Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 06:21 PM EST

PDB ID	:	2BMH
Title	:	MODELING PROTEIN-SUBSTRATE INTERACTIONS IN THE HEME DOMAIN OF CYTOCHROME P450BM-3
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	1994-05-17
Resolution	:	2.00 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*
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:

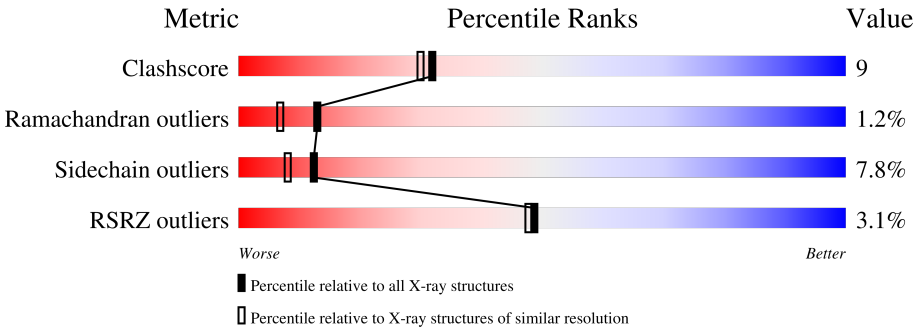
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 <=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	455	3% 77% 20% ·
1	B	455	4% 72% 25% ·

2 Entry composition

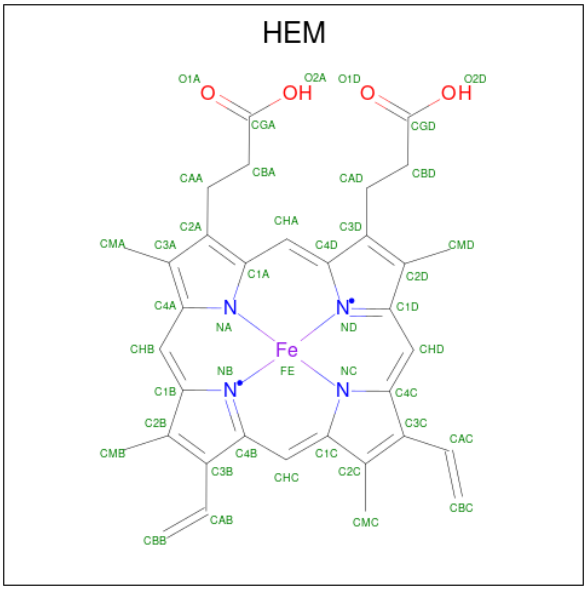
There are 3 unique types of molecules in this entry. The entry contains 7818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P450 BM-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3671	2345	623	686	17			
1	B	455	Total	C	N	O	S	0	0	0
			3671	2345	623	686	17			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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		

- Molecule 3 is water.

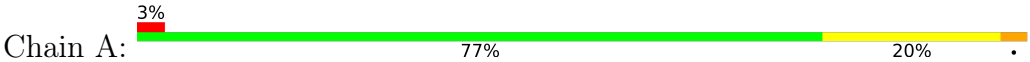
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	215	Total O 215 215	0	0
3	B	175	Total O 175 175	0	0

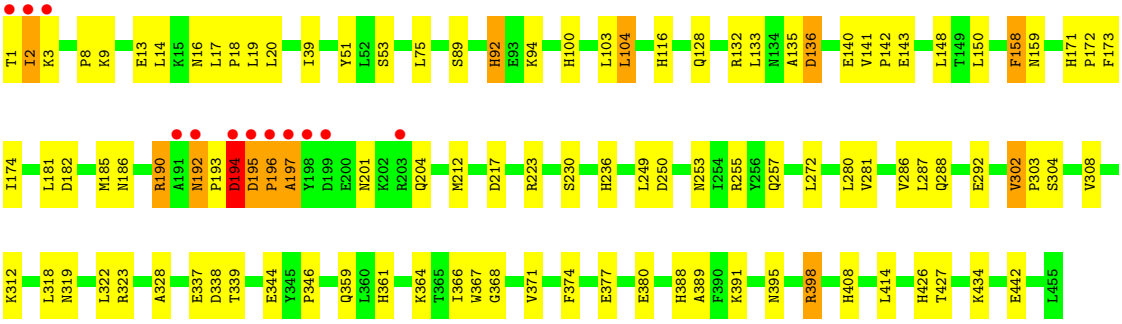
3 Residue-property plots (i)

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: CYTOCHROME P450 BM-3

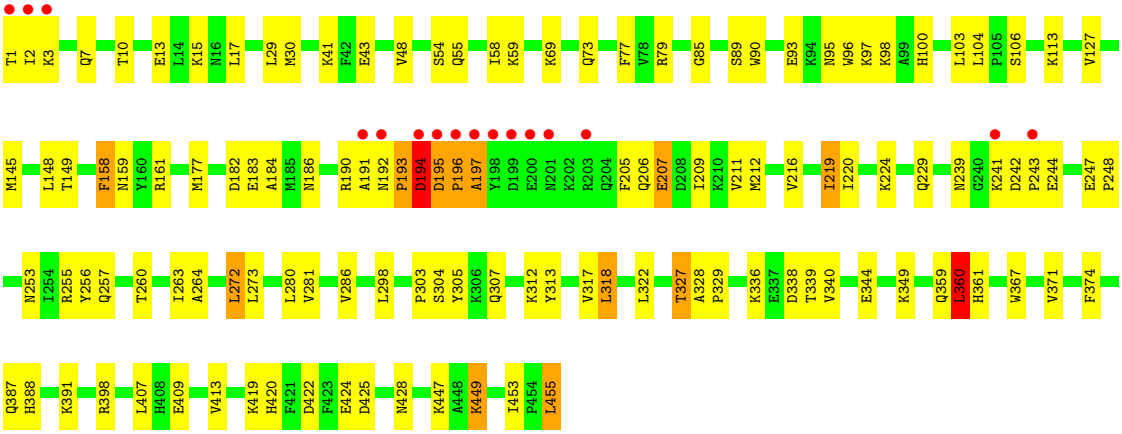
Chain A:





• Molecule 1: CYTOCHROME P450 BM-3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.53Å 154.03Å 62.43Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 48.39 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 70.3 (48.39-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.81 (at 2.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , (Not available) 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 86.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7818	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.39	0/3756	0.65	2/5077 (0.0%)
1	B	0.38	0/3756	0.70	4/5077 (0.1%)
All	All	0.39	0/7512	0.68	6/10154 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	244	GLU	CB-CA-C	-6.57	97.26	110.40
1	B	328	ALA	N-CA-C	-5.96	94.90	111.00
1	A	148	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	422	ASP	N-CA-C	-5.43	96.35	111.00
1	B	360	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	328	ALA	N-CA-C	-5.09	97.27	111.00

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	3671	0	3645	61	0
1	B	3671	0	3645	70	0
2	A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	0	0
3	A	215	0	0	2	0
3	B	175	0	0	4	0
All	All	7818	0	7350	131	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 9.

All (131) 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:190:ARG:HD2	1:A:196:PRO:HD2	1.49	0.95
1:A:16:ASN:HB3	1:A:19:LEU:HD12	1.57	0.84
1:B:256:TYR:O	1:B:260:THR:HG23	1.85	0.75
1:A:2:ILE:H	1:A:2:ILE:HD13	1.52	0.73
1:B:10:THR:HG23	1:B:15:LYS:HA	1.73	0.70
1:B:361:HIS:HE1	1:B:391:LYS:H	1.36	0.70
1:B:216:VAL:O	1:B:219:ILE:HG22	1.91	0.70
1:A:192:ASN:ND2	1:A:195:ASP:HB3	2.07	0.69
1:B:192:ASN:HD21	1:B:195:ASP:HB3	1.57	0.69
1:B:339:THR:HG22	1:B:340:VAL:H	1.58	0.69
1:A:89:SER:O	1:A:398:ARG:NH2	2.28	0.66
1:A:223:ARG:HH22	1:A:230:SER:HB2	1.62	0.65
1:A:361:HIS:HE1	1:A:391:LYS:H	1.43	0.64
1:A:190:ARG:NH2	1:A:197:ALA:HB2	2.12	0.64
1:B:190:ARG:HG3	1:B:196:PRO:HD2	1.80	0.63
1:B:190:ARG:HD2	1:B:196:PRO:HB2	1.80	0.63
1:B:194:ASP:O	1:B:195:ASP:HB2	1.99	0.62
1:A:116:HIS:HE1	1:A:303:PRO:O	1.83	0.61
1:A:192:ASN:HD21	1:A:195:ASP:HB3	1.66	0.60
1:B:192:ASN:ND2	1:B:195:ASP:HB3	2.15	0.60
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.83	0.60
1:B:127:VAL:HG11	1:B:455:LEU:HD21	1.83	0.59
1:B:253:ASN:O	1:B:257:GLN:HG2	2.02	0.59
1:A:171:HIS:HD2	1:A:173:PHE:H	1.49	0.59
1:B:298:LEU:HD22	1:B:303:PRO:HB3	1.85	0.59
1:B:190:ARG:HA	1:B:196:PRO:HD2	1.85	0.58
1:B:43:GLU:HG3	1:B:48:VAL:HG22	1.85	0.58
1:B:69:LYS:HD3	1:B:398:ARG:CZ	2.34	0.58
1:B:220:ILE:O	1:B:224:LYS:HG3	2.05	0.57
1:B:30:MET:HG2	1:B:359:GLN:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:HG2	1:B:242:ASP:HB2	1.85	0.56
1:A:434:LYS:HB2	1:A:442:GLU:HB2	1.87	0.56
1:B:97:LYS:HB2	3:B:783:HOH:O	2.05	0.56
1:B:205:PHE:CE2	1:B:209:ILE:HD11	2.40	0.56
1:A:17:LEU:HB3	1:A:18:PRO:HD3	1.88	0.56
1:B:387:GLN:HG2	1:B:388:HIS:CD2	2.41	0.56
1:A:141:VAL:HB	1:A:142:PRO:HD3	1.88	0.55
1:A:253:ASN:O	1:A:257:GLN:HG2	2.07	0.55
1:A:280:LEU:HD22	1:A:287:LEU:HA	1.88	0.54
1:B:190:ARG:CZ	1:B:197:ALA:HB3	2.36	0.54
1:B:85:GLY:HA3	1:B:260:THR:HG21	1.89	0.54
1:A:8:PRO:HB2	1:A:19:LEU:CD1	2.38	0.54
1:B:193:PRO:O	1:B:194:ASP:HB2	2.07	0.53
1:B:191:ALA:HB3	1:B:195:ASP:O	2.09	0.53
1:A:116:HIS:HD2	1:A:408:HIS:NE2	2.07	0.53
1:A:100:HIS:HD2	3:A:632:HOH:O	1.92	0.52
1:A:288:GLN:O	1:A:292:GLU:HG3	2.10	0.52
1:A:323:ARG:HA	1:A:361:HIS:CD2	2.45	0.52
1:B:424:GLU:HB2	1:B:449:LYS:HE2	1.92	0.52
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.92	0.52
1:B:158:PHE:CD1	1:B:158:PHE:N	2.79	0.51
1:A:92:HIS:H	1:A:92:HIS:CD2	2.27	0.51
1:A:140:GLU:HB3	1:A:143:GLU:OE1	2.12	0.50
1:A:194:ASP:O	1:A:195:ASP:HB2	2.11	0.50
1:A:135:ALA:O	1:A:136:ASP:HB3	2.12	0.50
1:B:420:HIS:HE1	3:B:552:HOH:O	1.93	0.50
1:A:181:LEU:O	1:A:185:MET:HG2	2.11	0.50
1:B:113:LYS:HE2	1:B:305:TYR:CE2	2.46	0.50
1:A:128:GLN:O	1:A:132:ARG:HG3	2.11	0.49
1:B:419:LYS:HE2	1:B:453:ILE:HG21	1.95	0.49
1:B:100:HIS:O	1:B:104:LEU:HB2	2.12	0.49
1:A:2:ILE:HG12	1:A:2:ILE:O	2.12	0.49
1:A:186:ASN:HB3	1:A:190:ARG:NH1	2.26	0.49
1:B:192:ASN:O	1:B:194:ASP:N	2.46	0.49
1:A:16:ASN:O	1:A:19:LEU:HB2	2.12	0.49
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.95	0.48
1:B:272:LEU:HG	1:B:322:LEU:HD13	1.95	0.48
1:A:377:GLU:O	1:A:380:GLU:HB2	2.12	0.48
1:B:55:GLN:O	1:B:59:LYS:HB2	2.14	0.48
1:B:183:GLU:HG2	1:B:205:PHE:CD1	2.48	0.48
1:B:219:ILE:HD13	1:B:219:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:HB3	1:A:359:GLN:HB3	1.96	0.47
1:A:426:HIS:CE1	1:A:427:THR:HG23	2.49	0.47
1:B:7:GLN:HG3	1:B:41:LYS:O	2.14	0.47
1:B:239:ASN:HD22	1:B:239:ASN:N	2.12	0.47
1:A:8:PRO:HB2	1:A:19:LEU:HD11	1.97	0.47
1:A:3:LYS:HD2	1:A:344:GLU:HA	1.97	0.47
1:B:1:THR:HG23	1:B:1:THR:O	2.15	0.46
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.96	0.46
1:B:161:ARG:HA	3:B:477:HOH:O	2.15	0.46
1:A:158:PHE:CD1	1:A:158:PHE:N	2.84	0.46
1:B:281:VAL:HG13	1:B:425:ASP:HB2	1.98	0.46
1:A:388:HIS:HD2	1:A:391:LYS:NZ	2.14	0.46
1:B:336:LYS:O	1:B:349:LYS:HG3	2.16	0.45
1:A:344:GLU:O	1:A:346:PRO:HD3	2.16	0.45
1:A:190:ARG:CZ	1:A:197:ALA:HB2	2.46	0.45
1:A:223:ARG:HH22	1:A:230:SER:CB	2.27	0.45
1:B:77:PHE:HB3	1:B:184:ALA:HB1	1.99	0.45
1:B:420:HIS:CE1	1:B:455:LEU:HD23	2.52	0.45
1:A:286:VAL:HG11	1:A:374:PHE:HE2	1.80	0.45
1:B:190:ARG:CD	1:B:196:PRO:HB2	2.45	0.44
1:B:205:PHE:O	1:B:209:ILE:HG13	2.17	0.44
1:B:327:THR:O	1:B:329:PRO:HD3	2.18	0.44
1:A:9:LYS:HE2	1:A:9:LYS:HB2	1.77	0.44
1:A:236:HIS:HB3	3:A:671:HOH:O	2.17	0.43
1:B:360:LEU:HD22	3:B:836:HOH:O	2.17	0.43
1:B:177:MET:HA	1:B:212:MET:SD	2.59	0.43
1:B:207:GLU:O	1:B:211:VAL:HG23	2.18	0.43
1:A:217:ASP:OD1	1:A:255:ARG:HD3	2.19	0.43
1:B:336:LYS:O	1:B:349:LYS:HE3	2.19	0.43
1:A:39:ILE:HA	1:A:51:TYR:O	2.18	0.43
1:A:194:ASP:O	1:A:195:ASP:CB	2.66	0.43
1:B:190:ARG:HG3	1:B:196:PRO:CD	2.49	0.43
1:B:79:ARG:HH12	1:B:89:SER:HA	1.82	0.42
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.93	0.42
1:A:302:VAL:HA	1:A:303:PRO:HD3	1.78	0.42
1:A:364:LYS:HA	1:A:368:GLY:O	2.20	0.42
1:B:54:SER:O	1:B:58:ILE:HG23	2.20	0.42
1:B:286:VAL:HG11	1:B:374:PHE:HE2	1.85	0.42
1:A:391:LYS:NZ	1:A:395:ASN:HD22	2.18	0.42
1:B:89:SER:OG	1:B:96:TRP:HB2	2.19	0.42
1:A:319:ASN:HD22	1:A:319:ASN:HA	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:HIS:O	1:A:104:LEU:HB2	2.19	0.41
1:B:2:ILE:HA	1:B:344:GLU:O	2.20	0.41
1:A:14:LEU:HG	1:A:18:PRO:HD3	2.01	0.41
1:A:173:PHE:CE2	1:A:212:MET:HA	2.55	0.41
1:B:195:ASP:N	1:B:196:PRO:O	2.54	0.41
1:B:242:ASP:HA	1:B:243:PRO:HD3	1.87	0.41
1:A:190:ARG:HH21	1:A:197:ALA:HB2	1.83	0.41
1:B:90:TRP:HB2	1:B:93:GLU:HG3	2.01	0.41
1:A:14:LEU:HD11	1:A:17:LEU:HD23	2.03	0.41
1:A:94:LYS:HA	1:A:94:LYS:HD2	1.87	0.41
1:A:150:LEU:HD13	1:A:174:ILE:HD13	2.03	0.41
1:B:263:ILE:HG13	1:B:264:ALA:N	2.36	0.41
1:A:304:SER:O	1:A:308:VAL:HG23	2.21	0.41
1:A:323:ARG:HG2	1:A:361:HIS:HB3	2.02	0.41
1:B:313:TYR:O	1:B:317:VAL:HG23	2.21	0.41
1:B:145:MET:O	1:B:149:THR:HG23	2.22	0.40
1:B:247:GLU:HA	1:B:248:PRO:HD3	1.83	0.40
1:B:304:SER:OG	1:B:307:GLN:HG3	2.22	0.40
1:B:103:LEU:O	1:B:106:SER:HB2	2.22	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	453/455 (100%)	427 (94%)	20 (4%)	6 (1%)	12	6
1	B	453/455 (100%)	426 (94%)	22 (5%)	5 (1%)	14	8
All	All	906/910 (100%)	853 (94%)	42 (5%)	11 (1%)	13	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	A	194	ASP
1	A	195	ASP
1	A	196	PRO
1	A	197	ALA
1	B	194	ASP
1	B	195	ASP
1	B	197	ALA
1	B	193	PRO
1	B	196	PRO
1	A	193	PRO

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	399/399 (100%)	368 (92%)	31 (8%)	12 8
1	B	399/399 (100%)	368 (92%)	31 (8%)	12 8
All	All	798/798 (100%)	736 (92%)	62 (8%)	12 8

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	2	ILE
1	A	13	GLU
1	A	20	LEU
1	A	75	LEU
1	A	92	HIS
1	A	103	LEU
1	A	104	LEU
1	A	133	LEU
1	A	158	PHE
1	A	159	ASN
1	A	172	PRO
1	A	182	ASP

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Mol	Chain	Res	Type
1	A	190	ARG
1	A	192	ASN
1	A	194	ASP
1	A	201	ASN
1	A	204	GLN
1	A	249	LEU
1	A	250	ASP
1	A	272	LEU
1	A	281	VAL
1	A	302	VAL
1	A	312	LYS
1	A	318	LEU
1	A	322	LEU
1	A	337	GLU
1	A	338	ASP
1	A	339	THR
1	A	398	ARG
1	A	414	LEU
1	B	3	LYS
1	B	13	GLU
1	B	17	LEU
1	B	29	LEU
1	B	73	GLN
1	B	95	ASN
1	B	158	PHE
1	B	159	ASN
1	B	182	ASP
1	B	186	ASN
1	B	194	ASP
1	B	206	GLN
1	B	207	GLU
1	B	219	ILE
1	B	229	GLN
1	B	241	LYS
1	B	255	ARG
1	B	272	LEU
1	B	273	LEU
1	B	280	LEU
1	B	312	LYS
1	B	318	LEU
1	B	327	THR
1	B	338	ASP

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Mol	Chain	Res	Type
1	B	360	LEU
1	B	407	LEU
1	B	409	GLU
1	B	428	ASN
1	B	447	LYS
1	B	449	LYS
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	92	HIS
1	A	95	ASN
1	A	100	HIS
1	A	116	HIS
1	A	128	GLN
1	A	138	HIS
1	A	171	HIS
1	A	192	ASN
1	A	204	GLN
1	A	229	GLN
1	A	239	ASN
1	A	266	HIS
1	A	319	ASN
1	A	361	HIS
1	A	388	HIS
1	A	395	ASN
1	A	403	GLN
1	B	27	GLN
1	B	95	ASN
1	B	100	HIS
1	B	101	ASN
1	B	116	HIS
1	B	192	ASN
1	B	201	ASN
1	B	213	ASN
1	B	229	GLN
1	B	239	ASN
1	B	266	HIS
1	B	359	GLN
1	B	361	HIS

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Mol	Chain	Res	Type
1	B	395	ASN
1	B	420	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	460	1,3	41,50,50	1.53	6 (14%)	45,82,82	1.10	2 (4%)
2	HEM	B	460	1,3	41,50,50	1.40	3 (7%)	45,82,82	1.28	7 (15%)

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	460	1,3	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	460	1,3	-	2/12/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	460	HEM	C3C-CAC	-4.04	1.39	1.47
2	A	460	HEM	C3C-CAC	-3.74	1.40	1.47
2	B	460	HEM	C3C-C2C	-3.49	1.35	1.40
2	A	460	HEM	C3C-C2C	-3.33	1.35	1.40
2	A	460	HEM	C2C-C1C	2.99	1.49	1.42
2	A	460	HEM	CAB-C3B	-2.83	1.39	1.47
2	B	460	HEM	CAB-C3B	-2.38	1.41	1.47
2	A	460	HEM	CMB-C2B	2.28	1.55	1.50
2	A	460	HEM	CMC-C2C	2.08	1.56	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	460	HEM	C4C-CHD-C1D	3.13	126.69	122.56
2	A	460	HEM	C3B-C2B-C1B	-2.94	104.30	106.49
2	B	460	HEM	CMD-C2D-C1D	2.67	129.10	125.04
2	A	460	HEM	C2B-C1B-NB	2.34	112.61	109.84
2	B	460	HEM	C1D-C2D-C3D	-2.33	104.50	106.96
2	B	460	HEM	CAD-C3D-C2D	-2.26	123.67	127.88
2	B	460	HEM	C4B-CHC-C1C	2.21	125.48	122.56
2	B	460	HEM	C4A-C3A-C2A	-2.15	105.50	107.00
2	B	460	HEM	C2B-C1B-NB	2.09	112.31	109.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

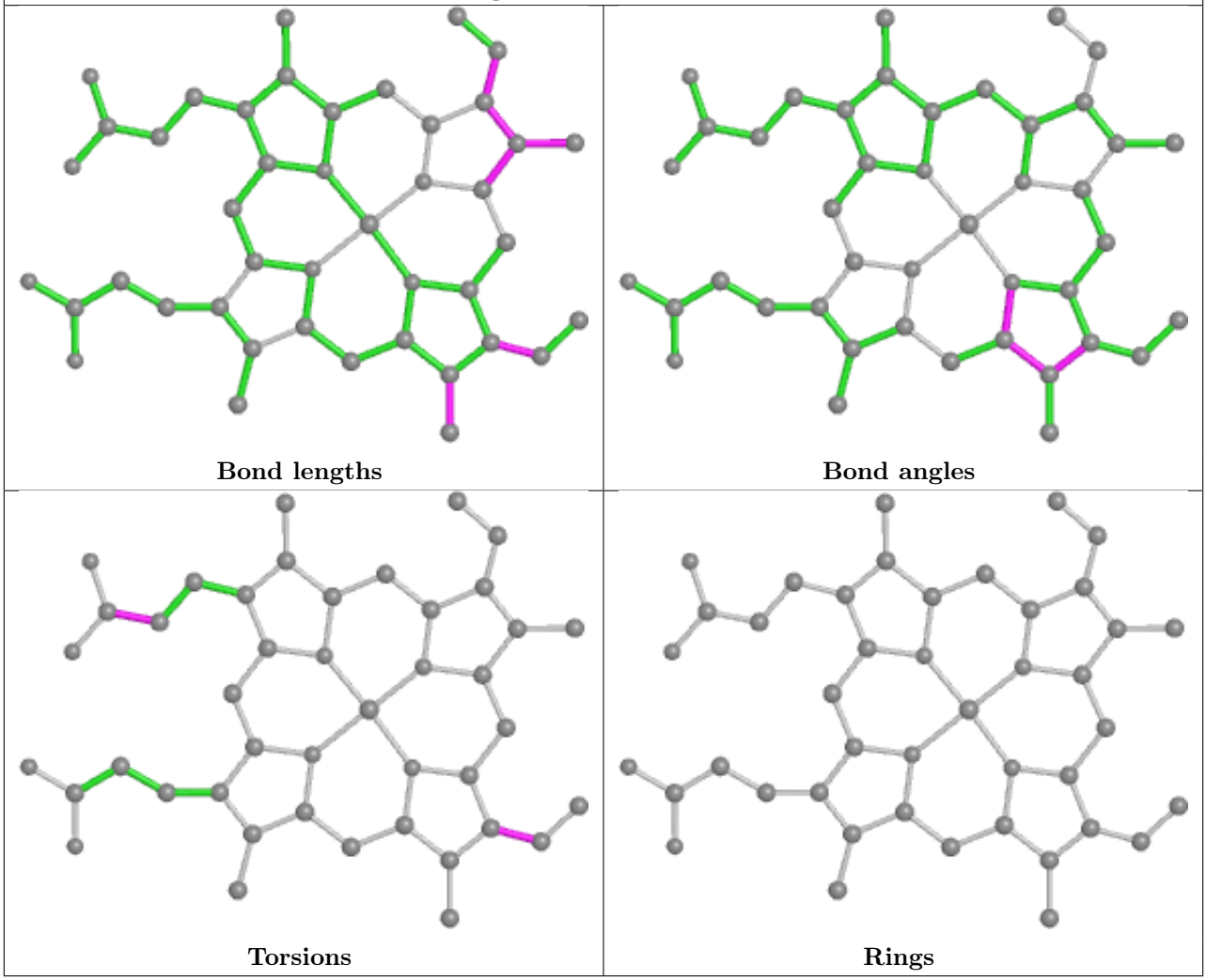
Mol	Chain	Res	Type	Atoms
2	A	460	HEM	C2B-C3B-CAB-CBB
2	A	460	HEM	CAD-CBD-CGD-O1D
2	A	460	HEM	CAD-CBD-CGD-O2D
2	B	460	HEM	CAD-CBD-CGD-O2D
2	B	460	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

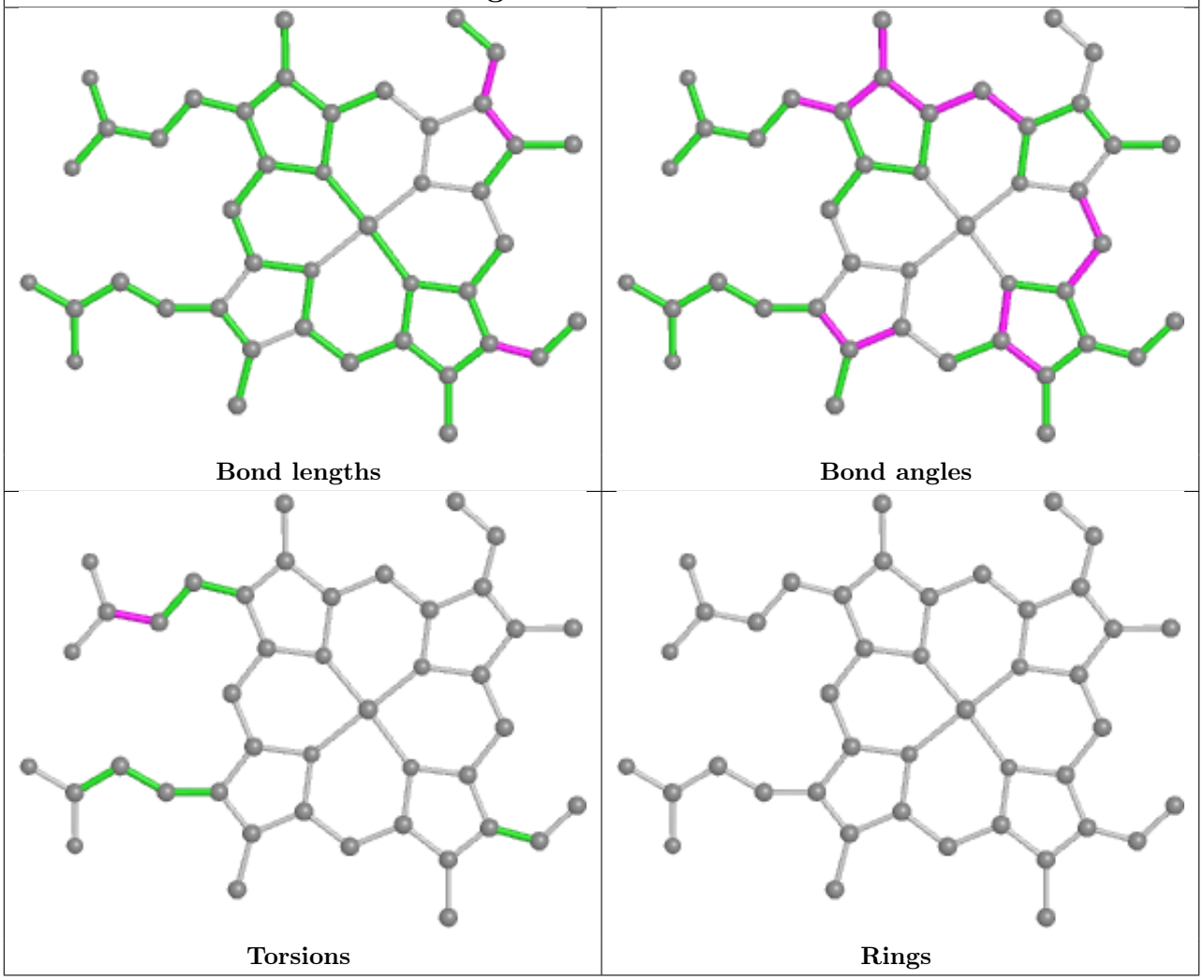
No monomer is involved in short contacts.

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 then 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 460



Ligand HEM B 460



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, 95^{th} 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	455/455 (100%)	-0.19	12 (2%)	56	54	6, 23, 67, 124	0
1	B	455/455 (100%)	-0.12	16 (3%)	44	43	7, 29, 68, 115	0
All	All	910/910 (100%)	-0.15	28 (3%)	49	48	6, 26, 68, 124	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	14.2
1	A	195	ASP	14.0
1	B	195	ASP	11.5
1	A	2	ILE	9.7
1	B	196	PRO	7.7
1	A	196	PRO	7.5
1	B	1	THR	5.3
1	B	191	ALA	5.1
1	A	191	ALA	4.6
1	B	2	ILE	4.5
1	B	192	ASN	3.8
1	A	198	TYR	3.8
1	B	200	GLU	3.5
1	A	197	ALA	3.4
1	B	197	ALA	3.3
1	A	199	ASP	3.2
1	B	194	ASP	3.2
1	B	203	ARG	3.1
1	B	198	TYR	2.8
1	B	243	PRO	2.6
1	B	201	ASN	2.6
1	A	192	ASN	2.5
1	A	203	ARG	2.5
1	B	199	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	ASP	2.1
1	A	3	LYS	2.1
1	B	241	LYS	2.0
1	B	3	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

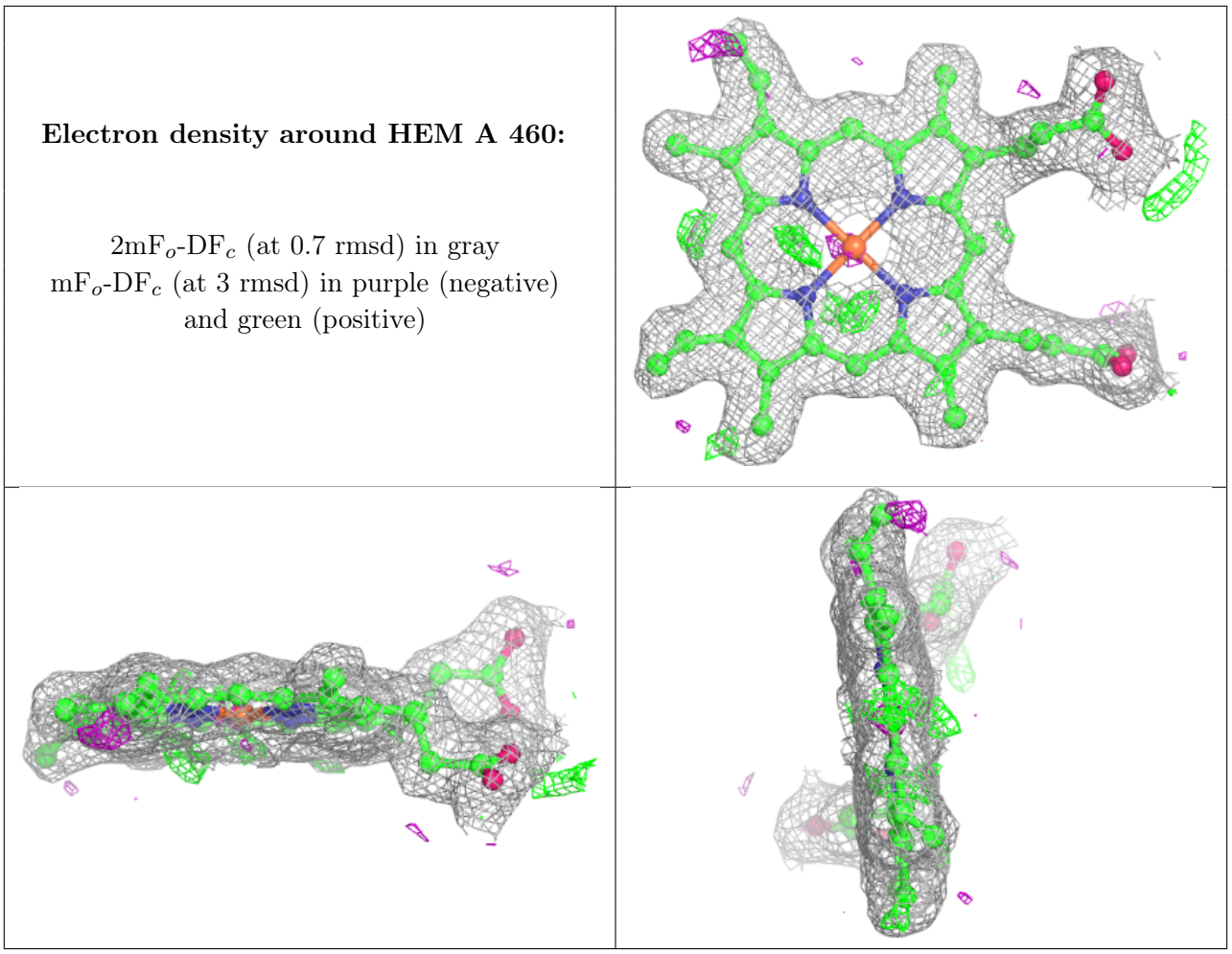
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	460	43/43	0.97	0.10	2,9,14,17	0
2	HEM	B	460	43/43	0.98	0.09	9,18,24,29	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.

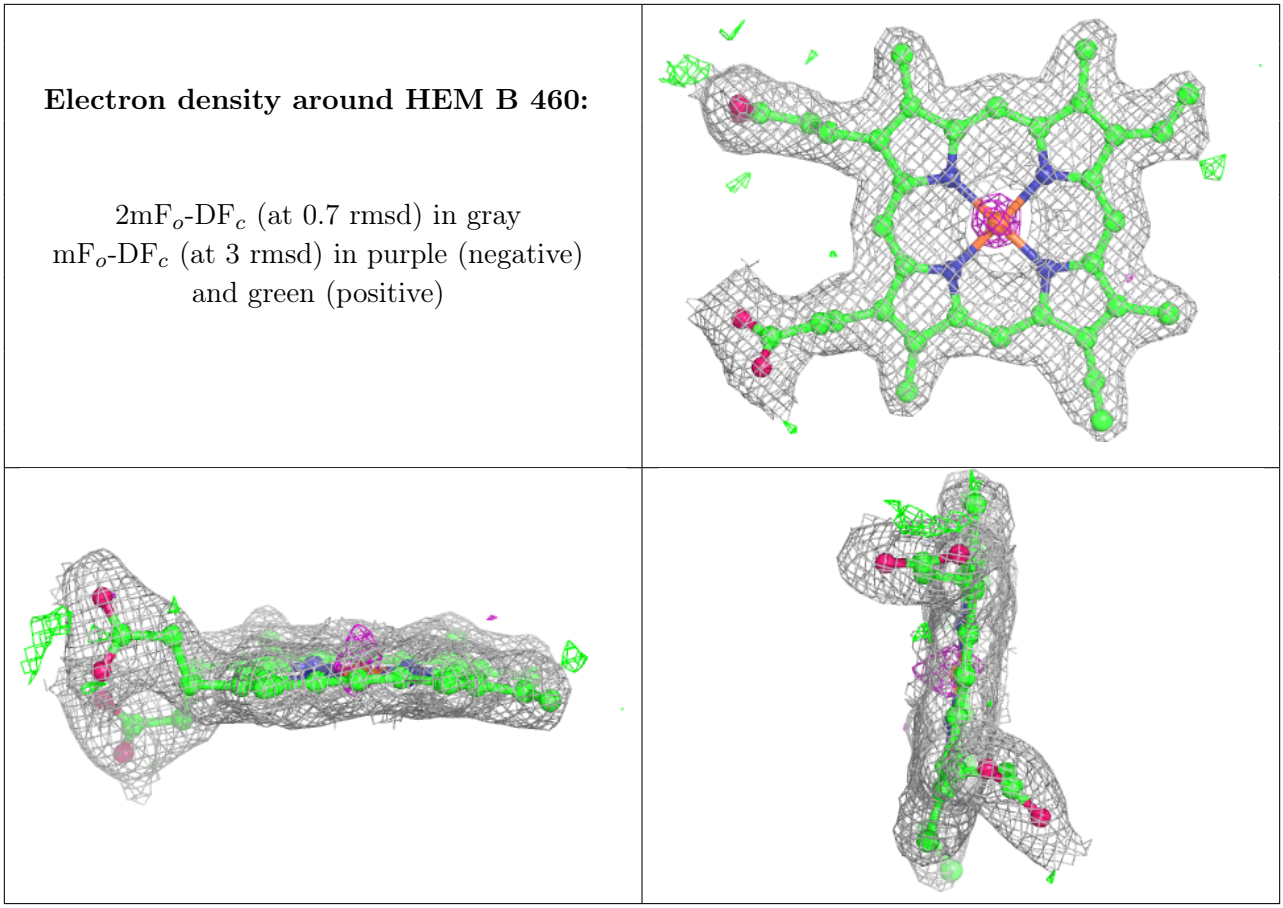
Electron density around HEM A 460:

$2mF_o$-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 460:

$2mF_o$-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

There are no such residues in this entry.