



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:55 AM UTC

PDB ID : 7NHM / pdb_00007nhm
EMDB ID : EMD-12333
Title : 70S ribosome from Staphylococcus aureus
Authors : Crowe-McAuliffe, C.; Murina, V.; Hauryliuk, V.; Wilson, D.N.
Deposited on : 2021-02-10
Resolution : 3.10 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:

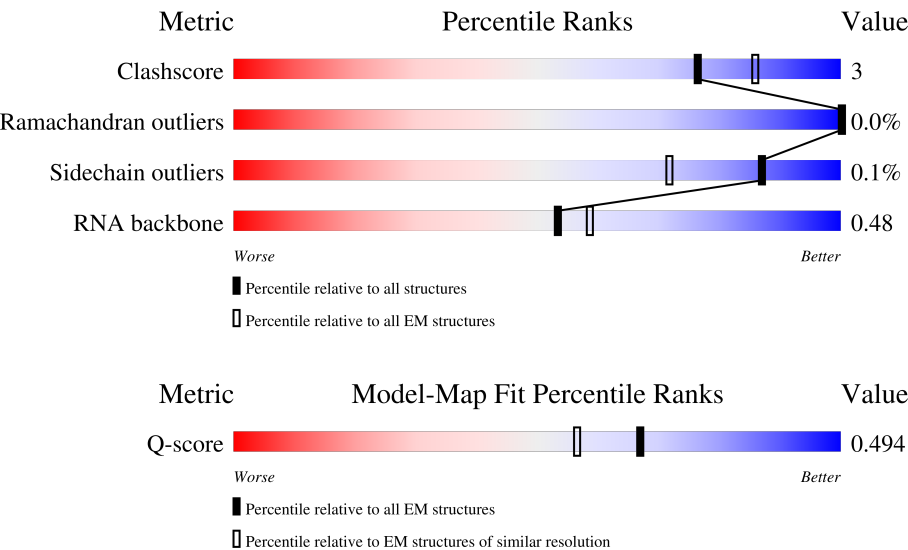
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.



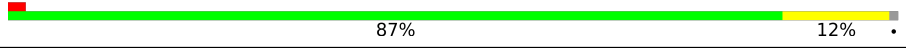
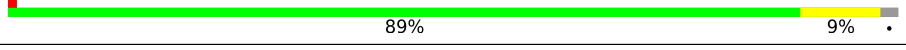
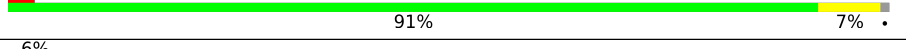
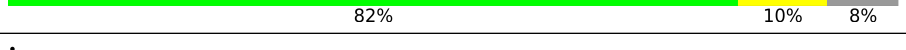
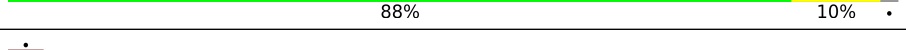
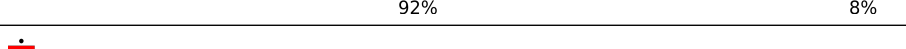
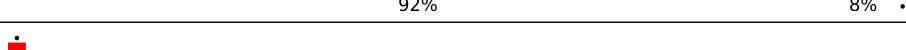
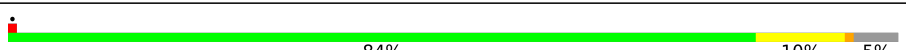
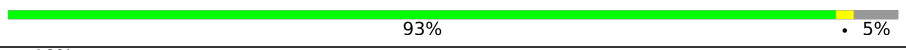
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. 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	Z	94	7% 82% 5% 13%
2	P	144	89% 5% 6%
3	A	2923	72% 21% . .

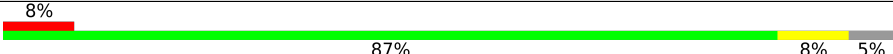
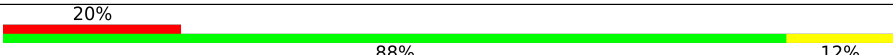
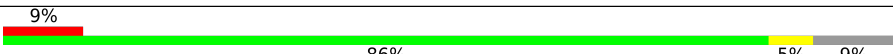
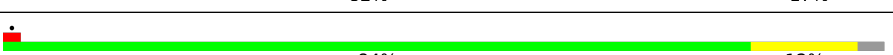
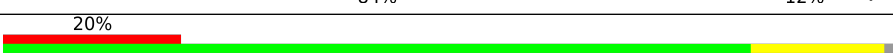
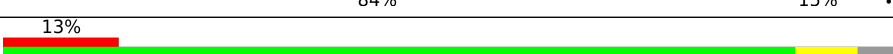
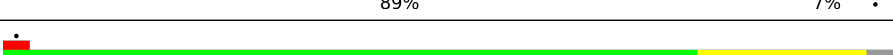
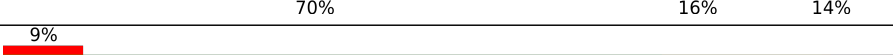
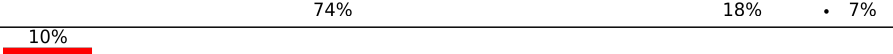
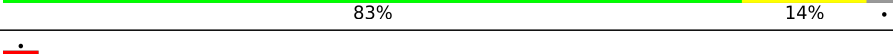
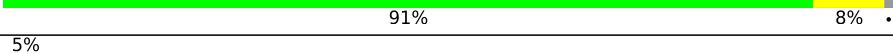
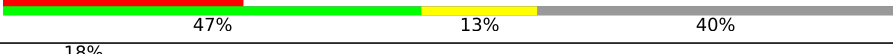
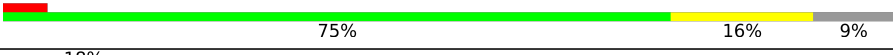
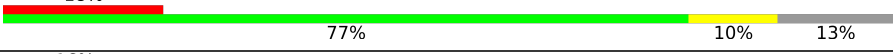
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	a	1551	
5	B	115	
6	G	277	
7	H	220	
8	I	207	
9	J	179	
10	K	178	
11	M	145	
12	N	122	
13	O	146	
14	Q	122	
15	R	119	
16	S	116	
17	T	118	
18	U	102	
19	V	117	
20	W	91	
21	X	105	
22	Y	217	
23	1	62	
24	2	69	
25	3	59	
26	5	58	
27	6	49	
28	8	66	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	7	45	
30	d	217	
31	e	200	
32	h	156	
33	k	102	
34	l	129	
35	o	60	
36	p	89	
37	q	91	
38	u	83	
39	9	37	
40	t	92	
41	n	121	
42	j	132	
43	f	166	
44	i	132	
45	s	80	
46	g	98	
47	b	15	
48	m	137	
49	r	87	
50	c	255	
51	D	77	
52	4	84	

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 140248 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 L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Z	82	Total	C	N	O	0	0
			626	386	122	118		

- Molecule 2 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	135	Total	C	N	O	S	0	0
			1081	693	205	180	3		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2824	Total	C	N	O	P	0	0
			60551	27035	11081	19611	2824		

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	1531	Total	C	N	O	P	0	0
			32794	14642	5986	10635	1531		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	175	Total	C	N	O	S	0	0
			1381	876	237	261	7		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	164	Total	C	N	O	S	0	0
			1284	799	232	250	3		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	142	Total	C	N	O	S	0	0
			1127	704	205	216	2		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	118	Total	C	N	O		0	0
			914	569	173	172			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	114	Total	C	N	O		0	0
			922	580	185	157			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	99	Total	C	N	O	S	0	0
			761	480	140	139	2		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	2	64	Total	C	N	O	0	0
			527	324	99	104		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	54	Total	C	N	O	S	0	0
			433	262	90	76	5		

- Molecule 27 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	47	Total	C	N	O	S	0	0
			389	232	79	74	4		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	42	Total	C	N	O	S	0	0
			360	220	88	51	1		

- Molecule 30 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	207	Total	C	N	O	S	0	0
			1634	1030	305	297	2		

- Molecule 31 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 32 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	148	Total	C	N	O	S	0	0
			1180	734	226	216	4		

- Molecule 33 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	102	Total	C	N	O	S	0	0
			814	513	149	150	2		

- Molecule 34 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 35 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	o	59	Total	C	N	O	S	0	0
			496	314	99	78	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	?	-	ALA	deletion	UNP Q2FW19

- Molecule 36 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 37 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 38 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 39 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	9	36	Total	C	N	O	S	0	0
			292	184	59	44	5		

- Molecule 40 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	t	79	Total	C	N	O	S	0	0
			646	416	116	112	2		

- Molecule 41 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	127	Total	C	N	O	S	0	0
			1008	624	201	182	1		

- Molecule 43 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 45 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 46 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 47 is a RNA chain called RNA (5'-R(P*GP*GP*AP*GP*GP*UP*NP*NP*NP*N P*NP*NP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
47	b	9	Total	C	N	O	P	0	0
			199	88	39	63	9		

- Molecule 48 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	79	Total	C	N	O	S	0	0
			651	413	116	121	1		

- Molecule 50 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 51 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	D	77	Total	C	N	O	P	0	0
			1644	733	298	536	77		

- Molecule 52 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	59	Total	C	N	O	S	0	0
			486	310	88	87	1		

- Molecule 53 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
53	A	9	Total	K	0
			9	9	
53	a	2	Total	K	0
			2	2	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	114	Total	Mg	0
			114	114	
54	a	25	Total	Mg	0
			25	25	

Continued on next page...

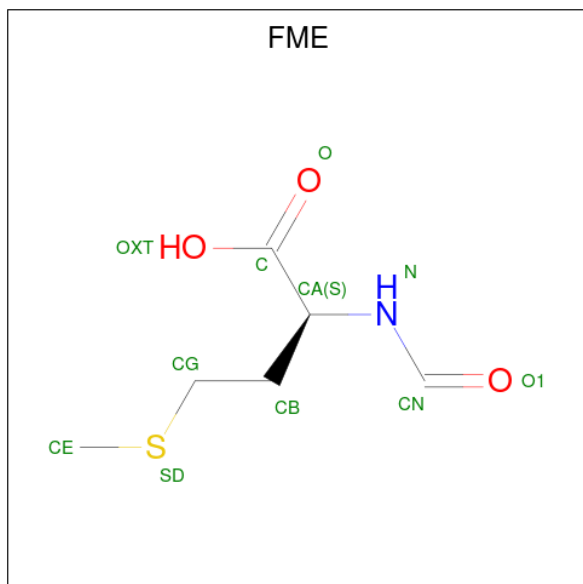
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
54	U	1	Total	Mg	0
			1	1	
54	D	1	Total	Mg	0
			1	1	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	5	1	Total	Zn	0
			1	1	
55	6	1	Total	Zn	0
			1	1	
55	o	1	Total	Zn	0
			1	1	
55	9	1	Total	Zn	0
			1	1	

- Molecule 56 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).

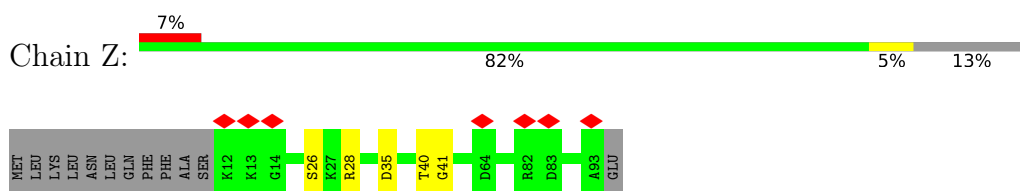


Mol	Chain	Residues	Atoms					AltConf
56	D	1	Total	C	N	O	S	0
			10	6	1	2	1	

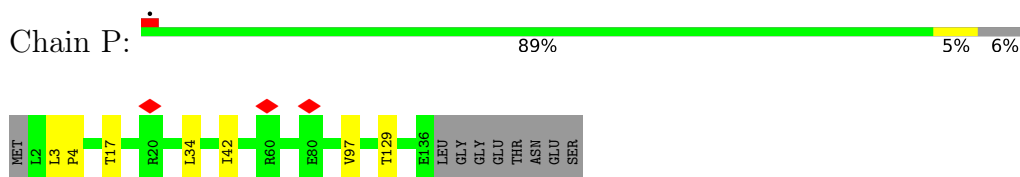
3 Residue-property plots

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.

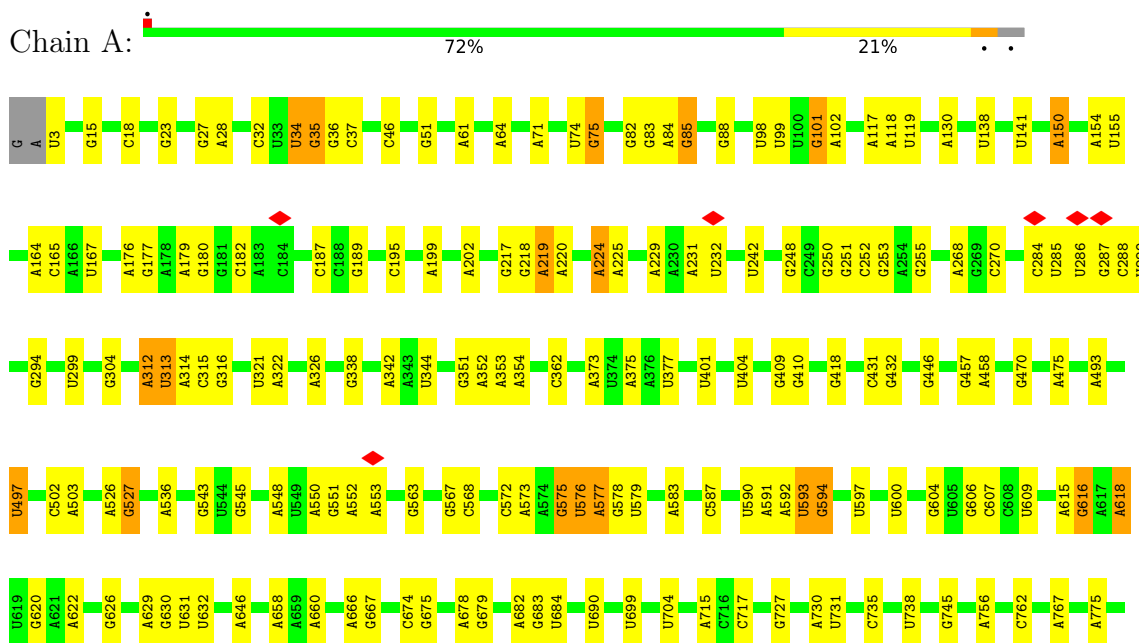
- Molecule 1: 50S ribosomal protein L27



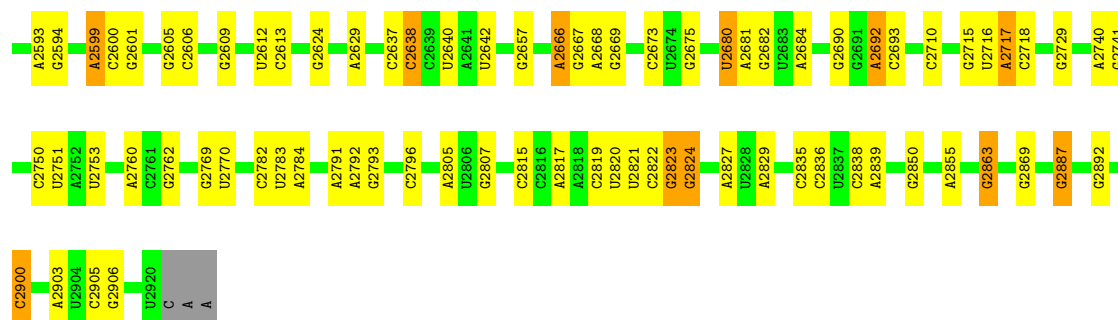
- Molecule 2: 50S ribosomal protein L16



- Molecule 3: 23S rRNA

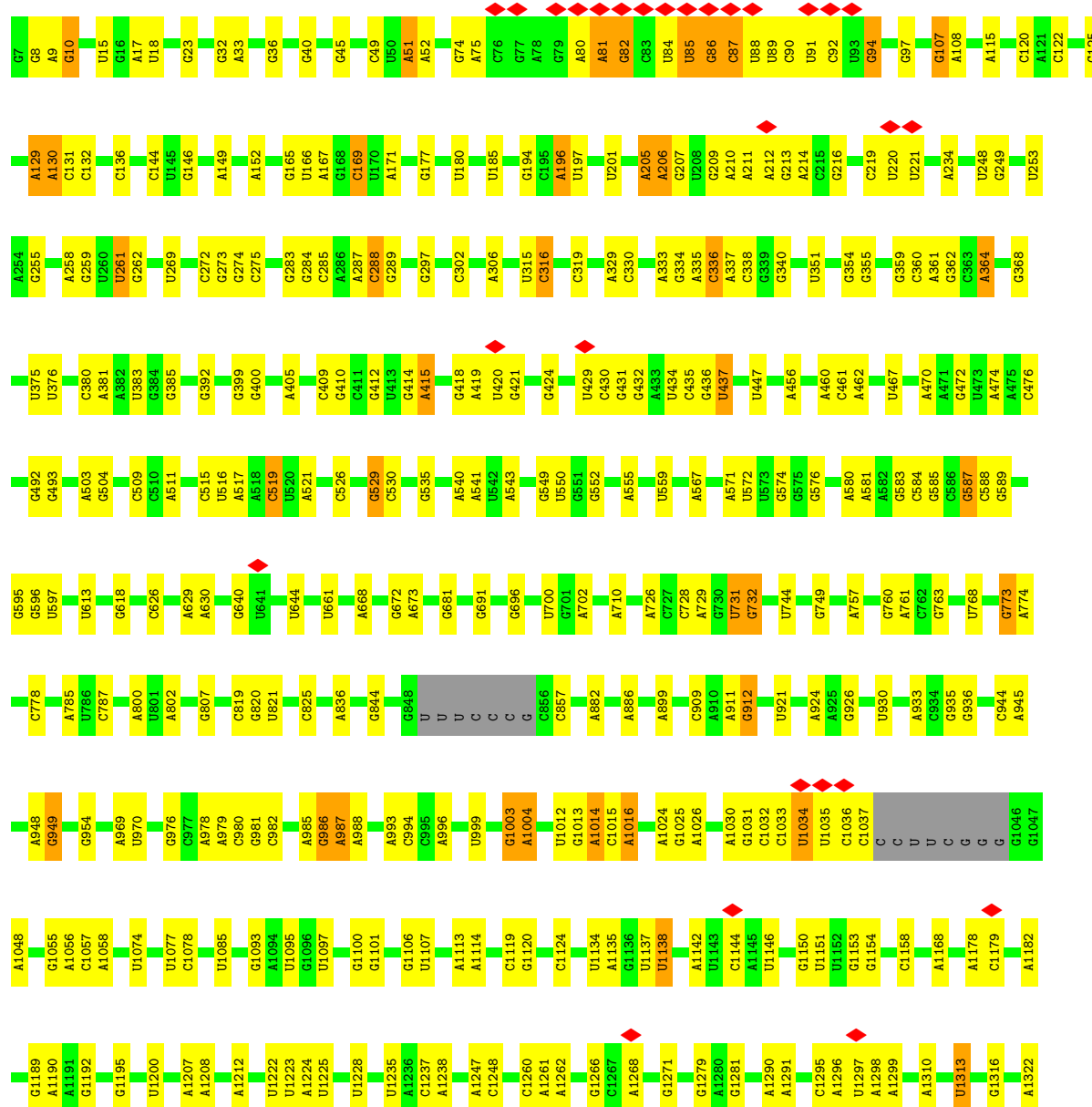


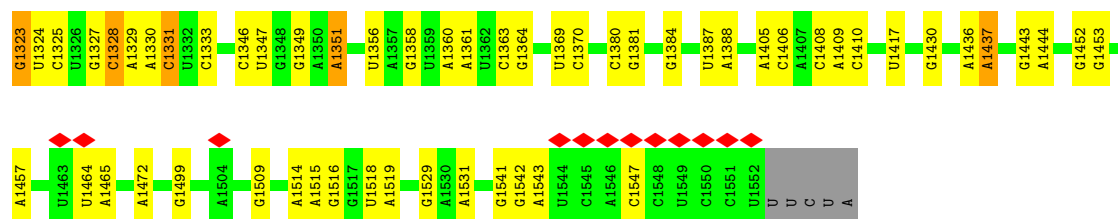




Molecule 4: 16S rRNA

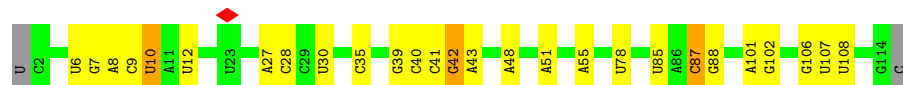
Chain a: 72% 24%





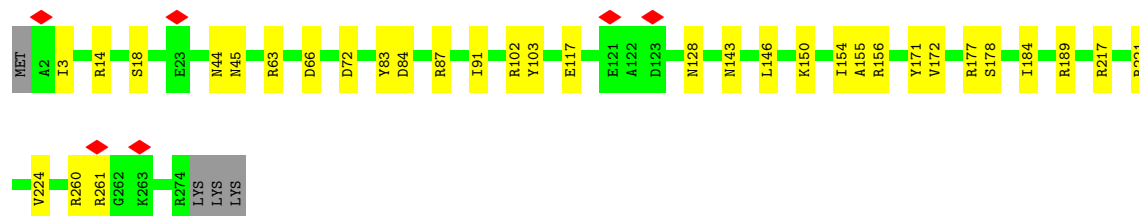
• Molecule 5: 5S rRNA

Chain B: 75% 21%



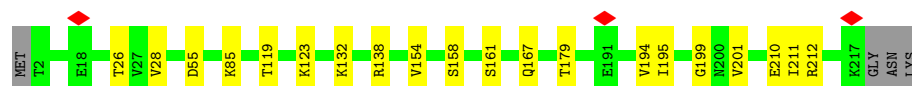
• Molecule 6: 50S ribosomal protein L2

Chain G: 87% 12%



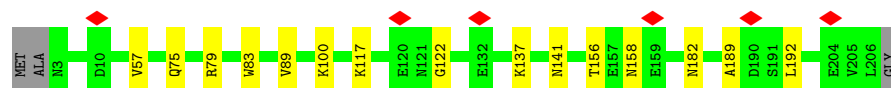
• Molecule 7: 50S ribosomal protein L3

Chain H: 89% 9%



• Molecule 8: 50S ribosomal protein L4

Chain I: 91% 7%

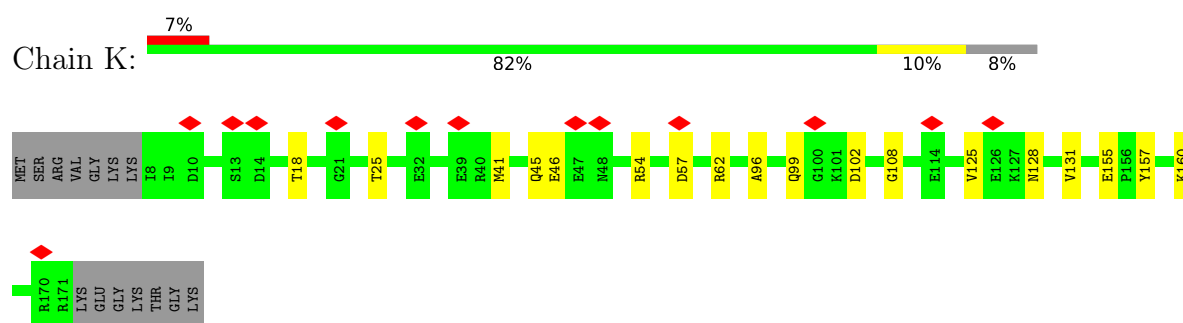


• Molecule 9: 50S ribosomal protein L5

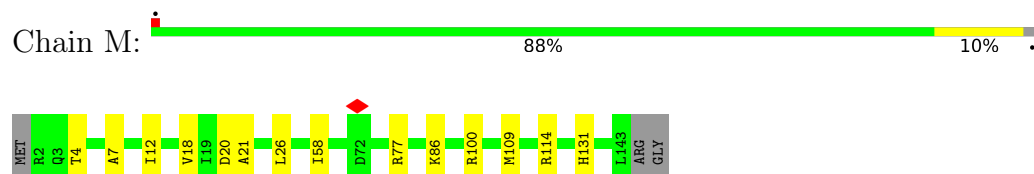
Chain J: 85% 13%



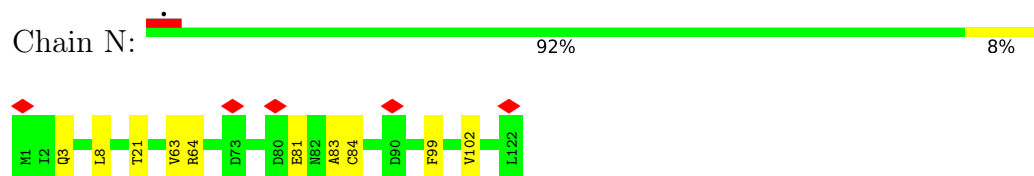
• Molecule 10: 50S ribosomal protein L6



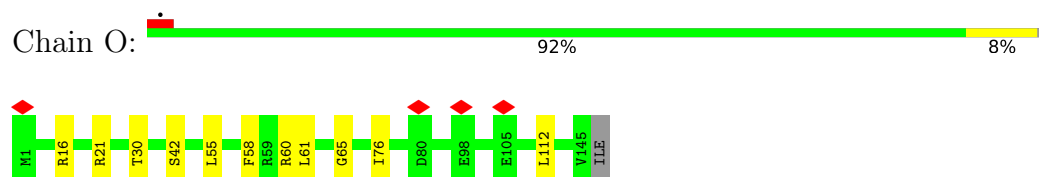
- Molecule 11: 50S ribosomal protein L13



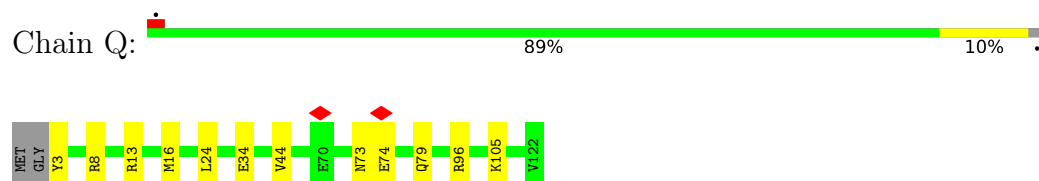
- Molecule 12: 50S ribosomal protein L14



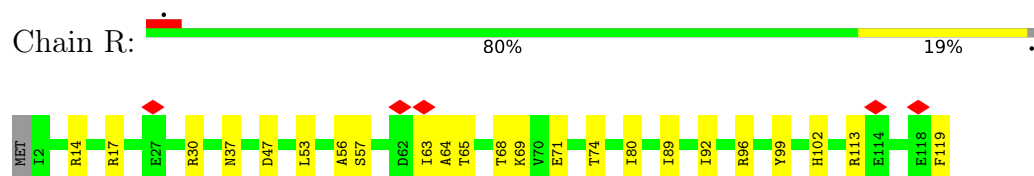
- Molecule 13: 50S ribosomal protein L15



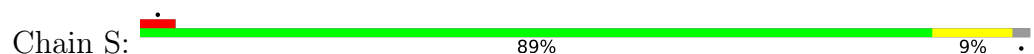
- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18

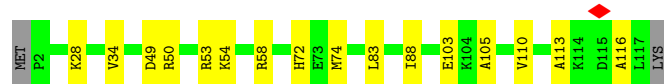
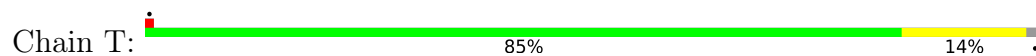


- Molecule 16: 50S ribosomal protein L19

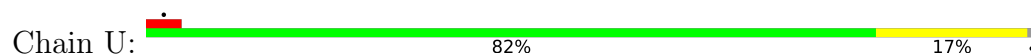




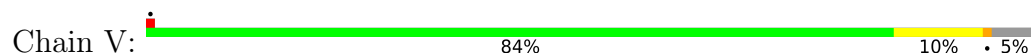
- Molecule 17: 50S ribosomal protein L20



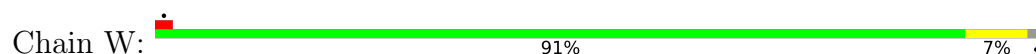
- Molecule 18: 50S ribosomal protein L21



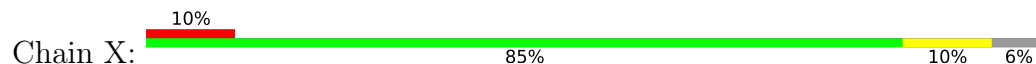
- Molecule 19: 50S ribosomal protein L22



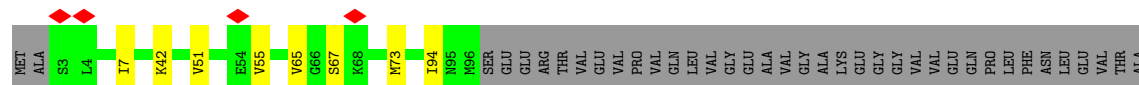
- Molecule 20: 50S ribosomal protein L23



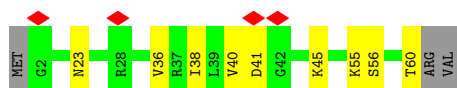
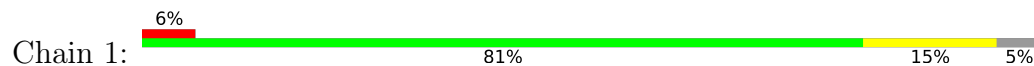
- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L28



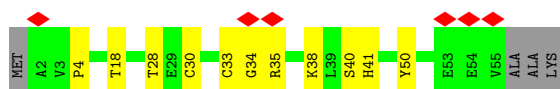
- Molecule 24: 50S ribosomal protein L29



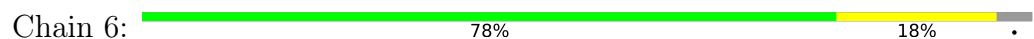
- Molecule 25: 50S ribosomal protein L30



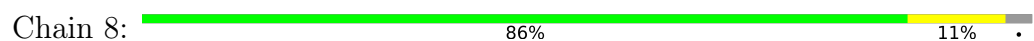
- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33 2



- Molecule 28: 50S ribosomal protein L35



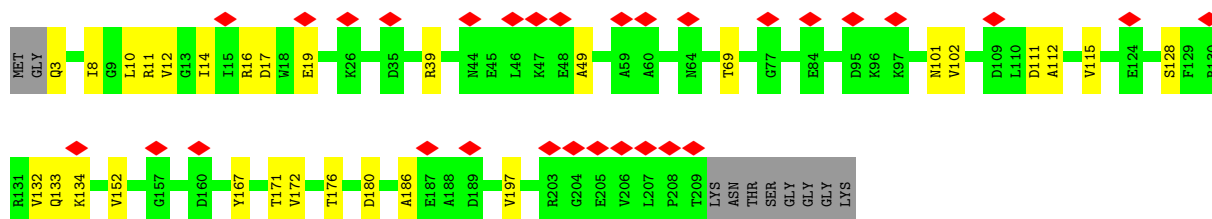
- Molecule 29: 50S ribosomal protein L34

Chain 7:  89% 7%



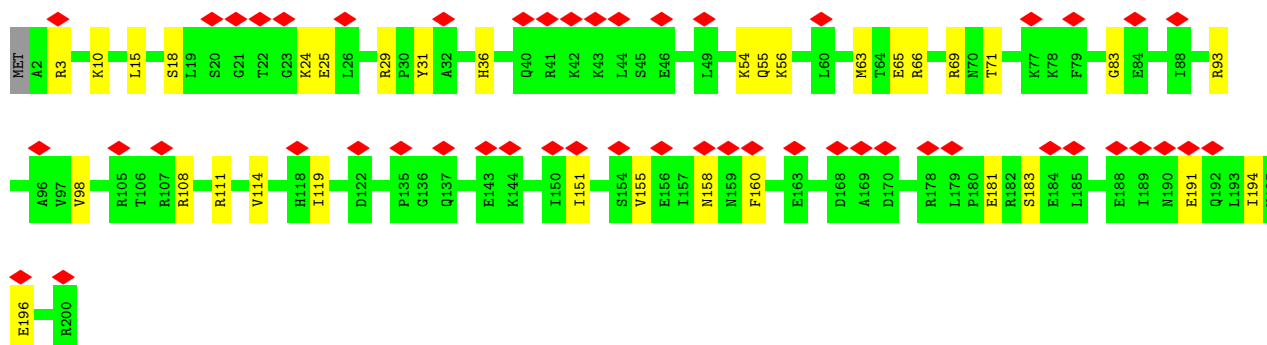
- Molecule 30: 30S ribosomal protein S3

Chain d:  14% 82% 13% 5%



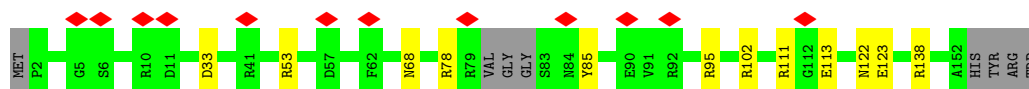
- Molecule 31: 30S ribosomal protein S4

Chain e:  25% 83% 16%



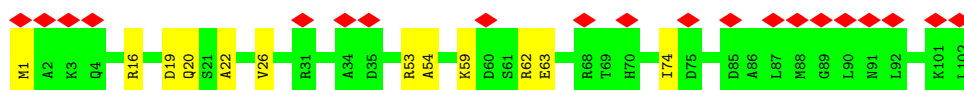
- Molecule 32: 30S ribosomal protein S7

Chain h:  8% 87% 8% 5%



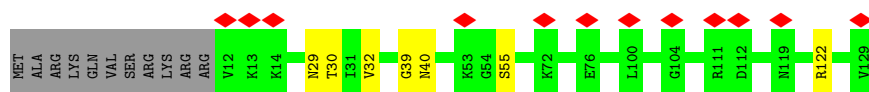
- Molecule 33: 30S ribosomal protein S10

Chain k:  20% 88% 12%



- Molecule 34: 30S ribosomal protein S11

Chain l:  9% 86% 5% 9%



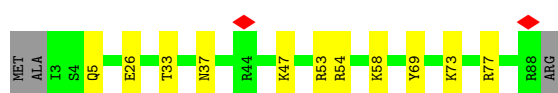
- Molecule 35: 30S ribosomal protein S14 type Z

Chain o: 82% 17%



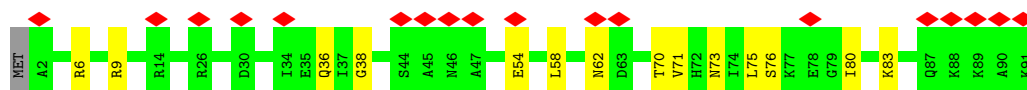
- Molecule 36: 30S ribosomal protein S15

Chain p: 84% 12%



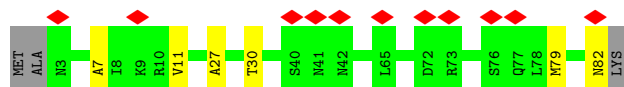
- Molecule 37: 30S ribosomal protein S16

Chain q: 20% 84% 15%



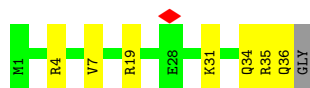
- Molecule 38: 30S ribosomal protein S20

Chain u: 13% 89% 7%



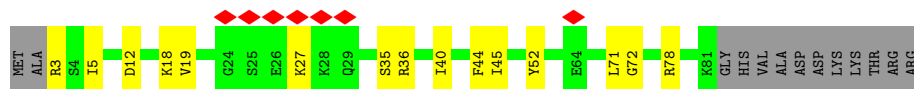
- Molecule 39: 50S ribosomal protein L36

Chain 9: 78% 19%

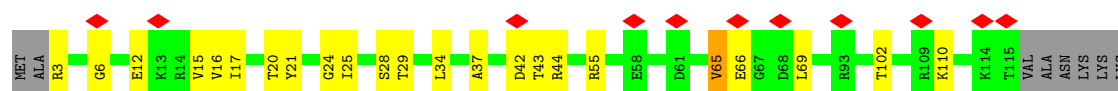
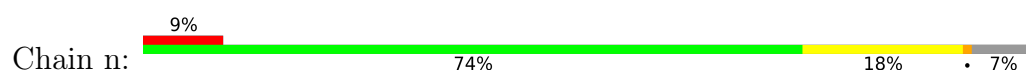


- Molecule 40: 30S ribosomal protein S19

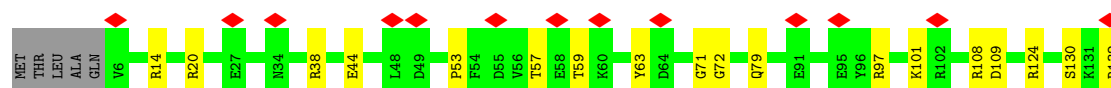
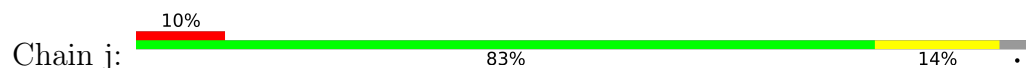
Chain t: 8% 70% 16% 14%



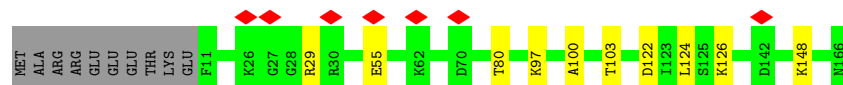
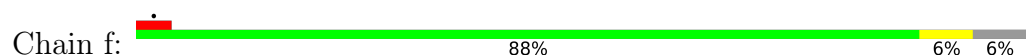
- Molecule 41: 30S ribosomal protein S13



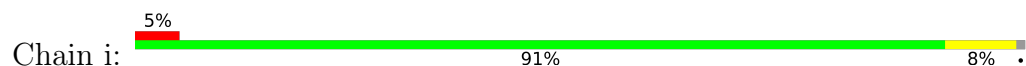
- Molecule 42: 30S ribosomal protein S9



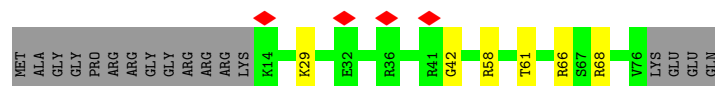
- Molecule 43: 30S ribosomal protein S5



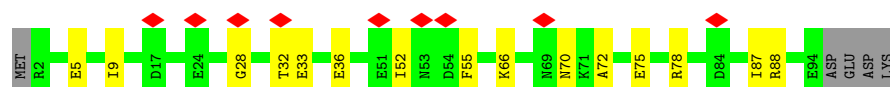
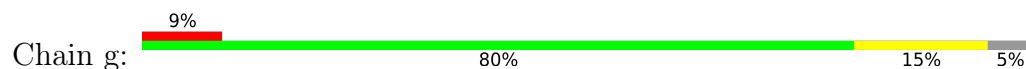
- Molecule 44: 30S ribosomal protein S8



- Molecule 45: 30S ribosomal protein S18



- Molecule 46: 30S ribosomal protein S6



- Molecule 47: RNA (5'-R(P*GP*GP*AP*GP*GP*UP*NP*NP*NP*NP*NP*NP*AP*UP*G)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35129	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 ($e^-/\text{\AA}^2$)	26.3	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-1900	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	366.432, 366.432, 366.432	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.041, 1.041, 1.041	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, FME, 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	Z	0.80	0/632	0.69	0/838
2	P	0.77	0/1105	0.62	0/1483
3	A	0.62	0/67815	0.51	1/105765 (0.0%)
4	a	0.46	0/36716	0.47	0/57253
5	B	0.47	0/2692	0.48	0/4193
6	G	0.83	0/2120	0.69	0/2847
7	H	0.80	0/1661	0.67	0/2227
8	I	0.77	0/1587	0.65	0/2143
9	J	0.56	0/1398	0.61	0/1877
10	K	0.46	0/1302	0.60	0/1757
11	M	0.72	0/1149	0.63	1/1549 (0.1%)
12	N	0.76	0/927	0.70	0/1243
13	O	0.80	0/1104	0.69	1/1471 (0.1%)
14	Q	0.74	0/956	0.61	0/1277
15	R	0.59	0/923	0.65	0/1234
16	S	0.73	0/934	0.62	0/1249
17	T	0.84	0/955	0.70	0/1265
18	U	0.75	0/803	0.62	0/1073
19	V	0.82	0/861	0.70	0/1159
20	W	0.73	0/733	0.69	0/978
21	X	0.58	0/770	0.62	0/1029
22	Y	0.51	0/746	0.67	0/1000
23	1	0.68	0/469	0.67	0/625
24	2	0.56	0/528	0.62	0/703
25	3	0.71	0/438	0.70	0/590
26	5	0.79	0/440	0.65	0/585
27	6	0.60	0/392	0.60	0/523
28	8	0.86	0/526	0.77	0/690
29	7	0.94	0/364	0.61	0/474
30	d	0.50	0/1657	0.63	0/2228
31	e	0.50	0/1647	0.66	0/2211
32	h	0.52	0/1195	0.62	0/1605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	k	0.52	0/826	0.62	0/1111
34	l	0.49	0/891	0.53	0/1203
35	o	0.58	0/506	0.64	0/671
36	p	0.58	0/730	0.58	0/975
37	q	0.48	0/723	0.59	0/971
38	u	0.44	0/606	0.56	0/810
39	9	0.71	0/295	0.71	0/388
40	t	0.47	0/663	0.59	0/889
41	n	0.50	0/909	0.60	0/1218
42	j	0.56	0/1024	0.65	0/1374
43	f	0.63	0/1174	0.60	0/1583
44	i	0.61	0/1044	0.61	0/1401
45	s	0.63	0/525	0.62	0/704
46	g	0.52	0/784	0.59	0/1052
47	b	0.34	0/222	0.66	0/343
48	m	0.54	0/1075	0.69	0/1439
49	r	0.51	0/659	0.64	0/881
50	c	0.43	0/1808	0.59	0/2426
51	D	0.34	0/1837	0.41	0/2862
52	4	0.43	0/496	0.53	0/661
All	All	0.59	0/152342	0.54	3/228106 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	131	HIS	N-CA-C	7.43	114.91	108.22
13	O	65	GLY	N-CA-C	6.51	119.77	110.46
3	A	3	U	N1-C1'-C2'	5.44	120.16	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	626	0	645	3	0
2	P	1081	0	1143	4	0
3	A	60551	0	30436	213	0
4	a	32794	0	16511	156	0
5	B	2408	0	1218	12	0
6	G	2085	0	2192	23	0
7	H	1637	0	1680	13	0
8	I	1564	0	1611	9	0
9	J	1381	0	1435	14	0
10	K	1284	0	1301	11	0
11	M	1127	0	1117	12	0
12	N	920	0	981	8	0
13	O	1090	0	1131	9	0
14	Q	952	0	999	8	0
15	R	914	0	956	16	0
16	S	922	0	994	8	0
17	T	943	0	1014	11	0
18	U	793	0	831	12	0
19	V	853	0	914	7	0
20	W	725	0	761	4	0
21	X	761	0	823	7	0
22	Y	738	0	787	5	0
23	1	463	0	501	6	0
24	2	527	0	554	7	0
25	3	436	0	473	1	0
26	5	433	0	441	9	0
27	6	389	0	388	6	0
28	8	521	0	586	8	0
29	7	360	0	406	1	0
30	d	1634	0	1699	19	0
31	e	1617	0	1646	23	0
32	h	1180	0	1221	7	0
33	k	814	0	863	9	0
34	l	876	0	895	6	0
35	o	496	0	520	8	0
36	p	721	0	751	8	0
37	q	712	0	744	8	0
38	u	606	0	650	3	0
39	9	292	0	336	6	0
40	t	646	0	653	14	0
41	n	902	0	950	20	0
42	j	1008	0	1031	14	0
43	f	1160	0	1223	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	i	1032	0	1082	8	0
45	s	516	0	548	4	0
46	g	773	0	772	11	0
47	b	199	0	99	1	0
48	m	1058	0	1130	16	0
49	r	651	0	689	10	0
50	c	1781	0	1844	13	0
51	D	1644	0	834	4	0
52	4	486	0	488	9	0
53	A	9	0	0	0	0
53	a	2	0	0	0	0
54	A	114	0	0	0	0
54	D	1	0	0	0	0
54	U	1	0	0	0	0
54	a	25	0	0	0	0
55	5	1	0	0	0	0
55	6	1	0	0	0	0
55	9	1	0	0	0	0
55	o	1	0	0	0	0
56	D	10	0	10	0	0
All	All	140248	0	93507	658	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 3.

All (658) 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)
3:A:2783:U:OP2	39:9:19:ARG:NH1	2.00	0.93
17:T:83:LEU:HD22	17:T:88:ILE:HD11	1.52	0.92
3:A:1708:A:H61	3:A:2023:C:N4	1.69	0.90
3:A:1112:G:O2'	3:A:1140:A:O2'	1.95	0.83
4:a:415:A:OP1	31:e:108:ARG:NH2	2.11	0.82
3:A:2007:G:O2'	3:A:2009:U:OP2	1.97	0.82
4:a:1237:C:O2'	41:n:110:LYS:NZ	2.13	0.81
4:a:1015:C:O2'	4:a:1016:A:O4'	1.96	0.81
4:a:1436:A:O2'	4:a:1437:A:O4'	1.98	0.81
3:A:1288:G:OP2	13:O:21:ARG:NH1	2.15	0.79
27:6:2:ARG:N	27:6:21:LYS:O	2.16	0.79
4:a:399:G:OP1	37:q:9:ARG:NH2	2.15	0.78
10:K:57:ASP:O	10:K:62:ARG:NH1	2.16	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1122:U:O2'	3:A:1132:A:OP1	2.01	0.78
4:a:80:A:OP2	4:a:81:A:N6	2.16	0.78
4:a:980:C:N4	42:j:132:ARG:OXT	2.16	0.78
5:B:41:C:O2	9:J:92:ARG:NH1	2.18	0.77
7:H:55:ASP:OD1	7:H:85:LYS:NZ	2.15	0.77
4:a:773:G:N2	4:a:821:U:OP2	2.17	0.77
3:A:1708:A:N6	3:A:2023:C:H42	1.83	0.77
3:A:2903:A:OP1	26:5:50:TYR:OH	2.03	0.77
4:a:1074:U:O4	30:d:3:GLN:NE2	2.18	0.76
3:A:1459:A:N6	3:A:1629:U:O2	2.18	0.76
13:O:55:LEU:O	13:O:60:ARG:NH2	2.19	0.76
4:a:1158:C:O2	42:j:20:ARG:NH1	2.19	0.76
30:d:11:ARG:NH2	30:d:176:THR:O	2.19	0.75
4:a:437:U:OP2	31:e:29:ARG:NH2	2.19	0.75
4:a:986:G:OP2	4:a:1369:U:O2'	2.05	0.75
3:A:1652:A:O2'	3:A:1654:A:OP2	2.05	0.75
3:A:2717:A:OP2	14:Q:13:ARG:NH2	2.20	0.75
4:a:819:C:O2'	4:a:911:A:N1	2.20	0.75
3:A:1879:U:O2	3:A:1917:A:N6	2.19	0.75
3:A:2710:C:OP1	16:S:53:ARG:NH1	2.20	0.74
27:6:9:CYS:SG	27:6:10:THR:N	2.60	0.74
52:4:16:ASP:O	52:4:20:ASN:N	2.20	0.74
4:a:434:U:OP1	31:e:31:TYR:OH	2.04	0.74
41:n:17:ILE:O	41:n:20:THR:OG1	2.04	0.74
6:G:63:ARG:NH1	6:G:83:TYR:O	2.21	0.74
4:a:152:A:N6	4:a:169:C:O2	2.21	0.74
19:V:1:MET:N	19:V:111:LYS:O	2.21	0.73
6:G:143:ASN:H	6:G:155:ALA:HB3	1.54	0.73
9:J:68:THR:OG1	9:J:85:ILE:O	2.04	0.73
4:a:700:U:O2'	4:a:702:A:N7	2.17	0.73
4:a:412:G:N7	31:e:3:ARG:NH1	2.37	0.73
46:g:36:GLU:OE2	46:g:66:LYS:NZ	2.21	0.73
4:a:1361:A:O2'	32:h:33:ASP:OD1	2.04	0.73
1:Z:35:ASP:OD2	3:A:900:G:O2'	2.06	0.73
3:A:1115:G:O2'	3:A:1133:G:OP2	2.07	0.73
30:d:17:ASP:OD1	33:k:16:ARG:NH2	2.21	0.73
3:A:2313:A:N6	27:6:19:THR:OG1	2.21	0.72
32:h:111:ARG:NH2	32:h:123:GLU:OE1	2.21	0.72
3:A:1708:A:H61	3:A:2023:C:H42	1.32	0.72
3:A:2255:G:OP1	6:G:261:ARG:NH2	2.22	0.72
3:A:2666:A:O2'	11:M:100:ARG:NH2	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:587:G:O2'	36:p:54:ARG:NH1	2.23	0.72
3:A:1038:C:OP1	17:T:53:ARG:NH2	2.22	0.71
4:a:644:U:OP1	49:r:8:LYS:NZ	2.22	0.71
4:a:1031:G:OP2	4:a:1032:C:N4	2.23	0.71
3:A:224:A:N1	3:A:268:A:O2'	2.23	0.71
3:A:593:U:O2'	3:A:594:G:OP1	2.07	0.71
3:A:2250:A:OP1	6:G:171:TYR:OH	2.07	0.71
4:a:541:A:O2'	4:a:543:A:OP2	2.06	0.71
12:N:64:ARG:NH1	12:N:81:GLU:OE2	2.23	0.71
3:A:791:U:O2'	3:A:2638:C:O2'	2.09	0.71
3:A:1038:C:O2'	18:U:10:LYS:NZ	2.22	0.71
42:j:132:ARG:NH2	51:D:36:A:OP1	2.23	0.71
7:H:210:GLU:OE1	7:H:212:ARG:NH2	2.24	0.71
3:A:575:G:O2'	3:A:577:A:N7	2.25	0.70
3:A:2285:C:O2'	3:A:2454:C:OP2	2.09	0.70
3:A:1377:U:OP2	20:W:58:TYR:OH	2.10	0.70
20:W:33:VAL:O	20:W:76:ARG:NH1	2.24	0.70
5:B:42:G:OP2	52:4:1:MET:N	2.23	0.70
3:A:1806:U:OP2	3:A:1811:A:N6	2.25	0.69
5:B:28:C:OP2	15:R:37:ASN:ND2	2.25	0.69
18:U:63:ASN:OD1	18:U:96:THR:OG1	2.08	0.69
4:a:383:U:OP1	37:q:70:THR:OG1	2.09	0.69
3:A:84:A:N1	3:A:98:U:O2'	2.25	0.69
3:A:2820:U:O2'	3:A:2824:G:N2	2.25	0.69
3:A:342:A:N3	3:A:362:C:O2'	2.24	0.69
13:O:61:LEU:O	28:8:13:ARG:NH1	2.25	0.69
24:2:7:ARG:NH1	24:2:59:GLU:OE1	2.24	0.69
30:d:16:ARG:NH2	30:d:180:ASP:OD1	2.25	0.69
4:a:9:A:N6	31:e:196:GLU:O	2.25	0.69
3:A:1089:C:O2'	3:A:1090:A:OP1	2.10	0.69
3:A:253:G:OP2	28:8:13:ARG:NH2	2.25	0.68
3:A:788:A:O2'	3:A:1703:U:OP1	2.12	0.68
4:a:1331:C:N3	40:t:36:ARG:NH1	2.40	0.68
3:A:2820:U:HO2'	3:A:2824:G:N2	1.92	0.68
3:A:2680:U:OP2	3:A:2681:A:O2'	2.12	0.67
3:A:2530:A:O2'	3:A:2532:G:OP2	2.10	0.67
4:a:509:C:OP1	48:m:127:ARG:NH2	2.26	0.67
31:e:18:SER:OG	31:e:25:GLU:OE1	2.10	0.67
3:A:527:G:O2'	3:A:552:A:N6	2.27	0.67
4:a:761:A:OP1	36:p:69:TYR:OH	2.11	0.67
4:a:691:G:N2	34:l:39:GLY:O	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1072:A:N3	3:A:2513:G:O2'	2.27	0.67
3:A:1432:A:O2'	3:A:1434:U:OP2	2.13	0.67
18:U:61:THR:OG1	18:U:98:ASP:OD2	2.12	0.67
3:A:2043:U:O2'	26:5:4:PRO:O	2.12	0.66
48:m:24:LEU:O	48:m:40:SER:OG	2.12	0.66
3:A:1229:G:OP1	13:O:30:THR:OG1	2.13	0.66
4:a:196:A:N6	49:r:66:THR:OG1	2.27	0.66
15:R:37:ASN:O	15:R:69:LYS:NZ	2.29	0.66
4:a:287:A:OP1	4:a:288:C:O2'	2.09	0.66
15:R:71:GLU:O	15:R:74:THR:OG1	2.14	0.66
45:s:58:ARG:O	45:s:61:THR:OG1	2.14	0.66
4:a:515:C:OP2	4:a:516:U:O2'	2.13	0.66
7:H:158:SER:O	7:H:161:SER:OG	2.11	0.66
3:A:1708:A:N6	3:A:2023:C:N4	2.40	0.66
4:a:530:C:OP2	48:m:79:TYR:OH	2.12	0.66
4:a:550:U:OP1	31:e:10:LYS:NZ	2.28	0.65
4:a:1003:G:O2'	4:a:1004:A:N7	2.29	0.65
8:I:122:GLY:O	8:I:192:LEU:N	2.29	0.65
4:a:595:G:OP1	44:i:86:ARG:NH2	2.28	0.65
16:S:33:ARG:NH1	16:S:84:GLU:OE2	2.29	0.65
23:l:40:VAL:HG23	23:l:41:ASP:H	1.62	0.65
42:j:108:ARG:NH1	42:j:109:ASP:O	2.30	0.65
3:A:1422:A:O2'	3:A:1433:U:O2	2.13	0.65
3:A:983:G:OP1	28:8:59:LYS:NZ	2.29	0.65
3:A:618:A:OP2	3:A:2526:C:O2'	2.15	0.64
4:a:129:A:O2'	4:a:197:U:O4	2.09	0.64
4:a:930:U:O2'	4:a:1093:G:O2'	2.05	0.64
4:a:1295:C:OP2	4:a:1296:A:O2'	2.11	0.64
3:A:252:C:O2	28:8:12:LYS:NZ	2.30	0.64
3:A:375:A:O2'	3:A:377:U:OP2	2.13	0.64
3:A:1916:A:N3	3:A:2113:U:O2'	2.23	0.64
4:a:410:G:OP2	31:e:66:ARG:NH1	2.31	0.64
4:a:435:C:OP2	4:a:436:G:O2'	2.12	0.64
4:a:409:C:O2'	4:a:629:A:N3	2.30	0.64
49:r:64:GLN:OE1	49:r:76:ARG:NH2	2.30	0.64
4:a:364:A:N3	4:a:376:U:O2'	2.30	0.64
4:a:948:A:N3	4:a:1387:U:O2'	2.29	0.64
42:j:38:ARG:NH1	42:j:44:GLU:OE1	2.30	0.64
37:q:73:ASN:O	37:q:76:SER:OG	2.14	0.64
3:A:2715:G:OP1	3:A:2740:A:N6	2.30	0.63
4:a:559:U:O2'	48:m:96:ARG:NH1	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:969:A:HO2'	4:a:994:C:HO2'	1.43	0.63
43:f:148:LYS:NZ	44:i:132:TRP:O	2.31	0.63
3:A:1039:C:O2	11:M:4:THR:OG1	2.13	0.63
4:a:10:G:OP2	43:f:126:LYS:NZ	2.23	0.63
4:a:205:A:N6	4:a:206:A:N6	2.46	0.63
3:A:1400:C:O2'	3:A:1836:A:N3	2.23	0.63
4:a:1351:A:O2'	51:D:32:G:O2'	2.14	0.63
5:B:48:A:OP1	15:R:68:THR:OG1	2.16	0.63
30:d:8:ILE:O	30:d:12:VAL:HG23	1.99	0.63
6:G:44:ASN:OD1	6:G:45:ASN:N	2.31	0.63
4:a:1200:U:OP1	33:k:53:ARG:NH2	2.32	0.63
32:h:68:ASN:O	32:h:138:ARG:NE	2.32	0.63
4:a:1262:A:N3	4:a:1380:C:O2'	2.26	0.62
41:n:12:GLU:O	41:n:44:ARG:NH1	2.32	0.62
3:A:1472:C:O2'	3:A:1616:A:OP2	2.15	0.62
50:c:57:LEU:HD12	50:c:217:MET:HE3	1.80	0.62
3:A:34:U:O2'	3:A:35:G:O4'	2.17	0.62
4:a:588:C:OP1	36:p:58:LYS:NZ	2.31	0.62
4:a:949:G:O5'	32:h:102:ARG:NH1	2.32	0.62
14:Q:8:ARG:NH1	14:Q:16:MET:SD	2.73	0.62
3:A:2751:U:OP1	7:H:132:LYS:NZ	2.30	0.62
3:A:607:C:O3'	18:U:76:TYR:OH	2.18	0.61
3:A:2318:U:OP1	3:A:2407:A:O2'	2.13	0.61
46:g:28:GLY:O	46:g:32:THR:OG1	2.07	0.61
3:A:1523:G:O2'	3:A:1607:A:O2'	2.16	0.61
14:Q:34:GLU:OE1	14:Q:105:LYS:NZ	2.33	0.61
4:a:1095:U:O2'	4:a:1114:A:OP2	2.14	0.61
17:T:50:ARG:O	17:T:54:LYS:NZ	2.34	0.61
3:A:1816:A:OP2	6:G:221:ARG:NH1	2.34	0.61
40:t:12:ASP:OD2	40:t:35:SER:OG	2.07	0.61
3:A:963:A:N3	5:B:78:U:O2'	2.33	0.61
3:A:1053:A:N3	3:A:1197:C:O2'	2.29	0.61
46:g:52:ILE:HG21	46:g:87:ILE:HG23	1.82	0.61
1:Z:26:SER:OG	1:Z:28:ARG:NH1	2.34	0.61
9:J:112:ARG:HD3	41:n:66:GLU:OE2	2.00	0.61
49:r:70:SER:OG	49:r:71:ALA:O	2.19	0.61
11:M:7:ALA:HB1	11:M:12:ILE:HD11	1.82	0.61
3:A:2024:A:OP2	7:H:138:ARG:NH1	2.34	0.61
3:A:923:A:O2'	3:A:924:G:O5'	2.19	0.60
4:a:82:G:H1	4:a:88:U:HO2'	1.44	0.60
38:u:7:ALA:O	38:u:11:VAL:N	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:1085:U:O2	50:c:103:ASN:ND2	2.34	0.60
4:a:1313:U:OP2	41:n:21:TYR:OH	2.13	0.60
4:a:988:A:O2'	4:a:1333:C:N3	2.31	0.60
4:a:519:C:O3'	31:e:36:HIS:NE2	2.35	0.60
6:G:146:LEU:HD11	6:G:154:ILE:HD11	1.83	0.60
15:R:96:ARG:NH1	15:R:99:TYR:O	2.35	0.60
3:A:2326:G:OP1	9:J:72:LYS:NZ	2.21	0.60
15:R:53:LEU:HD13	15:R:89:ILE:HD11	1.84	0.59
3:A:1711:G:O2'	3:A:2018:U:O4	2.20	0.59
3:A:826:A:OP1	6:G:217:ARG:NH2	2.34	0.59
3:A:1826:G:OP1	6:G:260:ARG:NE	2.33	0.59
10:K:45:GLN:OE1	10:K:46:GLU:O	2.20	0.59
3:A:1182:G:H21	11:M:109:MET:HE3	1.67	0.59
3:A:2815:C:O2'	3:A:2829:A:N3	2.30	0.59
4:a:1154:G:OP2	33:k:1:MET:N	2.23	0.59
6:G:177:ARG:O	6:G:178:SER:OG	2.21	0.59
3:A:1378:U:OP2	3:A:1431:U:O2'	2.18	0.59
6:G:146:LEU:HD21	6:G:154:ILE:HG13	1.85	0.59
37:q:54:GLU:OE2	37:q:83:LYS:NZ	2.36	0.59
3:A:545:G:N1	3:A:548:A:OP2	2.34	0.59
3:A:631:U:O5'	13:O:16:ARG:NH2	2.35	0.59
19:V:2:GLU:OE2	19:V:72:LYS:NZ	2.33	0.59
3:A:1198:G:OP2	17:T:58:ARG:NE	2.36	0.58
4:a:1329:A:OP1	40:t:3:ARG:NH1	2.36	0.58
30:d:19:GLU:O	30:d:39:ARG:NH2	2.36	0.58
3:A:2836:C:O2	3:A:2903:A:O2'	2.22	0.58
36:p:26:GLU:OE2	36:p:77:ARG:NH1	2.36	0.58
41:n:66:GLU:O	41:n:66:GLU:HG3	2.04	0.58
49:r:59:ASP:OD1	49:r:60:ILE:N	2.36	0.58
4:a:86:G:O2'	4:a:87:C:OP2	2.20	0.58
3:A:2323:U:O4	15:R:17:ARG:NH2	2.37	0.58
4:a:180:U:N3	4:a:209:G:N7	2.48	0.57
26:5:30:CYS:O	26:5:34:GLY:N	2.37	0.57
4:a:315:U:O2'	4:a:316:C:O5'	2.17	0.57
4:a:1055:G:O2'	4:a:1056:A:O4'	2.16	0.57
5:B:10:U:O2'	5:B:12:U:OP1	2.22	0.57
30:d:167:TYR:OH	43:f:55:GLU:OE2	2.21	0.57
4:a:1436:A:O2'	4:a:1437:A:O5'	2.23	0.57
3:A:1941:C:O2'	3:A:1942:U:O5'	2.23	0.57
4:a:681:G:O3'	46:g:88:ARG:NH2	2.37	0.57
8:I:156:THR:OG1	8:I:158:ASN:O	2.15	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:c:170:ARG:NH1	50:c:195:GLU:OE1	2.38	0.57
18:U:35:PHE:O	18:U:57:THR:OG1	2.21	0.57
3:A:620:G:O2'	3:A:1292:A:OP1	2.22	0.57
3:A:1989:C:O2'	3:A:1991:G:OP2	2.21	0.57
16:S:16:ARG:NH1	16:S:80:THR:O	2.37	0.57
31:e:114:VAL:HB	31:e:119:ILE:HD11	1.87	0.57
4:a:1443:G:OP1	16:S:108:LYS:N	2.38	0.56
7:H:154:VAL:O	7:H:167:GLN:NE2	2.38	0.56
35:o:24:CYS:SG	35:o:25:GLU:N	2.78	0.56
3:A:2770:U:OP2	3:A:2782:C:N4	2.39	0.56
42:j:14:ARG:HG2	42:j:79:GLN:HB2	1.87	0.56
30:d:128:SER:O	30:d:132:VAL:HG23	2.05	0.56
2:P:42:ILE:HD12	2:P:97:VAL:HG21	1.87	0.56
4:a:205:A:C6	4:a:206:A:N6	2.73	0.56
3:A:15:G:H4'	26:5:18:THR:HG22	1.88	0.56
15:R:56:ALA:HB3	15:R:80:ILE:HG23	1.86	0.56
50:c:90:PHE:HB3	50:c:151:ILE:HG22	1.86	0.56
3:A:82:G:N2	3:A:102:A:OP2	2.35	0.56
3:A:1216:U:HO2'	3:A:1217:U:C4'	2.19	0.56
6:G:72:ASP:OD2	6:G:189:ARG:NH2	2.38	0.55
43:f:80:THR:OG1	43:f:122:ASP:O	2.14	0.55
3:A:2669:G:OP2	11:M:86:LYS:NZ	2.31	0.55
45:s:29:LYS:NZ	46:g:5:GLU:OE2	2.37	0.55
2:P:17:THR:OG1	5:B:87:C:O2	2.13	0.55
3:A:593:U:OP2	18:U:64:LYS:NZ	2.24	0.55
44:i:110:GLU:OE1	44:i:121:ARG:NE	2.39	0.55
3:A:616:G:N2	3:A:2058:A:OP1	2.37	0.55
4:a:315:U:HO2'	4:a:316:C:C5'	2.20	0.55
4:a:351:U:O2'	4:a:354:G:O6	2.14	0.55
4:a:552:G:OP1	31:e:55:GLN:OE1	2.24	0.55
4:a:1327:G:N1	4:a:1330:A:OP2	2.36	0.55
31:e:65:GLU:OE2	31:e:69:ARG:NE	2.40	0.55
3:A:622:A:O2'	3:A:2046:U:OP1	2.24	0.55
4:a:691:G:N2	34:l:40:ASN:OD1	2.34	0.55
7:H:26:THR:OG1	7:H:199:GLY:O	2.25	0.55
51:D:59:A:O2'	51:D:61:U:OP2	2.20	0.55
3:A:1597:U:OP1	3:A:1762:U:O2'	2.19	0.55
4:a:122:C:OP1	4:a:319:C:O2'	2.24	0.55
4:a:820:G:OP1	4:a:912:G:N2	2.40	0.55
39:9:7:VAL:HG21	39:9:36:GLN:HB2	1.89	0.55
3:A:1130:A:O2'	3:A:1131:G:N7	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2060:A:O2'	3:A:2062:G:OP2	2.24	0.55
4:a:744:U:OP1	45:s:66:ARG:NH2	2.40	0.55
6:G:66:ASP:OD2	6:G:102:ARG:NH2	2.40	0.55
30:d:186:ALA:HB3	30:d:197:VAL:HG22	1.87	0.55
3:A:2822:C:O2'	3:A:2823:G:O4'	2.25	0.54
4:a:1237:C:O2'	41:n:102:THR:O	2.19	0.54
36:p:33:THR:O	36:p:37:ASN:ND2	2.40	0.54
3:A:418:G:O2'	3:A:446:G:O6	2.23	0.54
22:Y:73:MET:SD	22:Y:94:ILE:HD12	2.46	0.54
3:A:248:G:N7	28:8:8:ARG:NH2	2.52	0.54
27:6:8:ALA:N	27:6:46:ARG:O	2.41	0.54
52:4:47:ARG:NH1	52:4:48:LEU:O	2.40	0.54
41:n:37:ALA:HB1	41:n:55:ARG:HB3	1.88	0.54
4:a:166:U:O4	4:a:167:A:N6	2.41	0.54
4:a:702:A:OP1	34:l:55:SER:OG	2.26	0.54
4:a:1358:G:O2'	4:a:1384:G:O6	2.23	0.54
30:d:49:ALA:O	30:d:69:THR:OG1	2.26	0.54
3:A:2835:C:O2'	26:5:41:HIS:ND1	2.29	0.54
3:A:2392:G:O6	28:8:43:GLN:NE2	2.41	0.53
4:a:1024:A:P	40:t:18:LYS:HZ1	2.31	0.53
50:c:203:ASN:OD1	50:c:204:ASP:N	2.41	0.53
2:P:3:LEU:HD23	2:P:4:PRO:O	2.09	0.53
3:A:1785:G:OP1	3:A:1787:A:N6	2.41	0.53
4:a:1323:G:OP2	52:4:77:LYS:NZ	2.23	0.53
3:A:217:G:N2	3:A:219:A:N3	2.57	0.53
41:n:24:GLY:HA2	41:n:69:LEU:CD2	2.38	0.53
50:c:54:TYR:CD2	50:c:220:ALA:HB2	2.44	0.53
3:A:1844:G:O5'	6:G:156:ARG:NH2	2.42	0.53
3:A:2477:A:OP1	3:A:2524:A:O2'	2.11	0.53
41:n:25:ILE:CD1	41:n:65:VAL:HG21	2.39	0.53
4:a:921:U:OP2	48:m:107:ARG:NH2	2.42	0.53
48:m:26:LYS:O	48:m:72:ASN:ND2	2.41	0.53
3:A:2101:U:O2'	3:A:2624:G:O2'	2.25	0.52
9:J:114:PHE:O	9:J:115:GLN:NE2	2.43	0.52
24:2:2:LYS:NZ	24:2:5:GLU:OE1	2.41	0.52
44:i:3:MET:O	44:i:4:THR:OG1	2.22	0.52
3:A:351:G:H2'	3:A:352:A:C8	2.45	0.52
10:K:155:GLU:OE1	10:K:157:TYR:N	2.39	0.52
31:e:158:ASN:ND2	31:e:160:PHE:O	2.40	0.52
4:a:130:A:OP1	49:r:7:ARG:NH2	2.38	0.52
3:A:250:G:OP2	3:A:252:C:N4	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1712:A:O2'	3:A:1718:G:N7	2.36	0.52
3:A:18:C:O2'	3:A:597:U:OP1	2.26	0.52
4:a:731:U:O2'	4:a:732:G:OP1	2.27	0.52
17:T:72:HIS:NE2	17:T:103:GLU:OE2	2.43	0.52
3:A:2374:C:O2'	27:6:17:TYR:OH	2.23	0.52
4:a:107:G:P	4:a:334:G:H22	2.33	0.52
6:G:91:ILE:HD12	6:G:103:TYR:CD1	2.45	0.52
3:A:1070:A:OP2	3:A:1178:C:O2'	2.25	0.52
4:a:613:U:O2	4:a:640:G:N2	2.41	0.52
3:A:187:C:O2'	3:A:220:A:N3	2.37	0.52
3:A:590:U:OP1	3:A:1257:G:O2'	2.21	0.52
32:h:113:GLU:OE2	32:h:122:ASN:ND2	2.43	0.52
3:A:446:G:N7	23:1:55:LYS:NZ	2.55	0.51
4:a:269:U:N3	4:a:272:C:OP2	2.40	0.51
4:a:284:G:OP1	49:r:16:SER:OG	2.16	0.51
22:Y:65:VAL:O	22:Y:67:SER:N	2.42	0.51
4:a:418:G:OP2	31:e:24:LYS:NZ	2.44	0.51
3:A:579:U:O2'	17:T:49:ASP:OD2	2.19	0.51
3:A:2504:C:O2	39:9:4:ARG:NH2	2.42	0.51
4:a:672:G:H22	4:a:749:G:H1	1.58	0.51
4:a:774:A:OP2	4:a:820:G:N2	2.40	0.51
14:Q:73:ASN:ND2	14:Q:79:GLN:OE1	2.42	0.51
30:d:186:ALA:HB3	30:d:197:VAL:CG2	2.41	0.51
3:A:1073:A:H3'	3:A:1074:G:H8	1.76	0.51
12:N:8:LEU:HD22	12:N:84:CYS:SG	2.50	0.51
45:s:42:GLY:O	45:s:68:ARG:NH2	2.44	0.51
3:A:660:A:N3	8:I:182:ASN:ND2	2.56	0.51
4:a:152:A:N6	4:a:169:C:C2	2.76	0.51
28:8:9:GLY:O	28:8:13:ARG:NE	2.42	0.51
3:A:27:G:O2'	3:A:28:A:OP2	2.25	0.51
3:A:1324:A:N1	3:A:1692:C:O2'	2.42	0.51
19:V:24:ILE:HG22	19:V:71:VAL:HG11	1.92	0.51
3:A:32:C:N4	3:A:493:A:OP2	2.41	0.51
4:a:75:A:OP2	4:a:94:G:N2	2.30	0.51
4:a:205:A:N6	4:a:206:A:H62	2.09	0.51
9:J:34:ILE:HG23	9:J:155:VAL:O	2.10	0.51
31:e:63:MET:HE1	31:e:93:ARG:NH2	2.26	0.51
4:a:1190:A:OP2	42:j:97:ARG:NH2	2.44	0.50
3:A:312:A:O2'	3:A:313:U:O4'	2.12	0.50
4:a:529:G:N7	48:m:63:ARG:NH1	2.60	0.50
4:a:1266:G:OP1	35:o:36:LYS:NZ	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:1281:G:HO2'	4:a:1324:U:HO2'	1.58	0.50
3:A:1131:G:N2	3:A:1134:U:OP1	2.44	0.50
4:a:933:A:O2'	4:a:1410:C:OP2	2.15	0.50
15:R:64:ALA:O	15:R:65:THR:OG1	2.28	0.50
48:m:69:ARG:NH2	48:m:75:GLU:OE2	2.43	0.50
3:A:1577:G:O2'	3:A:1578:A:OP1	2.23	0.50
33:k:22:ALA:O	33:k:26:VAL:HG23	2.11	0.50
46:g:52:ILE:HG21	46:g:87:ILE:CG2	2.42	0.50
4:a:519:C:N3	4:a:549:G:N2	2.60	0.50
4:a:180:U:O2	4:a:210:A:N6	2.45	0.50
4:a:1026:A:O2'	4:a:1228:U:O2'	2.28	0.50
4:a:1322:A:OP1	52:4:73:ARG:NE	2.43	0.50
4:a:760:G:OP1	36:p:73:LYS:NZ	2.44	0.50
4:a:1328:C:H41	35:o:15:LYS:CD	2.24	0.50
13:O:76:ILE:HG23	13:O:112:LEU:HD12	1.93	0.50
38:u:27:ALA:O	38:u:30:THR:OG1	2.29	0.50
31:e:181:GLU:O	31:e:183:SER:N	2.45	0.50
3:A:629:A:H5'	8:I:89:VAL:HG21	1.94	0.49
4:a:1137:U:O2'	4:a:1138:U:O5'	2.29	0.49
40:t:27:LYS:NZ	40:t:45:ILE:O	2.45	0.49
3:A:1566:G:OP2	3:A:1567:A:O2'	2.08	0.49
4:a:1452:G:O2'	4:a:1472:A:N6	2.45	0.49
3:A:576:U:OP1	3:A:604:G:N2	2.45	0.49
3:A:2328:A:P	3:A:2336:A:H61	2.34	0.49
4:a:954:G:N1	4:a:1349:G:OP2	2.40	0.49
6:G:117:GLU:N	6:G:128:ASN:OD1	2.36	0.49
8:I:75:GLN:OE1	8:I:83:TRP:NE1	2.43	0.49
3:A:1131:G:O6	3:A:1133:G:N2	2.46	0.49
3:A:1604:C:OP2	3:A:1605:A:O2'	2.27	0.49
4:a:1100:G:H21	4:a:1178:A:H61	1.58	0.49
3:A:242:U:O2'	3:A:667:G:O2'	2.16	0.49
3:A:2277:G:N2	3:A:2303:G:OP1	2.43	0.49
4:a:787:C:O2'	34:l:122:ARG:NH1	2.46	0.49
9:J:112:ARG:CD	41:n:66:GLU:OE2	2.61	0.49
4:a:1013:G:N2	4:a:1014:A:O4'	2.43	0.49
17:T:105:ALA:HB1	18:U:40:PHE:HZ	1.77	0.49
3:A:632:U:OP2	13:O:16:ARG:NH2	2.42	0.49
29:7:21:LYS:O	29:7:24:SER:OG	2.29	0.49
4:a:1328:C:H41	35:o:15:LYS:HD3	1.77	0.49
10:K:54:ARG:NH2	10:K:57:ASP:OD1	2.39	0.49
3:A:1715:U:O2'	3:A:1717:G:N7	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:c:26:LYS:NZ	50:c:194:ASP:OD2	2.26	0.48
48:m:47:CYS:SG	48:m:93:VAL:HG21	2.54	0.48
4:a:302:C:OP1	4:a:618:G:O2'	2.29	0.48
7:H:119:THR:OG1	7:H:179:THR:HG22	2.12	0.48
17:T:74:MET:SD	17:T:110:VAL:HG13	2.52	0.48
37:q:58:LEU:O	37:q:62:ASN:OD1	2.31	0.48
3:A:2667:G:OP1	11:M:100:ARG:NH1	2.46	0.48
16:S:88:VAL:HG11	16:S:91:ARG:CZ	2.43	0.48
31:e:151:ILE:O	31:e:155:VAL:HG23	2.14	0.48
3:A:1658:A:N6	19:V:88:ARG:O	2.46	0.48
4:a:36:G:O2'	48:m:128:SER:O	2.17	0.48
40:t:36:ARG:NH2	40:t:72:GLY:O	2.46	0.48
24:2:9:LEU:O	24:2:60:ARG:NH2	2.46	0.48
41:n:24:GLY:HA2	41:n:69:LEU:HD22	1.95	0.48
4:a:51:A:O2'	4:a:368:G:N2	2.47	0.48
41:n:24:GLY:HA3	41:n:65:VAL:HG23	1.96	0.48
46:g:9:ILE:HD12	46:g:88:ARG:HB2	1.96	0.48
3:A:1008:C:O2'	3:A:2300:A:N3	2.44	0.48
3:A:2668:A:OP1	11:M:77:ARG:NH1	2.42	0.48
3:A:2750:C:P	7:H:123:LYS:HZ3	2.36	0.48
15:R:30:ARG:NE	15:R:47:ASP:OD2	2.40	0.48
21:X:77:GLU:OE1	21:X:96:LYS:NZ	2.43	0.48
3:A:735:C:O3'	6:G:217:ARG:NH1	2.47	0.48
9:J:139:PRO:O	52:4:29:LYS:NZ	2.40	0.48
4:a:285:C:OP1	49:r:47:LYS:NZ	2.41	0.47
4:a:288:C:O2	49:r:43:SER:N	2.47	0.47
21:X:94:ALA:O	21:X:98:GLY:N	2.47	0.47
3:A:2022:U:O2	12:N:3:GLN:NE2	2.42	0.47
3:A:85:G:O5'	21:X:26:THR:OG1	2.33	0.47
3:A:615:A:OP2	18:U:79:ARG:NH1	2.43	0.47
3:A:895:U:O2'	25:3:22:THR:HG22	2.13	0.47
3:A:1586:U:O2'	3:A:1587:C:O4'	2.19	0.47
5:B:35:C:O2	15:R:102:HIS:NE2	2.45	0.47
16:S:88:VAL:HG11	16:S:91:ARG:NH2	2.29	0.47
4:a:1100:G:N2	4:a:1178:A:H61	2.12	0.47
5:B:7:G:H1	5:B:108:U:H3	1.60	0.47
46:g:33:GLU:HB3	46:g:72:ALA:HB2	1.95	0.47
33:k:19:ASP:OD1	33:k:20:GLN:N	2.48	0.47
41:n:3:ARG:NH2	41:n:6:GLY:O	2.48	0.47
3:A:592:A:N3	3:A:592:A:O2'	2.44	0.47
3:A:2322:C:OP2	15:R:14:ARG:NH2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:778:C:O2'	4:a:909:C:N3	2.43	0.47
4:a:1408:C:OP2	43:f:29:ARG:NH2	2.47	0.47
9:J:123:ASP:OD2	9:J:127:ASN:ND2	2.46	0.47
16:S:51:LYS:HG2	16:S:62:THR:HG22	1.96	0.47
20:W:89:LEU:O	24:2:36:GLN:NE2	2.45	0.47
33:k:63:GLU:OE2	35:o:49:TYR:OH	2.25	0.47
49:r:22:THR:OG1	49:r:48:THR:O	2.30	0.47
4:a:936:G:H22	47:b:13:A:P	2.37	0.47
42:j:53:PRO:O	42:j:57:THR:HG22	2.13	0.47
18:U:88:HIS:NE2	18:U:90:GLN:OE1	2.45	0.47
52:4:25:SER:OG	52:4:26:GLY:N	2.48	0.47
3:A:2863:G:N3	16:S:2:THR:N	2.62	0.47
4:a:194:G:N2	4:a:197:U:OP2	2.42	0.47
13:O:58:PHE:CD2	28:8:10:ALA:HB2	2.49	0.47
44:i:12:THR:HG22	44:i:15:ARG:HH12	1.81	0.46
6:G:3:ILE:HG23	6:G:18:SER:O	2.15	0.46
6:G:84:ASP:OD2	6:G:87:ARG:NE	2.41	0.46
35:o:3:LYS:O	35:o:7:VAL:HG23	2.14	0.46
19:V:12:ILE:H	19:V:12:ILE:HG13	1.62	0.46
3:A:600:U:OP1	11:M:114:ARG:NH1	2.45	0.46
3:A:1092:A:H62	3:A:1154:G:H21	1.64	0.46
11:M:18:VAL:HG13	11:M:58:ILE:HD12	1.97	0.46
3:A:1710:G:H2'	3:A:1711:G:O4'	2.15	0.46
6:G:172:VAL:N	6:G:184:ILE:O	2.48	0.46
3:A:874:A:N7	3:A:2274:A:O2'	2.48	0.46
4:a:1134:U:O4	4:a:1135:A:N6	2.49	0.46
9:J:38:MET:SD	9:J:53:ALA:HB1	2.56	0.46
4:a:987:A:N6	4:a:1235:U:O4'	2.47	0.46
4:a:1138:U:N3	4:a:1291:A:OP1	2.44	0.46
10:K:99:GLN:N	10:K:102:ASP:O	2.47	0.46
21:X:48:THR:HG23	21:X:49:GLN:H	1.80	0.46
41:n:28:SER:OG	41:n:29:THR:N	2.48	0.45
3:A:830:U:H4'	3:A:1806:U:H4'	1.98	0.45
3:A:1938:U:O2'	3:A:1939:A:OP1	2.29	0.45
3:A:2370:U:O2'	3:A:2400:U:O2'	2.30	0.45
3:A:2505:A:OP1	39:9:31:LYS:NZ	2.26	0.45
4:a:15:U:N3	4:a:18:U:OP2	2.43	0.45
5:B:6:U:O2'	15:R:30:ARG:NH2	2.50	0.45
4:a:668:A:OP2	36:p:5:GLN:NE2	2.49	0.45
17:T:28:LYS:HG2	17:T:34:VAL:CG1	2.47	0.45
3:A:1101:A:OP2	3:A:1133:G:N2	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:m:66:ALA:N	48:m:78:ALA:O	2.50	0.45
3:A:1780:G:N2	3:A:1783:G:OP2	2.42	0.45
8:I:117:LYS:NZ	8:I:189:ALA:O	2.50	0.45
3:A:675:G:N1	3:A:678:A:OP2	2.46	0.45
4:a:1024:A:OP2	40:t:18:LYS:NZ	2.27	0.45
50:c:141:TYR:O	50:c:145:ILE:HG22	2.17	0.45
2:P:34:LEU:HD11	2:P:129:THR:OG1	2.17	0.45
3:A:1215:U:O2'	3:A:1217:U:OP2	2.29	0.45
11:M:20:ASP:OD1	11:M:21:ALA:N	2.47	0.45
19:V:28:ASN:OD1	19:V:29:ALA:N	2.49	0.45
3:A:1261:G:OP1	18:U:67:ARG:NH1	2.50	0.45
3:A:1440:A:O2'	3:A:1515:G:O2'	2.24	0.45
4:a:329:A:N7	4:a:336:C:O2'	2.48	0.45
50:c:93:ASN:OD1	50:c:94:GLN:N	2.50	0.45
3:A:2769:G:OP1	39:9:35:ARG:NH1	2.50	0.44
4:a:130:A:OP2	4:a:197:U:N3	2.50	0.44
14:Q:24:LEU:HD23	14:Q:44:VAL:HG21	2.00	0.44
3:A:37:C:H5'	3:A:497:U:H5''	1.98	0.44
3:A:850:G:OP2	3:A:851:C:N4	2.41	0.44
19:V:24:ILE:HD12	19:V:32:ALA:HB1	1.99	0.44
24:2:38:GLU:OE1	24:2:38:GLU:N	2.49	0.44
3:A:1064:A:N1	3:A:1185:U:O2'	2.35	0.44
3:A:2900:C:O3'	14:Q:96:ARG:NH1	2.50	0.44
4:a:1189:G:OP2	42:j:101:LYS:NZ	2.39	0.44
8:I:57:VAL:HG11	8:I:79:ARG:HB3	2.00	0.44
37:q:36:GLN:NE2	37:q:38:GLY:O	2.49	0.44
12:N:64:ARG:HG2	12:N:83:ALA:HB3	1.99	0.44
17:T:28:LYS:HG2	17:T:34:VAL:HG12	1.99	0.44
38:u:79:MET:O	38:u:82:ASN:OD1	2.35	0.44
40:t:3:ARG:HB2	40:t:5:ILE:HG22	1.99	0.44
41:n:15:VAL:CG1	41:n:34:LEU:HD21	2.47	0.44
48:m:123:ARG:NE	48:m:125:GLN:O	2.38	0.44
3:A:575:G:N2	3:A:2050:A:OP1	2.50	0.44
3:A:2599:A:OP1	3:A:2601:G:O2'	2.33	0.44
4:a:1119:C:OP1	30:d:171:THR:OG1	2.27	0.44
3:A:138:U:N3	3:A:141:U:OP2	2.46	0.44
4:a:1100:G:H21	4:a:1178:A:N6	2.15	0.44
41:n:15:VAL:HG11	41:n:34:LEU:HD21	2.00	0.44
46:g:75:GLU:OE1	46:g:78:ARG:NH2	2.45	0.44
52:4:49:ASP:OD1	52:4:50:ILE:N	2.50	0.44
3:A:1582:U:O2'	3:A:1583:G:O5'	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2231:C:OP2	6:G:150:LYS:NZ	2.34	0.44
4:a:272:C:H2'	4:a:273:G:O4'	2.18	0.44
42:j:130:SER:OG	42:j:132:ARG:O	2.35	0.44
50:c:120:MET:O	50:c:125:LEU:N	2.42	0.44
3:A:83:G:N1	3:A:101:G:O2'	2.43	0.44
3:A:2332:U:O2'	3:A:2333:U:OP2	2.31	0.44
3:A:2750:C:OP2	7:H:123:LYS:NZ	2.46	0.44
10:K:41:MET:HE1	10:K:54:ARG:HB2	2.00	0.44
3:A:1034:A:O2'	3:A:1036:C:OP2	2.35	0.44
4:a:1356:U:OP1	42:j:124:ARG:NH1	2.51	0.44
4:a:125:G:OP1	4:a:613:U:O2'	2.24	0.43
4:a:886:A:H1'	44:i:12:THR:HG21	2.00	0.43
3:A:1010:G:O4'	3:A:2294:A:N6	2.51	0.43
3:A:1037:A:H4'	18:U:71:ILE:HD11	2.00	0.43
4:a:1325:C:OP2	40:t:5:ILE:HD11	2.18	0.43
20:W:42:VAL:HA	20:W:45:ILE:HG22	2.00	0.43
31:e:15:LEU:HD13	31:e:56:LYS:HA	2.00	0.43
33:k:54:ALA:O	35:o:41:ARG:NH1	2.48	0.43
3:A:150:A:H61	3:A:179:A:H2	1.66	0.43
3:A:1109:U:O2	3:A:1113:A:O2'	2.22	0.43
36:p:47:LYS:O	36:p:53:ARG:NH1	2.47	0.43
44:i:46:ILE:HD13	44:i:62:LEU:HD22	1.99	0.43
3:A:1208:A:O2'	3:A:1262:U:O2	2.35	0.43
3:A:1459:A:H1'	3:A:1631:G:N2	2.33	0.43
4:a:1333:C:OP1	40:t:78:ARG:NH2	2.51	0.43
30:d:111:ASP:OD1	30:d:112:ALA:N	2.52	0.43
48:m:100:VAL:HG11	48:m:103:LEU:HD12	2.00	0.43
10:K:125:VAL:HG22	10:K:131:VAL:HG12	1.99	0.43
3:A:1073:A:H3'	3:A:1074:G:C8	2.53	0.43
3:A:2684:A:O3'	10:K:160:LYS:NZ	2.52	0.43
4:a:800:A:O2'	4:a:802:A:N7	2.45	0.43
41:n:42:ASP:OD1	41:n:43:THR:N	2.52	0.43
4:a:1260:C:O2'	42:j:72:GLY:O	2.31	0.43
4:a:1299:A:N3	4:a:1363:C:O2'	2.50	0.43
3:A:717:C:OP2	13:O:42:SER:OG	2.30	0.43
3:A:851:C:O2	3:A:2471:G:O2'	2.36	0.43
7:H:26:THR:HG21	7:H:201:VAL:HG22	2.01	0.43
12:N:3:GLN:O	12:N:21:THR:OG1	2.29	0.43
30:d:134:LYS:NZ	43:f:55:GLU:OE1	2.51	0.43
48:m:66:ALA:O	48:m:78:ALA:N	2.50	0.43
48:m:117:THR:HG23	48:m:117:THR:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2347:A:O2'	3:A:2348:G:OP2	2.36	0.43
12:N:63:VAL:HG11	12:N:102:VAL:HG22	2.01	0.43
34:l:29:ASN:OD1	34:l:30:THR:N	2.52	0.43
41:n:16:VAL:HG22	41:n:34:LEU:CD1	2.49	0.43
3:A:75:G:OP1	24:2:44:ARG:NH2	2.44	0.43
4:a:996:A:N3	40:t:52:TYR:OH	2.40	0.43
3:A:1861:U:O4	3:A:1927:A:N6	2.52	0.42
9:J:126:GLY:O	9:J:158:THR:OG1	2.19	0.42
24:2:6:ILE:HG22	24:2:56:VAL:HG11	2.01	0.42
31:e:98:VAL:HG21	31:e:119:ILE:HD13	2.01	0.42
32:h:78:ARG:O	32:h:85:TYR:N	2.46	0.42
46:g:70:ASN:O	46:g:70:ASN:ND2	2.52	0.42
3:A:745:G:O2'	3:A:1676:A:N3	2.50	0.42
3:A:1216:U:O2'	3:A:1217:U:O4'	2.35	0.42
4:a:571:A:O2'	4:a:574:G:O3'	2.37	0.42
8:I:137:LYS:O	8:I:141:ASN:OD1	2.37	0.42
21:X:26:THR:HG22	21:X:33:VAL:HG23	1.99	0.42
31:e:83:GLY:HA3	31:e:191:GLU:HB2	2.01	0.42
3:A:1898:C:OP2	3:A:1899:U:N3	2.52	0.42
3:A:2312:C:OP2	27:6:22:ASN:ND2	2.51	0.42
22:Y:51:VAL:O	22:Y:55:VAL:HG22	2.19	0.42
37:q:6:ARG:HA	37:q:71:VAL:HG21	2.02	0.42
41:n:25:ILE:HG13	41:n:65:VAL:HG21	2.01	0.42
17:T:113:ALA:O	17:T:116:ALA:HB3	2.19	0.42
34:l:32:VAL:O	34:l:32:VAL:HG13	2.20	0.42
4:a:1015:C:H2'	4:a:1034:U:O2'	2.18	0.42
12:N:63:VAL:CG1	12:N:102:VAL:HG22	2.50	0.42
39:9:7:VAL:HG13	39:9:34:GLN:OE1	2.19	0.42
3:A:1015:C:OP1	3:A:1033:G:N1	2.48	0.42
30:d:172:VAL:O	30:d:172:VAL:HG13	2.20	0.42
31:e:54:LYS:HA	31:e:194:ILE:HD13	2.00	0.42
3:A:1815:C:H5''	6:G:224:VAL:HG11	2.00	0.42
4:a:1261:A:OP1	42:j:71:GLY:N	2.46	0.42
18:U:38:VAL:HG11	18:U:56:ALA:HB3	2.02	0.42
3:A:674:C:O2	3:A:684:U:O2'	2.36	0.42
3:A:738:U:O2'	3:A:1390:A:N3	2.49	0.42
7:H:28:VAL:HG11	7:H:211:ILE:HD11	2.00	0.42
40:t:40:ILE:HD11	40:t:71:LEU:HD23	2.01	0.42
3:A:1725:G:O2'	3:A:1789:A:O2'	2.23	0.42
3:A:1739:G:N7	6:G:14:ARG:NH1	2.65	0.42
5:B:101:A:H2'	5:B:102:G:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:7:ILE:HG23	22:Y:42:LYS:O	2.19	0.42
30:d:10:LEU:O	30:d:14:ILE:HD12	2.20	0.42
40:t:19:VAL:HG21	40:t:44:PHE:CE1	2.55	0.42
50:c:87:ALA:HA	50:c:222:LEU:HD21	2.01	0.42
30:d:111:ASP:O	30:d:115:VAL:HG23	2.19	0.42
52:4:16:ASP:OD2	52:4:51:SER:OG	2.26	0.42
3:A:2500:U:OP1	3:A:2502:C:N4	2.52	0.41
4:a:330:C:OP2	4:a:336:C:N4	2.53	0.41
11:M:18:VAL:CG1	11:M:58:ILE:HD12	2.50	0.41
23:1:36:VAL:HG13	23:1:60:THR:HG23	2.01	0.41
50:c:46:THR:O	50:c:50:VAL:HG23	2.20	0.41
3:A:2546:U:O4'	3:A:2569:A:N6	2.53	0.41
3:A:2717:A:OP1	14:Q:3:TYR:OH	2.32	0.41
15:R:92:ILE:HD11	15:R:119:PHE:CD1	2.55	0.41
26:5:33:CYS:O	26:5:35:ARG:N	2.53	0.41
42:j:59:THR:HG21	42:j:63:TYR:HE2	1.86	0.41
3:A:2693:C:N4	10:K:108:GLY:O	2.54	0.41
4:a:85:U:O2'	4:a:86:G:OP1	2.38	0.41
21:X:9:VAL:CG1	21:X:68:VAL:HG13	2.50	0.41
21:X:9:VAL:HG13	21:X:68:VAL:HG13	2.01	0.41
50:c:187:VAL:HG21	50:c:199:VAL:HG13	2.02	0.41
3:A:2403:A:N3	15:R:113:ARG:NH2	2.68	0.41
3:A:2835:C:O2'	26:5:40:SER:OG	2.35	0.41
4:a:1331:C:O2	40:t:36:ARG:NH2	2.52	0.41
10:K:18:THR:OG1	10:K:25:THR:O	2.29	0.41
14:Q:74:GLU:OE1	14:Q:74:GLU:N	2.52	0.41
33:k:59:LYS:O	33:k:62:ARG:NE	2.53	0.41
4:a:1388:A:OP1	32:h:95:ARG:NH2	2.54	0.41
1:Z:40:THR:HG22	1:Z:41:GLY:N	2.36	0.41
3:A:943:C:HO2'	3:A:944:G:P	2.44	0.41
3:A:1506:C:HO2'	3:A:2729:G:HO2'	1.68	0.41
31:e:71:THR:OG1	31:e:93:ARG:NH2	2.54	0.41
33:k:22:ALA:HB1	33:k:74:ILE:HD11	2.03	0.41
43:f:100:ALA:O	43:f:103:THR:OG1	2.30	0.41
46:g:52:ILE:O	46:g:55:PHE:N	2.47	0.41
4:a:1369:U:OP2	4:a:1370:C:N4	2.43	0.41
9:J:50:LEU:O	9:J:54:VAL:HG23	2.20	0.41
9:J:111:VAL:HG12	9:J:113:ASP:H	1.85	0.41
15:R:57:SER:O	15:R:63:ILE:HG21	2.21	0.41
26:5:28:THR:O	26:5:38:LYS:N	2.46	0.41
37:q:75:LEU:HG	37:q:80:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:i:20:VAL:HG12	44:i:20:VAL:O	2.21	0.41
3:A:568:C:O2	3:A:597:U:O2'	2.38	0.41
3:A:2106:U:O2'	23:1:23:ASN:OD1	2.31	0.41
3:A:2682:G:N2	3:A:2692:A:OP2	2.54	0.41
4:a:261:U:O4'	4:a:283:G:N2	2.26	0.41
4:a:1516:G:OP2	4:a:1519:A:O2'	2.30	0.41
5:B:8:A:H61	5:B:107:U:H3	1.69	0.41
9:J:122:PHE:HE2	9:J:167:ARG:HE	1.69	0.41
23:1:55:LYS:O	23:1:56:SER:OG	2.22	0.41
3:A:2835:C:HO2'	26:5:41:HIS:CE1	2.29	0.40
10:K:96:ALA:N	10:K:128:ASN:O	2.53	0.40
3:A:704:U:O2'	8:I:100:LYS:O	2.32	0.40
3:A:1388:C:H2'	3:A:1389:U:O4'	2.20	0.40
3:A:1756:U:H2'	3:A:1757:U:O4'	2.20	0.40
22:Y:7:ILE:HD12	22:Y:42:LYS:O	2.22	0.40
35:o:16:TYR:HD2	35:o:18:VAL:HG12	1.86	0.40
43:f:97:LYS:N	43:f:124:LEU:O	2.48	0.40
51:D:7:A:H3'	51:D:8:U:H5'	2.03	0.40
3:A:1216:U:O2'	3:A:1217:U:O5'	2.35	0.40
3:A:2869:G:N7	3:A:2887:G:N2	2.57	0.40
4:a:412:G:OP1	31:e:111:ARG:NE	2.54	0.40
11:M:26:LEU:H	11:M:26:LEU:HD23	1.86	0.40
12:N:64:ARG:NH2	12:N:99:PHE:O	2.54	0.40
30:d:133:GLN:NE2	30:d:152:VAL:HG12	2.37	0.40
4:a:530:C:H41	48:m:63:ARG:NH2	2.19	0.40
3:A:609:U:O2'	3:A:854:G:OP2	2.33	0.40
3:A:838:A:OP2	3:A:2098:A:O2'	2.39	0.40
7:H:194:VAL:HG12	7:H:195:ILE:N	2.37	0.40
23:1:38:ILE:O	23:1:45:LYS:N	2.54	0.40
30:d:101:ASN:OD1	30:d:102:VAL:N	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	80/94 (85%)	72 (90%)	8 (10%)	0	100	100
2	P	133/144 (92%)	125 (94%)	8 (6%)	0	100	100
6	G	271/277 (98%)	251 (93%)	20 (7%)	0	100	100
7	H	214/220 (97%)	192 (90%)	22 (10%)	0	100	100
8	I	202/207 (98%)	186 (92%)	16 (8%)	0	100	100
9	J	173/179 (97%)	165 (95%)	8 (5%)	0	100	100
10	K	162/178 (91%)	147 (91%)	15 (9%)	0	100	100
11	M	140/145 (97%)	133 (95%)	7 (5%)	0	100	100
12	N	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
13	O	143/146 (98%)	135 (94%)	8 (6%)	0	100	100
14	Q	118/122 (97%)	115 (98%)	3 (2%)	0	100	100
15	R	116/119 (98%)	101 (87%)	15 (13%)	0	100	100
16	S	112/116 (97%)	100 (89%)	12 (11%)	0	100	100
17	T	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
18	U	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
19	V	109/117 (93%)	103 (94%)	6 (6%)	0	100	100
20	W	87/91 (96%)	77 (88%)	10 (12%)	0	100	100
21	X	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
22	Y	92/217 (42%)	77 (84%)	15 (16%)	0	100	100
23	1	57/62 (92%)	49 (86%)	8 (14%)	0	100	100
24	2	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
25	3	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
26	5	52/58 (90%)	43 (83%)	9 (17%)	0	100	100
27	6	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
28	8	62/66 (94%)	54 (87%)	8 (13%)	0	100	100
29	7	40/45 (89%)	39 (98%)	1 (2%)	0	100	100
30	d	205/217 (94%)	187 (91%)	18 (9%)	0	100	100
31	e	197/200 (98%)	175 (89%)	22 (11%)	0	100	100
32	h	144/156 (92%)	133 (92%)	10 (7%)	1 (1%)	18	49
33	k	100/102 (98%)	87 (87%)	13 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	l	116/129 (90%)	108 (93%)	8 (7%)	0	100	100
35	o	57/60 (95%)	57 (100%)	0	0	100	100
36	p	84/89 (94%)	80 (95%)	4 (5%)	0	100	100
37	q	88/91 (97%)	78 (89%)	10 (11%)	0	100	100
38	u	78/83 (94%)	75 (96%)	3 (4%)	0	100	100
39	9	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
40	t	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
41	n	111/121 (92%)	100 (90%)	11 (10%)	0	100	100
42	j	125/132 (95%)	114 (91%)	11 (9%)	0	100	100
43	f	154/166 (93%)	147 (96%)	7 (4%)	0	100	100
44	i	129/132 (98%)	118 (92%)	11 (8%)	0	100	100
45	s	61/80 (76%)	56 (92%)	5 (8%)	0	100	100
46	g	91/98 (93%)	83 (91%)	8 (9%)	0	100	100
48	m	133/137 (97%)	116 (87%)	17 (13%)	0	100	100
49	r	77/87 (88%)	67 (87%)	10 (13%)	0	100	100
50	c	219/255 (86%)	202 (92%)	17 (8%)	0	100	100
52	4	53/84 (63%)	51 (96%)	2 (4%)	0	100	100
All	All	5287/5775 (92%)	4856 (92%)	430 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	h	53	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	64/75 (85%)	64 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	112/119 (94%)	112 (100%)	0	100	100
6	G	220/224 (98%)	220 (100%)	0	100	100
7	H	174/177 (98%)	174 (100%)	0	100	100
8	I	168/169 (99%)	168 (100%)	0	100	100
9	J	154/158 (98%)	153 (99%)	1 (1%)	78	83
10	K	144/155 (93%)	144 (100%)	0	100	100
11	M	121/123 (98%)	121 (100%)	0	100	100
12	N	100/100 (100%)	100 (100%)	0	100	100
13	O	111/112 (99%)	111 (100%)	0	100	100
14	Q	101/102 (99%)	101 (100%)	0	100	100
15	R	94/95 (99%)	94 (100%)	0	100	100
16	S	100/102 (98%)	100 (100%)	0	100	100
17	T	96/98 (98%)	96 (100%)	0	100	100
18	U	86/86 (100%)	86 (100%)	0	100	100
19	V	90/94 (96%)	87 (97%)	3 (3%)	33	63
20	W	80/82 (98%)	80 (100%)	0	100	100
21	X	84/90 (93%)	84 (100%)	0	100	100
22	Y	83/190 (44%)	83 (100%)	0	100	100
23	1	49/52 (94%)	49 (100%)	0	100	100
24	2	58/62 (94%)	58 (100%)	0	100	100
25	3	51/53 (96%)	51 (100%)	0	100	100
26	5	49/51 (96%)	49 (100%)	0	100	100
27	6	45/47 (96%)	45 (100%)	0	100	100
28	8	55/57 (96%)	55 (100%)	0	100	100
29	7	38/40 (95%)	38 (100%)	0	100	100
30	d	169/175 (97%)	169 (100%)	0	100	100
31	e	174/175 (99%)	174 (100%)	0	100	100
32	h	126/132 (96%)	126 (100%)	0	100	100
33	k	91/91 (100%)	91 (100%)	0	100	100
34	l	94/104 (90%)	94 (100%)	0	100	100
35	o	52/53 (98%)	52 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	p	79/81 (98%)	79 (100%)	0	100	100
37	q	76/77 (99%)	76 (100%)	0	100	100
38	u	67/69 (97%)	67 (100%)	0	100	100
39	9	35/35 (100%)	35 (100%)	0	100	100
40	t	70/80 (88%)	70 (100%)	0	100	100
41	n	98/104 (94%)	97 (99%)	1 (1%)	68	79
42	j	105/109 (96%)	105 (100%)	0	100	100
43	f	122/131 (93%)	122 (100%)	0	100	100
44	i	112/113 (99%)	112 (100%)	0	100	100
45	s	56/68 (82%)	56 (100%)	0	100	100
46	g	81/86 (94%)	81 (100%)	0	100	100
48	m	117/119 (98%)	116 (99%)	1 (1%)	70	80
49	r	74/82 (90%)	74 (100%)	0	100	100
50	c	192/221 (87%)	192 (100%)	0	100	100
52	4	55/75 (73%)	55 (100%)	0	100	100
All	All	4572/4893 (93%)	4566 (100%)	6 (0%)	87	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	137	ILE
19	V	10	ILE
19	V	11	ARG
19	V	12	ILE
41	n	65	VAL
48	m	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
6	G	200	HIS
6	G	232	HIS
7	H	134	HIS
9	J	37	ASN
13	O	35	HIS
14	Q	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	6	26	ASN
30	d	68	HIS
35	o	31	HIS
36	p	9	ASN
36	p	50	HIS
41	n	105	ASN
42	j	16	ASN
44	i	16	ASN
44	i	18	ASN
49	r	49	HIS
52	4	20	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	2821/2923 (96%)	470 (16%)	9 (0%)
4	a	1528/1551 (98%)	262 (17%)	0
47	b	7/15 (46%)	1 (14%)	0
5	B	112/115 (97%)	13 (11%)	1 (0%)
51	D	76/77 (98%)	10 (13%)	0
All	All	4544/4681 (97%)	756 (16%)	10 (0%)

All (756) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	23	G
3	A	34	U
3	A	35	G
3	A	36	G
3	A	46	C
3	A	51	G
3	A	61	A
3	A	64	A
3	A	71	A
3	A	74	U
3	A	75	G
3	A	85	G
3	A	88	G
3	A	99	U
3	A	101	G
3	A	117	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	118	A
3	A	119	U
3	A	130	A
3	A	150	A
3	A	154	A
3	A	155	U
3	A	164	A
3	A	165	C
3	A	167	U
3	A	176	A
3	A	177	G
3	A	180	G
3	A	182	C
3	A	189	G
3	A	199	A
3	A	202	A
3	A	218	G
3	A	219	A
3	A	224	A
3	A	225	A
3	A	229	A
3	A	231	A
3	A	232	U
3	A	251	G
3	A	255	G
3	A	270	C
3	A	284	C
3	A	285	U
3	A	286	U
3	A	287	G
3	A	288	C
3	A	289	U
3	A	294	G
3	A	299	U
3	A	304	G
3	A	312	A
3	A	313	U
3	A	314	A
3	A	315	C
3	A	316	G
3	A	321	U
3	A	322	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	326	A
3	A	338	G
3	A	344	U
3	A	353	A
3	A	354	A
3	A	373	A
3	A	401	U
3	A	404	U
3	A	409	G
3	A	410	G
3	A	431	C
3	A	432	G
3	A	457	G
3	A	458	A
3	A	470	G
3	A	497	U
3	A	502	C
3	A	503	A
3	A	526	A
3	A	527	G
3	A	536	A
3	A	543	G
3	A	550	A
3	A	551	G
3	A	553	A
3	A	563	G
3	A	567	G
3	A	572	C
3	A	573	A
3	A	575	G
3	A	576	U
3	A	577	A
3	A	578	G
3	A	583	A
3	A	587	C
3	A	591	A
3	A	593	U
3	A	594	G
3	A	606	G
3	A	616	G
3	A	618	A
3	A	626	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	630	G
3	A	646	A
3	A	658	A
3	A	666	A
3	A	679	G
3	A	682	A
3	A	683	G
3	A	690	U
3	A	699	U
3	A	715	A
3	A	727	G
3	A	730	A
3	A	731	U
3	A	762	C
3	A	767	A
3	A	775	A
3	A	783	G
3	A	785	C
3	A	792	U
3	A	795	A
3	A	806	A
3	A	809	A
3	A	813	G
3	A	816	G
3	A	819	A
3	A	820	G
3	A	823	G
3	A	827	A
3	A	828	A
3	A	829	U
3	A	830	U
3	A	835	U
3	A	837	G
3	A	850	G
3	A	852	U
3	A	854	G
3	A	857	C
3	A	872	U
3	A	873	U
3	A	891	A
3	A	902	A
3	A	904	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	911	A
3	A	923	A
3	A	924	G
3	A	940	U
3	A	941	A
3	A	943	C
3	A	944	G
3	A	945	A
3	A	955	A
3	A	957	C
3	A	970	U
3	A	971	U
3	A	975	U
3	A	977	A
3	A	985	A
3	A	989	A
3	A	990	G
3	A	1001	A
3	A	1003	A
3	A	1005	G
3	A	1017	A
3	A	1018	A
3	A	1022	G
3	A	1027	A
3	A	1040	A
3	A	1049	C
3	A	1056	U
3	A	1057	A
3	A	1066	G
3	A	1069	G
3	A	1070	A
3	A	1077	U
3	A	1090	A
3	A	1091	G
3	A	1106	G
3	A	1112	G
3	A	1114	A
3	A	1123	C
3	A	1125	U
3	A	1127	U
3	A	1128	A
3	A	1129	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1130	A
3	A	1131	G
3	A	1132	A
3	A	1133	G
3	A	1141	U
3	A	1155	A
3	A	1156	G
3	A	1160	C
3	A	1172	A
3	A	1176	U
3	A	1177	A
3	A	1178	C
3	A	1183	G
3	A	1186	A
3	A	1215	U
3	A	1216	U
3	A	1217	U
3	A	1218	G
3	A	1225	G
3	A	1245	G
3	A	1250	G
3	A	1258	A
3	A	1276	G
3	A	1288	G
3	A	1291	A
3	A	1294	G
3	A	1302	G
3	A	1310	A
3	A	1312	A
3	A	1337	A
3	A	1339	U
3	A	1345	A
3	A	1358	A
3	A	1366	U
3	A	1378	U
3	A	1382	C
3	A	1401	G
3	A	1402	A
3	A	1405	G
3	A	1406	G
3	A	1416	U
3	A	1423	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1430	A
3	A	1432	A
3	A	1449	A
3	A	1452	C
3	A	1454	U
3	A	1455	U
3	A	1456	U
3	A	1457	U
3	A	1458	A
3	A	1459	A
3	A	1463	A
3	A	1464	U
3	A	1471	A
3	A	1472	C
3	A	1481	A
3	A	1490	G
3	A	1494	G
3	A	1497	A
3	A	1499	U
3	A	1504	U
3	A	1511	C
3	A	1522	G
3	A	1526	G
3	A	1527	A
3	A	1533	A
3	A	1536	C
3	A	1537	A
3	A	1547	C
3	A	1552	U
3	A	1553	A
3	A	1560	A
3	A	1561	G
3	A	1569	G
3	A	1574	G
3	A	1578	A
3	A	1581	U
3	A	1582	U
3	A	1583	G
3	A	1592	A
3	A	1594	U
3	A	1606	C
3	A	1607	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1616	A
3	A	1625	U
3	A	1630	A
3	A	1631	G
3	A	1634	A
3	A	1639	G
3	A	1651	C
3	A	1652	A
3	A	1654	A
3	A	1660	A
3	A	1671	A
3	A	1678	A
3	A	1683	U
3	A	1690	A
3	A	1691	G
3	A	1692	C
3	A	1704	C
3	A	1709	A
3	A	1718	G
3	A	1721	A
3	A	1726	A
3	A	1740	G
3	A	1759	G
3	A	1772	G
3	A	1786	A
3	A	1790	G
3	A	1791	G
3	A	1800	A
3	A	1803	G
3	A	1813	A
3	A	1818	A
3	A	1827	C
3	A	1828	U
3	A	1829	A
3	A	1835	U
3	A	1843	U
3	A	1846	A
3	A	1856	A
3	A	1860	C
3	A	1883	A
3	A	1885	G
3	A	1893	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1895	C
3	A	1896	U
3	A	1897	U
3	A	1899	U
3	A	1900	G
3	A	1909	C
3	A	1933	G
3	A	1939	A
3	A	1940	A
3	A	1942	U
3	A	1943	A
3	A	1955	A
3	A	1956	G
3	A	1957	G
3	A	1963	A
3	A	1965	A
3	A	1969	C
3	A	1982	U
3	A	1991	G
3	A	1994	C
3	A	1997	A
3	A	1998	A
3	A	1999	G
3	A	2014	G
3	A	2018	U
3	A	2020	U
3	A	2024	A
3	A	2040	A
3	A	2047	A
3	A	2050	A
3	A	2058	A
3	A	2059	G
3	A	2060	A
3	A	2070	C
3	A	2078	A
3	A	2079	G
3	A	2082	C
3	A	2083	G
3	A	2087	A
3	A	2088	G
3	A	2089	A
3	A	2096	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2114	G
3	A	2218	G
3	A	2225	A
3	A	2226	A
3	A	2231	C
3	A	2238	U
3	A	2239	A
3	A	2240	U
3	A	2241	C
3	A	2252	A
3	A	2265	G
3	A	2266	G
3	A	2290	C
3	A	2294	A
3	A	2295	A
3	A	2306	G
3	A	2310	C
3	A	2313	A
3	A	2314	A
3	A	2315	A
3	A	2326	G
3	A	2332	U
3	A	2333	U
3	A	2334	G
3	A	2335	G
3	A	2336	A
3	A	2337	A
3	A	2338	A
3	A	2339	U
3	A	2347	A
3	A	2352	G
3	A	2361	U
3	A	2362	A
3	A	2366	G
3	A	2372	G
3	A	2374	C
3	A	2377	C
3	A	2381	A
3	A	2404	A
3	A	2406	G
3	A	2410	G
3	A	2411	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2412	C
3	A	2418	G
3	A	2429	U
3	A	2430	C
3	A	2434	A
3	A	2450	U
3	A	2452	A
3	A	2456	G
3	A	2457	A
3	A	2468	C
3	A	2475	A
3	A	2479	C
3	A	2486	A
3	A	2529	G
3	A	2531	U
3	A	2532	G
3	A	2545	A
3	A	2547	C
3	A	2552	G
3	A	2562	G
3	A	2573	U
3	A	2575	G
3	A	2576	G
3	A	2581	U
3	A	2583	C
3	A	2593	A
3	A	2594	G
3	A	2599	A
3	A	2600	C
3	A	2605	G
3	A	2606	C
3	A	2609	G
3	A	2612	U
3	A	2613	C
3	A	2629	A
3	A	2637	C
3	A	2638	C
3	A	2640	U
3	A	2642	U
3	A	2657	G
3	A	2666	A
3	A	2673	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2675	G
3	A	2680	U
3	A	2690	G
3	A	2692	A
3	A	2716	U
3	A	2717	A
3	A	2718	C
3	A	2741	G
3	A	2753	U
3	A	2760	A
3	A	2762	G
3	A	2784	A
3	A	2791	A
3	A	2792	A
3	A	2793	G
3	A	2796	C
3	A	2805	A
3	A	2807	G
3	A	2817	A
3	A	2819	C
3	A	2821	U
3	A	2823	G
3	A	2824	G
3	A	2827	A
3	A	2838	C
3	A	2839	A
3	A	2850	G
3	A	2855	A
3	A	2863	G
3	A	2887	G
3	A	2892	G
3	A	2900	C
3	A	2905	C
3	A	2906	G
4	a	8	G
4	a	10	G
4	a	17	A
4	a	23	G
4	a	32	G
4	a	33	A
4	a	40	G
4	a	45	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	a	49	C
4	a	51	A
4	a	52	A
4	a	74	G
4	a	81	A
4	a	82	G
4	a	84	U
4	a	85	U
4	a	86	G
4	a	87	C
4	a	89	U
4	a	90	C
4	a	91	U
4	a	92	C
4	a	94	G
4	a	97	G
4	a	107	G
4	a	108	A
4	a	115	A
4	a	120	C
4	a	129	A
4	a	130	A
4	a	131	C
4	a	132	C
4	a	136	C
4	a	144	C
4	a	146	G
4	a	149	A
4	a	165	G
4	a	169	C
4	a	171	A
4	a	177	G
4	a	185	U
4	a	196	A
4	a	201	U
4	a	205	A
4	a	206	A
4	a	207	G
4	a	211	A
4	a	212	A
4	a	213	G
4	a	214	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	a	216	G
4	a	219	C
4	a	220	U
4	a	221	U
4	a	234	A
4	a	248	U
4	a	249	G
4	a	253	U
4	a	255	G
4	a	258	A
4	a	259	G
4	a	261	U
4	a	262	G
4	a	274	G
4	a	275	C
4	a	288	C
4	a	289	G
4	a	297	G
4	a	306	A
4	a	316	C
4	a	333	A
4	a	335	A
4	a	336	C
4	a	337	A
4	a	338	C
4	a	340	G
4	a	355	G
4	a	359	G
4	a	360	C
4	a	361	A
4	a	362	G
4	a	364	A
4	a	375	U
4	a	380	C
4	a	381	A
4	a	385	G
4	a	392	G
4	a	400	G
4	a	405	A
4	a	414	G
4	a	415	A
4	a	419	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	a	420	U
4	a	421	G
4	a	424	G
4	a	429	U
4	a	430	C
4	a	431	G
4	a	432	G
4	a	437	U
4	a	447	U
4	a	456	A
4	a	460	A
4	a	461	C
4	a	462	A
4	a	467	U
4	a	470	A
4	a	472	G
4	a	474	A
4	a	476	C
4	a	492	G
4	a	493	G
4	a	503	A
4	a	504	G
4	a	511	A
4	a	517	A
4	a	519	C
4	a	521	A
4	a	526	C
4	a	529	G
4	a	535	G
4	a	540	A
4	a	555	A
4	a	567	A
4	a	572	U
4	a	576	G
4	a	580	A
4	a	581	A
4	a	583	G
4	a	584	C
4	a	585	G
4	a	587	G
4	a	589	G
4	a	596	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	a	597	U
4	a	626	C
4	a	630	A
4	a	661	U
4	a	673	A
4	a	696	G
4	a	710	A
4	a	726	A
4	a	728	C
4	a	729	A
4	a	731	U
4	a	732	G
4	a	757	A
4	a	763	G
4	a	768	U
4	a	773	G
4	a	785	A
4	a	807	G
4	a	825	C
4	a	836	A
4	a	844	G
4	a	857	C
4	a	882	A
4	a	899	A
4	a	912	G
4	a	924	A
4	a	926	G
4	a	935	G
4	a	944	C
4	a	945	A
4	a	949	G
4	a	970	U
4	a	976	G
4	a	978	A
4	a	979	A
4	a	981	G
4	a	982	C
4	a	985	A
4	a	986	G
4	a	987	A
4	a	993	A
4	a	999	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	a	1003	G
4	a	1004	A
4	a	1012	U
4	a	1014	A
4	a	1016	A
4	a	1025	G
4	a	1030	A
4	a	1033	C
4	a	1034	U
4	a	1035	U
4	a	1036	C
4	a	1037	C
4	a	1048	A
4	a	1057	C
4	a	1058	A
4	a	1077	U
4	a	1078	C
4	a	1097	U
4	a	1101	G
4	a	1106	G
4	a	1107	U
4	a	1113	A
4	a	1120	G
4	a	1124	C
4	a	1138	U
4	a	1142	A
4	a	1144	C
4	a	1146	U
4	a	1150	G
4	a	1151	U
4	a	1153	G
4	a	1168	A
4	a	1179	C
4	a	1182	A
4	a	1192	G
4	a	1195	G
4	a	1207	A
4	a	1208	A
4	a	1212	A
4	a	1222	U
4	a	1223	U
4	a	1224	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	a	1225	U
4	a	1238	A
4	a	1247	A
4	a	1248	C
4	a	1268	A
4	a	1271	G
4	a	1279	G
4	a	1290	A
4	a	1297	U
4	a	1298	A
4	a	1310	A
4	a	1313	U
4	a	1316	G
4	a	1323	G
4	a	1328	C
4	a	1331	C
4	a	1346	C
4	a	1347	U
4	a	1351	A
4	a	1360	A
4	a	1364	G
4	a	1381	G
4	a	1405	A
4	a	1406	C
4	a	1409	A
4	a	1417	U
4	a	1430	G
4	a	1437	A
4	a	1444	A
4	a	1453	G
4	a	1457	A
4	a	1464	U
4	a	1465	A
4	a	1499	G
4	a	1509	G
4	a	1514	A
4	a	1515	A
4	a	1518	U
4	a	1529	G
4	a	1531	A
4	a	1541	G
4	a	1542	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	a	1543	A
4	a	1547	C
5	B	10	U
5	B	27	A
5	B	30	U
5	B	39	G
5	B	40	C
5	B	42	G
5	B	43	A
5	B	51	A
5	B	55	A
5	B	85	U
5	B	87	C
5	B	88	G
5	B	106	G
47	b	2	G
51	D	8	U
51	D	9	G
51	D	18	A
51	D	19	G
51	D	20	G
51	D	21	U
51	D	22	A
51	D	35	C
51	D	59	A
51	D	77	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	195	C
3	A	475	A
3	A	756	A
3	A	943	C
3	A	1128	A
3	A	1577	G
3	A	1938	U
3	A	1939	A
3	A	2337	A
5	B	9	C

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 157 ligands modelled in this entry, 156 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	FME	D	102	51	8,9,10	0.99	0	8,9,11	1.16	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	FME	D	102	51	-	3/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D	102	FME	C-CA-N	2.32	113.98	109.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	D	102	FME	CB-CA-N-CN
56	D	102	FME	O-C-CA-CB
56	D	102	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

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.

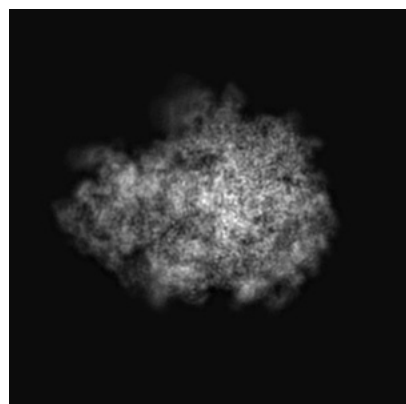
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12333. These allow visual inspection of the internal detail of the map and identification of artifacts.

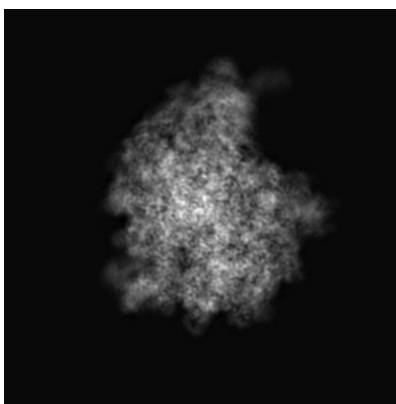
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

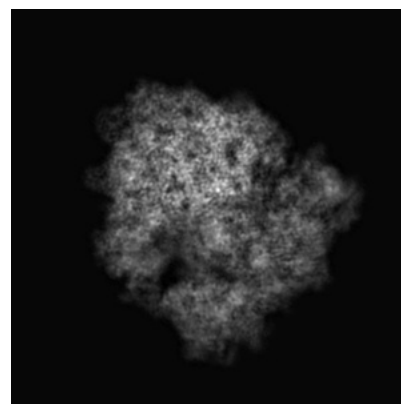
6.1.1 Primary map



X

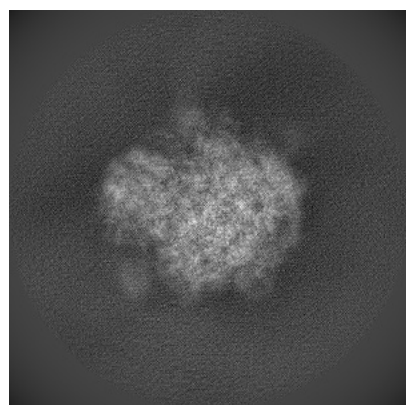


Y

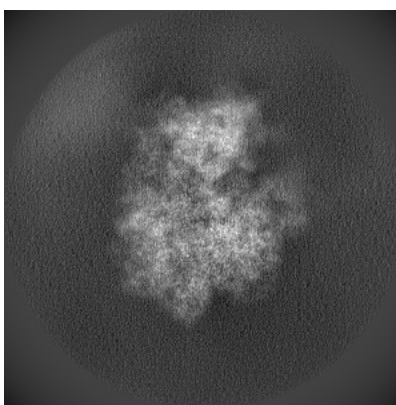


Z

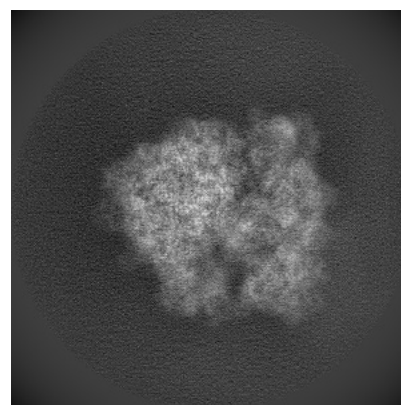
6.1.2 Raw map



X



Y

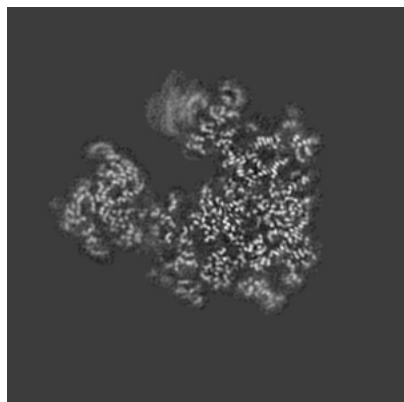


Z

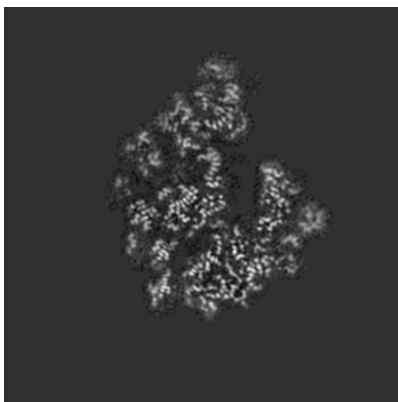
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

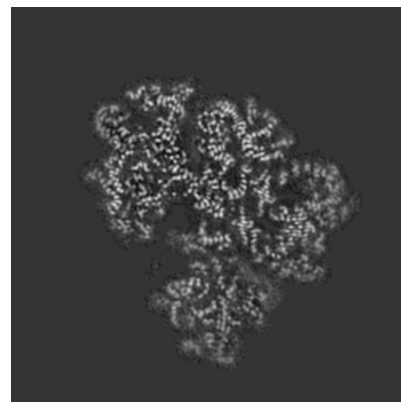
6.2.1 Primary map



X Index: 176

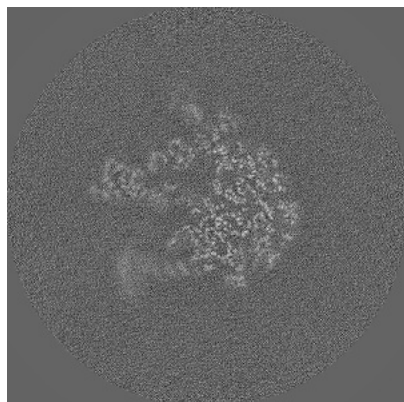


Y Index: 176

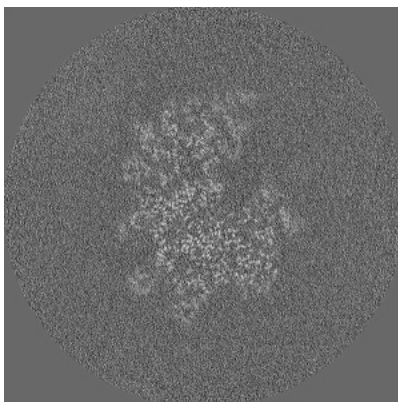


Z Index: 176

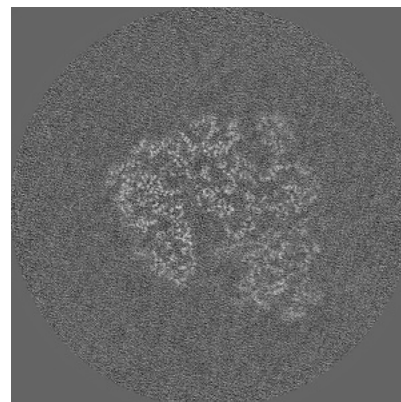
6.2.2 Raw map



X Index: 255



Y Index: 255

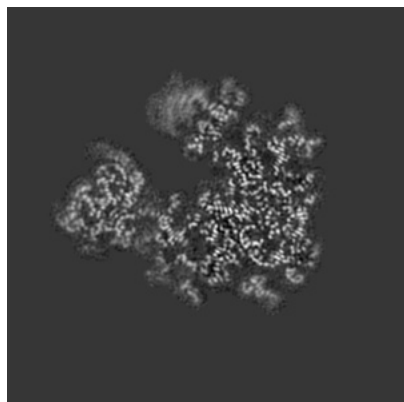


Z Index: 255

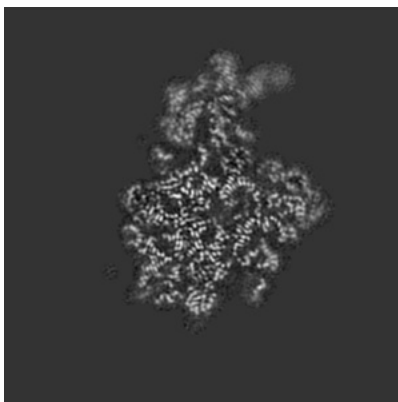
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

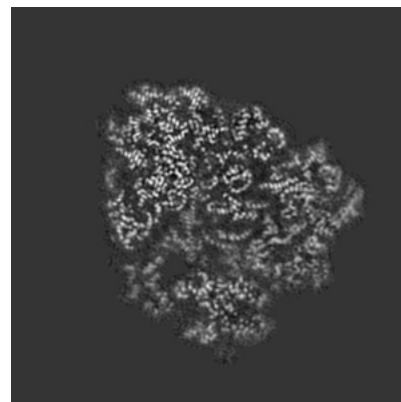
6.3.1 Primary map



X Index: 173

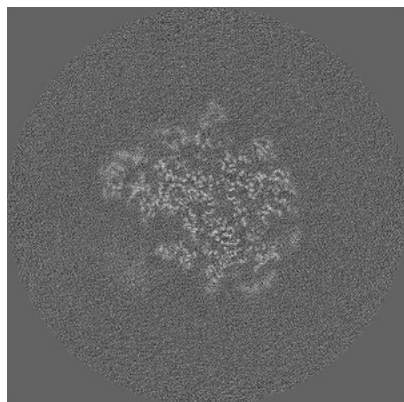


Y Index: 189

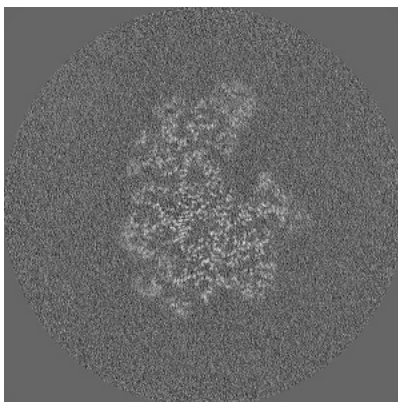


Z Index: 186

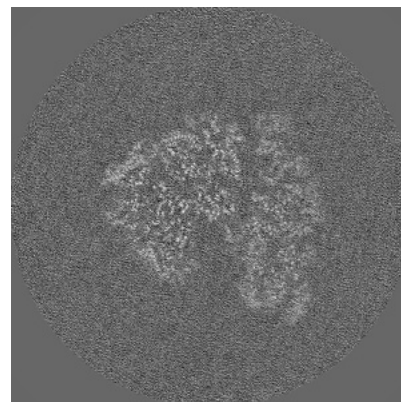
6.3.2 Raw map



X Index: 228



Y Index: 268

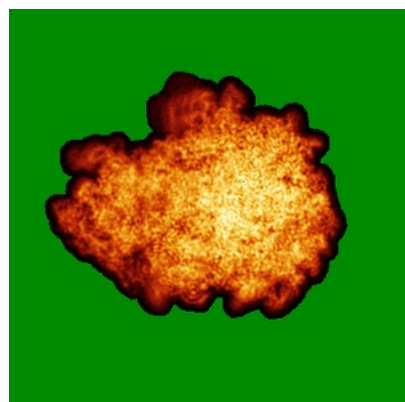


Z Index: 250

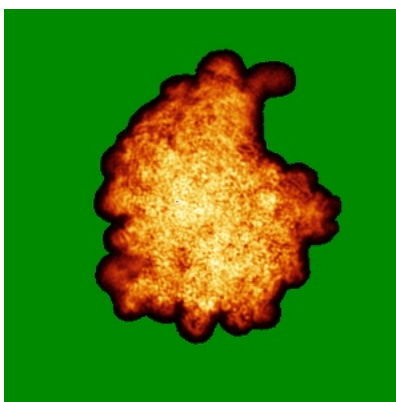
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

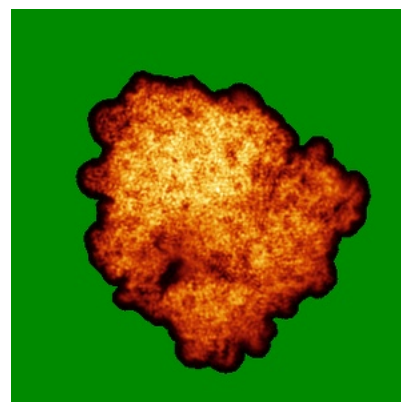
6.4.1 Primary map



X

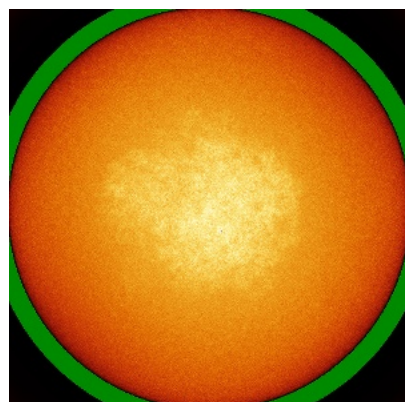


Y

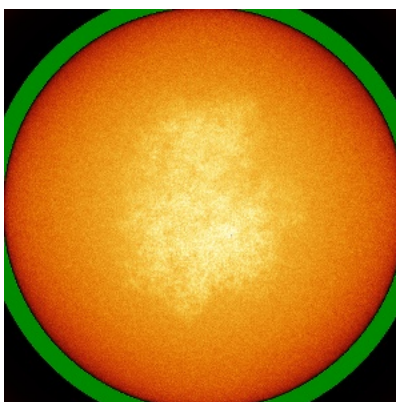


Z

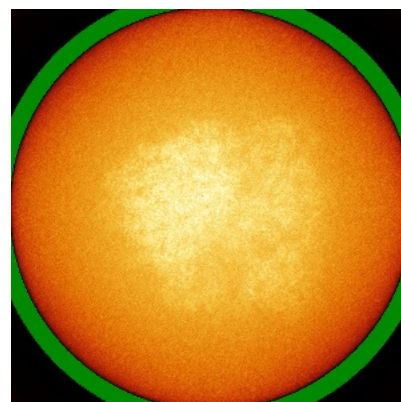
6.4.2 Raw map



X



Y

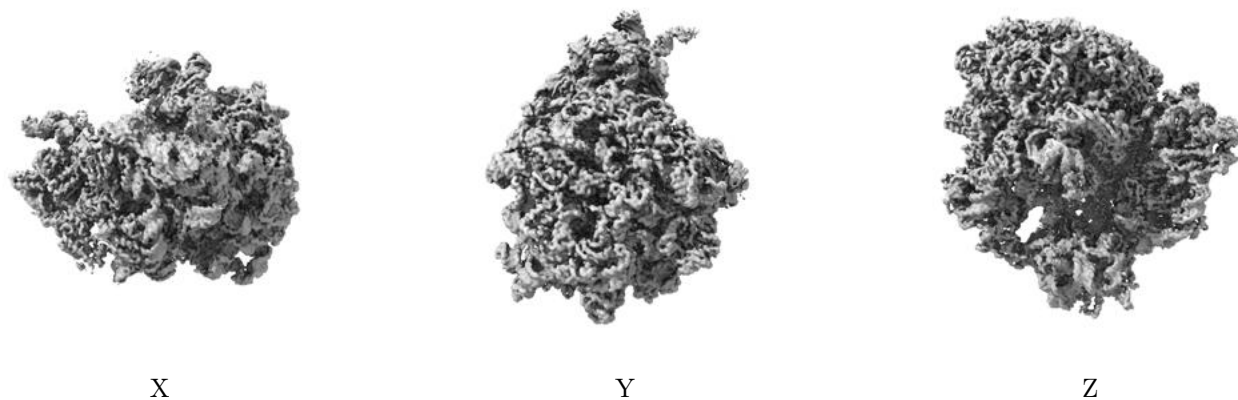


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

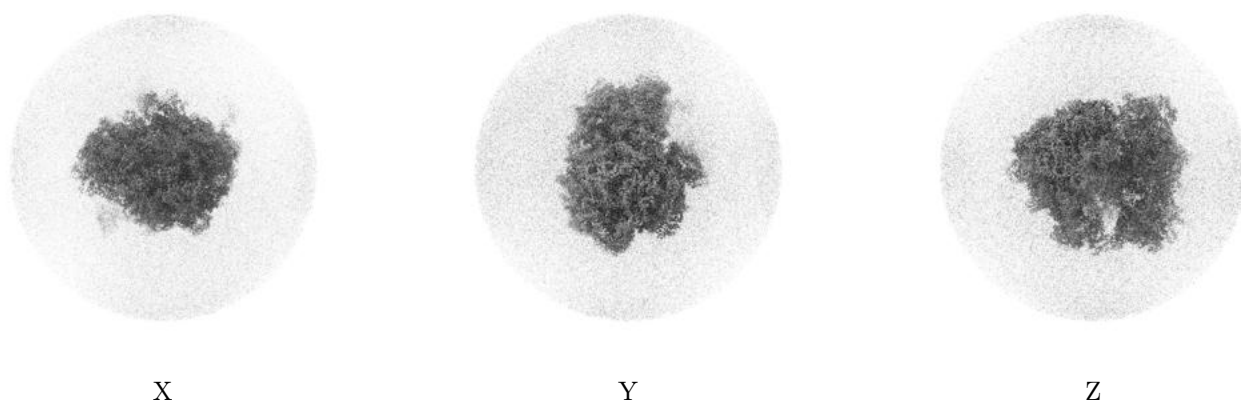
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

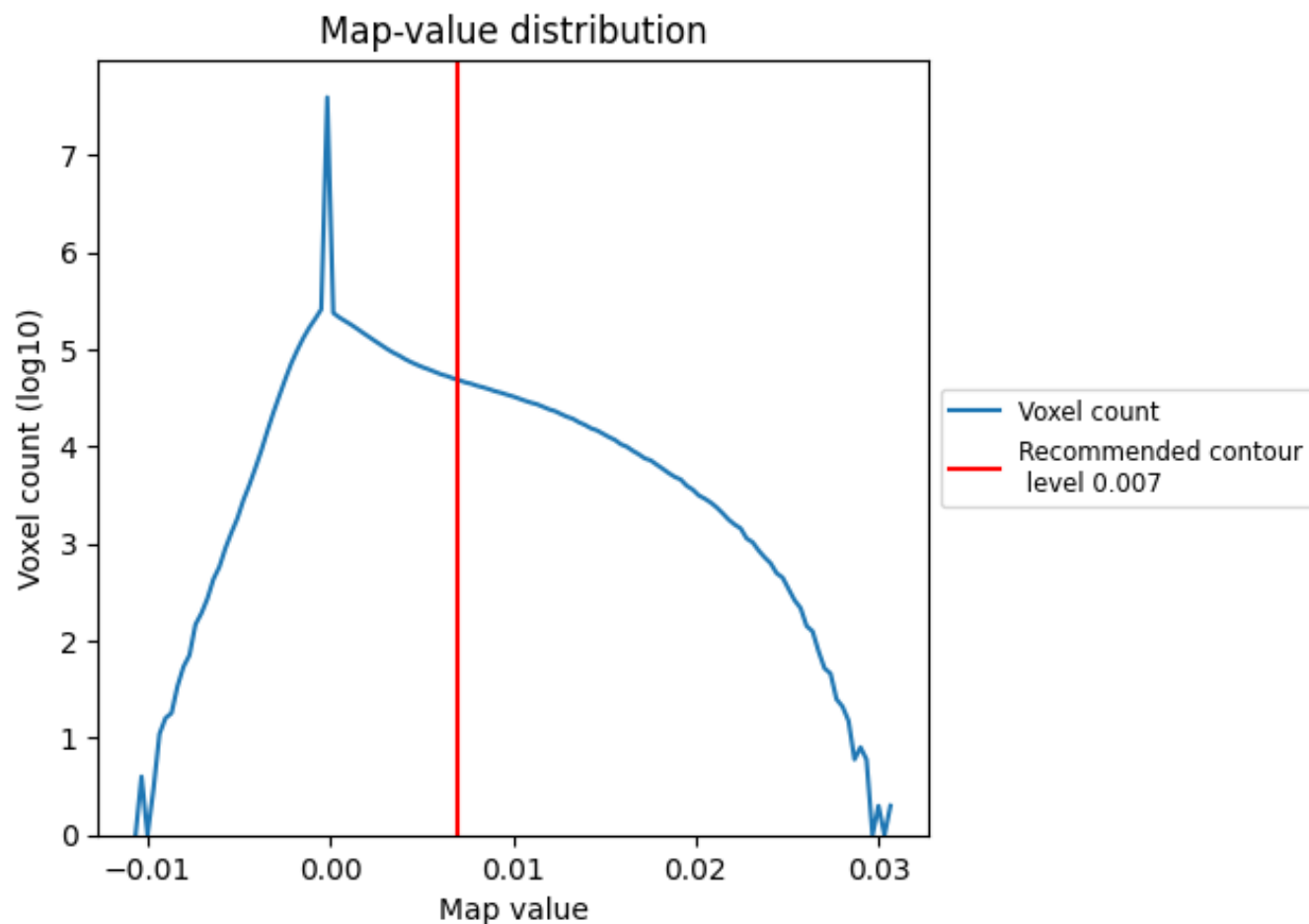
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

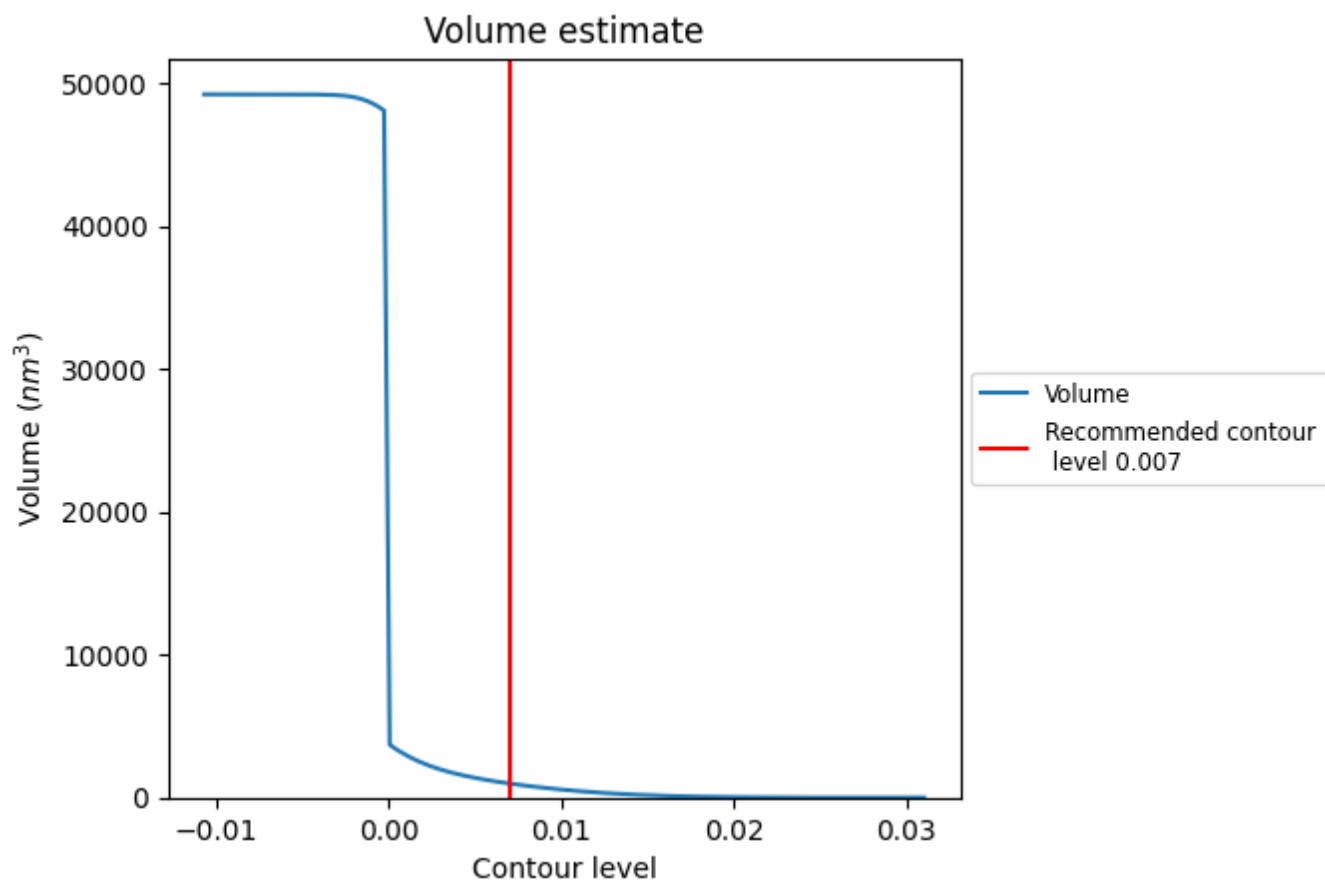
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

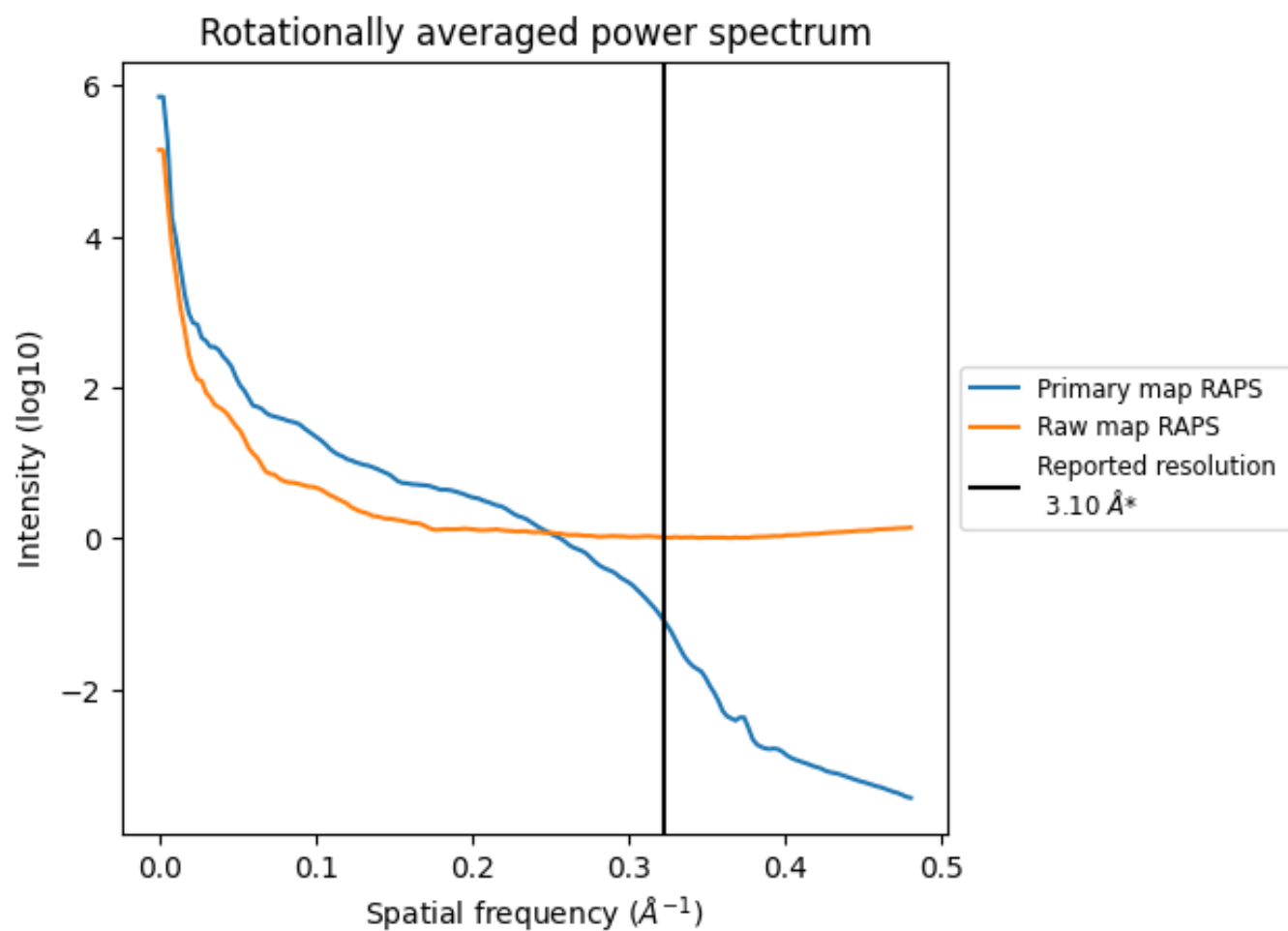
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 982 nm³; this corresponds to an approximate mass of 887 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 ⓘ

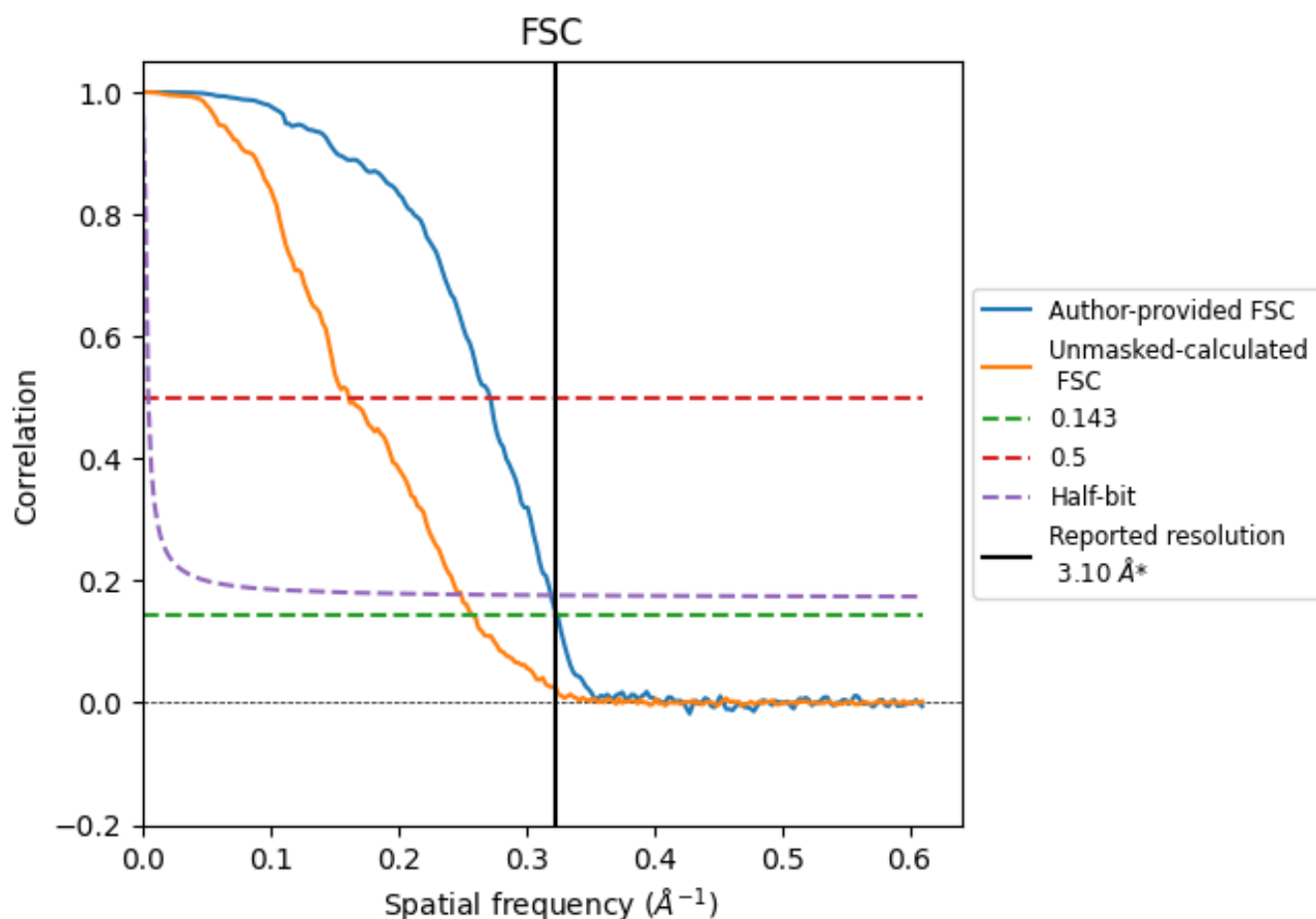


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

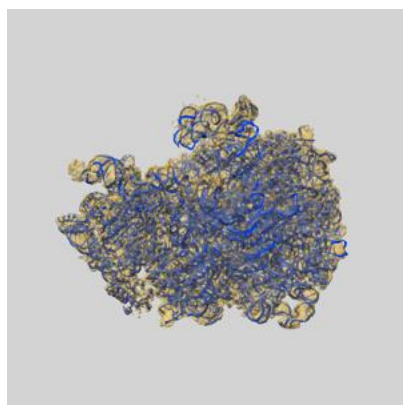
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.68	3.13
Unmasked-calculated*	3.87	6.19	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.1 by more than 10 %

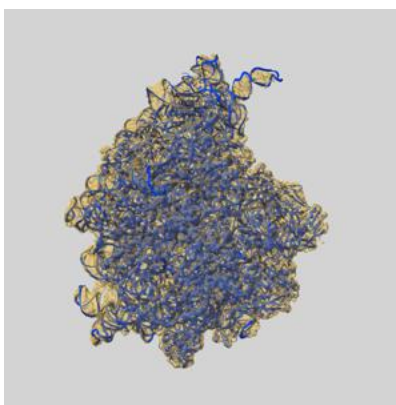
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12333 and PDB model 7NHM. Per-residue inclusion information can be found in section [3](#) on page [14](#).

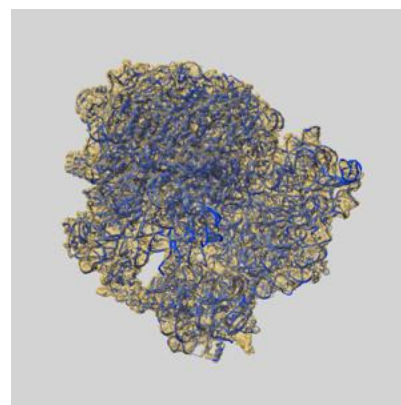
9.1 Map-model overlay [i](#)



X



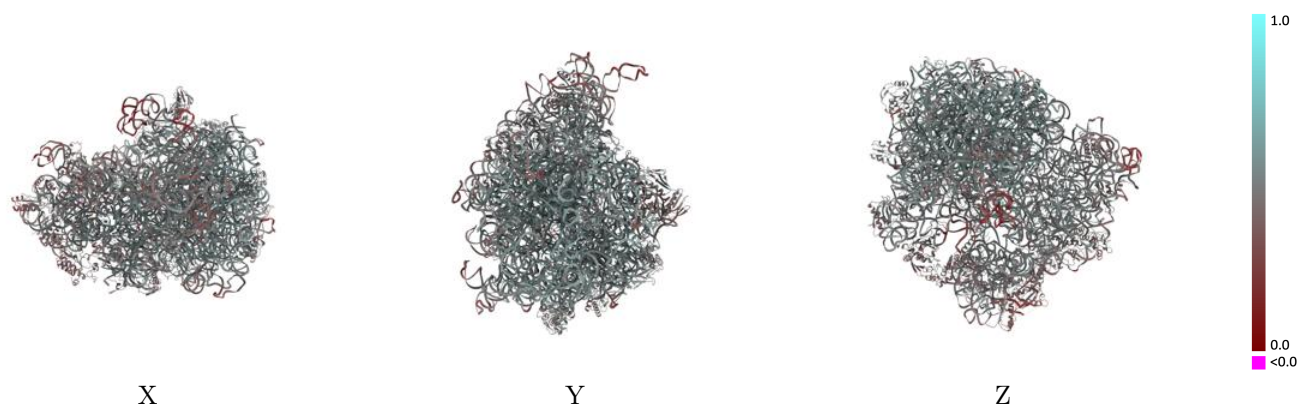
Y



Z

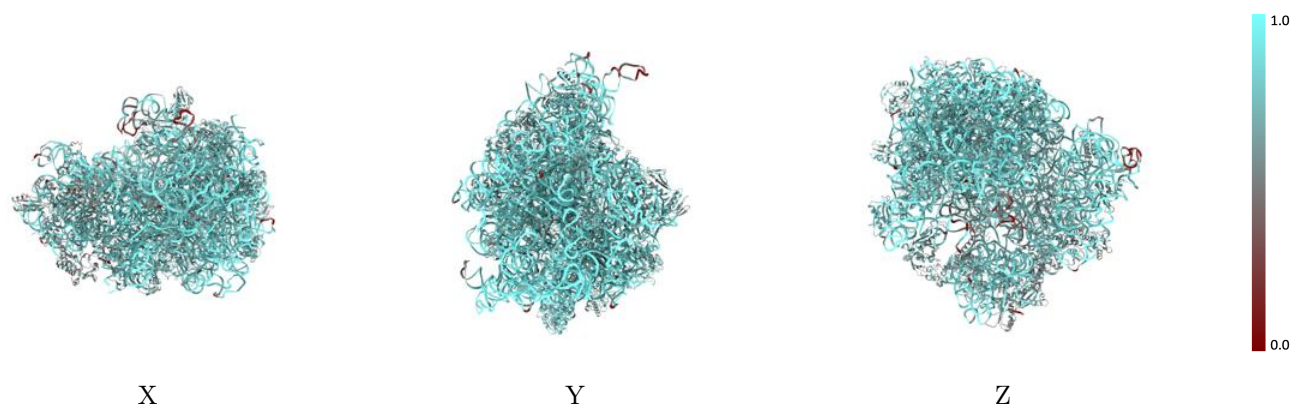
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



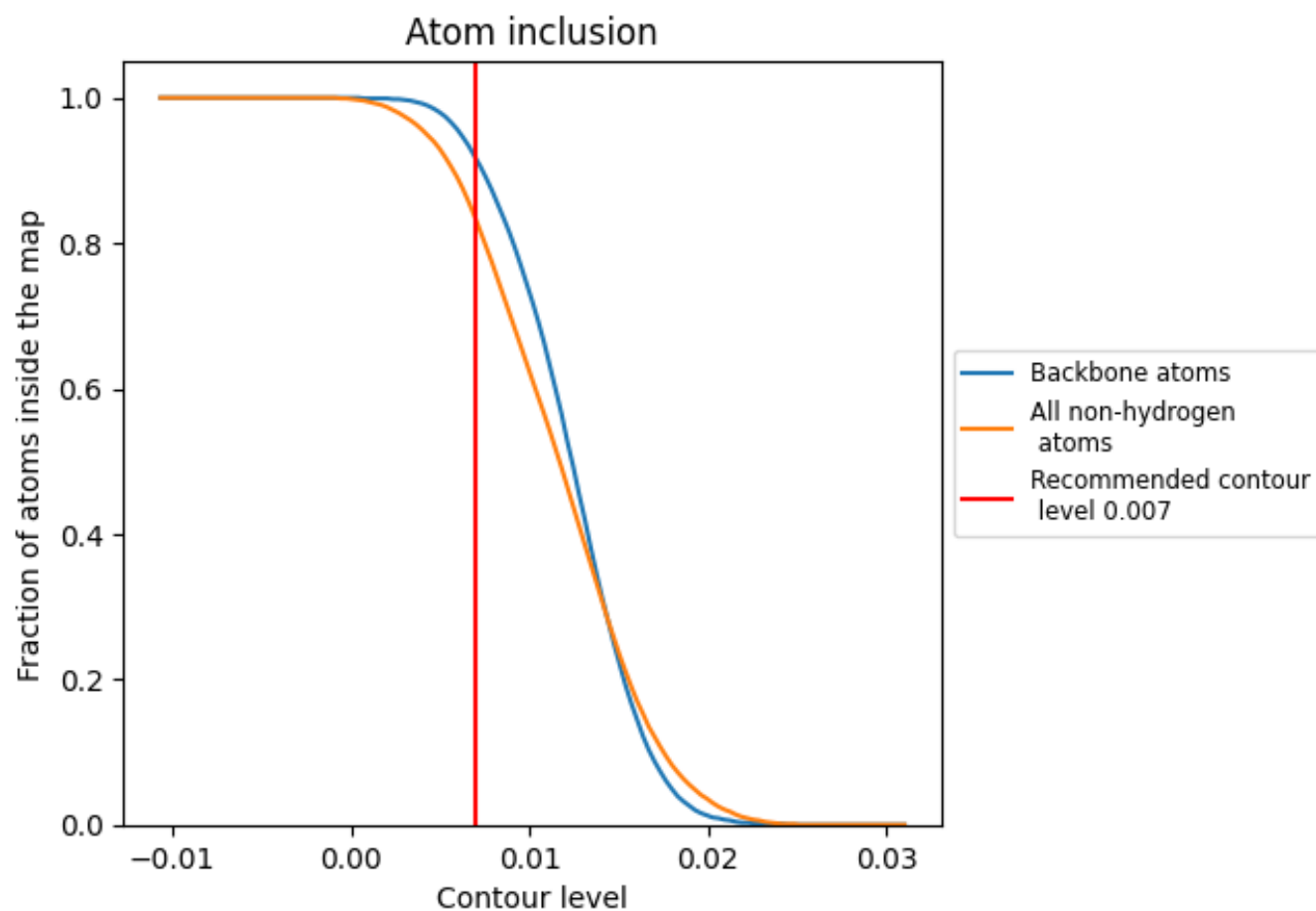
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.4940
1	 0.6800	 0.5010
2	 0.7240	 0.4500
3	 0.7240	 0.4990
4	 0.6370	 0.4010
5	 0.7300	 0.5120
6	 0.7820	 0.4780
7	 0.7790	 0.5460
8	 0.7730	 0.5370
9	 0.7280	 0.5210
A	 0.9170	 0.5200
B	 0.9270	 0.4840
D	 0.6210	 0.4700
G	 0.7390	 0.5310
H	 0.7560	 0.5230
I	 0.7310	 0.4900
J	 0.6380	 0.4240
K	 0.6650	 0.4340
M	 0.7270	 0.5050
N	 0.6760	 0.5150
O	 0.7370	 0.5080
P	 0.7250	 0.5090
Q	 0.7400	 0.4980
R	 0.6980	 0.4480
S	 0.7130	 0.4990
T	 0.7590	 0.5000
U	 0.7460	 0.5110
V	 0.7430	 0.5200
W	 0.7200	 0.4860
X	 0.6600	 0.4730
Y	 0.6510	 0.4520
Z	 0.7170	 0.5240
a	 0.8790	 0.4820
b	 0.4320	 0.3770
c	 0.5390	 0.4130



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.6140	 0.4330
e	 0.5640	 0.4110
f	 0.6790	 0.4870
g	 0.6550	 0.4530
h	 0.6290	 0.4160
i	 0.6880	 0.4690
j	 0.6510	 0.4560
k	 0.5570	 0.4010
l	 0.5980	 0.4400
m	 0.5980	 0.4580
n	 0.6340	 0.4280
o	 0.7080	 0.4690
p	 0.7160	 0.4410
q	 0.5680	 0.4380
r	 0.6460	 0.4600
s	 0.6910	 0.4750
t	 0.6380	 0.4300
u	 0.6140	 0.4070