Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 05:23 AM JST

PDB ID	:	5XYM
EMDB ID	:	EMD-6789
Title	:	Large subunit of Mycobacterium smegmatis
Authors	:	Li, Z.; Ge, X.; Zhang, Y.; Zheng, L.; Sanyal, S.; Gao, N.
Deposited on	:	2017-07-09
Resolution	:	3.08 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:

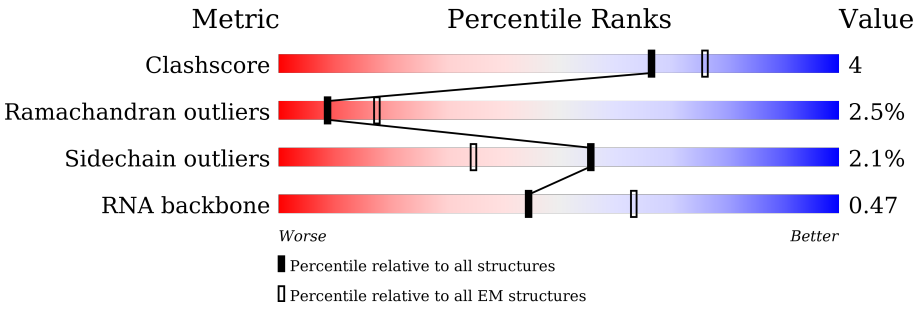
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.08 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	0	57	11% 89%
2	1	54	17% 37% 39% 6% 19%
3	2	47	6% 98%
4	3	64	92% 5%
5	4	37	5% 68% 30%
6	A	3164	65% 19% 16%
7	B	118	68% 27%

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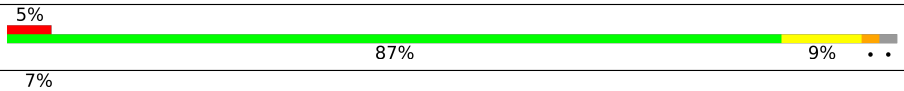
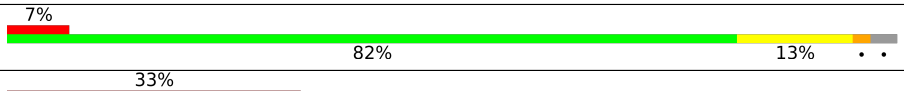
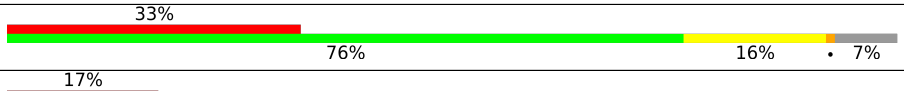
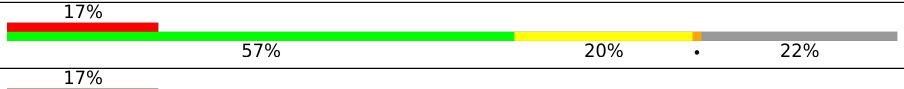
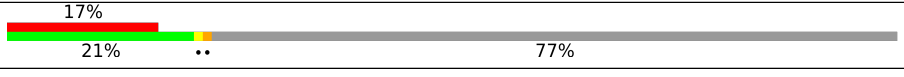
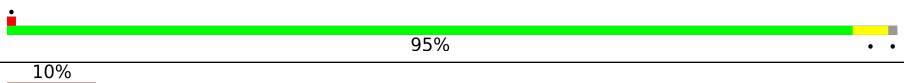
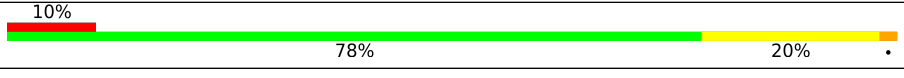
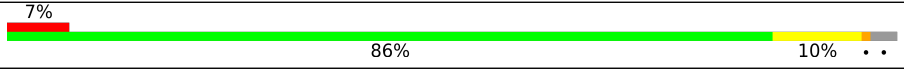
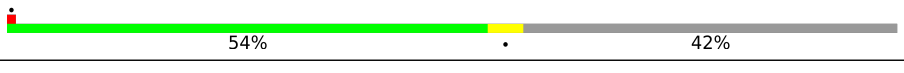
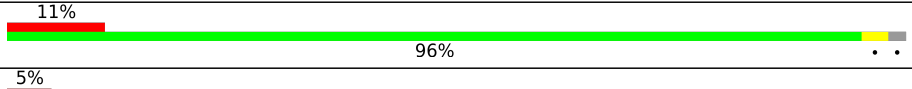
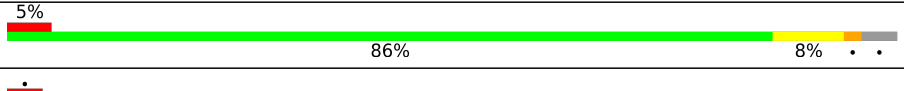
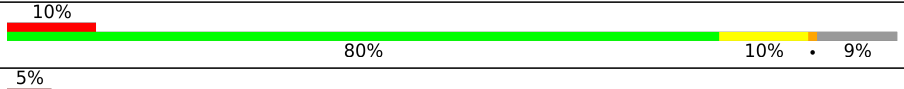
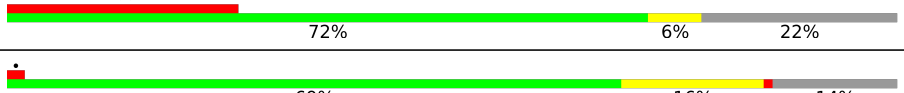
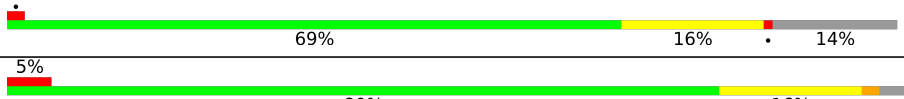
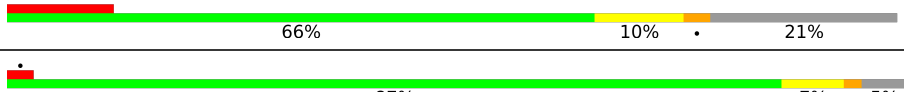
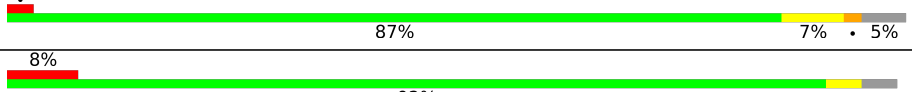
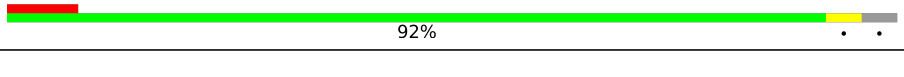
Mol	Chain	Length	Quality of chain
8	C	278	
9	D	217	
10	E	215	
11	F	187	
12	G	179	
13	H	151	
14	J	147	
15	K	122	
16	L	147	
17	M	138	
18	N	199	
19	O	127	
20	P	113	
21	Q	129	
22	R	103	
23	S	153	
24	T	100	
25	U	105	
26	V	215	
27	W	88	
28	X	64	
29	Y	77	
30	Z	61	
31	a	24	

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 84069 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 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	55	432	266	95	70	1	0	0

- Molecule 2 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	44	384	242	81	61	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	225	97	54	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	3	63	502	302	115	85	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	37	298	181	66	46	5	0	0

- Molecule 6 is a RNA chain called 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	A	2665	57277	25527	10588	18497	2665	0	0

- Molecule 7 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	116	Total	C	N	O	P	0	0
			2477	1106	457	798	116		

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	273	Total	C	N	O	S	0	0
			2097	1290	435	368	4		

- Molecule 9 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	212	Total	C	N	O	S	0	0
			1578	977	308	288	5		

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	208	Total	C	N	O	S	0	0
			1560	963	293	302	2		

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	174	Total	C	N	O	S	0	0
			1372	862	254	250	6		

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	139	Total	C	N	O	S	0	0
			1074	676	199	198	1		

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	34	Total	C	N	O	S	0	0
			255	164	43	47	1		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	144	Total	C	N	O	S	0	0
			1070	670	204	193	3		

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	134	Total	C	N	O	S	0	0
			1079	683	211	183	2		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	116	Total	C	N	O	S	0	0
			910	572	177	159	2		

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	107	Total	C	N	O	0	0
			815	500	173	142		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	P	111	Total	C	N	O	0	0
			888	559	166	163		

- Molecule 21 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Q	124	Total 988	C 613	N 203	O 172	0	0

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	R	100	Total 754	C 478	N 137	O 139	0	0

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	S	111	Total 850	C 528	N 168	O 154	0	0

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	T	91	Total 715	C 456	N 129	O 130	0	0

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	83	Total 636	C 399	N 120	O 115	S 2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	V	168	Total 1264	C 785	N 229	O 250	0	0

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	W	76	Total 563	C 347	N 117	O 99	0	0

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	62	Total	C	N	O	S	0	0
			465	280	102	79	4		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	61	Total	C	N	O	S	0	0
			516	316	100	99	1		

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Z	58	Total	C	N	O	0	0
			470	290	94	86		

- Molecule 31 is a protein called Uncharacterized protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	a	23	Total	C	N	O	0	0
			189	111	50	28		

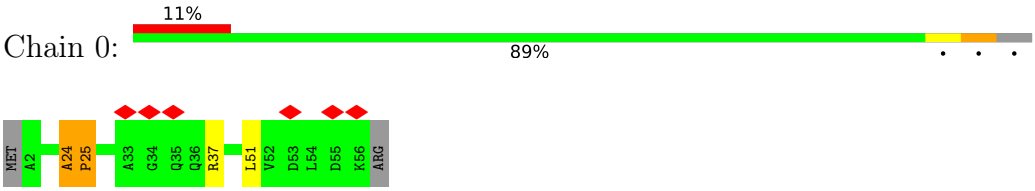
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	146	Total	Mg	0
			146	146	

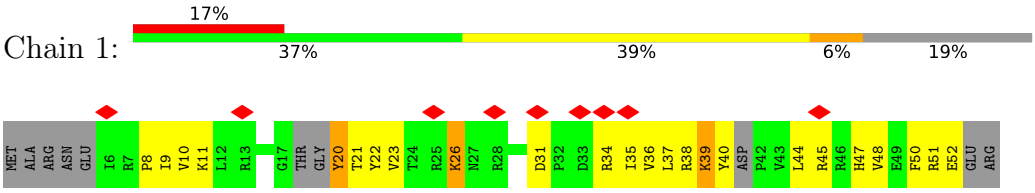
3 Residue-property plots (i)

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.

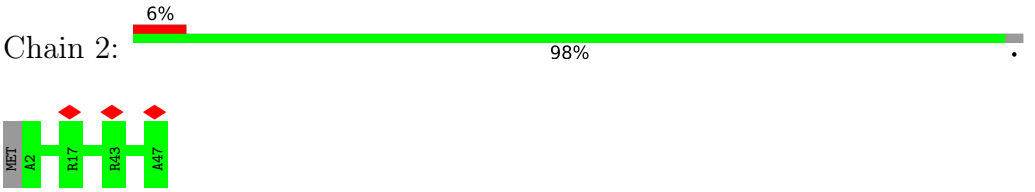
• Molecule 1: 50S ribosomal protein L32



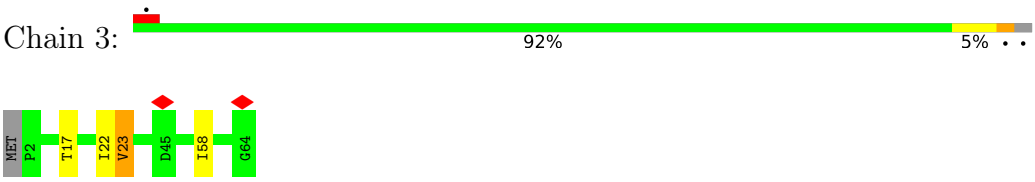
• Molecule 2: 50S ribosomal protein L33 2



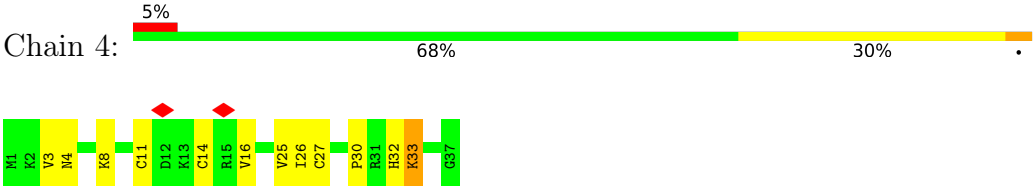
• Molecule 3: 50S ribosomal protein L34



• Molecule 4: 50S ribosomal protein L35

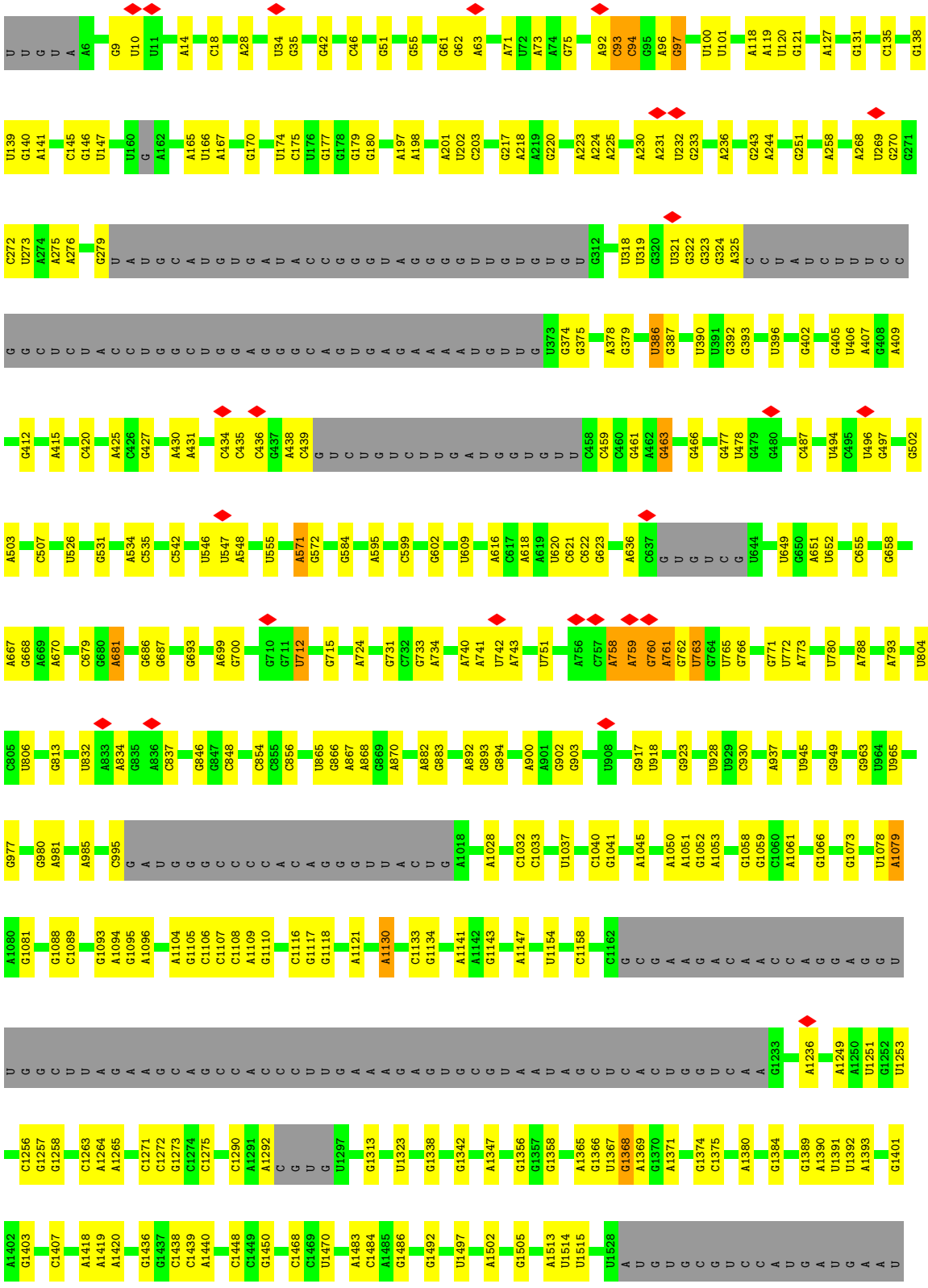


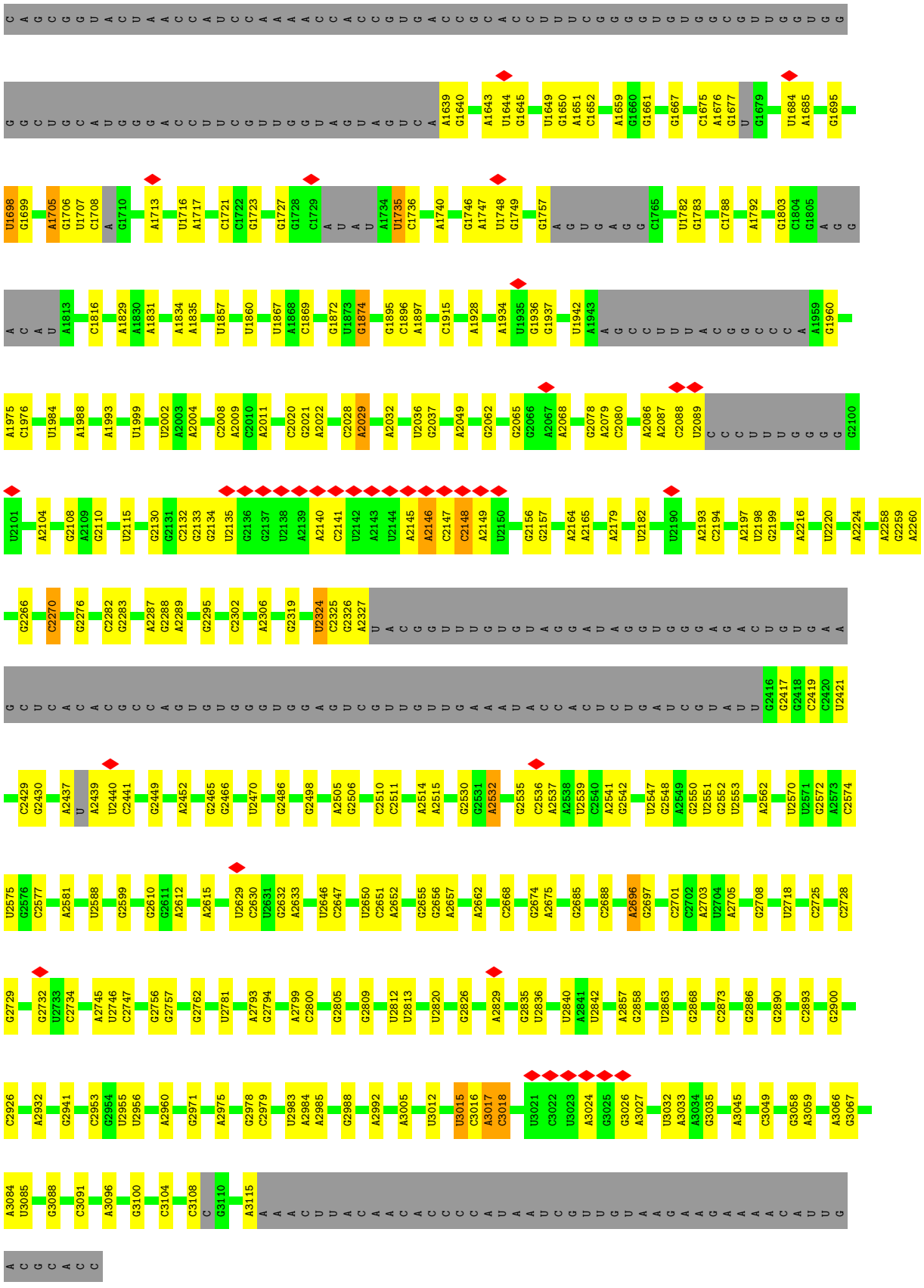
• Molecule 5: 50S ribosomal protein L36



• Molecule 6: 23S RNA

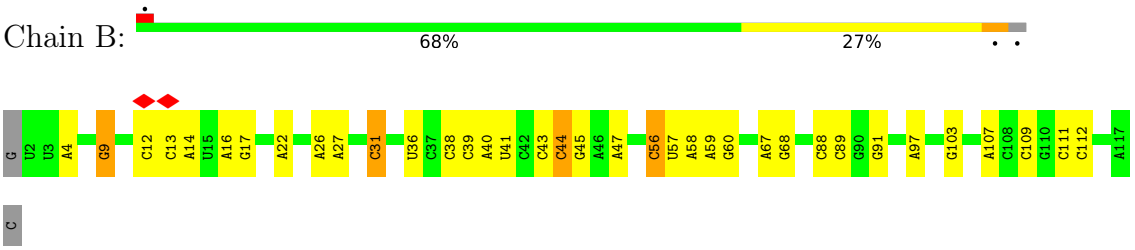
Chain A:





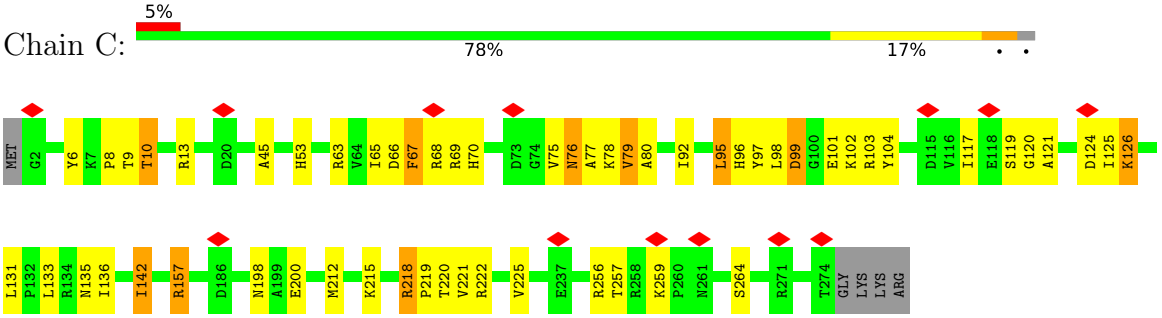
• Molecule 7: 5S RNA

Chain B:



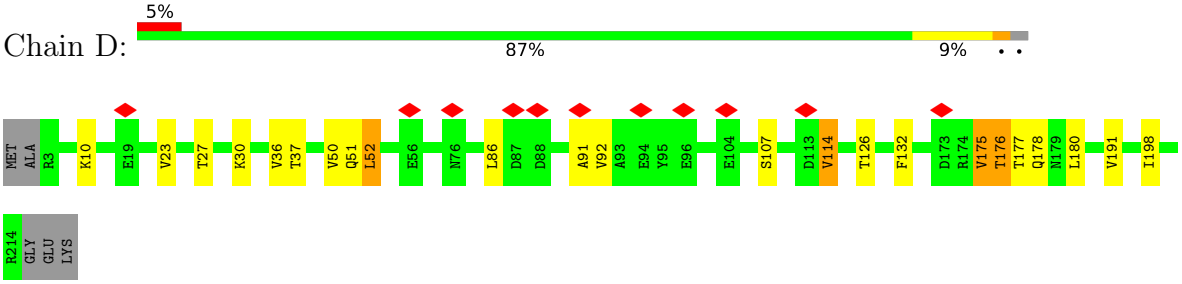
• Molecule 8: 50S ribosomal protein L2

Chain C:



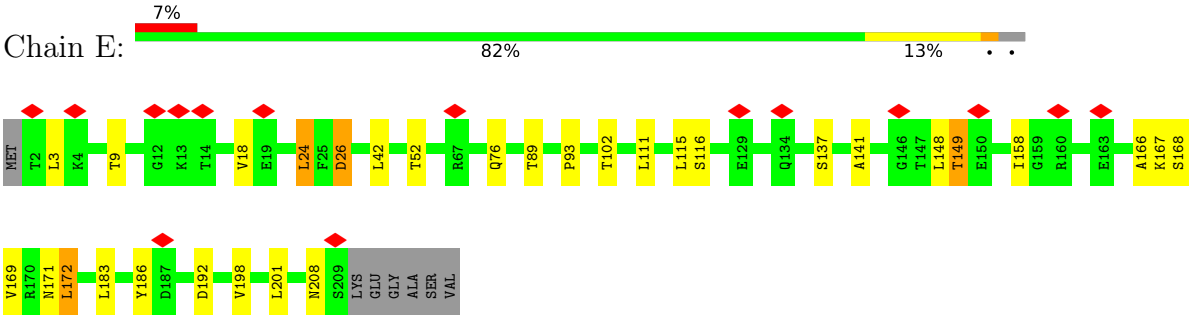
• Molecule 9: 50S ribosomal protein L3

Chain D:



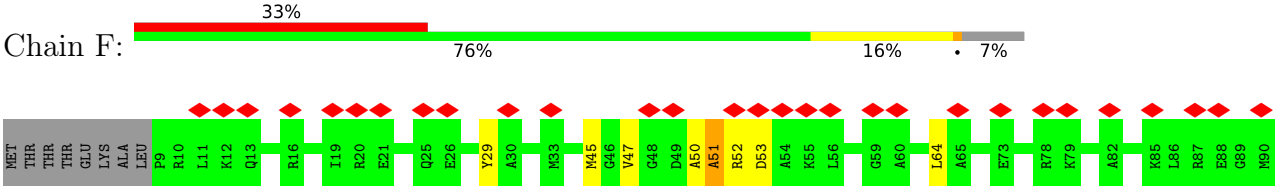
• Molecule 10: 50S ribosomal protein L4

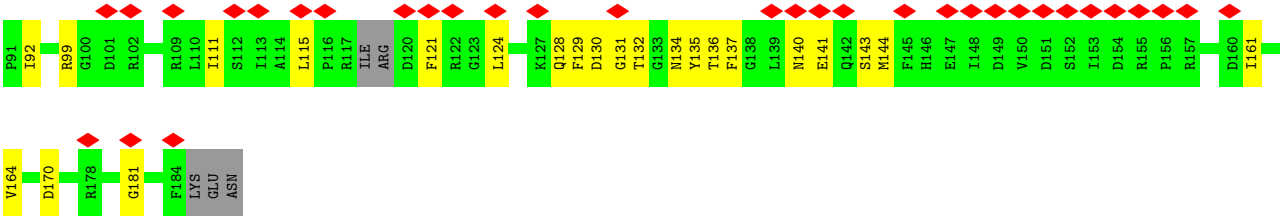
Chain E:



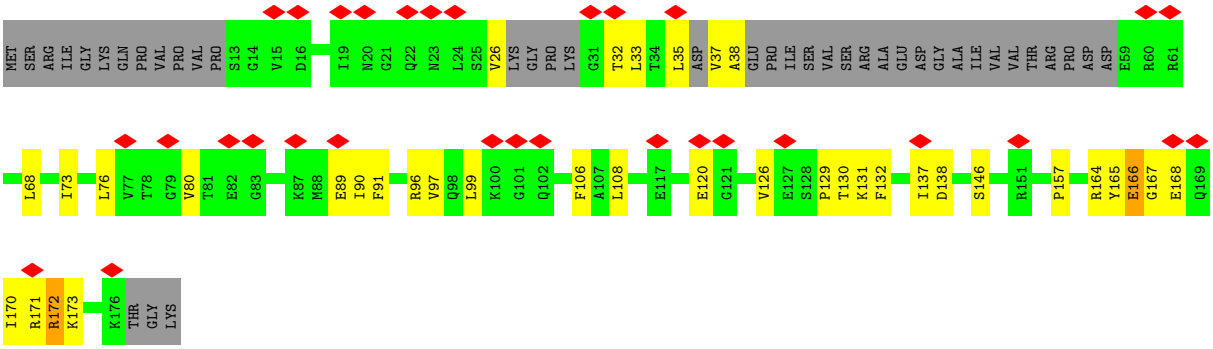
• Molecule 11: 50S ribosomal protein L5

Chain F:

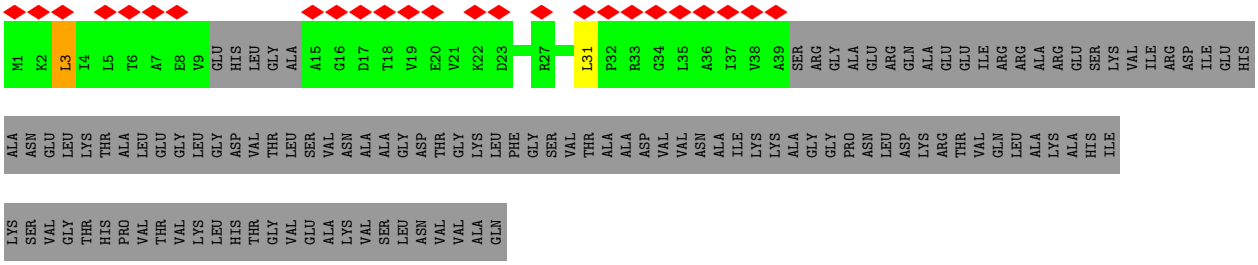




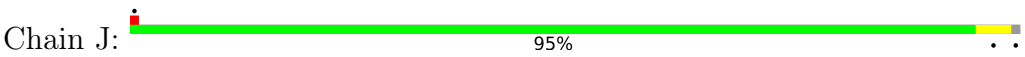
• Molecule 12: 50S ribosomal protein L6

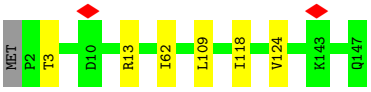


• Molecule 13: 50S ribosomal protein L9

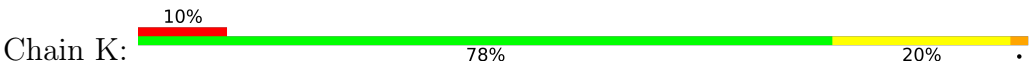


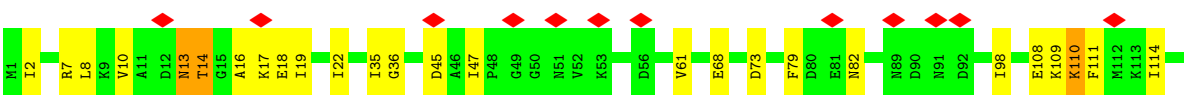
• Molecule 14: 50S ribosomal protein L13





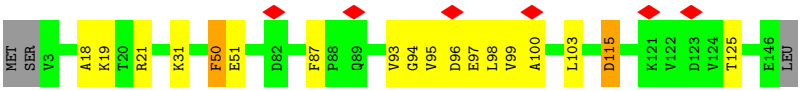
• Molecule 15: 50S ribosomal protein L14





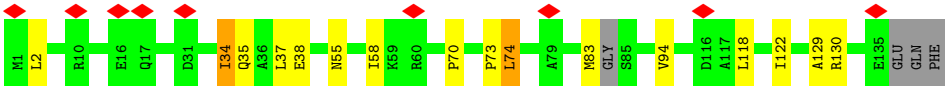
• Molecule 16: 50S ribosomal protein L15

Chain L:



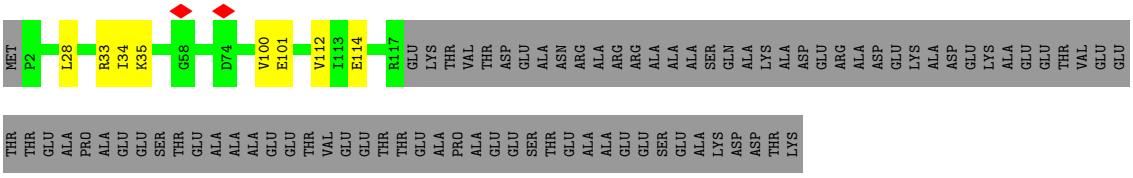
• Molecule 17: 50S ribosomal protein L16

Chain M:



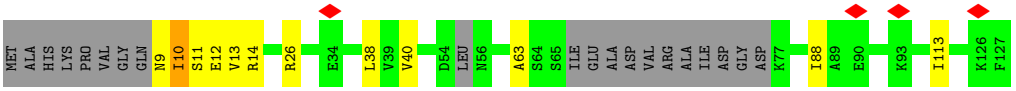
• Molecule 18: 50S ribosomal protein L17

Chain N:



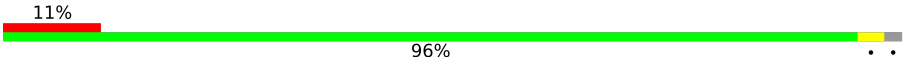
• Molecule 19: 50S ribosomal protein L18

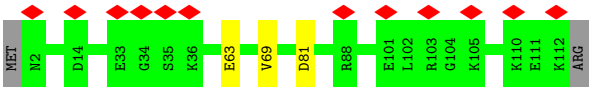
Chain O:



• Molecule 20: 50S ribosomal protein L19

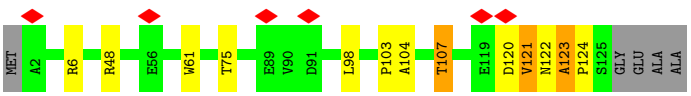
Chain P:





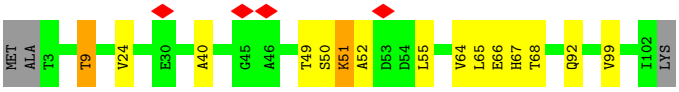
• Molecule 21: 50S ribosomal protein L20

Chain Q:



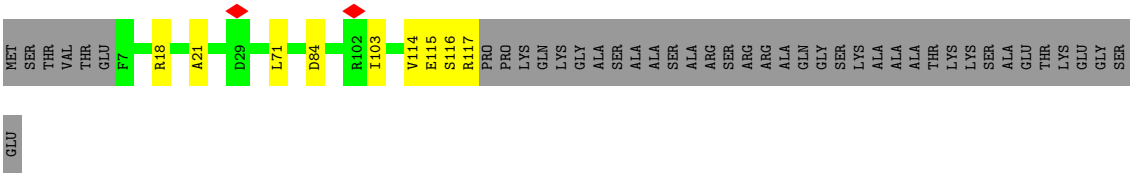
• Molecule 22: 50S ribosomal protein L21

Chain R:



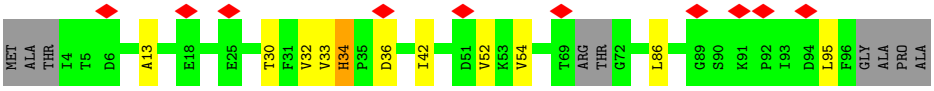
• Molecule 23: 50S ribosomal protein L22

Chain S:



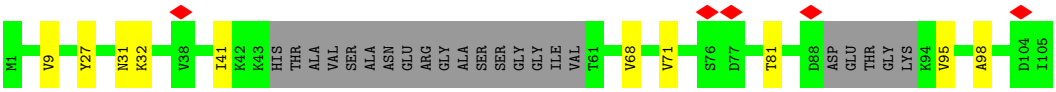
• Molecule 24: 50S ribosomal protein L23

Chain T:



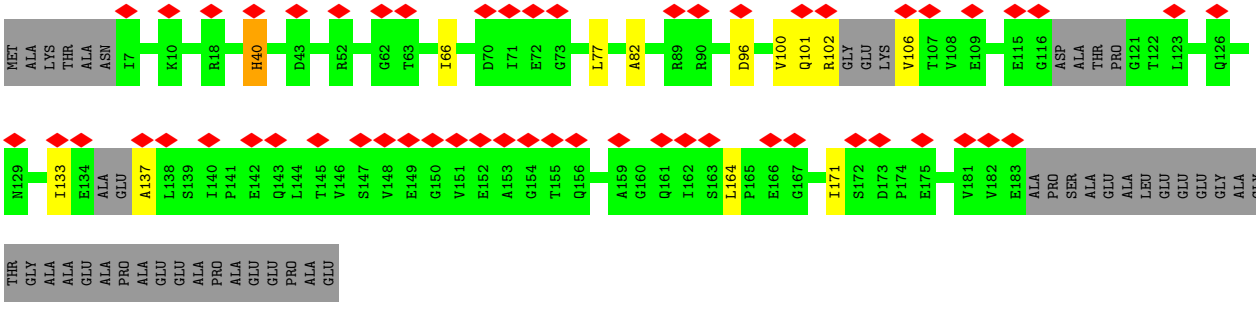
• Molecule 25: 50S ribosomal protein L24

Chain U:



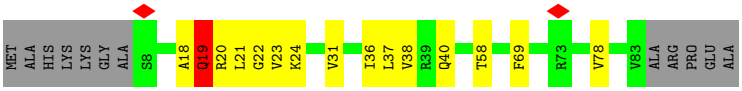
• Molecule 26: 50S ribosomal protein L25

Chain V:

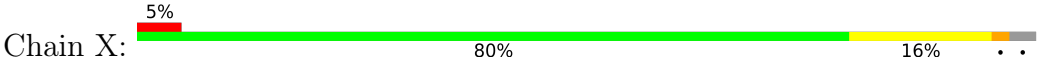


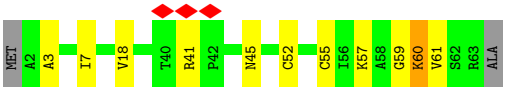
• Molecule 27: 50S ribosomal protein L27

Chain W:

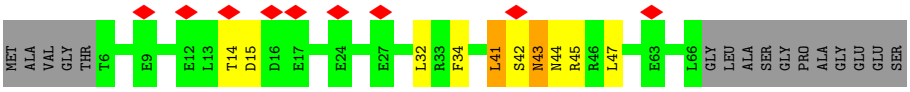


• Molecule 28: 50S ribosomal protein L28

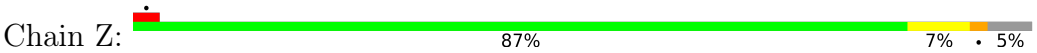


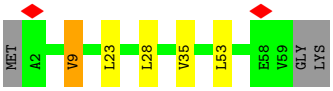


• Molecule 29: 50S ribosomal protein L29

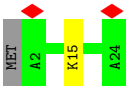


• Molecule 30: 50S ribosomal protein L30





• Molecule 31: Uncharacterized protein bL37



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71351	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.395	Depositor
Minimum map value	-0.243	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	369.6, 369.6, 369.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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: MG

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	0	0.37	0/436	0.66	0/583
2	1	0.37	0/389	0.69	0/518
3	2	0.38	0/380	0.69	0/500
4	3	0.37	0/507	0.64	0/672
5	4	0.48	0/302	0.80	0/401
6	A	0.19	0/64129	0.65	0/100026
7	B	0.19	0/2770	0.65	0/4316
8	C	0.41	0/2140	0.65	0/2879
9	D	0.37	0/1600	0.58	0/2153
10	E	0.39	0/1583	0.59	0/2142
11	F	0.37	0/1393	0.60	0/1874
12	G	0.38	0/1086	0.59	0/1456
13	H	0.37	0/256	0.52	0/344
14	J	0.36	0/1157	0.51	0/1567
15	K	0.36	0/946	0.61	0/1268
16	L	0.37	0/1083	0.58	0/1446
17	M	0.37	0/1104	0.57	0/1486
18	N	0.36	0/927	0.54	0/1244
19	O	0.36	0/821	0.58	0/1099
20	P	0.37	0/902	0.58	0/1212
21	Q	0.41	0/1000	0.65	0/1341
22	R	0.32	0/764	0.55	0/1030
23	S	0.35	0/862	0.58	0/1168
24	T	0.37	0/724	0.59	0/971
25	U	0.39	0/640	0.59	0/854
26	V	0.33	0/1274	0.52	0/1734
27	W	0.40	0/571	0.64	0/765
28	X	0.38	0/473	0.63	0/634
29	Y	0.40	0/519	0.70	0/693
30	Z	0.37	0/473	0.64	0/635
31	a	0.37	0/191	0.70	0/247
All	All	0.25	0/91402	0.64	0/137258

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	432	0	476	2	0
2	1	384	0	408	74	0
3	2	377	0	411	0	0
4	3	502	0	541	2	0
5	4	298	0	321	9	0
6	A	57277	0	28842	112	0
7	B	2477	0	1262	6	0
8	C	2097	0	2149	72	0
9	D	1578	0	1622	15	0
10	E	1560	0	1593	19	0
11	F	1372	0	1387	36	0
12	G	1074	0	1114	79	0
13	H	255	0	272	1	0
14	J	1130	0	1167	2	0
15	K	938	0	1000	29	0
16	L	1070	0	1140	22	0
17	M	1079	0	1118	18	0
18	N	910	0	953	8	0
19	O	815	0	851	12	0
20	P	888	0	913	2	0
21	Q	988	0	1038	18	0
22	R	754	0	802	15	0
23	S	850	0	889	4	0
24	T	715	0	756	8	0
25	U	636	0	689	6	0
26	V	1264	0	1296	11	0
27	W	563	0	576	8	0
28	X	465	0	476	4	0
29	Y	516	0	528	8	0
30	Z	470	0	497	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	189	0	205	0	0
32	A	146	0	0	0	0
All	All	84069	0	55292	546	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 (546) 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)
6:A:2145:A:O2'	6:A:2147:C:N4	1.57	1.35
2:1:26:LYS:NZ	2:1:34:ARG:HG2	1.41	1.34
2:1:22:TYR:OH	6:A:2575:U:H5'	1.28	1.29
12:G:89:GLU:HG3	12:G:166:GLU:OE1	1.34	1.25
2:1:26:LYS:CE	2:1:34:ARG:HH11	1.49	1.25
2:1:11:LYS:HG2	2:1:23:VAL:CG2	1.66	1.25
12:G:90:ILE:CG2	12:G:130:THR:HA	1.70	1.19
21:Q:123:ALA:HB1	21:Q:124:PRO:HA	1.23	1.18
2:1:26:LYS:HE3	2:1:34:ARG:NH1	1.59	1.17
8:C:121:ALA:O	8:C:135:ASN:ND2	1.77	1.17
6:A:758:A:N1	6:A:759:A:N6	1.92	1.15
6:A:405:G:N3	10:E:171:ASN:ND2	1.96	1.14
6:A:2542:G:H5'	11:F:134:ASN:ND2	1.59	1.13
6:A:1705:A:N1	6:A:1736:C:O2	1.82	1.11
6:A:2542:G:H5'	11:F:134:ASN:HD21	1.04	1.11
6:A:759:A:N3	6:A:760:G:C8	2.20	1.10
2:1:26:LYS:CE	2:1:34:ARG:NH1	2.12	1.10
11:F:135:TYR:CE2	11:F:137:PHE:HD2	1.71	1.08
12:G:96:ARG:HG3	12:G:129:PRO:HB3	1.33	1.08
8:C:101:GLU:OE2	8:C:103:ARG:CZ	2.02	1.07
11:F:131:GLY:HA2	11:F:170:ASP:OD1	1.55	1.06
6:A:2542:G:C5'	11:F:134:ASN:HD21	1.69	1.06
2:1:11:LYS:HG2	2:1:23:VAL:HG21	1.29	1.05
8:C:53:HIS:CE1	8:C:220:THR:HG23	1.91	1.05
2:1:26:LYS:HE2	2:1:34:ARG:HH11	1.14	1.04
8:C:101:GLU:OE2	8:C:103:ARG:NE	1.91	1.04
12:G:91:PHE:CE2	12:G:164:ARG:HD3	1.93	1.02
2:1:31:ASP:OD2	2:1:35:ILE:HG13	1.59	1.01
6:A:3017:A:O2'	6:A:3018:C:O4'	1.78	1.01
12:G:90:ILE:HG21	12:G:130:THR:HA	1.41	1.00
12:G:90:ILE:HG22	12:G:130:THR:CA	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:90:ILE:HG22	12:G:130:THR:HA	1.39	1.00
2:1:21:THR:HG1	2:1:22:TYR:HD2	1.04	0.99
6:A:758:A:N1	6:A:759:A:C6	2.31	0.97
2:1:22:TYR:OH	6:A:2575:U:C5'	2.11	0.97
2:1:11:LYS:HA	2:1:23:VAL:HG22	1.44	0.97
2:1:26:LYS:HZ1	2:1:34:ARG:HG2	1.14	0.97
12:G:91:PHE:CD2	12:G:164:ARG:HD3	2.00	0.96
6:A:759:A:H61	6:A:763:U:H3	1.12	0.96
11:F:135:TYR:HE2	11:F:137:PHE:CD2	1.85	0.95
15:K:110:LYS:HE2	15:K:110:LYS:N	1.82	0.95
11:F:135:TYR:HE2	11:F:137:PHE:HD2	1.07	0.95
12:G:33:LEU:HD12	12:G:80:VAL:HG23	1.49	0.94
2:1:36:VAL:CG2	2:1:51:ARG:HG2	1.98	0.92
12:G:91:PHE:CD2	12:G:164:ARG:CD	2.52	0.92
2:1:26:LYS:HZ3	2:1:34:ARG:HG2	1.33	0.92
2:1:31:ASP:OD2	2:1:35:ILE:CG1	2.18	0.92
12:G:90:ILE:HG23	12:G:130:THR:HG23	1.53	0.91
11:F:135:TYR:CE2	11:F:137:PHE:CD2	2.58	0.90
8:C:95:LEU:HD12	8:C:95:LEU:H	1.37	0.90
12:G:90:ILE:CG2	12:G:130:THR:CA	2.47	0.90
6:A:758:A:C2	6:A:759:A:C6	2.60	0.89
2:1:11:LYS:HG2	2:1:23:VAL:HG22	1.54	0.88
8:C:120:GLY:O	8:C:131:LEU:HD23	1.73	0.88
8:C:69:ARG:NH1	8:C:119:SER:OG	2.06	0.88
2:1:36:VAL:HG22	2:1:51:ARG:HG2	1.53	0.88
24:T:33:VAL:HG21	24:T:42:ILE:HD11	1.56	0.88
12:G:89:GLU:CG	12:G:166:GLU:OE1	2.21	0.87
6:A:2146:A:O2'	6:A:2147:C:H5'	1.73	0.87
12:G:33:LEU:HD21	12:G:137:ILE:HG13	1.54	0.87
11:F:131:GLY:HA2	11:F:170:ASP:CG	1.93	0.87
6:A:759:A:N6	6:A:763:U:H3	1.73	0.86
12:G:96:ARG:CG	12:G:129:PRO:HB3	2.05	0.86
12:G:99:LEU:HD23	12:G:126:VAL:HG12	1.55	0.86
8:C:96:HIS:CD2	8:C:102:LYS:HE2	2.10	0.86
6:A:2147:C:O2'	6:A:2148:C:H5'	1.74	0.86
16:L:96:ASP:O	16:L:99:VAL:HG22	1.75	0.85
5:4:11:CYS:SG	5:4:14:CYS:N	2.49	0.85
6:A:1271:C:O2'	21:Q:123:ALA:HB3	1.74	0.84
11:F:131:GLY:CA	11:F:170:ASP:OD1	2.25	0.84
12:G:126:VAL:HG23	12:G:131:LYS:O	1.77	0.84
12:G:90:ILE:CG2	12:G:130:THR:HG23	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1705:A:C2	6:A:1736:C:O2	2.30	0.84
11:F:50:ALA:O	11:F:52:ARG:N	2.09	0.84
2:1:11:LYS:CG	2:1:23:VAL:CG2	2.54	0.83
6:A:759:A:C2	6:A:760:G:C8	2.65	0.83
29:Y:41:LEU:HG	29:Y:42:SER:O	1.78	0.83
10:E:172:LEU:HD23	10:E:172:LEU:H	1.44	0.82
6:A:760:G:O2'	6:A:761:A:O5'	1.97	0.82
12:G:91:PHE:CE1	12:G:164:ARG:NH2	2.47	0.82
8:C:80:ALA:HB2	8:C:96:HIS:CE1	2.15	0.82
2:1:22:TYR:HH	6:A:2575:U:H5'	1.41	0.82
21:Q:123:ALA:CB	21:Q:124:PRO:HA	2.06	0.81
2:1:36:VAL:HG22	2:1:51:ARG:CG	2.11	0.81
2:1:21:THR:OG1	2:1:22:TYR:CD2	2.33	0.81
18:N:100:VAL:HG21	18:N:112:VAL:HG23	1.64	0.80
6:A:2146:A:C2'	6:A:2147:C:H5'	2.12	0.80
6:A:2148:C:O2'	6:A:2149:A:O5'	1.98	0.80
6:A:3017:A:O2'	6:A:3018:C:O5'	1.99	0.79
16:L:94:GLY:N	16:L:97:GLU:HG3	1.98	0.78
12:G:91:PHE:CD1	12:G:164:ARG:NH2	2.52	0.78
12:G:91:PHE:CD2	12:G:164:ARG:HD2	2.20	0.77
22:R:64:VAL:O	22:R:65:LEU:HD23	1.84	0.77
26:V:102:ARG:HA	26:V:137:ALA:HB3	1.66	0.77
2:1:11:LYS:CA	2:1:23:VAL:HG22	2.15	0.77
6:A:758:A:C2'	6:A:759:A:H5'	2.15	0.76
6:A:2145:A:O2'	6:A:2147:C:C4	2.36	0.76
2:1:26:LYS:CE	2:1:34:ARG:HG2	2.14	0.76
16:L:21:ARG:HG3	16:L:21:ARG:HH11	1.50	0.76
21:Q:120:ASP:O	21:Q:121:VAL:CG2	2.33	0.75
12:G:91:PHE:CZ	12:G:164:ARG:NH2	2.54	0.75
6:A:760:G:HO2'	6:A:761:A:P	2.07	0.75
8:C:66:ASP:O	8:C:68:ARG:N	2.18	0.75
12:G:170:ILE:HD12	12:G:170:ILE:H	1.51	0.75
17:M:37:LEU:O	17:M:38:GLU:HG2	1.86	0.75
6:A:2542:G:C5'	11:F:134:ASN:ND2	2.40	0.74
25:U:31:ASN:O	25:U:68:VAL:HG23	1.87	0.74
6:A:2530:G:H21	11:F:136:THR:HG21	1.52	0.74
6:A:759:A:N3	6:A:760:G:H8	1.86	0.73
15:K:17:LYS:HE2	15:K:45:ASP:OD2	1.87	0.73
2:1:45:ARG:NH2	6:A:740:A:H5'	2.04	0.73
8:C:96:HIS:HD2	8:C:102:LYS:HE2	1.51	0.73
21:Q:120:ASP:O	21:Q:121:VAL:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:110:LYS:HE2	15:K:110:LYS:CA	2.18	0.72
2:1:11:LYS:CG	2:1:23:VAL:HG22	2.16	0.72
26:V:40:HIS:CE1	26:V:101:GLN:CG	2.72	0.72
12:G:35:LEU:HD12	12:G:73:ILE:HD13	1.72	0.72
2:1:26:LYS:NZ	2:1:34:ARG:CG	2.37	0.72
12:G:35:LEU:HD12	12:G:76:LEU:HD13	1.70	0.72
22:R:40:ALA:O	22:R:55:LEU:HD11	1.90	0.72
2:1:31:ASP:OD2	2:1:35:ILE:CD1	2.38	0.71
16:L:94:GLY:H	16:L:97:GLU:HG3	1.54	0.71
26:V:40:HIS:CE1	26:V:101:GLN:HG3	2.26	0.71
12:G:33:LEU:HD12	12:G:80:VAL:CG2	2.22	0.70
15:K:13:ASN:O	15:K:14:THR:HG22	1.91	0.70
12:G:170:ILE:HD12	12:G:170:ILE:N	2.06	0.70
17:M:37:LEU:O	17:M:38:GLU:CG	2.39	0.70
27:W:18:ALA:C	27:W:19:GLN:HG2	2.10	0.70
22:R:40:ALA:O	22:R:55:LEU:CD1	2.39	0.70
2:1:21:THR:OG1	2:1:22:TYR:HD2	1.71	0.70
17:M:37:LEU:C	17:M:38:GLU:HG2	2.12	0.70
12:G:96:ARG:HG3	12:G:129:PRO:CB	2.17	0.70
16:L:95:VAL:HG22	16:L:125:THR:O	1.91	0.70
2:1:44:LEU:O	2:1:45:ARG:HB2	1.92	0.69
6:A:759:A:C2	6:A:760:G:N7	2.60	0.69
21:Q:123:ALA:HB1	21:Q:124:PRO:CA	2.14	0.69
12:G:89:GLU:OE2	12:G:131:LYS:HE3	1.92	0.69
2:1:36:VAL:HG22	2:1:51:ARG:CB	2.21	0.69
8:C:79:VAL:HA	8:C:95:LEU:HB3	1.75	0.69
2:1:22:TYR:HE1	6:A:2575:U:OP1	1.75	0.69
8:C:80:ALA:CB	8:C:96:HIS:CE1	2.76	0.68
12:G:37:VAL:HG12	12:G:38:ALA:N	2.07	0.68
6:A:2146:A:HO2'	6:A:2147:C:H5'	1.59	0.68
2:1:36:VAL:CG2	2:1:51:ARG:CG	2.70	0.68
12:G:33:LEU:HD22	12:G:138:ASP:OD1	1.93	0.68
12:G:35:LEU:CD1	12:G:76:LEU:HD13	2.24	0.67
8:C:63:ARG:HG3	8:C:63:ARG:HH11	1.59	0.67
2:1:11:LYS:CG	2:1:23:VAL:HG21	2.16	0.67
12:G:90:ILE:HG22	12:G:130:THR:C	2.14	0.67
16:L:18:ALA:O	16:L:19:LYS:HB3	1.95	0.67
2:1:26:LYS:HE3	2:1:34:ARG:HH12	1.57	0.67
8:C:95:LEU:HD12	8:C:103:ARG:O	1.95	0.67
6:A:2757:G:N7	12:G:173:LYS:NZ	2.42	0.66
12:G:33:LEU:HD21	12:G:137:ILE:CG1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:109:LYS:O	15:K:110:LYS:HB2	1.93	0.66
24:T:33:VAL:HG21	24:T:42:ILE:CD1	2.24	0.66
21:Q:120:ASP:C	21:Q:121:VAL:HG22	2.16	0.66
24:T:33:VAL:O	24:T:34:HIS:O	2.12	0.66
6:A:759:A:N3	6:A:760:G:N7	2.43	0.66
6:A:2146:A:H2'	6:A:2147:C:O4'	1.96	0.66
26:V:40:HIS:CE1	26:V:101:GLN:HG2	2.31	0.65
12:G:89:GLU:OE2	12:G:131:LYS:CE	2.44	0.65
2:1:36:VAL:HG21	2:1:51:ARG:NE	2.11	0.65
8:C:79:VAL:HA	8:C:95:LEU:HA	1.77	0.65
2:1:26:LYS:HZ1	2:1:34:ARG:CG	1.99	0.65
2:1:34:ARG:HB2	2:1:52:GLU:OE2	1.96	0.65
10:E:172:LEU:HD23	10:E:172:LEU:N	2.12	0.65
8:C:66:ASP:OD1	8:C:69:ARG:HA	1.97	0.65
12:G:91:PHE:CG	12:G:164:ARG:NH2	2.64	0.65
15:K:13:ASN:OD1	15:K:14:THR:N	2.29	0.65
8:C:76:ASN:N	8:C:76:ASN:HD22	1.94	0.65
12:G:90:ILE:HG22	12:G:130:THR:O	1.97	0.64
2:1:31:ASP:OD2	2:1:35:ILE:HD11	1.97	0.64
12:G:35:LEU:CD1	12:G:73:ILE:HD13	2.27	0.64
8:C:78:LYS:O	8:C:79:VAL:HG22	1.97	0.64
12:G:129:PRO:O	12:G:130:THR:HB	1.97	0.64
25:U:27:TYR:HD2	25:U:32:LYS:O	1.80	0.64
19:O:9:ASN:CB	19:O:13:VAL:HG23	2.27	0.64
9:D:86:LEU:HD11	9:D:92:VAL:HG13	1.79	0.64
11:F:45:MET:HG3	11:F:64:LEU:HD11	1.79	0.64
12:G:99:LEU:CD2	12:G:126:VAL:HG12	2.25	0.64
12:G:91:PHE:CE2	12:G:164:ARG:NH2	2.65	0.64
2:1:51:ARG:NH1	2:1:51:ARG:HB3	2.13	0.64
29:Y:43:ASN:OD1	29:Y:43:ASN:N	2.30	0.64
2:1:44:LEU:HD12	2:1:48:VAL:HG21	1.81	0.63
8:C:78:LYS:O	8:C:79:VAL:HG13	1.97	0.63
8:C:75:VAL:C	8:C:76:ASN:HD22	1.99	0.63
12:G:170:ILE:H	12:G:170:ILE:CD1	2.11	0.63
23:S:115:GLU:OE2	23:S:117:ARG:NH2	2.31	0.63
9:D:50:VAL:HG12	9:D:52:LEU:CD1	2.27	0.63
12:G:90:ILE:CG2	12:G:130:THR:CG2	2.77	0.63
5:4:30:PRO:O	5:4:33:LYS:HG2	1.99	0.62
22:R:50:SER:O	22:R:52:ALA:N	2.32	0.62
6:A:759:A:N1	6:A:763:U:C2	2.68	0.62
10:E:24:LEU:HD21	10:E:208:ASN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:35:GLN:NE2	17:M:130:ARG:NH1	2.48	0.62
12:G:171:ARG:HH11	12:G:171:ARG:HB3	1.63	0.62
27:W:22:GLY:H	27:W:24:LYS:NZ	1.98	0.62
2:1:10:VAL:O	2:1:23:VAL:HG13	2.00	0.62
12:G:89:GLU:OE2	12:G:131:LYS:NZ	2.33	0.62
6:A:758:A:C2	6:A:759:A:C5	2.88	0.61
10:E:137:SER:O	10:E:168:SER:OG	2.18	0.61
6:A:1271:C:O2'	21:Q:123:ALA:CB	2.46	0.61
25:U:81:THR:HG21	25:U:98:ALA:HB1	1.82	0.61
24:T:32:VAL:HG23	24:T:32:VAL:O	2.00	0.61
5:4:30:PRO:CG	12:G:171:ARG:HE	2.14	0.61
11:F:50:ALA:O	11:F:51:ALA:C	2.39	0.61
19:O:38:LEU:HD21	19:O:88:ILE:HD13	1.82	0.61
11:F:47:VAL:O	11:F:92:ILE:O	2.19	0.61
22:R:51:LYS:O	22:R:51:LYS:HG2	2.01	0.61
15:K:17:LYS:CE	15:K:45:ASP:OD2	2.49	0.60
8:C:218:ARG:HB2	8:C:219:PRO:CD	2.31	0.60
9:D:27:THR:HG21	9:D:198:ILE:HG12	1.82	0.60
10:E:26:ASP:HA	10:E:116:SER:HB3	1.84	0.60
15:K:110:LYS:HE2	15:K:110:LYS:H	1.67	0.60
8:C:101:GLU:OE2	8:C:103:ARG:NH2	2.35	0.60
22:R:49:THR:HG22	22:R:49:THR:O	2.01	0.60
11:F:47:VAL:O	11:F:47:VAL:HG13	2.01	0.60
11:F:131:GLY:HA2	11:F:170:ASP:OD2	2.00	0.59
2:1:51:ARG:HB3	2:1:51:ARG:CZ	2.32	0.59
6:A:406:U:O2	10:E:167:LYS:NZ	2.24	0.59
22:R:65:LEU:O	22:R:66:GLU:HG2	2.02	0.59
24:T:33:VAL:O	24:T:33:VAL:HG23	2.01	0.59
6:A:780:U:H5"	16:L:19:LYS:HB2	1.85	0.59
8:C:124:ASP:OD1	8:C:125:ILE:N	2.35	0.59
10:E:141:ALA:HB1	10:E:169:VAL:HG12	1.85	0.59
2:1:9:ILE:HG22	2:1:23:VAL:HG11	1.85	0.59
6:A:758:A:O2'	6:A:759:A:H5'	2.03	0.59
8:C:65:ILE:CG2	8:C:67:PHE:CE2	2.85	0.58
19:O:9:ASN:HB3	19:O:13:VAL:HG23	1.84	0.58
26:V:101:GLN:O	26:V:102:ARG:HG3	2.02	0.58
6:A:405:G:C2	10:E:171:ASN:ND2	2.70	0.58
2:1:36:VAL:CG1	2:1:51:ARG:HG2	2.33	0.58
15:K:110:LYS:HE2	15:K:110:LYS:HA	1.85	0.58
6:A:759:A:C2	6:A:760:G:H8	2.20	0.58
8:C:80:ALA:CB	8:C:96:HIS:HE1	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:122:ASN:O	21:Q:123:ALA:HB3	2.04	0.58
27:W:20:ARG:HD3	27:W:20:ARG:N	2.18	0.58
9:D:86:LEU:HD13	9:D:91:ALA:HB3	1.85	0.58
11:F:137:PHE:CZ	11:F:161:ILE:HD11	2.39	0.58
8:C:9:THR:C	8:C:10:THR:HG23	2.24	0.57
26:V:102:ARG:HA	26:V:137:ALA:CB	2.33	0.57
12:G:37:VAL:CG1	12:G:38:ALA:N	2.67	0.57
2:1:20:TYR:N	2:1:20:TYR:CD2	2.73	0.57
18:N:35:LYS:NZ	18:N:100:VAL:HG11	2.20	0.57
8:C:76:ASN:O	8:C:98:LEU:HD23	2.04	0.57
5:4:30:PRO:HG2	12:G:171:ARG:NE	2.19	0.57
17:M:37:LEU:O	17:M:38:GLU:CD	2.43	0.57
5:4:30:PRO:HG2	12:G:171:ARG:HE	1.68	0.57
8:C:67:PHE:CE2	8:C:157:ARG:NH1	2.73	0.56
15:K:10:VAL:HG21	15:K:16:ALA:HB3	1.86	0.56
9:D:36:VAL:HG12	9:D:52:LEU:HD12	1.87	0.56
6:A:1368:G:N7	16:L:21:ARG:NH2	2.53	0.56
12:G:157:PRO:HG3	12:G:173:LYS:HD2	1.88	0.56
8:C:9:THR:O	8:C:10:THR:HG23	2.06	0.56
5:4:27:CYS:HB2	5:4:32:HIS:HB2	1.87	0.56
25:U:27:TYR:O	25:U:31:ASN:N	2.39	0.56
2:1:26:LYS:HZ3	2:1:34:ARG:CG	2.12	0.56
9:D:36:VAL:HG12	9:D:52:LEU:CD1	2.36	0.56
8:C:53:HIS:ND1	8:C:220:THR:HG23	2.21	0.56
11:F:50:ALA:O	11:F:53:ASP:N	2.39	0.56
6:A:2696:A:N6	6:A:2708:G:O2'	2.39	0.56
8:C:76:ASN:O	8:C:98:LEU:CD2	2.54	0.56
12:G:90:ILE:HG22	12:G:130:THR:HG23	1.86	0.56
21:Q:120:ASP:OD2	21:Q:123:ALA:O	2.24	0.56
27:W:36:ILE:HD11	27:W:58:THR:HG21	1.88	0.56
2:1:22:TYR:CE1	6:A:2575:U:OP1	2.58	0.55
6:A:1705:A:N1	6:A:1736:C:C2	2.70	0.55
12:G:90:ILE:CG2	12:G:130:THR:CB	2.84	0.55
10:E:26:ASP:HA	10:E:116:SER:CB	2.37	0.55
12:G:33:LEU:CD1	12:G:80:VAL:HG23	2.30	0.55
19:O:9:ASN:C	19:O:10:ILE:HG13	2.27	0.55
2:1:40:TYR:HB2	2:1:47:HIS:CD2	2.41	0.55
17:M:34:ILE:HD12	17:M:122:ILE:HD13	1.89	0.55
8:C:95:LEU:HD12	8:C:95:LEU:N	2.08	0.55
12:G:171:ARG:HB3	12:G:171:ARG:NH1	2.23	0.55
5:4:30:PRO:CG	12:G:171:ARG:NE	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:111:LEU:HD11	10:E:183:LEU:HD23	1.89	0.54
21:Q:120:ASP:O	21:Q:121:VAL:HG23	2.05	0.54
12:G:90:ILE:HG22	12:G:130:THR:CG2	2.37	0.54
17:M:35:GLN:HG3	17:M:35:GLN:O	2.08	0.54
6:A:2532:A:N6	11:F:45:MET:O	2.41	0.54
11:F:129:PHE:CE2	11:F:135:TYR:HD1	2.26	0.54
6:A:2028:C:O2'	6:A:2029:A:O4'	2.26	0.54
8:C:77:ALA:HB1	8:C:95:LEU:HB2	1.90	0.54
8:C:120:GLY:O	8:C:131:LEU:CD2	2.54	0.54
2:1:34:ARG:O	2:1:52:GLU:OE2	2.26	0.53
2:1:47:HIS:CE1	6:A:2599:G:H1'	2.43	0.53
6:A:97:G:H1'	29:Y:45:ARG:HG3	1.90	0.53
19:O:9:ASN:HB2	19:O:13:VAL:HG23	1.90	0.53
8:C:125:ILE:O	8:C:126:LYS:HB2	2.09	0.53
12:G:35:LEU:HG	12:G:76:LEU:CD1	2.37	0.53
2:1:8:PRO:HD2	2:1:26:LYS:O	2.08	0.53
2:1:45:ARG:HH21	6:A:740:A:H5'	1.73	0.53
21:Q:120:ASP:C	21:Q:121:VAL:CG2	2.76	0.53
12:G:37:VAL:CG1	12:G:38:ALA:H	2.22	0.53
6:A:846:G:H4'	8:C:13:ARG:HH21	1.74	0.53
6:A:1874:G:H2'	6:A:1874:G:N3	2.24	0.53
6:A:758:A:H2'	6:A:759:A:H5'	1.91	0.53
18:N:33:ARG:HG2	18:N:114:GLU:HB3	1.90	0.52
6:A:2148:C:O2'	6:A:2149:A:P	2.68	0.52
9:D:50:VAL:HG12	9:D:52:LEU:HD13	1.90	0.52
12:G:171:ARG:NH1	12:G:171:ARG:CB	2.73	0.52
12:G:171:ARG:O	12:G:172:ARG:HB3	2.10	0.52
6:A:3017:A:C2	6:A:3018:C:C4	2.98	0.52
8:C:79:VAL:HA	8:C:95:LEU:CB	2.40	0.52
15:K:110:LYS:HA	15:K:110:LYS:CE	2.40	0.52
22:R:66:GLU:CD	22:R:68:THR:HG22	2.29	0.52
23:S:71:LEU:HD23	23:S:116:SER:HB2	1.92	0.52
12:G:157:PRO:CG	12:G:173:LYS:HD2	2.39	0.52
16:L:87:PHE:CZ	16:L:93:VAL:HG13	2.45	0.52
8:C:79:VAL:CG1	8:C:117:ILE:HD12	2.40	0.51
2:1:11:LYS:CB	2:1:23:VAL:HG22	2.40	0.51
8:C:79:VAL:HG12	8:C:117:ILE:HD12	1.92	0.51
15:K:36:GLY:HA3	15:K:109:LYS:HE3	1.92	0.51
29:Y:42:SER:HB2	29:Y:43:ASN:OD1	2.11	0.51
5:4:11:CYS:N	5:4:14:CYS:SG	2.83	0.51
8:C:6:TYR:CE1	8:C:13:ARG:NH1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:99:VAL:HG23	16:L:100:ALA:N	2.26	0.51
2:1:51:ARG:CB	2:1:51:ARG:NH1	2.73	0.51
11:F:134:ASN:OD1	11:F:164:VAL:HA	2.11	0.51
12:G:90:ILE:HD11	12:G:108:LEU:HD11	1.93	0.51
12:G:91:PHE:CE2	12:G:164:ARG:CD	2.77	0.51
6:A:62:G:N3	6:A:62:G:H2'	2.26	0.51
17:M:37:LEU:HD11	17:M:130:ARG:HB2	1.93	0.51
6:A:3015:U:O2'	6:A:3033:A:N3	2.43	0.51
21:Q:123:ALA:CB	21:Q:124:PRO:CA	2.83	0.51
29:Y:41:LEU:O	29:Y:42:SER:HB2	2.11	0.51
2:1:10:VAL:C	2:1:23:VAL:HG13	2.32	0.50
15:K:16:ALA:O	15:K:17:LYS:HB2	2.11	0.50
8:C:79:VAL:HA	8:C:95:LEU:CA	2.41	0.50
27:W:37:LEU:HD13	27:W:78:VAL:HG11	1.93	0.50
6:A:463:G:N7	28:X:57:LYS:HE3	2.26	0.50
6:A:2148:C:HO2'	6:A:2149:A:H8	1.58	0.50
6:A:3017:A:O2'	6:A:3018:C:C4'	2.60	0.50
8:C:65:ILE:HG21	8:C:67:PHE:CE2	2.46	0.50
8:C:78:LYS:C	8:C:79:VAL:HG13	2.30	0.50
11:F:47:VAL:C	11:F:92:ILE:O	2.50	0.50
15:K:108:GLU:O	15:K:110:LYS:HE3	2.11	0.50
18:N:33:ARG:NE	18:N:114:GLU:OE1	2.44	0.50
15:K:110:LYS:CA	15:K:110:LYS:CE	2.85	0.49
27:W:20:ARG:N	27:W:20:ARG:CD	2.72	0.49
6:A:846:G:H5'	8:C:13:ARG:NH2	2.27	0.49
16:L:21:ARG:HG3	16:L:21:ARG:NH1	2.23	0.49
1:0:24:ALA:HB1	1:0:25:PRO:HA	1.94	0.49
6:A:655:C:O2'	21:Q:48:ARG:NH2	2.46	0.49
6:A:2858:G:N2	6:A:3015:U:C2	2.80	0.49
8:C:221:VAL:HG12	8:C:222:ARG:N	2.28	0.49
6:A:712:U:O2	6:A:712:U:O4'	2.30	0.49
8:C:63:ARG:HG3	8:C:63:ARG:NH1	2.23	0.48
25:U:9:VAL:HG13	25:U:71:VAL:HG13	1.95	0.48
6:A:758:A:N1	6:A:759:A:C5	2.80	0.48
8:C:6:TYR:CZ	8:C:13:ARG:NH1	2.81	0.48
11:F:50:ALA:C	11:F:52:ARG:N	2.65	0.48
11:F:135:TYR:CD2	11:F:137:PHE:HD2	2.26	0.48
16:L:21:ARG:HH11	16:L:21:ARG:CG	2.20	0.48
2:1:38:ARG:O	2:1:39:LYS:HG3	2.12	0.48
27:W:18:ALA:O	27:W:19:GLN:HG2	2.12	0.48
29:Y:32:LEU:CD1	29:Y:41:LEU:HD22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:22:TYR:O	2:1:23:VAL:HG23	2.14	0.48
7:B:56:C:O4'	7:B:56:C:O2	2.30	0.48
6:A:1698:U:O2	6:A:1698:U:O4'	2.31	0.48
6:A:2530:G:H4'	11:F:129:PHE:O	2.13	0.48
8:C:76:ASN:N	8:C:76:ASN:ND2	2.60	0.48
17:M:35:GLN:NE2	17:M:130:ARG:HH11	2.10	0.48
6:A:760:G:O2'	6:A:761:A:H3'	2.12	0.48
14:J:109:LEU:HD22	14:J:118:ILE:HG21	1.96	0.48
21:Q:120:ASP:C	21:Q:122:ASN:H	2.17	0.48
11:F:130:ASP:OD2	11:F:134:ASN:HB2	2.13	0.48
8:C:67:PHE:CZ	8:C:157:ARG:NH1	2.81	0.48
6:A:1705:A:N6	6:A:1735:U:H3	2.12	0.47
7:B:9:G:OP1	19:O:26:ARG:NH1	2.47	0.47
8:C:95:LEU:CD1	8:C:103:ARG:O	2.62	0.47
17:M:37:LEU:C	17:M:38:GLU:CG	2.82	0.47
7:B:31:C:H4'	19:O:11:SER:HB3	1.97	0.47
28:X:7:ILE:HD13	28:X:61:VAL:HG11	1.95	0.47
9:D:23:VAL:HG23	15:K:73:ASP:HA	1.96	0.47
11:F:135:TYR:CD2	11:F:135:TYR:C	2.88	0.47
6:A:980:G:H2'	6:A:981:A:O4'	2.14	0.47
10:E:52:THR:HG21	10:E:93:PRO:HD2	1.97	0.47
22:R:49:THR:O	22:R:55:LEU:HD21	2.15	0.47
26:V:66:ILE:HD11	26:V:77:LEU:HD11	1.97	0.47
2:1:9:ILE:CG2	2:1:23:VAL:HG11	2.45	0.47
2:1:47:HIS:HE1	6:A:2599:G:H1'	1.78	0.47
8:C:65:ILE:HG21	8:C:67:PHE:CZ	2.49	0.47
1:0:51:LEU:HD12	18:N:112:VAL:HG21	1.95	0.47
6:A:1999:U:H5	6:A:2004:A:N7	2.13	0.47
16:L:98:LEU:HD22	16:L:103:LEU:HD12	1.96	0.47
7:B:47:A:OP1	19:O:14:ARG:NH2	2.48	0.46
16:L:94:GLY:H	16:L:97:GLU:CG	2.23	0.46
17:M:34:ILE:CG2	17:M:118:LEU:HD22	2.45	0.46
18:N:33:ARG:O	18:N:34:ILE:HG23	2.15	0.46
6:A:1130:A:N3	6:A:1275:C:O2'	2.46	0.46
6:A:2008:C:H5"	8:C:225:VAL:HG21	1.96	0.46
2:1:36:VAL:HG13	2:1:51:ARG:HG2	1.97	0.46
8:C:53:HIS:CE1	8:C:220:THR:CG2	2.81	0.46
12:G:33:LEU:CD2	12:G:138:ASP:OD1	2.60	0.46
10:E:115:LEU:HD11	10:E:183:LEU:HD21	1.98	0.46
6:A:93:C:H3'	6:A:94:C:H5"	1.98	0.46
6:A:832:U:O2'	6:A:834:A:N7	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:167:GLY:O	12:G:168:GLU:HB3	2.14	0.46
2:1:36:VAL:HG21	2:1:51:ARG:HE	1.79	0.46
9:D:10:LYS:HG3	9:D:198:ILE:HD11	1.97	0.46
19:O:63:ALA:HB3	19:O:88:ILE:HG23	1.97	0.46
2:1:44:LEU:O	2:1:45:ARG:CB	2.61	0.46
2:1:44:LEU:CD1	2:1:48:VAL:HG21	2.45	0.46
15:K:98:ILE:HD13	15:K:114:ILE:HG23	1.98	0.46
16:L:94:GLY:N	16:L:97:GLU:CG	2.75	0.46
6:A:2498:G:OP1	27:W:18:ALA:HB1	2.16	0.46
6:A:3017:A:O2'	6:A:3018:C:C5'	2.64	0.46
9:D:177:THR:HG21	9:D:180:LEU:HD22	1.98	0.46
22:R:64:VAL:C	22:R:65:LEU:HD23	2.35	0.46
6:A:759:A:N6	6:A:763:U:N3	2.53	0.46
12:G:146:SER:HB3	12:G:165:TYR:HE1	1.81	0.46
17:M:35:GLN:HE21	17:M:130:ARG:HD2	1.80	0.46
26:V:133:ILE:HB	26:V:171:ILE:HB	1.98	0.46
8:C:65:ILE:CG2	8:C:67:PHE:CD2	2.98	0.45
8:C:133:LEU:HA	8:C:136:ILE:HD12	1.98	0.45
12:G:80:VAL:HG22	12:G:137:ILE:HD11	1.98	0.45
6:A:1108:C:O2'	6:A:1121:A:N3	2.45	0.45
2:1:38:ARG:O	2:1:39:LYS:CB	2.64	0.45
12:G:130:THR:O	12:G:130:THR:HG22	2.15	0.45
24:T:13:ALA:O	24:T:32:VAL:HG22	2.16	0.45
23:S:114:VAL:O	23:S:114:VAL:HG23	2.15	0.45
10:E:52:THR:HB	10:E:89:THR:HG21	1.98	0.45
6:A:571:A:O4'	25:U:41:ILE:HG21	2.17	0.45
6:A:2179:A:C5	15:K:22:ILE:HD12	2.52	0.45
15:K:7:ARG:HG2	15:K:18:GLU:OE2	2.16	0.45
6:A:1079:A:H62	17:M:83:MET:HE1	1.82	0.45
6:A:1440:A:OP1	23:S:18:ARG:NH1	2.50	0.45
10:E:18:VAL:HG11	10:E:201:LEU:HD22	1.99	0.45
10:E:158:ILE:HD11	10:E:166:ALA:HA	1.99	0.45
16:L:50:PHE:O	16:L:50:PHE:CD2	2.70	0.45
8:C:92:ILE:HD12	8:C:104:TYR:CD1	2.52	0.45
11:F:128:GLN:O	11:F:129:PHE:CD2	2.70	0.45
2:1:48:VAL:O	2:1:50:PHE:CD2	2.70	0.44
15:K:79:PHE:CD1	20:P:69:VAL:HG12	2.51	0.44
2:1:22:TYR:O	2:1:23:VAL:CG2	2.66	0.44
6:A:2148:C:O2'	6:A:2149:A:C5'	2.65	0.44
12:G:97:VAL:HG12	12:G:106:PHE:CE1	2.53	0.44
15:K:61:VAL:HG21	15:K:111:PHE:CE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:122:ILE:HD12	17:M:129:ALA:HB3	1.99	0.44
6:A:1079:A:N6	17:M:83:MET:CE	2.80	0.44
10:E:42:LEU:HD13	10:E:186:TYR:CE1	2.53	0.44
16:L:21:ARG:NH1	16:L:21:ARG:CG	2.78	0.44
2:1:36:VAL:HG21	2:1:51:ARG:HG2	1.91	0.44
6:A:3091:C:O2	6:A:3091:C:O4'	2.31	0.44
30:Z:28:LEU:HD21	30:Z:35:VAL:HG12	1.97	0.44
7:B:60:G:H4'	19:O:12:GLU:CG	2.47	0.44
2:1:36:VAL:CG2	2:1:51:ARG:NE	2.77	0.44
6:A:2148:C:O2'	6:A:2149:A:H8	1.99	0.44
17:M:74:LEU:HD22	17:M:94:VAL:HG21	1.99	0.44
28:X:55:CYS:SG	28:X:60:LYS:HD3	2.58	0.44
12:G:35:LEU:CD1	12:G:76:LEU:CD1	2.95	0.44
6:A:18:C:O2'	6:A:649:U:OP1	2.36	0.43
12:G:26:VAL:HG22	12:G:32:THR:HG22	1.99	0.43
2:1:52:GLU:HG3	2:1:52:GLU:O	2.18	0.43
15:K:17:LYS:HG2	15:K:47:ILE:HG12	2.00	0.43
24:T:95:LEU:HD23	29:Y:34:PHE:CD2	2.53	0.43
6:A:386:U:O2	6:A:386:U:O4'	2.35	0.43
6:A:2009:A:OP2	8:C:222:ARG:NH2	2.51	0.43
22:R:52:ALA:O	22:R:55:LEU:HB2	2.18	0.43
8:C:136:ILE:HD13	8:C:142:ILE:HD11	1.99	0.43
6:A:3017:A:C2'	6:A:3018:C:O5'	2.66	0.43
15:K:2:ILE:HG23	15:K:8:LEU:HD21	2.00	0.43
2:1:51:ARG:CB	2:1:51:ARG:HH11	2.32	0.43
14:J:3:THR:HG21	21:Q:61:TRP:HE1	1.83	0.43
19:O:40:VAL:HG11	19:O:113:ILE:HD12	2.01	0.43
4:3:17:THR:HG23	4:3:23:VAL:HG21	1.99	0.43
6:A:2985:A:C4	12:G:68:LEU:HD21	2.54	0.43
6:A:758:A:N6	6:A:759:A:H62	2.17	0.43
9:D:30:LYS:HB3	9:D:191:VAL:HG12	2.00	0.43
18:N:35:LYS:HZ2	18:N:100:VAL:HG11	1.81	0.43
6:A:846:G:H5'	8:C:13:ARG:HH22	1.83	0.42
8:C:212:MET:HA	8:C:215:LYS:HD3	2.01	0.42
10:E:42:LEU:HD12	10:E:42:LEU:HA	1.87	0.42
15:K:8:LEU:HD22	15:K:82:ASN:HB3	2.01	0.42
16:L:99:VAL:CG2	16:L:100:ALA:N	2.82	0.42
8:C:75:VAL:CG2	8:C:97:TYR:CD1	3.03	0.42
21:Q:104:ALA:HA	21:Q:107:THR:HG22	2.01	0.42
5:4:30:PRO:HD3	12:G:171:ARG:HD3	2.00	0.42
19:O:9:ASN:HB2	19:O:13:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:758:A:C6	6:A:759:A:N6	2.73	0.42
6:A:2324:U:H2'	6:A:2325:C:C6	2.53	0.42
9:D:126:THR:HG23	9:D:132:PHE:CD2	2.54	0.42
9:D:37:THR:OG1	9:D:51:GLN:HG2	2.19	0.42
15:K:17:LYS:CG	15:K:47:ILE:HG12	2.49	0.42
16:L:51:GLU:O	16:L:51:GLU:HG3	2.20	0.42
24:T:52:VAL:HG11	24:T:86:LEU:HD13	2.02	0.42
11:F:47:VAL:O	11:F:47:VAL:HG22	2.19	0.42
16:L:94:GLY:CA	16:L:97:GLU:CG	2.98	0.42
6:A:681:A:N7	6:A:1369:A:N1	2.67	0.42
11:F:111:ILE:HG21	11:F:181:GLY:O	2.20	0.42
13:H:3:LEU:HD22	13:H:31:LEU:HD21	2.01	0.42
15:K:18:GLU:HG2	15:K:19:ILE:N	2.34	0.42
22:R:9:THR:HG21	22:R:24:VAL:CG1	2.50	0.42
6:A:406:U:O2'	6:A:425:A:N3	2.52	0.42
12:G:33:LEU:CD1	12:G:80:VAL:CG2	2.94	0.42
15:K:122:LEU:HD21	20:P:69:VAL:HG21	2.00	0.42
30:Z:23:LEU:HD21	30:Z:53:LEU:HD23	2.02	0.42
6:A:2032:A:HO2'	8:C:45:ALA:H	1.67	0.42
8:C:9:THR:O	8:C:10:THR:OG1	2.28	0.42
22:R:40:ALA:O	22:R:55:LEU:HD13	2.18	0.42
28:X:7:ILE:CD1	28:X:61:VAL:HG11	2.50	0.42
9:D:114:VAL:HG11	9:D:180:LEU:HD23	2.01	0.41
11:F:115:LEU:HD22	11:F:124:LEU:HD11	2.01	0.41
12:G:165:TYR:O	12:G:166:GLU:CB	2.68	0.41
6:A:618:A:C2	6:A:2270:C:H4'	2.55	0.41
8:C:66:ASP:OD1	8:C:69:ARG:CG	2.68	0.41
10:E:26:ASP:HA	10:E:116:SER:OG	2.21	0.41
11:F:129:PHE:CE2	11:F:135:TYR:CD1	3.07	0.41
4:3:22:ILE:HG21	4:3:58:ILE:HG21	2.02	0.41
16:L:95:VAL:HG23	16:L:125:THR:OG1	2.20	0.41
29:Y:32:LEU:HD11	29:Y:41:LEU:CD2	2.50	0.41
2:1:36:VAL:HG22	2:1:51:ARG:HA	2.03	0.41
8:C:98:LEU:HD13	8:C:98:LEU:HA	1.78	0.41
22:R:66:GLU:CD	22:R:68:THR:CG2	2.88	0.41
8:C:80:ALA:HB2	8:C:96:HIS:ND1	2.33	0.41
8:C:99:ASP:OD2	8:C:99:ASP:N	2.54	0.41
6:A:758:A:O2'	6:A:759:A:C5'	2.69	0.41
6:A:2179:A:C4	15:K:22:ILE:HD12	2.55	0.41
9:D:175:VAL:O	9:D:176:THR:HG23	2.21	0.41
18:N:100:VAL:CG2	18:N:112:VAL:HG23	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:759:A:O2'	6:A:760:G:P	2.79	0.41
16:L:94:GLY:H	16:L:97:GLU:HB2	1.86	0.41
6:A:3017:A:N6	6:A:3115:A:H2'	2.36	0.41
8:C:75:VAL:HG23	8:C:97:TYR:CD1	2.56	0.40
17:M:55:ASN:HA	17:M:58:ILE:HG22	2.01	0.40
26:V:82:ALA:HB3	26:V:96:ASP:HB2	2.02	0.40
26:V:100:VAL:HG21	26:V:137:ALA:HB2	2.03	0.40
26:V:101:GLN:O	26:V:102:ARG:CB	2.69	0.40
8:C:9:THR:O	8:C:10:THR:CB	2.69	0.40
8:C:218:ARG:CB	8:C:219:PRO:CD	2.99	0.40
21:Q:103:PRO:O	21:Q:104:ALA:HB3	2.22	0.40
22:R:66:GLU:HG3	22:R:67:HIS:N	2.36	0.40
2:1:26:LYS:HE2	2:1:34:ARG:HG2	2.01	0.40
6:A:3049:C:O2	6:A:3049:C:O4'	2.35	0.40
8:C:221:VAL:CG1	8:C:222:ARG:N	2.85	0.40
12:G:35:LEU:HG	12:G:76:LEU:HD12	2.03	0.40
12:G:37:VAL:HG12	12:G:38:ALA:H	1.77	0.40
12:G:171:ARG:O	12:G:172:ARG:CB	2.70	0.40
2:1:37:LEU:O	2:1:38:ARG:HG2	2.21	0.40
6:A:1079:A:H61	17:M:83:MET:HE3	1.86	0.40
7:B:44:C:O2	11:F:99:ARG:NH2	2.54	0.40
15:K:2:ILE:HD12	15:K:8:LEU:HD21	2.03	0.40
11:F:130:ASP:OD1	11:F:132:THR:N	2.39	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	0	53/57 (93%)	45 (85%)	5 (9%)	3 (6%)	1 9
2	1	38/54 (70%)	32 (84%)	5 (13%)	1 (3%)	5 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	2	44/47 (94%)	39 (89%)	5 (11%)	0	100 100
4	3	61/64 (95%)	57 (93%)	3 (5%)	1 (2%)	9 35
5	4	35/37 (95%)	27 (77%)	4 (11%)	4 (11%)	0 2
8	C	271/278 (98%)	235 (87%)	26 (10%)	10 (4%)	3 17
9	D	210/217 (97%)	188 (90%)	18 (9%)	4 (2%)	8 31
10	E	206/215 (96%)	186 (90%)	16 (8%)	4 (2%)	8 31
11	F	170/187 (91%)	150 (88%)	14 (8%)	6 (4%)	3 18
12	G	131/179 (73%)	118 (90%)	12 (9%)	1 (1%)	19 52
13	H	30/151 (20%)	27 (90%)	2 (7%)	1 (3%)	4 19
14	J	144/147 (98%)	133 (92%)	9 (6%)	2 (1%)	11 38
15	K	120/122 (98%)	103 (86%)	15 (12%)	2 (2%)	9 34
16	L	142/147 (97%)	126 (89%)	14 (10%)	2 (1%)	11 38
17	M	130/138 (94%)	119 (92%)	8 (6%)	3 (2%)	6 26
18	N	114/199 (57%)	107 (94%)	7 (6%)	0	100 100
19	O	101/127 (80%)	90 (89%)	10 (10%)	1 (1%)	15 47
20	P	109/113 (96%)	98 (90%)	9 (8%)	2 (2%)	8 32
21	Q	122/129 (95%)	116 (95%)	3 (2%)	3 (2%)	5 25
22	R	98/103 (95%)	90 (92%)	5 (5%)	3 (3%)	4 21
23	S	109/153 (71%)	104 (95%)	3 (3%)	2 (2%)	8 32
24	T	87/100 (87%)	80 (92%)	5 (6%)	2 (2%)	6 26
25	U	77/105 (73%)	69 (90%)	7 (9%)	1 (1%)	12 40
26	V	160/215 (74%)	150 (94%)	8 (5%)	2 (1%)	12 40
27	W	74/88 (84%)	61 (82%)	7 (10%)	6 (8%)	1 4
28	X	60/64 (94%)	50 (83%)	4 (7%)	6 (10%)	0 3
29	Y	59/77 (77%)	51 (86%)	6 (10%)	2 (3%)	3 19
30	Z	56/61 (92%)	49 (88%)	6 (11%)	1 (2%)	8 32
31	a	21/24 (88%)	18 (86%)	2 (10%)	1 (5%)	2 12
All	All	3032/3598 (84%)	2718 (90%)	238 (8%)	76 (2%)	9 25

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	142	ILE

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Mol	Chain	Res	Type
9	D	175	VAL
10	E	149	THR
11	F	51	ALA
15	K	13	ASN
21	Q	121	VAL
22	R	51	LYS
25	U	95	VAL
27	W	31	VAL
27	W	38	VAL
27	W	40	GLN
30	Z	9	VAL
5	4	3	VAL
5	4	16	VAL
8	C	67	PHE
8	C	79	VAL
8	C	256	ARG
8	C	264	SER
10	E	198	VAL
15	K	35	ILE
17	M	74	LEU
24	T	34	HIS
28	X	59	GLY
31	a	15	LYS
8	C	70	HIS
8	C	198	ASN
10	E	76	GLN
11	F	140	ASN
16	L	31	LYS
16	L	115	ASP
19	O	10	ILE
20	P	63	GLU
20	P	81	ASP
24	T	36	ASP
28	X	3	ALA
29	Y	14	THR
8	C	259	LYS
9	D	107	SER
10	E	102	THR
11	F	29	TYR
12	G	120	GLU
14	J	62	ILE
21	Q	123	ALA

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Mol	Chain	Res	Type
22	R	92	GLN
23	S	21	ALA
28	X	60	LYS
29	Y	15	ASP
1	0	37	ARG
2	1	39	LYS
8	C	126	LYS
9	D	178	GLN
11	F	141	GLU
11	F	143	SER
13	H	3	LEU
14	J	13	ARG
21	Q	6	ARG
26	V	40	HIS
26	V	164	LEU
27	W	19	GLN
27	W	69	PHE
28	X	41	ARG
1	0	24	ALA
4	3	23	VAL
5	4	8	LYS
11	F	144	MET
22	R	99	VAL
23	S	103	ILE
28	X	18	VAL
28	X	45	ASN
5	4	4	ASN
9	D	114	VAL
17	M	70	PRO
8	C	10	THR
17	M	73	PRO
27	W	23	VAL
1	0	25	PRO

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	0	44/46 (96%)	44 (100%)	0	100	100
2	1	42/50 (84%)	40 (95%)	2 (5%)	25	57
3	2	35/36 (97%)	35 (100%)	0	100	100
4	3	53/54 (98%)	53 (100%)	0	100	100
5	4	35/35 (100%)	32 (91%)	3 (9%)	10	36
8	C	214/218 (98%)	206 (96%)	8 (4%)	34	65
9	D	160/163 (98%)	158 (99%)	2 (1%)	69	86
10	E	168/173 (97%)	160 (95%)	8 (5%)	25	57
11	F	143/156 (92%)	142 (99%)	1 (1%)	84	92
12	G	116/150 (77%)	113 (97%)	3 (3%)	46	72
13	H	26/116 (22%)	26 (100%)	0	100	100
14	J	119/120 (99%)	118 (99%)	1 (1%)	81	91
15	K	100/100 (100%)	97 (97%)	3 (3%)	41	70
16	L	111/114 (97%)	109 (98%)	2 (2%)	59	80
17	M	113/116 (97%)	111 (98%)	2 (2%)	59	80
18	N	95/158 (60%)	93 (98%)	2 (2%)	53	77
19	O	79/94 (84%)	79 (100%)	0	100	100
20	P	98/100 (98%)	98 (100%)	0	100	100
21	Q	97/99 (98%)	94 (97%)	3 (3%)	40	69
22	R	81/83 (98%)	80 (99%)	1 (1%)	71	87
23	S	87/117 (74%)	86 (99%)	1 (1%)	73	88
24	T	79/85 (93%)	77 (98%)	2 (2%)	47	74
25	U	71/86 (83%)	71 (100%)	0	100	100
26	V	140/168 (83%)	139 (99%)	1 (1%)	84	92
27	W	56/63 (89%)	54 (96%)	2 (4%)	35	66
28	X	50/51 (98%)	49 (98%)	1 (2%)	55	78
29	Y	57/66 (86%)	53 (93%)	4 (7%)	15	43
30	Z	52/54 (96%)	51 (98%)	1 (2%)	57	79
31	a	18/19 (95%)	18 (100%)	0	100	100
All	All	2539/2890 (88%)	2486 (98%)	53 (2%)	56	77

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	20	TYR
2	1	26	LYS
5	4	25	VAL
5	4	26	ILE
5	4	33	LYS
8	C	8	PRO
8	C	76	ASN
8	C	95	LEU
8	C	99	ASP
8	C	157	ARG
8	C	200	GLU
8	C	218	ARG
8	C	257	THR
9	D	52	LEU
9	D	176	THR
10	E	3	LEU
10	E	9	THR
10	E	24	LEU
10	E	26	ASP
10	E	148	LEU
10	E	149	THR
10	E	172	LEU
10	E	192	ASP
11	F	121	PHE
12	G	132	PHE
12	G	166	GLU
12	G	172	ARG
14	J	124	VAL
15	K	14	THR
15	K	68	GLU
15	K	110	LYS
16	L	50	PHE
16	L	115	ASP
17	M	2	LEU
17	M	34	ILE
18	N	28	LEU
18	N	101	GLU
21	Q	75	THR
21	Q	98	LEU
21	Q	107	THR
22	R	9	THR
23	S	84	ASP
24	T	30	THR

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Mol	Chain	Res	Type
24	T	54	VAL
26	V	106	VAL
27	W	19	GLN
27	W	21	LEU
28	X	52	CYS
29	Y	41	LEU
29	Y	43	ASN
29	Y	44	ASN
29	Y	47	LEU
30	Z	9	VAL

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

Mol	Chain	Res	Type
2	1	47	HIS
8	C	53	HIS
8	C	76	ASN
8	C	96	HIS
9	D	21	ASN
10	E	182	GLN
10	E	190	ASN
11	F	13	GLN
14	J	147	GLN
17	M	35	GLN
19	O	56	ASN
23	S	64	ASN
26	V	40	HIS
26	V	64	ASN
31	a	17	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	A	2647/3164 (83%)	564 (21%)	36 (1%)
7	B	115/118 (97%)	33 (28%)	1 (0%)
All	All	2762/3282 (84%)	597 (21%)	37 (1%)

All (597) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	9	G
6	A	10	U
6	A	14	A
6	A	28	A
6	A	34	U
6	A	35	G
6	A	42	G
6	A	46	C
6	A	51	G
6	A	55	G
6	A	61	G
6	A	63	A
6	A	71	A
6	A	73	A
6	A	75	G
6	A	92	A
6	A	93	C
6	A	94	C
6	A	96	A
6	A	97	G
6	A	100	U
6	A	101	U
6	A	118	A
6	A	119	A
6	A	120	U
6	A	121	G
6	A	127	A
6	A	131	G
6	A	135	C
6	A	138	G
6	A	139	U
6	A	140	G
6	A	141	A
6	A	146	G
6	A	147	U
6	A	165	A
6	A	166	U
6	A	167	A
6	A	170	G
6	A	174	U
6	A	175	C
6	A	177	G
6	A	180	G

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Mol	Chain	Res	Type
6	A	197	A
6	A	198	A
6	A	201	A
6	A	202	U
6	A	203	C
6	A	217	G
6	A	218	A
6	A	220	G
6	A	223	A
6	A	224	A
6	A	225	A
6	A	230	A
6	A	231	A
6	A	232	U
6	A	233	G
6	A	236	A
6	A	243	G
6	A	244	A
6	A	251	G
6	A	258	A
6	A	269	U
6	A	270	G
6	A	272	C
6	A	273	U
6	A	275	A
6	A	276	A
6	A	279	G
6	A	318	U
6	A	319	U
6	A	321	U
6	A	322	G
6	A	324	G
6	A	325	A
6	A	374	G
6	A	375	G
6	A	378	A
6	A	379	G
6	A	386	U
6	A	387	G
6	A	390	U
6	A	392	G
6	A	393	G

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Mol	Chain	Res	Type
6	A	396	U
6	A	402	G
6	A	407	A
6	A	409	A
6	A	412	G
6	A	415	A
6	A	420	C
6	A	427	G
6	A	430	A
6	A	431	A
6	A	434	C
6	A	435	C
6	A	436	C
6	A	438	A
6	A	439	C
6	A	459	C
6	A	461	G
6	A	463	G
6	A	466	G
6	A	477	G
6	A	478	U
6	A	487	C
6	A	494	U
6	A	496	U
6	A	497	G
6	A	502	G
6	A	503	A
6	A	507	C
6	A	526	U
6	A	531	G
6	A	534	A
6	A	535	C
6	A	542	C
6	A	546	U
6	A	547	U
6	A	548	A
6	A	555	U
6	A	571	A
6	A	572	G
6	A	584	G
6	A	595	A
6	A	599	C

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Mol	Chain	Res	Type
6	A	609	U
6	A	616	A
6	A	620	U
6	A	621	C
6	A	622	C
6	A	623	G
6	A	636	A
6	A	651	A
6	A	652	U
6	A	658	G
6	A	667	A
6	A	668	G
6	A	670	A
6	A	679	C
6	A	681	A
6	A	687	G
6	A	693	G
6	A	699	A
6	A	700	G
6	A	712	U
6	A	715	G
6	A	724	A
6	A	731	G
6	A	733	G
6	A	734	A
6	A	741	A
6	A	742	U
6	A	743	A
6	A	751	U
6	A	758	A
6	A	759	A
6	A	760	G
6	A	761	A
6	A	762	G
6	A	763	U
6	A	765	U
6	A	766	G
6	A	771	G
6	A	772	U
6	A	773	A
6	A	788	A
6	A	793	A

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Mol	Chain	Res	Type
6	A	804	U
6	A	806	U
6	A	813	G
6	A	837	C
6	A	848	C
6	A	854	C
6	A	856	C
6	A	865	U
6	A	866	G
6	A	867	A
6	A	868	A
6	A	870	A
6	A	882	A
6	A	883	G
6	A	892	A
6	A	893	G
6	A	894	G
6	A	900	A
6	A	902	G
6	A	903	G
6	A	917	G
6	A	918	U
6	A	923	G
6	A	928	U
6	A	930	C
6	A	937	A
6	A	945	U
6	A	949	G
6	A	963	G
6	A	965	U
6	A	977	G
6	A	985	A
6	A	995	C
6	A	1028	A
6	A	1032	C
6	A	1033	C
6	A	1037	U
6	A	1040	C
6	A	1041	G
6	A	1045	A
6	A	1050	A
6	A	1051	A

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Mol	Chain	Res	Type
6	A	1052	G
6	A	1053	A
6	A	1058	G
6	A	1059	G
6	A	1061	A
6	A	1066	G
6	A	1073	G
6	A	1078	U
6	A	1079	A
6	A	1081	G
6	A	1088	G
6	A	1089	C
6	A	1093	G
6	A	1094	A
6	A	1095	G
6	A	1096	A
6	A	1104	A
6	A	1105	G
6	A	1106	C
6	A	1107	C
6	A	1109	A
6	A	1110	G
6	A	1116	C
6	A	1117	G
6	A	1118	G
6	A	1130	A
6	A	1133	C
6	A	1134	G
6	A	1141	A
6	A	1143	G
6	A	1147	A
6	A	1154	U
6	A	1158	C
6	A	1236	A
6	A	1249	A
6	A	1251	U
6	A	1253	U
6	A	1256	C
6	A	1257	G
6	A	1258	G
6	A	1263	C
6	A	1264	A

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Mol	Chain	Res	Type
6	A	1265	A
6	A	1272	C
6	A	1273	G
6	A	1290	C
6	A	1292	A
6	A	1313	G
6	A	1323	U
6	A	1338	G
6	A	1342	G
6	A	1347	A
6	A	1356	G
6	A	1358	G
6	A	1365	A
6	A	1366	G
6	A	1367	U
6	A	1368	G
6	A	1371	A
6	A	1374	G
6	A	1375	C
6	A	1380	A
6	A	1384	G
6	A	1389	G
6	A	1390	A
6	A	1391	U
6	A	1392	U
6	A	1393	A
6	A	1401	G
6	A	1403	G
6	A	1407	C
6	A	1418	A
6	A	1419	A
6	A	1420	A
6	A	1436	G
6	A	1439	C
6	A	1448	C
6	A	1450	G
6	A	1468	C
6	A	1470	U
6	A	1483	A
6	A	1484	C
6	A	1486	G
6	A	1492	G

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Mol	Chain	Res	Type
6	A	1497	U
6	A	1502	A
6	A	1505	G
6	A	1513	A
6	A	1514	U
6	A	1515	U
6	A	1640	G
6	A	1643	A
6	A	1644	U
6	A	1645	G
6	A	1649	U
6	A	1650	G
6	A	1651	A
6	A	1652	C
6	A	1659	A
6	A	1661	G
6	A	1667	G
6	A	1675	C
6	A	1676	A
6	A	1677	G
6	A	1684	U
6	A	1685	A
6	A	1695	G
6	A	1698	U
6	A	1699	G
6	A	1705	A
6	A	1706	G
6	A	1707	U
6	A	1708	C
6	A	1713	A
6	A	1716	U
6	A	1717	A
6	A	1721	C
6	A	1723	G
6	A	1727	G
6	A	1735	U
6	A	1740	A
6	A	1746	G
6	A	1747	A
6	A	1748	U
6	A	1749	G
6	A	1757	G

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Mol	Chain	Res	Type
6	A	1782	U
6	A	1783	G
6	A	1788	C
6	A	1792	A
6	A	1803	G
6	A	1816	C
6	A	1829	A
6	A	1831	A
6	A	1834	A
6	A	1835	A
6	A	1857	U
6	A	1860	U
6	A	1867	U
6	A	1869	C
6	A	1872	G
6	A	1874	G
6	A	1895	G
6	A	1896	C
6	A	1897	A
6	A	1915	C
6	A	1928	A
6	A	1934	A
6	A	1936	G
6	A	1937	G
6	A	1942	U
6	A	1960	G
6	A	1976	C
6	A	1984	U
6	A	1988	A
6	A	1993	A
6	A	2002	U
6	A	2011	A
6	A	2020	C
6	A	2021	G
6	A	2022	A
6	A	2029	A
6	A	2036	U
6	A	2037	G
6	A	2049	A
6	A	2062	G
6	A	2065	G
6	A	2068	A

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Mol	Chain	Res	Type
6	A	2078	G
6	A	2079	A
6	A	2080	C
6	A	2086	A
6	A	2087	A
6	A	2088	C
6	A	2089	U
6	A	2104	A
6	A	2108	G
6	A	2110	G
6	A	2115	U
6	A	2130	G
6	A	2132	C
6	A	2133	G
6	A	2134	G
6	A	2135	U
6	A	2140	A
6	A	2141	C
6	A	2146	A
6	A	2148	C
6	A	2156	G
6	A	2157	G
6	A	2164	A
6	A	2165	A
6	A	2182	U
6	A	2193	A
6	A	2194	C
6	A	2197	A
6	A	2198	U
6	A	2199	G
6	A	2216	A
6	A	2220	U
6	A	2224	A
6	A	2258	A
6	A	2259	G
6	A	2260	A
6	A	2266	G
6	A	2270	C
6	A	2276	G
6	A	2282	C
6	A	2283	G
6	A	2287	A

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Mol	Chain	Res	Type
6	A	2288	G
6	A	2289	A
6	A	2295	G
6	A	2302	C
6	A	2306	A
6	A	2319	G
6	A	2324	U
6	A	2326	G
6	A	2327	A
6	A	2417	G
6	A	2419	C
6	A	2421	U
6	A	2430	G
6	A	2437	A
6	A	2440	U
6	A	2441	C
6	A	2449	G
6	A	2452	A
6	A	2465	G
6	A	2466	G
6	A	2470	U
6	A	2486	G
6	A	2505	A
6	A	2506	G
6	A	2510	C
6	A	2511	C
6	A	2514	A
6	A	2515	A
6	A	2532	A
6	A	2535	G
6	A	2536	C
6	A	2537	A
6	A	2539	U
6	A	2541	A
6	A	2547	U
6	A	2548	G
6	A	2550	G
6	A	2552	G
6	A	2553	U
6	A	2562	A
6	A	2570	U
6	A	2572	G

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Mol	Chain	Res	Type
6	A	2574	C
6	A	2577	C
6	A	2581	A
6	A	2588	U
6	A	2610	G
6	A	2612	A
6	A	2615	A
6	A	2629	U
6	A	2630	C
6	A	2632	G
6	A	2633	A
6	A	2646	U
6	A	2647	C
6	A	2650	U
6	A	2651	C
6	A	2652	A
6	A	2655	G
6	A	2656	G
6	A	2657	A
6	A	2662	A
6	A	2668	C
6	A	2674	G
6	A	2675	A
6	A	2688	C
6	A	2696	A
6	A	2697	G
6	A	2701	C
6	A	2703	A
6	A	2705	A
6	A	2718	U
6	A	2725	C
6	A	2728	C
6	A	2729	G
6	A	2732	G
6	A	2734	C
6	A	2745	A
6	A	2746	U
6	A	2747	C
6	A	2756	G
6	A	2762	G
6	A	2781	U
6	A	2793	A

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Mol	Chain	Res	Type
6	A	2794	G
6	A	2799	A
6	A	2800	C
6	A	2805	G
6	A	2809	G
6	A	2812	U
6	A	2813	U
6	A	2820	U
6	A	2826	G
6	A	2829	A
6	A	2835	G
6	A	2836	U
6	A	2840	U
6	A	2842	U
6	A	2857	A
6	A	2863	U
6	A	2868	G
6	A	2873	C
6	A	2886	G
6	A	2890	G
6	A	2893	C
6	A	2900	G
6	A	2926	C
6	A	2932	A
6	A	2941	G
6	A	2953	C
6	A	2955	U
6	A	2956	U
6	A	2960	A
6	A	2971	G
6	A	2975	A
6	A	2978	G
6	A	2979	C
6	A	2984	A
6	A	2988	G
6	A	2992	A
6	A	3005	A
6	A	3012	U
6	A	3015	U
6	A	3016	C
6	A	3017	A
6	A	3018	C

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Mol	Chain	Res	Type
6	A	3024	A
6	A	3026	G
6	A	3027	A
6	A	3032	U
6	A	3035	G
6	A	3045	A
6	A	3058	G
6	A	3059	A
6	A	3066	A
6	A	3067	G
6	A	3084	A
6	A	3085	U
6	A	3088	G
6	A	3096	A
6	A	3100	G
6	A	3104	C
6	A	3108	C
7	B	4	A
7	B	9	G
7	B	12	C
7	B	13	C
7	B	14	A
7	B	16	A
7	B	17	G
7	B	22	A
7	B	26	A
7	B	27	A
7	B	31	C
7	B	36	U
7	B	38	C
7	B	39	C
7	B	40	A
7	B	41	U
7	B	43	C
7	B	44	C
7	B	45	G
7	B	56	C
7	B	57	U
7	B	58	A
7	B	59	A
7	B	67	A
7	B	68	G

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Mol	Chain	Res	Type
7	B	88	C
7	B	89	C
7	B	91	G
7	B	97	A
7	B	103	G
7	B	107	A
7	B	109	C
7	B	112	C

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	9	G
6	A	92	A
6	A	93	C
6	A	119	A
6	A	145	C
6	A	179	G
6	A	201	A
6	A	268	A
6	A	323	G
6	A	434	C
6	A	602	G
6	A	686	G
6	A	759	A
6	A	760	G
6	A	761	A
6	A	762	G
6	A	882	A
6	A	902	G
6	A	1078	U
6	A	1105	G
6	A	1264	A
6	A	1438	C
6	A	1639	A
6	A	1975	A
6	A	2148	C
6	A	2429	C
6	A	2439	A
6	A	2547	U
6	A	2551	U
6	A	2552	G

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Mol	Chain	Res	Type
6	A	2685	G
6	A	2953	C
6	A	2978	G
6	A	2983	U
6	A	3016	C
6	A	3017	A
7	B	111	C

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 146 ligands modelled in this entry, 146 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

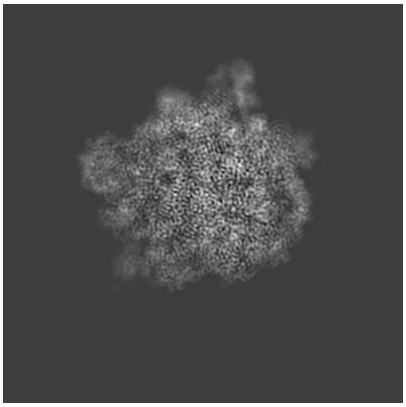
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6789. These allow visual inspection of the internal detail of the map and identification of artifacts.

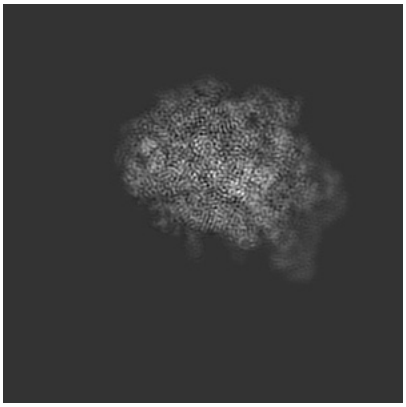
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

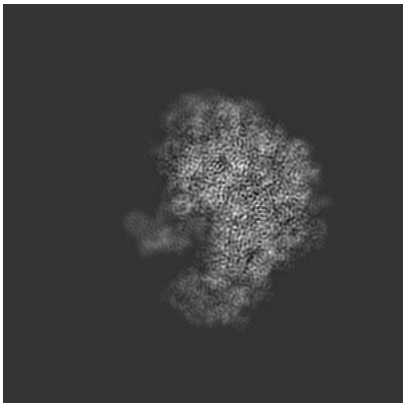
6.1.1 Primary map



X



Y

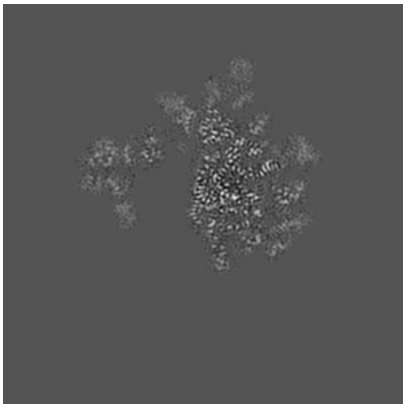


Z

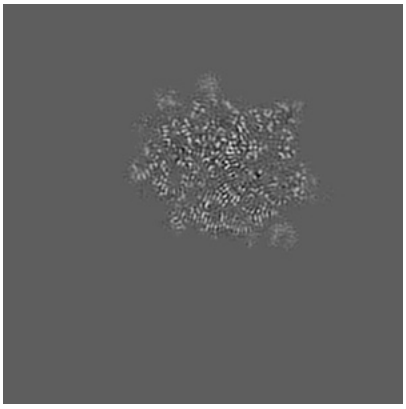
The images above show the map projected in three orthogonal directions.

6.2 Central slices

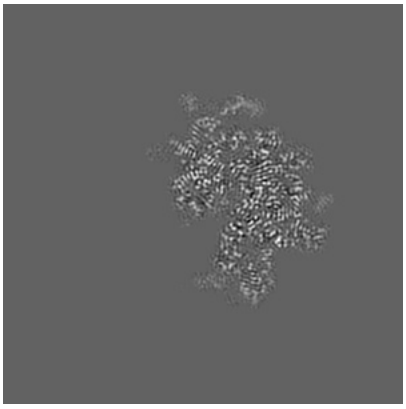
6.2.1 Primary map



X Index: 140



Y Index: 140

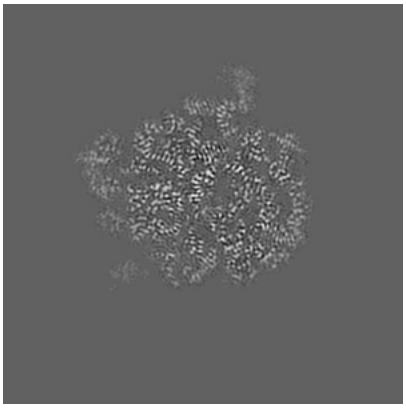


Z Index: 140

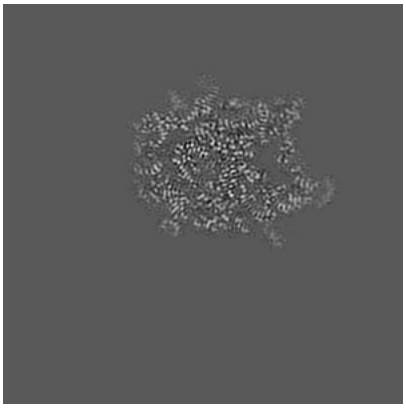
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

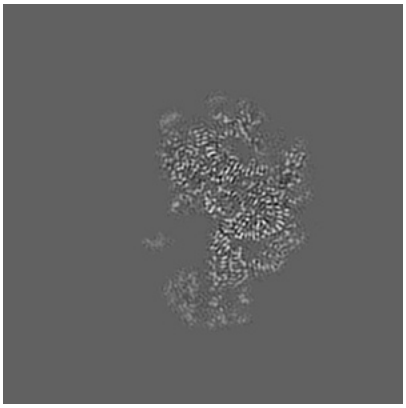
6.3.1 Primary map



X Index: 162



Y Index: 145

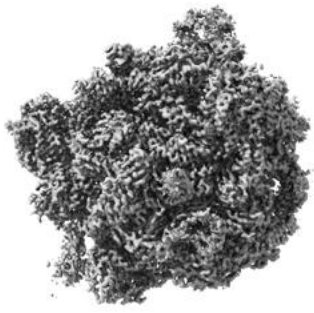


Z Index: 164

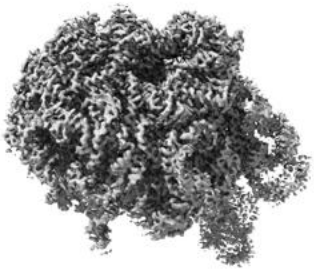
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

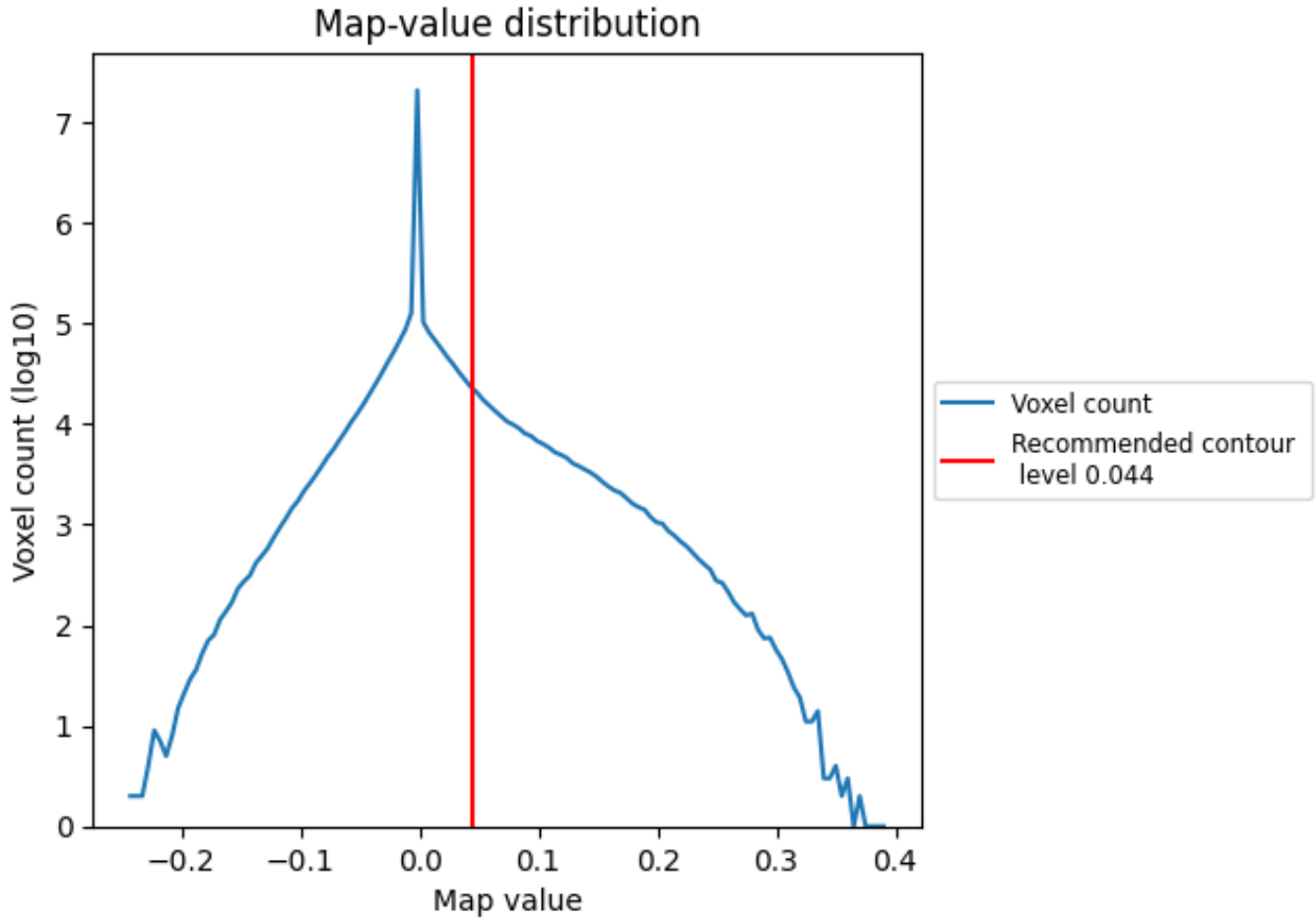
6.5 Mask visualisation (i)

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

7 Map analysis

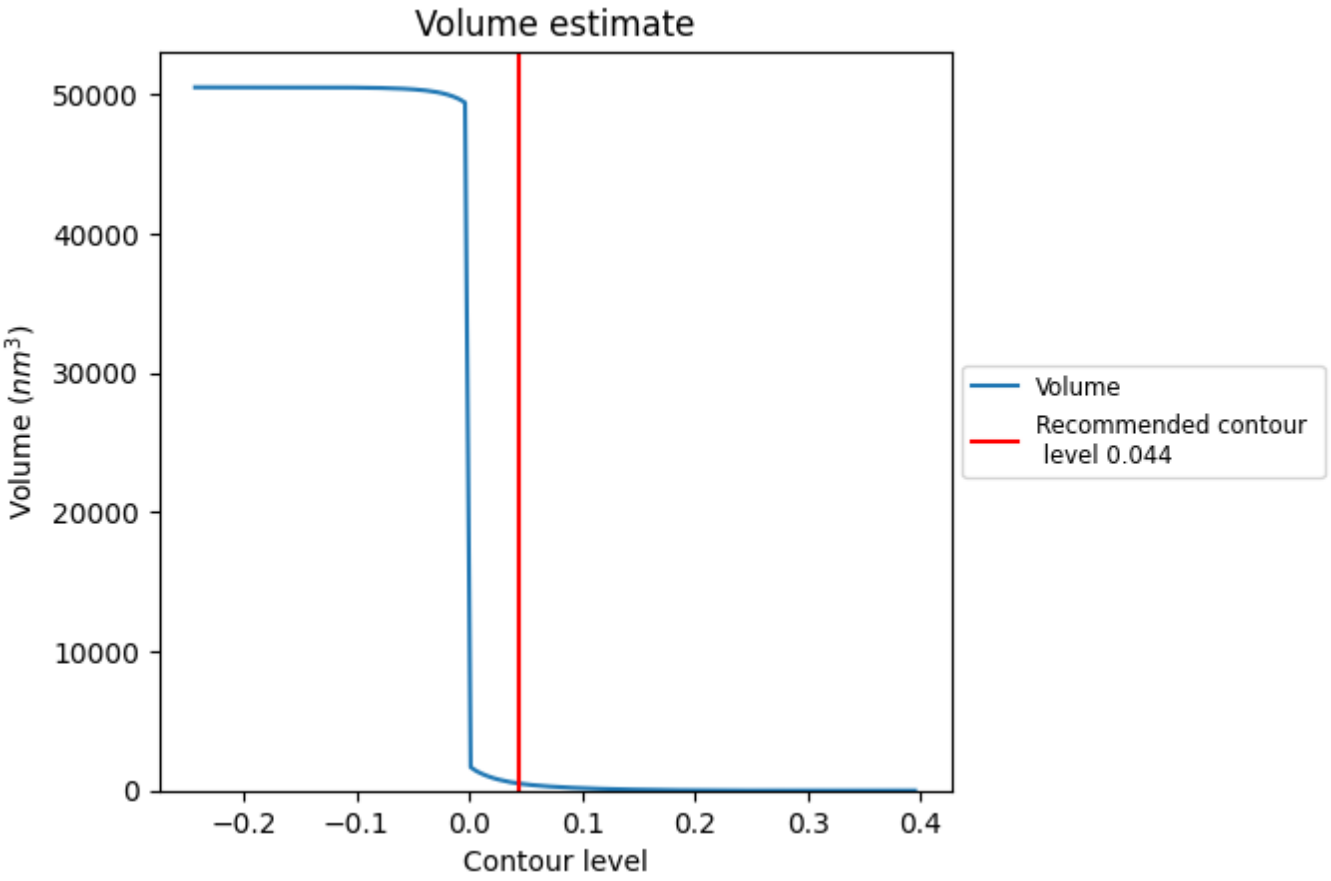
This section contains the results of statistical analysis of the map.

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.

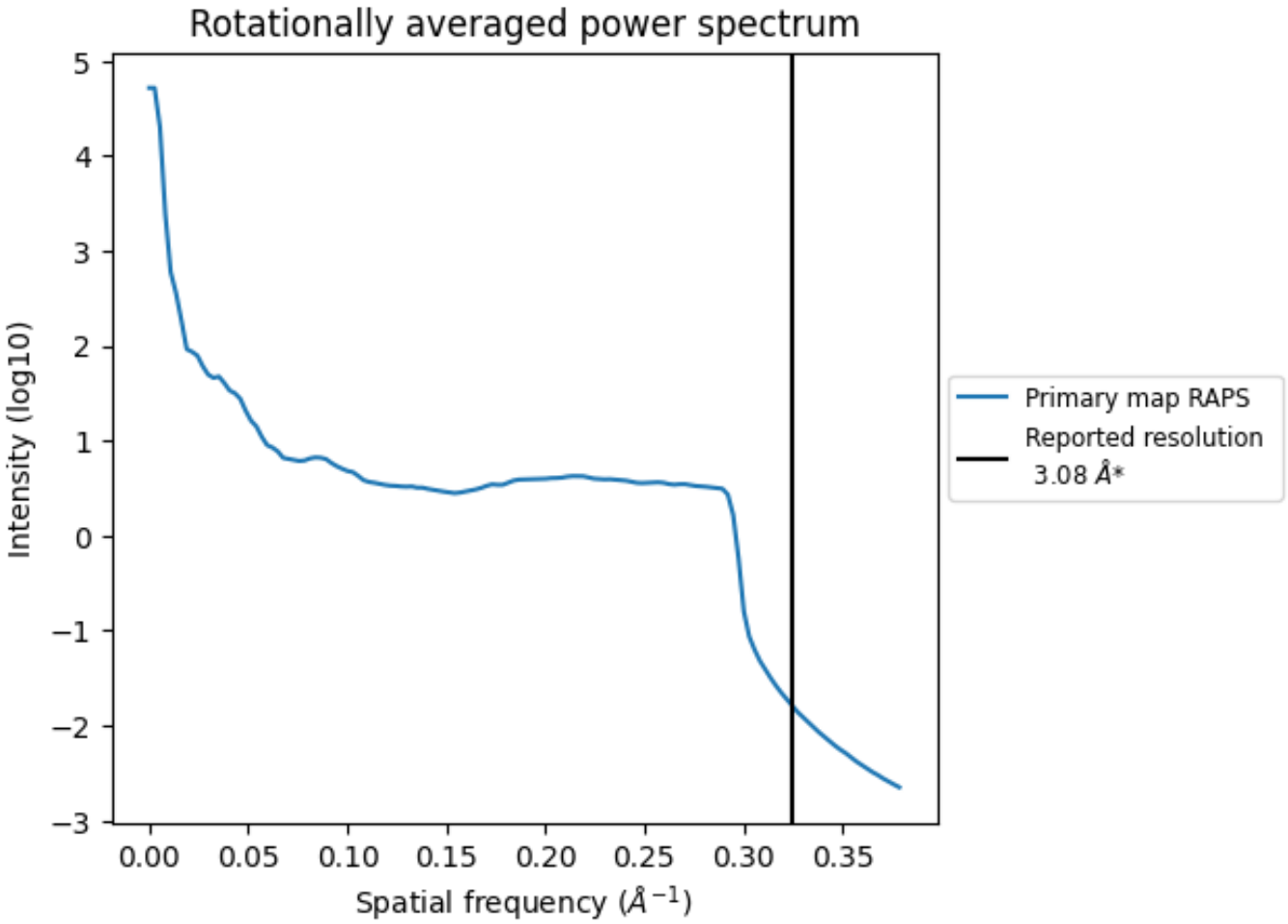
7.2 Volume estimate



The volume at the recommended contour level is 509 nm^3; this corresponds to an approximate mass of 460 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)

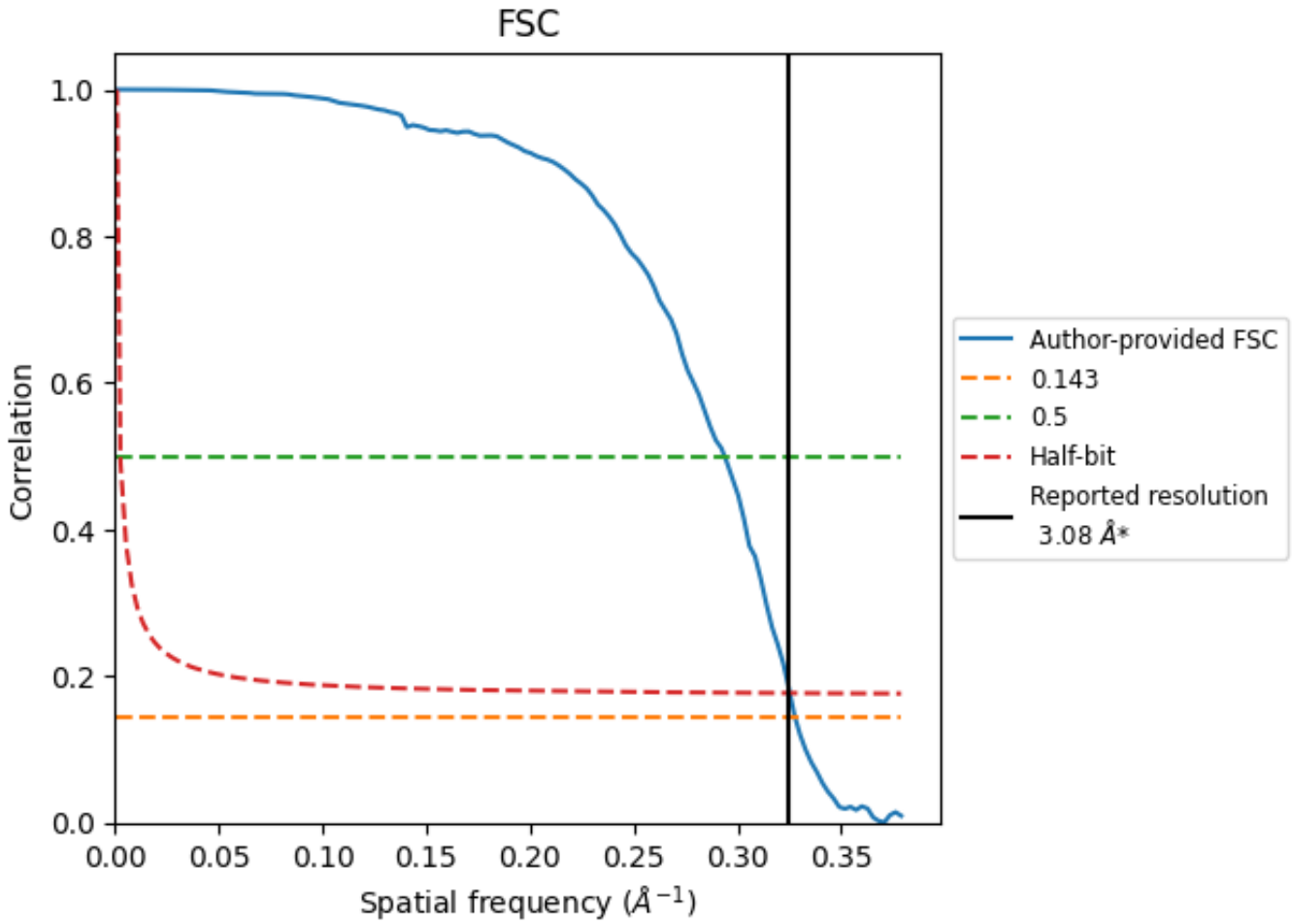


*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

8.2 Resolution estimates (i)

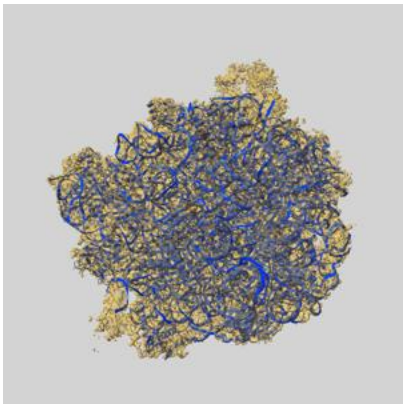
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.05	3.40	3.08
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

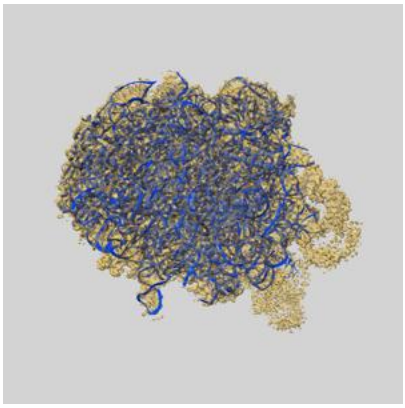
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6789 and PDB model 5XYM. Per-residue inclusion information can be found in section 3 on page 9.

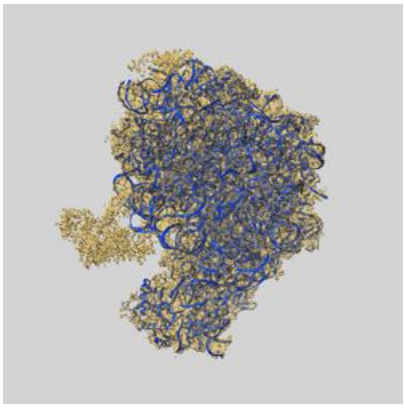
9.1 Map-model overlay



X



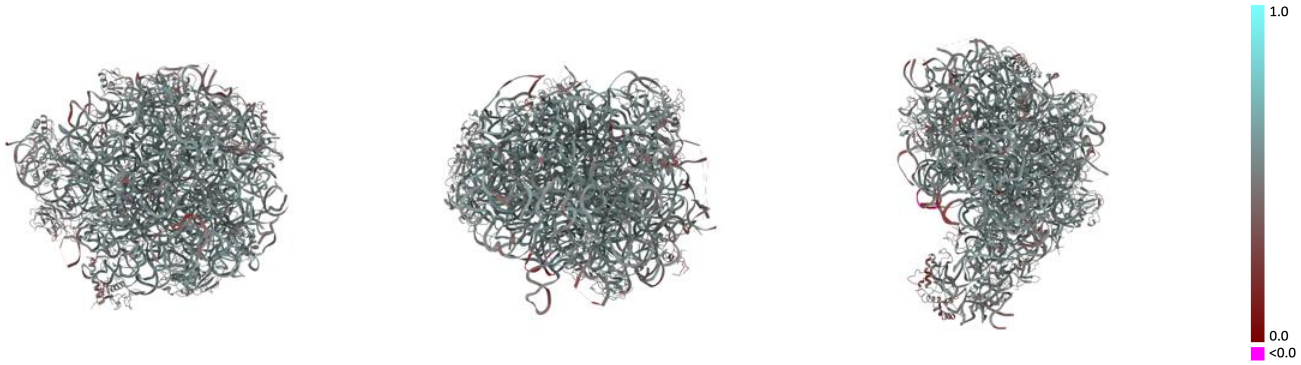
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.044 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.

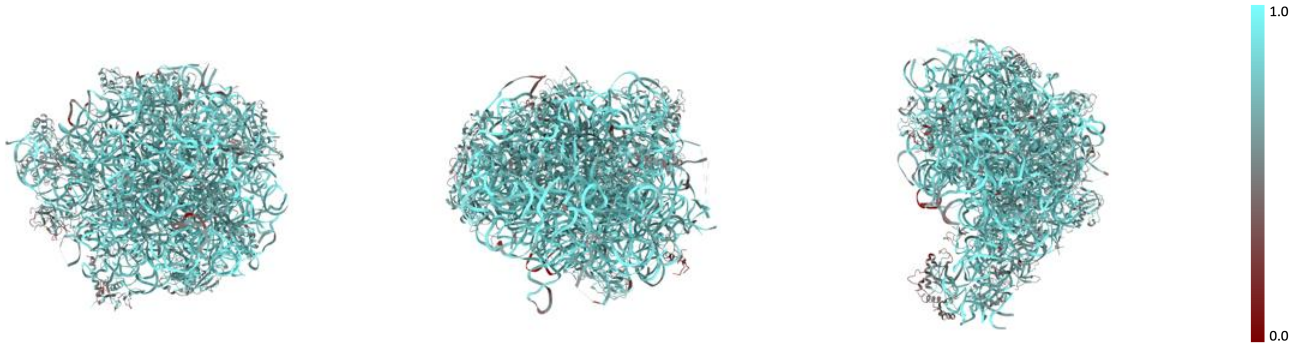
9.2 Q-score mapped to coordinate model (i)



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.

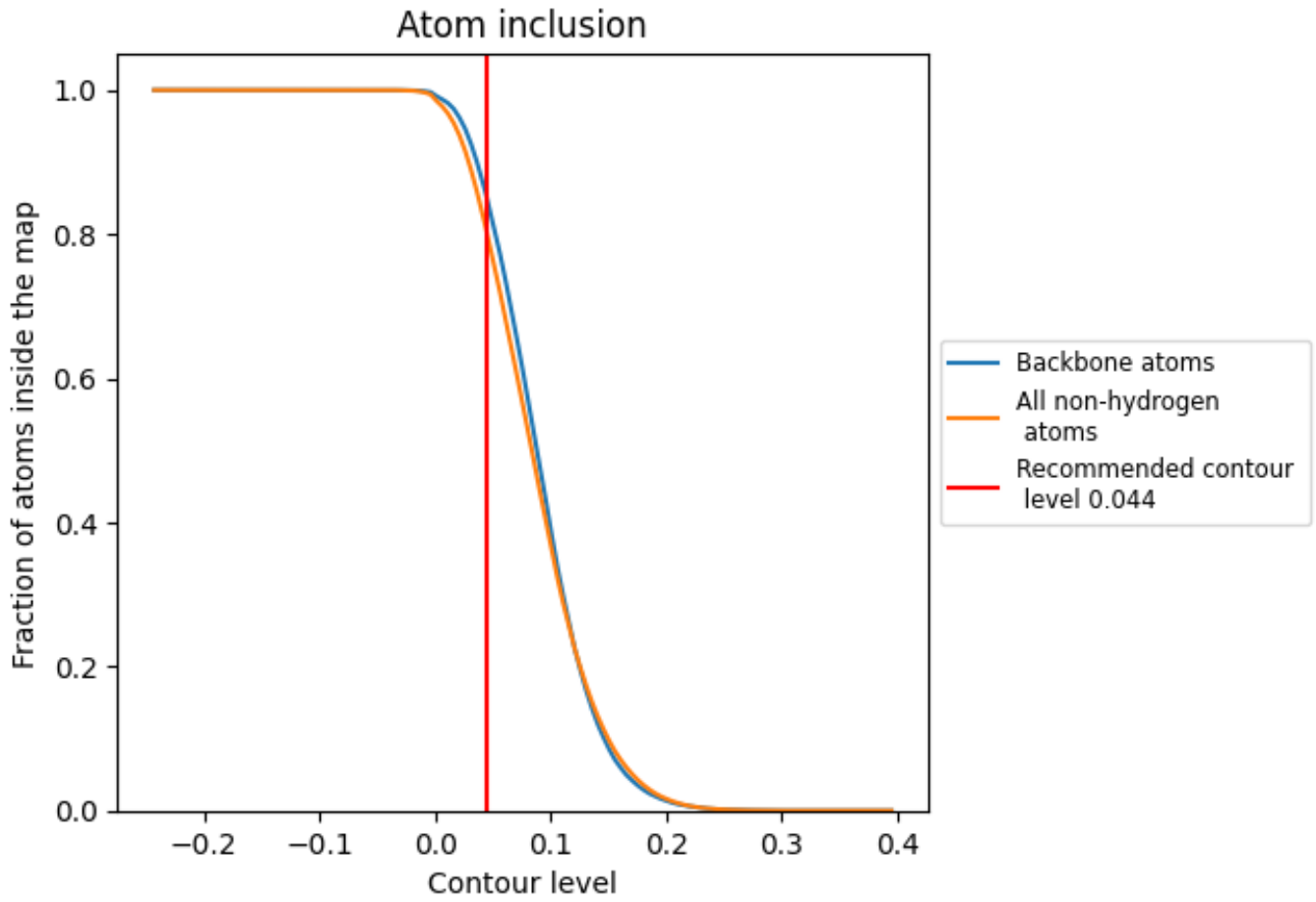
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.044).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 81% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8089	0.5180
0	0.6886	0.4860
1	0.5485	0.4390
2	0.7679	0.5310
3	0.7479	0.5220
4	0.7587	0.4990
A	0.8582	0.5290
B	0.8147	0.4940
C	0.7517	0.5280
D	0.7533	0.5230
E	0.7009	0.4950
F	0.4782	0.3860
G	0.5971	0.4380
H	0.2771	0.3490
J	0.7527	0.5150
K	0.6549	0.4930
L	0.7174	0.5050
M	0.7273	0.5130
N	0.7706	0.5260
O	0.6960	0.4910
P	0.6825	0.4920
Q	0.7600	0.5290
R	0.7221	0.5120
S	0.7302	0.5240
T	0.6961	0.5070
U	0.6490	0.4750
V	0.5342	0.4380
W	0.7651	0.5250
X	0.7299	0.4990
Y	0.6707	0.4650
Z	0.7231	0.5050
a	0.7709	0.5310