Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 02:57 PM JST

PDB ID	:	4ZRC
Title	:	Crystal structure of MSM-13, a putative T1-like thiolase from Mycobacterium smegmatis
Authors	:	Janardan, N.; Harijan, R.K.; Keima, T.R.; Wierenga, R.; Murthy, M.R.N.
Deposited on	:	2015-05-12
Resolution	:	2.70 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

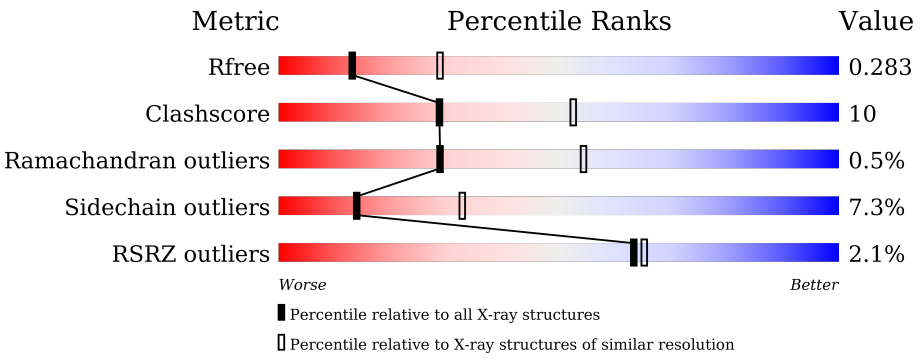
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	413	2% 77% 15% • • 5%
1	B	413	2% 77% 16% • • •
1	C	413	2% 76% 18% • •
1	D	413	3% 74% 19% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11586 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 Beta-ketothiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	2794	1721	513	544	16	0	0	0
1	B	397	2885	1780	531	558	16	0	0	0
1	C	396	2904	1790	537	561	16	0	0	0
1	D	395	2900	1790	535	559	16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP A0QUH3
A	-4	HIS	-	expression tag	UNP A0QUH3
A	-3	HIS	-	expression tag	UNP A0QUH3
A	-2	HIS	-	expression tag	UNP A0QUH3
A	-1	HIS	-	expression tag	UNP A0QUH3
A	0	HIS	-	expression tag	UNP A0QUH3
B	-5	HIS	-	expression tag	UNP A0QUH3
B	-4	HIS	-	expression tag	UNP A0QUH3
B	-3	HIS	-	expression tag	UNP A0QUH3
B	-2	HIS	-	expression tag	UNP A0QUH3
B	-1	HIS	-	expression tag	UNP A0QUH3
B	0	HIS	-	expression tag	UNP A0QUH3
C	-5	HIS	-	expression tag	UNP A0QUH3
C	-4	HIS	-	expression tag	UNP A0QUH3
C	-3	HIS	-	expression tag	UNP A0QUH3
C	-2	HIS	-	expression tag	UNP A0QUH3
C	-1	HIS	-	expression tag	UNP A0QUH3
C	0	HIS	-	expression tag	UNP A0QUH3
D	-5	HIS	-	expression tag	UNP A0QUH3
D	-4	HIS	-	expression tag	UNP A0QUH3
D	-3	HIS	-	expression tag	UNP A0QUH3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	expression tag	UNP A0QUH3
D	-1	HIS	-	expression tag	UNP A0QUH3
D	0	HIS	-	expression tag	UNP A0QUH3

- Molecule 2 is water.

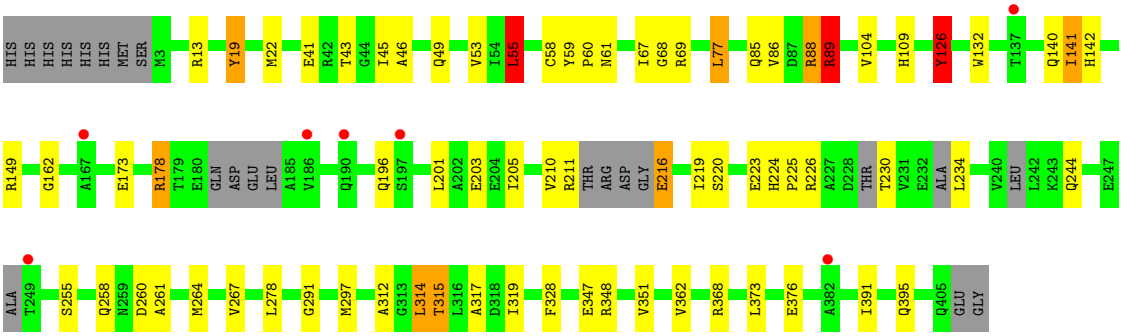
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	31	31	31	0	0
			Total	O		
2	B	25	25	25	0	0
			Total	O		
2	C	32	32	32	0	0
			Total	O		
2	D	15	15	15	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

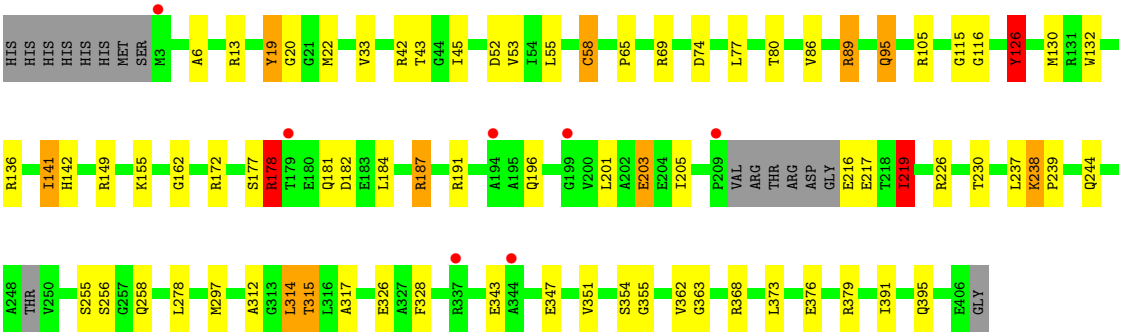
• Molecule 1: Beta-ketothiolase

Chain A:



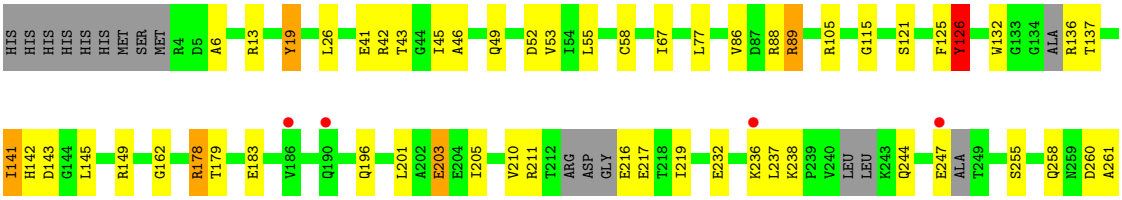
• Molecule 1: Beta-ketothiolase

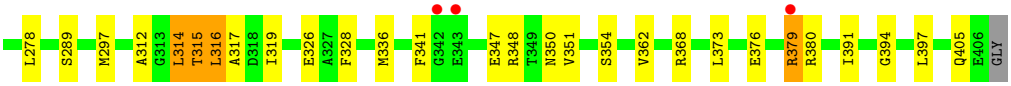
Chain B:



• Molecule 1: Beta-ketothiolase

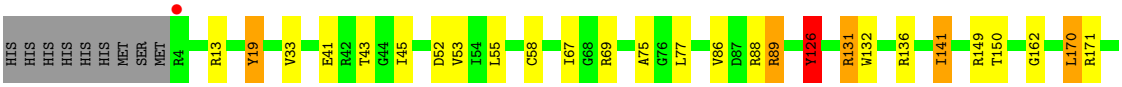
Chain C:

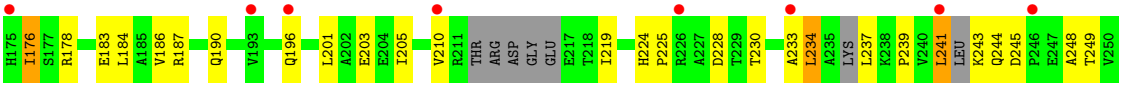


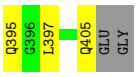


- Molecule 1: Beta-ketothiolase

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.46Å 104.14Å 104.57Å 90.00° 107.53° 90.00°	Depositor
Resolution (Å)	47.52 – 2.70 69.05 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.52-2.70) 99.0 (69.05-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.223 , 0.283 0.223 , 0.283	Depositor DCC
R_{free} test set	2129 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 17.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11586	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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)

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	0.68	5/2831 (0.2%)	0.83	6/3837 (0.2%)
1	B	0.65	5/2927 (0.2%)	0.81	4/3970 (0.1%)
1	C	0.64	2/2944 (0.1%)	0.79	1/3987 (0.0%)
1	D	0.68	4/2942 (0.1%)	0.87	3/3989 (0.1%)
All	All	0.66	16/11644 (0.1%)	0.82	14/15783 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	178	ARG	CZ-NH1	-12.12	1.17	1.33
1	D	126	TYR	CE1-CZ	-8.96	1.26	1.38
1	A	126	TYR	CE1-CZ	-8.21	1.27	1.38
1	B	126	TYR	CE1-CZ	-7.21	1.29	1.38
1	B	95	GLN	CD-NE2	-6.81	1.15	1.32
1	A	126	TYR	CG-CD2	-6.55	1.30	1.39
1	A	89	ARG	CZ-NH1	-6.52	1.24	1.33
1	D	126	TYR	CG-CD1	-6.25	1.31	1.39
1	D	126	TYR	CG-CD2	-6.23	1.31	1.39
1	C	126	TYR	CE1-CZ	-6.09	1.30	1.38
1	A	126	TYR	CE2-CZ	-6.03	1.30	1.38
1	B	126	TYR	CG-CD1	-5.87	1.31	1.39
1	B	126	TYR	CG-CD2	-5.86	1.31	1.39
1	C	126	TYR	CG-CD2	-5.70	1.31	1.39
1	A	126	TYR	CG-CD1	-5.34	1.32	1.39
1	B	95	GLN	CD-OE1	-5.03	1.12	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	178	ARG	NE-CZ-NH2	21.32	130.96	120.30
1	B	219	ILE	CG1-CB-CG2	-9.85	89.72	111.40
1	D	178	ARG	NH1-CZ-NH2	-7.74	110.89	119.40
1	A	89	ARG	NE-CZ-NH2	7.70	124.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	C	178	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	B	178	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	A	88	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	69	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	55	LEU	CD1-CG-CD2	-5.32	94.54	110.50
1	A	89	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
1	B	58	CYS	CA-CB-SG	-5.16	104.71	114.00
1	A	69	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	131	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2794	0	2683	61	0
1	B	2885	0	2824	65	1
1	C	2904	0	2861	63	1
1	D	2900	0	2871	68	0
2	A	31	0	0	4	0
2	B	25	0	0	1	0
2	C	32	0	0	3	0
2	D	15	0	0	0	0
All	All	11586	0	11239	221	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 10.

All (221) 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:89:ARG:NH1	1:B:65:PRO:HB3	1.69	1.06
1:A:89:ARG:HH11	1:B:65:PRO:HB3	1.24	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:CYS:HB3	1:A:89:ARG:HH21	1.38	0.89
1:C:19:TYR:HE1	1:D:132:TRP:CH2	1.92	0.88
1:A:89:ARG:HH11	1:B:65:PRO:CB	1.88	0.87
1:D:53:VAL:HG12	1:D:55:LEU:HD13	1.57	0.86
1:C:53:VAL:HG12	1:C:55:LEU:HD13	1.61	0.82
1:A:132:TRP:CH2	1:B:19:TYR:HE1	1.99	0.81
1:C:132:TRP:CH2	1:D:19:TYR:HE1	2.00	0.78
1:C:19:TYR:HE1	1:D:132:TRP:HH2	1.33	0.76
1:B:53:VAL:HG12	1:B:55:LEU:HD13	1.65	0.76
1:D:171:ARG:HA	1:D:176:ILE:HD12	1.68	0.76
1:D:45:ILE:HD11	1:D:278:LEU:HD21	1.68	0.75
1:D:230:THR:OG1	1:D:233:ALA:HB3	1.89	0.72
1:A:45:ILE:HD11	1:A:278:LEU:HD21	1.72	0.71
1:D:77:LEU:HD12	1:D:77:LEU:H	1.57	0.70
1:C:89:ARG:HB2	1:C:391:ILE:HG23	1.74	0.70
1:C:19:TYR:CE1	1:D:132:TRP:CH2	2.80	0.68
1:A:53:VAL:HG12	1:A:55:LEU:CD1	2.24	0.68
1:A:19:TYR:HD1	1:A:19:TYR:C	1.97	0.68
1:C:19:TYR:HD1	1:C:19:TYR:C	1.96	0.67
1:A:53:VAL:HG12	1:A:55:LEU:HD12	1.75	0.67
1:C:126:TYR:CE1	1:C:142:HIS:HB2	2.31	0.66
1:A:77:LEU:HD12	1:A:77:LEU:H	1.61	0.66
1:D:184:LEU:HA	1:D:187:ARG:HH21	1.60	0.66
1:A:126:TYR:CE1	1:A:142:HIS:HB2	2.30	0.65
1:A:55:LEU:HD13	1:A:68:GLY:HA2	1.79	0.65
1:B:45:ILE:HD11	1:B:278:LEU:HD21	1.79	0.64
1:A:55:LEU:HD21	1:A:264:MET:CE	2.28	0.64
1:D:149:ARG:O	1:D:162:GLY:HA2	1.96	0.64
1:A:149:ARG:O	1:A:162:GLY:HA2	1.98	0.64
1:C:88:ARG:NH2	1:D:52:ASP:OD1	2.30	0.64
1:C:19:TYR:CE1	1:D:132:TRP:HH2	2.16	0.64
1:B:126:TYR:HD1	1:B:126:TYR:C	2.01	0.63
1:A:19:TYR:C	1:A:19:TYR:CD1	2.72	0.63
1:B:126:TYR:CE1	1:B:142:HIS:HB2	2.34	0.63
1:B:141:ILE:HD11	1:C:141:ILE:HD11	1.80	0.63
1:A:141:ILE:HD11	1:D:141:ILE:HD11	1.79	0.62
1:C:77:LEU:H	1:C:77:LEU:HD12	1.64	0.62
1:C:132:TRP:CZ2	1:D:19:TYR:HE1	2.17	0.62
1:C:19:TYR:C	1:C:19:TYR:CD1	2.72	0.62
1:B:149:ARG:O	1:B:162:GLY:HA2	1.99	0.62
1:B:19:TYR:C	1:B:19:TYR:HD1	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:HD1	1:B:126:TYR:O	1.84	0.61
1:A:88:ARG:NH2	1:B:52:ASP:OD1	2.33	0.61
1:C:136:ARG:HG2	1:C:137:THR:HG23	1.82	0.61
1:B:53:VAL:HG12	1:B:55:LEU:CD1	2.30	0.61
1:B:89:ARG:HB2	1:B:391:ILE:HG23	1.81	0.61
1:B:19:TYR:C	1:B:19:TYR:CD1	2.73	0.61
1:A:291:GLY:O	1:B:80:THR:HA	2.01	0.61
1:D:170:LEU:HD23	1:D:331:GLN:HA	1.83	0.61
1:A:132:TRP:HH2	1:B:19:TYR:HE1	1.49	0.60
1:D:391:ILE:HB	1:D:395:GLN:HB2	1.83	0.60
1:C:132:TRP:CH2	1:D:19:TYR:CE1	2.89	0.60
1:A:58:CYS:HB3	1:A:89:ARG:NH2	2.12	0.59
1:B:77:LEU:HD12	1:B:77:LEU:H	1.66	0.59
1:B:126:TYR:C	1:B:126:TYR:CD1	2.76	0.59
1:D:53:VAL:HG12	1:D:55:LEU:CD1	2.32	0.59
1:C:211:ARG:HA	1:C:216:GLU:HA	1.85	0.58
1:C:142:HIS:ND1	2:C:503:HOH:O	2.31	0.58
1:A:230:THR:O	1:A:234:LEU:CB	2.51	0.58
1:D:19:TYR:CD1	1:D:19:TYR:C	2.77	0.58
1:B:141:ILE:HD11	1:C:141:ILE:CD1	2.33	0.58
1:C:149:ARG:O	1:C:162:GLY:HA2	2.04	0.57
1:D:19:TYR:C	1:D:19:TYR:HD1	2.07	0.57
1:D:89:ARG:HB2	1:D:391:ILE:HG23	1.86	0.57
1:B:55:LEU:HA	1:B:115:GLY:O	2.04	0.57
1:C:45:ILE:HD11	1:C:278:LEU:HD21	1.86	0.57
1:A:13:ARG:HD3	1:A:368:ARG:HG3	1.86	0.56
1:D:13:ARG:HD3	1:D:368:ARG:HG3	1.88	0.56
1:D:379:ARG:HB2	1:D:379:ARG:HH11	1.70	0.56
1:A:55:LEU:HD21	1:A:264:MET:HE1	1.88	0.56
1:B:13:ARG:CD	1:B:368:ARG:HG3	2.37	0.55
1:C:379:ARG:HH11	1:C:379:ARG:HB2	1.72	0.55
1:B:13:ARG:HD3	1:B:368:ARG:HG3	1.87	0.55
1:B:141:ILE:CD1	1:C:141:ILE:HD11	2.36	0.55
1:D:13:ARG:CD	1:D:368:ARG:HG3	2.36	0.55
1:A:61:ASN:HB2	1:B:126:TYR:CE2	2.42	0.55
1:D:43:THR:OG1	1:D:45:ILE:HG12	2.07	0.55
1:A:142:HIS:ND1	2:A:501:HOH:O	2.33	0.54
1:B:58:CYS:O	1:B:89:ARG:NH2	2.41	0.54
1:D:126:TYR:CD1	1:D:126:TYR:C	2.81	0.54
1:A:319:ILE:O	1:A:348:ARG:NH1	2.40	0.53
1:C:315:THR:HG23	1:C:317:ALA:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:TRP:HH2	1:B:19:TYR:CE1	2.27	0.53
1:A:104:VAL:HG21	1:A:267:VAL:HG12	1.91	0.53
1:A:132:TRP:CZ2	1:B:19:TYR:HE1	2.26	0.53
1:A:132:TRP:CH2	1:B:19:TYR:CE1	2.90	0.52
1:A:43:THR:OG1	1:A:45:ILE:HG12	2.09	0.52
1:D:19:TYR:HD2	1:D:258:GLN:NE2	2.08	0.52
1:A:88:ARG:HH22	1:B:52:ASP:CG	2.14	0.52
1:A:13:ARG:CD	1:A:368:ARG:HG3	2.38	0.51
1:B:312:ALA:HB1	1:B:314:LEU:HD12	1.91	0.51
1:C:149:ARG:NH2	1:C:258:GLN:OE1	2.44	0.51
1:B:178:ARG:HD2	1:B:182:ASP:OD2	2.09	0.51
1:C:55:LEU:HA	1:C:115:GLY:O	2.11	0.51
1:C:58:CYS:O	1:C:89:ARG:NH2	2.44	0.51
1:A:141:ILE:HD11	1:D:141:ILE:CD1	2.41	0.51
1:D:126:TYR:C	1:D:126:TYR:HD1	2.13	0.51
1:C:13:ARG:HD3	1:C:368:ARG:HG3	1.93	0.51
1:A:351:VAL:HG21	1:A:376:GLU:HG2	1.92	0.50
1:A:86:VAL:HG12	1:B:86:VAL:HG12	1.92	0.50
1:A:141:ILE:CD1	1:D:141:ILE:HD11	2.41	0.50
1:A:149:ARG:NH2	1:A:258:GLN:OE1	2.44	0.50
1:B:255:SER:HB2	1:B:328:PHE:CD2	2.45	0.50
1:C:13:ARG:CD	1:C:368:ARG:HG3	2.41	0.50
1:D:315:THR:HG23	1:D:317:ALA:H	1.77	0.50
1:D:239:PRO:HA	1:D:251:THR:HG22	1.92	0.50
1:B:326:GLU:OE1	1:B:354:SER:HB3	2.12	0.50
1:D:19:TYR:CD2	1:D:258:GLN:NE2	2.80	0.49
1:C:26:LEU:HD11	1:C:210:VAL:HG12	1.93	0.49
1:A:196:GLN:HG3	1:A:201:LEU:HD22	1.94	0.49
1:D:228:ASP:O	1:D:230:THR:HG23	2.13	0.49
1:A:55:LEU:HD21	1:A:264:MET:HE2	1.95	0.49
1:C:312:ALA:HB1	1:C:314:LEU:HD12	1.95	0.49
1:A:315:THR:HG23	1:A:317:ALA:H	1.77	0.49
1:D:149:ARG:NH2	1:D:258:GLN:OE1	2.46	0.49
1:D:319:ILE:O	1:D:348:ARG:NH1	2.40	0.49
1:C:52:ASP:OD1	1:D:88:ARG:NH2	2.46	0.49
1:A:55:LEU:CD1	1:A:68:GLY:HA2	2.42	0.48
1:C:53:VAL:HG12	1:C:55:LEU:CD1	2.38	0.48
1:D:241:LEU:O	1:D:243:LYS:N	2.47	0.48
1:A:19:TYR:HE1	1:B:132:TRP:CH2	2.32	0.48
1:B:256:SER:HB2	1:B:355:GLY:O	2.13	0.48
1:B:130:MET:HE1	1:B:141:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ARG:HD2	1:B:191:ARG:HH21	1.78	0.48
1:C:247:GLU:OE1	1:C:247:GLU:N	2.47	0.48
1:B:126:TYR:HE1	1:B:142:HIS:CD2	2.32	0.48
1:D:326:GLU:OE1	1:D:354:SER:HB3	2.13	0.48
1:C:86:VAL:HG12	1:D:86:VAL:HG12	1.96	0.47
1:C:316:LEU:HD11	1:C:341:PHE:HE1	1.79	0.47
1:C:394:GLY:O	1:D:69:ARG:NH2	2.47	0.47
1:D:58:CYS:O	1:D:89:ARG:NH2	2.46	0.47
1:D:77:LEU:H	1:D:77:LEU:CD1	2.27	0.47
1:D:230:THR:HG1	1:D:233:ALA:HB3	1.79	0.47
1:B:43:THR:OG1	1:B:45:ILE:HG12	2.15	0.47
1:C:132:TRP:HH2	1:D:19:TYR:CE1	2.30	0.47
1:C:326:GLU:OE1	1:C:354:SER:HB3	2.14	0.47
1:C:219:ILE:HG21	1:C:219:ILE:HD13	1.66	0.47
1:D:13:ARG:O	1:D:205:ILE:HA	2.15	0.47
1:D:312:ALA:HB1	1:D:314:LEU:HD12	1.97	0.46
1:B:177:SER:O	1:B:181:GLN:HG3	2.15	0.46
1:C:319:ILE:O	1:C:348:ARG:NH1	2.47	0.46
1:D:260:ASP:O	1:D:261:ALA:HB2	2.16	0.46
1:D:379:ARG:HB2	1:D:379:ARG:NH1	2.28	0.46
1:D:255:SER:HB2	1:D:328:PHE:CD2	2.50	0.46
1:A:312:ALA:HB1	1:A:314:LEU:HD12	1.98	0.46
2:A:525:HOH:O	1:B:155:LYS:HE3	2.14	0.46
1:D:289:SER:HB3	1:D:397:LEU:HD12	1.98	0.46
1:D:171:ARG:NH1	1:D:248:ALA:HA	2.31	0.46
1:C:260:ASP:O	1:C:261:ALA:HB2	2.16	0.45
1:A:260:ASP:O	1:A:261:ALA:HB2	2.15	0.45
1:B:19:TYR:HD1	1:B:20:GLY:N	2.14	0.45
1:A:211:ARG:HA	1:A:216:GLU:HA	1.98	0.45
1:D:234:LEU:O	1:D:237:LEU:N	2.49	0.45
1:D:351:VAL:HG21	1:D:376:GLU:HG2	1.99	0.45
1:A:89:ARG:HB2	1:A:391:ILE:HG23	1.99	0.45
1:A:255:SER:HB2	1:A:328:PHE:CD2	2.51	0.45
1:B:178:ARG:HH21	1:B:239:PRO:HG3	1.81	0.45
1:A:59:TYR:N	1:A:60:PRO:CD	2.80	0.45
1:C:46:ALA:O	1:C:49:GLN:HB2	2.17	0.45
1:A:19:TYR:HE1	1:B:132:TRP:HH2	1.65	0.45
1:A:224:HIS:N	1:A:225:PRO:CD	2.80	0.45
1:B:22:MET:SD	1:B:219:ILE:HD13	2.57	0.45
1:B:149:ARG:NH2	1:B:258:GLN:OE1	2.49	0.45
1:B:351:VAL:HG21	1:B:376:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:SER:O	1:D:131:ARG:HD2	2.17	0.44
1:C:351:VAL:HG21	1:C:376:GLU:HG2	1.98	0.44
1:C:43:THR:OG1	1:C:45:ILE:HG12	2.17	0.44
1:D:196:GLN:HG3	1:D:201:LEU:HD22	2.00	0.44
1:A:109:HIS:HE1	2:B:503:HOH:O	2.00	0.44
1:C:145:LEU:O	2:C:501:HOH:O	2.21	0.43
1:B:33:VAL:HG21	1:B:74:ASP:HB3	2.00	0.43
1:B:219:ILE:HD13	1:B:219:ILE:HG21	1.36	0.43
1:D:33:VAL:HG22	1:D:75:ALA:HB2	1.99	0.43
1:C:196:GLN:HG3	1:C:201:LEU:HD22	2.00	0.43
1:C:132:TRP:CZ2	1:D:19:TYR:CE1	3.02	0.43
1:B:6:ALA:HB2	1:B:105:ARG:HG3	2.00	0.43
1:B:238:LYS:HG2	1:B:238:LYS:O	2.18	0.43
1:C:179:THR:O	1:C:183:GLU:HG3	2.19	0.43
1:C:238:LYS:NZ	1:C:238:LYS:HB3	2.34	0.43
1:B:391:ILE:HB	1:B:395:GLN:HB2	2.01	0.42
1:C:6:ALA:HB2	1:C:105:ARG:HG3	2.01	0.42
1:D:171:ARG:HD2	1:D:249:THR:HG23	2.01	0.42
1:B:141:ILE:HG13	1:C:141:ILE:HG13	2.01	0.42
1:B:196:GLN:HG3	1:B:201:LEU:HD22	2.01	0.42
1:C:289:SER:HB3	1:C:397:LEU:HD12	2.01	0.42
1:A:391:ILE:HB	1:A:395:GLN:HB2	2.00	0.42
1:A:53:VAL:HG12	1:A:55:LEU:HD11	1.98	0.42
1:C:255:SER:HB2	1:C:328:PHE:CD2	2.55	0.42
1:D:219:ILE:HD13	1:D:219:ILE:HG21	1.67	0.42
1:D:352:ARG:HD2	1:D:372:THR:HG23	2.02	0.42
1:A:67:ILE:HG22	1:A:85:GLN:HB2	2.01	0.42
1:C:13:ARG:O	1:C:205:ILE:HA	2.20	0.42
1:C:350:ASN:N	2:C:506:HOH:O	2.50	0.42
1:C:58:CYS:HB3	1:C:89:ARG:NH2	2.35	0.42
1:A:46:ALA:O	1:A:49:GLN:HB2	2.20	0.41
1:C:42:ARG:NH1	1:C:203:GLU:O	2.52	0.41
1:A:13:ARG:O	1:A:205:ILE:HA	2.20	0.41
1:A:173:GLU:HG2	2:A:527:HOH:O	2.20	0.41
1:D:245:ASP:HB3	1:D:248:ALA:HB2	2.01	0.41
1:A:140:GLN:NE2	2:A:502:HOH:O	2.34	0.41
1:B:184:LEU:HA	1:B:187:ARG:HH21	1.85	0.41
1:D:184:LEU:CA	1:D:187:ARG:HH21	2.30	0.41
1:A:22:MET:SD	1:A:223:GLU:HB2	2.60	0.41
1:B:42:ARG:NH1	1:B:203:GLU:O	2.54	0.41
1:B:116:GLY:HA3	1:B:363:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:HIS:N	1:D:225:PRO:CD	2.84	0.41
1:B:187:ARG:HG2	1:B:191:ARG:HH21	1.86	0.41
1:C:125:PHE:CE2	1:C:143:ASP:HB2	2.55	0.41
1:D:293:ALA:HB3	1:D:296:LEU:HB2	2.02	0.41
1:A:219:ILE:HD13	1:A:219:ILE:HG21	1.84	0.41
1:B:95:GLN:NE2	1:B:95:GLN:HA	2.36	0.41
1:B:315:THR:HG23	1:B:317:ALA:H	1.86	0.40
1:C:232:GLU:H	1:C:232:GLU:CD	2.24	0.40
1:C:196:GLN:HG3	1:C:201:LEU:CD2	2.51	0.40
1:B:13:ARG:O	1:B:205:ILE:HA	2.22	0.40
1:D:256:SER:HB2	1:D:355:GLY:O	2.21	0.40
1:C:336:MET:O	1:C:341:PHE:HB2	2.21	0.40
1:B:196:GLN:HG3	1:B:201:LEU:CD2	2.52	0.40
1:D:186:VAL:HG12	1:D:190:GLN:OE1	2.21	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)
1:B:343:GLU:OE1	1:C:380:ARG:O[1_554]	2.02	0.18

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	377/413 (91%)	348 (92%)	26 (7%)	3 (1%)	19	43
1	B	391/413 (95%)	369 (94%)	21 (5%)	1 (0%)	41	66
1	C	386/413 (94%)	361 (94%)	23 (6%)	2 (0%)	29	54
1	D	387/413 (94%)	357 (92%)	28 (7%)	2 (0%)	29	54
All	All	1541/1652 (93%)	1435 (93%)	98 (6%)	8 (0%)	29	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	VAL
1	B	362	VAL
1	D	67	ILE
1	C	362	VAL
1	D	362	VAL
1	A	89	ARG
1	C	67	ILE
1	A	77	LEU

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	270/315 (86%)	252 (93%)	18 (7%)	16	37
1	B	285/315 (90%)	262 (92%)	23 (8%)	11	27
1	C	291/315 (92%)	272 (94%)	19 (6%)	17	38
1	D	293/315 (93%)	270 (92%)	23 (8%)	12	29
All	All	1139/1260 (90%)	1056 (93%)	83 (7%)	14	33

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TYR
1	A	41	GLU
1	A	55	LEU
1	A	89	ARG
1	A	126	TYR
1	A	141	ILE
1	A	178	ARG
1	A	203	GLU
1	A	210	VAL
1	A	216	GLU
1	A	220	SER
1	A	226	ARG

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Mol	Chain	Res	Type
1	A	244	GLN
1	A	297	MET
1	A	314	LEU
1	A	315	THR
1	A	347	GLU
1	A	373	LEU
1	B	19	TYR
1	B	89	ARG
1	B	126	TYR
1	B	136	ARG
1	B	141	ILE
1	B	172	ARG
1	B	178	ARG
1	B	187	ARG
1	B	203	GLU
1	B	216	GLU
1	B	217	GLU
1	B	219	ILE
1	B	226	ARG
1	B	230	THR
1	B	237	LEU
1	B	238	LYS
1	B	244	GLN
1	B	297	MET
1	B	314	LEU
1	B	315	THR
1	B	347	GLU
1	B	373	LEU
1	B	379	ARG
1	C	19	TYR
1	C	41	GLU
1	C	89	ARG
1	C	126	TYR
1	C	141	ILE
1	C	178	ARG
1	C	203	GLU
1	C	217	GLU
1	C	236	LYS
1	C	237	LEU
1	C	244	GLN
1	C	297	MET
1	C	314	LEU

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Mol	Chain	Res	Type
1	C	315	THR
1	C	316	LEU
1	C	347	GLU
1	C	373	LEU
1	C	379	ARG
1	C	405	GLN
1	D	19	TYR
1	D	41	GLU
1	D	89	ARG
1	D	126	TYR
1	D	136	ARG
1	D	141	ILE
1	D	150	THR
1	D	170	LEU
1	D	176	ILE
1	D	183	GLU
1	D	203	GLU
1	D	210	VAL
1	D	234	LEU
1	D	241	LEU
1	D	244	GLN
1	D	297	MET
1	D	314	LEU
1	D	315	THR
1	D	316	LEU
1	D	347	GLU
1	D	373	LEU
1	D	379	ARG
1	D	405	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	GLN
1	B	181	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	391/413 (94%)	-0.15	7 (1%)	68	70	17, 42, 73, 103	0
1	B	397/413 (96%)	-0.18	7 (1%)	68	70	20, 41, 77, 90	0
1	C	396/413 (95%)	-0.13	7 (1%)	68	70	17, 43, 72, 94	0
1	D	395/413 (95%)	-0.05	12 (3%)	50	51	16, 44, 74, 97	0
All	All	1579/1652 (95%)	-0.13	33 (2%)	63	65	16, 43, 75, 103	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	MET	4.5
1	C	342	GLY	3.9
1	A	249	THR	3.8
1	D	241	LEU	3.6
1	D	246	PRO	3.5
1	C	379	ARG	3.1
1	D	226	ARG	2.9
1	B	199	GLY	2.9
1	C	343	GLU	2.8
1	D	175	HIS	2.8
1	A	167	ALA	2.7
1	B	344	ALA	2.7
1	C	190	GLN	2.7
1	D	341	PHE	2.5
1	A	137	THR	2.5
1	B	179	THR	2.4
1	D	196	GLN	2.3
1	A	197	SER	2.3
1	B	209	PRO	2.3
1	D	210	VAL	2.3
1	D	193	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	247	GLU	2.2
1	D	233	ALA	2.2
1	B	337	ARG	2.2
1	D	276	LEU	2.2
1	A	186	VAL	2.1
1	D	4	ARG	2.1
1	D	379	ARG	2.1
1	C	186	VAL	2.1
1	A	382	ALA	2.0
1	C	236	LYS	2.0
1	B	194	ALA	2.0
1	A	190	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.