Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2016 – 07:14 PM EDT

PDB ID	:	5SYI
Title	:	Structure of D141A variant of B. pseudomallei KatG complexed with INH
Authors	:	Loewen, P.C.
Deposited on	:	2016-08-11
Resolution	:	1.70 Å(reported)

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 (i)

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

The reported resolution of this entry is 1.70 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		0.181
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		2.4%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
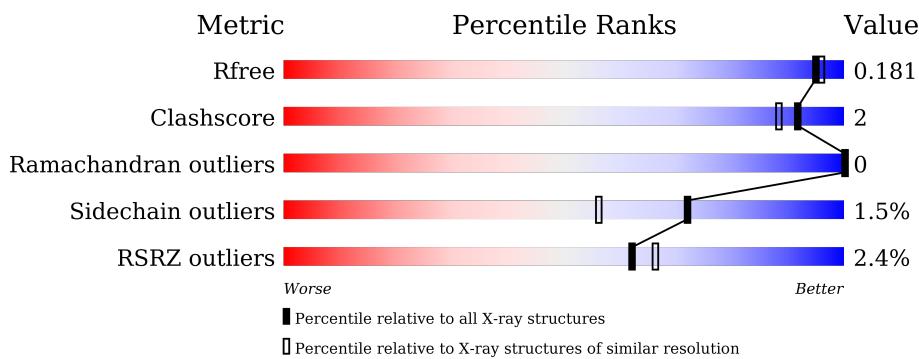
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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% ▮ 86% 11% ··
1	B	728	2% ▮ 85% 11% ··
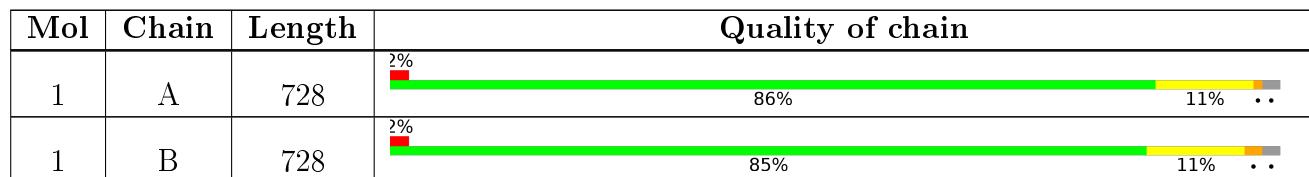
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NIZ	B	805	-	X	-	X
6	NIZ	B	806	-	X	-	-
7	MPD	A	807	-	-	-	X
7	MPD	B	807	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12740 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 5523	C 3490	N 984	O 1035	S 14	0	4	0
1	B	713	Total 5526	C 3494	N 984	O 1034	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: $C_{34}H_{32}FeN_4O_4$).
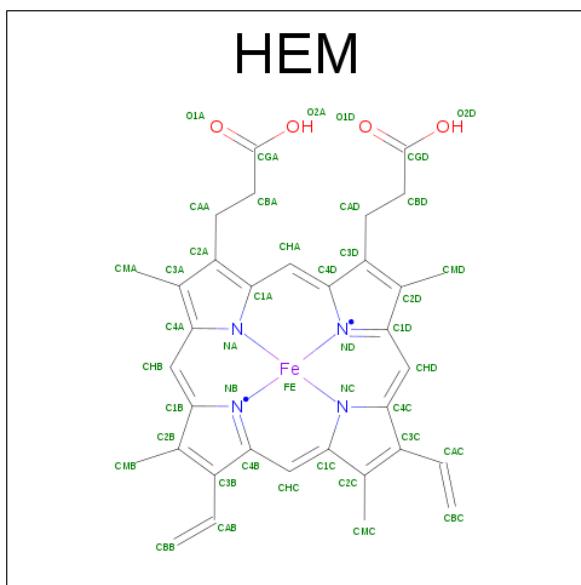
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

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

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).
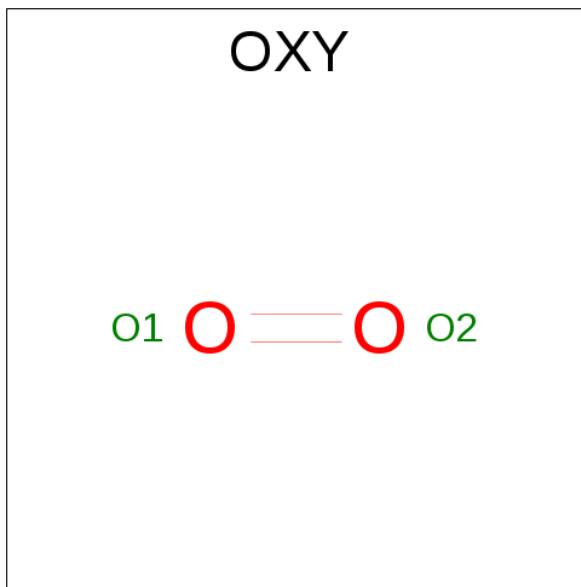
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	1	2	2	0	0
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is pyridine-4-carbohydrazide (three-letter code: NIZ) (formula: $C_6H_7N_3O$).
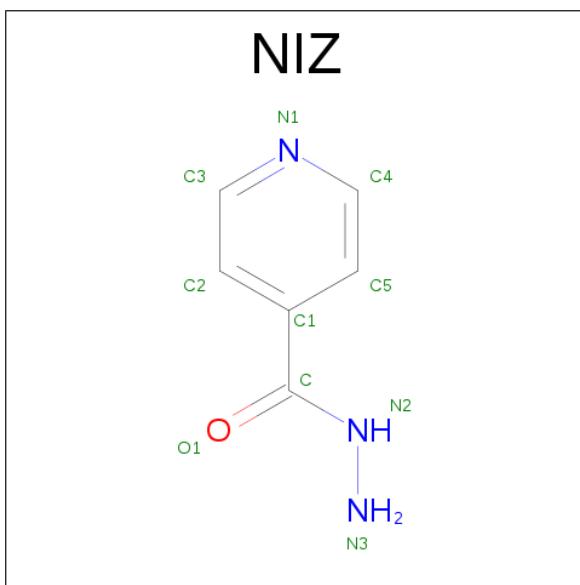
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 10	C 6	N 3	O 1	0	0
6	B	1	Total 10	C 6	N 3	O 1	0	0
6	B	1	Total 10	C 6	N 3	O 1	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
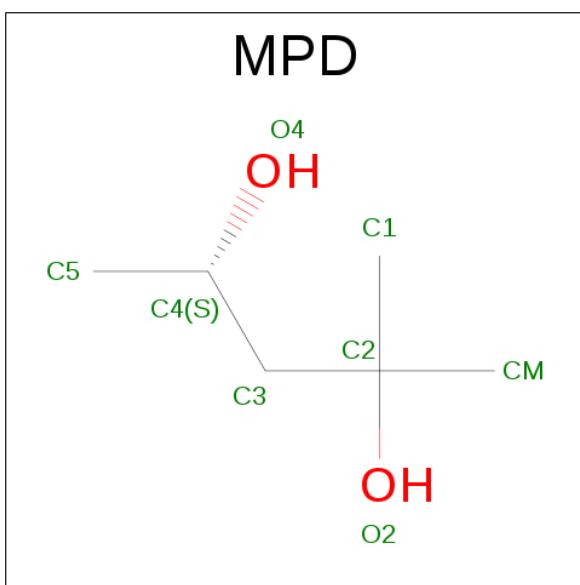
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 8	C 6	O 2	0	0
7	A	1	Total 8	C 6	O 2	0	0
7	B	1	Total 8	C 6	O 2	0	0
7	B	1	Total 8	C 6	O 2	0	0

• Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
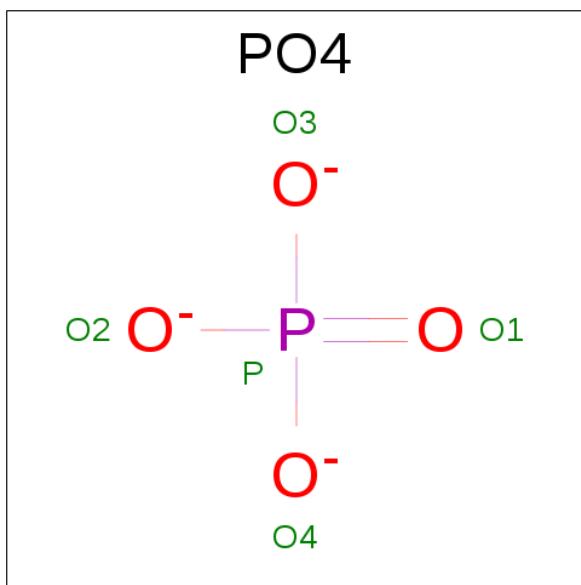
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 5	O 4	P 1	0	0
8	B	1	Total 5	O 4	P 1	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	783	Total 783	O 783	0	0
9	B	742	Total 742	O 742	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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
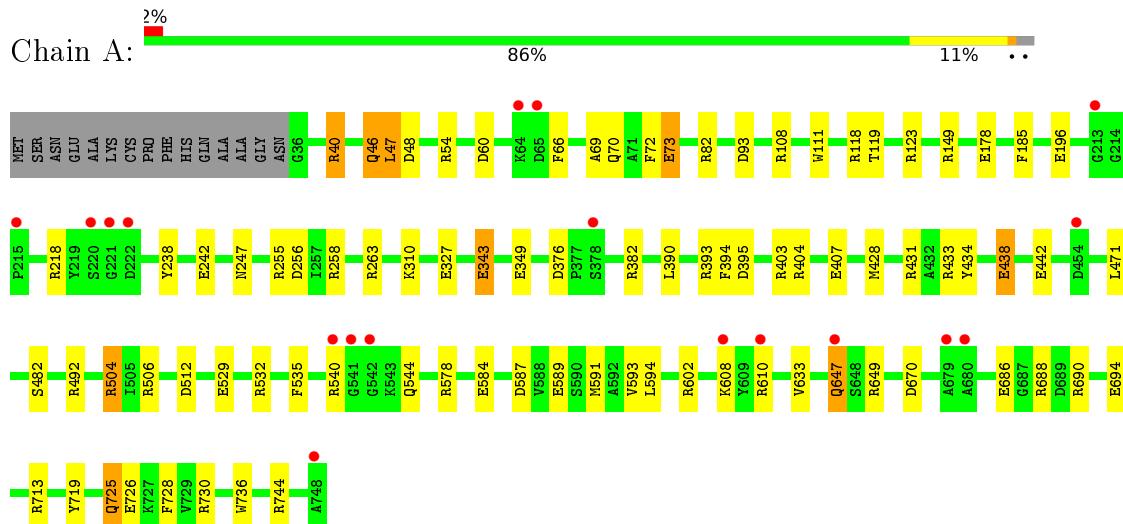
- Molecule 1: Catalase-peroxidase
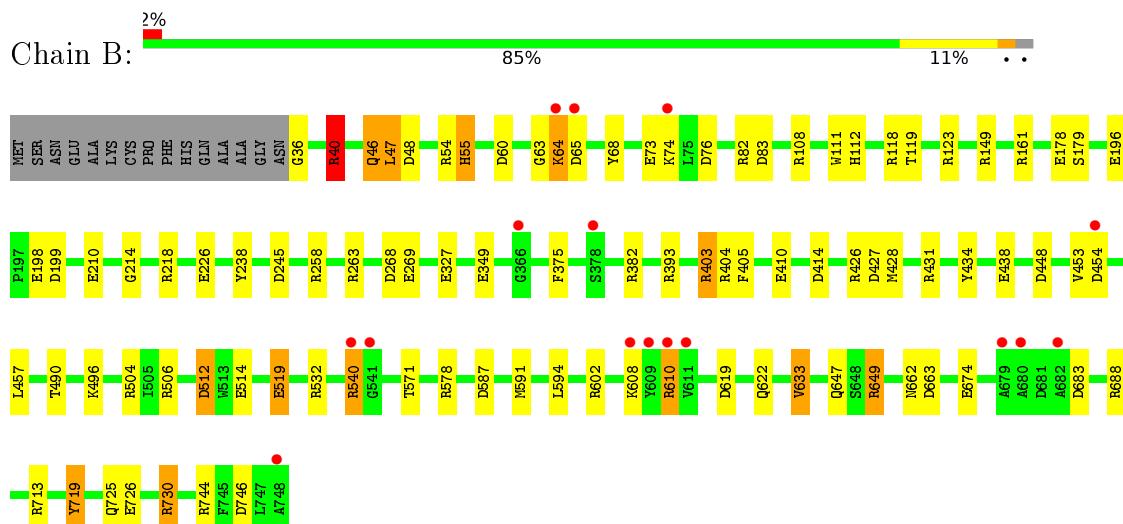
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.77Å　　115.59Å　　174.57Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	20.00　–　1.70 40.83　–　1.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-1.70) 99.4 (40.83-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	2.70 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145　,　0.170 0.158　,　0.181	Depositor DCC
R_{free} test set	11136 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.5	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12740	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, 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	1.52	52/5677 (0.9%)	1.50	67/7718 (0.9%)
1	B	1.51	47/5685 (0.8%)	1.38	72/7729 (0.9%)
All	All	1.51	99/11362 (0.9%)	1.44	139/15447 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	GLU	CD-OE1	12.09	1.39	1.25
1	A	532	ARG	CD-NE	-10.38	1.28	1.46
1	A	438	GLU	CD-OE1	-9.78	1.14	1.25
1	A	584	GLU	CG-CD	8.80	1.65	1.51
1	A	327	GLU	CD-OE1	8.72	1.35	1.25
1	B	730[A]	ARG	CZ-NH1	8.36	1.44	1.33
1	B	730[B]	ARG	CZ-NH1	8.36	1.44	1.33
1	A	343	GLU	CD-OE2	8.33	1.34	1.25
1	B	63	GLY	N-CA	8.17	1.58	1.46
1	B	434	TYR	CE2-CZ	-8.08	1.28	1.38
1	B	426	ARG	CZ-NH2	7.92	1.43	1.33
1	A	255	ARG	CD-NE	7.90	1.59	1.46
1	B	410	GLU	CG-CD	7.84	1.63	1.51
1	B	82	ARG	CZ-NH2	-7.78	1.23	1.33
1	A	196	GLU	CG-CD	7.77	1.63	1.51
1	B	438	GLU	CD-OE1	-7.75	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	GLU	CG-CD	7.62	1.63	1.51
1	A	532	ARG	CZ-NH2	-7.44	1.23	1.33
1	A	647	GLN	CG-CD	7.42	1.68	1.51
1	B	512	ASP	CG-OD2	7.35	1.42	1.25
1	B	327	GLU	CG-CD	7.25	1.62	1.51
1	A	442	GLU	CD-OE2	-7.15	1.17	1.25
1	B	540	ARG	C-O	7.04	1.36	1.23
1	A	349	GLU	CD-OE2	-6.97	1.18	1.25
1	B	726	GLU	CG-CD	6.91	1.62	1.51
1	B	496	LYS	CE-NZ	-6.87	1.31	1.49
1	A	532	ARG	NE-CZ	-6.80	1.24	1.33
1	A	438	GLU	CD-OE2	6.72	1.33	1.25
1	B	36	GLY	N-CA	6.71	1.56	1.46
1	B	327	GLU	CD-OE1	6.65	1.32	1.25
1	B	179	SER	C-O	6.60	1.35	1.23
1	A	327	GLU	CG-CD	6.57	1.61	1.51
1	A	725	GLN	CG-CD	6.46	1.66	1.51
1	A	686	GLU	CG-CD	6.42	1.61	1.51
1	A	178	GLU	CG-CD	6.34	1.61	1.51
1	A	434	TYR	CE2-CZ	-6.30	1.30	1.38
1	A	196	GLU	CB-CG	-6.29	1.40	1.52
1	B	514	GLU	CD-OE2	-6.29	1.18	1.25
1	A	540	ARG	C-O	6.27	1.35	1.23
1	A	73	GLU	CG-CD	6.24	1.61	1.51
1	A	255	ARG	CG-CD	6.22	1.67	1.51
1	A	728	PHE	CG-CD2	-6.22	1.29	1.38
1	B	198	GLU	CD-OE2	6.18	1.32	1.25
1	A	46	GLN	CG-CD	6.16	1.65	1.51
1	B	602	ARG	CZ-NH2	-6.13	1.25	1.33
1	B	512	ASP	CB-CG	6.10	1.64	1.51
1	B	454	ASP	CB-CG	6.03	1.64	1.51
1	B	226	GLU	CD-OE2	-6.03	1.19	1.25
1	B	532	ARG	NE-CZ	-6.02	1.25	1.33
1	A	434	TYR	CG-CD1	-6.01	1.31	1.39
1	B	633[A]	VAL	CB-CG2	-5.98	1.40	1.52
1	B	633[B]	VAL	CB-CG2	-5.98	1.40	1.52
1	B	226	GLU	CB-CG	-5.92	1.40	1.52
1	A	434	TYR	CE1-CZ	-5.79	1.31	1.38
1	A	584	GLU	CD-OE2	5.79	1.32	1.25
1	B	119	THR	CB-CG2	-5.72	1.33	1.52
1	A	736	TRP	CG-CD1	-5.70	1.28	1.36
1	B	196	GLU	CB-CG	-5.66	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	GLN	CG-CD	5.59	1.64	1.51
1	B	674	GLU	CG-CD	5.56	1.60	1.51
1	B	65	ASP	CB-CG	5.55	1.63	1.51
1	B	269	GLU	CD-OE1	-5.47	1.19	1.25
1	A	256	ASP	CB-CG	5.45	1.63	1.51
1	A	242	GLU	CD-OE2	5.43	1.31	1.25
1	A	407	GLU	CG-CD	5.39	1.60	1.51
1	A	726	GLU	CD-OE2	5.38	1.31	1.25
1	B	68	TYR	CE1-CZ	5.37	1.45	1.38
1	A	70	GLN	CG-CD	5.37	1.63	1.51
1	B	349	GLU	CD-OE2	-5.35	1.19	1.25
1	A	247	ASN	CG-ND2	-5.34	1.19	1.32
1	A	688	ARG	CZ-NH1	-5.34	1.26	1.33
1	A	726	GLU	CG-CD	5.33	1.59	1.51
1	A	428	MET	CG-SD	-5.31	1.67	1.81
1	B	519	GLU	CD-OE2	5.30	1.31	1.25
1	A	47	LEU	CB-CG	-5.30	1.37	1.52
1	A	633	VAL	CB-CG1	-5.29	1.41	1.52
1	A	434	TYR	CB-CG	-5.29	1.43	1.51
1	B	434	TYR	CE1-CZ	-5.27	1.31	1.38
1	A	694	GLU	CG-CD	5.25	1.59	1.51
1	B	746	ASP	CB-CG	5.24	1.62	1.51
1	A	482	SER	CB-OG	5.23	1.49	1.42
1	B	453	VAL	C-O	-5.22	1.13	1.23
1	B	719	TYR	CD1-CE1	5.20	1.47	1.39
1	B	214	GLY	CA-C	-5.17	1.43	1.51
1	B	210	GLU	CD-OE2	5.17	1.31	1.25
1	B	438	GLU	CD-OE2	5.17	1.31	1.25
1	A	535	PHE	CG-CD1	-5.12	1.31	1.38
1	A	376	ASP	CB-CG	5.11	1.62	1.51
1	A	255	ARG	NE-CZ	5.10	1.39	1.33
1	A	394	PHE	CG-CD2	5.06	1.46	1.38
1	A	688	ARG	CZ-NH2	-5.05	1.26	1.33
1	B	619	ASP	CG-OD1	-5.05	1.13	1.25
1	A	82	ARG	CZ-NH2	-5.05	1.26	1.33
1	B	457	LEU	C-O	5.03	1.32	1.23
1	A	719	TYR	CD1-CE1	5.03	1.46	1.39
1	A	719	TYR	CE1-CZ	5.01	1.45	1.38
1	A	584	GLU	CD-OE1	5.01	1.31	1.25
1	B	178	GLU	CG-CD	5.01	1.59	1.51
1	A	649	ARG	CZ-NH2	5.00	1.39	1.33

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	532	ARG	NE-CZ-NH2	-44.01	98.30	120.30
1	A	532	ARG	NE-CZ-NH1	34.08	137.34	120.30
1	A	255	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	A	532	ARG	CD-NE-CZ	11.08	139.12	123.60
1	A	713	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	B	512	ASP	CB-CG-OD1	-10.82	108.56	118.30
1	A	54	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	A	404	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	B	431	ARG	NE-CZ-NH2	10.64	125.62	120.30
1	A	149	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	403[A]	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	A	403[B]	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	B	393	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	B	123	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	B	268	ASP	CB-CG-OD1	9.98	127.28	118.30
1	A	578	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	B	218	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	B	108	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	A	434	TYR	CB-CG-CD1	9.29	126.57	121.00
1	B	82	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	404	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	48	ASP	CB-CG-OD1	8.71	126.14	118.30
1	B	54	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	B	48	ASP	CB-CG-OD1	8.65	126.08	118.30
1	B	123	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	744	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	149	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	B	578	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	434	TYR	CB-CG-CD1	8.29	125.98	121.00
1	B	46	GLN	CA-CB-CG	8.23	131.51	113.40
1	A	431	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	A	218	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	690	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	B	76	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	B	108	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	683	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	578	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	54	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	602	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	46	GLN	CA-CB-CG	7.27	129.39	113.40
1	B	414	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	670	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	B	65	ASP	CB-CG-OD2	-7.17	111.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	404	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	60	ASP	CB-CG-OD1	7.03	124.62	118.30
1	B	73	GLU	OE1-CD-OE2	7.03	131.73	123.30
1	B	263	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	123	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	108	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	54	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	218	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	48	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	428	MET	CA-CB-CG	-6.74	101.83	113.30
1	B	258	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	504	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	382	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	B	426	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	404	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	47	LEU	N-CA-CB	-6.55	97.30	110.40
1	A	178	GLU	OE1-CD-OE2	6.52	131.13	123.30
1	A	730	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	633[A]	VAL	CG1-CB-CG2	-6.50	100.49	110.90
1	B	633[B]	VAL	CG1-CB-CG2	-6.50	100.49	110.90
1	B	587	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	60	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	47	LEU	N-CA-CB	-6.33	97.75	110.40
1	A	587	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	403	ARG	CG-CD-NE	-6.28	98.62	111.80
1	B	54	ARG	CG-CD-NE	-6.22	98.73	111.80
1	B	149	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	571	THR	CA-CB-CG2	-6.21	103.71	112.40
1	A	263	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	492	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	434	TYR	CZ-CE2-CD2	6.14	125.33	119.80
1	A	258	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	427	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	82	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	123	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	376	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	434	TYR	CZ-CE2-CD2	6.03	125.22	119.80
1	B	68	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	A	532	ARG	CB-CG-CD	-6.00	96.00	111.60
1	B	245	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	149	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	375	PHE	CB-CG-CD1	-5.91	116.66	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	688	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	66	PHE	CG-CD2-CE2	-5.88	114.33	120.80
1	A	504	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	433	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	713	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	405	PHE	CB-CG-CD2	5.79	124.85	120.80
1	A	584	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	A	263	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	405	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	B	540	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	93	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	255	ARG	CD-NE-CZ	5.62	131.46	123.60
1	B	161	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	730[A]	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	730[B]	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	713	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	185	PHE	CB-CG-CD1	5.49	124.64	120.80
1	A	395	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	40	ARG	CA-CB-CG	5.49	125.47	113.40
1	A	40	ARG	CA-CB-CG	5.46	125.41	113.40
1	A	82	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	730	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	506	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	70	GLN	CA-CB-CG	5.38	125.23	113.40
1	A	438	GLU	CG-CD-OE1	-5.38	107.55	118.30
1	B	263	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	529	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	B	83	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	55	HIS	CB-CA-C	5.30	120.99	110.40
1	B	431	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	428	MET	CA-CB-CG	-5.25	104.37	113.30
1	A	390	LEU	CB-CG-CD2	5.22	119.88	111.00
1	A	310	LYS	CD-CE-NZ	-5.20	99.75	111.70
1	B	268	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	B	719	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	A	72	PHE	CG-CD1-CE1	5.14	126.45	120.80
1	A	382	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	649	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	578	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	60	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	649	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	663	ASP	CB-CG-OD2	-5.05	113.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	649	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	448	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	393	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	683	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	82	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	532	ARG	CG-CD-NE	-5.02	101.25	111.80
1	B	610	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	490	THR	CA-CB-CG2	-5.01	105.39	112.40
1	B	199	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	B	506	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	A	744	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	A	512	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	438	GLU	Sidechain
1	A	47	LEU	Mainchain

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	5523	0	5351	12	0
1	B	5526	0	5360	18	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	1	0
5	B	2	0	0	1	0
6	A	10	0	7	2	0
6	B	20	0	14	4	0
7	A	16	0	28	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	16	0	28	4	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	A	783	0	0	11	1
9	B	742	0	0	8	1
All	All	12740	0	10848	47	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 2.

All (47) 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:A:806:MPD:O4	7:A:806:MPD:H11	1.44	1.14
5:B:804:OXY:O1	6:B:806:NIZ:N2	1.85	1.08
1:A:119[B]:THR:HG21	9:A:1012:HOH:O	1.73	0.88
7:A:806:MPD:H53	9:A:1185:HOH:O	1.75	0.85
5:A:804:OXY:O1	6:A:805:NIZ:N2	2.11	0.84
7:A:806:MPD:HO4	7:A:806:MPD:H11	1.46	0.80
7:A:806:MPD:C1	7:A:806:MPD:O4	2.25	0.80
1:B:47:LEU:O	9:B:901:HOH:O	2.00	0.79
7:A:806:MPD:H51	9:A:1600:HOH:O	1.83	0.77
7:A:807:MPD:C5	7:A:807:MPD:H12	2.14	0.77
1:B:622:GLN:OE1	6:B:805:NIZ:O1	2.08	0.72
1:A:343:GLU:OE1	9:A:901:HOH:O	2.12	0.67
7:B:807:MPD:HM1	9:B:1374:HOH:O	1.93	0.67
1:B:55:HIS:HD2	9:B:1287:HOH:O	1.81	0.62
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.81	0.62
1:A:593:VAL:HG13	9:A:926:HOH:O	2.00	0.62
7:A:807:MPD:H52	7:A:807:MPD:H12	1.83	0.59
1:B:519:GLU:OE1	9:B:902:HOH:O	2.16	0.59
1:B:40:ARG:NH1	9:B:908:HOH:O	2.35	0.58
1:B:730[A]:ARG:HD2	9:B:1519:HOH:O	2.04	0.58
7:B:808:MPD:HM2	7:B:808:MPD:C5	2.34	0.58
7:B:808:MPD:HM2	7:B:808:MPD:H52	1.84	0.58
1:B:403:ARG:NH1	9:B:910:HOH:O	2.38	0.57
1:B:591:MET:SD	1:B:594:LEU:HD12	2.46	0.56
1:A:69:ALA:O	1:A:73:GLU:HG3	2.06	0.56
1:A:647:GLN:HG2	9:A:1127:HOH:O	2.04	0.56
1:B:512:ASP:OD1	9:B:903:HOH:O	2.18	0.55
1:A:343:GLU:HG3	9:A:901:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:MET:SD	1:A:594:LEU:HD12	2.48	0.53
7:A:807:MPD:H53	7:A:807:MPD:H12	1.88	0.53
7:B:807:MPD:O2	7:B:807:MPD:O4	2.27	0.50
1:B:662:ASN:H	1:B:725:GLN:HE22	1.60	0.48
1:B:64:LYS:HD3	1:B:64:LYS:O	2.15	0.46
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.99	0.46
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.61	0.44
1:B:622:GLN:HE22	6:B:805:NIZ:C1	2.30	0.44
1:A:504:ARG:HD2	9:A:932:HOH:O	2.18	0.43
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.48	0.43
1:A:544:GLN:OE1	9:A:902:HOH:O	2.21	0.43
7:A:807:MPD:C5	7:A:807:MPD:C1	2.88	0.43
7:A:807:MPD:HM3	9:A:1039:HOH:O	2.17	0.43
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.62	0.43
1:B:540:ARG:HA	1:B:540:ARG:NH1	2.34	0.42
6:A:805:NIZ:H4	9:A:1191:HOH:O	2.20	0.42
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.55	0.41
1:A:471:LEU:HA	1:A:471:LEU:HD23	1.94	0.41
1:B:112:HIS:NE2	6:B:806:NIZ:N2	2.69	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:1132:HOH:O	9:B:1056:HOH:O[2_444]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	715/728 (98%)	706 (99%)	9 (1%)	0	100 | 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	716/728 (98%)	709 (99%)	7 (1%)	0	100	100
All	All	1431/1456 (98%)	1415 (99%)	16 (1%)	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	553/560 (99%)	546 (99%)	7 (1%)	76	62
1	B	554/560 (99%)	545 (98%)	9 (2%)	70	54
All	All	1107/1120 (99%)	1091 (99%)	16 (1%)	72	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	118	ARG
1	A	589	GLU
1	A	608	LYS
1	A	610	ARG
1	A	725	GLN
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	74	LYS
1	B	118	ARG
1	B	608	LYS
1	B	610	ARG
1	B	647	GLN
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	B	46	GLN
1	B	55	HIS
1	B	227	ASN
1	B	622	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	1,6	24,50,50	1.79	6 (25%)	16,82,82	2.20	6 (37%)
5	OXY	A	804	-	1,1,1	0.32	0	0,0,0	0.00	-
6	NIZ	A	805	2	10,10,10	3.80	6 (60%)	12,12,12	1.73	3 (25%)
7	MPD	A	806	-	6,7,7	1.28	0	6,10,10	1.53	1 (16%)
7	MPD	A	807	-	6,7,7	0.76	0	6,10,10	1.94	2 (33%)
8	PO4	A	808	-	4,4,4	0.99	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	HEM	B	801	1,6	24,50,50	2.03	6 (25%)	16,82,82	2.45	8 (50%)
5	OXY	B	804	-	1,1,1	0.04	0	0,0,0	0.00	-
6	NIZ	B	805	-	10,10,10	4.65	7 (70%)	12,12,12	4.09	9 (75%)
6	NIZ	B	806	2	10,10,10	3.98	4 (40%)	12,12,12	2.98	8 (66%)
7	MPD	B	807	-	6,7,7	0.67	0	6,10,10	1.39	2 (33%)
7	MPD	B	808	-	6,7,7	1.12	0	6,10,10	0.99	1 (16%)
8	PO4	B	809	-	4,4,4	1.67	1 (25%)	6,6,6	0.66	0

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	1,6	-	0/6/54/54	0/0/8/8
5	OXY	A	804	-	-	0/0/0/0	0/0/0/0
6	NIZ	A	805	2	-	0/6/6/6	0/1/1/1
7	MPD	A	806	-	-	0/5/5/5	0/0/0/0
7	MPD	A	807	-	-	0/5/5/5	0/0/0/0
8	PO4	A	808	-	-	0/0/0/0	0/0/0/0
2	HEM	B	801	1,6	-	0/6/54/54	0/0/8/8
5	OXY	B	804	-	-	0/0/0/0	0/0/0/0
6	NIZ	B	805	-	-	0/6/6/6	0/1/1/1
6	NIZ	B	806	2	-	0/6/6/6	0/1/1/1
7	MPD	B	807	-	-	0/5/5/5	0/0/0/0
7	MPD	B	808	-	-	0/5/5/5	0/0/0/0
8	PO4	B	809	-	-	0/0/0/0	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-6.95	1.31	1.40
2	A	801	HEM	CAD-C3D	-4.60	1.46	1.52
6	B	805	NIZ	N3-N2	-4.42	1.35	1.41
2	B	801	HEM	C3C-CAC	-3.73	1.39	1.47
2	A	801	HEM	CMD-C2D	-3.03	1.45	1.51
8	B	809	PO4	P-O3	-3.01	1.44	1.53
2	B	801	HEM	C4C-NC	-2.69	1.33	1.36
6	A	805	NIZ	O1-C	-2.46	1.18	1.23
6	B	805	NIZ	C1-C	-2.31	1.45	1.50
2	B	801	HEM	C4A-CHB	-2.20	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	CMD-C2D	-2.06	1.47	1.51
2	B	801	HEM	CMB-C2B	2.22	1.56	1.51
2	A	801	HEM	C1C-NC	2.36	1.39	1.36
2	A	801	HEM	CAA-C2A	2.58	1.56	1.52
2	A	801	HEM	CMA-C3A	2.59	1.57	1.51
6	B	805	NIZ	C2-C3	2.67	1.44	1.38
6	A	805	NIZ	C4-N1	3.13	1.42	1.33
6	A	805	NIZ	C5-C1	3.20	1.44	1.39
2	A	801	HEM	C4D-ND	3.46	1.41	1.36
6	B	805	NIZ	C-N2	3.70	1.37	1.33
6	B	806	NIZ	C3-N1	3.79	1.44	1.33
6	A	805	NIZ	C3-N1	3.95	1.45	1.33
6	B	806	NIZ	C4-N1	4.76	1.47	1.33
6	B	806	NIZ	C2-C1	5.00	1.47	1.39
6	A	805	NIZ	C2-C1	5.73	1.48	1.39
6	B	805	NIZ	C2-C1	6.02	1.49	1.39
6	B	805	NIZ	C5-C1	6.81	1.50	1.39
6	A	805	NIZ	C-N2	8.14	1.40	1.33
6	B	806	NIZ	C-N2	9.16	1.41	1.33
6	B	805	NIZ	C4-N1	9.31	1.60	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	805	NIZ	C5-C4-N1	-6.03	113.20	123.64
2	A	801	HEM	CAA-CBA-CGA	-5.50	102.08	112.78
6	B	805	NIZ	O1-C-C1	-5.09	112.22	120.95
6	B	805	NIZ	C3-C2-C1	-4.35	114.21	119.07
2	A	801	HEM	C3B-CAB-CBB	-3.49	119.38	126.40
2	B	801	HEM	C3B-CAB-CBB	-3.41	119.53	126.40
7	A	807	MPD	CM-C2-C1	-3.38	102.34	110.41
6	B	805	NIZ	C-N2-N3	-3.02	117.97	121.77
6	B	806	NIZ	O1-C-N2	-2.96	119.03	122.28
6	B	806	NIZ	C5-C1-C	-2.93	111.28	120.62
6	B	806	NIZ	O1-C-C1	-2.78	116.19	120.95
6	B	806	NIZ	C3-C2-C1	-2.56	116.20	119.07
6	A	805	NIZ	O1-C-C1	-2.55	116.58	120.95
2	B	801	HEM	CAA-CBA-CGA	-2.52	107.88	112.78
6	B	805	NIZ	O1-C-N2	-2.49	119.55	122.28
6	A	805	NIZ	C5-C4-N1	-2.34	119.58	123.64
6	B	806	NIZ	C4-C5-C1	-2.15	116.66	119.07
2	A	801	HEM	CMA-C3A-C4A	-2.06	124.81	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	806	NIZ	C-N2-N3	-2.02	119.22	121.77
6	B	805	NIZ	C5-C1-C	-2.01	114.19	120.62
7	B	807	MPD	O2-C2-C1	-2.01	100.63	108.01
2	A	801	HEM	CMB-C2B-C3B	2.00	129.01	125.09
7	B	807	MPD	CM-C2-C1	2.03	115.25	110.41
7	A	807	MPD	O2-C2-CM	2.04	115.52	108.01
2	B	801	HEM	C3C-CAC-CBC	2.14	130.70	126.40
7	B	808	MPD	CM-C2-C1	2.28	115.85	110.41
2	A	801	HEM	CAD-CBD-CGD	2.56	117.77	112.78
7	A	806	MPD	CM-C2-C1	2.65	116.73	110.41
6	A	805	NIZ	C1-C-N2	2.97	119.93	116.41
2	B	801	HEM	CBA-CAA-C2A	3.06	117.87	112.49
2	A	801	HEM	CBD-CAD-C3D	3.21	118.11	112.47
2	B	801	HEM	CAD-CBD-CGD	3.33	119.26	112.78
6	B	805	NIZ	C3-N1-C4	3.36	124.92	116.84
2	B	801	HEM	CMD-C2D-C3D	3.65	132.86	125.24
2	B	801	HEM	CBD-CAD-C3D	3.72	118.99	112.47
6	B	806	NIZ	C2-C1-C5	3.74	123.74	118.61
2	B	801	HEM	CMB-C2B-C3B	4.03	132.97	125.09
6	B	805	NIZ	C2-C1-C5	4.80	125.18	118.61
6	B	806	NIZ	C1-C-N2	7.02	124.70	116.41
6	B	805	NIZ	C1-C-N2	7.97	125.83	116.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	OXY	1	0
6	A	805	NIZ	2	0
7	A	806	MPD	5	0
7	A	807	MPD	5	0
5	B	804	OXY	1	0
6	B	805	NIZ	2	0
6	B	806	NIZ	2	0
7	B	807	MPD	2	0
7	B	808	MPD	2	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(Å^2)	Q<0.9
1	A	713/728 (97%)	-0.33	18 (2%)	61	65	12, 20, 37, 80	0
1	B	713/728 (97%)	-0.34	16 (2%)	65	70	12, 19, 37, 82	0
All	All	1426/1456 (97%)	-0.34	34 (2%)	62	66	12, 20, 37, 82	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	8.4
1	B	610	ARG	5.5
1	B	748	ALA	5.0
1	B	540	ARG	4.7
1	A	540	ARG	4.5
1	A	541	GLY	4.4
1	B	679	ALA	4.3
1	A	680	ALA	4.2
1	A	608	LYS	4.0
1	B	541	GLY	3.9
1	A	454	ASP	3.7
1	A	679	ALA	3.5
1	A	610	ARG	3.5
1	B	608	LYS	3.3
1	B	65	ASP	3.0
1	A	221	GLY	2.9
1	A	215	PRO	2.9
1	B	680	ALA	2.9
1	B	454	ASP	2.7
1	B	682	ALA	2.6
1	A	222	ASP	2.6
1	A	542	GLY	2.3
1	A	64	LYS	2.3
1	B	366	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	609	TYR	2.3
1	A	647	GLN	2.3
1	A	213	GLY	2.3
1	B	64	LYS	2.3
1	A	220	SER	2.2
1	B	611	VAL	2.2
1	B	74	LYS	2.1
1	B	378	SER	2.1
1	A	378	SER	2.1
1	A	65	ASP	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 (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(Å²)	Q<0.9
6	NIZ	B	805	10/10	0.74	0.25	7.92	26,39,48,49	0
7	MPD	A	807	8/8	0.90	0.12	2.98	42,50,57,68	0
7	MPD	B	807	8/8	0.90	0.12	2.14	46,54,59,60	0
6	NIZ	A	805	10/10	0.90	0.11	1.08	28,32,35,35	0
6	NIZ	B	806	10/10	0.88	0.13	1.01	26,30,34,35	0
2	HEM	A	801	43/43	0.99	0.09	0.52	12,15,19,20	0
2	HEM	B	801	43/43	0.99	0.10	0.37	12,14,17,20	0
4	CL	B	803	1/1	0.98	0.05	-2.38	31,31,31,31	0
3	NA	B	802	1/1	0.99	0.03	-3.07	17,17,17,17	0
3	NA	A	802	1/1	0.99	0.03	-3.14	16,16,16,16	0
4	CL	A	803	1/1	0.99	0.04	-3.44	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	OXY	B	804	2/2	0.96	0.08	-	26,26,26,40	0
8	PO4	B	809	5/5	0.96	0.21	-	35,46,50,54	0
8	PO4	A	808	5/5	0.96	0.23	-	44,54,60,61	0
7	MPD	B	808	8/8	0.79	0.21	-	44,63,71,74	0
7	MPD	A	806	8/8	0.77	0.20	-	38,41,55,59	0
5	OXY	A	804	2/2	0.96	0.07	-	23,23,23,38	0

6.5 Other polymers (i)

There are no such residues in this entry.