



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 02:06 pm BST

PDB ID : 4BFL / pdb_00004bfl
Title : Structure of natively expressed catalase HP1I
Authors : Gabrielsen, M.; Schuttelkopf, A.W.
Deposited on : 2013-03-19
Resolution : 1.64 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

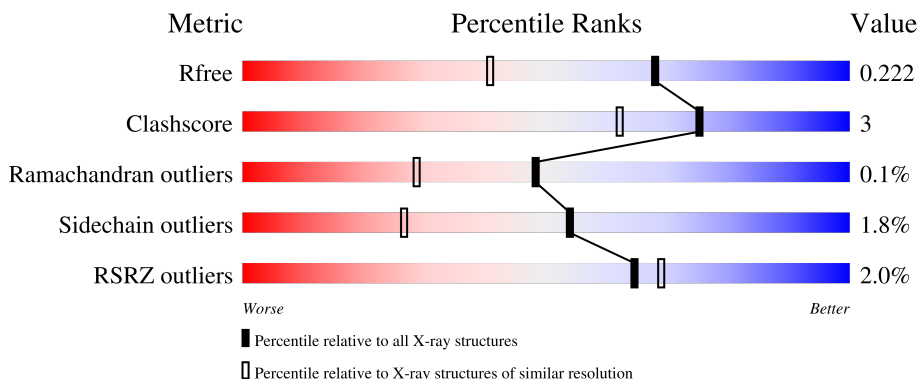
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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}	164625	1015 (1.64-1.64)
Clashscore	180529	1093 (1.64-1.64)
Ramachandran outliers	177936	1077 (1.64-1.64)
Sidechain outliers	177891	1077 (1.64-1.64)
RSRZ outliers	164620	1015 (1.64-1.64)

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	753	 2% 91% 7% ..
1	B	753	 % 91% 8% .
1	C	753	 3% 90% 8% ..
1	D	753	 % 88% 9% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25666 atoms, of which 18 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 CATALASE HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	744	Total	C	N	O	S	0	3	0
			5889	3733	1033	1110	13			
1	B	745	Total	C	N	O	S	0	3	0
			5899	3741	1036	1109	13			
1	C	743	Total	C	N	O	S	0	4	0
			5895	3736	1034	1112	13			
1	D	735	Total	C	N	O	S	0	1	0
			5807	3683	1016	1095	13			

- 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	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O		
			10	2	6	2		
3	B	1	Total	C	H	O		
			10	2	6	2		
3	C	1	Total	C	H	O		
			10	2	6	2		

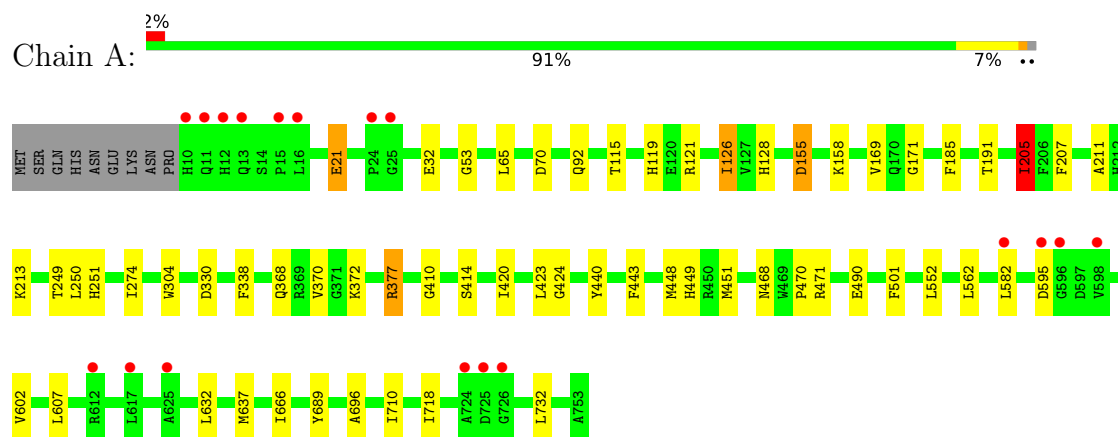
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	588	Total	O		
			588	588	0	0
4	B	572	Total	O		
			572	572	0	0
4	C	437	Total	O		
			437	437	0	0
4	D	377	Total	O		
			377	377	0	0

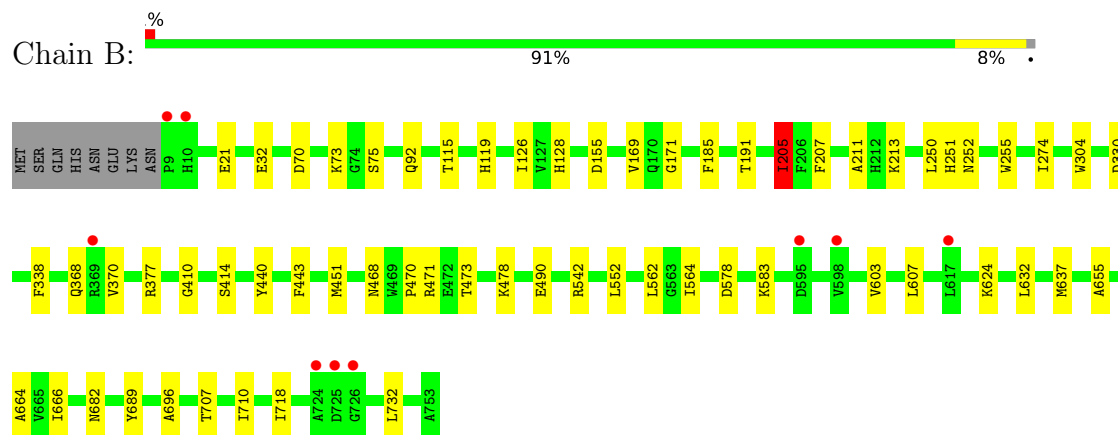
3 Residue-property plots

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

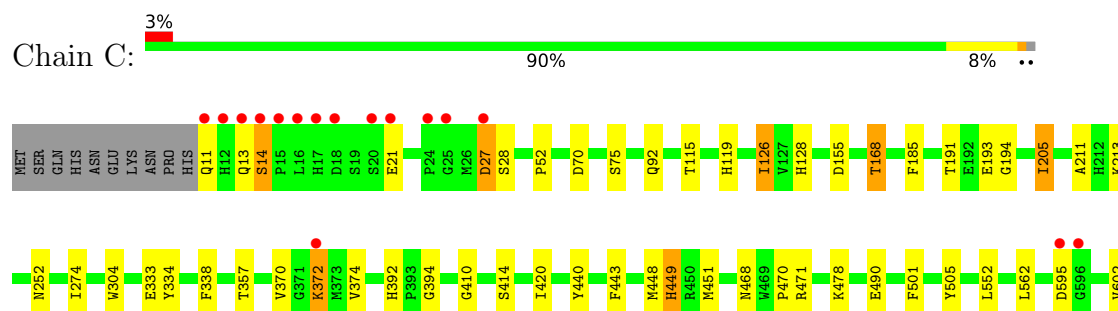
• Molecule 1: CATALASE HPII

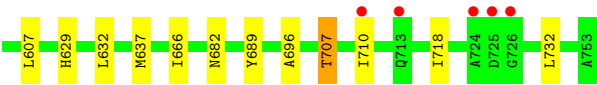


• Molecule 1: CATALASE HPII

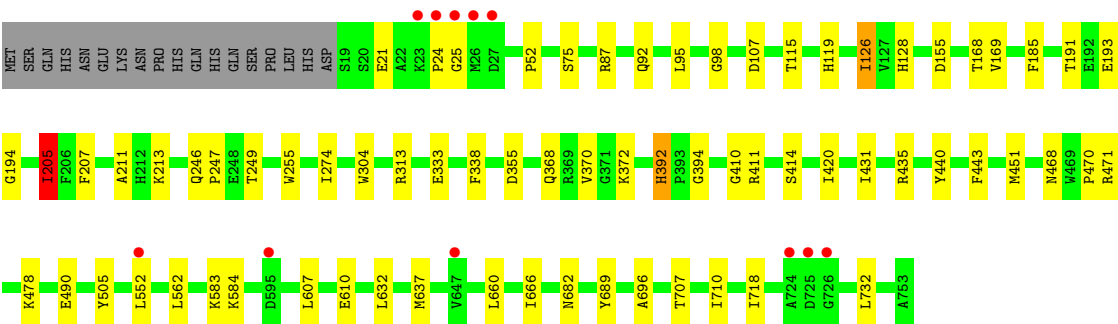
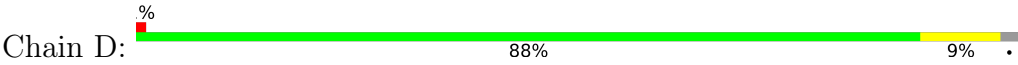


• Molecule 1: CATALASE HPII





● Molecule 1: CATALASE HP11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.40Å 171.67Å 123.21Å 90.00° 104.67° 90.00°	Depositor
Resolution (Å)	48.95 – 1.64 48.95 – 1.64	Depositor EDS
% Data completeness (in resolution range)	80.8 (48.95-1.64) 81.0 (48.95-1.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.64Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.174 , 0.202 0.192 , 0.222	Depositor DCC
R_{free} test set	14727 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	1.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25666	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: EDO, HEM

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	0.79	1/6054 (0.0%)	1.17	11/8231 (0.1%)
1	B	0.78	1/6065 (0.0%)	1.16	12/8247 (0.1%)
1	C	0.79	0/6056	1.17	16/8232 (0.2%)
1	D	0.79	1/5965 (0.0%)	1.16	12/8109 (0.1%)
All	All	0.79	3/24140 (0.0%)	1.17	51/32819 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ILE	CG1-CD1	-6.18	1.27	1.51
1	B	205	ILE	CG1-CD1	-6.06	1.28	1.51
1	D	205	ILE	CG1-CD1	-5.74	1.29	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	PHE	CA-CB-CG	7.56	121.36	113.80
1	A	338	PHE	CA-CB-CG	7.36	121.16	113.80
1	C	13	GLN	N-CA-C	7.33	121.94	112.26
1	C	27	ASP	CA-CB-CG	7.30	119.90	112.60
1	D	338	PHE	CA-CB-CG	7.16	120.96	113.80
1	D	155	ASP	CA-CB-CG	7.16	119.75	112.60
1	A	155	ASP	CA-CB-CG	7.13	119.73	112.60
1	C	155	ASP	CA-CB-CG	7.13	119.73	112.60
1	B	155	ASP	CA-CB-CG	7.05	119.65	112.60
1	B	338	PHE	CA-CB-CG	7.00	120.80	113.80
1	B	578	ASP	CA-CB-CG	6.23	118.83	112.60
1	D	355	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	414	SER	N-CA-C	5.98	118.29	111.11
1	B	414	SER	N-CA-C	5.89	118.18	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	TRP	N-CA-C	5.79	118.08	111.02
1	A	185	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	250	LEU	N-CA-C	5.68	118.21	111.33
1	A	330	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	185	PHE	CA-CB-CG	5.65	119.45	113.80
1	C	185	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	595	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	330	ASP	CA-CB-CG	5.58	118.19	112.60
1	B	250	LEU	N-CA-C	5.58	117.36	111.28
1	D	185	PHE	CA-CB-CG	5.56	119.36	113.80
1	D	168	THR	N-CA-C	-5.53	101.26	109.94
1	A	70	ASP	CA-CB-CG	5.49	118.08	112.60
1	D	304	TRP	N-CA-C	5.45	117.67	111.02
1	D	98	GLY	CA-C-N	5.44	131.93	121.54
1	D	98	GLY	C-N-CA	5.44	131.93	121.54
1	C	414	SER	N-CA-C	5.40	117.59	111.11
1	D	583	LYS	N-CA-C	-5.39	105.83	112.90
1	D	414	SER	N-CA-C	5.35	117.53	111.11
1	C	304	TRP	N-CA-C	5.34	117.54	111.02
1	A	171	GLY	N-CA-C	5.34	118.20	112.33
1	C	505	TYR	N-CA-C	5.33	120.44	113.88
1	A	501	PHE	CA-CB-CG	5.29	119.09	113.80
1	D	431	ILE	N-CA-C	-5.28	103.78	108.95
1	C	70	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	501	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	52	PRO	CA-C-N	5.21	125.87	120.03
1	C	52	PRO	C-N-CA	5.21	125.87	120.03
1	B	70	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	168	THR	N-CA-C	-5.12	101.87	109.96
1	B	171	GLY	N-CA-C	5.11	117.95	112.33
1	A	304	TRP	N-CA-C	5.11	117.24	111.11
1	C	357	THR	N-CA-C	-5.10	106.75	113.17
1	D	505	TYR	N-CA-C	5.05	120.09	113.88
1	C	595	ASP	CA-C-N	5.02	125.49	120.98
1	C	595	ASP	C-N-CA	5.02	125.49	120.98
1	B	655	ALA	CA-C-N	5.00	125.53	119.98
1	B	655	ALA	C-N-CA	5.00	125.53	119.98

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	5889	0	5694	44	0
1	B	5899	0	5718	28	0
1	C	5895	0	5704	48	0
1	D	5807	0	5627	42	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	B	8	12	12	0	0
3	C	4	6	6	0	0
4	A	588	0	0	2	0
4	B	572	0	0	0	0
4	C	437	0	0	2	0
4	D	377	0	0	4	0
All	All	25648	18	22881	135	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 3.

All (135) 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:449[B]:HIS:CE1	1:C:449[B]:HIS:CE1	2.39	1.10
1:A:21:GLU:HG3	1:D:247:PRO:HD2	1.57	0.86
1:C:448:MET:HG3	1:C:449[B]:HIS:ND1	1.91	0.86
1:B:682:ASN:OD1	1:B:707:THR:HG21	1.79	0.83
1:D:682:ASN:OD1	1:D:707:THR:HG21	1.79	0.80
1:D:191:THR:HB	1:D:194:GLY:O	1.80	0.80
1:B:451:MET:HE2	1:D:451:MET:HE2	1.63	0.79
1:D:191:THR:HG21	4:D:2095:HOH:O	1.82	0.78
1:C:448:MET:HG3	1:C:449[B]:HIS:CE1	2.18	0.78
1:D:191:THR:HG22	1:D:193:GLU:H	1.49	0.77
1:A:449[B]:HIS:CE1	1:C:449[B]:HIS:ND1	2.52	0.76
1:A:65:LEU:HD21	1:A:377[A]:ARG:NH1	2.04	0.73
1:C:191:THR:HB	1:C:194:GLY:O	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASP:CG	1:C:28:SER:H	1.99	0.71
1:A:65:LEU:CD2	1:A:377[A]:ARG:NH1	2.55	0.70
1:A:451:MET:HE2	1:C:451:MET:HE2	1.73	0.68
1:C:448:MET:HG3	1:C:449[B]:HIS:HD1	1.58	0.67
1:A:65:LEU:HD21	1:A:377[A]:ARG:HH12	1.59	0.67
1:C:710:ILE:HD13	1:C:718:ILE:HG13	1.77	0.66
1:A:710:ILE:HD13	1:A:718:ILE:HG13	1.77	0.66
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.78	0.66
1:D:710:ILE:HD13	1:D:718:ILE:HG13	1.78	0.66
1:A:424:GLY:HA3	1:C:449[B]:HIS:HE1	1.64	0.62
1:A:274:ILE:HD12	2:A:1754:HEM:HMB1	1.82	0.62
1:B:542:ARG:HG2	1:C:14:SER:H	1.68	0.58
1:A:213:LYS:HD3	1:D:92:GLN:HA	1.85	0.58
1:A:92:GLN:HA	1:D:213:LYS:HD3	1.86	0.57
1:C:666:ILE:HD11	1:C:732:LEU:HD22	1.87	0.57
1:A:449[B]:HIS:ND1	1:C:449[B]:HIS:CE1	2.72	0.57
1:B:92:GLN:HA	1:C:213:LYS:HD3	1.85	0.56
1:B:666:ILE:HD11	1:B:732:LEU:HD22	1.87	0.56
1:C:274:ILE:HD12	2:C:1754:HEM:HMB1	1.88	0.56
1:B:689:TYR:CE1	1:B:710:ILE:HD11	2.41	0.56
1:D:666:ILE:HD11	1:D:732:LEU:HD22	1.88	0.56
1:A:423:LEU:O	1:C:449[B]:HIS:NE2	2.38	0.56
1:D:205:ILE:HD11	1:D:255:TRP:CD1	2.41	0.56
1:A:666:ILE:HD11	1:A:732:LEU:HD22	1.89	0.55
1:A:689:TYR:CE1	1:A:710:ILE:HD11	2.41	0.55
1:D:392:HIS:HD1	1:D:394:GLY:H	1.55	0.55
1:D:689:TYR:CE1	1:D:710:ILE:HD11	2.42	0.55
1:C:689:TYR:CE1	1:C:710:ILE:HD11	2.42	0.55
1:B:213:LYS:HD3	1:C:92:GLN:HA	1.88	0.55
1:C:126:ILE:CG2	2:C:1754:HEM:HMD1	2.37	0.54
1:A:65:LEU:CD2	1:A:377[A]:ARG:HH12	2.19	0.53
1:C:490:GLU:HG2	1:D:490:GLU:HG2	1.90	0.53
1:B:603[B]:VAL:HG12	1:B:664:ALA:HB3	1.91	0.53
1:A:710:ILE:CD1	1:A:718:ILE:HG13	2.40	0.52
1:A:562:LEU:HA	1:D:637:MET:HB2	1.92	0.52
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.44	0.52
1:A:448:MET:HG3	1:A:449[B]:HIS:CE1	2.45	0.52
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.92	0.51
1:C:710:ILE:CD1	1:C:718:ILE:HG13	2.40	0.51
1:C:602:VAL:HG22	1:C:629:HIS:HB2	1.91	0.51
1:D:126:ILE:CG2	2:D:1754:HEM:HMD1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:ILE:CD1	1:D:718:ILE:HG13	2.40	0.51
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.41	0.50
1:A:423:LEU:O	1:C:449[B]:HIS:CE1	2.64	0.50
1:C:128:HIS:HA	1:C:168:THR:O	2.11	0.50
1:A:65:LEU:HD22	1:A:377[A]:ARG:NH1	2.26	0.50
1:D:607:LEU:HD11	1:D:632:LEU:HB3	1.94	0.50
1:B:607:LEU:HD11	1:B:632:LEU:HB3	1.94	0.50
1:A:449[B]:HIS:HE1	1:C:449[B]:HIS:CE1	2.21	0.49
1:C:191:THR:HG22	1:C:193:GLU:H	1.78	0.49
1:A:637:MET:HB2	1:D:562:LEU:HA	1.96	0.48
1:B:689:TYR:HE1	1:B:710:ILE:HD11	1.78	0.48
1:C:372[B]:LYS:HE2	1:C:374:VAL:CG2	2.44	0.48
1:A:696:ALA:HB2	1:A:732:LEU:HD13	1.96	0.48
1:C:392:HIS:HD1	1:C:394:GLY:H	1.61	0.48
1:B:637:MET:HB2	1:C:562:LEU:HA	1.95	0.47
1:B:473:THR:HG21	1:D:87:ARG:HH11	1.79	0.47
1:D:696:ALA:HB2	1:D:732:LEU:HD13	1.97	0.47
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.50	0.47
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.96	0.47
2:C:1754:HEM:CMC	2:C:1754:HEM:HBC2	2.46	0.46
1:D:191:THR:CG2	4:D:2095:HOH:O	2.53	0.46
1:B:468:ASN:O	1:B:471:ARG:HG3	2.16	0.46
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.98	0.46
1:C:468:ASN:O	1:C:471:ARG:HG3	2.16	0.46
1:C:696:ALA:HB2	1:C:732:LEU:HD13	1.98	0.46
1:B:115:THR:O	1:B:119:HIS:HD2	1.99	0.45
1:B:696:ALA:HB2	1:B:732:LEU:HD13	1.97	0.45
1:C:191:THR:HG21	4:C:2107:HOH:O	2.16	0.45
1:C:689:TYR:HE1	1:C:710:ILE:HD11	1.81	0.45
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.47	0.45
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.47	0.45
1:B:562:LEU:HA	1:C:637:MET:HB2	1.98	0.45
1:D:115:THR:O	1:D:119:HIS:HD2	1.99	0.45
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.52	0.45
1:C:115:THR:O	1:C:119:HIS:HD2	2.00	0.45
1:A:53:GLY:C	1:A:377[A]:ARG:HE	2.24	0.45
1:D:24:PRO:HA	1:D:25:GLY:HA2	1.85	0.45
1:D:468:ASN:O	1:D:471:ARG:HG3	2.16	0.45
1:C:607:LEU:HD11	1:C:632:LEU:HB3	1.99	0.44
1:D:274:ILE:HD12	2:D:1754:HEM:HMB1	1.99	0.44
1:A:155:ASP:HB3	1:A:158:LYS:HG3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:TYR:HE1	1:A:710:ILE:HD11	1.79	0.44
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.52	0.44
1:C:682:ASN:HB3	1:C:707:THR:HG21	1.98	0.44
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.53	0.44
1:A:115:THR:O	1:A:119:HIS:HD2	2.01	0.44
1:C:27:ASP:CG	1:C:28:SER:N	2.73	0.43
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.48	0.43
1:C:205:ILE:HD11	1:C:252:ASN:N	2.32	0.43
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.53	0.43
1:A:468:ASN:O	1:A:471:ARG:HG3	2.18	0.43
1:B:274:ILE:HD12	2:B:1754:HEM:HMB1	1.99	0.43
1:C:191:THR:CG2	4:C:2107:HOH:O	2.66	0.43
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.43
1:A:420:ILE:HG21	1:C:119:HIS:CE1	2.54	0.42
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.54	0.42
4:A:2253:HOH:O	1:D:52:PRO:HG3	2.20	0.42
1:C:334:TYR:N	1:C:372[A]:LYS:HZ1	2.18	0.42
1:A:121:ARG:CZ	1:D:126:ILE:HD12	2.49	0.42
1:D:689:TYR:HE1	1:D:710:ILE:HD11	1.81	0.42
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.50	0.42
1:B:205:ILE:HD13	1:B:251:HIS:CG	2.55	0.41
1:D:333:GLU:HB3	1:D:372:LYS:CE	2.50	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.41
1:D:435:ARG:HD3	4:D:2231:HOH:O	2.18	0.41
1:D:584:LYS:HD2	4:D:2315:HOH:O	2.21	0.41
1:A:602:VAL:HG21	4:A:2127:HOH:O	2.21	0.41
1:C:333:GLU:HB3	1:C:372[A]:LYS:NZ	2.35	0.41
1:D:333:GLU:HB3	1:D:372:LYS:HE3	2.02	0.41
1:A:205:ILE:HD13	1:A:251:HIS:CG	2.55	0.41
1:B:564:ILE:HG23	1:C:11:GLN:HG3	2.01	0.41
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.55	0.41
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.56	0.41
1:B:207:PHE:CD1	1:B:252:ASN:HB3	2.56	0.41
1:D:95:LEU:HB3	1:D:107:ASP:HB2	2.03	0.41
1:C:372[B]:LYS:HE2	1:C:374:VAL:HG23	2.03	0.41
1:A:126:ILE:CG2	2:A:1754:HEM:HMD1	2.51	0.40
1:A:21:GLU:HG3	1:D:246:GLN:HA	2.03	0.40
1:A:372:LYS:HE2	1:A:372:LYS:HB3	1.97	0.40
1:B:205:ILE:HD11	1:B:255:TRP:CD1	2.57	0.40
1:D:411:ARG:HG2	2:D:1754:HEM:C2C	2.56	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	745/753 (99%)	725 (97%)	20 (3%)	0	100	100
1	B	746/753 (99%)	724 (97%)	21 (3%)	1 (0%)	48	29
1	C	745/753 (99%)	725 (97%)	18 (2%)	2 (0%)	37	19
1	D	734/753 (98%)	717 (98%)	16 (2%)	1 (0%)	48	29
All	All	2970/3012 (99%)	2891 (97%)	75 (2%)	4 (0%)	48	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	SER
1	B	75	SER
1	C	75	SER
1	D	75	SER

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	627/636 (99%)	615 (98%)	12 (2%)	52	24
1	B	630/636 (99%)	616 (98%)	14 (2%)	47	18
1	C	628/636 (99%)	616 (98%)	12 (2%)	52	24
1	D	618/636 (97%)	608 (98%)	10 (2%)	58	32
All	All	2503/2544 (98%)	2455 (98%)	48 (2%)	54	24

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	32	GLU
1	A	126	ILE
1	A	191	THR
1	A	205	ILE
1	A	368	GLN
1	A	370	VAL
1	A	377[A]	ARG
1	A	377[B]	ARG
1	A	440	TYR
1	A	552	LEU
1	A	582	LEU
1	B	21	GLU
1	B	32	GLU
1	B	73	LYS
1	B	126	ILE
1	B	191	THR
1	B	205	ILE
1	B	368	GLN
1	B	370	VAL
1	B	377	ARG
1	B	440	TYR
1	B	478	LYS
1	B	552	LEU
1	B	583	LYS
1	B	624	LYS
1	C	21	GLU
1	C	126	ILE
1	C	205	ILE
1	C	370	VAL
1	C	372[A]	LYS
1	C	372[B]	LYS
1	C	440	TYR
1	C	449[A]	HIS
1	C	449[B]	HIS
1	C	478	LYS
1	C	552	LEU
1	C	707	THR
1	D	21	GLU
1	D	126	ILE
1	D	205	ILE
1	D	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	370	VAL
1	D	392	HIS
1	D	440	TYR
1	D	478	LYS
1	D	552	LEU
1	D	610	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	492	ASN
1	A	556	GLN
1	B	368	GLN
1	B	492	ASN
1	C	492	ASN
1	C	682	ASN
1	D	419	GLN
1	D	492	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	A	1754	1	41,50,50	2.04	10 (24%)	45,82,82	1.69	10 (22%)
3	EDO	B	1755	-	3,3,3	0.88	0	2,2,2	0.34	0
2	HEM	B	1754	1	41,50,50	1.79	11 (26%)	45,82,82	1.99	12 (26%)
2	HEM	C	1754	1	41,50,50	1.79	12 (29%)	45,82,82	1.88	15 (33%)
3	EDO	C	1755	-	3,3,3	0.61	0	2,2,2	0.46	0
2	HEM	D	1754	1	41,50,50	1.80	11 (26%)	45,82,82	1.76	12 (26%)
3	EDO	B	1756	-	3,3,3	0.49	0	2,2,2	0.04	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
2	HEM	A	1754	1	-	2/12/54/54	-
3	EDO	B	1755	-	-	0/1/1/1	-
2	HEM	B	1754	1	-	2/12/54/54	-
2	HEM	C	1754	1	-	2/12/54/54	-
3	EDO	C	1755	-	-	1/1/1/1	-
2	HEM	D	1754	1	-	3/12/54/54	-
3	EDO	B	1756	-	-	1/1/1/1	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1754	HEM	C3B-C4B	5.54	1.55	1.44
2	B	1754	HEM	O1D-CGD	4.98	1.38	1.22
2	C	1754	HEM	C4D-C3D	4.95	1.53	1.45
2	A	1754	HEM	C4D-C3D	4.72	1.53	1.45
2	D	1754	HEM	O1D-CGD	4.58	1.37	1.22
2	D	1754	HEM	CAA-C2A	-4.51	1.45	1.52
2	A	1754	HEM	O1D-CGD	3.81	1.34	1.22
2	B	1754	HEM	C4D-ND	-3.78	1.33	1.40
2	A	1754	HEM	C1B-NB	-3.74	1.33	1.40
2	D	1754	HEM	O2D-CGD	-3.57	1.18	1.30
2	C	1754	HEM	O1D-CGD	3.55	1.33	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1754	HEM	C4D-ND	-3.49	1.34	1.40
2	C	1754	HEM	C1B-NB	-3.47	1.34	1.40
2	D	1754	HEM	C4A-NA	3.43	1.43	1.36
2	B	1754	HEM	C1A-NA	3.35	1.43	1.36
2	C	1754	HEM	C1D-C2D	3.27	1.50	1.44
2	C	1754	HEM	CHB-C1B	3.15	1.43	1.35
2	B	1754	HEM	C1B-NB	-3.07	1.35	1.40
2	B	1754	HEM	C4A-NA	3.07	1.42	1.36
2	C	1754	HEM	C4A-NA	2.96	1.42	1.36
2	A	1754	HEM	C1A-NA	2.96	1.42	1.36
2	B	1754	HEM	C4D-C3D	2.74	1.49	1.45
2	D	1754	HEM	C4D-ND	-2.73	1.35	1.40
2	C	1754	HEM	C1A-NA	2.67	1.41	1.36
2	D	1754	HEM	CHB-C1B	2.62	1.41	1.35
2	D	1754	HEM	C3B-C4B	2.58	1.50	1.44
2	D	1754	HEM	C1B-NB	-2.56	1.35	1.40
2	C	1754	HEM	C3B-C4B	2.54	1.49	1.44
2	A	1754	HEM	O2A-CGA	2.53	1.39	1.30
2	B	1754	HEM	CHA-C4D	2.50	1.41	1.35
2	C	1754	HEM	O2D-CGD	-2.44	1.22	1.30
2	B	1754	HEM	O2D-CGD	-2.32	1.22	1.30
2	A	1754	HEM	C3D-C2D	-2.29	1.31	1.36
2	B	1754	HEM	CHB-C1B	2.27	1.40	1.35
2	A	1754	HEM	CHB-C1B	2.26	1.40	1.35
2	C	1754	HEM	CAB-C3B	2.24	1.53	1.47
2	C	1754	HEM	C4B-NB	-2.20	1.34	1.38
2	D	1754	HEM	CBD-CAD	2.17	1.58	1.52
2	C	1754	HEM	C4D-ND	-2.16	1.36	1.40
2	D	1754	HEM	O1A-CGA	2.15	1.29	1.22
2	A	1754	HEM	C1D-C2D	2.11	1.48	1.44
2	D	1754	HEM	C4D-C3D	2.10	1.48	1.45
2	B	1754	HEM	C3B-C4B	2.09	1.49	1.44
2	B	1754	HEM	C1B-C2B	2.03	1.48	1.44

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1754	HEM	CHD-C1D-C2D	-5.25	116.78	124.98
2	B	1754	HEM	C4B-C3B-C2B	-4.97	103.17	107.11
2	B	1754	HEM	CHD-C1D-ND	4.88	129.73	124.43
2	C	1754	HEM	CHD-C1D-ND	4.57	129.39	124.43
2	A	1754	HEM	CHD-C1D-ND	4.22	129.02	124.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1754	HEM	CHD-C1D-C2D	-4.06	118.64	124.98
2	D	1754	HEM	C4B-C3B-C2B	-3.92	104.01	107.11
2	D	1754	HEM	CHD-C1D-ND	3.91	128.68	124.43
2	D	1754	HEM	C4A-C3A-C2A	-3.82	104.34	107.00
2	C	1754	HEM	CBD-CAD-C3D	-3.37	103.26	112.63
2	A	1754	HEM	CAA-CBA-CGA	-3.34	104.39	113.76
2	D	1754	HEM	CHD-C1D-C2D	-3.29	119.84	124.98
2	C	1754	HEM	C4B-C3B-C2B	-3.23	104.55	107.11
2	A	1754	HEM	C4B-C3B-C2B	-3.22	104.56	107.11
2	A	1754	HEM	CBD-CAD-C3D	-3.19	103.78	112.63
2	A	1754	HEM	CHD-C1D-C2D	-3.15	120.06	124.98
2	D	1754	HEM	CAA-CBA-CGA	-3.11	105.05	113.76
2	B	1754	HEM	C1D-C2D-C3D	-3.05	103.75	106.96
2	B	1754	HEM	C4B-CHC-C1C	3.05	126.58	122.56
2	D	1754	HEM	CBD-CAD-C3D	-2.99	104.32	112.63
2	B	1754	HEM	C2D-C1D-ND	2.95	113.42	109.88
2	C	1754	HEM	C4C-CHD-C1D	-2.93	118.70	122.56
2	D	1754	HEM	C4B-CHC-C1C	2.81	126.27	122.56
2	C	1754	HEM	CMB-C2B-C1B	-2.80	120.78	125.04
2	A	1754	HEM	C2B-C1B-NB	2.75	113.10	109.84
2	D	1754	HEM	O2D-CGD-CBD	2.72	122.76	114.03
2	B	1754	HEM	CAA-CBA-CGA	-2.69	106.20	113.76
2	C	1754	HEM	CHB-C1B-NB	2.57	127.55	124.38
2	C	1754	HEM	CAA-CBA-CGA	-2.52	106.69	113.76
2	D	1754	HEM	CBA-CAA-C2A	2.47	116.84	112.62
2	C	1754	HEM	CMD-C2D-C1D	-2.38	121.41	125.04
2	B	1754	HEM	O2D-CGD-CBD	2.36	121.61	114.03
2	A	1754	HEM	CHB-C1B-C2B	-2.35	120.21	126.72
2	B	1754	HEM	CBB-CAB-C3B	-2.32	116.08	127.62
2	C	1754	HEM	CBB-CAB-C3B	-2.29	116.21	127.62
2	C	1754	HEM	O2D-CGD-CBD	2.27	121.32	114.03
2	C	1754	HEM	CMD-C2D-C3D	2.26	132.25	126.12
2	C	1754	HEM	CAD-C3D-C4D	2.25	128.59	124.66
2	C	1754	HEM	CAD-CBD-CGD	-2.23	108.81	113.60
2	A	1754	HEM	O2D-CGD-CBD	2.21	121.13	114.03
2	A	1754	HEM	CMC-C2C-C3C	2.21	128.81	124.68
2	D	1754	HEM	CHB-C1B-NB	2.12	127.00	124.38
2	B	1754	HEM	CHC-C4B-NB	-2.12	122.13	124.43
2	A	1754	HEM	C4B-CHC-C1C	2.10	125.33	122.56
2	B	1754	HEM	O2D-CGD-O1D	-2.05	118.18	123.30
2	D	1754	HEM	O2D-CGD-O1D	-2.05	118.19	123.30
2	B	1754	HEM	CBA-CAA-C2A	2.04	116.11	112.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1754	HEM	CMC-C2C-C3C	2.04	128.49	124.68
2	D	1754	HEM	CHB-C1B-C2B	-2.03	121.11	126.72

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1756	EDO	O1-C1-C2-O2
3	C	1755	EDO	O1-C1-C2-O2
2	C	1754	HEM	CAA-CBA-CGA-O1A
2	C	1754	HEM	CAA-CBA-CGA-O2A
2	A	1754	HEM	CAA-CBA-CGA-O1A
2	B	1754	HEM	CAA-CBA-CGA-O1A
2	A	1754	HEM	CAA-CBA-CGA-O2A
2	B	1754	HEM	CAA-CBA-CGA-O2A
2	D	1754	HEM	CAA-CBA-CGA-O2A
2	D	1754	HEM	CAA-CBA-CGA-O1A
2	D	1754	HEM	CAD-CBD-CGD-O2D

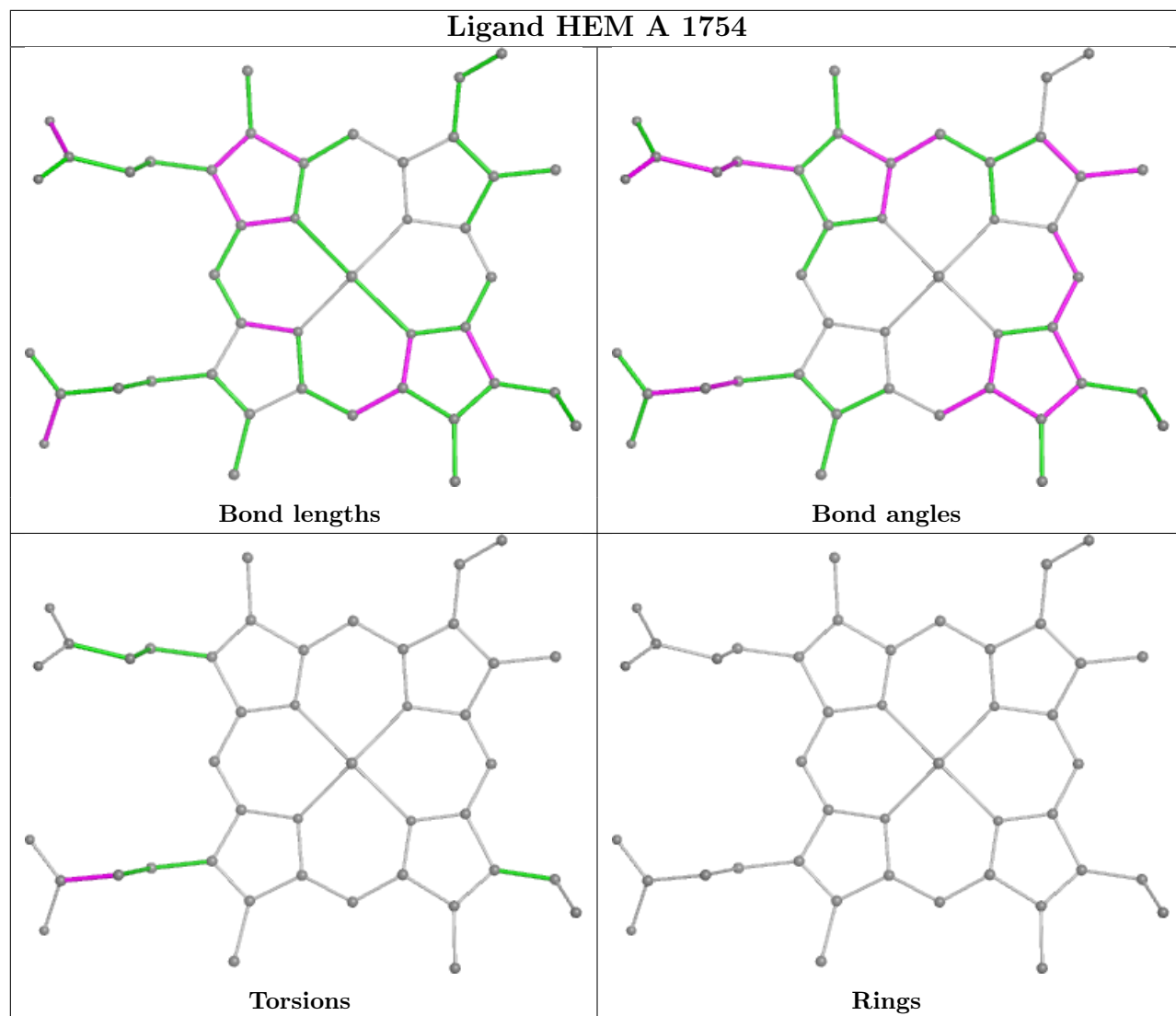
There are no ring outliers.

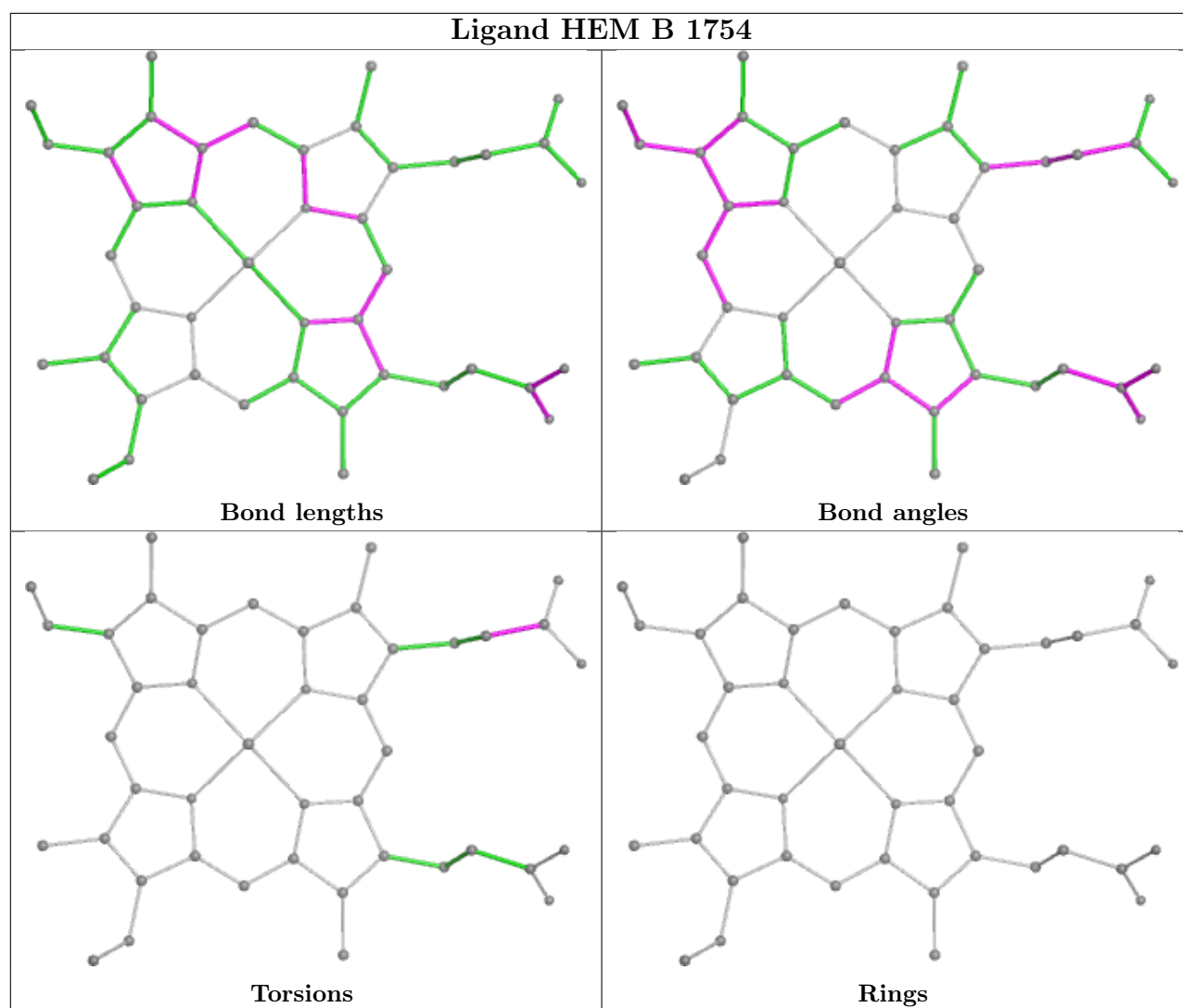
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1754	HEM	2	0
2	B	1754	HEM	1	0
2	C	1754	HEM	3	0
2	D	1754	HEM	3	0

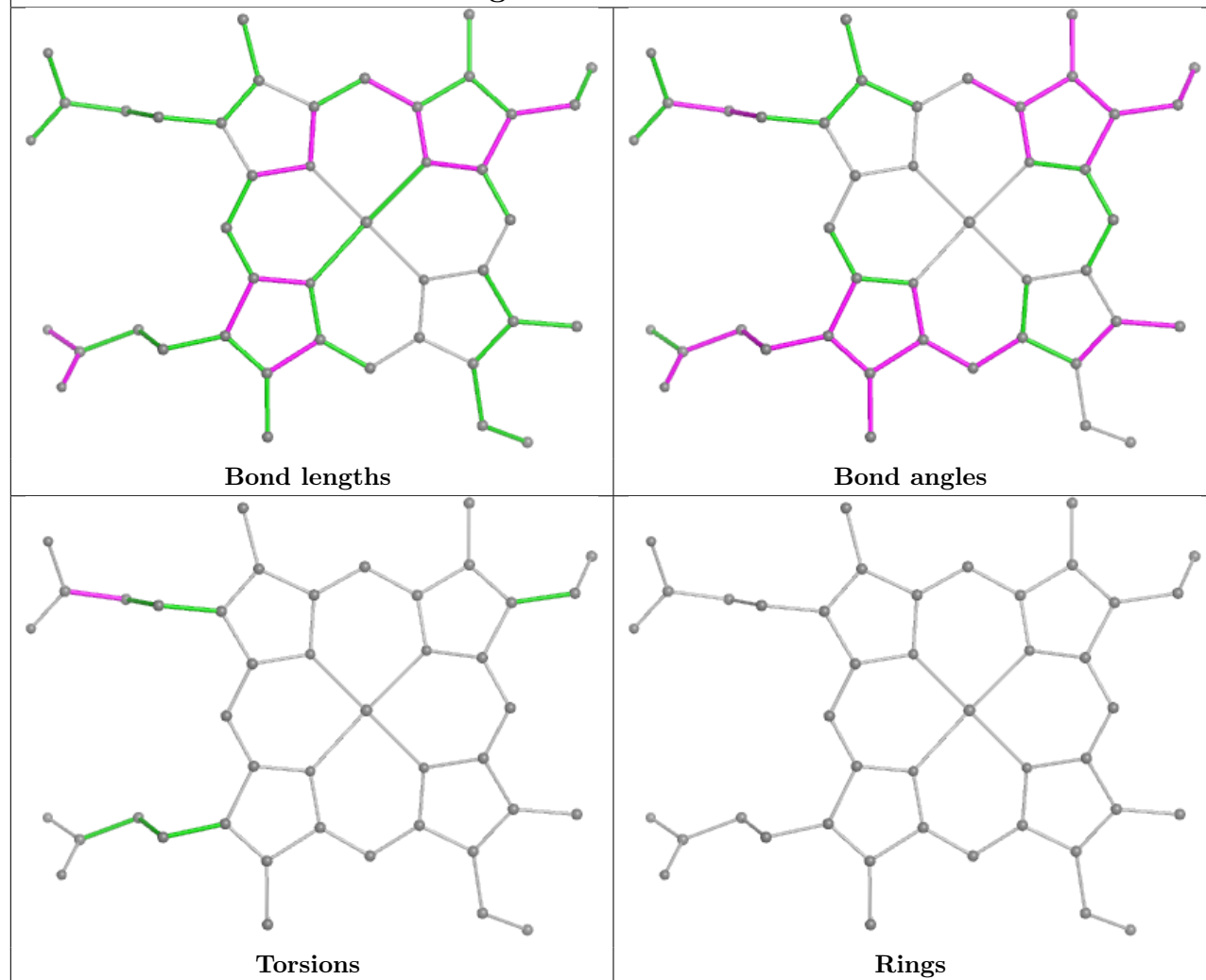
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

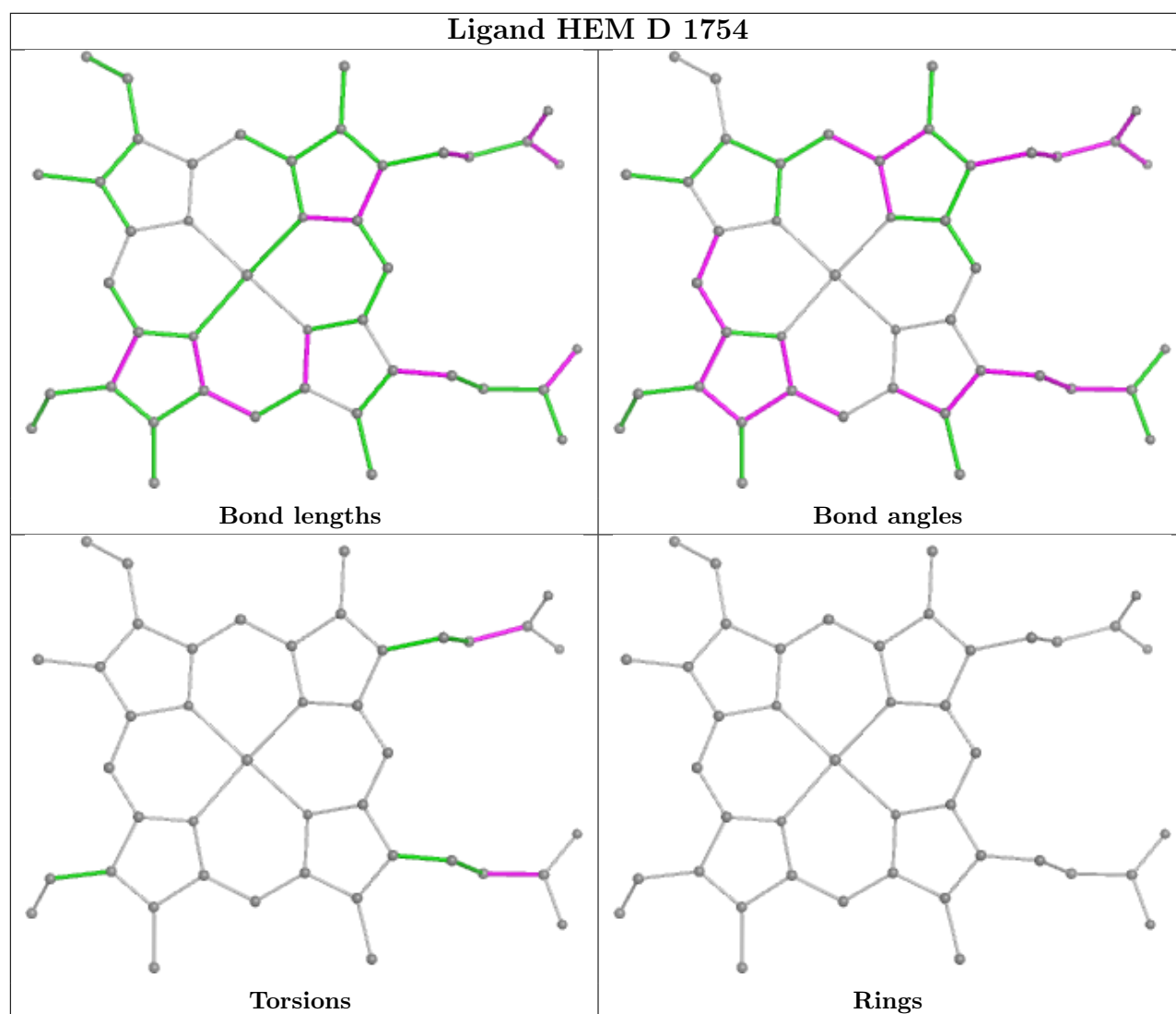
Ligand HEM A 1754





Ligand HEM C 1754





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	744/753 (98%)	0.00	18 (2%) 59 63	9, 27, 50, 70	3 (0%)
1	B	745/753 (98%)	-0.03	9 (1%) 76 80	9, 26, 48, 65	3 (0%)
1	C	743/753 (98%)	-0.07	21 (2%) 55 58	11, 24, 48, 72	4 (0%)
1	D	735/753 (97%)	0.00	11 (1%) 71 76	10, 26, 50, 68	1 (0%)
All	All	2967/3012 (98%)	-0.02	59 (1%) 64 69	9, 26, 49, 72	11 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	4.4
1	C	24	PRO	4.2
1	C	25	GLY	3.9
1	C	16	LEU	3.7
1	A	582	LEU	3.6
1	D	552	LEU	3.6
1	B	9	PRO	3.6
1	B	724	ALA	3.5
1	A	16	LEU	3.4
1	A	12	HIS	3.3
1	A	726	GLY	3.3
1	D	24	PRO	3.3
1	C	20	SER	3.2
1	A	10	HIS	3.2
1	B	726	GLY	3.0
1	C	724	ALA	3.0
1	D	724	ALA	3.0
1	C	11	GLN	2.9
1	A	596	GLY	2.9
1	C	13	GLN	2.9
1	A	13	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	595	ASP	2.8
1	C	14	SER	2.8
1	C	372[A]	LYS	2.7
1	D	27	ASP	2.7
1	A	24	PRO	2.7
1	C	18	ASP	2.7
1	C	17	HIS	2.7
1	C	21	GLU	2.6
1	C	27	ASP	2.6
1	A	725	ASP	2.5
1	C	12	HIS	2.5
1	D	26	MET	2.5
1	C	15	PRO	2.5
1	B	725	ASP	2.5
1	D	725	ASP	2.5
1	C	596	GLY	2.4
1	D	25	GLY	2.4
1	B	595	ASP	2.4
1	B	10	HIS	2.3
1	D	647	VAL	2.3
1	A	625	ALA	2.3
1	A	595	ASP	2.2
1	A	25	GLY	2.2
1	A	724	ALA	2.2
1	B	617	LEU	2.2
1	A	617	LEU	2.1
1	B	598	VAL	2.1
1	D	23	LYS	2.1
1	A	612	ARG	2.1
1	B	369	ARG	2.1
1	C	713	GLN	2.1
1	C	725	ASP	2.1
1	A	598	VAL	2.1
1	C	710	ILE	2.0
1	A	11	GLN	2.0
1	D	595	ASP	2.0
1	D	726	GLY	2.0
1	A	15	PRO	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

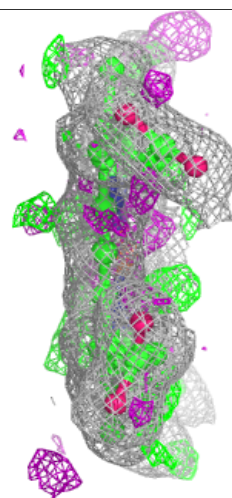
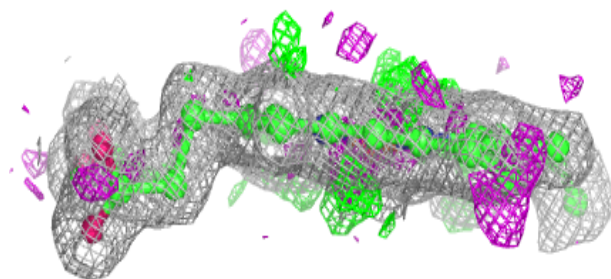
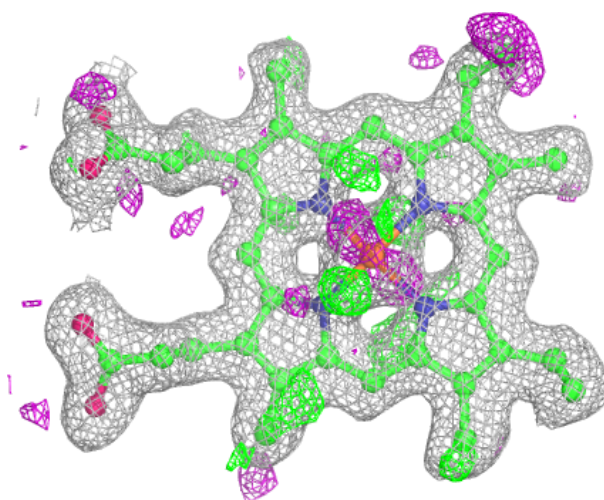
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	B	1756	4/4	0.85	0.12	39,41,42,42	0
3	EDO	B	1755	4/4	0.86	0.09	19,19,20,20	0
3	EDO	C	1755	4/4	0.86	0.10	33,34,35,35	0
2	HEM	A	1754	43/43	0.97	0.07	12,13,15,18	0
2	HEM	C	1754	43/43	0.97	0.06	12,13,15,16	0
2	HEM	D	1754	43/43	0.97	0.07	11,12,15,16	0
2	HEM	B	1754	43/43	0.98	0.06	11,12,15,17	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.

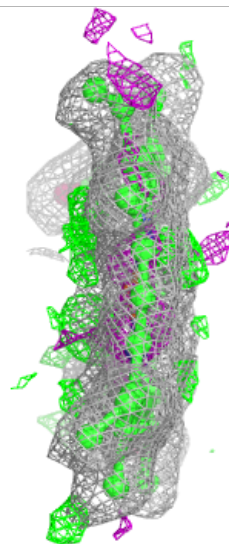
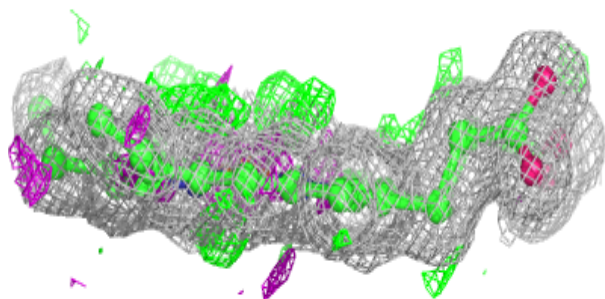
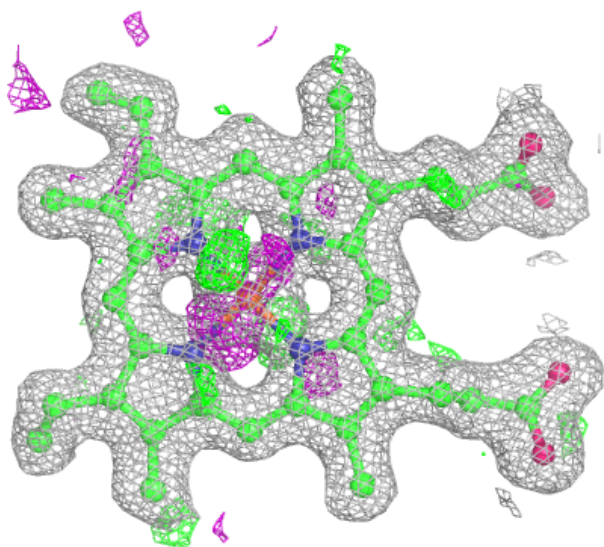
Electron density around HEM A 1754:

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



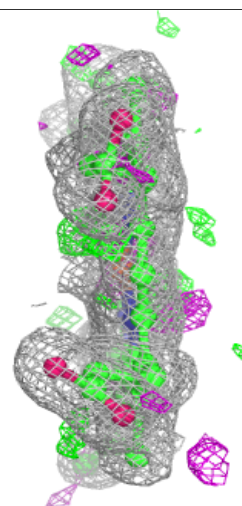
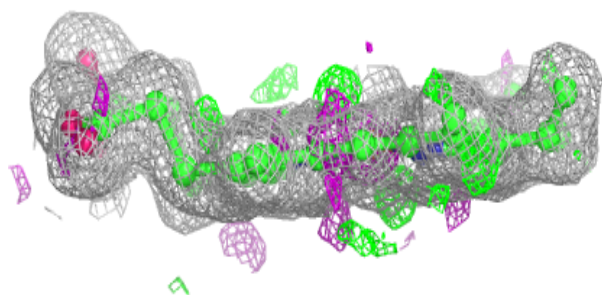
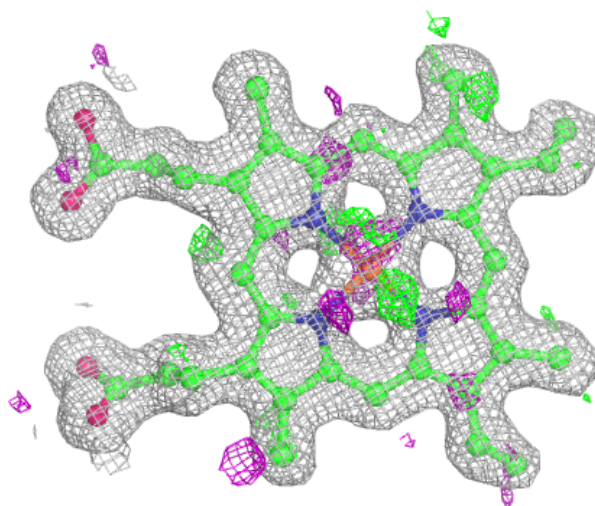
Electron density around HEM C 1754:

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



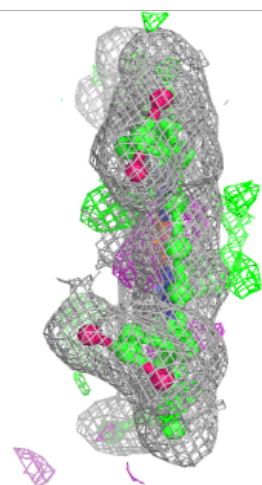
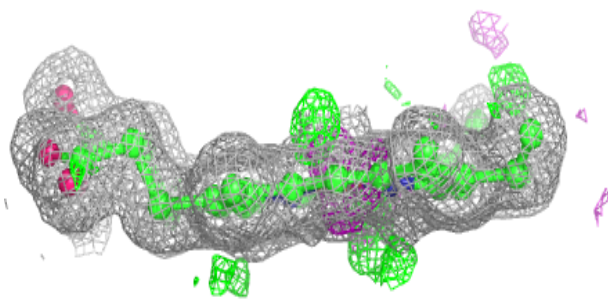
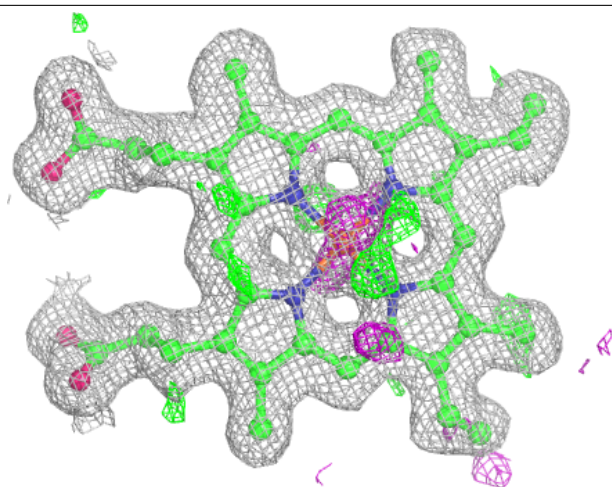
Electron density around HEM D 1754:

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



Electron density around HEM B 1754:

$2mF_o-DF_c$ (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.