



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:30 am BST

PDB ID : 5KSN  
Title : Crystal structure of the S324G variant of catalase-peroxidase from *B. pseudo-mallei* with INH bound  
Authors : Loewen, P.C.  
Deposited on : 2016-07-08  
Resolution : 1.87 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.

---

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

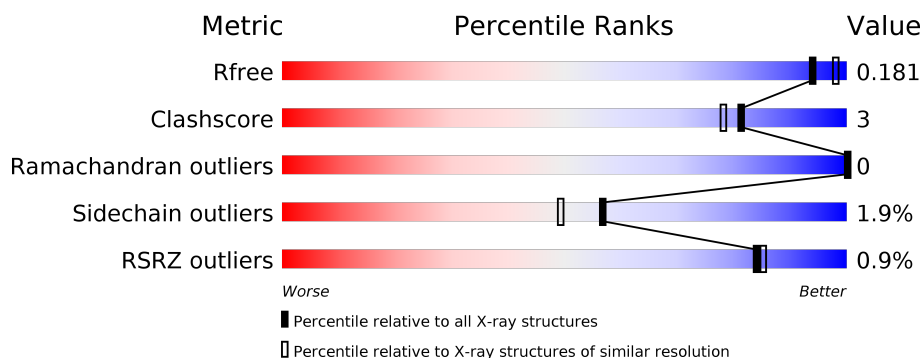
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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></div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	B	728	<div> <div></div> <div>86%</div> <div>11%</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
8	NIZ	A	809	-	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.

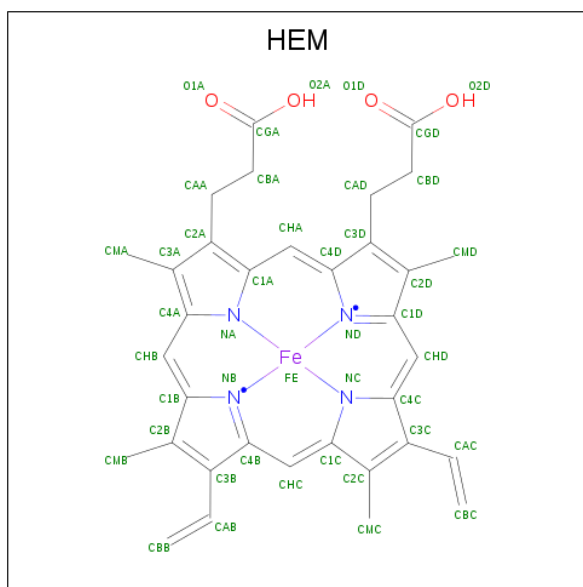
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total 5555	C 3508	N 989	O 1044	S 14	0	7	0
1	B	713	Total 5581	C 3523	N 994	O 1050	S 14	0	10	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	GLY	SER	engineered mutation	UNP Q3JNW6
B	324	GLY	SER	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		

*Continued on next page...*

*Continued from previous page...*

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

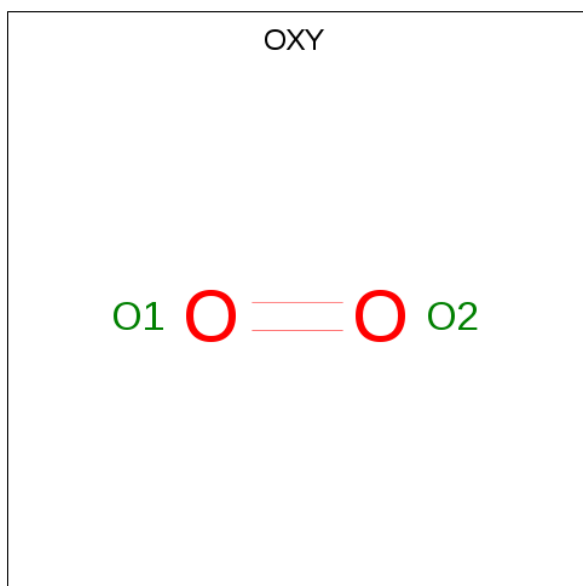
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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>).



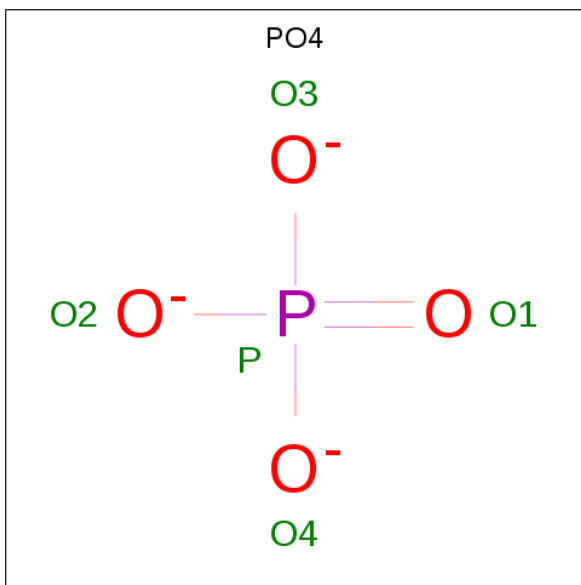
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	A	1	Total	O		
			2	2	0	0

*Continued on next page...*

*Continued from previous page...*

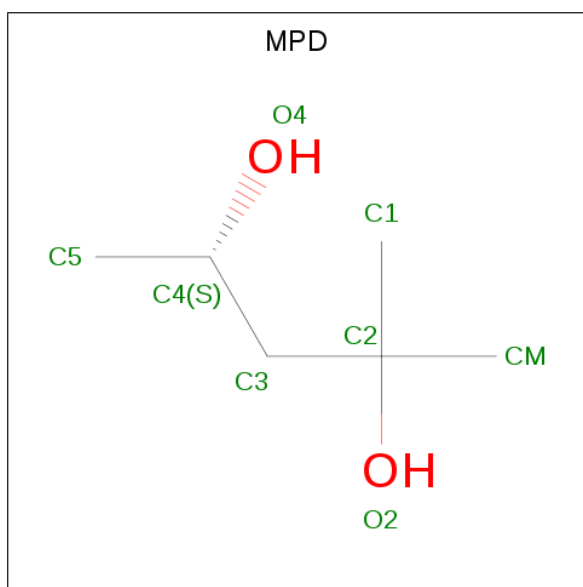
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



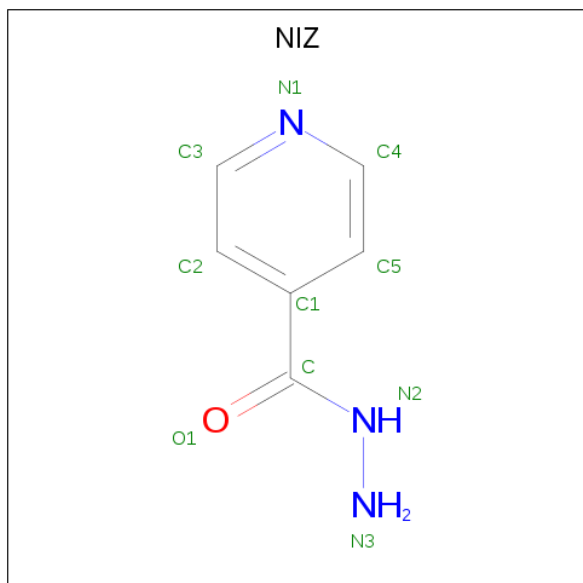
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

- Molecule 8 is pyridine-4-carbohydrazide (three-letter code: NIZ) (formula:  $C_6H_7N_3O$ ).



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

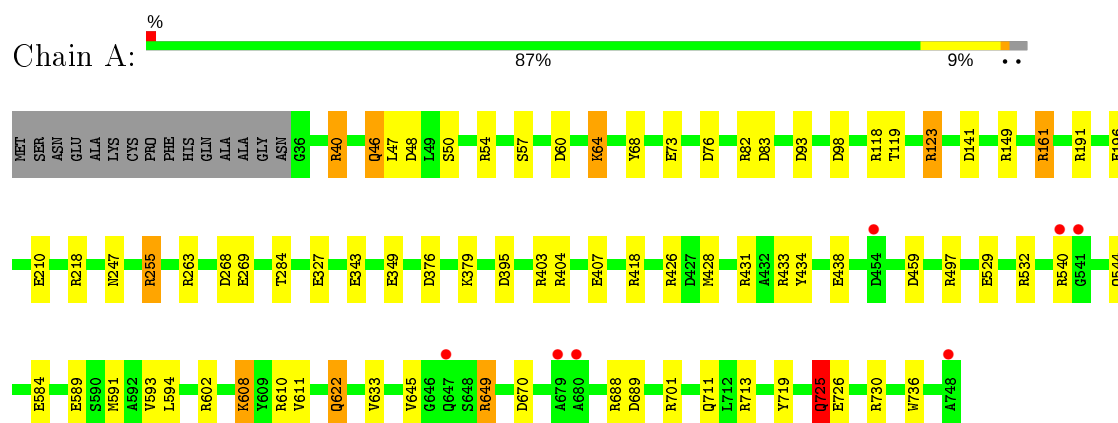
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	786	Total	O	0	0
			786	786		
9	B	821	Total	O	0	0
			821	821		

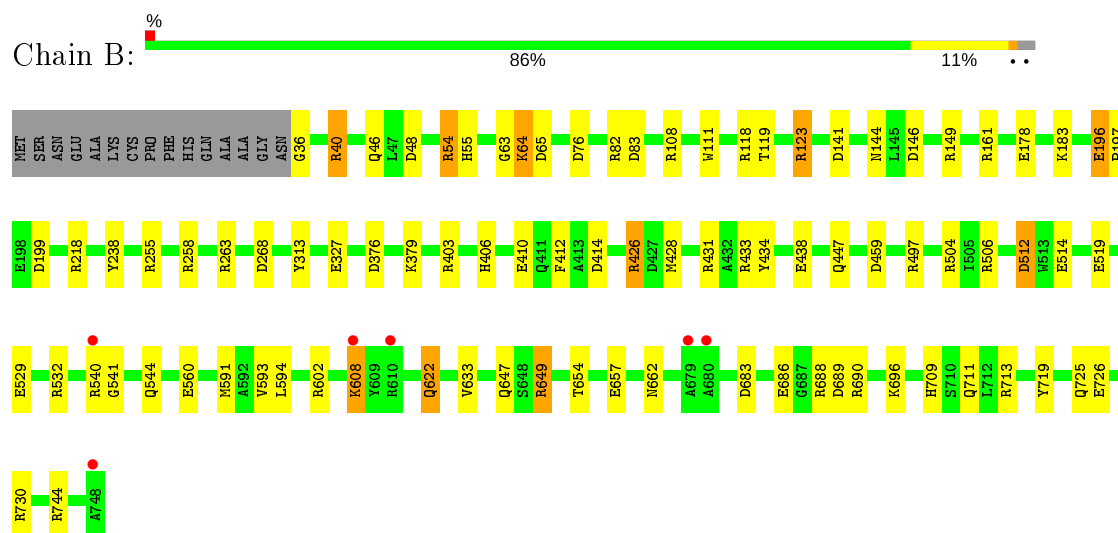
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	100.43Å 115.28Å 174.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 1.87 48.05 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.05-1.87) 98.6 (48.05-1.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.141 , 0.171 0.154 , 0.181	Depositor DCC
$R_{free}$ test set	8235 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12903	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 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, OXY, CL, NA, PO4, NIZ, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.34	28/5706 (0.5%)	1.27	61/7757 (0.8%)
1	B	1.36	31/5735 (0.5%)	1.19	44/7795 (0.6%)
All	All	1.35	59/11441 (0.5%)	1.23	105/15552 (0.7%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	410	GLU	CG-CD	9.37	1.66	1.51
1	B	426	ARG	CZ-NH2	9.01	1.44	1.33
1	A	589	GLU	CD-OE2	8.09	1.34	1.25
1	B	438	GLU	CD-OE1	-7.85	1.17	1.25
1	B	434	TYR	CE1-CZ	-7.68	1.28	1.38
1	B	410	GLU	CD-OE2	7.67	1.34	1.25
1	A	50	SER	CB-OG	-7.60	1.32	1.42
1	B	514	GLU	CD-OE2	-7.40	1.17	1.25
1	B	532	ARG	CZ-NH1	-7.39	1.23	1.33
1	B	512	ASP	CG-OD2	7.34	1.42	1.25
1	A	438	GLU	CD-OE1	-7.15	1.17	1.25
1	A	46	GLN	CG-CD	7.02	1.67	1.51
1	B	313	TYR	CG-CD1	7.00	1.48	1.39
1	B	726	GLU	CG-CD	6.92	1.62	1.51
1	B	434	TYR	CG-CD1	-6.78	1.30	1.39
1	B	541	GLY	C-O	6.77	1.34	1.23
1	A	57	SER	CB-OG	6.74	1.51	1.42
1	A	343	GLU	CD-OE1	6.74	1.33	1.25
1	A	584	GLU	CG-CD	6.67	1.61	1.51
1	A	327	GLU	CD-OE1	6.56	1.32	1.25
1	B	196	GLU	CB-CG	-6.43	1.40	1.52
1	A	68	TYR	CG-CD2	-6.37	1.30	1.39
1	A	688	ARG	CZ-NH2	-6.35	1.24	1.33
1	B	532	ARG	CD-NE	-6.30	1.35	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	TYR	CE2-CZ	-6.25	1.30	1.38
1	A	428	MET	CG-SD	-6.19	1.65	1.81
1	A	434	TYR	CG-CD2	-6.18	1.31	1.39
1	B	560	GLU	CD-OE1	-6.17	1.18	1.25
1	A	589	GLU	CD-OE1	6.04	1.32	1.25
1	A	269	GLU	CD-OE1	-6.03	1.19	1.25
1	A	196	GLU	CB-CG	-6.00	1.40	1.52
1	A	434	TYR	CE1-CZ	-5.99	1.30	1.38
1	B	726	GLU	CD-OE2	5.94	1.32	1.25
1	A	418	ARG	CZ-NH1	-5.74	1.25	1.33
1	A	161	ARG	NE-CZ	5.70	1.40	1.33
1	B	82	ARG	CZ-NH2	-5.56	1.25	1.33
1	A	82	ARG	CZ-NH2	-5.55	1.25	1.33
1	B	63	GLY	N-CA	5.51	1.54	1.46
1	B	730	ARG	CZ-NH2	5.41	1.40	1.33
1	B	36	GLY	N-CA	5.38	1.54	1.46
1	A	210	GLU	CD-OE1	-5.37	1.19	1.25
1	B	686	GLU	CG-CD	5.35	1.59	1.51
1	A	736	TRP	CG-CD1	-5.34	1.29	1.36
1	B	434	TYR	CE2-CZ	-5.24	1.31	1.38
1	B	327	GLU	CD-OE1	5.24	1.31	1.25
1	B	434	TYR	CG-CD2	-5.24	1.32	1.39
1	B	255[A]	ARG	CZ-NH1	-5.21	1.26	1.33
1	B	255[B]	ARG	CZ-NH1	-5.21	1.26	1.33
1	A	711	GLN	CG-CD	5.18	1.62	1.51
1	B	161[A]	ARG	CZ-NH1	5.17	1.39	1.33
1	B	161[B]	ARG	CZ-NH1	5.17	1.39	1.33
1	B	199	ASP	C-O	5.15	1.33	1.23
1	A	247	ASN	CG-ND2	-5.14	1.20	1.32
1	A	73	GLU	CG-CD	5.10	1.59	1.51
1	A	540	ARG	C-O	5.09	1.33	1.23
1	A	327	GLU	CD-OE2	5.08	1.31	1.25
1	B	602	ARG	CZ-NH2	-5.08	1.26	1.33
1	B	327	GLU	CG-CD	5.03	1.59	1.51
1	A	349	GLU	CG-CD	-5.03	1.44	1.51

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	NE-CZ-NH1	19.12	129.86	120.30
1	A	255[A]	ARG	NE-CZ-NH2	-16.83	111.88	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-16.83	111.88	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255[A]	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	A	255[B]	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	A	48	ASP	CB-CG-OD1	10.85	128.06	118.30
1	A	60	ASP	CB-CG-OD2	-10.21	109.11	118.30
1	B	40	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	376	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	B	688	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	A	649	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	433	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	649	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	149	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	B	108	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	263	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	40	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	B	512	ASP	CB-CG-OD2	8.47	125.92	118.30
1	B	48	ASP	CB-CG-OD1	8.46	125.91	118.30
1	B	649	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	688	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	532	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	B	218	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	B	268	ASP	CB-CG-OD1	7.91	125.42	118.30
1	B	688	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	B	258	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	A	404	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	161	ARG	CD-NE-CZ	7.64	134.30	123.60
1	A	497	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	670	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	B	649	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	713	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	123	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	B	683	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	B	512	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	A	54	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	433	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	689	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	A	730	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	B	108	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	532	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	268	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	B	541	GLY	N-CA-C	-6.98	95.65	113.10
1	B	65	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	434	TYR	CB-CG-CD1	6.79	125.08	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	689	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	83	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	46	GLN	CA-CB-CG	6.62	127.95	113.40
1	B	123	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	263	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	744	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	149	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	161	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	414	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	725[A]	GLN	CB-CG-CD	6.45	128.37	111.60
1	A	725[B]	GLN	CB-CG-CD	6.45	128.37	111.60
1	A	76	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	161	ARG	NH1-CZ-NH2	-6.35	112.41	119.40
1	A	689	ASP	CB-CG-OD1	6.34	124.01	118.30
1	B	713	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	263	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	60	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	83	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	54	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	395	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	730	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	404	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	428	MET	CA-CB-CG	-5.90	103.26	113.30
1	A	255[A]	ARG	CG-CD-NE	-5.90	99.42	111.80
1	A	255[B]	ARG	CG-CD-NE	-5.90	99.42	111.80
1	A	540	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	497	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	532	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	376	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	504	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	431	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	412	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	A	532	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	433	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	161[A]	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	161[B]	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	403	ARG	CG-CD-NE	-5.60	100.03	111.80
1	A	529	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	A	459	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	98	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	B	506	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	701	ARG	NE-CZ-NH1	5.40	123.00	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529[A]	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	B	529[B]	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	A	268	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	191	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	263	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	47	LEU	N-CA-CB	-5.29	99.82	110.40
1	B	327	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	A	268	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	82	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	93	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	54	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	459	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	218	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	349	GLU	OE1-CD-OE2	5.05	129.37	123.30
1	A	407[A]	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	407[B]	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	426	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	713	ARG	NE-CZ-NH2	-5.00	117.80	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	5555	0	5368	23	0
1	B	5581	0	5391	30	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	1	0
6	A	5	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5	0	0	0	0
7	A	16	0	28	3	0
7	B	16	0	28	1	0
8	A	10	0	7	2	0
8	B	10	0	7	1	0
9	A	786	0	0	5	1
9	B	821	0	0	13	1
All	All	12903	0	10889	58	1

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 (58) 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:A:725[A]:GLN:NE2	1:A:726[A]:GLU:HG3	1.45	1.30
1:A:622[A]:GLN:NE2	8:A:809:NIZ:O1	1.91	1.04
1:B:622[A]:GLN:NE2	8:B:809:NIZ:O1	1.96	0.97
1:A:725[A]:GLN:NE2	1:A:726[A]:GLU:CG	2.30	0.94
1:A:119[B]:THR:HG21	9:A:1114:HOH:O	1.74	0.87
1:B:119[B]:THR:HG21	9:B:1087:HOH:O	1.73	0.87
1:B:403:ARG:NH1	9:B:903:HOH:O	2.07	0.86
1:B:647:GLN:HG2	9:B:928:HOH:O	1.76	0.85
1:A:544:GLN:OE1	9:A:901:HOH:O	2.02	0.75
1:B:519:GLU:OE1	9:B:902:HOH:O	2.05	0.75
1:A:725[A]:GLN:HE22	1:A:726[A]:GLU:HG3	1.50	0.73
1:A:593:VAL:HG13	9:A:988:HOH:O	1.90	0.72
1:B:178:GLU:OE1	9:B:904:HOH:O	2.08	0.71
1:B:123:ARG:HH21	1:B:622[A]:GLN:HE21	1.39	0.69
1:B:76:ASP:OD1	9:B:905:HOH:O	2.12	0.67
7:A:807:MPD:O4	7:A:807:MPD:HM1	1.95	0.67
1:A:725[A]:GLN:CD	1:A:726[A]:GLU:HG3	2.14	0.66
1:B:512:ASP:OD1	9:B:906:HOH:O	2.14	0.64
1:A:255[A]:ARG:NH2	9:A:902:HOH:O	2.11	0.64
1:A:123:ARG:HH21	1:A:622[A]:GLN:HE21	1.43	0.64
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.80	0.61
1:A:622[A]:GLN:HE22	8:A:809:NIZ:C	2.01	0.60
1:B:657[A]:GLU:CD	9:B:926:HOH:O	2.39	0.60
1:B:662:ASN:H	1:B:725:GLN:HE22	1.53	0.56
7:A:807:MPD:O4	7:A:807:MPD:CM	2.52	0.56
1:B:123:ARG:HH21	1:B:622[A]:GLN:NE2	2.05	0.55

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725[A]:GLN:HE22	1:A:726[A]:GLU:CG	2.13	0.54
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.91	0.54
1:B:544:GLN:NE2	9:B:913:HOH:O	2.40	0.54
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.92	0.53
1:A:725[A]:GLN:NE2	9:A:903:HOH:O	2.22	0.52
1:B:46:GLN:NE2	9:B:901:HOH:O	1.96	0.52
1:A:608:LYS:HE2	1:A:608:LYS:HA	1.91	0.51
5:B:805:OXY:O1	9:B:908:HOH:O	2.19	0.51
1:B:696:LYS:HE2	9:B:973:HOH:O	2.12	0.50
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.48	0.49
1:B:608:LYS:HE2	1:B:608:LYS:HA	1.95	0.49
1:A:64:LYS:HE3	1:A:64:LYS:O	2.14	0.48
1:B:64:LYS:HE3	1:B:64:LYS:O	2.14	0.48
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.60	0.48
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.46	0.46
1:A:123:ARG:NH2	1:A:622[B]:GLN:OE1	2.49	0.46
1:B:196:GLU:HB2	1:B:197:PRO:HD2	1.98	0.45
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.17	0.45
7:B:807:MPD:O4	7:B:807:MPD:H12	2.17	0.44
1:B:119[B]:THR:HG23	1:B:593:VAL:HG11	1.98	0.44
1:B:591:MET:SD	1:B:594:LEU:HD12	2.57	0.44
1:B:426:ARG:HA	1:B:426:ARG:HD2	1.88	0.44
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.17	0.44
1:B:709:HIS:CE1	1:B:711[A]:GLN:HB2	2.53	0.44
7:A:808:MPD:O4	7:A:808:MPD:H11	2.18	0.43
1:A:610:ARG:HG2	1:A:611:VAL:HG23	2.02	0.41
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.55	0.41
1:B:406:HIS:HD2	9:B:1408:HOH:O	2.02	0.41
1:A:591:MET:SD	1:A:594:LEU:HD12	2.61	0.41
1:A:602:ARG:HB3	1:A:645:VAL:HG23	2.03	0.41
1:B:654:THR:HG23	1:B:657[A]:GLU:HG3	2.02	0.40
1:A:284:THR:HG22	2:A:801:HEM:CAA	2.51	0.40

All (1) 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)
9:A:1251:HOH:O	9:B:1149:HOH:O[2_444]	2.01	0.19

## 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	718/728 (99%)	710 (99%)	8 (1%)	0	100	100
1	B	721/728 (99%)	711 (99%)	10 (1%)	0	100	100
All	All	1439/1456 (99%)	1421 (99%)	18 (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	556/560 (99%)	543 (98%)	13 (2%)	50	41
1	B	559/560 (100%)	548 (98%)	11 (2%)	55	47
All	All	1115/1120 (100%)	1091 (98%)	24 (2%)	57	43

All (24) 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	161	ARG
1	A	379	LYS
1	A	608	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	622[A]	GLN
1	A	622[B]	GLN
1	A	649	ARG
1	A	725[A]	GLN
1	A	725[B]	GLN
1	B	40	ARG
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	183	LYS
1	B	379	LYS
1	B	608	LYS
1	B	622[A]	GLN
1	B	622[B]	GLN
1	B	649	ARG
1	B	690	ARG

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	247	ASN
1	A	520	GLN
1	A	544	GLN
1	B	227	ASN
1	B	520	GLN
1	B	544	GLN
1	B	647	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 ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	OXY	B	804	-	1,1,1	0.19	0	-		
5	OXY	A	804	-	1,1,1	0.05	0	-		
7	MPD	B	807	-	7,7,7	0.52	0	9,10,10	1.48	1 (11%)
2	HEM	B	801	1,9	27,50,50	1.50	4 (14%)	17,82,82	2.18	6 (35%)
8	NIZ	A	809	-	10,10,10	2.86	4 (40%)	12,12,12	3.42	9 (75%)
6	PO4	A	806	-	4,4,4	1.78	1 (25%)	6,6,6	2.51	2 (33%)
5	OXY	B	805	-	1,1,1	0.23	0	-		
6	PO4	B	806	-	4,4,4	1.00	0	6,6,6	1.98	3 (50%)
5	OXY	A	805	-	1,1,1	0.31	0	-		
7	MPD	A	808	-	7,7,7	0.73	0	9,10,10	1.76	2 (22%)
7	MPD	A	807	-	7,7,7	0.54	0	9,10,10	1.12	0
8	NIZ	B	809	-	10,10,10	2.97	4 (40%)	12,12,12	3.15	7 (58%)
2	HEM	A	801	1,9	27,50,50	1.21	3 (11%)	17,82,82	1.96	7 (41%)
7	MPD	B	808	-	7,7,7	0.70	0	9,10,10	1.62	4 (44%)

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	B	807	-	-	3/5/5/5	-
2	HEM	B	801	1,9	-	0/6/54/54	-
8	NIZ	A	809	-	-	0/6/6/6	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	A	807	-	-	0/5/5/5	-
7	MPD	A	808	-	-	0/5/5/5	-
8	NIZ	B	809	-	-	0/6/6/6	0/1/1/1
2	HEM	A	801	1,9	-	0/6/54/54	-
7	MPD	B	808	-	-	3/5/5/5	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	809	NIZ	N3-N2	-7.07	1.31	1.41
8	B	809	NIZ	N3-N2	-6.34	1.32	1.41
2	B	801	HEM	C3B-C2B	-5.23	1.33	1.40
8	B	809	NIZ	C4-N1	4.26	1.46	1.33
8	B	809	NIZ	C5-C1	4.06	1.46	1.39
8	A	809	NIZ	C4-N1	3.06	1.42	1.33
8	A	809	NIZ	O1-C	-2.72	1.17	1.23
2	A	801	HEM	C3C-CAC	2.67	1.53	1.47
2	B	801	HEM	C2A-C3A	-2.52	1.30	1.37
2	B	801	HEM	C3C-C2C	-2.51	1.36	1.40
8	A	809	NIZ	C1-C	-2.51	1.45	1.50
6	A	806	PO4	P-O4	-2.48	1.47	1.54
2	A	801	HEM	C4B-CHC	-2.46	1.34	1.41
8	B	809	NIZ	C2-C3	2.33	1.43	1.38
2	B	801	HEM	CMD-C2D	-2.13	1.47	1.51
2	A	801	HEM	C1D-ND	2.12	1.40	1.36

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	809	NIZ	O1-C-C1	-6.30	109.70	120.94
8	B	809	NIZ	C1-C-N2	5.73	122.82	116.27
2	B	801	HEM	CAA-CBA-CGA	-5.39	103.63	112.67
8	B	809	NIZ	C5-C4-N1	-5.31	114.38	123.62
6	A	806	PO4	O4-P-O3	5.23	124.75	107.97
8	A	809	NIZ	O1-C-N2	4.89	128.60	122.50
7	A	808	MPD	CM-C2-C1	-4.21	101.81	110.57
8	A	809	NIZ	C1-C-N2	4.10	120.96	116.27
8	A	809	NIZ	C-N2-N3	3.97	127.99	121.59
8	B	809	NIZ	O1-C-C1	-3.78	114.19	120.94
2	A	801	HEM	CAA-CBA-CGA	-3.75	106.38	112.67
8	B	809	NIZ	C3-C2-C1	-3.71	114.99	119.05
8	A	809	NIZ	C5-C1-C2	3.71	123.87	118.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CMB-C2B-C3B	3.61	131.42	124.68
7	B	807	MPD	CM-C2-C1	-3.40	103.48	110.57
8	A	809	NIZ	C5-C4-N1	-3.17	118.10	123.62
8	B	809	NIZ	C4-C5-C1	3.07	122.41	119.05
6	A	806	PO4	O4-P-O1	-3.03	99.82	110.89
6	B	806	PO4	O4-P-O1	-2.98	100.00	110.89
2	A	801	HEM	CAD-CBD-CGD	2.93	117.59	112.67
8	B	809	NIZ	C4-N1-C3	2.84	123.53	116.85
8	A	809	NIZ	C4-N1-C3	2.83	123.52	116.85
2	A	801	HEM	C1D-C2D-C3D	-2.80	105.05	107.00
8	B	809	NIZ	C-N2-N3	2.79	126.07	121.59
7	B	808	MPD	O2-C2-C3	-2.64	99.87	109.80
2	B	801	HEM	CMA-C3A-C2A	2.57	129.79	124.94
2	B	801	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
2	A	801	HEM	CBD-CAD-C3D	2.43	116.95	112.48
2	A	801	HEM	CMB-C2B-C3B	2.41	129.19	124.68
2	A	801	HEM	CBA-CAA-C2A	2.38	116.87	112.49
2	B	801	HEM	CAD-CBD-CGD	2.30	116.53	112.67
7	B	808	MPD	CM-C2-C3	2.27	120.54	109.96
7	B	808	MPD	O2-C2-C1	-2.25	100.86	108.08
7	A	808	MPD	C1-C2-C3	2.20	120.20	109.96
2	B	801	HEM	CBD-CAD-C3D	2.18	116.49	112.48
8	A	809	NIZ	C3-C2-C1	-2.17	116.68	119.05
6	B	806	PO4	O4-P-O2	2.17	114.93	107.97
2	A	801	HEM	C4A-C3A-C2A	2.11	108.47	107.00
6	B	806	PO4	O3-P-O1	2.11	118.62	110.89
8	A	809	NIZ	C2-C3-N1	-2.05	120.04	123.62
7	B	808	MPD	O2-C2-CM	2.05	114.64	108.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

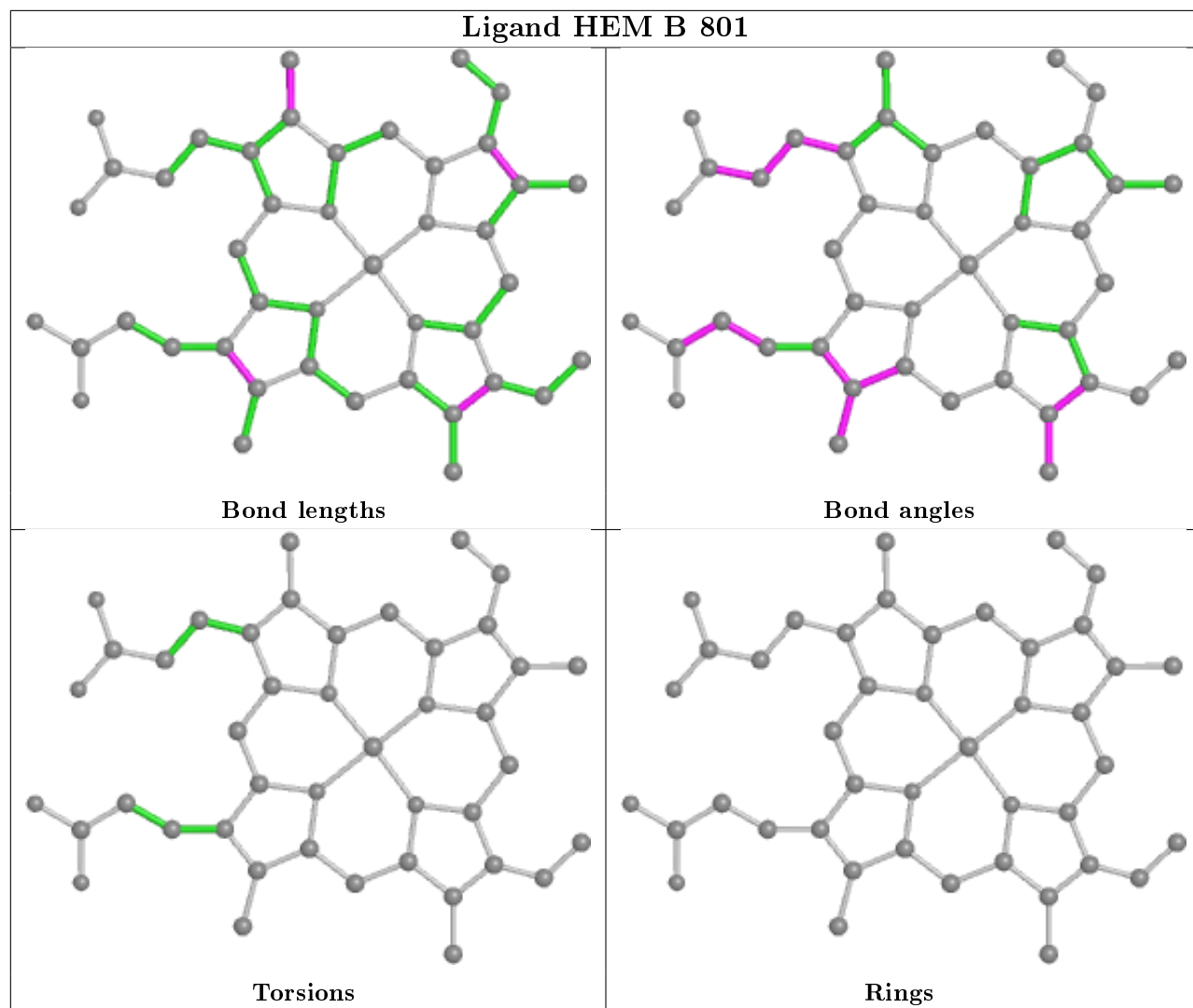
Mol	Chain	Res	Type	Atoms
7	B	807	MPD	C1-C2-C3-C4
7	B	807	MPD	O2-C2-C3-C4
7	B	808	MPD	O2-C2-C3-C4
7	B	808	MPD	CM-C2-C3-C4
7	B	807	MPD	CM-C2-C3-C4
7	B	808	MPD	C2-C3-C4-O4

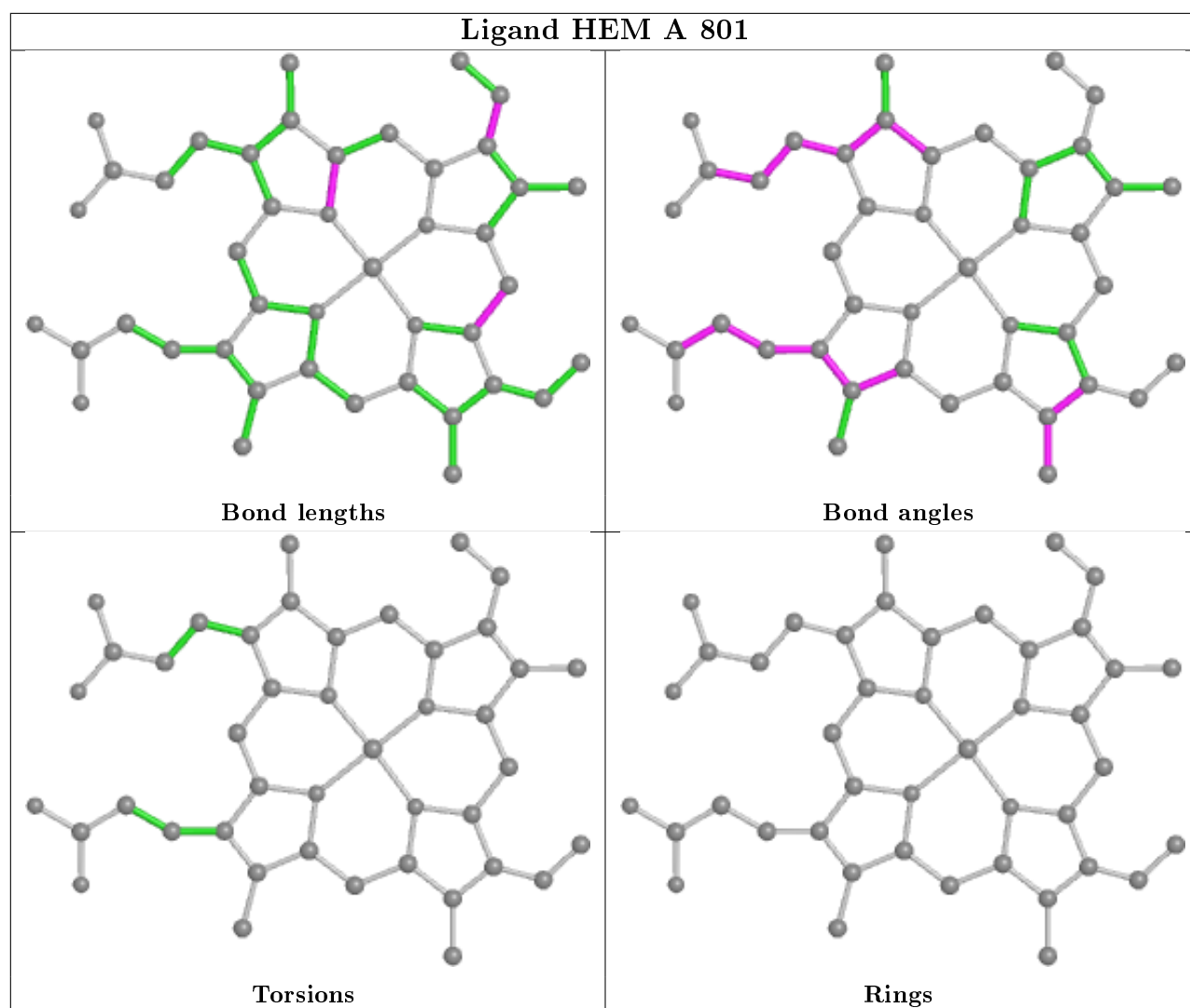
There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	807	MPD	1	0
8	A	809	NIZ	2	0
5	B	805	OXY	1	0
7	A	808	MPD	1	0
7	A	807	MPD	2	0
8	B	809	NIZ	1	0
2	A	801	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	713/728 (97%)	-0.51	7 (0%) 82 83	12, 18, 35, 74	0
1	B	713/728 (97%)	-0.53	6 (0%) 86 87	12, 17, 34, 67	0
All	All	1426/1456 (97%)	-0.52	13 (0%) 84 85	12, 18, 34, 74	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	4.2
1	A	541	GLY	4.0
1	A	540	ARG	3.5
1	B	748	ALA	3.4
1	A	679	ALA	3.3
1	B	540	ARG	3.1
1	A	680	ALA	3.1
1	B	610	ARG	2.5
1	B	608	LYS	2.3
1	A	454	ASP	2.3
1	B	679	ALA	2.2
1	B	680	ALA	2.2
1	A	647	GLN	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

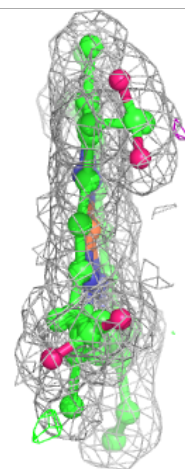
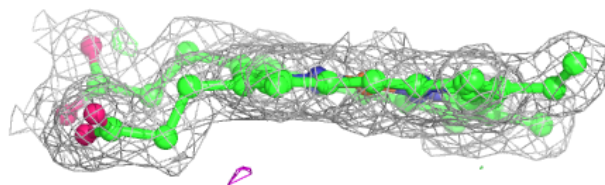
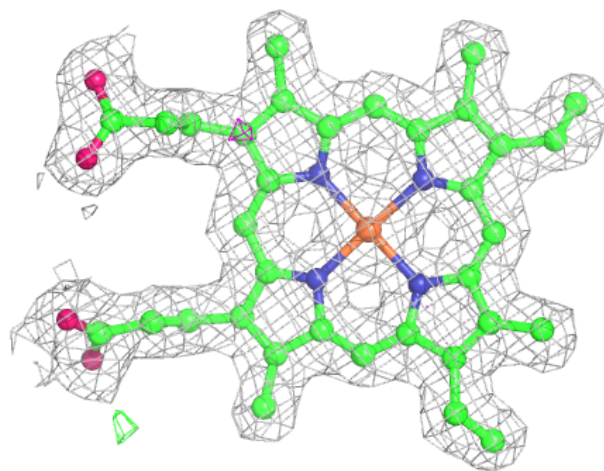
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

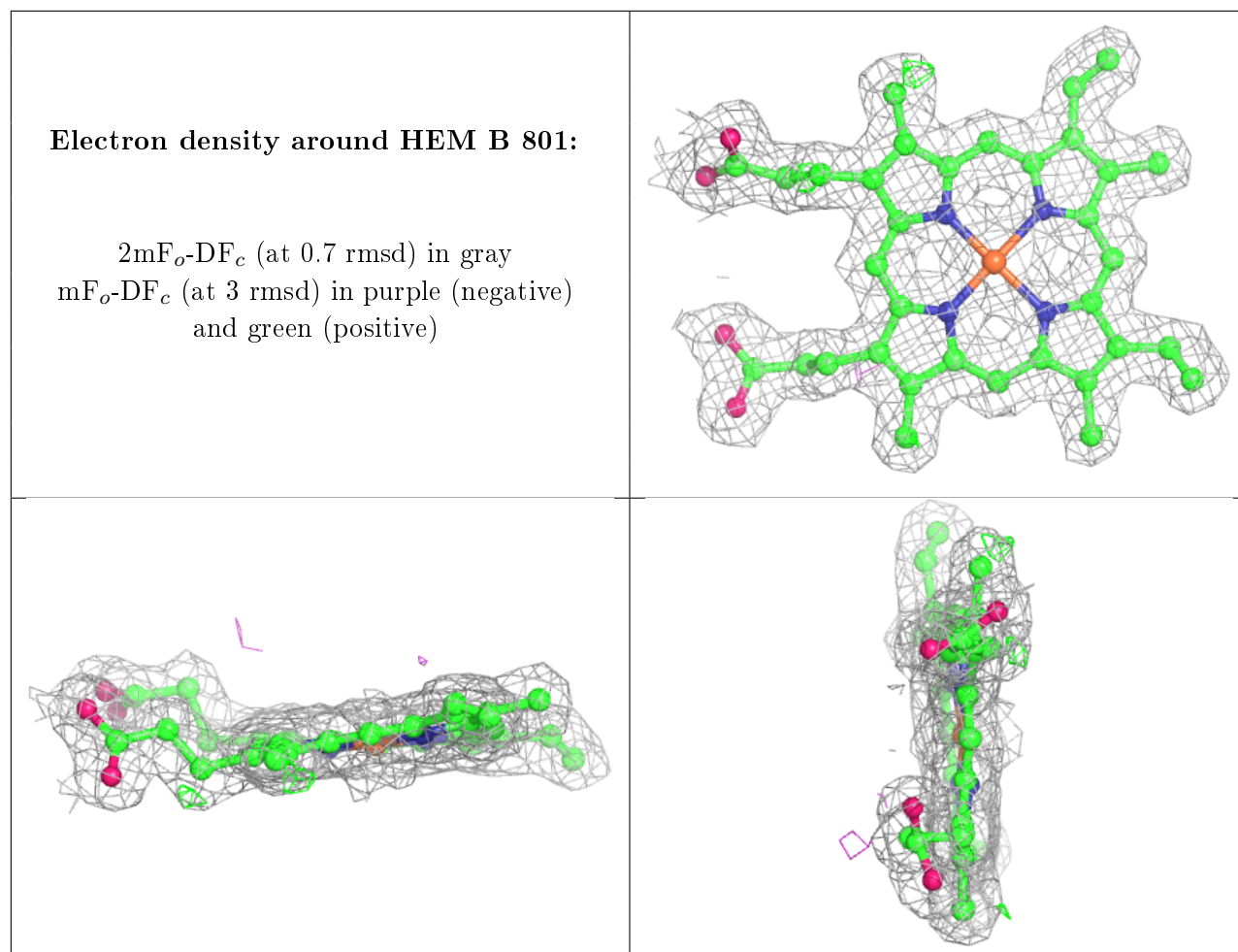
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NIZ	A	809	10/10	0.81	0.45	17,20,22,24	10
8	NIZ	B	809	10/10	0.91	0.13	21,24,29,29	10
7	MPD	A	808	8/8	0.93	0.14	35,40,54,56	0
7	MPD	B	807	8/8	0.93	0.14	39,42,47,48	0
7	MPD	B	808	8/8	0.93	0.12	40,43,45,47	0
6	PO4	A	806	5/5	0.94	0.14	40,50,59,59	0
7	MPD	A	807	8/8	0.95	0.14	50,58,59,64	0
6	PO4	B	806	5/5	0.95	0.21	39,50,56,61	0
5	OXY	B	805	2/2	0.95	0.10	31,31,31,39	0
5	OXY	A	805	2/2	0.97	0.10	32,32,32,38	0
5	OXY	B	804	2/2	0.99	0.10	24,24,24,27	0
4	CL	B	803	1/1	0.99	0.07	23,23,23,23	0
3	NA	A	802	1/1	0.99	0.06	15,15,15,15	0
4	CL	A	803	1/1	0.99	0.07	25,25,25,25	0
5	OXY	A	804	2/2	0.99	0.16	25,25,25,33	0
2	HEM	A	801	43/43	0.99	0.07	12,14,17,18	0
2	HEM	B	801	43/43	0.99	0.09	12,13,14,15	0
3	NA	B	802	1/1	1.00	0.04	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around HEM A 801:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.