



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 04:40 PM EDT

PDB ID : 5SW6 / pdb_00005sw6
Title : Crystal structure of an oxoferryl species of catalase-peroxidase KatG at pH5.6
Authors : Loewen, P.C.
Deposited on : 2016-08-08
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

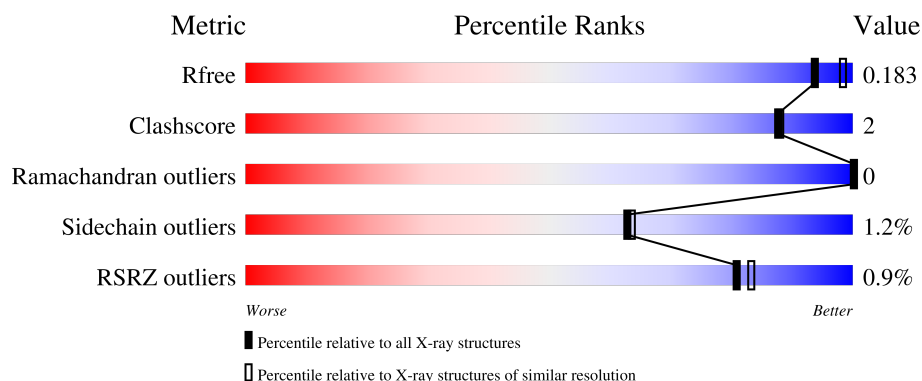
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	728	% 87% 10% .
1	B	728	% 87% 10% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12683 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 Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5534	3498	984	1038	14			
1	B	713	Total	C	N	O	S	0	5	0
			5518	3486	981	1037	14			

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

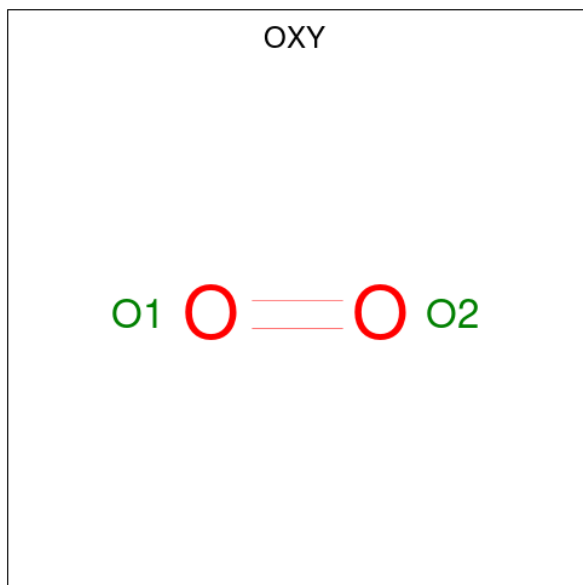


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		

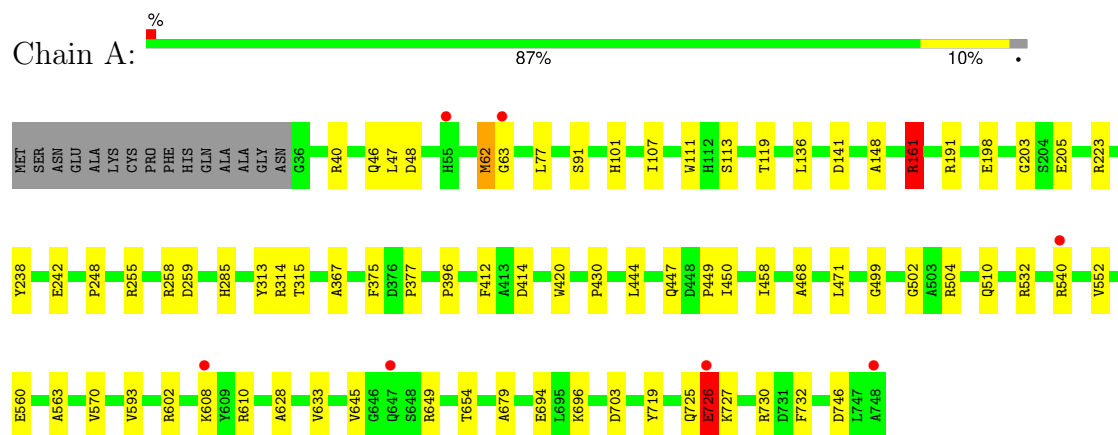
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	725	Total	O	0	0
			725	725		
8	B	776	Total	O	0	0
			776	776		

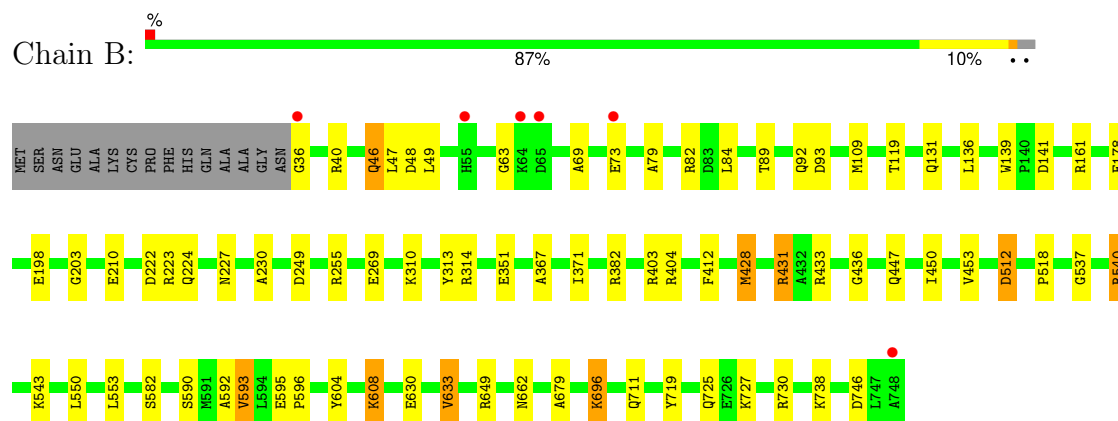
3 Residue-property plots

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-peroxidase



• Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.21Å 114.66Å 174.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-1.90) 98.8 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.141 , 0.175 0.154 , 0.183	Depositor DCC
R_{free} test set	15522 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12683	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: PO4, MPD, NA, O, HEM, OXY

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	1.65	51/5694 (0.9%)	1.26	13/7742 (0.2%)
1	B	1.65	51/5669 (0.9%)	1.28	16/7708 (0.2%)
All	All	1.65	102/11363 (0.9%)	1.27	29/15450 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	GLN	CD-OE1	10.18	1.42	1.23
1	B	203	GLY	C-O	9.16	1.30	1.23
1	A	285	HIS	C-O	8.29	1.33	1.24
1	A	203	GLY	C-O	7.93	1.29	1.23
1	A	628	ALA	N-CA	-7.88	1.38	1.46
1	A	532	ARG	NE-CZ	-7.80	1.24	1.33
1	A	458	ILE	CA-CB	-7.57	1.46	1.54
1	B	382	ARG	CZ-NH1	7.38	1.43	1.32
1	A	285	HIS	N-CA	7.35	1.55	1.46
1	B	109	MET	CA-C	7.31	1.62	1.52
1	B	512	ASP	CG-OD2	7.09	1.38	1.25
1	B	604	TYR	N-CA	-7.02	1.37	1.46
1	B	550	LEU	CA-C	-6.98	1.43	1.52
1	B	161	ARG	CD-NE	-6.81	1.36	1.46
1	B	727	LYS	N-CA	-6.76	1.38	1.46
1	B	590	SER	C-O	-6.74	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	LEU	CA-C	-6.72	1.43	1.52
1	B	139	TRP	CA-CB	6.71	1.63	1.53
1	A	725	GLN	CG-CD	6.69	1.68	1.52
1	B	79	ALA	N-CA	6.67	1.54	1.46
1	A	191	ARG	CA-C	6.67	1.61	1.52
1	B	82	ARG	CA-C	6.64	1.61	1.52
1	A	570	VAL	CA-C	-6.56	1.45	1.52
1	B	367	ALA	C-O	-6.48	1.15	1.23
1	B	224	GLN	C-O	6.43	1.32	1.24
1	A	62	MET	SD-CE	-6.41	1.63	1.79
1	B	518	PRO	N-CA	-6.26	1.39	1.47
1	A	732	PHE	N-CA	6.24	1.53	1.46
1	A	161	ARG	CD-NE	-6.23	1.37	1.46
1	A	113	SER	CA-C	6.21	1.60	1.52
1	B	136	LEU	CA-C	-6.19	1.44	1.52
1	B	746	ASP	C-O	-6.14	1.16	1.24
1	B	249	ASP	N-CA	6.11	1.53	1.46
1	B	131	GLN	CA-C	6.11	1.61	1.52
1	B	82	ARG	CZ-NH2	-6.05	1.25	1.33
1	A	726	GLU	CG-CD	6.01	1.67	1.52
1	A	77	LEU	N-CA	-6.00	1.38	1.46
1	A	447	GLN	N-CA	6.00	1.54	1.46
1	B	230	ALA	N-CA	-5.95	1.39	1.46
1	A	205	GLU	C-O	5.93	1.31	1.23
1	A	377	PRO	C-O	-5.86	1.16	1.24
1	A	63	GLY	N-CA	5.85	1.52	1.45
1	A	258	ARG	N-CA	-5.85	1.39	1.46
1	B	92	GLN	N-CA	-5.83	1.38	1.46
1	B	36	GLY	N-CA	5.79	1.54	1.45
1	A	414	ASP	CG-OD1	-5.75	1.14	1.25
1	B	436	GLY	C-O	-5.75	1.16	1.24
1	A	471	LEU	CA-C	5.72	1.60	1.52
1	B	592	ALA	CA-C	-5.71	1.45	1.52
1	B	596	PRO	CA-CB	-5.71	1.46	1.53
1	B	582	SER	C-O	5.67	1.31	1.23
1	A	107	ILE	N-CA	5.66	1.53	1.46
1	A	430	PRO	C-O	5.66	1.30	1.23
1	B	161	ARG	CZ-NH1	5.63	1.40	1.32
1	A	259	ASP	CA-C	5.61	1.59	1.52
1	B	89	THR	N-CA	-5.59	1.39	1.46
1	A	449	PRO	N-CA	-5.58	1.40	1.47
1	B	540	ARG	C-O	5.54	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	537	GLY	N-CA	5.53	1.52	1.45
1	B	47	LEU	CB-CG	-5.50	1.42	1.53
1	B	84	LEU	C-O	5.48	1.30	1.24
1	A	563	ALA	N-CA	-5.46	1.39	1.46
1	A	420	TRP	C-O	5.44	1.30	1.24
1	A	502	GLY	C-O	5.44	1.32	1.24
1	B	543	LYS	C-O	-5.43	1.17	1.23
1	B	412	PHE	N-CA	5.42	1.52	1.46
1	B	453	VAL	C-O	-5.42	1.18	1.24
1	A	148	ALA	C-O	-5.41	1.17	1.24
1	A	375	PHE	C-O	-5.38	1.17	1.24
1	A	654	THR	C-O	-5.34	1.17	1.23
1	B	679	ALA	N-CA	5.31	1.52	1.46
1	A	628	ALA	C-O	5.30	1.30	1.24
1	B	371	ILE	CA-C	5.28	1.58	1.52
1	A	560	GLU	N-CA	5.26	1.52	1.46
1	B	178	GLU	CD-OE2	5.26	1.35	1.25
1	B	227	ASN	CA-C	-5.25	1.47	1.53
1	A	694	GLU	CA-C	5.22	1.59	1.52
1	A	552	VAL	N-CA	5.21	1.52	1.46
1	A	499	GLY	C-O	5.19	1.28	1.23
1	A	315	THR	C-O	-5.19	1.17	1.24
1	A	91	SER	C-O	-5.17	1.17	1.23
1	A	679	ALA	N-CA	5.17	1.52	1.46
1	B	210	GLU	CA-C	5.16	1.59	1.52
1	B	738	LYS	N-CA	-5.15	1.40	1.46
1	B	550	LEU	CA-CB	5.14	1.61	1.53
1	A	101	HIS	C-O	-5.13	1.18	1.23
1	A	727	LYS	N-CA	-5.13	1.40	1.46
1	B	431	ARG	CD-NE	5.10	1.53	1.46
1	B	730	ARG	CZ-NH2	5.10	1.40	1.33
1	B	593	VAL	CA-C	-5.09	1.46	1.52
1	B	553	LEU	N-CA	-5.09	1.40	1.46
1	A	412	PHE	C-N	-5.07	1.27	1.33
1	A	396	PRO	N-CA	-5.06	1.40	1.47
1	B	198	GLU	CG-CD	5.06	1.64	1.52
1	A	746	ASP	C-O	-5.05	1.17	1.24
1	B	63	GLY	N-CA	5.05	1.51	1.45
1	A	444	LEU	CA-C	-5.03	1.46	1.52
1	B	223	ARG	C-O	-5.03	1.17	1.23
1	A	367	ALA	C-O	-5.03	1.17	1.23
1	A	191	ARG	CZ-NH2	-5.02	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	ALA	C-O	-5.01	1.18	1.24
1	B	222	ASP	CA-CB	5.00	1.59	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	NE-CZ-NH2	-10.35	109.88	119.20
1	B	161	ARG	NE-CZ-NH1	9.44	130.94	121.50
1	B	161	ARG	NE-CZ-NH2	-8.75	111.33	119.20
1	A	450	ILE	CB-CA-C	-7.51	102.84	110.13
1	A	161	ARG	NE-CZ-NH1	7.26	128.76	121.50
1	B	93	ASP	N-CA-C	6.68	119.39	111.71
1	B	630	GLU	N-CA-C	6.68	118.21	111.07
1	B	46	GLN	N-CA-C	-6.40	102.54	110.41
1	B	310	LYS	CB-CG-CD	-6.39	96.60	111.30
1	B	595	GLU	CA-C-N	-6.29	113.03	120.13
1	B	595	GLU	C-N-CA	-6.29	113.03	120.13
1	A	161	ARG	CD-NE-CZ	6.17	133.04	124.40
1	B	633	VAL	CG1-CB-CG2	-6.03	97.53	110.80
1	A	198	GLU	CG-CD-OE1	6.01	132.22	118.40
1	A	48	ASP	N-CA-C	5.93	118.78	107.75
1	B	351	GLU	CB-CG-CD	-5.89	102.59	112.60
1	B	48	ASP	N-CA-C	5.86	118.64	107.75
1	A	223	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	510	GLN	N-CA-C	5.55	117.33	111.28
1	A	47	LEU	N-CA-CB	-5.53	101.70	110.06
1	B	198	GLU	CG-CD-OE1	5.42	130.85	118.40
1	B	428	MET	CA-CB-CG	-5.41	103.28	114.10
1	B	608	LYS	CB-CA-C	5.36	119.16	110.22
1	A	46	GLN	N-CA-C	-5.32	103.51	110.53
1	A	703	ASP	N-CA-C	5.31	116.88	111.14
1	A	198	GLU	CB-CG-CD	5.28	121.57	112.60
1	B	230	ALA	N-CA-C	5.18	119.35	112.30
1	B	450	ILE	CA-CB-CG1	-5.18	101.59	110.40
1	A	113	SER	N-CA-C	-5.04	105.68	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain

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	5534	0	5366	16	0
1	B	5518	0	5337	20	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	1	0
4	B	2	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	16	0	28	5	0
7	B	8	0	14	2	0
8	A	725	0	0	8	1
8	B	776	0	0	9	1
All	All	12683	0	10805	44	1

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 2.

All (44) 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:119[B]:THR:HG22	1:B:593:VAL:HG21	1.54	0.90
1:A:255:ARG:NH2	8:A:901:HOH:O	2.06	0.88
1:A:119[B]:THR:HG21	8:A:1061:HOH:O	1.77	0.83
1:B:512:ASP:OD1	8:B:901:HOH:O	2.05	0.74
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.73	0.71
1:A:593:VAL:HG13	8:A:1011:HOH:O	1.92	0.70
7:A:807:MPD:O4	7:A:807:MPD:CM	2.43	0.67
7:B:806:MPD:O4	7:B:806:MPD:H12	1.94	0.66
7:A:808:MPD:H11	7:A:808:MPD:H53	1.77	0.65
1:B:119[B]:THR:HG23	8:B:1092:HOH:O	1.94	0.65
7:B:806:MPD:O4	7:B:806:MPD:C1	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LYS:HE2	8:B:922:HOH:O	2.02	0.60
4:A:803:OXY:O2	8:A:902:HOH:O	2.18	0.57
1:B:711[A]:GLN:NE2	8:B:907:HOH:O	2.40	0.55
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.38	0.54
1:A:161:ARG:NH2	8:A:906:HOH:O	2.36	0.54
1:A:62:MET:HE1	1:A:161:ARG:HD3	1.89	0.54
1:B:403[A]:ARG:NH1	8:B:913:HOH:O	2.42	0.53
1:A:504:ARG:HD2	8:A:976:HOH:O	2.09	0.52
1:A:696:LYS:HE2	8:A:1183:HOH:O	2.11	0.51
1:B:255:ARG:HD2	8:B:1345:HOH:O	2.11	0.50
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.95	0.49
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.42	0.48
1:B:662:ASN:H	1:B:725:GLN:HE22	1.59	0.48
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.58	0.47
1:B:725:GLN:NE2	8:B:923:HOH:O	2.48	0.47
1:A:313:TYR:CZ	1:A:314:ARG:HD3	2.50	0.47
1:B:313:TYR:CZ	1:B:314:ARG:HD3	2.51	0.46
1:B:633:VAL:CG2	1:B:719:TYR:CZ	2.99	0.46
1:B:49:LEU:HD12	1:B:711[B]:GLN:CD	2.41	0.46
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.16	0.45
7:A:808:MPD:HM2	8:A:1126:HOH:O	2.16	0.45
7:A:807:MPD:O4	7:A:807:MPD:HM1	2.18	0.43
1:B:696:LYS:CE	8:B:922:HOH:O	2.66	0.42
1:B:255:ARG:HB2	8:B:1586:HOH:O	2.20	0.42
1:A:726:GLU:HG2	1:A:730:ARG:NH1	2.35	0.42
7:A:808:MPD:H53	7:A:808:MPD:C1	2.48	0.42
1:B:540:ARG:HA	1:B:540:ARG:NH1	2.35	0.42
1:A:602:ARG:HB3	1:A:645:VAL:HG23	2.01	0.41
1:A:313:TYR:CE2	1:A:314:ARG:HD3	2.55	0.41
1:B:69:ALA:O	1:B:73:GLU:HG2	2.20	0.41
1:B:269:GLU:OE1	1:B:404:ARG:NH2	2.48	0.41
1:B:428:MET:O	1:B:433:ARG:HD3	2.21	0.41
1:A:242:GLU:O	1:A:248:PRO:HA	2.21	0.40

All (1) 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)
8:A:1470:HOH:O	8:B:1563:HOH:O[4_445]	1.97	0.23

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	717/728 (98%)	706 (98%)	11 (2%)	0	100	100
1	B	714/728 (98%)	704 (99%)	10 (1%)	0	100	100
All	All	1431/1456 (98%)	1410 (98%)	21 (2%)	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	556/561 (99%)	549 (99%)	7 (1%)	61	61
1	B	553/561 (99%)	547 (99%)	6 (1%)	65	67
All	All	1109/1122 (99%)	1096 (99%)	13 (1%)	63	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	141	ASP
1	A	540	ARG
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	A	726	GLU
1	B	40	ARG

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Mol	Chain	Res	Type
1	B	46	GLN
1	B	141	ASP
1	B	608	LYS
1	B	649	ARG
1	B	696	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	70	GLN
1	A	85	HIS
1	A	227	ASN
1	A	520	GLN
1	A	737	ASN
1	B	46	GLN
1	B	55	HIS
1	B	520	GLN
1	B	544	GLN
1	B	725	GLN
1	B	737	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](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z > 2$
5	PO4	A	805	-	4,4,4	0.50	0	6,6,6	1.21	1 (16%)
4	OXY	A	803	-	1,1,1	0.08	0	-		
7	MPD	A	807	-	7,7,7	1.57	2 (28%)	9,10,10	2.49	4 (44%)
2	HEM	B	801	6,1	50,50,50	1.97	17 (34%)	67,82,82	2.23	20 (29%)
7	MPD	A	808	-	7,7,7	0.82	0	9,10,10	1.16	1 (11%)
4	OXY	A	804	-	1,1,1	0.19	0	-		
2	HEM	A	801	6,1	50,50,50	1.39	8 (16%)	67,82,82	1.52	15 (22%)
4	OXY	B	804	-	1,1,1	0.02	0	-		
7	MPD	B	806	-	7,7,7	0.79	0	9,10,10	1.88	3 (33%)
5	PO4	B	805	-	4,4,4	1.02	0	6,6,6	1.48	1 (16%)

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
7	MPD	A	807	-	-	1/5/5/5	-
2	HEM	B	801	6,1	-	2/14/54/54	-
7	MPD	A	808	-	-	2/5/5/5	-
2	HEM	A	801	6,1	-	2/14/54/54	-
7	MPD	B	806	-	-	3/5/5/5	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C4B-NB	-4.81	1.29	1.38
2	B	801	HEM	C1B-NB	-4.25	1.32	1.40
2	A	801	HEM	FE-NA	3.93	2.08	1.95
2	B	801	HEM	FE-NB	3.70	2.06	1.94
2	B	801	HEM	CHB-C1B	3.44	1.45	1.38
2	B	801	HEM	C4A-NA	-3.22	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	CHA-C4D	-3.10	1.32	1.38
2	B	801	HEM	C4A-C3A	3.03	1.50	1.43
2	A	801	HEM	C3C-C2C	2.94	1.43	1.37
2	B	801	HEM	C1A-NA	-2.87	1.34	1.39
2	A	801	HEM	FE-NC	2.83	2.04	1.95
7	A	807	MPD	O2-C2	-2.81	1.37	1.44
2	B	801	HEM	C1C-NC	-2.79	1.34	1.39
2	B	801	HEM	C3B-C4B	2.71	1.50	1.44
2	B	801	HEM	C2A-C3A	-2.61	1.32	1.38
2	A	801	HEM	C1C-NC	-2.61	1.34	1.39
2	A	801	HEM	FE-NB	2.61	2.02	1.94
2	A	801	HEM	CMB-C2B	2.60	1.56	1.50
7	A	807	MPD	C5-C4	2.55	1.62	1.51
2	B	801	HEM	C1A-C2A	2.52	1.49	1.44
2	B	801	HEM	C1D-ND	-2.47	1.34	1.38
2	B	801	HEM	O1A-CGA	2.47	1.30	1.22
2	B	801	HEM	O1D-CGD	2.27	1.29	1.22
2	B	801	HEM	FE-NC	2.24	2.02	1.95
2	B	801	HEM	CHD-C1D	2.11	1.44	1.39
2	A	801	HEM	O1D-CGD	2.07	1.28	1.22
2	A	801	HEM	C1B-NB	-2.00	1.36	1.40

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C4B-C3B-C2B	-7.06	100.79	107.28
2	B	801	HEM	C3B-C4B-NB	5.73	113.58	109.47
2	B	801	HEM	CMA-C3A-C4A	-4.75	118.19	125.42
2	B	801	HEM	CMA-C3A-C2A	4.40	134.95	125.62
7	A	807	MPD	O4-C4-C3	-4.24	94.48	111.35
2	B	801	HEM	C2D-C1D-ND	4.12	114.67	109.90
2	B	801	HEM	CHD-C4C-NC	3.70	128.48	124.45
2	A	801	HEM	CAA-CBA-CGA	-3.63	104.04	113.67
2	B	801	HEM	CAA-CBA-CGA	-3.62	104.06	113.67
2	A	801	HEM	C3B-C2B-C1B	3.53	109.06	106.41
2	B	801	HEM	CMD-C2D-C1D	3.46	130.44	125.03
2	A	801	HEM	C1B-NB-C4B	3.32	109.14	105.21
7	A	807	MPD	CM-C2-C3	3.20	124.02	110.20
2	B	801	HEM	CAA-C2A-C1A	2.99	130.77	124.94
2	B	801	HEM	O2A-CGA-CBA	2.96	123.35	114.00
2	B	801	HEM	C4D-C3D-C2D	-2.96	102.59	106.89
2	B	801	HEM	C3D-C4D-ND	2.83	113.28	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	807	MPD	O4-C4-C5	2.77	121.39	109.45
2	A	801	HEM	C4B-C3B-C2B	-2.76	104.74	107.28
2	A	801	HEM	C2B-C1B-NB	-2.73	106.70	109.84
7	B	806	MPD	C1-C2-C3	2.72	121.92	110.20
2	A	801	HEM	CHC-C4B-NB	2.68	127.31	124.42
2	B	801	HEM	CHA-C4D-C3D	-2.67	120.30	125.23
2	A	801	HEM	CHB-C1B-NB	2.66	127.66	124.37
2	A	801	HEM	O1D-CGD-CBD	-2.59	114.88	123.09
2	A	801	HEM	CHD-C4C-NC	2.57	127.25	124.45
2	B	801	HEM	CHC-C1C-NC	-2.56	121.67	124.45
7	B	806	MPD	O2-C2-CM	2.53	115.88	107.99
2	A	801	HEM	C3D-C4D-ND	2.52	112.93	110.17
2	A	801	HEM	C2D-C1D-ND	2.50	112.79	109.90
2	B	801	HEM	CMC-C2C-C1C	2.49	129.12	124.73
2	B	801	HEM	C4D-ND-C1D	-2.47	102.28	105.21
7	A	807	MPD	CM-C2-C1	2.46	116.14	110.63
2	B	801	HEM	O1A-CGA-CBA	-2.44	115.34	123.09
2	B	801	HEM	CHC-C4B-C3B	-2.44	120.20	125.07
2	A	801	HEM	C4C-NC-C1C	2.34	109.64	105.82
7	B	806	MPD	O2-C2-C3	-2.34	100.50	109.27
7	A	808	MPD	O4-C4-C3	-2.34	102.05	111.35
2	A	801	HEM	CMB-C2B-C1B	-2.32	121.41	125.03
2	A	801	HEM	C4D-ND-C1D	-2.24	102.56	105.21
2	A	801	HEM	CMD-C2D-C1D	2.19	128.45	125.03
5	B	805	PO4	O3-P-O1	2.18	118.64	110.95
2	B	801	HEM	CAC-C3C-C4C	-2.05	119.93	124.82
2	B	801	HEM	CAD-C3D-C4D	2.04	128.25	124.70
5	A	805	PO4	O4-P-O3	2.00	114.14	107.91

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	807	MPD	CM-C2-C3-C4
7	B	806	MPD	C1-C2-C3-C4
7	A	808	MPD	O2-C2-C3-C4
7	B	806	MPD	O2-C2-C3-C4
7	B	806	MPD	CM-C2-C3-C4
7	A	808	MPD	C2-C3-C4-C5
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A

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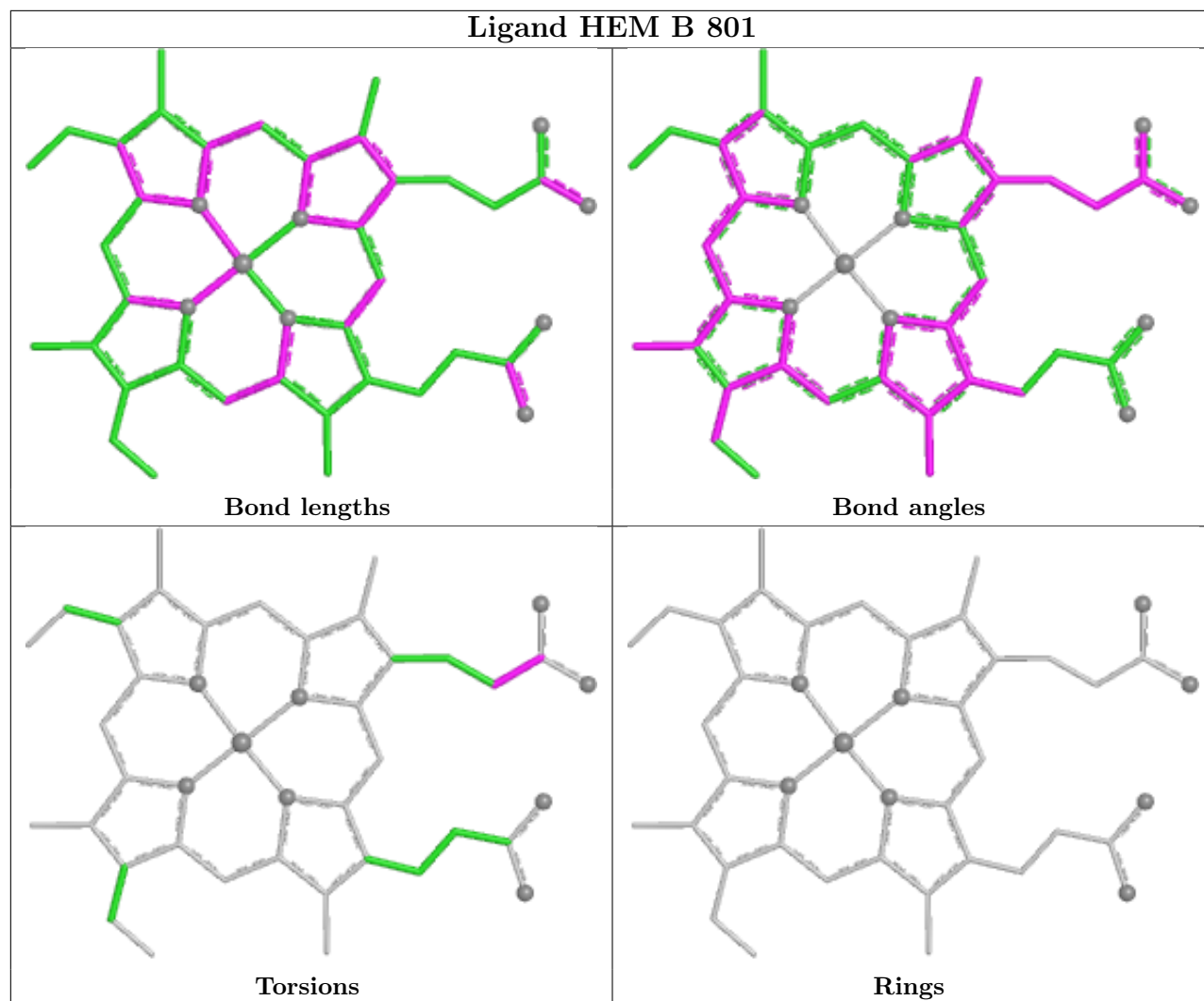
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	CAA-CBA-CGA-O1A

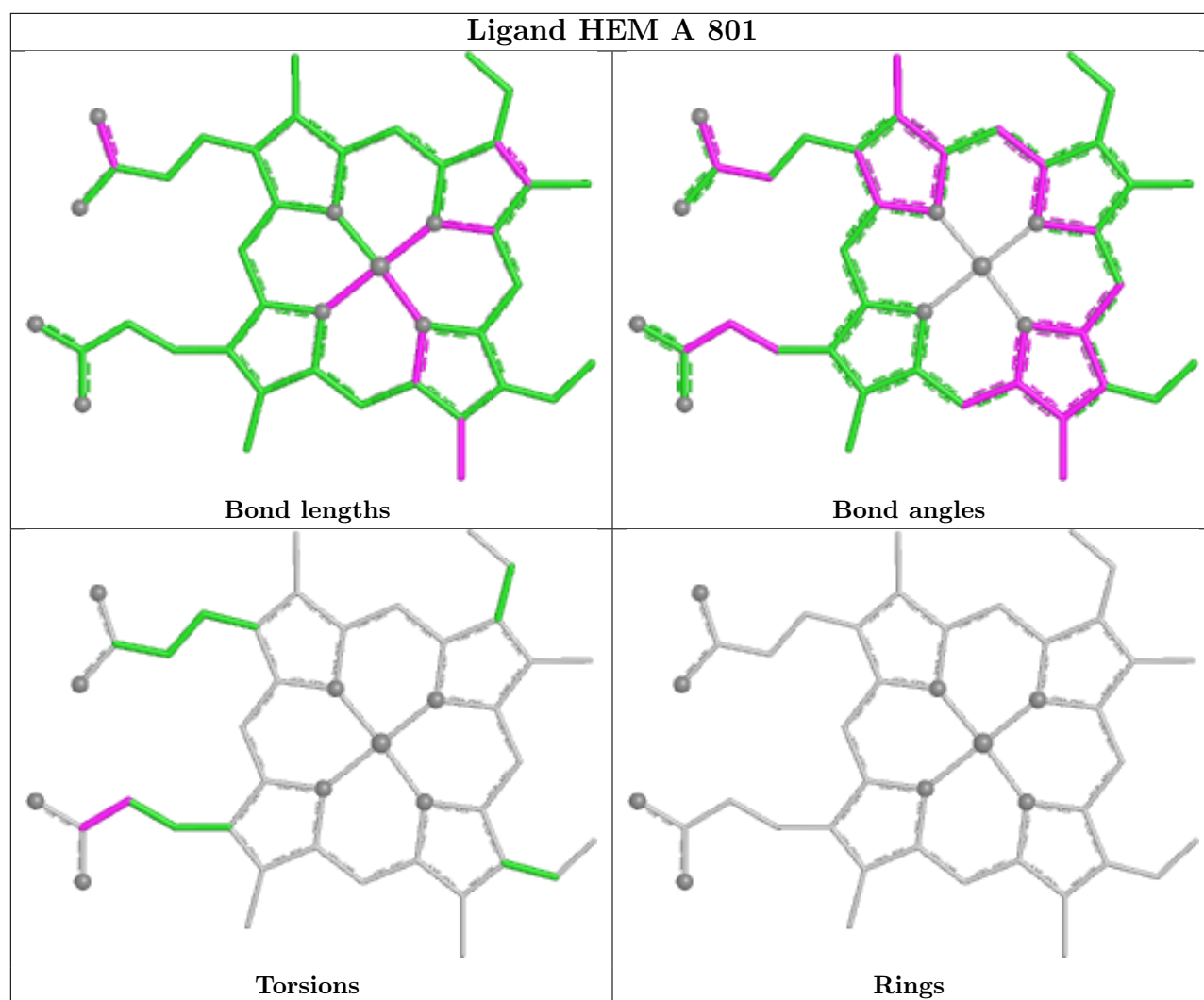
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	OXY	1	0
7	A	807	MPD	2	0
7	A	808	MPD	3	0
7	B	806	MPD	2	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	713/728 (97%)	-0.48	7 (0%) 79 82	8, 18, 37, 68	6 (0%)
1	B	713/728 (97%)	-0.56	6 (0%) 82 85	8, 17, 35, 70	3 (0%)
All	All	1426/1456 (97%)	-0.52	13 (0%) 81 83	8, 18, 36, 70	9 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	4.1
1	A	748	ALA	3.7
1	B	55	HIS	3.4
1	B	65	ASP	2.9
1	A	55	HIS	2.5
1	A	608	LYS	2.3
1	A	540	ARG	2.3
1	A	647	GLN	2.2
1	B	64	LYS	2.2
1	B	36	GLY	2.1
1	A	726	GLU	2.0
1	A	63	GLY	2.0
1	B	73	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

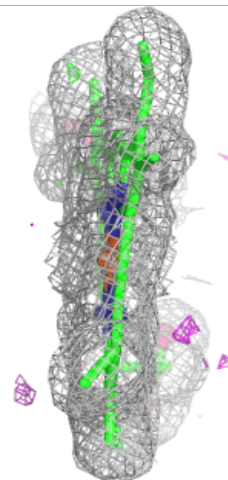
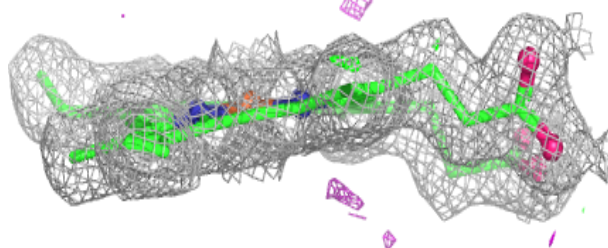
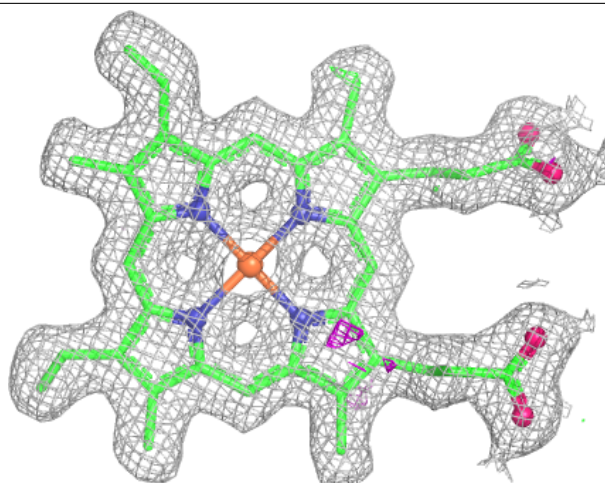
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

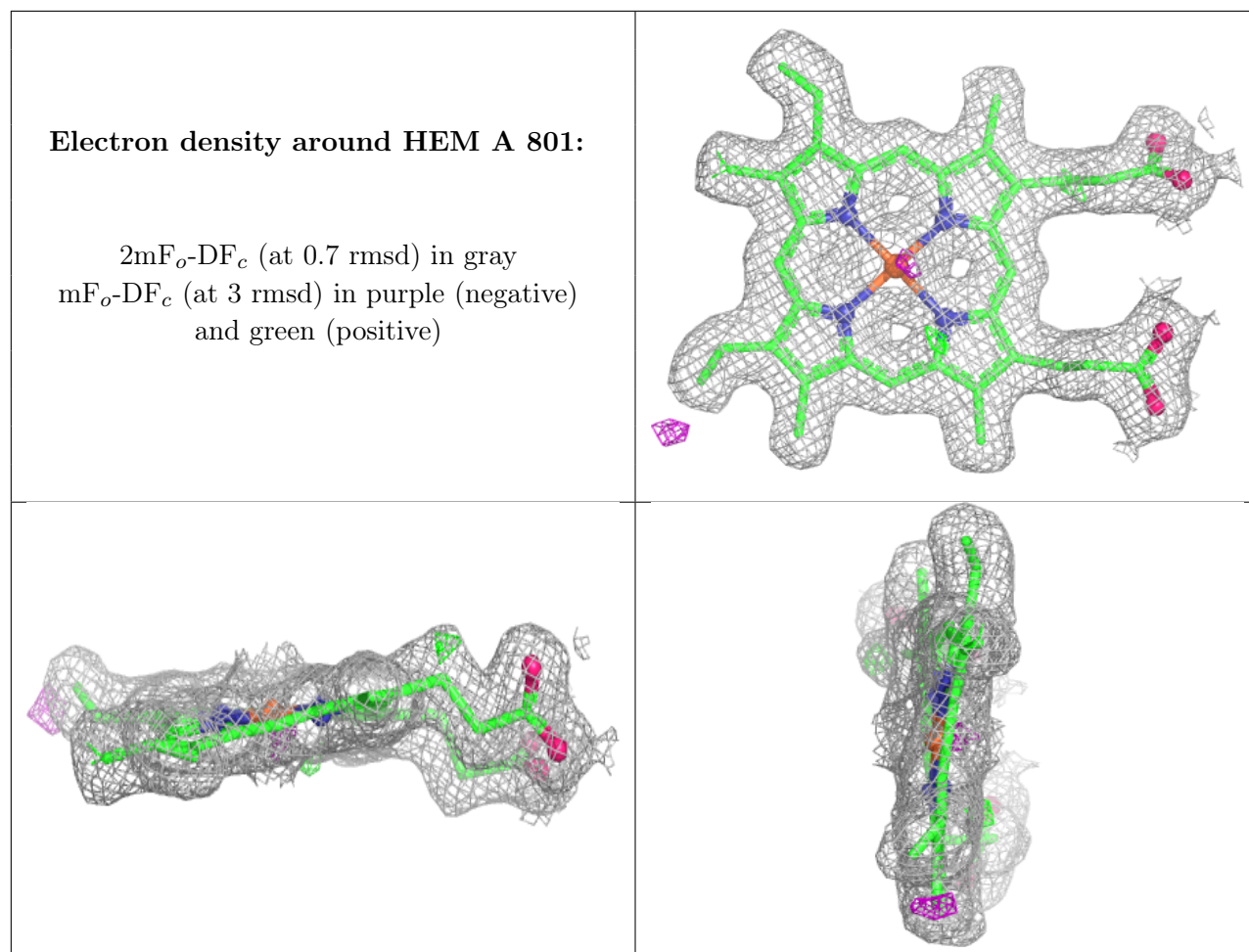
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MPD	A	807	8/8	0.75	0.22	44,47,66,67	0
7	MPD	A	808	8/8	0.83	0.14	37,39,47,49	0
5	PO4	B	805	5/5	0.87	0.10	53,54,67,70	0
7	MPD	B	806	8/8	0.90	0.14	45,50,55,56	0
4	OXY	A	804	2/2	0.91	0.15	32,32,32,42	0
4	OXY	B	804	2/2	0.93	0.20	35,35,35,36	0
5	PO4	A	805	5/5	0.93	0.12	44,56,58,63	0
4	OXY	A	803	2/2	0.94	0.15	28,28,28,35	0
6	O	B	803	1/1	0.98	0.05	19,19,19,19	0
6	O	A	806	1/1	0.99	0.11	24,24,24,24	0
2	HEM	B	801	43/43	0.99	0.04	11,12,13,14	0
3	NA	A	802	1/1	0.99	0.04	13,13,13,13	0
3	NA	B	802	1/1	0.99	0.07	14,14,14,14	0
2	HEM	A	801	43/43	0.99	0.04	12,14,16,17	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 B 801:

$2mF_o-DF_c$ (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.