



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 05:49 PM EDT

PDB ID : 5SXQ / pdb_00005sxq
Title : Crystal structure of B. pseudomallei KatG with isonicotinic acid hydrazide bound
Authors : Loewen, P.C.
Deposited on : 2016-08-10
Resolution : 2.10 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

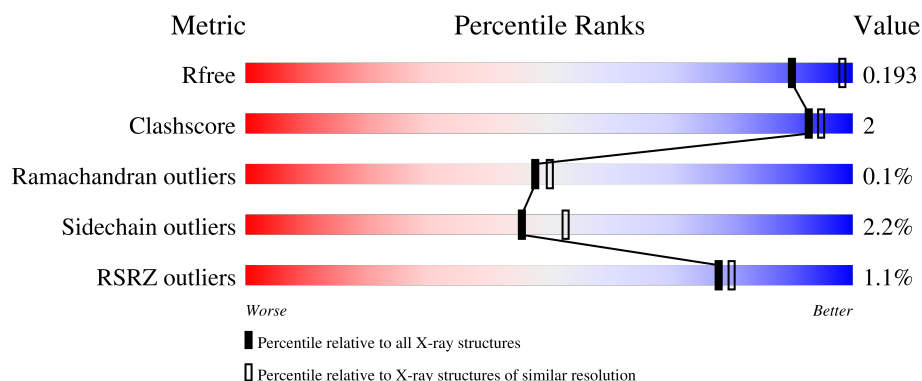
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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.

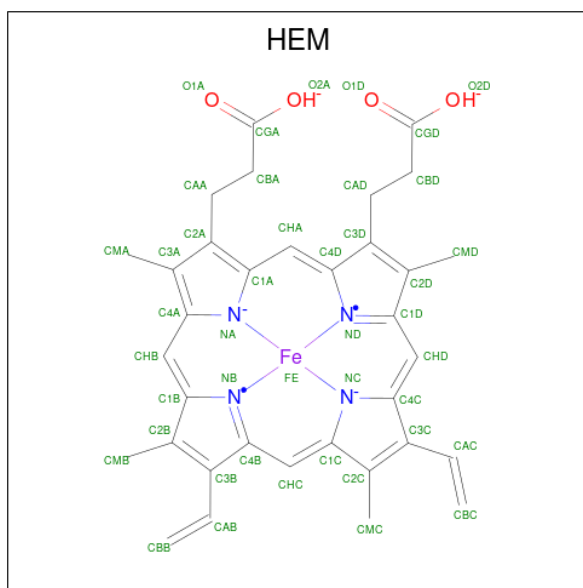
Mol	Chain	Length	Quality of chain
1	A	728	
1	B	728	

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 5528	C 3493	N 984	O 1037	S 14	0	5	0
1	B	713	Total 5522	C 3488	N 984	O 1036	S 14	0	4	0

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

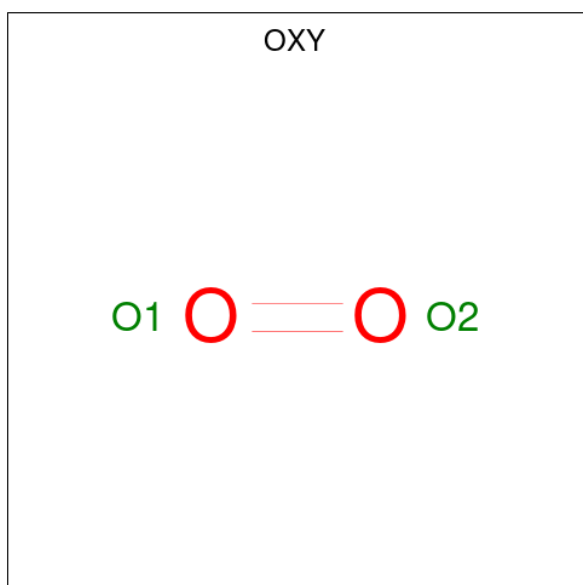
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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).



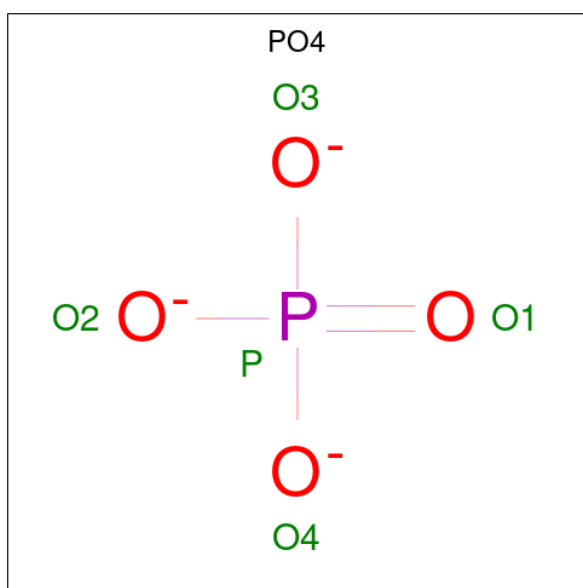
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



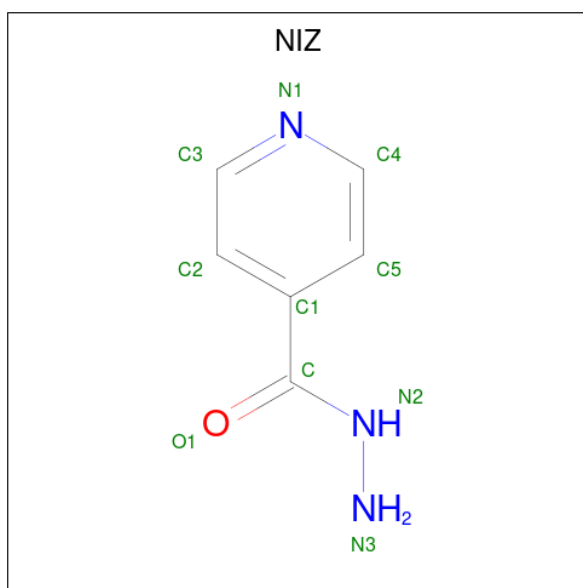
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 8 is pyridine-4-carbohydrazide (CCD ID: NIZ) (formula: C₆H₇N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			10	6	3	1		
8	B	1	Total	C	N	O	0	0
			10	6	3	1		

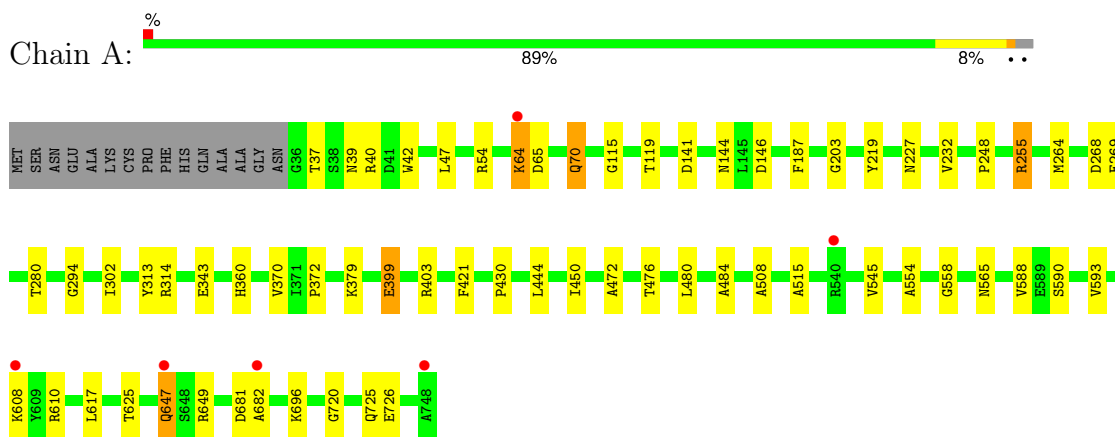
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	576	Total	O	0	0
			576	576		
9	B	594	Total	O	0	0
			594	594		

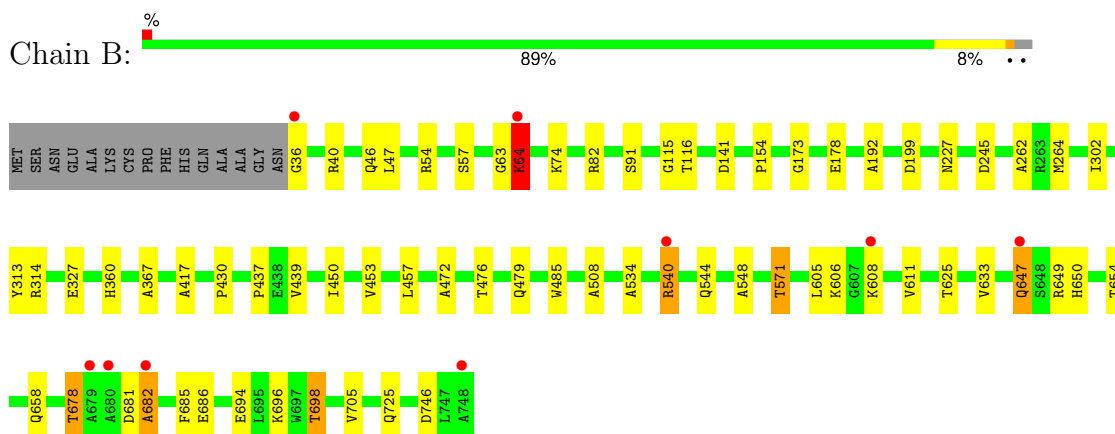
3 Residue-property plots [i](#)

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	100.07Å 113.32Å 174.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.10) 99.3 (20.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.152 , 0.187 0.163 , 0.193	Depositor DCC
R_{free} test set	5724 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.2	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	0.96	EDS
Total number of atoms	12364	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: OXY, MPD, HEM, NA, PO4, NIZ, CL

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	1.57	37/5687 (0.7%)	1.20	10/7732 (0.1%)
1	B	1.58	41/5680 (0.7%)	1.20	8/7722 (0.1%)
All	All	1.57	78/11367 (0.7%)	1.20	18/15454 (0.1%)

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	681	ASP	CA-C	10.36	1.64	1.52
1	A	681	ASP	CA-C	9.02	1.62	1.52
1	A	682	ALA	N-CA	8.16	1.57	1.46
1	B	647	GLN	CA-C	7.91	1.64	1.53
1	A	203	GLY	C-O	7.76	1.29	1.23
1	A	269	GLU	N-CA	-7.64	1.36	1.46
1	B	439	VAL	C-O	-7.49	1.14	1.24
1	B	227	ASN	C-O	-7.44	1.14	1.24
1	A	647	GLN	CA-C	7.40	1.63	1.53
1	A	720	GLY	C-O	-7.02	1.17	1.24
1	A	421	PHE	CA-C	6.98	1.61	1.52
1	B	437	PRO	C-O	-6.97	1.15	1.24
1	B	64	LYS	N-CA	6.87	1.55	1.46
1	A	472	ALA	C-O	-6.84	1.15	1.24
1	A	484	ALA	CA-C	6.76	1.61	1.52
1	B	571	THR	C-O	-6.63	1.15	1.24
1	B	91	SER	C-O	-6.52	1.16	1.23
1	A	248	PRO	CA-C	-6.46	1.47	1.53
1	B	508	ALA	CA-C	6.43	1.60	1.53
1	B	682	ALA	N-CA	6.41	1.54	1.46
1	B	74	LYS	C-O	-6.23	1.15	1.24
1	B	485	TRP	N-CA	6.19	1.53	1.46
1	B	698	THR	C-O	-6.17	1.16	1.23
1	B	192	ALA	C-O	-6.14	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	TRP	C-O	-6.12	1.16	1.24
1	A	47	LEU	C-O	6.09	1.31	1.23
1	B	430	PRO	C-O	5.95	1.30	1.23
1	A	268	ASP	C-O	-5.95	1.17	1.24
1	B	746	ASP	C-O	-5.93	1.16	1.24
1	A	64	LYS	N-CA	5.89	1.54	1.46
1	B	63	GLY	N-CA	5.89	1.53	1.45
1	A	255	ARG	CD-NE	5.89	1.54	1.46
1	B	245	ASP	C-O	-5.88	1.15	1.23
1	A	343	GLU	CA-C	-5.86	1.45	1.52
1	B	705	VAL	N-CA	-5.84	1.39	1.46
1	A	399	GLU	C-O	-5.79	1.17	1.24
1	B	450	ILE	N-CA	-5.77	1.41	1.46
1	B	654	THR	CA-C	5.72	1.59	1.52
1	A	187	PHE	C-O	5.64	1.30	1.23
1	A	37	THR	N-CA	5.57	1.53	1.46
1	B	327	GLU	C-O	-5.52	1.16	1.23
1	B	678	THR	C-O	5.52	1.31	1.23
1	A	294	GLY	C-O	-5.49	1.18	1.23
1	A	617	LEU	C-O	-5.48	1.17	1.24
1	B	116	THR	CA-C	5.46	1.60	1.52
1	A	370	VAL	C-O	-5.43	1.18	1.24
1	B	658	GLN	CD-NE2	-5.39	1.22	1.33
1	B	685	PHE	CA-C	-5.39	1.46	1.52
1	A	47	LEU	CB-CG	-5.39	1.42	1.53
1	A	430	PRO	N-CA	-5.36	1.40	1.47
1	B	199	ASP	C-O	5.35	1.30	1.24
1	B	544	GLN	CD-OE1	5.35	1.33	1.23
1	B	694	GLU	CA-C	5.34	1.59	1.52
1	A	565	ASN	C-O	-5.34	1.17	1.24
1	A	558	GLY	N-CA	5.34	1.52	1.45
1	B	548	ALA	C-O	-5.33	1.18	1.24
1	A	515	ALA	C-O	-5.31	1.17	1.24
1	B	534	ALA	CA-C	5.30	1.59	1.52
1	B	606	LYS	C-O	-5.26	1.17	1.24
1	A	590	SER	C-O	-5.25	1.17	1.24
1	B	367	ALA	C-O	-5.24	1.16	1.23
1	B	472	ALA	C-O	-5.23	1.17	1.24
1	A	70	GLN	CD-NE2	5.23	1.44	1.33
1	A	430	PRO	C-O	5.23	1.29	1.23
1	A	372	PRO	C-O	5.22	1.29	1.23
1	A	508	ALA	CA-C	5.21	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	654	THR	C-O	-5.20	1.17	1.23
1	B	417	ALA	CA-C	5.16	1.59	1.52
1	A	444	LEU	N-CA	5.15	1.52	1.46
1	B	36	GLY	N-CA	5.15	1.53	1.45
1	A	682	ALA	CA-C	5.11	1.59	1.52
1	A	725	GLN	CA-C	5.11	1.59	1.52
1	A	476	THR	CB-CG2	5.10	1.69	1.52
1	A	545	VAL	C-O	5.10	1.29	1.24
1	B	605	LEU	C-O	-5.08	1.18	1.24
1	B	82	ARG	CZ-NH2	-5.03	1.26	1.33
1	B	173	GLY	C-O	5.03	1.29	1.23
1	B	476	THR	CA-C	5.00	1.60	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ARG	CG-CD-NE	-6.89	96.84	112.00
1	B	571	THR	N-CA-CB	6.67	121.42	110.69
1	B	571	THR	CB-CA-C	-6.40	97.86	109.38
1	B	450	ILE	CB-CA-C	-6.00	104.31	110.13
1	A	588	VAL	N-CA-C	5.67	116.40	110.62
1	A	343	GLU	OE1-CD-OE2	5.62	136.38	122.90
1	A	450	ILE	CB-CA-C	-5.56	104.73	110.13
1	A	54	ARG	CG-CD-NE	-5.53	99.83	112.00
1	A	343	GLU	CG-CD-OE2	-5.41	105.95	118.40
1	A	65	ASP	N-CA-C	5.28	119.57	113.18
1	B	611	VAL	N-CA-C	5.20	113.10	108.63
1	B	262	ALA	N-CA-C	-5.18	105.81	111.82
1	B	479	GLN	N-CA-C	5.16	116.59	111.07
1	A	39	ASN	CA-C-N	5.13	127.15	120.28
1	A	39	ASN	C-N-CA	5.13	127.15	120.28
1	A	70	GLN	CA-CB-CG	5.12	124.34	114.10
1	B	450	ILE	CA-C-O	-5.11	116.34	119.51
1	A	280	THR	N-CA-C	-5.05	106.63	112.89

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	5528	0	5355	13	0
1	B	5522	0	5344	17	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	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	8	0	14	1	0
6	B	8	0	14	2	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	10	0	7	1	0
8	B	10	0	7	1	0
9	A	576	0	0	2	0
9	B	594	0	0	5	0
All	All	12364	0	10801	33	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 2.

All (33) 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:64:LYS:HE3	9:B:1421:HOH:O	1.66	0.95
1:A:119[B]:THR:HG21	9:A:985:HOH:O	1.77	0.83
6:B:806:MPD:O4	6:B:806:MPD:H12	1.85	0.76
1:A:360:HIS:ND1	9:A:901:HOH:O	2.23	0.71
1:B:57:SER:HB2	1:B:64:LYS:HD2	1.83	0.60
1:A:625:THR:HG22	8:A:808:NIZ:H4	1.86	0.57
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.87	0.55
6:A:806:MPD:O4	6:A:806:MPD:HM1	2.10	0.51
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:806:MPD:O4	6:B:806:MPD:C1	2.56	0.50
1:A:399:GLU:OE2	1:A:403[B]:ARG:NH2	2.42	0.48
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.43	0.47
1:B:725:GLN:CD	9:B:920:HOH:O	2.56	0.47
1:B:64:LYS:N	1:B:64:LYS:HD3	2.30	0.47
1:B:360:HIS:ND1	9:B:905:HOH:O	2.36	0.46
1:B:115:GLY:O	1:B:264:MET:SD	2.75	0.45
1:B:678:THR:HG22	1:B:686:GLU:HG3	1.99	0.45
1:A:115:GLY:O	1:A:264:MET:SD	2.75	0.44
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.17	0.44
1:B:540:ARG:HA	1:B:540:ARG:NE	2.32	0.44
1:B:625:THR:HG22	8:B:808:NIZ:H4	1.99	0.44
1:B:178:GLU:OE1	9:B:901:HOH:O	2.21	0.44
1:B:650:HIS:HD2	1:B:698:THR:OG1	2.01	0.43
1:B:725:GLN:NE2	9:B:920:HOH:O	2.51	0.43
1:B:302:ILE:HD13	1:B:302:ILE:HG21	1.84	0.42
1:A:313:TYR:CE2	1:A:314:ARG:HD3	2.54	0.42
1:B:47:LEU:HD12	1:B:47:LEU:HA	1.85	0.42
1:B:313:TYR:CE2	1:B:314:ARG:HD3	2.56	0.41
1:A:219:TYR:OH	1:A:232:VAL:HG12	2.20	0.41
1:B:453:VAL:HG11	1:B:457:LEU:HD21	2.01	0.41
1:A:480:LEU:HD22	1:A:554:ALA:HB1	2.03	0.41
1:A:227:ASN:HD22	1:A:227:ASN:HA	1.66	0.41
1:A:302:ILE:HD13	1:A:302:ILE:HG21	1.89	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	716/728 (98%)	704 (98%)	12 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	715/728 (98%)	701 (98%)	13 (2%)	1 (0%)	48	50
All	All	1431/1456 (98%)	1405 (98%)	25 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	682	ALA

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	555/561 (99%)	543 (98%)	12 (2%)	45	53
1	B	554/561 (99%)	541 (98%)	13 (2%)	44	51
All	All	1109/1122 (99%)	1084 (98%)	25 (2%)	45	51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	70	GLN
1	A	141	ASP
1	A	255	ARG
1	A	379	LYS
1	A	608	LYS
1	A	610	ARG
1	A	647	GLN
1	A	649	ARG
1	A	696	LYS
1	A	726	GLU
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS

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Mol	Chain	Res	Type
1	B	141	ASP
1	B	154	PRO
1	B	540	ARG
1	B	571	THR
1	B	608	LYS
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	647	GLN
1	B	649	ARG
1	B	696	LYS

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

Mol	Chain	Res	Type
1	A	70	GLN
1	A	227	ASN
1	A	247	ASN
1	A	544	GLN
1	A	737	ASN
1	B	46	GLN
1	B	647	GLN
1	B	650	HIS
1	B	741	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	OXY	A	805	-	1,1,1	0.16	0	-		
5	OXY	B	804	-	1,1,1	0.13	0	-		
2	HEM	B	801	9,1	50,50,50	1.78	11 (22%)	67,82,82	1.65	14 (20%)
7	PO4	A	807	-	4,4,4	0.93	0	6,6,6	1.09	1 (16%)
5	OXY	B	805	-	1,1,1	0.06	0	-		
7	PO4	B	807	-	4,4,4	0.80	0	6,6,6	2.10	3 (50%)
6	MPD	A	806	-	7,7,7	0.99	0	9,10,10	1.10	0
5	OXY	A	804	-	1,1,1	0.13	0	-		
8	NIZ	A	808	-	10,10,10	2.68	3 (30%)	12,12,12	1.84	3 (25%)
6	MPD	B	806	-	7,7,7	0.79	0	9,10,10	2.07	4 (44%)
8	NIZ	B	808	-	10,10,10	2.38	4 (40%)	12,12,12	1.85	3 (25%)
2	HEM	A	801	9,1	50,50,50	2.04	14 (28%)	67,82,82	1.66	14 (20%)

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	B	801	9,1	-	2/14/54/54	-
6	MPD	A	806	-	-	2/5/5/5	-
8	NIZ	A	808	-	-	0/6/6/6	0/1/1/1
6	MPD	B	806	-	-	3/5/5/5	-
8	NIZ	B	808	-	-	0/6/6/6	0/1/1/1
2	HEM	A	801	9,1	-	2/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4D-ND	-5.79	1.30	1.40
8	A	808	NIZ	C-N2	5.30	1.39	1.33
2	B	801	HEM	C1B-NB	-5.02	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	FE-NC	4.86	2.11	1.95
2	A	801	HEM	FE-NB	4.68	2.09	1.94
2	B	801	HEM	C4D-ND	-4.63	1.32	1.40
8	A	808	NIZ	C2-C1	4.45	1.46	1.39
2	A	801	HEM	C1B-NB	-4.22	1.32	1.40
8	B	808	NIZ	C2-C1	4.13	1.45	1.39
8	B	808	NIZ	C-N2	4.06	1.38	1.33
2	B	801	HEM	FE-NB	3.90	2.06	1.94
2	B	801	HEM	FE-NC	3.60	2.07	1.95
2	A	801	HEM	FE-NA	3.43	2.06	1.95
2	A	801	HEM	C4A-NA	-3.36	1.33	1.39
2	B	801	HEM	C2A-C3A	-3.07	1.30	1.38
2	B	801	HEM	CBA-CGA	2.81	1.57	1.50
2	A	801	HEM	C4B-NB	-2.75	1.33	1.38
8	A	808	NIZ	C2-C3	2.73	1.43	1.38
8	B	808	NIZ	O1-C	2.71	1.29	1.23
2	B	801	HEM	C1A-NA	-2.55	1.34	1.39
2	A	801	HEM	C1A-NA	-2.51	1.34	1.39
2	A	801	HEM	C4D-C3D	2.41	1.49	1.45
2	B	801	HEM	C4B-NB	-2.36	1.34	1.38
2	A	801	HEM	C3D-C2D	-2.27	1.31	1.36
2	B	801	HEM	CHA-C4D	-2.26	1.34	1.38
2	A	801	HEM	C1C-C2C	-2.19	1.41	1.45
2	B	801	HEM	C3B-C4B	2.14	1.49	1.44
8	B	808	NIZ	C2-C3	2.10	1.42	1.38
2	A	801	HEM	C3C-C2C	2.09	1.41	1.37
2	A	801	HEM	CHC-C4B	-2.08	1.34	1.39
2	B	801	HEM	CHB-C1B	2.07	1.42	1.38
2	A	801	HEM	O1A-CGA	2.02	1.28	1.22

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CHC-C4B-NB	5.55	130.40	124.42
2	A	801	HEM	C1B-NB-C4B	4.93	111.04	105.21
2	B	801	HEM	C1B-NB-C4B	4.16	110.13	105.21
8	B	808	NIZ	O1-C-N2	3.91	127.16	122.46
2	A	801	HEM	C4B-C3B-C2B	-3.83	103.76	107.28
2	B	801	HEM	CHB-C1B-NB	3.80	129.06	124.37
7	B	807	PO4	O3-P-O2	-3.60	96.72	107.91
6	B	806	MPD	CM-C2-C1	-3.57	102.64	110.63
2	A	801	HEM	CHC-C4B-NB	3.51	128.20	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	808	NIZ	C1-C-N2	-3.38	112.58	116.33
2	A	801	HEM	CAD-C3D-C4D	3.35	130.54	124.70
6	B	806	MPD	O2-C2-CM	3.34	118.39	107.99
2	A	801	HEM	CHB-C1B-NB	3.31	128.46	124.37
2	A	801	HEM	C3B-C2B-C1B	3.28	108.87	106.41
8	A	808	NIZ	C-N2-N3	3.24	126.59	121.50
6	B	806	MPD	O2-C2-C3	-3.11	97.64	109.27
2	A	801	HEM	CMB-C2B-C1B	-3.09	120.21	125.03
8	A	808	NIZ	O1-C-N2	3.07	126.15	122.46
2	B	801	HEM	C3B-C4B-NB	-3.00	107.31	109.47
2	A	801	HEM	CBD-CAD-C3D	2.99	120.81	112.53
2	B	801	HEM	CHA-C4D-ND	2.92	127.97	124.37
2	B	801	HEM	CHD-C1D-ND	2.71	127.34	124.42
8	A	808	NIZ	C2-C3-N1	-2.66	119.06	123.60
2	A	801	HEM	C3D-C4D-ND	2.56	112.98	110.17
2	A	801	HEM	CAA-CBA-CGA	-2.50	107.04	113.67
7	B	807	PO4	O3-P-O1	2.50	119.79	110.95
2	A	801	HEM	CHD-C4C-C3C	2.49	129.41	125.21
2	B	801	HEM	C4A-CHB-C1B	-2.41	120.59	126.25
2	A	801	HEM	C4C-NC-C1C	2.37	109.69	105.82
2	B	801	HEM	CAA-CBA-CGA	-2.31	107.54	113.67
2	B	801	HEM	CHA-C4D-C3D	-2.26	121.05	125.23
2	A	801	HEM	CHA-C4D-C3D	-2.24	121.09	125.23
7	A	807	PO4	O4-P-O3	2.23	114.84	107.91
6	B	806	MPD	C1-C2-C3	2.20	119.68	110.20
2	B	801	HEM	C4B-C3B-C2B	-2.19	105.26	107.28
8	B	808	NIZ	C-N2-N3	2.16	124.89	121.50
2	B	801	HEM	CMA-C3A-C2A	2.14	130.16	125.62
2	B	801	HEM	C3B-C2B-C1B	2.09	107.98	106.41
2	B	801	HEM	O1A-CGA-CBA	-2.08	116.48	123.09
2	A	801	HEM	C4D-C3D-C2D	-2.07	103.88	106.89
2	B	801	HEM	C4D-C3D-C2D	-2.07	103.88	106.89
7	B	807	PO4	O4-P-O1	-2.02	103.82	110.95

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	806	MPD	C1-C2-C3-C4
6	B	806	MPD	O2-C2-C3-C4
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A

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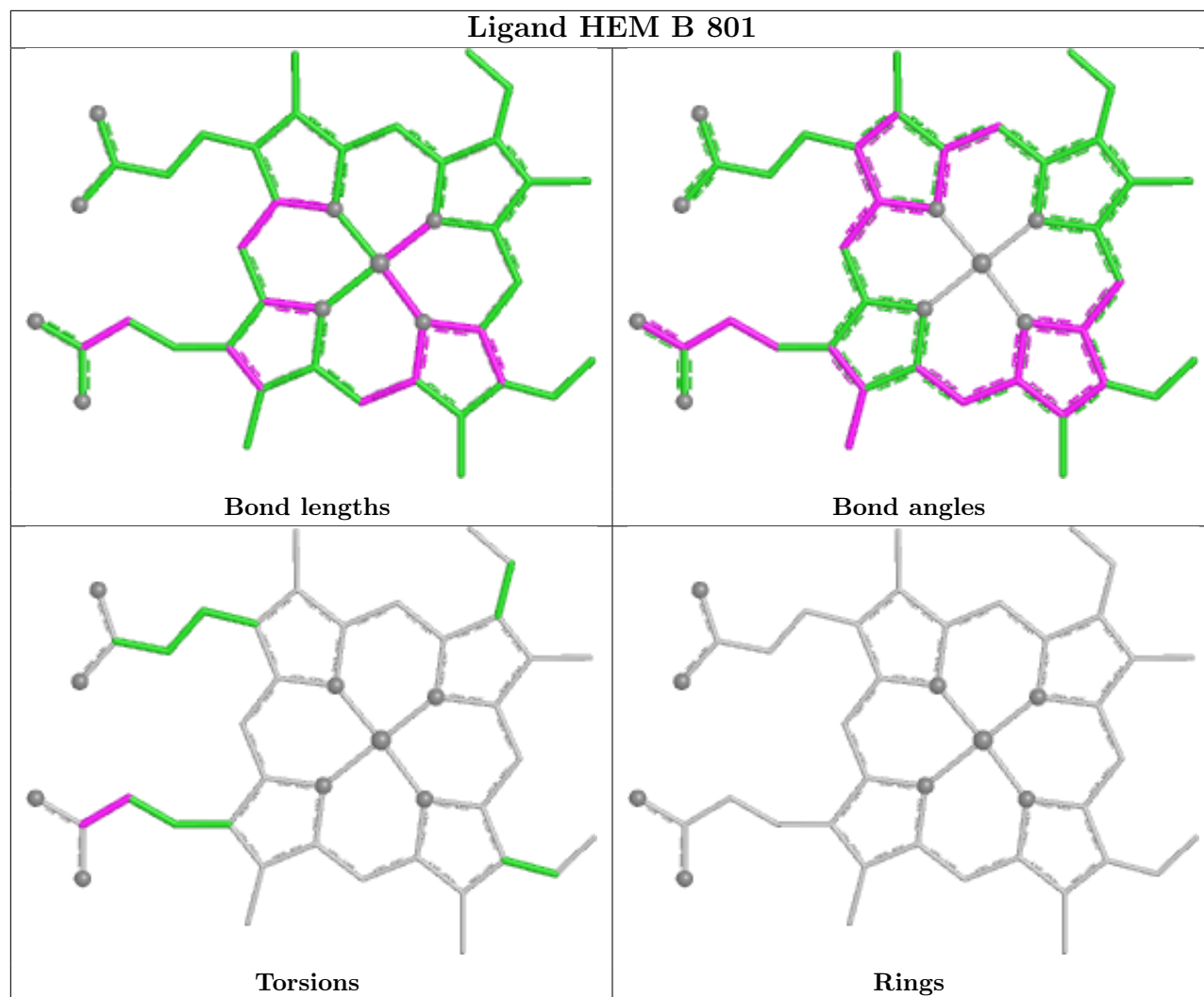
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
6	A	806	MPD	O2-C2-C3-C4
6	A	806	MPD	C2-C3-C4-O4
6	B	806	MPD	CM-C2-C3-C4

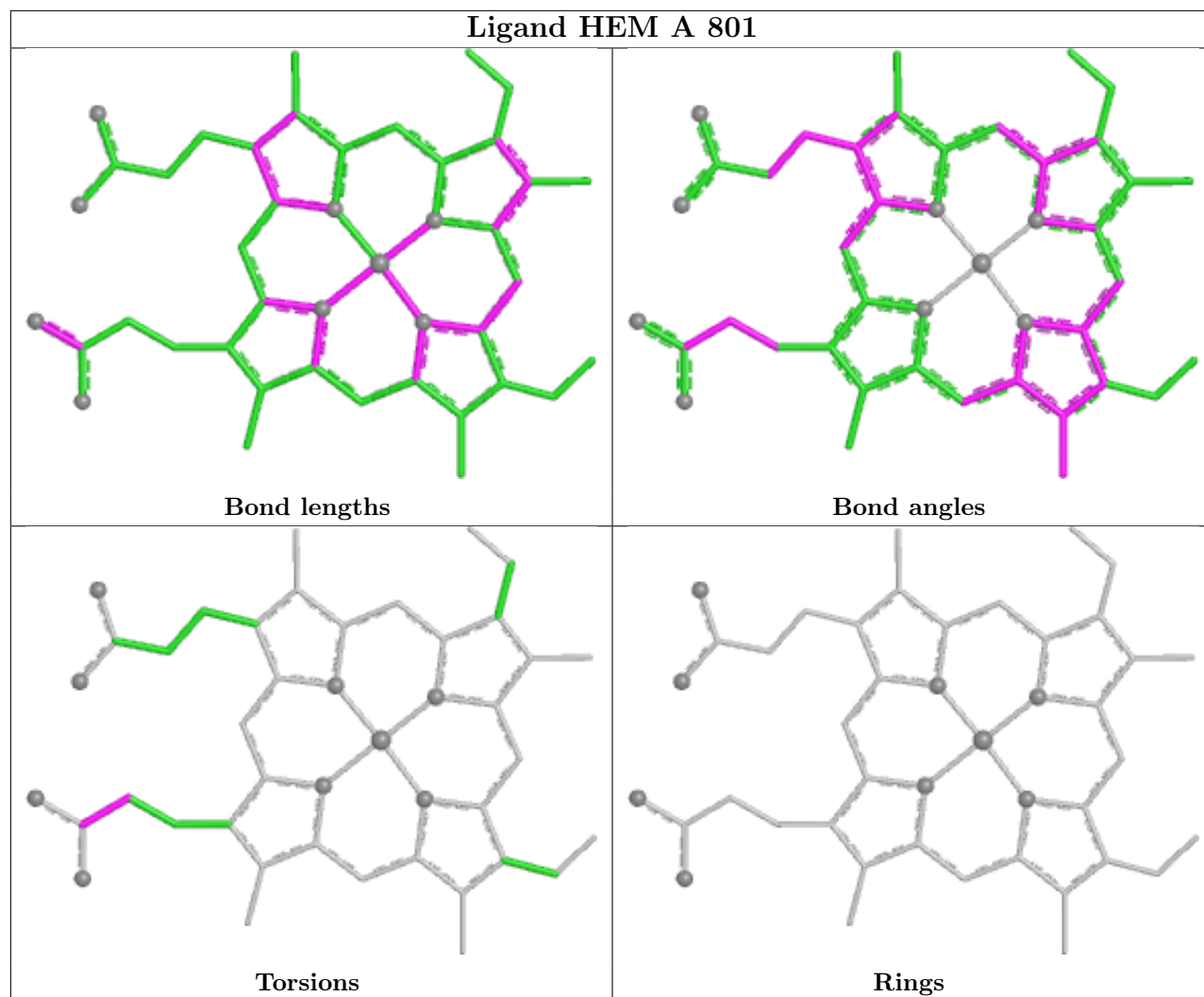
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	806	MPD	1	0
8	A	808	NIZ	1	0
6	B	806	MPD	2	0
8	B	808	NIZ	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%)	-0.48	6 (0%) 82 84	11, 26, 47, 89	5 (0%)
1	B	713/728 (97%)	-0.61	9 (1%) 75 77	11, 23, 45, 93	4 (0%)
All	All	1426/1456 (97%)	-0.55	15 (1%) 78 80	11, 24, 46, 93	9 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	3.7
1	A	682	ALA	3.3
1	B	679	ALA	3.2
1	B	540	ARG	3.0
1	B	36	GLY	3.0
1	A	647	GLN	2.8
1	B	64	LYS	2.6
1	B	680	ALA	2.6
1	B	682	ALA	2.6
1	A	64	LYS	2.4
1	B	647	GLN	2.4
1	B	608	LYS	2.4
1	A	748	ALA	2.3
1	A	540	ARG	2.2
1	A	608	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

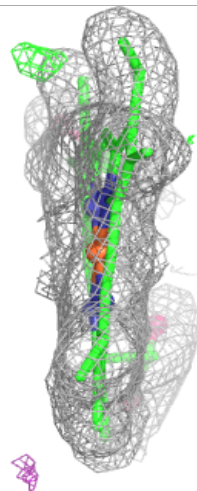
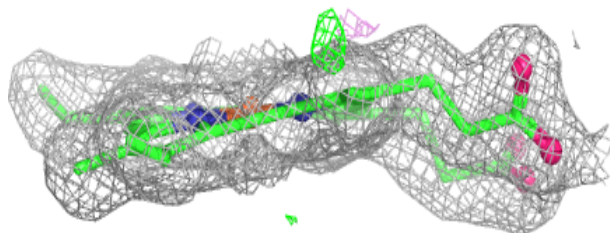
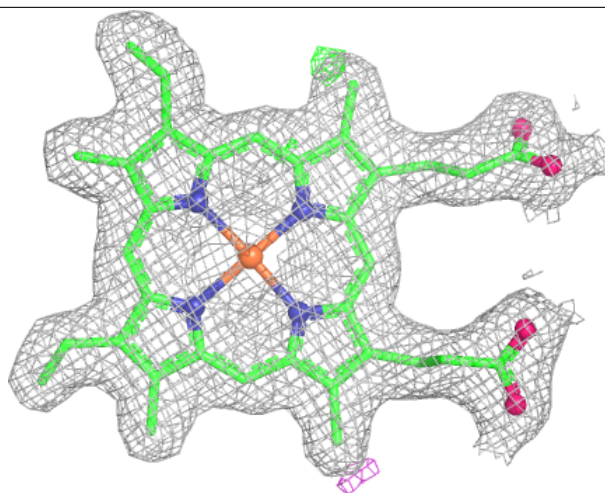
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

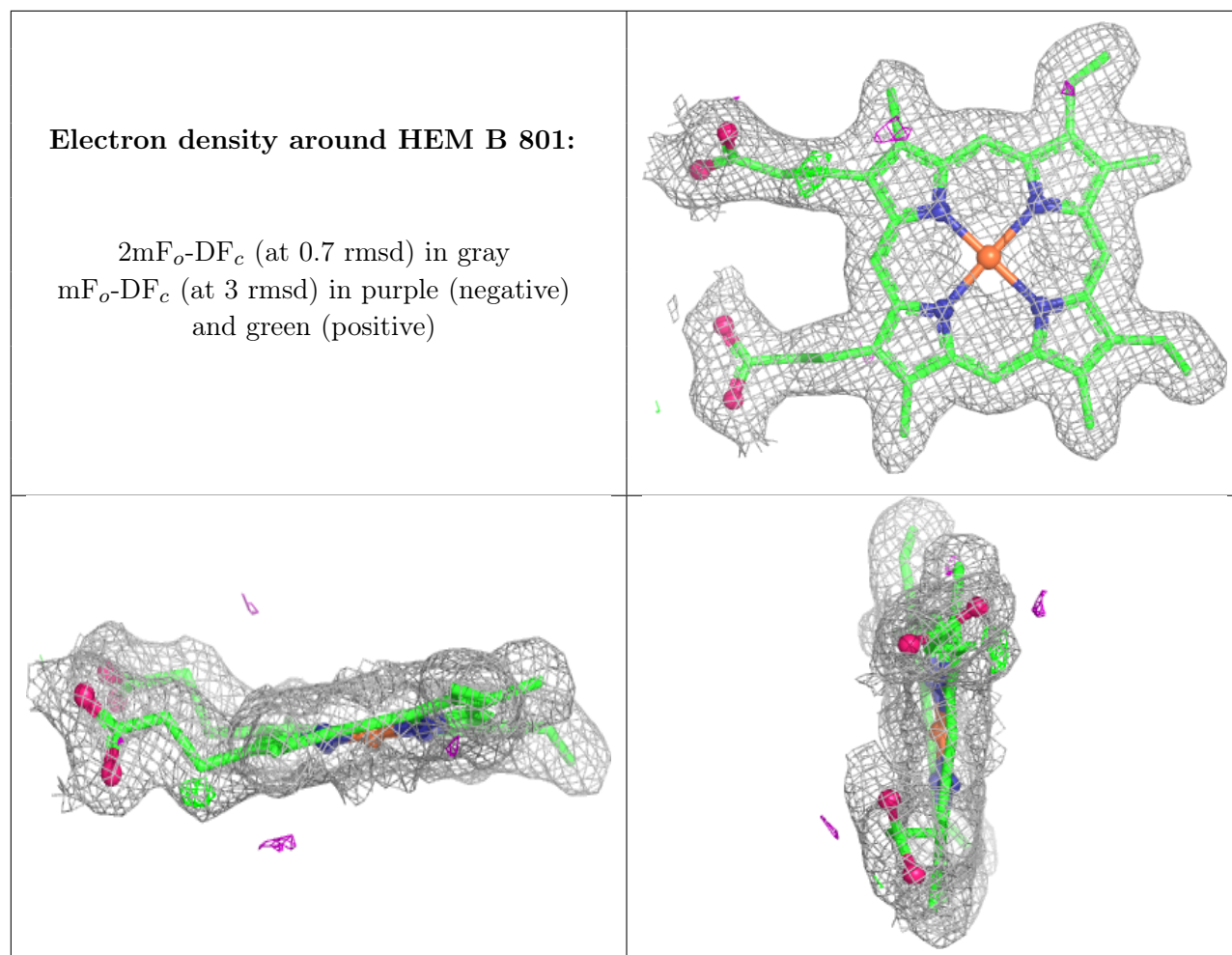
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NIZ	A	808	10/10	0.82	0.13	40,49,54,55	0
6	MPD	A	806	8/8	0.85	0.21	65,74,82,82	0
7	PO4	B	807	5/5	0.86	0.14	55,62,73,77	0
6	MPD	B	806	8/8	0.87	0.16	48,58,61,70	0
5	OXY	A	805	2/2	0.91	0.11	40,40,40,52	0
7	PO4	A	807	5/5	0.91	0.10	57,62,71,74	0
8	NIZ	B	808	10/10	0.91	0.09	36,39,41,41	0
5	OXY	B	805	2/2	0.93	0.12	37,37,37,53	0
5	OXY	B	804	2/2	0.96	0.14	26,26,26,32	0
2	HEM	A	801	43/43	0.98	0.05	19,22,24,25	0
4	CL	A	803	1/1	0.98	0.04	31,31,31,31	0
5	OXY	A	804	2/2	0.98	0.13	34,34,34,40	0
2	HEM	B	801	43/43	0.99	0.04	16,17,19,20	0
4	CL	B	803	1/1	0.99	0.05	28,28,28,28	0
3	NA	B	802	1/1	0.99	0.09	20,20,20,20	0
3	NA	A	802	1/1	1.00	0.04	18,18,18,18	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.