



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:43 PM UTC

PDB ID : 2WE7 / pdb_00002we7
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 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

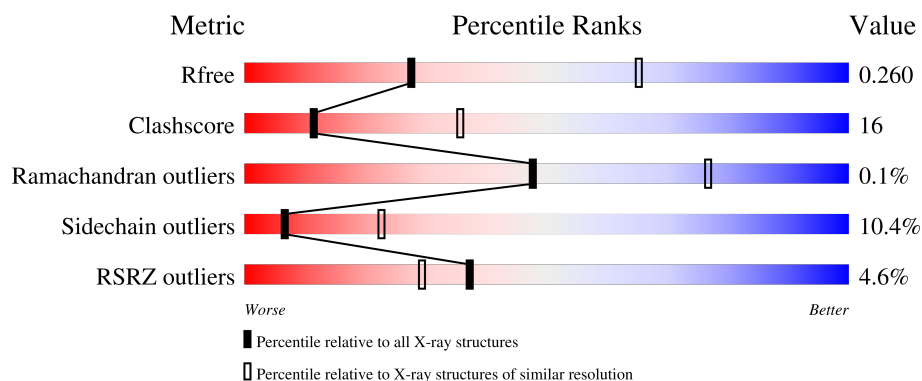
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	8% 65% 19% • • 11%
1	B	386	8% 58% 25% • • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5046 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 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		

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) 98.5 (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 0.207 , 0.260	Depositor DCC
R_{free} test set	1135 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.24	15/2614 (0.6%)	1.11	15/3557 (0.4%)
1	B	0.85	1/2503 (0.0%)	1.05	9/3408 (0.3%)
All	All	1.07	16/5117 (0.3%)	1.08	24/6965 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	VAL	CA-CB	-7.62	1.44	1.54
1	A	212	ALA	CA-CB	-6.91	1.43	1.52
1	A	251	VAL	C-O	-6.12	1.17	1.24
1	A	253	VAL	C-O	-5.84	1.17	1.24
1	A	213	ILE	CA-CB	-5.79	1.46	1.54
1	A	145	LEU	C-O	-5.75	1.17	1.23
1	B	28	VAL	CA-CB	-5.70	1.49	1.55
1	A	251	VAL	CA-CB	-5.67	1.47	1.54
1	A	213	ILE	C-O	-5.44	1.17	1.24
1	A	252	VAL	C-O	-5.43	1.18	1.24
1	A	296	PRO	CA-C	-5.26	1.46	1.52
1	A	172	LEU	CA-C	-5.22	1.46	1.52
1	A	146	VAL	C-O	-5.12	1.18	1.24
1	A	211	GLY	C-O	-5.09	1.17	1.23
1	A	63	VAL	CA-CB	-5.06	1.47	1.54
1	A	328	ALA	CA-CB	-5.02	1.45	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLY	N-CA-C	-8.80	99.88	112.55
1	A	296	PRO	N-CA-C	-7.98	98.42	111.11
1	B	191	GLY	N-CA-C	-7.15	100.94	112.31
1	A	204[A]	ARG	CA-C-N	-6.99	113.46	120.31
1	A	204[A]	ARG	C-N-CA	-6.99	113.46	120.31
1	A	204[B]	ARG	CA-C-N	-6.99	113.46	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204[B]	ARG	C-N-CA	-6.99	113.46	120.31
1	B	307	ARG	N-CA-C	-6.76	103.93	111.71
1	A	298	ILE	N-CA-C	-6.60	99.08	108.65
1	A	297	ASP	N-CA-C	6.60	119.33	110.35
1	A	286	VAL	CA-C-N	-6.46	112.53	119.24
1	A	286	VAL	C-N-CA	-6.46	112.53	119.24
1	B	324	GLU	N-CA-C	5.94	117.75	111.28
1	B	296	PRO	N-CA-C	-5.67	102.19	111.15
1	B	310	HIS	N-CA-C	-5.42	105.38	111.28
1	A	336	LEU	N-CA-C	-5.39	103.27	110.55
1	A	28	VAL	N-CA-CB	-5.38	104.85	112.12
1	A	150	ASP	N-CA-C	5.33	120.44	113.30
1	A	149	THR	CB-CA-C	-5.26	102.05	110.79
1	B	75	THR	CA-C-N	5.25	125.19	119.78
1	B	75	THR	C-N-CA	5.25	125.19	119.78
1	B	214	ASP	N-CA-C	-5.20	105.61	111.28
1	A	141	ILE	N-CA-C	5.19	115.78	109.30
1	B	28	VAL	CB-CA-C	-5.07	105.82	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2562	0	2555	53	0
1	B	2463	0	2437	108	0
2	A	20	0	0	2	0
2	B	1	0	0	0	0
All	All	5046	0	4992	161	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 16.

All (161) 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:114:LEU:O	1:A:114:LEU:HD12	1.34	1.21
1:A:189:ARG:CG	1:A:189:ARG:HH11	1.56	1.17
1:B:27:VAL:HG23	1:B:38:ALA:HA	1.21	1.14
1:A:189:ARG:HH11	1:A:189:ARG:HG3	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:A:114:LEU:HD12	1:A:114:LEU:C	1.87	0.89
1:B:28:VAL:CG1	1:B:180:VAL:HG21	2.03	0.87
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:CG	1:A:189:ARG:NH1	2.30	0.82
1:B:27:VAL:HG23	1:B:27:VAL:O	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:CG2	1:B:27:VAL:O	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:O	1:B:269:ILE:HG13	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:O	1:B:269:ILE:CG1	2.38	0.72
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:151:GLU:OE1	1:B:151:GLU:C	2.35	0.70
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:295:LEU:O	1:A:296:PRO:C	2.43	0.60
1:A:5:VAL:HG12	1:A:41:SER:OG	2.03	0.59
1:B:102:PHE:CD1	1:B:133:ILE:HG22	2.36	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:295:LEU:O	1:B:296:PRO:C	2.45	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:A:67:ALA:O	1:A:71:VAL:HG23	2.06	0.55
1:B:50:VAL:CG2	1:B:64:TYR:HE2	2.19	0.55
1:B:310:HIS:HE1	1:B:314:LEU:HD21	1.70	0.55
1:B:342:THR:HG22	1:B:345:GLU:CD	2.32	0.55
1:B:15:VAL:HG11	1:B:22:ALA:HB2	1.88	0.55
1:B:26:THR:O	1:B:101:VAL:HA	2.06	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:A:226:LEU:HD21	1:A:355:ILE:HD11	1.90	0.53
1:B:272:ARG:HA	1:B:299:ALA:HB2	1.90	0.53
1:B:311:GLU:O	1:B:312:ASP:C	2.48	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:A:35:PRO:CG	1:A:56:GLY:H	2.20	0.52
1:B:27:VAL:HG22	1:B:39:GLY:N	2.24	0.52
1:A:27:VAL:HG23	1:A:54:VAL:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:A:204[B]:ARG:NH1	2.22	0.51
1:B:315:ALA:HA	1:B:318:ARG:HD2	1.91	0.51
1:B:60:GLU:O	1:B:61:GLY:C	2.53	0.50
1:B:151:GLU:N	1:B:170:ARG:HH21	2.09	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:186:ASP:OD2	1:B:186:ASP:O	2.30	0.50
1:B:309:THR:O	1:B:309:THR:OG1	2.30	0.50
1:B:214:ASP:OD1	1:B:214:ASP:N	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:273:THR:CG2	1:B:274:VAL:N	2.74	0.49
1:B:148:HIS:O	1:B:170:ARG:NE	2.44	0.49
1:B:150:ASP:OD2	1:B:150:ASP:O	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:306:SER:OG	1:B:309:THR:HG22	2.13	0.48
1:A:189:ARG:O	1:A:190:ARG:CB	2.45	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:A:254:ASP:OD1	1:A:255:TRP:N	2.47	0.47
1:B:151:GLU:H	1:B:170:ARG:HH21	1.63	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:150:ASP:O	1:B:150:ASP:CG	2.55	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: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:123:ALA:O	1:B:124:GLN:HB2	2.15	0.45
1:B:310:HIS:HE1	1:B:314:LEU:CD2	2.29	0.45
1:A:66:LEU:HD22	1:A:79:GLN:HG3	1.98	0.45
1:A:285:ASP:OD2	1:A:313:ARG:HD3	2.16	0.45
1:B:27:VAL:HA	1:B:100:ASP:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLY:O	1:B:185:PRO:C	2.59	0.45
1:B:297:ASP:N	1:B:297:ASP:OD1	2.46	0.45
1:B:358:ARG:O	1:B:358:ARG:HG2	2.18	0.44
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.67	0.44
1:A:281:ASP:HA	1:A:282:PRO:HD3	1.86	0.44
1:B:316:ARG:HA	1:B:319:GLU:CD	2.43	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:B:332:SER:HA	1:B:333:PRO:C	2.43	0.43
1:A:259:TYR:O	1:A:263:GLN:HG2	2.18	0.43
1:B:47:ASP:CG	1:B:49:THR:CG2	2.90	0.43
1:A:338:LEU:HD22	1:A:349:SER:HB2	1.99	0.43
1:B:317:LEU:HD22	1:B:327:LEU:HD21	2.00	0.43
1:B:214:ASP:O	1:B:215:PHE:C	2.58	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:A:295:LEU:C	1:A:296:PRO:O	2.55	0.43
1:B:55:SER:HG	1:B:57:GLY:C	2.27	0.43
1:B:337:ASP:OD2	1:B:337:ASP:C	2.59	0.42
1:B:80:ARG:HG3	1:B:100:ASP:OD1	2.18	0.42
1:B:171:GLY:O	1:B:174:ALA:HB3	2.20	0.42
1:A:298:ILE:HG21	1:A:298:ILE:HD13	1.85	0.41
1:B:338:LEU:HA	1:B:338:LEU:HD12	1.78	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:A:286:VAL:O	1:A:287:PRO:C	2.62	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:65:ASP:OD2	1:B:65:ASP:N	2.53	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
1:B:27:VAL:HG21	1:B:37:PRO:C	2.45	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%)	36	65
All	All	671/772 (87%)	653 (97%)	17 (2%)	1 (0%)	48	77

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%)	234 (89%)	28 (11%)	6	22
1	B	250/285 (88%)	225 (90%)	25 (10%)	7	24
All	All	512/570 (90%)	459 (90%)	53 (10%)	7	23

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	28	VAL
1	A	29	ARG
1	A	30	THR
1	A	42	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	43	VAL
1	A	49	THR
1	A	54	VAL
1	A	79	GLN
1	A	98	ILE
1	A	114	LEU
1	A	122	GLU
1	A	145	LEU
1	A	150	ASP
1	A	152	VAL
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	196	VAL
1	A	207	MSE
1	A	241	THR
1	A	247	THR
1	A	272	ARG
1	A	327	LEU
1	A	338	LEU
1	B	11	THR
1	B	27	VAL
1	B	49	THR
1	B	51	SER
1	B	65	ASP
1	B	66	LEU
1	B	69	GLU
1	B	99	LEU
1	B	110	THR
1	B	134	THR
1	B	149	THR
1	B	152	VAL
1	B	192	GLU
1	B	194	MSE
1	B	196	VAL
1	B	206	ARG
1	B	214	ASP
1	B	233	CYS
1	B	247	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	ILE
1	B	309	THR
1	B	310	HIS
1	B	311	GLU
1	B	338	LEU
1	B	342	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	108	GLN
1	A	148	HIS
1	B	257	HIS
1	B	310	HIS

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 oligosaccharides 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 ⓘ

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	339/386 (87%)	-0.62	2 (0%) 85 81	5, 21, 47, 73	3 (0%)
1	B	331/386 (85%)	0.76	29 (8%) 15 13	20, 73, 100, 106	0
All	All	670/772 (86%)	0.06	31 (4%) 37 29	5, 47, 96, 106	3 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	PRO	4.8
1	B	247	THR	4.0
1	B	238	VAL	3.8
1	B	186	ASP	3.5
1	B	359	TRP	3.4
1	A	4	GLY	3.3
1	B	239	PHE	3.0
1	B	214	ASP	3.0
1	B	150	ASP	3.0
1	B	179	GLU	3.0
1	B	270	ASP	2.9
1	B	4	GLY	2.9
1	B	243	ALA	2.8
1	B	240	ALA	2.7
1	B	246	PRO	2.7
1	B	96	GLY	2.5
1	B	9	LEU	2.4
1	B	98	ILE	2.3
1	B	253	VAL	2.3
1	B	151	GLU	2.3
1	B	338	LEU	2.3
1	B	343	PRO	2.3
1	B	54	VAL	2.2
1	B	56	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	99	LEU	2.1
1	B	245	PHE	2.1
1	B	121	ILE	2.1
1	A	359	TRP	2.1
1	B	248	ALA	2.1
1	B	174	ALA	2.1
1	B	358	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 oligosaccharides 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.