



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2017 – 12:18 PM EDT

PDB ID : 5SXT  
Title : Crystal structure of the S324T variant of Burkholderia pseudomallei KatG with isonicotinic acid hydrazide bound  
Authors : Loewen, P.C.  
Deposited on : unknown  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

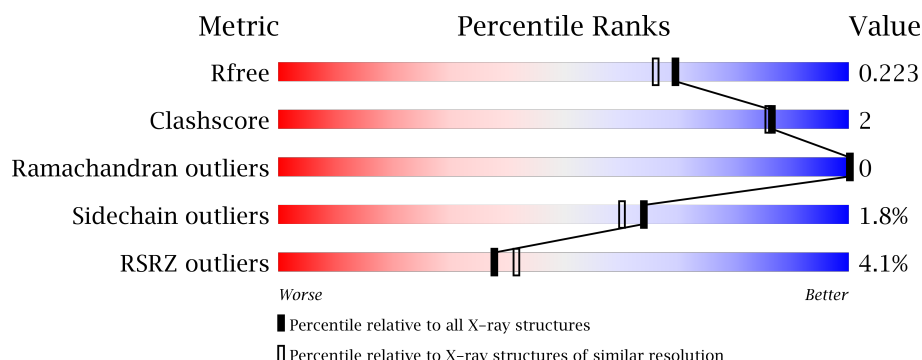
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>4%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>9%</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	OXY	B	805	-	-	-	X
7	MPD	A	806	-	-	-	X
7	MPD	B	807	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12424 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	5	0
			5528	3494	984	1036	14			
1	B	713	Total	C	N	O	S	0	4	0
			5522	3489	984	1035	14			

There are 2 discrepancies between the modelled and reference sequences:

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

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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

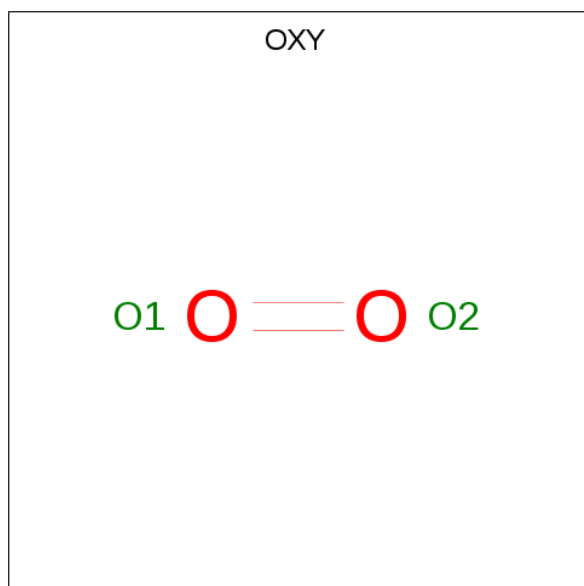
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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>).



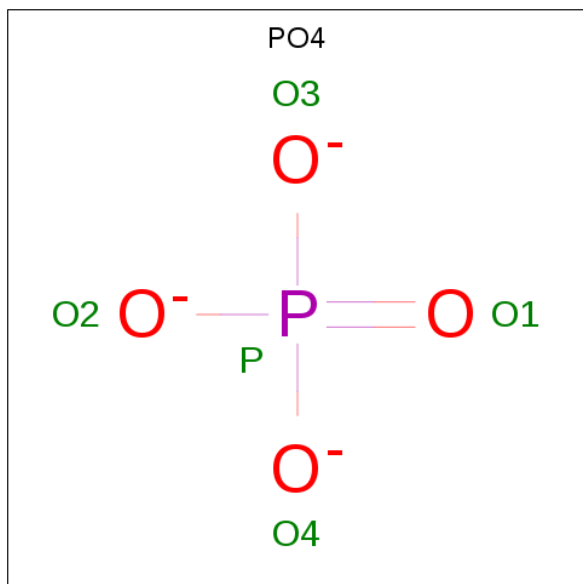
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

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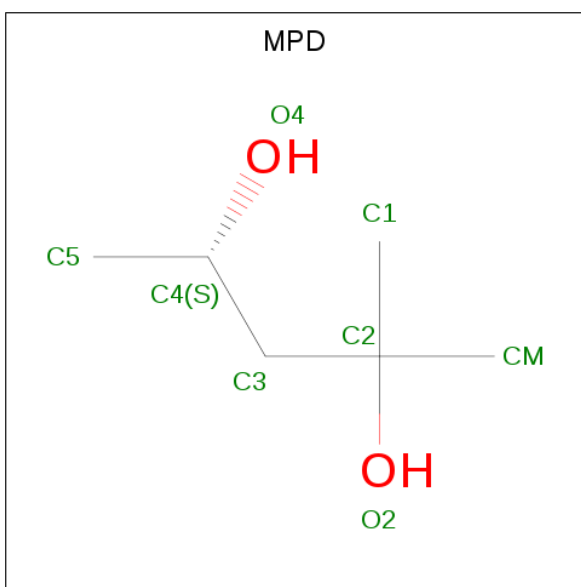
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			2	2		

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



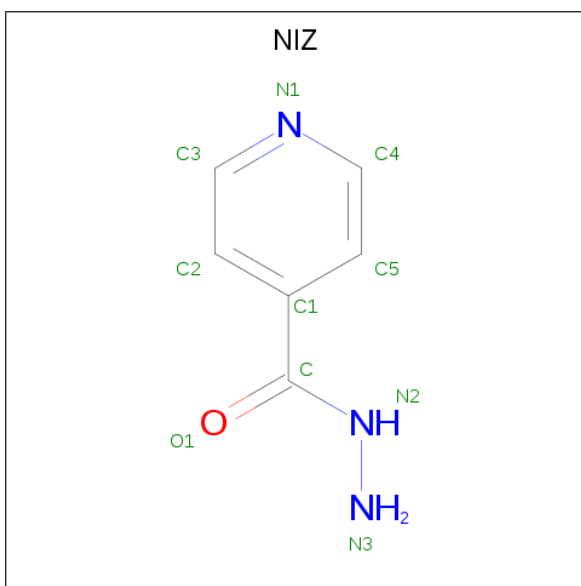
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- 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	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.

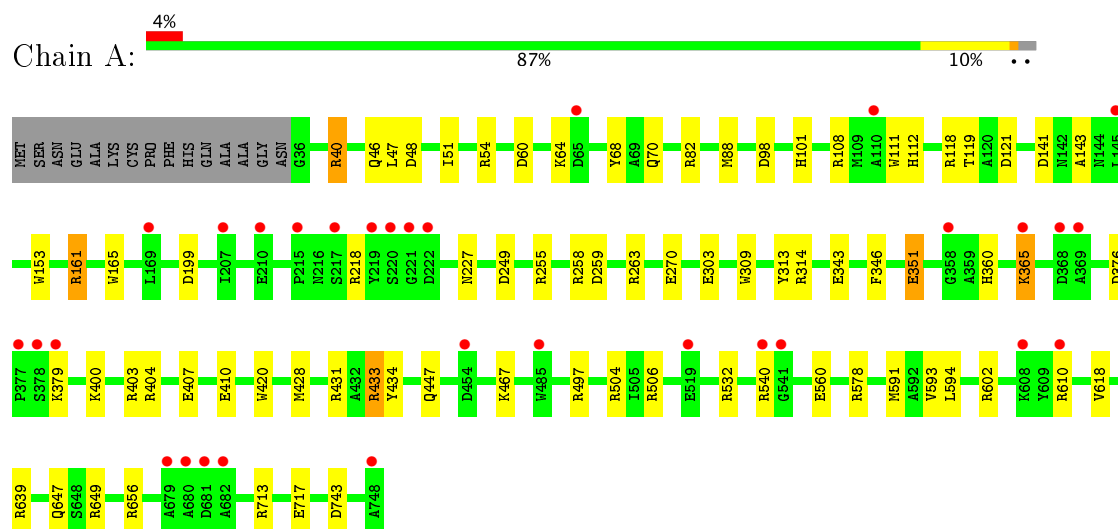
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	611	Total 611	O 611	0	0
9	B	621	Total 621	O 621	0	0



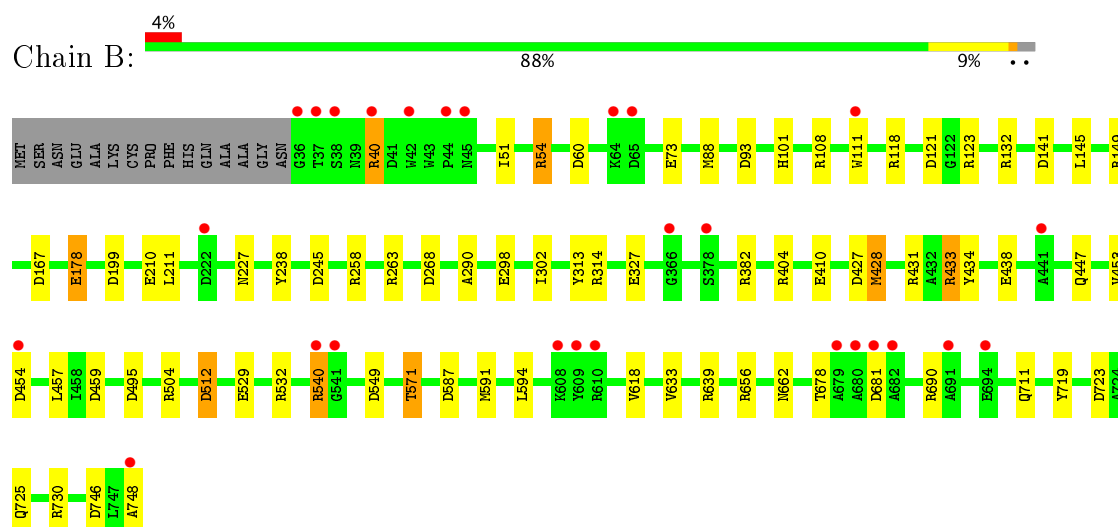
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Catalase-peroxidase



#### • Molecule 1: Catalase-peroxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.22Å 112.60Å 173.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 32.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.90) 100.0 (32.82-1.90)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.182 , 0.216 0.190 , 0.223	Depositor DCC
$R_{free}$ test set	7613 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.23	14/5687 (0.2%)	1.13	37/7734 (0.5%)
1	B	1.25	11/5680 (0.2%)	1.11	30/7724 (0.4%)
All	All	1.24	25/11367 (0.2%)	1.12	67/15458 (0.4%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	GLU	CG-CD	7.10	1.62	1.51
1	B	178	GLU	CG-CD	6.51	1.61	1.51
1	B	73	GLU	CG-CD	6.28	1.61	1.51
1	A	68	TYR	CG-CD2	-6.16	1.31	1.39
1	B	746	ASP	CB-CG	6.03	1.64	1.51
1	B	438	GLU	CD-OE2	5.98	1.32	1.25
1	B	327	GLU	CG-CD	5.92	1.60	1.51
1	B	210	GLU	CD-OE1	5.83	1.32	1.25
1	A	578	ARG	CZ-NH2	-5.79	1.25	1.33
1	A	410	GLU	CD-OE2	5.64	1.31	1.25
1	A	743	ASP	CB-CG	5.64	1.63	1.51
1	A	165	TRP	CZ3-CH2	-5.63	1.31	1.40
1	B	512	ASP	CG-OD2	5.48	1.38	1.25
1	A	351	GLU	CG-CD	5.47	1.60	1.51
1	A	153	TRP	CE3-CZ3	5.16	1.47	1.38
1	A	717	GLU	CD-OE2	-5.15	1.20	1.25
1	A	420	TRP	CZ3-CH2	-5.12	1.31	1.40
1	A	153	TRP	CZ3-CH2	-5.12	1.31	1.40
1	A	407	GLU	CG-CD	5.11	1.59	1.51
1	A	258	ARG	CZ-NH1	5.11	1.39	1.33
1	A	434	TYR	CE1-CZ	-5.11	1.31	1.38
1	B	434	TYR	CE1-CZ	-5.10	1.31	1.38
1	A	270	GLU	CD-OE2	5.03	1.31	1.25
1	B	504	ARG	CZ-NH1	-5.02	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	ASP	CB-CG	-5.01	1.41	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	B	108	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	B	433	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	433	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	263	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	404	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	532	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	108	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	161	ARG	NE-CZ-NH1	-7.77	116.41	120.30
1	A	258	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	161	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	602	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	433	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	639	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	506	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	713	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	60	ASP	CB-CG-OD1	7.13	124.72	118.30
1	B	258	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	578	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	B	532	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	82	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	82	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	149	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	713	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	218	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	259	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	438	GLU	OE1-CD-OE2	6.62	131.25	123.30
1	A	434	TYR	CB-CG-CD1	6.62	124.97	121.00
1	B	730	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	B	123	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	263	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	60	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	255	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	40	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	587	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	404	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	571	THR	CB-CA-C	-6.16	94.97	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	145	LEU	CB-CG-CD2	6.04	121.27	111.00
1	A	639	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	382	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	268	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	108	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	167	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	578	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	649	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	121	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	40	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	132	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	428	MET	CA-CB-CG	-5.52	103.91	113.30
1	A	98	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	48	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	258	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	433	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	121	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	459	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	263	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	54	ARG	CG-CD-NE	-5.34	100.59	111.80
1	B	549	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	376	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	649	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	497	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	73	GLU	OE1-CD-OE2	-5.19	117.08	123.30
1	A	249	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	723	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	108	ARG	CD-NE-CZ	5.12	130.78	123.60
1	A	303	GLU	OE1-CD-OE2	-5.12	117.16	123.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5528	0	5357	23	0
1	B	5522	0	5346	30	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	4	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	8	0	14	0	0
7	B	8	0	14	3	0
8	A	10	0	7	0	0
8	B	10	0	7	0	0
9	A	611	0	0	9	0
9	B	621	0	0	8	0
All	All	12424	0	10805	54	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (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)
7:B:807:MPD:HM3	7:B:807:MPD:O4	1.80	0.81
1:A:343:GLU:HG3	9:A:1368:HOH:O	1.79	0.80
1:B:512:ASP:OD1	9:B:901:HOH:O	2.02	0.77
1:A:119[B]:THR:HG21	9:A:945:HOH:O	1.85	0.74
1:A:360:HIS:ND1	9:A:901:HOH:O	2.21	0.74
1:B:540:ARG:NH1	1:B:540:ARG:HA	2.13	0.63
1:B:662:ASN:H	1:B:725:GLN:HE22	1.47	0.62
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.82	0.61
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.83	0.60
1:B:633[A]:VAL:HG21	1:B:719:TYR:CZ	2.38	0.58
1:A:54:ARG:NE	1:A:199:ASP:OD2	2.33	0.57
1:B:178:GLU:OE1	9:B:902:HOH:O	2.16	0.57
1:B:633[A]:VAL:CG2	1:B:719:TYR:CE1	2.88	0.57
1:B:54:ARG:NE	1:B:199:ASP:OD2	2.38	0.56
1:A:161:ARG:NH1	9:A:912:HOH:O	2.41	0.54
1:B:662:ASN:N	1:B:725:GLN:HE22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:807:MPD:CM	7:B:807:MPD:O4	2.48	0.52
1:B:51:ILE:HD11	1:B:618:VAL:HG12	1.92	0.52
1:A:88:MET:HB3	1:A:101:HIS:CE1	2.45	0.52
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.55	0.51
1:B:711[A]:GLN:NE2	9:B:914:HOH:O	2.44	0.51
1:A:161:ARG:CZ	9:A:912:HOH:O	2.60	0.50
1:B:725:GLN:CD	9:B:964:HOH:O	2.52	0.47
1:B:227:ASN:ND2	9:B:918:HOH:O	2.46	0.47
1:B:453:VAL:HG11	1:B:457:LEU:HD21	1.97	0.46
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.45	0.46
1:A:51:ILE:HD11	1:A:618:VAL:HG12	1.98	0.45
1:A:647:GLN:HG2	9:A:1149:HOH:O	2.16	0.45
1:B:748:ALA:C	9:B:1472:HOH:O	2.55	0.45
1:B:454:ASP:N	1:B:454:ASP:OD1	2.49	0.45
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.17	0.45
1:B:591:MET:SD	1:B:594:LEU:HD12	2.57	0.45
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.18	0.44
1:B:211:LEU:HB2	9:B:1403:HOH:O	2.16	0.44
1:A:46:GLN:NE2	1:B:298:GLU:O	2.46	0.44
1:A:111:TRP:CD1	1:A:112:HIS:HD2	2.36	0.43
1:A:400:LYS:HE2	9:A:1396:HOH:O	2.18	0.43
1:A:365:LYS:HA	9:A:1443:HOH:O	2.18	0.43
1:B:313:TYR:CE2	1:B:314:ARG:HD3	2.53	0.43
1:B:410:GLU:HB2	9:B:1366:HOH:O	2.19	0.43
1:B:88:MET:HB3	1:B:101:HIS:CE1	2.54	0.42
1:A:428:MET:O	1:A:433:ARG:HD3	2.20	0.42
1:A:591:MET:SD	1:A:594:LEU:HD12	2.59	0.42
1:A:504:ARG:HD2	9:A:960:HOH:O	2.19	0.42
1:A:467:LYS:NZ	1:A:560:GLU:OE2	2.53	0.42
1:A:313:TYR:CE2	1:A:314:ARG:HD3	2.55	0.42
1:B:678:THR:OG1	1:B:681:ASP:O	2.36	0.42
1:A:346:PHE:CZ	1:A:403[A]:ARG:HG2	2.55	0.41
1:B:428:MET:O	1:B:433:ARG:HD3	2.20	0.41
1:A:47:LEU:HA	1:A:47:LEU:HD12	1.86	0.41
1:B:427:ASP:HA	1:B:495:ASP:HB2	2.02	0.41
1:A:143:ALA:HA	1:A:309:TRP:CZ3	2.56	0.41
1:B:211:LEU:HD22	1:B:245:ASP:HA	2.03	0.40
1:B:290:ALA:HB1	7:B:807:MPD:H4	2.03	0.40

There are no symmetry-related clashes.

## 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	716/728 (98%)	705 (98%)	11 (2%)	0	100	100
1	B	715/728 (98%)	706 (99%)	9 (1%)	0	100	100
All	All	1431/1456 (98%)	1411 (99%)	20 (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	555/561 (99%)	543 (98%)	12 (2%)	57	51
1	B	554/561 (99%)	546 (99%)	8 (1%)	71	69
All	All	1109/1122 (99%)	1089 (98%)	20 (2%)	64	60

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

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	70	GLN
1	A	118	ARG
1	A	141	ASP
1	A	227	ASN
1	A	351	GLU
1	A	365	LYS

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Mol	Chain	Res	Type
1	A	379	LYS
1	A	540	ARG
1	A	610	ARG
1	A	656	ARG
1	B	40	ARG
1	B	118	ARG
1	B	141	ASP
1	B	302	ILE
1	B	540	ARG
1	B	571	THR
1	B	656	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	85	HIS
1	A	647	GLN
1	B	46	GLN
1	B	227	ASN
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	A	801	1,9	28,50,50	1.71	3 (10%)	17,82,82	2.17	5 (29%)
5	OXY	A	804	-	1,1,1	0.01	0	0,0,0	0.00	-
6	PO4	A	805	-	4,4,4	0.59	0	6,6,6	0.90	0
7	MPD	A	806	-	7,7,7	0.65	0	9,10,10	2.02	4 (44%)
8	NIZ	A	807	-	10,10,10	1.10	1 (10%)	12,12,12	1.60	3 (25%)
2	HEM	B	801	1,9	28,50,50	2.26	7 (25%)	17,82,82	1.94	4 (23%)
5	OXY	B	804	-	1,1,1	0.06	0	0,0,0	0.00	-
5	OXY	B	805	-	1,1,1	0.15	0	0,0,0	0.00	-
6	PO4	B	806	-	4,4,4	0.46	0	6,6,6	1.58	2 (33%)
7	MPD	B	807	-	7,7,7	0.82	0	9,10,10	1.42	1 (11%)
8	NIZ	B	808	-	10,10,10	1.80	2 (20%)	12,12,12	2.17	6 (50%)

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	A	801	1,9	-	0/6/54/54	0/0/8/8
5	OXY	A	804	-	-	0/0/0/0	0/0/0/0
6	PO4	A	805	-	-	0/0/0/0	0/0/0/0
7	MPD	A	806	-	-	0/5/5/5	0/0/0/0
8	NIZ	A	807	-	-	0/6/6/6	0/1/1/1
2	HEM	B	801	1,9	-	0/6/54/54	0/0/8/8
5	OXY	B	804	-	-	0/0/0/0	0/0/0/0
5	OXY	B	805	-	-	0/0/0/0	0/0/0/0
6	PO4	B	806	-	-	0/0/0/0	0/0/0/0
7	MPD	B	807	-	-	0/5/5/5	0/0/0/0
8	NIZ	B	808	-	-	0/6/6/6	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C2B	-5.92	1.32	1.40
2	A	801	HEM	C1C-NC	-3.90	1.32	1.36
2	B	801	HEM	C4B-NB	-3.88	1.27	1.36
2	B	801	HEM	C3B-C2B	-2.64	1.36	1.40
8	B	808	NIZ	N3-N2	-2.48	1.38	1.41
2	B	801	HEM	C1D-CHD	-2.25	1.34	1.40
2	B	801	HEM	CAA-C2A	-2.17	1.48	1.52
2	B	801	HEM	CMC-C2C	-2.01	1.47	1.51
8	A	807	NIZ	C2-C1	2.38	1.43	1.39
2	A	801	HEM	C4C-NC	3.21	1.40	1.36
8	B	808	NIZ	C4-N1	3.54	1.44	1.33
2	B	801	HEM	C1A-NA	4.26	1.45	1.36
2	B	801	HEM	C4C-NC	8.38	1.46	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CAA-CBA-CGA	-4.33	105.27	112.66
2	B	801	HEM	C1D-C2D-C3D	-4.30	104.00	107.00
8	B	808	NIZ	O1-C-C1	-3.83	114.14	120.94
7	B	807	MPD	O2-C2-C3	-3.51	95.95	109.88
7	A	806	MPD	CM-C2-C1	-3.23	103.22	110.42
2	A	801	HEM	C4A-C3A-C2A	-3.07	104.86	107.00
8	B	808	NIZ	C2-C3-N1	-2.86	118.63	123.63
7	A	806	MPD	O2-C2-C3	-2.71	99.12	109.88
6	B	806	PO4	O4-P-O1	-2.45	100.52	110.97
8	A	807	NIZ	C2-C3-N1	-2.44	119.37	123.63
8	A	807	NIZ	O1-C-C1	-2.42	116.65	120.94
2	B	801	HEM	CAA-CBA-CGA	-2.40	108.55	112.66
8	B	808	NIZ	C5-C4-N1	-2.16	119.87	123.63
2	A	801	HEM	C3C-C4C-NC	-2.05	107.07	110.94
7	A	806	MPD	CM-C2-C3	2.15	120.76	110.08
8	A	807	NIZ	C1-C-N2	2.20	118.85	116.33
8	B	808	NIZ	C3-N1-C4	2.30	122.36	116.83
2	A	801	HEM	CMA-C3A-C2A	2.36	129.39	124.94
6	B	806	PO4	O4-P-O3	2.38	116.65	107.90
8	B	808	NIZ	O1-C-N2	2.69	125.54	122.45
8	B	808	NIZ	C1-C-N2	3.23	120.03	116.33
2	B	801	HEM	CBD-CAD-C3D	3.26	118.68	112.47
7	A	806	MPD	O2-C2-C1	3.29	119.42	108.00
2	B	801	HEM	CMB-C2B-C3B	3.86	132.06	124.89
2	A	801	HEM	CBD-CAD-C3D	5.24	122.47	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	807	MPD	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	713/728 (97%)	0.09	31 (4%) 36 39	16, 24, 44, 78	0
1	B	713/728 (97%)	-0.07	27 (3%) 41 45	16, 22, 41, 70	0
All	All	1426/1456 (97%)	0.01	58 (4%) 38 42	16, 23, 43, 78	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	7.3
1	A	679	ALA	7.0
1	A	541	GLY	6.7
1	B	748	ALA	5.9
1	B	679	ALA	4.7
1	B	608	LYS	4.6
1	A	222	ASP	4.4
1	A	540	ARG	4.0
1	B	680	ALA	4.0
1	B	540	ARG	3.8
1	B	454	ASP	3.6
1	A	610	ARG	3.6
1	A	221	GLY	3.4
1	B	44	PRO	3.3
1	A	215	PRO	3.2
1	B	610	ARG	3.1
1	A	219	TYR	3.1
1	B	541	GLY	3.1
1	B	36	GLY	3.1
1	A	110	ALA	3.1
1	A	680	ALA	3.1
1	A	454	ASP	3.0
1	B	65	ASP	3.0
1	B	37	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	210	GLU	2.8
1	A	145	LEU	2.7
1	B	609	TYR	2.7
1	A	377	PRO	2.7
1	A	169	LEU	2.7
1	A	378	SER	2.7
1	A	365	LYS	2.6
1	B	694	GLU	2.6
1	B	682	ALA	2.6
1	A	608	LYS	2.6
1	B	38	SER	2.5
1	A	217	SER	2.4
1	A	681	ASP	2.4
1	B	222	ASP	2.4
1	A	220	SER	2.4
1	A	379	LYS	2.4
1	A	682	ALA	2.3
1	B	366	GLY	2.3
1	B	378	SER	2.3
1	A	358	GLY	2.3
1	B	42	TRP	2.3
1	B	441	ALA	2.3
1	B	691	ALA	2.3
1	B	45	ASN	2.2
1	B	40	ARG	2.2
1	A	369	ALA	2.2
1	A	485	TRP	2.2
1	A	368	ASP	2.2
1	A	65	ASP	2.2
1	B	64	LYS	2.1
1	B	111	TRP	2.1
1	A	207	ILE	2.1
1	B	681	ASP	2.0
1	A	519	GLU	2.0

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

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

### 6.3 Carbohydrates [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MPD	A	806	8/8	0.85	0.22	4.98	58,60,63,65	0
7	MPD	B	807	8/8	0.88	0.19	4.46	44,51,61,65	0
5	OXY	B	805	2/2	0.95	0.25	3.66	37,37,37,47	0
2	HEM	A	801	43/43	0.98	0.16	1.40	17,19,22,23	0
8	NIZ	A	807	10/10	0.85	0.16	0.99	40,44,47,48	0
8	NIZ	B	808	10/10	0.91	0.14	0.30	31,36,41,44	0
2	HEM	B	801	43/43	0.97	0.13	0.14	14,16,17,18	0
3	NA	A	802	1/1	0.98	0.06	-1.50	20,20,20,20	0
3	NA	B	802	1/1	0.98	0.04	-4.34	18,18,18,18	0
4	CL	A	803	1/1	0.98	0.07	-	34,34,34,34	0
5	OXY	A	804	2/2	0.79	0.24	-	42,42,42,46	0
6	PO4	B	806	5/5	0.92	0.21	-	46,53,60,62	0
6	PO4	A	805	5/5	0.82	0.24	-	75,82,86,87	0
4	CL	B	803	1/1	0.98	0.06	-	31,31,31,31	0
5	OXY	B	804	2/2	0.96	0.17	-	30,30,30,32	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.