



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2016 – 07:47 PM EDT

PDB ID : 5SXS  
Title : Crystal structure of catalase-peroxidase KatG with isonicotinic acid hydrazide and AMP bound  
Authors : Loewen, P.C.  
Deposited on : 2016-08-10  
Resolution : 1.89 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027939

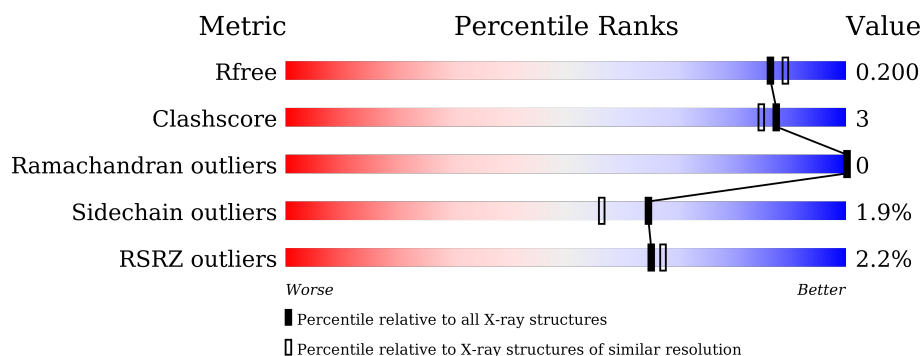
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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))
$R_{free}$	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (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. 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>88%</div> <div>9%</div> <div>..</div> </div>
1	B	728	<div> <div>2%</div> <div>88%</div> <div>9%</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
10	AMP	B	809	-	-	-	X
4	CL	A	803	-	-	-	X
4	CL	B	803	-	-	-	X
7	MRD	A	807	-	-	-	X
9	MPD	B	807	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 12576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5537	3497	988	1038	14			
1	B	713	Total	C	N	O	S	0	4	0
			5522	3489	982	1037	14			

- 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

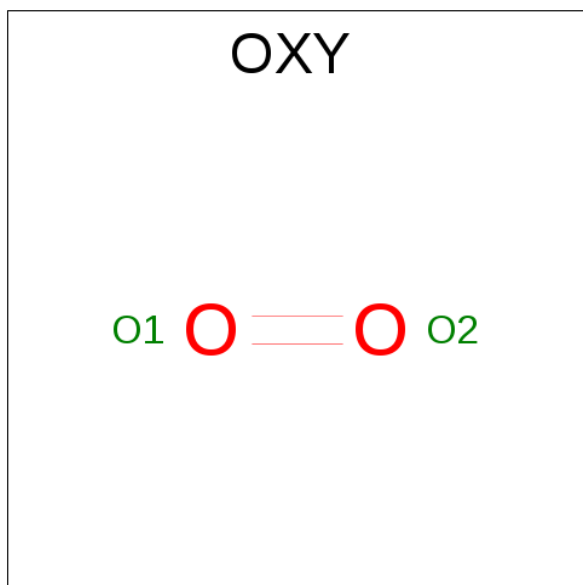
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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).

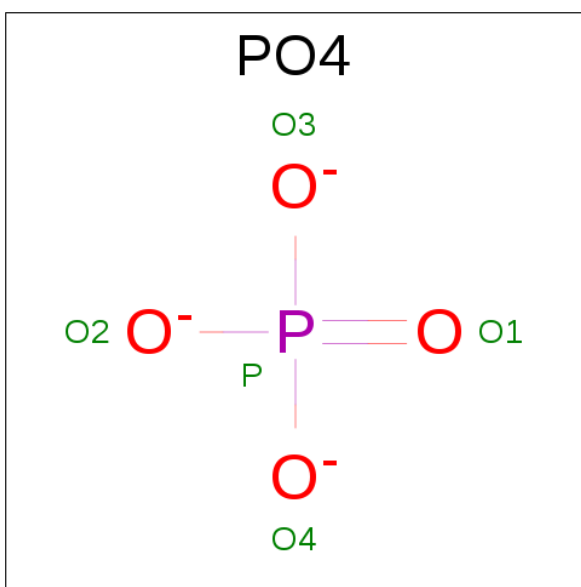
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

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



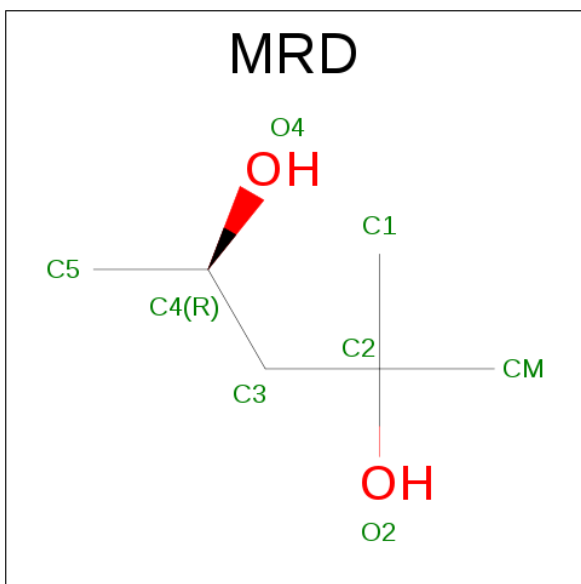
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0

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



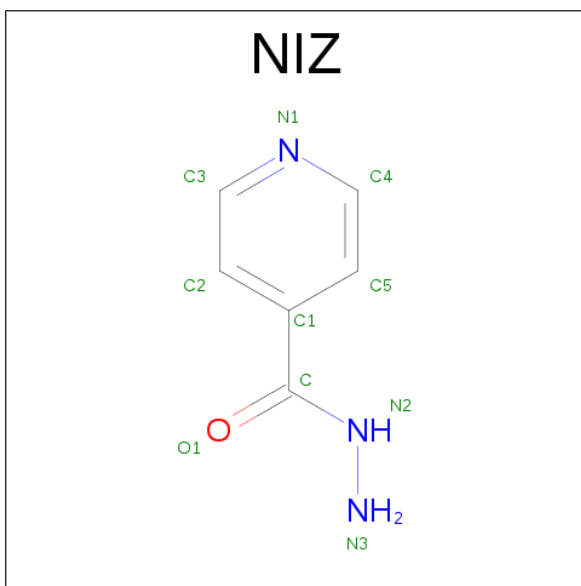
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



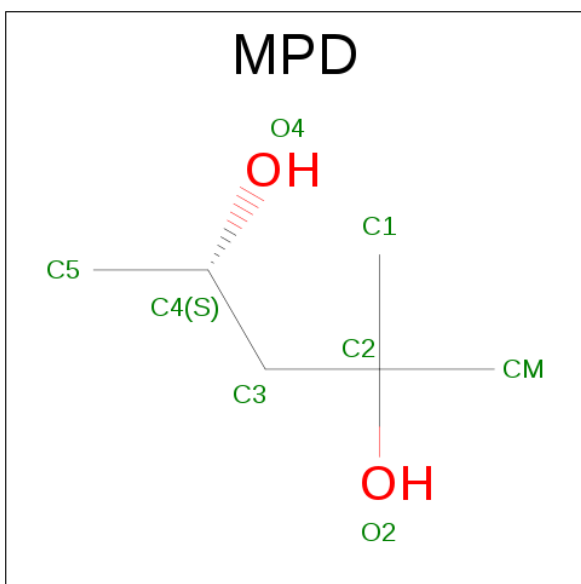
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		

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



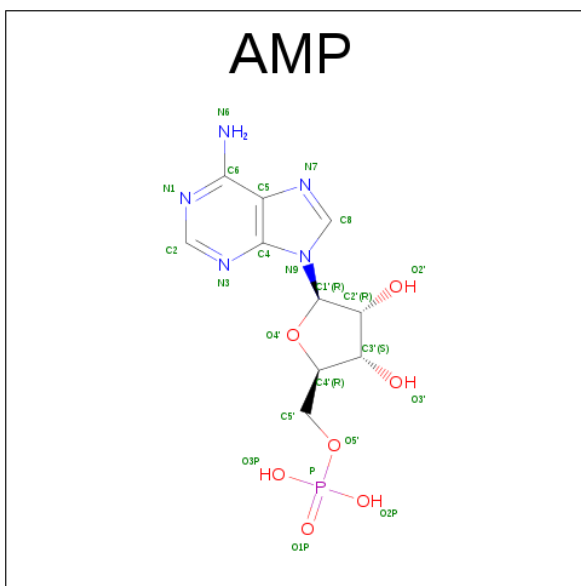
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



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

- Molecule 10 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 11 is water.

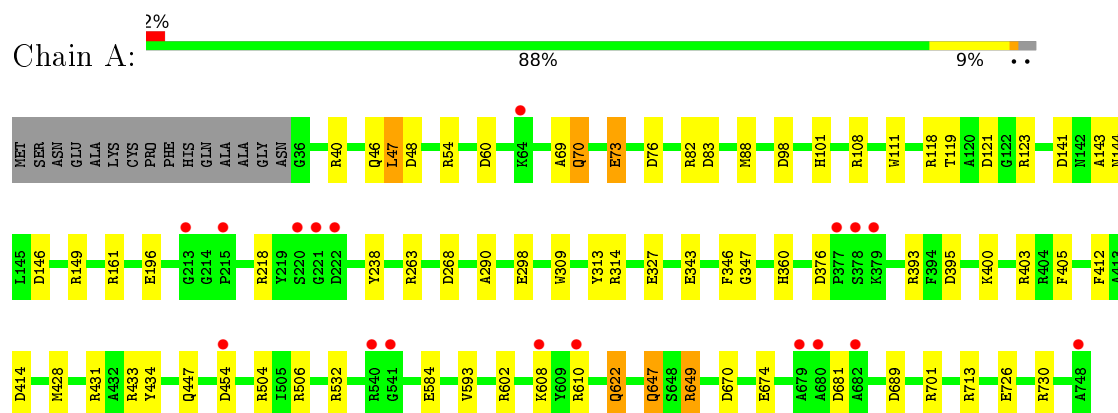
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	651	Total	O	0	0
			651	651		
11	B	709	Total	O	0	0
			709	709		



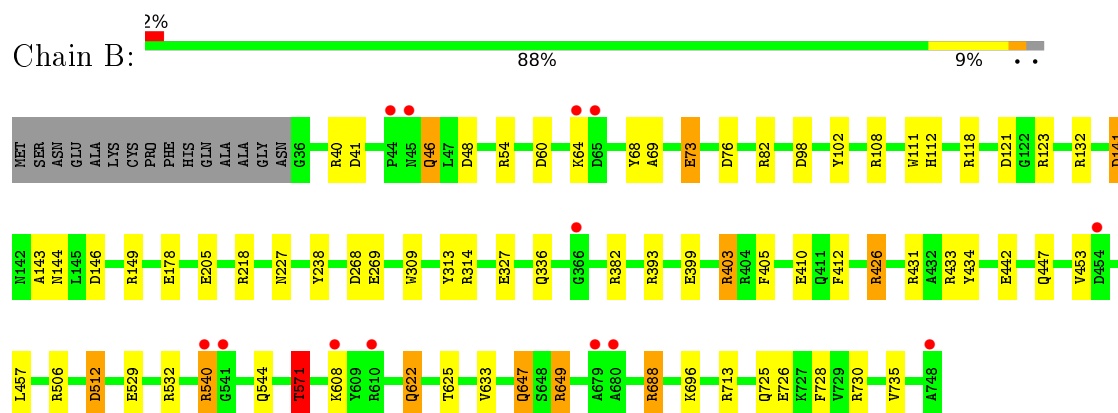
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	100.44Å 114.17Å 174.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.89 34.87 – 1.89	Depositor EDS
% Data completeness (in resolution range)	90.1 (20.00-1.89) 90.2 (34.87-1.89)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.162 , 0.193 0.172 , 0.200	Depositor DCC
$R_{free}$ test set	7127 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.8	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	0.96	EDS
Total number of atoms	12576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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, MRD, AMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.16	16/5707 (0.3%)	1.11	43/7758 (0.6%)
1	B	1.20	21/5678 (0.4%)	1.11	40/7720 (0.5%)
All	All	1.18	37/11385 (0.3%)	1.11	83/15478 (0.5%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	GLU	CD-OE1	11.83	1.38	1.25
1	B	529	GLU	CG-CD	9.88	1.66	1.51
1	B	327	GLU	CG-CD	8.33	1.64	1.51
1	B	399	GLU	CD-OE1	7.51	1.33	1.25
1	B	726	GLU	CG-CD	7.22	1.62	1.51
1	B	327	GLU	CD-OE1	7.17	1.33	1.25
1	A	196	GLU	CG-CD	6.41	1.61	1.51
1	A	726	GLU	CG-CD	6.35	1.61	1.51
1	B	327	GLU	CD-OE2	6.27	1.32	1.25
1	A	343	GLU	CD-OE2	6.25	1.32	1.25
1	A	347	GLY	C-O	-6.25	1.13	1.23
1	A	327	GLU	CD-OE1	6.16	1.32	1.25
1	B	726	GLU	CD-OE1	6.11	1.32	1.25
1	A	584	GLU	CG-CD	6.01	1.60	1.51
1	A	73	GLU	CD-OE2	5.98	1.32	1.25
1	A	46	GLN	CG-CD	5.91	1.64	1.51
1	B	434	TYR	CE1-CZ	-5.89	1.30	1.38
1	B	434	TYR	CG-CD1	-5.87	1.31	1.39
1	A	454	ASP	CB-CG	5.85	1.64	1.51
1	B	205	GLU	CD-OE1	5.84	1.32	1.25
1	B	726	GLU	CB-CG	5.73	1.63	1.52
1	A	647	GLN	CG-CD	5.61	1.64	1.51
1	A	73	GLU	CD-OE1	5.49	1.31	1.25
1	B	647	GLN	CG-CD	5.45	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	GLU	CD-OE1	5.44	1.31	1.25
1	B	442	GLU	CD-OE1	-5.42	1.19	1.25
1	B	426	ARG	CZ-NH2	5.42	1.40	1.33
1	A	434	TYR	CG-CD1	-5.32	1.32	1.39
1	A	428	MET	CG-SD	-5.31	1.67	1.81
1	B	269	GLU	CD-OE1	-5.29	1.19	1.25
1	B	512	ASP	CG-OD2	5.24	1.37	1.25
1	A	674	GLU	CD-OE2	-5.16	1.20	1.25
1	B	336	GLN	CG-CD	5.14	1.62	1.51
1	B	728	PHE	CB-CG	-5.09	1.42	1.51
1	B	46	GLN	CG-CD	5.08	1.62	1.51
1	B	102	TYR	CG-CD1	-5.08	1.32	1.39
1	B	68	TYR	CE1-CZ	5.06	1.45	1.38

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLU	OE1-CD-OE2	14.69	140.93	123.30
1	B	393	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	B	433	ARG	NE-CZ-NH1	10.91	125.75	120.30
1	A	532	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	A	433	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	B	529	GLU	OE1-CD-OE2	-8.56	113.03	123.30
1	B	76	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	B	82	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	602	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	A	433	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	B	713	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	713	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	506	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	B	54	ARG	CG-CD-NE	-7.51	96.03	111.80
1	A	263	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	54	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	B	82	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	60	ASP	CB-CG-OD1	7.18	124.77	118.30
1	A	82	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	433	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	76	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	121	ASP	CB-CG-OD1	6.84	124.45	118.30
1	B	532	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	726	GLU	OE1-CD-OE2	-6.73	115.23	123.30
1	B	54	ARG	NE-CZ-NH2	-6.65	116.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	73	GLU	OE1-CD-OE2	6.56	131.18	123.30
1	A	602	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	A	713	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	82	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	48	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	649	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	268	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	B	268	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	60	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	701	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	83	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	343	GLU	CG-CD-OE2	-6.04	106.21	118.30
1	A	395	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	132	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	506	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	48	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	393	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	108	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	504	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	108	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	98	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	54	ARG	CG-CD-NE	-5.75	99.72	111.80
1	B	512	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	B	121	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	218	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	688	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	681	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	149	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	726	GLU	CG-CD-OE1	5.64	129.59	118.30
1	A	60	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	54	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	149	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	98	ASP	CB-CG-OD1	-5.58	113.27	118.30
1	A	730	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	506	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	73	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	A	414	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	730	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	149	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	730	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	426	ARG	NE-CZ-NH1	-5.33	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	649	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	382	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	571	THR	CB-CA-C	-5.26	97.39	111.60
1	B	735	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	A	47	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	A	70	GLN	CA-CB-CG	5.20	124.83	113.40
1	A	584	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	B	218	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	689	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	670	ASP	CB-CG-OD1	5.12	122.90	118.30
1	A	268	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	73	GLU	CB-CA-C	-5.07	100.25	110.40
1	A	54	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	41	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	434	TYR	CB-CG-CD1	5.02	124.01	121.00

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	5537	0	5360	22	0
1	B	5522	0	5343	29	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	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	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	10	0	7	2	0
9	B	8	0	14	3	0
10	B	23	0	12	0	0
11	A	651	0	0	7	1
11	B	709	0	0	12	1
All	All	12576	0	10810	57	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 (57) 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:161[B]:ARG:NH1	11:A:901:HOH:O	2.01	0.93
1:B:622[A]:GLN:NE2	8:B:806:NIZ:O1	2.04	0.91
1:A:161[B]:ARG:CZ	11:A:901:HOH:O	2.20	0.88
1:A:119[B]:THR:HG21	11:A:1066:HOH:O	1.74	0.87
7:A:807:MRD:H1C2	7:A:807:MRD:O4	1.76	0.84
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.64	0.79
1:B:571:THR:HG23	11:B:1118:HOH:O	1.86	0.74
9:B:807:MPD:H11	9:B:807:MPD:O4	1.89	0.73
7:A:807:MRD:O4	7:A:807:MRD:C1	2.31	0.73
1:B:178:GLU:OE1	11:B:901:HOH:O	2.06	0.72
1:B:571:THR:CG2	11:B:1118:HOH:O	2.37	0.72
1:B:512:ASP:OD1	11:B:902:HOH:O	2.08	0.71
1:B:540:ARG:HA	1:B:540:ARG:NE	2.05	0.71
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.23	0.69
1:B:69:ALA:O	1:B:73:GLU:HG2	1.98	0.64
1:A:69:ALA:O	1:A:73:GLU:HG2	1.98	0.63
9:B:807:MPD:O4	9:B:807:MPD:C1	2.49	0.60
1:B:123:ARG:NH2	1:B:622[B]:GLN:OE1	2.36	0.58
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.34	0.56
1:A:290:ALA:HB1	7:A:807:MRD:H5C3	1.86	0.56
1:B:123:ARG:HH21	1:B:622[A]:GLN:HE21	1.56	0.54
1:B:696:LYS:HE2	11:B:967:HOH:O	2.08	0.54
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.10	0.51
1:A:360:HIS:ND1	11:A:906:HOH:O	2.35	0.50
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.12	0.50
1:A:47:LEU:O	11:A:902:HOH:O	2.19	0.50
1:A:313:TYR:CE2	1:A:314:ARG:HD3	2.47	0.49
1:A:290:ALA:CB	7:A:807:MRD:H5C3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.58	0.49
1:A:346:PHE:CE2	1:A:403[A]:ARG:NE	2.82	0.47
1:A:400:LYS:HE2	11:A:1466:HOH:O	2.15	0.46
1:B:313:TYR:CE2	1:B:314:ARG:HD3	2.50	0.46
1:B:405:PHE:HB3	1:B:412:PHE:HB2	1.97	0.46
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.15	0.46
1:B:725:GLN:NE2	11:B:931:HOH:O	2.49	0.46
1:A:123:ARG:HH21	1:A:622[A]:GLN:NE2	2.15	0.45
1:A:647:GLN:HG2	11:A:1112:HOH:O	2.15	0.45
1:B:571:THR:HG22	11:B:1118:HOH:O	2.09	0.45
1:B:410:GLU:HB2	11:B:1383:HOH:O	2.17	0.45
1:B:544:GLN:OE1	11:B:903:HOH:O	2.21	0.44
1:A:88:MET:HB3	1:A:101:HIS:CE1	2.53	0.44
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.53	0.43
1:B:123:ARG:HH21	1:B:622[A]:GLN:NE2	2.17	0.43
1:B:403:ARG:NH1	11:B:938:HOH:O	2.51	0.43
7:A:807:MRD:H1C2	7:A:807:MRD:HA	1.81	0.43
1:A:346:PHE:CD2	1:A:403[A]:ARG:CZ	3.03	0.42
1:B:426:ARG:HA	1:B:426:ARG:HD2	1.90	0.42
1:B:453:VAL:HG11	1:B:457:LEU:HD21	2.00	0.42
1:A:405:PHE:HB3	1:A:412:PHE:HB2	1.99	0.42
1:B:625:THR:HG22	8:B:806:NIZ:H4	2.01	0.42
1:B:112:HIS:CE1	1:B:141:ASP:O	2.73	0.41
1:B:143:ALA:HA	1:B:309:TRP:CH2	2.55	0.41
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.20	0.41
9:B:807:MPD:H11	9:B:807:MPD:HO4	1.82	0.41
1:B:647:GLN:HG2	11:B:1038:HOH:O	2.19	0.40
1:B:688:ARG:NE	11:B:905:HOH:O	2.38	0.40
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.64	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)
11:A:1166:HOH:O	11:B:979:HOH:O[2_444]	2.14	0.06



## 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%)	708 (99%)	10 (1%)	0	100	100
1	B	715/728 (98%)	707 (99%)	8 (1%)	0	100	100
All	All	1433/1456 (98%)	1415 (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	557/561 (99%)	548 (98%)	9 (2%)	70	63
1	B	554/561 (99%)	539 (97%)	15 (3%)	52	40
All	All	1111/1122 (99%)	1087 (98%)	24 (2%)	65	50

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	70	GLN
1	A	118	ARG
1	A	141	ASP
1	A	608	LYS
1	A	610	ARG
1	A	622[A]	GLN
1	A	622[B]	GLN

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Mol	Chain	Res	Type
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	227	ASN
1	B	403	ARG
1	B	540	ARG
1	B	571	THR
1	B	608	LYS
1	B	622[A]	GLN
1	B	622[B]	GLN
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	649	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	227	ASN
1	A	247	ASN
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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	HEM	A	801	1,11	24,50,50	1.22	3 (12%)	16,82,82	2.14	5 (31%)
5	OXY	A	804	-	1,1,1	0.40	0	0,0,0	0.00	-
5	OXY	A	805	-	1,1,1	0.14	0	0,0,0	0.00	-
6	PO4	A	806	-	4,4,4	0.31	0	6,6,6	0.38	0
7	MRD	A	807	-	6,7,7	0.57	0	6,10,10	1.39	1 (16%)
2	HEM	B	801	1,11	24,50,50	2.08	5 (20%)	16,82,82	2.02	5 (31%)
5	OXY	B	804	-	1,1,1	0.01	0	0,0,0	0.00	-
5	OXY	B	805	-	1,1,1	0.04	0	0,0,0	0.00	-
8	NIZ	B	806	-	10,10,10	1.79	2 (20%)	12,12,12	1.82	4 (33%)
9	MPD	B	807	-	6,7,7	0.71	0	6,10,10	1.23	0
6	PO4	B	808	-	4,4,4	1.10	0	6,6,6	0.32	0
10	AMP	B	809	-	22,25,25	1.82	5 (22%)	22,38,38	3.31	9 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	801	1,11	-	0/6/54/54	0/0/8/8
5	OXY	A	804	-	-	0/0/0/0	0/0/0/0
5	OXY	A	805	-	-	0/0/0/0	0/0/0/0
6	PO4	A	806	-	-	0/0/0/0	0/0/0/0
7	MRD	A	807	-	-	0/5/5/5	0/0/0/0
2	HEM	B	801	1,11	-	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
8	NIZ	B	806	-	-	0/6/6/6	0/1/1/1
9	MPD	B	807	-	-	0/5/5/5	0/0/0/0
6	PO4	B	808	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	AMP	B	809	-	-	0/6/26/26	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-5.45	1.29	1.36
2	B	801	HEM	C3B-C2B	-5.24	1.33	1.40
2	B	801	HEM	C3C-C2C	-3.51	1.35	1.40
2	A	801	HEM	C3B-C2B	-2.83	1.36	1.40
2	A	801	HEM	C1D-CHD	-2.53	1.33	1.40
2	A	801	HEM	CAA-C2A	-2.34	1.48	1.52
2	B	801	HEM	C2A-C3A	-2.11	1.31	1.37
10	B	809	AMP	C8-N7	2.25	1.39	1.34
10	B	809	AMP	C4-N3	3.06	1.40	1.35
8	B	806	NIZ	C5-C1	3.06	1.44	1.39
10	B	809	AMP	C5-C4	3.62	1.48	1.40
8	B	806	NIZ	C-N2	3.68	1.37	1.33
10	B	809	AMP	C2'-C1'	3.70	1.59	1.53
2	B	801	HEM	C4C-NC	3.87	1.41	1.36
10	B	809	AMP	C2-N3	4.05	1.39	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	809	AMP	N3-C2-N1	-10.10	120.94	128.87
10	B	809	AMP	C1'-N9-C4	-5.65	120.50	126.81
2	A	801	HEM	CAA-CBA-CGA	-4.02	104.95	112.78
2	B	801	HEM	CAA-CBA-CGA	-3.64	105.71	112.78
10	B	809	AMP	O2P-P-O5'	-3.37	96.90	106.72
10	B	809	AMP	C4'-O4'-C1'	-3.20	106.25	109.64
2	B	801	HEM	C3B-CAB-CBB	-3.18	120.01	126.40
2	B	801	HEM	CMA-C3A-C4A	-3.02	123.18	128.31
10	B	809	AMP	O5'-P-O1P	-2.74	100.21	107.08
8	B	806	NIZ	O1-C-C1	-2.54	116.60	120.95
2	A	801	HEM	C3C-C4C-NC	-2.21	106.77	110.94
8	B	806	NIZ	C2-C3-N1	-2.12	119.97	123.64
10	B	809	AMP	O3'-C3'-C4'	2.17	117.50	111.01
8	B	806	NIZ	C3-N1-C4	2.29	122.34	116.84
7	A	807	MRD	C1-C2-C3	2.31	122.35	109.98
2	A	801	HEM	CAD-CBD-CGD	2.38	117.41	112.78
2	A	801	HEM	CMC-C2C-C3C	3.24	131.42	125.09
2	B	801	HEM	CBD-CAD-C3D	3.31	118.28	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CAD-CBD-CGD	3.35	119.30	112.78
8	B	806	NIZ	C1-C-N2	4.10	121.26	116.41
10	B	809	AMP	C2-N1-C6	4.22	126.31	118.77
10	B	809	AMP	O2P-P-O1P	4.24	124.45	110.63
10	B	809	AMP	N6-C6-N1	4.94	126.80	118.52
2	A	801	HEM	CBD-CAD-C3D	4.98	121.21	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	807	MRD	5	0
8	B	806	NIZ	2	0
9	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%)	-0.23	18 (2%) 61 63	15, 23, 45, 83	0
1	B	713/728 (97%)	-0.33	13 (1%) 71 73	15, 21, 40, 73	0
All	All	1426/1456 (97%)	-0.28	31 (2%) 65 67	15, 22, 43, 83	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	ARG	5.3
1	B	680	ALA	5.3
1	A	748	ALA	5.1
1	A	541	GLY	5.1
1	A	610	ARG	4.4
1	B	540	ARG	4.3
1	B	679	ALA	4.2
1	A	608	LYS	3.8
1	B	608	LYS	3.7
1	B	541	GLY	3.6
1	A	215	PRO	3.5
1	A	680	ALA	3.4
1	B	610	ARG	3.4
1	A	679	ALA	3.1
1	A	378	SER	3.0
1	B	65	ASP	2.9
1	A	220	SER	2.9
1	A	221	GLY	2.8
1	A	454	ASP	2.7
1	B	748	ALA	2.7
1	A	379	LYS	2.5
1	A	222	ASP	2.5
1	B	64	LYS	2.5
1	A	213	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	366	GLY	2.4
1	B	454	ASP	2.4
1	A	682	ALA	2.3
1	A	64	LYS	2.2
1	A	377	PRO	2.2
1	B	44	PRO	2.2
1	B	45	ASN	2.0

## 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 [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	MRD	A	807	8/8	0.92	0.16	7.40	48,55,61,62	0
4	CL	A	803	1/1	0.99	0.15	3.62	25,25,25,25	1
10	AMP	B	809	23/23	0.95	0.15	2.72	29,32,51,54	0
4	CL	B	803	1/1	0.99	0.12	2.59	20,20,20,20	1
9	MPD	B	807	8/8	0.89	0.15	2.41	42,46,53,54	0
2	HEM	A	801	43/43	0.98	0.13	0.89	18,20,23,24	0
2	HEM	B	801	43/43	0.99	0.13	0.39	14,15,17,18	0
8	NIZ	B	806	10/10	0.90	0.12	0.04	36,42,48,49	0
3	NA	A	802	1/1	0.99	0.05	-2.82	16,16,16,16	0
3	NA	B	802	1/1	0.99	0.05	-6.72	18,18,18,18	0
6	PO4	A	806	5/5	0.92	0.19	-	57,59,66,67	0
5	OXY	A	805	2/2	0.93	0.32	-	47,47,47,52	0
6	PO4	B	808	5/5	0.95	0.19	-	45,54,57,61	0
5	OXY	B	804	2/2	0.98	0.09	-	26,26,26,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	OXY	A	804	2/2	0.98	0.12	-	34,34,34,35	0
5	OXY	B	805	2/2	0.95	0.18	-	36,36,36,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.