



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:17 PM BST

PDB ID : 5GAO  
EMDB ID: : EMD-8013  
Title : Head region of the yeast spliceosomal U4/U6.U5 tri-snRNP  
Authors : Nguyen, T.H.D.; Galej, W.P.; Bai, X.C.; Oubridge, C.; Scheres, S.H.W.; Newman, A.J.; Nagai, K.  
Deposited on : 2015-12-15  
Resolution : 3.60 Å(reported)  
Based on PDB ID : 4BGD

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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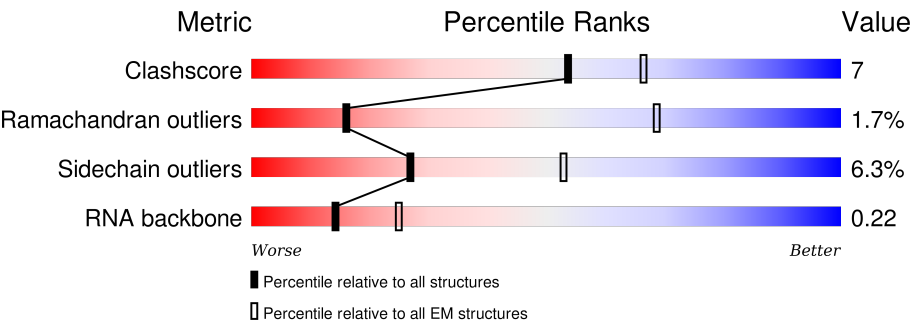
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	k	196	<div><div>39%</div><div>.</div><div>59%</div></div>
2	l	146	<div><div>60%</div><div>.</div><div>38%</div></div>
3	m	110	<div><div>80%</div><div>5%</div><div>15%</div></div>
4	n	101	<div><div>79%</div><div>.</div><div>19%</div></div>
5	p	94	<div><div>76%</div><div>5%</div><div>19%</div></div>
6	q	86	<div><div>83%</div><div>.</div><div>16%</div></div>
7	r	77	<div><div>86%</div><div>.</div><div>10%</div></div>
8	E	338	<div><div>98%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
9	B	2163	<div><div></div><div>59%</div><div>18%</div><div>•</div><div>21%</div></div>
10	V	96	<div><div></div><div>17%</div><div>35%</div><div>7%</div><div>41%</div></div>
11	A	267	<div><div></div><div>76%</div><div>17%</div><div>•</div><div>•</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 23073 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	k	80	Total	C	N	O	S	0	0
			635	406	115	111	3		

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	91	Total	C	N	O	S	0	0
			720	455	129	134	2		

- Molecule 3 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	m	94	Total	C	N	O	S	0	0
			737	474	140	119	4		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	p	76	Total	C	N	O	S	0	0
			580	382	93	102	3		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	q	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	r	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

- Molecule 8 is a protein called Snu66.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	338	Total	C	N	O		0	0
			1763	1063	352	348			

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	1710	Total	C	N	O	S	1	0
			13690	8772	2283	2579	56		

- Molecule 10 is a RNA chain called Saccharomyces cerevisiae strain UOA\_M2 chromosome 5 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	57	Total	C	N	O	P	0	0
			1209	542	212	398	57		

- Molecule 11 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	255	Total	C	N	O	S	0	0
			2015	1300	329	380	6		

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- Molecule 1: Small nuclear ribonucleoprotein-associated protein B











## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	Not provided	Depositor

## 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  >2	RMSZ	# Z  >2
1	k	0.42	0/640	0.66	0/860
10	V	0.33	0/1350	0.77	0/2097
11	A	0.48	0/2064	0.67	0/2801
2	l	0.44	0/725	0.68	0/980
3	m	0.44	0/749	0.64	0/1009
4	n	0.37	0/634	0.57	0/859
5	p	0.48	0/590	0.61	0/802
6	q	0.42	0/585	0.63	0/791
7	r	0.38	0/529	0.57	0/711
8	E	0.41	0/1751	0.53	0/2411
9	B	0.46	0/13989	0.72	1/18966 (0.0%)
All	All	0.45	0/23606	0.69	1/32287 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	k	0	1
9	B	0	5
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	643	ARG	NE-CZ-NH1	5.31	122.96	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	B	1200	PRO	Peptide
9	B	1484	TYR	Peptide
9	B	1517	ASN	Peptide
9	B	790	ASP	Peptide
9	B	791	PRO	Peptide
1	k	84	LEU	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	k	635	0	681	0	0
2	l	720	0	772	0	0
3	m	737	0	767	0	0
4	n	625	0	647	0	0
5	p	580	0	602	0	0
6	q	573	0	572	0	0
7	r	526	0	555	0	0
8	E	1763	0	1764	3	0
9	B	13690	0	13704	234	0
10	V	1209	0	612	15	0
11	A	2015	0	1970	28	0
All	All	23073	0	22646	267	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 7.

All (267) 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)
9:B:1700:ILE:HD11	9:B:1740:LEU:HD13	1.37	1.06
9:B:1208:ALA:HB2	9:B:1218:PHE:CD2	2.23	0.74
9:B:1220:ILE:HD13	9:B:1241:LEU:HD11	1.71	0.72
9:B:1183:ILE:CD1	9:B:1192:VAL:HG11	2.19	0.71
9:B:1224:ALA:HB3	9:B:1264:VAL:HA	1.72	0.71
9:B:632:ILE:HG22	9:B:670:LEU:HD11	1.70	0.71
9:B:1177:ALA:HB2	10:V:99:G:H5"	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1085:SER:OG	9:B:1140:TRP:NE1	2.22	0.70
9:B:1124:PRO:O	9:B:1128:LEU:N	2.23	0.69
9:B:1125:THR:HG21	9:B:1251:ILE:HD11	1.76	0.68
9:B:1294:SER:OG	9:B:1297:TRP:N	2.30	0.65
9:B:1782:ILE:HD11	9:B:1791:VAL:HG21	1.78	0.64
9:B:1880:LEU:HD23	9:B:1927:PHE:CZ	2.31	0.64
9:B:924:VAL:HG12	9:B:998:ALA:HB2	1.79	0.64
9:B:1109:LEU:HD22	9:B:1131:LEU:HD12	1.80	0.63
9:B:2031:LEU:HD23	9:B:2038:LEU:HD23	1.82	0.62
9:B:1291:THR:HG22	9:B:1293:ILE:HD11	1.82	0.62
9:B:804:HIS:CE1	9:B:813:ARG:HB2	2.35	0.62
9:B:1253:TYR:CE1	9:B:1272:PHE:CG	2.87	0.62
11:A:2204:ALA:O	11:A:2229:GLN:NE2	2.34	0.61
9:B:1372:LYS:HB3	9:B:1708:GLY:HA2	1.83	0.61
9:B:1485:GLY:O	9:B:1488:TYR:N	2.34	0.60
9:B:631:LEU:HD22	9:B:654:THR:HG21	1.84	0.60
9:B:1261:PRO:O	9:B:1264:VAL:HG22	2.02	0.59
11:A:2182:VAL:HG23	11:A:2338:GLN:HB3	1.84	0.59
8:E:368:ALA:HB1	9:B:1184:ARG:NH1	2.18	0.59
9:B:499:LEU:HD23	9:B:503:GLN:HB3	1.85	0.59
9:B:1399:ASN:O	9:B:1405:ILE:HD11	2.04	0.58
9:B:1396:VAL:HG13	9:B:1445:LEU:HD11	1.84	0.58
9:B:1982:MET:O	9:B:1986:GLY:N	2.36	0.58
9:B:707:PHE:CZ	9:B:902:LEU:HD12	2.38	0.57
9:B:2113:ALA:HB2	9:B:2130:PHE:HB3	1.87	0.57
9:B:1585:LEU:CD2	9:B:1683:LEU:HD23	2.34	0.57
9:B:1521:PHE:O	9:B:1521:PHE:HD1	1.88	0.57
9:B:518:LEU:HD12	9:B:519:ILE:N	2.20	0.57
9:B:740:ILE:HG23	9:B:827:VAL:HG13	1.87	0.56
9:B:1215:VAL:HG21	9:B:1735:PHE:CZ	2.40	0.56
9:B:1582:SER:HB3	9:B:1677:THR:HG21	1.88	0.56
9:B:2013:VAL:HG13	9:B:2018:ASP:HB2	1.86	0.56
10:V:75:U:O2	10:V:75:U:H2'	2.06	0.55
9:B:1682:ILE:HD12	9:B:1722:ILE:CG1	2.36	0.55
9:B:1080:LEU:HD11	9:B:1084:PHE:CZ	2.41	0.55
9:B:637:HIS:HB2	9:B:674:LEU:HD12	1.88	0.55
9:B:1080:LEU:HD11	9:B:1084:PHE:CE1	2.42	0.55
9:B:1061:ALA:HA	11:A:2395:PHE:CD1	2.42	0.55
9:B:1080:LEU:CD1	9:B:1084:PHE:CE1	2.89	0.55
11:A:2227:VAL:HG12	11:A:2374:PHE:CE1	2.42	0.54
9:B:561:ALA:O	9:B:609:PRO:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:593:ARG:HB3	10:V:82:C:OP1	2.06	0.54
9:B:1704:LEU:O	9:B:1708:GLY:N	2.38	0.54
9:B:1122:GLY:N	9:B:1249:ASP:O	2.41	0.54
9:B:1641:TYR:C	9:B:1670:CYS:SG	2.87	0.53
9:B:639:LEU:HA	9:B:644:GLY:HA3	1.91	0.53
9:B:933:ASN:O	9:B:936:VAL:HG22	2.08	0.53
9:B:774:ASP:HB3	9:B:778:LYS:HB2	1.89	0.53
9:B:633:ILE:HG21	9:B:636:ILE:HD13	1.90	0.53
9:B:1894:LEU:HD21	9:B:1922:VAL:HA	1.90	0.53
9:B:567:VAL:O	9:B:571:VAL:HG23	2.09	0.53
9:B:1080:LEU:HG	9:B:1084:PHE:CZ	2.44	0.53
9:B:1208:ALA:HA	9:B:1218:PHE:HA	1.91	0.53
9:B:636:ILE:HG22	9:B:671:SER:HB2	1.91	0.53
9:B:574:PHE:CB	9:B:585:VAL:HG11	2.38	0.52
9:B:1243:LEU:HG	9:B:1252:LEU:HD12	1.91	0.52
9:B:1482:GLY:O	9:B:1483:VAL:HG13	2.09	0.52
11:A:2208:TYR:CE2	11:A:2244:ILE:HD11	2.45	0.52
9:B:1032:PHE:CD2	9:B:1080:LEU:HD23	2.44	0.52
9:B:508:HIS:O	9:B:512:GLU:N	2.40	0.52
9:B:1583:VAL:HG22	9:B:1681:ILE:HB	1.91	0.52
9:B:708:CYS:SG	9:B:709:GLY:N	2.83	0.51
9:B:1682:ILE:HD12	9:B:1722:ILE:HG13	1.93	0.51
8:E:513:ALA:HB3	9:B:1463:LYS:CE	2.41	0.51
9:B:1863:ILE:O	9:B:1867:VAL:HG23	2.11	0.51
9:B:632:ILE:CG2	9:B:670:LEU:HD11	2.40	0.51
9:B:1394:ARG:HB3	9:B:1468:LEU:HD23	1.91	0.51
9:B:1929:LEU:HD21	9:B:1943:PHE:CD1	2.45	0.51
9:B:1930:LEU:HD22	9:B:1983:LEU:HD21	1.91	0.51
10:V:81:C:C2	10:V:82:C:C6	2.98	0.51
9:B:1585:LEU:HD21	9:B:1683:LEU:HD23	1.92	0.51
11:A:2197:SER:OG	11:A:2261:THR:HG21	2.11	0.50
9:B:1367:PHE:HZ	9:B:1515:LEU:HD11	1.76	0.50
9:B:1220:ILE:HD12	9:B:1270:LEU:HB3	1.94	0.50
9:B:1201:LYS:HA	9:B:1302:PHE:CZ	2.47	0.50
9:B:594:LEU:CD2	9:B:620:ASN:HD21	2.25	0.50
9:B:614:ILE:HG21	10:V:81:C:H5"	1.94	0.50
9:B:1986:GLY:O	9:B:1987:VAL:HG13	2.12	0.49
9:B:630:LEU:CD2	9:B:632:ILE:HD11	2.42	0.49
9:B:912:PHE:CE2	9:B:916:LEU:HA	2.47	0.49
9:B:1652:VAL:HA	9:B:1655:LEU:HD12	1.94	0.49
9:B:1459:TRP:CG	9:B:1498:ILE:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:503:GLN:O	9:B:507:PHE:N	2.45	0.49
9:B:574:PHE:HB3	9:B:585:VAL:HG11	1.95	0.49
9:B:1621:ILE:HD12	9:B:1630:ARG:HG3	1.94	0.49
9:B:1369:GLY:C	9:B:1512:SER:O	2.51	0.49
9:B:1477:HIS:N	9:B:1512:SER:OG	2.46	0.49
9:B:2103:LEU:HB3	9:B:2113:ALA:HB3	1.94	0.49
9:B:917:VAL:HG12	9:B:981:LEU:HD21	1.95	0.49
9:B:1950:ILE:O	9:B:1954:VAL:HG13	2.12	0.49
9:B:1183:ILE:O	9:B:1183:ILE:HG22	2.13	0.49
9:B:1770:VAL:O	9:B:1774:THR:HG23	2.13	0.49
9:B:1994:LEU:HD13	9:B:2008:CYS:SG	2.53	0.49
9:B:1368:VAL:O	9:B:1533:TYR:O	2.30	0.49
9:B:632:ILE:HG12	9:B:668:ILE:HD13	1.94	0.48
8:E:513:ALA:HB3	9:B:1463:LYS:HE3	1.95	0.48
9:B:589:THR:O	9:B:589:THR:HG23	2.12	0.48
11:A:2194:ILE:HD11	11:A:2293:ILE:HG21	1.94	0.48
9:B:2044:PHE:O	9:B:2048:TYR:HB2	2.13	0.48
9:B:1101:ILE:O	9:B:1105:ALA:N	2.45	0.48
9:B:1200:PRO:HG2	9:B:1297:TRP:CD1	2.48	0.48
9:B:1179:VAL:HG13	9:B:1183:ILE:HD12	1.96	0.48
10:V:83:A:O2'	10:V:84:G:O5'	2.28	0.48
9:B:527:LYS:HA	9:B:530:ILE:HD12	1.96	0.48
9:B:1544:LEU:HD13	9:B:1707:VAL:HG12	1.96	0.48
9:B:1486:ALA:O	9:B:1490:THR:OG1	2.31	0.48
11:A:2223:THR:HG22	11:A:2224:VAL:O	2.14	0.48
9:B:483:LEU:HB3	9:B:487:CYS:HB2	1.95	0.48
11:A:2182:VAL:HG23	11:A:2338:GLN:CB	2.43	0.48
9:B:2113:ALA:HB1	9:B:2128:LEU:HB3	1.95	0.47
9:B:1751:HIS:HA	9:B:1810:CYS:SG	2.54	0.47
9:B:1546:ILE:HD11	9:B:1707:VAL:HG11	1.96	0.47
9:B:1215:VAL:HG21	9:B:1735:PHE:HZ	1.79	0.47
9:B:2011:ILE:O	9:B:2011:ILE:HG22	2.14	0.47
11:A:2259:ILE:HD11	11:A:2293:ILE:HD11	1.96	0.47
9:B:631:LEU:HD23	9:B:633:ILE:HD11	1.96	0.47
9:B:634:ASP:CA	9:B:670:LEU:HD12	2.45	0.47
9:B:1782:ILE:HD11	9:B:1791:VAL:CG2	2.45	0.47
10:V:74:U:C2'	10:V:74:U:O2	2.63	0.47
9:B:1011:ASN:O	9:B:1014:SER:N	2.48	0.47
9:B:1521:PHE:CD1	9:B:1521:PHE:C	2.89	0.47
9:B:1438:LEU:O	9:B:1442:SER:N	2.41	0.47
11:A:2311:GLY:HA2	11:A:2329:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:517:MET:SD	9:B:666:ARG:NH2	2.88	0.47
10:V:75:U:O2	10:V:75:U:C2'	2.63	0.46
9:B:1147:ARG:NH2	9:B:1157:ILE:HD13	2.30	0.46
9:B:1396:VAL:HG13	9:B:1445:LEU:CD1	2.44	0.46
9:B:1201:LYS:HA	9:B:1302:PHE:CE1	2.51	0.46
11:A:2228:PRO:HA	11:A:2357:TRP:O	2.16	0.46
10:V:79:A:O2'	10:V:80:A:O4'	2.19	0.46
9:B:1786:PRO:HB2	9:B:1791:VAL:HB	1.96	0.46
9:B:1253:TYR:CZ	9:B:1272:PHE:CB	2.98	0.46
9:B:1085:SER:HB2	9:B:1087:LEU:HD13	1.98	0.46
9:B:1812:ASN:HA	9:B:1815:VAL:HG22	1.98	0.46
9:B:1057:LEU:O	9:B:1060:LYS:N	2.49	0.46
9:B:1080:LEU:CG	9:B:1084:PHE:CZ	2.99	0.46
9:B:644:GLY:N	9:B:645:PRO:HD2	2.31	0.46
9:B:708:CYS:SG	9:B:890:THR:N	2.89	0.46
9:B:1140:TRP:HE3	9:B:1141:PRO:HD2	1.80	0.45
9:B:614:ILE:HD11	9:B:1009:TYR:CD2	2.51	0.45
9:B:592:SER:HB3	10:V:83:A:P	2.55	0.45
9:B:744:VAL:HG23	9:B:745:HIS:N	2.30	0.45
9:B:1075:LYS:O	9:B:1078:VAL:HG12	2.17	0.45
9:B:872:LEU:O	9:B:875:ALA:N	2.49	0.45
9:B:1656:TYR:CE1	9:B:1677:THR:HG22	2.51	0.45
11:A:2329:PHE:O	11:A:2330:GLU:CB	2.65	0.45
11:A:2354:GLY:O	11:A:2355:ASN:CB	2.64	0.45
9:B:632:ILE:C	9:B:633:ILE:HD12	2.37	0.45
9:B:2001:ASN:N	9:B:2001:ASN:OD1	2.50	0.45
9:B:480:ILE:HD12	9:B:491:PHE:CD2	2.52	0.45
9:B:1142:THR:HG21	11:A:2389:PRO:HA	1.98	0.45
9:B:1157:ILE:HD12	9:B:1158:LYS:N	2.32	0.45
9:B:556:LYS:O	9:B:628:VAL:HA	2.16	0.45
9:B:2113:ALA:HB2	9:B:2130:PHE:CB	2.46	0.45
9:B:1743:GLU:HB2	9:B:1789:TYR:OH	2.17	0.45
9:B:1981:GLN:NE2	9:B:2149:TYR:O	2.49	0.45
9:B:708:CYS:SG	9:B:889:ILE:HA	2.57	0.44
9:B:1113:PHE:HZ	9:B:1240:LEU:HD13	1.82	0.44
9:B:1216:MET:O	9:B:1273:THR:HA	2.18	0.44
11:A:2166:LEU:HB3	11:A:2169:ILE:HD11	2.00	0.44
9:B:1773:PHE:CD2	9:B:1803:LEU:HD21	2.52	0.44
9:B:1095:ASN:O	9:B:1098:ILE:HG22	2.15	0.44
9:B:1456:SER:O	9:B:1457:ARG:C	2.56	0.44
11:A:2152:TRP:CG	11:A:2153:ARG:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1939:LEU:HD13	9:B:1947:LEU:HD22	1.99	0.44
9:B:634:ASP:HA	9:B:670:LEU:HD12	1.99	0.44
9:B:1194:ASP:O	9:B:1198:ARG:HB2	2.18	0.44
9:B:1432:PRO:HB3	9:B:1454:LEU:HD21	1.99	0.44
9:B:1426:ASN:HD22	9:B:1442:SER:HB2	1.83	0.44
9:B:1062:PRO:HD3	11:A:2395:PHE:CG	2.53	0.44
9:B:1396:VAL:HG21	9:B:1468:LEU:HD13	2.00	0.44
9:B:1080:LEU:CD1	9:B:1084:PHE:CZ	3.01	0.44
9:B:1585:LEU:CD1	9:B:1591:CYS:HA	2.48	0.43
9:B:1521:PHE:HD1	9:B:1521:PHE:C	2.21	0.43
9:B:809:THR:HA	9:B:1092:PHE:CD1	2.53	0.43
9:B:1236:LEU:HD22	9:B:1258:PHE:HB3	2.00	0.43
9:B:651:VAL:HG11	9:B:683:PHE:CE1	2.54	0.43
9:B:1253:TYR:CD1	9:B:1272:PHE:CD2	3.06	0.43
9:B:571:VAL:HG21	9:B:587:GLU:HB3	2.00	0.43
9:B:890:THR:OG1	9:B:891:ASP:N	2.51	0.43
9:B:2044:PHE:O	9:B:2048:TYR:CB	2.67	0.43
9:B:931:CYS:SG	9:B:934:ASP:N	2.83	0.43
10:V:134:U:C5	10:V:135:A:C8	3.06	0.43
9:B:1853:ALA:HB2	9:B:1863:ILE:HG13	2.01	0.43
11:A:2189:LEU:HD22	11:A:2224:VAL:HG23	2.00	0.43
9:B:726:CYS:O	9:B:730:VAL:HG23	2.17	0.43
9:B:1257:LEU:HD22	9:B:1270:LEU:HD12	1.99	0.43
9:B:1704:LEU:HA	9:B:1707:VAL:HG23	2.00	0.43
9:B:1960:VAL:O	9:B:1964:ILE:N	2.52	0.43
9:B:1092:PHE:CD1	9:B:1095:ASN:HB3	2.54	0.43
9:B:978:LEU:CD1	9:B:996:ILE:HD12	2.49	0.43
9:B:1867:VAL:HG22	9:B:1964:ILE:HD11	2.01	0.43
9:B:1065:ILE:CG1	9:B:1077:ASN:HD21	2.31	0.43
9:B:1571:SER:OG	9:B:1663:VAL:HG21	2.18	0.43
9:B:580:PHE:CE2	9:B:581:LEU:HG	2.54	0.43
9:B:558:VAL:HG21	9:B:612:TRP:CH2	2.54	0.43
9:B:2002:ASN:HA	9:B:2005:LEU:HD12	2.01	0.42
9:B:1595:ALA:HB1	9:B:1632:PRO:HB3	2.01	0.42
9:B:836:TRP:HA	9:B:836:TRP:CE3	2.54	0.42
9:B:1113:PHE:CZ	9:B:1129:LEU:HD13	2.55	0.42
9:B:562:PRO:HB3	9:B:638:LEU:HD22	2.02	0.42
9:B:1819:PHE:HZ	9:B:1863:ILE:HB	1.84	0.42
9:B:557:ILE:HD12	9:B:604:VAL:HG22	2.02	0.42
9:B:833:THR:HG22	10:V:77:U:H3'	2.00	0.42
11:A:2224:VAL:HG11	11:A:2349:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:936:VAL:HG11	9:B:971:GLU:CD	2.40	0.42
11:A:2165:ARG:HB3	11:A:2300:VAL:HG13	2.00	0.42
9:B:1453:GLU:O	9:B:1494:ARG:NH1	2.51	0.42
9:B:532:LEU:HD21	9:B:577:ARG:HB3	2.02	0.42
9:B:594:LEU:HB2	10:V:83:A:H3'	2.01	0.42
9:B:1095:ASN:O	9:B:1099:VAL:HG23	2.19	0.42
9:B:1781:ARG:O	9:B:1784:VAL:HG22	2.20	0.42
9:B:634:ASP:CB	9:B:670:LEU:HD12	2.50	0.42
9:B:456:VAL:HG12	9:B:457:LYS:N	2.35	0.42
11:A:2159:ASN:HA	11:A:2162:LEU:HD13	2.00	0.42
9:B:613:ASP:HA	9:B:616:THR:HG22	2.02	0.42
11:A:2188:ASN:OD1	11:A:2189:LEU:N	2.53	0.42
9:B:1584:PHE:CE1	9:B:1666:ILE:HD12	2.55	0.42
9:B:1156:VAL:HG13	9:B:1183:ILE:CG2	2.51	0.41
9:B:932:ARG:O	9:B:936:VAL:HG13	2.19	0.41
11:A:2204:ALA:O	11:A:2238:ILE:HD11	2.20	0.41
9:B:1682:ILE:HD13	9:B:1703:LEU:HD22	2.01	0.41
9:B:2140:LEU:HD11	9:B:2160:ILE:HD11	2.02	0.41
9:B:1001:LEU:HD23	9:B:1015:MET:CE	2.50	0.41
10:V:81:C:H2'	10:V:81:C:O2	2.20	0.41
9:B:1884:SER:HA	9:B:1926:VAL:HG11	2.02	0.41
9:B:594:LEU:HD22	9:B:620:ASN:HD21	1.84	0.41
9:B:2117:VAL:HG21	9:B:2119:LEU:HD21	2.03	0.41
9:B:2037:GLN:O	9:B:2041:VAL:HG23	2.19	0.41
9:B:1955:VAL:HG21	9:B:2091:TYR:OH	2.20	0.41
9:B:1880:LEU:HD23	9:B:1927:PHE:CE2	2.55	0.41
9:B:1922:VAL:O	9:B:1926:VAL:HG23	2.20	0.41
9:B:1785:ASN:O	9:B:1787:SER:N	2.53	0.41
9:B:1243:LEU:HD22	9:B:1272:PHE:CE2	2.55	0.41
9:B:1533:TYR:HB3	9:B:1535:PHE:CZ	2.56	0.41
9:B:1065:ILE:HG13	9:B:1077:ASN:HD21	1.85	0.41
10:V:135:A:C2	10:V:136:U:C2	3.09	0.41
9:B:1846:THR:O	9:B:1847:LEU:HD23	2.21	0.41
9:B:1750:ILE:HG21	9:B:1773:PHE:HZ	1.86	0.41
9:B:1939:LEU:CD1	9:B:1947:LEU:HD22	2.51	0.41
9:B:1210:PRO:O	9:B:1785:ASN:ND2	2.43	0.41
11:A:2321:ILE:HG22	11:A:2322:MET:H	1.84	0.41
11:A:2396:SER:O	11:A:2398:LEU:N	2.54	0.41
9:B:1744:SER:OG	9:B:1746:LEU:N	2.54	0.41
9:B:1067:GLU:HB2	9:B:1074:ALA:HB2	2.01	0.41
9:B:898:TYR:O	9:B:901:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1087:LEU:HD22	11:A:2395:PHE:CE2	2.55	0.40
9:B:1476:ALA:HB1	9:B:1521:PHE:CZ	2.56	0.40
9:B:1631:ALA:HB3	9:B:1632:PRO:HD3	2.02	0.40
9:B:770:LEU:O	9:B:772:LYS:N	2.54	0.40
9:B:1331:THR:HG23	9:B:1346:LYS:O	2.21	0.40
9:B:1791:VAL:HG11	9:B:1799:ILE:HG12	2.03	0.40
11:A:2247:LEU:HD11	11:A:2374:PHE:O	2.20	0.40
9:B:808:LEU:HD23	9:B:813:ARG:HA	2.03	0.40
9:B:788:VAL:HG12	9:B:788:VAL:O	2.21	0.40
9:B:1500:THR:O	9:B:1500:THR:HG22	2.21	0.40
9:B:1183:ILE:O	9:B:1183:ILE:CG2	2.68	0.40
9:B:1745:TYR:O	9:B:1746:LEU:C	2.60	0.40
9:B:1145:PRO:HD2	9:B:1167:TRP:CE3	2.57	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 PDB entries followed by that with respect to all EM entries.

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	k	76/196 (39%)	67 (88%)	8 (10%)	1 (1%)	15	60
2	l	87/146 (60%)	74 (85%)	12 (14%)	1 (1%)	17	64
3	m	92/110 (84%)	80 (87%)	10 (11%)	2 (2%)	8	51
4	n	80/101 (79%)	70 (88%)	10 (12%)	0	100	100
5	p	72/94 (77%)	64 (89%)	8 (11%)	0	100	100
6	q	70/86 (81%)	60 (86%)	10 (14%)	0	100	100
7	r	65/77 (84%)	58 (89%)	6 (9%)	1 (2%)	13	57
8	E	308/338 (91%)	266 (86%)	38 (12%)	4 (1%)	15	60
9	B	1707/2163 (79%)	1499 (88%)	174 (10%)	34 (2%)	9	53
11	A	253/267 (95%)	213 (84%)	34 (13%)	6 (2%)	7	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2810/3578 (78%)	2451 (87%)	310 (11%)	49 (2%)	16	55

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	B	448	LEU
9	B	771	THR
9	B	792	SER
9	B	985	GLU
9	B	1370	SER
9	B	1481	GLN
9	B	1483	VAL
11	A	2330	GLU
1	k	81	VAL
9	B	1009	TYR
9	B	1051	LYS
9	B	1069	ILE
9	B	1147	ARG
9	B	1637	VAL
9	B	1697	PRO
11	A	2321	ILE
11	A	2355	ASN
11	A	2398	LEU
8	E	101	ALA
9	B	875	ALA
9	B	1972	ASN
9	B	1991	ASP
11	A	2197	SER
2	l	97	LEU
3	m	66	ASN
8	E	212	ALA
8	E	512	ALA
9	B	928	ASN
9	B	958	PRO
9	B	1024	GLU
9	B	1088	LYS
9	B	1201	LYS
9	B	1296	ASN
9	B	1480	SER
9	B	1485	GLY
9	B	1750	ILE
7	r	59	LEU

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Mol	Chain	Res	Type
8	E	411	ALA
9	B	744	VAL
9	B	1275	GLU
9	B	1317	PHE
9	B	1401	SER
9	B	1185	SER
9	B	1335	GLY
11	A	2388	ARG
9	B	2030	ILE
9	B	1910	PRO
3	m	81	GLY
9	B	1785	ASN

### 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 PDB entries followed by that with respect to all EM entries.

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	k	71/176 (40%)	69 (97%)	2 (3%)	51	82
2	l	85/129 (66%)	82 (96%)	3 (4%)	43	79
3	m	78/103 (76%)	74 (95%)	4 (5%)	29	70
4	n	69/89 (78%)	67 (97%)	2 (3%)	50	82
5	p	65/83 (78%)	60 (92%)	5 (8%)	16	56
6	q	63/77 (82%)	62 (98%)	1 (2%)	70	90
7	r	57/66 (86%)	55 (96%)	2 (4%)	43	79
8	E	20/20 (100%)	18 (90%)	2 (10%)	9	43
9	B	1536/1955 (79%)	1428 (93%)	108 (7%)	19	60
11	A	220/236 (93%)	206 (94%)	14 (6%)	22	63
All	All	2264/2934 (77%)	2121 (94%)	143 (6%)	27	64

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	k	25	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	k	48	CYS
2	l	78	ASN
2	l	110	GLN
2	l	113	LEU
3	m	41	ARG
3	m	52	HIS
3	m	82	LYS
3	m	94	LEU
4	n	20	SER
4	n	43	GLN
5	p	18	PHE
5	p	77	LEU
5	p	79	LYS
5	p	81	LEU
5	p	88	THR
6	q	79	LEU
7	r	69	ILE
7	r	71	LEU
8	E	550	GLN
8	E	552	PHE
9	B	453	PHE
9	B	463	ILE
9	B	491	PHE
9	B	505	LYS
9	B	518	LEU
9	B	539	LEU
9	B	543	TYR
9	B	566	LEU
9	B	610	GLU
9	B	645	PRO
9	B	670	LEU
9	B	684	LEU
9	B	717	LYS
9	B	726	CYS
9	B	768	HIS
9	B	778	LYS
9	B	782	LYS
9	B	784	GLU
9	B	793	LEU
9	B	815	LEU
9	B	818	ASP
9	B	831	THR

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Mol	Chain	Res	Type
9	B	836	TRP
9	B	864	SER
9	B	870	GLN
9	B	872	LEU
9	B	897	TYR
9	B	901	VAL
9	B	902	LEU
9	B	920	LEU
9	B	921	ASN
9	B	928	ASN
9	B	942	THR
9	B	944	LEU
9	B	948	MET
9	B	963	ASP
9	B	978	LEU
9	B	1000	ASP
9	B	1006	SER
9	B	1015	MET
9	B	1016	ASP
9	B	1052	ARG
9	B	1054	LEU
9	B	1057	LEU
9	B	1077	ASN
9	B	1085	SER
9	B	1086	GLN
9	B	1088	LYS
9	B	1128	LEU
9	B	1131	LEU
9	B	1132	CYS
9	B	1137	THR
9	B	1138	LYS
9	B	1139	MET
9	B	1152	CYS
9	B	1160	LEU
9	B	1198	ARG
9	B	1202	MET
9	B	1246	THR
9	B	1253	TYR
9	B	1260	THR
9	B	1262	ASP
9	B	1268	PHE
9	B	1270	LEU

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Mol	Chain	Res	Type
9	B	1277	LYS
9	B	1280	ASN
9	B	1284	LEU
9	B	1370	SER
9	B	1400	PRO
9	B	1411	ASP
9	B	1453	GLU
9	B	1483	VAL
9	B	1490	THR
9	B	1491	LEU
9	B	1493	SER
9	B	1498	ILE
9	B	1514	CYS
9	B	1515	LEU
9	B	1519	ARG
9	B	1521	PHE
9	B	1540	ARG
9	B	1578	ARG
9	B	1590	ASP
9	B	1610	LEU
9	B	1648	ASP
9	B	1651	ILE
9	B	1675	CYS
9	B	1687	LEU
9	B	1689	ASP
9	B	1694	LYS
9	B	1696	MET
9	B	1705	GLU
9	B	1707	VAL
9	B	1722	ILE
9	B	1724	THR
9	B	1744	SER
9	B	1847	LEU
9	B	1849	ASN
9	B	1860	PHE
9	B	1887	VAL
9	B	1917	THR
9	B	1933	TYR
9	B	1975	THR
9	B	1987	VAL
9	B	2000	PHE
9	B	2024	ASP

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Mol	Chain	Res	Type
9	B	2098	SER
9	B	2131	ASP
11	A	2155	SER
11	A	2164	LEU
11	A	2168	ASN
11	A	2170	TYR
11	A	2188	ASN
11	A	2190	LEU
11	A	2228	PRO
11	A	2238	ILE
11	A	2251	GLU
11	A	2306	ASN
11	A	2309	ASP
11	A	2340	LEU
11	A	2356	VAL
11	A	2381	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	25	GLN
2	l	78	ASN
2	l	110	GLN
5	p	86	ASN
9	B	620	ASN
9	B	739	GLN
9	B	804	HIS
9	B	1280	ASN
9	B	1513	ASN
9	B	1727	ASN
9	B	1959	ASN
9	B	2069	GLN
11	A	2237	GLN
11	A	2306	ASN
11	A	2394	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	V	55/96 (57%)	34 (61%)	5 (9%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	V	74	U
10	V	75	U
10	V	78	A
10	V	80	A
10	V	81	C
10	V	83	A
10	V	84	G
10	V	85	A
10	V	86	C
10	V	87	C
10	V	88	G
10	V	89	U
10	V	90	C
10	V	91	U
10	V	94	U
10	V	98	G
10	V	100	U
10	V	101	C
10	V	102	A
10	V	103	A
10	V	129	A
10	V	130	A
10	V	131	G
10	V	132	A
10	V	136	U
10	V	137	G
10	V	138	U
10	V	143	A
10	V	144	A
10	V	145	U
10	V	147	U
10	V	149	U
10	V	151	G
10	V	152	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	V	80	A
10	V	83	A
10	V	88	G
10	V	143	A

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Mol	Chain	Res	Type
10	V	150	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	132:ALA	C	150:ALA	N	37.33
1	E	170:ALA	C	180:ALA	N	34.57
1	E	102:ALA	C	120:ALA	N	31.59
1	E	299:ALA	C	310:ALA	N	27.52
1	E	226:ALA	C	240:ALA	N	26.36
1	E	250:ALA	C	270:ALA	N	25.18
1	E	420:ALA	C	487:ALA	N	24.74
1	E	280:ALA	C	290:ALA	N	24.21
1	E	318:ALA	C	330:ALA	N	14.53
1	E	194:ALA	C	210:ALA	N	14.15
1	E	57:ALA	C	70:ALA	N	11.23

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	25:ALA	C	40:ALA	N	8.77
1	E	91:ALA	C	96:ALA	N	7.75
1	E	79:ALA	C	82:ALA	N	5.51