



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:27 pm BST

PDB ID : 2A9E
Title : Helicobacter pylori catalase compound I
Authors : Loewen, P.C.; Carpena, X.; Fita, I.
Deposited on : 2005-07-11
Resolution : 1.76 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

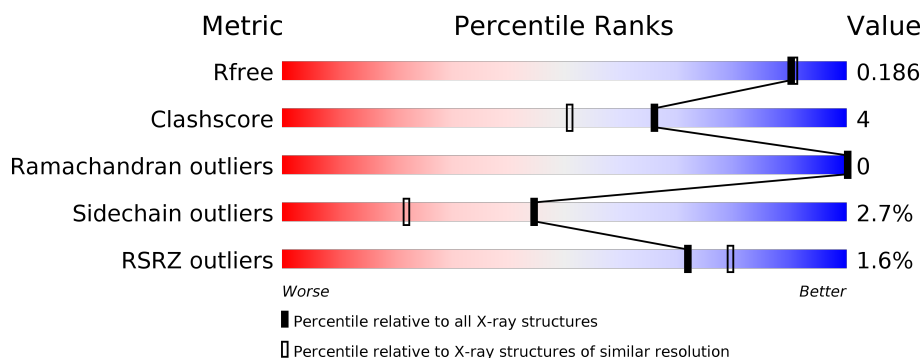
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	505	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	505	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9112 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 KatA Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	11	0
			4072	2599	706	753	14			
1	B	491	Total	C	N	O	S	0	11	0
			4064	2594	703	753	14			

There are 8 discrepancies between the modelled and reference sequences:

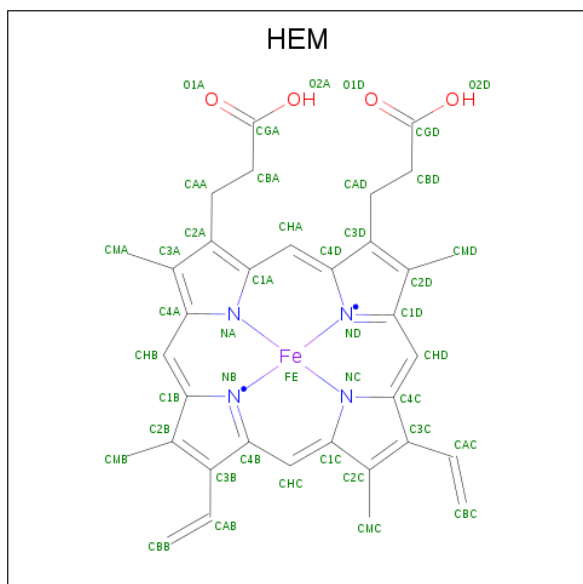
Chain	Residue	Modelled	Actual	Comment	Reference
A	162	MHO	MET	MODIFIED RESIDUE	UNP P77872
A	181	MHO	MET	MODIFIED RESIDUE	UNP P77872
A	292	MHO	MET	MODIFIED RESIDUE	UNP P77872
A	372	MHO	MET	MODIFIED RESIDUE	UNP P77872
B	162	MHO	MET	MODIFIED RESIDUE	UNP P77872
B	181	MHO	MET	MODIFIED RESIDUE	UNP P77872
B	292	MHO	MET	MODIFIED RESIDUE	UNP P77872
B	372	MHO	MET	MODIFIED RESIDUE	UNP P77872

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



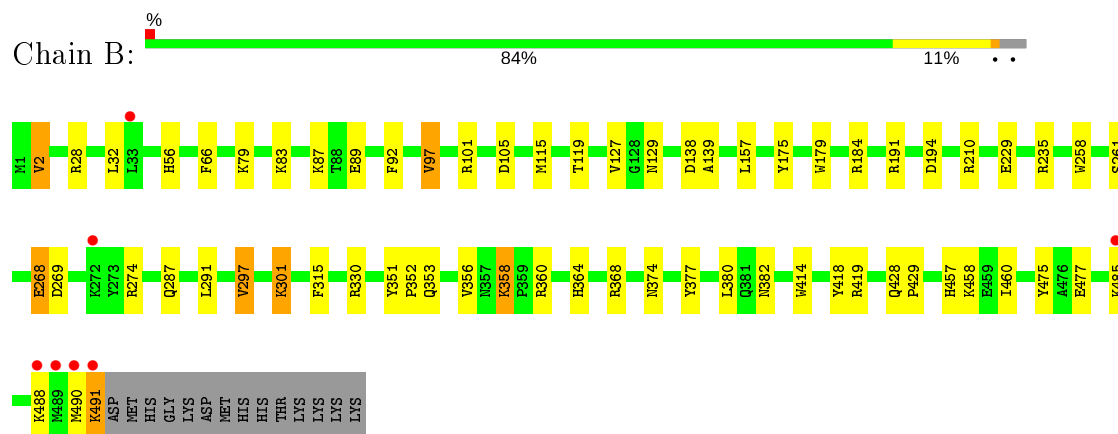
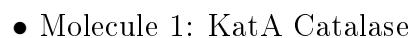
- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	440	Total 440	O 440	0	0
5	B	444	Total 444	O 444	0	0

- Molecule 1: KatA Catalase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.39 Å 154.29 Å 95.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.00 – 1.76 37.06 – 1.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.00-1.76) 96.6 (37.06-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.76 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.137 , 0.178 0.148 , 0.186	Depositor DCC
R_{free} test set	4674 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9112	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MHO, ACT, O, 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	1.23	11/4211 (0.3%)	1.05	13/5694 (0.2%)
1	B	1.30	16/4200 (0.4%)	1.12	25/5680 (0.4%)
All	All	1.26	27/8411 (0.3%)	1.08	38/11374 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	LYS	CE-NZ	8.05	1.69	1.49
1	A	376	TYR	CB-CG	7.92	1.63	1.51
1	A	229	GLU	CG-CD	7.47	1.63	1.51
1	A	466	GLU	CB-CG	-6.62	1.39	1.52
1	A	376	TYR	CG-CD1	6.51	1.47	1.39
1	B	360	ARG	CZ-NH1	6.51	1.41	1.33
1	B	297[A]	VAL	CB-CG1	6.23	1.66	1.52
1	B	297[B]	VAL	CB-CG1	6.23	1.66	1.52
1	A	477	GLU	CG-CD	6.13	1.61	1.51
1	B	419	ARG	C-O	6.10	1.34	1.23
1	B	229	GLU	CG-CD	6.02	1.60	1.51
1	A	376	TYR	CE1-CZ	5.96	1.46	1.38
1	B	477	GLU	CG-CD	5.84	1.60	1.51
1	B	97	VAL	CB-CG2	5.73	1.64	1.52
1	B	235	ARG	CB-CG	-5.55	1.37	1.52
1	A	392	LYS	CD-CE	5.54	1.65	1.51
1	B	301	LYS	CD-CE	5.51	1.65	1.51
1	B	89	GLU	CB-CG	5.43	1.62	1.52
1	B	268[A]	GLU	CB-CG	5.29	1.62	1.52
1	B	268[B]	GLU	CB-CG	5.29	1.62	1.52
1	A	339	TYR	CE1-CZ	5.17	1.45	1.38
1	B	97	VAL	CB-CG1	5.17	1.63	1.52
1	A	401	LYS	CB-CG	-5.13	1.38	1.52
1	A	270	ALA	CA-CB	5.09	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	GLU	CD-OE1	5.08	1.31	1.25
1	B	358	LYS	CG-CD	5.06	1.69	1.52
1	B	179	TRP	CE3-CZ3	5.02	1.47	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	B	28	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	B	330	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	A	210	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	B	184	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	194	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	2	VAL	CG1-CB-CG2	6.97	122.05	110.90
1	A	101[A]	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	A	101[B]	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	B	101[A]	ARG	N-CA-C	6.87	129.54	111.00
1	B	101[B]	ARG	N-CA-C	6.87	129.54	111.00
1	B	83	LYS	CD-CE-NZ	6.58	126.84	111.70
1	A	191	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	194	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	191	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	360	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	356	VAL	CG1-CB-CG2	6.33	121.03	110.90
1	B	301	LYS	CD-CE-NZ	6.26	126.11	111.70
1	A	194	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	210	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	210	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	368	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	368	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	101[A]	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	A	101[B]	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	B	269	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	B	380	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	B	101[A]	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	101[B]	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	360[A]	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	360[B]	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	269	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	28	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	191	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	138	ASP	CB-CG-OD2	-5.15	113.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	184	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	105	ASP	CB-CG-OD1	5.01	122.81	118.30

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	4072	0	3893	35	1
1	B	4064	0	3874	35	0
2	A	4	0	3	0	0
3	A	43	0	30	4	0
3	B	43	0	30	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	440	0	0	8	3
5	B	444	0	0	3	3
All	All	9112	0	7830	64	4

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 4.

All (64) 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:B:358:LYS:NZ	1:B:358:LYS:CE	1.69	1.49
1:A:32[A]:LEU:HD23	1:B:32[A]:LEU:HD23	1.20	1.15
1:A:101[B]:ARG:O	5:A:1321:HOH:O	1.69	1.07
1:A:89:GLU:OE1	5:A:1133:HOH:O	1.75	1.02
1:A:32[A]:LEU:HD23	1:B:32[A]:LEU:CD2	1.92	0.98
1:A:32[A]:LEU:CD2	1:B:32[A]:LEU:CD2	2.66	0.74
1:A:353:GLN:HE22	1:A:374:ASN:H	1.41	0.69
1:A:360[A]:ARG:NH1	5:A:1327:HOH:O	1.82	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274[A]:ARG:HH22	1:B:287:GLN:NE2	1.93	0.65
1:B:364:HIS:HD2	5:B:888:HOH:O	1.80	0.64
1:B:353:GLN:HE22	1:B:374:ASN:H	1.44	0.64
1:A:1:MET:HE3	1:A:3:ASN:HD21	1.68	0.58
1:A:32[A]:LEU:CD2	1:B:32[A]:LEU:HD23	2.12	0.58
1:A:139:ALA:HB2	3:A:550:HEM:HBB1	1.87	0.57
1:A:118:TYR:CD1	1:A:360[B]:ARG:HD3	2.39	0.57
1:B:491:LYS:NZ	1:B:491:LYS:HB2	2.21	0.56
1:B:490:MET:H	1:B:491:LYS:C	2.10	0.55
1:B:490:MET:N	1:B:491:LYS:C	2.61	0.54
1:A:32[A]:LEU:CD2	1:B:32[A]:LEU:HD21	2.38	0.53
1:B:258:TRP:HB2	1:B:297[B]:VAL:HG23	1.90	0.53
1:A:1:MET:CE	1:A:3:ASN:HD21	2.23	0.52
1:B:428:GLN:N	1:B:429:PRO:HD2	2.25	0.52
1:A:139:ALA:CB	3:A:550:HEM:HBB1	2.42	0.50
1:B:457:HIS:HB2	1:B:460:ILE:HD12	1.93	0.49
1:B:491:LYS:HZ2	1:B:491:LYS:HB2	1.77	0.49
1:A:287:GLN:HG2	5:A:1255:HOH:O	2.13	0.49
1:B:428:GLN:N	1:B:429:PRO:CD	2.76	0.49
1:A:56:HIS:CE1	1:A:97:VAL:HG22	2.48	0.48
1:A:490:MET:N	1:A:491:LYS:HA	2.29	0.48
1:A:409:LYS:HG3	5:A:1143:HOH:O	2.15	0.47
1:B:79:LYS:HE3	5:B:937:HOH:O	2.15	0.47
1:A:129:ASN:CG	3:A:550:HEM:HAC	2.35	0.47
1:A:135:PHE:CE2	1:A:176:GLN:HG3	2.51	0.46
1:A:268[B]:GLU:HG2	5:A:1248:HOH:O	2.13	0.46
1:B:261[B]:SER:OG	1:B:291:LEU:HD22	2.14	0.46
1:A:327:SER:HB2	1:A:328:PRO:HD2	1.97	0.46
1:B:139:ALA:CB	3:B:550:HEM:CBB	2.94	0.46
1:B:66:PHE:O	1:B:87:LYS:HA	2.17	0.45
1:B:351:TYR:N	1:B:352:PRO:CD	2.80	0.45
1:B:129:ASN:CG	3:B:550:HEM:HAC	2.38	0.44
1:B:92:PHE:CZ	1:B:297[A]:VAL:HG11	2.52	0.44
1:A:135:PHE:CZ	1:A:176:GLN:HG3	2.53	0.44
1:A:95:SER:O	1:A:111:ARG:HA	2.17	0.44
1:A:360[A]:ARG:CD	5:A:1327:HOH:O	2.67	0.43
1:A:364:HIS:HD2	5:A:1105:HOH:O	2.02	0.42
1:B:56:HIS:CE1	1:B:97:VAL:HG22	2.54	0.42
1:A:236:LYS:HE3	1:A:237:HIS:CE1	2.54	0.42
1:A:204:ILE:HD12	1:A:400:PRO:HG2	2.02	0.42
1:B:92:PHE:CZ	1:B:297[B]:VAL:HG11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ALA:CB	3:B:550:HEM:HBB1	2.49	0.42
1:B:358:LYS:HD2	5:B:875:HOH:O	2.19	0.42
1:B:92:PHE:CZ	1:B:115:MET:HG2	2.55	0.41
1:A:147:HIS:HB3	1:B:382:ASN:OD1	2.21	0.41
1:A:358:LYS:HE2	1:A:358:LYS:HB3	1.82	0.41
1:A:23:ILE:HG22	1:A:32[A]:LEU:HD12	2.03	0.41
1:B:139:ALA:HB2	3:B:550:HEM:HBB1	2.02	0.41
1:A:56:HIS:HA	1:A:96:THR:O	2.21	0.41
1:A:66:PHE:O	1:A:87:LYS:HA	2.20	0.41
1:B:92:PHE:CE1	1:B:115:MET:HG2	2.55	0.41
1:A:139:ALA:CB	3:A:550:HEM:CBB	2.98	0.41
1:B:488:LYS:O	1:B:491:LYS:HG3	2.22	0.40
1:B:139:ALA:HA	3:B:550:HEM:HBB1	2.04	0.40
1:B:127:VAL:HG22	1:B:315:PHE:HB3	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1339:HOH:O	5:B:993:HOH:O[2_565]	2.02	0.18
5:A:1295:HOH:O	5:A:1295:HOH:O[2_565]	2.13	0.07
5:A:1318:HOH:O	5:B:916:HOH:O[2_565]	2.14	0.06
1:A:372:MHO:OD1	5:B:688:HOH:O[2_565]	2.19	0.01

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	496/505 (98%)	478 (96%)	18 (4%)	0	100	100
1	B	495/505 (98%)	478 (97%)	17 (3%)	0	100	100
All	All	991/1010 (98%)	956 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	435/438 (99%)	424 (98%)	11 (2%)	47	25
1	B	434/438 (99%)	421 (97%)	13 (3%)	41	18
All	All	869/876 (99%)	845 (97%)	24 (3%)	44	20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	119	THR
1	A	175	TYR
1	A	267	GLU
1	A	271	LYS
1	A	377	TYR
1	A	414	TRP
1	A	418	TYR
1	A	475	TYR
1	A	485	LYS
1	A	490	MET
1	B	2	VAL
1	B	119	THR
1	B	175	TYR
1	B	268[A]	GLU
1	B	268[B]	GLU
1	B	301	LYS
1	B	377	TYR
1	B	414	TRP
1	B	418	TYR
1	B	458	LYS
1	B	475	TYR
1	B	485	LYS
1	B	491	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	149	GLN
1	A	237	HIS
1	A	353	GLN
1	A	364	HIS
1	B	287	GLN
1	B	353	GLN
1	B	364	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MHO	A	292	1	7,8,9	3.68	2 (28%)	4,9,11	2.49	2 (50%)
1	MHO	A	181	1	7,8,9	3.28	2 (28%)	4,9,11	3.38	3 (75%)
1	MHO	B	162	1	7,8,9	3.29	3 (42%)	4,9,11	5.11	3 (75%)
1	MHO	B	181	1	7,8,9	2.02	2 (28%)	4,9,11	2.01	2 (50%)
1	MHO	A	162	1	7,8,9	3.50	3 (42%)	4,9,11	4.05	3 (75%)
1	MHO	B	372	1	7,8,9	3.27	2 (28%)	4,9,11	3.47	2 (50%)
1	MHO	B	292	1	7,8,9	3.95	1 (14%)	4,9,11	2.38	1 (25%)
1	MHO	A	372	1	7,8,9	2.76	2 (28%)	4,9,11	1.99	1 (25%)

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
1	MHO	A	292	1	-	0/6/7/9	-
1	MHO	A	181	1	-	1/6/7/9	-
1	MHO	B	162	1	-	2/6/7/9	-
1	MHO	B	181	1	-	1/6/7/9	-
1	MHO	A	162	1	-	2/6/7/9	-
1	MHO	B	372	1	-	2/6/7/9	-
1	MHO	B	292	1	-	0/6/7/9	-
1	MHO	A	372	1	-	3/6/7/9	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	MHO	OD1-SD	10.09	1.77	1.50
1	A	292	MHO	OD1-SD	9.17	1.75	1.50
1	A	181	MHO	OD1-SD	8.15	1.72	1.50
1	B	372	MHO	OD1-SD	8.00	1.72	1.50
1	A	162	MHO	OD1-SD	7.92	1.72	1.50
1	B	162	MHO	OD1-SD	7.58	1.71	1.50
1	A	372	MHO	OD1-SD	6.61	1.68	1.50
1	B	181	MHO	OD1-SD	4.44	1.62	1.50
1	A	162	MHO	CB-CA	3.39	1.58	1.53
1	B	162	MHO	CB-CA	3.21	1.57	1.53
1	B	372	MHO	CG-SD	-3.11	1.66	1.80
1	A	162	MHO	CG-SD	-3.10	1.66	1.80
1	A	181	MHO	CG-SD	-2.88	1.67	1.80
1	B	181	MHO	CG-SD	-2.87	1.67	1.80
1	A	292	MHO	CG-SD	-2.63	1.68	1.80
1	B	162	MHO	CG-SD	-2.57	1.68	1.80
1	A	372	MHO	CB-CA	2.31	1.56	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	MHO	CE-SD-CG	8.85	117.84	97.71
1	A	162	MHO	CE-SD-CG	5.99	111.34	97.71
1	A	181	MHO	OD1-SD-CG	-5.07	92.06	106.03
1	B	372	MHO	CE-SD-CG	4.93	108.92	97.71
1	B	372	MHO	OD1-SD-CE	4.59	115.55	106.25
1	B	162	MHO	OD1-SD-CG	-4.48	93.67	106.03
1	B	292	MHO	OD1-SD-CE	4.34	115.04	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	MHO	OD1-SD-CG	-4.32	94.12	106.03
1	A	372	MHO	CE-SD-CG	3.95	106.70	97.71
1	A	162	MHO	OD1-SD-CE	3.91	114.18	106.25
1	A	162	MHO	OD1-SD-CG	-3.66	95.94	106.03
1	A	181	MHO	OD1-SD-CE	-3.43	99.30	106.25
1	B	181	MHO	OD1-SD-CG	-2.63	98.78	106.03
1	A	181	MHO	CB-CG-SD	2.44	119.70	111.39
1	B	162	MHO	OD1-SD-CE	-2.44	101.31	106.25
1	B	181	MHO	OD1-SD-CE	-2.40	101.39	106.25
1	A	292	MHO	OD1-SD-CE	-2.33	101.52	106.25

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	372	MHO	CB-CG-SD-OD1
1	B	162	MHO	CB-CG-SD-OD1
1	A	162	MHO	CB-CG-SD-OD1
1	A	372	MHO	CB-CG-SD-OD1
1	A	181	MHO	CA-CB-CG-SD
1	A	372	MHO	CA-CB-CG-SD
1	B	162	MHO	C-CA-CB-CG
1	A	372	MHO	CB-CG-SD-CE
1	A	162	MHO	CB-CG-SD-CE
1	B	181	MHO	CA-CB-CG-SD
1	B	372	MHO	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	372	MHO	0	1

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	900	-	1,3,3	4.96	1 (100%)	0,3,3	0.00	-
3	HEM	B	550	1,4	27,50,50	1.86	8 (29%)	17,82,82	2.41	9 (52%)
3	HEM	A	550	1,4	27,50,50	1.93	9 (33%)	17,82,82	3.03	9 (52%)

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
3	HEM	B	550	1,4	-	0/6/54/54	-
3	HEM	A	550	1,4	-	0/6/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ACT	CH3-C	-4.96	1.42	1.48
3	A	550	HEM	C3C-CAC	4.36	1.56	1.47
3	B	550	HEM	C4D-C3D	4.13	1.51	1.42
3	B	550	HEM	C3D-C2D	3.60	1.48	1.37
3	A	550	HEM	C3B-C2B	-3.45	1.35	1.40
3	B	550	HEM	C3B-C2B	-3.42	1.35	1.40
3	A	550	HEM	C3D-C2D	3.34	1.47	1.37
3	B	550	HEM	CMC-C2C	3.17	1.59	1.51
3	A	550	HEM	CMC-C2C	3.07	1.58	1.51
3	B	550	HEM	C1C-C2C	2.98	1.49	1.42
3	A	550	HEM	C1C-C2C	2.91	1.49	1.42
3	A	550	HEM	C1D-ND	2.81	1.41	1.36
3	A	550	HEM	CMB-C2B	2.51	1.57	1.51
3	A	550	HEM	CMA-C3A	2.38	1.56	1.51
3	B	550	HEM	C3C-CAC	2.33	1.52	1.47
3	B	550	HEM	CMA-C3A	2.29	1.56	1.51
3	B	550	HEM	CMD-C2D	2.11	1.56	1.51
3	A	550	HEM	CAA-C2A	2.03	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	HEM	C1D-C2D-C3D	-8.55	101.05	107.00
3	B	550	HEM	CAD-CBD-CGD	-4.57	105.01	112.67
3	B	550	HEM	CMA-C3A-C4A	-4.18	122.04	128.46
3	A	550	HEM	CBA-CAA-C2A	-3.59	105.87	112.49
3	A	550	HEM	CMA-C3A-C4A	-3.57	122.97	128.46
3	B	550	HEM	C4C-C3C-C2C	3.54	109.37	106.90
3	A	550	HEM	CMD-C2D-C1D	3.32	133.56	128.46
3	A	550	HEM	CMA-C3A-C2A	3.00	130.60	124.94
3	B	550	HEM	C1D-C2D-C3D	-2.84	105.02	107.00
3	A	550	HEM	C3C-C4C-NC	-2.82	105.61	110.94
3	B	550	HEM	CMC-C2C-C3C	2.71	129.74	124.68
3	A	550	HEM	CAD-CBD-CGD	-2.70	108.13	112.67
3	A	550	HEM	CAA-CBA-CGA	2.65	117.11	112.67
3	B	550	HEM	CMA-C3A-C2A	2.63	129.90	124.94
3	B	550	HEM	C3B-C4B-NB	-2.44	106.06	109.21
3	B	550	HEM	CMB-C2B-C3B	2.32	129.03	124.68
3	A	550	HEM	C4C-C3C-C2C	2.26	108.48	106.90
3	B	550	HEM	CBD-CAD-C3D	-2.23	108.37	112.48

There are no chirality outliers.

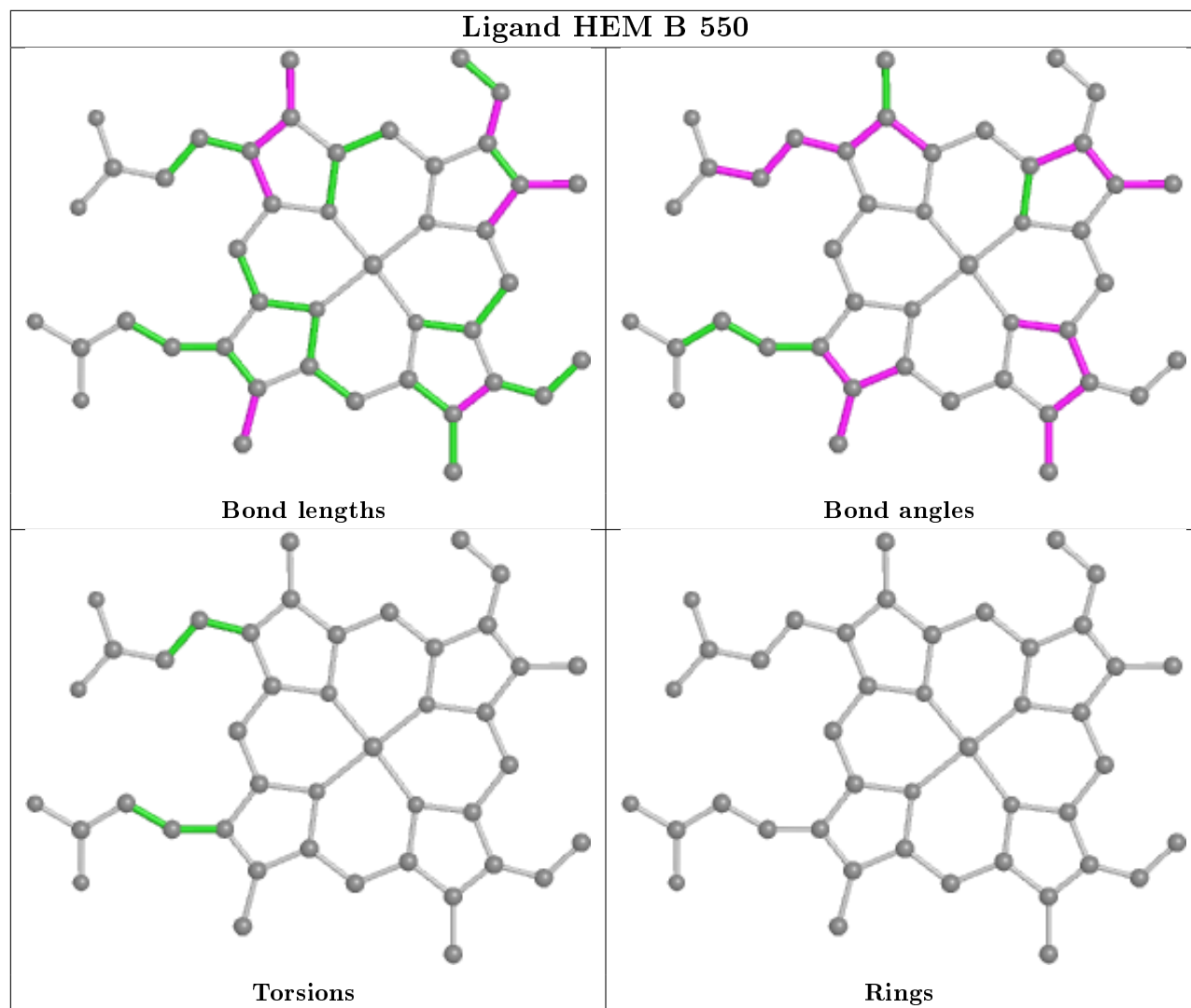
There are no torsion outliers.

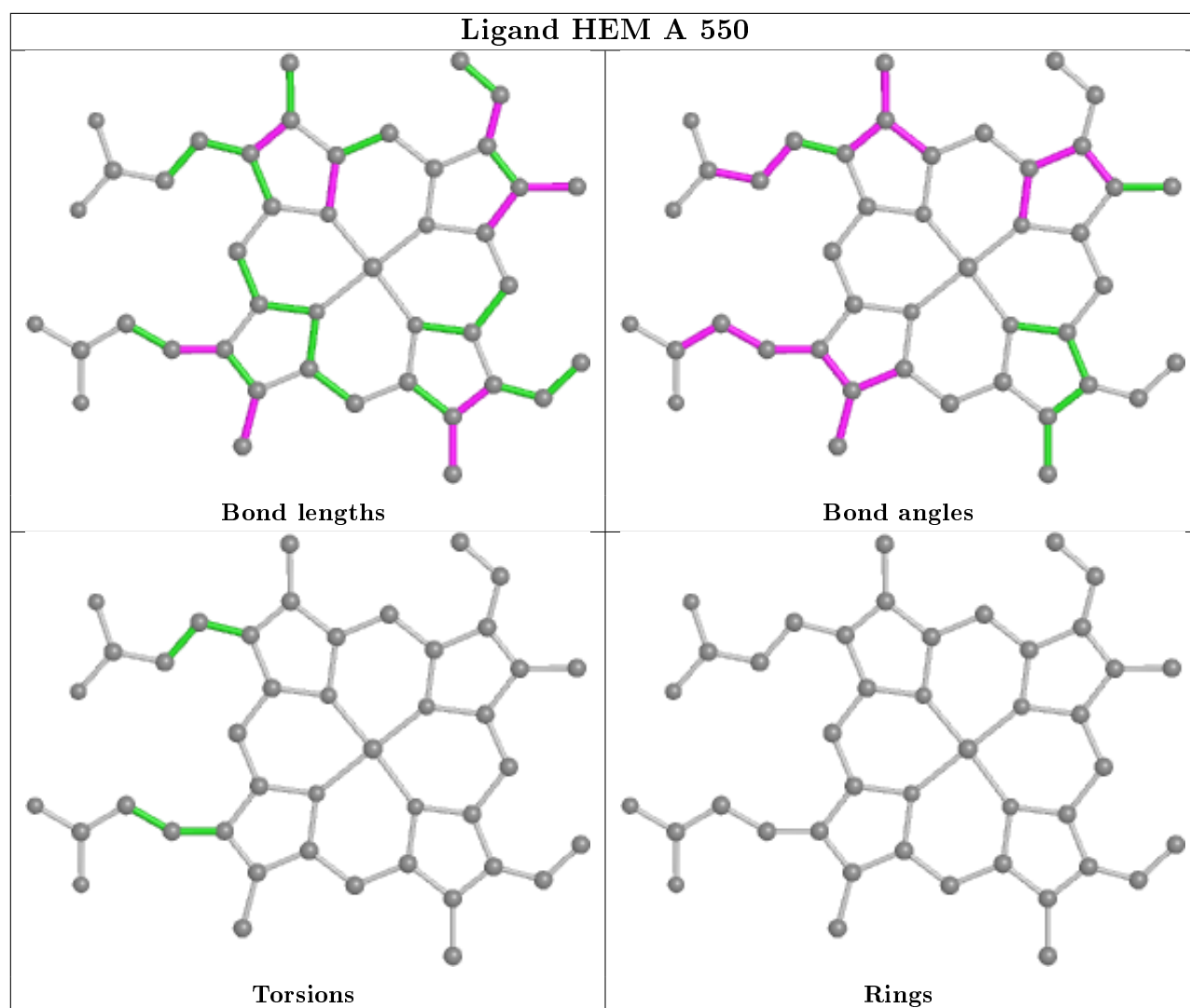
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	550	HEM	5	0
3	A	550	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	487/505 (96%)	-0.07	9 (1%) 68 76	3, 5, 14, 46	1 (0%)
1	B	487/505 (96%)	-0.17	7 (1%) 75 82	3, 6, 14, 45	2 (0%)
All	All	974/1010 (96%)	-0.12	16 (1%) 72 79	3, 6, 14, 46	3 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	MET	8.5
1	B	491	LYS	7.6
1	A	489	MET	7.1
1	B	490	MET	6.8
1	A	491	LYS	6.2
1	B	489	MET	6.1
1	A	488	LYS	4.3
1	A	272	LYS	4.2
1	A	2	VAL	4.1
1	B	488	LYS	3.0
1	A	287	GLN	2.9
1	B	33	LEU	2.5
1	A	487	GLN	2.5
1	B	272	LYS	2.4
1	A	376	TYR	2.3
1	B	485	LYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MHO	A	292	9/10	0.95	0.09	4,7,19,23	0
1	MHO	A	372	9/10	0.96	0.09	6,9,18,20	0
1	MHO	B	181	9/10	0.97	0.08	2,4,9,10	0
1	MHO	A	162	9/10	0.97	0.09	3,4,12,20	0
1	MHO	B	372	9/10	0.97	0.11	7,8,15,20	0
1	MHO	B	292	9/10	0.97	0.08	4,7,21,23	0
1	MHO	B	162	9/10	0.97	0.10	2,3,12,15	0
1	MHO	A	181	9/10	0.98	0.07	3,4,10,11	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

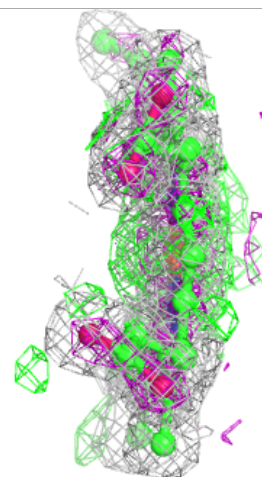
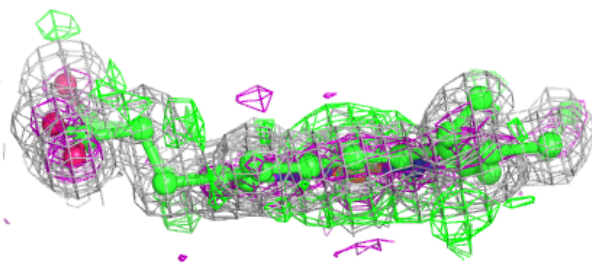
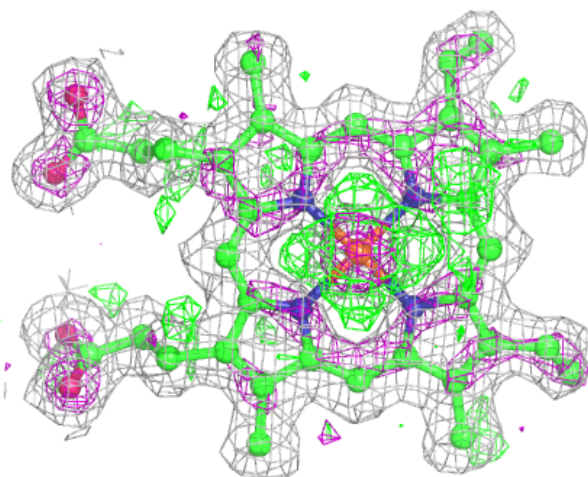
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	O	B	551	1/1	0.95	0.16	10,10,10,10	0
2	ACT	A	900	4/4	0.96	0.14	10,11,11,14	0
3	HEM	B	550	43/43	0.98	0.09	2,2,8,12	0
3	HEM	A	550	43/43	0.98	0.10	2,3,8,18	1
4	O	A	551	1/1	0.98	0.12	16,16,16,16	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.

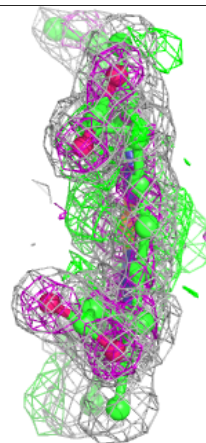
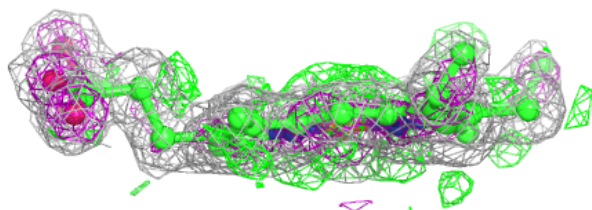
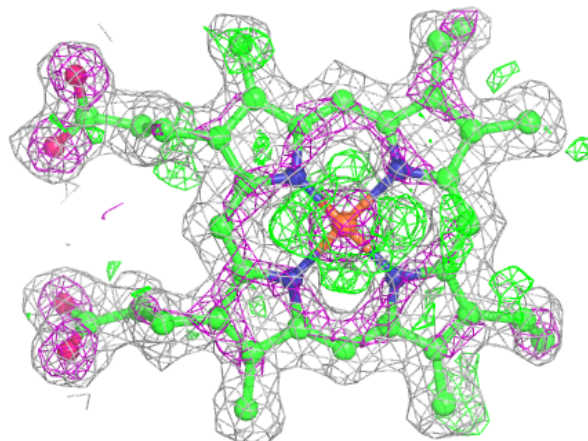
Electron density around HEM B 550:

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



Electron density around HEM A 550:

$2mF_o-DF_c$ (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.