



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:22 AM UTC

PDB ID : 1TM0 / pdb_00001tm0
Title : Crystal Structure of the putative proline racemase from Brucella melitensis, Northeast Structural Genomics Target LR31
Authors : Forouhar, F.; Chen, Y.; Xiao, R.; Ho, C.K.; Ma, L.-C.; Cooper, B.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-06-10
Resolution : 2.80 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

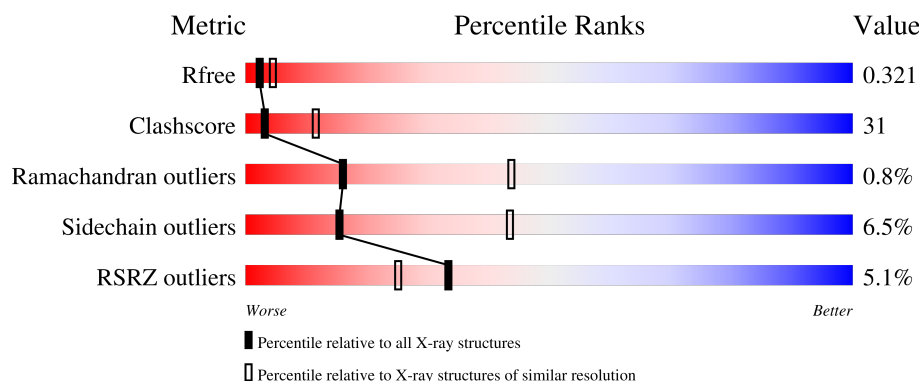
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	350	5% 49% 36% • 11%
1	B	350	4% 45% 40% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4718 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 PROLINE RACEMASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	Se	0	0	0
			2342	1471	416	439	6	10			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2342	1471	416	439	6	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8YFD6
A	76	MSE	MET	modified residue	UNP Q8YFD6
A	81	MSE	MET	modified residue	UNP Q8YFD6
A	89	MSE	MET	modified residue	UNP Q8YFD6
A	109	MSE	MET	modified residue	UNP Q8YFD6
A	116	MSE	MET	modified residue	UNP Q8YFD6
A	164	MSE	MET	modified residue	UNP Q8YFD6
A	263	MSE	MET	modified residue	UNP Q8YFD6
A	272	MSE	MET	modified residue	UNP Q8YFD6
A	321	MSE	MET	modified residue	UNP Q8YFD6
A	343	LEU	-	cloning artifact	UNP Q8YFD6
A	344	GLU	-	cloning artifact	UNP Q8YFD6
A	345	HIS	-	expression tag	UNP Q8YFD6
A	346	HIS	-	expression tag	UNP Q8YFD6
A	347	HIS	-	expression tag	UNP Q8YFD6
A	348	HIS	-	expression tag	UNP Q8YFD6
A	349	HIS	-	expression tag	UNP Q8YFD6
A	350	HIS	-	expression tag	UNP Q8YFD6
B	1	MSE	MET	modified residue	UNP Q8YFD6
B	76	MSE	MET	modified residue	UNP Q8YFD6
B	81	MSE	MET	modified residue	UNP Q8YFD6
B	89	MSE	MET	modified residue	UNP Q8YFD6
B	109	MSE	MET	modified residue	UNP Q8YFD6
B	116	MSE	MET	modified residue	UNP Q8YFD6
B	164	MSE	MET	modified residue	UNP Q8YFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	263	MSE	MET	modified residue	UNP Q8YFD6
B	272	MSE	MET	modified residue	UNP Q8YFD6
B	321	MSE	MET	modified residue	UNP Q8YFD6
B	343	LEU	-	cloning artifact	UNP Q8YFD6
B	344	GLU	-	cloning artifact	UNP Q8YFD6
B	345	HIS	-	expression tag	UNP Q8YFD6
B	346	HIS	-	expression tag	UNP Q8YFD6
B	347	HIS	-	expression tag	UNP Q8YFD6
B	348	HIS	-	expression tag	UNP Q8YFD6
B	349	HIS	-	expression tag	UNP Q8YFD6
B	350	HIS	-	expression tag	UNP Q8YFD6

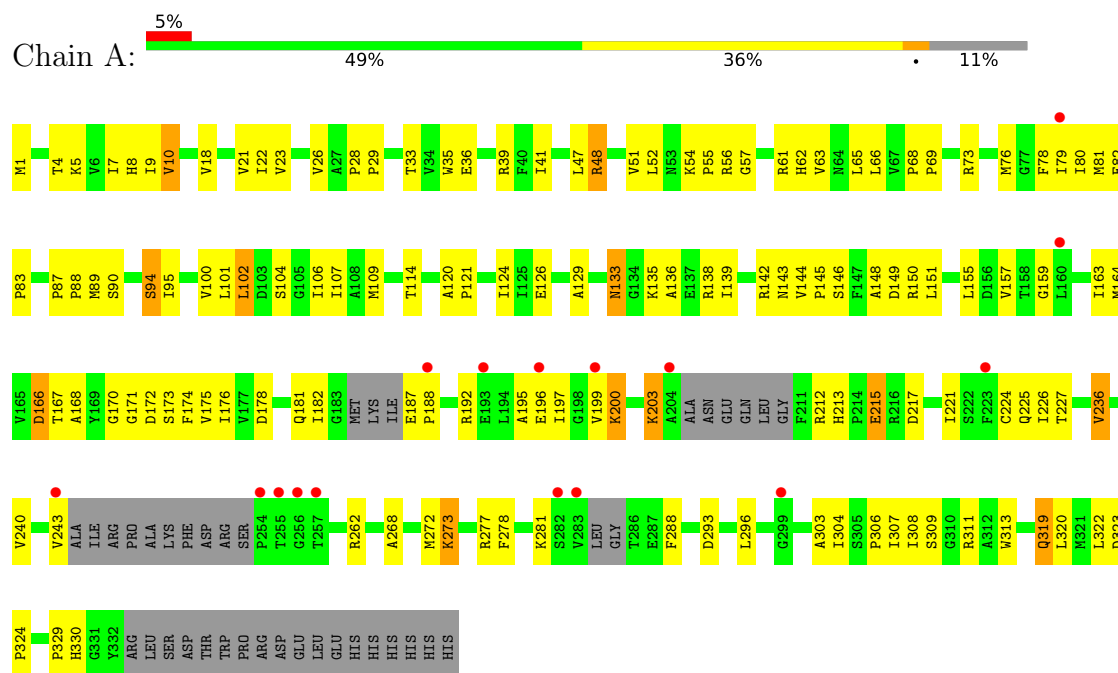
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	23	Total O 23 23	0	0

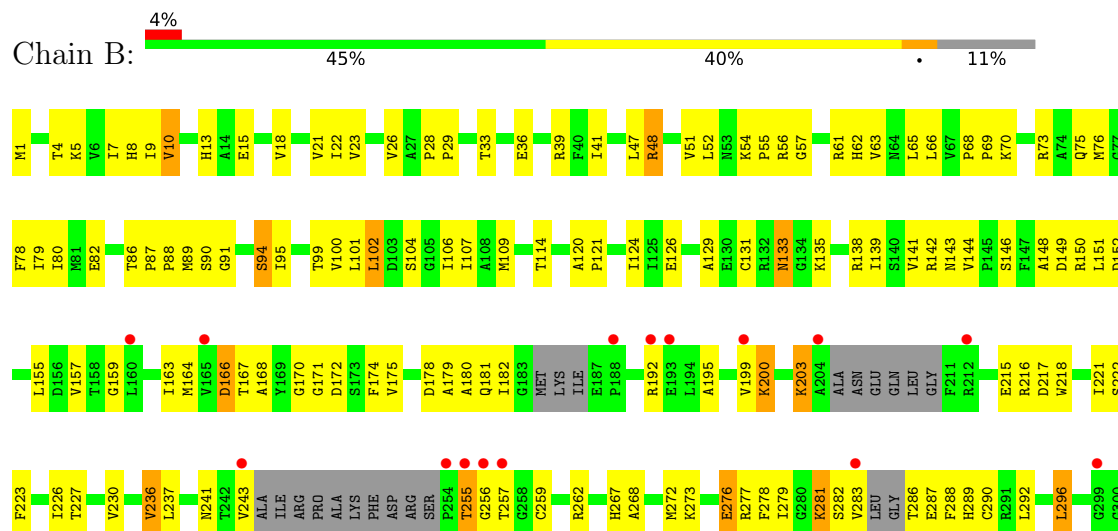
3 Residue-property plots [i](#)

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: PROLINE RACEMASE



• Molecule 1: PROLINE RACEMASE



K301	P302	A303	I304	S305	P306	I307	I308	S309	G310	R311	A312	Q319	L320	M321	L322	D323	P324	Y332	ARG	LEU	SER	ASP	THR	TRP	PRO	ARG	ASP	GLU	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.03Å 77.36Å 77.42Å 90.00° 124.11° 90.00°	Depositor
Resolution (Å)	28.57 – 2.80 28.57 – 2.84	Depositor EDS
% Data completeness (in resolution range)	84.3 (28.57-2.80) 89.5 (28.57-2.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.312 0.253 , 0.321	Depositor DCC
R_{free} test set	2766 reflections (9.46%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.015 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.016 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.014 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.014 for $-h+k-l, -l, -k$ 0.015 for $-h-k-l, l, k$ 0.015 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.014 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.016 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.016 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.469 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4718	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.53	0/2379	0.93	4/3209 (0.1%)
1	B	0.55	0/2379	0.96	5/3209 (0.2%)
All	All	0.54	0/4758	0.94	9/6418 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	SER	N-CA-C	-6.53	104.57	112.54
1	A	94	SER	N-CA-C	-6.31	104.85	112.54
1	B	322	LEU	N-CA-C	6.10	118.35	107.80
1	B	26	VAL	N-CA-C	5.62	115.95	107.80
1	B	171	GLY	N-CA-C	-5.56	107.37	114.37
1	A	171	GLY	N-CA-C	-5.55	107.38	114.37
1	A	26	VAL	N-CA-C	5.40	115.63	107.80
1	A	236	VAL	N-CA-C	5.32	114.96	106.88
1	B	222	SER	N-CA-C	5.15	116.58	111.07

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	2342	0	2344	138	0
1	B	2342	0	2344	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	11	0	0	1	0
2	B	23	0	0	4	0
All	All	4718	0	4688	292	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 31.

All (292) 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:143:ASN:HD22	1:A:144:VAL:N	1.50	1.08
1:B:143:ASN:HD22	1:B:144:VAL:N	1.50	1.08
1:A:143:ASN:ND2	1:A:144:VAL:H	1.56	1.02
1:B:143:ASN:ND2	1:B:144:VAL:H	1.57	1.02
1:A:272:MSE:HE1	1:A:278:PHE:HB2	1.42	1.01
1:B:308:ILE:H	1:B:308:ILE:HD12	1.23	1.01
1:B:301:LYS:HG3	1:B:302:PRO:HD2	1.42	1.01
1:A:164:MSE:H	1:A:181:GLN:HE22	1.07	1.00
1:B:164:MSE:H	1:B:181:GLN:HE22	1.06	0.96
1:B:175:VAL:HG21	1:B:199:VAL:HG21	1.50	0.93
1:A:200:LYS:HD2	1:A:221:ILE:H	1.36	0.90
1:B:296:LEU:HD11	1:B:305:SER:HB2	1.55	0.87
1:B:143:ASN:HB2	1:B:308:ILE:HD11	1.57	0.85
1:B:150:ARG:NH1	1:B:203:LYS:HG2	1.94	0.82
1:A:7:ILE:HD11	1:A:320:LEU:HD23	1.63	0.80
1:B:164:MSE:N	1:B:181:GLN:HE22	1.79	0.80
1:A:164:MSE:N	1:A:181:GLN:HE22	1.80	0.78
1:B:157:VAL:HG22	1:B:159:GLY:H	1.49	0.77
1:B:179:ALA:HB2	1:B:226:ILE:HG22	1.66	0.77
1:B:259:CYS:HB3	2:B:351:HOH:O	1.85	0.77
1:A:143:ASN:HD22	1:A:144:VAL:H	0.79	0.76
1:A:175:VAL:HG21	1:A:199:VAL:HG21	1.64	0.76
1:A:150:ARG:NH1	1:A:203:LYS:HG3	2.01	0.76
1:B:143:ASN:HD22	1:B:144:VAL:H	0.79	0.76
1:A:143:ASN:ND2	1:A:144:VAL:HG22	2.00	0.76
1:B:195:ALA:O	1:B:199:VAL:HG23	1.86	0.75
1:A:157:VAL:HG22	1:A:159:GLY:H	1.50	0.75
1:A:155:LEU:HD13	1:A:203:LYS:HE2	1.66	0.75
1:B:62:HIS:CD2	1:B:82:GLU:HG2	2.22	0.75
1:A:104:SER:HB3	1:A:106:ILE:HD12	1.69	0.74
1:B:7:ILE:HD11	1:B:320:LEU:HD23	1.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASN:ND2	1:B:144:VAL:HG22	2.02	0.74
1:A:62:HIS:CD2	1:A:82:GLU:HG2	2.23	0.74
1:B:104:SER:HB3	1:B:106:ILE:HD12	1.70	0.73
1:B:304:ILE:O	1:B:306:PRO:HD3	1.89	0.71
1:B:290:CYS:HA	1:B:307:ILE:O	1.89	0.71
1:B:150:ARG:HH11	1:B:203:LYS:HG2	1.56	0.70
1:B:141:VAL:O	1:B:308:ILE:HD12	1.91	0.70
1:B:143:ASN:ND2	1:B:144:VAL:N	2.26	0.70
1:A:195:ALA:O	1:A:199:VAL:HG23	1.91	0.70
1:A:143:ASN:ND2	1:A:144:VAL:N	2.26	0.69
1:B:164:MSE:H	1:B:181:GLN:NE2	1.86	0.69
1:B:114:THR:HG23	1:B:129:ALA:HB3	1.75	0.69
1:B:4:THR:HG23	1:B:5:LYS:HG2	1.74	0.69
1:A:164:MSE:H	1:A:181:GLN:NE2	1.87	0.68
1:A:35:TRP:HZ2	1:A:217:ASP:HB3	1.58	0.68
1:A:114:THR:HG23	1:A:129:ALA:HB3	1.75	0.66
1:A:4:THR:HG23	1:A:5:LYS:HG2	1.77	0.66
1:A:143:ASN:HD21	1:A:144:VAL:HG22	1.62	0.65
1:B:54:LYS:HB3	1:B:55:PRO:HA	1.78	0.65
1:A:187:GLU:HB2	1:A:188:PRO:HD2	1.80	0.64
1:A:54:LYS:HB3	1:A:55:PRO:HA	1.79	0.64
1:B:82:GLU:OE2	1:B:87:PRO:HG3	1.99	0.63
1:A:18:VAL:O	1:A:62:HIS:HB2	1.99	0.63
1:A:41:ILE:HG13	1:A:79:ILE:CD1	2.29	0.62
1:B:41:ILE:HG13	1:B:79:ILE:CD1	2.29	0.62
1:A:126:GLU:HG3	1:A:142:ARG:HD2	1.80	0.62
1:B:73:ARG:NH2	1:B:124:ILE:HD13	2.14	0.62
1:A:133:ASN:N	1:A:133:ASN:HD22	1.97	0.62
1:B:143:ASN:HD21	1:B:144:VAL:HG22	1.64	0.61
1:B:126:GLU:HG3	1:B:142:ARG:HD2	1.81	0.61
1:B:200:LYS:HD3	1:B:221:ILE:HB	1.81	0.61
1:B:133:ASN:N	1:B:133:ASN:HD22	1.99	0.60
1:B:91:GLY:H	1:B:257:THR:HG23	1.66	0.60
1:B:18:VAL:O	1:B:62:HIS:HB2	2.02	0.60
1:B:102:LEU:HB3	1:B:109:MSE:HE3	1.84	0.59
1:A:73:ARG:NH2	1:A:124:ILE:HD13	2.16	0.59
1:B:241:ASN:HD22	1:B:262:ARG:HH11	1.51	0.59
1:B:139:ILE:O	1:B:309:SER:HA	2.03	0.59
1:A:102:LEU:HB3	1:A:109:MSE:HE3	1.84	0.59
1:B:88:PRO:HA	1:B:121:PRO:HB2	1.85	0.59
1:B:273:LYS:O	1:B:276:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ASP:HB3	1:B:167:THR:OG1	2.03	0.58
1:A:57:GLY:HA3	1:A:61:ARG:HH11	1.68	0.58
1:A:35:TRP:CZ2	1:A:217:ASP:HB3	2.38	0.58
1:B:237:LEU:HD22	1:B:272:MSE:HE3	1.85	0.58
1:A:82:GLU:OE2	1:A:87:PRO:HG3	2.02	0.57
1:B:308:ILE:HD12	1:B:308:ILE:N	2.06	0.57
1:A:47:LEU:O	1:A:51:VAL:HG22	2.04	0.57
1:A:150:ARG:HH11	1:A:203:LYS:HG3	1.66	0.57
1:A:80:ILE:HG12	1:A:90:SER:HB3	1.86	0.57
1:A:273:LYS:HE2	1:A:273:LYS:HA	1.87	0.57
1:B:7:ILE:CD1	1:B:320:LEU:HD23	2.35	0.57
1:A:65:LEU:HB3	1:A:79:ILE:HG12	1.86	0.57
1:A:88:PRO:HA	1:A:121:PRO:HB2	1.85	0.57
1:B:237:LEU:HD12	1:B:237:LEU:N	2.19	0.57
1:A:151:LEU:HA	1:A:166:ASP:HB3	1.86	0.56
1:B:138:ARG:NH2	1:B:311:ARG:HG3	2.19	0.56
1:A:149:ASP:HB3	1:A:167:THR:OG1	2.05	0.56
1:A:199:VAL:HG13	1:A:203:LYS:HE3	1.88	0.56
1:B:151:LEU:HA	1:B:166:ASP:HB3	1.87	0.56
1:B:57:GLY:HA3	1:B:61:ARG:HH11	1.69	0.55
1:A:146:SER:OG	1:A:170:GLY:HA2	2.06	0.55
1:A:95:ILE:HD12	1:A:139:ILE:HB	1.89	0.55
1:A:69:PRO:HG3	1:A:76:MSE:HA	1.89	0.55
1:B:28:PRO:HB3	1:B:68:PRO:HD2	1.89	0.55
1:B:47:LEU:O	1:B:51:VAL:HG22	2.07	0.55
1:B:323:ASP:OD2	1:B:324:PRO:HD2	2.06	0.55
1:B:33:THR:HG23	1:B:36:GLU:H	1.72	0.55
1:B:69:PRO:HG3	1:B:76:MSE:HA	1.89	0.55
1:A:28:PRO:HB3	1:A:68:PRO:HD2	1.89	0.54
1:A:62:HIS:NE2	1:A:82:GLU:HG2	2.22	0.54
1:B:80:ILE:HG12	1:B:90:SER:HB3	1.89	0.54
1:B:175:VAL:HG12	1:B:223:PHE:O	2.06	0.54
1:B:114:THR:CG2	1:B:129:ALA:HB3	2.36	0.54
1:A:293:ASP:HB2	1:A:307:ILE:CG1	2.38	0.54
1:A:200:LYS:HD2	1:A:221:ILE:N	2.17	0.54
1:B:70:LYS:NZ	2:B:361:HOH:O	2.39	0.54
1:B:62:HIS:NE2	1:B:82:GLU:HG2	2.22	0.54
1:B:146:SER:OG	1:B:170:GLY:HA2	2.08	0.54
1:A:114:THR:CG2	1:A:129:ALA:HB3	2.38	0.53
1:B:179:ALA:HB2	1:B:226:ILE:CG2	2.38	0.53
1:B:308:ILE:H	1:B:308:ILE:CD1	2.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HB3	1:B:79:ILE:HG12	1.88	0.53
1:B:203:LYS:HZ3	1:B:203:LYS:HB2	1.73	0.53
1:B:95:ILE:HD12	1:B:139:ILE:HB	1.89	0.53
1:A:240:VAL:HG13	1:A:281:LYS:HD2	1.91	0.53
1:B:192:ARG:HD2	1:B:243:VAL:HG22	1.91	0.53
1:B:7:ILE:CG1	1:B:320:LEU:HD23	2.39	0.53
1:B:41:ILE:HD12	1:B:47:LEU:HD23	1.91	0.52
1:A:33:THR:HG23	1:A:36:GLU:H	1.74	0.52
1:A:7:ILE:CD1	1:A:320:LEU:HD23	2.37	0.52
1:A:41:ILE:HD12	1:A:47:LEU:HD23	1.91	0.52
1:B:99:THR:OG1	1:B:312:ALA:HB3	2.09	0.52
1:A:9:ILE:HG23	1:A:21:VAL:O	2.09	0.52
1:B:10:VAL:HG11	1:B:100:VAL:HG11	1.92	0.52
1:A:212:ARG:HD3	1:A:212:ARG:N	2.25	0.52
1:B:9:ILE:HG23	1:B:21:VAL:O	2.10	0.52
1:A:10:VAL:HG11	1:A:100:VAL:HG11	1.90	0.52
1:B:199:VAL:HA	1:B:203:LYS:NZ	2.26	0.51
1:A:236:VAL:HG22	1:A:277:ARG:HD2	1.93	0.51
1:A:304:ILE:O	1:A:306:PRO:HD3	2.10	0.51
1:B:227:THR:HG22	1:B:241:ASN:HB2	1.94	0.50
1:A:175:VAL:HG13	1:A:175:VAL:O	2.12	0.50
1:A:23:VAL:HG21	1:B:8:HIS:CE1	2.47	0.50
1:A:304:ILE:HG13	1:A:306:PRO:HD3	1.93	0.50
1:B:104:SER:HB3	1:B:106:ILE:CD1	2.40	0.50
1:B:15:GLU:OE2	1:B:286:THR:HB	2.12	0.49
1:A:52:LEU:HD21	1:A:63:VAL:HG12	1.94	0.49
1:B:255:THR:HG22	1:B:256:GLY:N	2.27	0.49
1:B:237:LEU:HD22	1:B:272:MSE:CE	2.42	0.49
1:B:292:LEU:HD11	1:B:304:ILE:HG21	1.95	0.49
1:A:329:PRO:HG2	1:A:330:HIS:CD2	2.48	0.49
1:B:175:VAL:HG13	1:B:175:VAL:O	2.12	0.48
1:A:145:PRO:HB3	1:A:296:LEU:HD11	1.94	0.48
1:B:279:ILE:O	1:B:279:ILE:HG22	2.13	0.48
1:B:52:LEU:HD21	1:B:63:VAL:HG12	1.94	0.48
1:B:199:VAL:HG13	1:B:203:LYS:HZ3	1.77	0.48
1:A:104:SER:HB3	1:A:106:ILE:CD1	2.41	0.48
1:A:323:ASP:OD2	1:A:324:PRO:HD2	2.12	0.48
1:B:159:GLY:HA2	2:B:366:HOH:O	2.13	0.48
1:A:293:ASP:HB2	1:A:307:ILE:HG13	1.95	0.47
1:B:90:SER:O	1:B:94:SER:HB3	2.14	0.47
1:A:4:THR:O	1:A:5:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:O	1:A:319:GLN:HA	2.15	0.47
1:B:287:GLU:HG3	1:B:289:HIS:CE1	2.49	0.47
1:B:287:GLU:HG3	1:B:289:HIS:HE1	1.78	0.47
1:A:90:SER:O	1:A:94:SER:HB3	2.14	0.47
1:A:151:LEU:HD11	1:A:268:ALA:HB1	1.96	0.47
1:A:178:ASP:HA	1:A:227:THR:O	2.14	0.47
1:B:172:ASP:HB3	1:B:174:PHE:CE1	2.49	0.47
1:A:224:CYS:O	1:A:243:VAL:HG23	2.15	0.47
1:B:323:ASP:OD2	1:B:324:PRO:CD	2.63	0.47
1:A:10:VAL:HG11	1:A:100:VAL:CG1	2.45	0.47
1:A:48:ARG:HB3	1:A:48:ARG:NH1	2.30	0.47
1:A:192:ARG:O	1:A:196:GLU:HG3	2.14	0.47
1:A:199:VAL:CG1	1:A:221:ILE:HG13	2.45	0.47
1:A:311:ARG:HB2	1:A:313:TRP:CH2	2.50	0.47
1:A:4:THR:HG22	1:A:322:LEU:O	2.14	0.47
1:A:176:ILE:HG13	1:A:225:GLN:NE2	2.29	0.47
1:B:101:LEU:HB3	1:B:107:ILE:HG12	1.97	0.47
1:B:78:PHE:CZ	1:B:120:ALA:HB2	2.50	0.47
1:A:78:PHE:CZ	1:A:120:ALA:HB2	2.50	0.47
1:A:172:ASP:HB3	1:A:174:PHE:CE1	2.50	0.46
1:B:172:ASP:HB3	1:B:174:PHE:HE1	1.80	0.46
1:B:200:LYS:HD2	1:B:221:ILE:H	1.80	0.46
1:A:41:ILE:HG13	1:A:79:ILE:HD12	1.98	0.46
1:B:216:ARG:C	1:B:218:TRP:H	2.22	0.46
1:A:164:MSE:N	1:A:181:GLN:NE2	2.57	0.46
1:A:311:ARG:HG3	1:A:311:ARG:HH11	1.79	0.46
1:B:308:ILE:N	1:B:308:ILE:CD1	2.74	0.46
1:A:138:ARG:NH2	1:A:311:ARG:HG2	2.30	0.46
1:A:61:ARG:HB3	2:A:351:HOH:O	2.16	0.46
1:B:4:THR:O	1:B:5:LYS:HB3	2.16	0.46
1:B:272:MSE:HE1	1:B:278:PHE:HD2	1.81	0.46
1:A:172:ASP:HB3	1:A:174:PHE:HE1	1.80	0.45
1:B:192:ARG:NH1	1:B:243:VAL:HG13	2.30	0.45
1:A:304:ILE:C	1:A:306:PRO:HD3	2.41	0.45
1:B:22:ILE:HB	1:B:65:LEU:HD12	1.98	0.45
1:B:75:GLN:HG3	2:B:372:HOH:O	2.15	0.45
1:A:262:ARG:NH1	1:A:262:ARG:HG2	2.30	0.45
1:A:323:ASP:OD2	1:A:324:PRO:CD	2.64	0.45
1:B:120:ALA:HB1	1:B:121:PRO:CD	2.46	0.45
1:B:163:ILE:HG21	1:B:181:GLN:O	2.15	0.45
1:A:8:HIS:CE1	1:B:23:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:HG11	1:B:100:VAL:CG1	2.47	0.45
1:B:91:GLY:N	1:B:257:THR:HG23	2.31	0.45
1:B:199:VAL:HA	1:B:203:LYS:HZ1	1.82	0.45
1:A:188:PRO:HB2	1:A:226:ILE:HD12	1.99	0.45
1:B:163:ILE:CG2	1:B:181:GLN:HB3	2.47	0.45
1:A:163:ILE:HG21	1:A:181:GLN:O	2.17	0.44
1:B:282:SER:HA	1:B:286:THR:O	2.18	0.44
1:B:7:ILE:O	1:B:319:GLN:HA	2.17	0.44
1:A:323:ASP:OD2	1:A:323:ASP:C	2.61	0.44
1:B:227:THR:HG22	1:B:241:ASN:CB	2.48	0.44
1:B:236:VAL:HA	1:B:277:ARG:O	2.18	0.44
1:A:262:ARG:HG2	1:A:262:ARG:HH11	1.82	0.44
1:A:172:ASP:OD2	1:A:173:SER:N	2.50	0.44
1:B:79:ILE:O	1:B:79:ILE:HG13	2.17	0.44
1:B:120:ALA:HB1	1:B:121:PRO:HD2	2.00	0.44
1:B:157:VAL:HG13	1:B:157:VAL:O	2.18	0.44
1:A:323:ASP:OD2	1:A:324:PRO:N	2.50	0.43
1:B:100:VAL:O	1:B:101:LEU:C	2.59	0.43
1:A:65:LEU:HB3	1:A:79:ILE:CG1	2.47	0.43
1:A:135:LYS:C	1:A:135:LYS:HD3	2.44	0.43
1:A:163:ILE:CG2	1:A:181:GLN:HB3	2.49	0.43
1:B:48:ARG:NH1	1:B:48:ARG:HB3	2.33	0.43
1:A:101:LEU:HB3	1:A:107:ILE:HG12	2.00	0.43
1:B:7:ILE:HG12	1:B:320:LEU:HB2	2.00	0.43
1:B:273:LYS:N	1:B:276:GLU:OE1	2.45	0.43
1:B:281:LYS:HG2	1:B:282:SER:N	2.34	0.43
1:A:146:SER:O	1:A:303:ALA:HB1	2.18	0.43
1:A:213:HIS:CE1	1:A:215:GLU:HB3	2.53	0.43
1:B:151:LEU:HD11	1:B:268:ALA:HB1	1.98	0.43
1:B:164:MSE:N	1:B:181:GLN:NE2	2.56	0.43
1:B:267:HIS:O	1:B:267:HIS:CG	2.71	0.43
1:B:304:ILE:C	1:B:306:PRO:HD3	2.42	0.43
1:A:157:VAL:HG22	1:A:159:GLY:N	2.27	0.43
1:B:157:VAL:HG22	1:B:159:GLY:N	2.27	0.43
1:B:272:MSE:HE1	1:B:278:PHE:CD2	2.53	0.43
1:B:51:VAL:HG23	1:B:52:LEU:N	2.34	0.42
1:B:65:LEU:HB3	1:B:79:ILE:CG1	2.48	0.42
1:B:255:THR:HG22	1:B:256:GLY:H	1.84	0.42
1:B:52:LEU:CD2	1:B:63:VAL:HG12	2.49	0.42
1:B:69:PRO:HG3	1:B:76:MSE:CA	2.49	0.42
1:B:114:THR:HG22	1:B:131:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:VAL:HG22	1:B:277:ARG:NE	2.35	0.42
1:A:51:VAL:HG23	1:A:52:LEU:N	2.34	0.42
1:A:120:ALA:HB1	1:A:121:PRO:HD2	2.01	0.42
1:B:135:LYS:HD3	1:B:135:LYS:C	2.44	0.42
1:A:22:ILE:HB	1:A:65:LEU:HD12	2.00	0.42
1:A:28:PRO:HA	1:A:29:PRO:HD3	1.95	0.42
1:A:196:GLU:HG2	1:A:224:CYS:HB2	2.00	0.42
1:B:148:ALA:HA	1:B:168:ALA:HA	2.01	0.42
1:B:192:ARG:NH1	1:B:243:VAL:HG22	2.35	0.42
1:A:69:PRO:HG3	1:A:76:MSE:CA	2.49	0.42
1:A:139:ILE:O	1:A:309:SER:HA	2.19	0.42
1:B:41:ILE:HG13	1:B:79:ILE:HD12	1.98	0.42
1:A:120:ALA:HB1	1:A:121:PRO:CD	2.50	0.42
1:A:320:LEU:H	1:A:320:LEU:HD22	1.84	0.42
1:B:13:HIS:O	1:B:13:HIS:CD2	2.73	0.42
1:A:133:ASN:N	1:A:133:ASN:ND2	2.68	0.41
1:B:155:LEU:HD13	1:B:203:LYS:HZ1	1.86	0.41
1:A:4:THR:O	1:A:5:LYS:CB	2.67	0.41
1:A:79:ILE:O	1:A:79:ILE:HG13	2.20	0.41
1:A:164:MSE:HG2	1:A:181:GLN:NE2	2.35	0.41
1:A:65:LEU:O	1:A:78:PHE:HA	2.20	0.41
1:B:178:ASP:C	1:B:180:ALA:H	2.28	0.41
1:B:200:LYS:CD	1:B:221:ILE:H	2.33	0.41
1:B:292:LEU:HD11	1:B:304:ILE:CG2	2.51	0.41
1:A:148:ALA:HA	1:A:168:ALA:HA	2.02	0.41
1:A:157:VAL:HG13	1:A:157:VAL:O	2.19	0.41
1:A:196:GLU:O	1:A:197:ILE:C	2.64	0.41
1:B:307:ILE:O	1:B:307:ILE:HG22	2.20	0.41
1:A:138:ARG:NH2	1:A:311:ARG:CG	2.83	0.41
1:B:73:ARG:NH2	1:B:124:ILE:HG21	2.36	0.41
1:A:52:LEU:CD2	1:A:63:VAL:HG12	2.50	0.41
1:B:65:LEU:O	1:B:78:PHE:HA	2.21	0.41
1:A:56:ARG:NH2	1:A:56:ARG:HG3	2.35	0.41
1:A:63:VAL:HG13	1:A:81:MSE:HE3	2.03	0.41
1:A:66:LEU:HD22	1:A:76:MSE:HG2	2.03	0.41
1:A:100:VAL:O	1:A:101:LEU:C	2.62	0.41
1:A:164:MSE:HG2	1:A:181:GLN:HE22	1.85	0.41
1:B:56:ARG:HG2	1:B:320:LEU:HD12	2.03	0.41
1:B:199:VAL:HG13	1:B:203:LYS:NZ	2.36	0.41
1:A:48:ARG:O	1:A:52:LEU:HB2	2.21	0.41
1:B:296:LEU:HD11	1:B:305:SER:CB	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:O	1:A:7:ILE:HG13	2.20	0.40
1:A:52:LEU:HD13	1:A:83:PRO:HA	2.02	0.40
1:A:95:ILE:HD13	1:A:95:ILE:HA	1.89	0.40
1:A:136:ALA:HB1	1:A:139:ILE:HD11	2.03	0.40
1:B:56:ARG:NH2	1:B:56:ARG:HG3	2.36	0.40
1:B:66:LEU:HD22	1:B:76:MSE:HG2	2.03	0.40
1:B:151:LEU:O	1:B:152:ASP:C	2.64	0.40
1:A:200:LYS:CD	1:A:221:ILE:HB	2.52	0.40
1:B:86:THR:O	1:B:86:THR:OG1	2.39	0.40
1:A:320:LEU:HD22	1:A:320:LEU:N	2.37	0.40
1:B:28:PRO:HB3	1:B:68:PRO:CD	2.51	0.40
1:B:28:PRO:HA	1:B:29:PRO:HD3	1.95	0.40
1:B:230:VAL:O	1:B:230:VAL:HG13	2.20	0.40
1:A:225:GLN:HB3	1:A:243:VAL:HB	2.04	0.40
1:B:141:VAL:HB	1:B:308:ILE:HD13	2.03	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	301/350 (86%)	264 (88%)	36 (12%)	1 (0%)	36	66
1	B	301/350 (86%)	264 (88%)	33 (11%)	4 (1%)	9	31
All	All	602/700 (86%)	528 (88%)	69 (12%)	5 (1%)	16	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	THR
1	A	215	GLU
1	B	215	GLU

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Mol	Chain	Res	Type
1	B	217	ASP
1	B	281	LYS

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	255/279 (91%)	240 (94%)	15 (6%)	18	48
1	B	255/279 (91%)	237 (93%)	18 (7%)	13	39
All	All	510/558 (91%)	477 (94%)	33 (6%)	15	43

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	10	VAL
1	A	39	ARG
1	A	48	ARG
1	A	89	MSE
1	A	102	LEU
1	A	133	ASN
1	A	166	ASP
1	A	182	ILE
1	A	200	LYS
1	A	203	LYS
1	A	273	LYS
1	A	288	PHE
1	A	308	ILE
1	A	319	GLN
1	B	1	MSE
1	B	10	VAL
1	B	39	ARG
1	B	48	ARG
1	B	89	MSE
1	B	102	LEU

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Mol	Chain	Res	Type
1	B	133	ASN
1	B	166	ASP
1	B	182	ILE
1	B	200	LYS
1	B	203	LYS
1	B	236	VAL
1	B	276	GLU
1	B	283	VAL
1	B	288	PHE
1	B	296	LEU
1	B	308	ILE
1	B	319	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	37	GLN
1	A	43	ASN
1	A	49	ASN
1	A	53	ASN
1	A	93	ASN
1	A	133	ASN
1	A	143	ASN
1	A	181	GLN
1	A	213	HIS
1	A	225	GLN
1	A	319	GLN
1	A	330	HIS
1	B	13	HIS
1	B	37	GLN
1	B	43	ASN
1	B	49	ASN
1	B	53	ASN
1	B	93	ASN
1	B	133	ASN
1	B	143	ASN
1	B	181	GLN
1	B	241	ASN
1	B	330	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 [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	301/350 (86%)	0.41	16 (5%) 32 24	4, 29, 64, 78	0
1	B	301/350 (86%)	0.41	15 (4%) 34 26	5, 28, 66, 77	0
All	All	602/700 (86%)	0.41	31 (5%) 33 25	4, 28, 66, 78	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	GLY	4.4
1	A	254	PRO	4.2
1	A	257	THR	3.8
1	B	255	THR	3.1
1	A	256	GLY	3.0
1	A	188	PRO	3.0
1	A	193	GLU	2.8
1	B	257	THR	2.8
1	A	283	VAL	2.7
1	B	193	GLU	2.7
1	B	283	VAL	2.7
1	B	188	PRO	2.6
1	B	243	VAL	2.6
1	A	160	LEU	2.6
1	B	204	ALA	2.5
1	A	243	VAL	2.4
1	A	199	VAL	2.3
1	A	223	PHE	2.3
1	B	199	VAL	2.2
1	B	299	GLY	2.2
1	A	79	ILE	2.2
1	B	254	PRO	2.2
1	B	160	LEU	2.2
1	A	282	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	255	THR	2.1
1	A	196	GLU	2.1
1	B	165	VAL	2.0
1	A	299	GLY	2.0
1	B	212	ARG	2.0
1	B	192	ARG	2.0
1	A	204	ALA	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.