



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:35 am BST

PDB ID : 5SXW  
Title : Crystal structure of the E198A variant of catalase-peroxidase KatG of *Burkholderia pseudomallei*  
Authors : Loewen, P.C.  
Deposited on : 2016-08-10  
Resolution : 1.60 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

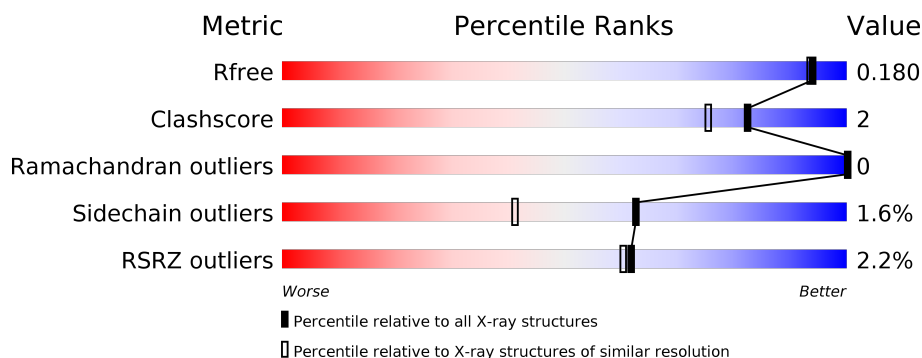
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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>81%</div> <div>15%</div> <div>••</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>12%</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
5	PO4	A	804	-	X	-	-



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.

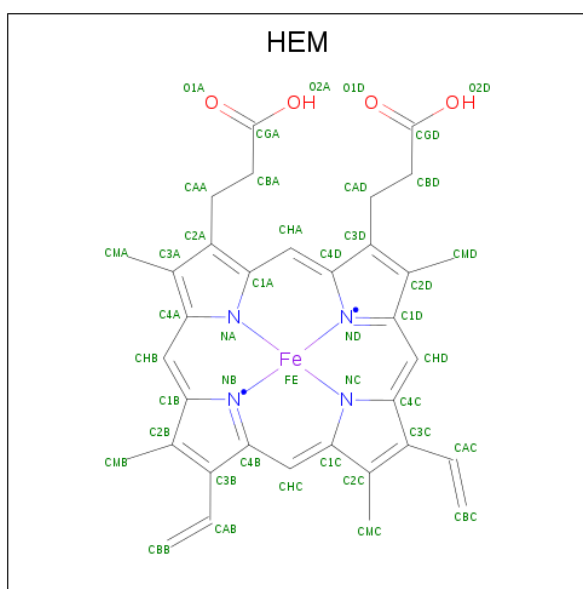
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total 5526	C 3490	N 984	O 1038	S 14	0	6	0
1	B	714	Total 5538	C 3496	N 986	O 1042	S 14	0	8	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (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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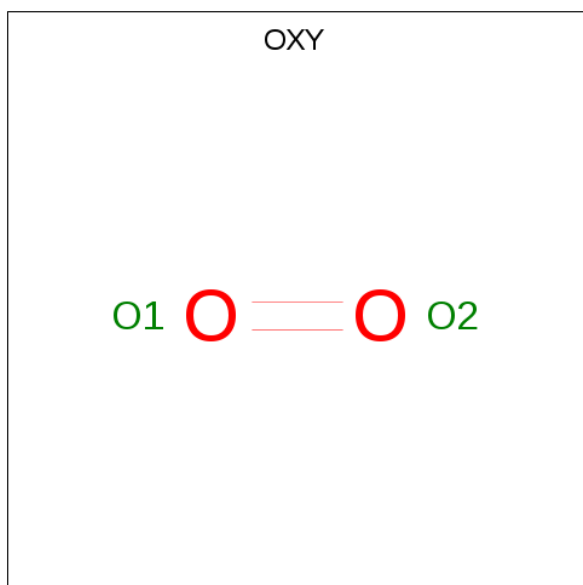
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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



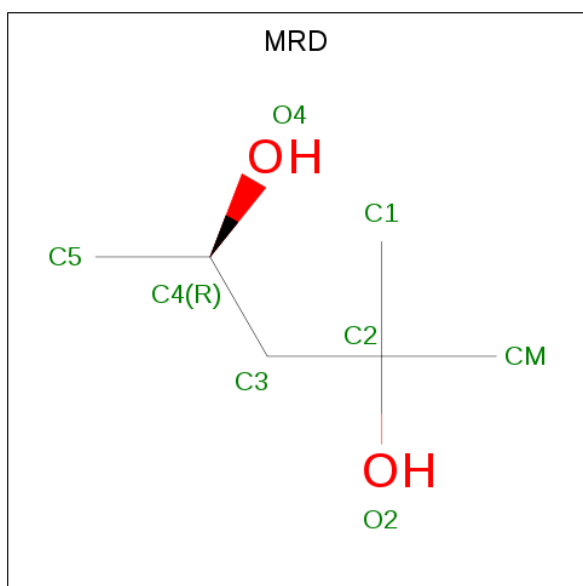
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O		
			2	2	0	0
4	B	1	Total	O		
			2	2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



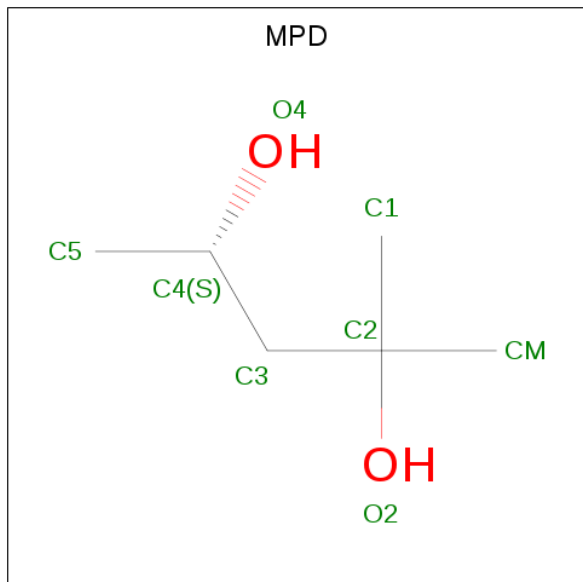
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



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

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



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

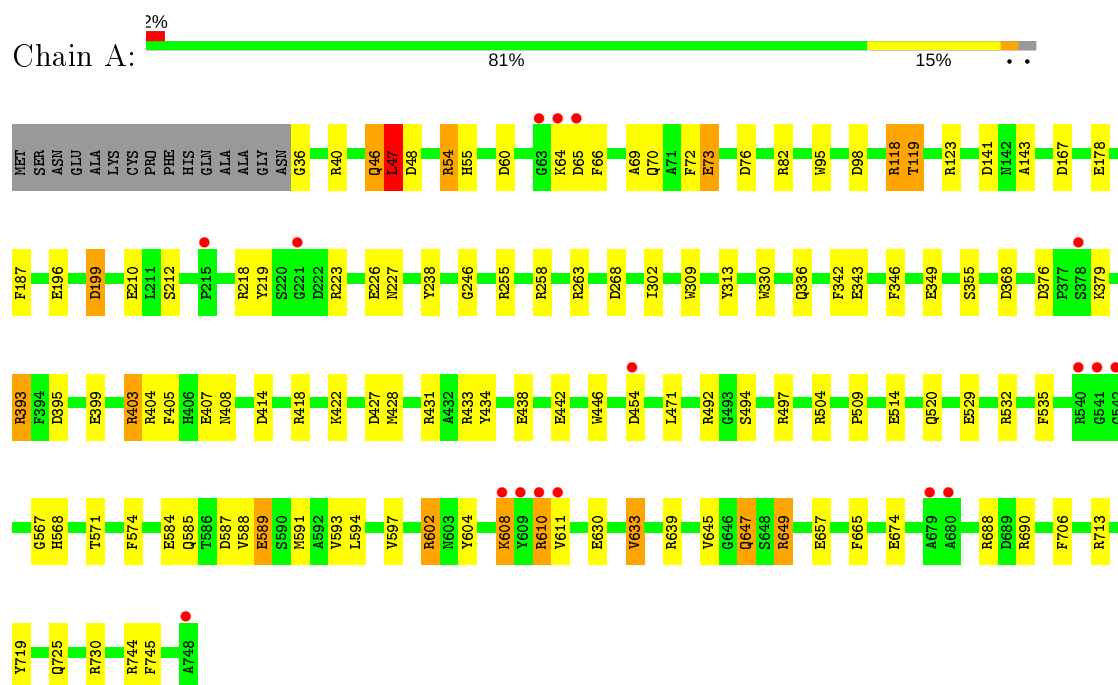
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	955	Total	O	0	0
			955	955		
8	B	911	Total	O	0	0
			911	911		

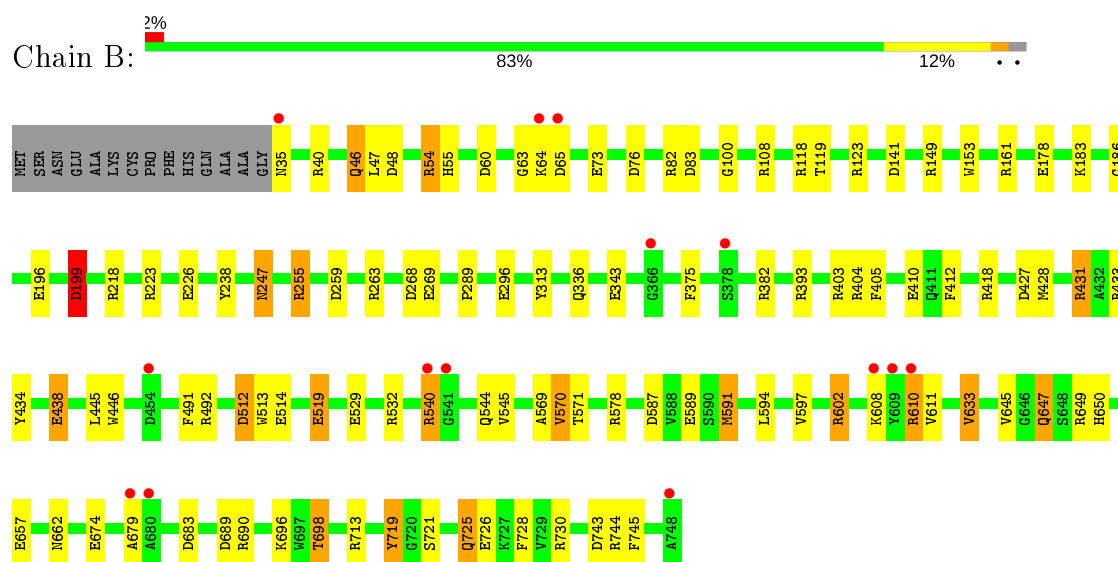
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	100.34Å 116.02Å 174.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 29.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.60) 99.9 (29.00-1.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.143 , 0.169 0.158 , 0.180	Depositor DCC
$R_{free}$ test set	13409 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: TOX, OXY, NA, PO4, MPD, MRD, 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	1.66	68/5666 (1.2%)	1.74	92/7701 (1.2%)
1	B	1.64	67/5688 (1.2%)	1.57	85/7732 (1.1%)
All	All	1.65	135/11354 (1.2%)	1.66	177/15433 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	GLU	CD-OE2	18.30	1.45	1.25
1	A	438	GLU	CD-OE2	13.53	1.40	1.25
1	A	532	ARG	CD-NE	-12.58	1.25	1.46
1	A	255	ARG	CD-NE	10.61	1.64	1.46
1	A	438	GLU	CD-OE1	-10.11	1.14	1.25
1	A	725	GLN	CD-NE2	10.05	1.57	1.32
1	A	196	GLU	CG-CD	9.55	1.66	1.51
1	B	73	GLU	CG-CD	9.29	1.65	1.51
1	A	336	GLN	CG-CD	9.24	1.72	1.51
1	B	726	GLU	CD-OE2	9.18	1.35	1.25
1	B	46	GLN	CG-CD	8.96	1.71	1.51
1	A	343	GLU	CD-OE1	8.19	1.34	1.25
1	B	438	GLU	CD-OE2	8.12	1.34	1.25
1	B	730	ARG	CZ-NH2	7.97	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	410	GLU	CG-CD	7.94	1.63	1.51
1	B	532	ARG	NE-CZ	-7.91	1.22	1.33
1	A	532	ARG	CZ-NH2	-7.86	1.22	1.33
1	A	584	GLU	CG-CD	7.79	1.63	1.51
1	B	226	GLU	CB-CG	-7.72	1.37	1.52
1	B	178	GLU	CD-OE2	7.67	1.34	1.25
1	B	269	GLU	CD-OE2	-7.64	1.17	1.25
1	B	446	TRP	CD2-CE2	7.62	1.50	1.41
1	B	512	ASP	CG-OD2	7.61	1.42	1.25
1	B	226	GLU	CG-CD	7.58	1.63	1.51
1	A	196	GLU	CB-CG	-7.55	1.37	1.52
1	A	226	GLU	CG-CD	7.55	1.63	1.51
1	B	343	GLU	CD-OE2	7.54	1.33	1.25
1	B	63	GLY	N-CA	7.52	1.57	1.46
1	A	647	GLN	CG-CD	7.46	1.68	1.51
1	B	196	GLU	CG-CD	7.46	1.63	1.51
1	A	494	SER	CA-CB	-7.29	1.42	1.52
1	B	512	ASP	CB-CG	7.29	1.67	1.51
1	A	725	GLN	CG-CD	7.24	1.67	1.51
1	B	514	GLU	CD-OE2	-7.21	1.17	1.25
1	B	418	ARG	CZ-NH1	-7.20	1.23	1.33
1	B	196	GLU	CB-CG	-7.19	1.38	1.52
1	B	571	THR	CA-C	-7.14	1.34	1.52
1	A	349	GLU	CD-OE2	-7.10	1.17	1.25
1	A	199	ASP	C-O	7.06	1.36	1.23
1	B	647	GLN	CG-CD	7.06	1.67	1.51
1	B	434	TYR	CE2-CZ	-7.02	1.29	1.38
1	B	674	GLU	CG-CD	6.97	1.62	1.51
1	A	633[A]	VAL	CB-CG1	-6.92	1.38	1.52
1	A	633[B]	VAL	CB-CG1	-6.92	1.38	1.52
1	B	657	GLU	CD-OE2	6.75	1.33	1.25
1	A	535	PHE	CG-CD1	-6.68	1.28	1.38
1	A	178	GLU	CG-CD	6.68	1.61	1.51
1	B	199	ASP	C-O	6.61	1.35	1.23
1	A	567	GLY	CA-C	-6.61	1.41	1.51
1	A	219	TYR	CE1-CZ	-6.57	1.30	1.38
1	B	725	GLN	CD-OE1	6.52	1.38	1.24
1	A	446	TRP	CD1-NE1	-6.44	1.26	1.38
1	B	403	ARG	CZ-NH1	-6.42	1.24	1.33
1	A	255	ARG	CG-CD	6.41	1.68	1.51
1	A	330	TRP	CZ3-CH2	-6.38	1.29	1.40
1	A	399	GLU	CD-OE2	6.26	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	ARG	CG-CD	6.19	1.67	1.51
1	B	247[A]	ASN	CG-ND2	6.19	1.48	1.32
1	B	247[B]	ASN	CG-ND2	6.19	1.48	1.32
1	A	95	TRP	CZ3-CH2	-6.14	1.30	1.40
1	B	434	TYR	CE1-CZ	-6.07	1.30	1.38
1	B	296	GLU	CD-OE1	6.07	1.32	1.25
1	A	418	ARG	CZ-NH1	-6.06	1.25	1.33
1	A	602	ARG	CZ-NH2	-6.03	1.25	1.33
1	A	255	ARG	NE-CZ	6.00	1.40	1.33
1	B	491	PHE	CG-CD1	-6.00	1.29	1.38
1	B	532	ARG	CG-CD	5.95	1.66	1.51
1	A	123	ARG	CZ-NH2	5.92	1.40	1.33
1	B	540	ARG	C-O	5.91	1.34	1.23
1	A	226	GLU	CB-CG	-5.87	1.41	1.52
1	B	76	ASP	CB-CG	5.85	1.64	1.51
1	A	223	ARG	CG-CD	-5.84	1.37	1.51
1	B	153	TRP	CE3-CZ3	-5.81	1.28	1.38
1	A	70	GLN	CG-CD	5.80	1.64	1.51
1	B	633[A]	VAL	CB-CG2	-5.80	1.40	1.52
1	B	633[B]	VAL	CB-CG2	-5.80	1.40	1.52
1	A	454	ASP	CB-CG	5.75	1.63	1.51
1	B	434	TYR	CB-CG	-5.74	1.43	1.51
1	B	513	TRP	CZ3-CH2	-5.74	1.30	1.40
1	A	376	ASP	CB-CG	5.73	1.63	1.51
1	A	657	GLU	CG-CD	5.73	1.60	1.51
1	B	721	SER	CA-CB	-5.71	1.44	1.52
1	A	434	TYR	CG-CD2	-5.71	1.31	1.39
1	A	46	GLN	CG-CD	5.70	1.64	1.51
1	A	212	SER	CB-OG	-5.70	1.34	1.42
1	B	519	GLU	CD-OE2	5.69	1.31	1.25
1	B	446	TRP	N-CA	-5.67	1.35	1.46
1	B	223	ARG	CG-CD	-5.65	1.37	1.51
1	A	343	GLU	CB-CG	-5.64	1.41	1.52
1	A	73	GLU	CG-CD	5.61	1.60	1.51
1	B	589	GLU	CD-OE2	5.59	1.31	1.25
1	A	688	ARG	CZ-NH1	-5.59	1.25	1.33
1	A	36	GLY	N-CA	5.58	1.54	1.46
1	B	514	GLU	CD-OE1	-5.57	1.19	1.25
1	A	442	GLU	CD-OE2	-5.56	1.19	1.25
1	B	65	ASP	CB-CG	5.55	1.63	1.51
1	B	730	ARG	CG-CD	5.53	1.65	1.51
1	A	355	SER	CA-CB	5.51	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	GLU	CG-CD	5.49	1.60	1.51
1	A	568	HIS	CA-CB	-5.49	1.41	1.53
1	A	589	GLU	CD-OE2	5.44	1.31	1.25
1	A	119[A]	THR	CB-CG2	-5.41	1.34	1.52
1	A	119[B]	THR	CB-CG2	-5.41	1.34	1.52
1	B	289	PRO	N-CA	-5.37	1.38	1.47
1	B	82	ARG	CZ-NH2	-5.37	1.26	1.33
1	A	431	ARG	CD-NE	5.36	1.55	1.46
1	B	73	GLU	CB-CG	5.35	1.62	1.52
1	B	100	GLY	N-CA	-5.33	1.38	1.46
1	B	719	TYR	CZ-OH	5.33	1.47	1.37
1	B	336	GLN	CG-CD	5.30	1.63	1.51
1	B	446	TRP	CZ3-CH2	-5.29	1.31	1.40
1	B	657	GLU	CG-CD	5.29	1.59	1.51
1	B	602	ARG	CZ-NH2	-5.27	1.26	1.33
1	B	255[A]	ARG	CZ-NH1	-5.27	1.26	1.33
1	B	255[B]	ARG	CZ-NH1	-5.27	1.26	1.33
1	B	313	TYR	CE1-CZ	-5.27	1.31	1.38
1	A	414	ASP	CG-OD1	-5.24	1.13	1.25
1	A	210	GLU	CD-OE2	5.21	1.31	1.25
1	B	54	ARG	CB-CG	-5.21	1.38	1.52
1	B	35	ASN	CA-C	5.19	1.66	1.52
1	A	520	GLN	CD-OE1	5.17	1.35	1.24
1	A	442	GLU	CG-CD	5.16	1.59	1.51
1	A	246	GLY	N-CA	-5.15	1.38	1.46
1	A	532	ARG	NE-CZ	-5.14	1.26	1.33
1	A	408	ASN	C-O	5.14	1.33	1.23
1	A	47	LEU	CB-CG	-5.13	1.37	1.52
1	A	72	PHE	CG-CD2	-5.10	1.31	1.38
1	B	226	GLU	CD-OE2	-5.08	1.20	1.25
1	A	434	TYR	CG-CD1	-5.05	1.32	1.39
1	A	263	ARG	CZ-NH1	5.04	1.39	1.33
1	A	713	ARG	CZ-NH1	-5.04	1.26	1.33
1	B	375	PHE	CG-CD1	-5.02	1.31	1.38
1	A	588	VAL	N-CA	-5.02	1.36	1.46
1	B	679	ALA	N-CA	5.01	1.56	1.46
1	A	630	GLU	CD-OE2	5.00	1.31	1.25

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-50.66	94.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH1	41.67	141.14	120.30
1	A	492	ARG	NE-CZ-NH2	-14.41	113.09	120.30
1	B	82	ARG	NE-CZ-NH2	-14.35	113.13	120.30
1	B	76	ASP	CB-CG-OD2	-13.97	105.72	118.30
1	B	123	ARG	NE-CZ-NH1	13.80	127.20	120.30
1	A	532	ARG	CD-NE-CZ	13.61	142.65	123.60
1	A	404	ARG	NE-CZ-NH1	13.58	127.09	120.30
1	A	492	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	B	434	TYR	CB-CG-CD1	12.29	128.37	121.00
1	A	263	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	B	82	ARG	NE-CZ-NH1	11.85	126.23	120.30
1	A	434	TYR	CB-CG-CD1	11.72	128.03	121.00
1	A	730	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	B	512	ASP	CB-CG-OD1	-11.40	108.04	118.30
1	B	60	ASP	CB-CG-OD2	-11.21	108.22	118.30
1	A	713	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	B	263	ARG	NE-CZ-NH2	-11.15	114.72	120.30
1	B	54	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	649	ARG	NE-CZ-NH1	10.97	125.79	120.30
1	A	60	ASP	CB-CG-OD2	-10.58	108.78	118.30
1	B	393	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	B	427	ASP	CB-CG-OD2	-10.46	108.89	118.30
1	A	123	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	A	433	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	B	123	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	B	218	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	B	108	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	B	730	ARG	NE-CZ-NH1	-9.94	115.33	120.30
1	B	744	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	A	376	ASP	CB-CG-OD2	-9.62	109.65	118.30
1	A	123	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	454	ASP	CB-CG-OD2	9.45	126.81	118.30
1	A	60	ASP	CB-CG-OD1	9.21	126.58	118.30
1	B	54	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	B	161	ARG	NE-CZ-NH1	9.01	124.80	120.30
1	A	438	GLU	OE1-CD-OE2	8.94	134.03	123.30
1	B	54	ARG	CG-CD-NE	-8.91	93.09	111.80
1	B	48	ASP	CB-CG-OD1	8.90	126.31	118.30
1	A	255	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	649	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	438	GLU	CG-CD-OE1	-8.60	101.10	118.30
1	A	690	ARG	NE-CZ-NH1	-8.52	116.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ASP	CB-CG-OD1	8.52	125.97	118.30
1	B	108	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	438	GLU	OE1-CD-OE2	8.38	133.35	123.30
1	A	48	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	403	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	B	255[A]	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	B	255[B]	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	B	649	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	B	728	PHE	CB-CG-CD1	-8.06	115.16	120.80
1	B	744	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	A	730	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	584	GLU	OE1-CD-OE2	-7.85	113.88	123.30
1	A	46	GLN	CA-CB-CG	7.84	130.66	113.40
1	B	690	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	A	82	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	118	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	744	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	B	73	GLU	CG-CD-OE2	7.65	133.60	118.30
1	B	492	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	A	395	ASP	CB-CG-OD1	7.47	125.03	118.30
1	B	434	TYR	CZ-CE2-CD2	7.43	126.49	119.80
1	B	382	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	713	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	82	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	604	TYR	CZ-CE2-CD2	-7.39	113.15	119.80
1	A	587	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	167	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	633[A]	VAL	CA-CB-CG1	7.21	121.72	110.90
1	A	633[B]	VAL	CA-CB-CG1	7.21	121.72	110.90
1	B	438	GLU	CG-CD-OE1	-7.20	103.89	118.30
1	B	428	MET	CA-CB-CG	-7.18	101.10	113.30
1	B	434	TYR	CD1-CG-CD2	-7.17	110.01	117.90
1	B	683	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	B	719	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	A	404	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	497	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	649	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	76	ASP	OD1-CG-OD2	6.97	136.53	123.30
1	B	404	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	418	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	602	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	427	ASP	OD1-CG-OD2	6.85	136.32	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	570	VAL	CG1-CB-CG2	-6.81	100.01	110.90
1	A	431	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	587	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	574	PHE	CB-CG-CD2	-6.66	116.14	120.80
1	A	238	TYR	CZ-CE2-CD2	6.51	125.66	119.80
1	A	65	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	54	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	B	743	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	66	PHE	CG-CD2-CE2	-6.45	113.70	120.80
1	B	433	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	263	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	46	GLN	CA-CB-CG	6.29	127.23	113.40
1	A	118	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	604	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	A	571	THR	OG1-CB-CG2	-6.26	95.59	110.00
1	A	255	ARG	CD-NE-CZ	6.21	132.29	123.60
1	A	434	TYR	CZ-CE2-CD2	6.19	125.37	119.80
1	B	674	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	A	588	VAL	CG1-CB-CG2	6.13	120.71	110.90
1	A	47	LEU	N-CA-CB	-6.12	98.16	110.40
1	B	578	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	46	GLN	N-CA-C	-6.09	94.55	111.00
1	A	376	ASP	OD1-CG-OD2	6.05	134.79	123.30
1	A	218	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	529[A]	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	B	529[B]	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	A	178	GLU	OE1-CD-OE2	6.00	130.49	123.30
1	B	393	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	268	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	35	ASN	CB-CA-C	5.97	122.33	110.40
1	B	83	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	639	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	405	PHE	CB-CG-CD2	5.93	124.95	120.80
1	A	393	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	591	MET	CG-SD-CE	-5.89	90.77	100.20
1	A	302	ILE	CG1-CB-CG2	5.89	124.36	111.40
1	B	698	THR	CA-CB-CG2	-5.89	104.16	112.40
1	A	434	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	238	TYR	CB-CG-CD2	5.87	124.52	121.00
1	B	689	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	726	GLU	CG-CD-OE2	5.84	129.97	118.30
1	B	492	ARG	NE-CZ-NH2	-5.83	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	B	578	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	54	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	713	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	187	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	A	258	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	382	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	540	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	98	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	405	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	B	405	PHE	CB-CG-CD1	-5.62	116.86	120.80
1	B	313	TYR	CG-CD1-CE1	-5.59	116.83	121.30
1	B	745	PHE	CZ-CE2-CD2	-5.57	113.42	120.10
1	B	597	VAL	CA-CB-CG1	-5.56	102.56	110.90
1	A	342	PHE	CB-CG-CD1	-5.53	116.93	120.80
1	B	226	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	A	46	GLN	N-CA-C	-5.51	96.13	111.00
1	A	427	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	514	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	B	412	PHE	CD1-CE1-CZ	5.44	126.63	120.10
1	A	597	VAL	CA-CB-CG1	-5.43	102.75	110.90
1	B	149	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	259	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	745	PHE	CB-CG-CD1	-5.38	117.03	120.80
1	B	405	PHE	CB-CG-CD2	5.37	124.56	120.80
1	A	54	ARG	CG-CD-NE	-5.34	100.59	111.80
1	A	674	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	A	529	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	A	690	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	B	532	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	73	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	B	431	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	258	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	368	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	649	ARG	CB-CG-CD	-5.20	98.08	111.60
1	A	587	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	445	LEU	O-C-N	-5.19	114.40	122.70
1	B	199	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	434	TYR	CG-CD1-CE1	5.14	125.41	121.30
1	B	54	ARG	CB-CA-C	-5.13	100.14	110.40
1	B	65	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	149	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	MET	CA-CB-CG	-5.10	104.62	113.30
1	A	665	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
1	A	454	ASP	OD1-CG-OD2	-5.09	113.63	123.30
1	A	706	PHE	CB-CG-CD1	5.09	124.36	120.80
1	B	47	LEU	N-CA-CB	-5.08	100.25	110.40
1	B	545	VAL	CA-CB-CG1	5.04	118.47	110.90
1	B	183	LYS	CD-CE-NZ	5.03	123.26	111.70
1	A	313	TYR	CB-CG-CD1	-5.01	117.99	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ASP	Mainchain
1	A	393	ARG	Sidechain
1	A	47	LEU	Mainchain
1	A	471	LEU	Mainchain
1	B	199	ASP	Mainchain
1	B	438	GLU	Sidechain

## 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	5526	0	5342	23	0
1	B	5538	0	5348	25	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	2	0	0	0	0
4	B	2	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	8	0	14	2	0
7	A	8	0	14	2	0
7	B	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	955	0	0	12	2
8	B	911	0	0	12	2
All	All	13056	0	10792	54	2

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 (54) 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:569:ALA:O	1:B:570:VAL:HG23	1.63	0.99
1:A:119[B]:THR:HG21	8:A:1227:HOH:O	1.67	0.94
1:B:119[B]:THR:HG21	8:B:1263:HOH:O	1.68	0.93
1:B:544:GLN:OE1	8:B:901:HOH:O	1.88	0.90
1:B:431:ARG:HD2	8:B:1576:HOH:O	1.78	0.83
1:A:589:GLU:HG2	8:A:1552:HOH:O	1.79	0.82
1:B:569:ALA:O	1:B:570:VAL:CG2	2.29	0.80
1:B:431:ARG:CD	8:B:1576:HOH:O	2.29	0.77
1:B:610:ARG:HD3	1:B:611:VAL:HG23	1.74	0.70
6:A:805:MRD:H1C2	6:A:805:MRD:O4	1.93	0.68
1:A:610:ARG:HD3	1:A:611:VAL:HG23	1.76	0.67
1:A:633[B]:VAL:CG2	1:A:719:TYR:CZ	2.77	0.67
1:A:76:ASP:OD1	8:A:903:HOH:O	2.12	0.66
1:B:512:ASP:OD1	8:B:902:HOH:O	2.14	0.65
1:B:647:GLN:HG2	8:B:1043:HOH:O	1.97	0.65
1:B:255[B]:ARG:NH2	8:B:907:HOH:O	2.28	0.62
1:B:512:ASP:HB2	8:B:1460:HOH:O	2.00	0.62
1:A:647:GLN:HG2	8:A:1101:HOH:O	2.01	0.61
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.85	0.60
1:A:407:GLU:HG2	8:A:1547:HOH:O	2.02	0.59
1:A:422:LYS:NZ	8:A:906:HOH:O	2.38	0.57
1:B:54:ARG:HG3	1:B:199:ASP:OD2	2.07	0.54
1:A:585:GLN:NE2	8:A:911:HOH:O	2.40	0.54
1:B:591:MET:SD	1:B:594:LEU:HD12	2.48	0.54
1:B:662:ASN:H	1:B:725:GLN:HE22	1.57	0.53
6:A:805:MRD:C1	6:A:805:MRD:O4	2.57	0.53
4:B:803:OXY:O2	8:B:903:HOH:O	2.19	0.51
1:B:519:GLU:OE1	8:B:904:HOH:O	2.19	0.50
1:A:69:ALA:O	1:A:73:GLU:HG3	2.12	0.49
1:A:591:MET:SD	1:A:594:LEU:HD12	2.53	0.49
1:A:504:ARG:HD2	8:A:1062:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:806:MPD:HM2	8:A:1605:HOH:O	2.14	0.47
1:A:633[B]:VAL:HG23	1:A:719:TYR:CE1	2.49	0.47
1:A:593:VAL:HG13	8:A:922:HOH:O	2.14	0.47
1:A:633[B]:VAL:CG2	1:A:719:TYR:CE1	2.98	0.47
7:B:804:MPD:H11	7:B:804:MPD:O4	2.15	0.46
1:A:509:PRO:HD2	1:A:591:MET:HG2	1.98	0.46
1:A:54:ARG:HB3	1:A:55:HIS:CD2	2.51	0.46
1:B:633[A]:VAL:CG2	1:B:719:TYR:CE1	3.01	0.44
1:B:186:GLY:HA2	8:B:911:HOH:O	2.17	0.44
1:A:633[B]:VAL:HG21	1:A:719:TYR:CZ	2.51	0.43
1:A:47:LEU:HB2	8:A:908:HOH:O	2.18	0.43
1:B:247[A]:ASN:ND2	8:B:929:HOH:O	2.51	0.43
1:B:650:HIS:HD2	1:B:698:THR:OG1	2.01	0.43
1:A:602:ARG:HB3	1:A:645:VAL:HG23	2.01	0.42
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.54	0.42
1:A:346:PHE:CZ	1:A:403:ARG:HG2	2.55	0.41
7:A:806:MPD:C1	8:A:1091:HOH:O	2.68	0.41
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.56	0.41
1:B:602:ARG:HB3	1:B:645:VAL:HG23	2.02	0.41
1:A:608:LYS:HD3	1:A:608:LYS:HA	1.91	0.41
1:B:569:ALA:C	1:B:570:VAL:HG23	2.38	0.40
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1330:HOH:O	8:B:1223:HOH:O[2_444]	2.03	0.17
8:A:1547:HOH:O	8:B:1138:HOH:O[2_444]	2.08	0.12

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	705 (99%)	10 (1%)	0	100	100
1	B	718/728 (99%)	707 (98%)	11 (2%)	0	100	100
All	All	1433/1456 (98%)	1412 (98%)	21 (2%)	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	553/559 (99%)	543 (98%)	10 (2%)	59	36
1	B	555/559 (99%)	547 (99%)	8 (1%)	67	47
All	All	1108/1118 (99%)	1090 (98%)	18 (2%)	62	41

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	64	LYS
1	A	118	ARG
1	A	141	ASP
1	A	227	ASN
1	A	379	LYS
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	227	ASN
1	A	247	ASN
1	B	46	GLN
1	B	227	ASN
1	B	544	GLN
1	B	647	GLN
1	B	650	HIS
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	1.87	2 (20%)	10,23,25	1.81	3 (30%)
1	TOX	A	111[A]	2	10,17,18	1.87	2 (20%)	10,23,25	1.81	3 (30%)
1	TOX	B	111[B]	-	10,17,18	2.53	4 (40%)	10,23,25	1.57	2 (20%)
1	TOX	B	111[A]	2	10,17,18	2.53	4 (40%)	10,23,25	1.57	2 (20%)

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

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

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	-5.99	1.33	1.39
1	B	111[A]	TOX	CD1-NE1	-5.99	1.33	1.39
1	A	111[B]	TOX	CD1-NE1	-4.53	1.34	1.39
1	A	111[A]	TOX	CD1-NE1	-4.53	1.34	1.39
1	B	111[B]	TOX	CZ2-CE2	-3.21	1.34	1.41
1	B	111[A]	TOX	CZ2-CE2	-3.21	1.34	1.41
1	A	111[B]	TOX	CE3-CD2	-3.03	1.36	1.42
1	A	111[A]	TOX	CE3-CD2	-3.03	1.36	1.42
1	B	111[B]	TOX	O-C	2.59	1.30	1.19
1	B	111[A]	TOX	O-C	2.59	1.30	1.19
1	B	111[B]	TOX	CE3-CD2	-2.27	1.37	1.42
1	B	111[A]	TOX	CE3-CD2	-2.27	1.37	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[B]	TOX	CZ2-CE2-CD2	-3.68	115.94	120.94
1	A	111[A]	TOX	CZ2-CE2-CD2	-3.68	115.94	120.94
1	B	111[B]	TOX	CZ3-CE3-CD2	-3.47	116.08	120.89
1	B	111[A]	TOX	CZ3-CE3-CD2	-3.47	116.08	120.89
1	A	111[B]	TOX	CB-CA-C	2.33	115.83	111.47
1	A	111[A]	TOX	CB-CA-C	2.33	115.83	111.47
1	A	111[B]	TOX	CB-CG-CD1	-2.27	125.17	127.97
1	A	111[A]	TOX	CB-CG-CD1	-2.27	125.17	127.97
1	B	111[B]	TOX	CE3-CD2-CG	-2.24	130.30	134.42
1	B	111[A]	TOX	CE3-CD2-CG	-2.24	130.30	134.42

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	A	111[B]	TOX	C-CA-CB-CG

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

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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	1.70	2 (28%)	9,10,10	1.19	1 (11%)
5	PO4	A	804	-	4,4,4	2.12	2 (50%)	6,6,6	3.24	3 (50%)
2	HEM	B	801	1	27,50,50	1.76	4 (14%)	17,82,82	2.34	9 (52%)
6	MRD	A	805	-	7,7,7	0.72	0	9,10,10	1.71	4 (44%)
4	OXY	A	803	-	1,1,1	0.84	0	-	-	-
5	PO4	B	805	-	4,4,4	1.86	1 (25%)	6,6,6	2.53	2 (33%)
7	MPD	B	804	-	7,7,7	0.66	0	9,10,10	2.04	4 (44%)
4	OXY	B	803	-	1,1,1	1.45	0	-	-	-
2	HEM	A	801	1	27,50,50	1.21	4 (14%)	17,82,82	2.21	7 (41%)

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	-	-	0/5/5/5	-
6	MRD	A	805	-	-	1/5/5/5	-
2	HEM	B	801	1	-	0/6/54/54	-
7	MPD	B	804	-	-	3/5/5/5	-
2	HEM	A	801	1	-	0/6/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-5.07	1.33	1.40
2	B	801	HEM	C4A-NA	4.34	1.45	1.36
2	B	801	HEM	C3C-C2C	-3.58	1.35	1.40
7	A	806	MPD	O2-C2	3.45	1.53	1.44
5	A	804	PO4	P-O4	-3.22	1.44	1.54
2	A	801	HEM	CAD-C3D	-3.13	1.46	1.52
5	B	805	PO4	P-O3	-3.09	1.45	1.54
2	A	801	HEM	CAA-C2A	2.70	1.56	1.52
2	A	801	HEM	C1D-ND	2.57	1.41	1.36
2	A	801	HEM	C1C-C2C	2.47	1.48	1.42
5	A	804	PO4	P-O1	2.41	1.56	1.50
7	A	806	MPD	C3-C2	-2.12	1.47	1.53
2	B	801	HEM	C3B-CAB	2.05	1.52	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	PO4	O3-P-O1	-6.47	87.22	110.89
5	B	805	PO4	O3-P-O2	4.24	121.57	107.97
2	A	801	HEM	CAA-CBA-CGA	-3.87	106.18	112.67
2	B	801	HEM	CAD-CBD-CGD	3.78	119.02	112.67
5	B	805	PO4	O2-P-O1	-3.62	97.65	110.89
2	B	801	HEM	C4A-C3A-C2A	3.58	109.49	107.00
2	A	801	HEM	CMD-C2D-C3D	3.45	131.44	124.94
2	A	801	HEM	CMD-C2D-C1D	-3.42	123.20	128.46
7	B	804	MPD	O2-C2-C3	-3.32	97.32	109.80
2	A	801	HEM	CBD-CAD-C3D	3.21	118.40	112.48
2	B	801	HEM	CAA-CBA-CGA	-3.11	107.45	112.67
5	A	804	PO4	O4-P-O1	3.11	122.27	110.89
2	A	801	HEM	C4A-C3A-C2A	3.08	109.14	107.00
7	B	804	MPD	O4-C4-C5	3.06	122.63	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CMB-C2B-C3B	3.05	130.39	124.68
6	A	805	MRD	CM-C2-C1	-2.99	104.34	110.57
2	B	801	HEM	CMD-C2D-C3D	2.95	130.51	124.94
7	A	806	MPD	CM-C2-C1	-2.87	104.60	110.57
2	B	801	HEM	CMD-C2D-C1D	-2.82	124.13	128.46
2	A	801	HEM	C1D-C2D-C3D	-2.76	105.08	107.00
2	A	801	HEM	CMB-C2B-C3B	2.75	129.81	124.68
2	B	801	HEM	CMA-C3A-C4A	-2.64	124.40	128.46
6	A	805	MRD	O2-C2-CM	2.62	116.48	108.08
2	B	801	HEM	CBD-CAD-C3D	2.59	117.25	112.48
2	B	801	HEM	C1D-C2D-C3D	-2.52	105.25	107.00
7	B	804	MPD	C1-C2-C3	2.34	120.86	109.96
5	A	804	PO4	O2-P-O1	2.28	119.25	110.89
6	A	805	MRD	C1-C2-C3	2.16	120.02	109.96
7	B	804	MPD	O2-C2-CM	2.01	114.54	108.08
6	A	805	MRD	CM-C2-C3	-2.01	100.61	109.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	804	MPD	C1-C2-C3-C4
7	B	804	MPD	O2-C2-C3-C4
7	B	804	MPD	CM-C2-C3-C4
6	A	805	MRD	C2-C3-C4-O4

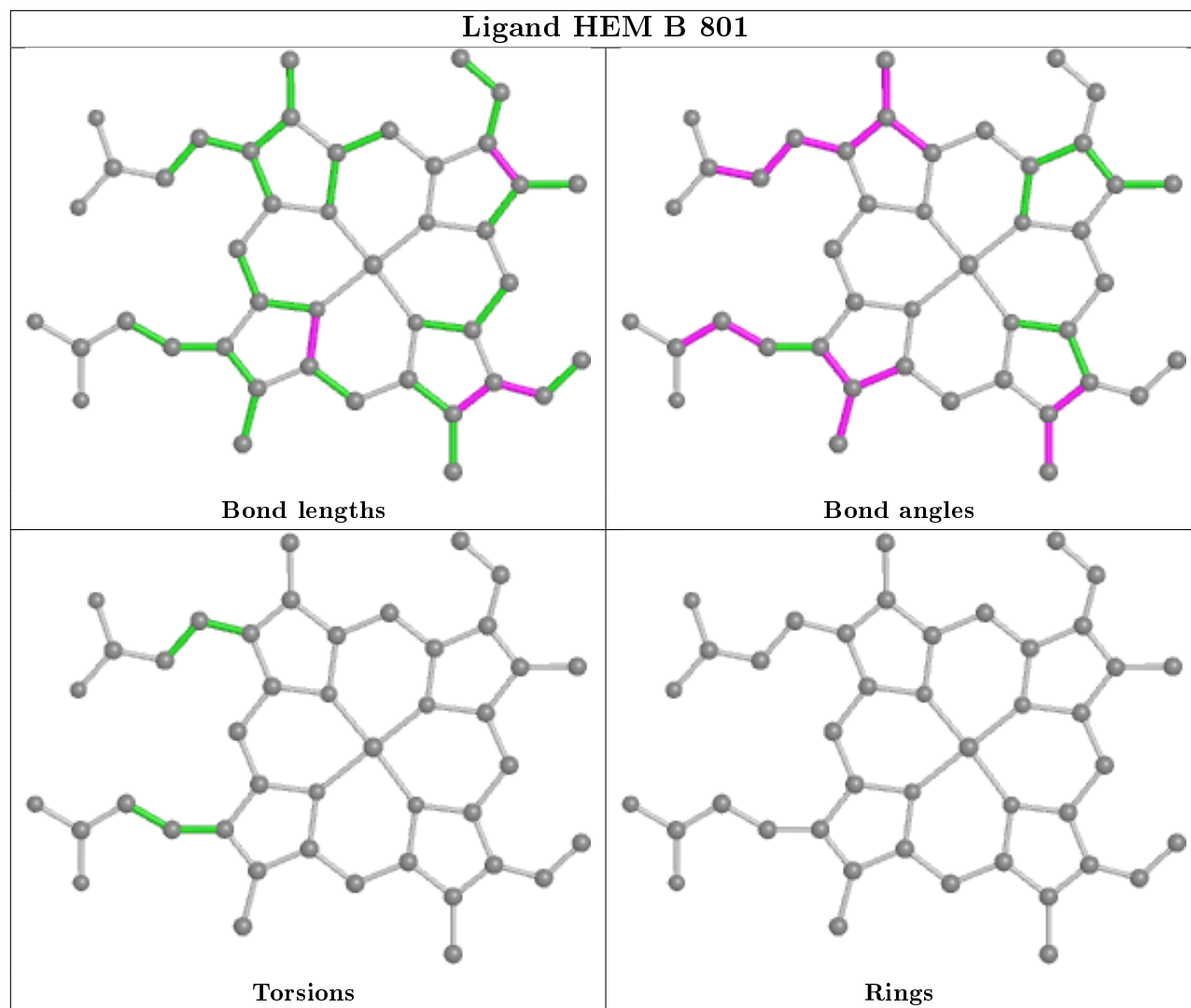
There are no ring outliers.

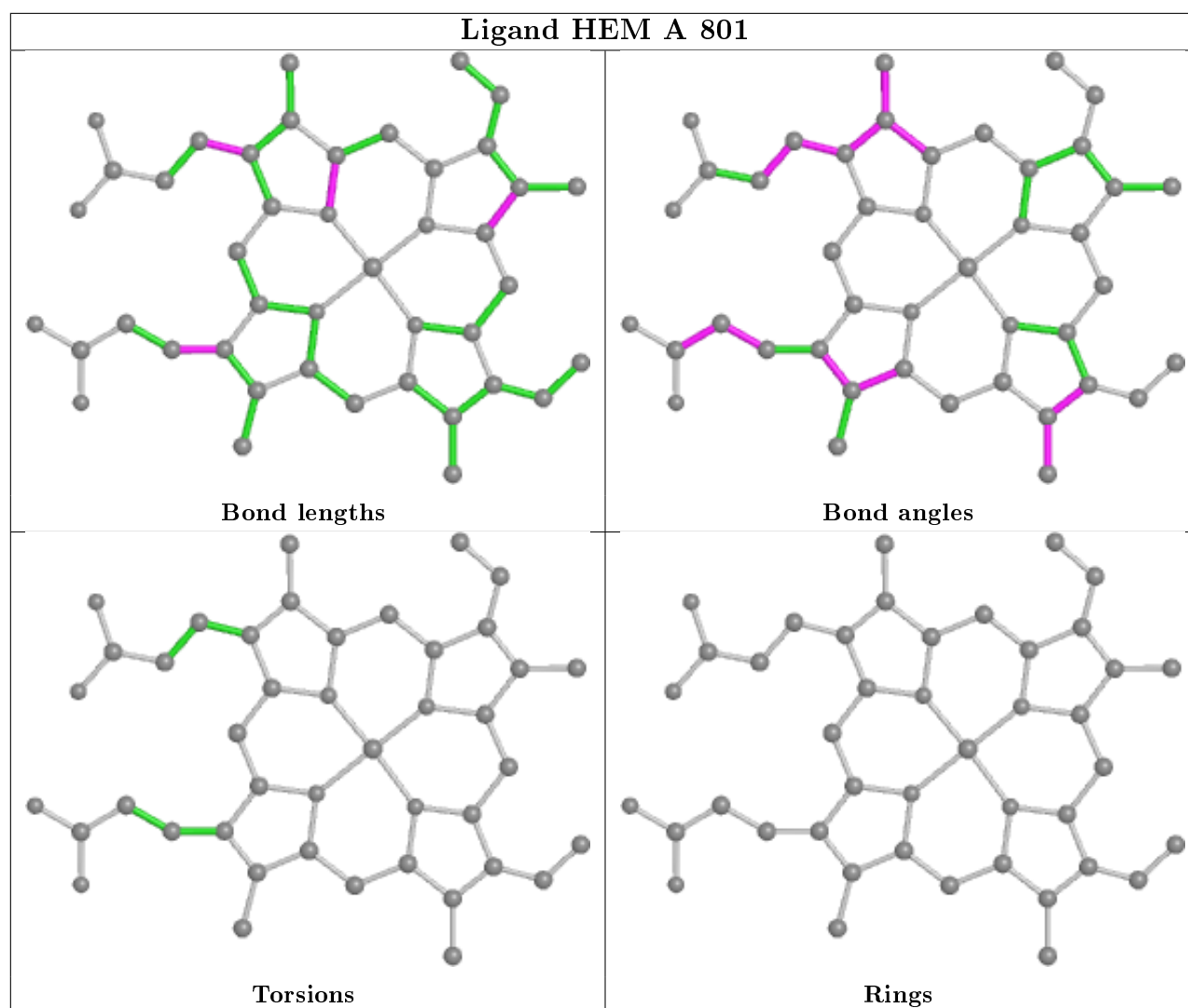
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	806	MPD	2	0
6	A	805	MRD	2	0
7	B	804	MPD	1	0
4	B	803	OXY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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%)	-0.39	17 (2%) 59 56	12, 17, 34, 81	1 (0%)
1	B	713/728 (97%)	-0.39	14 (1%) 65 64	11, 18, 34, 94	1 (0%)
All	All	1425/1456 (97%)	-0.39	31 (2%) 62 60	11, 18, 34, 94	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	7.0
1	B	610	ARG	6.9
1	A	540	ARG	5.7
1	B	748	ALA	5.5
1	A	541	GLY	4.4
1	B	608	LYS	4.4
1	B	541	GLY	4.2
1	B	540	ARG	4.1
1	A	610	ARG	3.7
1	B	65	ASP	3.6
1	B	679	ALA	3.6
1	A	454	ASP	3.4
1	B	35	ASN	3.4
1	B	64	LYS	3.3
1	A	608	LYS	3.2
1	B	454	ASP	3.1
1	A	64	LYS	3.0
1	A	680	ALA	2.9
1	B	680	ALA	2.8
1	A	65	ASP	2.7
1	A	542	GLY	2.6
1	A	609	TYR	2.4
1	B	609	TYR	2.3
1	A	679	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	378	SER	2.2
1	B	366	GLY	2.2
1	A	611	VAL	2.2
1	A	378	SER	2.1
1	A	63	GLY	2.1
1	A	221	GLY	2.0
1	A	215	PRO	2.0

## 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[B]	16/17	0.97	0.10	10,12,14,19	2
1	TOX	A	111[A]	16/17	0.97	0.10	10,12,16,19	2
1	TOX	B	111[B]	16/17	0.97	0.10	11,12,14,21	1
1	TOX	B	111[A]	16/17	0.97	0.10	11,12,17,21	1

## 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
7	MPD	A	806	8/8	0.87	0.13	32,35,46,52	0
4	OXY	A	803	2/2	0.92	0.14	28,28,28,31	0
6	MRD	A	805	8/8	0.92	0.11	45,50,61,62	0
7	MPD	B	804	8/8	0.92	0.12	50,53,57,61	0
4	OXY	B	803	2/2	0.92	0.13	24,24,24,28	0
5	PO4	A	804	5/5	0.95	0.17	38,42,51,57	0
5	PO4	B	805	5/5	0.95	0.21	37,51,57,63	0

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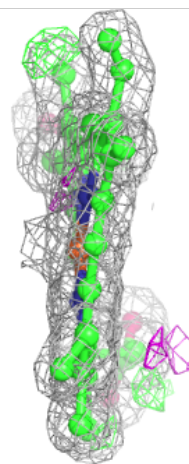
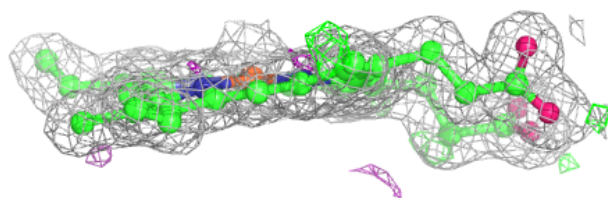
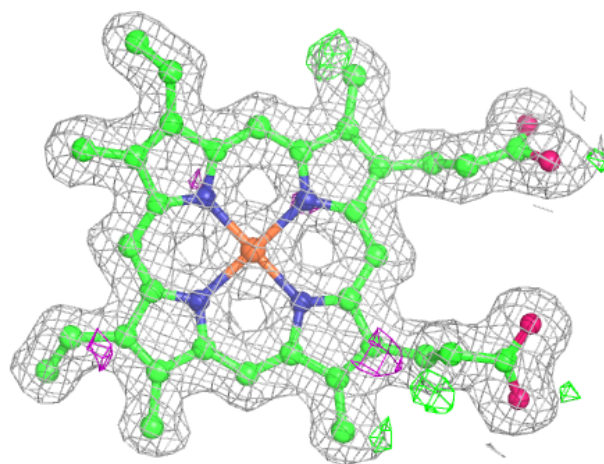
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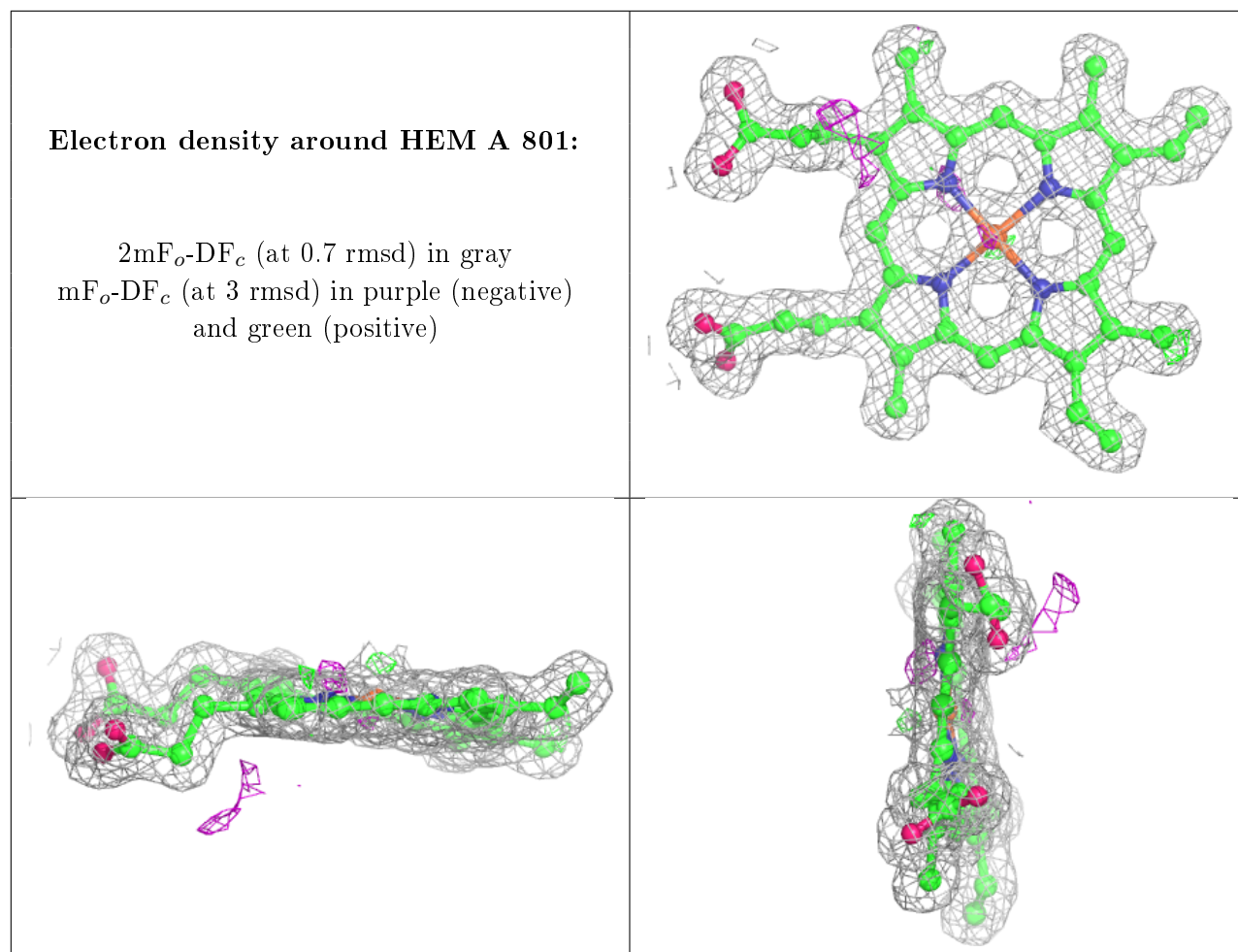
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	A	802	1/1	0.98	0.05	18,18,18,18	0
3	NA	B	802	1/1	0.98	0.05	20,20,20,20	0
2	HEM	B	801	43/43	0.99	0.09	12,13,15,18	0
2	HEM	A	801	43/43	0.99	0.10	11,13,15,15	0

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<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.