W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 10:34 am GMT

PDB ID	:	5E27
Title	:	The structure of Resuscitation Promoting Factor B from M. tuberculosis reveals unexpected ubiquitin-like domains
Authors	:	Ruggiero, A.; Squeglia, F.; Romano, M.; Vitagliano, L.; De Simone, A.; Berisio, R.
Deposited on	:	2015-09-30
Resolution	:	2.60 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.
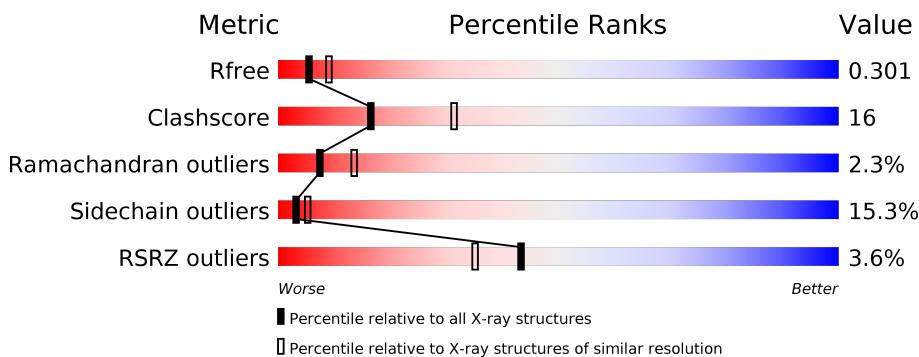
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 <=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	248	3% / 59% / 26% / 6% / 9%
1	B	248	3% / 59% / 22% / 8% / 11%
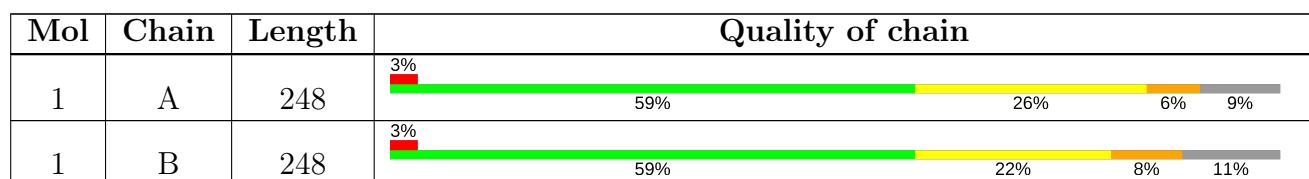
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3387 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 Resuscitation-promoting factor RpfB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	2	0
			1682	1049	310	318	5			
1	B	220	Total	C	N	O	S	0	0	0
			1629	1018	297	309	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	40	Total	O	0	0
			40	40		

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 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: Resuscitation-promoting factor RpfB
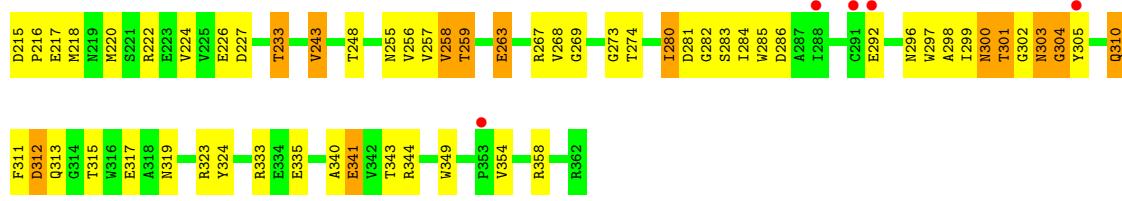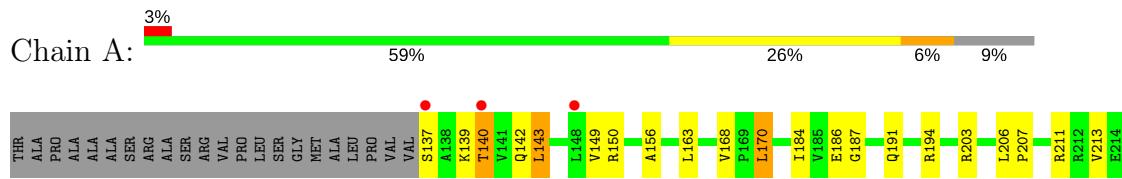
• Molecule 1: Resuscitation-promoting factor RpfB
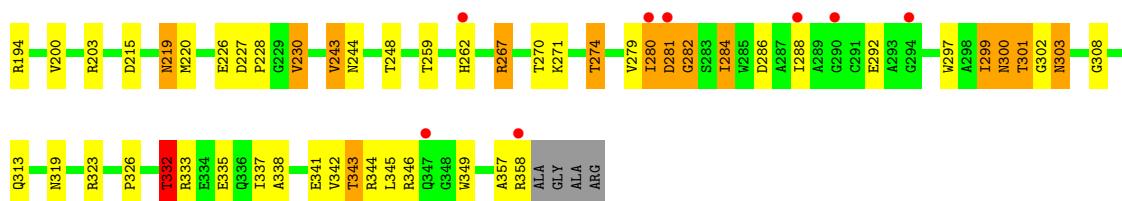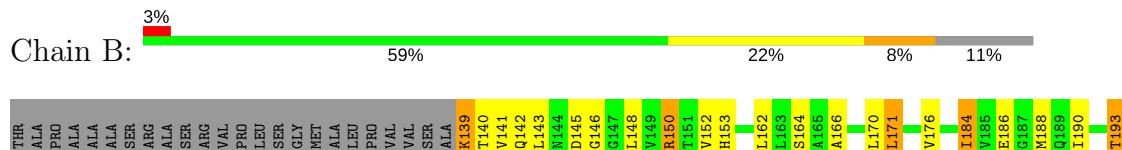
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	102.38Å 126.99Å 86.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 14.95 – 2.65	Depositor EDS
% Data completeness (in resolution range)	92.9 (15.00-2.60) 94.7 (14.95-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.15 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.222 , 0.291 0.234 , 0.301	Depositor DCC
R_{free} test set	786 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3387	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.00 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.2437e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

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	0.88	1/1720 (0.1%)	0.83	3/2356 (0.1%)
1	B	0.82	0/1664	0.86	1/2282 (0.0%)
All	All	0.85	1/3384 (0.0%)	0.84	4/4638 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	GLU	CG-CD	5.90	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	ASP	C-N-CD	6.15	141.31	128.40
1	B	203	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	143	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	319	ASN	CB-CA-C	5.20	120.80	110.40

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	1682	0	1667	52	0
1	B	1629	0	1612	53	0
2	A	36	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	40	0	0	4	0
All	All	3387	0	3279	105	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 (105) 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:303:ASN:OD1	1:A:304:GLY:N	1.95	0.99
1:A:305:TYR:CB	1:A:310:GLN:HG3	1.97	0.93
1:A:305:TYR:HB3	1:A:310:GLN:HG3	1.53	0.91
1:A:233:THR:HG22	1:A:258:VAL:HG22	1.58	0.84
1:B:220:MET:H	1:B:274:THR:CG2	1.92	0.83
1:A:313:GLN:O	1:A:317:GLU:HG3	1.81	0.81
1:B:140:THR:OG1	1:B:153:HIS:HD2	1.66	0.78
1:A:305:TYR:HB2	1:A:310:GLN:HG3	1.69	0.74
1:B:332:THR:HG22	1:B:335:GLU:H	1.56	0.70
1:A:163:LEU:HD13	1:A:170:LEU:HD13	1.73	0.70
1:B:220:MET:H	1:B:274:THR:HG21	1.55	0.70
1:A:281:ASP:OD1	1:A:284:ILE:HD12	1.93	0.69
1:B:194:ARG:H	1:B:244:ASN:ND2	1.92	0.68
1:B:274:THR:HG23	1:B:274:THR:O	1.94	0.67
1:A:203:ARG:NH2	1:A:258:VAL:HG21	2.11	0.66
1:A:156:ALA:O	1:A:184:ILE:HD12	1.95	0.66
1:B:297:TRP:CE2	1:B:333:ARG:HG3	2.31	0.66
1:A:280:ILE:O	1:A:281:ASP:HB2	1.97	0.65
1:B:141:VAL:HG11	1:B:190:ILE:HD12	1.78	0.63
1:A:324:TYR:CD1	1:A:335:GLU:HG2	2.33	0.63
2:A:424:HOH:O	1:B:193:THR:HB	1.98	0.63
1:B:342:VAL:HG12	1:B:342:VAL:O	1.99	0.61
1:B:150:ARG:NH2	1:B:166:ALA:HB1	2.16	0.60
1:A:282:GLY:O	1:A:286:ASP:N	2.23	0.60
1:A:137:SER:O	1:A:139:LYS:HD2	2.02	0.59
1:A:220:MET:HG3	1:A:274:THR:OG1	2.01	0.59
1:B:230:VAL:CG1	1:B:262:HIS:HB2	2.33	0.59
1:B:280:ILE:HG22	1:B:281:ASP:N	2.18	0.58
1:A:149:VAL:HG12	1:A:150:ARG:N	2.18	0.58
1:A:297:TRP:CZ2	1:A:333:ARG:HG3	2.39	0.58
1:B:284:ILE:HD12	1:B:349:TRP:CH2	2.39	0.57
1:B:139:LYS:HG3	2:B:408:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:CD1	1:A:170:LEU:HD13	2.34	0.56
1:B:297:TRP:CE3	1:B:308:GLY:HA3	2.40	0.56
1:B:184:ILE:HG13	1:B:188:MET:CE	2.37	0.55
1:A:300:ASN:C	1:A:300:ASN:HD22	2.09	0.55
1:A:273:GLY:O	1:A:323:ARG:HD2	2.07	0.55
1:B:139:LYS:HA	2:B:408:HOH:O	2.07	0.55
1:B:140:THR:OG1	1:B:153:HIS:CD2	2.55	0.55
1:A:140:THR:HB	1:A:187:GLY:H	1.73	0.54
1:A:203:ARG:HH21	1:A:258:VAL:HG21	1.71	0.54
1:A:226:GLU:OE2	1:A:267[A]:ARG:NH1	2.42	0.53
1:B:288:ILE:O	1:B:292:GLU:CB	2.56	0.53
1:A:191:GLN:HG3	2:B:427:HOH:O	2.08	0.53
1:B:343:THR:C	1:B:345:LEU:H	2.12	0.53
1:B:194:ARG:H	1:B:244:ASN:HD21	1.55	0.53
1:A:243:VAL:HG13	1:A:248:THR:HG21	1.91	0.52
1:A:344:ARG:HD2	1:A:349:TRP:CE2	2.43	0.52
1:B:319:ASN:OD1	1:B:343:THR:OG1	2.04	0.52
1:A:299:ILE:O	1:A:299:ILE:HG23	2.10	0.52
1:B:200:VAL:HG23	1:B:200:VAL:O	2.09	0.51
1:B:288:ILE:O	1:B:292:GLU:HB2	2.10	0.51
1:B:219:ASN:HA	1:B:274:THR:HG21	1.93	0.51
1:A:186:GLU:HA	1:A:186:GLU:OE2	2.10	0.51
1:A:213:VAL:HG23	1:A:267[A]:ARG:HG3	1.93	0.50
1:B:357:ALA:N	2:B:403:HOH:O	2.44	0.50
1:B:338:ALA:O	1:B:342:VAL:HG23	2.11	0.50
1:B:343:THR:C	1:B:345:LEU:N	2.65	0.50
1:A:222:ARG:HB2	2:A:430:HOH:O	2.12	0.50
1:B:271:LYS:O	1:B:274:THR:HB	2.11	0.50
1:B:274:THR:CG2	1:B:274:THR:O	2.59	0.50
1:B:170:LEU:O	1:B:171:LEU:HD13	2.12	0.50
1:B:281:ASP:O	1:B:282:GLY:C	2.51	0.50
1:A:344:ARG:HD2	1:A:349:TRP:CZ2	2.47	0.49
1:A:168:VAL:HB	1:A:194:ARG:NH2	2.28	0.48
1:B:301:THR:O	1:B:303:ASN:N	2.47	0.48
1:A:285:TRP:CZ2	1:A:341:GLU:HG3	2.49	0.48
1:A:149:VAL:HG12	1:A:150:ARG:H	1.79	0.48
1:B:281:ASP:O	1:B:284:ILE:HG22	2.14	0.47
1:B:184:ILE:HG13	1:B:188:MET:HE2	1.96	0.47
1:A:280:ILE:HA	1:A:280:ILE:HD12	1.67	0.47
1:A:303:ASN:OD1	1:A:305:TYR:N	2.39	0.47
1:B:341:GLU:C	1:B:343:THR:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TRP:CE2	1:A:333:ARG:HG3	2.50	0.46
1:A:302:GLY:O	1:A:303:ASN:HB3	2.15	0.46
1:A:281:ASP:OD1	1:A:284:ILE:CD1	2.64	0.45
1:B:299:ILE:O	1:B:300:ASN:HB2	2.16	0.45
1:B:319:ASN:OD1	1:B:343:THR:HG23	2.16	0.45
1:B:162:LEU:HD12	1:B:184:ILE:HD12	1.99	0.45
1:A:218:MET:HG2	1:A:269:GLY:CA	2.47	0.45
1:A:312:ASP:OD2	1:A:312:ASP:C	2.55	0.45
1:B:219:ASN:N	1:B:219:ASN:HD22	2.14	0.44
1:A:258:VAL:CG2	1:A:259:THR:N	2.81	0.44
1:B:215:ASP:HB2	1:B:267:ARG:HD2	1.99	0.44
1:A:206:LEU:HD12	1:A:207:PRO:HD2	1.99	0.44
1:A:296:ASN:ND2	1:A:298:ALA:H	2.16	0.44
1:A:149:VAL:CG1	1:A:150:ARG:N	2.80	0.43
1:A:211:ARG:HD3	1:A:263:GLU:OE1	2.19	0.43
1:B:220:MET:H	1:B:274:THR:HG23	1.81	0.43
1:A:301:THR:HG23	1:A:302:GLY:H	1.84	0.43
1:B:230:VAL:HG13	1:B:262:HIS:HB2	2.01	0.43
1:B:279:VAL:HG12	1:B:337:ILE:HG21	2.01	0.43
1:B:244:ASN:HA	1:B:244:ASN:HD22	1.66	0.42
1:B:319:ASN:OD1	1:B:343:THR:CG2	2.66	0.42
1:B:243:VAL:HG13	1:B:248:THR:HG21	2.00	0.42
1:B:145:ASP:O	1:B:146:GLY:C	2.58	0.42
1:A:285:TRP:HZ2	1:A:341:GLU:HG3	1.84	0.42
1:A:215:ASP:HA	1:A:216:PRO:HD3	1.90	0.41
1:B:227:ASP:HA	1:B:228:PRO:HD2	1.90	0.41
1:B:313:GLN:NE2	1:B:326:PRO:O	2.51	0.41
1:A:358:ARG:CZ	1:A:358:ARG:HB2	2.51	0.41
1:B:280:ILE:CG2	1:B:281:ASP:N	2.83	0.41
1:A:215:ASP:C	1:A:217:GLU:H	2.24	0.40
1:B:226:GLU:OE1	1:B:267:ARG:NH1	2.54	0.40
1:A:340:ALA:O	1:A:343:THR:N	2.50	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	226/248 (91%)	205 (91%)	18 (8%)	3 (1%)	14	29
1	B	218/248 (88%)	194 (89%)	17 (8%)	7 (3%)	5	7
All	All	444/496 (90%)	399 (90%)	35 (8%)	10 (2%)	7	13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	GLU
1	A	303	ASN
1	B	302	GLY
1	B	332	THR
1	B	300	ASN
1	B	186	GLU
1	B	344	ARG
1	A	304	GLY
1	B	282	GLY
1	B	280	ILE

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	172/187 (92%)	149 (87%)	23 (13%)	4	8
1	B	169/187 (90%)	140 (83%)	29 (17%)	2	3
All	All	341/374 (91%)	289 (85%)	52 (15%)	3	5

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	THR
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	143	LEU
1	A	170	LEU
1	A	224	VAL
1	A	233	THR
1	A	243	VAL
1	A	255	ASN
1	A	256	VAL
1	A	257	VAL
1	A	258	VAL
1	A	259	THR
1	A	268	VAL
1	A	280	ILE
1	A	283	SER
1	A	292	GLU
1	A	300	ASN
1	A	301	THR
1	A	310	GLN
1	A	311	PHE
1	A	312	ASP
1	A	315	THR
1	A	354	VAL
1	B	139	LYS
1	B	142	GLN
1	B	143	LEU
1	B	148	LEU
1	B	150	ARG
1	B	152	VAL
1	B	164	SER
1	B	171	LEU
1	B	176	VAL
1	B	184	ILE
1	B	193	THR
1	B	219	ASN
1	B	230	VAL
1	B	243	VAL
1	B	259	THR
1	B	267	ARG
1	B	270	THR
1	B	274	THR
1	B	281	ASP
1	B	284	ILE
1	B	286	ASP

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Mol	Chain	Res	Type
1	B	299	ILE
1	B	301	THR
1	B	303	ASN
1	B	323	ARG
1	B	332	THR
1	B	343	THR
1	B	346	ARG
1	B	358	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	219	ASN
1	A	296	ASN
1	A	300	ASN
1	B	153	HIS
1	B	172	GLN
1	B	219	ASN
1	B	244	ASN
1	B	255	ASN
1	B	303	ASN
1	B	336	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	226/248 (91%)	-0.02	8 (3%)	44	36	18, 33, 56, 67	0
1	B	220/248 (88%)	-0.10	8 (3%)	43	35	21, 32, 70, 76	0
All	All	446/496 (89%)	-0.06	16 (3%)	43	35	18, 32, 64, 76	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	GLY	3.3
1	A	137	SER	3.1
1	B	288	ILE	2.8
1	B	347	GLN	2.8
1	B	290	GLY	2.6
1	A	148	LEU	2.5
1	A	353	PRO	2.4
1	A	292	GLU	2.4
1	A	140	THR	2.4
1	B	358	ARG	2.3
1	B	280	ILE	2.3
1	B	281	ASP	2.3
1	A	305	TYR	2.2
1	B	262	HIS	2.2
1	A	288	ILE	2.1
1	A	291	CYS	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.