



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 04:55 PM EDT

PDB ID : 5SXX / pdb_00005sxx
Title : Crystal structure of the E198A variant of Burkholderia pseudomallei catalase-peroxidase KatG with INH
Authors : Loewen, P.C.
Deposited on : 2016-08-10
Resolution : 1.70 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

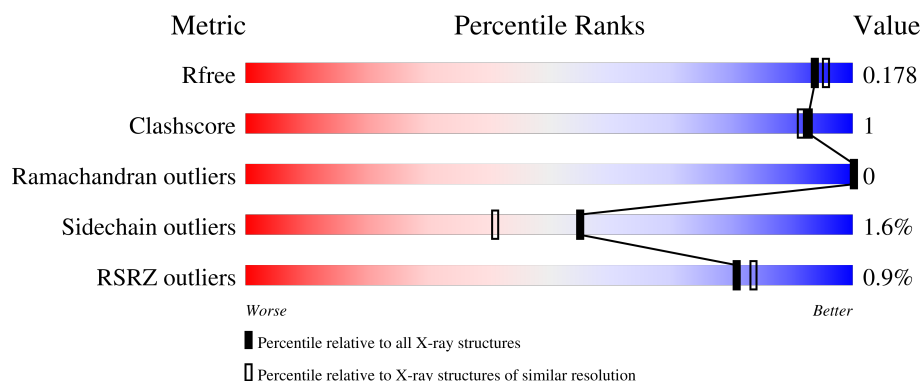
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

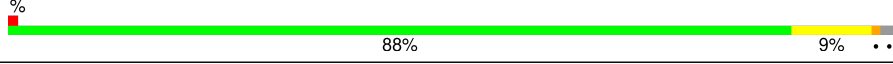
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	
1	B	728	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	A	806	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12723 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.

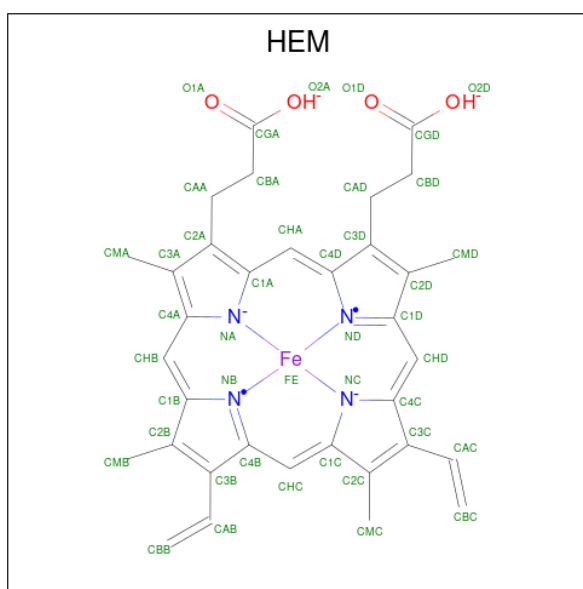
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	5	0
			5524	3491	984	1035	14			
1	B	713	Total	C	N	O	S	0	5	0
			5526	3491	987	1034	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ALA	GLU	engineered mutation	UNP Q3JNW6
B	198	ALA	GLU	engineered mutation	UNP Q3JNW6

- 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		

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

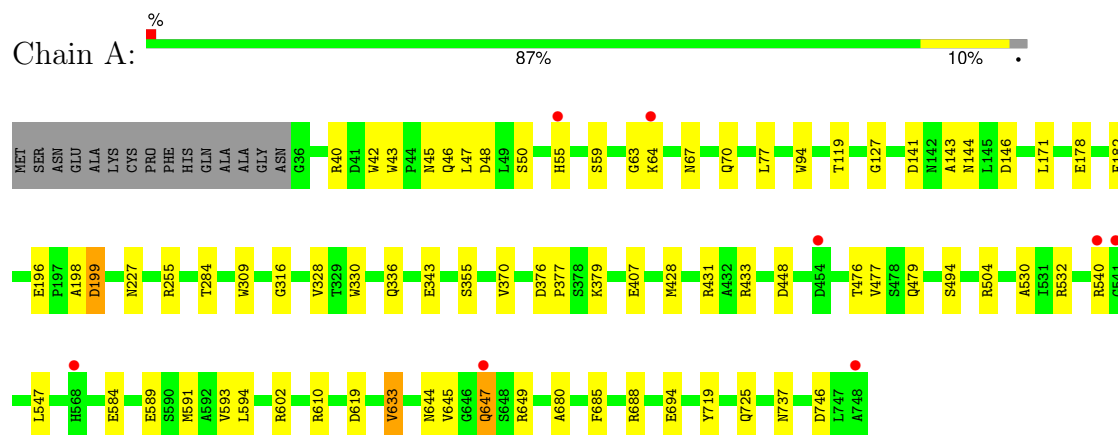
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	780	Total	O	0	0
			780	780		
8	B	769	Total	O	0	0
			769	769		

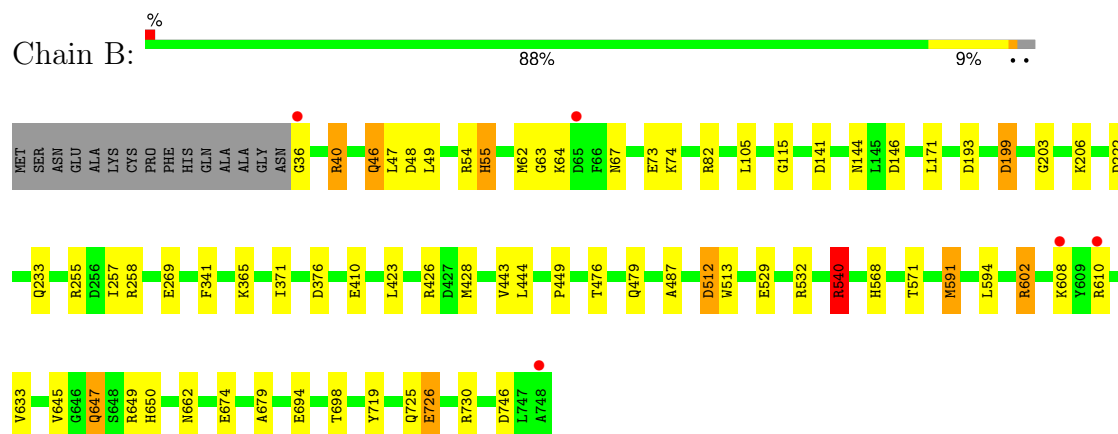
3 Residue-property plots [i](#)

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: 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	100.57Å 115.94Å 174.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-1.70) 91.4 (20.00-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.142 , 0.169 0.155 , 0.178	Depositor DCC
R_{free} test set	10170 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12723	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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, HEM, OXY, CL, MPD, NA

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	1.70	54/5683 (1.0%)	1.32	16/7727 (0.2%)
1	B	1.69	51/5687 (0.9%)	1.32	21/7731 (0.3%)
All	All	1.70	105/11370 (0.9%)	1.32	37/15458 (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
1	B	0	1
All	All	0	2

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	532	ARG	CD-NE	-11.20	1.30	1.46
1	A	532	ARG	CD-NE	-10.67	1.31	1.46
1	A	448	ASP	CA-CB	8.96	1.58	1.52
1	A	255	ARG	CD-NE	8.90	1.58	1.46
1	B	36	GLY	N-CA	8.49	1.59	1.45
1	B	746	ASP	C-O	-8.23	1.13	1.24
1	A	448	ASP	C-O	7.94	1.27	1.23
1	B	63	GLY	N-CA	7.72	1.55	1.45
1	A	199	ASP	N-CA	7.63	1.57	1.46
1	A	532	ARG	NE-CZ	-7.62	1.24	1.33
1	B	540	ARG	C-O	7.51	1.33	1.23
1	B	532	ARG	CZ-NH2	-7.49	1.23	1.33
1	A	647	GLN	CA-C	7.38	1.63	1.53
1	B	512	ASP	CG-OD2	7.26	1.39	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLY	N-CA	7.16	1.54	1.45
1	B	82	ARG	CZ-NH2	-7.11	1.24	1.33
1	A	532	ARG	CZ-NH2	-7.04	1.24	1.33
1	B	602	ARG	CZ-NH2	-6.99	1.24	1.33
1	B	647	GLN	CA-C	6.94	1.62	1.53
1	B	679	ALA	N-CA	6.74	1.54	1.46
1	A	644	ASN	C-O	-6.69	1.15	1.23
1	A	376	ASP	N-CA	6.68	1.54	1.46
1	B	199	ASP	C-O	6.56	1.32	1.23
1	B	376	ASP	N-CA	6.55	1.54	1.46
1	B	258	ARG	N-CA	-6.44	1.38	1.46
1	A	255	ARG	NE-CZ	6.33	1.40	1.33
1	B	371	ILE	N-CA	6.31	1.53	1.46
1	B	591	MET	SD-CE	-6.27	1.63	1.79
1	A	540	ARG	C-O	6.23	1.31	1.23
1	B	443	VAL	CA-C	-6.22	1.45	1.52
1	A	725	GLN	CD-NE2	6.21	1.46	1.33
1	B	532	ARG	NE-CZ	-6.03	1.26	1.33
1	A	47	LEU	CB-CG	-5.99	1.41	1.53
1	B	54	ARG	CA-C	-5.98	1.44	1.53
1	B	365	LYS	N-CA	5.92	1.53	1.46
1	A	584	GLU	C-O	-5.91	1.16	1.24
1	A	45	ASN	C-O	-5.88	1.16	1.24
1	A	619	ASP	C-O	-5.88	1.17	1.24
1	B	63	GLY	C-O	5.87	1.30	1.23
1	A	43	TRP	CA-CB	5.80	1.59	1.53
1	A	316	GLY	N-CA	5.76	1.53	1.45
1	A	746	ASP	C-O	-5.76	1.16	1.24
1	B	105	LEU	CA-C	5.71	1.60	1.52
1	B	74	LYS	N-CA	-5.69	1.38	1.46
1	B	171	LEU	CA-CB	-5.67	1.44	1.53
1	A	694	GLU	CA-C	5.67	1.60	1.52
1	B	674	GLU	N-CA	-5.65	1.39	1.46
1	A	182	PHE	C-O	-5.64	1.17	1.24
1	B	694	GLU	CA-C	5.63	1.60	1.52
1	A	377	PRO	C-O	-5.63	1.16	1.24
1	B	199	ASP	N-CA	5.62	1.54	1.46
1	A	530	ALA	N-CA	5.61	1.53	1.46
1	B	193	ASP	C-O	5.59	1.30	1.23
1	A	448	ASP	N-CA	5.58	1.50	1.46
1	B	67	ASN	CG-ND2	-5.52	1.21	1.33
1	A	94	TRP	CA-C	5.52	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	341	PHE	C-O	5.52	1.30	1.24
1	A	644	ASN	N-CA	-5.48	1.39	1.46
1	A	688	ARG	CA-C	-5.44	1.46	1.52
1	B	444	LEU	N-CA	-5.44	1.39	1.45
1	B	40	ARG	N-CA	5.41	1.53	1.46
1	A	370	VAL	C-O	-5.40	1.17	1.24
1	A	685	PHE	N-CA	-5.39	1.39	1.46
1	A	336	GLN	CD-NE2	5.38	1.44	1.33
1	A	433	ARG	CZ-NH2	-5.38	1.26	1.33
1	B	410	GLU	CD-OE2	5.37	1.35	1.25
1	B	647	GLN	CA-CB	5.35	1.61	1.53
1	B	730	ARG	CZ-NH2	5.34	1.40	1.33
1	A	46	GLN	CA-CB	5.33	1.61	1.53
1	A	77	LEU	N-CA	-5.33	1.40	1.46
1	A	59	SER	C-O	-5.33	1.17	1.24
1	B	46	GLN	CG-CD	5.29	1.65	1.52
1	B	47	LEU	CB-CG	-5.28	1.43	1.53
1	A	196	GLU	CG-CD	5.25	1.65	1.52
1	A	476	THR	CA-C	5.23	1.60	1.53
1	B	257	ILE	CA-C	-5.23	1.46	1.52
1	B	49	LEU	CB-CG	-5.22	1.43	1.53
1	A	67	ASN	CA-C	5.20	1.59	1.52
1	A	680	ALA	N-CA	5.20	1.52	1.46
1	A	477	VAL	CA-CB	-5.19	1.48	1.54
1	B	203	GLY	C-O	5.19	1.27	1.23
1	A	547	LEU	N-CA	-5.18	1.39	1.46
1	A	737	ASN	CA-C	5.18	1.59	1.52
1	A	428	MET	CG-SD	-5.17	1.67	1.80
1	B	222	ASP	CA-CB	5.15	1.59	1.52
1	A	355	SER	CA-CB	5.14	1.59	1.53
1	B	730	ARG	CZ-NH1	5.13	1.40	1.32
1	B	476	THR	CA-C	5.13	1.60	1.53
1	A	584	GLU	CG-CD	5.13	1.64	1.52
1	B	529	GLU	CG-CD	5.13	1.64	1.52
1	B	726	GLU	CG-CD	5.12	1.64	1.52
1	A	328	VAL	C-O	5.10	1.29	1.24
1	A	178	GLU	N-CA	5.09	1.52	1.46
1	A	55	HIS	CA-CB	5.09	1.61	1.53
1	A	431	ARG	CD-NE	5.08	1.53	1.46
1	A	494	SER	CA-CB	-5.07	1.45	1.53
1	B	115	GLY	C-O	-5.05	1.17	1.23
1	A	343	GLU	N-CA	5.05	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	HIS	CA-CB	5.05	1.61	1.53
1	B	233	GLN	CA-C	5.04	1.58	1.52
1	A	42	TRP	C-O	-5.02	1.18	1.24
1	A	171	LEU	CA-C	5.01	1.59	1.52
1	B	479	GLN	CA-C	5.01	1.59	1.52
1	B	513	TRP	CA-C	-5.01	1.46	1.52
1	B	269	GLU	N-CA	-5.00	1.40	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-15.57	105.19	119.20
1	B	532	ARG	NE-CZ-NH2	-12.52	107.93	119.20
1	B	46	GLN	N-CA-C	-9.88	97.78	110.53
1	A	46	GLN	N-CA-C	-8.73	99.67	110.41
1	A	532	ARG	NE-CZ-NH1	8.51	130.01	121.50
1	B	532	ARG	NE-CZ-NH1	8.11	129.61	121.50
1	A	532	ARG	CD-NE-CZ	7.85	135.40	124.40
1	B	428	MET	CA-CB-CG	-6.97	100.16	114.10
1	B	54	ARG	CG-CD-NE	-6.65	97.37	112.00
1	B	532	ARG	CD-NE-CZ	6.59	133.63	124.40
1	A	55	HIS	CB-CA-C	6.33	121.20	111.39
1	A	127	GLY	N-CA-C	6.25	121.55	114.67
1	A	428	MET	CA-CB-CG	-6.25	101.61	114.10
1	B	255[A]	ARG	NE-CZ-NH1	6.02	127.52	121.50
1	B	255[B]	ARG	NE-CZ-NH1	6.02	127.52	121.50
1	A	47	LEU	N-CA-CB	-5.89	100.69	110.23
1	A	330	TRP	N-CA-C	5.85	118.89	111.69
1	B	48	ASP	N-CA-C	5.83	118.59	107.75
1	B	199	ASP	CA-C-N	-5.78	115.65	123.10
1	B	199	ASP	C-N-CA	-5.78	115.65	123.10
1	A	70	GLN	CA-CB-CG	5.40	124.89	114.10
1	B	487	ALA	N-CA-C	5.38	116.83	111.07
1	B	532	ARG	CG-CD-NE	-5.31	100.31	112.00
1	B	47	LEU	N-CA-CB	-5.28	101.68	110.23
1	B	55	HIS	CB-CA-C	5.26	119.83	111.51
1	B	449	PRO	CB-CA-C	-5.24	104.12	110.98
1	A	479	GLN	N-CA-C	5.23	116.98	111.28
1	A	584	GLU	CB-CG-CD	5.21	121.46	112.60
1	B	46	GLN	N-CA-CB	5.11	117.75	110.44
1	A	46	GLN	N-CA-CB	5.09	117.36	110.38
1	B	62	MET	CA-C-N	-5.08	114.46	121.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	MET	C-N-CA	-5.08	114.46	121.06
1	B	529	GLU	CB-CG-CD	5.06	121.21	112.60
1	A	477	VAL	N-CA-C	-5.06	105.57	110.42
1	A	198	ALA	CA-C-N	-5.03	115.33	123.23
1	A	198	ALA	C-N-CA	-5.03	115.33	123.23
1	B	206	LYS	CG-CD-CE	5.01	122.82	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ASP	Mainchain
1	B	199	ASP	Mainchain

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	5524	0	5354	13	0
1	B	5526	0	5356	16	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	8	0	14	2	0
7	B	8	0	14	0	0
8	A	780	0	0	5	1
8	B	769	0	0	5	1
All	All	12723	0	10798	32	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 1.

All (32) 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:119[B]:THR:HG21	8:A:997:HOH:O	1.66	0.94
1:B:512:ASP:OD1	8:B:904:HOH:O	2.11	0.67
1:B:55:HIS:HD2	8:B:1335:HOH:O	1.82	0.61
1:A:633[B]:VAL:CG2	1:A:719:TYR:CZ	2.84	0.60
5:B:805:OXY:O2	8:B:905:HOH:O	2.17	0.58
1:B:568:HIS:ND1	1:B:726:GLU:OE1	2.37	0.57
7:A:807:MPD:O4	7:A:807:MPD:H12	2.05	0.57
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.88	0.56
1:B:662:ASN:H	1:B:725:GLN:HE22	1.55	0.54
1:B:647:GLN:HG2	8:B:940:HOH:O	2.07	0.53
1:A:593:VAL:HG13	8:A:929:HOH:O	2.10	0.52
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.41	0.51
1:A:591:MET:SD	1:A:594:LEU:HD12	2.51	0.51
1:B:591:MET:SD	1:B:594:LEU:HD12	2.51	0.50
7:A:807:MPD:O4	7:A:807:MPD:C1	2.60	0.50
1:A:589:GLU:HG2	8:A:1407:HOH:O	2.12	0.49
1:A:284:THR:HG22	2:A:801:HEM:HAA1	1.97	0.46
1:A:407:GLU:HG2	8:A:1411:HOH:O	2.14	0.46
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.17	0.45
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.52	0.44
1:B:55:HIS:CD2	8:B:1335:HOH:O	2.64	0.43
1:B:73:GLU:HA	1:B:73:GLU:OE1	2.17	0.43
1:B:426[A]:ARG:HA	1:B:426[A]:ARG:HD2	1.89	0.43
1:A:48:ASP:OD1	1:A:50[B]:SER:OG	2.29	0.43
1:A:602:ARG:HB3	1:A:645:VAL:HG23	2.01	0.43
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.19	0.43
1:B:650:HIS:HD2	1:B:698:THR:OG1	2.02	0.42
1:A:504:ARG:HD2	8:A:979:HOH:O	2.19	0.42
1:B:423:LEU:HD12	1:B:426[B]:ARG:CZ	2.50	0.42
1:B:602:ARG:HB3	1:B:645:VAL:HG23	2.03	0.41
1:A:633[B]:VAL:HG21	1:A:719:TYR:CZ	2.57	0.40
1:B:423:LEU:HD12	1:B:426[B]:ARG:NH2	2.37	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:1135:HOH:O	8:B:1181:HOH:O[2_444]	2.02	0.18

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	716/728 (98%)	708 (99%)	8 (1%)	0	100	100
1	B	716/728 (98%)	707 (99%)	9 (1%)	0	100	100
All	All	1432/1456 (98%)	1415 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	554/560 (99%)	544 (98%)	10 (2%)	51	36
1	B	554/560 (99%)	545 (98%)	9 (2%)	55	41
All	All	1108/1120 (99%)	1089 (98%)	19 (2%)	55	38

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	141	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	227	ASN
1	A	379	LYS
1	A	610	ARG
1	A	633[A]	VAL
1	A	633[B]	VAL
1	A	647	GLN
1	A	649	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	141	ASP
1	B	540	ARG
1	B	571	THR
1	B	608	LYS
1	B	610	ARG
1	B	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	70	GLN
1	A	227	ASN
1	A	292	ASN
1	A	520	GLN
1	A	568	HIS
1	A	647	GLN
1	A	737	ASN
1	B	55	HIS
1	B	520	GLN
1	B	544	GLN
1	B	650	HIS
1	B	725	GLN
1	B	737	ASN

5.3.3 RNA ⓘ

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	$\# Z > 2$
6	PO4	B	806	-	4,4,4	0.82	0	6,6,6	3.60	2 (33%)
6	PO4	A	806	-	4,4,4	1.70	1 (25%)	6,6,6	2.87	3 (50%)
7	MPD	A	807	-	7,7,7	0.40	0	9,10,10	2.36	4 (44%)
5	OXY	A	805	-	1,1,1	0.29	0	-		
5	OXY	B	804	-	1,1,1	0.13	0	-		
7	MPD	B	807	-	7,7,7	0.44	0	9,10,10	1.10	1 (11%)
5	OXY	A	804	-	1,1,1	0.01	0	-		
2	HEM	A	801	8,1	50,50,50	1.66	10 (20%)	67,82,82	2.01	20 (29%)
2	HEM	B	801	8,1	50,50,50	1.87	13 (26%)	67,82,82	1.43	11 (16%)
5	OXY	B	805	-	1,1,1	0.34	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
7	MPD	A	807	-	-	3/5/5/5	-
2	HEM	A	801	8,1	-	3/14/54/54	-
2	HEM	B	801	8,1	-	3/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	B	807	-	-	3/5/5/5	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1D-ND	-4.15	1.30	1.38
2	A	801	HEM	C4C-NC	-3.93	1.32	1.39
2	B	801	HEM	C1A-NA	-3.83	1.32	1.39
2	B	801	HEM	C4A-NA	3.77	1.46	1.39
2	A	801	HEM	FE-NC	3.76	2.07	1.95
2	A	801	HEM	FE-NB	3.70	2.06	1.94
2	B	801	HEM	CHC-C1C	3.59	1.45	1.38
2	B	801	HEM	C4C-NC	-3.48	1.33	1.39
2	A	801	HEM	CMD-C2D	-3.34	1.43	1.50
2	A	801	HEM	FE-NA	3.09	2.05	1.95
2	B	801	HEM	FE-ND	3.04	2.04	1.94
2	B	801	HEM	C4B-NB	-3.01	1.32	1.38
2	A	801	HEM	O1A-CGA	3.00	1.31	1.22
6	A	806	PO4	P-O4	-2.98	1.46	1.54
2	B	801	HEM	FE-NC	2.96	2.04	1.95
2	B	801	HEM	CHB-C1B	2.92	1.44	1.38
2	A	801	HEM	C1A-NA	-2.91	1.34	1.39
2	A	801	HEM	C2A-C3A	-2.88	1.31	1.38
2	B	801	HEM	C1C-C2C	-2.81	1.39	1.45
2	B	801	HEM	C3C-C4C	-2.77	1.41	1.46
2	B	801	HEM	FE-NB	2.76	2.03	1.94
2	A	801	HEM	CBD-CGD	2.47	1.56	1.50
2	B	801	HEM	O1D-CGD	2.32	1.29	1.22
2	A	801	HEM	CHD-C1D	2.10	1.44	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C3B-C2B-C1B	6.73	111.47	106.41
6	B	806	PO4	O2-P-O1	-6.38	88.40	110.95
6	A	806	PO4	O3-P-O1	-5.73	90.67	110.95
6	B	806	PO4	O3-P-O2	5.53	125.13	107.91
2	A	801	HEM	C2B-C1B-NB	-4.90	104.21	109.84
7	A	807	MPD	CM-C2-C1	-4.29	101.02	110.63
2	A	801	HEM	C1B-NB-C4B	4.15	110.13	105.21
2	A	801	HEM	O1D-CGD-CBD	-3.61	111.65	123.09
2	A	801	HEM	CHD-C1D-ND	-3.48	120.67	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CHC-C1C-NC	3.46	128.22	124.45
2	B	801	HEM	C4C-C3C-C2C	-3.27	103.98	106.81
2	A	801	HEM	CHC-C4B-NB	3.19	127.86	124.42
2	A	801	HEM	C4B-C3B-C2B	-3.16	104.37	107.28
7	A	807	MPD	C1-C2-C3	3.14	123.75	110.20
2	A	801	HEM	C2D-C1D-ND	3.12	113.51	109.90
2	A	801	HEM	O1A-CGA-CBA	-3.07	113.36	123.09
7	A	807	MPD	O2-C2-C3	-3.07	97.80	109.27
2	B	801	HEM	CHC-C4B-NB	2.94	127.59	124.42
7	A	807	MPD	O2-C2-CM	2.92	117.09	107.99
2	B	801	HEM	CHC-C1C-NC	2.87	127.58	124.45
2	A	801	HEM	CHB-C1B-NB	2.86	127.90	124.37
2	B	801	HEM	C2A-C1A-NA	2.83	113.29	110.15
2	A	801	HEM	CAD-C3D-C2D	-2.75	122.72	127.87
2	A	801	HEM	C1D-C2D-C3D	-2.74	104.10	106.98
2	B	801	HEM	CHA-C4D-ND	2.72	127.73	124.37
6	A	806	PO4	O4-P-O3	2.72	116.36	107.91
2	A	801	HEM	C3B-C4B-NB	-2.70	107.53	109.47
2	B	801	HEM	C1D-C2D-C3D	-2.70	104.14	106.98
2	B	801	HEM	C1C-CHC-C4B	-2.67	120.35	126.02
2	B	801	HEM	CAA-CBA-CGA	-2.63	106.69	113.67
2	A	801	HEM	CHD-C4C-NC	2.59	127.28	124.45
2	A	801	HEM	O2A-CGA-CBA	2.47	121.80	114.00
2	A	801	HEM	CAA-CBA-CGA	-2.37	107.37	113.67
2	B	801	HEM	C2D-C1D-ND	2.36	112.63	109.90
2	B	801	HEM	CMB-C2B-C1B	-2.35	121.36	125.03
2	A	801	HEM	CAD-C3D-C4D	2.24	128.61	124.70
2	A	801	HEM	O2D-CGD-O1D	2.22	129.05	123.33
2	B	801	HEM	C3D-C4D-ND	-2.13	107.83	110.17
6	A	806	PO4	O4-P-O1	2.09	118.35	110.95
7	B	807	MPD	C1-C2-C3	2.05	119.03	110.20
2	A	801	HEM	CMB-C2B-C1B	-2.02	121.87	125.03

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	807	MPD	C1-C2-C3-C4
7	A	807	MPD	O2-C2-C3-C4
7	B	807	MPD	C1-C2-C3-C4
7	B	807	MPD	O2-C2-C3-C4
7	A	807	MPD	CM-C2-C3-C4

Continued on next page...

Continued from previous page...

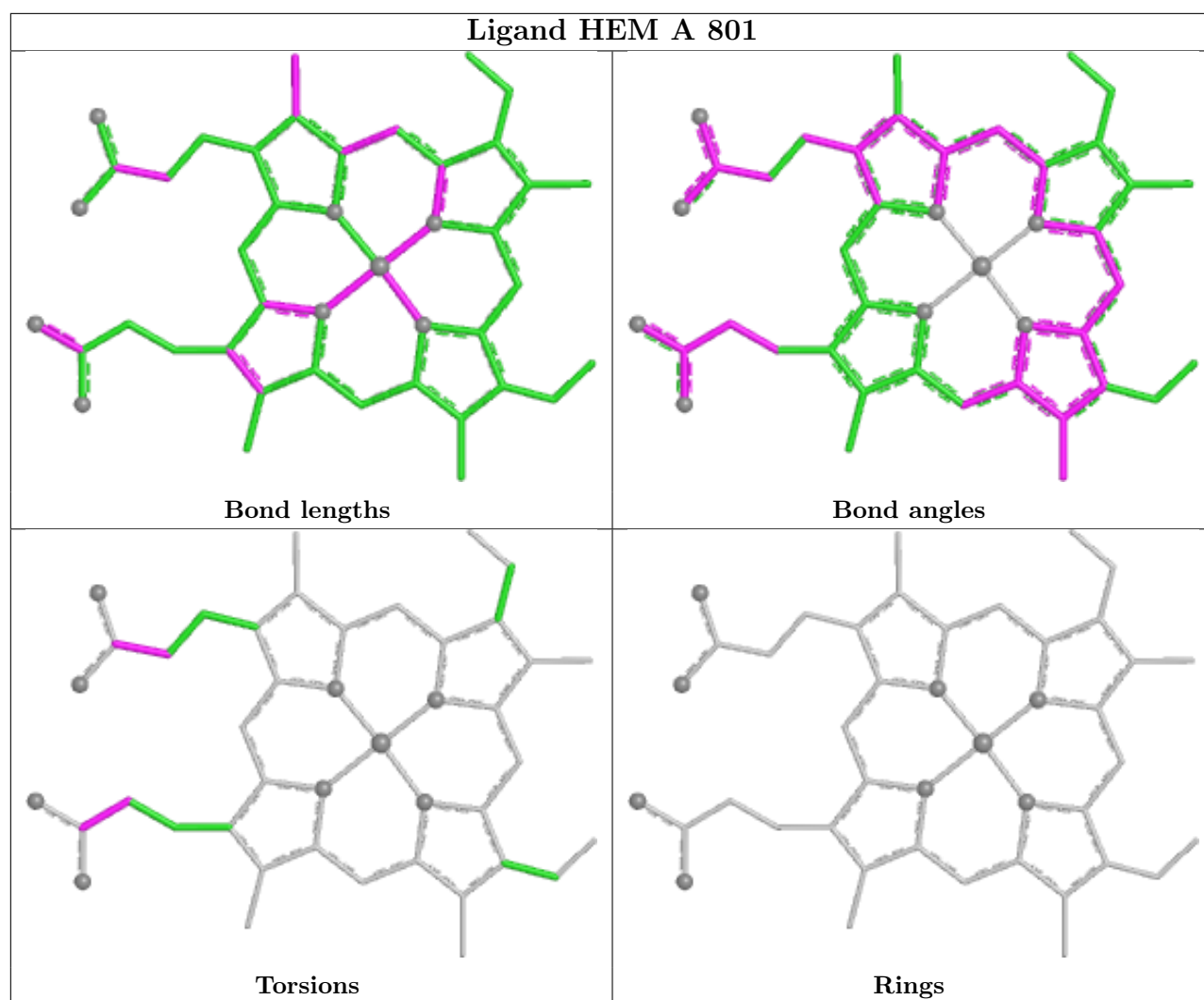
Mol	Chain	Res	Type	Atoms
7	B	807	MPD	CM-C2-C3-C4
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	CAD-CBD-CGD-O2D

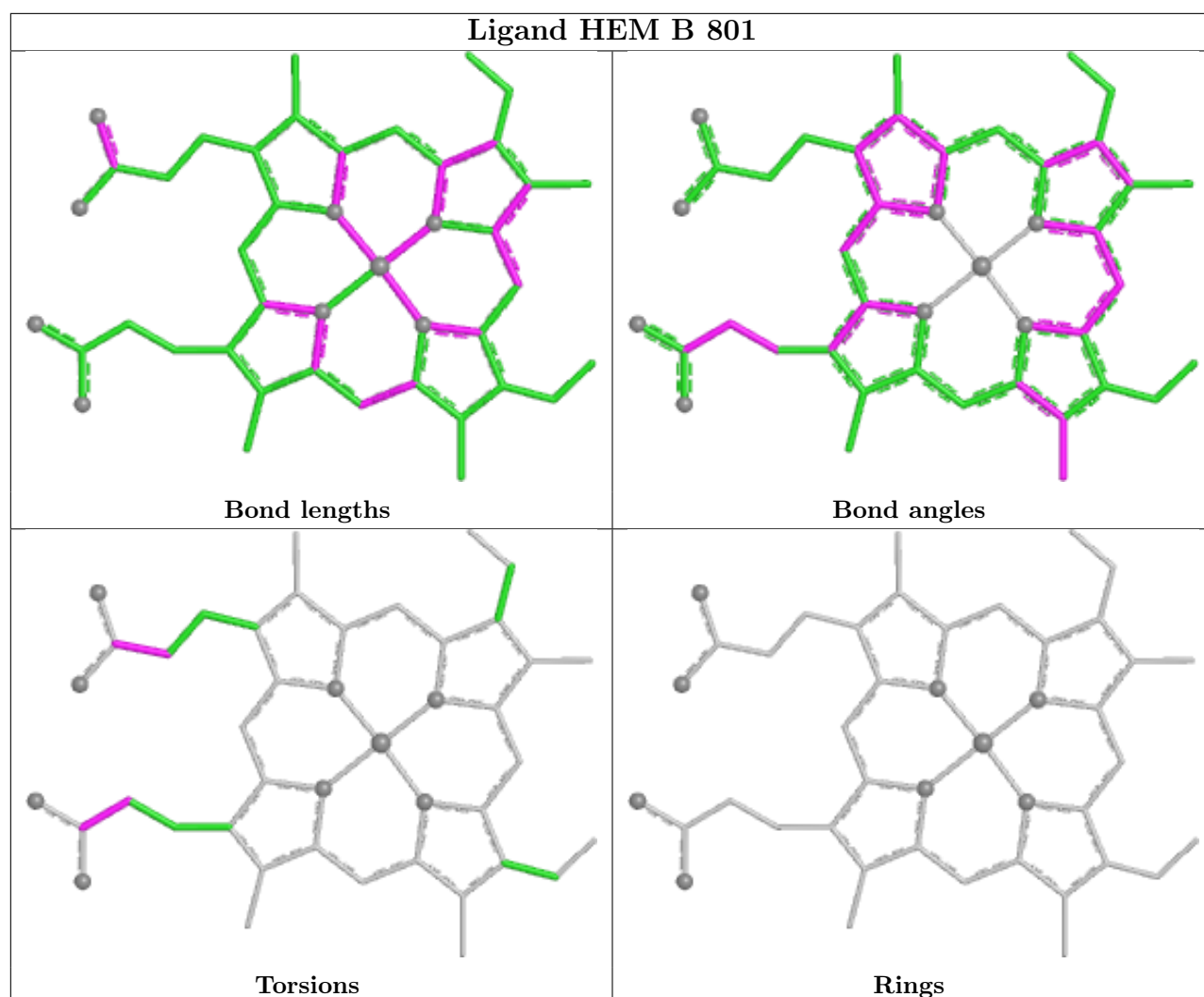
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	807	MPD	2	0
2	A	801	HEM	1	0
5	B	805	OXY	1	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%)	-0.50	8 (1%) 78 81	8, 18, 38, 81	5 (0%)
1	B	713/728 (97%)	-0.53	5 (0%) 84 86	8, 18, 36, 82	5 (0%)
All	All	1426/1456 (97%)	-0.51	13 (0%) 81 83	8, 18, 37, 82	10 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.6
1	B	748	ALA	3.9
1	B	610	ARG	2.6
1	B	65	ASP	2.6
1	A	541	GLY	2.5
1	A	540	ARG	2.4
1	A	55	HIS	2.3
1	B	608	LYS	2.2
1	A	454	ASP	2.2
1	A	64	LYS	2.2
1	A	568	HIS	2.0
1	A	647	GLN	2.0
1	B	36	GLY	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

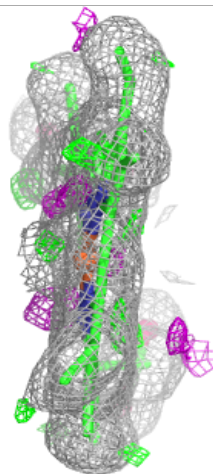
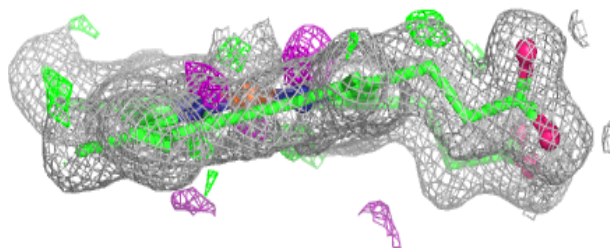
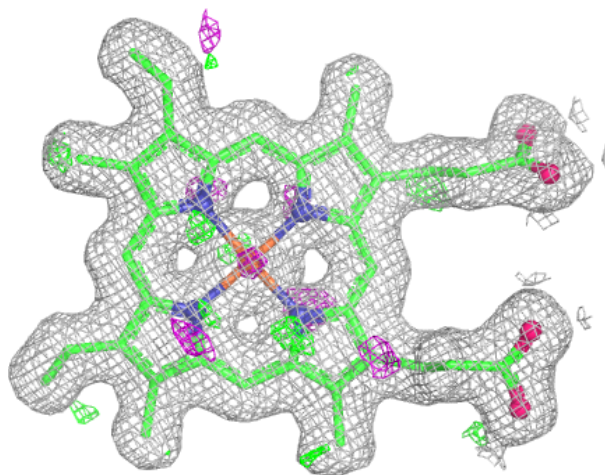
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

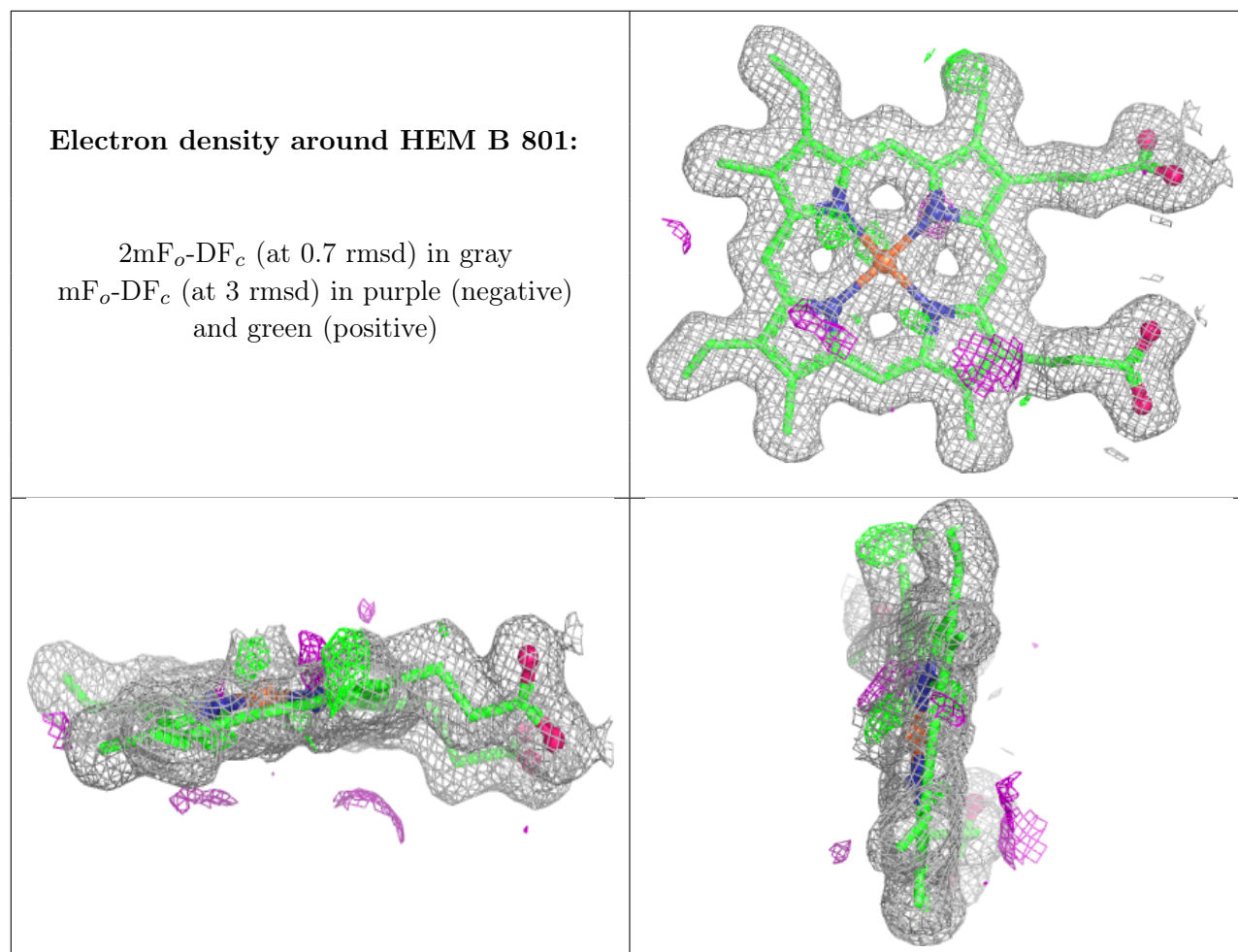
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	OXY	A	805	2/2	0.79	0.21	34,34,34,60	0
4	CL	A	803	1/1	0.89	0.20	62,62,62,62	0
5	OXY	B	805	2/2	0.89	0.23	34,34,34,42	0
6	PO4	B	806	5/5	0.90	0.09	41,49,57,60	0
7	MPD	A	807	8/8	0.90	0.12	49,57,65,67	0
7	MPD	B	807	8/8	0.90	0.13	49,58,63,64	0
6	PO4	A	806	5/5	0.93	0.08	42,55,57,65	0
4	CL	B	803	1/1	0.94	0.19	54,54,54,54	0
5	OXY	B	804	2/2	0.96	0.20	25,25,25,26	0
5	OXY	A	804	2/2	0.97	0.15	26,26,26,32	0
3	NA	B	802	1/1	0.98	0.09	19,19,19,19	0
3	NA	A	802	1/1	0.99	0.07	17,17,17,17	0
2	HEM	A	801	43/43	0.99	0.04	10,13,15,17	0
2	HEM	B	801	43/43	0.99	0.04	10,12,15,17	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 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 [i](#)

There are no such residues in this entry.