



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:02 pm BST

PDB ID : 5KQ2  
Title : Crystal structure of the A357D variant of catalase-peroxidase from *B. pseudo-mallei*  
Authors : Loewen, P.C.  
Deposited on : 2016-07-05  
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](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	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

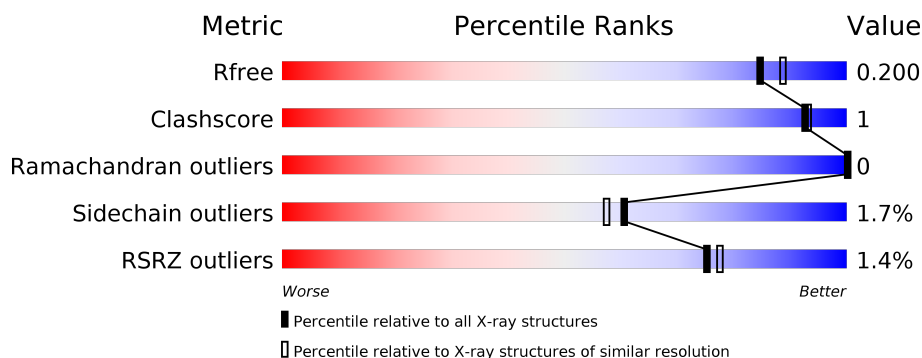
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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>90%</div> <div>7%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </div> </div>

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
4	CL	B	803	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12676 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
			5570	3513	992	1051	14			
1	B	713	Total	C	N	O	S	0	5	0
			5545	3500	986	1045	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	ASP	ALA	conflict	UNP Q3JNW6
B	357	ASP	ALA	conflict	UNP Q3JNW6

- 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		

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

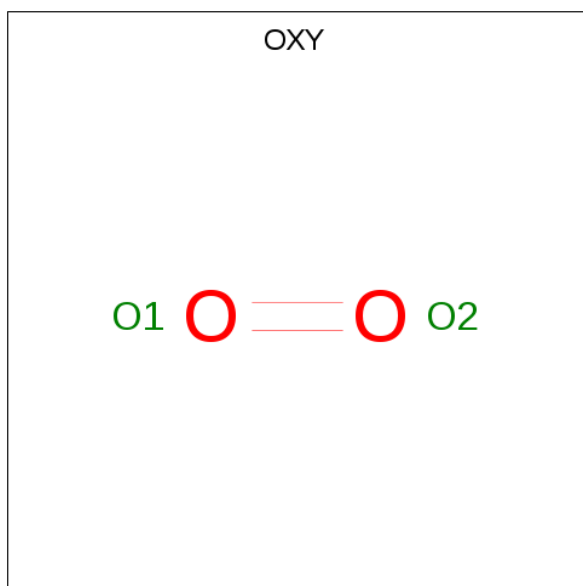
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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>).



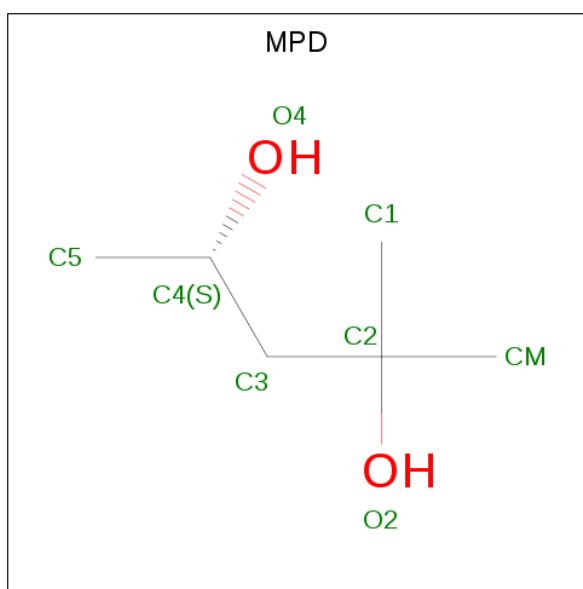
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



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 (three-letter code: MPD) (formula:  $\text{C}_6\text{H}_{14}\text{O}_2$ ).



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

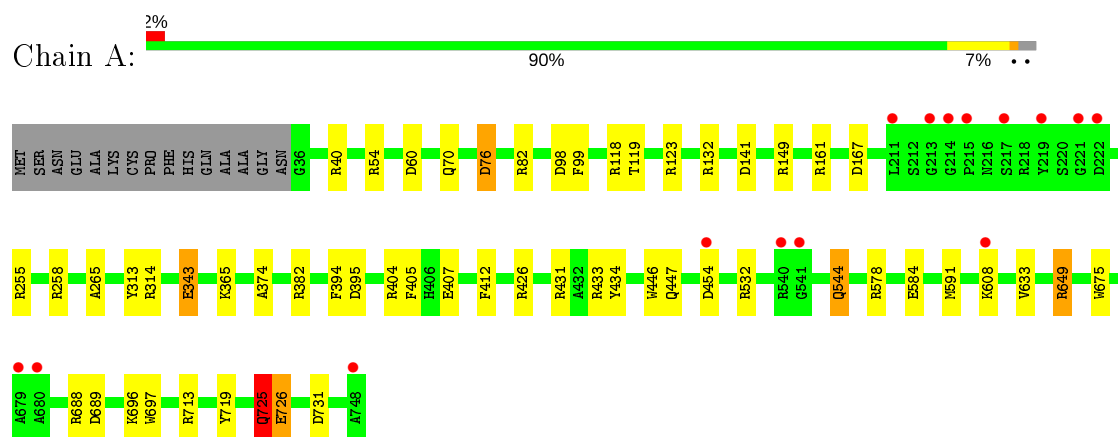
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	707	Total O 707 707	0	0
8	B	718	Total O 718 718	0	0

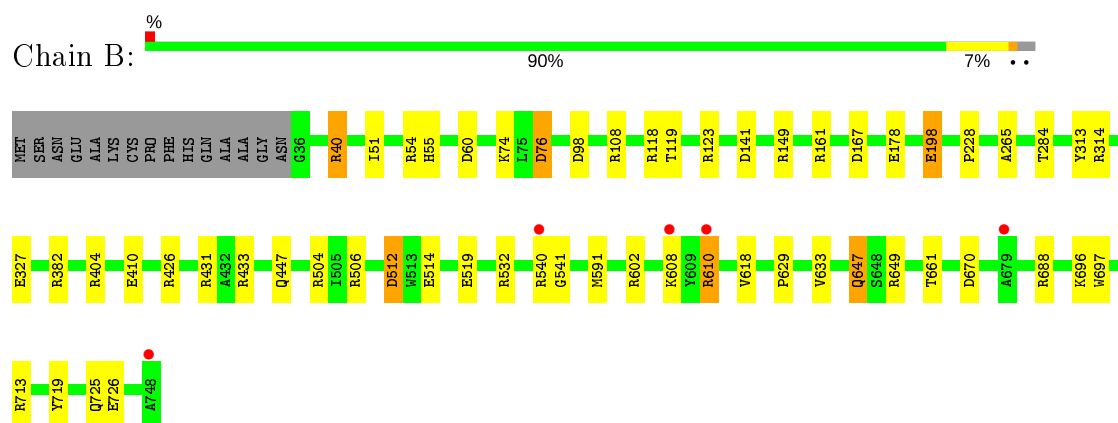
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	100.83Å 114.13Å 174.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 1.90 47.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.78-1.90) 96.9 (47.78-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.156 , 0.191 0.167 , 0.200	Depositor DCC
$R_{free}$ test set	7663 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TOX, OXY, CL, NA, PO4, MPD, 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	1.19	12/5696 (0.2%)	1.10	39/7740 (0.5%)
1	B	1.16	10/5674 (0.2%)	1.10	37/7712 (0.5%)
All	All	1.17	22/11370 (0.2%)	1.10	76/15452 (0.5%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	GLU	CG-CD	8.92	1.65	1.51
1	B	512	ASP	CG-OD2	8.48	1.44	1.25
1	B	514	GLU	CD-OE2	-6.74	1.18	1.25
1	B	512	ASP	CB-CG	6.66	1.65	1.51
1	A	584	GLU	CG-CD	6.63	1.61	1.51
1	A	544	GLN	CD-OE1	6.36	1.38	1.24
1	B	726	GLU	CG-CD	6.27	1.61	1.51
1	B	602	ARG	CZ-NH2	-6.21	1.25	1.33
1	A	365	LYS	N-CA	6.17	1.58	1.46
1	B	410	GLU	CG-CD	6.16	1.61	1.51
1	A	407	GLU	CD-OE1	6.02	1.32	1.25
1	A	725	GLN	CG-CD	5.89	1.64	1.51
1	A	697	TRP	CG-CD1	-5.65	1.28	1.36
1	A	434	TYR	CE1-CZ	-5.54	1.31	1.38
1	B	327	GLU	CD-OE1	5.53	1.31	1.25
1	B	426	ARG	CZ-NH2	5.47	1.40	1.33
1	A	454	ASP	CB-CG	5.28	1.62	1.51
1	A	675	TRP	CE3-CZ3	5.28	1.47	1.38
1	A	343	GLU	CD-OE1	5.21	1.31	1.25
1	A	446	TRP	CE3-CZ3	5.21	1.47	1.38
1	B	647	GLN	CG-CD	5.11	1.62	1.51
1	B	697	TRP	CG-CD1	-5.09	1.29	1.36

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ASP	CB-CG-OD2	10.77	127.99	118.30
1	B	512	ASP	CB-CG-OD1	-10.02	109.28	118.30
1	A	433	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	433	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	A	76	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	B	149	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	149	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	B	161[A]	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	B	161[B]	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	258	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	649	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	A	688	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	426	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	B	532	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	578	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	98	ASP	CB-CG-OD1	-7.22	111.80	118.30
1	B	670	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	532	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	B	167	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	649	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	B	591	MET	CG-SD-CE	-6.76	89.38	100.20
1	B	433	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	161	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	149	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	B	382	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	404	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	404	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	108	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	713	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	649	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	40	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	108	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	54	ARG	CG-CD-NE	-6.15	98.89	111.80
1	B	713	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	407	GLU	OE1-CD-OE2	-6.13	115.95	123.30
1	A	82	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	132	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	255[A]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	688	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	731	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	161	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	434	TYR	CB-CG-CD1	5.88	124.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	610	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	98	ASP	CB-CG-OD2	5.84	123.55	118.30
1	B	504	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	382	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	404	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	60	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	454	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	433	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	591	MET	CG-SD-CE	-5.59	91.26	100.20
1	B	123	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	713	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	149	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	504	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	167	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	123	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	649	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	395	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	426[A]	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	532	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	60	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	541	GLY	N-CA-C	-5.38	99.64	113.10
1	B	76	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	689	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	688	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	540	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	506	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	123	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	407	GLU	CG-CD-OE1	5.14	128.58	118.30
1	B	532	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	382	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	670	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	98	ASP	CB-CG-OD2	5.05	122.85	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	5570	0	5369	13	0
1	B	5545	0	5354	19	0
2	A	43	0	30	0	0
2	B	43	0	30	1	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	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	24	0	42	2	0
7	B	8	0	14	0	0
8	A	707	0	0	3	0
8	B	718	0	0	7	0
All	All	12676	0	10839	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 1.

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:519:GLU:OE1	8:B:901:HOH:O	1.99	0.79
1:B:647:GLN:HG2	8:B:1350:HOH:O	1.85	0.76
1:B:198:GLU:OE1	8:B:902:HOH:O	2.06	0.74
1:A:343:GLU:HG3	8:A:1441:HOH:O	1.89	0.73
1:A:76:ASP:OD2	8:A:903:HOH:O	2.06	0.72
1:B:76:ASP:OD2	8:B:903:HOH:O	2.10	0.70
1:B:512:ASP:OD1	8:B:904:HOH:O	2.12	0.67
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.37	0.60
1:B:198:GLU:HG2	4:B:803:CL:CL	2.40	0.58
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.38	0.54
1:B:178:GLU:OE1	8:B:905:HOH:O	2.18	0.54
1:B:198:GLU:CG	4:B:803:CL:CL	2.94	0.52
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.93	0.51
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.45	0.51
1:A:725:GLN:HE22	1:A:726[A]:GLU:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.95	0.49
1:A:394:PHE:CZ	7:A:806:MPD:HM1	2.49	0.48
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.43	0.47
1:B:51:ILE:HD11	1:B:618:VAL:HG12	1.96	0.47
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.50	0.47
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.15	0.46
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.16	0.46
1:A:725:GLN:NE2	1:A:726[A]:GLU:HG3	2.30	0.46
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.16	0.45
1:B:313:TYR:CE2	1:B:314:ARG:HD3	2.53	0.43
1:B:178:GLU:HG2	8:B:1034:HOH:O	2.19	0.42
1:A:119[A]:THR:HG22	1:A:265:ALA:HB2	2.00	0.42
1:A:313:TYR:CE2	1:A:314:ARG:HD3	2.54	0.42
7:A:808:MPD:H11	8:A:1331:HOH:O	2.18	0.42
1:B:661:THR:HA	1:B:725:GLN:HE22	1.85	0.42
1:B:284:THR:HG22	2:B:801:HEM:HAA1	2.02	0.42
1:A:405:PHE:HB3	1:A:412:PHE:HB2	2.00	0.41
1:A:99:PHE:CD2	1:A:374:ALA:HA	2.55	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	717/728 (98%)	711 (99%)	6 (1%)	0	100	100
1	B	715/728 (98%)	705 (99%)	10 (1%)	0	100	100
All	All	1432/1456 (98%)	1416 (99%)	16 (1%)	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	557/561 (99%)	546 (98%)	11 (2%)	55	51
1	B	555/561 (99%)	546 (98%)	9 (2%)	62	60
All	All	1112/1122 (99%)	1092 (98%)	20 (2%)	60	55

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	70	GLN
1	A	118	ARG
1	A	141	ASP
1	A	544	GLN
1	A	608	LYS
1	A	649	ARG
1	A	696	LYS
1	A	725	GLN
1	A	726[A]	GLU
1	A	726[B]	GLU
1	B	40	ARG
1	B	74	LYS
1	B	118	ARG
1	B	141	ASP
1	B	198	GLU
1	B	228	PRO
1	B	608	LYS
1	B	610	ARG
1	B	696	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	B	227	ASN

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Mol	Chain	Res	Type
1	B	406	HIS
1	B	647	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TOX	A	111	1,2	10,17,18	2.58	3 (30%)	10,23,25	2.10	3 (30%)
1	TOX	B	111	1,2	10,17,18	2.93	5 (50%)	10,23,25	2.25	4 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TOX	A	111	1,2	-	2/4/8/10	0/2/2/2
1	TOX	B	111	1,2	-	2/4/8/10	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TOX	CD1-NE1	-6.56	1.32	1.39
1	A	111	TOX	CE3-CD2	-4.83	1.32	1.42
1	B	111	TOX	O-C	4.70	1.38	1.19
1	A	111	TOX	O-C	4.18	1.36	1.19
1	A	111	TOX	CD1-NE1	-3.89	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TOX	CE3-CD2	-2.24	1.37	1.42
1	B	111	TOX	CH2-CZ2	2.09	1.41	1.36
1	B	111	TOX	CA-N	-2.06	1.41	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TOX	CB-CA-C	5.00	120.84	111.47
1	B	111	TOX	CZ3-CH2-CZ2	-4.87	113.61	120.44
1	B	111	TOX	CB-CA-C	2.76	116.65	111.47
1	B	111	TOX	CH2-CZ2-CE2	2.72	124.66	119.44
1	A	111	TOX	CZ3-CH2-CZ2	-2.48	116.96	120.44
1	A	111	TOX	CH2-CZ3-CE3	2.40	123.81	120.44
1	B	111	TOX	CH2-CZ3-CE3	2.18	123.50	120.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111	TOX	N-CA-CB-CG
1	A	111	TOX	C-CA-CB-CG
1	B	111	TOX	N-CA-CB-CG
1	B	111	TOX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
7	MPD	A	806	-	7,7,7	0.66	0	9,10,10	1.61	1 (11%)
6	PO4	B	805	-	4,4,4	0.98	0	6,6,6	1.13	0
7	MPD	B	806	-	7,7,7	0.68	0	9,10,10	2.01	2 (22%)
5	OXY	A	804	-	1,1,1	0.12	0	-	-	-
7	MPD	A	807	-	7,7,7	0.65	0	9,10,10	1.10	1 (11%)
5	OXY	B	804	-	1,1,1	0.45	0	-	-	-
2	HEM	A	801	1	27,50,50	0.93	0	17,82,82	2.17	5 (29%)
2	HEM	B	801	1	27,50,50	0.99	1 (3%)	17,82,82	2.62	8 (47%)
6	PO4	A	805	-	4,4,4	0.42	0	6,6,6	2.43	2 (33%)
7	MPD	A	808	-	7,7,7	0.47	0	9,10,10	1.48	2 (22%)

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	806	-	-	4/5/5/5	-
7	MPD	A	807	-	-	0/5/5/5	-
2	HEM	A	801	1	-	0/6/54/54	-
2	HEM	B	801	1	-	0/6/54/54	-
7	MPD	B	806	-	-	0/5/5/5	-
7	MPD	A	808	-	-	4/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C4D-C3D	2.04	1.47	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C4C-C3C-C2C	-5.53	103.04	106.90
2	B	801	HEM	CBD-CAD-C3D	5.07	121.82	112.48
2	A	801	HEM	CBD-CAD-C3D	4.92	121.55	112.48
6	A	805	PO4	O4-P-O3	4.47	122.30	107.97
2	A	801	HEM	CAA-CBA-CGA	-4.19	105.64	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	806	MPD	O4-C4-C3	-3.99	95.27	111.36
7	B	806	MPD	CM-C2-C1	3.86	118.62	110.57
2	B	801	HEM	C1D-C2D-C3D	-3.82	104.34	107.00
2	B	801	HEM	CMA-C3A-C4A	-3.02	123.82	128.46
2	B	801	HEM	CMA-C3A-C2A	3.00	130.61	124.94
7	B	806	MPD	O4-C4-C3	-2.92	99.57	111.36
2	B	801	HEM	CAD-CBD-CGD	2.79	117.35	112.67
2	A	801	HEM	CAD-CBD-CGD	2.77	117.31	112.67
7	A	808	MPD	O2-C2-CM	-2.64	99.61	108.08
2	A	801	HEM	C1D-C2D-C3D	-2.62	105.18	107.00
2	A	801	HEM	C4A-C3A-C2A	-2.36	105.36	107.00
6	A	805	PO4	O4-P-O2	-2.35	100.42	107.97
7	A	807	MPD	CM-C2-C1	2.30	115.36	110.57
2	B	801	HEM	C4A-C3A-C2A	-2.28	105.41	107.00
2	B	801	HEM	CBA-CAA-C2A	2.10	116.35	112.49
7	A	808	MPD	O4-C4-C3	-2.05	103.09	111.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	808	MPD	O2-C2-C3-C4
7	A	808	MPD	C2-C3-C4-O4
7	A	806	MPD	C1-C2-C3-C4
7	A	806	MPD	O2-C2-C3-C4
7	A	808	MPD	C2-C3-C4-C5
7	A	806	MPD	C2-C3-C4-C5
7	A	808	MPD	CM-C2-C3-C4
7	A	806	MPD	C2-C3-C4-O4

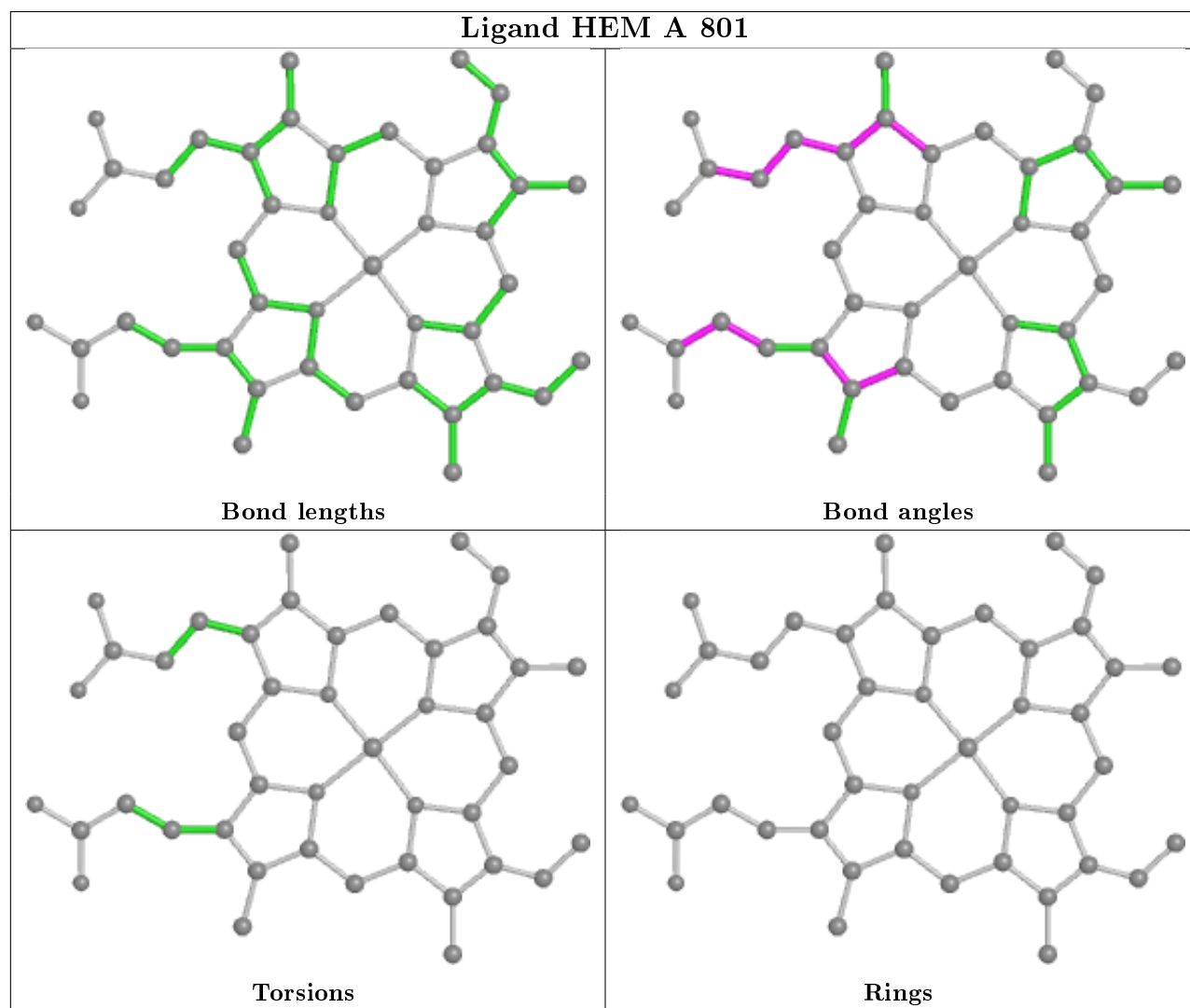
There are no ring outliers.

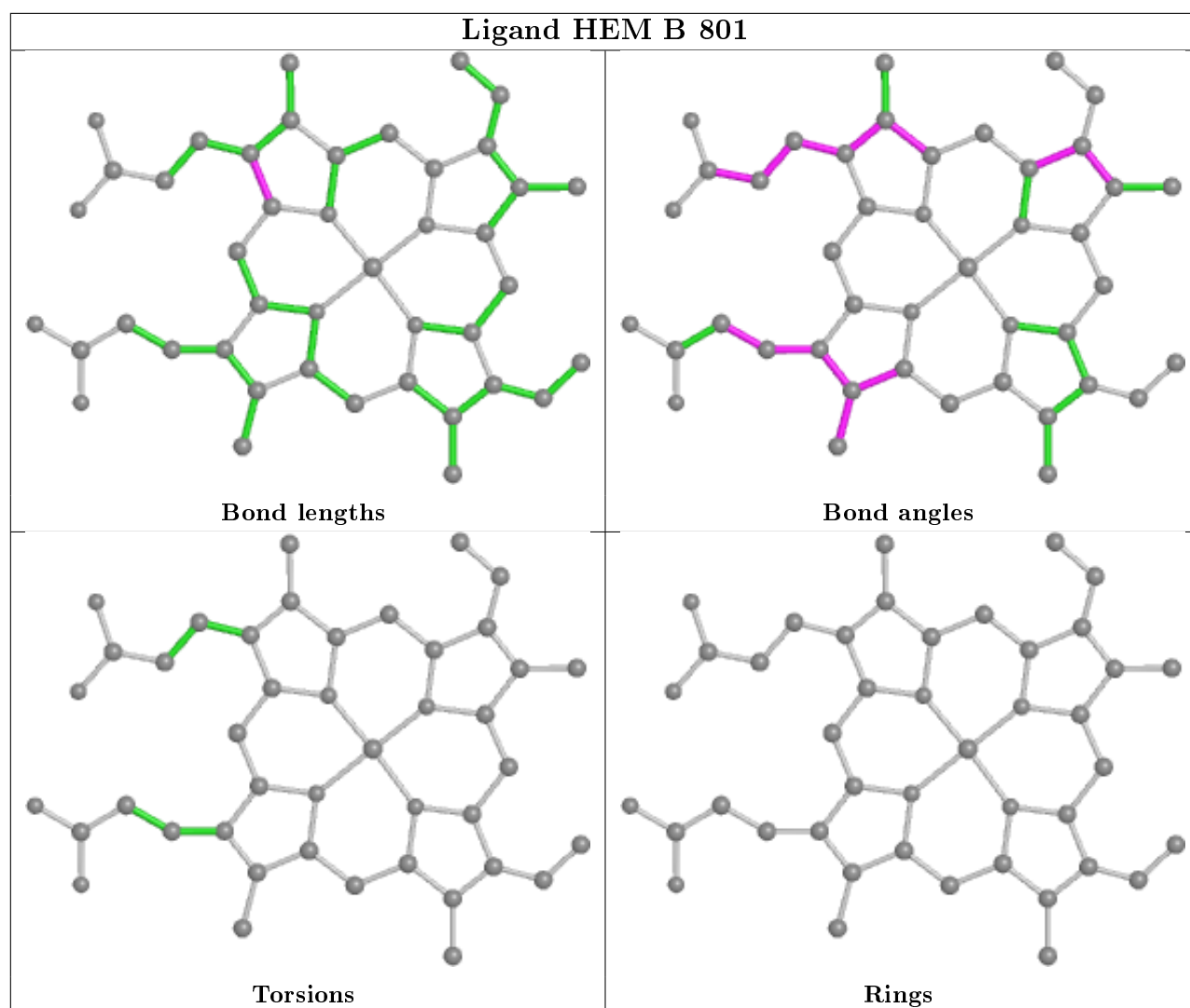
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	806	MPD	1	0
2	B	801	HEM	1	0
7	A	808	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	712/728 (97%)	-0.38	15 (2%) 63 66	15, 24, 44, 80	0
1	B	712/728 (97%)	-0.44	5 (0%) 87 88	17, 24, 42, 76	0
All	All	1424/1456 (97%)	-0.41	20 (1%) 75 77	15, 24, 44, 80	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	3.8
1	A	215	PRO	3.5
1	B	540	ARG	3.4
1	B	608	LYS	3.3
1	A	541	GLY	3.2
1	A	679	ALA	3.2
1	A	213	GLY	3.1
1	A	221	GLY	3.1
1	A	540	ARG	2.7
1	A	748	ALA	2.7
1	A	222	ASP	2.7
1	A	608	LYS	2.6
1	A	454	ASP	2.5
1	A	680	ALA	2.5
1	A	214	GLY	2.4
1	A	219	TYR	2.2
1	B	610	ARG	2.2
1	A	217	SER	2.2
1	B	679	ALA	2.1
1	A	211	LEU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
1	TOX	A	111	16/17	0.97	0.11	17,20,30,30	2
1	TOX	B	111	16/17	0.97	0.12	16,21,31,37	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

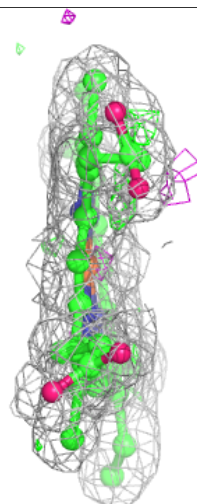
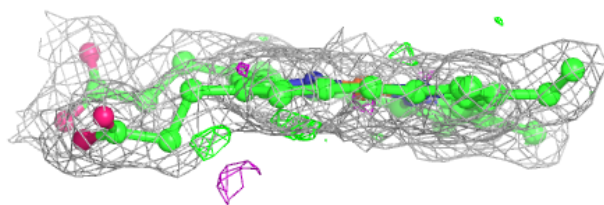
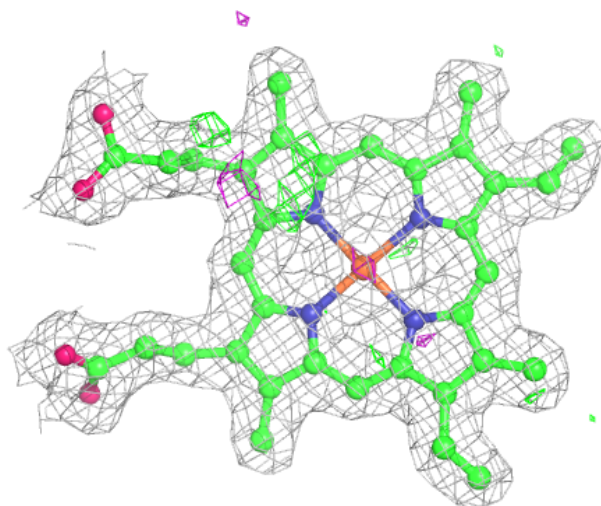
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	PO4	A	805	5/5	0.83	0.18	69,78,80,82	0
7	MPD	A	806	8/8	0.86	0.18	42,54,59,60	0
5	OXY	A	804	2/2	0.90	0.24	52,52,52,52	0
7	MPD	A	807	8/8	0.90	0.18	61,68,79,79	0
7	MPD	B	806	8/8	0.92	0.15	43,49,60,61	0
7	MPD	A	808	8/8	0.93	0.16	49,52,65,72	0
5	OXY	B	804	2/2	0.94	0.14	35,35,35,38	0
4	CL	A	803	1/1	0.94	0.11	44,44,44,44	0
6	PO4	B	805	5/5	0.95	0.21	43,55,59,64	0
3	NA	A	802	1/1	0.97	0.06	20,20,20,20	0
4	CL	B	803	1/1	0.98	0.10	39,39,39,39	0
2	HEM	A	801	43/43	0.98	0.09	18,21,24,27	0
2	HEM	B	801	43/43	0.99	0.11	16,19,20,24	0
3	NA	B	802	1/1	1.00	0.03	22,22,22,22	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:**

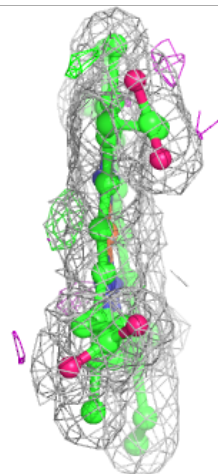
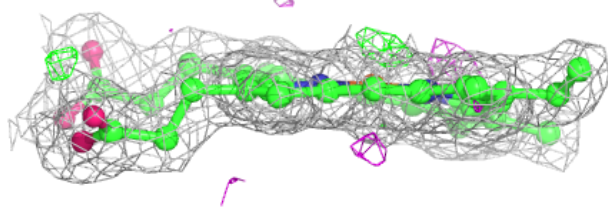
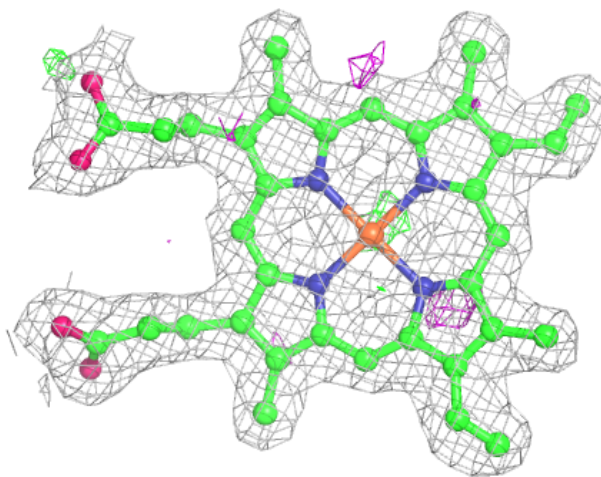
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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 [i](#)

There are no such residues in this entry.