Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 08:45 am GMT

PDB ID	:	5ANB
EMDB ID	:	EMD-3146
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	:	4.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

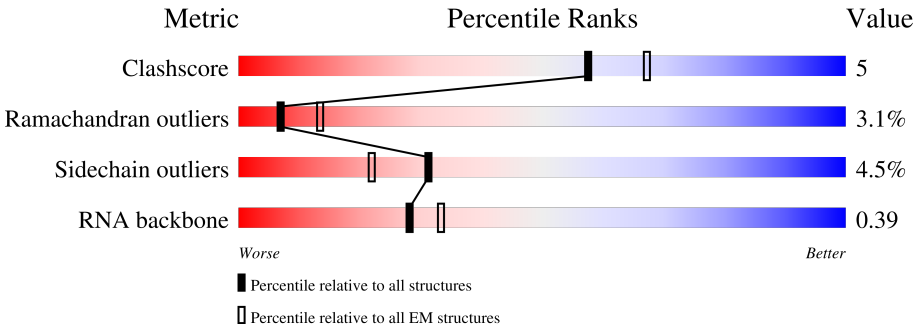
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	75% 20%
2	B	188	84% 16%
3	C	205	54% 95% 5%
4	D	166	45% 92% 7%
5	E	136	85% 13%
6	F	217	78% 20%
7	G	69	83% 17%

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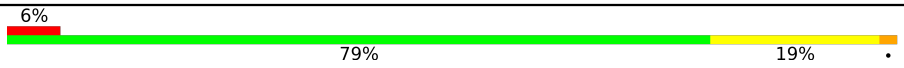
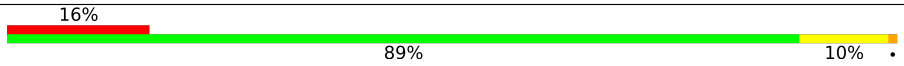
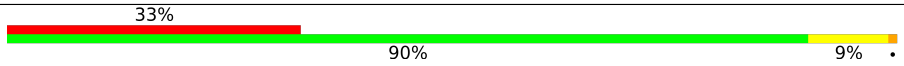
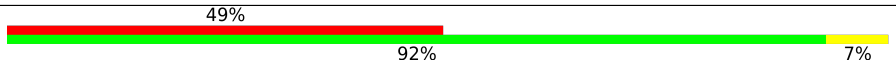
Mol	Chain	Length	Quality of chain
8	H	52	
9	I	224	
10	J	250	
11	K	1120	
12	N	3741	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 48493 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 protein called ELONGATION FACTOR TU GTP-BINDING DOMAIN-CONTAINING PROTEIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	1120	Total	C	N	O	S	0	0
			8800	5547	1518	1682	53		

- Molecule 12 is a RNA chain called 26S RIBOSOMAL RNA.

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

There is a discrepancy between the modelled and reference sequences:

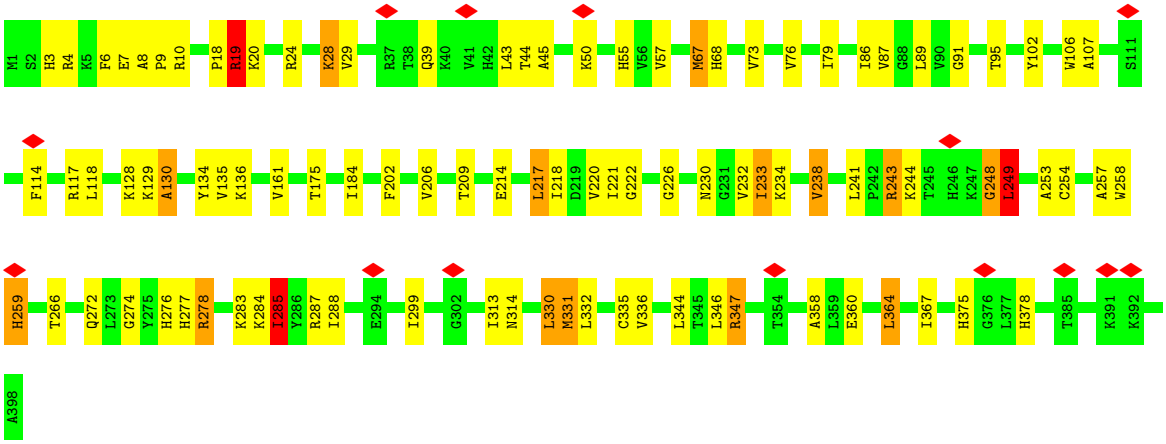
Chain	Residue	Modelled	Actual	Comment	Reference
N	3119	C	G	conflict	GB FR733594.

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

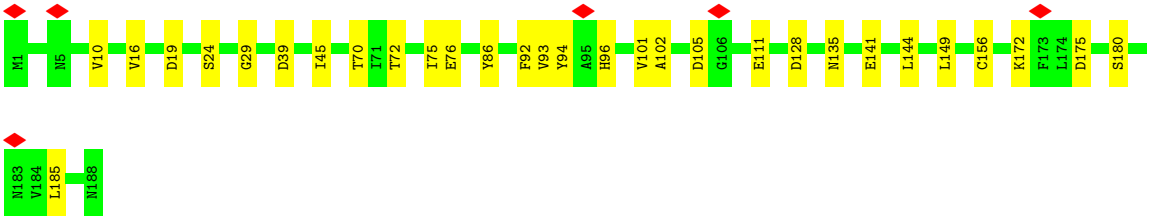
• Molecule 1: 60S RIBOSOMAL PROTEIN L3

Chain A:



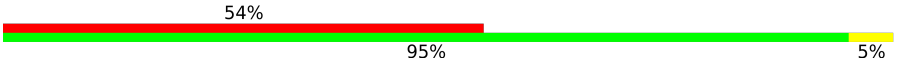
• Molecule 2: 60S RIBOSOMAL PROTEIN L9

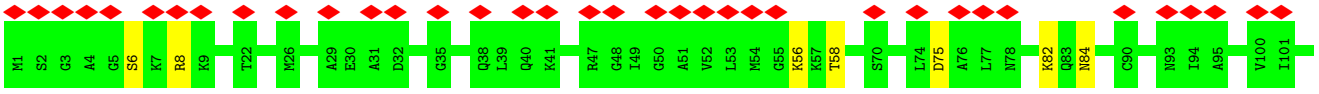
Chain B:

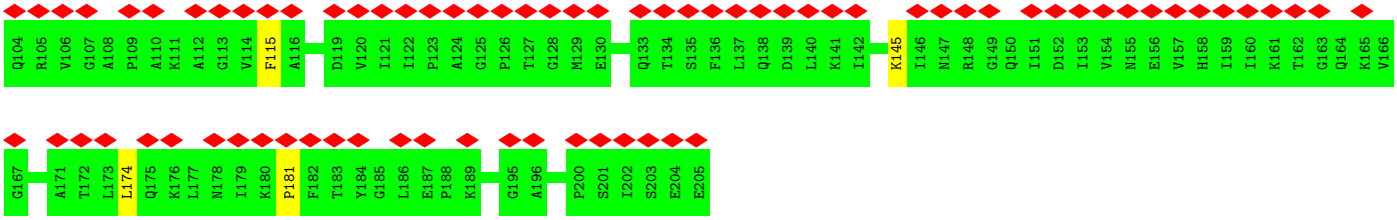


• Molecule 3: 60S ACIDIC RIBOSOMAL PROTEIN P0

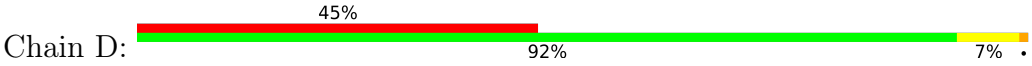
Chain C:

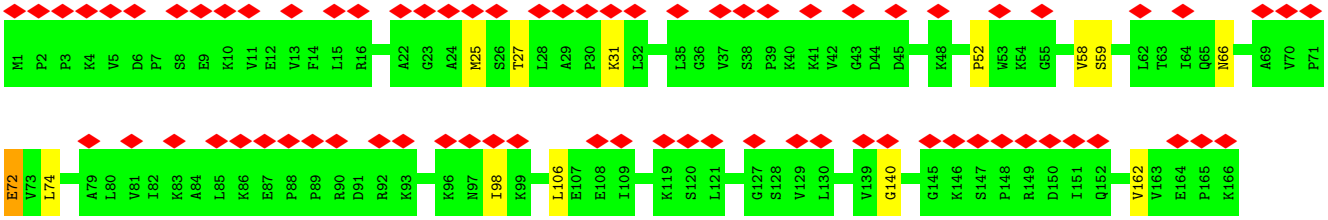




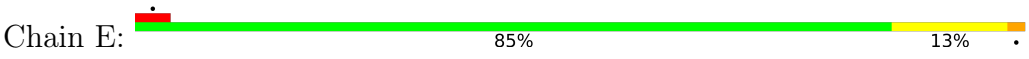


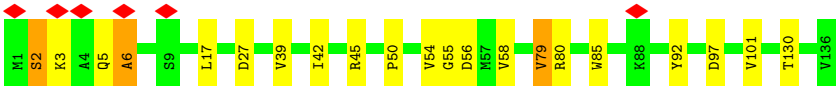
• Molecule 4: 60S RIBOSOMAL PROTEIN L12



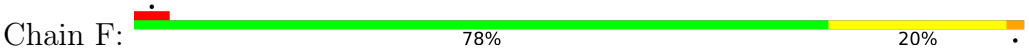


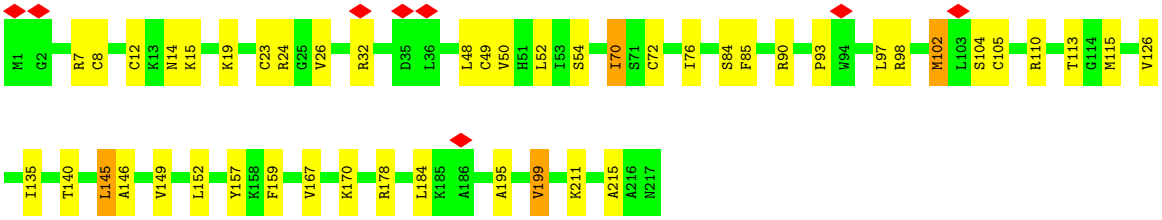
• Molecule 5: 60S RIBOSOMAL PROTEIN L23



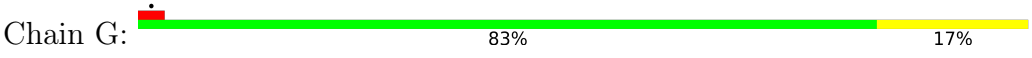


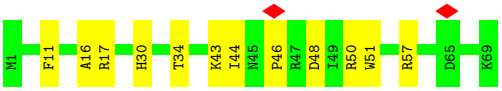
• Molecule 6: 60S RIBOSOMAL PROTEIN L10



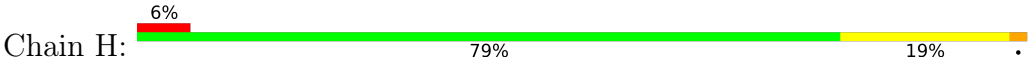


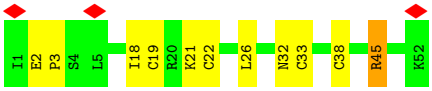
• Molecule 7: 60S RIBOSOMAL PROTEIN L24





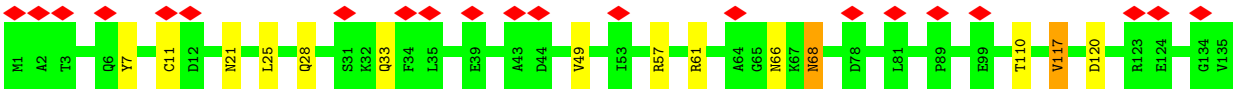
• Molecule 8: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

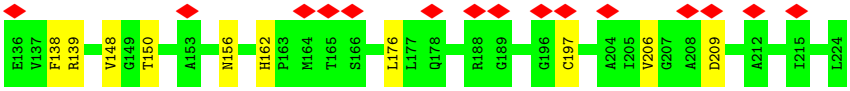




• Molecule 9: EUKARYOTIC TRANSLATION INITIATION FACTOR 6

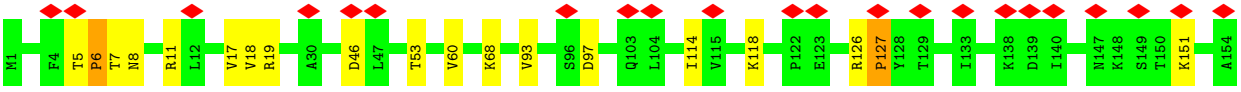
Chain I:

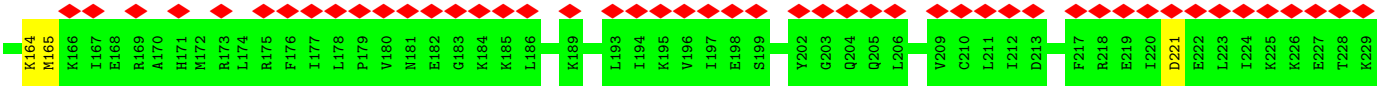


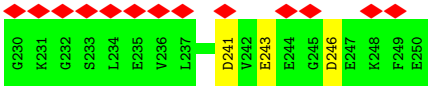


• Molecule 10: RIBOSOME MATURATION PROTEIN SBDS

Chain J:

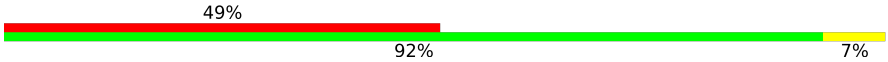


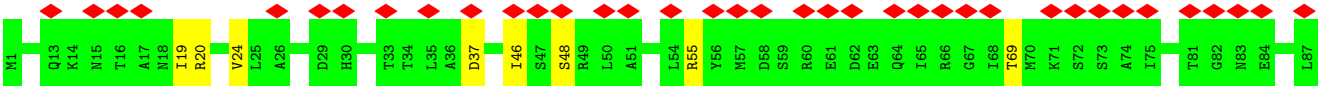


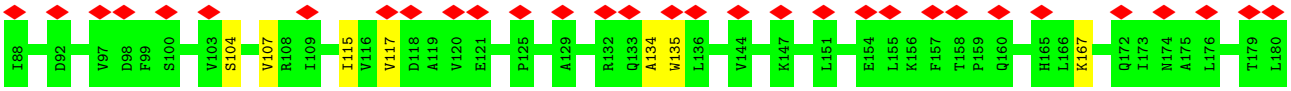


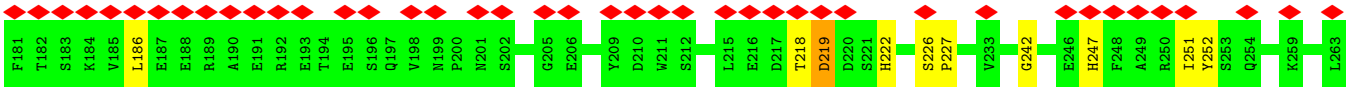
• Molecule 11: ELONGATION FACTOR TU GTP-BINDING DOMAIN-CONTAINING PROTEIN 1

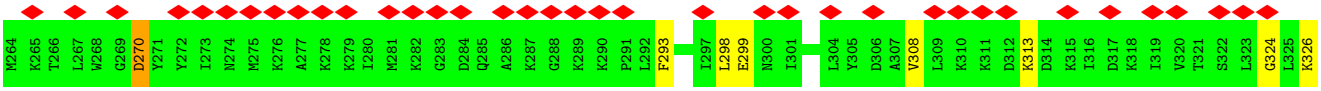
Chain K:

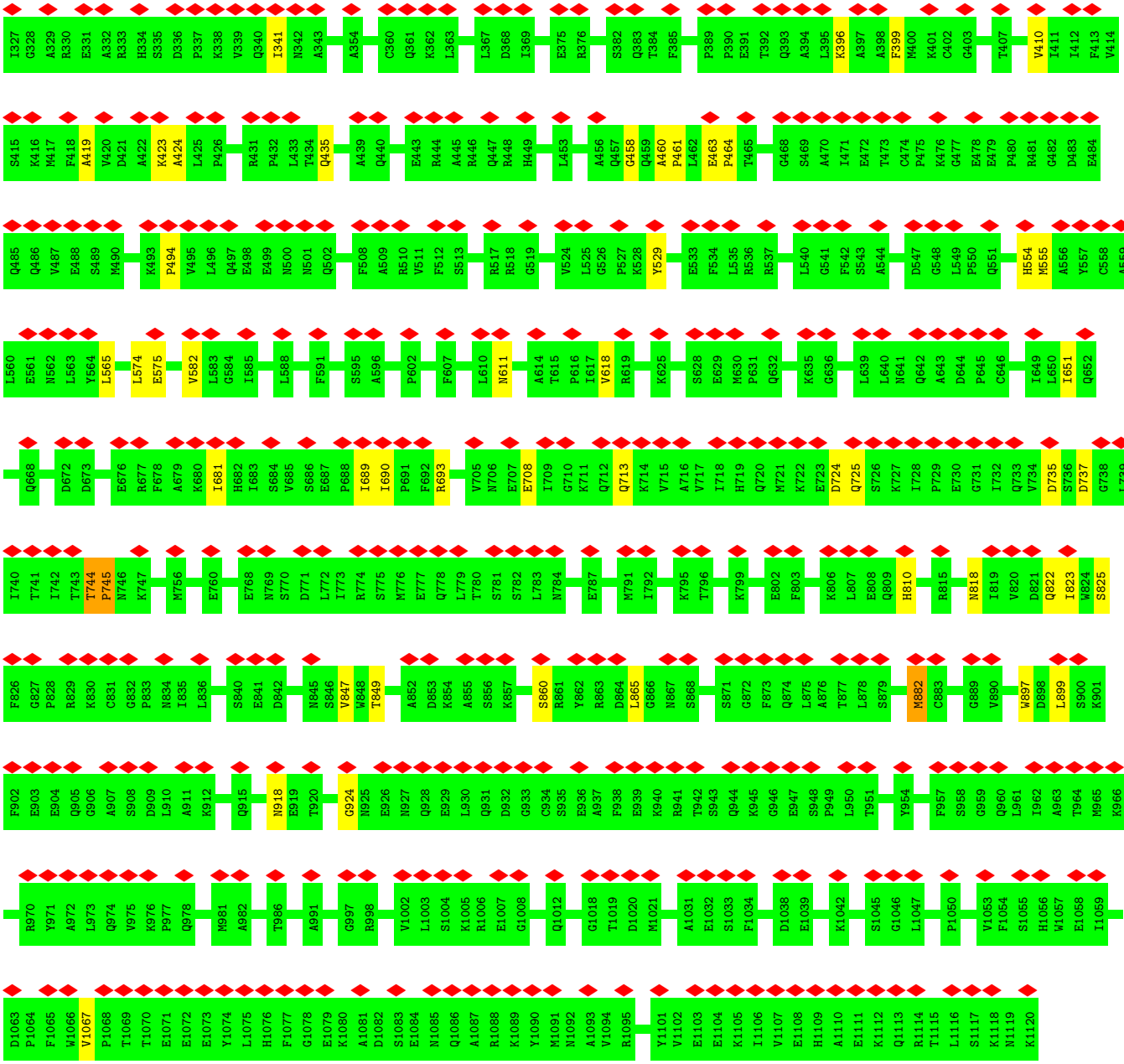






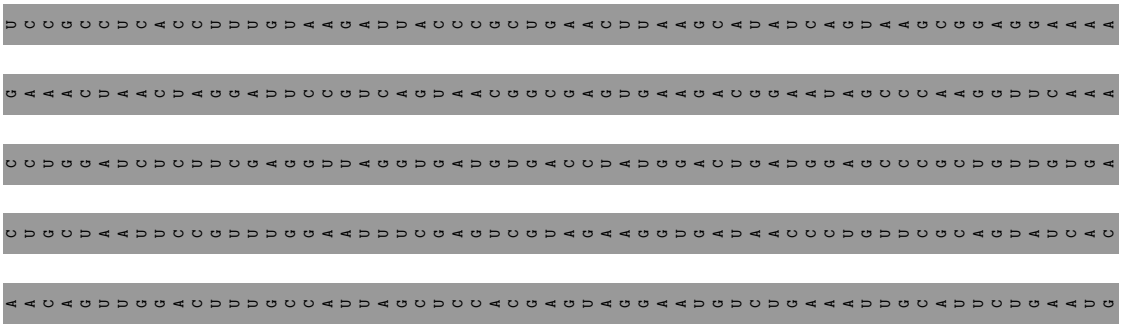


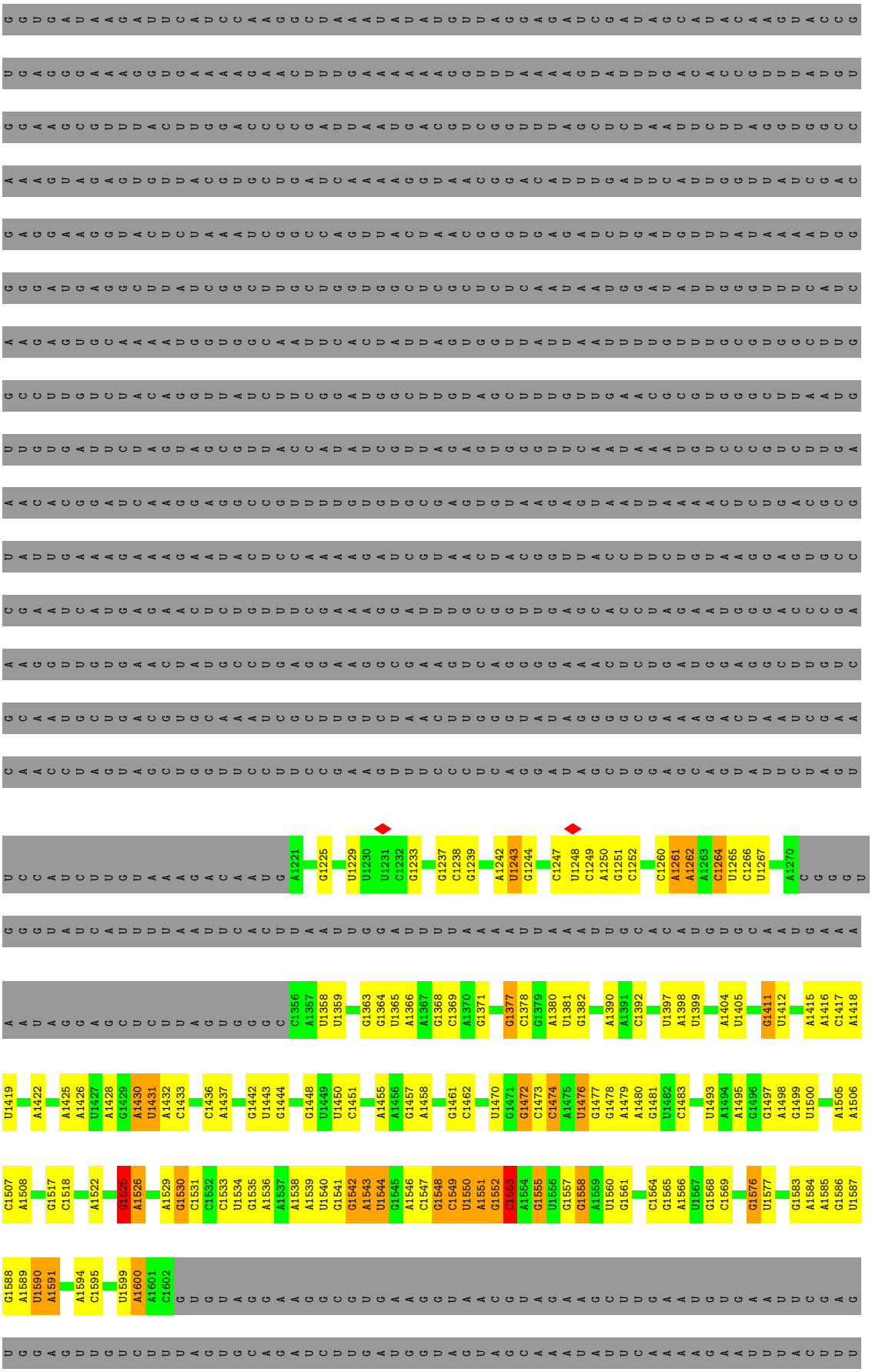


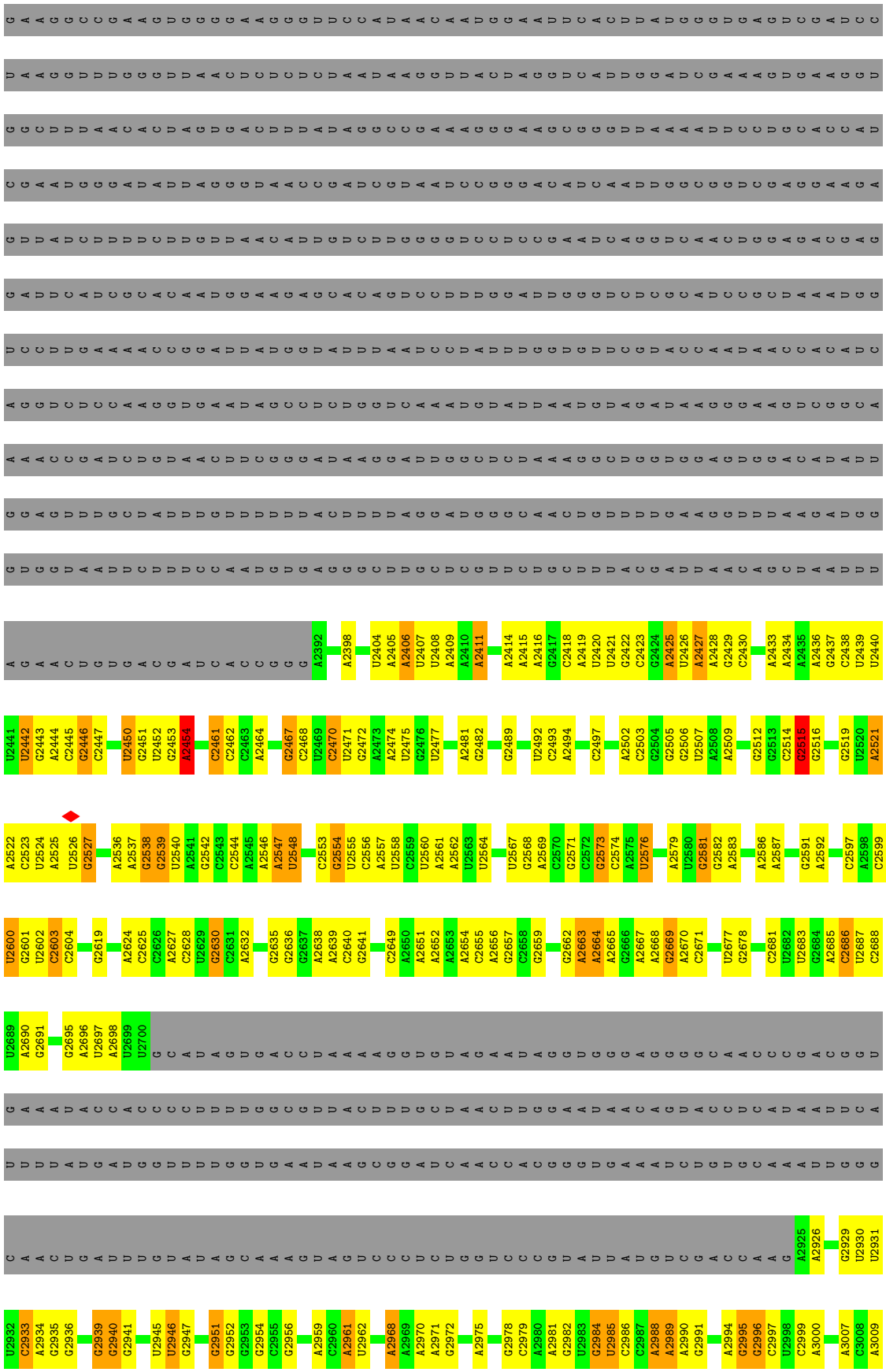


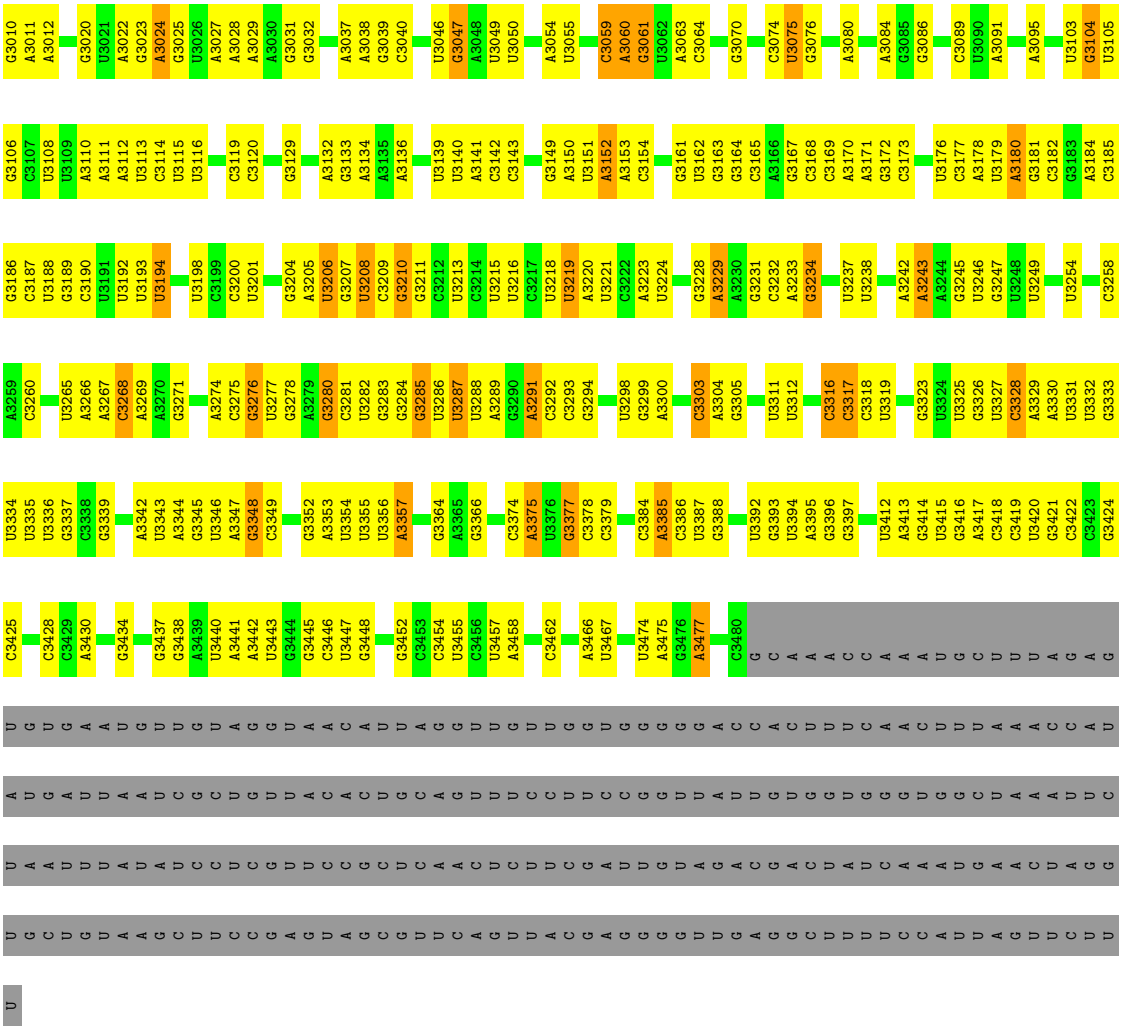
• Molecule 12: 26S RIBOSOMAL RNA

Chain N:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11970	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	105263	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.646	Depositor
Minimum map value	-0.444	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	399.0, 399.0, 399.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.53	0/3241	0.85	3/4339 (0.1%)
2	B	0.41	0/1510	0.72	0/2030
3	C	0.38	0/1592	0.57	0/2142
4	D	0.38	0/1265	0.61	0/1702
5	E	0.44	0/1032	0.75	0/1386
6	F	0.46	0/1752	0.77	0/2345
7	G	0.52	0/600	0.78	0/801
8	H	0.43	0/433	0.79	0/571
9	I	0.40	0/1706	0.66	0/2325
10	J	0.43	0/2038	0.67	0/2727
11	K	0.41	0/8969	0.64	0/12124
12	N	0.38	1/27702 (0.0%)	0.79	12/43160 (0.0%)
All	All	0.41	1/51840 (0.0%)	0.75	15/75652 (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	1
2	B	0	1
6	F	0	1
10	J	0	1
11	K	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	3316	C	O3'-P	5.09	1.67	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	2995	G	C2'-C3'-O3'	9.35	130.07	109.50
12	N	2515	G	C2'-C3'-O3'	7.63	126.29	109.50
1	A	249	LEU	CA-CB-CG	7.36	132.22	115.30
12	N	3303	C	C2'-C3'-O3'	7.04	124.98	109.50
12	N	1525	G	C2'-C3'-O3'	6.83	124.63	113.70
12	N	3291	A	C5'-C4'-O4'	6.20	116.54	109.10
12	N	2597	C	C1'-O4'-C4'	-6.07	105.05	109.90
12	N	2454	A	C2'-C3'-O3'	5.76	122.92	113.70
12	N	2603	C	N1-C1'-C2'	5.55	121.21	114.00
12	N	1553	C	N1-C1'-C2'	5.51	121.16	114.00
1	A	19	ARG	NE-CZ-NH1	5.45	123.03	120.30
12	N	3316	C	N1-C1'-C2'	5.44	121.07	114.00
1	A	347	ARG	NE-CZ-NH1	5.32	122.96	120.30
12	N	2470	C	C2'-C3'-O3'	5.27	122.13	113.70
12	N	2597	C	C5'-C4'-O4'	5.17	115.31	109.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	TRP	Peptide
2	B	96	HIS	Peptide
6	F	70	ILE	Peptide
10	J	126	ARG	Peptide
11	K	226	SER	Peptide

5.2 Too-close contacts (i)

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	51	0
2	B	1491	0	1555	13	0
3	C	1571	0	1657	1	0
4	D	1245	0	1338	0	0
5	E	1017	0	1076	11	0
6	F	1721	0	1778	22	0
7	G	586	0	601	3	0
8	H	427	0	483	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1686	0	1685	9	0
10	J	2015	0	2112	10	0
11	K	8800	0	8840	16	0
12	N	24758	0	12487	311	0
All	All	48493	0	36931	427	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 5.

All (427) 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)
12:N:2989:A:N6	12:N:3046:U:N3	2.19	0.89
12:N:2989:A:N6	12:N:3046:U:H3	1.73	0.87
6:F:50:VAL:HG12	6:F:167:VAL:HG22	1.57	0.86
5:E:45:ARG:NH1	12:N:3379:C:OP1	2.13	0.79
1:A:285:ILE:HD11	1:A:330:LEU:HG	1.68	0.75
12:N:1415:A:N7	12:N:1416:A:C6	2.55	0.74
2:B:10:VAL:HG21	2:B:75:ILE:HD11	1.70	0.73
12:N:1568:G:N2	12:N:1569:C:C2	2.59	0.70
12:N:2939:G:H2'	12:N:2939:G:N3	2.07	0.68
12:N:2437:G:N2	12:N:2438:C:C2	2.65	0.65
12:N:1261:A:H2'	12:N:1264:C:C5	2.32	0.65
1:A:220:VAL:HG11	1:A:336:VAL:HG13	1.79	0.65
12:N:1432:A:C8	12:N:1433:C:C6	2.84	0.65
5:E:79:VAL:HG13	5:E:80:ARG:HG3	1.79	0.64
12:N:2423:C:O2'	12:N:2427:A:N3	2.30	0.64
12:N:2663:A:H8	12:N:3206:U:O2	1.81	0.63
1:A:107:ALA:HB2	1:A:202:PHE:CG	2.34	0.63
12:N:3276:G:N7	12:N:3277:U:C5	2.67	0.63
12:N:2425:A:H61	12:N:2442:U:H3	1.48	0.62
12:N:3441:A:H2'	12:N:3442:A:O4'	1.99	0.62
6:F:19:LYS:HD2	6:F:26:VAL:HG21	1.81	0.62
1:A:50:LYS:HA	1:A:79:ILE:HG22	1.79	0.62
12:N:2406:A:N3	12:N:2406:A:H3'	2.15	0.62
12:N:2506:G:H2'	12:N:2507:U:O4'	2.00	0.62
12:N:1568:G:C2	12:N:1569:C:C6	2.89	0.61
1:A:7:GLU:OE2	1:A:9:PRO:HB3	2.01	0.61
12:N:2429:G:N1	12:N:2430:C:C2	2.70	0.60
12:N:3374:C:H2'	12:N:3375:A:O4'	2.02	0.60
5:E:5:GLN:HA	5:E:6:ALA:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:ILE:HG21	5:E:50:PRO:HA	1.84	0.59
12:N:1261:A:H2'	12:N:1264:C:C4	2.38	0.59
12:N:2951:G:O2'	12:N:3198:U:OP1	2.20	0.59
8:H:33:CYS:SG	8:H:38:CYS:SG	3.01	0.59
12:N:1472:G:N2	12:N:1473:C:C2	2.70	0.59
12:N:3335:U:H2'	12:N:3336:U:O4'	2.02	0.59
12:N:1553:C:C2	12:N:1555:G:N7	2.72	0.58
12:N:3328:C:O4'	12:N:3328:C:O2	2.21	0.58
1:A:8:ALA:HB1	12:N:3215:U:OP2	2.02	0.58
12:N:3172:G:N2	12:N:3173:C:C2	2.72	0.58
12:N:1404:A:C2	12:N:1405:U:C6	2.91	0.58
12:N:3215:U:H2'	12:N:3216:U:O4'	2.04	0.58
12:N:3397:G:C2	12:N:3419:C:C2	2.91	0.58
6:F:24:ARG:NH1	12:N:2981:A:OP1	2.37	0.57
1:A:45:ALA:HB3	1:A:184:ILE:HG22	1.85	0.57
12:N:3209:C:C2	12:N:3285:G:C2	2.93	0.57
1:A:55:HIS:HE1	7:G:16:ALA:HB3	1.69	0.57
1:A:364:LEU:HD13	1:A:367:ILE:HD11	1.87	0.57
5:E:130:THR:HG22	9:I:150:THR:HG23	1.87	0.57
1:A:254:CYS:SG	1:A:257:ALA:N	2.77	0.57
11:K:270:ASP:OD1	11:K:270:ASP:N	2.38	0.57
11:K:247:HIS:CE1	11:K:251:ILE:HD11	2.39	0.57
12:N:3276:G:C8	12:N:3277:U:C5	2.93	0.56
12:N:2467:G:C6	12:N:2468:C:C4	2.93	0.56
12:N:1568:G:N1	12:N:1569:C:C4	2.73	0.56
6:F:135:ILE:HD12	6:F:159:PHE:CE2	2.42	0.55
12:N:3167:G:N2	12:N:3168:C:C2	2.75	0.55
12:N:1450:U:H2'	12:N:1451:C:C6	2.42	0.55
10:J:7:THR:HB	12:N:3208:U:N1	2.21	0.55
12:N:2986:C:H1'	12:N:3027:A:C2	2.42	0.55
1:A:243:ARG:HA	12:N:2602:U:H5'	1.88	0.55
10:J:164:LYS:N	10:J:165:MET:HA	2.22	0.54
12:N:3299:G:H2'	12:N:3300:A:C8	2.41	0.54
10:J:18:VAL:HG22	10:J:93:VAL:HG23	1.90	0.54
12:N:3385:A:C2	12:N:3386:C:C6	2.95	0.54
12:N:2437:G:N1	12:N:2438:C:C4	2.75	0.54
1:A:209:THR:HG22	1:A:288:ILE:HG21	1.89	0.54
2:B:102:ALA:HB3	2:B:111:GLU:HG3	1.90	0.54
12:N:2635:G:H2'	12:N:2636:G:C8	2.43	0.54
12:N:2670:A:N3	12:N:2670:A:O5'	2.40	0.54
12:N:3039:G:N2	12:N:3040:C:C2	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:396:LYS:HA	11:K:399:PHE:CE2	2.43	0.54
6:F:115:MET:HB2	12:N:2951:G:C4	2.42	0.53
12:N:2670:A:C2	12:N:2670:A:OP1	2.61	0.53
12:N:3114:C:H2'	12:N:3115:U:C6	2.43	0.53
6:F:105:CYS:SG	6:F:113:THR:HG21	2.48	0.53
12:N:3343:U:H2'	12:N:3344:A:O4'	2.08	0.53
12:N:3242:A:N6	12:N:3243:A:C2	2.77	0.53
12:N:1525:G:H2'	12:N:1526:A:C8	2.44	0.53
12:N:1530:G:C6	12:N:1531:C:C4	2.97	0.53
12:N:2411:A:H1'	12:N:2547:A:N6	2.23	0.53
12:N:2978:G:N2	12:N:2979:C:C2	2.76	0.53
12:N:3352:G:H2'	12:N:3353:A:C8	2.44	0.53
2:B:144:LEU:HD22	2:B:156:CYS:SG	2.49	0.53
12:N:2988:A:H4'	12:N:2989:A:O4'	2.08	0.53
12:N:3325:U:H2'	12:N:3326:G:O4'	2.09	0.53
1:A:76:VAL:HG23	1:A:332:LEU:O	2.09	0.52
12:N:3285:G:C5	12:N:3286:U:C4	2.97	0.52
9:I:25:LEU:HA	9:I:49:VAL:HG22	1.91	0.52
12:N:1415:A:N7	12:N:1416:A:C5	2.77	0.52
12:N:1590:U:H2'	12:N:1591:A:C2	2.45	0.52
1:A:134:TYR:O	1:A:134:TYR:CD2	2.63	0.52
12:N:2968:A:N6	12:N:2975:A:OP2	2.42	0.52
12:N:3059:C:O2	12:N:3059:C:O4'	2.28	0.52
5:E:27:ASP:HB2	5:E:101:VAL:HG23	1.92	0.51
12:N:2567:U:C2	12:N:2568:G:C8	2.98	0.51
6:F:52:LEU:HD13	6:F:152:LEU:HB3	1.92	0.51
11:K:107:VAL:HG11	11:K:134:ALA:HB2	1.91	0.51
12:N:1398:A:C6	12:N:1399:U:C4	2.99	0.51
1:A:364:LEU:CD1	1:A:367:ILE:HD11	2.41	0.51
12:N:3189:G:N2	12:N:3190:C:C2	2.79	0.51
12:N:3242:A:H2'	12:N:3243:A:O4'	2.11	0.51
12:N:1358:U:C4	12:N:1359:U:C4	2.99	0.51
12:N:1243:U:O2	12:N:1243:U:O4'	2.28	0.51
12:N:2933:C:C2	12:N:2934:A:C8	2.99	0.51
1:A:248:GLY:CA	1:A:249:LEU:HD22	2.41	0.51
1:A:253:ALA:HB1	12:N:3280:G:C4	2.46	0.51
5:E:5:GLN:CA	5:E:6:ALA:HB2	2.41	0.51
6:F:170:LYS:O	6:F:178:ARG:NH2	2.44	0.51
1:A:76:VAL:HG21	1:A:331:MET:SD	2.51	0.51
12:N:3334:U:O2	12:N:3334:U:O4'	2.29	0.50
1:A:284:LYS:NZ	1:A:360:GLU:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:19:CYS:SG	8:H:22:CYS:HB2	2.51	0.50
12:N:1363:G:H2'	12:N:1364:G:O4'	2.12	0.50
12:N:2477:U:O4'	12:N:2477:U:O2	2.29	0.50
12:N:3288:U:H2'	12:N:3289:A:O4'	2.11	0.50
12:N:2553:C:C2	12:N:2564:U:O4'	2.64	0.50
12:N:2662:G:N2	12:N:3318:C:C2	2.80	0.50
12:N:3172:G:N1	12:N:3173:C:C4	2.79	0.50
12:N:3352:G:H2'	12:N:3353:A:H8	1.77	0.50
1:A:114:PHE:CE2	1:A:136:LYS:HB3	2.47	0.50
12:N:1542:G:C2	12:N:1543:A:C2	3.00	0.50
12:N:2467:G:C2	12:N:2468:C:C2	2.99	0.50
12:N:2568:G:C6	12:N:2569:A:N7	2.79	0.50
12:N:3347:A:N1	12:N:3379:C:O2'	2.35	0.50
12:N:3353:A:H2'	12:N:3354:U:O4'	2.12	0.50
12:N:2670:A:O5'	12:N:2670:A:C4	2.64	0.49
1:A:91:GLY:HA2	1:A:161:VAL:HG12	1.94	0.49
12:N:1530:G:C2	12:N:1531:C:C2	3.01	0.49
12:N:2683:U:HO2'	12:N:3298:U:H3	1.54	0.49
12:N:1442:G:C2	12:N:1533:C:C2	2.99	0.49
2:B:102:ALA:HB3	2:B:111:GLU:CG	2.43	0.49
12:N:1590:U:H2'	12:N:1591:A:N3	2.27	0.49
6:F:157:TYR:CG	12:N:3169:C:H4'	2.47	0.49
12:N:3387:U:C2	12:N:3388:G:C8	2.99	0.49
12:N:2526:U:H2'	12:N:2527:G:O4'	2.12	0.49
12:N:2999:C:H2'	12:N:2999:C:O2	2.12	0.49
1:A:6:PHE:O	12:N:3249:U:OP1	2.30	0.49
1:A:243:ARG:HA	12:N:2602:U:H4'	1.95	0.49
1:A:287:ARG:HD3	1:A:364:LEU:HD21	1.95	0.49
6:F:97:LEU:HD21	6:F:126:VAL:HG11	1.95	0.49
12:N:1472:G:N1	12:N:1473:C:C4	2.80	0.49
12:N:2420:U:C2	12:N:2421:U:C6	3.01	0.49
12:N:2581:G:C2	12:N:2582:G:N7	2.80	0.49
12:N:3112:A:C6	12:N:3113:U:C5	3.01	0.49
12:N:3161:G:C5	12:N:3162:U:C5	3.01	0.49
12:N:3445:G:C2	12:N:3446:C:C2	3.01	0.49
12:N:2686:C:C4	12:N:2687:U:C5	3.00	0.49
12:N:2996:G:C2	12:N:2997:C:C2	3.01	0.49
12:N:3354:U:N3	12:N:3355:U:C5	2.81	0.49
12:N:3445:G:C2	12:N:3462:C:C2	3.01	0.49
1:A:253:ALA:HB3	12:N:3213:U:O2	2.12	0.48
12:N:2418:C:C2	12:N:2419:A:C8	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:3163:G:H1'	12:N:3194:U:C2	2.47	0.48
1:A:257:ALA:O	1:A:259:HIS:N	2.44	0.48
3:C:115:PHE:CD1	3:C:174:LEU:HD11	2.48	0.48
12:N:2547:A:O2'	12:N:2548:U:OP1	2.25	0.48
12:N:2996:G:C6	12:N:2997:C:C4	3.00	0.48
6:F:7:ARG:NH2	12:N:3161:G:OP2	2.46	0.48
1:A:184:ILE:HG13	1:A:184:ILE:O	2.12	0.48
12:N:1251:G:N2	12:N:1252:C:C2	2.81	0.48
12:N:3293:C:H2'	12:N:3294:G:C8	2.49	0.48
12:N:3394:U:O2	12:N:3394:U:O4'	2.30	0.48
12:N:3445:G:C6	12:N:3446:C:C4	3.01	0.48
1:A:18:PRO:O	1:A:19:ARG:C	2.52	0.48
12:N:2416:A:C2	12:N:2454:A:O4'	2.66	0.48
12:N:3474:U:H2'	12:N:3475:A:O4'	2.14	0.48
1:A:226:GLY:HA2	1:A:274:GLY:HA3	1.93	0.48
12:N:2696:A:C2	12:N:2697:U:C4	3.02	0.48
10:J:114:ILE:HD13	10:J:151:LYS:HA	1.96	0.48
12:N:2419:A:O4'	12:N:2509:A:C2	2.67	0.48
12:N:3218:U:H2'	12:N:3219:U:O4'	2.13	0.48
12:N:1568:G:C6	12:N:1569:C:C4	3.02	0.48
12:N:3412:U:O4	12:N:3413:A:N6	2.47	0.48
11:K:744:THR:HB	11:K:745:PRO:HD3	1.96	0.48
12:N:1371:G:O2'	12:N:2975:A:N3	2.40	0.48
12:N:2571:G:OP2	12:N:2571:G:N2	2.38	0.48
1:A:24:ARG:HD3	1:A:28:LYS:HB2	1.96	0.47
12:N:1560:U:H2'	12:N:1561:G:O4'	2.14	0.47
12:N:2561:A:C6	12:N:2562:A:C6	3.01	0.47
12:N:3442:A:H2'	12:N:3443:U:O4'	2.13	0.47
8:H:45:ARG:NH2	12:N:3180:A:OP1	2.47	0.47
12:N:2671:C:O2	12:N:3152:A:N1	2.47	0.47
12:N:3024:A:H2'	12:N:3025:G:O4'	2.14	0.47
12:N:3039:G:C6	12:N:3040:C:C4	3.02	0.47
12:N:3387:U:H2'	12:N:3388:G:O4'	2.14	0.47
9:I:68:ASN:OD1	9:I:68:ASN:N	2.47	0.47
12:N:3103:U:N3	12:N:3104:G:O6	2.48	0.47
12:N:3281:C:H2'	12:N:3282:U:O4'	2.14	0.47
1:A:79:ILE:HD11	1:A:330:LEU:HB3	1.96	0.47
12:N:1568:G:C2	12:N:1569:C:C5	3.03	0.47
12:N:3446:C:H2'	12:N:3447:U:C6	2.49	0.47
12:N:1517:G:C2	12:N:1518:C:C2	3.02	0.47
12:N:3063:A:H2'	12:N:3064:C:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:HIS:CE1	7:G:16:ALA:HB3	2.49	0.47
6:F:211:LYS:O	6:F:215:ALA:N	2.48	0.47
12:N:1476:U:O2	12:N:1476:U:O4'	2.32	0.47
12:N:1541:G:O6	12:N:2632:A:O2'	2.31	0.47
12:N:3267:A:H2'	12:N:3268:C:O4'	2.15	0.47
12:N:3342:A:C2	12:N:3477:A:C4	3.02	0.47
2:B:72:THR:O	2:B:75:ILE:HG13	2.14	0.47
2:B:93:VAL:HG13	2:B:175:ASP:HA	1.96	0.47
10:J:6:PRO:HB2	12:N:3153:A:C2	2.49	0.47
12:N:1568:G:N2	12:N:1569:C:N1	2.62	0.47
12:N:2554:G:C4	12:N:2555:U:C5	3.02	0.47
12:N:3377:G:C2	12:N:3378:C:C2	3.03	0.47
12:N:1568:G:N3	12:N:1569:C:C6	2.83	0.47
12:N:2624:A:H8	12:N:2625:C:C6	2.33	0.47
12:N:1493:U:O2	12:N:1495:A:C8	2.68	0.47
12:N:1517:G:C6	12:N:1518:C:C4	3.03	0.47
7:G:44:ILE:HG21	7:G:48:ASP:OD2	2.15	0.46
1:A:218:ILE:HG21	1:A:346:LEU:HD22	1.96	0.46
6:F:184:LEU:HD22	6:F:199:VAL:HG13	1.97	0.46
11:K:293:PHE:CD1	11:K:298:LEU:HD13	2.50	0.46
12:N:2414:A:H2'	12:N:2415:A:O4'	2.15	0.46
12:N:2502:A:C5	12:N:2503:C:C5	3.04	0.46
12:N:2978:G:C6	12:N:2979:C:C4	3.04	0.46
12:N:3054:A:H2'	12:N:3055:U:O4'	2.16	0.46
12:N:3209:C:H1'	12:N:3285:G:N2	2.30	0.46
8:H:22:CYS:SG	8:H:38:CYS:SG	3.10	0.46
12:N:1261:A:C2'	12:N:1264:C:C5	2.99	0.46
12:N:1529:A:C2	12:N:1530:G:N7	2.83	0.46
12:N:2683:U:O2'	12:N:3298:U:N3	2.37	0.46
11:K:308:VAL:HG21	11:K:341:ILE:HA	1.97	0.46
12:N:3169:C:O2	12:N:3169:C:O4'	2.33	0.46
12:N:3189:G:C6	12:N:3190:C:N4	2.84	0.46
9:I:28:GLN:O	9:I:57:ARG:NH1	2.48	0.46
1:A:217:LEU:HA	1:A:283:LYS:O	2.16	0.46
10:J:7:THR:HB	12:N:3208:U:C2	2.51	0.46
12:N:2515:G:C8	12:N:2538:G:C8	3.04	0.46
11:K:565:LEU:HD13	11:K:574:LEU:HD11	1.98	0.46
12:N:3075:U:C2	12:N:3076:G:C8	3.04	0.46
12:N:3161:G:C4	12:N:3162:U:C6	3.04	0.46
12:N:2695:G:C6	12:N:2696:A:N7	2.84	0.45
12:N:2696:A:H2'	12:N:2697:U:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:197:CYS:HB3	9:I:206:VAL:HG23	1.97	0.45
12:N:1431:U:O2	12:N:1431:U:O4'	2.34	0.45
12:N:2416:A:N1	12:N:2454:A:O4'	2.49	0.45
12:N:3032:G:C2	12:N:3089:C:C2	3.05	0.45
12:N:3186:G:C2	12:N:3187:C:C2	3.04	0.45
12:N:3189:G:C2	12:N:3190:C:C2	3.04	0.45
12:N:3209:C:C2	12:N:3285:G:N1	2.84	0.45
6:F:146:ALA:HA	6:F:149:VAL:HG12	1.96	0.45
9:I:138:PHE:CD2	9:I:176:LEU:HD11	2.52	0.45
12:N:3445:G:N2	12:N:3446:C:C2	2.84	0.45
5:E:39:VAL:HG22	5:E:58:VAL:HG12	1.99	0.45
6:F:48:LEU:HD11	6:F:167:VAL:CG1	2.46	0.45
12:N:1251:G:C6	12:N:1252:C:C4	3.05	0.45
12:N:1461:G:C2	12:N:1462:C:C2	3.04	0.45
12:N:2695:G:C5	12:N:2696:A:N7	2.85	0.45
12:N:3164:G:C2	12:N:3165:C:C2	3.04	0.45
12:N:3377:G:C6	12:N:3378:C:C4	3.05	0.45
10:J:7:THR:HG23	12:N:3287:U:C6	2.51	0.45
12:N:2686:C:H2'	12:N:2687:U:O4'	2.17	0.45
12:N:2978:G:C2	12:N:2979:C:C2	3.04	0.45
12:N:3027:A:C6	12:N:3028:A:C6	3.05	0.45
12:N:2649:C:O2	12:N:2649:C:O4'	2.35	0.45
12:N:3184:A:H2'	12:N:3185:C:C6	2.51	0.45
10:J:7:THR:HG22	10:J:7:THR:O	2.16	0.45
12:N:2557:A:C5	12:N:2558:U:C5	3.05	0.45
12:N:2544:C:C2	12:N:2573:G:N2	2.85	0.45
12:N:3039:G:C2	12:N:3040:C:C2	3.05	0.45
12:N:3228:G:C6	12:N:3229:A:N7	2.85	0.45
12:N:3415:U:O2	12:N:3415:U:O4'	2.33	0.45
6:F:15:LYS:HD2	12:N:1262:A:C1'	2.47	0.44
12:N:1430:A:C2	12:N:1544:U:N3	2.85	0.44
12:N:2600:U:O2	12:N:2600:U:O4'	2.31	0.44
12:N:3186:G:C6	12:N:3187:C:C4	3.05	0.44
5:E:2:SER:N	5:E:3:LYS:HA	2.31	0.44
12:N:1411:G:C6	12:N:1412:U:C4	3.05	0.44
12:N:3059:C:C5	12:N:3061:G:C4	3.06	0.44
12:N:3200:C:OP2	12:N:3201:U:OP2	2.35	0.44
12:N:3418:C:C2	12:N:3419:C:C5	3.06	0.44
5:E:92:TYR:CE2	12:N:3387:U:O4'	2.71	0.44
8:H:2:GLU:N	8:H:3:PRO:HD2	2.32	0.44
11:K:865:LEU:HD12	11:K:899:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:1404:A:C2	12:N:1405:U:N1	2.85	0.44
12:N:3223:A:C5	12:N:3224:U:C5	3.06	0.44
12:N:2669:G:O2'	12:N:2670:A:H2'	2.17	0.44
6:F:48:LEU:HD11	6:F:167:VAL:HG13	2.00	0.44
12:N:2591:G:C2	12:N:2592:A:C8	3.05	0.44
1:A:117:ARG:HB2	1:A:117:ARG:CZ	2.48	0.44
2:B:75:ILE:HD12	2:B:76:GLU:N	2.32	0.44
12:N:1550:U:O2'	12:N:1551:A:OP1	2.27	0.44
1:A:285:ILE:HD13	1:A:331:MET:O	2.18	0.44
6:F:184:LEU:HD13	6:F:199:VAL:HG22	1.99	0.44
12:N:3237:U:C2	12:N:3238:U:C6	3.05	0.44
12:N:1546:A:H2'	12:N:1547:C:O4'	2.18	0.44
12:N:2429:G:C6	12:N:2430:C:C4	3.06	0.44
12:N:2961:A:H2'	12:N:2962:U:O4'	2.18	0.44
1:A:313:ILE:HD12	1:A:314:ASN:N	2.33	0.43
2:B:70:THR:HG23	12:N:3448:G:O2'	2.18	0.43
12:N:2635:G:C6	12:N:2636:G:C6	3.05	0.43
12:N:3119:C:H2'	12:N:3120:C:O4'	2.18	0.43
12:N:3167:G:N1	12:N:3168:C:C4	2.86	0.43
12:N:3356:U:C4	12:N:3357:A:C5	3.06	0.43
12:N:3417:A:C6	12:N:3418:C:C4	3.06	0.43
12:N:3336:U:C2	12:N:3337:G:C8	3.06	0.43
12:N:3397:G:N2	12:N:3419:C:C2	2.87	0.43
12:N:2450:U:C2	12:N:2451:G:C8	3.06	0.43
12:N:2521:A:C8	12:N:2527:G:N2	2.86	0.43
12:N:3074:C:H2'	12:N:3075:U:O4'	2.17	0.43
12:N:2568:G:C6	12:N:2569:A:C5	3.06	0.43
12:N:2697:U:H2'	12:N:2698:A:O4'	2.18	0.43
5:E:54:VAL:HG11	5:E:85:TRP:CH2	2.52	0.43
12:N:1568:G:C2	12:N:1569:C:C2	3.06	0.43
12:N:2492:U:H2'	12:N:2493:C:O4'	2.19	0.43
12:N:2548:U:O2	12:N:2576:U:H4'	2.19	0.43
12:N:3317:C:C2	12:N:3318:C:C5	3.07	0.43
12:N:2940:G:C6	12:N:2941:G:C5	3.07	0.43
12:N:3060:A:H5"	12:N:3061:G:OP2	2.18	0.43
12:N:1237:G:C5	12:N:1238:C:C5	3.06	0.43
12:N:2514:C:H2'	12:N:2539:G:C8	2.53	0.43
12:N:2568:G:C4	12:N:2569:A:C8	3.07	0.43
12:N:3210:G:C6	12:N:3211:G:C5	3.06	0.43
12:N:3246:U:C2	12:N:3247:G:C8	3.06	0.43
2:B:92:PHE:CE2	2:B:101:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:1425:A:N7	12:N:1551:A:OP1	2.52	0.43
12:N:2935:G:H2'	12:N:2936:G:O4'	2.19	0.43
12:N:2961:A:C2	12:N:2962:U:H1'	2.53	0.43
12:N:3424:G:C6	12:N:3425:C:C4	3.07	0.43
1:A:19:ARG:HG2	1:A:276:HIS:CE1	2.53	0.43
1:A:248:GLY:C	1:A:249:LEU:HD22	2.39	0.43
1:A:336:VAL:HG11	1:A:344:LEU:HD22	2.01	0.43
12:N:1479:A:C2	12:N:1483:C:C5	3.06	0.43
12:N:3181:G:C6	12:N:3182:C:C4	3.07	0.43
1:A:134:TYR:O	1:A:134:TYR:CG	2.71	0.43
2:B:92:PHE:CD2	2:B:101:VAL:HG21	2.54	0.43
10:J:19:ARG:NH1	12:N:2574:C:O2	2.52	0.43
11:K:882:MET:SD	11:K:882:MET:N	2.90	0.43
12:N:1534:U:H2'	12:N:1535:G:O4'	2.19	0.43
12:N:2627:A:C5	12:N:2628:C:C5	3.06	0.42
12:N:3445:G:C2	12:N:3462:C:O2	2.71	0.42
1:A:313:ILE:HG22	1:A:367:ILE:HG21	2.01	0.42
6:F:102:MET:HA	6:F:113:THR:HG22	2.01	0.42
12:N:2461:C:H2'	12:N:2462:C:O4'	2.19	0.42
12:N:2564:U:C5	12:N:3254:U:H1'	2.55	0.42
12:N:2586:A:H2'	12:N:2587:A:O4'	2.19	0.42
12:N:3152:A:C2	12:N:3153:A:C4	3.08	0.42
12:N:3164:G:C6	12:N:3165:C:C4	3.07	0.42
8:H:18:ILE:HD13	12:N:3229:A:H4'	2.00	0.42
9:I:117:VAL:HG12	9:I:139:ARG:HA	2.01	0.42
12:N:1250:A:C4	12:N:1251:G:C8	3.07	0.42
12:N:2537:A:H2'	12:N:2538:G:O4'	2.19	0.42
12:N:2655:C:H2'	12:N:2656:A:C8	2.54	0.42
1:A:43:LEU:HD22	1:A:184:ILE:CD1	2.49	0.42
11:K:115:ILE:HG22	11:K:117:VAL:HG13	2.00	0.42
12:N:1576:G:C5	12:N:1577:U:C5	3.08	0.42
12:N:2497:C:O2	12:N:2497:C:O4'	2.36	0.42
12:N:3059:C:N4	12:N:3061:G:C6	2.88	0.42
12:N:3265:U:O2	12:N:3267:A:C8	2.73	0.42
6:F:145:LEU:HD13	6:F:145:LEU:N	2.34	0.42
12:N:3172:G:C2	12:N:3173:C:C2	3.08	0.42
2:B:86:TYR:CE2	2:B:149:LEU:HB2	2.55	0.42
8:H:45:ARG:HE	12:N:3180:A:P	2.42	0.42
12:N:1557:G:H2'	12:N:1558:G:O4'	2.19	0.42
12:N:2446:G:C2	12:N:2447:C:C2	3.08	0.42
12:N:2929:G:C5	12:N:2930:U:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:3419:C:C4	12:N:3420:U:C5	3.08	0.42
1:A:128:LYS:O	1:A:130:ALA:N	2.53	0.42
11:K:618:VAL:HG12	11:K:690:ILE:HG21	2.02	0.42
12:N:1418:A:C5	12:N:1419:U:C5	3.08	0.42
12:N:1552:G:C2'	12:N:1553:C:O5'	2.68	0.42
11:K:460:ALA:HB3	11:K:461:PRO:HD3	2.02	0.42
12:N:2425:A:N6	12:N:2442:U:H3	2.14	0.42
12:N:2481:A:C5	12:N:2482:G:C8	3.08	0.42
12:N:3209:C:O2	12:N:3285:G:C2	2.73	0.42
12:N:3276:G:C5	12:N:3277:U:C5	3.07	0.42
2:B:172:LYS:HD2	12:N:3234:G:H5'	2.02	0.41
12:N:3281:C:C2	12:N:3282:U:C6	3.08	0.41
12:N:3345:G:C5	12:N:3346:U:C5	3.08	0.41
12:N:1461:G:C6	12:N:1462:C:C4	3.08	0.41
12:N:3189:G:C6	12:N:3190:C:C4	3.08	0.41
12:N:2422:G:C2	12:N:2423:C:C2	3.08	0.41
12:N:3060:A:OP2	12:N:3061:G:N2	2.53	0.41
12:N:3167:G:C2	12:N:3168:C:C2	3.08	0.41
1:A:107:ALA:HB2	1:A:202:PHE:CD2	2.55	0.41
1:A:221:ILE:HG22	1:A:222:GLY:N	2.35	0.41
1:A:233:ILE:HD12	1:A:238:VAL:HG22	2.03	0.41
9:I:21:ASN:HD21	9:I:156:ASN:ND2	2.19	0.41
11:K:247:HIS:NE2	11:K:251:ILE:HD11	2.34	0.41
12:N:2664:A:H8	12:N:2664:A:H5"	1.85	0.41
12:N:3047:G:C8	12:N:3084:A:C2	3.09	0.41
12:N:3223:A:O2'	12:N:3266:A:N3	2.41	0.41
12:N:1377:G:C6	12:N:1378:C:C4	3.08	0.41
12:N:2404:U:C6	12:N:2408:U:C5	3.09	0.41
12:N:2984:G:H4'	12:N:2985:U:OP2	2.21	0.41
9:I:66:ASN:HD21	9:I:110:THR:HG23	1.85	0.41
11:K:565:LEU:HD12	11:K:582:VAL:O	2.20	0.41
12:N:2467:G:H2'	12:N:2468:C:O4'	2.21	0.41
12:N:1247:C:H2'	12:N:1248:U:C6	2.56	0.41
12:N:1599:U:C2	12:N:1600:A:C8	3.09	0.41
12:N:2437:G:C2	12:N:2438:C:C2	3.08	0.41
12:N:1461:G:C6	12:N:1462:C:N4	2.88	0.41
12:N:2630:G:C8	12:N:3318:C:O2'	2.73	0.41
2:B:16:VAL:HG12	2:B:29:GLY:CA	2.51	0.41
6:F:48:LEU:HB3	6:F:140:THR:HG23	2.03	0.41
6:F:76:ILE:HG13	6:F:85:PHE:CD1	2.56	0.41
12:N:1237:G:C6	12:N:1238:C:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:1472:G:C6	12:N:1473:C:N4	2.89	0.41
12:N:1552:G:H2'	12:N:1553:C:O5'	2.21	0.41
12:N:2452:U:H2'	12:N:2453:G:O4'	2.21	0.41
12:N:2945:U:C2	12:N:2946:U:C6	3.08	0.41
12:N:3039:G:N1	12:N:3040:C:C4	2.89	0.41
12:N:1251:G:C2	12:N:1252:C:C2	3.08	0.41
12:N:1364:G:H5"	12:N:1365:U:OP2	2.21	0.41
12:N:1418:A:C6	12:N:1419:U:C4	3.09	0.41
12:N:1430:A:H2'	12:N:1544:U:O2	2.21	0.41
12:N:2555:U:N3	12:N:2556:C:C5	2.89	0.41
12:N:3348:G:C2	12:N:3349:C:C2	3.09	0.41
1:A:57:VAL:HG22	1:A:73:VAL:HG22	2.03	0.40
12:N:1251:G:N1	12:N:1252:C:C4	2.88	0.40
12:N:1548:G:C2	12:N:1549:C:C2	3.09	0.40
12:N:2930:U:C4	12:N:2931:U:C5	3.09	0.40
12:N:3416:G:C6	12:N:3417:A:C5	3.09	0.40
1:A:29:VAL:HB	1:A:347:ARG:CZ	2.52	0.40
12:N:3049:U:N3	12:N:3050:U:C5	2.90	0.40
12:N:3206:U:O2	12:N:3206:U:O4'	2.39	0.40
1:A:43:LEU:HD11	1:A:206:VAL:HG11	2.02	0.40
11:K:104:SER:O	11:K:107:VAL:HG12	2.20	0.40
12:N:2984:G:H5"	12:N:2985:U:O4'	2.21	0.40
12:N:2690:A:H2'	12:N:2691:G:O4'	2.21	0.40
12:N:3245:G:C6	12:N:3246:U:C4	3.09	0.40
12:N:3420:U:H2'	12:N:3421:G:O4'	2.21	0.40
1:A:243:ARG:HA	12:N:2602:U:C4'	2.52	0.40
10:J:17:VAL:HG13	10:J:60:VAL:HG12	2.03	0.40
12:N:1473:C:C2'	12:N:1474:C:OP1	2.70	0.40
12:N:3139:U:H2'	12:N:3140:U:C6	2.57	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%)	306 (77%)	65 (16%)	25 (6%)	1 19
2	B	186/188 (99%)	167 (90%)	16 (9%)	3 (2%)	9 43
3	C	203/205 (99%)	180 (89%)	21 (10%)	2 (1%)	15 52
4	D	164/166 (99%)	138 (84%)	21 (13%)	5 (3%)	4 31
5	E	134/136 (98%)	117 (87%)	13 (10%)	4 (3%)	4 31
6	F	215/217 (99%)	169 (79%)	39 (18%)	7 (3%)	4 29
7	G	67/69 (97%)	58 (87%)	7 (10%)	2 (3%)	4 31
8	H	50/52 (96%)	40 (80%)	9 (18%)	1 (2%)	7 39
9	I	222/224 (99%)	200 (90%)	21 (10%)	1 (0%)	29 67
10	J	248/250 (99%)	225 (91%)	17 (7%)	6 (2%)	6 35
11	K	1118/1120 (100%)	921 (82%)	160 (14%)	37 (3%)	4 29
All	All	3003/3025 (99%)	2521 (84%)	389 (13%)	93 (3%)	7 31

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	130	ALA
5	E	6	ALA
6	F	195	ALA
7	G	46	PRO
9	I	120	ASP
10	J	5	THR
10	J	6	PRO
10	J	127	PRO
11	K	219	ASP
11	K	227	PRO
11	K	464	PRO
11	K	689	ILE
11	K	725	GLN
1	A	3	HIS
1	A	39	GLN
1	A	67	MET
1	A	238	VAL
1	A	358	ALA
7	G	43	LYS
11	K	46	ILE
11	K	48	SER
11	K	313	LYS

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Mol	Chain	Res	Type
11	K	458	GLY
1	A	102	TYR
1	A	233	ILE
1	A	259	HIS
1	A	278	ARG
1	A	285	ILE
1	A	335	CYS
5	E	55	GLY
6	F	14	ASN
6	F	93	PRO
6	F	104	SER
8	H	21	LYS
10	J	46	ASP
11	K	218	THR
11	K	222	HIS
11	K	423	LYS
11	K	555	MET
11	K	611	ASN
11	K	735	ASP
11	K	825	SER
11	K	918	ASN
1	A	118	LEU
1	A	378	HIS
3	C	84	ASN
3	C	181	PRO
4	D	72	GLU
10	J	118	LYS
10	J	246	ASP
11	K	19	ILE
11	K	242	GLY
11	K	326	LYS
11	K	419	ALA
11	K	424	ALA
11	K	529	TYR
11	K	554	HIS
11	K	713	GLN
11	K	744	THR
11	K	745	PRO
11	K	849	THR
11	K	860	SER
11	K	924	GLY
11	K	1067	VAL

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Mol	Chain	Res	Type
1	A	10	ARG
1	A	19	ARG
1	A	44	THR
1	A	135	VAL
1	A	232	VAL
1	A	241	LEU
1	A	244	LYS
2	B	141	GLU
5	E	56	ASP
6	F	199	VAL
11	K	410	VAL
11	K	494	PRO
1	A	375	HIS
2	B	39	ASP
5	E	17	LEU
6	F	90	ARG
11	K	24	VAL
11	K	651	ILE
1	A	87	VAL
4	D	162	VAL
11	K	324	GLY
1	A	248	GLY
11	K	847	VAL
4	D	52	PRO
4	D	58	VAL
4	D	140	GLY
2	B	45	ILE
6	F	70	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	312 (93%)	25 (7%)	13 41
2	B	168/168 (100%)	160 (95%)	8 (5%)	25 53
3	C	172/172 (100%)	165 (96%)	7 (4%)	30 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	139/139 (100%)	130 (94%)	9 (6%)	17 45
5	E	108/108 (100%)	105 (97%)	3 (3%)	43 65
6	F	180/180 (100%)	168 (93%)	12 (7%)	16 44
7	G	65/65 (100%)	58 (89%)	7 (11%)	6 26
8	H	48/48 (100%)	45 (94%)	3 (6%)	18 46
9	I	190/190 (100%)	181 (95%)	9 (5%)	26 53
10	J	228/228 (100%)	219 (96%)	9 (4%)	32 58
11	K	975/975 (100%)	950 (97%)	25 (3%)	46 67
All	All	2610/2610 (100%)	2493 (96%)	117 (4%)	31 54

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	20	LYS
1	A	28	LYS
1	A	67	MET
1	A	68	HIS
1	A	86	ILE
1	A	89	LEU
1	A	95	THR
1	A	106	TRP
1	A	175	THR
1	A	214	GLU
1	A	217	LEU
1	A	230	ASN
1	A	234	LYS
1	A	243	ARG
1	A	249	LEU
1	A	266	THR
1	A	272	GLN
1	A	277	HIS
1	A	278	ARG
1	A	285	ILE
1	A	299	ILE
1	A	330	LEU
1	A	331	MET
1	A	364	LEU
2	B	19	ASP

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Mol	Chain	Res	Type
2	B	24	SER
2	B	94	TYR
2	B	105	ASP
2	B	128	ASP
2	B	135	ASN
2	B	180	SER
2	B	185	LEU
3	C	6	SER
3	C	8	ARG
3	C	56	LYS
3	C	58	THR
3	C	75	ASP
3	C	82	LYS
3	C	145	LYS
4	D	25	MET
4	D	27	THR
4	D	31	LYS
4	D	59	SER
4	D	66	ASN
4	D	72	GLU
4	D	74	LEU
4	D	98	ILE
4	D	106	LEU
5	E	2	SER
5	E	79	VAL
5	E	97	ASP
6	F	8	CYS
6	F	12	CYS
6	F	23	CYS
6	F	32	ARG
6	F	49	CYS
6	F	54	SER
6	F	72	CYS
6	F	84	SER
6	F	98	ARG
6	F	102	MET
6	F	110	ARG
6	F	145	LEU
7	G	11	PHE
7	G	17	ARG
7	G	30	HIS
7	G	34	THR

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Mol	Chain	Res	Type
7	G	50	ARG
7	G	51	TRP
7	G	57	ARG
8	H	26	LEU
8	H	32	ASN
8	H	45	ARG
9	I	7	TYR
9	I	11	CYS
9	I	33	GLN
9	I	61	ARG
9	I	68	ASN
9	I	117	VAL
9	I	148	VAL
9	I	162	HIS
9	I	209	ASP
10	J	8	ASN
10	J	11	ARG
10	J	53	THR
10	J	68	LYS
10	J	97	ASP
10	J	127	PRO
10	J	221	ASP
10	J	241	ASP
10	J	243	GLU
11	K	20	ARG
11	K	37	ASP
11	K	55	ARG
11	K	69	THR
11	K	135	TRP
11	K	167	LYS
11	K	186	LEU
11	K	219	ASP
11	K	252	TYR
11	K	270	ASP
11	K	299	GLU
11	K	435	GLN
11	K	463	GLU
11	K	575	GLU
11	K	681	ILE
11	K	693	ARG
11	K	708	GLU
11	K	724	ASP

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Mol	Chain	Res	Type
11	K	737	ASP
11	K	810	HIS
11	K	818	ASN
11	K	822	GLN
11	K	823	ILE
11	K	882	MET
11	K	897	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	137	GLN
1	A	176	GLN
1	A	180	HIS
1	A	207	ASN
1	A	314	ASN
2	B	77	ASN
2	B	135	ASN
3	C	84	ASN
3	C	118	ASN
3	C	178	ASN
5	E	5	GLN
5	E	10	ASN
5	E	24	ASN
6	F	163	GLN
7	G	61	ASN
9	I	9	ASN
9	I	21	ASN
9	I	66	ASN
9	I	82	GLN
10	J	103	GLN
11	K	4	ASN
11	K	11	GLN
11	K	30	HIS
11	K	138	ASN
11	K	199	ASN
11	K	204	GLN
11	K	334	HIS
11	K	340	GLN
11	K	668	GLN
11	K	818	ASN

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Mol	Chain	Res	Type
11	K	978	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	N	1158/3741 (30%)	320 (27%)	46 (3%)

All (320) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	N	1225	G
12	N	1229	U
12	N	1233	G
12	N	1239	G
12	N	1242	A
12	N	1243	U
12	N	1244	G
12	N	1249	C
12	N	1260	C
12	N	1261	A
12	N	1262	A
12	N	1264	C
12	N	1266	C
12	N	1267	U
12	N	1366	A
12	N	1368	G
12	N	1369	C
12	N	1377	G
12	N	1380	A
12	N	1381	U
12	N	1382	G
12	N	1390	A
12	N	1392	C
12	N	1397	U
12	N	1411	G
12	N	1417	C
12	N	1422	A
12	N	1426	A
12	N	1428	A
12	N	1430	A
12	N	1431	U

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Mol	Chain	Res	Type
12	N	1436	C
12	N	1437	A
12	N	1443	U
12	N	1444	G
12	N	1448	G
12	N	1455	A
12	N	1457	G
12	N	1458	A
12	N	1470	U
12	N	1472	G
12	N	1474	C
12	N	1476	U
12	N	1477	G
12	N	1478	G
12	N	1480	A
12	N	1481	G
12	N	1497	G
12	N	1498	A
12	N	1499	G
12	N	1500	U
12	N	1505	A
12	N	1506	A
12	N	1507	C
12	N	1508	A
12	N	1522	A
12	N	1525	G
12	N	1526	A
12	N	1530	G
12	N	1536	A
12	N	1539	A
12	N	1540	U
12	N	1542	G
12	N	1543	A
12	N	1544	U
12	N	1548	G
12	N	1549	C
12	N	1551	A
12	N	1552	G
12	N	1553	C
12	N	1555	G
12	N	1558	G
12	N	1564	C

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Mol	Chain	Res	Type
12	N	1566	A
12	N	1576	G
12	N	1584	A
12	N	1585	A
12	N	1586	G
12	N	1587	U
12	N	1588	G
12	N	1589	A
12	N	1590	U
12	N	1591	A
12	N	1594	A
12	N	1595	C
12	N	1600	A
12	N	2398	A
12	N	2405	A
12	N	2406	A
12	N	2407	U
12	N	2409	A
12	N	2411	A
12	N	2425	A
12	N	2426	U
12	N	2427	A
12	N	2428	A
12	N	2433	A
12	N	2434	A
12	N	2436	A
12	N	2439	U
12	N	2440	U
12	N	2442	U
12	N	2444	A
12	N	2445	C
12	N	2446	G
12	N	2450	U
12	N	2454	A
12	N	2461	C
12	N	2464	A
12	N	2467	G
12	N	2471	U
12	N	2472	G
12	N	2474	A
12	N	2475	U
12	N	2489	G

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Mol	Chain	Res	Type
12	N	2494	A
12	N	2505	G
12	N	2512	G
12	N	2515	G
12	N	2516	G
12	N	2519	G
12	N	2521	A
12	N	2522	A
12	N	2523	C
12	N	2524	U
12	N	2525	A
12	N	2527	G
12	N	2536	A
12	N	2538	G
12	N	2539	G
12	N	2540	U
12	N	2542	G
12	N	2546	A
12	N	2547	A
12	N	2548	U
12	N	2554	G
12	N	2560	U
12	N	2573	G
12	N	2576	U
12	N	2579	A
12	N	2581	G
12	N	2583	A
12	N	2599	C
12	N	2600	U
12	N	2601	G
12	N	2603	C
12	N	2604	C
12	N	2619	G
12	N	2630	G
12	N	2638	A
12	N	2639	A
12	N	2640	C
12	N	2641	G
12	N	2651	A
12	N	2652	A
12	N	2654	A
12	N	2657	G

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Mol	Chain	Res	Type
12	N	2659	G
12	N	2663	A
12	N	2664	A
12	N	2665	A
12	N	2667	A
12	N	2668	A
12	N	2669	G
12	N	2677	U
12	N	2678	G
12	N	2681	C
12	N	2685	A
12	N	2686	C
12	N	2688	C
12	N	2926	A
12	N	2933	C
12	N	2939	G
12	N	2940	G
12	N	2946	U
12	N	2947	G
12	N	2951	G
12	N	2952	G
12	N	2954	G
12	N	2959	A
12	N	2961	A
12	N	2968	A
12	N	2970	A
12	N	2971	A
12	N	2972	G
12	N	2982	G
12	N	2984	G
12	N	2985	U
12	N	2988	A
12	N	2989	A
12	N	2990	A
12	N	2991	G
12	N	2994	A
12	N	2996	G
12	N	3000	A
12	N	3007	A
12	N	3009	A
12	N	3010	G
12	N	3011	A

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Mol	Chain	Res	Type
12	N	3012	A
12	N	3020	G
12	N	3022	A
12	N	3023	G
12	N	3024	A
12	N	3029	A
12	N	3031	G
12	N	3037	A
12	N	3038	A
12	N	3047	G
12	N	3059	C
12	N	3060	A
12	N	3061	G
12	N	3070	G
12	N	3075	U
12	N	3080	A
12	N	3086	G
12	N	3091	A
12	N	3095	A
12	N	3104	G
12	N	3105	U
12	N	3106	G
12	N	3108	U
12	N	3110	A
12	N	3111	A
12	N	3116	U
12	N	3129	G
12	N	3132	A
12	N	3133	G
12	N	3134	A
12	N	3136	A
12	N	3141	A
12	N	3142	C
12	N	3143	C
12	N	3149	G
12	N	3150	A
12	N	3151	U
12	N	3152	A
12	N	3154	C
12	N	3170	A
12	N	3171	A
12	N	3176	U

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Mol	Chain	Res	Type
12	N	3177	C
12	N	3178	A
12	N	3179	U
12	N	3180	A
12	N	3188	U
12	N	3192	U
12	N	3193	U
12	N	3194	U
12	N	3204	G
12	N	3205	A
12	N	3206	U
12	N	3207	G
12	N	3208	U
12	N	3210	G
12	N	3220	A
12	N	3221	U
12	N	3229	A
12	N	3231	G
12	N	3232	C
12	N	3233	A
12	N	3234	G
12	N	3243	A
12	N	3258	C
12	N	3260	C
12	N	3268	C
12	N	3269	A
12	N	3271	G
12	N	3274	A
12	N	3275	C
12	N	3276	G
12	N	3278	G
12	N	3280	G
12	N	3284	G
12	N	3285	G
12	N	3287	U
12	N	3292	C
12	N	3303	C
12	N	3304	A
12	N	3305	G
12	N	3311	U
12	N	3312	U
12	N	3316	C

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Mol	Chain	Res	Type
12	N	3317	C
12	N	3319	U
12	N	3323	G
12	N	3327	U
12	N	3328	C
12	N	3329	A
12	N	3330	A
12	N	3331	U
12	N	3332	U
12	N	3333	G
12	N	3339	G
12	N	3348	G
12	N	3357	A
12	N	3364	G
12	N	3366	G
12	N	3375	A
12	N	3377	G
12	N	3384	C
12	N	3385	A
12	N	3392	U
12	N	3393	G
12	N	3395	A
12	N	3396	G
12	N	3414	G
12	N	3422	C
12	N	3428	C
12	N	3430	A
12	N	3434	G
12	N	3437	G
12	N	3438	G
12	N	3440	U
12	N	3452	G
12	N	3454	C
12	N	3455	U
12	N	3458	A
12	N	3466	A
12	N	3467	U

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	N	1265	U

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Mol	Chain	Res	Type
12	N	1443	U
12	N	1457	G
12	N	1477	G
12	N	1525	G
12	N	1536	A
12	N	1538	A
12	N	1540	U
12	N	1542	G
12	N	1550	U
12	N	1565	G
12	N	1583	G
12	N	1588	G
12	N	2411	A
12	N	2426	U
12	N	2443	G
12	N	2445	C
12	N	2470	C
12	N	2515	G
12	N	2538	G
12	N	2546	A
12	N	2547	A
12	N	2560	U
12	N	2651	A
12	N	2664	A
12	N	2951	G
12	N	2956	G
12	N	2995	G
12	N	3022	A
12	N	3060	A
12	N	3105	U
12	N	3134	A
12	N	3170	A
12	N	3205	A
12	N	3206	U
12	N	3219	U
12	N	3231	G
12	N	3283	G
12	N	3291	A
12	N	3303	C
12	N	3316	C
12	N	3384	C
12	N	3392	U

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Mol	Chain	Res	Type
12	N	3452	G
12	N	3457	U
12	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

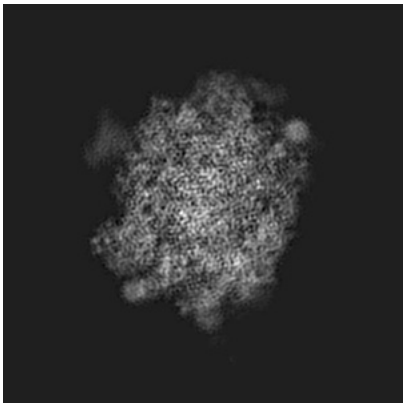
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3146. These allow visual inspection of the internal detail of the map and identification of artifacts.

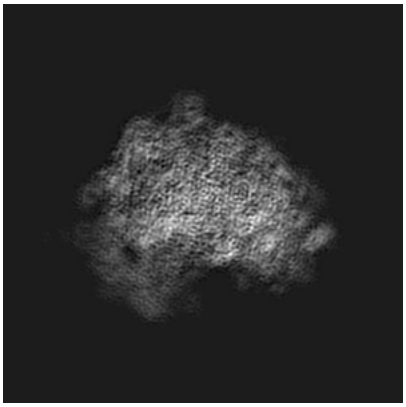
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

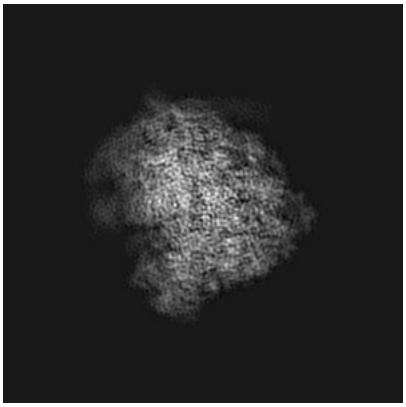
6.1.1 Primary map



X



Y

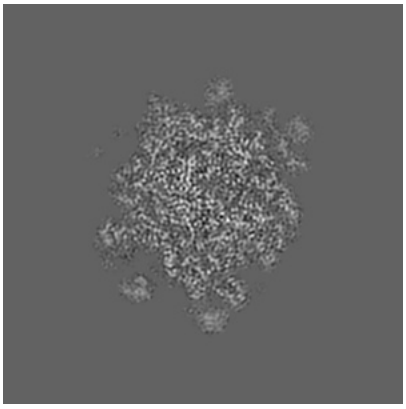


Z

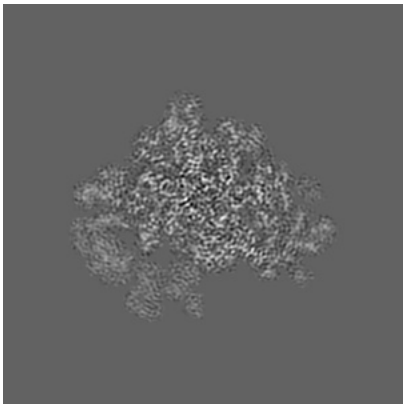
The images above show the map projected in three orthogonal directions.

6.2 Central slices

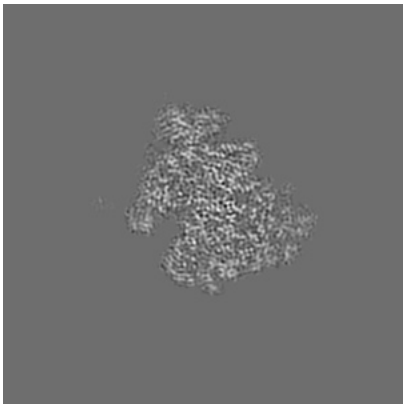
6.2.1 Primary map



X Index: 150



Y Index: 150

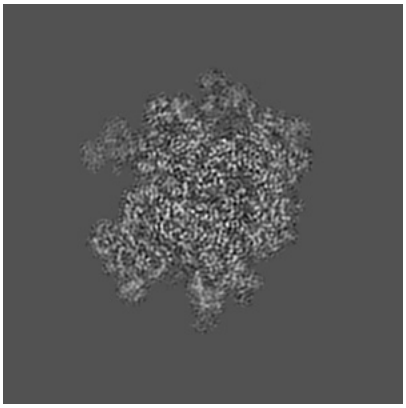


Z Index: 150

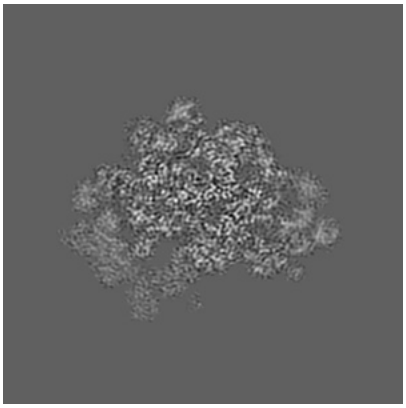
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

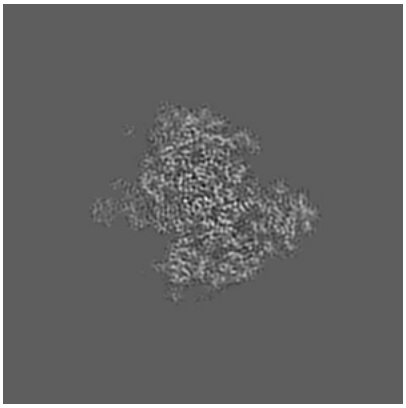
6.3.1 Primary map



X Index: 137



Y Index: 155

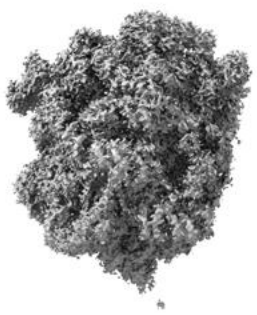


Z Index: 140

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

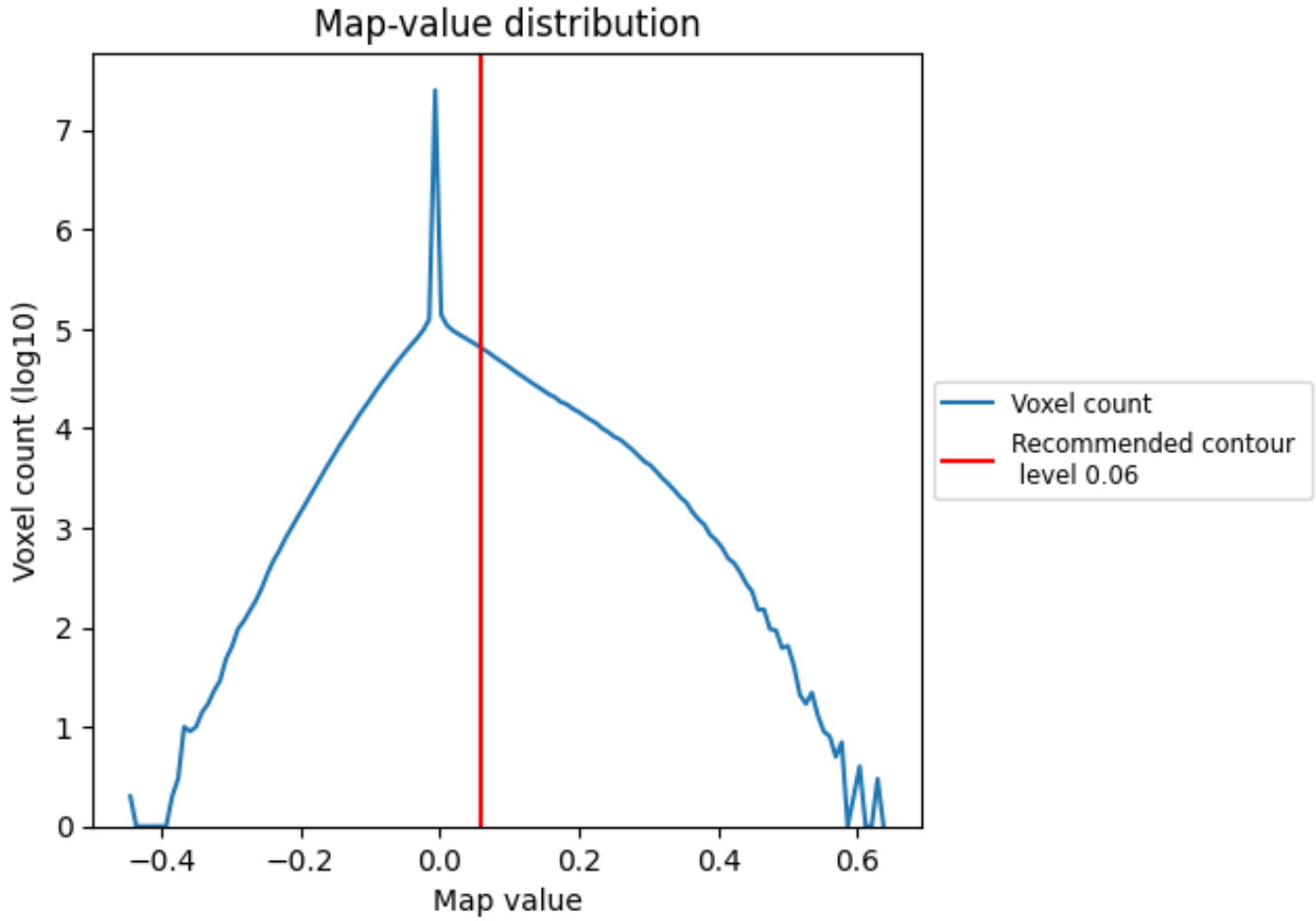
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

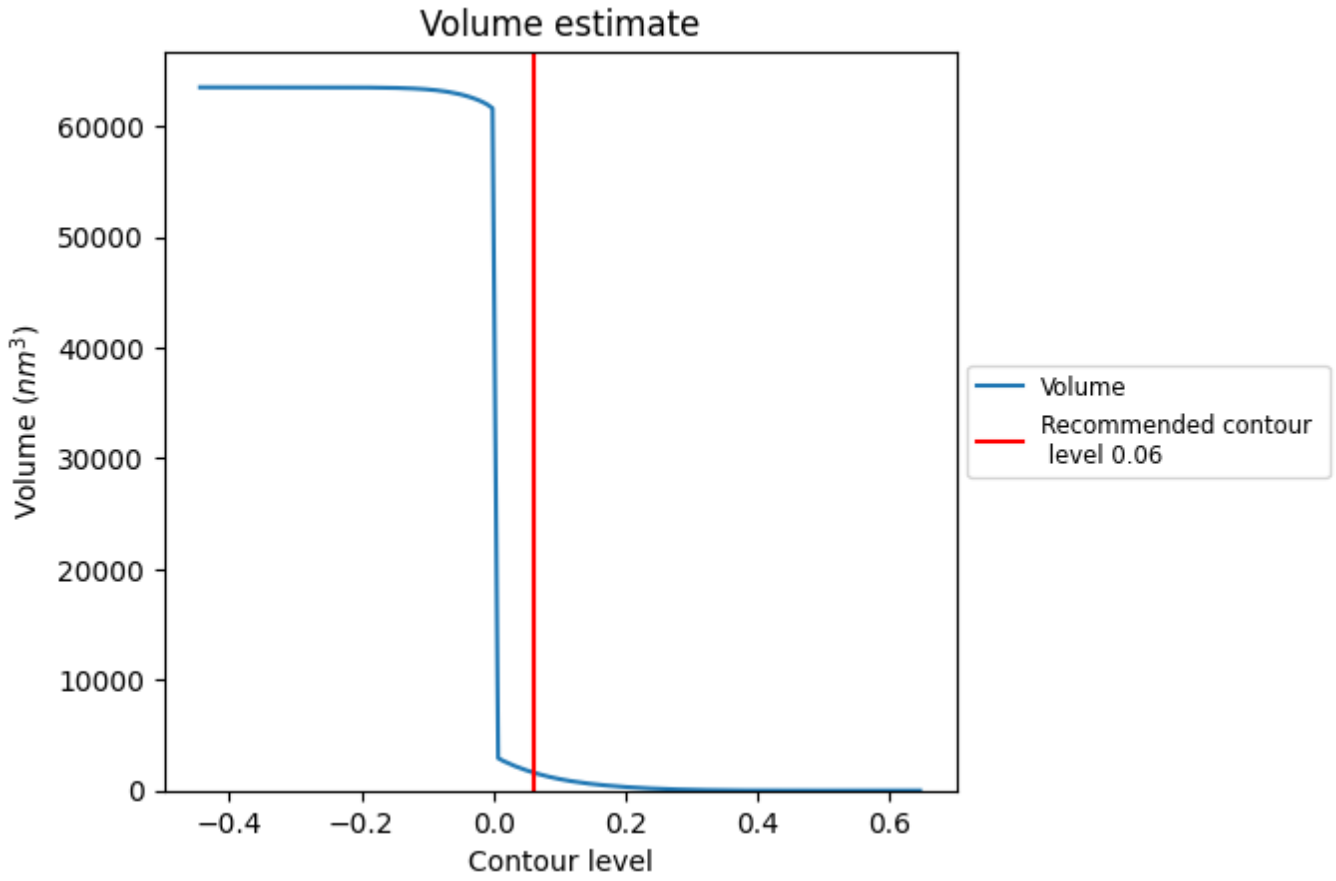
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

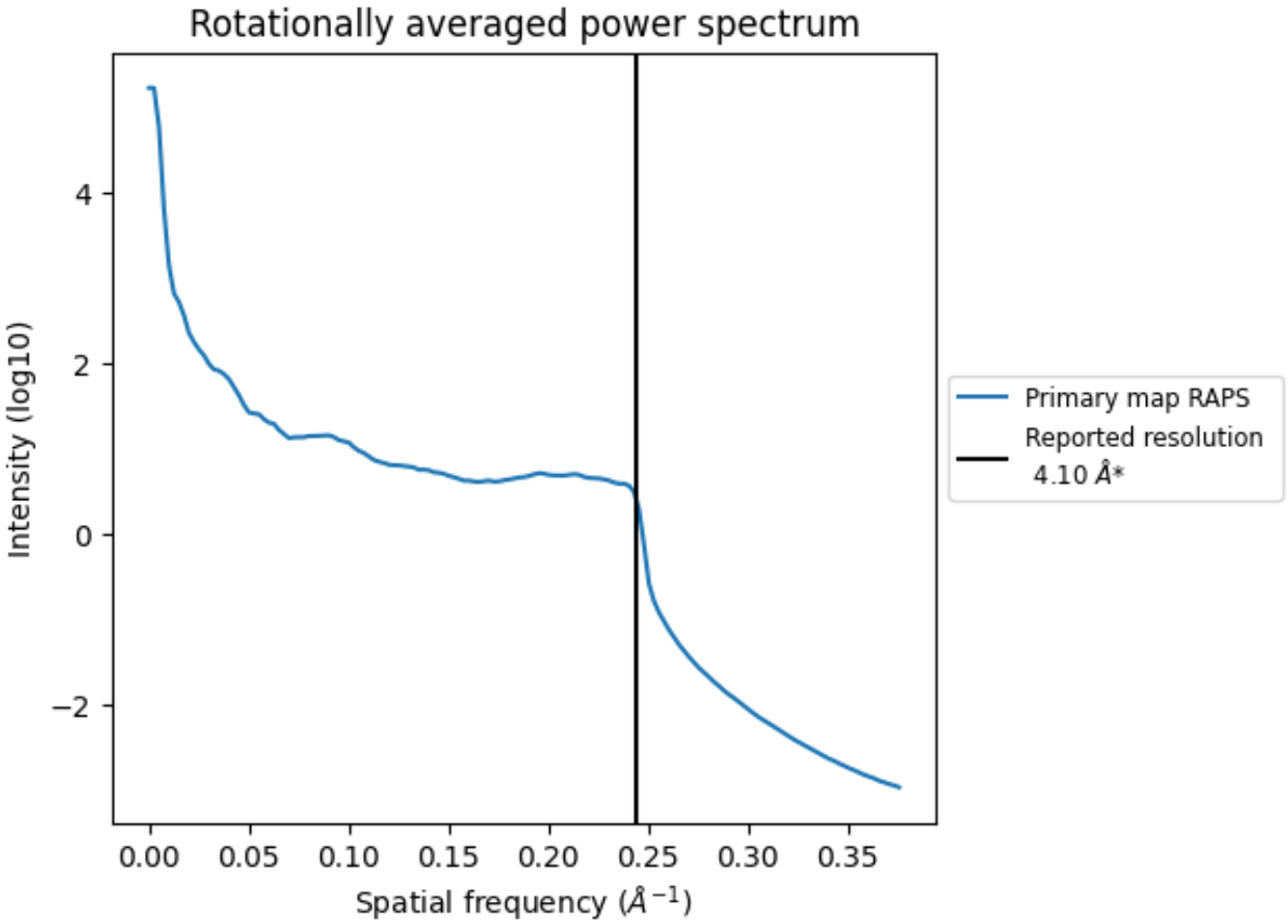
7.2 Volume estimate (i)



The volume at the recommended contour level is 1641 nm^3; this corresponds to an approximate mass of 1483 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

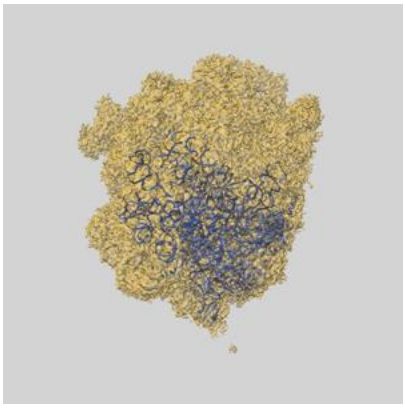
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

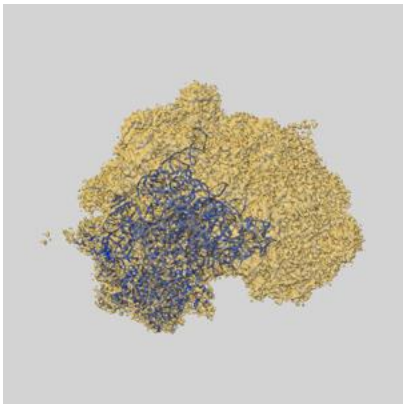
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3146 and PDB model 5ANB. Per-residue inclusion information can be found in section 3 on page 6.

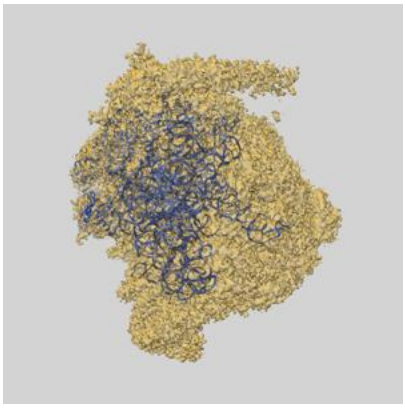
9.1 Map-model overlay



X



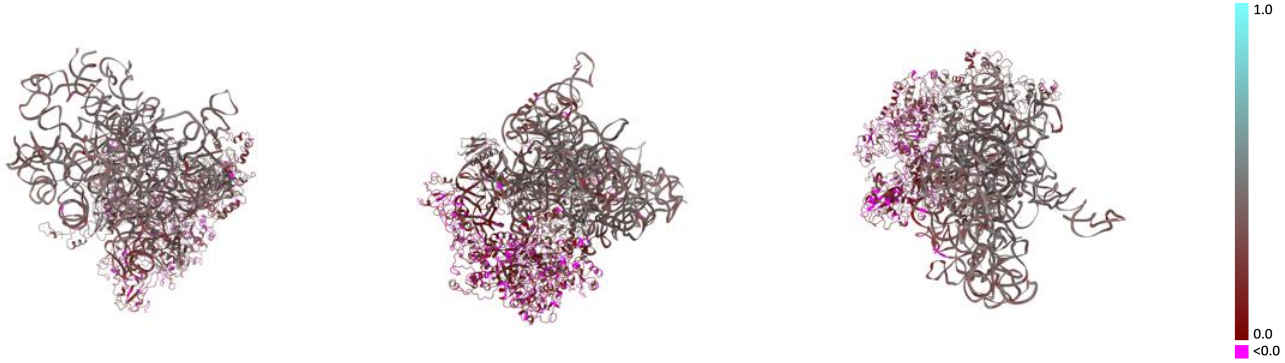
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

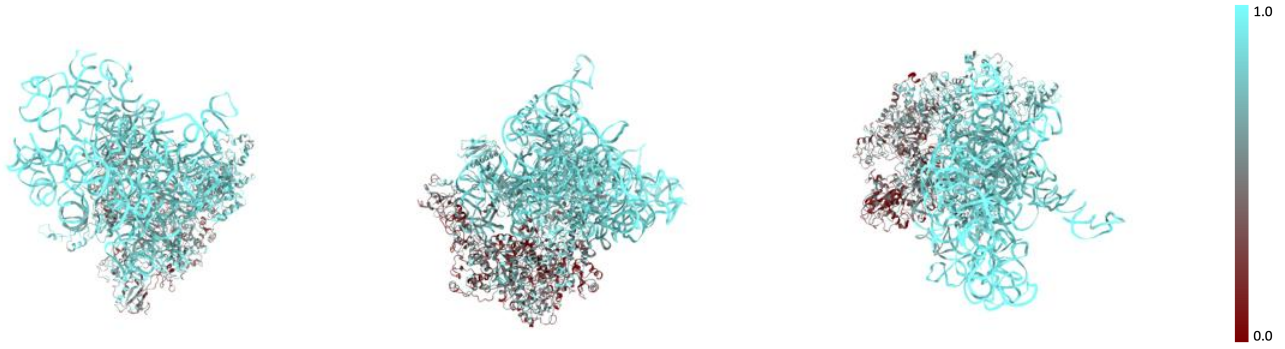
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

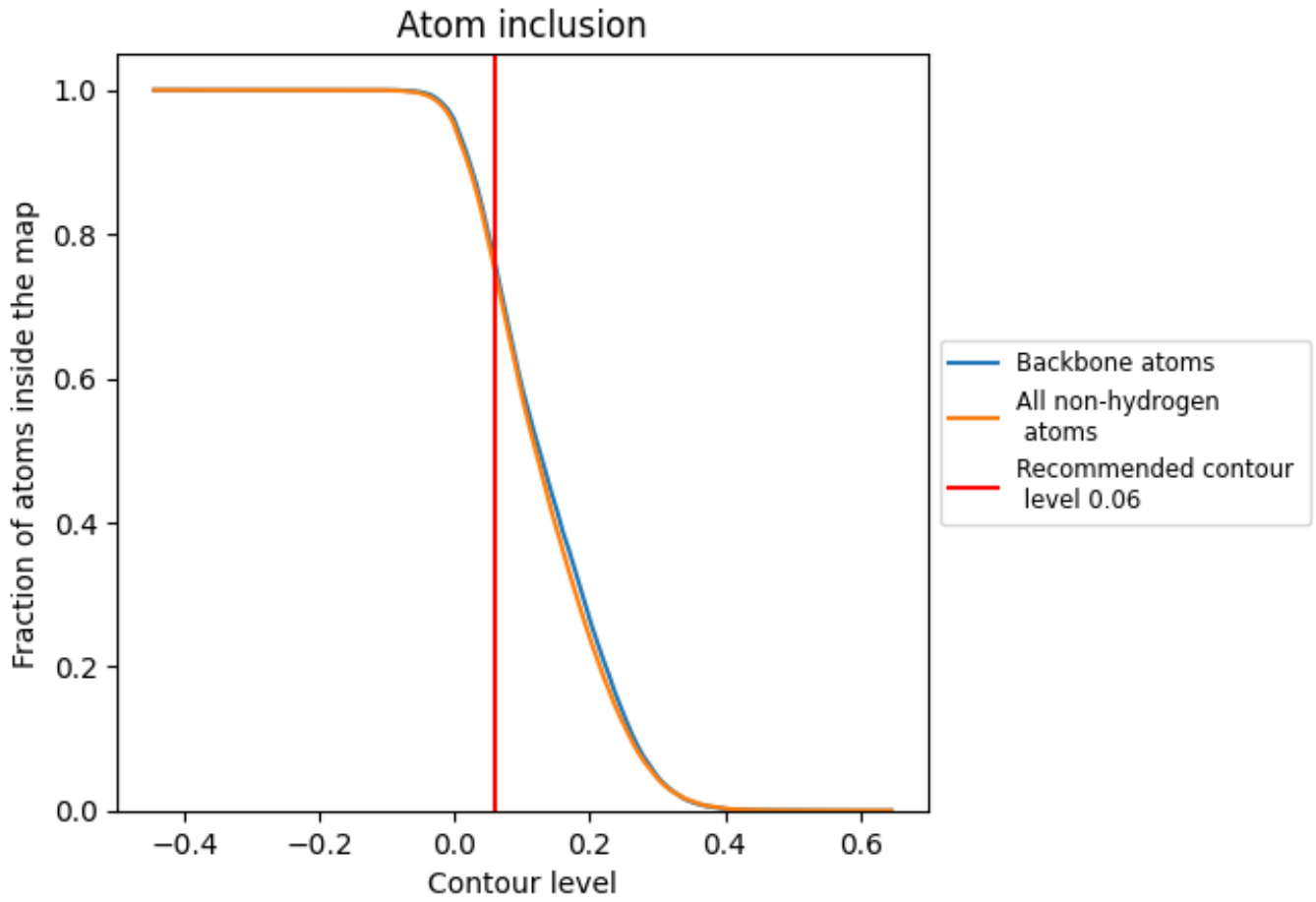
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7487	0.2980
A	0.8223	0.3540
B	0.7936	0.3380
C	0.3800	0.1330
D	0.4586	0.1310
E	0.7934	0.3840
F	0.8067	0.3690
G	0.8042	0.3130
H	0.7627	0.3590
I	0.6578	0.2510
J	0.5237	0.2240
K	0.4131	0.1290
N	0.9086	0.3660