



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:20 AM GMT

PDB ID : 2WE7
Title : CRYSTAL STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS
RV0376C HOMOLOGUE FROM MYCOBACTERIUM SMEGMATIS
Authors : Cho, H.J.; Kang, B.S.
Deposited on : 2009-03-29
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

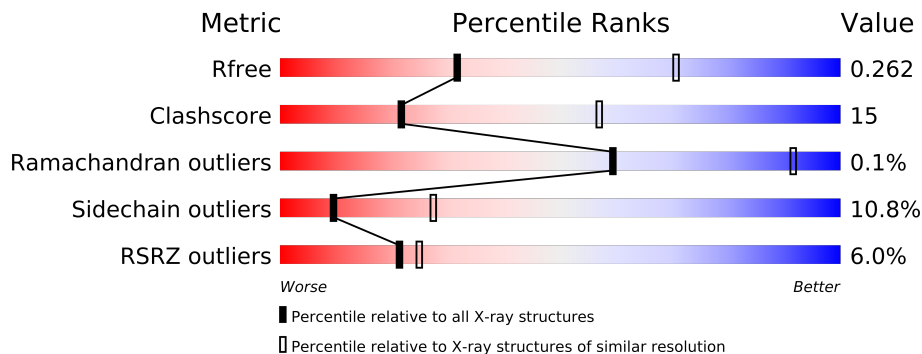
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	386	
1	B	386	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5046 atoms, of which 0 are hydrogen and 0 are deuterium.

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 XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	Se	0	3	0
			2562	1604	462	489	3	4			
1	B	335	Total	C	N	O	S	Se	0	0	0
			2463	1545	436	475	3	4			

- Molecule 2 is water.

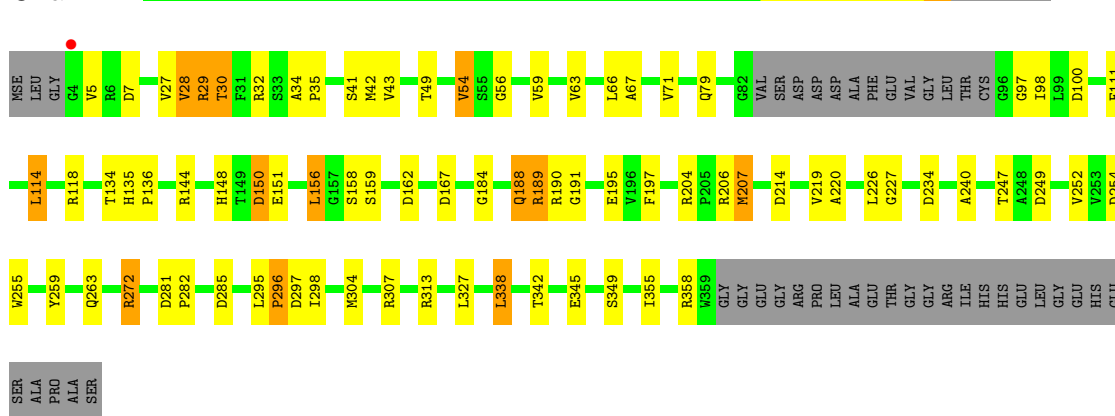
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	1	Total	O	0	0
			1	1		

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.

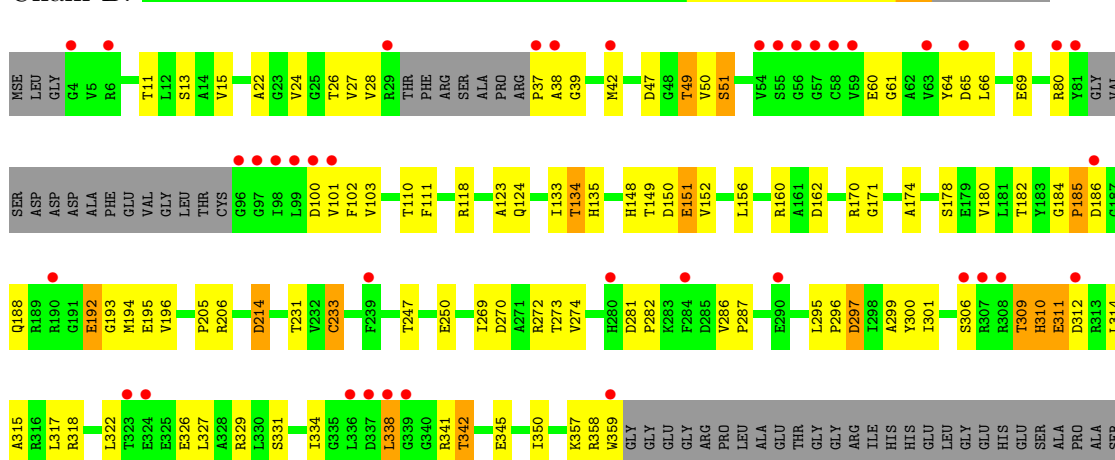
• Molecule 1: XANTHINE DEHYDROGENASE

Chain A:



• Molecule 1: XANTHINE DEHYDROGENASE

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.04Å 101.04Å 316.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.29 – 2.90 38.29 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.29-2.90) 98.6 (38.29-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	45.39 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.252 0.208 , 0.262	Depositor DCC
R_{free} test set	1135 reflections (5.49%)	DCC
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 9.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 21801 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5046	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.95	2/2614 (0.1%)	0.78	2/3557 (0.1%)
1	B	0.63	1/2503 (0.0%)	0.67	0/3408
All	All	0.81	3/5117 (0.1%)	0.73	2/6965 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	VAL	CB-CG1	-5.52	1.41	1.52
1	B	233	CYS	CB-SG	-5.38	1.73	1.81
1	A	252	VAL	CB-CG2	-5.12	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLY	N-CA-C	-5.29	99.88	113.10
1	A	296	PRO	N-CA-C	-5.26	98.42	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2562	0	2555	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2463	0	2437	101	0
2	A	20	0	0	2	0
2	B	1	0	0	0	0
All	All	5046	0	4992	152	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (152) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:114:LEU:O	1:A:114:LEU:HD12	1.34	1.21
1:A:189:ARG:HH11	1:A:189:ARG:CG	1.56	1.17
1:B:27:VAL:HG23	1:B:38:ALA:HA	1.21	1.14
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.16	1.05
1:B:342:THR:HG22	1:B:345:GLU:HG3	1.37	1.04
1:B:28:VAL:CG1	1:B:180:VAL:CG2	2.40	0.99
1:B:47:ASP:OD1	1:B:49:THR:HG23	1.66	0.95
1:B:27:VAL:CG2	1:B:38:ALA:HA	1.96	0.94
1:B:28:VAL:HG12	1:B:180:VAL:HG21	1.49	0.93
1:A:134:THR:HB	1:A:195:GLU:HG2	1.51	0.90
1:B:28:VAL:CG1	1:B:180:VAL:HG21	2.03	0.87
1:A:114:LEU:HD12	1:A:114:LEU:C	1.87	0.84
1:B:342:THR:HG22	1:B:345:GLU:CG	2.07	0.84
1:A:189:ARG:O	1:A:190:ARG:HB2	1.74	0.83
1:A:189:ARG:NH1	1:A:189:ARG:CG	2.30	0.82
1:B:27:VAL:O	1:B:27:VAL:HG23	1.79	0.82
1:A:189:ARG:HG3	1:A:189:ARG:NH1	1.87	0.81
1:B:28:VAL:HG12	1:B:180:VAL:CG2	2.05	0.81
1:B:310:HIS:CE1	1:B:314:LEU:HD11	2.16	0.80
1:B:27:VAL:O	1:B:27:VAL:CG2	2.32	0.78
1:A:189:ARG:HH11	1:A:189:ARG:HG2	1.45	0.78
1:A:204[B]:ARG:HG3	1:A:204[B]:ARG:HH11	1.48	0.78
1:B:28:VAL:CG1	1:B:180:VAL:HG22	2.13	0.77
1:A:30:THR:CG2	1:A:34:ALA:HB3	2.13	0.77
1:B:310:HIS:CE1	1:B:314:LEU:HG	2.20	0.76
1:B:269:ILE:HG13	1:B:269:ILE:O	1.83	0.76
1:B:27:VAL:HG21	1:B:37:PRO:O	1.85	0.76
1:A:30:THR:HG22	1:A:34:ALA:HB3	1.66	0.76
1:B:50:VAL:HG12	1:B:51:SER:N	2.00	0.74
1:B:310:HIS:CE1	1:B:314:LEU:CG	2.72	0.73
1:B:47:ASP:OD1	1:B:49:THR:CG2	2.36	0.72
1:B:269:ILE:CG1	1:B:269:ILE:O	2.38	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:310:HIS:CE1	1:B:314:LEU:CD1	2.72	0.71
1:A:59:VAL:O	1:A:63:VAL:HG23	1.90	0.71
1:B:182:THR:HG22	1:B:195:GLU:HG2	1.71	0.70
1:B:342:THR:CG2	1:B:345:GLU:HG3	2.18	0.70
1:A:35:PRO:HG3	1:A:56:GLY:H	1.57	0.70
1:B:28:VAL:HG13	1:B:180:VAL:HG22	1.74	0.69
1:B:192:GLU:HG2	1:B:193:GLY:N	2.07	0.69
1:B:42:MSE:HE2	1:B:50:VAL:HG11	1.73	0.69
1:A:207:MSE:HE1	1:A:219:VAL:O	1.91	0.69
1:A:184:GLY:HA3	1:A:188:GLN:HG2	1.77	0.67
1:A:358:ARG:HB3	2:A:2020:HOH:O	1.94	0.66
1:B:151:GLU:C	1:B:151:GLU:OE1	2.35	0.66
1:A:29:ARG:NH1	1:A:100:ASP:OD2	2.29	0.66
1:B:184:GLY:O	1:B:186:ASP:N	2.30	0.65
1:B:134:THR:O	1:B:194:MSE:HA	1.96	0.65
1:A:32:ARG:HB2	1:A:97:GLY:HA2	1.79	0.65
1:B:151:GLU:OE1	1:B:152:VAL:N	2.30	0.65
1:B:286:VAL:HB	1:B:287:PRO:HD3	1.79	0.65
1:B:341:ARG:N	1:B:345:GLU:OE1	2.31	0.63
1:B:50:VAL:CG1	1:B:51:SER:N	2.62	0.62
1:B:27:VAL:HG22	1:B:39:GLY:H	1.65	0.62
1:B:160:ARG:NH2	1:B:188:GLN:HB3	2.15	0.60
1:B:102:PHE:CD1	1:B:133:ILE:HG22	2.36	0.59
1:A:5:VAL:HG12	1:A:41:SER:OG	2.03	0.59
1:B:50:VAL:CG2	1:B:64:TYR:CE2	2.86	0.59
1:B:270:ASP:OD1	1:B:272:ARG:HG2	2.03	0.58
1:A:234:ASP:HB3	1:A:240:ALA:HB2	1.84	0.58
1:B:331:SER:OG	1:B:357:LYS:HE3	2.03	0.57
1:B:28:VAL:HG13	1:B:180:VAL:CG2	2.29	0.57
1:B:13:SER:OG	1:B:118:ARG:NH1	2.38	0.56
1:B:27:VAL:CG2	1:B:38:ALA:CA	2.76	0.56
1:B:310:HIS:HE1	1:B:314:LEU:HD21	1.70	0.55
1:B:50:VAL:CG2	1:B:64:TYR:HE2	2.19	0.55
1:A:67:ALA:O	1:A:71:VAL:HG23	2.06	0.55
1:A:295:LEU:O	1:A:296:PRO:C	2.43	0.55
1:B:26:THR:O	1:B:101:VAL:HA	2.06	0.55
1:B:15:VAL:HG11	1:B:22:ALA:HB2	1.88	0.55
1:B:270:ASP:OD1	1:B:272:ARG:N	2.28	0.55
1:A:28:VAL:HG22	1:A:197:PHE:CG	2.43	0.54
1:A:156:LEU:HB2	1:A:162:ASP:OD1	2.07	0.54
1:B:272:ARG:HA	1:B:299:ALA:HB2	1.90	0.53
1:A:226:LEU:HD21	1:A:355:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:295:LEU:O	1:B:296:PRO:C	2.45	0.53
1:B:50:VAL:HG21	1:B:64:TYR:CD2	2.44	0.53
1:B:273:THR:HG22	1:B:274:VAL:N	2.23	0.53
1:B:50:VAL:HG23	1:B:64:TYR:HE2	1.74	0.52
1:B:27:VAL:HG22	1:B:39:GLY:N	2.24	0.52
1:A:35:PRO:CG	1:A:56:GLY:H	2.20	0.52
1:A:27:VAL:HG23	1:A:54:VAL:HG22	1.91	0.52
1:A:134:THR:CB	1:A:195:GLU:HG2	2.33	0.52
1:B:27:VAL:HG23	1:B:38:ALA:CA	2.15	0.51
1:A:204[B]:ARG:NH1	1:A:204[B]:ARG:HG3	2.22	0.51
1:B:315:ALA:HA	1:B:318:ARG:HD2	1.91	0.51
1:B:151:GLU:N	1:B:170:ARG:HH21	2.09	0.50
1:B:342:THR:HG22	1:B:345:GLU:CD	2.32	0.50
1:B:273:THR:CG2	1:B:274:VAL:N	2.74	0.50
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.76	0.50
1:B:27:VAL:CG2	1:B:37:PRO:O	2.59	0.50
1:B:306:SER:OG	1:B:309:THR:CG2	2.59	0.50
1:B:309:THR:OG1	1:B:309:THR:O	2.30	0.50
1:B:186:ASP:OD2	1:B:186:ASP:O	2.30	0.50
1:B:214:ASP:N	1:B:214:ASP:OD1	2.37	0.49
1:B:306:SER:O	1:B:310:HIS:N	2.43	0.49
1:B:310:HIS:HE1	1:B:314:LEU:CG	2.24	0.49
1:B:148:HIS:O	1:B:170:ARG:NE	2.44	0.49
1:B:150:ASP:O	1:B:150:ASP:OD2	2.30	0.49
1:B:273:THR:O	1:B:299:ALA:HB3	2.13	0.48
1:A:148:HIS:HB2	1:A:151:GLU:HG2	1.95	0.48
1:B:311:GLU:O	1:B:312:ASP:C	2.48	0.48
1:A:189:ARG:O	1:A:190:ARG:CB	2.45	0.48
1:B:306:SER:OG	1:B:309:THR:HG22	2.13	0.48
1:B:310:HIS:ND1	1:B:314:LEU:HG	2.28	0.48
1:B:274:VAL:HG22	1:B:300:TYR:HB3	1.95	0.47
1:B:151:GLU:H	1:B:170:ARG:HH21	1.63	0.47
1:A:254:ASP:OD1	1:A:255:TRP:N	2.47	0.47
1:A:184:GLY:HA3	1:A:188:GLN:CG	2.44	0.47
1:B:135:HIS:NE2	1:B:185:PRO:O	2.46	0.47
1:B:27:VAL:CG2	1:B:39:GLY:H	2.26	0.47
1:B:134:THR:OG1	1:B:195:GLU:HB2	2.15	0.46
1:B:334:ILE:HG12	1:B:350:ILE:HG12	1.96	0.46
1:B:24:VAL:O	1:B:103:VAL:HA	2.15	0.46
1:B:231:THR:HG23	1:B:250:GLU:HB3	1.97	0.46
1:A:189:ARG:NH1	1:A:189:ARG:HG2	2.16	0.46
1:B:60:GLU:O	1:B:61:GLY:C	2.53	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:342:THR:HG23	1:A:345:GLU:OE2	2.15	0.46
1:A:135:HIS:CG	1:A:136:PRO:HD2	2.51	0.46
1:B:310:HIS:HE1	1:B:314:LEU:CD2	2.29	0.45
1:B:123:ALA:O	1:B:124:GLN:HB2	2.15	0.45
1:A:66:LEU:HD22	1:A:79:GLN:HG3	1.98	0.45
1:B:27:VAL:HA	1:B:100:ASP:O	2.16	0.45
1:A:285:ASP:OD2	1:A:313:ARG:HD3	2.16	0.45
1:B:297:ASP:N	1:B:297:ASP:OD1	2.46	0.45
1:B:358:ARG:HG2	1:B:358:ARG:O	2.18	0.44
1:A:156:LEU:HA	1:A:156:LEU:HD12	1.67	0.44
1:A:281:ASP:HA	1:A:282:PRO:HD3	1.86	0.44
1:A:304:MSE:HE3	2:A:2015:HOH:O	2.17	0.44
1:B:156:LEU:HB2	1:B:162:ASP:OD1	2.17	0.44
1:A:204[A]:ARG:HG2	1:A:227:GLY:O	2.18	0.43
1:B:322:LEU:HD21	1:B:326:GLU:HB2	1.99	0.43
1:A:259:TYR:O	1:A:263:GLN:HG2	2.18	0.43
1:B:317:LEU:HD22	1:B:327:LEU:HD21	2.00	0.43
1:A:338:LEU:HD22	1:A:349:SER:HB2	1.99	0.43
1:B:42:MSE:CE	1:B:50:VAL:HG11	2.44	0.43
1:B:326:GLU:HA	1:B:329:ARG:HH22	1.84	0.43
1:B:80:ARG:HG3	1:B:100:ASP:OD1	2.18	0.42
1:B:150:ASP:CG	1:B:150:ASP:O	2.55	0.42
1:B:171:GLY:O	1:B:174:ALA:HB3	2.20	0.42
1:B:338:LEU:HA	1:B:338:LEU:HD12	1.78	0.41
1:A:298:ILE:HD13	1:A:298:ILE:HG21	1.85	0.41
1:B:27:VAL:CG2	1:B:39:GLY:N	2.83	0.41
1:B:231:THR:HA	1:B:250:GLU:O	2.20	0.41
1:B:65:ASP:OD2	1:B:65:ASP:N	2.53	0.41
1:B:50:VAL:CG2	1:B:64:TYR:CD2	3.04	0.41
1:A:207:MSE:CE	1:A:220:ALA:HA	2.50	0.41
1:A:207:MSE:CE	1:A:219:VAL:HG12	2.51	0.41
1:A:114:LEU:O	1:A:114:LEU:CD1	2.30	0.41
1:A:150:ASP:OD1	1:A:150:ASP:N	2.52	0.40
1:B:184:GLY:O	1:B:185:PRO:C	2.59	0.40
1:B:205:PRO:HB3	1:B:272:ARG:HG3	2.03	0.40
1:B:281:ASP:HA	1:B:282:PRO:HD2	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/386 (89%)	335 (98%)	7 (2%)	0	100	100
1	B	329/386 (85%)	318 (97%)	10 (3%)	1 (0%)	50	85
All	All	671/772 (87%)	653 (97%)	17 (2%)	1 (0%)	59	91

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/285 (92%)	231 (88%)	31 (12%)	8	22
1	B	250/285 (88%)	225 (90%)	25 (10%)	11	32
All	All	512/570 (90%)	456 (89%)	56 (11%)	9	26

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	28	VAL
1	A	29	ARG
1	A	30	THR
1	A	42	MSE
1	A	43	VAL
1	A	49	THR
1	A	54	VAL

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Mol	Chain	Res	Type
1	A	98	ILE
1	A	111	PHE
1	A	114	LEU
1	A	118	ARG
1	A	144	ARG
1	A	150	ASP
1	A	156	LEU
1	A	158	SER
1	A	159	SER
1	A	167	ASP
1	A	188	GLN
1	A	189	ARG
1	A	206	ARG
1	A	207	MSE
1	A	214	ASP
1	A	247	THR
1	A	249[A]	ASP
1	A	249[B]	ASP
1	A	272	ARG
1	A	297	ASP
1	A	307	ARG
1	A	327	LEU
1	A	338	LEU
1	B	11	THR
1	B	49	THR
1	B	51	SER
1	B	66	LEU
1	B	69	GLU
1	B	110	THR
1	B	111	PHE
1	B	134	THR
1	B	149	THR
1	B	151	GLU
1	B	178	SER
1	B	192	GLU
1	B	196	VAL
1	B	206	ARG
1	B	214	ASP
1	B	233	CYS
1	B	247	THR
1	B	297	ASP
1	B	301	ILE

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Mol	Chain	Res	Type
1	B	309	THR
1	B	310	HIS
1	B	311	GLU
1	B	338	LEU
1	B	342	THR
1	B	359	TRP

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

Mol	Chain	Res	Type
1	A	108	GLN
1	B	310	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	343/386 (88%)	-0.26	1 (0%) 91 95	5, 22, 47, 73	0
1	B	335/386 (86%)	0.79	40 (11%) 5 7	20, 73, 100, 106	0
All	All	678/772 (87%)	0.26	41 (6%) 21 25	5, 47, 96, 106	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	LEU	6.0
1	B	359	TRP	5.6
1	B	98	ILE	5.6
1	B	56	GLY	4.7
1	B	239	PHE	4.6
1	B	96	GLY	4.5
1	B	58	CYS	4.4
1	B	99	LEU	4.1
1	B	42	MSE	3.7
1	B	37	PRO	3.6
1	B	280	HIS	3.6
1	B	100	ASP	3.5
1	B	337	ASP	3.2
1	B	307	ARG	3.2
1	B	339	GLY	3.2
1	B	190	ARG	3.1
1	B	101	VAL	3.1
1	B	29	ARG	3.0
1	B	97	GLY	2.9
1	B	81	TYR	2.9
1	B	80	ARG	2.9
1	B	4	GLY	2.8
1	B	57	GLY	2.7
1	B	186	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	59	VAL	2.7
1	A	4	GLY	2.7
1	B	308	ARG	2.7
1	B	65	ASP	2.6
1	B	54	VAL	2.6
1	B	55	SER	2.5
1	B	290	GLU	2.5
1	B	323	THR	2.5
1	B	336	LEU	2.5
1	B	306	SER	2.4
1	B	38	ALA	2.4
1	B	63	VAL	2.3
1	B	69	GLU	2.3
1	B	312	ASP	2.2
1	B	6	ARG	2.2
1	B	324	GLU	2.2
1	B	284	PHE	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.