



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:18 PM UTC

PDB ID : 4M09 / pdb_00004m09
Title : Crystal Structure of Mutant Chlorite Dismutase from Candidatus Nitrospira defluvii W146Y R173Q
Authors : Gysel, K.; Hagmueller, A.; Djinovic-Carugo, K.
Deposited on : 2013-08-01
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

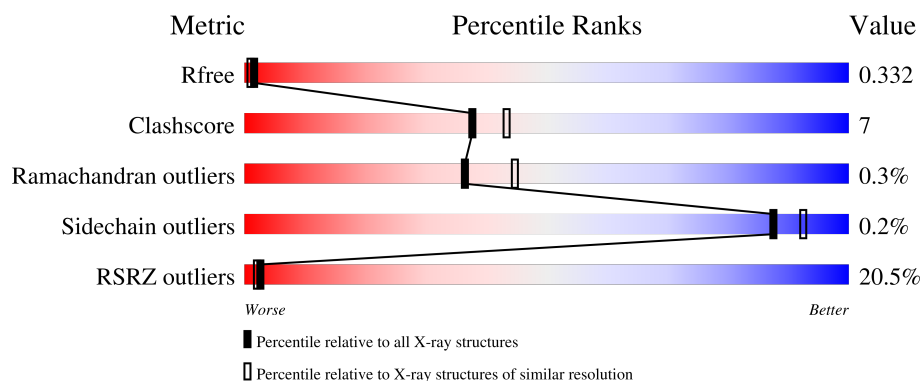
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	23% 83%16%
1	B	241	20% 79%19%
1	C	241	21% 83%15%
1	D	241	18% 84%14%
1	E	241	19% 78%20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10015 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 Chlorite dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1915	1220	332	357	6			
1	B	238	Total	C	N	O	S	0	0	0
			1915	1220	332	357	6			
1	C	236	Total	C	N	O	S	0	0	0
			1902	1213	330	353	6			
1	D	236	Total	C	N	O	S	0	0	0
			1902	1213	330	353	6			
1	E	237	Total	C	N	O	S	0	0	0
			1910	1217	331	356	6			

There are 25 discrepancies between the modelled and reference sequences:

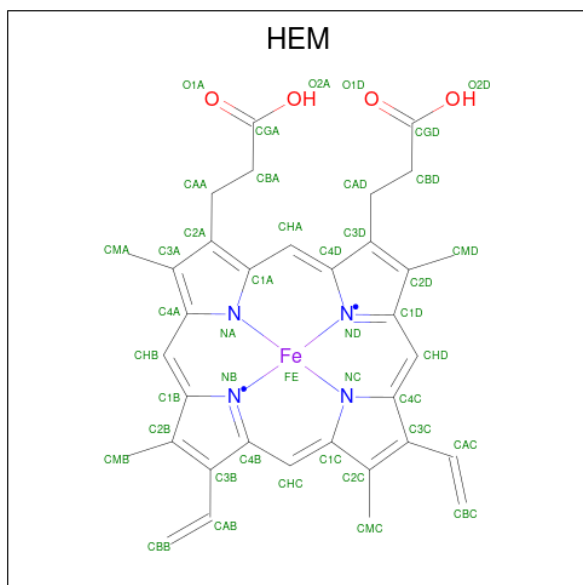
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP B3U4H7
A	-1	ALA	-	expression tag	UNP B3U4H7
A	0	MET	-	expression tag	UNP B3U4H7
A	146	TYR	TRP	engineered mutation	UNP B3U4H7
A	173	GLN	ARG	engineered mutation	UNP B3U4H7
B	-2	GLY	-	expression tag	UNP B3U4H7
B	-1	ALA	-	expression tag	UNP B3U4H7
B	0	MET	-	expression tag	UNP B3U4H7
B	146	TYR	TRP	engineered mutation	UNP B3U4H7
B	173	GLN	ARG	engineered mutation	UNP B3U4H7
C	-2	GLY	-	expression tag	UNP B3U4H7
C	-1	ALA	-	expression tag	UNP B3U4H7
C	0	MET	-	expression tag	UNP B3U4H7
C	146	TYR	TRP	engineered mutation	UNP B3U4H7
C	173	GLN	ARG	engineered mutation	UNP B3U4H7
D	-2	GLY	-	expression tag	UNP B3U4H7
D	-1	ALA	-	expression tag	UNP B3U4H7
D	0	MET	-	expression tag	UNP B3U4H7
D	146	TYR	TRP	engineered mutation	UNP B3U4H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	173	GLN	ARG	engineered mutation	UNP B3U4H7
E	-2	GLY	-	expression tag	UNP B3U4H7
E	-1	ALA	-	expression tag	UNP B3U4H7
E	0	MET	-	expression tag	UNP B3U4H7
E	146	TYR	TRP	engineered mutation	UNP B3U4H7
E	173	GLN	ARG	engineered mutation	UNP B3U4H7

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



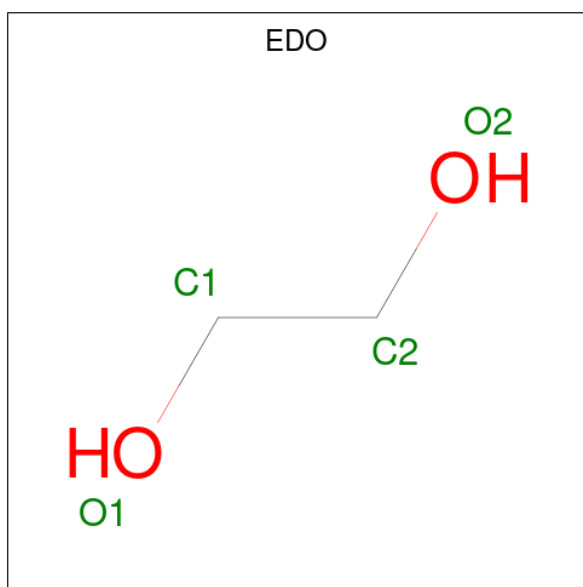
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



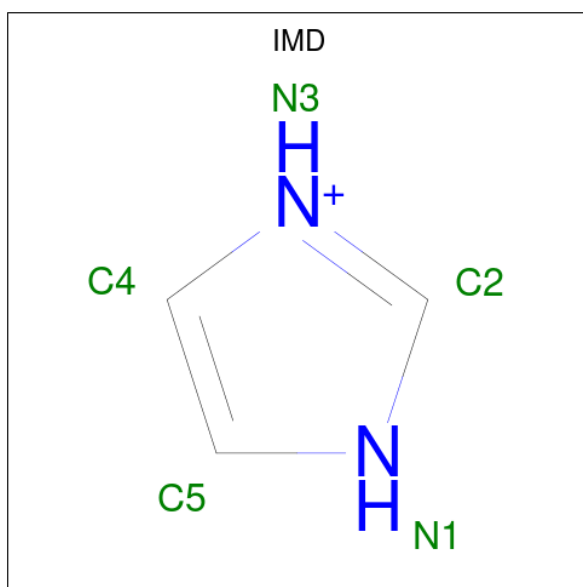
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

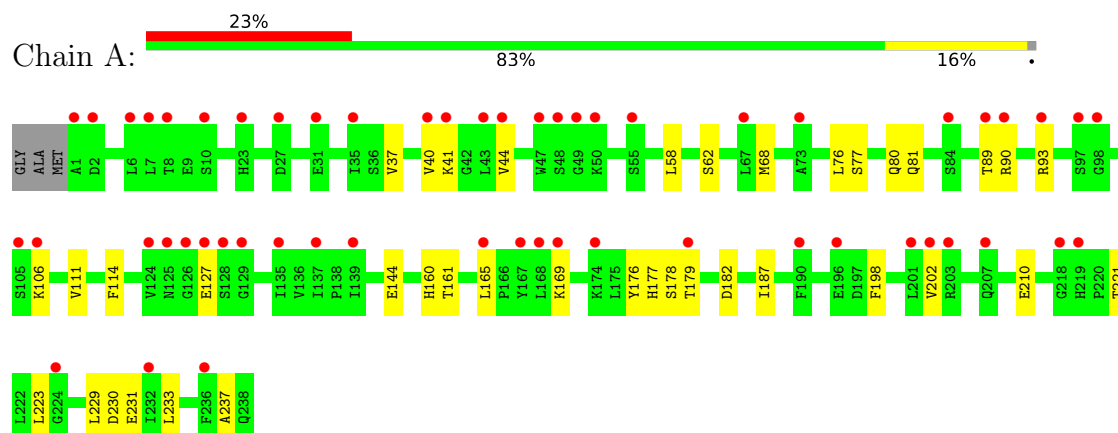
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total	O	0	0
			38	38		
6	B	38	Total	O	0	0
			38	38		
6	C	36	Total	O	0	0
			36	36		
6	D	27	Total	O	0	0
			27	27		
6	E	26	Total	O	0	0
			26	26		

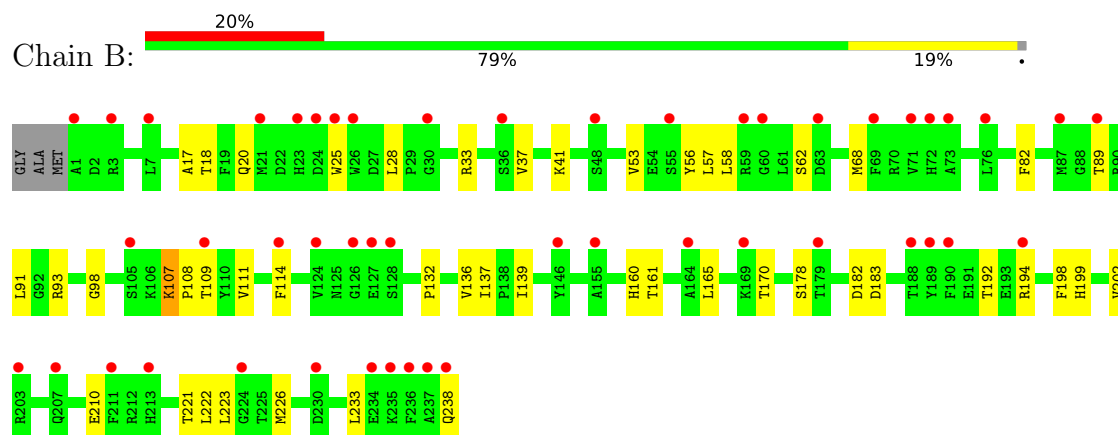
3 Residue-property plots [i](#)

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.

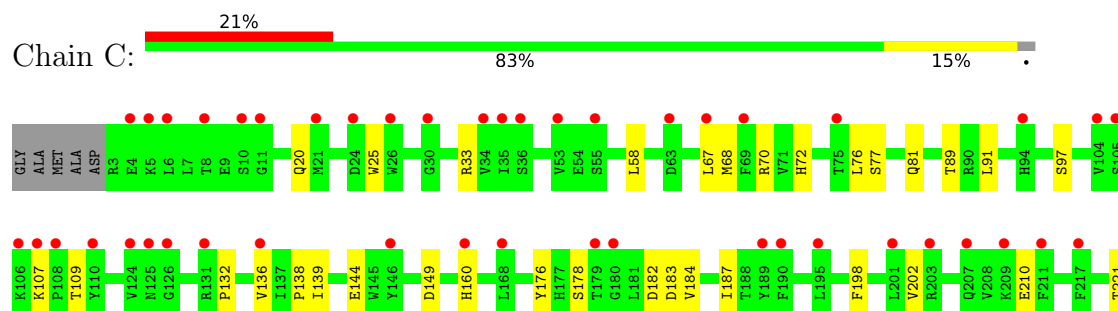
• Molecule 1: Chlorite dismutase

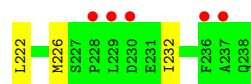


• Molecule 1: Chlorite dismutase

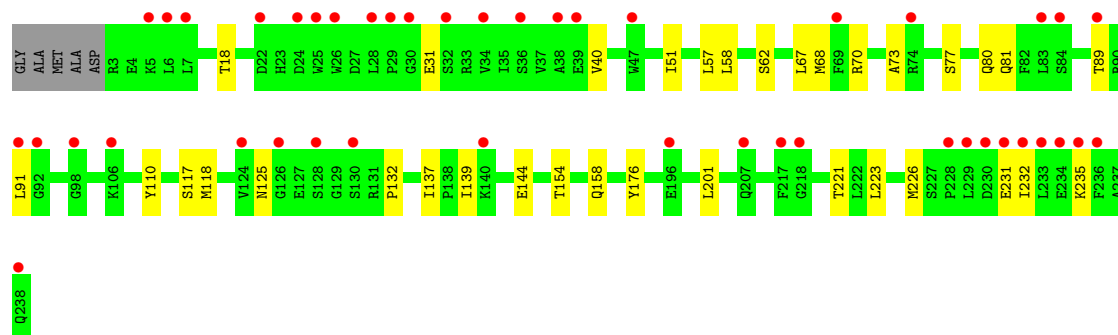
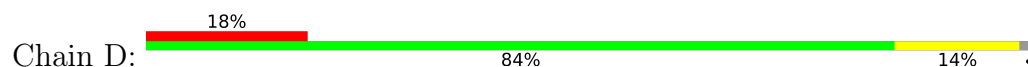


• Molecule 1: Chlorite dismutase

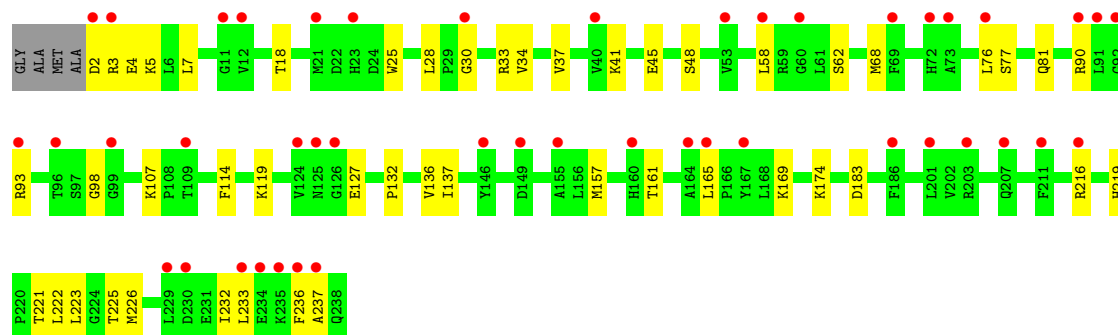
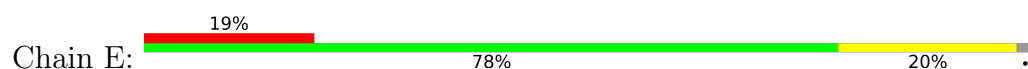




● Molecule 1: Chlorite dismutase



● Molecule 1: Chlorite dismutase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.10Å 114.98Å 118.87Å 90.00° 118.08° 90.00°	Depositor
Resolution (Å)	44.38 – 2.45 44.38 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.38-2.45) 98.3 (44.38-2.45)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.45Å)	Xtriage
Refinement program	PHENIX dev_1388	Depositor
R, R_{free}	0.277 , 0.333 0.278 , 0.332	Depositor DCC
R_{free} test set	2975 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10015	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, SO4, HEM, EDO

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	0.29	0/1960	0.73	0/2650
1	B	0.27	0/1960	0.73	2/2650 (0.1%)
1	C	0.27	0/1947	0.73	2/2632 (0.1%)
1	D	0.26	0/1947	0.68	0/2632
1	E	0.28	0/1955	0.72	3/2643 (0.1%)
All	All	0.27	0/9769	0.72	7/13207 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	LYS	CA-C-N	6.31	126.33	119.90
1	C	107	LYS	C-N-CA	6.31	126.33	119.90
1	E	107	LYS	CA-C-N	6.24	126.26	119.90
1	E	107	LYS	C-N-CA	6.24	126.26	119.90
1	B	107	LYS	CA-C-N	5.87	125.88	119.90
1	B	107	LYS	C-N-CA	5.87	125.88	119.90
1	E	4	GLU	N-CA-C	5.50	119.83	113.18

There are no chirality outliers.

There are no planarity outliers.

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	1915	0	1887	25	0
1	B	1915	0	1887	34	0
1	C	1902	0	1875	22	0
1	D	1902	0	1875	19	0
1	E	1910	0	1879	31	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
2	E	43	0	30	3	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
3	E	5	0	0	1	0
4	A	4	0	6	2	0
4	B	4	0	6	0	0
4	C	12	0	18	0	0
4	D	4	0	6	0	0
4	E	12	0	18	1	0
5	A	5	0	5	0	0
5	D	5	0	5	0	0
6	A	38	0	0	0	0
6	B	38	0	0	2	0
6	C	36	0	0	3	0
6	D	27	0	0	0	0
6	E	26	0	0	1	0
All	All	10015	0	9617	136	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 7.

All (136) 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:93:ARG:NH1	4:A:303:EDO:O1	2.14	0.81
1:E:233:LEU:HA	1:E:236:PHE:HD2	1.51	0.76
1:E:28:LEU:O	1:E:33:ARG:NH1	2.21	0.73
1:B:28:LEU:O	1:B:33:ARG:NH1	2.22	0.73
1:B:33:ARG:NH2	1:B:238:GLN:O	2.22	0.72
2:E:301:HEM:HHC	2:E:301:HEM:HBB2	1.72	0.70
2:A:301:HEM:HHC	2:A:301:HEM:HBB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ILE:HG22	1:E:236:PHE:HE2	1.61	0.66
1:A:179:THR:O	1:B:199:HIS:ND1	2.22	0.66
1:E:7:LEU:O	1:E:174:LYS:NZ	2.29	0.66
1:D:139:ILE:HD11	2:D:301:HEM:HAC	1.79	0.65
1:D:201:LEU:HD21	2:D:301:HEM:HAB	1.80	0.62
1:B:139:ILE:HD11	2:B:301:HEM:HAC	1.80	0.61
1:C:58:LEU:HD11	1:C:68:MET:HB2	1.81	0.61
1:C:97:SER:OG	6:C:413:HOH:O	2.16	0.61
1:B:58:LEU:HD11	1:B:68:MET:HB2	1.82	0.60
1:A:58:LEU:HD11	1:A:68:MET:HB2	1.84	0.60
1:B:192:THR:HG22	1:B:194:ARG:H	1.66	0.59
1:E:30:GLY:H	4:E:302:EDO:H12	1.66	0.59
2:D:301:HEM:HBC2	2:D:301:HEM:HMC1	1.84	0.59
1:A:160:HIS:ND1	1:A:210:GLU:OE1	2.36	0.58
1:D:132:PRO:HD2	1:D:226:MET:HB3	1.85	0.58
1:B:136:VAL:HB	1:B:222:LEU:HB2	1.86	0.57
1:E:137:ILE:HG12	1:E:221:THR:HG23	1.85	0.57
1:A:80:GLN:NE2	1:B:57:LEU:O	2.38	0.55
1:A:90:ARG:HG3	1:A:93:ARG:HE	1.71	0.55
2:D:301:HEM:HMB1	2:D:301:HEM:HBB2	1.88	0.55
1:C:20:GLN:NE2	6:C:431:HOH:O	2.31	0.55
2:C:301:HEM:HBB2	2:C:301:HEM:HMB2	1.89	0.54
1:B:37:VAL:HG12	1:B:41:LYS:HE3	1.90	0.54
1:B:25:TRP:CE2	1:B:33:ARG:HD2	2.43	0.54
1:D:144:GLU:N	1:D:144:GLU:OE2	2.40	0.54
2:A:301:HEM:HMC1	2:A:301:HEM:HBC2	1.89	0.54
1:E:62:SER:OG	1:E:223:LEU:O	2.25	0.54
1:D:58:LEU:HB3	1:D:62:SER:HB2	1.90	0.53
2:E:301:HEM:HMC1	2:E:301:HEM:HBC2	1.90	0.53
1:B:160:HIS:ND1	1:B:210:GLU:OE1	2.33	0.53
1:C:132:PRO:HD2	1:C:226:MET:HB3	1.90	0.53
1:C:25:TRP:CE2	1:C:33:ARG:HD3	2.43	0.53
1:B:132:PRO:HD2	1:B:226:MET:HB3	1.89	0.53
1:C:160:HIS:ND1	1:C:210:GLU:OE1	2.38	0.53
1:B:62:SER:OG	1:B:223:LEU:O	2.26	0.52
1:D:117:SER:N	3:D:304:SO4:O4	2.37	0.52
1:B:137:ILE:HG12	1:B:221:THR:HG23	1.92	0.52
1:A:62:SER:OG	1:A:223:LEU:O	2.25	0.52
1:B:89:THR:HG22	1:B:91:LEU:H	1.74	0.52
1:E:18:THR:OG1	1:E:98:GLY:O	2.27	0.52
1:C:77:SER:O	1:C:81:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLU:OE1	1:C:144:GLU:N	2.42	0.51
1:E:233:LEU:HA	1:E:236:PHE:CD2	2.39	0.51
3:A:302:SO4:O1	1:B:20:GLN:NE2	2.44	0.51
1:A:37:VAL:HG12	1:A:41:LYS:HE3	1.92	0.50
1:E:58:LEU:HD11	1:E:68:MET:HB2	1.94	0.50
1:E:232:ILE:HG22	1:E:236:PHE:CE2	2.44	0.50
1:B:170:THR:O	1:B:192:THR:HG23	2.12	0.50
1:B:25:TRP:O	1:B:33:ARG:HD3	2.12	0.50
1:E:2:ASP:O	1:E:3:ARG:HB2	2.11	0.49
1:B:18:THR:OG1	1:B:98:GLY:O	2.27	0.49
1:E:37:VAL:HG12	1:E:41:LYS:HE3	1.95	0.49
2:B:301:HEM:HMB2	2:B:301:HEM:HBB2	1.94	0.48
1:C:139:ILE:HD11	2:C:301:HEM:HAC	1.94	0.48
1:D:57:LEU:HD13	1:D:232:ILE:HG23	1.96	0.48
1:D:40:VAL:HG21	1:D:91:LEU:HD23	1.96	0.48
1:E:90:ARG:O	1:E:93:ARG:HG2	2.13	0.48
1:C:221:THR:OG1	1:E:183:ASP:OD1	2.25	0.48
1:A:230:ASP:OD2	1:A:231:GLU:N	2.46	0.48
2:E:301:HEM:HBA1	2:E:301:HEM:HHA	1.96	0.47
1:A:179:THR:HB	1:B:199:HIS:CE1	2.49	0.47
1:B:139:ILE:CD1	2:B:301:HEM:HAC	2.45	0.47
1:D:110:TYR:HB3	1:D:154:THR:HG23	1.97	0.47
1:E:132:PRO:HD2	1:E:226:MET:HB3	1.97	0.47
1:E:219:HIS:NE2	3:E:305:SO4:O4	2.48	0.47
1:E:127:GLU:HB2	1:E:169:LYS:O	2.14	0.46
1:E:30:GLY:O	1:E:34:VAL:HG23	2.16	0.46
1:E:77:SER:O	1:E:81:GLN:HG2	2.15	0.46
2:B:301:HEM:HMC1	2:B:301:HEM:HBC2	1.97	0.46
1:B:37:VAL:HG22	1:B:233:LEU:HB3	1.98	0.46
1:C:109:THR:N	2:C:301:HEM:O1A	2.48	0.46
1:A:127:GLU:HB2	1:A:169:LYS:O	2.16	0.46
1:C:89:THR:HG22	1:C:91:LEU:H	1.81	0.46
1:D:80:GLN:NE2	1:E:225:THR:OG1	2.42	0.45
1:A:144:GLU:OE1	1:A:144:GLU:N	2.47	0.45
1:E:161:THR:O	1:E:165:LEU:HG	2.17	0.45
1:E:216:ARG:NH2	1:E:219:HIS:O	2.30	0.44
1:C:176:TYR:HB2	1:C:187:ILE:HB	1.99	0.44
1:D:137:ILE:HG12	1:D:221:THR:HG23	1.99	0.44
1:C:178:SER:OG	1:C:182:ASP:OD1	2.35	0.44
1:E:90:ARG:HG3	1:E:93:ARG:HE	1.83	0.44
1:C:136:VAL:HB	1:C:222:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASP:OD1	6:C:427:HOH:O	2.20	0.44
1:B:68:MET:O	6:B:427:HOH:O	2.21	0.43
1:D:77:SER:O	1:D:81:GLN:HG2	2.18	0.43
1:C:67:LEU:HD12	1:C:232:ILE:HG21	1.99	0.43
1:A:106:LYS:HD2	1:A:177:HIS:CG	2.53	0.43
1:A:77:SER:O	1:A:81:GLN:HG2	2.17	0.43
1:B:161:THR:O	1:B:165:LEU:HG	2.17	0.43
1:B:198:PHE:O	1:B:202:VAL:HG23	2.17	0.43
1:C:198:PHE:O	1:C:202:VAL:HG23	2.19	0.43
1:E:76:LEU:HD23	1:E:76:LEU:HA	1.86	0.43
1:A:40:VAL:HG22	1:A:89:THR:HG21	1.99	0.43
1:A:221:THR:OG1	1:C:183:ASP:OD1	2.27	0.43
1:B:111:VAL:HA	1:B:114:PHE:CD2	2.53	0.43
1:D:51:ILE:HG22	1:D:73:ALA:HB2	2.00	0.43
1:A:111:VAL:HA	1:A:114:PHE:CD2	2.54	0.43
1:B:109:THR:N	2:B:301:HEM:O1A	2.44	0.43
1:E:157:MET:HE1	6:E:418:HOH:O	2.18	0.43
1:A:198:PHE:O	1:A:202:VAL:HG23	2.19	0.43
1:B:107:LYS:HA	1:B:108:PRO:HD3	1.92	0.43
1:C:70:ARG:HG2	1:C:72:HIS:CE1	2.53	0.43
1:D:231:GLU:O	1:D:235:LYS:HG2	2.19	0.42
1:D:70:ARG:NH1	1:D:176:TYR:OH	2.52	0.42
1:A:37:VAL:HG13	1:A:233:LEU:HB3	2.01	0.42
1:E:2:ASP:CG	1:E:5:LYS:HB2	2.44	0.42
1:D:67:LEU:HD23	1:D:68:MET:N	2.34	0.42
1:A:161:THR:O	1:A:165:LEU:HG	2.19	0.42
1:D:62:SER:OG	1:D:223:LEU:O	2.33	0.42
1:B:17:ALA:O	1:B:68:MET:HA	2.20	0.42
1:E:114:PHE:O	1:E:119:LYS:HE3	2.19	0.42
1:B:182:ASP:HB2	1:B:183:ASP:H	1.71	0.42
1:D:89:THR:HG22	1:D:91:LEU:H	1.85	0.42
1:E:25:TRP:CE2	1:E:33:ARG:HD2	2.55	0.42
1:A:93:ARG:NH2	4:A:303:EDO:O2	2.40	0.41
1:B:56:TYR:O	6:B:427:HOH:O	2.22	0.41
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.86	0.41
1:C:138:PRO:HB2	1:C:184:VAL:HG11	2.02	0.41
1:E:45:GLU:HA	1:E:48:SER:HB3	2.02	0.41
1:D:118:MET:HE1	1:D:158:GLN:HG3	2.02	0.41
1:E:136:VAL:HB	1:E:222:LEU:HB2	2.02	0.41
1:A:178:SER:OG	1:A:182:ASP:OD1	2.38	0.41
1:B:178:SER:OG	1:B:182:ASP:OD1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.81	0.40
1:A:44:VAL:HG21	1:A:229:LEU:CD2	2.51	0.40
1:A:176:TYR:HB2	1:A:187:ILE:HB	2.03	0.40
1:B:53:VAL:HG21	1:B:82:PHE:CZ	2.56	0.40
1:B:93:ARG:NH2	3:B:302:SO4:O2	2.54	0.40
2:C:301:HEM:HMC1	2:C:301:HEM:HBC2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	30	37
1	B	236/241 (98%)	228 (97%)	8 (3%)	0	100	100
1	C	234/241 (97%)	227 (97%)	7 (3%)	0	100	100
1	D	234/241 (97%)	221 (94%)	12 (5%)	1 (0%)	30	37
1	E	235/241 (98%)	227 (97%)	7 (3%)	1 (0%)	30	37
All	All	1175/1205 (98%)	1130 (96%)	42 (4%)	3 (0%)	36	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	ALA
1	E	237	ALA
1	D	125	ASN

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	205/206 (100%)	205 (100%)	0	100	100
1	B	205/206 (100%)	205 (100%)	0	100	100
1	C	204/206 (99%)	204 (100%)	0	100	100
1	D	204/206 (99%)	202 (99%)	2 (1%)	68	77
1	E	205/206 (100%)	205 (100%)	0	100	100
All	All	1023/1030 (99%)	1021 (100%)	2 (0%)	87	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	18	THR
1	D	31	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	162	GLN
1	C	213	HIS
1	D	238	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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
2	HEM	C	301	1	50,50,50	1.94	10 (20%)	67,82,82	1.19	4 (5%)
4	EDO	E	304	-	3,3,3	0.43	0	2,2,2	0.37	0
5	IMD	D	302	2	5,5,5	0.62	0	5,5,5	0.48	0
3	SO4	B	302	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	305	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.05	0
4	EDO	D	305	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	C	305	-	3,3,3	0.42	0	2,2,2	0.38	0
3	SO4	E	305	-	4,4,4	0.24	0	6,6,6	0.07	0
2	HEM	B	301	1	50,50,50	1.94	10 (20%)	67,82,82	1.27	4 (5%)
3	SO4	B	303	-	4,4,4	0.23	0	6,6,6	0.07	0
2	HEM	A	301	1	50,50,50	1.94	9 (18%)	67,82,82	1.42	8 (11%)
5	IMD	A	304	-	5,5,5	0.64	0	5,5,5	0.43	0
4	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.23	0
2	HEM	D	301	5,1	50,50,50	1.94	10 (20%)	67,82,82	1.26	3 (4%)
4	EDO	E	302	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	B	304	-	3,3,3	0.43	0	2,2,2	0.38	0
3	SO4	D	303	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	C	303	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	304	-	4,4,4	0.24	0	6,6,6	0.07	0
2	HEM	E	301	1	50,50,50	1.93	10 (20%)	67,82,82	1.35	5 (7%)
4	EDO	E	303	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	C	306	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	C	304	-	3,3,3	0.42	0	2,2,2	0.37	0
3	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.08	0

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
4	EDO	C	305	-	-	0/1/1/1	-
2	HEM	C	301	1	-	4/14/54/54	-
4	EDO	C	306	-	-	0/1/1/1	-
4	EDO	E	304	-	-	0/1/1/1	-
5	IMD	D	302	2	-	-	0/1/1/1
4	EDO	C	304	-	-	0/1/1/1	-
4	EDO	E	302	-	-	0/1/1/1	-
2	HEM	B	301	1	-	4/14/54/54	-
4	EDO	B	304	-	-	0/1/1/1	-
2	HEM	A	301	1	-	8/14/54/54	-
5	IMD	A	304	-	-	-	0/1/1/1
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
2	HEM	E	301	1	-	4/14/54/54	-
4	EDO	D	305	-	-	0/1/1/1	-
2	HEM	D	301	5,1	-	2/14/54/54	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	HEM	C3D-C2D	8.09	1.54	1.36
2	D	301	HEM	C3D-C2D	8.06	1.54	1.36
2	B	301	HEM	C3D-C2D	7.91	1.53	1.36
2	E	301	HEM	C3D-C2D	7.91	1.53	1.36
2	A	301	HEM	C3D-C2D	7.79	1.53	1.36
2	C	301	HEM	FE-ND	4.90	2.10	1.94
2	A	301	HEM	FE-ND	4.89	2.09	1.94
2	B	301	HEM	FE-NB	4.65	2.09	1.94
2	E	301	HEM	FE-ND	4.58	2.09	1.94
2	D	301	HEM	FE-NB	4.44	2.08	1.94
2	A	301	HEM	FE-NB	4.41	2.08	1.94
2	E	301	HEM	FE-NB	4.40	2.08	1.94
2	D	301	HEM	FE-ND	4.27	2.08	1.94
2	B	301	HEM	FE-ND	4.23	2.07	1.94
2	C	301	HEM	FE-NB	4.16	2.07	1.94
2	D	301	HEM	FE-NC	3.85	2.07	1.95
2	B	301	HEM	FE-NC	3.77	2.07	1.95
2	B	301	HEM	FE-NA	3.58	2.07	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	HEM	FE-NA	3.51	2.06	1.95
2	E	301	HEM	FE-NA	3.40	2.06	1.95
2	C	301	HEM	FE-NA	3.38	2.06	1.95
2	A	301	HEM	FE-NC	3.31	2.06	1.95
2	E	301	HEM	FE-NC	3.29	2.06	1.95
2	C	301	HEM	FE-NC	3.24	2.05	1.95
2	A	301	HEM	CAC-C3C	3.18	1.55	1.47
2	C	301	HEM	CAB-C3B	3.15	1.55	1.47
2	D	301	HEM	CAC-C3C	3.14	1.55	1.47
2	B	301	HEM	CAB-C3B	3.13	1.55	1.47
2	E	301	HEM	CAC-C3C	3.13	1.55	1.47
2	D	301	HEM	FE-NA	3.13	2.05	1.95
2	D	301	HEM	CAB-C3B	3.12	1.55	1.47
2	B	301	HEM	CAC-C3C	3.09	1.55	1.47
2	C	301	HEM	CAC-C3C	3.06	1.55	1.47
2	E	301	HEM	CAB-C3B	2.97	1.55	1.47
2	A	301	HEM	CAB-C3B	2.94	1.55	1.47
2	B	301	HEM	CMC-C2C	2.19	1.55	1.50
2	D	301	HEM	CMC-C2C	2.17	1.55	1.50
2	C	301	HEM	CMC-C2C	2.17	1.55	1.50
2	E	301	HEM	CMC-C2C	2.17	1.55	1.50
2	A	301	HEM	CMC-C2C	2.16	1.55	1.50
2	C	301	HEM	CMB-C2B	2.11	1.55	1.50
2	B	301	HEM	CMB-C2B	2.10	1.55	1.50
2	D	301	HEM	CMB-C2B	2.09	1.55	1.50
2	C	301	HEM	CMD-C2D	2.08	1.55	1.50
2	E	301	HEM	CMD-C2D	2.06	1.55	1.50
2	B	301	HEM	CMD-C2D	2.04	1.55	1.50
2	D	301	HEM	CMD-C2D	2.02	1.54	1.50
2	A	301	HEM	CMB-C2B	2.01	1.54	1.50
2	E	301	HEM	CMB-C2B	2.01	1.54	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	HEM	C4D-ND-C1D	5.73	111.99	105.21
2	D	301	HEM	C4D-ND-C1D	5.65	111.90	105.21
2	A	301	HEM	C4D-ND-C1D	5.62	111.86	105.21
2	E	301	HEM	C4D-ND-C1D	5.53	111.75	105.21
2	C	301	HEM	C4D-ND-C1D	5.43	111.64	105.21
2	E	301	HEM	C3B-C2B-C1B	2.80	108.51	106.41
2	A	301	HEM	CAD-C3D-C4D	2.73	129.46	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	HEM	C3B-C4B-NB	-2.72	107.52	109.47
2	A	301	HEM	C3B-C2B-C1B	2.71	108.45	106.41
2	E	301	HEM	C3B-C4B-NB	-2.56	107.63	109.47
2	A	301	HEM	C1B-NB-C4B	2.49	108.15	105.21
2	E	301	HEM	C1B-NB-C4B	2.47	108.14	105.21
2	D	301	HEM	C2A-C1A-NA	-2.26	107.64	110.15
2	D	301	HEM	C3B-C2B-C1B	2.20	108.07	106.41
2	B	301	HEM	C2A-C1A-NA	-2.19	107.72	110.15
2	A	301	HEM	C2A-C1A-NA	-2.19	107.73	110.15
2	B	301	HEM	CHA-C4D-ND	2.12	126.99	124.37
2	C	301	HEM	CAD-CBD-CGD	-2.05	108.22	113.67
2	E	301	HEM	C2A-C1A-NA	-2.05	107.88	110.15
2	B	301	HEM	C3B-C2B-C1B	2.05	107.95	106.41
2	C	301	HEM	C3B-C2B-C1B	2.04	107.94	106.41
2	A	301	HEM	CHD-C1D-ND	2.03	126.61	124.42
2	A	301	HEM	CAA-CBA-CGA	-2.01	108.34	113.67
2	C	301	HEM	C1B-NB-C4B	2.00	107.58	105.21

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	HEM	C1A-C2A-CAA-CBA
2	A	301	HEM	C4D-C3D-CAD-CBD
2	A	301	HEM	C1A-C2A-CAA-CBA
2	A	301	HEM	C3D-CAD-CBD-CGD
2	C	301	HEM	C4D-C3D-CAD-CBD
2	E	301	HEM	C3A-C2A-CAA-CBA
2	A	301	HEM	C4B-C3B-CAB-CBB
2	E	301	HEM	C4B-C3B-CAB-CBB
2	A	301	HEM	C2D-C3D-CAD-CBD
2	C	301	HEM	C2D-C3D-CAD-CBD
2	D	301	HEM	C2D-C3D-CAD-CBD
2	D	301	HEM	C4D-C3D-CAD-CBD
2	C	301	HEM	CAA-CBA-CGA-O2A
2	C	301	HEM	CAA-CBA-CGA-O1A
2	A	301	HEM	CAD-CBD-CGD-O1D
2	A	301	HEM	CAD-CBD-CGD-O2D
2	B	301	HEM	CAD-CBD-CGD-O2D
2	A	301	HEM	C3A-C2A-CAA-CBA
4	A	303	EDO	O1-C1-C2-O2
2	B	301	HEM	CAA-CBA-CGA-O2A

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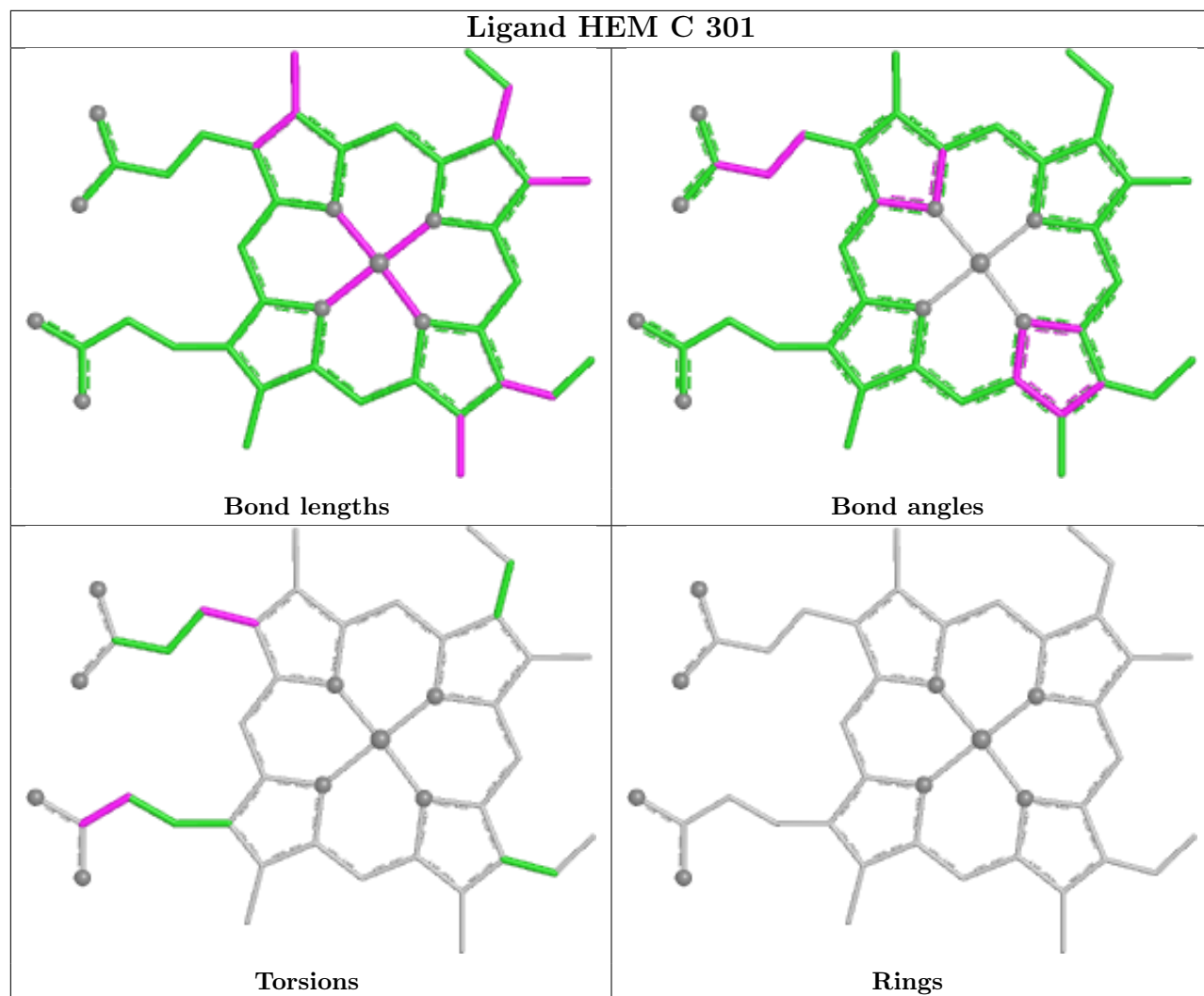
Mol	Chain	Res	Type	Atoms
2	B	301	HEM	CAD-CBD-CGD-O1D
2	B	301	HEM	CAA-CBA-CGA-O1A
2	E	301	HEM	CAD-CBD-CGD-O2D

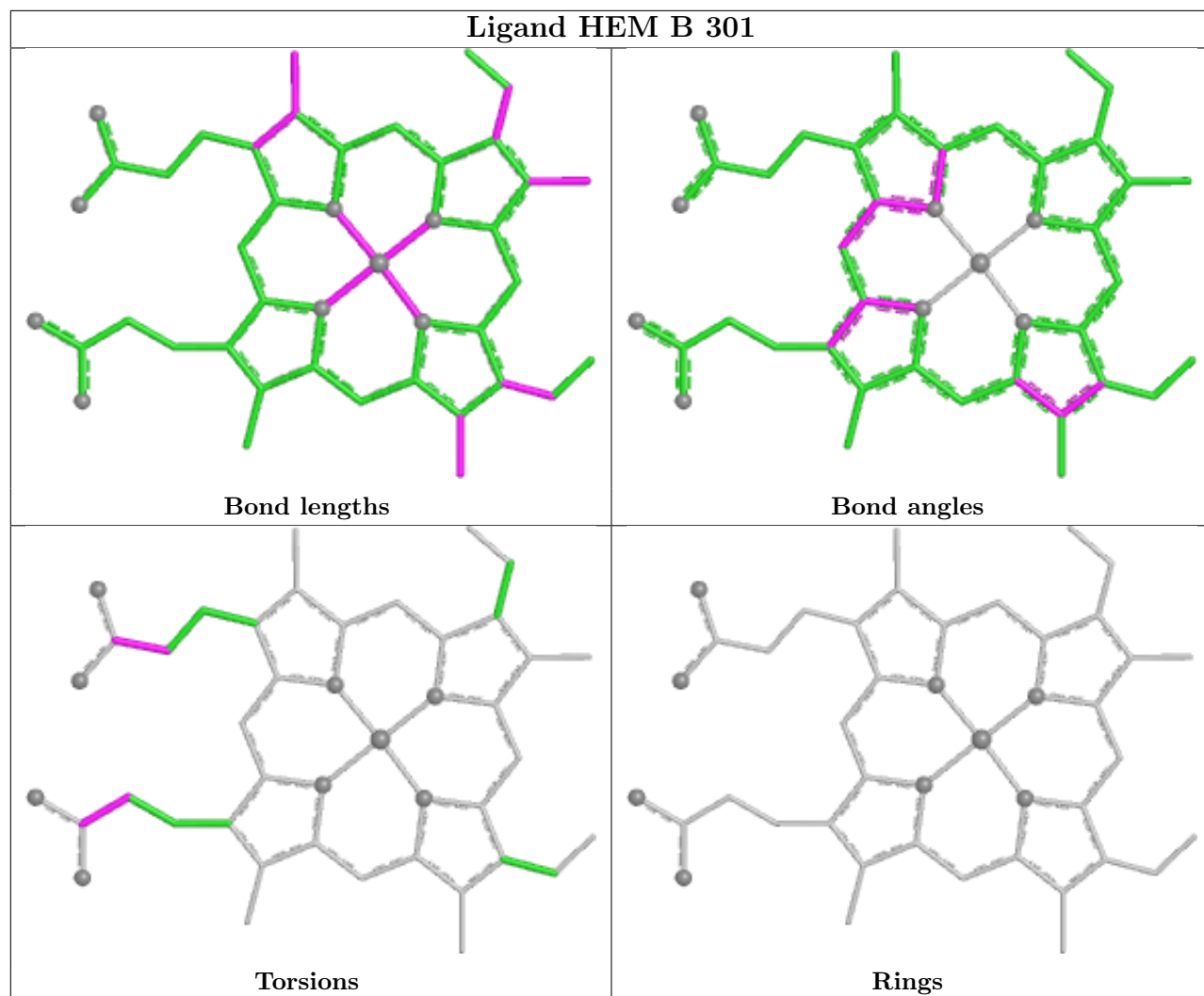
There are no ring outliers.

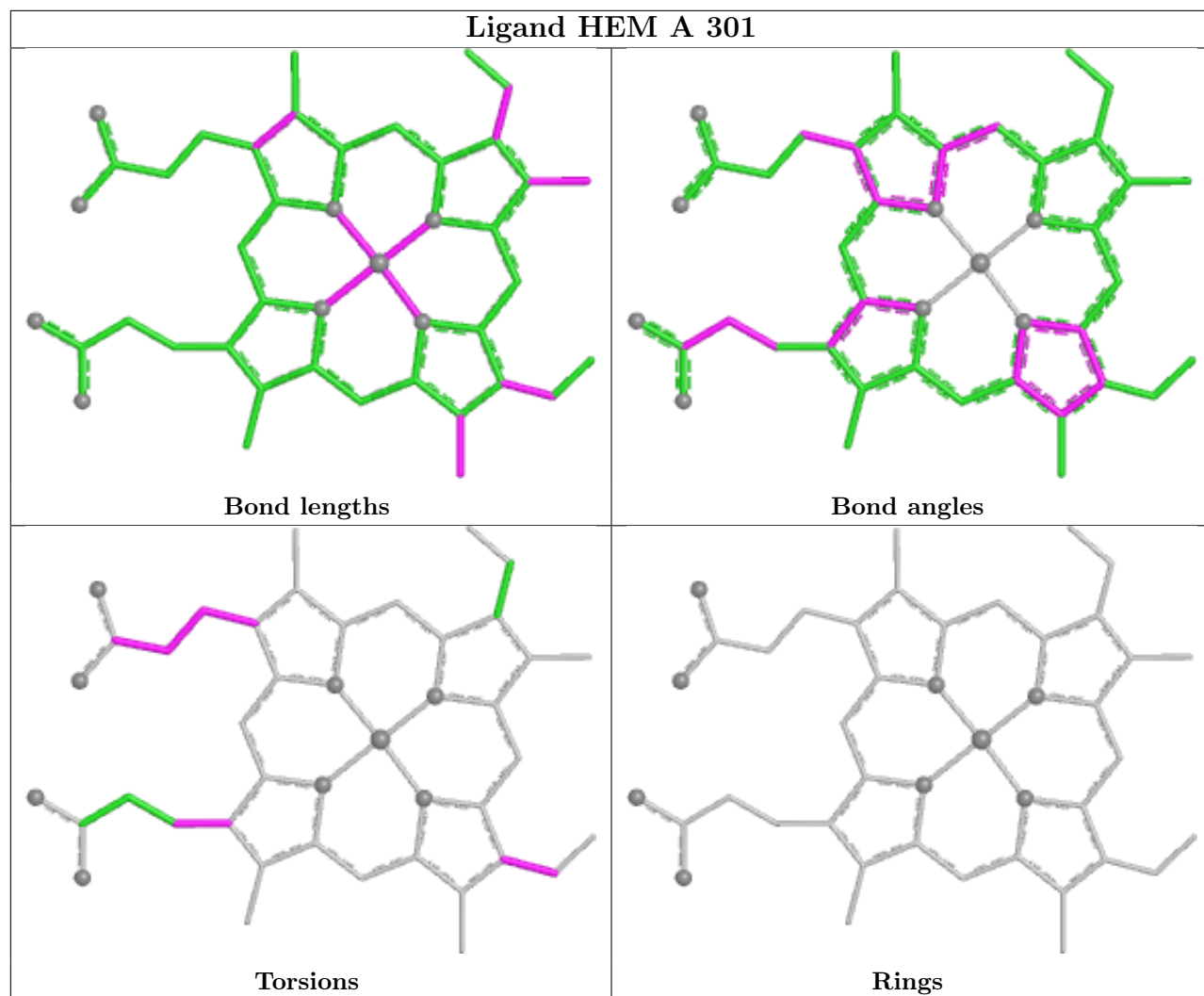
11 monomers are involved in 25 short contacts:

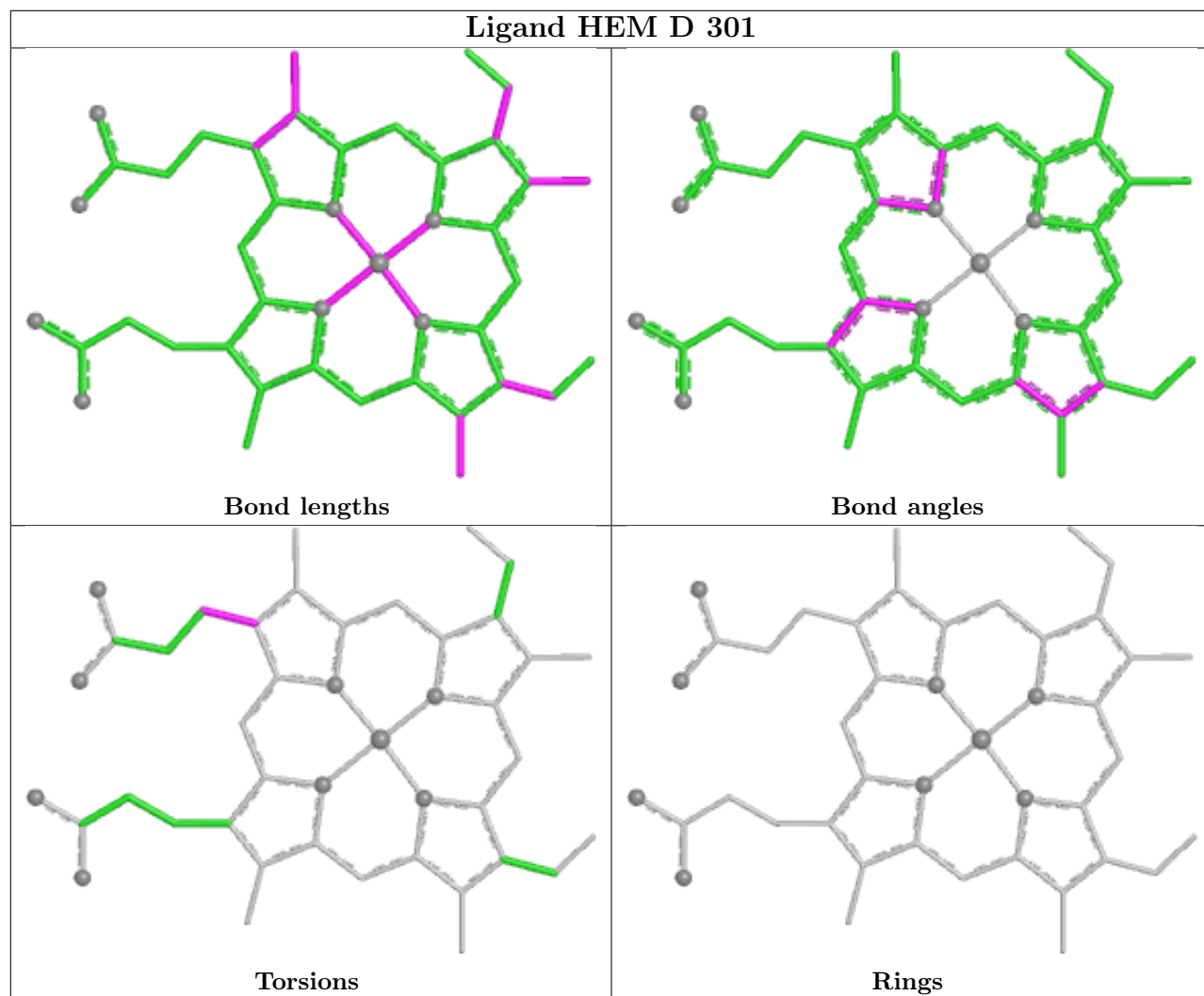
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	HEM	4	0
3	B	302	SO4	1	0
3	A	302	SO4	1	0
3	E	305	SO4	1	0
2	B	301	HEM	5	0
2	A	301	HEM	2	0
4	A	303	EDO	2	0
2	D	301	HEM	4	0
4	E	302	EDO	1	0
3	D	304	SO4	1	0
2	E	301	HEM	3	0

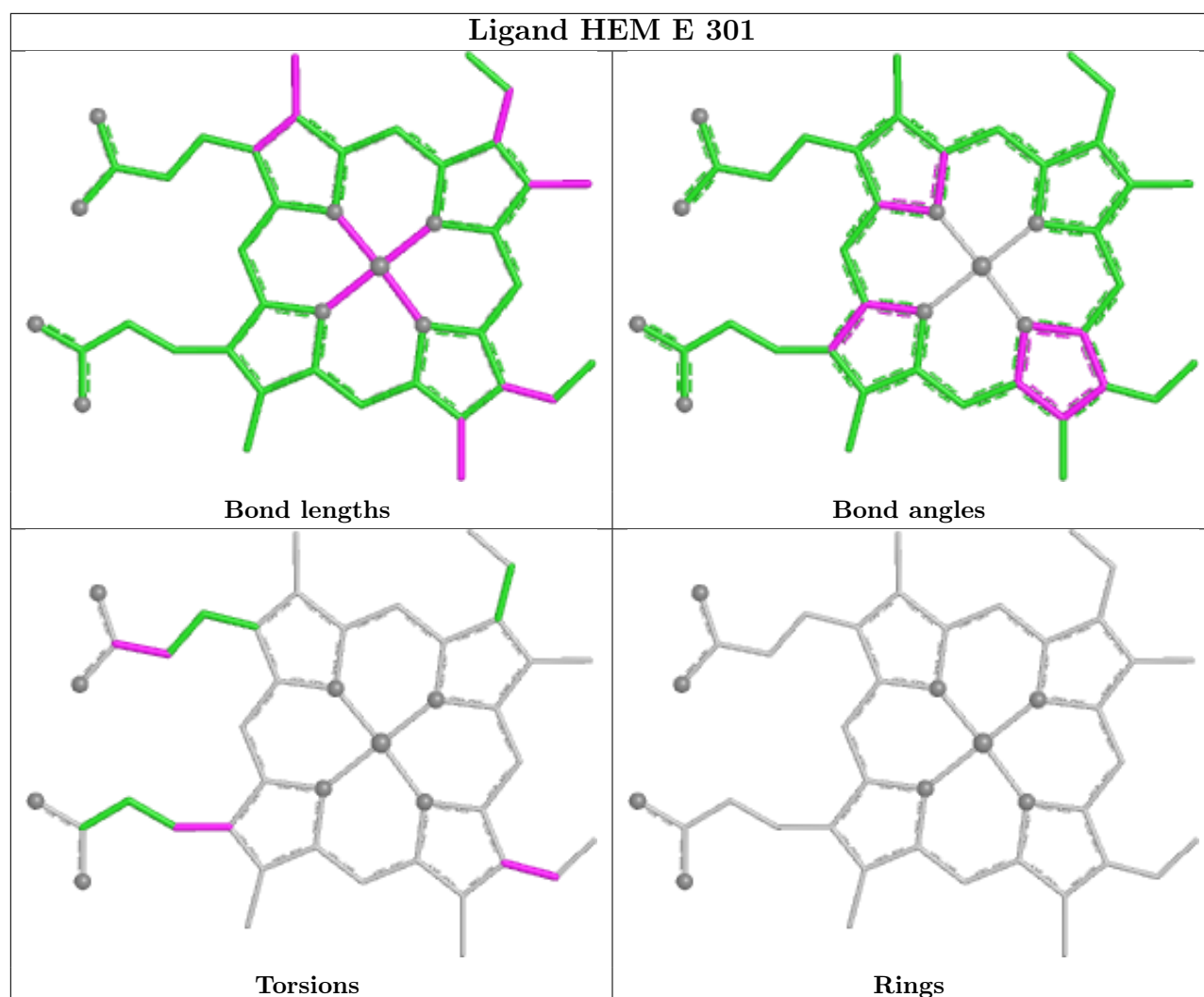
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	238/241 (98%)	1.31	55 (23%) 2 1	31, 63, 114, 150	0
1	B	238/241 (98%)	1.37	49 (20%) 2 2	30, 62, 113, 146	1 (0%)
1	C	236/241 (97%)	1.33	50 (21%) 2 2	32, 65, 114, 136	1 (0%)
1	D	236/241 (97%)	1.28	44 (18%) 3 2	36, 66, 110, 131	1 (0%)
1	E	237/241 (98%)	1.29	45 (18%) 3 2	29, 65, 112, 149	1 (0%)
All	All	1185/1205 (98%)	1.31	243 (20%) 2 2	29, 64, 113, 150	4 (0%)

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	232	ILE	6.1
1	E	236	PHE	5.6
1	C	26	TRP	5.3
1	B	236	PHE	4.5
1	D	236	PHE	4.5
1	A	236	PHE	4.4
1	C	217	PHE	4.4
1	B	124	VAL	4.3
1	B	48	SER	4.3
1	D	26	TRP	4.2
1	D	229	LEU	4.2
1	B	238	GLN	4.1
1	D	69	PHE	4.1
1	B	237	ALA	3.9
1	B	211	PHE	3.9
1	E	203	ARG	3.9
1	D	89	THR	3.7
1	B	3	ARG	3.7
1	B	203	ARG	3.7
1	E	23	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	3.6
1	C	6	LEU	3.6
1	E	93	ARG	3.6
1	E	146	TYR	3.6
1	D	218	GLY	3.5
1	C	124	VAL	3.4
1	A	93	ARG	3.4
1	E	124	VAL	3.4
1	E	69	PHE	3.4
1	B	21	MET	3.3
1	C	229	LEU	3.3
1	A	55	SER	3.3
1	E	167	TYR	3.3
1	E	11	GLY	3.3
1	E	207	GLN	3.3
1	E	234	GLU	3.3
1	A	207	GLN	3.2
1	B	146	TYR	3.2
1	E	73	ALA	3.2
1	B	26	TRP	3.2
1	C	69	PHE	3.2
1	E	211	PHE	3.1
1	D	24	ASP	3.1
1	D	91	LEU	3.1
1	B	72	HIS	3.1
1	D	29	PRO	3.1
1	D	6	LEU	3.1
1	E	201	LEU	3.1
1	A	168	LEU	3.0
1	B	63	ASP	3.0
1	E	164	ALA	3.0
1	E	76	LEU	3.0
1	B	190	PHE	3.0
1	B	169	LYS	3.0
1	E	237	ALA	2.9
1	E	230	ASP	2.9
1	C	207	GLN	2.9
1	D	98	GLY	2.9
1	D	39	GLU	2.9
1	E	72	HIS	2.8
1	A	1	ALA	2.8
1	C	230	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	47	TRP	2.8
1	D	230	ASP	2.8
1	D	106	LYS	2.8
1	A	137	ILE	2.8
1	A	174	LYS	2.8
1	C	189	TYR	2.8
1	E	60	GLY	2.8
1	A	31	GLU	2.8
1	C	34	VAL	2.8
1	E	96	THR	2.8
1	D	126	GLY	2.7
1	C	146	TYR	2.7
1	A	84	SER	2.7
1	A	126	GLY	2.7
1	E	92	GLY	2.7
1	B	7	LEU	2.7
1	C	195	LEU	2.7
1	C	35	ILE	2.7
1	C	108	PRO	2.7
1	A	125	ASN	2.7
1	B	105	SER	2.7
1	A	47	TRP	2.7
1	B	234	GLU	2.7
1	D	234	GLU	2.7
1	A	218	GLY	2.7
1	C	105	SER	2.7
1	B	23	HIS	2.7
1	B	213	HIS	2.7
1	C	126	GLY	2.6
1	D	228	PRO	2.6
1	D	84	SER	2.6
1	D	231	GLU	2.6
1	B	189	TYR	2.6
1	B	126	GLY	2.6
1	C	30	GLY	2.6
1	B	71	VAL	2.6
1	A	201	LEU	2.6
1	E	233	LEU	2.6
1	A	202	VAL	2.6
1	A	35	ILE	2.6
1	C	94	HIS	2.6
1	C	237	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	32	SER	2.6
1	E	2	ASP	2.5
1	E	12	VAL	2.5
1	C	106	LYS	2.5
1	D	22	ASP	2.5
1	D	25	TRP	2.5
1	C	75	THR	2.5
1	C	203	ARG	2.5
1	E	126	GLY	2.5
1	C	211	PHE	2.5
1	C	107	LYS	2.5
1	E	235	LYS	2.5
1	E	90	ARG	2.5
1	A	105	SER	2.5
1	B	235	LYS	2.5
1	D	28	LEU	2.5
1	D	83	LEU	2.5
1	E	58	LEU	2.5
1	E	165	LEU	2.5
1	D	124	VAL	2.5
1	A	10	SER	2.5
1	B	89	THR	2.5
1	C	236	PHE	2.4
1	D	34	VAL	2.4
1	B	155	ALA	2.4
1	B	30	GLY	2.4
1	C	11	GLY	2.4
1	D	140	LYS	2.4
1	A	7	LEU	2.4
1	A	67	LEU	2.4
1	A	219	HIS	2.4
1	A	124	VAL	2.4
1	B	55	SER	2.4
1	C	10	SER	2.4
1	E	109	THR	2.4
1	D	36	SER	2.4
1	D	128	SER	2.4
1	A	129	GLY	2.4
1	C	168	LEU	2.4
1	B	69	PHE	2.4
1	C	55	SER	2.3
1	A	27	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	127	GLU	2.3
1	A	203	ARG	2.3
1	B	36	SER	2.3
1	D	92	GLY	2.3
1	C	228	PRO	2.3
1	C	8	THR	2.3
1	B	194	ARG	2.3
1	A	167	TYR	2.3
1	E	40	VAL	2.3
1	B	73	ALA	2.3
1	E	125	ASN	2.3
1	C	131	ARG	2.3
1	B	109	THR	2.3
1	C	5	LYS	2.3
1	C	110	TYR	2.3
1	A	224	GLY	2.2
1	C	190	PHE	2.2
1	E	3	ARG	2.2
1	D	38	ALA	2.2
1	A	23	HIS	2.2
1	B	207	GLN	2.2
1	C	180	GLY	2.2
1	E	99	GLY	2.2
1	A	169	LYS	2.2
1	E	160	HIS	2.2
1	A	8	THR	2.2
1	B	76	LEU	2.2
1	D	233	LEU	2.2
1	E	30	GLY	2.2
1	E	229	LEU	2.2
1	C	63	ASP	2.2
1	C	53	VAL	2.2
1	A	50	LYS	2.2
1	A	73	ALA	2.2
1	B	164	ALA	2.2
1	C	125	ASN	2.2
1	C	21	MET	2.2
1	D	207	GLN	2.2
1	A	165	LEU	2.2
1	C	67	LEU	2.2
1	A	97	SER	2.2
1	A	128	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	24	ASP	2.2
1	D	196	GLU	2.2
1	B	25	TRP	2.2
1	A	41	LYS	2.2
1	A	106	LYS	2.2
1	D	217	PHE	2.2
1	A	6	LEU	2.1
1	B	179	THR	2.1
1	C	201	LEU	2.1
1	D	7	LEU	2.1
1	A	232	ILE	2.1
1	A	48	SER	2.1
1	D	74	ARG	2.1
1	E	53	VAL	2.1
1	B	188	THR	2.1
1	B	224	GLY	2.1
1	A	90	ARG	2.1
1	D	5	LYS	2.1
1	C	179	THR	2.1
1	D	30	GLY	2.1
1	A	135	ILE	2.1
1	B	128	SER	2.1
1	B	230	ASP	2.1
1	A	190	PHE	2.1
1	D	238	GLN	2.1
1	A	49	GLY	2.1
1	E	216	ARG	2.1
1	A	196	GLU	2.1
1	B	127	GLU	2.1
1	C	4	GLU	2.1
1	A	139	ILE	2.1
1	A	2	ASP	2.1
1	C	36	SER	2.1
1	E	21	MET	2.1
1	C	160	HIS	2.1
1	A	44	VAL	2.0
1	B	114	PHE	2.0
1	E	155	ALA	2.0
1	E	91	LEU	2.0
1	A	98	GLY	2.0
1	C	209	LYS	2.0
1	C	24	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	149	ASP	2.0
1	B	87	MET	2.0
1	A	40	VAL	2.0
1	B	59	ARG	2.0
1	C	104	VAL	2.0
1	C	136	VAL	2.0
1	E	186	PHE	2.0
1	A	43	LEU	2.0
1	B	60	GLY	2.0
1	D	235	LYS	2.0
1	A	89	THR	2.0
1	A	179	THR	2.0
1	D	130	SER	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	304	5/5	0.52	0.14	115,120,133,138	0
3	SO4	D	303	5/5	0.67	0.15	110,119,126,130	0
4	EDO	E	302	4/4	0.68	0.20	72,75,83,86	0
3	SO4	B	302	5/5	0.70	0.10	95,108,114,117	0
4	EDO	A	303	4/4	0.72	0.21	64,74,81,91	0
3	SO4	C	303	5/5	0.72	0.18	113,114,118,121	0
3	SO4	E	305	5/5	0.74	0.14	96,104,110,115	0
3	SO4	C	302	5/5	0.75	0.13	84,97,112,117	0
4	EDO	E	303	4/4	0.75	0.24	54,72,77,79	0
4	EDO	C	306	4/4	0.76	0.23	56,65,75,88	0

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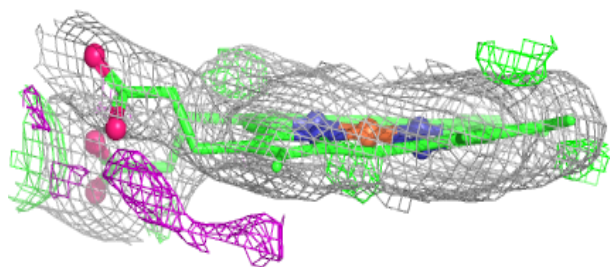
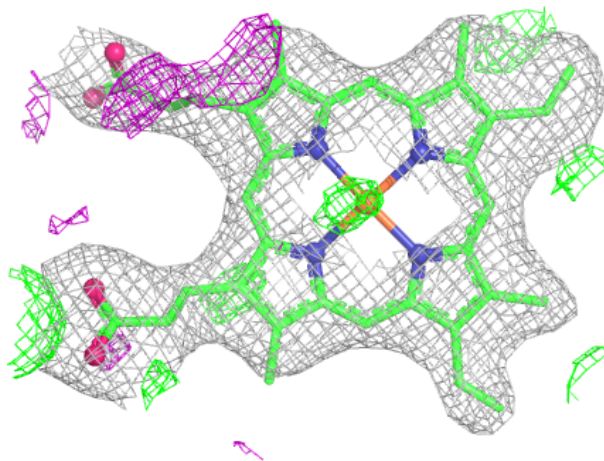
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	303	5/5	0.76	0.15	133,134,138,146	0
4	EDO	C	304	4/4	0.76	0.27	66,74,79,79	0
3	SO4	A	305	5/5	0.77	0.16	148,152,156,156	0
4	EDO	D	305	4/4	0.79	0.18	46,49,60,68	0
4	EDO	C	305	4/4	0.83	0.13	69,75,79,80	0
4	EDO	B	304	4/4	0.84	0.18	43,44,50,51	0
4	EDO	E	304	4/4	0.88	0.10	59,61,64,67	0
5	IMD	A	304	5/5	0.89	0.21	35,51,60,62	0
5	IMD	D	302	5/5	0.90	0.13	67,69,77,79	0
3	SO4	A	302	5/5	0.91	0.11	18,28,51,61	5
2	HEM	D	301	43/43	0.94	0.14	29,57,71,73	0
2	HEM	C	301	43/43	0.95	0.12	13,38,56,70	0
2	HEM	B	301	43/43	0.95	0.11	6,35,59,66	0
2	HEM	A	301	43/43	0.96	0.10	11,31,61,72	0
2	HEM	E	301	43/43	0.96	0.12	10,33,60,77	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.

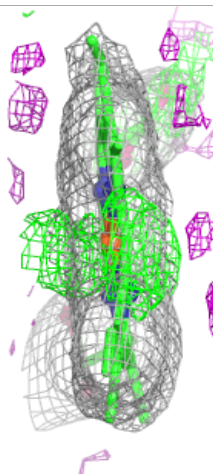
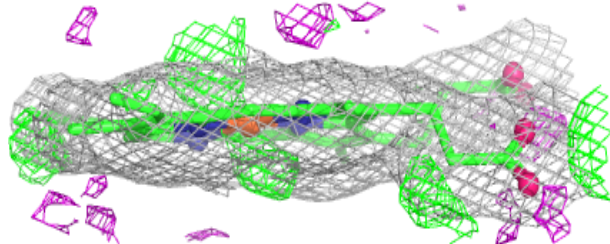
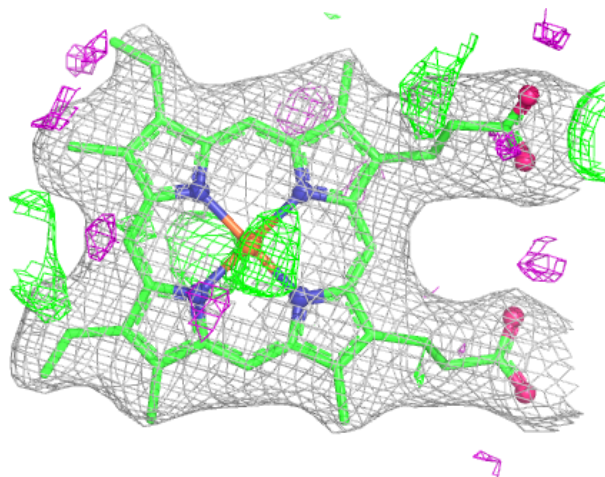
Electron density around HEM D 301:

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



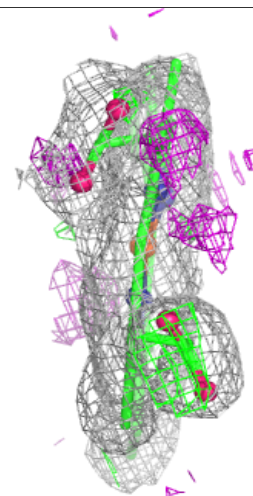
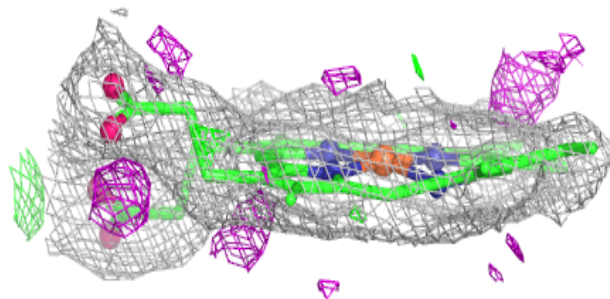
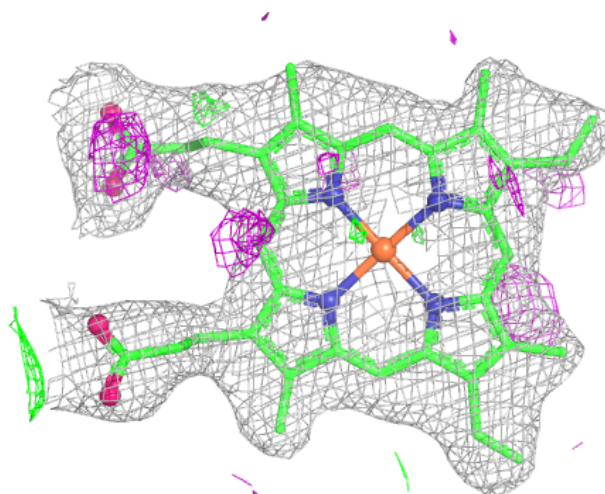
Electron density around HEM C 301:

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



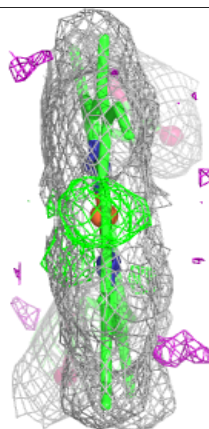
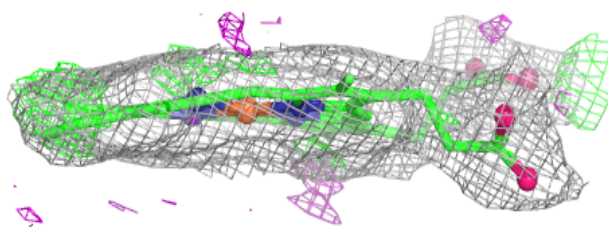
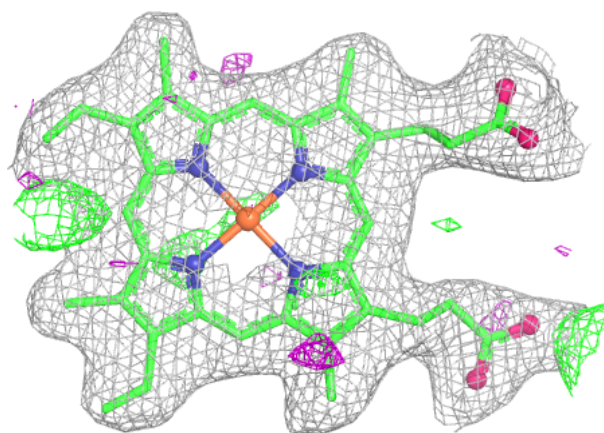
Electron density around HEM B 301:

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



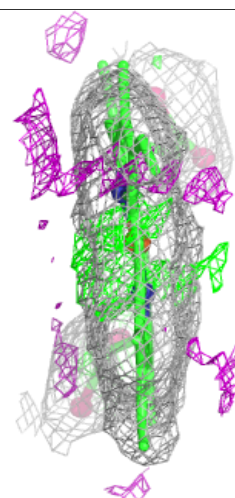
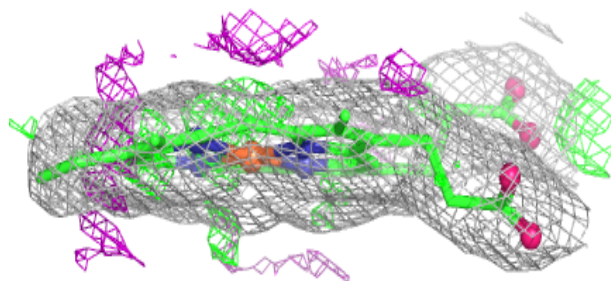
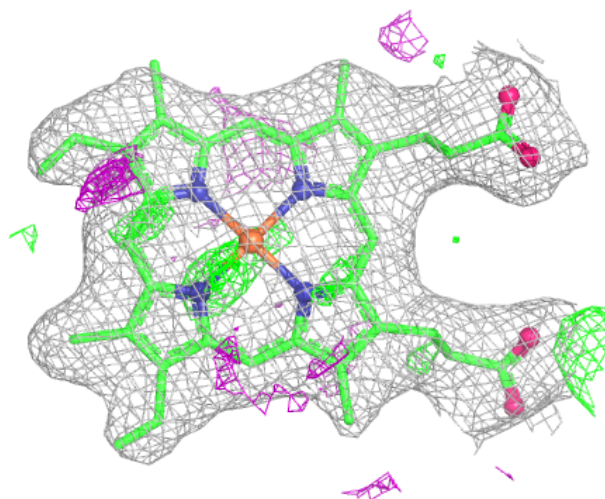
Electron density around HEM A 301:

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



Electron density around HEM E 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.