



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:16 PM BST

PDB ID : 5AN9
EMDB ID: : EMD-3145
Title : Mechanism of eIF6 release from the nascent 60S ribosomal subunit
Authors : Weis, F.; Giudice, E.; Churcher, M.; Jin, L.; Hilcenko, C.; Wong, C.C.;
Traynor, D.; Kay, R.R.; Warren, A.J.
Deposited on : 2015-09-06
Resolution : 3.30 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 : 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

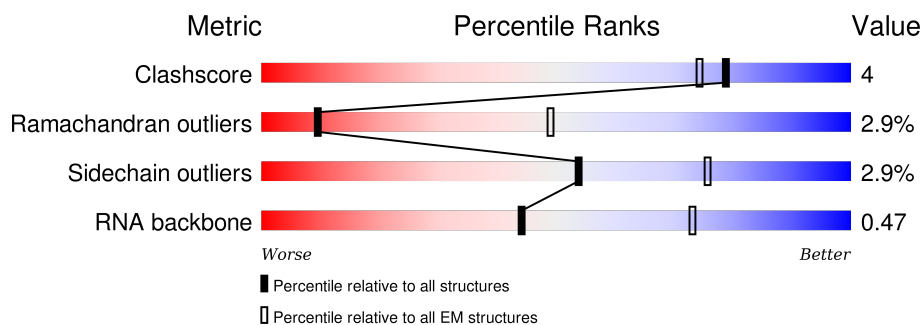
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	A	398	82% 15% .
2	B	188	88% 12%
3	C	205	97% .
4	D	166	96% . .
5	E	136	85% 15% .
6	F	217	86% 13%
7	G	69	91% 9%
8	H	52	83% 13% . .

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Mol	Chain	Length	Quality of chain
9	I	224	<div><div></div><div>92%</div><div>7%</div></div>
10	J	250	<div><div></div><div>96%</div><div></div></div>
11	N	3741	<div><div></div><div>21%</div><div>9%</div><div></div><div>69%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 39693 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 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	398	Total	C	N	O	S	0	0
			3176	2018	599	547	12		

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	188	Total	C	N	O	S	0	0
			1491	944	264	277	6		

- Molecule 3 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	205	Total	C	N	O	S	0	0
			1571	998	271	294	8		

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	166	Total	C	N	O	S	0	0
			1245	790	220	228	7		

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	136	Total	C	N	O	S	0	0
			1017	640	188	181	8		

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	217	Total	C	N	O	S	0	0
			1721	1079	332	297	13		

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	69	Total	C	N	O	S	0	0
			586	378	105	99	4		

- Molecule 8 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	52	Total	C	N	O	S	0	0
			427	269	88	64	6		

- Molecule 9 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	224	Total	C	N	O	S	0	0
			1686	1048	290	338	10		

- Molecule 10 is a protein called RIBOSOME MATURATION PROTEIN SBDS.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	250	Total	C	N	O	S	0	0
			2015	1272	352	380	11		

- Molecule 11 is a RNA chain called 26S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	1162	Total	C	N	O	P	0	0
			24758	11082	4431	8087	1158		

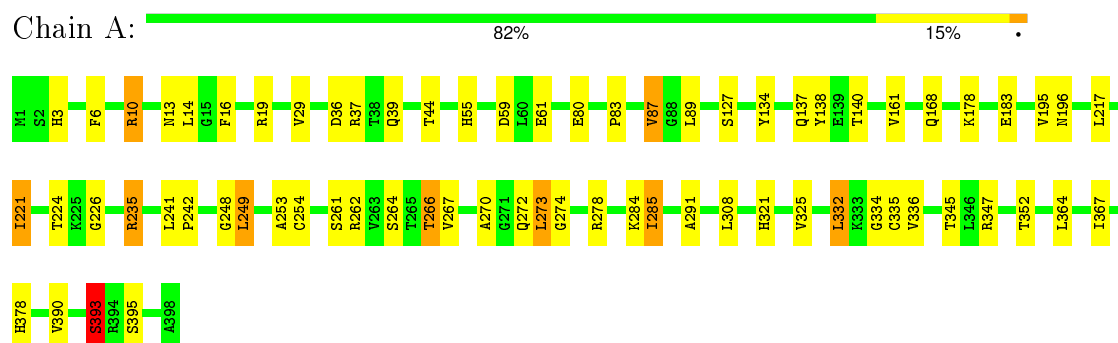
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	3119	C	G	CONFLICT	GB FR733594.

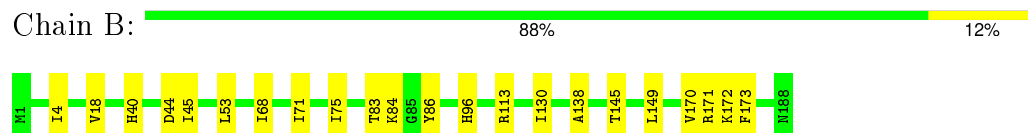
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

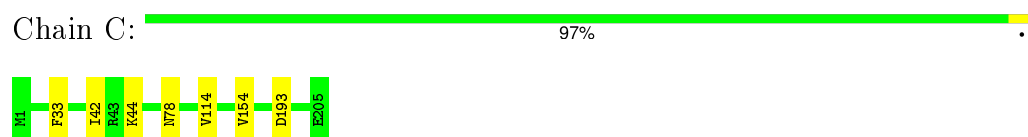
• Molecule 1: 60S RIBOSOMAL PROTEIN L3



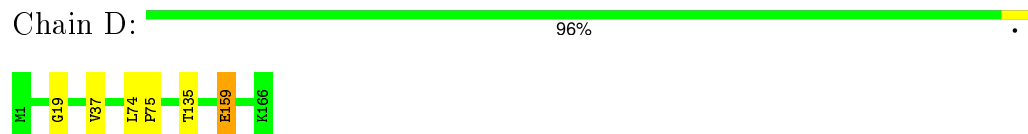
• Molecule 2: 60S RIBOSOMAL PROTEIN L9



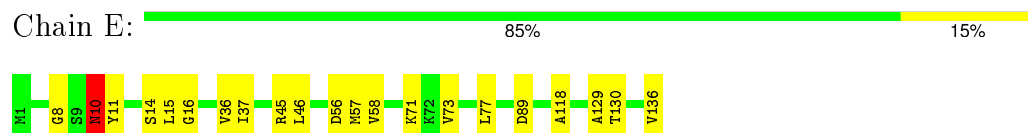
• Molecule 3: 60S ACIDIC RIBOSOMAL PROTEIN P0



• Molecule 4: 60S RIBOSOMAL PROTEIN L12



• Molecule 5: 60S RIBOSOMAL PROTEIN L23









C3165	C3275	C3422	C	C	U
A3166	G3278	U3425	A	U	C
G3167	A3279	U3426	G	C	C
C3168	G3280	A3427	G	G	G
C3169	C3281	C3428	U	A	A
	U3282	C3429	A	U	G
G3172	G3283	A3430	C	C	U
C3173	G3284		A	C	C
	G3285	A3442	C	C	A
U3176	U3286	U3443	G	U	G
C3177	U3287	G3444	U	C	C
A3178	U3288	G3445	A	C	U
		C3446	A	A	U
G3181			G	G	C
C3182	A3304		U	C	A
	G3305	C3453	U	U	A
			U	U	G
G3186	C3316	C3456	U	C	U
C3187	C3317	U3457	U	C	U
U3188	C3318	A3458	U	C	A
G3189	U3319		G	D	C
C3190		C3462	U	U	C
	G3323		C	C	A
U3193		A3466	G	C	U
	C3328	U3467	U	G	U
G3204	A3329		G	U	G
A3205	A3330	A3477	G	U	U
	U3331		A	A	U
U3208	U3332	C3480	C	C	G
C3209		G	U	U	A
G3210	G3339	C	C	U	C
C3211		A	A	A	C
U3213	A3347	A	C	U	U
C3214	G3348	A	U	G	G
U3215	C3349	C	U	U	G
U3216		C	C	U	U
	G3364	A	C	G	C
U3219		A	A	G	G
A3220	C3378	A	A	U	U
	C3379	U	C	G	U
G3228		G	U	U	U
A3229	C3384	C	U	C	U
A3230		U	A	U	A
G3231	C3391	U	A	A	A
C3232	U3392	U	A	A	C
		A	A	A	U
G3245	A3395	G	C	C	C
U3246	G3396	A	A	U	U
	G3397	A	U	C	G
		U	A	U	U
G3251		G	A	A	U
	A3401	U	U	U	G
C3261	U3402	U	G	A	C
C3262		G	A	U	A
	G3414	A	U	U	U
C3268	U3415	A	U	U	U
A3269	G3416	U	A	A	A
A3270	A3417	G	A	U	A
G3271	C3418	U	A	U	C
C3272	C3419	U	C	U	C
		G	G	U	C

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4K X 4K)	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	A	0.45	0/3241	0.78	1/4339 (0.0%)
10	J	0.38	0/2038	0.64	0/2727
11	N	0.35	0/27702	0.74	7/43160 (0.0%)
2	B	0.37	0/1510	0.68	0/2030
3	C	0.38	0/1592	0.57	0/2142
4	D	0.37	0/1265	0.58	0/1702
5	E	0.36	0/1032	0.69	0/1386
6	F	0.38	0/1752	0.70	0/2345
7	G	0.44	0/600	0.67	0/801
8	H	0.39	0/433	0.77	0/571
9	I	0.37	0/1706	0.62	0/2325
All	All	0.36	0/42871	0.72	8/63528 (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	A	0	2
5	E	0	1
9	I	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	2995	G	C2'-C3'-O3'	8.84	128.96	109.50
11	N	1582	A	C2'-C3'-O3'	7.68	126.41	109.50
11	N	1565	G	C4'-C3'-O3'	6.44	125.88	113.00
11	N	1519	C	C2'-C3'-O3'	6.32	123.81	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	2515	G	C2'-C3'-O3'	6.02	123.33	113.70
11	N	1542	G	C2'-C3'-O3'	5.82	123.01	113.70
11	N	1525	G	C2'-C3'-O3'	5.72	122.86	113.70
1	A	235	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	PHE	Peptide
1	A	393	SER	Peptide
5	E	10	ASN	Peptide
9	I	118	HIS	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	3176	0	3319	26	0
2	B	1491	0	1555	8	0
3	C	1571	0	1657	1	0
4	D	1245	0	1338	1	0
5	E	1017	0	1076	11	0
6	F	1721	0	1778	14	0
7	G	586	0	601	2	0
8	H	427	0	483	5	0
9	I	1686	0	1685	7	0
10	J	2015	0	2112	2	0
11	N	24758	0	12487	174	0
All	All	39693	0	28091	238	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 4.

All (238) 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:285:ILE:CD1	1:A:332:LEU:HD23	2.24	0.68
11:N:1415:A:N3	11:N:1564:C:O2'	2.26	0.67
6:F:96:VAL:HG12	6:F:125:THR:HG22	1.78	0.64
6:F:14:ASN:ND2	11:N:1363:G:OP2	2.29	0.64
5:E:36:VAL:HG13	5:E:58:VAL:HG13	1.79	0.63
6:F:190:LEU:HD11	6:F:197:VAL:HG11	1.81	0.63
1:A:221:ILE:HG23	1:A:345:THR:HG23	1.81	0.62
11:N:1385:G:N2	11:N:1393:C:C2	2.67	0.62
11:N:2425:A:H61	11:N:2442:U:H3	1.48	0.61
11:N:2437:G:N2	11:N:2438:C:C2	2.68	0.61
1:A:134:TYR:O	1:A:138:TYR:OH	2.18	0.61
5:E:129:ALA:HB1	9:I:58:ILE:HD12	1.82	0.61
2:B:83:THR:HG23	2:B:84:LYS:HG2	1.82	0.61
5:E:130:THR:HG21	9:I:195:ALA:HB2	1.83	0.59
11:N:2676:U:H3	11:N:3134:A:H61	1.49	0.59
11:N:2411:A:H1'	11:N:2547:A:N6	2.18	0.59
11:N:1568:G:N2	11:N:1569:C:C2	2.71	0.58
11:N:1600:A:H2'	11:N:1601:A:C8	2.38	0.58
11:N:1378:C:O2'	11:N:1390:A:N3	2.33	0.58
11:N:3024:A:H2'	11:N:3025:G:O4'	2.03	0.58
11:N:3445:G:C2	11:N:3462:C:C2	2.93	0.57
9:I:199:VAL:HG11	9:I:222:PHE:CE2	2.39	0.56
1:A:285:ILE:HD11	1:A:332:LEU:HD23	1.88	0.56
8:H:23:TYR:O	11:N:3228:G:O2'	2.23	0.55
11:N:2419:A:HO2'	11:N:2509:A:HO2'	1.54	0.55
11:N:1385:G:C2	11:N:1393:C:C2	2.94	0.55
1:A:29:VAL:HG22	1:A:347:ARG:NH1	2.21	0.55
1:A:87:VAL:HG22	1:A:87:VAL:O	2.06	0.55
1:A:226:GLY:HA2	1:A:274:GLY:O	2.07	0.54
11:N:2616:A:C5	11:N:2617:C:C5	2.96	0.54
5:E:130:THR:HG22	9:I:150:THR:HG23	1.90	0.53
11:N:3167:G:N2	11:N:3168:C:C2	2.77	0.53
5:E:36:VAL:HG22	5:E:58:VAL:HG11	1.90	0.53
11:N:2437:G:N1	11:N:2438:C:C4	2.77	0.53
1:A:248:GLY:O	1:A:249:LEU:HB2	2.08	0.53
11:N:3378:C:OP2	11:N:3428:C:N4	2.41	0.52
11:N:1461:G:C6	11:N:1462:C:C4	2.97	0.52
11:N:3251:G:C2	11:N:3262:C:C2	2.97	0.52
11:N:1442:G:C2	11:N:1533:C:C2	2.98	0.52
11:N:1461:G:C2	11:N:1462:C:C2	2.98	0.52
11:N:3172:G:N2	11:N:3173:C:C2	2.78	0.52
11:N:3106:G:N2	11:N:3107:C:C2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:3251:G:N2	11:N:3262:C:C2	2.78	0.52
11:N:2404:U:C6	11:N:2408:U:C5	2.98	0.52
11:N:2602:U:O4'	11:N:2602:U:O2	2.27	0.52
11:N:2429:G:N1	11:N:2430:C:C2	2.79	0.52
8:H:18:ILE:HD12	8:H:25:ARG:HA	1.92	0.51
11:N:1258:C:H2'	11:N:1259:U:O4'	2.10	0.51
11:N:3176:U:O2	11:N:3176:U:O4'	2.27	0.51
1:A:80:GLU:HG3	1:A:325:VAL:HG12	1.92	0.50
9:I:53:ILE:HD12	9:I:59:VAL:HG13	1.93	0.50
11:N:3378:C:OP2	11:N:3428:C:C4	2.63	0.50
5:E:10:ASN:HA	5:E:11:TYR:HB2	1.93	0.50
11:N:3022:A:N3	11:N:3022:A:H2'	2.27	0.50
1:A:241:LEU:HB3	1:A:242:PRO:HD2	1.94	0.50
5:E:36:VAL:HG13	5:E:58:VAL:CG1	2.42	0.50
11:N:2999:C:H2'	11:N:2999:C:O2	2.11	0.49
8:H:25:ARG:HD3	11:N:3229:A:OP1	2.12	0.49
8:H:19:CYS:SG	8:H:20:ARG:N	2.84	0.49
6:F:31:ILE:HD13	6:F:65:ILE:HG21	1.93	0.49
11:N:1386:G:N2	11:N:1392:C:C2	2.81	0.49
11:N:2477:U:O4'	11:N:2477:U:O2	2.30	0.49
1:A:89:LEU:HD21	1:A:195:VAL:HG13	1.93	0.49
11:N:2642:G:H2'	11:N:2643:G:C8	2.48	0.49
11:N:3127:G:H1'	11:N:3128:U:C6	2.48	0.49
11:N:3032:G:C2	11:N:3089:C:C2	3.01	0.49
11:N:1541:G:O6	11:N:2632:A:O2'	2.14	0.49
2:B:40:HIS:CE1	2:B:71:ILE:HD11	2.49	0.48
2:B:86:TYR:CE2	2:B:149:LEU:HB2	2.48	0.48
11:N:2536:A:H2'	11:N:2537:A:C8	2.48	0.48
11:N:1568:G:C6	11:N:1569:C:C4	3.00	0.48
11:N:3445:G:C6	11:N:3446:C:C4	3.02	0.48
11:N:2996:G:C2	11:N:2997:C:C2	3.02	0.48
11:N:2404:U:OP2	11:N:2409:A:N6	2.46	0.48
11:N:1530:G:C6	11:N:1531:C:C4	3.01	0.48
11:N:2992:G:H4'	11:N:3084:A:O2'	2.13	0.48
6:F:10:ARG:HG2	6:F:11:TYR:CE2	2.49	0.48
11:N:1438:A:N3	11:N:3188:U:O2'	2.41	0.48
11:N:2939:G:H2'	11:N:2939:G:N3	2.29	0.48
2:B:68:ILE:HA	2:B:71:ILE:HD12	1.96	0.47
11:N:2996:G:C6	11:N:2997:C:C4	3.01	0.47
11:N:2978:G:C6	11:N:2979:C:C4	3.02	0.47
11:N:3422:C:O2	11:N:3422:C:H2'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:3318:C:H2'	11:N:3319:U:O4'	2.15	0.47
11:N:2419:A:O4'	11:N:2509:A:C2	2.67	0.47
11:N:1366:A:H2'	11:N:1367:A:C8	2.49	0.47
10:J:134:GLU:O	10:J:137:MET:HG3	2.13	0.47
6:F:26:VAL:HG12	6:F:122:PRO:HB2	1.96	0.47
1:A:183:GLU:OE1	11:N:3339:G:H4'	2.15	0.47
6:F:31:ILE:HD13	6:F:65:ILE:CG2	2.45	0.47
11:N:3204:G:H5''	11:N:3205:A:H5'	1.97	0.47
11:N:3039:G:N2	11:N:3040:C:C2	2.83	0.47
11:N:3456:C:H2'	11:N:3456:C:O2	2.14	0.47
11:N:2506:G:H2'	11:N:2507:U:O4'	2.15	0.47
11:N:3104:G:C4	11:N:3106:G:C8	3.02	0.47
11:N:3209:C:C2	11:N:3285:G:C2	3.03	0.46
11:N:3215:U:H2'	11:N:3216:U:C6	2.50	0.46
11:N:2992:G:C6	11:N:2993:C:C4	3.04	0.46
11:N:1240:U:O4'	11:N:1240:U:O2	2.33	0.46
11:N:2978:G:C2	11:N:2979:C:C2	3.04	0.46
11:N:3045:U:H2'	11:N:3046:U:C6	2.50	0.46
11:N:3169:C:O4'	11:N:3169:C:O2	2.33	0.46
11:N:2989:A:C8	11:N:2991:G:C8	3.04	0.46
11:N:2467:G:C6	11:N:2468:C:C4	3.03	0.46
11:N:1385:G:C2	11:N:1393:C:N3	2.83	0.46
11:N:2933:C:C2	11:N:2934:A:C8	3.03	0.46
11:N:3445:G:C2	11:N:3446:C:C2	3.04	0.46
11:N:2442:U:O2	11:N:2442:U:H2'	2.15	0.45
11:N:2945:U:H2'	11:N:2946:U:O4'	2.16	0.45
11:N:3415:U:O4'	11:N:3415:U:O2	2.31	0.45
1:A:80:GLU:CG	1:A:325:VAL:HG12	2.47	0.45
11:N:1548:G:C2	11:N:1549:C:C2	3.04	0.45
11:N:3186:G:C6	11:N:3187:C:C4	3.04	0.45
11:N:2619:G:C6	11:N:2620:C:C4	3.05	0.45
4:D:135:THR:HG21	11:N:1489:C:O2'	2.16	0.45
11:N:2992:G:H2'	11:N:2993:C:O4'	2.17	0.45
11:N:1548:G:C6	11:N:1549:C:C4	3.03	0.45
11:N:3043:G:C2	11:N:3044:C:C2	3.04	0.45
11:N:2948:G:C6	11:N:2949:C:C4	3.05	0.45
11:N:2470:C:H4'	11:N:2471:U:OP1	2.17	0.45
11:N:3039:G:C6	11:N:3040:C:C4	3.05	0.45
11:N:2948:G:C2	11:N:2949:C:C2	3.05	0.45
7:G:31:PHE:CD2	7:G:37:GLU:HG2	2.52	0.45
11:N:1568:G:N1	11:N:1569:C:C4	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:3043:G:C6	11:N:3044:C:C4	3.05	0.45
11:N:3271:G:C2	11:N:3272:G:C8	3.05	0.45
6:F:43:THR:HG21	6:F:197:VAL:HG13	1.98	0.44
2:B:18:VAL:HG11	2:B:53:LEU:HD12	1.99	0.44
11:N:1564:C:H2'	11:N:1565:G:C8	2.52	0.44
11:N:2429:G:C6	11:N:2430:C:C4	3.05	0.44
11:N:1530:G:C2	11:N:1531:C:C2	3.05	0.44
11:N:1404:A:C2	11:N:1405:U:C6	3.06	0.44
11:N:2544:C:C2	11:N:2573:G:C2	3.05	0.44
11:N:2544:C:C2	11:N:2573:G:N2	2.85	0.44
6:F:61:SER:HA	6:F:126:VAL:HG23	1.99	0.44
11:N:2578:A:O2'	11:N:2581:G:N3	2.48	0.44
11:N:3047:G:N3	11:N:3047:G:H5''	2.33	0.44
11:N:3189:G:C2	11:N:3190:C:C2	3.05	0.44
11:N:2602:U:H2'	11:N:2603:C:O4'	2.18	0.44
11:N:1426:A:C8	11:N:1428:A:H1'	2.53	0.44
11:N:1427:U:O2	11:N:1428:A:C8	2.70	0.44
11:N:3211:G:C6	11:N:3212:C:C4	3.06	0.44
11:N:2657:G:C6	11:N:2658:C:C4	3.06	0.44
11:N:3039:G:C2	11:N:3040:C:C2	3.06	0.44
11:N:3189:G:C6	11:N:3190:C:C4	3.06	0.44
3:C:114:VAL:HG23	11:N:1464:G:C5'	2.48	0.44
11:N:3155:U:H2'	11:N:3156:G:O4'	2.18	0.44
1:A:253:ALA:HB1	11:N:3280:G:N3	2.32	0.44
11:N:3401:A:H2'	11:N:3402:U:O4'	2.18	0.44
11:N:3397:G:N2	11:N:3419:C:C2	2.86	0.43
11:N:3164:G:C6	11:N:3165:C:C4	3.06	0.43
11:N:3186:G:C2	11:N:3187:C:C2	3.06	0.43
11:N:2657:G:C2	11:N:2658:C:C2	3.06	0.43
11:N:3397:G:C2	11:N:3419:C:C2	3.06	0.43
11:N:1550:U:O2'	11:N:1551:A:OP1	2.24	0.43
11:N:2957:G:C6	11:N:2958:C:C4	3.07	0.43
11:N:1593:U:O2	11:N:1593:U:O4'	2.36	0.43
1:A:83:PRO:O	1:A:168:GLN:HG3	2.19	0.43
11:N:1568:G:C2	11:N:1569:C:C6	3.07	0.43
11:N:2615:U:C4	11:N:2616:A:N7	2.86	0.43
1:A:364:LEU:HD13	1:A:367:ILE:HD11	2.00	0.43
11:N:1568:G:C2	11:N:1569:C:C2	3.07	0.43
11:N:2992:G:C2	11:N:2993:C:C2	3.07	0.43
11:N:3164:G:C2	11:N:3165:C:C2	3.06	0.43
11:N:1265:U:HO2'	11:N:1266:C:H6	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:3425:C:H2'	11:N:3426:U:O4'	2.19	0.43
6:F:91:VAL:O	6:F:91:VAL:HG13	2.18	0.43
6:F:31:ILE:HD11	6:F:93:PRO:HD3	2.01	0.43
1:A:332:LEU:HD13	1:A:336:VAL:HG11	2.01	0.42
11:N:2470:C:C2	11:N:2505:G:C2	3.07	0.42
1:A:217:LEU:HD23	1:A:284:LYS:HA	2.01	0.42
1:A:235:ARG:NE	1:A:272:GLN:O	2.38	0.42
11:N:2599:C:H2'	11:N:2600:U:O4'	2.19	0.42
11:N:3181:G:C6	11:N:3182:C:C4	3.06	0.42
10:J:71:LEU:HD22	10:J:83:ILE:HD13	2.02	0.42
8:H:19:CYS:SG	8:H:22:CYS:HB3	2.59	0.42
2:B:53:LEU:HD22	2:B:75:ILE:CD1	2.50	0.42
11:N:3211:G:C2	11:N:3212:C:C2	3.07	0.42
11:N:3245:G:C6	11:N:3246:U:C4	3.08	0.42
11:N:3167:G:N1	11:N:3168:C:C4	2.88	0.42
6:F:91:VAL:HG22	6:F:127:ALA:HB1	2.00	0.42
9:I:119:PRO:HG2	9:I:141:THR:HG23	2.02	0.42
11:N:2437:G:C6	11:N:2438:C:C4	3.07	0.42
11:N:3445:G:N2	11:N:3446:C:C2	2.88	0.42
11:N:2477:U:H2'	11:N:2478:C:O4'	2.19	0.42
11:N:1525:G:H2'	11:N:1526:A:C8	2.55	0.42
2:B:170:VAL:HA	2:B:173:PHE:CE2	2.54	0.42
11:N:1387:U:OP2	11:N:1431:U:N3	2.51	0.42
2:B:45:ILE:HG23	2:B:45:ILE:O	2.19	0.42
6:F:49:CYS:SG	6:F:51:HIS:CE1	3.12	0.42
11:N:3106:G:C2	11:N:3107:C:C2	3.08	0.41
11:N:2978:G:N2	11:N:2979:C:C2	2.88	0.41
11:N:2467:G:C2	11:N:2468:C:C2	3.07	0.41
11:N:2616:A:C6	11:N:2617:C:C4	3.08	0.41
11:N:3106:G:C6	11:N:3107:C:C4	3.07	0.41
11:N:2993:C:H2'	11:N:2994:A:C8	2.54	0.41
11:N:3280:G:N2	11:N:3281:C:C2	2.89	0.41
11:N:2690:A:H2'	11:N:2691:G:O4'	2.20	0.41
11:N:1417:C:H4'	11:N:1417:C:OP1	2.20	0.41
1:A:253:ALA:HB3	11:N:3213:U:O2	2.20	0.41
11:N:2437:G:C2	11:N:2438:C:C2	3.08	0.41
11:N:3172:G:C2	11:N:3173:C:C2	3.09	0.41
11:N:2631:C:C2	11:N:2632:A:C8	3.08	0.41
11:N:3230:A:C2	11:N:3232:C:H5'	2.56	0.41
6:F:50:VAL:HG21	6:F:148:VAL:HG23	2.02	0.41
1:A:37:ARG:NH1	1:A:352:THR:OG1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:3422:C:C2'	11:N:3422:C:O2	2.68	0.41
11:N:3457:U:H4'	11:N:3458:A:OP1	2.21	0.41
5:E:57:MET:HE3	5:E:77:LEU:HD21	2.02	0.41
7:G:22:VAL:HG22	7:G:28:VAL:HG12	2.02	0.41
11:N:1377:G:C2	11:N:1378:C:C2	3.09	0.41
11:N:3172:G:N1	11:N:3173:C:C4	2.89	0.41
11:N:3348:G:C6	11:N:3349:C:C4	3.09	0.41
11:N:3348:G:C2	11:N:3349:C:C2	3.08	0.41
11:N:1586:G:N3	11:N:1586:G:H2'	2.35	0.41
1:A:10:ARG:NH1	1:A:266:THR:OG1	2.54	0.41
11:N:2957:G:C2	11:N:2958:C:C2	3.09	0.41
11:N:3181:G:N1	11:N:3182:C:C2	2.89	0.41
11:N:1542:G:C4	11:N:1543:A:C2	3.09	0.41
11:N:2943:G:H2'	11:N:2944:U:O4'	2.21	0.41
11:N:1374:C:C4	11:N:1375:U:C4	3.09	0.41
11:N:3158:C:C4	11:N:3159:U:C4	3.09	0.41
11:N:3347:A:N1	11:N:3379:C:O2'	2.43	0.41
11:N:3442:A:H2'	11:N:3443:U:O4'	2.21	0.41
1:A:161:VAL:HG11	1:A:195:VAL:HG22	2.03	0.40
1:A:272:GLN:CG	1:A:273:LEU:N	2.84	0.40
5:E:71:LYS:NZ	11:N:2560:U:OP2	2.54	0.40
11:N:3220:A:N3	11:N:3220:A:H2'	2.36	0.40
5:E:37:ILE:CD1	5:E:73:VAL:HG23	2.51	0.40
11:N:2672:C:H2'	11:N:2673:C:C6	2.56	0.40
5:E:136:VAL:HG13	9:I:75:THR:HG21	2.02	0.40
11:N:1583:G:H5'	11:N:1584:A:OP2	2.22	0.40
11:N:2534:U:H2'	11:N:2535:U:C6	2.56	0.40
11:N:3209:C:H1'	11:N:3285:G:N2	2.36	0.40
11:N:2452:U:H2'	11:N:2453:G:O4'	2.21	0.40
1:A:264:SER:O	1:A:267:VAL:HG12	2.21	0.40
11:N:3417:A:C6	11:N:3418:C:C4	3.08	0.40
1:A:13:ASN:OD1	1:A:14:LEU:N	2.55	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 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	A	396/398 (100%)	328 (83%)	50 (13%)	18 (4%)	3	21
2	B	186/188 (99%)	169 (91%)	14 (8%)	3 (2%)	12	48
3	C	203/205 (99%)	185 (91%)	15 (7%)	3 (2%)	13	49
4	D	164/166 (99%)	142 (87%)	17 (10%)	5 (3%)	5	33
5	E	134/136 (98%)	114 (85%)	13 (10%)	7 (5%)	2	18
6	F	215/217 (99%)	188 (87%)	21 (10%)	6 (3%)	6	34
7	G	67/69 (97%)	62 (92%)	4 (6%)	1 (2%)	13	49
8	H	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	4	24
9	I	222/224 (99%)	199 (90%)	17 (8%)	6 (3%)	6	35
10	J	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	16	54
All	All	1885/1905 (99%)	1659 (88%)	172 (9%)	54 (3%)	9	34

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LEU
2	B	138	ALA
5	E	46	LEU
9	I	119	PRO
1	A	285	ILE
1	A	321	HIS
1	A	334	GLY
1	A	393	SER
5	E	10	ASN
6	F	199	VAL
6	F	211	LYS
8	H	22	CYS
9	I	121	ILE
1	A	39	GLN
1	A	127	SER
1	A	261	SER
1	A	291	ALA
3	C	33	PHE
3	C	78	ASN
5	E	118	ALA

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Mol	Chain	Res	Type
8	H	20	ARG
9	I	45	HIS
9	I	105	GLY
1	A	44	THR
1	A	140	THR
1	A	270	ALA
1	A	378	HIS
4	D	19	GLY
4	D	75	PRO
5	E	8	GLY
5	E	14	SER
5	E	16	GLY
6	F	177	ASN
9	I	120	ASP
10	J	46	ASP
1	A	3	HIS
1	A	87	VAL
1	A	308	LEU
1	A	335	CYS
2	B	4	ILE
2	B	96	HIS
3	C	154	VAL
5	E	89	ASP
6	F	194	GLY
7	G	60	LYS
10	J	141	HIS
1	A	10	ARG
4	D	159	GLU
10	J	123	GLU
6	F	91	VAL
9	I	117	VAL
6	F	33	ILE
4	D	37	VAL
4	D	74	LEU

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	A	337/337 (100%)	317 (94%)	20 (6%)	24	63
2	B	168/168 (100%)	162 (96%)	6 (4%)	42	76
3	C	172/172 (100%)	169 (98%)	3 (2%)	68	86
4	D	139/139 (100%)	138 (99%)	1 (1%)	88	94
5	E	108/108 (100%)	104 (96%)	4 (4%)	41	76
6	F	180/180 (100%)	176 (98%)	4 (2%)	60	84
7	G	65/65 (100%)	64 (98%)	1 (2%)	72	88
8	H	48/48 (100%)	44 (92%)	4 (8%)	14	47
9	I	190/190 (100%)	189 (100%)	1 (0%)	92	95
10	J	228/228 (100%)	224 (98%)	4 (2%)	66	85
All	All	1635/1635 (100%)	1587 (97%)	48 (3%)	54	80

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	19	ARG
1	A	36	ASP
1	A	55	HIS
1	A	59	ASP
1	A	61	GLU
1	A	137	GLN
1	A	178	LYS
1	A	196	ASN
1	A	221	ILE
1	A	224	THR
1	A	254	CYS
1	A	262	ARG
1	A	266	THR
1	A	273	LEU
1	A	278	ARG
1	A	332	LEU
1	A	390	VAL
1	A	393	SER
1	A	395	SER
2	B	44	ASP
2	B	113	ARG
2	B	130	ILE
2	B	145	THR

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Mol	Chain	Res	Type
2	B	171	ARG
2	B	172	LYS
3	C	42	ILE
3	C	44	LYS
3	C	193	ASP
4	D	159	GLU
5	E	10	ASN
5	E	15	LEU
5	E	45	ARG
5	E	56	ASP
6	F	24	ARG
6	F	131	ILE
6	F	145	LEU
6	F	168	SER
7	G	34	THR
8	H	20	ARG
8	H	26	LEU
8	H	34	ARG
8	H	42	ASN
9	I	112	ASP
10	J	119	CYS
10	J	128	TYR
10	J	137	MET
10	J	139	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	166	HIS
1	A	230	ASN
1	A	298	GLN
1	A	353	GLN
2	B	40	HIS
2	B	114	ASN
2	B	135	ASN
2	B	147	ASN
3	C	93	ASN
3	C	164	GLN
4	D	103	ASN
6	F	133	GLN
6	F	177	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	N	1158/3741 (30%)	216 (18%)	36 (3%)

All (216) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	N	1225	G
11	N	1229	U
11	N	1230	U
11	N	1231	U
11	N	1233	G
11	N	1236	G
11	N	1241	A
11	N	1243	U
11	N	1244	G
11	N	1245	C
11	N	1250	A
11	N	1262	A
11	N	1366	A
11	N	1368	G
11	N	1381	U
11	N	1382	G
11	N	1388	U
11	N	1390	A
11	N	1397	U
11	N	1417	C
11	N	1427	U
11	N	1428	A
11	N	1431	U
11	N	1436	C
11	N	1444	G
11	N	1457	G
11	N	1458	A
11	N	1467	C
11	N	1470	U
11	N	1474	C
11	N	1476	U
11	N	1477	G
11	N	1478	G
11	N	1479	A
11	N	1480	A
11	N	1481	G

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Mol	Chain	Res	Type
11	N	1484	G
11	N	1497	G
11	N	1498	A
11	N	1499	G
11	N	1500	U
11	N	1501	G
11	N	1507	C
11	N	1520	A
11	N	1522	A
11	N	1526	A
11	N	1530	G
11	N	1540	U
11	N	1542	G
11	N	1543	A
11	N	1544	U
11	N	1548	G
11	N	1550	U
11	N	1551	A
11	N	1552	G
11	N	1553	C
11	N	1558	G
11	N	1566	A
11	N	1576	G
11	N	1583	G
11	N	1584	A
11	N	1585	A
11	N	1586	G
11	N	1587	U
11	N	1588	G
11	N	1589	A
11	N	1590	U
11	N	1591	A
11	N	1592	A
11	N	1594	A
11	N	1601	A
11	N	1602	C
11	N	2398	A
11	N	2407	U
11	N	2416	A
11	N	2425	A
11	N	2436	A
11	N	2440	U

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Mol	Chain	Res	Type
11	N	2442	U
11	N	2451	G
11	N	2454	A
11	N	2458	C
11	N	2471	U
11	N	2474	A
11	N	2476	G
11	N	2489	G
11	N	2495	A
11	N	2505	G
11	N	2510	A
11	N	2515	G
11	N	2516	G
11	N	2519	G
11	N	2523	C
11	N	2524	U
11	N	2528	A
11	N	2539	G
11	N	2540	U
11	N	2547	A
11	N	2548	U
11	N	2554	G
11	N	2572	C
11	N	2573	G
11	N	2576	U
11	N	2579	A
11	N	2581	G
11	N	2601	G
11	N	2602	U
11	N	2606	U
11	N	2630	G
11	N	2638	A
11	N	2639	A
11	N	2640	C
11	N	2641	G
11	N	2654	A
11	N	2659	G
11	N	2663	A
11	N	2668	A
11	N	2669	G
11	N	2670	A
11	N	2671	C

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Mol	Chain	Res	Type
11	N	2676	U
11	N	2677	U
11	N	2678	G
11	N	2685	A
11	N	2688	C
11	N	2926	A
11	N	2927	C
11	N	2939	G
11	N	2940	G
11	N	2947	G
11	N	2959	A
11	N	2981	A
11	N	2985	U
11	N	2989	A
11	N	2990	A
11	N	2991	G
11	N	2996	G
11	N	3000	A
11	N	3007	A
11	N	3010	G
11	N	3014	U
11	N	3016	U
11	N	3022	A
11	N	3024	A
11	N	3027	A
11	N	3029	A
11	N	3036	A
11	N	3037	A
11	N	3038	A
11	N	3046	U
11	N	3047	G
11	N	3059	C
11	N	3060	A
11	N	3061	G
11	N	3062	U
11	N	3070	G
11	N	3086	G
11	N	3095	A
11	N	3105	U
11	N	3110	A
11	N	3111	A
11	N	3116	U

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Mol	Chain	Res	Type
11	N	3120	C
11	N	3129	G
11	N	3132	A
11	N	3133	G
11	N	3134	A
11	N	3135	A
11	N	3136	A
11	N	3143	C
11	N	3150	A
11	N	3151	U
11	N	3167	G
11	N	3172	G
11	N	3178	A
11	N	3186	G
11	N	3190	C
11	N	3193	U
11	N	3204	G
11	N	3205	A
11	N	3208	U
11	N	3220	A
11	N	3231	G
11	N	3232	C
11	N	3261	C
11	N	3268	C
11	N	3269	A
11	N	3271	G
11	N	3275	C
11	N	3278	G
11	N	3279	A
11	N	3280	G
11	N	3287	U
11	N	3288	U
11	N	3304	A
11	N	3305	G
11	N	3316	C
11	N	3323	G
11	N	3328	C
11	N	3329	A
11	N	3331	U
11	N	3332	U
11	N	3348	G
11	N	3364	G

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Mol	Chain	Res	Type
11	N	3392	U
11	N	3395	A
11	N	3414	G
11	N	3422	C
11	N	3428	C
11	N	3429	C
11	N	3430	A
11	N	3445	G
11	N	3453	C
11	N	3458	A
11	N	3466	A
11	N	3467	U

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	N	1381	U
11	N	1391	A
11	N	1427	U
11	N	1443	U
11	N	1456	A
11	N	1457	G
11	N	1476	U
11	N	1519	C
11	N	1525	G
11	N	1542	G
11	N	1550	U
11	N	1565	G
11	N	1582	A
11	N	1583	G
11	N	2411	A
11	N	2470	C
11	N	2515	G
11	N	2527	G
11	N	2547	A
11	N	2571	G
11	N	2575	A
11	N	2995	G
11	N	3047	G
11	N	3061	G
11	N	3070	G
11	N	3150	A

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Mol	Chain	Res	Type
11	N	3151	U
11	N	3219	U
11	N	3231	G
11	N	3283	G
11	N	3316	C
11	N	3384	C
11	N	3391	C
11	N	3429	C
11	N	3457	U
11	N	3477	A

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](#)

There are no chain breaks in this entry.