



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:26 PM GMT

PDB ID : 3RB9
Title : Crystal structure of the M. tuberculosis beta clamp
Authors : Kukshal, V.; Ramachandran, R.
Deposited on : 2011-03-29
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

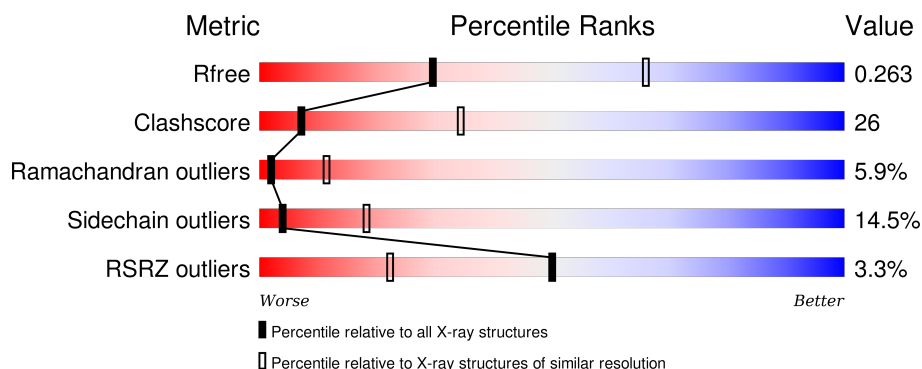
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

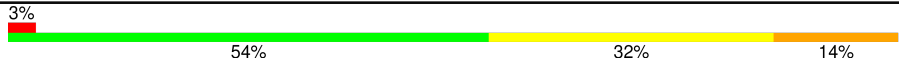
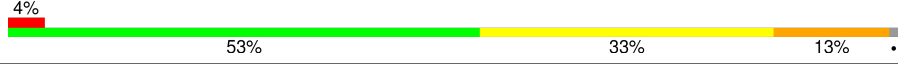
The reported resolution of this entry is 3.00 Å.

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	395	 3% 54% 32% 14%
1	B	395	 4% 53% 33% 13% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5813 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.

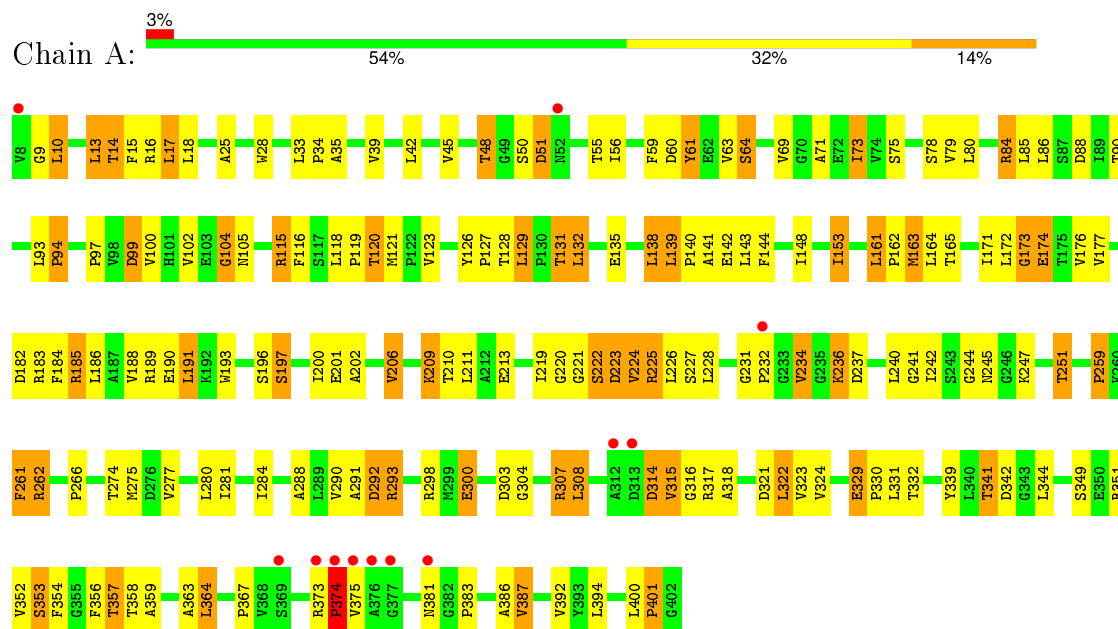
- Molecule 1 is a protein called DNA polymerase III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2912	1841	499	566	6			
1	B	393	Total	C	N	O	S	0	0	0
			2901	1834	497	564	6			

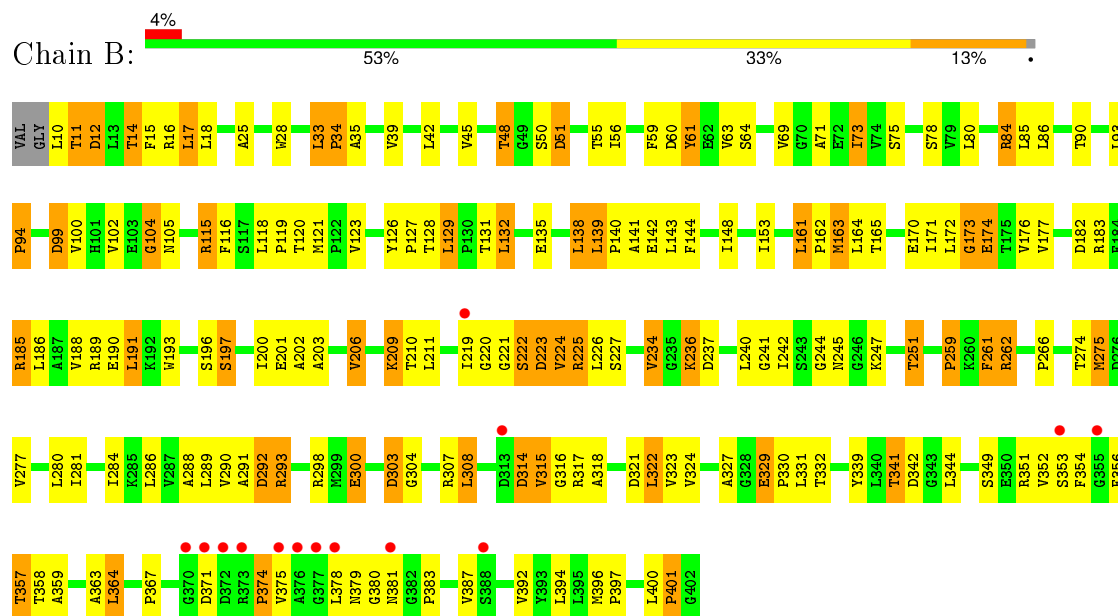
3 Residue-property plots

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: DNA polymerase III subunit beta



• Molecule 1: DNA polymerase III subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.90Å 233.25Å 124.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.81 – 3.00 21.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (21.81-3.00) 99.9 (21.80-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.250 0.227 , 0.263	Depositor DCC
R_{free} test set	1093 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 59.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 21312 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5813	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	0/2963	0.68	3/4043 (0.1%)
1	B	0.49	0/2952	0.68	1/4028 (0.0%)
All	All	0.50	0/5915	0.68	4/8071 (0.0%)

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	401	PRO	N-CA-C	5.96	127.60	112.10
1	B	401	PRO	N-CA-C	5.90	127.44	112.10
1	A	13	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	13	LEU	CB-CG-CD2	5.10	119.67	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	314	ASP	Peptide
1	B	11	THR	Peptide
1	B	314	ASP	Peptide

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	2912	0	2960	157	0
1	B	2901	0	2948	158	0
All	All	5813	0	5908	307	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 26.

All (307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:THR:HG21	1:B:251:THR:HB	1.40	1.00
1:A:210:THR:HG21	1:A:251:THR:HB	1.42	1.00
1:B:327:ALA:HB2	1:B:375:VAL:HG13	1.49	0.93
1:A:162:PRO:HA	1:A:165:THR:HG22	1.52	0.91
1:B:162:PRO:HA	1:B:165:THR:HG22	1.52	0.90
1:B:143:LEU:HD21	1:B:191:LEU:HD11	1.52	0.89
1:A:364:LEU:HD12	1:A:394:LEU:HD13	1.55	0.89
1:A:143:LEU:HD21	1:A:191:LEU:HD11	1.55	0.89
1:A:206:VAL:HG21	1:A:211:LEU:HD13	1.57	0.86
1:B:364:LEU:HD12	1:B:394:LEU:HD13	1.55	0.86
1:B:206:VAL:HG21	1:B:211:LEU:HD13	1.59	0.85
1:A:14:THR:HG23	1:A:75:SER:HB3	1.58	0.83
1:B:200:ILE:HD11	1:B:234:VAL:HG11	1.65	0.79
1:B:138:LEU:HD12	1:B:223:ASP:OD1	1.83	0.79
1:B:162:PRO:O	1:B:163:MET:HB3	1.83	0.79
1:B:14:THR:HG23	1:B:75:SER:HB3	1.64	0.78
1:A:162:PRO:O	1:A:163:MET:HB3	1.83	0.78
1:A:200:ILE:HD11	1:A:234:VAL:HG11	1.66	0.76
1:A:210:THR:HG21	1:A:251:THR:CB	2.16	0.75
1:A:138:LEU:HD12	1:A:223:ASP:OD1	1.87	0.74
1:B:182:ASP:O	1:B:183:ARG:HB2	1.87	0.74
1:B:162:PRO:HA	1:B:165:THR:CG2	2.16	0.74
1:A:162:PRO:HA	1:A:165:THR:CG2	2.18	0.73
1:B:210:THR:HG21	1:B:251:THR:CB	2.17	0.73
1:B:262:ARG:HH11	1:B:262:ARG:HG2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HH11	1:A:262:ARG:HG2	1.53	0.72
1:A:182:ASP:O	1:A:183:ARG:HB2	1.88	0.72
1:B:176:VAL:HG12	1:B:191:LEU:HB3	1.71	0.71
1:B:143:LEU:CD2	1:B:191:LEU:HD11	2.20	0.71
1:A:48:THR:HG22	1:A:78:SER:HB3	1.74	0.69
1:A:63:VAL:HG12	1:A:64:SER:N	2.07	0.69
1:A:143:LEU:CD2	1:A:191:LEU:HD11	2.23	0.68
1:B:17:LEU:HD13	1:B:71:ALA:HB2	1.75	0.68
1:A:39:VAL:HG22	1:A:42:LEU:HD12	1.76	0.67
1:A:104:GLY:O	1:A:105:ASN:HB3	1.94	0.67
1:A:307:ARG:HB2	1:A:321:ASP:OD1	1.95	0.67
1:B:48:THR:HG22	1:B:78:SER:HB3	1.76	0.66
1:B:104:GLY:O	1:B:105:ASN:HB3	1.95	0.66
1:A:171:ILE:HG13	1:A:202:ALA:H	1.61	0.66
1:A:39:VAL:HG22	1:A:42:LEU:CD1	2.26	0.65
1:B:171:ILE:HG13	1:B:202:ALA:H	1.59	0.65
1:B:292:ASP:O	1:B:293:ARG:HD2	1.97	0.65
1:B:303:ASP:CG	1:B:304:GLY:H	1.99	0.65
1:A:80:LEU:HD23	1:A:121:MET:HB2	1.78	0.65
1:A:17:LEU:HD13	1:A:71:ALA:HB2	1.78	0.64
1:A:291:ALA:O	1:A:292:ASP:CB	2.45	0.64
1:A:303:ASP:CG	1:A:304:GLY:H	2.01	0.64
1:B:291:ALA:O	1:B:292:ASP:CB	2.46	0.64
1:B:374:PRO:O	1:B:375:VAL:HB	1.98	0.64
1:A:119:PRO:HG2	1:B:314:ASP:HB2	1.80	0.64
1:B:307:ARG:HB2	1:B:321:ASP:OD1	1.97	0.64
1:B:39:VAL:HG22	1:B:42:LEU:HD12	1.81	0.63
1:A:173:GLY:O	1:A:174:GLU:HB3	1.98	0.63
1:A:236:LYS:O	1:A:237:ASP:HB2	1.98	0.63
1:B:236:LYS:O	1:B:237:ASP:HB2	1.97	0.63
1:B:291:ALA:O	1:B:292:ASP:HB3	1.99	0.62
1:A:291:ALA:O	1:A:292:ASP:HB3	1.98	0.62
1:A:292:ASP:O	1:A:293:ARG:HD2	1.99	0.62
1:A:176:VAL:HG12	1:A:191:LEU:HB3	1.81	0.62
1:B:80:LEU:HD23	1:B:121:MET:HB2	1.81	0.62
1:B:173:GLY:O	1:B:174:GLU:HB3	1.98	0.62
1:A:63:VAL:HG12	1:A:64:SER:H	1.65	0.62
1:B:10:LEU:HG	1:B:11:THR:N	2.16	0.61
1:B:300:GLU:HG3	1:B:332:THR:OG1	2.00	0.61
1:B:327:ALA:HB2	1:B:375:VAL:CG1	2.28	0.61
1:B:63:VAL:HG12	1:B:64:SER:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:HB3	1:A:374:PRO:O	2.01	0.61
1:B:42:LEU:HD22	1:B:59:PHE:O	2.01	0.61
1:A:373:ARG:HG2	1:A:375:VAL:HB	1.81	0.61
1:A:161:LEU:HD13	1:A:164:LEU:HD12	1.83	0.60
1:A:129:LEU:HD23	1:A:129:LEU:H	1.67	0.60
1:A:357:THR:OG1	1:A:358:THR:N	2.35	0.59
1:B:210:THR:CG2	1:B:251:THR:HB	2.23	0.59
1:B:60:ASP:O	1:B:61:TYR:HB2	2.02	0.59
1:B:357:THR:OG1	1:B:358:THR:N	2.32	0.59
1:A:210:THR:CG2	1:A:251:THR:HB	2.26	0.59
1:A:277:VAL:HG23	1:A:351:ARG:HA	1.85	0.58
1:A:86:LEU:O	1:A:90:THR:HG23	2.02	0.58
1:B:141:ALA:HA	1:B:224:VAL:HG12	1.85	0.58
1:A:102:VAL:HG12	1:A:104:GLY:H	1.68	0.58
1:A:162:PRO:CA	1:A:165:THR:HG22	2.31	0.58
1:B:141:ALA:HA	1:B:224:VAL:CG1	2.34	0.58
1:B:161:LEU:HD13	1:B:164:LEU:HD12	1.84	0.58
1:A:300:GLU:HG3	1:A:332:THR:OG1	2.04	0.58
1:A:219:ILE:HG13	1:A:220:GLY:H	1.69	0.58
1:A:85:LEU:HD21	1:A:118:LEU:HD22	1.85	0.58
1:A:266:PRO:HD2	1:A:364:LEU:HD13	1.85	0.57
1:B:226:LEU:HD12	1:B:240:LEU:HD11	1.84	0.57
1:A:141:ALA:HA	1:A:224:VAL:HG12	1.86	0.57
1:A:119:PRO:CG	1:B:314:ASP:HB2	2.35	0.57
1:B:196:SER:O	1:B:197:SER:CB	2.52	0.57
1:A:363:ALA:O	1:A:394:LEU:HD12	2.05	0.57
1:B:259:PRO:O	1:B:261:PHE:HB3	2.05	0.57
1:B:39:VAL:HG22	1:B:42:LEU:CD1	2.35	0.57
1:B:102:VAL:HG12	1:B:104:GLY:H	1.70	0.56
1:A:288:ALA:O	1:A:291:ALA:HB2	2.06	0.56
1:B:266:PRO:HD2	1:B:364:LEU:HD13	1.88	0.56
1:A:73:ILE:HG13	1:A:73:ILE:O	2.04	0.56
1:B:277:VAL:HG23	1:B:351:ARG:HA	1.87	0.56
1:B:129:LEU:H	1:B:129:LEU:HD23	1.70	0.56
1:A:226:LEU:HD12	1:A:240:LEU:HD11	1.87	0.56
1:B:262:ARG:HG2	1:B:262:ARG:NH1	2.21	0.56
1:B:73:ILE:HG13	1:B:73:ILE:O	2.06	0.56
1:B:219:ILE:HG13	1:B:220:GLY:H	1.69	0.56
1:B:139:LEU:HD11	1:B:144:PHE:HB2	1.88	0.56
1:A:60:ASP:O	1:A:61:TYR:HB2	2.04	0.55
1:B:242:ILE:N	1:B:242:ILE:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:O	1:A:132:LEU:CB	2.55	0.55
1:B:352:VAL:HG22	1:B:353:SER:N	2.21	0.55
1:B:242:ILE:H	1:B:242:ILE:HD12	1.72	0.55
1:B:308:LEU:HD21	1:B:322:LEU:HD11	1.87	0.55
1:B:131:THR:O	1:B:132:LEU:HB3	2.06	0.55
1:A:196:SER:O	1:A:197:SER:CB	2.54	0.55
1:A:143:LEU:HD21	1:A:191:LEU:CD1	2.34	0.55
1:B:298:ARG:O	1:B:308:LEU:HA	2.06	0.55
1:B:379:ASN:N	1:B:380:GLY:HA3	2.22	0.55
1:B:288:ALA:O	1:B:291:ALA:HB2	2.06	0.55
1:B:173:GLY:O	1:B:174:GLU:CB	2.54	0.55
1:A:173:GLY:O	1:A:174:GLU:CB	2.55	0.55
1:A:352:VAL:HG22	1:A:353:SER:N	2.21	0.55
1:B:162:PRO:CA	1:B:165:THR:HG22	2.32	0.54
1:A:262:ARG:NH1	1:A:262:ARG:HG2	2.21	0.54
1:B:131:THR:O	1:B:132:LEU:CB	2.54	0.54
1:B:307:ARG:O	1:B:307:ARG:HG2	2.08	0.54
1:A:308:LEU:HD21	1:A:322:LEU:HD11	1.88	0.54
1:A:307:ARG:O	1:A:307:ARG:HG2	2.05	0.54
1:B:280:LEU:O	1:B:284:ILE:HG13	2.08	0.54
1:A:141:ALA:HA	1:A:224:VAL:CG1	2.37	0.54
1:B:45:VAL:O	1:B:80:LEU:HD12	2.08	0.54
1:B:222:SER:O	1:B:223:ASP:HB2	2.06	0.53
1:A:222:SER:O	1:A:223:ASP:HB2	2.07	0.53
1:A:172:LEU:O	1:A:173:GLY:O	2.27	0.53
1:A:298:ARG:O	1:A:308:LEU:HA	2.08	0.53
1:B:48:THR:HG22	1:B:78:SER:CB	2.39	0.53
1:A:131:THR:O	1:A:132:LEU:HB3	2.09	0.53
1:A:314:ASP:OD2	1:A:316:GLY:CA	2.57	0.53
1:A:45:VAL:O	1:A:80:LEU:HD12	2.08	0.53
1:B:123:VAL:O	1:B:123:VAL:HG22	2.08	0.53
1:B:363:ALA:O	1:B:394:LEU:HD12	2.09	0.52
1:B:85:LEU:HD21	1:B:118:LEU:HD22	1.91	0.52
1:A:280:LEU:O	1:A:284:ILE:HG13	2.09	0.52
1:B:371:ASP:OD2	1:B:374:PRO:HG2	2.09	0.52
1:A:139:LEU:HD11	1:A:144:PHE:HB2	1.92	0.52
1:A:161:LEU:HD12	1:A:161:LEU:O	2.09	0.52
1:A:25:ALA:HB1	1:A:56:ILE:HD13	1.91	0.52
1:A:17:LEU:HD21	1:A:69:VAL:HG11	1.92	0.52
1:A:50:SER:O	1:A:51:ASP:C	2.48	0.52
1:B:50:SER:O	1:B:51:ASP:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:TRP:NE1	1:A:247:LYS:HB3	2.25	0.52
1:A:16:ARG:NH2	1:A:99:ASP:OD2	2.43	0.52
1:B:379:ASN:N	1:B:380:GLY:CA	2.73	0.51
1:A:115:ARG:HB2	1:A:115:ARG:CZ	2.41	0.51
1:B:314:ASP:OD2	1:B:316:GLY:CA	2.58	0.51
1:A:9:GLY:O	1:A:10:LEU:HB2	2.11	0.51
1:A:48:THR:HG22	1:A:78:SER:CB	2.39	0.51
1:A:42:LEU:HD22	1:A:59:PHE:O	2.11	0.51
1:A:259:PRO:O	1:A:261:PHE:HB3	2.11	0.51
1:A:277:VAL:HG13	1:A:344:LEU:HD22	1.93	0.51
1:A:18:LEU:HG	1:A:18:LEU:O	2.11	0.51
1:B:17:LEU:HD12	1:B:18:LEU:H	1.75	0.51
1:B:327:ALA:CB	1:B:375:VAL:HG13	2.31	0.50
1:A:56:ILE:H	1:A:56:ILE:HD12	1.75	0.50
1:B:15:PHE:CZ	1:B:100:VAL:HG21	2.46	0.50
1:A:123:VAL:HG22	1:A:123:VAL:O	2.11	0.50
1:A:314:ASP:HB2	1:B:119:PRO:HG2	1.93	0.50
1:B:354:PHE:HB3	1:B:356:PHE:CZ	2.46	0.50
1:B:143:LEU:HD21	1:B:191:LEU:CD1	2.36	0.50
1:A:354:PHE:HB3	1:A:356:PHE:CZ	2.47	0.49
1:B:200:ILE:HD11	1:B:234:VAL:CG1	2.40	0.49
1:B:200:ILE:HD12	1:B:201:GLU:H	1.77	0.49
1:B:17:LEU:HD13	1:B:71:ALA:CB	2.42	0.49
1:B:25:ALA:HB1	1:B:56:ILE:HD13	1.93	0.49
1:A:188:VAL:HB	1:A:392:VAL:HG12	1.94	0.49
1:A:290:VAL:O	1:A:290:VAL:HG23	2.11	0.49
1:B:56:ILE:HD12	1:B:56:ILE:H	1.78	0.49
1:A:162:PRO:O	1:A:163:MET:CB	2.59	0.49
1:A:200:ILE:HD12	1:A:201:GLU:H	1.78	0.49
1:A:329:GLU:CD	1:A:329:GLU:H	2.16	0.49
1:B:16:ARG:NH2	1:B:99:ASP:OD2	2.46	0.49
1:B:290:VAL:HG23	1:B:290:VAL:O	2.12	0.49
1:B:172:LEU:O	1:B:173:GLY:O	2.31	0.48
1:B:115:ARG:HB2	1:B:115:ARG:CZ	2.42	0.48
1:B:329:GLU:CD	1:B:329:GLU:H	2.15	0.48
1:B:93:LEU:O	1:B:94:PRO:O	2.31	0.48
1:A:219:ILE:HG13	1:A:220:GLY:N	2.27	0.48
1:B:140:PRO:HB3	1:B:142:GLU:OE2	2.14	0.48
1:A:63:VAL:CG1	1:A:64:SER:N	2.76	0.48
1:B:63:VAL:HG12	1:B:64:SER:H	1.75	0.48
1:B:308:LEU:HD23	1:B:308:LEU:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:N	1:A:242:ILE:HD12	2.28	0.48
1:B:17:LEU:HD21	1:B:69:VAL:HG11	1.95	0.48
1:A:93:LEU:O	1:A:94:PRO:O	2.32	0.48
1:A:331:LEU:HD11	1:A:359:ALA:HB2	1.95	0.48
1:A:303:ASP:CG	1:A:304:GLY:N	2.67	0.48
1:B:314:ASP:O	1:B:315:VAL:HG23	2.13	0.48
1:B:162:PRO:O	1:B:163:MET:CB	2.59	0.47
1:A:48:THR:HG23	1:A:78:SER:HB2	1.96	0.47
1:B:161:LEU:HD12	1:B:161:LEU:O	2.13	0.47
1:B:188:VAL:HB	1:B:392:VAL:HG12	1.96	0.47
1:A:339:TYR:CD1	1:A:339:TYR:N	2.82	0.47
1:A:17:LEU:HD12	1:A:18:LEU:H	1.80	0.47
1:A:15:PHE:CZ	1:A:100:VAL:HG21	2.49	0.47
1:B:303:ASP:CG	1:B:304:GLY:N	2.66	0.47
1:A:206:VAL:CG2	1:A:211:LEU:HD13	2.38	0.47
1:B:12:ASP:HB3	1:B:102:VAL:HB	1.96	0.47
1:B:219:ILE:HG13	1:B:220:GLY:N	2.29	0.47
1:A:9:GLY:O	1:A:10:LEU:CB	2.62	0.47
1:B:28:TRP:NE1	1:B:247:LYS:HB3	2.30	0.47
1:B:364:LEU:HD12	1:B:394:LEU:CD1	2.38	0.47
1:B:378:LEU:C	1:B:380:GLY:HA3	2.36	0.47
1:A:228:LEU:N	1:A:228:LEU:HD12	2.30	0.47
1:A:104:GLY:O	1:A:105:ASN:CB	2.61	0.46
1:A:140:PRO:HB3	1:A:142:GLU:OE2	2.15	0.46
1:B:148:ILE:HD12	1:B:211:LEU:HD23	1.97	0.46
1:A:17:LEU:HD21	1:A:69:VAL:CG1	2.44	0.46
1:A:373:ARG:HA	1:A:374:PRO:C	2.35	0.46
1:B:352:VAL:CG2	1:B:353:SER:N	2.78	0.46
1:B:104:GLY:O	1:B:105:ASN:CB	2.61	0.46
1:A:240:LEU:HD12	1:A:241:GLY:H	1.79	0.46
1:A:266:PRO:HD2	1:A:364:LEU:CD1	2.44	0.46
1:B:18:LEU:HG	1:B:18:LEU:O	2.16	0.46
1:B:185:ARG:NH2	1:B:342:ASP:OD2	2.48	0.46
1:B:281:ILE:HG12	1:B:341:THR:HG22	1.98	0.46
1:A:177:VAL:HG12	1:A:190:GLU:HG3	1.97	0.46
1:A:116:PHE:CD1	1:B:318:ALA:HB2	2.51	0.46
1:A:116:PHE:CE1	1:B:318:ALA:HB2	2.50	0.46
1:B:339:TYR:N	1:B:339:TYR:CD1	2.84	0.46
1:A:153:ILE:H	1:A:153:ILE:HG12	1.51	0.45
1:A:144:PHE:O	1:A:148:ILE:HG12	2.17	0.45
1:A:84:ARG:HD3	1:A:85:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HD21	1:B:69:VAL:CG1	2.46	0.45
1:A:352:VAL:CG2	1:A:353:SER:N	2.79	0.45
1:B:86:LEU:O	1:B:90:THR:HG23	2.15	0.45
1:B:135:GLU:CD	1:B:225:ARG:HH12	2.20	0.45
1:A:17:LEU:HD13	1:A:71:ALA:CB	2.44	0.45
1:A:314:ASP:OD2	1:A:316:GLY:HA2	2.17	0.45
1:B:236:LYS:O	1:B:237:ASP:CB	2.65	0.45
1:B:206:VAL:CG2	1:B:211:LEU:HD13	2.39	0.45
1:B:331:LEU:HD11	1:B:359:ALA:HB2	1.99	0.45
1:A:261:PHE:C	1:A:261:PHE:CD1	2.91	0.44
1:B:349:SER:HB3	1:B:367:PRO:HB3	1.99	0.44
1:B:400:LEU:HA	1:B:401:PRO:HD3	1.60	0.44
1:B:374:PRO:O	1:B:375:VAL:CB	2.65	0.44
1:A:349:SER:HB3	1:A:367:PRO:HB3	1.99	0.44
1:A:200:ILE:HD11	1:A:234:VAL:CG1	2.42	0.44
1:B:277:VAL:HG13	1:B:344:LEU:HD22	1.99	0.44
1:A:126:TYR:HA	1:A:127:PRO:HD3	1.82	0.44
1:A:221:GLY:O	1:A:223:ASP:N	2.50	0.44
1:A:277:VAL:HG23	1:A:351:ARG:CA	2.47	0.44
1:B:177:VAL:HG12	1:B:190:GLU:HG3	2.00	0.43
1:A:274:THR:HG22	1:A:351:ARG:HH22	1.82	0.43
1:A:314:ASP:O	1:A:315:VAL:HG23	2.18	0.43
1:A:307:ARG:O	1:A:307:ARG:CG	2.66	0.43
1:B:144:PHE:O	1:B:148:ILE:HG12	2.19	0.43
1:B:221:GLY:O	1:B:223:ASP:N	2.51	0.43
1:A:242:ILE:H	1:A:242:ILE:HD12	1.84	0.43
1:A:48:THR:CG2	1:A:78:SER:CB	2.97	0.43
1:B:240:LEU:HD12	1:B:241:GLY:H	1.83	0.43
1:A:39:VAL:CG2	1:A:42:LEU:HG	2.49	0.43
1:A:148:ILE:HD12	1:A:211:LEU:HD23	2.00	0.42
1:A:48:THR:CG2	1:A:78:SER:HB2	2.49	0.42
1:B:266:PRO:HD2	1:B:364:LEU:CD1	2.49	0.42
1:A:102:VAL:HG12	1:A:104:GLY:N	2.34	0.42
1:A:400:LEU:HA	1:A:401:PRO:HD3	1.55	0.42
1:A:185:ARG:NH2	1:A:342:ASP:OD2	2.52	0.42
1:B:63:VAL:CG1	1:B:64:SER:N	2.82	0.42
1:B:380:GLY:O	1:B:381:ASN:HB2	2.20	0.42
1:A:184:PHE:C	1:A:185:ARG:HG3	2.39	0.42
1:B:34:PRO:HB2	1:B:35:ALA:H	1.57	0.42
1:B:126:TYR:HA	1:B:127:PRO:HD3	1.81	0.42
1:B:48:THR:HG23	1:B:78:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ALA:O	1:B:291:ALA:CB	2.67	0.42
1:A:105:ASN:O	1:A:120:THR:HB	2.20	0.42
1:B:135:GLU:HB2	1:B:225:ARG:HH22	1.85	0.42
1:B:170:GLU:HG2	1:B:203:ALA:HB1	2.02	0.42
1:A:172:LEU:O	1:A:173:GLY:C	2.59	0.42
1:B:84:ARG:HD3	1:B:85:LEU:N	2.35	0.41
1:A:288:ALA:O	1:A:291:ALA:CB	2.67	0.41
1:A:274:THR:HG22	1:A:351:ARG:NH2	2.35	0.41
1:A:281:ILE:HG12	1:A:341:THR:HG22	2.03	0.41
1:A:244:GLY:O	1:A:245:ASN:HB3	2.20	0.41
1:A:231:GLY:HA3	1:A:232:PRO:HD3	1.80	0.41
1:A:221:GLY:C	1:A:223:ASP:N	2.74	0.41
1:A:318:ALA:HB2	1:B:116:PHE:CD1	2.56	0.41
1:B:396:MET:HA	1:B:397:PRO:HD3	1.96	0.41
1:A:386:ALA:C	1:A:387:VAL:HG13	2.41	0.41
1:A:277:VAL:HG12	1:A:281:ILE:HD12	2.02	0.41
1:B:244:GLY:O	1:B:245:ASN:HB3	2.21	0.41
1:A:79:VAL:HG22	1:A:80:LEU:N	2.36	0.41
1:B:141:ALA:CA	1:B:224:VAL:HG12	2.50	0.41
1:A:177:VAL:CG1	1:A:190:GLU:HG3	2.51	0.41
1:B:33:LEU:N	1:B:34:PRO:HD3	2.36	0.41
1:A:209:LYS:HE3	1:A:209:LYS:HB2	1.90	0.41
1:B:209:LYS:HE3	1:B:209:LYS:HB2	1.90	0.41
1:A:236:LYS:O	1:A:237:ASP:CB	2.66	0.40
1:B:286:LEU:HD12	1:B:289:LEU:HD12	2.03	0.40
1:B:48:THR:CG2	1:B:78:SER:HB2	2.51	0.40
1:B:274:THR:HG22	1:B:351:ARG:HH22	1.86	0.40
1:B:277:VAL:HG23	1:B:351:ARG:CA	2.49	0.40
1:B:275:MET:H	1:B:275:MET:HG2	1.82	0.40
1:A:16:ARG:NH1	1:A:97:PRO:HB2	2.36	0.40
1:A:88:ASP:HB3	1:B:289:LEU:HD22	2.03	0.40
1:A:135:GLU:CD	1:A:225:ARG:HH12	2.25	0.40
1:B:262:ARG:CG	1:B:262:ARG:NH1	2.83	0.40
1:B:314:ASP:OD2	1:B:316:GLY:HA2	2.22	0.40
1:B:172:LEU:O	1:B:173:GLY:C	2.59	0.40
1:A:314:ASP:HB2	1:B:119:PRO:CG	2.51	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	393/395 (100%)	317 (81%)	53 (14%)	23 (6%)	2	11
1	B	391/395 (99%)	319 (82%)	49 (12%)	23 (6%)	2	11
All	All	784/790 (99%)	636 (81%)	102 (13%)	46 (6%)	2	11

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	94	PRO
1	A	132	LEU
1	A	173	GLY
1	A	197	SER
1	A	222	SER
1	A	223	ASP
1	A	292	ASP
1	A	317	ARG
1	A	374	PRO
1	B	12	ASP
1	B	94	PRO
1	B	132	LEU
1	B	173	GLY
1	B	197	SER
1	B	223	ASP
1	B	292	ASP
1	B	317	ARG
1	B	374	PRO
1	A	34	PRO
1	A	51	ASP
1	A	104	GLY
1	A	174	GLU
1	A	330	PRO
1	B	34	PRO

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Mol	Chain	Res	Type
1	B	51	ASP
1	B	104	GLY
1	B	128	THR
1	B	174	GLU
1	B	222	SER
1	B	330	PRO
1	A	61	TYR
1	A	128	THR
1	A	163	MET
1	A	236	LYS
1	A	259	PRO
1	A	383	PRO
1	B	61	TYR
1	B	163	MET
1	B	236	LYS
1	B	259	PRO
1	B	383	PRO
1	A	387	VAL
1	B	387	VAL
1	A	35	ALA
1	B	303	ASP

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	311/311 (100%)	262 (84%)	49 (16%)	3	15
1	B	310/311 (100%)	269 (87%)	41 (13%)	5	22
All	All	621/622 (100%)	531 (86%)	90 (14%)	4	18

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	THR

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Mol	Chain	Res	Type
1	A	17	LEU
1	A	33	LEU
1	A	48	THR
1	A	55	THR
1	A	64	SER
1	A	73	ILE
1	A	84	ARG
1	A	99	ASP
1	A	115	ARG
1	A	120	THR
1	A	129	LEU
1	A	131	THR
1	A	138	LEU
1	A	139	LEU
1	A	153	ILE
1	A	161	LEU
1	A	185	ARG
1	A	186	LEU
1	A	189	ARG
1	A	191	LEU
1	A	193	TRP
1	A	206	VAL
1	A	209	LYS
1	A	213	GLU
1	A	224	VAL
1	A	225	ARG
1	A	227	SER
1	A	234	VAL
1	A	251	THR
1	A	261	PHE
1	A	262	ARG
1	A	275	MET
1	A	293	ARG
1	A	300	GLU
1	A	307	ARG
1	A	308	LEU
1	A	315	VAL
1	A	322	LEU
1	A	323	VAL
1	A	324	VAL
1	A	329	GLU
1	A	341	THR

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Mol	Chain	Res	Type
1	A	353	SER
1	A	357	THR
1	A	364	LEU
1	A	374	PRO
1	A	381	ASN
1	B	14	THR
1	B	17	LEU
1	B	33	LEU
1	B	48	THR
1	B	55	THR
1	B	73	ILE
1	B	84	ARG
1	B	99	ASP
1	B	115	ARG
1	B	120	THR
1	B	129	LEU
1	B	138	LEU
1	B	139	LEU
1	B	153	ILE
1	B	161	LEU
1	B	185	ARG
1	B	186	LEU
1	B	189	ARG
1	B	191	LEU
1	B	193	TRP
1	B	206	VAL
1	B	209	LYS
1	B	224	VAL
1	B	225	ARG
1	B	227	SER
1	B	234	VAL
1	B	251	THR
1	B	261	PHE
1	B	262	ARG
1	B	275	MET
1	B	293	ARG
1	B	300	GLU
1	B	308	LEU
1	B	315	VAL
1	B	322	LEU
1	B	323	VAL
1	B	324	VAL

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Mol	Chain	Res	Type
1	B	329	GLU
1	B	341	THR
1	B	357	THR
1	B	364	LEU

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

Mol	Chain	Res	Type
1	A	101	HIS
1	A	263	GLN
1	B	101	HIS
1	B	263	GLN
1	B	379	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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	395/395 (100%)	-0.31	12 (3%)	54 25	71, 102, 161, 242	0
1	B	393/395 (99%)	-0.30	14 (3%)	46 20	72, 101, 159, 233	0
All	All	788/790 (99%)	-0.31	26 (3%)	50 22	71, 102, 161, 242	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	ASN	7.7
1	A	375	VAL	4.3
1	B	373	ARG	4.3
1	B	378	LEU	4.0
1	A	313	ASP	3.6
1	B	313	ASP	3.5
1	A	376	ALA	3.5
1	A	8	VAL	3.0
1	B	370	GLY	2.8
1	B	377	GLY	2.7
1	B	371	ASP	2.7
1	B	372	ASP	2.7
1	A	232	PRO	2.6
1	B	375	VAL	2.6
1	A	369	SER	2.5
1	B	355	GLY	2.3
1	A	377	GLY	2.3
1	B	376	ALA	2.2
1	B	388	SER	2.2
1	A	312	ALA	2.2
1	B	381	ASN	2.2
1	A	373	ARG	2.1
1	B	353	SER	2.0
1	A	52	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	219	ILE	2.0
1	A	374	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.