



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 08:39 PM BST

PDB ID : 5SXQ  
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](mailto: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.

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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 : 2.13  
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) : 2.13

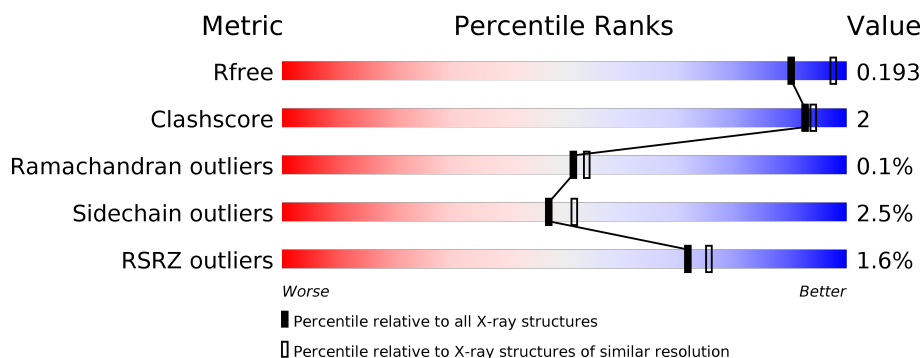
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>••</div> </div> </div>
1	B	728	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>••</div> </div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12364 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
			5528	3493	984	1037	14			
1	B	713	Total	C	N	O	S	0	4	0
			5522	3488	984	1036	14			

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



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

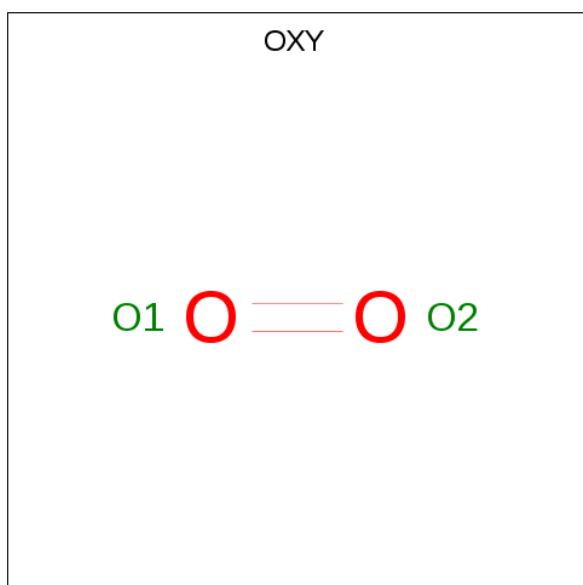
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

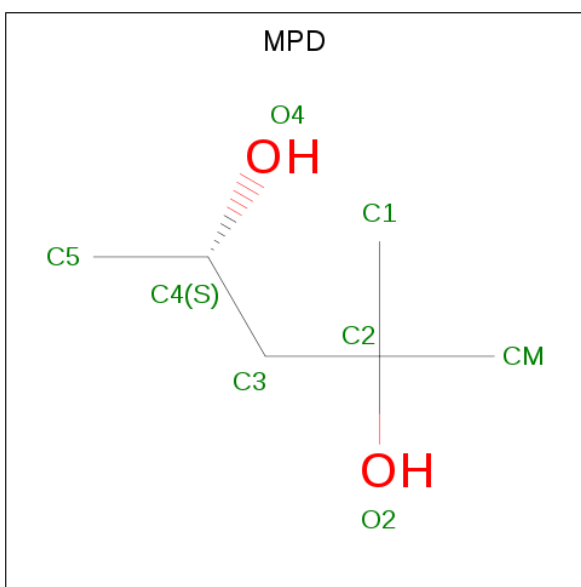
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



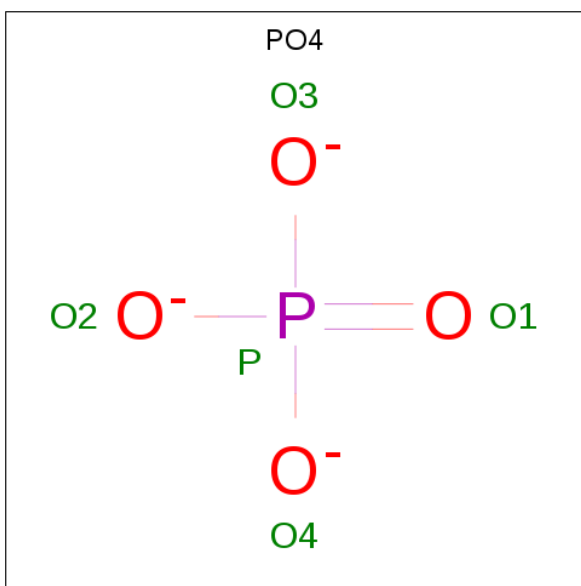
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



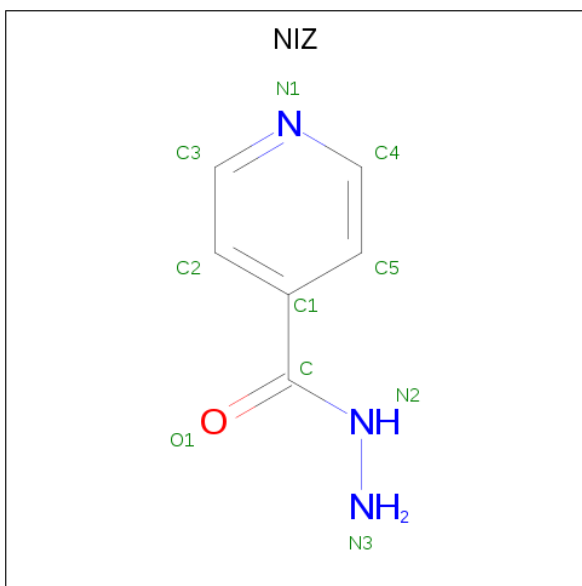
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is PHOSPHATE ION (three-letter code: 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 (three-letter code: NIZ) (formula: C<sub>6</sub>H<sub>7</sub>N<sub>3</sub>O).



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		

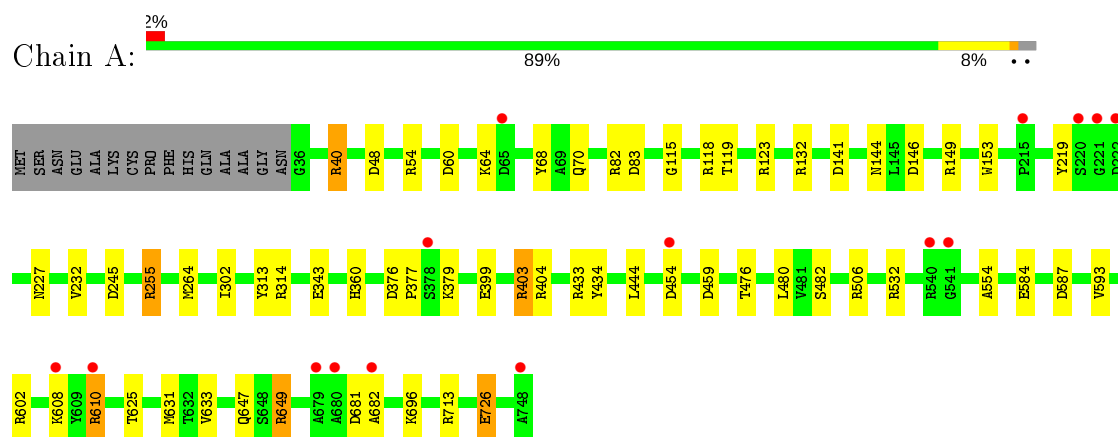
- Molecule 9 is water.

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

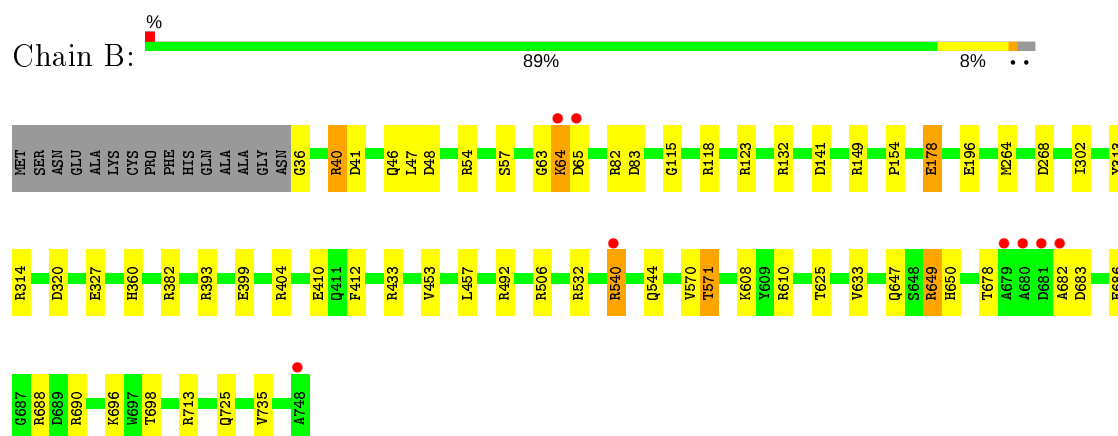
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	100.07Å 113.32Å 174.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 32.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.10) 99.4 (32.98-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, OXY, CL, NA, PO4, NIZ, 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	11/5687 (0.2%)	1.12	44/7732 (0.6%)
1	B	1.23	9/5680 (0.2%)	1.10	36/7722 (0.5%)
All	All	1.23	20/11367 (0.2%)	1.11	80/15454 (0.5%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	TYR	CE1-CZ	-8.55	1.27	1.38
1	B	410	GLU	CG-CD	7.68	1.63	1.51
1	A	343	GLU	CD-OE1	6.94	1.33	1.25
1	A	68	TYR	CG-CD2	-6.42	1.30	1.39
1	A	482	SER	CB-OG	5.93	1.50	1.42
1	A	153	TRP	CG-CD1	-5.89	1.28	1.36
1	B	327	GLU	CG-CD	5.60	1.60	1.51
1	A	682	ALA	N-CA	5.42	1.57	1.46
1	A	726	GLU	CG-CD	5.35	1.59	1.51
1	A	584	GLU	CG-CD	5.31	1.59	1.51
1	B	327	GLU	CD-OE2	5.29	1.31	1.25
1	B	647	GLN	CG-CD	5.29	1.63	1.51
1	B	63	GLY	N-CA	5.24	1.53	1.46
1	B	178	GLU	CD-OE2	5.24	1.31	1.25
1	A	647	GLN	CG-CD	5.17	1.62	1.51
1	A	476	THR	CB-CG2	5.16	1.69	1.52
1	B	399	GLU	CD-OE1	5.16	1.31	1.25
1	B	36	GLY	N-CA	5.16	1.53	1.46
1	B	65	ASP	CB-CG	5.09	1.62	1.51
1	A	726	GLU	CD-OE2	5.08	1.31	1.25

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLU	OE1-CD-OE2	10.90	136.38	123.30
1	B	532	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	A	255	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	A	48	ASP	CB-CG-OD2	-9.72	109.55	118.30
1	B	433	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	403[A]	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	A	403[B]	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	B	132	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	688	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	A	713	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	48	ASP	CB-CG-OD1	8.32	125.79	118.30
1	A	602	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	B	713	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	B	82	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	54	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	149	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	532	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	602	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	48	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	A	54	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	433	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	54	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	B	433	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	B	54	ARG	CG-CD-NE	-7.12	96.84	111.80
1	B	123	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	40	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	649	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	40	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	376	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	506	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	320	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	B	54	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	735	VAL	CG1-CB-CG2	-6.23	100.94	110.90
1	A	713	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	343	GLU	CG-CD-OE2	-6.17	105.95	118.30
1	B	268	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	123	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	393	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	454	ASP	CB-CG-OD2	5.89	123.61	118.30
1	A	631	MET	CG-SD-CE	5.88	109.61	100.20
1	A	681	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	B	571	THR	N-CA-CB	5.86	121.42	110.30
1	B	492	ARG	NE-CZ-NH1	5.81	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	83	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	610	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	433	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	54	ARG	CG-CD-NE	-5.70	99.83	111.80
1	B	48	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	382	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	404	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	506	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	683	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	403[A]	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	403[B]	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	713	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	532	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	434	TYR	CB-CG-CD1	5.51	124.31	121.00
1	A	610	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	649	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	82	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	444	LEU	CB-CG-CD1	5.43	120.23	111.00
1	A	60	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	149	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	149	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	196	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	245	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	633[A]	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	A	633[B]	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	A	532	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	83	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	404	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	132	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	404	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	41	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	570	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	B	412	PHE	CB-CG-CD1	5.09	124.36	120.80
1	B	571	THR	CB-CA-C	-5.09	97.86	111.60
1	A	459	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	587	ASP	CB-CG-OD1	5.00	122.80	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	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:HM1	6:A:806:MPD:O4	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: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:NE	1:B:540:ARG:HA	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:CD	9:B:920:HOH:O	2.56	0.43
1:B:725:GLN:NE2	9:B:920:HOH:O	2.51	0.43
1:B:302:ILE:HG21	1:B:302:ILE:HD13	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%)	51	54
All	All	1431/1456 (98%)	1405 (98%)	25 (2%)	1 (0%)	51	54

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%)	542 (98%)	13 (2%)	50	55
1	B	554/561 (99%)	539 (97%)	15 (3%)	44	48
All	All	1109/1122 (99%)	1081 (98%)	28 (2%)	47	52

All (28) 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	118	ARG
1	A	141	ASP
1	A	255	ARG
1	A	377	PRO
1	A	379	LYS
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	A	696	LYS
1	A	726	GLU
1	B	40	ARG
1	B	46	GLN

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Mol	Chain	Res	Type
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	154	PRO
1	B	540	ARG
1	B	544	GLN
1	B	571	THR
1	B	608	LYS
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	649	ARG
1	B	690	ARG
1	B	696	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	227	ASN
1	A	247	ASN
1	A	647	GLN
1	B	46	GLN
1	B	647	GLN
1	B	650	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	B	804	-	1,1,1	0.19	0	-		
8	NIZ	B	808	-	10,10,10	2.33	3 (30%)	12,12,12	1.78	3 (25%)
2	HEM	A	801	1,9	27,50,50	1.25	2 (7%)	17,82,82	1.89	3 (17%)
2	HEM	B	801	1,9	27,50,50	1.53	5 (18%)	17,82,82	1.84	5 (29%)
8	NIZ	A	808	-	10,10,10	2.58	3 (30%)	12,12,12	1.80	3 (25%)
6	MPD	B	806	-	7,7,7	0.75	0	9,10,10	2.11	4 (44%)
7	PO4	B	807	-	4,4,4	0.75	0	6,6,6	2.03	2 (33%)
5	OXY	B	805	-	1,1,1	0.03	0	-		
6	MPD	A	806	-	7,7,7	0.93	0	9,10,10	1.12	1 (11%)
7	PO4	A	807	-	4,4,4	0.88	0	6,6,6	1.04	1 (16%)
5	OXY	A	805	-	1,1,1	0.14	0	-		
5	OXY	A	804	-	1,1,1	0.11	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
8	NIZ	B	808	-	-	0/6/6/6	0/1/1/1
2	HEM	A	801	1,9	-	0/6/54/54	-
2	HEM	B	801	1,9	-	0/6/54/54	-
8	NIZ	A	808	-	-	0/6/6/6	0/1/1/1
6	MPD	B	806	-	-	2/5/5/5	-
6	MPD	A	806	-	-	2/5/5/5	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	808	NIZ	C-N2	5.24	1.39	1.33
2	B	801	HEM	C3B-C2B	-4.68	1.33	1.40
8	B	808	NIZ	C-N2	4.02	1.38	1.33
8	A	808	NIZ	C2-C1	4.01	1.46	1.39
8	B	808	NIZ	C2-C1	3.73	1.45	1.39
8	B	808	NIZ	O1-C	3.13	1.29	1.23
2	B	801	HEM	CAA-C2A	-2.97	1.47	1.52
2	A	801	HEM	C4D-C3D	2.90	1.49	1.42
8	A	808	NIZ	C2-C3	2.59	1.43	1.38
2	B	801	HEM	C4D-C3D	2.49	1.48	1.42
2	A	801	HEM	C4B-CHC	-2.36	1.34	1.41
2	B	801	HEM	C2A-C3A	-2.28	1.30	1.37
2	B	801	HEM	C4B-CHC	-2.15	1.35	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CBD-CAD-C3D	4.52	120.81	112.48
6	B	806	MPD	CM-C2-C1	-3.81	102.64	110.57
8	B	808	NIZ	O1-C-N2	3.73	127.16	122.50
7	B	807	PO4	O3-P-O2	-3.50	96.72	107.97
2	A	801	HEM	CAA-CBA-CGA	-3.36	107.04	112.67
6	B	806	MPD	O2-C2-C3	-3.24	97.64	109.80
8	B	808	NIZ	C1-C-N2	-3.23	112.58	116.27
6	B	806	MPD	O2-C2-CM	3.21	118.39	108.08
2	B	801	HEM	CMA-C3A-C4A	-3.15	123.63	128.46
8	A	808	NIZ	C-N2-N3	3.11	126.59	121.59
2	A	801	HEM	CMB-C2B-C3B	3.09	130.45	124.68
2	B	801	HEM	CAA-CBA-CGA	-3.06	107.54	112.67
2	B	801	HEM	CAD-CBD-CGD	2.93	117.58	112.67
8	A	808	NIZ	O1-C-N2	2.92	126.15	122.50
2	B	801	HEM	CMA-C3A-C2A	2.77	130.16	124.94
8	A	808	NIZ	C2-C3-N1	-2.62	119.06	123.62
7	B	807	PO4	O3-P-O1	2.43	119.79	110.89
2	B	801	HEM	CBD-CAD-C3D	2.29	116.70	112.48
7	A	807	PO4	O4-P-O3	2.14	114.84	107.97
6	B	806	MPD	C1-C2-C3	2.09	119.68	109.96
8	B	808	NIZ	C-N2-N3	2.05	124.89	121.59
6	A	806	MPD	O2-C2-C3	-2.05	102.10	109.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

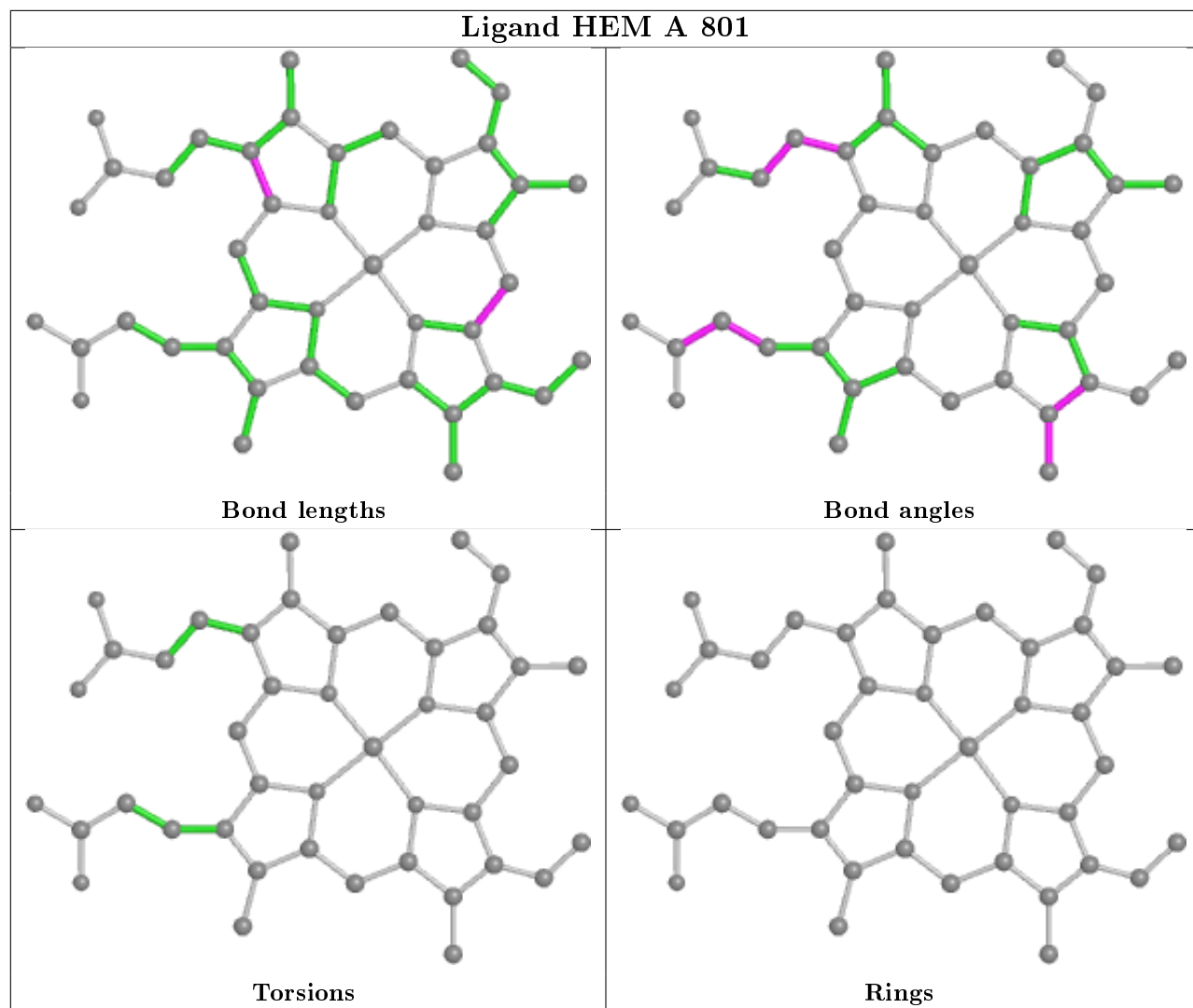
Mol	Chain	Res	Type	Atoms
6	B	806	MPD	C1-C2-C3-C4
6	B	806	MPD	O2-C2-C3-C4
6	A	806	MPD	O2-C2-C3-C4
6	A	806	MPD	C2-C3-C4-O4

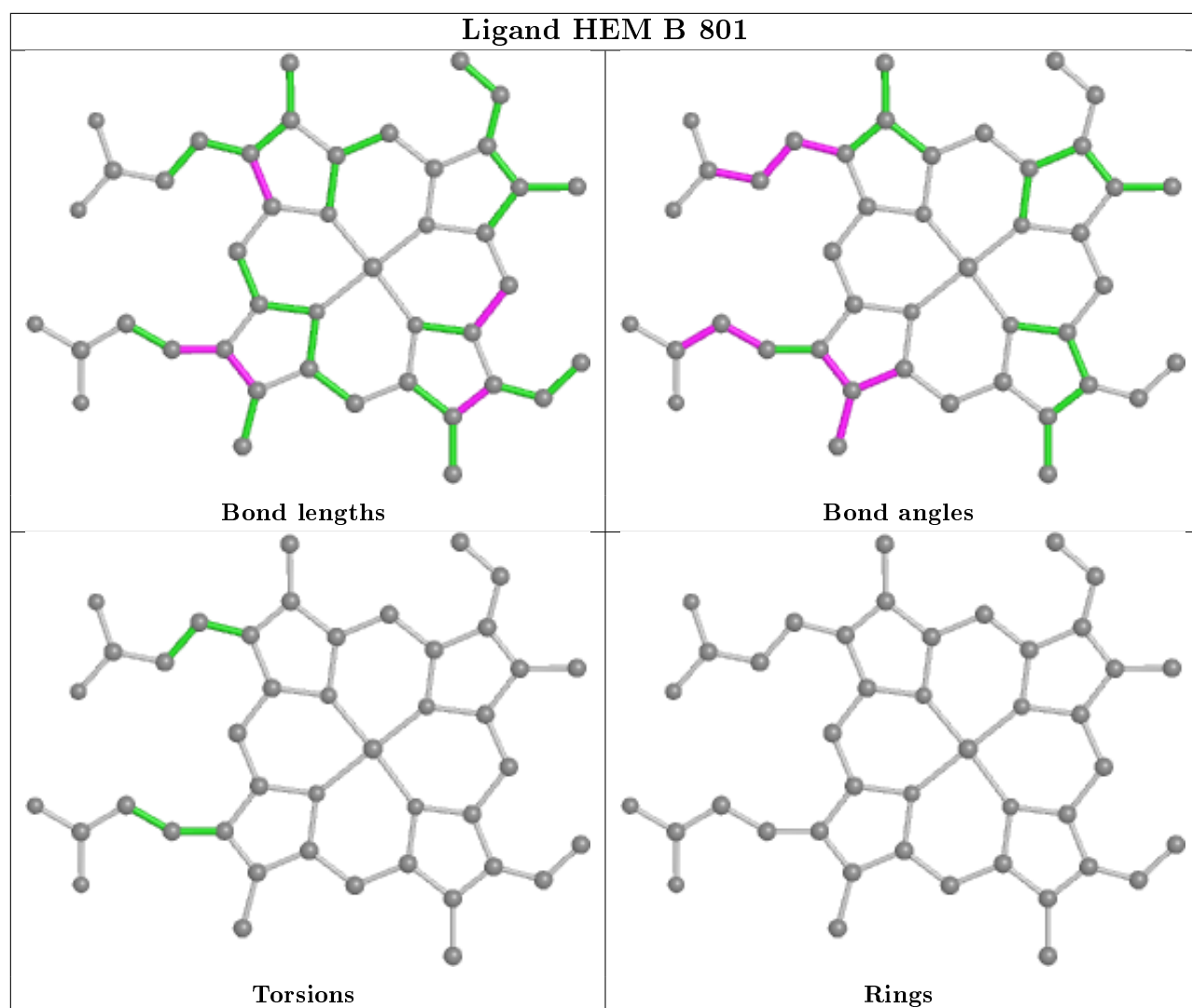
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	808	NIZ	1	0
8	A	808	NIZ	1	0
6	B	806	MPD	2	0
6	A	806	MPD	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	713/728 (97%)	-0.45	15 (2%) 63 68	16, 26, 47, 89	0
1	B	713/728 (97%)	-0.57	8 (1%) 80 84	16, 23, 45, 93	0
All	All	1426/1456 (97%)	-0.51	23 (1%) 72 75	16, 24, 46, 93	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	GLY	5.5
1	A	748	ALA	5.4
1	B	748	ALA	5.1
1	B	679	ALA	4.7
1	A	540	ARG	4.4
1	B	540	ARG	4.1
1	A	215	PRO	3.6
1	A	679	ALA	3.4
1	A	608	LYS	3.2
1	B	64	LYS	3.1
1	A	680	ALA	3.1
1	B	680	ALA	3.0
1	A	222	ASP	3.0
1	A	610	ARG	2.9
1	A	682	ALA	2.7
1	A	378	SER	2.6
1	B	65	ASP	2.5
1	B	681	ASP	2.4
1	A	65	ASP	2.4
1	A	454	ASP	2.2
1	A	221	GLY	2.2
1	A	220	SER	2.1
1	B	682	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

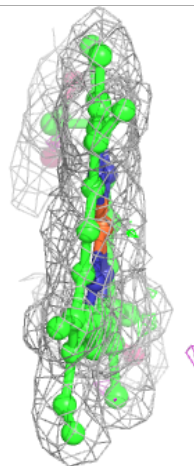
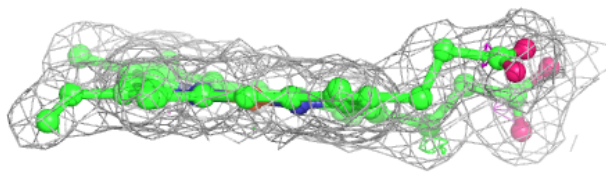
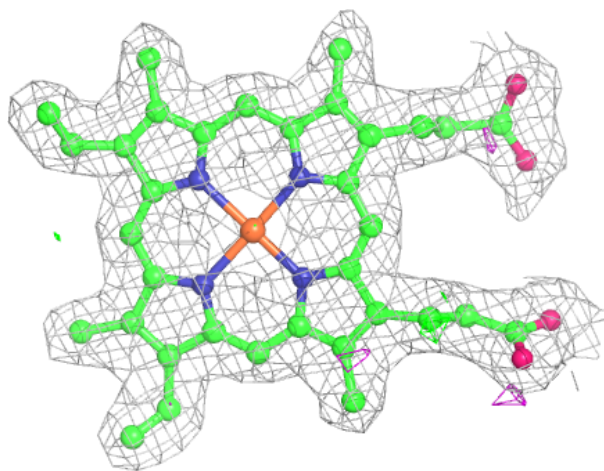
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MPD	A	806	8/8	0.85	0.25	65,74,82,82	0
8	NIZ	A	808	10/10	0.87	0.16	40,49,54,55	0
7	PO4	B	807	5/5	0.89	0.20	55,62,73,77	0
6	MPD	B	806	8/8	0.91	0.16	48,58,61,70	0
8	NIZ	B	808	10/10	0.93	0.10	36,39,41,41	0
7	PO4	A	807	5/5	0.94	0.20	57,62,71,74	0
5	OXY	B	805	2/2	0.95	0.19	37,37,37,53	0
5	OXY	A	805	2/2	0.96	0.24	40,40,40,52	0
5	OXY	B	804	2/2	0.97	0.10	26,26,26,32	0
4	CL	B	803	1/1	0.99	0.07	28,28,28,28	0
2	HEM	B	801	43/43	0.99	0.14	16,17,19,20	0
4	CL	A	803	1/1	0.99	0.06	31,31,31,31	0
2	HEM	A	801	43/43	0.99	0.14	19,22,24,25	0
3	NA	B	802	1/1	0.99	0.04	20,20,20,20	0
5	OXY	A	804	2/2	0.99	0.09	34,34,34,40	0
3	NA	A	802	1/1	1.00	0.03	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.

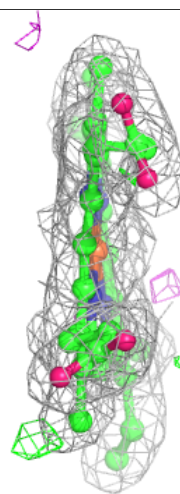
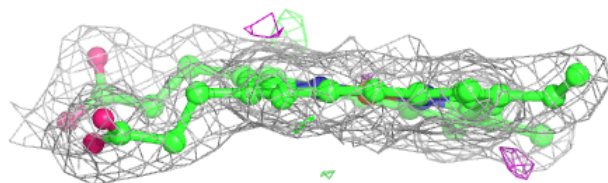
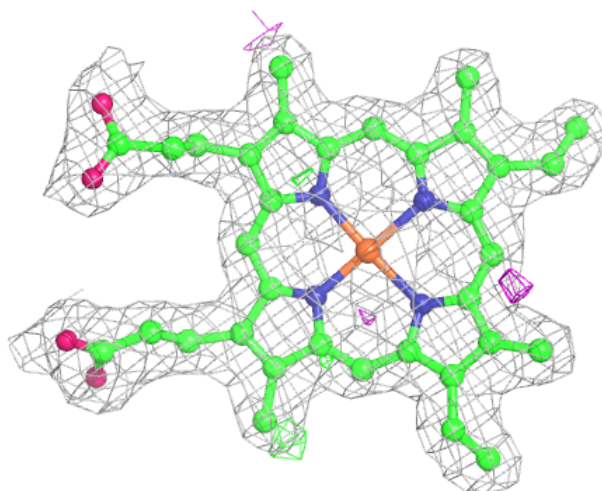
**Electron density around HEM B 801:**

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



**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.