



wwPDB EM Map/Model Validation Report ⓘ

Oct 3, 2016 – 08:54 PM EDT

PDB ID : 5GAM
EMDB ID: : EMD-8011
Title : Foot 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 : 3.70 Å(reported)

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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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) : rb-20027939

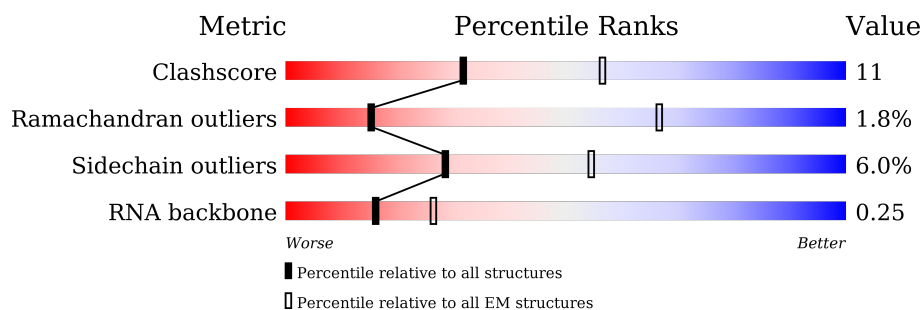
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 ≥ 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	U	178	24% 30% 24% . 21%
2	A	735	62% 17% . 19%
3	C	1008	57% 25% . 15%
4	W	31	35% 32% 13% 19%
5	b	196	41% 59%
6	e	94	74% 5% 20%
7	f	86	80% . 16%
8	g	77	87% .. 10%

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Mol	Chain	Length	Quality of chain
9	x	18	<div><div></div><div>100%</div></div>
10	d	101	<div><div></div><div>78%</div><div></div><div>19%</div></div>
11	h	146	<div><div></div><div>52%</div><div></div><div>44%</div></div>
12	j	110	<div><div></div><div>81%</div><div></div><div>5%</div><div>15%</div></div>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 19123 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 RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

- Molecule 2 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	593	Total	C	N	O	S	0	0
			4702	3052	817	817	16		

- Molecule 3 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	855	Total	C	N	O	S	0	0
			6450	4195	1089	1143	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	530	SER	GLU	conflict	UNP P36048
C	531	LYS	ASP	conflict	UNP P36048
C	532	THR	ASP	conflict	UNP P36048

- Molecule 4 is a RNA chain called U6 snRNA, 5' end.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	25	Total	C	N	O	P	0	0
			532	237	91	179	25		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

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

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

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 9 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	x	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D1.

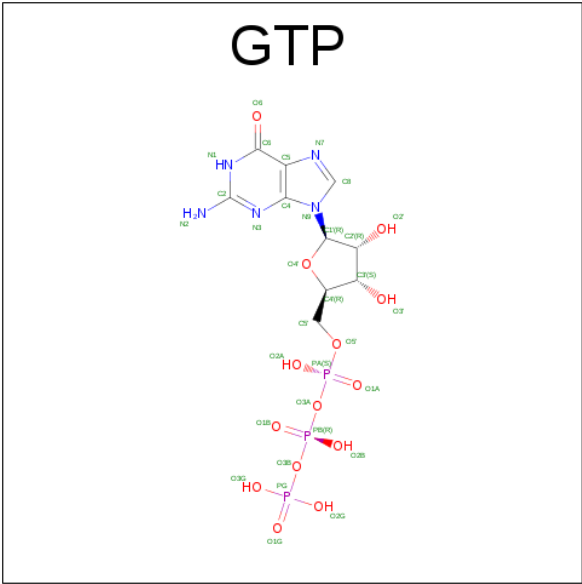
Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:


C₁₀H₁₆N₅O₁₄P₃).

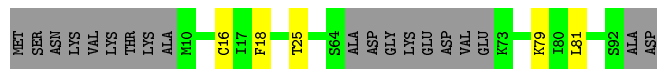


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	C	1	32	10	5	14	3	0




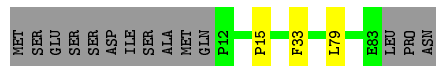
- Molecule 6: Small nuclear ribonucleoprotein E

Chain e:  74% 5% 20%




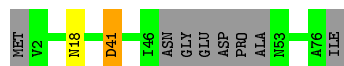
- Molecule 7: Small nuclear ribonucleoprotein F

Chain f:  80% 16%



- Molecule 8: Small nuclear ribonucleoprotein G

Chain g:  87% 10%



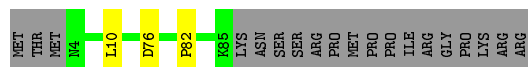
- Molecule 9: Unknown polypeptide

Chain x:  100%

There are no outlier residues recorded for this chain.

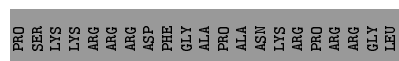
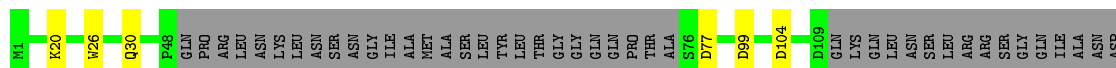
- Molecule 10: Small nuclear ribonucleoprotein Sm D3

Chain d:  78% 19%




- Molecule 11: Small nuclear ribonucleoprotein Sm D1

Chain h:  52% 44%



- Molecule 12: Small nuclear ribonucleoprotein Sm D2

Chain j:  81% 5% 15%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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	U	0.38	0/3351	0.87	3/5213 (0.1%)
10	d	0.36	0/634	0.66	0/859
11	h	0.36	0/649	0.59	0/880
12	j	0.41	0/753	0.67	0/1013
2	A	0.42	0/4840	0.74	2/6596 (0.0%)
3	C	0.44	0/6590	0.78	1/8975 (0.0%)
4	W	0.26	0/592	0.73	0/918
5	b	0.36	0/636	0.64	0/856
6	e	0.39	0/585	0.60	0/795
7	f	0.43	0/585	0.62	0/791
8	g	0.35	0/532	0.62	0/715
All	All	0.41	0/19747	0.76	6/27611 (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
2	A	0	5
3	C	0	4
8	g	0	1
All	All	0	10

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	82	A	C2'-C3'-O3'	7.10	125.12	109.50
1	U	128	A	C2'-C3'-O3'	6.70	124.43	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	62	G	C4'-C3'-O3'	5.50	124.01	113.00
2	A	425	ASP	CB-CG-OD2	5.26	123.03	118.30
3	C	659	LEU	CA-CB-CG	5.17	127.19	115.30
2	A	615	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	460	PRO	Peptide
2	A	464	GLU	Peptide
2	A	466	GLU	Peptide
2	A	553	ASN	Peptide
2	A	556	TYR	Peptide
3	C	498	THR	Peptide
3	C	607	LEU	Peptide
3	C	811	GLU	Peptide
3	C	958	PRO	Peptide
8	g	41	ASP	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	U	2999	0	1515	103	0
2	A	4702	0	4527	109	0
3	C	6450	0	6420	186	0
4	W	532	0	269	4	0
5	b	631	0	670	0	0
6	e	575	0	597	0	0
7	f	573	0	572	0	0
8	g	529	0	557	0	0
9	x	90	0	20	0	0
10	d	625	0	647	0	0
11	h	644	0	686	0	0
12	j	741	0	778	0	0
13	C	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19123	0	17270	377	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 11.

All (377) 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)
2:A:139:LEU:HD13	2:A:193:TYR:CD2	1.31	1.63
2:A:139:LEU:CD1	2:A:193:TYR:CD2	2.15	1.29
1:U:42:A:H3'	1:U:43:G:H5''	1.24	1.15
2:A:139:LEU:HD13	2:A:193:TYR:CE2	1.87	1.08
2:A:139:LEU:CD1	2:A:193:TYR:HD2	1.60	1.07
1:U:42:A:C3'	1:U:43:G:H5''	1.88	1.03
1:U:42:A:H2'	1:U:43:G:C4'	1.98	0.94
1:U:41:A:C8	1:U:75:A:C2	2.56	0.93
2:A:468:LEU:HD21	3:C:382:TYR:HB3	1.51	0.92
1:U:42:A:H3'	1:U:43:G:C5'	1.99	0.91
2:A:468:LEU:CD1	3:C:281:PRO:HG3	2.00	0.91
1:U:74:U:H2'	1:U:76:U:OP2	1.77	0.85
2:A:460:PRO:HB3	3:C:376:PHE:CD1	2.10	0.85
1:U:41:A:C8	1:U:75:A:N1	2.46	0.82
1:U:74:U:O2'	1:U:76:U:OP2	1.98	0.82
1:U:74:U:C2'	1:U:76:U:OP2	2.30	0.79
1:U:74:U:H2'	1:U:75:A:H4'	1.62	0.79
2:A:461:LEU:HD22	3:C:404:PHE:CE1	2.19	0.78
3:C:472:VAL:HG22	3:C:486:VAL:HG22	1.66	0.77
1:U:42:A:C2'	1:U:43:G:H5''	2.14	0.77
2:A:461:LEU:HD11	3:C:380:PRO:HB3	1.67	0.77
2:A:708:TRP:CE2	2:A:712:LEU:HD11	2.19	0.77
1:U:41:A:H2'	1:U:42:A:C8	2.19	0.77
3:C:387:TYR:HB3	3:C:396:LEU:HD12	1.67	0.76
3:C:324:ILE:HG23	3:C:377:ILE:HD11	1.68	0.75
1:U:43:G:H4'	1:U:43:G:OP1	1.85	0.75
2:A:658:ASN:HD22	2:A:684:LYS:HB2	1.53	0.74
3:C:836:SER:O	3:C:840:PRO:HD2	1.87	0.74
1:U:17:C:H2'	1:U:18:A:C8	2.24	0.73
1:U:42:A:C3'	1:U:43:G:C5'	2.62	0.73
3:C:200:CYS:HB3	3:C:436:VAL:HG21	1.72	0.72
2:A:469:ILE:HG23	2:A:473:THR:CG2	2.20	0.71
1:U:74:U:C2'	1:U:75:A:H4'	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:390:LEU:HD22	2:A:391:TYR:CE1	2.26	0.70
3:C:868:VAL:HG11	3:C:876:VAL:HG21	1.73	0.70
1:U:41:A:N9	1:U:75:A:C2	2.60	0.70
2:A:467:GLU:N	2:A:467:GLU:OE1	2.21	0.70
3:C:872:LEU:HD13	3:C:922:THR:HG22	1.74	0.69
1:U:24:G:H2'	1:U:25:G:O4'	1.92	0.69
1:U:45:A:N3	1:U:45:A:H2'	2.07	0.68
1:U:42:A:H2'	1:U:43:G:O4'	1.93	0.68
1:U:42:A:H2'	1:U:43:G:C5'	2.24	0.68
2:A:171:ALA:HB1	2:A:201:PHE:HB3	1.77	0.67
2:A:458:PHE:CE2	3:C:336:ILE:HD11	2.30	0.67
3:C:774:LEU:HD13	3:C:803:VAL:HG23	1.78	0.66
1:U:46:C:H4'	3:C:111:LYS:HG3	1.77	0.66
1:U:45:A:H3'	1:U:46:C:C6	2.31	0.65
2:A:462:LEU:HD23	3:C:403:ASN:HD22	1.61	0.65
3:C:236:LEU:HD11	3:C:435:LEU:HD21	1.79	0.65
3:C:761:ALA:O	3:C:765:VAL:HG13	1.97	0.65
2:A:715:LEU:O	2:A:719:ILE:HG23	1.97	0.64
3:C:345:THR:HA	3:C:348:LEU:HD12	1.78	0.64
3:C:149:LEU:HD21	3:C:435:LEU:HD11	1.77	0.64
1:U:45:A:C5'	1:U:46:C:H5	2.11	0.64
2:A:468:LEU:HD11	3:C:281:PRO:HG3	1.80	0.64
1:U:133:C:H2'	1:U:133:C:O2	1.97	0.64
3:C:360:ARG:HA	3:C:361:THR:HG22	1.79	0.64
1:U:46:C:H4'	3:C:111:LYS:CG	2.28	0.64
2:A:673:VAL:HG22	2:A:714:PHE:CE1	2.32	0.63
3:C:323:THR:HG21	3:C:438:ALA:HB2	1.78	0.63
2:A:468:LEU:HD12	3:C:281:PRO:HG3	1.79	0.63
3:C:387:TYR:CE1	3:C:399:LEU:CD1	2.82	0.63
3:C:864:VAL:HG22	3:C:930:LEU:CD2	2.27	0.63
2:A:470:LEU:HB3	2:A:471:PRO:HD2	1.81	0.62
3:C:659:LEU:HD21	3:C:668:ILE:HD13	1.82	0.62
1:U:45:A:H5''	1:U:46:C:H5	1.65	0.62
1:U:42:A:H2'	1:U:43:G:H5''	1.81	0.62
1:U:41:A:C2	1:U:42:A:C6	2.88	0.62
3:C:472:VAL:HG13	3:C:484:SER:OG	2.00	0.61
3:C:501:ILE:CD1	3:C:567:ILE:HG23	2.31	0.61
1:U:40:C:N3	1:U:115:G:C6	2.69	0.61
3:C:387:TYR:CZ	3:C:399:LEU:HD11	2.35	0.61
3:C:501:ILE:HD11	3:C:567:ILE:HD12	1.82	0.61
1:U:20:U:H2'	1:U:21:G:C1'	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:193:TYR:HB3	2:A:200:THR:HG23	1.82	0.61
1:U:128:A:H2'	1:U:129:G:O4'	2.01	0.60
3:C:857:LEU:HG	3:C:967:VAL:HG22	1.83	0.60
2:A:330:LEU:HD22	2:A:385:VAL:HG23	1.84	0.60
1:U:45:A:H3'	1:U:46:C:H6	1.65	0.60
2:A:176:LEU:HD23	2:A:715:LEU:HD12	1.84	0.60
3:C:235:VAL:HG23	3:C:261:VAL:HG11	1.83	0.59
1:U:22:G:C2	1:U:131:A:C2	2.90	0.59
3:C:387:TYR:CZ	3:C:399:LEU:CD1	2.85	0.59
3:C:762:SER:O	3:C:765:VAL:HG22	2.02	0.59
2:A:462:LEU:HD23	3:C:403:ASN:ND2	2.17	0.59
3:C:223:ASP:OD2	3:C:631:GLY:N	2.36	0.59
1:U:19:A:H2'	1:U:20:U:C1'	2.32	0.59
2:A:175:LEU:HD13	2:A:571:LEU:HD12	1.85	0.58
2:A:222:ILE:HD11	2:A:317:PRO:HG2	1.84	0.58
1:U:42:A:H2'	1:U:43:G:H4'	1.83	0.58
2:A:194:HIS:HD2	2:A:196:SER:H	1.52	0.58
3:C:193:LEU:HD11	3:C:213:LEU:HB3	1.86	0.57
3:C:605:ILE:HD13	3:C:656:LEU:HD11	1.85	0.57
2:A:403:TYR:CD2	3:C:189:LEU:HD11	2.40	0.57
1:U:25:G:H4'	1:U:26:A:O4'	2.03	0.57
2:A:569:LEU:HD21	2:A:637:VAL:HG21	1.86	0.57
1:U:33:U:O4	2:A:284:ARG:NH2	2.37	0.57
2:A:461:LEU:N	2:A:461:LEU:HD12	2.19	0.57
3:C:318:LEU:HD21	3:C:421:LEU:HD13	1.87	0.57
3:C:864:VAL:HG21	3:C:906:VAL:HG23	1.86	0.57
1:U:23:C:H2'	1:U:24:G:O4'	2.05	0.57
1:U:42:A:C2'	1:U:43:G:C5'	2.81	0.57
2:A:172:ILE:HD11	2:A:626:LEU:CD2	2.34	0.57
3:C:241:VAL:HG11	3:C:273:LEU:HD23	1.85	0.57
1:U:38:A:H2'	1:U:39:U:C6	2.40	0.57
3:C:387:TYR:CE1	3:C:399:LEU:HD12	2.40	0.56
1:U:12:C:O2'	1:U:13:A:O4'	2.23	0.56
4:W:29:U:H2'	4:W:30:G:O4'	2.04	0.56
3:C:108:GLN:O	3:C:111:LYS:HD3	2.04	0.56
2:A:673:VAL:HG22	2:A:714:PHE:CZ	2.40	0.56
2:A:461:LEU:H	2:A:461:LEU:HD12	1.71	0.56
2:A:459:ALA:HB1	2:A:463:ALA:CB	2.35	0.56
3:C:472:VAL:HG22	3:C:486:VAL:CG2	2.35	0.56
3:C:656:LEU:HD22	3:C:670:ILE:HD11	1.87	0.56
1:U:79:C:C2	1:U:114:G:N2	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:314:ALA:HB2	3:C:321:THR:HG22	1.87	0.56
3:C:723:LEU:HD12	3:C:773:VAL:HG11	1.88	0.56
2:A:656:ILE:O	2:A:660:ILE:HD12	2.06	0.56
2:A:639:PHE:HA	2:A:644:VAL:HG11	1.87	0.56
3:C:133:ILE:HD13	3:C:560:GLN:HB3	1.88	0.56
1:U:26:A:O5'	1:U:26:A:C8	2.59	0.56
1:U:31:G:O2'	1:U:32:G:H5'	2.06	0.56
3:C:234:LEU:HD13	3:C:439:ILE:HG23	1.88	0.55
2:A:199:ILE:HG23	2:A:199:ILE:O	2.06	0.55
3:C:602:VAL:HG11	3:C:908:VAL:HG21	1.88	0.55
2:A:193:TYR:N	2:A:193:TYR:CD1	2.73	0.55
2:A:193:TYR:N	2:A:193:TYR:HD1	2.05	0.55
3:C:774:LEU:HD22	3:C:803:VAL:HB	1.89	0.54
1:U:26:A:C6	1:U:129:G:H1'	2.42	0.54
3:C:152:LEU:HB2	3:C:432:GLN:HE22	1.72	0.54
3:C:710:VAL:HG22	3:C:820:LEU:HD23	1.89	0.54
3:C:626:SER:HB3	3:C:634:ILE:HD12	1.90	0.54
3:C:320:PHE:CE2	3:C:425:LEU:HD13	2.43	0.54
1:U:41:A:C4	1:U:75:A:C2	2.96	0.54
3:C:187:ARG:NH1	3:C:654:CYS:SG	2.73	0.54
3:C:688:SER:HB3	3:C:821:LEU:HD12	1.88	0.53
1:U:20:U:H2'	1:U:21:G:O4'	2.09	0.53
3:C:423:HIS:CE1	3:C:427:LEU:HD11	2.43	0.53
3:C:288:LEU:HD13	3:C:313:PHE:CE2	2.43	0.53
1:U:40:C:O2	1:U:115:G:C2	2.62	0.53
2:A:318:LEU:HD11	2:A:703:PHE:CE1	2.44	0.53
2:A:636:HIS:CE1	2:A:653:ILE:HD11	2.45	0.52
1:U:73:U:H2'	1:U:74:U:C1'	2.40	0.52
3:C:251:GLN:HG2	3:C:933:TRP:CD2	2.44	0.52
2:A:305:LEU:HD21	2:A:476:ALA:HB2	1.91	0.52
3:C:269:LYS:HA	13:C:1101:GTP:O6	2.10	0.52
3:C:241:VAL:CG1	3:C:273:LEU:HD23	2.40	0.52
3:C:774:LEU:HD21	3:C:813:ILE:HB	1.91	0.52
3:C:545:LEU:HB3	3:C:546:GLY:HA3	1.90	0.52
1:U:19:A:H2'	1:U:20:U:N1	2.24	0.52
2:A:674:MET:HA	2:A:677:ILE:HD12	1.91	0.51
3:C:862:TYR:CD2	3:C:908:VAL:HG22	2.46	0.51
1:U:18:A:H3'	1:U:19:A:H8	1.75	0.51
3:C:320:PHE:CD2	3:C:425:LEU:HD13	2.46	0.51
2:A:176:LEU:HD13	2:A:632:ILE:CD1	2.40	0.51
3:C:197:THR:O	3:C:198:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:132:A:C2'	1:U:133:C:OP1	2.58	0.51
1:U:22:G:N1	1:U:131:A:C2	2.79	0.51
3:C:124:LEU:HD22	3:C:553:VAL:HG11	1.93	0.51
2:A:461:LEU:CD1	3:C:380:PRO:HB3	2.40	0.51
3:C:615:LEU:N	3:C:616:PRO:HD2	2.25	0.51
2:A:497:GLN:HB3	2:A:712:LEU:HD13	1.93	0.51
3:C:675:THR:HG23	3:C:909:ILE:HG12	1.91	0.51
2:A:390:LEU:HG	3:C:605:ILE:HD11	1.92	0.50
1:U:40:C:C2	1:U:115:G:N1	2.79	0.50
1:U:70:A:H3'	1:U:71:A:H5''	1.91	0.50
2:A:459:ALA:HB1	2:A:463:ALA:HB3	1.93	0.50
2:A:139:LEU:CD1	2:A:193:TYR:CE2	2.74	0.50
3:C:138:VAL:HG12	3:C:214:ASP:HA	1.93	0.50
3:C:239:ILE:HD13	3:C:245:VAL:HG22	1.94	0.50
2:A:591:LEU:HD13	2:A:599:LEU:HD11	1.94	0.50
3:C:780:PRO:HD2	3:C:783:ILE:HD13	1.93	0.50
3:C:680:SER:O	3:C:856:ILE:N	2.45	0.50
1:U:129:G:H4'	1:U:130:A:C4'	2.42	0.50
3:C:628:TYR:O	3:C:630:PRO:HD3	2.11	0.50
2:A:526:LEU:O	2:A:530:VAL:HG23	2.12	0.50
3:C:255:GLN:HG3	3:C:598:ILE:HD13	1.93	0.50
1:U:74:U:H2'	1:U:76:U:P	2.52	0.50
3:C:314:ALA:CB	3:C:321:THR:HG22	2.42	0.49
2:A:390:LEU:HD22	2:A:391:TYR:CD1	2.47	0.49
2:A:625:LEU:HD22	2:A:715:LEU:HD21	1.94	0.49
3:C:235:VAL:CG2	3:C:261:VAL:HG11	2.42	0.49
2:A:315:SER:O	2:A:318:LEU:N	2.44	0.49
3:C:322:PHE:HE2	3:C:381:LEU:HD11	1.77	0.49
3:C:862:TYR:CE2	3:C:908:VAL:HG13	2.48	0.49
3:C:869:HIS:CD2	3:C:925:LEU:HD22	2.47	0.49
2:A:288:GLU:OE2	2:A:296:THR:HG22	2.12	0.49
3:C:208:ARG:NH1	3:C:440:THR:OG1	2.46	0.49
3:C:864:VAL:HG22	3:C:930:LEU:HD22	1.94	0.49
3:C:712:ALA:HB2	3:C:818:TYR:CD2	2.47	0.49
3:C:659:LEU:HD23	3:C:660:ARG:N	2.28	0.48
1:U:78:A:N6	1:U:81:A:C2	2.81	0.48
1:U:128:A:N3	1:U:128:A:H2'	2.28	0.48
2:A:462:LEU:CD2	3:C:403:ASN:ND2	2.77	0.48
2:A:657:LEU:HD13	2:A:708:TRP:HA	1.94	0.48
2:A:630:LYS:O	2:A:634:ASP:N	2.40	0.48
3:C:154:VAL:O	3:C:157:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:712:ALA:HB1	3:C:816:VAL:CG1	2.44	0.48
2:A:636:HIS:CD2	2:A:649:LEU:HD21	2.49	0.48
3:C:236:LEU:HD21	3:C:439:ILE:CG1	2.44	0.48
3:C:768:PHE:HB3	3:C:775:ILE:HA	1.96	0.48
3:C:288:LEU:HD13	3:C:313:PHE:HE2	1.79	0.48
2:A:194:HIS:CD2	2:A:196:SER:H	2.30	0.48
2:A:424:PHE:CZ	3:C:900:LEU:HD21	2.49	0.48
3:C:775:ILE:O	3:C:818:TYR:N	2.47	0.48
3:C:602:VAL:HG12	3:C:602:VAL:O	2.14	0.47
2:A:468:LEU:O	2:A:468:LEU:HD23	2.14	0.47
3:C:502:LEU:HD12	3:C:591:PHE:CD1	2.49	0.47
3:C:605:ILE:HD12	3:C:652:MET:HG3	1.96	0.47
3:C:315:SER:HB3	3:C:320:PHE:CE2	2.50	0.47
1:U:13:A:H2'	1:U:14:G:C8	2.49	0.47
1:U:22:G:C5	1:U:23:C:C5	3.02	0.47
1:U:74:U:H3'	1:U:75:A:H5''	1.95	0.47
2:A:172:ILE:HG23	2:A:629:MET:CG	2.45	0.47
3:C:387:TYR:CE1	3:C:399:LEU:HD11	2.48	0.47
3:C:493:LEU:HD23	3:C:542:ILE:HD11	1.97	0.47
3:C:567:ILE:HG22	3:C:571:TYR:CE1	2.50	0.47
2:A:168:LEU:HA	2:A:199:ILE:HD11	1.96	0.47
3:C:270:LEU:HD11	3:C:313:PHE:HB3	1.96	0.47
3:C:457:SER:OG	3:C:592:PHE:HA	2.15	0.47
3:C:873:LEU:HD22	3:C:900:LEU:HD13	1.96	0.47
3:C:934:HIS:O	3:C:935:LYS:CB	2.63	0.47
1:U:74:U:H2'	1:U:75:A:C4'	2.38	0.47
3:C:988:THR:HB	3:C:989:LEU:CB	2.45	0.47
2:A:460:PRO:HB3	3:C:376:PHE:CE1	2.47	0.47
3:C:361:THR:O	3:C:361:THR:HG23	2.15	0.47
1:U:25:G:H2'	1:U:25:G:N3	2.30	0.47
2:A:644:VAL:HG22	2:A:645:ASP:H	1.80	0.47
2:A:719:ILE:N	2:A:720:PRO:CD	2.78	0.47
3:C:236:LEU:HD21	3:C:439:ILE:HG12	1.97	0.47
3:C:567:ILE:HG22	3:C:571:TYR:CD1	2.49	0.47
2:A:507:LEU:HD23	2:A:526:LEU:CD2	2.46	0.46
3:C:873:LEU:N	3:C:874:PRO:CD	2.77	0.46
1:U:21:G:C2	1:U:132:A:C2	3.03	0.46
3:C:324:ILE:HD13	3:C:324:ILE:N	2.29	0.46
3:C:944:VAL:HG23	3:C:967:VAL:HG21	1.98	0.46
1:U:75:A:H5'	1:U:76:U:C5	2.50	0.46
3:C:223:ASP:OD2	3:C:630:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:492:LEU:HD12	3:C:492:LEU:O	2.15	0.46
3:C:470:ALA:HB3	3:C:577:LEU:HD11	1.98	0.46
2:A:709:ARG:HA	2:A:712:LEU:HD12	1.97	0.46
3:C:154:VAL:HG11	3:C:177:TYR:CD2	2.51	0.46
3:C:360:ARG:HA	3:C:361:THR:CG2	2.46	0.46
1:U:115:G:N3	1:U:115:G:H2'	2.31	0.46
1:U:26:A:N6	1:U:129:G:H1'	2.30	0.46
2:A:330:LEU:HD21	2:A:386:ALA:HB2	1.98	0.46
3:C:816:VAL:HG11	3:C:818:TYR:CE1	2.50	0.46
3:C:866:ILE:HD13	3:C:918:LEU:HD11	1.96	0.46
3:C:582:SER:OG	3:C:583:LYS:N	2.48	0.46
3:C:191:ILE:HG22	3:C:192:LYS:HG3	1.98	0.46
1:U:87:G:H2'	1:U:88:U:C6	2.51	0.46
3:C:242:VAL:HG21	3:C:272:ARG:HG2	1.97	0.45
2:A:209:ILE:HB	2:A:212:VAL:HB	1.97	0.45
2:A:499:VAL:HG12	2:A:501:LEU:HD21	1.98	0.45
3:C:470:ALA:HB3	3:C:577:LEU:CD1	2.46	0.45
3:C:879:LEU:HD11	3:C:921:SER:OG	2.17	0.45
3:C:408:LEU:HD11	3:C:424:VAL:HG22	1.99	0.45
3:C:152:LEU:HD11	3:C:319:GLY:HA2	1.97	0.45
3:C:856:ILE:HD13	3:C:939:LYS:HG3	1.97	0.45
3:C:324:ILE:HG23	3:C:377:ILE:CD1	2.44	0.45
3:C:625:ILE:HG22	3:C:634:ILE:HD11	1.97	0.45
3:C:866:ILE:HB	3:C:902:VAL:HG13	1.97	0.45
1:U:38:A:H2'	1:U:39:U:C5	2.52	0.45
2:A:469:ILE:HG23	2:A:473:THR:HG23	1.99	0.45
3:C:655:LEU:C	3:C:655:LEU:HD23	2.37	0.45
1:U:101:C:OP1	2:A:672:LYS:N	2.46	0.45
4:W:27:U:H2'	4:W:28:U:C6	2.51	0.45
2:A:458:PHE:O	2:A:458:PHE:CG	2.70	0.45
2:A:168:LEU:N	2:A:169:PRO:HD2	2.32	0.45
2:A:631:LEU:HD21	2:A:663:LEU:HD13	1.99	0.44
3:C:632:VAL:HG22	3:C:651:TYR:HE2	1.82	0.44
1:U:21:G:N2	1:U:132:A:N3	2.65	0.44
2:A:458:PHE:O	2:A:458:PHE:CD2	2.70	0.44
1:U:101:C:OP1	2:A:671:TYR:N	2.51	0.44
2:A:168:LEU:CD2	2:A:578:MET:HG2	2.48	0.44
2:A:199:ILE:HG13	2:A:201:PHE:HD2	1.82	0.44
2:A:578:MET:HG3	2:A:579:LEU:N	2.33	0.44
2:A:172:ILE:HG23	2:A:629:MET:HG3	1.99	0.44
1:U:41:A:N7	1:U:75:A:N1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:5:G:C6	4:W:6:C:N4	2.85	0.44
3:C:133:ILE:HA	3:C:209:MET:O	2.17	0.44
3:C:572:ILE:HG22	3:C:573:LYS:HG3	1.99	0.44
1:U:74:U:H3'	1:U:75:A:C5'	2.48	0.44
4:W:5:G:C2	4:W:6:C:C2	3.05	0.44
2:A:210:GLU:N	2:A:211:PRO:HD2	2.32	0.44
3:C:129:ILE:HG22	3:C:130:PRO:O	2.17	0.44
3:C:385:PHE:CE1	3:C:425:LEU:HD11	2.53	0.44
1:U:18:A:H2'	1:U:19:A:H5'	1.99	0.44
1:U:19:A:H2'	1:U:20:U:O4'	2.18	0.44
2:A:172:ILE:HD11	2:A:626:LEU:HD21	2.00	0.44
2:A:459:ALA:HB1	2:A:460:PRO:HD2	2.00	0.44
2:A:538:LEU:HD12	2:A:538:LEU:N	2.32	0.44
1:U:41:A:C2	1:U:42:A:N1	2.86	0.44
1:U:18:A:H3'	1:U:19:A:C8	2.51	0.44
3:C:324:ILE:HD12	3:C:377:ILE:HD13	2.00	0.43
2:A:458:PHE:CZ	3:C:336:ILE:HD11	2.54	0.43
3:C:416:ASP:HB3	3:C:417:PRO:HD2	2.01	0.43
3:C:918:LEU:HD22	3:C:926:GLY:O	2.18	0.43
3:C:862:TYR:CG	3:C:908:VAL:HG22	2.53	0.43
3:C:577:LEU:HD12	3:C:577:LEU:C	2.39	0.43
1:U:32:G:C2	1:U:34:C:C2	3.06	0.43
1:U:44:A:C2	1:U:70:A:N6	2.87	0.43
2:A:484:PHE:C	2:A:484:PHE:CD1	2.90	0.43
3:C:468:LEU:HD12	3:C:468:LEU:C	2.38	0.43
3:C:883:ARG:NH2	3:C:914:PHE:CG	2.87	0.43
1:U:19:A:C2'	1:U:20:U:O4'	2.67	0.43
1:U:32:G:C6	1:U:34:C:C4	3.06	0.43
2:A:404:ASN:CG	2:A:405:ASN:N	2.72	0.43
3:C:285:TYR:HB2	3:C:374:VAL:HG22	2.01	0.43
1:U:93:G:C6	1:U:94:C:N4	2.86	0.43
3:C:629:TYR:HB3	3:C:651:TYR:OH	2.19	0.43
1:U:93:G:C2	1:U:94:C:N3	2.87	0.43
1:U:98:U:C4	1:U:99:U:C5	3.07	0.43
3:C:142:LEU:HD22	3:C:143:HIS:N	2.33	0.43
3:C:242:VAL:HG22	3:C:277:LEU:HD11	2.00	0.43
2:A:461:LEU:O	3:C:403:ASN:ND2	2.48	0.43
2:A:308:MET:HG3	2:A:479:LEU:HD11	2.00	0.43
3:C:360:ARG:HD3	3:C:361:THR:HG22	2.01	0.43
3:C:597:TYR:O	3:C:599:THR:N	2.51	0.43
1:U:42:A:C5	1:U:43:G:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:186:ALA:HB2	2:A:640:ARG:HH12	1.84	0.42
3:C:138:VAL:HG22	3:C:146:LYS:HB2	2.01	0.42
3:C:444:GLN:N	3:C:445:PRO:HA	2.34	0.42
3:C:864:VAL:HG21	3:C:906:VAL:CG2	2.49	0.42
1:U:74:U:C2	1:U:75:A:H4'	2.54	0.42
2:A:172:ILE:HA	2:A:571:LEU:HD11	2.02	0.42
3:C:957:ALA:HB1	3:C:961:SER:OG	2.20	0.42
2:A:342:LEU:HD11	2:A:398:VAL:HG21	2.00	0.42
3:C:567:ILE:O	3:C:568:SER:CB	2.67	0.42
3:C:866:ILE:HG22	3:C:868:VAL:CG1	2.49	0.42
3:C:191:ILE:HG23	3:C:221:PHE:CE2	2.55	0.42
1:U:82:A:C2'	1:U:83:C:OP1	2.68	0.42
2:A:503:LYS:HA	2:A:506:PHE:CE2	2.54	0.42
3:C:306:PRO:HG2	3:C:349:TRP:CE3	2.55	0.42
3:C:911:SER:O	3:C:912:ALA:C	2.58	0.42
3:C:962:LEU:HD11	3:C:966:PHE:CZ	2.54	0.42
1:U:111:C:N3	2:A:716:ARG:NH1	2.67	0.42
2:A:173:LEU:HA	2:A:715:LEU:HD13	2.01	0.42
3:C:472:VAL:HB	3:C:575:ALA:HB3	2.02	0.42
3:C:617:LYS:CB	3:C:666:ILE:HD11	2.50	0.42
1:U:42:A:C6	1:U:43:G:C5	3.07	0.42
1:U:68:A:O2'	1:U:69:G:H8	2.02	0.42
2:A:284:ARG:N	2:A:285:PRO:HA	2.34	0.42
2:A:631:LEU:HD23	2:A:656:ILE:HG23	2.00	0.42
1:U:79:C:N4	1:U:114:G:C6	2.88	0.42
3:C:379:ILE:N	3:C:380:PRO:HD2	2.34	0.41
3:C:629:TYR:CE2	3:C:655:LEU:HA	2.55	0.41
3:C:888:ILE:HG23	3:C:902:VAL:HG23	2.01	0.41
1:U:43:G:C2'	1:U:44:A:H5'	2.49	0.41
1:U:79:C:C4	1:U:114:G:N1	2.88	0.41
3:C:142:LEU:HD21	3:C:189:LEU:HD22	2.02	0.41
3:C:472:VAL:N	3:C:575:ALA:O	2.54	0.41
3:C:774:LEU:HD13	3:C:803:VAL:CG2	2.47	0.41
1:U:25:G:H4'	1:U:26:A:C5'	2.51	0.41
2:A:346:ILE:O	2:A:347:PRO:C	2.58	0.41
3:C:869:HIS:HB2	3:C:872:LEU:HD12	2.03	0.41
2:A:305:LEU:N	2:A:306:PRO:CD	2.84	0.41
2:A:719:ILE:N	2:A:720:PRO:HD3	2.36	0.41
3:C:500:ARG:HB3	3:C:578:TYR:CZ	2.55	0.41
3:C:129:ILE:N	3:C:129:ILE:HD12	2.35	0.41
1:U:18:A:C2'	1:U:19:A:H5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:74:U:N1	1:U:75:A:H4'	2.36	0.41
3:C:412:ALA:HA	3:C:415:TYR:CE1	2.56	0.41
2:A:708:TRP:NE1	2:A:712:LEU:HD11	2.35	0.41
3:C:195:GLY:O	3:C:478:TYR:OH	2.39	0.41
3:C:780:PRO:HD2	3:C:783:ILE:HG21	2.02	0.41
2:A:641:LEU:HD12	2:A:642:GLY:O	2.21	0.41
1:U:31:G:H2'	1:U:32:G:C8	2.55	0.41
3:C:138:VAL:CG1	3:C:214:ASP:HA	2.50	0.41
2:A:410:ILE:HG23	2:A:412:GLN:HE21	1.85	0.40
3:C:539:VAL:HG13	3:C:564:ILE:HG23	2.02	0.40
1:U:132:A:H2'	1:U:133:C:OP1	2.21	0.40
1:U:16:U:H3'	1:U:17:C:C6	2.56	0.40
1:U:46:C:H4'	3:C:111:LYS:HG2	2.01	0.40
3:C:797:GLN:HA	3:C:800:TYR:CD2	2.55	0.40
3:C:245:VAL:HG21	3:C:295:ILE:HG13	2.03	0.40
3:C:774:LEU:HD11	3:C:813:ILE:C	2.41	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	
2	A	587/735 (80%)	511 (87%)	67 (11%)	9 (2%)	13	59
3	C	847/1008 (84%)	730 (86%)	93 (11%)	24 (3%)	6	47
5	b	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
6	e	71/94 (76%)	66 (93%)	5 (7%)	0	100	100
7	f	70/86 (81%)	62 (89%)	6 (9%)	2 (3%)	6	46
8	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
10	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	15	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
12	j	92/110 (84%)	86 (94%)	6 (6%)	0	100	100
All	All	1966/2553 (77%)	1734 (88%)	196 (10%)	36 (2%)	15	56

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	247	PRO
2	A	615	LEU
3	C	269	LYS
3	C	356	LYS
3	C	367	VAL
3	C	369	LYS
3	C	371	PRO
3	C	432	GLN
3	C	568	SER
3	C	912	ALA
3	C	935	LYS
2	A	404	ASN
2	A	644	VAL
3	C	428	ILE
3	C	446	PHE
3	C	535	PRO
3	C	884	ARG
7	f	33	PHE
2	A	286	LEU
2	A	360	GLU
3	C	598	ILE
3	C	767	SER
3	C	886	SER
2	A	262	ASP
2	A	426	PRO
3	C	180	ASN
3	C	309	ASN
3	C	361	THR
3	C	596	ASP
3	C	370	TYR
7	f	15	PRO
10	d	82	PRO
2	A	260	PRO
3	C	458	ILE

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Mol	Chain	Res	Type
3	C	464	PRO
3	C	951	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 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	
2	A	482/677 (71%)	460 (95%)	22 (5%)	33	73
3	C	673/910 (74%)	618 (92%)	55 (8%)	14	53
5	b	70/176 (40%)	70 (100%)	0	100	100
6	e	65/83 (78%)	60 (92%)	5 (8%)	16	56
7	f	63/77 (82%)	62 (98%)	1 (2%)	70	90
8	g	58/66 (88%)	56 (97%)	2 (3%)	44	79
10	d	69/89 (78%)	67 (97%)	2 (3%)	50	81
11	h	77/129 (60%)	71 (92%)	6 (8%)	16	56
12	j	79/103 (77%)	74 (94%)	5 (6%)	22	64
All	All	1636/2310 (71%)	1538 (94%)	98 (6%)	28	66

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	162	LEU
2	A	175	LEU
2	A	193	TYR
2	A	228	LYS
2	A	254	HIS
2	A	284	ARG
2	A	287	GLU
2	A	340	LYS
2	A	364	TYR
2	A	374	ILE
2	A	402	TRP
2	A	409	CYS

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Mol	Chain	Res	Type
2	A	461	LEU
2	A	468	LEU
2	A	551	LEU
2	A	571	LEU
2	A	578	MET
2	A	615	LEU
2	A	617	ASN
2	A	655	TYR
2	A	705	GLN
2	A	716	ARG
3	C	111	LYS
3	C	112	ASN
3	C	113	ILE
3	C	160	ARG
3	C	173	LYS
3	C	176	ARG
3	C	179	ASP
3	C	183	GLN
3	C	207	SER
3	C	211	ASN
3	C	219	VAL
3	C	255	GLN
3	C	260	ASN
3	C	327	PHE
3	C	342	ASP
3	C	347	ARG
3	C	359	PHE
3	C	361	THR
3	C	400	LEU
3	C	406	VAL
3	C	421	LEU
3	C	431	GLN
3	C	468	LEU
3	C	469	TRP
3	C	475	THR
3	C	476	VAL
3	C	478	TYR
3	C	534	THR
3	C	537	CYS
3	C	576	THR
3	C	577	LEU
3	C	590	LYS

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Mol	Chain	Res	Type
3	C	658	ASP
3	C	659	LEU
3	C	674	LEU
3	C	678	SER
3	C	707	SER
3	C	723	LEU
3	C	760	LEU
3	C	762	SER
3	C	770	ASN
3	C	772	ASN
3	C	784	SER
3	C	791	TYR
3	C	851	LEU
3	C	861	ILE
3	C	869	HIS
3	C	883	ARG
3	C	902	VAL
3	C	922	THR
3	C	928	CYS
3	C	933	TRP
3	C	961	SER
3	C	971	ARG
3	C	988	THR
6	e	16	CYS
6	e	18	PHE
6	e	25	THR
6	e	79	LYS
6	e	81	LEU
7	f	79	LEU
8	g	18	ASN
8	g	41	ASP
10	d	10	LEU
10	d	76	ASP
11	h	20	LYS
11	h	26	TRP
11	h	30	GLN
11	h	77	ASP
11	h	99	ASP
11	h	104	ASP
12	j	24	PHE
12	j	49	ARG
12	j	77	THR

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Mol	Chain	Res	Type
12	j	99	ASP
12	j	100	SER

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

Mol	Chain	Res	Type
2	A	146	HIS
2	A	194	HIS
2	A	310	ASN
2	A	326	ASN
2	A	344	ASN
2	A	392	ASN
2	A	404	ASN
2	A	412	GLN
2	A	558	GLN
2	A	559	GLN
2	A	576	HIS
2	A	617	ASN
2	A	658	ASN
3	C	112	ASN
3	C	260	ASN
3	C	289	ASN
3	C	418	GLN
3	C	423	HIS
3	C	431	GLN
3	C	776	ASN
6	e	34	GLN
7	f	77	ASN
8	g	66	ASN
11	h	30	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	139/178 (78%)	81 (58%)	23 (16%)
4	W	24/31 (77%)	11 (45%)	4 (16%)
All	All	163/209 (77%)	92 (56%)	27 (16%)

All (92) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	5	A
1	U	7	C
1	U	8	U
1	U	9	U
1	U	10	U
1	U	12	C
1	U	13	A
1	U	14	G
1	U	15	A
1	U	16	U
1	U	17	C
1	U	18	A
1	U	19	A
1	U	22	G
1	U	23	C
1	U	25	G
1	U	26	A
1	U	27	G
1	U	28	G
1	U	32	G
1	U	34	C
1	U	35	A
1	U	38	A
1	U	39	U
1	U	40	C
1	U	41	A
1	U	43	G
1	U	44	A
1	U	45	A
1	U	46	C
1	U	51	G
1	U	52	G
1	U	53	C
1	U	65	U
1	U	66	A
1	U	68	A
1	U	69	G
1	U	70	A
1	U	71	A
1	U	72	C
1	U	74	U
1	U	75	A
1	U	76	U

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Mol	Chain	Res	Type
1	U	77	A
1	U	78	A
1	U	79	C
1	U	80	G
1	U	81	A
1	U	82	A
1	U	83	C
1	U	84	A
1	U	94	C
1	U	95	C
1	U	96	U
1	U	97	U
1	U	101	C
1	U	103	A
1	U	105	A
1	U	112	C
1	U	115	G
1	U	119	U
1	U	120	G
1	U	121	U
1	U	122	C
1	U	123	U
1	U	125	C
1	U	127	U
1	U	128	A
1	U	129	G
1	U	130	A
1	U	133	C
1	U	134	A
1	U	135	G
1	U	136	G
1	U	139	A
1	U	141	G
1	U	167	A
1	U	170	U
1	U	171	U
1	U	172	U
1	U	173	U
4	W	2	U
4	W	7	G
4	W	8	A
4	W	17	U

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Mol	Chain	Res	Type
4	W	25	C
4	W	26	A
4	W	27	U
4	W	28	U
4	W	29	U
4	W	30	G
4	W	31	G

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	U	6	G
1	U	7	C
1	U	21	G
1	U	25	G
1	U	26	A
1	U	27	G
1	U	33	U
1	U	38	A
1	U	40	C
1	U	51	G
1	U	62	G
1	U	68	A
1	U	78	A
1	U	82	A
1	U	83	C
1	U	95	C
1	U	114	G
1	U	127	U
1	U	128	A
1	U	129	G
1	U	132	A
1	U	133	C
1	U	172	U
4	W	16	C
4	W	25	C
4	W	26	A
4	W	27	U

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	GTP	C	1101	-	26,34,34	0.99	2 (7%)	29,54,54	1.79	7 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GTP	C	1101	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	1101	GTP	C5-C4	2.70	1.46	1.40
13	C	1101	GTP	C6-C5	2.93	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	1101	GTP	N3-C2-N1	-3.85	122.31	127.56
13	C	1101	GTP	C5-C6-N1	-3.36	119.14	123.52
13	C	1101	GTP	C6-C5-C4	-3.18	117.22	120.86
13	C	1101	GTP	C1'-N9-C4	-2.42	124.11	126.81
13	C	1101	GTP	O3G-PG-O2G	2.23	115.63	107.44
13	C	1101	GTP	O4'-C1'-N9	2.67	113.16	108.11
13	C	1101	GTP	C6-N1-C2	4.79	121.49	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	1101	GTP	1	0

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.