Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:24 AM EDT

PDB ID	:	3GKU
Title	:	Crystal structure of a probable RNA-binding protein from Clostridium symbiosum ATCC 14940
Authors	:	Tan, K.; Keigher, L.; Jedrzejczak, R.; Babnigg, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-03-11
Resolution	:	2.95 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 (i) 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 (i)) were used in the production of this report:

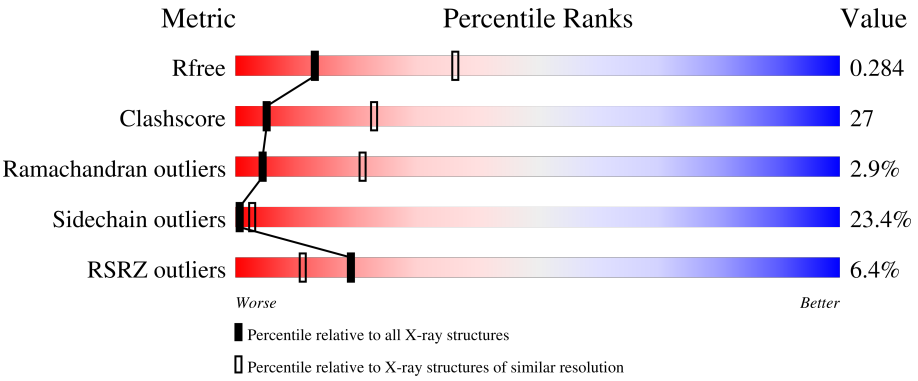
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	225	44% 39% 8% 8%
1	B	225	9% 44% 30% 11% 14%
1	C	225	6% 27% 25% 7% 40%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4131 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 Probable RNA-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	Se	0	0	0
			1636	1020	287	323	6			
1	B	193	Total	C	N	O	Se	0	0	0
			1500	934	263	297	6			
1	C	134	Total	C	N	O	Se	0	0	0
			995	619	163	208	5			

There are 9 discrepancies between the modelled and reference sequences:

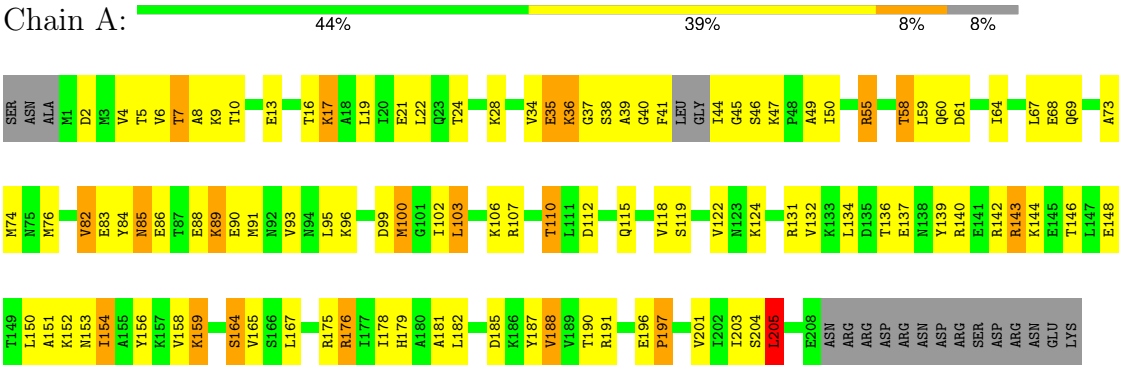
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	PDB 3GKU
A	-1	ASN	-	EXPRESSION TAG	PDB 3GKU
A	0	ALA	-	EXPRESSION TAG	PDB 3GKU
B	-2	SER	-	EXPRESSION TAG	PDB 3GKU
B	-1	ASN	-	EXPRESSION TAG	PDB 3GKU
B	0	ALA	-	EXPRESSION TAG	PDB 3GKU
C	-2	SER	-	EXPRESSION TAG	PDB 3GKU
C	-1	ASN	-	EXPRESSION TAG	PDB 3GKU
C	0	ALA	-	EXPRESSION TAG	PDB 3GKU

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.

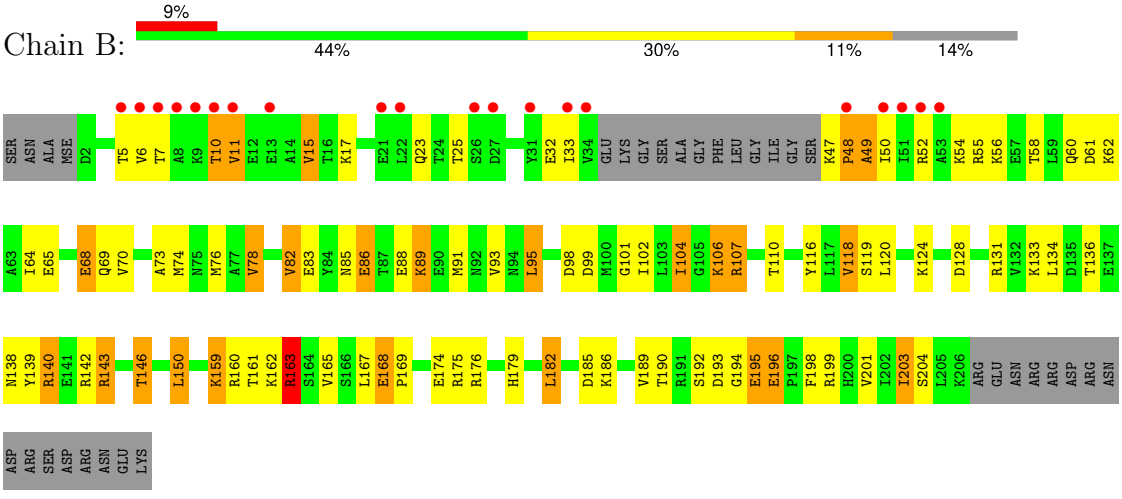
• Molecule 1: Probable RNA-binding protein

Chain A:



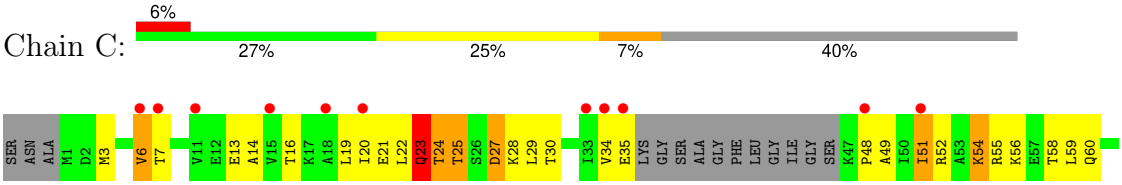
• Molecule 1: Probable RNA-binding protein

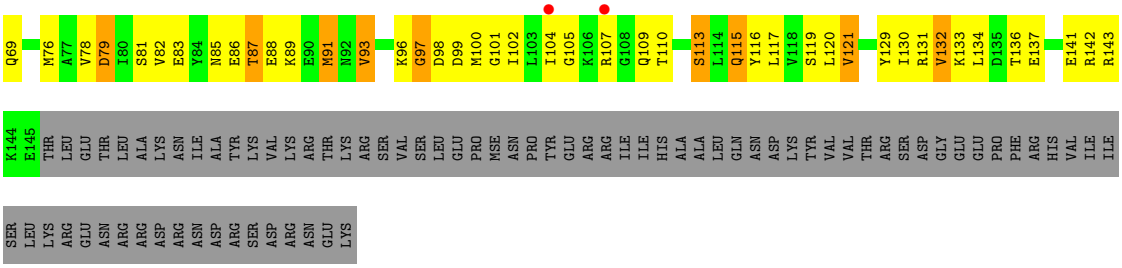
Chain B:



• Molecule 1: Probable RNA-binding protein

Chain C:




Q69
M76 A77 V78 D79 I80 S81 V82 E83 Y84 N85 E86 T87 E88 K89 E90 M91 N92 V93
K96 G97 D98 D99 M100 G101 I102 L103 I104 G105 K106 R107 G108 Q109 T110
S113 L114 Q115 Y116 L117 V118 S119 L120 V121
Y129 I130 R131 V132 K133 L134 D135 T136 E137
E141 R142 R143
K144 E145 THR LEU GLU THR LEU ALA LYS ASN ILE ALA TYR LYS VAL LYS ARG THR LYS ARG SER VAL SER LEU GLU PRO MSE ASN PRO TYR GLU ARG ARG ILE ILE HIS ALA ALA LEU GLN ASN ASP LYS TYR VAL VAL THR ARG SER ASP GLY GLU GLU PRO PHE ARG HIS VAL ILE ILE
SER LEU LYS ARG GLU ASN ARG ARG ASP ARG ASN ASP ARG SER ASP ARG ASN GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.99Å 126.99Å 106.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.72 – 2.95 40.73 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.72-2.95) 99.8 (40.73-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.220 , 0.287 0.219 , 0.284	Depositor DCC
R_{free} test set	1084 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4131	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.03	0/1645	0.98	2/2200 (0.1%)
1	B	0.82	0/1508	0.84	0/2027
1	C	0.67	0/994	0.80	1/1337 (0.1%)
All	All	0.88	0/4147	0.89	3/5564 (0.1%)

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	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	GLY	N-CA-C	6.51	129.37	113.10
1	A	205	LEU	CA-CB-CG	5.38	127.69	115.30
1	A	67	LEU	CB-CG-CD1	-5.36	101.89	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	24	THR	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	1636	0	1673	87	0
1	B	1500	0	1483	65	0
1	C	995	0	949	73	0
All	All	4131	0	4105	221	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 27.

All (221) 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:103:LEU:HD23	1:A:103:LEU:H	1.02	1.13
1:C:100:MSE:HE2	1:C:136:THR:HG22	1.24	1.12
1:A:110:THR:HG22	1:B:116:TYR:HE2	1.08	1.10
1:C:97:GLY:HA2	1:C:100:MSE:HG2	1.29	1.10
1:C:100:MSE:HE2	1:C:136:THR:CG2	1.86	1.05
1:A:103:LEU:H	1:A:103:LEU:CD2	1.74	0.99
1:A:110:THR:HG22	1:B:116:TYR:CE2	1.97	0.98
1:B:95:LEU:H	1:B:95:LEU:CD2	1.75	0.98
1:A:106:LYS:O	1:A:110:THR:HG23	1.63	0.98
1:C:100:MSE:CE	1:C:136:THR:CG2	2.43	0.96
1:C:82:VAL:HG21	1:C:91:MSE:HE2	1.48	0.96
1:C:101:GLY:O	1:C:104:ILE:HB	1.65	0.95
1:A:69:GLN:HG2	1:B:73:ALA:HB2	1.51	0.92
1:B:95:LEU:H	1:B:95:LEU:HD22	1.36	0.89
1:C:97:GLY:HA2	1:C:100:MSE:CG	2.02	0.89
1:A:103:LEU:HD23	1:A:103:LEU:N	1.84	0.89
1:B:78:VAL:HG21	1:B:95:LEU:HB2	1.54	0.87
1:A:58:THR:HG22	1:A:61:ASP:H	1.40	0.87
1:B:182:LEU:HD23	1:B:203:ILE:HD13	1.55	0.86
1:B:95:LEU:HD22	1:B:95:LEU:N	1.92	0.84
1:C:100:MSE:CE	1:C:136:THR:HG21	2.08	0.84
1:A:74:MSE:HE2	1:A:76:MSE:SE	2.28	0.83
1:B:82:VAL:HB	1:B:93:VAL:HG22	1.61	0.83
1:B:95:LEU:CD2	1:B:95:LEU:N	2.36	0.82
1:C:97:GLY:CA	1:C:100:MSE:HG2	2.07	0.82
1:A:73:ALA:HB2	1:B:69:GLN:HG2	1.62	0.81
1:C:76:MSE:HE1	1:C:102:ILE:HG21	1.63	0.80
1:B:182:LEU:HD23	1:B:203:ILE:CD1	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HD13	1:A:165:VAL:HG11	1.65	0.79
1:C:60:GLN:HA	1:C:91:MSE:HE1	1.66	0.78
1:C:23:GLN:OE1	1:C:23:GLN:HA	1.84	0.78
1:C:119:SER:HA	1:C:132:VAL:HG21	1.65	0.78
1:C:100:MSE:CE	1:C:136:THR:HG22	2.04	0.76
1:A:10:THR:OG1	1:A:13:GLU:HG3	1.85	0.76
1:C:100:MSE:HE3	1:C:136:THR:HG21	1.65	0.76
1:A:44:ILE:O	1:A:46:SER:N	2.18	0.75
1:B:95:LEU:H	1:B:95:LEU:HD23	1.52	0.74
1:B:78:VAL:CG2	1:B:95:LEU:HB2	2.18	0.74
1:A:39:ALA:HA	1:A:46:SER:HA	1.70	0.74
1:C:58:THR:HG21	1:C:60:GLN:HG2	1.68	0.73
1:C:119:SER:HB2	1:C:132:VAL:CG2	2.18	0.73
1:A:175:ARG:HG2	1:A:201:VAL:HG23	1.69	0.72
1:A:93:VAL:HG13	1:A:134:LEU:HD12	1.74	0.70
1:C:51:ILE:HG12	1:C:52:ARG:N	2.05	0.70
1:A:136:THR:O	1:A:137:GLU:C	2.29	0.70
1:C:35:GLU:HG2	1:C:49:ALA:HA	1.74	0.69
1:C:137:GLU:HA	1:C:137:GLU:OE1	1.93	0.69
1:C:117:LEU:O	1:C:121:VAL:HG23	1.93	0.69
1:C:24:THR:HB	1:C:55:ARG:HH11	1.57	0.68
1:A:154:ILE:HD13	1:A:165:VAL:CG1	2.23	0.68
1:C:27:ASP:OD1	1:C:27:ASP:N	2.23	0.68
1:A:142:ARG:O	1:A:146:THR:HG23	1.93	0.68
1:C:119:SER:HB2	1:C:132:VAL:HG23	1.76	0.68
1:A:58:THR:O	1:A:61:ASP:HB2	1.94	0.67
1:C:58:THR:HG22	1:C:60:GLN:H	1.58	0.67
1:A:196:GLU:HG3	1:A:197:PRO:HA	1.77	0.67
1:B:179:HIS:ND1	1:B:190:THR:OG1	2.24	0.67
1:C:22:LEU:CB	1:C:55:ARG:HH12	2.09	0.66
1:C:25:THR:HB	1:C:27:ASP:OD1	1.95	0.65
1:A:91:MSE:HB3	1:A:132:VAL:HG12	1.79	0.65
1:A:93:VAL:HG13	1:A:134:LEU:CD1	2.27	0.65
1:C:58:THR:HG21	1:C:60:GLN:CG	2.27	0.64
1:B:182:LEU:CD2	1:B:203:ILE:CD1	2.75	0.64
1:A:139:TYR:CZ	1:A:143:ARG:HG2	2.34	0.63
1:A:34:VAL:HB	1:A:50:ILE:HB	1.81	0.63
1:C:119:SER:CA	1:C:132:VAL:HG21	2.30	0.61
1:A:144:LYS:HE2	1:A:148:GLU:OE2	2.01	0.61
1:A:164:SER:OG	1:A:204:SER:HB3	2.01	0.61
1:A:112:ASP:OD1	1:A:140:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASP:O	1:A:102:ILE:HG12	2.01	0.60
1:B:193:ASP:OD2	1:B:194:GLY:N	2.34	0.60
1:A:24:THR:OG1	1:A:28:LYS:HB2	2.01	0.60
1:A:84:TYR:CE2	1:A:86:GLU:HG2	2.37	0.59
1:A:205:LEU:CD2	1:A:205:LEU:H	2.15	0.59
1:C:119:SER:CB	1:C:132:VAL:HG21	2.31	0.59
1:C:22:LEU:O	1:C:24:THR:N	2.30	0.59
1:B:65:GLU:OE1	1:B:65:GLU:HA	2.01	0.59
1:B:58:THR:HG22	1:B:60:GLN:N	2.18	0.58
1:A:85:ASN:C	1:A:85:ASN:HD22	2.07	0.58
1:B:58:THR:HG22	1:B:60:GLN:H	1.68	0.58
1:A:205:LEU:H	1:A:205:LEU:HD22	1.67	0.57
1:C:58:THR:HG22	1:C:59:LEU:N	2.21	0.56
1:C:129:TYR:HE2	1:C:131:ARG:HD2	1.69	0.56
1:B:64:ILE:O	1:B:68:GLU:HB2	2.05	0.56
1:C:141:GLU:C	1:C:143:ARG:H	2.08	0.56
1:B:70:VAL:O	1:B:74:MSE:HG3	2.06	0.56
1:B:32:GLU:HB2	1:B:52:ARG:HB2	1.88	0.55
1:A:100:MSE:HA	1:A:100:MSE:CE	2.37	0.55
1:A:103:LEU:O	1:A:107:ARG:HG3	2.06	0.55
1:C:79:ASP:HB2	1:C:96:LYS:CB	2.36	0.55
1:B:93:VAL:CG1	1:B:134:LEU:CD1	2.85	0.55
1:A:38:SER:O	1:A:46:SER:HA	2.06	0.55
1:C:107:ARG:HB2	1:C:107:ARG:HH11	1.72	0.55
1:B:142:ARG:O	1:B:146:THR:HG23	2.07	0.54
1:C:119:SER:CB	1:C:132:VAL:CG2	2.86	0.54
1:B:85:ASN:ND2	1:B:88:GLU:HG2	2.21	0.54
1:B:101:GLY:O	1:B:104:ILE:HG12	2.08	0.54
1:C:119:SER:HB2	1:C:132:VAL:HG21	1.86	0.54
1:A:176:ARG:O	1:A:176:ARG:HG3	2.07	0.53
1:B:169:PRO:HB3	1:B:198:PHE:HA	1.91	0.53
1:C:115:GLN:HG3	1:C:134:LEU:HB2	1.90	0.53
1:A:7:THR:O	1:A:8:ALA:HB2	2.09	0.53
1:B:86:GLU:O	1:B:89:LYS:HD3	2.09	0.53
1:A:37:GLY:CA	1:A:47:LYS:O	2.58	0.52
1:C:3:MSE:HG3	1:C:54:LYS:HG2	1.92	0.52
1:A:58:THR:HG21	1:A:60:GLN:HG2	1.92	0.51
1:B:150:LEU:HD23	1:B:150:LEU:O	2.10	0.51
1:C:6:VAL:HG13	1:C:51:ILE:HD11	1.92	0.51
1:B:95:LEU:N	1:B:95:LEU:HD23	2.17	0.51
1:C:3:MSE:HE2	1:C:54:LYS:NZ	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:O	1:A:89:LYS:N	2.42	0.50
1:A:102:ILE:HG13	1:A:103:LEU:HD22	1.92	0.50
1:C:16:THR:O	1:C:20:ILE:HG13	2.12	0.50
1:A:88:GLU:OE2	1:A:88:GLU:HA	2.07	0.50
1:B:161:THR:C	1:B:163:ARG:H	2.15	0.50
1:B:58:THR:CG2	1:B:60:GLN:OE1	2.60	0.50
1:C:115:GLN:HG3	1:C:134:LEU:CB	2.42	0.49
1:A:154:ILE:CD1	1:A:165:VAL:HB	2.42	0.49
1:A:58:THR:HG23	1:A:60:GLN:OE1	2.13	0.49
1:A:119:SER:HB2	1:A:132:VAL:CG2	2.42	0.49
1:A:167:LEU:N	1:A:167:LEU:CD1	2.75	0.49
1:B:5:THR:HG23	1:B:52:ARG:HE	1.77	0.49
1:B:5:THR:HG23	1:B:52:ARG:NE	2.28	0.49
1:C:89:LYS:HG2	1:C:130:ILE:HD12	1.95	0.48
1:C:105:GLY:HA2	1:C:110:THR:HG23	1.95	0.48
1:C:107:ARG:HB2	1:C:107:ARG:NH1	2.27	0.48
1:A:7:THR:O	1:A:17:LYS:HE2	2.13	0.48
1:C:129:TYR:CE2	1:C:131:ARG:HD2	2.48	0.48
1:A:102:ILE:HG13	1:A:103:LEU:N	2.29	0.48
1:A:60:GLN:O	1:A:64:ILE:HG13	2.14	0.48
1:B:139:TYR:CZ	1:B:143:ARG:HG2	2.49	0.48
1:C:51:ILE:CG1	1:C:52:ARG:N	2.76	0.48
1:B:93:VAL:HG12	1:B:134:LEU:CD1	2.43	0.48
1:C:14:ALA:HB3	1:C:51:ILE:HG23	1.96	0.48
1:C:141:GLU:C	1:C:143:ARG:N	2.68	0.47
1:A:100:MSE:HA	1:A:100:MSE:HE3	1.96	0.47
1:C:82:VAL:HG22	1:C:83:GLU:N	2.29	0.47
1:C:82:VAL:HA	1:C:93:VAL:HA	1.96	0.47
1:A:90:GLU:HB3	1:A:131:ARG:HB3	1.97	0.47
1:C:85:ASN:ND2	1:C:88:GLU:HB2	2.29	0.47
1:B:11:VAL:O	1:B:15:VAL:N	2.48	0.46
1:A:41:PHE:HA	1:A:44:ILE:HA	1.98	0.46
1:A:103:LEU:CD2	1:A:103:LEU:N	2.52	0.46
1:A:10:THR:HG1	1:A:13:GLU:HG3	1.80	0.46
1:A:55:ARG:HE	1:A:55:ARG:HB2	1.60	0.46
1:A:35:GLU:O	1:A:49:ALA:HA	2.16	0.46
1:A:151:ALA:HB1	1:A:182:LEU:HD13	1.97	0.46
1:A:178:ILE:O	1:A:181:ALA:N	2.48	0.46
1:C:109:GLN:O	1:C:113:SER:HB2	2.16	0.46
1:B:65:GLU:OE1	1:B:65:GLU:CA	2.64	0.46
1:A:38:SER:O	1:A:47:LYS:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:CG2	1:A:60:GLN:HG2	2.46	0.46
1:A:6:VAL:HG12	1:A:7:THR:N	2.31	0.45
1:B:10:THR:HG23	1:B:11:VAL:H	1.81	0.45
1:A:37:GLY:HA3	1:A:47:LYS:O	2.16	0.45
1:B:182:LEU:HD12	1:B:182:LEU:HA	1.81	0.45
1:B:159:LYS:HD2	1:B:159:LYS:C	2.37	0.45
1:B:58:THR:HB	1:B:61:ASP:CG	2.37	0.45
1:C:101:GLY:HA2	1:C:104:ILE:HD12	1.99	0.45
1:B:139:TYR:O	1:B:140:ARG:C	2.54	0.44
1:A:40:GLY:C	1:A:44:ILE:HA	2.38	0.44
1:A:88:GLU:O	1:A:89:LYS:CB	2.63	0.44
1:A:95:LEU:O	1:A:136:THR:HG23	2.18	0.44
1:B:106:LYS:HB2	1:B:106:LYS:HE2	1.74	0.44
1:A:36:LYS:H	1:A:36:LYS:HG2	1.62	0.44
1:A:158:VAL:O	1:A:159:LYS:C	2.55	0.44
1:A:82:VAL:HG23	1:A:83:GLU:N	2.33	0.44
1:A:76:MSE:HE2	1:A:102:ILE:HD11	2.00	0.43
1:B:76:MSE:HE2	1:B:102:ILE:HB	1.98	0.43
1:C:116:TYR:CD2	1:C:116:TYR:C	2.92	0.43
1:A:178:ILE:O	1:A:179:HIS:C	2.57	0.43
1:C:58:THR:HB	1:C:60:GLN:HG3	2.00	0.43
1:B:93:VAL:CG1	1:B:134:LEU:HD12	2.47	0.43
1:C:3:MSE:HE2	1:C:54:LYS:HZ3	1.81	0.43
1:B:7:THR:HG23	1:B:49:ALA:O	2.18	0.43
1:C:97:GLY:HA2	1:C:100:MSE:SE	2.69	0.43
1:A:58:THR:CG2	1:A:59:LEU:N	2.82	0.42
1:A:182:LEU:HD23	1:A:190:THR:CG2	2.48	0.42
1:B:139:TYR:HA	1:B:142:ARG:NH2	2.34	0.42
1:A:153:ASN:O	1:A:156:TYR:HB3	2.19	0.42
1:B:150:LEU:C	1:B:150:LEU:CD2	2.87	0.42
1:C:82:VAL:CG2	1:C:83:GLU:N	2.82	0.42
1:A:158:VAL:HG21	1:A:203:ILE:HG22	2.01	0.42
1:C:6:VAL:HG13	1:C:51:ILE:CD1	2.50	0.42
1:A:159:LYS:HD2	1:A:187:TYR:HB2	2.02	0.42
1:B:138:ASN:O	1:B:139:TYR:C	2.57	0.42
1:A:205:LEU:CD2	1:A:205:LEU:N	2.82	0.42
1:B:85:ASN:ND2	1:B:88:GLU:CG	2.83	0.41
1:A:190:THR:HG22	1:A:203:ILE:HG12	2.01	0.41
1:A:59:LEU:HD22	1:A:122:VAL:HG13	2.02	0.41
1:C:104:ILE:HG22	1:C:105:GLY:N	2.35	0.41
1:A:115:GLN:OE1	1:A:134:LEU:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:HG2	1:B:201:VAL:HG23	2.01	0.41
1:C:60:GLN:CA	1:C:91:MSE:HE1	2.41	0.41
1:A:85:ASN:ND2	1:A:88:GLU:H	2.19	0.41
1:C:86:GLU:O	1:C:87:THR:C	2.56	0.41
1:C:136:THR:OG1	1:C:137:GLU:N	2.53	0.41
1:B:118:VAL:CG1	1:B:119:SER:N	2.84	0.41
1:B:161:THR:C	1:B:163:ARG:N	2.74	0.41
1:A:58:THR:HB	1:A:61:ASP:OD2	2.21	0.41
1:A:185:ASP:OD2	1:A:188:VAL:N	2.52	0.41
1:B:48:PRO:O	1:B:49:ALA:HB2	2.21	0.41
1:B:54:LYS:HE2	1:B:56:LYS:HA	2.03	0.41
1:B:91:MSE:HE3	1:B:91:MSE:HB2	1.93	0.41
1:B:189:VAL:HG13	1:B:204:SER:O	2.21	0.41
1:C:29:LEU:HG	1:C:30:THR:N	2.36	0.41
1:C:141:GLU:O	1:C:143:ARG:N	2.54	0.41
1:A:58:THR:HB	1:A:61:ASP:CG	2.41	0.41
1:B:167:LEU:HD13	1:B:201:VAL:HB	2.02	0.41
1:C:105:GLY:HA3	1:C:110:THR:H	1.86	0.41
1:B:7:THR:HA	1:B:49:ALA:O	2.20	0.40
1:B:47:LYS:N	1:B:48:PRO:CD	2.85	0.40
1:C:24:THR:OG1	1:C:28:LYS:CB	2.69	0.40
1:C:59:LEU:HD23	1:C:59:LEU:HA	1.89	0.40
1:B:168:GLU:H	1:B:168:GLU:HG3	1.39	0.40
1:C:58:THR:CG2	1:C:60:GLN:H	2.30	0.40
1:C:97:GLY:O	1:C:98:ASP:C	2.60	0.40
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.79	0.40
1:A:178:ILE:HG22	1:A:179:HIS:N	2.36	0.40
1:B:93:VAL:HG12	1:B:134:LEU:HD12	2.03	0.40
1:B:195:GLU:O	1:B:196:GLU:C	2.59	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	202/225 (90%)	179 (89%)	22 (11%)	1 (0%)	29 64
1	B	189/225 (84%)	161 (85%)	17 (9%)	11 (6%)	1 7
1	C	130/225 (58%)	110 (85%)	17 (13%)	3 (2%)	6 27
All	All	521/675 (77%)	450 (86%)	56 (11%)	15 (3%)	4 21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLY
1	B	107	ARG
1	C	23	GLN
1	C	48	PRO
1	B	17	LYS
1	B	23	GLN
1	B	163	ARG
1	B	186	LYS
1	B	162	LYS
1	B	185	ASP
1	C	142	ARG
1	B	49	ALA
1	B	48	PRO
1	B	11	VAL
1	B	104	ILE

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	181/195 (93%)	147 (81%)	34 (19%)	1 7
1	B	161/195 (83%)	117 (73%)	44 (27%)	0 1
1	C	103/195 (53%)	77 (75%)	26 (25%)	0 2
All	All	445/585 (76%)	341 (77%)	104 (23%)	1 3

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	4	VAL
1	A	5	THR
1	A	7	THR
1	A	9	LYS
1	A	16	THR
1	A	17	LYS
1	A	19	LEU
1	A	21	GLU
1	A	35	GLU
1	A	36	LYS
1	A	55	ARG
1	A	58	THR
1	A	68	GLU
1	A	82	VAL
1	A	85	ASN
1	A	89	LYS
1	A	96	LYS
1	A	100	MSE
1	A	103	LEU
1	A	110	THR
1	A	118	VAL
1	A	124	LYS
1	A	143	ARG
1	A	150	LEU
1	A	152	LYS
1	A	154	ILE
1	A	159	LYS
1	A	164	SER
1	A	176	ARG
1	A	188	VAL
1	A	191	ARG
1	A	197	PRO
1	A	205	LEU
1	B	6	VAL
1	B	10	THR
1	B	15	VAL
1	B	25	THR
1	B	33	ILE
1	B	50	ILE
1	B	55	ARG
1	B	62	LYS
1	B	68	GLU

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Mol	Chain	Res	Type
1	B	78	VAL
1	B	82	VAL
1	B	83	GLU
1	B	86	GLU
1	B	89	LYS
1	B	95	LEU
1	B	98	ASP
1	B	99	ASP
1	B	106	LYS
1	B	107	ARG
1	B	110	THR
1	B	118	VAL
1	B	120	LEU
1	B	124	LYS
1	B	128	ASP
1	B	131	ARG
1	B	133	LYS
1	B	136	THR
1	B	140	ARG
1	B	143	ARG
1	B	146	THR
1	B	150	LEU
1	B	159	LYS
1	B	160	ARG
1	B	163	ARG
1	B	165	VAL
1	B	168	GLU
1	B	174	GLU
1	B	176	ARG
1	B	182	LEU
1	B	192	SER
1	B	195	GLU
1	B	196	GLU
1	B	199	ARG
1	B	203	ILE
1	C	6	VAL
1	C	7	THR
1	C	13	GLU
1	C	19	LEU
1	C	21	GLU
1	C	23	GLN
1	C	25	THR

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Mol	Chain	Res	Type
1	C	27	ASP
1	C	34	VAL
1	C	51	ILE
1	C	54	LYS
1	C	56	LYS
1	C	69	GLN
1	C	78	VAL
1	C	79	ASP
1	C	81	SER
1	C	87	THR
1	C	91	MSE
1	C	93	VAL
1	C	99	ASP
1	C	113	SER
1	C	115	GLN
1	C	120	LEU
1	C	121	VAL
1	C	132	VAL
1	C	133	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	153	ASN
1	A	183	GLN
1	A	200	HIS
1	B	75	ASN
1	B	153	ASN
1	B	200	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 monosaccharides 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, 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	199/225 (88%)	-0.18	0 100 100	17, 32, 56, 70	0
1	B	187/225 (83%)	0.34	20 (10%) 6 3	27, 46, 82, 92	0
1	C	128/225 (56%)	0.39	13 (10%) 6 4	38, 56, 71, 76	0
All	All	514/675 (76%)	0.15	33 (6%) 19 11	17, 44, 72, 92	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	VAL	5.5
1	B	8	ALA	4.8
1	B	9	LYS	4.7
1	B	7	THR	4.4
1	B	51	ILE	4.3
1	B	48	PRO	4.2
1	B	50	ILE	4.2
1	C	34	VAL	3.8
1	B	11	VAL	3.7
1	C	6	VAL	3.7
1	B	34	VAL	3.5
1	B	33	ILE	3.4
1	B	5	THR	2.9
1	C	11	VAL	2.8
1	C	104	ILE	2.8
1	B	52	ARG	2.8
1	C	33	ILE	2.7
1	B	31	TYR	2.7
1	C	51	ILE	2.6
1	B	21	GLU	2.5
1	B	27	ASP	2.5
1	B	53	ALA	2.4
1	C	15	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	10	THR	2.3
1	C	35	GLU	2.3
1	C	7	THR	2.3
1	C	48	PRO	2.2
1	B	13	GLU	2.2
1	C	20	ILE	2.1
1	B	26	SER	2.1
1	C	18	ALA	2.1
1	C	107	ARG	2.0
1	B	22	LEU	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 monosaccharides 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.