



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:44 pm BST

PDB ID : 5KT8  
Title : Crystal structure of the W139F variant of the catalase-peroxidase from *B. pseudomallei* treated with isoniazid  
Authors : Loewen, P.C.  
Deposited on : 2016-07-11  
Resolution : 2.00 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

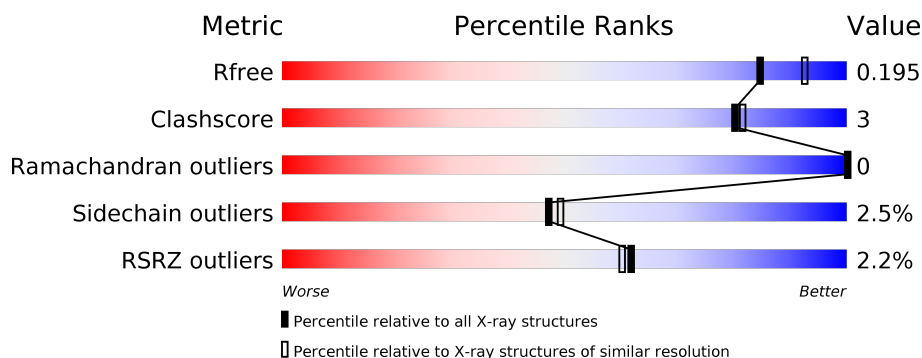
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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>91%</div> <div>6% ..</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9% ..</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
6	MPD	B	805	-	-	X	-
7	NIZ	B	809	-	X	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12425 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	6	0
			5538	3497	988	1039	14			
1	B	713	Total	C	N	O	S	0	8	0
			5541	3501	986	1040	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	PHE	TRP	engineered mutation	UNP Q3JNW6
B	139	PHE	TRP	engineered mutation	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

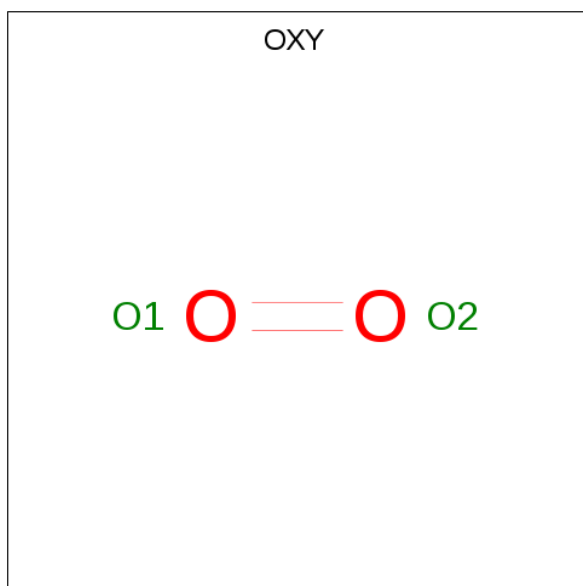
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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).

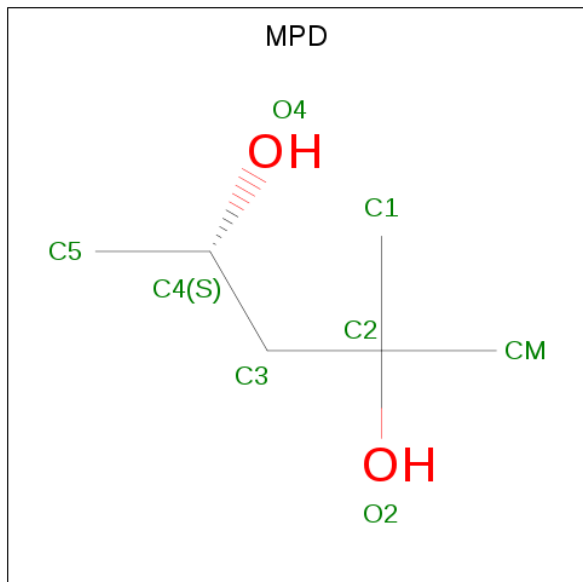
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl		
			1	1	0	0
4	A	1	Total	Cl		
			1	1	0	0

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



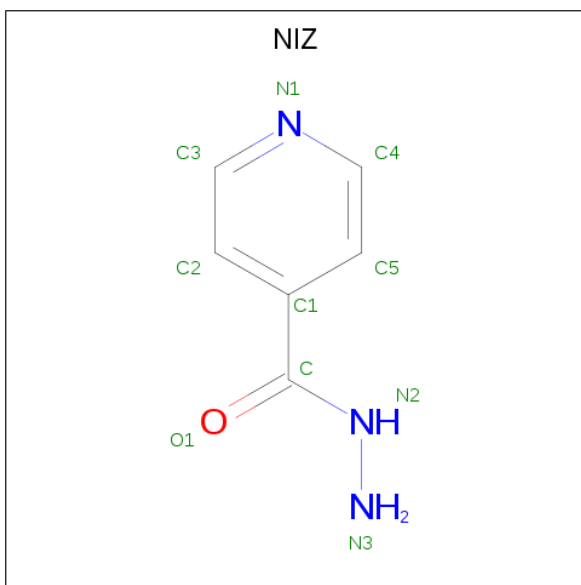
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



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

- Molecule 7 is pyridine-4-carbohydrazide (three-letter code: NIZ) (formula:  $C_6H_7N_3O$ ).



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

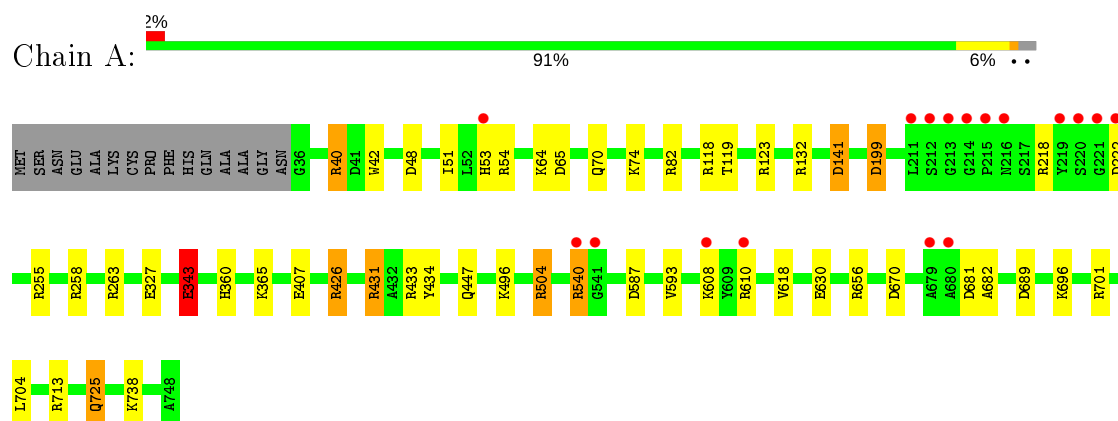
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	599	Total	O	0	0
			599	599		
8	B	587	Total	O	0	0
			587	587		

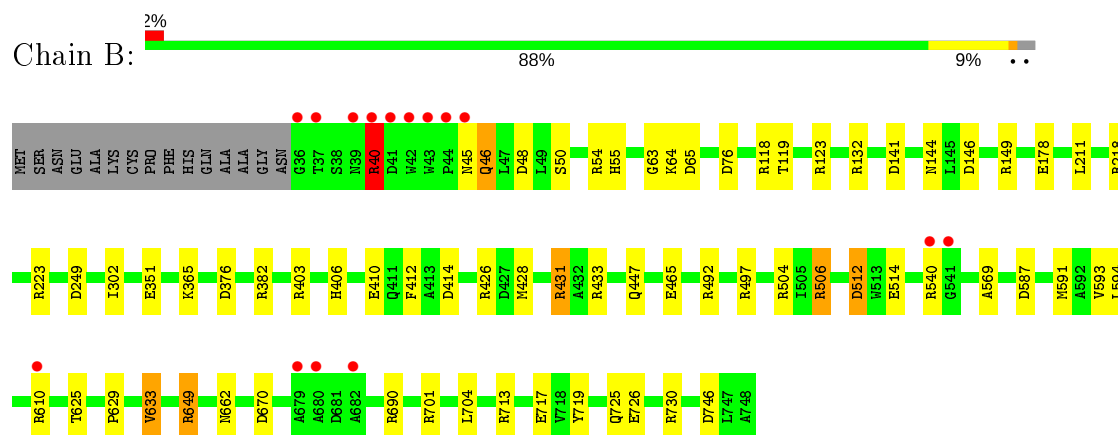
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	100.65Å 112.78Å 174.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.00 48.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.36-2.00) 94.0 (48.36-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.150 , 0.186 0.162 , 0.195	Depositor DCC
$R_{free}$ test set	6269 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12425	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, MPD, 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	1.16	8/5675 (0.1%)	1.10	37/7710 (0.5%)
1	B	1.16	8/5685 (0.1%)	1.10	40/7724 (0.5%)
All	All	1.16	16/11360 (0.1%)	1.10	77/15434 (0.5%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	GLU	CG-CD	8.52	1.64	1.51
1	B	514	GLU	CD-OE2	-8.34	1.16	1.25
1	A	407	GLU	CD-OE1	8.19	1.34	1.25
1	A	725	GLN	CG-CD	7.26	1.67	1.51
1	A	426[A]	ARG	CZ-NH2	6.62	1.41	1.33
1	A	426[B]	ARG	CZ-NH2	6.62	1.41	1.33
1	B	512	ASP	CG-OD2	6.25	1.39	1.25
1	B	63	GLY	N-CA	6.17	1.55	1.46
1	B	410	GLU	CG-CD	5.93	1.60	1.51
1	B	730	ARG	CZ-NH2	5.50	1.40	1.33
1	B	465	GLU	CD-OE1	5.47	1.31	1.25
1	B	726	GLU	CG-CD	5.39	1.60	1.51
1	A	343	GLU	CD-OE1	5.30	1.31	1.25
1	A	327	GLU	CG-CD	5.13	1.59	1.51
1	A	42	TRP	CB-CG	5.09	1.59	1.50
1	B	746	ASP	CB-CG	5.01	1.62	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426[A]	ARG	NE-CZ-NH1	-12.61	114.00	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-12.61	114.00	120.30
1	B	713	ARG	NE-CZ-NH1	9.41	125.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426[A]	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	B	426[B]	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	B	433	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	A	433	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	B	512	ASP	CB-CG-OD2	8.12	125.61	118.30
1	B	40	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	B	504	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	504	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	149	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	65	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	132	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	263	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	497	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	249	ASP	CB-CG-OD1	7.16	124.75	118.30
1	A	431	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	A	434	TYR	CB-CG-CD1	6.81	125.09	121.00
1	B	382	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	218	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	704	LEU	CB-CG-CD1	6.54	122.12	111.00
1	A	587	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	199	ASP	CB-CG-OD1	-6.36	112.57	118.30
1	A	123	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	258	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	497	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	407	GLU	CG-CD-OE1	6.22	130.74	118.30
1	A	255[A]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	343	GLU	CA-CB-CG	6.18	126.99	113.40
1	B	218	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	B	433	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	65	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	B	512	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	A	132	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	504	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	492	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	48	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	587	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	82	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	414	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	123	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	717	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	B	376	ASP	CB-CG-OD2	-5.76	113.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	670	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	506	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	633[A]	VAL	CG1-CB-CG2	-5.64	101.88	110.90
1	B	633[B]	VAL	CG1-CB-CG2	-5.64	101.88	110.90
1	B	132	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	670	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	412	PHE	CB-CG-CD1	5.62	124.73	120.80
1	A	263	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	222	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	587	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	713	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	681	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	656	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	407	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	B	670	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	40	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	496	LYS	CD-CE-NZ	-5.28	99.56	111.70
1	B	506	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	701	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	713	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	76	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	B	431	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	B	701	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	689	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	141	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	149	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	412	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	B	428	MET	CA-CB-CG	-5.07	104.68	113.30
1	B	403	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	704[A]	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	B	704[B]	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	A	540	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	5538	0	5356	19	0
1	B	5541	0	5370	29	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	2	0	0	0	0
5	B	2	0	0	0	0
6	A	24	0	42	6	0
6	B	32	0	56	12	0
7	B	10	0	7	1	0
8	A	599	0	0	12	0
8	B	587	0	0	11	0
All	All	12425	0	10891	60	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 3.

All (60) 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:506:ARG:HE	6:B:805:MPD:H12	1.27	0.96
1:A:119[B]:THR:HG21	8:A:983:HOH:O	1.76	0.85
1:A:53[B]:HIS:ND1	8:A:903:HOH:O	2.13	0.80
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.62	0.80
1:B:178:GLU:OE1	8:B:902:HOH:O	2.00	0.77
1:B:48:ASP:OD1	1:B:50[B]:SER:OG	2.09	0.70
6:B:805:MPD:H51	8:B:1261:HOH:O	1.91	0.69
1:A:53[B]:HIS:CE1	8:A:903:HOH:O	2.47	0.67
6:B:806:MPD:HM2	6:B:806:MPD:O4	1.95	0.65
1:B:119[B]:THR:HG21	8:B:1436:HOH:O	1.98	0.64
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.80	0.63
1:A:504:ARG:HD2	8:A:1024:HOH:O	1.98	0.63
1:A:360:HIS:ND1	8:A:906:HOH:O	2.31	0.62
1:A:593:VAL:HG13	8:A:955:HOH:O	2.00	0.62
6:A:807:MPD:H52	6:A:807:MPD:HM2	1.82	0.61
1:B:119[B]:THR:HG23	8:B:1105:HOH:O	1.99	0.61
1:A:343:GLU:HG2	8:A:1328:HOH:O	2.01	0.60
1:B:629:PRO:O	1:B:633[B]:VAL:HG12	2.03	0.58
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:HIS:HE1	8:B:1355:HOH:O	1.88	0.57
6:B:807:MPD:H53	6:B:807:MPD:H12	1.88	0.56
1:B:662:ASN:H	1:B:725:GLN:HE22	1.53	0.55
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.43	0.54
6:A:805:MPD:O4	6:A:805:MPD:H11	2.07	0.54
1:B:46:GLN:NE2	8:B:908:HOH:O	2.41	0.54
1:A:426[A]:ARG:NE	8:A:904:HOH:O	2.13	0.53
6:B:807:MPD:H53	6:B:807:MPD:C1	2.39	0.53
1:A:696:LYS:HE2	8:A:927:HOH:O	2.08	0.53
1:A:343:GLU:CG	8:A:1328:HOH:O	2.56	0.52
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.35	0.52
1:B:406:HIS:CE1	8:B:1355:HOH:O	2.62	0.51
1:B:625:THR:HG22	7:B:809:NIZ:H4	1.92	0.51
1:B:506:ARG:NE	6:B:805:MPD:H12	2.11	0.51
6:B:807:MPD:H11	6:B:807:MPD:O4	2.10	0.51
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.45	0.50
6:B:805:MPD:C1	6:B:805:MPD:H52	2.42	0.50
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.11	0.49
6:A:807:MPD:C5	6:A:807:MPD:HM2	2.42	0.49
1:B:55:HIS:HD2	8:B:1299:HOH:O	1.97	0.48
1:B:54:ARG:HB3	1:B:55:HIS:ND1	2.29	0.48
1:A:682:ALA:O	8:A:905:HOH:O	2.20	0.46
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.99	0.46
6:B:808:MPD:HM1	6:B:808:MPD:O4	2.16	0.46
6:A:807:MPD:C5	6:A:807:MPD:CM	2.94	0.46
1:A:54:ARG:NE	1:A:199:ASP:OD2	2.37	0.45
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.17	0.45
1:B:55:HIS:CD2	8:B:1299:HOH:O	2.70	0.44
1:A:630:GLU:HG3	6:A:807:MPD:H51	2.00	0.43
1:B:40:ARG:HH11	1:B:40:ARG:HA	1.82	0.43
6:B:805:MPD:H11	6:B:805:MPD:H52	2.01	0.42
1:B:569:ALA:H	6:B:808:MPD:H52	1.83	0.42
1:B:211:LEU:HB2	8:B:1321:HOH:O	2.20	0.41
1:B:649[A]:ARG:HA	1:B:649[A]:ARG:HD3	1.89	0.41
1:A:738:LYS:NZ	8:A:936:HOH:O	2.54	0.41
1:A:630:GLU:CG	6:A:807:MPD:H51	2.50	0.41
1:B:506:ARG:HE	6:B:805:MPD:C1	2.15	0.41
1:A:51:ILE:HD11	1:A:618:VAL:HG12	2.01	0.41
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.20	0.40
1:B:591:MET:SD	1:B:594:LEU:HD12	2.60	0.40
1:B:431:ARG:HG3	8:B:1192:HOH:O	2.21	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	715/728 (98%)	704 (98%)	11 (2%)	0	100	100
1	B	717/728 (98%)	704 (98%)	13 (2%)	0	100	100
All	All	1432/1456 (98%)	1408 (98%)	24 (2%)	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%)	542 (98%)	12 (2%)	52	55
1	B	556/560 (99%)	540 (97%)	16 (3%)	42	43
All	All	1110/1120 (99%)	1082 (98%)	28 (2%)	47	49

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	74	LYS
1	A	118	ARG

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Mol	Chain	Res	Type
1	A	141	ASP
1	A	343	GLU
1	A	365	LYS
1	A	540	ARG
1	A	608	LYS
1	A	610	ARG
1	A	725	GLN
1	B	40	ARG
1	B	45	ASN
1	B	46	GLN
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	223	ARG
1	B	302	ILE
1	B	351	GLU
1	B	365	LYS
1	B	512	ASP
1	B	540	ARG
1	B	610	ARG
1	B	649[A]	ARG
1	B	649[B]	ARG
1	B	690	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	247	ASN
1	A	339	HIS
1	A	544	GLN
1	A	647	GLN
1	B	46	GLN
1	B	544	GLN
1	B	725	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

4 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[B]	-	10,17,18	2.20	3 (30%)	10,23,25	2.26	4 (40%)
1	TOX	B	111[B]	-	10,17,18	3.36	3 (30%)	10,23,25	1.21	2 (20%)
1	TOX	B	111[A]	2	10,17,18	3.36	3 (30%)	10,23,25	1.21	2 (20%)
1	TOX	A	111[A]	2	10,17,18	2.20	3 (30%)	10,23,25	2.26	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[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	2/4/8/10	0/2/2/2
1	TOX	A	111[A]	2	-	2/4/8/10	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[B]	TOX	CD1-NE1	-7.90	1.31	1.39
1	B	111[A]	TOX	CD1-NE1	-7.90	1.31	1.39
1	B	111[B]	TOX	O-C	5.48	1.41	1.19
1	B	111[A]	TOX	O-C	5.48	1.41	1.19
1	A	111[B]	TOX	O-C	5.33	1.41	1.19
1	A	111[A]	TOX	O-C	5.33	1.41	1.19
1	A	111[B]	TOX	CH2-CZ2	3.13	1.43	1.36
1	A	111[A]	TOX	CH2-CZ2	3.13	1.43	1.36
1	B	111[B]	TOX	CE3-CD2	-3.05	1.36	1.42
1	B	111[A]	TOX	CE3-CD2	-3.05	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[B]	TOX	CE3-CD2	-2.06	1.38	1.42
1	A	111[A]	TOX	CE3-CD2	-2.06	1.38	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[B]	TOX	CB-CG-CD1	-4.16	122.82	127.97
1	A	111[A]	TOX	CB-CG-CD1	-4.16	122.82	127.97
1	A	111[B]	TOX	CB-CG-CD2	3.82	132.19	126.25
1	A	111[A]	TOX	CB-CG-CD2	3.82	132.19	126.25
1	A	111[B]	TOX	CB-CA-C	2.81	116.73	111.47
1	A	111[A]	TOX	CB-CA-C	2.81	116.73	111.47
1	B	111[B]	TOX	CZ3-CH2-CZ2	-2.71	116.64	120.44
1	B	111[A]	TOX	CZ3-CH2-CZ2	-2.71	116.64	120.44
1	B	111[B]	TOX	CH2-CZ3-CE3	2.24	123.58	120.44
1	B	111[A]	TOX	CH2-CZ3-CE3	2.24	123.58	120.44
1	A	111[B]	TOX	CZ3-CH2-CZ2	-2.06	117.55	120.44
1	A	111[A]	TOX	CZ3-CH2-CZ2	-2.06	117.55	120.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates 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
2	HEM	B	801	1	27,50,50	1.53	5 (18%)	17,82,82	2.24	6 (35%)
5	OXY	A	804	-	1,1,1	0.15	0	-		
5	OXY	B	804	-	1,1,1	0.41	0	-		
6	MPD	A	806	-	7,7,7	0.80	0	9,10,10	1.83	3 (33%)
7	NIZ	B	809	-	10,10,10	2.44	4 (40%)	12,12,12	3.27	9 (75%)
6	MPD	B	808	-	7,7,7	0.63	0	9,10,10	1.55	2 (22%)
6	MPD	B	805	-	7,7,7	1.14	1 (14%)	9,10,10	1.31	1 (11%)
6	MPD	A	805	-	7,7,7	1.01	0	9,10,10	1.59	3 (33%)
2	HEM	A	801	1	27,50,50	1.13	2 (7%)	17,82,82	1.71	3 (17%)
6	MPD	B	806	-	7,7,7	0.54	0	9,10,10	1.18	1 (11%)
6	MPD	A	807	-	7,7,7	0.78	0	9,10,10	1.56	3 (33%)
6	MPD	B	807	-	7,7,7	1.03	0	9,10,10	1.63	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
2	HEM	B	801	1	-	0/6/54/54	-
6	MPD	A	806	-	-	0/5/5/5	-
7	NIZ	B	809	-	-	1/6/6/6	0/1/1/1
6	MPD	B	808	-	-	5/5/5/5	-
6	MPD	B	805	-	-	1/5/5/5	-
6	MPD	A	805	-	-	3/5/5/5	-
2	HEM	A	801	1	-	0/6/54/54	-
6	MPD	B	806	-	-	4/5/5/5	-
6	MPD	A	807	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	B	807	-	-	2/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	809	NIZ	C5-C1	5.09	1.48	1.39
2	A	801	HEM	C3B-C2B	-3.79	1.35	1.40
7	B	809	NIZ	C-N2	3.56	1.37	1.33
2	B	801	HEM	CAA-C2A	-3.47	1.46	1.52
2	B	801	HEM	C1A-NA	3.38	1.43	1.36
2	B	801	HEM	C4A-NA	3.18	1.42	1.36
7	B	809	NIZ	C4-N1	3.02	1.42	1.33
2	B	801	HEM	C1B-C2B	2.84	1.49	1.42
7	B	809	NIZ	C2-C1	2.76	1.44	1.39
6	B	805	MPD	C3-C2	2.16	1.59	1.53
2	A	801	HEM	CMD-C2D	2.13	1.56	1.51
2	B	801	HEM	C3B-C2B	-2.04	1.37	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	809	NIZ	O1-C-C1	-5.85	110.50	120.94
7	B	809	NIZ	C1-C-N2	5.48	122.53	116.27
2	B	801	HEM	CBD-CAD-C3D	4.66	121.07	112.48
2	B	801	HEM	CAA-CBA-CGA	-4.63	104.90	112.67
2	A	801	HEM	CBD-CAD-C3D	4.27	120.34	112.48
7	B	809	NIZ	C4-N1-C3	3.78	125.74	116.85
6	A	806	MPD	CM-C2-C1	-3.76	102.74	110.57
6	B	807	MPD	O2-C2-C3	-3.67	96.01	109.80
7	B	809	NIZ	C5-C1-C2	3.51	123.58	118.59
2	B	801	HEM	CMA-C3A-C4A	-3.40	123.24	128.46
2	B	801	HEM	C4A-C3A-C2A	3.02	109.10	107.00
7	B	809	NIZ	C5-C4-N1	-3.02	118.37	123.62
6	B	808	MPD	CM-C2-C1	-2.99	104.35	110.57
7	B	809	NIZ	O1-C-N2	2.92	126.14	122.50
2	B	801	HEM	CAD-CBD-CGD	2.73	117.25	112.67
6	B	808	MPD	O4-C4-C3	2.67	122.13	111.36
2	A	801	HEM	CMC-C2C-C3C	2.61	129.56	124.68
6	A	805	MPD	CM-C2-C1	-2.57	105.22	110.57
7	B	809	NIZ	C3-C2-C1	-2.56	116.25	119.05
6	A	807	MPD	CM-C2-C3	2.56	121.86	109.96
7	B	809	NIZ	C2-C3-N1	-2.54	119.19	123.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	806	MPD	CM-C2-C1	2.46	115.71	110.57
6	A	805	MPD	O2-C2-CM	-2.46	100.20	108.08
6	A	805	MPD	C1-C2-C3	2.44	121.33	109.96
6	B	807	MPD	C1-C2-C3	2.40	121.12	109.96
2	A	801	HEM	CAA-CBA-CGA	-2.25	108.89	112.67
6	A	807	MPD	O2-C2-C3	-2.25	101.34	109.80
6	A	807	MPD	O2-C2-CM	-2.14	101.22	108.08
6	A	806	MPD	O4-C4-C3	-2.09	102.93	111.36
6	A	806	MPD	O2-C2-CM	2.06	114.67	108.08
2	B	801	HEM	CMB-C2B-C3B	2.05	128.51	124.68
6	B	805	MPD	CM-C2-C1	-2.02	106.36	110.57
7	B	809	NIZ	C4-C5-C1	-2.01	116.85	119.05

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	809	NIZ	C1-C-N2-N3
6	B	808	MPD	O2-C2-C3-C4
6	B	808	MPD	CM-C2-C3-C4
6	B	808	MPD	C2-C3-C4-C5
6	A	805	MPD	C2-C3-C4-O4
6	A	805	MPD	C2-C3-C4-C5
6	B	806	MPD	O2-C2-C3-C4
6	B	806	MPD	CM-C2-C3-C4
6	A	807	MPD	C2-C3-C4-O4
6	A	807	MPD	C2-C3-C4-C5
6	B	808	MPD	C1-C2-C3-C4
6	A	805	MPD	C1-C2-C3-C4
6	B	806	MPD	C1-C2-C3-C4
6	B	805	MPD	C2-C3-C4-C5
6	B	807	MPD	C2-C3-C4-C5
6	B	808	MPD	C2-C3-C4-O4
6	B	807	MPD	C2-C3-C4-O4
6	B	806	MPD	C2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 19 short contacts:

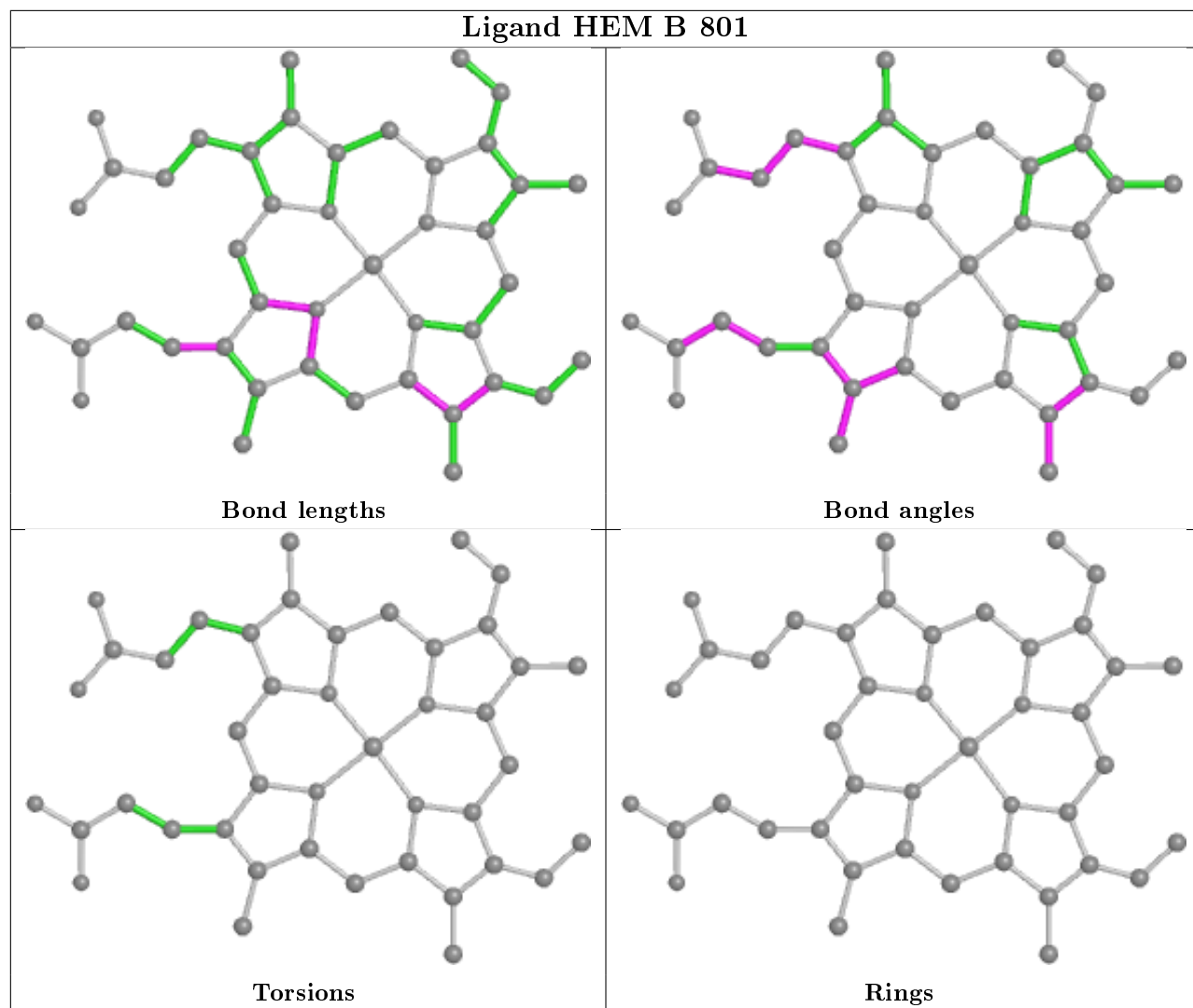
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	809	NIZ	1	0

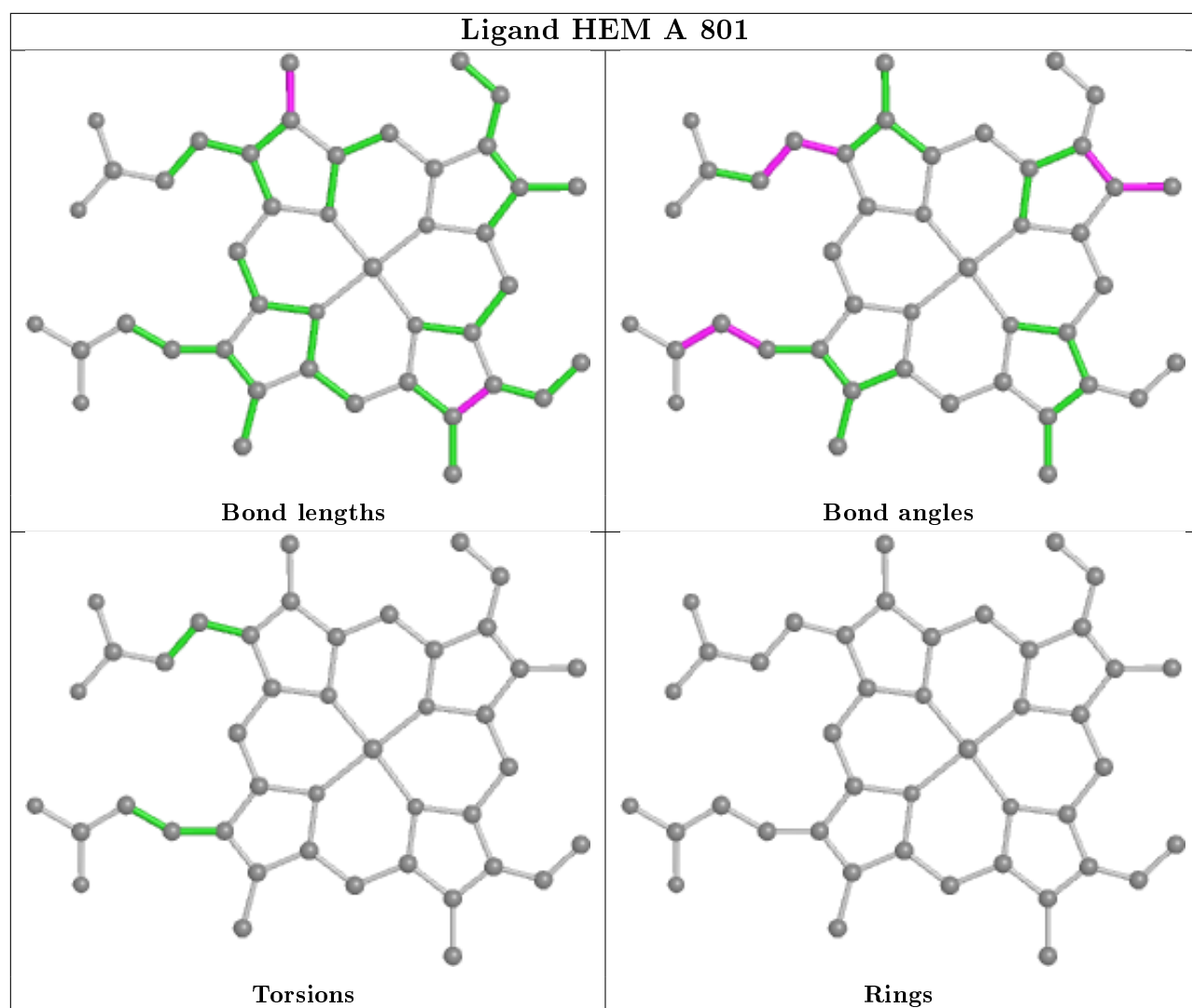
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	808	MPD	2	0
6	B	805	MPD	6	0
6	A	805	MPD	1	0
6	B	806	MPD	1	0
6	A	807	MPD	5	0
6	B	807	MPD	3	0

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%)	-0.44	17 (2%) 59 57	21, 28, 54, 87	0
1	B	712/728 (97%)	-0.55	15 (2%) 63 62	20, 27, 49, 99	0
All	All	1424/1456 (97%)	-0.50	32 (2%) 62 60	20, 27, 52, 99	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	GLY	5.6
1	A	679	ALA	4.3
1	A	213	GLY	3.9
1	B	40	ARG	3.9
1	A	215	PRO	3.7
1	A	222	ASP	3.7
1	B	679	ALA	3.7
1	B	42	TRP	3.6
1	B	680	ALA	3.5
1	A	610	ARG	3.5
1	A	540	ARG	3.3
1	B	540	ARG	3.2
1	B	37	THR	3.1
1	B	45	ASN	3.0
1	A	221	GLY	3.0
1	B	39	ASN	2.9
1	B	44	PRO	2.9
1	A	219	TYR	2.9
1	A	608	LYS	2.8
1	A	211	LEU	2.8
1	A	541	GLY	2.7
1	B	610	ARG	2.7
1	A	212	SER	2.6
1	A	680	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	43	TRP	2.3
1	A	220	SER	2.3
1	B	541	GLY	2.3
1	B	682	ALA	2.2
1	A	216	ASN	2.1
1	A	53[A]	HIS	2.1
1	A	214	GLY	2.0
1	B	41	ASP	2.0

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

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[B]	16/17	0.98	0.12	21,23,26,26	2
1	TOX	B	111[B]	16/17	0.98	0.13	19,21,24,27	1
1	TOX	B	111[A]	16/17	0.98	0.13	19,21,25,27	1
1	TOX	A	111[A]	16/17	0.98	0.12	21,23,26,26	2

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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(Å <sup>2</sup> )	Q<0.9
7	NIZ	B	809	10/10	0.84	0.21	46,52,57,58	0
6	MPD	B	807	8/8	0.87	0.21	58,64,74,77	0
6	MPD	A	805	8/8	0.88	0.19	44,47,64,65	0
6	MPD	A	806	8/8	0.88	0.19	51,60,72,80	0
6	MPD	B	808	8/8	0.89	0.18	55,68,68,69	0
6	MPD	B	805	8/8	0.89	0.22	49,54,58,59	0

*Continued on next page...*

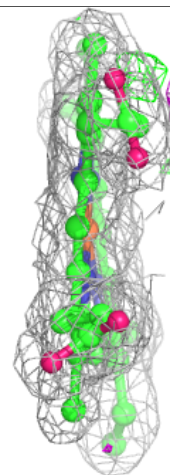
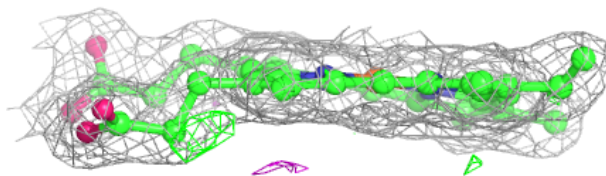
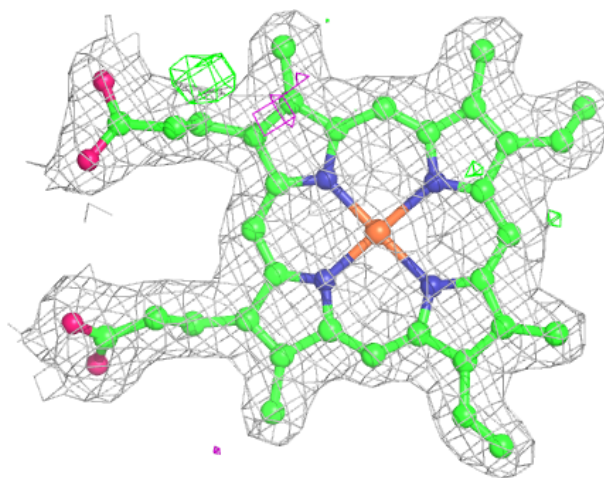
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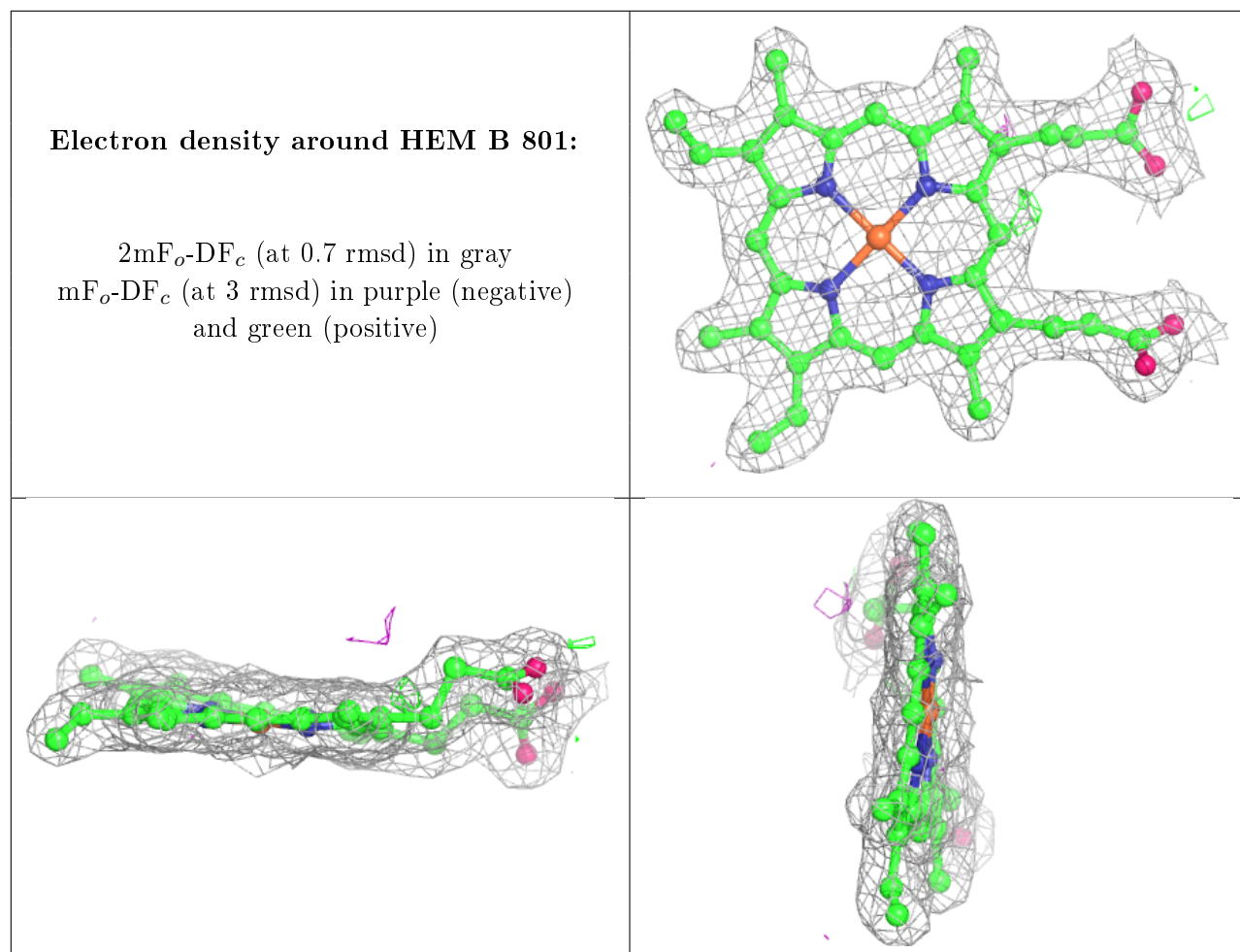
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MPD	A	807	8/8	0.91	0.16	56,68,69,70	0
6	MPD	B	806	8/8	0.92	0.17	49,55,62,63	0
5	OXY	A	804	2/2	0.96	0.20	42,42,42,49	0
5	OXY	B	804	2/2	0.96	0.17	37,37,37,42	0
2	HEM	A	801	43/43	0.99	0.10	20,24,26,28	0
3	NA	A	802	1/1	0.99	0.07	25,25,25,25	0
4	CL	A	803	1/1	0.99	0.10	42,42,42,42	0
2	HEM	B	801	43/43	0.99	0.12	19,21,23,27	0
4	CL	B	803	1/1	0.99	0.10	36,36,36,36	0
3	NA	B	802	1/1	0.99	0.04	24,24,24,24	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<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.