Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:22 AM GMT

PDB ID	:	2WUS
Title	:	BACTERIAL ACTIN MREB ASSEMBLES IN COMPLEX WITH CELL SHAPE PROTEIN RODZ
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Deposited on	:	2009-10-08
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
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 (1)) were used in the production of this report:

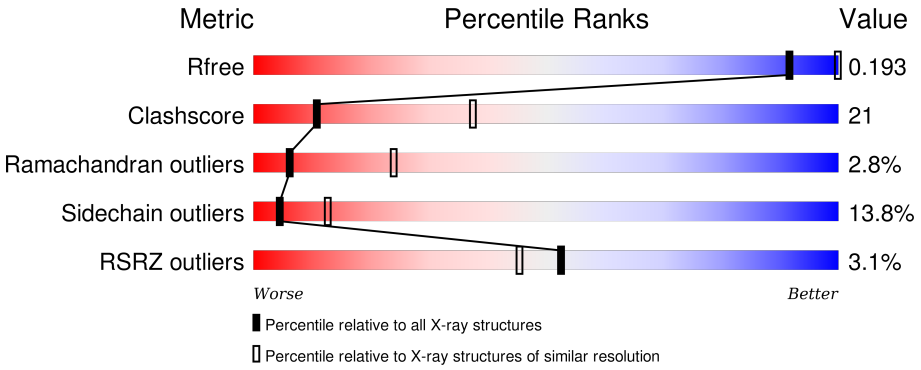
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	344	% 57% 33% 7% •
1	B	344	7% 52% 39% 5% • •
2	R	112	49% 21% 7% • 22%
2	S	112	% 33% 37% • • 27%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6399 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 ROD SHAPE-DETERMINING PROTEIN MREB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2500	1580	430	482	8			
1	B	333	Total	C	N	O	S	0	0	0
			2481	1568	425	480	8			

- Molecule 2 is a protein called PUTATIVE UNCHARACTERIZED PROTEIN.

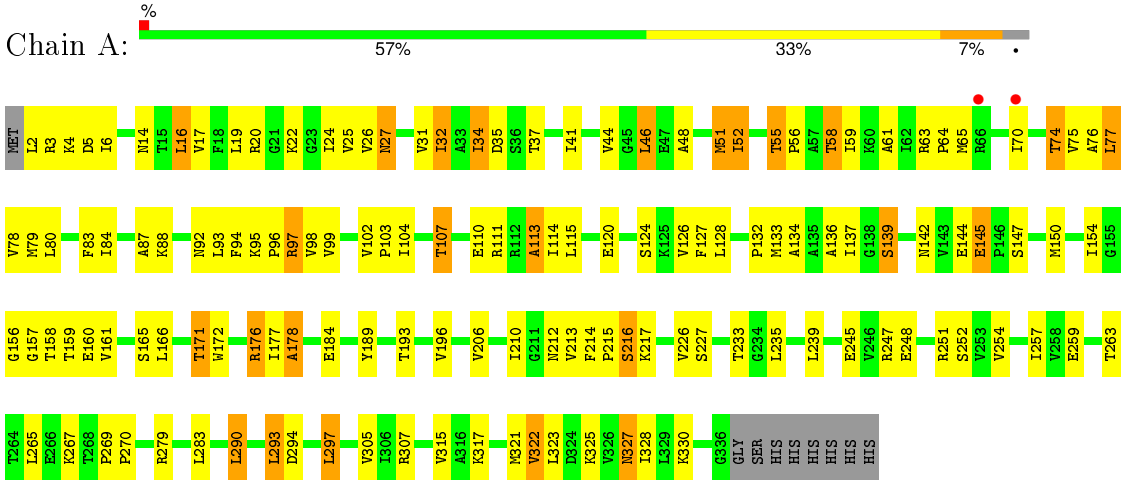
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	87	Total	C	N	O	S	0	0	0
			729	463	119	146	1			
2	S	82	Total	C	N	O	S	0	0	0
			689	440	114	134	1			

3 Residue-property plots (i)

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.

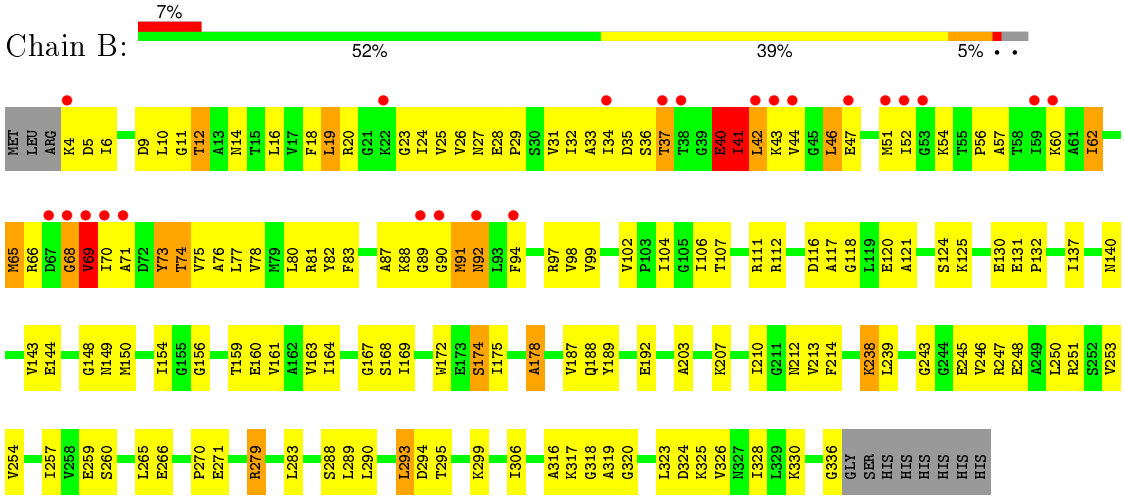
- Molecule 1: ROD SHAPE-DETERMINING PROTEIN MREB

Chain A:



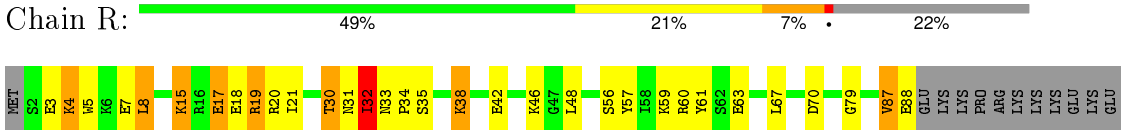
- Molecule 1: ROD SHAPE-DETERMINING PROTEIN MREB

Chain B:



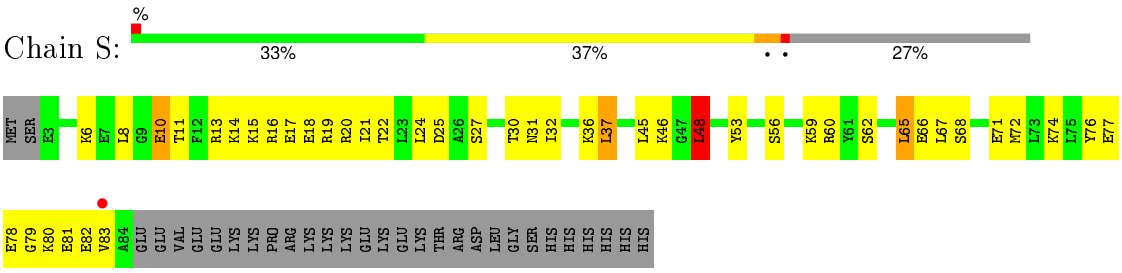
- Molecule 2: PUTATIVE UNCHARACTERIZED PROTEIN

Chain R:



• Molecule 2: PUTATIVE UNCHARACTERIZED PROTEIN

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.81Å 109.84Å 112.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.26 – 2.90 39.26 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.8 (39.26-2.90) 95.1 (39.26-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.197 , 0.288 0.198 , 0.193	Depositor DCC
R_{free} test set	1135 reflections (5.46%)	DCC
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.6	EDS
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 21917 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6399	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	0/2523	0.65	1/3411 (0.0%)
1	B	0.41	0/2504	0.60	1/3386 (0.0%)
2	R	0.46	0/739	0.63	0/986
2	S	0.41	0/699	0.57	0/932
All	All	0.44	0/6465	0.62	2/8715 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	306	ILE	CB-CA-C	-5.04	101.52	111.60

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	2500	0	2643	96	0
1	B	2481	0	2619	122	0
2	R	729	0	733	24	0
2	S	689	0	701	36	0
All	All	6399	0	6696	276	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 21.

All (276) 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:6:ILE:HD11	1:B:98:VAL:HG22	1.43	0.97
1:A:19:LEU:HD12	1:A:22:LYS:HB2	1.47	0.96
2:R:32:ILE:HG22	2:R:33:ASN:H	1.40	0.86
1:B:33:ALA:HB3	1:B:43:LYS:HB2	1.60	0.84
1:B:73:TYR:HB3	1:B:75:VAL:HG23	1.60	0.83
1:B:25:VAL:HG23	1:B:26:VAL:HG23	1.61	0.83
1:B:40:GLU:O	1:B:41:ILE:HB	1.79	0.82
1:B:34:ILE:HG22	1:B:41:ILE:HA	1.62	0.82
1:A:32:ILE:HD13	1:A:75:VAL:HG13	1.63	0.80
1:B:5:ASP:HB3	1:B:323:LEU:HD13	1.62	0.80
1:B:66:ARG:HD3	1:B:71:ALA:HB3	1.65	0.79
1:B:18:PHE:CE1	1:B:23:GLY:HA2	2.21	0.76
1:A:196:VAL:HG21	1:A:239:LEU:HD21	1.68	0.76
2:S:11:THR:HG23	2:S:14:LYS:HE2	1.70	0.74
1:A:74:THR:O	1:A:78:VAL:HG23	1.89	0.73
1:A:64:PRO:HG2	1:A:79:MET:SD	2.28	0.73
1:A:145:GLU:HG2	1:A:147:SER:H	1.53	0.73
1:B:36:SER:HB2	1:B:60:LYS:HE2	1.72	0.72
2:R:30:THR:O	2:R:32:ILE:N	2.21	0.72
1:B:32:ILE:HD11	1:B:41:ILE:HD11	1.72	0.72
1:A:159:THR:HG21	1:A:257:ILE:HG23	1.72	0.71
1:B:41:ILE:HG23	1:B:41:ILE:O	1.90	0.70
2:R:33:ASN:OD1	2:R:35:SER:HB3	1.90	0.70
1:A:52:ILE:HD11	1:A:61:ALA:HB2	1.73	0.70
1:B:42:LEU:H	1:B:42:LEU:HD23	1.57	0.70
1:A:233:THR:HB	1:A:235:LEU:HD12	1.72	0.70
1:A:297:LEU:HB3	1:A:305:VAL:HG21	1.72	0.69
1:B:11:GLY:O	1:B:65:MET:HG3	1.91	0.69
1:B:104:ILE:HD11	1:B:132:PRO:HG2	1.74	0.68
2:S:22:THR:HG22	2:S:24:LEU:N	2.09	0.67
1:B:77:LEU:CD1	1:B:120:GLU:HB3	2.23	0.67
1:B:6:ILE:CD1	1:B:98:VAL:HG22	2.23	0.66
1:B:81:ARG:HG3	1:B:81:ARG:HH21	1.60	0.66
1:B:46:LEU:HD13	1:B:47:GLU:H	1.62	0.65
1:B:99:VAL:HB	1:B:319:ALA:O	1.96	0.65
2:S:68:SER:HB3	2:S:71:GLU:HG2	1.78	0.64
1:B:75:VAL:O	1:B:78:VAL:HG22	1.99	0.63
1:B:34:ILE:HD11	1:B:62:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASN:HD21	1:A:247:ARG:HH21	1.48	0.62
1:B:70:ILE:O	1:B:70:ILE:HG22	2.00	0.61
2:R:59:LYS:HE2	2:R:63:GLU:OE1	1.99	0.61
1:A:77:LEU:HD11	1:A:120:GLU:OE1	2.01	0.61
2:R:87:VAL:HG12	2:R:88:GLU:N	2.16	0.61
1:B:5:ASP:HB2	1:B:20:ARG:HD2	1.83	0.60
1:B:106:ILE:HG23	1:B:111:ARG:HD2	1.81	0.60
1:B:77:LEU:HD21	1:B:81:ARG:NH1	2.16	0.59
2:S:74:LYS:O	2:S:78:GLU:HG3	2.03	0.59
1:A:65:MET:SD	1:A:70:ILE:HG22	2.42	0.59
1:B:118:GLY:O	1:B:121:ALA:HB3	2.03	0.59
2:S:30:THR:O	2:S:32:ILE:N	2.31	0.59
2:S:22:THR:HG22	2:S:25:ASP:H	1.68	0.59
1:B:42:LEU:HD12	1:B:43:LYS:HG2	1.84	0.59
1:B:43:LYS:HE3	1:B:51:MET:SD	2.43	0.59
1:B:74:THR:O	1:B:74:THR:HG23	2.02	0.59
1:A:215:PRO:O	1:A:216:SER:HB3	2.03	0.59
1:B:77:LEU:HD11	1:B:120:GLU:HB3	1.84	0.58
2:S:20:ARG:O	2:S:20:ARG:HG3	2.03	0.58
2:R:32:ILE:HG22	2:R:33:ASN:N	2.16	0.58
2:R:15:LYS:O	2:R:15:LYS:HD3	2.02	0.58
1:A:5:ASP:OD2	1:A:97:ARG:NH2	2.36	0.58
1:B:189:TYR:OH	1:B:245:GLU:HB2	2.04	0.58
1:B:214:PHE:HE1	1:B:299:LYS:HD3	1.69	0.58
2:R:18:GLU:C	2:R:19:ARG:HG3	2.24	0.57
1:B:77:LEU:HD12	1:B:120:GLU:HB3	1.86	0.57
1:B:43:LYS:HE3	1:B:51:MET:CE	2.35	0.57
1:B:212:ASN:HD21	1:B:247:ARG:HB2	1.70	0.57
1:A:95:LYS:HB2	1:A:124:SER:HB3	1.87	0.57
2:R:19:ARG:HB2	2:R:21:ILE:HG13	1.86	0.56
1:B:44:VAL:HG12	1:B:82:TYR:HD2	1.69	0.56
1:B:270:PRO:HD2	1:B:271:GLU:OE2	2.05	0.56
2:R:30:THR:HB	2:R:32:ILE:HG13	1.88	0.56
1:A:171:THR:HG22	1:A:267:LYS:HE3	1.87	0.56
2:S:45:LEU:O	2:S:48:LEU:HB2	2.05	0.56
1:B:16:LEU:HD12	1:B:24:ILE:HD12	1.86	0.56
1:B:188:GLN:O	1:B:192:GLU:HG3	2.06	0.56
1:B:32:ILE:HD11	1:B:41:ILE:CD1	2.36	0.55
2:R:4:LYS:O	2:R:7:GLU:HG2	2.06	0.55
1:A:136:ALA:O	1:A:139:SER:O	2.24	0.55
1:A:19:LEU:CD1	1:A:22:LYS:HB2	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASN:ND2	1:A:247:ARG:HD3	2.21	0.54
1:A:32:ILE:HB	1:A:44:VAL:HG22	1.90	0.54
1:A:92:ASN:ND2	1:A:94:PHE:H	2.05	0.54
2:S:56:SER:O	2:S:60:ARG:HD3	2.07	0.54
2:R:30:THR:C	2:R:32:ILE:H	2.09	0.54
2:S:65:LEU:HD13	2:S:67:LEU:HD12	1.89	0.54
1:A:70:ILE:HD11	1:A:113:ALA:CB	2.38	0.53
2:S:30:THR:C	2:S:32:ILE:H	2.12	0.53
1:A:55:THR:HG22	1:A:58:THR:OG1	2.08	0.53
1:B:90:GLY:O	1:B:91:MET:HB2	2.08	0.53
2:R:19:ARG:O	2:R:21:ILE:N	2.38	0.53
1:A:189:TYR:CE1	1:A:193:THR:HG21	2.43	0.53
1:A:254:VAL:HG23	1:A:257:ILE:HD12	1.91	0.53
1:B:283:LEU:HD21	1:B:293:LEU:HD13	1.91	0.53
1:B:92:ASN:N	1:B:92:ASN:HD22	2.07	0.53
1:A:157:GLY:HA2	1:A:176:ARG:NH1	2.24	0.52
1:B:150:MET:HE1	1:B:265:LEU:HG	1.90	0.52
1:A:51:MET:SD	1:A:59:ILE:HD11	2.49	0.52
1:B:34:ILE:HG22	1:B:41:ILE:CA	2.37	0.52
1:B:214:PHE:CE1	1:B:299:LYS:HD3	2.44	0.52
1:A:99:VAL:HG22	1:A:127:PHE:HB2	1.92	0.52
1:B:102:VAL:O	1:B:130:GLU:HA	2.10	0.52
1:B:14:ASN:HA	1:B:29:PRO:HA	1.90	0.52
1:A:25:VAL:HG23	1:A:26:VAL:HG23	1.92	0.52
1:B:65:MET:SD	1:B:70:ILE:HG23	2.50	0.51
1:A:102:VAL:HG11	1:A:128:LEU:HD13	1.90	0.51
1:B:137:ILE:HD11	1:B:328:ILE:HD13	1.91	0.51
2:S:76:TYR:O	2:S:79:GLY:N	2.44	0.51
1:A:104:ILE:HD11	1:A:132:PRO:HG2	1.93	0.50
1:B:54:LYS:C	1:B:56:PRO:HD3	2.31	0.50
2:R:17:GLU:C	2:R:19:ARG:H	2.15	0.50
1:B:12:THR:HA	1:B:65:MET:HB2	1.93	0.50
1:B:9:ASP:HB2	1:B:316:ALA:HB2	1.92	0.50
1:B:175:ILE:HD13	1:B:260:SER:HB2	1.94	0.50
2:S:22:THR:HG22	2:S:24:LEU:H	1.76	0.50
1:B:107:THR:O	1:B:111:ARG:HG3	2.12	0.49
2:R:5:TRP:O	2:R:8:LEU:HB3	2.12	0.49
2:S:62:SER:OG	2:S:72:MET:HG3	2.12	0.49
1:B:125:LYS:HD2	1:B:336:GLY:HA2	1.93	0.49
2:S:78:GLU:HA	2:S:80:LYS:HG2	1.94	0.49
2:S:17:GLU:C	2:S:19:ARG:H	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:24:LEU:C	2:S:24:LEU:HD13	2.33	0.48
1:B:32:ILE:HD11	1:B:41:ILE:CG1	2.43	0.48
1:A:98:VAL:HB	1:A:126:VAL:HG22	1.95	0.48
1:A:134:ALA:HB3	1:A:315:VAL:HG13	1.96	0.48
1:B:5:ASP:HB2	1:B:20:ARG:CD	2.42	0.48
2:S:16:ARG:CG	2:S:21:ILE:HG22	2.44	0.48
2:S:6:LYS:O	2:S:10:GLU:HB2	2.13	0.48
1:A:16:LEU:HD12	1:A:24:ILE:CG2	2.43	0.48
2:S:71:GLU:HG3	2:S:72:MET:N	2.29	0.48
1:B:81:ARG:HG3	1:B:81:ARG:NH2	2.26	0.48
1:A:48:ALA:O	1:A:52:ILE:HB	2.13	0.48
1:B:46:LEU:HD13	1:B:47:GLU:N	2.27	0.48
1:A:294:ASP:HA	1:A:305:VAL:HG11	1.94	0.48
1:B:187:VAL:HG23	1:B:203:ALA:HB2	1.96	0.48
2:S:24:LEU:HD13	2:S:24:LEU:O	2.14	0.48
1:B:78:VAL:O	1:B:81:ARG:HB3	2.13	0.47
1:B:131:GLU:HB2	1:B:132:PRO:HD3	1.97	0.47
2:R:38:LYS:O	2:R:42:GLU:HG2	2.14	0.47
1:A:216:SER:O	1:A:217:LYS:C	2.53	0.47
2:S:16:ARG:HG3	2:S:21:ILE:HG22	1.96	0.47
2:R:56:SER:O	2:R:60:ARG:HG3	2.13	0.47
1:B:43:LYS:HG3	1:B:51:MET:SD	2.55	0.47
1:A:76:ALA:O	1:A:77:LEU:C	2.53	0.47
2:S:15:LYS:O	2:S:15:LYS:HD3	2.15	0.47
1:B:210:ILE:HD11	1:B:246:VAL:HG21	1.97	0.47
1:B:279:ARG:HG2	2:S:53:TYR:CE2	2.50	0.47
2:R:33:ASN:O	2:R:34:PRO:C	2.53	0.46
1:B:154:ILE:HG23	1:B:159:THR:OG1	2.15	0.46
1:A:79:MET:HG2	1:A:83:PHE:HE1	1.80	0.46
1:A:215:PRO:O	1:A:216:SER:CB	2.63	0.46
1:B:28:GLU:HG3	1:B:83:PHE:HE2	1.80	0.46
2:S:11:THR:O	2:S:14:LYS:HG2	2.14	0.46
2:S:79:GLY:C	2:S:81:GLU:H	2.19	0.46
1:B:294:ASP:OD2	1:B:294:ASP:N	2.47	0.46
1:A:52:ILE:CD1	1:A:61:ALA:HB2	2.45	0.46
1:A:5:ASP:HB3	1:A:323:LEU:CD1	2.45	0.46
2:S:36:LYS:HG2	2:S:48:LEU:HD21	1.97	0.46
1:A:177:ILE:O	1:A:178:ALA:HB2	2.16	0.46
1:B:10:LEU:HB3	1:B:65:MET:HE3	1.98	0.46
1:B:172:TRP:HZ3	1:B:174:SER:HB2	1.80	0.46
1:B:104:ILE:HD13	1:B:169:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HD23	1:B:118:GLY:HA2	1.98	0.46
1:B:46:LEU:HD22	1:B:47:GLU:N	2.32	0.45
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.51	0.45
1:A:154:ILE:HG23	1:A:159:THR:OG1	2.17	0.45
1:A:58:THR:O	1:A:59:ILE:HG13	2.17	0.45
1:B:144:GLU:HA	1:B:144:GLU:OE1	2.16	0.45
1:B:32:ILE:CD1	1:B:41:ILE:HD11	2.45	0.45
1:A:79:MET:HG2	1:A:83:PHE:CE1	2.52	0.45
1:A:251:ARG:HA	1:A:254:VAL:HG12	1.99	0.45
1:B:210:ILE:HD12	1:B:243:GLY:HA2	1.98	0.45
1:A:165:SER:O	1:A:166:LEU:HB2	2.16	0.45
1:A:206:VAL:CG2	1:A:226:VAL:HG11	2.47	0.45
1:A:76:ALA:O	1:A:79:MET:N	2.50	0.45
1:B:40:GLU:HB2	1:B:41:ILE:H	1.58	0.45
1:B:6:ILE:HD11	1:B:98:VAL:CG2	2.30	0.45
1:B:20:ARG:NH1	1:B:324:ASP:HB2	2.31	0.45
1:A:95:LYS:HA	1:A:96:PRO:HD3	1.79	0.45
1:B:137:ILE:HG13	1:B:143:VAL:HG21	1.98	0.45
1:B:325:LYS:HD3	1:B:328:ILE:HD12	1.99	0.45
1:B:175:ILE:CD1	1:B:257:ILE:HA	2.47	0.45
2:R:5:TRP:O	2:R:8:LEU:CB	2.65	0.45
1:A:70:ILE:HD11	1:A:113:ALA:HB1	1.98	0.45
1:B:212:ASN:ND2	1:B:247:ARG:HB2	2.31	0.45
1:A:133:MET:O	1:A:137:ILE:HG13	2.16	0.45
1:A:137:ILE:HD13	1:A:322:VAL:HG23	1.97	0.45
1:A:325:LYS:CB	1:A:328:ILE:HG22	2.46	0.45
1:A:103:PRO:HA	1:A:160:GLU:OE2	2.17	0.45
1:B:34:ILE:CD1	1:B:62:ILE:HD11	2.46	0.44
1:B:26:VAL:CG1	1:B:28:GLU:HG2	2.46	0.44
1:A:115:LEU:HD23	1:A:126:VAL:HG12	1.97	0.44
1:B:161:VAL:O	1:B:172:TRP:HA	2.16	0.44
2:S:32:ILE:CG2	2:S:37:LEU:HD13	2.47	0.44
1:A:16:LEU:HD12	1:A:24:ILE:HG23	2.00	0.44
1:A:150:MET:HE1	1:A:265:LEU:HD23	1.99	0.44
1:A:317:LYS:HZ2	1:A:317:LYS:HB2	1.83	0.44
2:R:32:ILE:HD13	2:R:57:TYR:CD2	2.52	0.44
1:A:210:ILE:O	1:A:210:ILE:HG13	2.18	0.44
1:A:84:ILE:O	1:A:88:LYS:HB2	2.16	0.44
1:B:92:ASN:OD1	1:B:94:PHE:HB2	2.18	0.44
1:B:137:ILE:HD11	1:B:328:ILE:HG21	2.00	0.44
1:A:4:LYS:HB3	1:A:4:LYS:HE2	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASN:H	1:B:92:ASN:HD22	1.65	0.43
2:R:32:ILE:CG2	2:R:33:ASN:H	2.21	0.43
1:B:10:LEU:HB3	1:B:65:MET:CE	2.48	0.43
2:S:45:LEU:O	2:S:46:LYS:C	2.56	0.43
1:B:143:VAL:O	1:B:167:GLY:N	2.45	0.43
1:B:207:LYS:HB3	1:B:207:LYS:HE2	1.75	0.43
1:A:17:VAL:HG11	1:A:87:ALA:HB2	1.99	0.43
1:A:156:GLY:HA2	1:A:178:ALA:O	2.18	0.43
1:A:107:THR:HG23	1:A:110:GLU:OE2	2.19	0.43
1:A:161:VAL:O	1:A:172:TRP:HA	2.18	0.43
1:B:4:LYS:HG3	1:B:19:LEU:HD21	2.00	0.43
1:A:142:ASN:O	1:A:145:GLU:CD	2.56	0.43
1:B:74:THR:C	1:B:76:ALA:N	2.71	0.43
1:A:2:LEU:HB2	1:A:95:LYS:O	2.18	0.43
1:B:82:TYR:C	1:B:82:TYR:CD1	2.88	0.43
1:B:91:MET:HG2	1:B:91:MET:O	2.19	0.43
1:A:150:MET:CE	1:A:265:LEU:CD2	2.97	0.43
1:A:283:LEU:HD21	1:A:293:LEU:HD13	2.01	0.43
2:S:77:GLU:C	2:S:79:GLY:H	2.22	0.42
1:A:19:LEU:HD13	1:A:20:ARG:O	2.19	0.42
1:A:322:VAL:HG22	1:A:328:ILE:HG23	2.02	0.42
2:S:65:LEU:CD1	2:S:67:LEU:HD12	2.50	0.42
1:A:34:ILE:HG22	1:A:41:ILE:HA	2.01	0.42
1:A:206:VAL:HG23	1:A:226:VAL:HG11	2.01	0.42
1:A:70:ILE:HD11	1:A:113:ALA:HB3	2.00	0.42
1:B:117:ALA:O	1:B:121:ALA:HB2	2.19	0.42
1:A:17:VAL:HG11	1:A:87:ALA:CB	2.50	0.42
2:R:17:GLU:C	2:R:19:ARG:N	2.73	0.42
1:A:251:ARG:O	1:A:254:VAL:HG12	2.20	0.42
1:B:52:ILE:C	1:B:54:LYS:H	2.23	0.42
1:B:41:ILE:HD11	1:B:75:VAL:HG13	2.02	0.42
1:B:77:LEU:HD23	1:B:77:LEU:C	2.40	0.41
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.66	0.41
1:A:6:ILE:HG22	1:A:19:LEU:HD23	2.01	0.41
2:R:5:TRP:CD1	2:R:79:GLY:HA3	2.55	0.41
1:A:307:ARG:HG2	1:A:307:ARG:NH2	2.35	0.41
1:B:87:ALA:C	1:B:89:GLY:H	2.22	0.41
1:A:269:PRO:HA	1:A:270:PRO:HD3	1.83	0.41
1:B:74:THR:C	1:B:76:ALA:H	2.24	0.41
2:S:79:GLY:C	2:S:81:GLU:N	2.73	0.41
1:B:283:LEU:HG	1:B:288:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:20:ARG:O	2:S:20:ARG:CG	2.68	0.41
1:A:171:THR:HG21	1:A:267:LYS:HG3	2.02	0.41
1:B:238:LYS:HG2	1:B:239:LEU:N	2.32	0.41
1:A:19:LEU:HD22	1:A:20:ARG:N	2.35	0.41
1:A:52:ILE:O	1:A:56:PRO:HG3	2.21	0.41
1:A:171:THR:HG22	1:A:267:LYS:CE	2.50	0.41
1:B:148:GLY:HA2	1:B:164:ILE:O	2.21	0.41
2:R:19:ARG:C	2:R:21:ILE:H	2.20	0.41
1:B:159:THR:HB	1:B:175:ILE:HG13	2.03	0.41
1:A:294:ASP:N	1:A:294:ASP:OD2	2.54	0.41
1:B:88:LYS:C	1:B:90:GLY:H	2.24	0.41
1:A:98:VAL:O	1:A:126:VAL:HA	2.21	0.41
1:B:279:ARG:HG2	2:S:53:TYR:CZ	2.55	0.41
1:A:325:LYS:O	1:A:328:ILE:HG22	2.21	0.41
1:B:318:GLY:C	1:B:320:GLY:H	2.23	0.41
1:B:149:ASN:O	1:B:163:VAL:HA	2.21	0.41
1:B:12:THR:HA	1:B:65:MET:CB	2.51	0.41
1:B:68:GLY:O	1:B:69:VAL:HG13	2.21	0.41
1:B:106:ILE:O	1:B:106:ILE:HG23	2.20	0.41
1:A:327:ASN:HD22	1:A:327:ASN:HA	1.52	0.41
2:S:22:THR:CG2	2:S:24:LEU:H	2.34	0.40
2:S:80:LYS:O	2:S:83:VAL:HG12	2.20	0.40
1:A:19:LEU:HD12	1:A:22:LYS:CB	2.34	0.40
1:B:69:VAL:HB	1:B:70:ILE:H	1.62	0.40
1:B:156:GLY:O	1:B:178:ALA:O	2.40	0.40
1:B:5:ASP:HB3	1:B:323:LEU:CD1	2.43	0.40
1:B:251:ARG:O	1:B:254:VAL:HG12	2.22	0.40
1:B:19:LEU:HD22	1:B:20:ARG:N	2.36	0.40
1:A:214:PHE:HA	1:A:215:PRO:HD3	1.84	0.40
1:A:31:VAL:CG2	1:A:63:ARG:NH2	2.84	0.40
1:B:290:LEU:HD23	1:B:290:LEU:HA	1.84	0.40
1:A:14:ASN:HB3	1:A:27:ASN:ND2	2.37	0.40
1:B:250:LEU:O	1:B:253:VAL:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	333/344 (97%)	296 (89%)	33 (10%)	4 (1%)	16 48
1	B	331/344 (96%)	282 (85%)	38 (12%)	11 (3%)	5 20
2	R	85/112 (76%)	76 (89%)	5 (6%)	4 (5%)	3 11
2	S	80/112 (71%)	63 (79%)	13 (16%)	4 (5%)	3 9
All	All	829/912 (91%)	717 (86%)	89 (11%)	23 (3%)	6 24

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	ALA
1	A	216	SER
1	B	40	GLU
1	B	41	ILE
1	B	57	ALA
1	B	91	MET
2	R	31	ASN
2	R	87	VAL
2	S	66	GLU
1	B	69	VAL
1	B	140	ASN
1	B	178	ALA
1	A	77	LEU
1	B	65	MET
1	B	73	TYR
2	R	20	ARG
2	S	31	ASN
2	S	48	LEU
1	A	113	ALA
1	B	37	THR
2	S	18	GLU
2	R	32	ILE
1	B	68	GLY

5.3.2 Protein sidechains (i)

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	272/280 (97%)	232 (85%)	40 (15%)	4 11
1	B	270/280 (96%)	237 (88%)	33 (12%)	6 18
2	R	80/104 (77%)	66 (82%)	14 (18%)	2 7
2	S	75/104 (72%)	66 (88%)	9 (12%)	6 18
All	All	697/768 (91%)	601 (86%)	96 (14%)	4 13

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	16	LEU
1	A	27	ASN
1	A	32	ILE
1	A	34	ILE
1	A	35	ASP
1	A	37	THR
1	A	46	LEU
1	A	51	MET
1	A	52	ILE
1	A	55	THR
1	A	58	THR
1	A	74	THR
1	A	93	LEU
1	A	97	ARG
1	A	107	THR
1	A	111	ARG
1	A	114	ILE
1	A	139	SER
1	A	144	GLU
1	A	145	GLU
1	A	158	THR
1	A	171	THR
1	A	176	ARG

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Mol	Chain	Res	Type
1	A	184	GLU
1	A	213	VAL
1	A	227	SER
1	A	245	GLU
1	A	248	GLU
1	A	252	SER
1	A	259	GLU
1	A	263	THR
1	A	279	ARG
1	A	290	LEU
1	A	293	LEU
1	A	297	LEU
1	A	321	MET
1	A	322	VAL
1	A	327	ASN
1	A	330	LYS
1	B	12	THR
1	B	19	LEU
1	B	27	ASN
1	B	31	VAL
1	B	35	ASP
1	B	37	THR
1	B	40	GLU
1	B	41	ILE
1	B	42	LEU
1	B	46	LEU
1	B	62	ILE
1	B	69	VAL
1	B	74	THR
1	B	92	ASN
1	B	97	ARG
1	B	112	ARG
1	B	116	ASP
1	B	124	SER
1	B	160	GLU
1	B	168	SER
1	B	174	SER
1	B	213	VAL
1	B	238	LYS
1	B	248	GLU
1	B	259	GLU
1	B	266	GLU

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Mol	Chain	Res	Type
1	B	279	ARG
1	B	289	LEU
1	B	293	LEU
1	B	295	THR
1	B	317	LYS
1	B	326	VAL
1	B	330	LYS
2	R	3	GLU
2	R	4	LYS
2	R	8	LEU
2	R	15	LYS
2	R	17	GLU
2	R	19	ARG
2	R	30	THR
2	R	32	ILE
2	R	38	LYS
2	R	46	LYS
2	R	48	LEU
2	R	61	TYR
2	R	67	LEU
2	R	70	ASP
2	S	8	LEU
2	S	10	GLU
2	S	13	ARG
2	S	27	SER
2	S	37	LEU
2	S	48	LEU
2	S	59	LYS
2	S	65	LEU
2	S	82	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	50	ASN
1	A	85	ASN
1	A	92	ASN
1	A	212	ASN
1	A	327	ASN
1	B	85	ASN
1	B	92	ASN

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Mol	Chain	Res	Type
1	B	212	ASN
1	B	298	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, 95^{th} 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	335/344 (97%)	-0.46	2 (0%) 90 89	9, 32, 64, 123	0
1	B	333/344 (96%)	-0.07	23 (6%) 20 14	12, 47, 133, 170	0
2	R	87/112 (77%)	-0.44	0 100 100	12, 36, 76, 98	0
2	S	82/112 (73%)	-0.10	1 (1%) 81 78	17, 48, 91, 128	0
All	All	837/912 (91%)	-0.27	26 (3%) 52 45	9, 39, 108, 170	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	GLY	5.8
1	B	90	GLY	5.8
1	B	71	ALA	5.2
1	B	60	LYS	4.1
1	B	53	GLY	4.0
1	B	52	ILE	3.6
1	B	47	GLU	3.4
2	S	83	VAL	3.4
1	B	89	GLY	3.4
1	B	51	MET	3.3
1	A	70	ILE	2.8
1	A	66	ARG	2.8
1	B	59	ILE	2.8
1	B	22	LYS	2.6
1	B	37	THR	2.5
1	B	44	VAL	2.5
1	B	42	LEU	2.5
1	B	43	LYS	2.5
1	B	4	LYS	2.5
1	B	38	THR	2.4
1	B	94	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	69	VAL	2.3
1	B	92	ASN	2.2
1	B	67	ASP	2.2
1	B	34	ILE	2.1
1	B	70	ILE	2.0

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.