WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2017 – 07:39 AM EDT

PDB ID	:	5SYJ
Title	:	Crystal structure of the D141A variant of B. pseudomallei KatGin complex with isoniazid
Authors	:	Loewen, P.C.
Deposited on	:	unknown
Resolution	:	1.88 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	Percentile Ranks	Value
Rfree		0.179
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		1.7%

Worse — *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
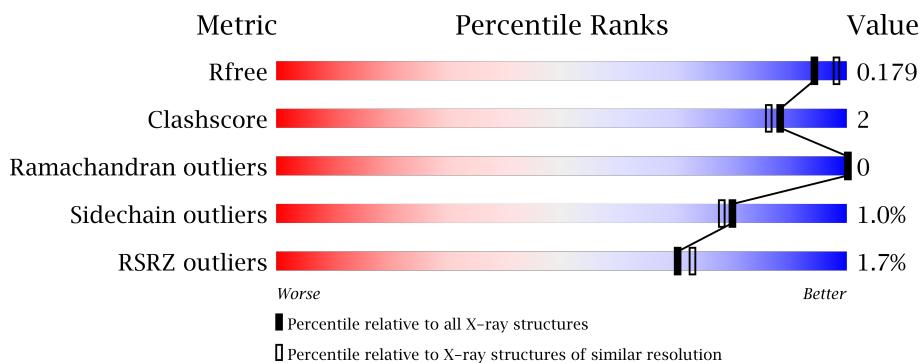
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	7505 (1.90-1.86)
Clashscore	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)
RSRZ outliers	101464	7571 (1.90-1.86)

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 >=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 <=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	2% ▮ 88% ··· 10% ··
1	B	728	.% ▮ 87% ··· 9% ··
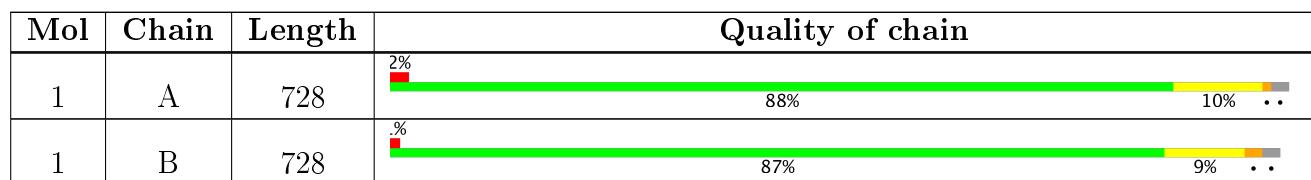
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	805	-	-	-	X
5	MPD	A	806	-	-	-	X
5	MPD	B	804	-	-	-	X
5	MPD	B	805	-	-	-	X
5	MPD	B	807	-	-	-	X
7	NIZ	A	809	-	X	-	X
7	NIZ	A	810	-	X	-	X
7	NIZ	B	810	-	X	X	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12427 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 5539	C 3500	N 990	O 1035	S 14	0	7	0
1	B	713	Total 5525	C 3492	N 984	O 1035	S 14	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q3JNW6
B	141	ALA	ASP	engineered mutation	UNP Q3JNW6

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
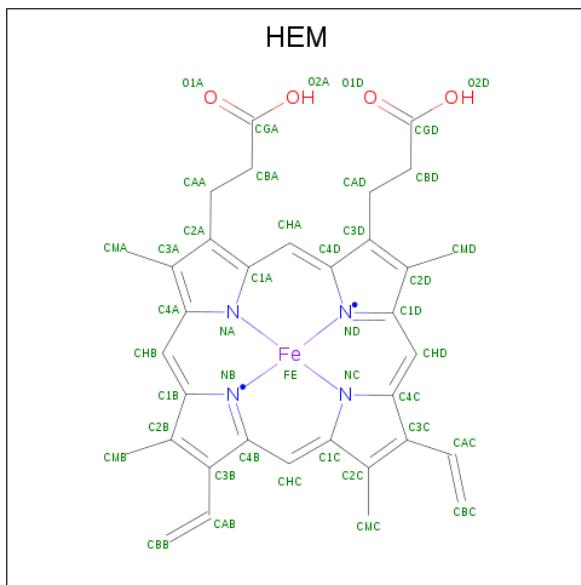
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
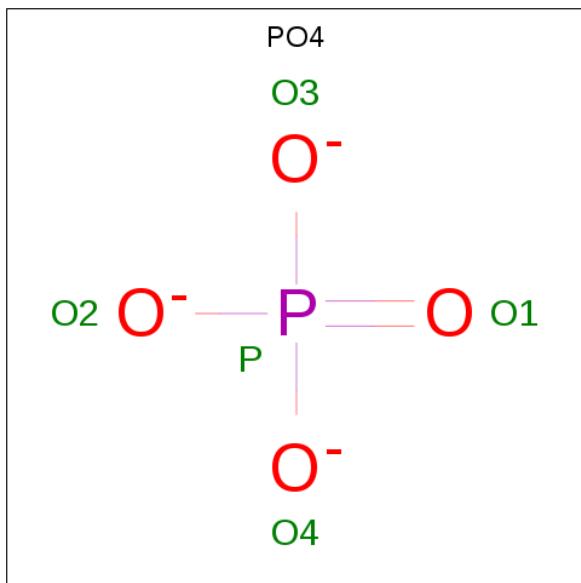
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	P 1	0	0
6	B	1	Total 5	O 4	P 1	0	0

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

NIZ

N1

N

C3   C4

C2   C5

C1

C

O1   O   NH   N2

NH₂

N3
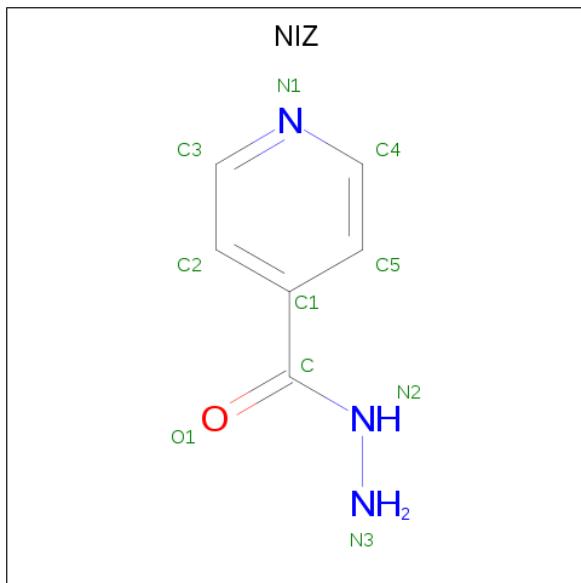
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 10	C 6	N 3	O 1	0	0
7	A	1	Total 10	C 6	N 3	O 1	0	0
7	B	1	Total 10	C 6	N 3	O 1	0	0
7	B	1	Total 10	C 6	N 3	O 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	576	Total 576	O 576	0	0
8	B	583	Total 583	O 583	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
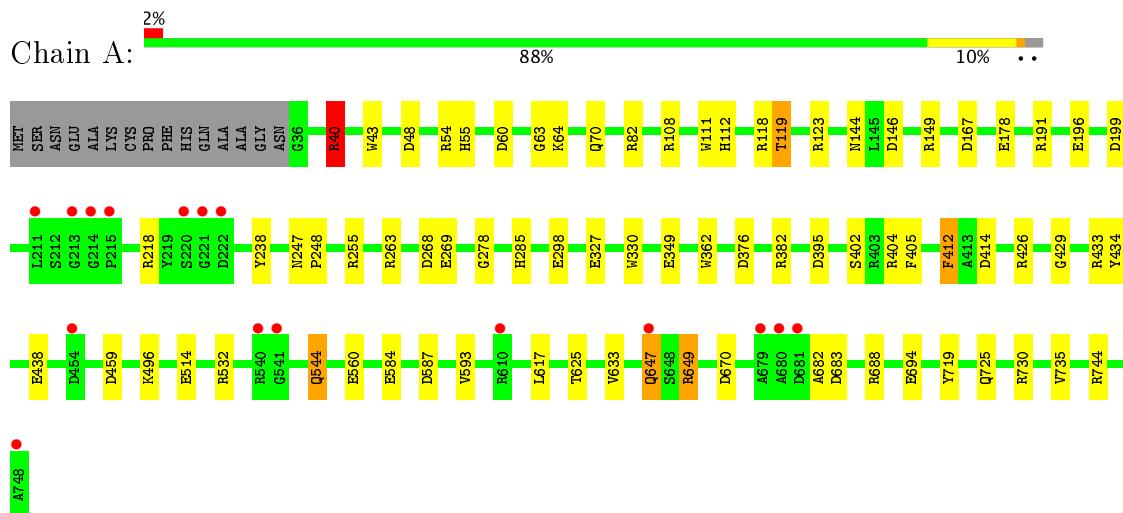
- Molecule 1: Catalase-peroxidase
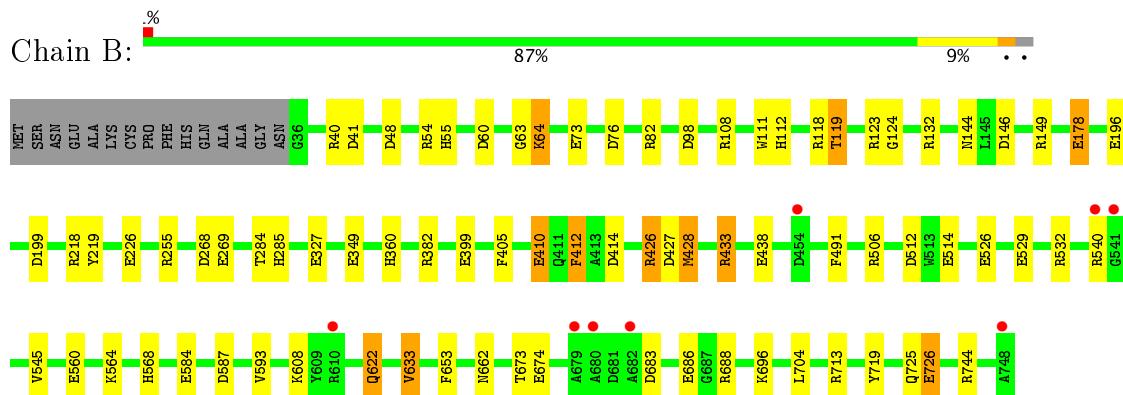
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.64Å 114.64Å 174.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.88 47.95 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-1.88) 98.4 (47.95-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.140 , 0.170 0.152 , 0.179	Depositor DCC
R_{free} test set	8131 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.0	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12427	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, 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	1.43	39/5706 (0.7%)	1.25	48/7756 (0.6%)
1	B	1.41	37/5684 (0.7%)	1.28	56/7728 (0.7%)
All	All	1.42	76/11390 (0.7%)	1.27	104/15484 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	GLU	CG-CD	10.33	1.67	1.51
1	B	63	GLY	N-CA	10.17	1.61	1.46
1	A	63	GLY	N-CA	9.08	1.59	1.46
1	B	269	GLU	CD-OE1	-8.87	1.15	1.25
1	B	327	GLU	CD-OE1	8.58	1.35	1.25
1	A	544	GLN	CD-NE2	8.23	1.53	1.32
1	B	726	GLU	CD-OE2	8.03	1.34	1.25
1	B	119[A]	THR	CB-CG2	-7.93	1.26	1.52
1	B	119[B]	THR	CB-CG2	-7.93	1.26	1.52
1	B	327	GLU	CD-OE2	7.49	1.33	1.25
1	A	584	GLU	CG-CD	7.12	1.62	1.51
1	A	255	ARG	CD-NE	6.73	1.57	1.46
1	A	298	GLU	CD-OE2	6.67	1.32	1.25
1	A	438	GLU	CD-OE1	-6.66	1.18	1.25
1	B	73	GLU	CD-OE1	6.65	1.32	1.25
1	B	410	GLU	CG-CD	6.63	1.61	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	438	GLU	CD-OE1	-6.56	1.18	1.25
1	A	119[A]	THR	CB-CG2	-6.47	1.30	1.52
1	A	119[B]	THR	CB-CG2	-6.47	1.30	1.52
1	B	532	ARG	CD-NE	-6.43	1.35	1.46
1	A	532	ARG	NE-CZ	-6.43	1.24	1.33
1	B	412	PHE	CG-CD1	6.36	1.48	1.38
1	B	327	GLU	CG-CD	6.21	1.61	1.51
1	B	726	GLU	CG-CD	6.18	1.61	1.51
1	A	196	GLU	CG-CD	6.15	1.61	1.51
1	A	285	HIS	C-O	6.03	1.34	1.23
1	B	686	GLU	CD-OE1	5.95	1.32	1.25
1	B	399	GLU	CD-OE1	5.89	1.32	1.25
1	A	278	GLY	N-CA	5.89	1.54	1.46
1	A	429	GLY	C-O	-5.87	1.14	1.23
1	A	178	GLU	CG-CD	5.82	1.60	1.51
1	B	512	ASP	CG-OD2	5.68	1.38	1.25
1	A	70	GLN	CD-OE1	5.67	1.36	1.24
1	B	426[A]	ARG	CZ-NH2	5.65	1.40	1.33
1	B	426[B]	ARG	CZ-NH2	5.65	1.40	1.33
1	A	560	GLU	CD-OE2	-5.64	1.19	1.25
1	B	560	GLU	CD-OE1	-5.63	1.19	1.25
1	B	219	TYR	CG-CD2	5.61	1.46	1.39
1	A	330	TRP	CG-CD1	-5.57	1.28	1.36
1	A	82	ARG	CZ-NH2	-5.55	1.25	1.33
1	B	674	GLU	CD-OE2	-5.53	1.19	1.25
1	B	269	GLU	CG-CD	5.51	1.60	1.51
1	B	285	HIS	C-O	5.50	1.33	1.23
1	A	327	GLU	CG-CD	5.47	1.60	1.51
1	A	43	TRP	CG-CD1	5.46	1.44	1.36
1	B	196	GLU	CB-CG	-5.41	1.41	1.52
1	A	514	GLU	CD-OE2	-5.41	1.19	1.25
1	A	434	TYR	CE2-CZ	-5.39	1.31	1.38
1	B	686	GLU	CG-CD	5.39	1.60	1.51
1	A	255	ARG	CG-CD	5.37	1.65	1.51
1	A	434	TYR	CG-CD1	-5.37	1.32	1.39
1	B	526	GLU	CG-CD	5.33	1.59	1.51
1	A	362	TRP	CE3-CZ3	5.32	1.47	1.38
1	A	532	ARG	CD-NE	-5.32	1.37	1.46
1	A	269	GLU	CG-CD	5.30	1.59	1.51
1	A	402	SER	CB-OG	5.29	1.49	1.42
1	B	514	GLU	CD-OE2	-5.28	1.19	1.25
1	B	178	GLU	CG-CD	5.28	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	491	PHE	CG-CD1	-5.24	1.30	1.38
1	A	349	GLU	CD-OE1	-5.23	1.19	1.25
1	A	694	GLU	CG-CD	5.22	1.59	1.51
1	B	532	ARG	NE-CZ	-5.22	1.26	1.33
1	A	426[A]	ARG	CZ-NH2	5.19	1.39	1.33
1	A	426[B]	ARG	CZ-NH2	5.19	1.39	1.33
1	A	349	GLU	CD-OE2	-5.17	1.20	1.25
1	A	496	LYS	CE-NZ	-5.16	1.36	1.49
1	A	40	ARG	NE-CZ	5.15	1.39	1.33
1	B	427	ASP	CB-CG	5.13	1.62	1.51
1	A	725	GLN	N-CA	5.09	1.56	1.46
1	A	40	ARG	CD-NE	5.08	1.55	1.46
1	B	64	LYS	C-O	-5.08	1.13	1.23
1	B	82	ARG	CZ-NH2	-5.05	1.26	1.33
1	A	725	GLN	CD-NE2	5.03	1.45	1.32
1	A	298	GLU	CB-CG	5.03	1.61	1.52
1	B	124	GLY	C-O	5.02	1.31	1.23
1	B	219	TYR	CE1-CZ	5.01	1.45	1.38

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-17.51	111.55	120.30
1	A	426[A]	ARG	NE-CZ-NH1	-16.04	112.28	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-16.04	112.28	120.30
1	B	532	ARG	NE-CZ-NH2	-15.72	112.44	120.30
1	B	255	ARG	NE-CZ-NH1	14.97	127.79	120.30
1	B	255	ARG	NE-CZ-NH2	-14.67	112.97	120.30
1	B	382	ARG	NE-CZ-NH2	-13.47	113.56	120.30
1	A	433	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	B	123	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	A	60	ASP	CB-CG-OD2	-9.99	109.31	118.30
1	B	268	ASP	CB-CG-OD1	9.90	127.22	118.30
1	B	433	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	A	532	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	A	48	ASP	CB-CG-OD1	9.51	126.86	118.30
1	B	532	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	B	688	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	426[A]	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	A	426[B]	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	B	132	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	B	688	ARG	NE-CZ-NH1	8.79	124.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	404	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	54	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	633[A]	VAL	CG1-CB-CG2	-8.32	97.58	110.90
1	B	633[B]	VAL	CG1-CB-CG2	-8.32	97.58	110.90
1	B	382	ARG	CG-CD-NE	-8.27	94.44	111.80
1	A	670	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	A	268	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	B	529	GLU	OE1-CD-OE2	-8.04	113.66	123.30
1	B	54	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	B	48	ASP	CB-CG-OD1	7.83	125.35	118.30
1	B	713	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	B	744	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	B	268	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	82	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	123	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	76	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	376	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	B	704	LEU	CB-CG-CD1	-7.29	98.60	111.00
1	A	54	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	149	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	395	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	459	ASP	CB-CG-OD1	6.94	124.54	118.30
1	B	426[A]	ARG	NE-CZ-NH1	-6.89	116.85	120.30
1	B	426[B]	ARG	NE-CZ-NH1	-6.89	116.85	120.30
1	A	587	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	108	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	149	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	B	414	ASP	CB-CG-OD1	6.84	124.45	118.30
1	B	149	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	B	108	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	123	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	60	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	255	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	55	HIS	CB-CA-C	6.19	122.79	110.40
1	B	199	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	B	686	GLU	OE1-CD-OE2	6.18	130.72	123.30
1	A	382	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	584	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	A	199	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	B	108	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	268	ASP	CB-CG-OD1	6.03	123.73	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	TYR	CB-CG-CD1	6.03	124.62	121.00
1	A	263	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	218	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	744	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	730	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	98	ASP	CB-CG-OD2	-5.91	112.99	118.30
1	B	726	GLU	CG-CD-OE2	5.91	130.11	118.30
1	A	584	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	B	60	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	412	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	B	54	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	167	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	414	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	269	GLU	OE1-CD-OE2	-5.81	116.33	123.30
1	B	433	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	735	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	B	683	ASP	CB-CG-OD1	5.73	123.45	118.30
1	B	744	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	255	ARG	CG-CD-NE	-5.62	99.99	111.80
1	A	617	LEU	CB-CG-CD1	5.56	120.45	111.00
1	A	688	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	545	VAL	CG1-CB-CG2	-5.52	102.06	110.90
1	A	382	ARG	CG-CD-NE	-5.52	100.21	111.80
1	B	587	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	149	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	532	ARG	CG-CD-NE	-5.47	100.31	111.80
1	B	532	ARG	CG-CD-NE	-5.38	100.49	111.80
1	B	55	HIS	CB-CA-C	5.37	121.15	110.40
1	B	713	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	226	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	A	191	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	532	ARG	CD-NE-CZ	5.30	131.02	123.60
1	B	349	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	48	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	73	GLU	OE1-CD-OE2	5.18	129.51	123.30
1	B	428	MET	CA-CB-CG	-5.17	104.51	113.30
1	B	653	PHE	CB-CG-CD1	5.17	124.42	120.80
1	A	196	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	A	382	ARG	CD-NE-CZ	5.07	130.70	123.60
1	B	41	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	218	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	683	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	622	GLN	Sidechain

5.2 Too-close contacts (i)

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	5539	0	5374	18	0
1	B	5525	0	5356	26	0
2	A	43	0	30	0	0
2	B	43	0	30	1	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	32	0	56	3	0
5	B	32	0	56	4	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	20	0	14	4	0
7	B	20	0	14	6	0
8	A	576	0	0	6	0
8	B	583	0	0	6	0
All	All	12427	0	10930	50	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 (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:GLN:NE2	7:B:809:NIZ:O1	2.07	0.88
5:A:805:MPD:O2	5:A:805:MPD:H53	1.80	0.80
1:B:119[B]:THR:HG23	8:B:1093:HOH:O	1.80	0.79
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:GLU:OE1	8:B:903:HOH:O	2.07	0.71
1:A:649:ARG:NH2	8:A:905:HOH:O	2.28	0.67
5:B:804:MPD:H53	5:B:804:MPD:H11	1.76	0.66
1:B:119[B]:THR:HG21	8:B:1435:HOH:O	1.95	0.66
7:B:810:NIZ:H4	8:B:1072:HOH:O	1.98	0.64
1:A:647:GLN:HG3	8:A:1212:HOH:O	1.99	0.62
1:B:360:HIS:ND1	8:B:906:HOH:O	2.32	0.59
1:A:40:ARG:HG3	8:A:1337:HOH:O	2.07	0.55
1:B:622:GLN:HE21	7:B:809:NIZ:H5	1.73	0.54
5:B:804:MPD:H53	5:B:804:MPD:C1	2.39	0.53
7:A:810:NIZ:H4	8:A:1059:HOH:O	2.09	0.52
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.45	0.52
1:B:662:ASN:H	1:B:725:GLN:HE22	1.57	0.51
1:A:40:ARG:HD2	1:B:40:ARG:CZ	2.40	0.51
1:A:111:TRP:HE1	7:A:810:NIZ:H7	1.60	0.50
1:A:683:ASP:HA	8:A:903:HOH:O	2.12	0.49
1:A:633[B]:VAL:CG2	1:A:719:TYR:CZ	2.98	0.47
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.97	0.47
1:A:625:THR:HG22	7:A:809:NIZ:H4	1.96	0.47
1:B:564:LYS:HG3	5:B:807:MPD:HM3	1.96	0.47
1:A:682:ALA:O	8:A:903:HOH:O	2.20	0.46
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.59	0.46
1:A:112:HIS:NE2	7:A:810:NIZ:N2	2.64	0.46
5:B:804:MPD:C1	5:B:804:MPD:C5	2.94	0.46
1:A:247:ASN:HD22	1:A:248:PRO:HD2	1.80	0.45
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.52	0.44
1:B:696:LYS:HE2	8:B:942:HOH:O	2.18	0.44
5:A:805:MPD:O2	5:A:805:MPD:C5	2.46	0.43
1:B:112:HIS:NE2	7:B:810:NIZ:N3	2.66	0.43
1:B:284:THR:HG22	2:B:801:HEM:HAA1	2.01	0.43
1:B:112:HIS:NE2	7:B:810:NIZ:N2	2.66	0.43
1:A:649:ARG:HD2	1:A:649:ARG:HA	1.73	0.42
1:B:426[B]:ARG:HD2	1:B:426[B]:ARG:HA	1.88	0.42
1:A:405:PHE:HB3	1:A:412:PHE:HB2	2.00	0.42
1:B:673:THR:OG1	1:B:696:LYS:HE3	2.18	0.42
1:B:568:HIS:ND1	1:B:726:GLU:OE1	2.44	0.42
1:B:112:HIS:CE1	7:B:810:NIZ:C	3.02	0.42
1:B:405:PHE:HB3	1:B:412:PHE:HB2	2.02	0.42
1:A:111:TRP:CD1	1:A:112:HIS:HD2	2.38	0.42
5:A:804:MPD:H4	5:A:804:MPD:HM2	1.63	0.42
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HD2	1:B:40:ARG:NE	2.35	0.41
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.19	0.41
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	2.02	0.41
1:B:111:TRP:CD1	1:B:112:HIS:HD2	2.39	0.40
1:B:428:MET:O	1:B:433:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	718/728 (99%)	706 (98%)	12 (2%)	0	100	100
1	B	716/728 (98%)	706 (99%)	10 (1%)	0	100	100
All	All	1434/1456 (98%)	1412 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	556/560 (99%)	550 (99%)	6 (1%)	78	75
1	B	554/560 (99%)	549 (99%)	5 (1%)	82	81
All	All	1110/1120 (99%)	1099 (99%)	11 (1%)	80	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	118	ARG
1	A	544	GLN
1	A	647	GLN
1	A	649	ARG
1	B	64	LYS
1	B	118	ARG
1	B	410	GLU
1	B	540	ARG
1	B	608	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	B	46	GLN
1	B	227	ASN
1	B	406	HIS
1	B	650	HIS
1	B	725	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	1,7	28,50,50	1.20	3 (10%)	17,82,82	2.11	7 (41%)
5	MPD	A	804	-	7,7,7	1.14	1 (14%)	9,10,10	1.90	2 (22%)
5	MPD	A	805	-	7,7,7	0.72	0	9,10,10	1.64	2 (22%)
5	MPD	A	806	-	7,7,7	1.45	1 (14%)	9,10,10	1.33	1 (11%)
6	PO4	A	807	-	4,4,4	0.67	0	6,6,6	1.36	1 (16%)
5	MPD	A	808	-	7,7,7	0.67	0	9,10,10	2.00	3 (33%)
7	NIZ	A	809	-	10,10,10	3.64	6 (60%)	12,12,12	2.32	7 (58%)
7	NIZ	A	810	2	10,10,10	4.60	6 (60%)	12,12,12	3.82	9 (75%)
2	HEM	B	801	1	28,50,50	1.75	8 (28%)	17,82,82	2.11	4 (23%)
5	MPD	B	804	-	7,7,7	1.30	1 (14%)	9,10,10	3.81	6 (66%)
5	MPD	B	805	-	7,7,7	0.81	0	9,10,10	1.68	3 (33%)
5	MPD	B	806	-	7,7,7	0.68	0	9,10,10	1.26	1 (11%)
5	MPD	B	807	-	7,7,7	1.10	0	9,10,10	1.11	1 (11%)
6	PO4	B	808	-	4,4,4	1.17	1 (25%)	6,6,6	0.96	0
7	NIZ	B	809	-	10,10,10	2.07	3 (30%)	12,12,12	3.67	7 (58%)
7	NIZ	B	810	-	10,10,10	5.18	8 (80%)	12,12,12	4.70	9 (75%)

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	1,7	-	0/6/54/54	0/0/8/8
5	MPD	A	804	-	-	0/5/5/5	0/0/0/0
5	MPD	A	805	-	-	0/5/5/5	0/0/0/0
5	MPD	A	806	-	-	0/5/5/5	0/0/0/0
6	PO4	A	807	-	-	0/0/0/0	0/0/0/0
5	MPD	A	808	-	-	0/5/5/5	0/0/0/0
7	NIZ	A	809	-	-	0/6/6/6	0/1/1/1
7	NIZ	A	810	2	-	0/6/6/6	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	801	1	-	0/6/54/54	0/0/8/8
5	MPD	B	804	-	-	0/5/5/5	0/0/0/0
5	MPD	B	805	-	-	0/5/5/5	0/0/0/0
5	MPD	B	806	-	-	0/5/5/5	0/0/0/0
5	MPD	B	807	-	-	0/5/5/5	0/0/0/0
6	PO4	B	808	-	-	0/0/0/0	0/0/0/0
7	NIZ	B	809	-	-	0/6/6/6	0/1/1/1
7	NIZ	B	810	-	-	0/6/6/6	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-3.92	1.35	1.40
2	B	801	HEM	C1B-NB	-3.01	1.33	1.36
7	A	809	NIZ	N3-N2	-2.82	1.37	1.41
2	A	801	HEM	C3B-C2B	-2.68	1.36	1.40
5	B	804	MPD	O2-C2	-2.62	1.37	1.44
2	B	801	HEM	C1D-CHD	-2.47	1.33	1.40
2	B	801	HEM	C4B-NB	-2.47	1.30	1.36
7	B	809	NIZ	N3-N2	-2.30	1.38	1.41
2	A	801	HEM	C4A-CHB	2.01	1.45	1.40
6	B	808	PO4	P-O1	2.01	1.54	1.50
2	B	801	HEM	CMB-C2B	2.02	1.55	1.51
5	A	804	MPD	C5-C4	2.11	1.61	1.51
7	A	809	NIZ	C2-C3	2.13	1.43	1.38
2	A	801	HEM	C1C-NC	2.14	1.39	1.36
7	B	810	NIZ	C5-C4	2.31	1.43	1.38
2	B	801	HEM	C4A-NA	2.33	1.41	1.36
7	B	810	NIZ	C3-N1	2.55	1.41	1.33
7	A	810	NIZ	C4-N1	2.65	1.41	1.33
7	A	810	NIZ	C3-N1	2.73	1.41	1.33
5	A	806	MPD	C1-C2	3.13	1.62	1.52
7	B	809	NIZ	C4-N1	3.30	1.43	1.33
7	B	810	NIZ	C4-N1	3.43	1.43	1.33
2	B	801	HEM	C1A-NA	3.49	1.43	1.36
2	B	801	HEM	C4D-ND	3.76	1.41	1.36
7	A	809	NIZ	C4-N1	3.93	1.45	1.33
7	B	809	NIZ	C5-C1	4.22	1.46	1.39
7	B	810	NIZ	O1-C	4.46	1.32	1.23
7	A	809	NIZ	C5-C1	4.73	1.47	1.39
7	A	810	NIZ	N3-N2	5.10	1.49	1.41
7	A	809	NIZ	C2-C1	5.34	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	810	NIZ	C2-C1	5.53	1.48	1.39
7	B	810	NIZ	N3-N2	5.79	1.50	1.41
7	A	810	NIZ	C5-C1	6.47	1.50	1.39
7	B	810	NIZ	C5-C1	6.66	1.50	1.39
7	B	810	NIZ	C2-C1	6.68	1.50	1.39
7	A	809	NIZ	C-N2	7.14	1.40	1.33
7	A	810	NIZ	C-N2	9.71	1.42	1.33
7	B	810	NIZ	C-N2	10.08	1.43	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	810	NIZ	C3-C2-C1	-7.35	110.83	119.05
7	A	810	NIZ	O1-C-C1	-7.32	107.95	120.94
7	B	810	NIZ	O1-C-C1	-7.20	108.16	120.94
5	B	804	MPD	O2-C2-C3	-6.72	83.21	109.88
7	B	810	NIZ	C-N2-N3	-6.69	113.32	121.84
5	B	804	MPD	O2-C2-CM	-6.38	85.91	108.00
7	B	809	NIZ	O1-C-N2	-5.17	116.50	122.45
5	B	804	MPD	O4-C4-C3	-4.39	91.17	111.28
5	A	804	MPD	O4-C4-C3	-4.02	92.90	111.28
2	B	801	HEM	CAA-CBA-CGA	-3.92	105.96	112.66
2	A	801	HEM	CMA-C3A-C4A	-3.88	122.51	128.46
5	A	808	MPD	O2-C2-C3	-3.86	94.57	109.88
2	A	801	HEM	CAA-CBA-CGA	-3.76	106.24	112.66
7	A	810	NIZ	C3-C2-C1	-3.46	115.18	119.05
7	B	809	NIZ	C5-C4-N1	-3.43	117.64	123.63
7	A	809	NIZ	C2-C3-N1	-3.42	117.66	123.63
7	A	809	NIZ	O1-C-C1	-3.41	114.89	120.94
5	A	808	MPD	CM-C2-C1	-3.39	102.85	110.42
7	B	809	NIZ	C3-C2-C1	-3.39	115.26	119.05
5	B	805	MPD	O2-C2-C3	-3.38	96.46	109.88
7	A	809	NIZ	C4-C5-C1	-3.25	115.41	119.05
7	B	810	NIZ	C4-C5-C1	-3.16	115.52	119.05
5	A	805	MPD	O2-C2-CM	-3.06	97.39	108.00
7	B	809	NIZ	C-N2-N3	-2.69	118.41	121.84
7	B	810	NIZ	C5-C1-C	-2.63	112.15	120.61
7	A	810	NIZ	C4-C5-C1	-2.62	116.12	119.05
7	B	809	NIZ	O1-C-C1	-2.52	116.47	120.94
7	A	810	NIZ	C5-C4-N1	-2.40	119.44	123.63
5	B	806	MPD	O2-C2-C1	-2.38	99.77	108.00
6	A	807	PO4	O3-P-O1	-2.25	101.37	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	810	NIZ	C5-C4-N1	-2.23	119.73	123.63
5	B	807	MPD	O2-C2-C1	-2.19	100.39	108.00
5	B	805	MPD	O2-C2-C1	-2.08	100.78	108.00
5	B	804	MPD	O4-C4-C5	2.05	118.84	109.46
7	A	809	NIZ	O1-C-N2	2.12	124.89	122.45
2	A	801	HEM	CMB-C2B-C3B	2.24	129.05	124.89
5	A	808	MPD	O2-C2-CM	2.27	115.86	108.00
5	B	805	MPD	CM-C2-C3	2.27	121.36	110.08
7	A	809	NIZ	C1-C-N2	2.28	118.95	116.33
2	A	801	HEM	CMC-C2C-C3C	2.37	129.30	124.89
5	A	805	MPD	O2-C2-C1	2.40	116.32	108.00
2	B	801	HEM	CAD-CBD-CGD	2.57	117.06	112.66
7	A	810	NIZ	C-N2-N3	2.59	125.13	121.84
5	A	804	MPD	O4-C4-C5	2.61	121.43	109.46
7	A	809	NIZ	C3-N1-C4	2.64	123.20	116.83
2	A	801	HEM	CAD-CBD-CGD	2.68	117.24	112.66
5	A	806	MPD	CM-C2-C1	2.72	116.48	110.42
5	B	804	MPD	CM-C2-C1	2.85	116.78	110.42
2	A	801	HEM	CBD-CAD-C3D	2.91	118.02	112.47
7	A	810	NIZ	C3-N1-C4	2.98	124.01	116.83
7	A	809	NIZ	C-N2-N3	3.03	125.69	121.84
5	B	804	MPD	CM-C2-C3	3.13	125.63	110.08
7	B	809	NIZ	C2-C1-C5	3.20	123.01	118.58
2	A	801	HEM	CMA-C3A-C2A	3.26	131.08	124.94
2	B	801	HEM	CBD-CAD-C3D	3.28	118.73	112.47
7	A	810	NIZ	C2-C1-C5	3.56	123.50	118.58
7	B	810	NIZ	O1-C-N2	4.27	127.36	122.45
7	A	810	NIZ	O1-C-N2	4.75	127.92	122.45
7	B	810	NIZ	C2-C1-C5	5.09	125.62	118.58
2	B	801	HEM	CMB-C2B-C3B	5.19	134.52	124.89
7	B	810	NIZ	C1-C-N2	6.42	123.70	116.33
7	A	810	NIZ	C1-C-N2	6.61	123.91	116.33
7	B	809	NIZ	C1-C-N2	9.13	126.80	116.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	MPD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	805	MPD	2	0
7	A	809	NIZ	1	0
7	A	810	NIZ	3	0
2	B	801	HEM	1	0
5	B	804	MPD	3	0
5	B	807	MPD	1	0
7	B	809	NIZ	2	0
7	B	810	NIZ	4	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 (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, 95th 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(Å²)	Q<0.9
1	A	713/728 (97%)	-0.36	16 (2%)	62	65	18, 26, 47, 79	0
1	B	713/728 (97%)	-0.41	8 (1%)	80	82	17, 24, 43, 77	0
All	All	1426/1456 (97%)	-0.39	24 (1%)	70	73	17, 25, 45, 79	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	GLY	6.0
1	B	679	ALA	5.2
1	A	680	ALA	4.0
1	B	748	ALA	3.8
1	A	679	ALA	3.8
1	B	541	GLY	3.7
1	B	540	ARG	3.6
1	A	540	ARG	3.6
1	A	748	ALA	3.6
1	A	213	GLY	3.3
1	A	220	SER	3.0
1	A	215	PRO	3.0
1	A	222	ASP	3.0
1	A	647	GLN	2.9
1	B	680	ALA	2.9
1	A	214	GLY	2.7
1	A	211	LEU	2.6
1	A	221	GLY	2.6
1	B	454	ASP	2.4
1	B	682	ALA	2.3
1	B	610	ARG	2.2
1	A	454	ASP	2.0
1	A	681	ASP	2.0
1	A	610	ARG	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, 95th 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^2)	Q<0.9
7	NIZ	A	810	10/10	0.73	0.24	9.80	46,56,61,64	0
5	MPD	A	806	8/8	0.81	0.18	7.32	46,65,70,71	0
5	MPD	A	805	8/8	0.83	0.27	6.32	56,62,80,81	0
7	NIZ	A	809	10/10	0.89	0.15	5.06	39,44,52,58	0
7	NIZ	B	810	10/10	0.77	0.22	3.37	37,47,54,58	0
5	MPD	B	807	8/8	0.88	0.21	3.15	49,58,62,65	0
5	MPD	B	805	8/8	0.95	0.11	2.99	47,49,53,55	0
5	MPD	B	804	8/8	0.92	0.16	2.41	45,58,67,71	0
5	MPD	B	806	8/8	0.89	0.16	0.77	47,63,73,76	0
7	NIZ	B	809	10/10	0.92	0.11	0.63	32,36,40,41	0
2	HEM	B	801	43/43	0.99	0.11	0.33	15,19,21,23	0
2	HEM	A	801	43/43	0.99	0.08	-0.37	19,21,25,27	0
3	NA	B	802	1/1	1.00	0.05	-2.61	20,20,20,20	0
4	CL	B	803	1/1	0.99	0.08	-2.69	30,30,30,30	0
3	NA	A	802	1/1	1.00	0.06	-5.11	21,21,21,21	0
5	MPD	A	804	8/8	0.82	0.21	-	54,57,69,69	0
6	PO4	A	807	5/5	0.83	0.22	-	59,93,95,99	0
6	PO4	B	808	5/5	0.84	0.37	-	51,76,92,94	0
5	MPD	A	808	8/8	0.79	0.28	-	59,72,80,81	0
4	CL	A	803	1/1	0.99	0.08	-	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.