CA-CB-CC-CD
12	B	202	OPC	CAY-CAZ-CBA-CBB
12	H	30	OPC	CBS-CBT-CBU-CBV
12	B	202	OPC	CAS-CAT-CAU-CAV
13	B	203	SQD	C33-C34-C35-C36
10	A	305	UMQ	O1'-CA-CB-CC
10	A	304	UMQ	CG-CH-CI-CJ
12	B	202	OPC	CBT-CBU-CBV-CBW
13	B	203	SQD	C31-C32-C33-C34
12	H	30	OPC	CBU-CBV-CBW-CBX
13	B	203	SQD	C44-C45-C46-O48
12	H	30	OPC	CBY-CBZ-CCA-CCB
10	A	304	UMQ	CI-CJ-CK-CL
12	H	30	OPC	CBW-CBX-CBY-CBZ
13	B	203	SQD	C12-C13-C14-C15
13	B	203	SQD	C14-C15-C16-C17
11	B	201	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	B	201	CLA	C2-C3-C5-C6
12	H	30	OPC	CBM-CBN-CBO-CBP
13	B	203	SQD	C25-C26-C27-C28
10	A	304	UMQ	CB-CA-O1'-C1'
13	B	203	SQD	C13-C14-C15-C16
12	B	202	OPC	CBL-CBM-CBN-CBO
13	B	203	SQD	O6-C44-C45-O47
15	G	101	BCR	C23-C24-C25-C26
10	A	304	UMQ	CB-CC-CD-CF
13	B	203	SQD	C16-C17-C18-C19
10	A	304	UMQ	CC-CD-CF-CG
10	A	305	UMQ	CD-CF-CG-CH
15	G	101	BCR	C6-C7-C8-C9
13	B	203	SQD	O6-C44-C45-C46
10	A	305	UMQ	CF-CG-CH-CI
10	A	305	UMQ	C2'-C1'-O1'-CA
12	B	202	OPC	CBC-CBD-CBE-CBF
12	H	30	OPC	CAL-OAK-PAJ-OAB
12	B	202	OPC	CAL-OAK-PAJ-OAB
10	A	306	UMQ	O5'-C1'-O1'-CA
12	H	30	OPC	OAK-CAL-CAM-CBI
12	H	30	OPC	OAK-CAL-CAM-OAN
12	H	30	OPC	CBP-CBQ-CBR-CBS
12	B	202	OPC	CBP-CBQ-CBR-CBS
13	B	203	SQD	C29-C30-C31-C32
11	B	201	CLA	C2A-CAA-CBA-CGA
10	A	306	UMQ	CI-CJ-CK-CL
12	H	30	OPC	CAH-OAI-PAJ-OAK
12	B	202	OPC	CAZ-CBA-CBB-CBC
11	B	201	CLA	C11-C12-C13-C15
9	A	301	HEM	C2A-CAA-CBA-CGA
12	H	30	OPC	CAR-CAS-CAT-CAU
15	G	101	BCR	C11-C10-C9-C34
11	B	201	CLA	C6-C7-C8-C10
12	H	30	OPC	CBC-CBD-CBE-CBF
12	H	30	OPC	CAH-CAG-NAF-CBG
15	G	101	BCR	C11-C10-C9-C8
10	A	305	UMQ	CI-CJ-CK-CL
12	H	30	OPC	OBJ-CBK-CBL-CBM
12	H	30	OPC	OAN-CAO-CAP-CAQ
12	B	202	OPC	CBM-CBN-CBO-CBP
12	B	202	OPC	OAN-CAO-CAP-CAQ

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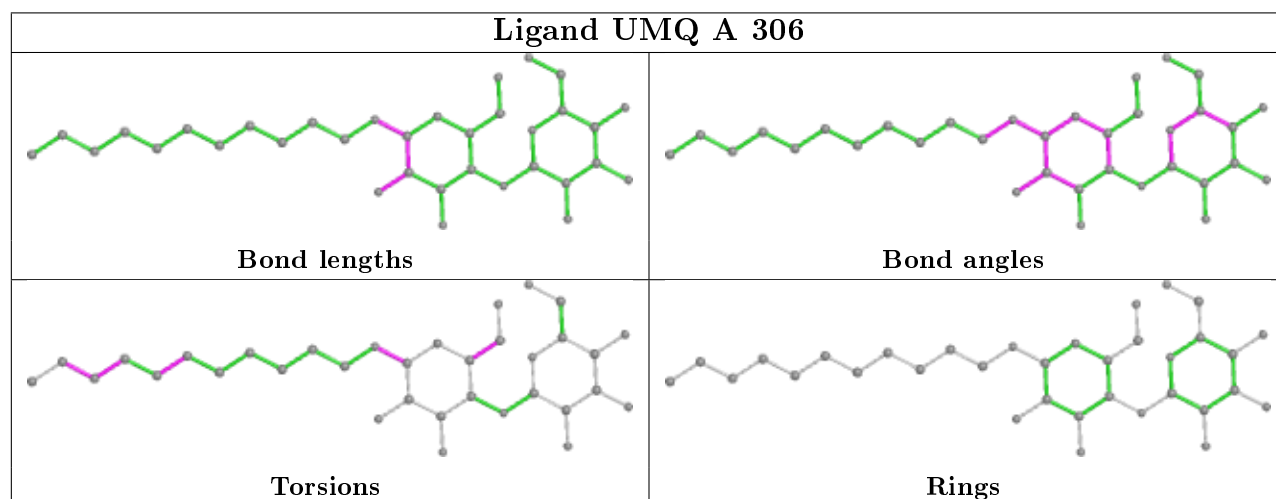
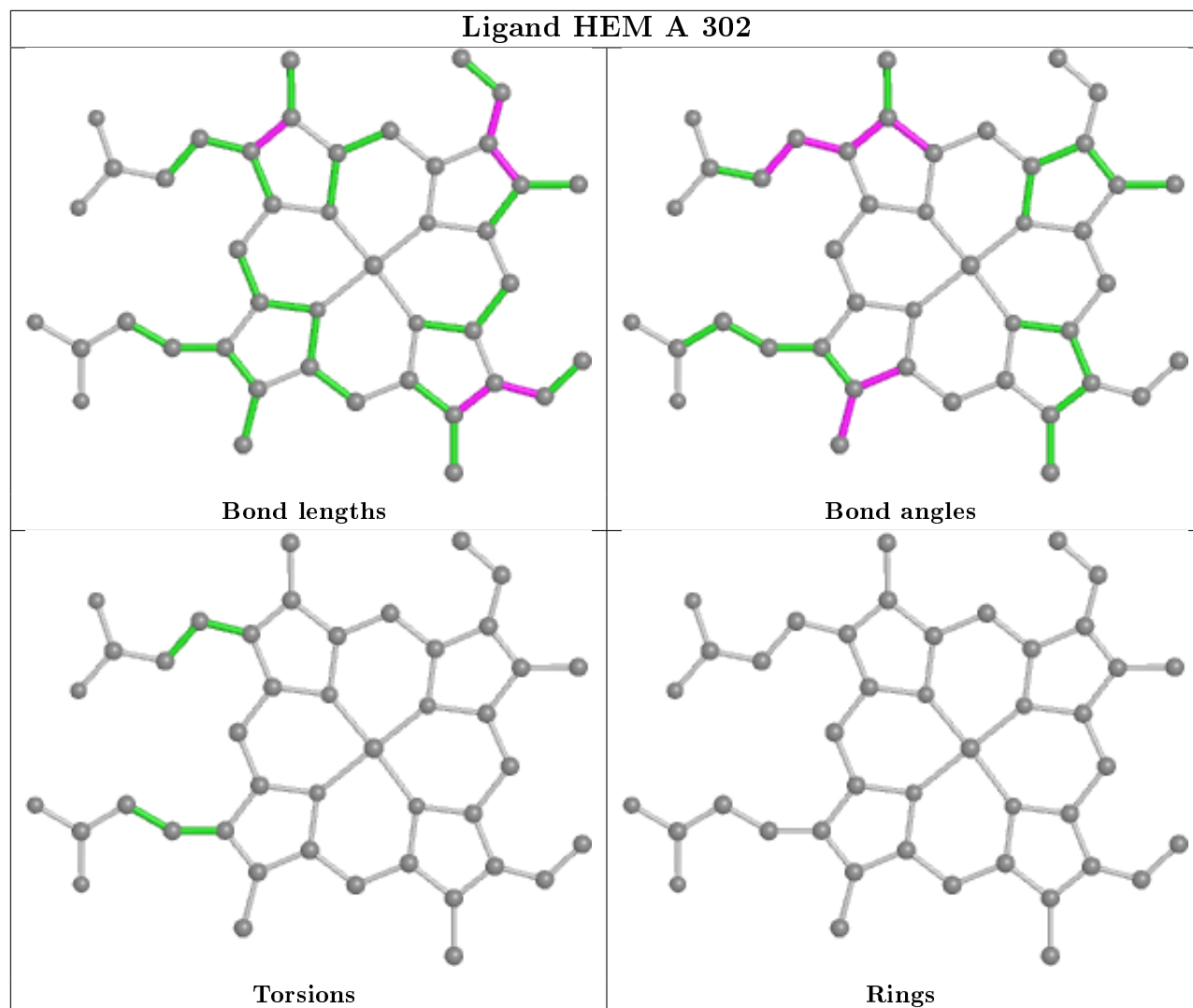
Mol	Chain	Res	Type	Atoms
13	B	203	SQD	O48-C23-C24-C25
12	B	202	OPC	CBR-CBS-CBT-CBU
12	B	202	OPC	OAD-CAO-CAP-CAQ
12	H	30	OPC	OAD-CAO-CAP-CAQ
13	B	203	SQD	O10-C23-C24-C25
12	H	30	OPC	OCC-CBK-CBL-CBM
13	B	203	SQD	C17-C18-C19-C20
13	B	203	SQD	C35-C36-C37-C38
12	H	30	OPC	CBR-CBS-CBT-CBU
12	H	30	OPC	CAH-OAI-PAJ-OAB
12	H	30	OPC	CAH-CAG-NAF-CAE
11	B	201	CLA	C6-C7-C8-C9
11	B	201	CLA	C11-C12-C13-C14

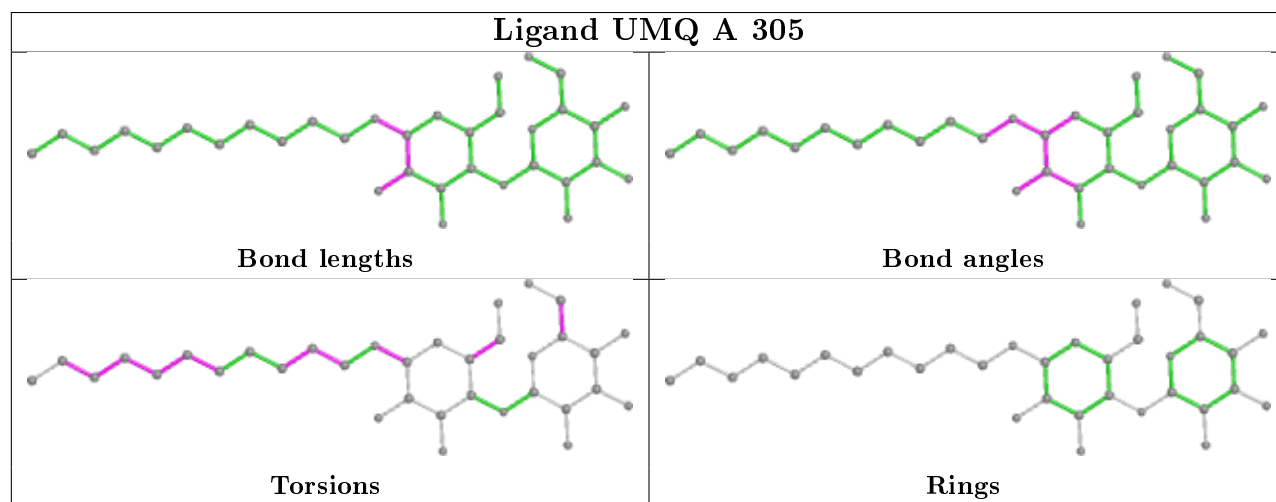
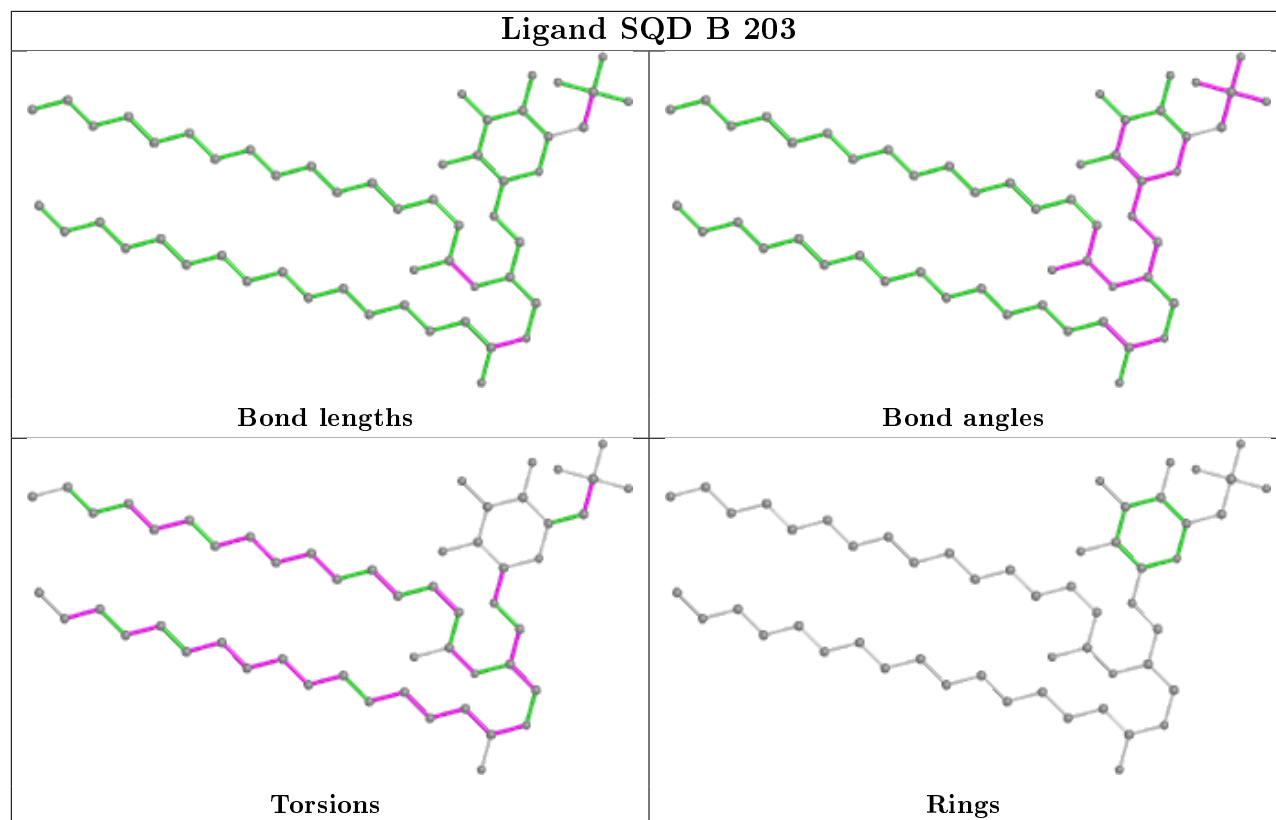
There are no ring outliers.

11 monomers are involved in 31 short contacts:

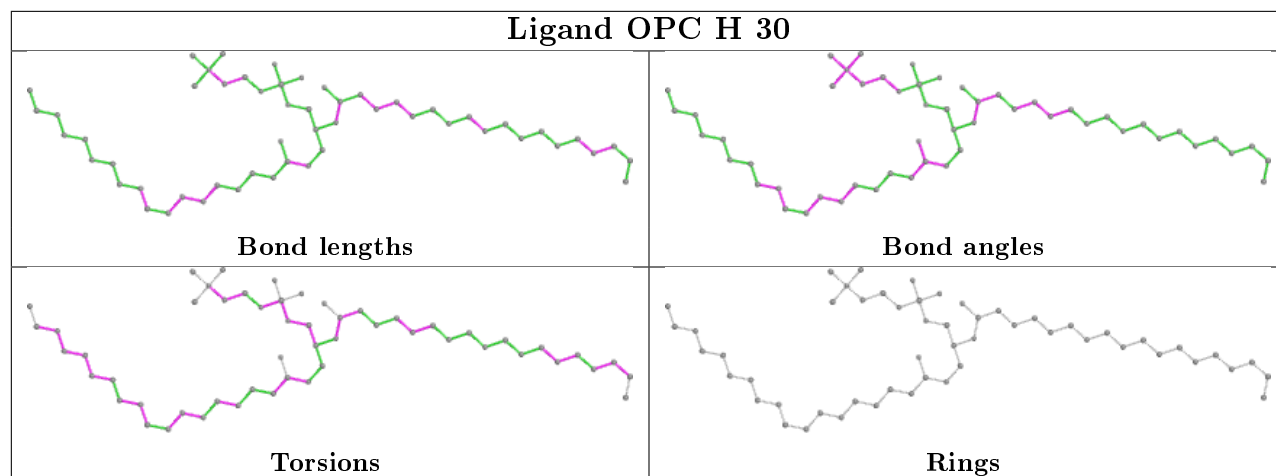
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	306	UMQ	2	0
13	B	203	SQD	1	0
14	D	200	FES	1	0
10	A	305	UMQ	1	0
12	H	30	OPC	4	0
9	A	303	HEM	6	0
10	A	304	UMQ	1	0
11	B	201	CLA	1	0
9	A	301	HEM	2	0
9	C	301	HEM	6	0
15	G	101	BCR	7	0

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.

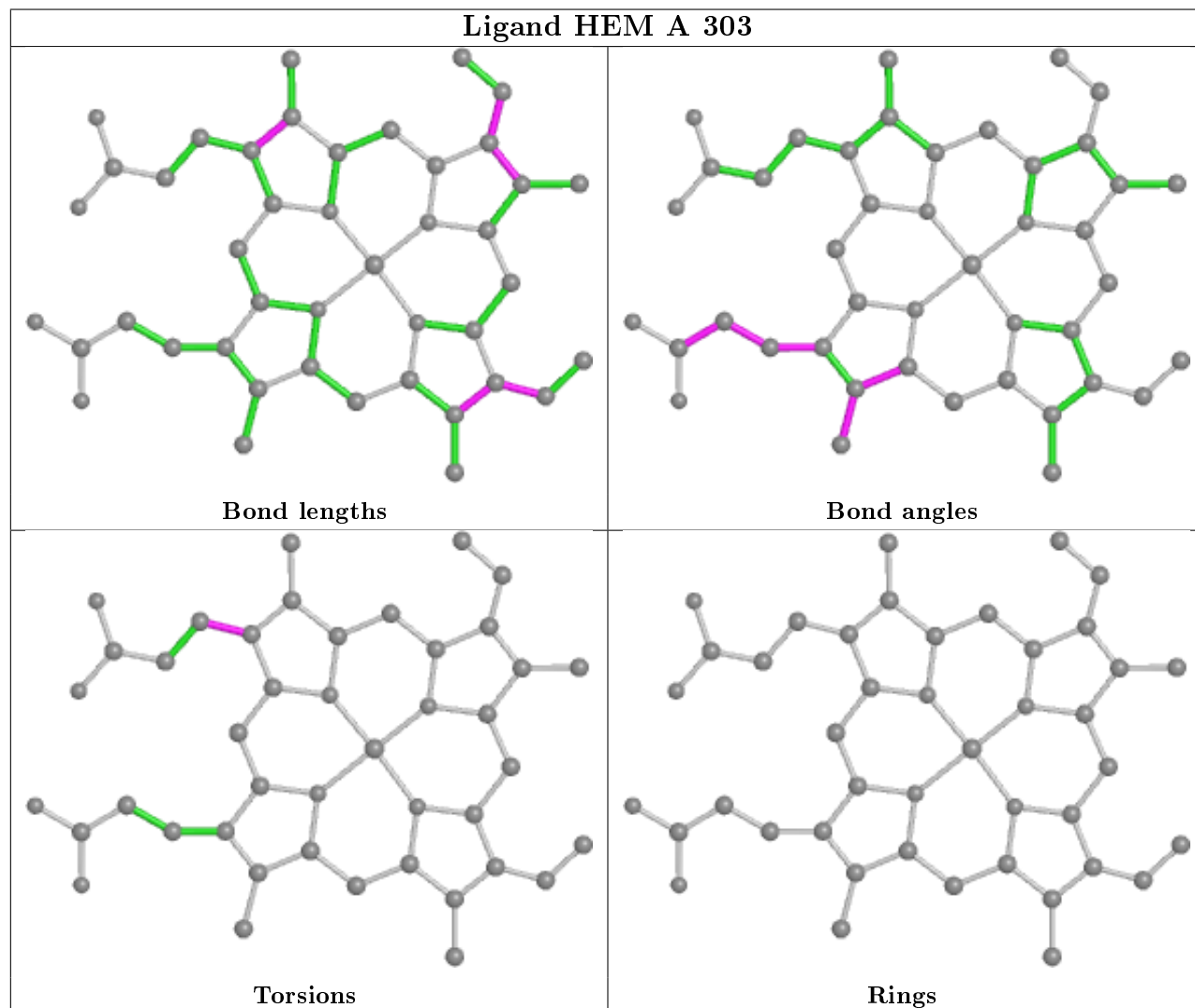


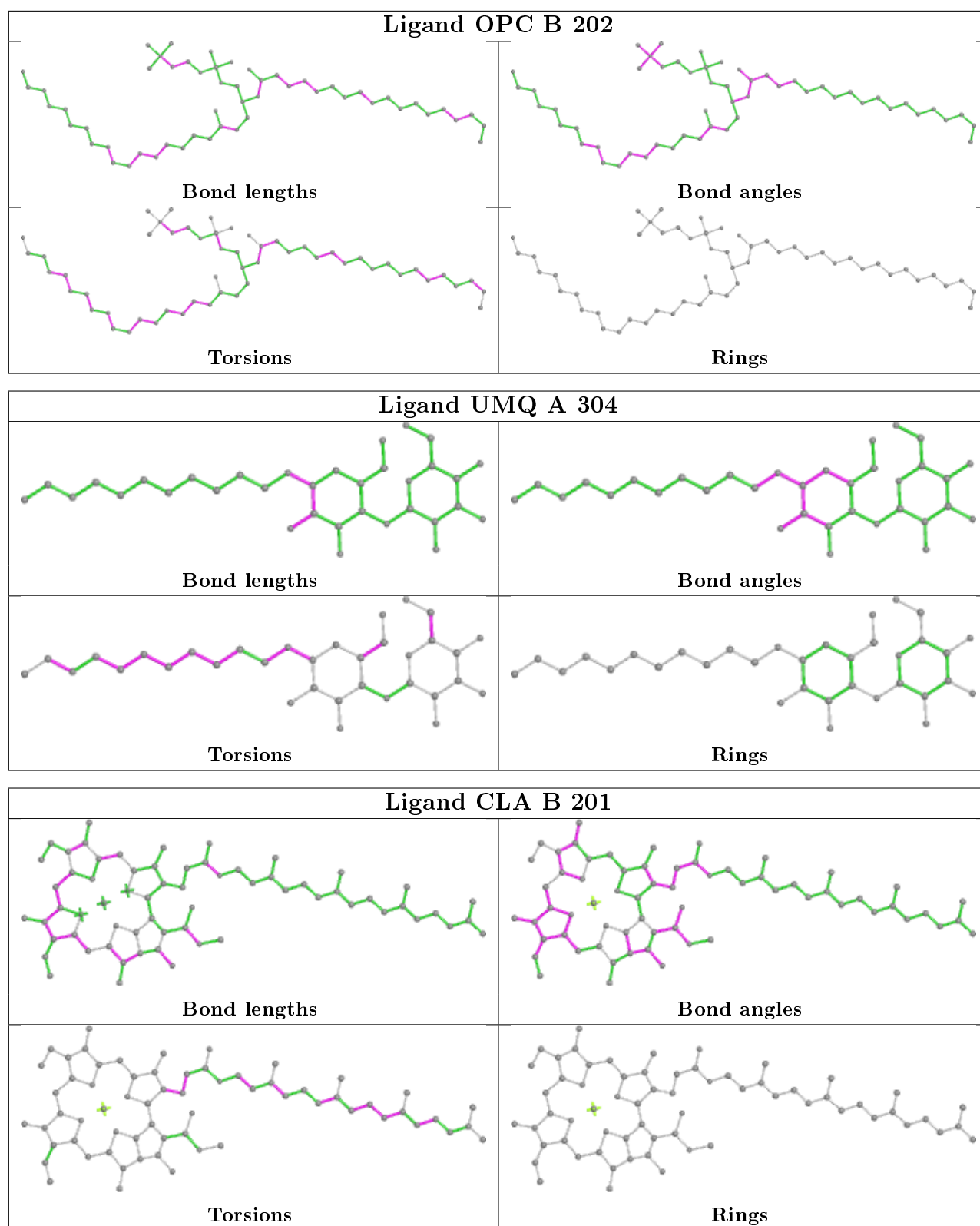


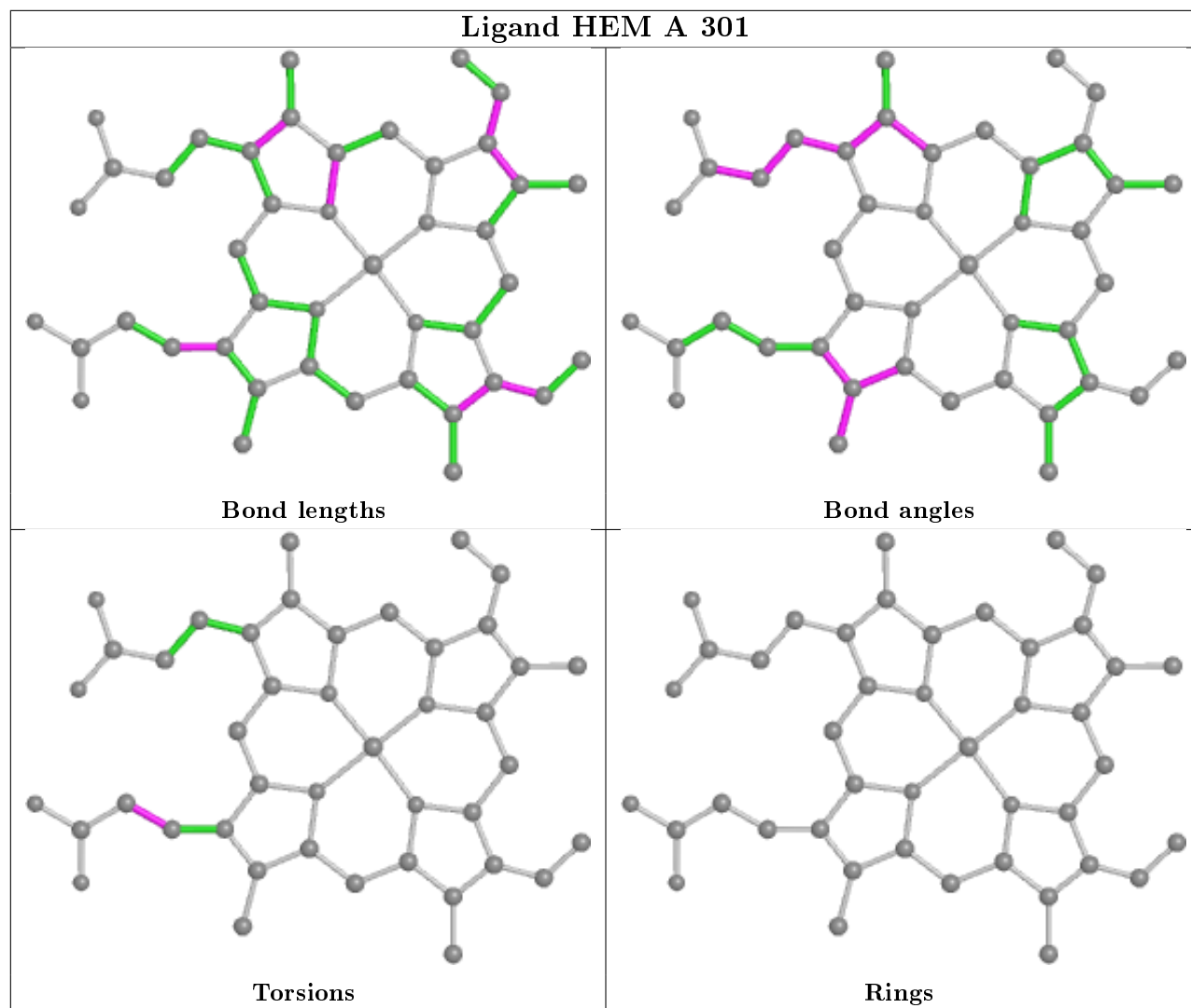
## Ligand OPC H 30

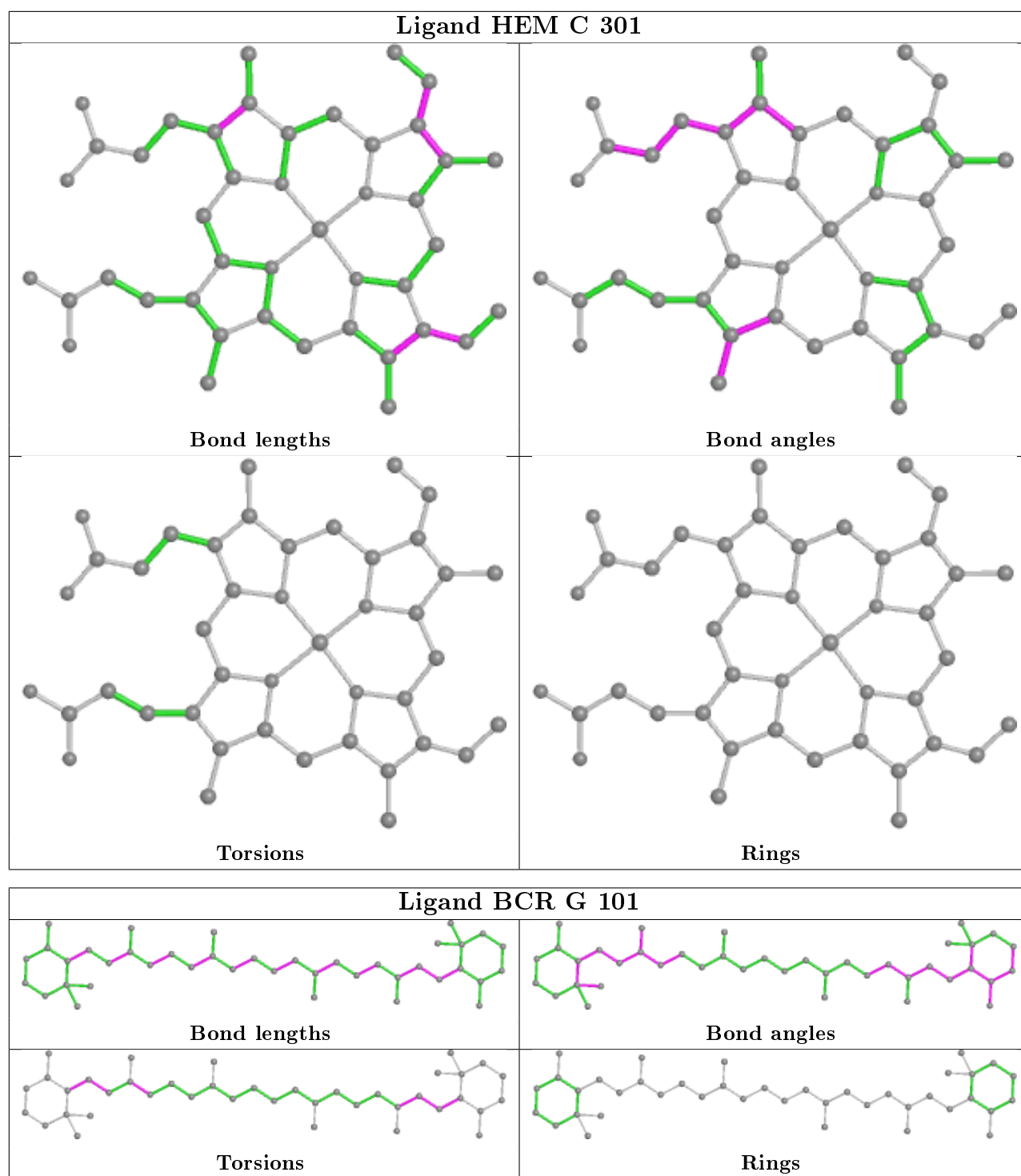


## Ligand HEM A 303









## 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, 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%)	-0.39	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

All (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
3	C	224	ALA	6.3
4	D	157	ASN	5.6
4	D	73	HIS	5.5
3	C	184	ALA	5.1
4	D	69	PHE	5.0
3	C	186	GLN	4.8
4	D	72	SER	4.8
4	D	49	GLY	4.7
4	D	50	ALA	4.7
4	D	56	ALA	4.6
3	C	194	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	160	PHE	4.6
3	C	189	GLU	4.4
3	C	206	VAL	4.4
4	D	70	LEU	4.3
3	C	199	ILE	4.2
3	C	220	SER	4.1
4	D	175	GLU	4.1
4	D	155	THR	4.1
3	C	219	VAL	4.0
3	C	177	THR	3.9
3	C	183	ILE	3.8
3	C	181	SER	3.6
1	A	1	MET	3.6
4	D	57	LYS	3.6
3	C	179	THR	3.6
4	D	158	ASP	3.6
4	D	160	ILE	3.6
3	C	195	TYR	3.6
4	D	77	ASP	3.5
4	D	67	SER	3.4
3	C	196	LEU	3.4
3	C	178	GLY	3.4
4	D	140	VAL	3.3
3	C	207	VAL	3.3
4	D	66	VAL	3.3
3	C	188	GLY	3.3
4	D	74	ASN	3.3
4	D	64	VAL	3.3
3	C	202	GLU	3.3
3	C	227	ALA	3.2
4	D	159	LYS	3.2
4	D	48	GLY	3.1
4	D	55	THR	3.0
1	A	2	ALA	2.9
3	C	205	GLU	2.8
3	C	190	ASP	2.8
4	D	63	ASP	2.8
3	C	213	ALA	2.8
3	C	198	ASP	2.6
4	D	71	GLU	2.6
4	D	176	PRO	2.6
4	D	52	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	226	THR	2.6
4	D	17	GLN	2.6
4	D	47	ALA	2.5
4	D	154	LYS	2.4
3	C	208	SER	2.4
4	D	51	GLY	2.4
3	C	176	ALA	2.4
3	C	168	ASN	2.4
4	D	169	ASP	2.4
4	D	141	ARG	2.4
4	D	145	PRO	2.4
5	E	31	LEU	2.4
4	D	99	ILE	2.3
4	D	65	SER	2.3
4	D	168	THR	2.3
4	D	13	MET	2.3
2	B	2	ALA	2.3
3	C	187	GLU	2.3
4	D	68	LYS	2.2
3	C	193	VAL	2.1
4	D	171	ARG	2.1
4	D	16	ARG	2.1
4	D	177	TRP	2.1
3	C	212	PRO	2.1
3	C	209	ASP	2.1

## 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 ⓘ

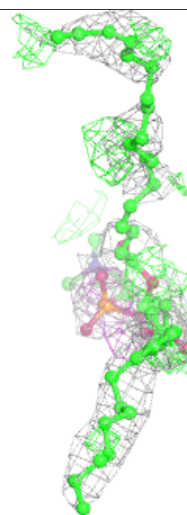
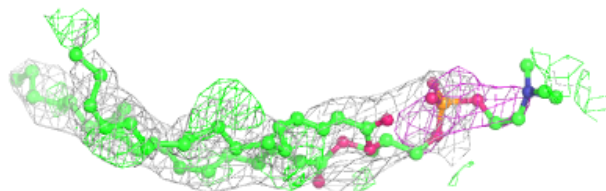
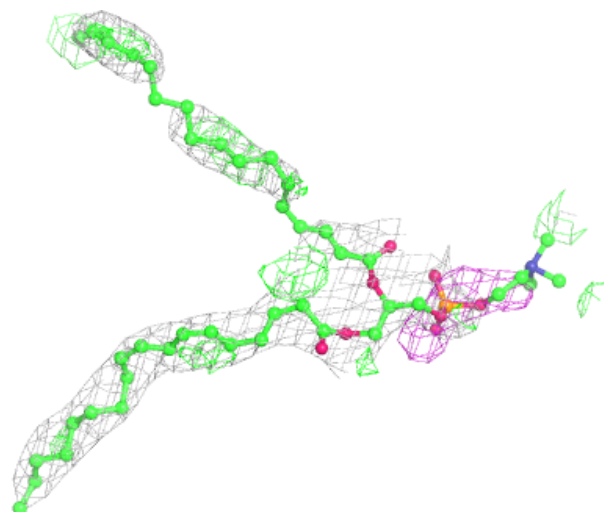
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

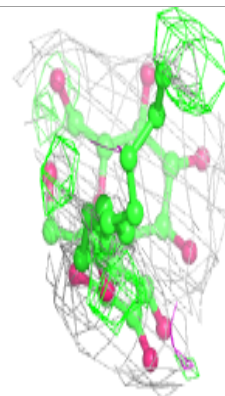
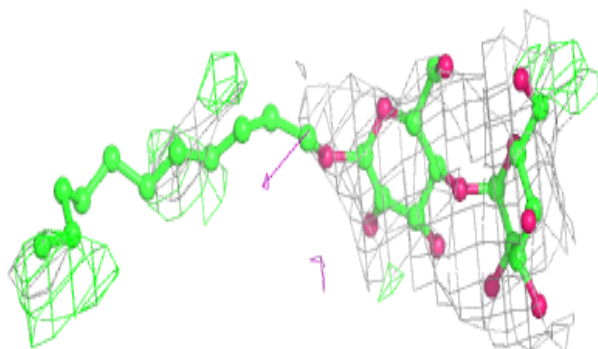
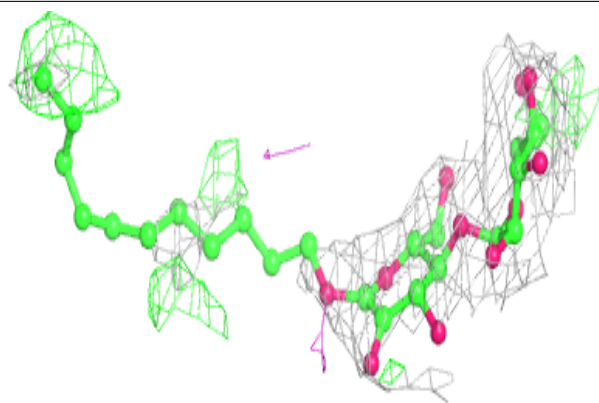
**Electron density around OPC H 30:**

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

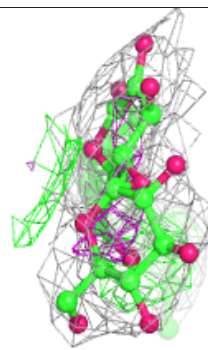
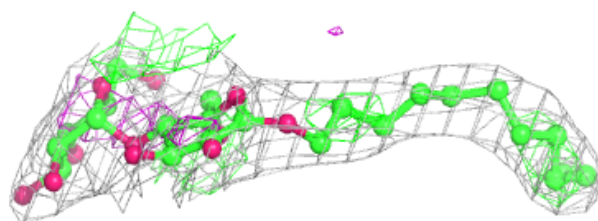
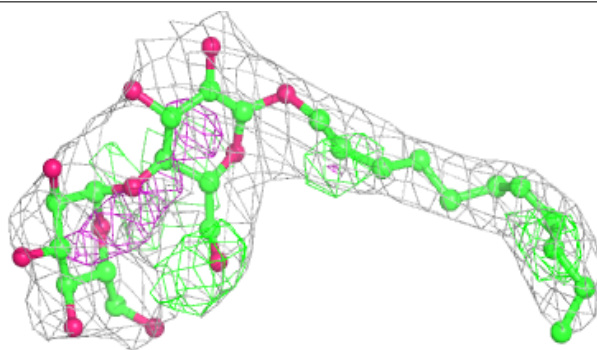


**Electron density around UMQ A 305:**

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

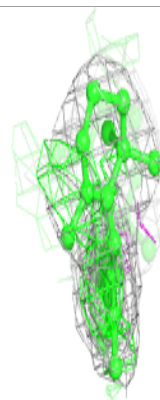
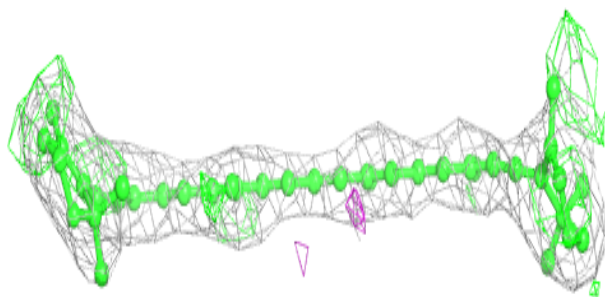
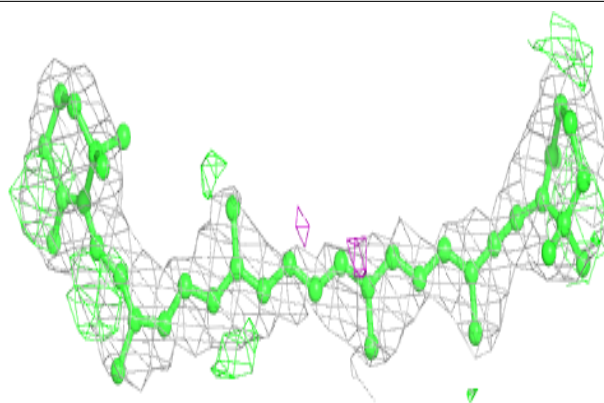
**Electron density around UMQ A 304:**

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

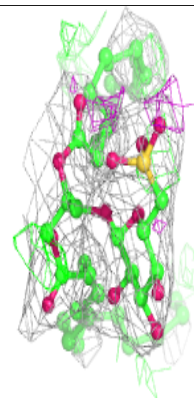
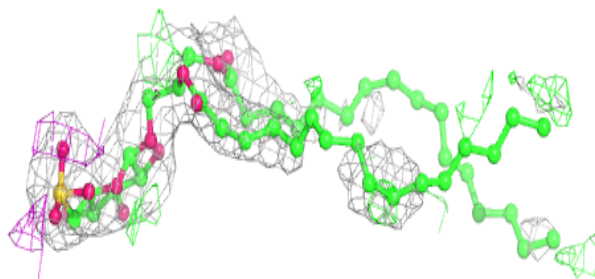
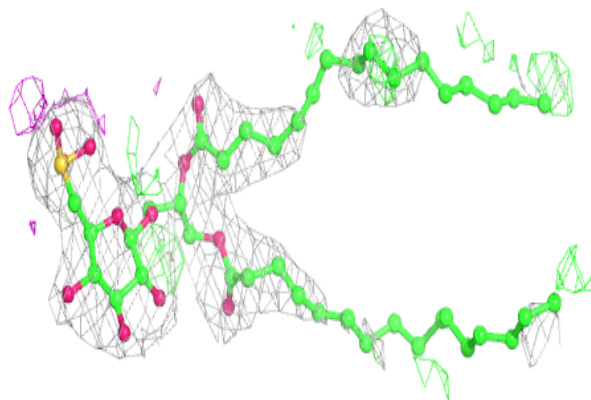


**Electron density around BCR G 101:**

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

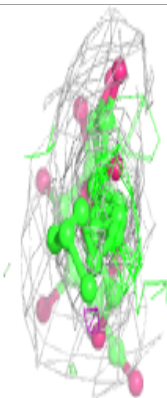
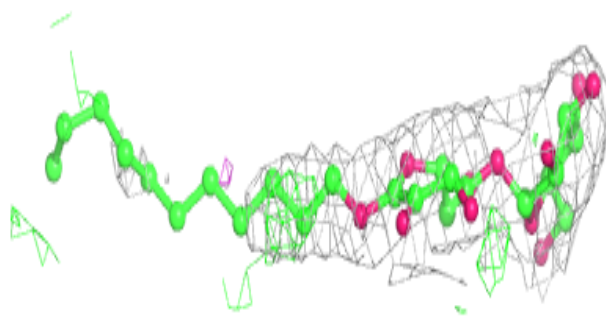
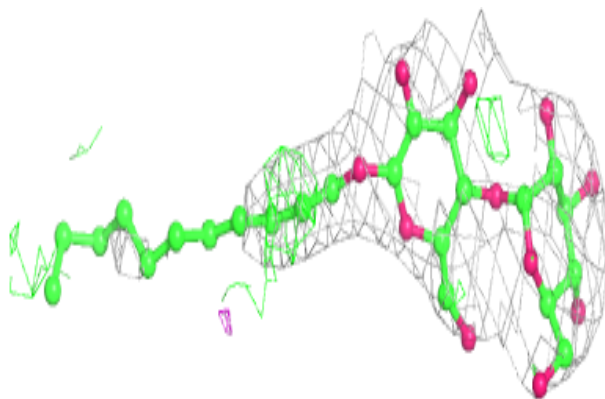
**Electron density around SQD B 203:**

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

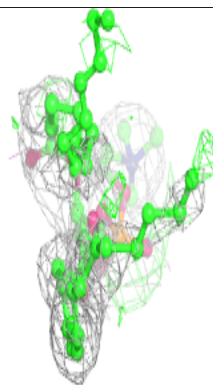
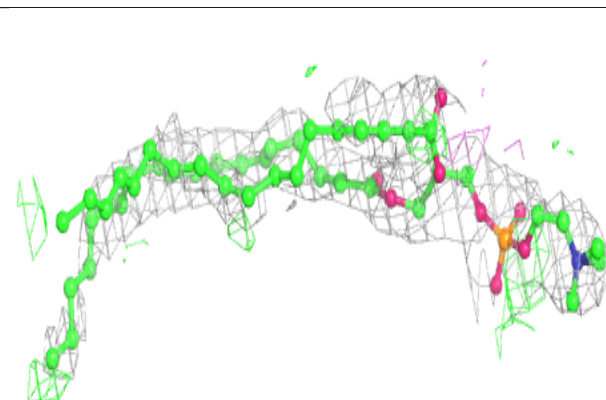
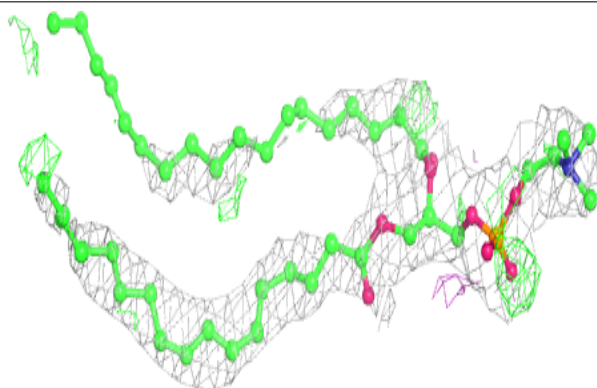


**Electron density around UMQ A 306:**

$2mF_o-DF_c$  (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:**

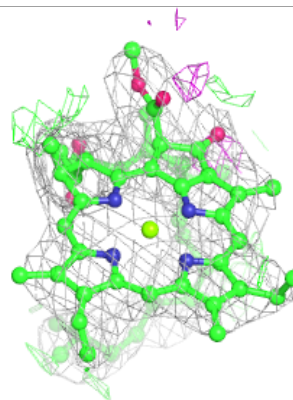
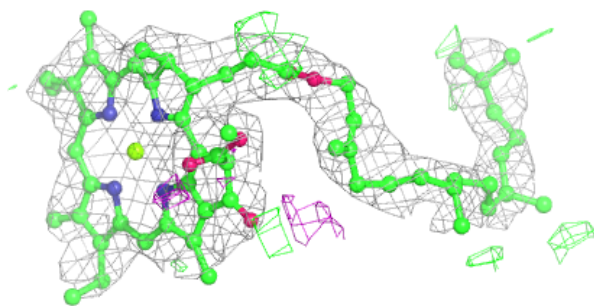
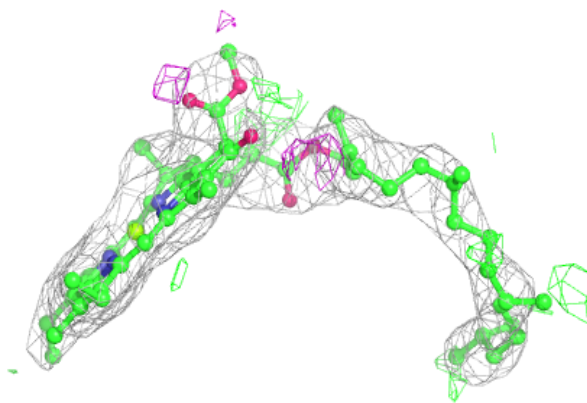
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





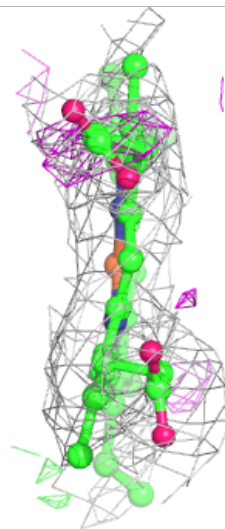
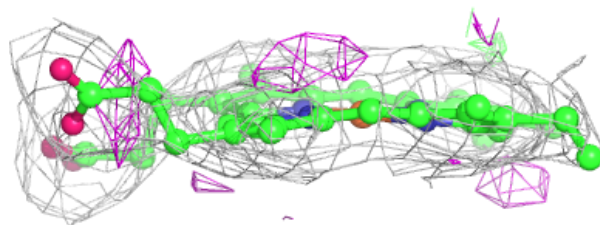
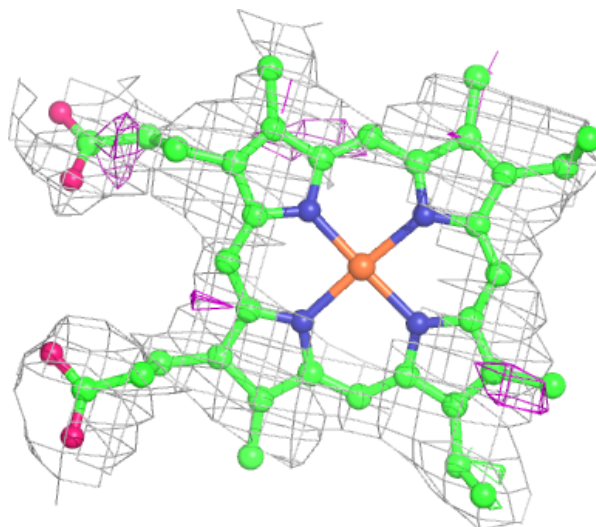
**Electron density around CLA B 201:**

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



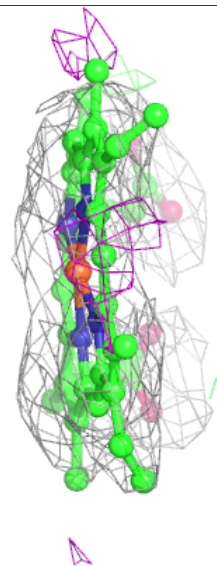
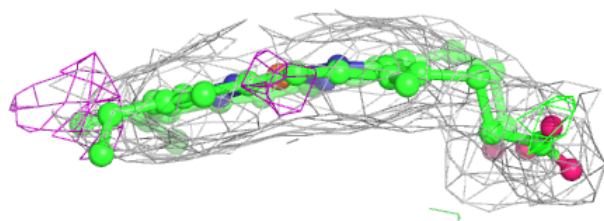
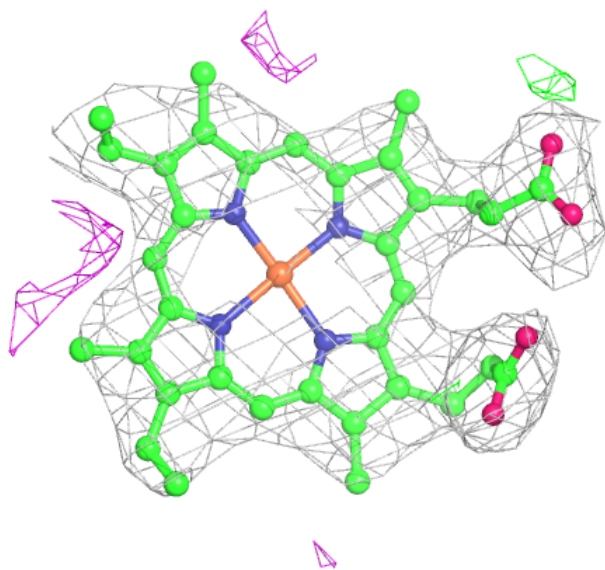
**Electron density around HEM C 301:**

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



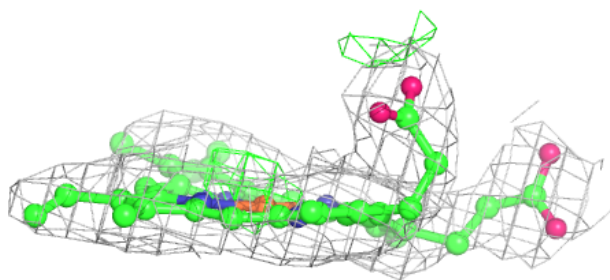
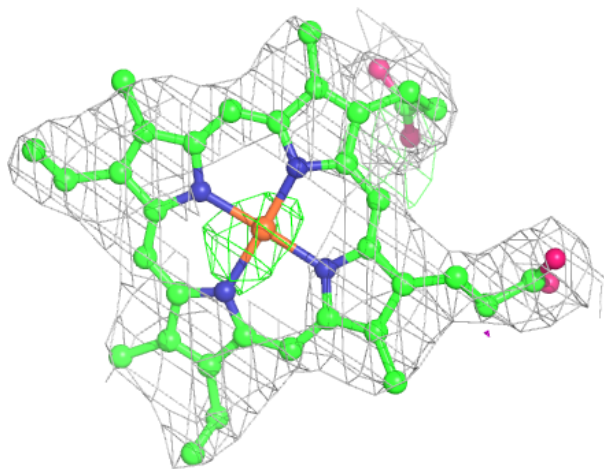
**Electron density around HEM A 303:**

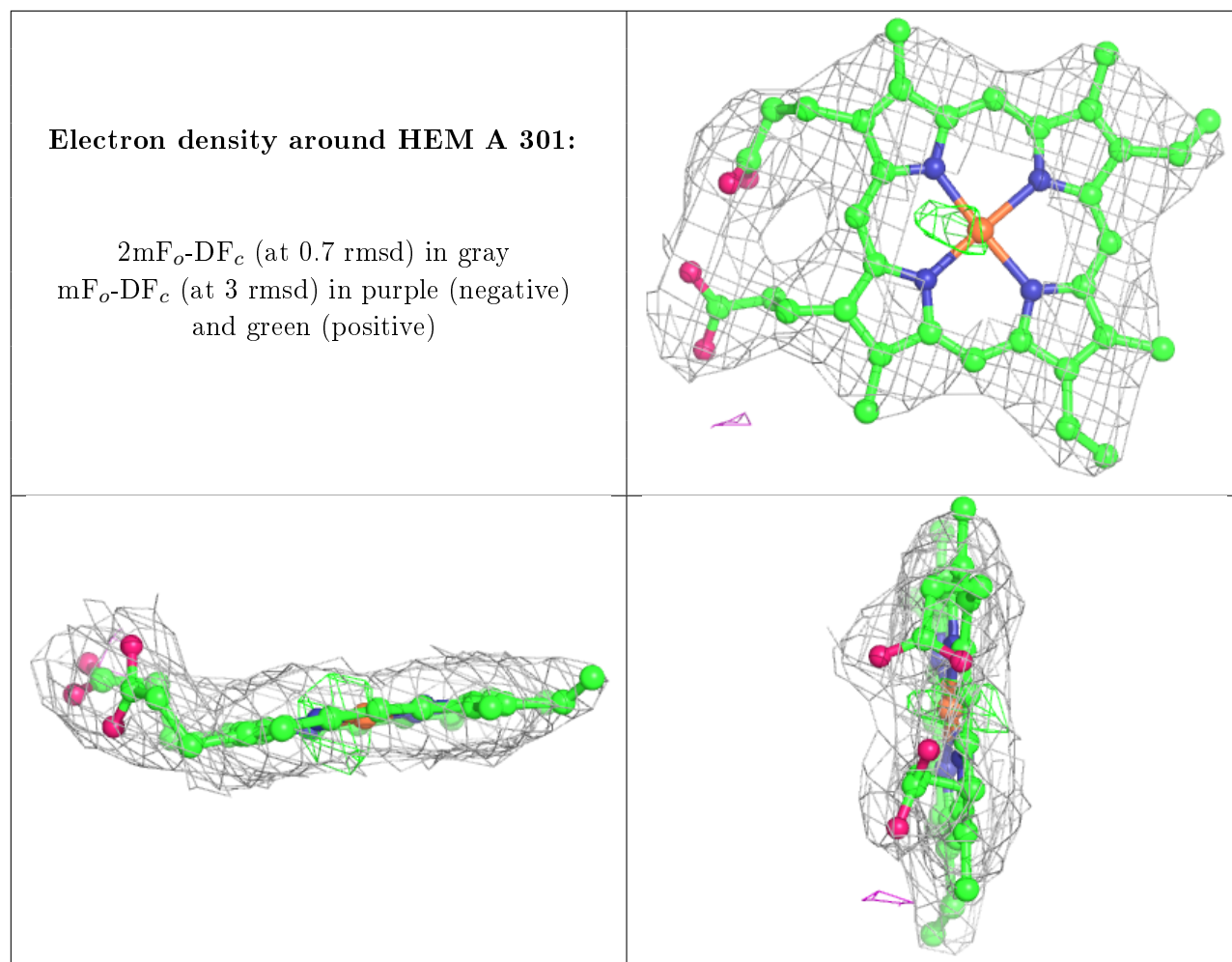
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.