



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 12:35 pm BST

PDB ID : 9FBV / pdb_00009fbv
EMDB ID : EMD-50296
Title : 70S Escherichia coli ribosome with P-site initiator tRNA.
Authors : Koller, T.O.; Wilson, D.N.
Deposited on : 2024-05-14
Resolution : 2.40 Å (reported)
Based on initial model : 7K00

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:

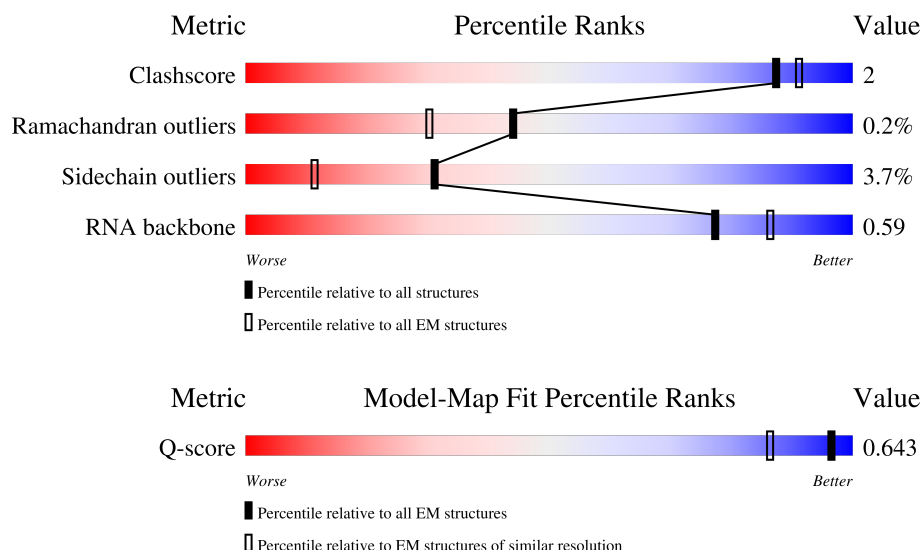
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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

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

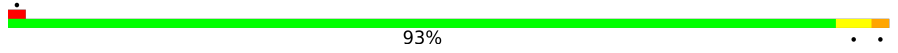
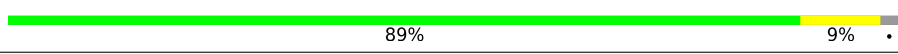
The reported resolution of this entry is 2.40 Å.

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.



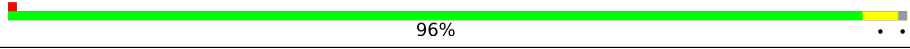
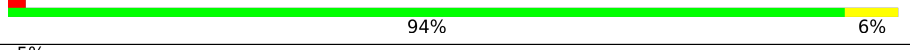
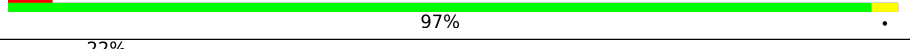
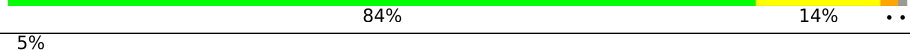
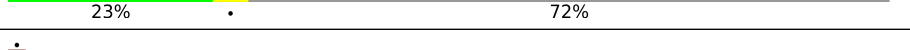
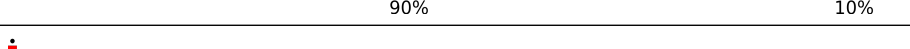
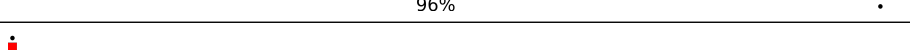
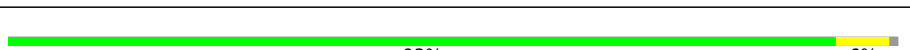
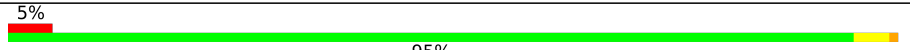
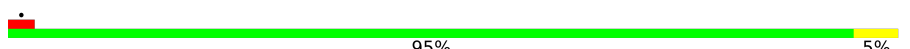
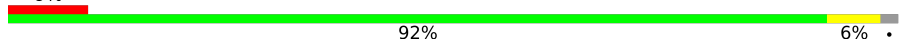
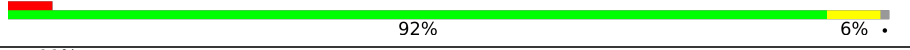
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	0	55	
2	1	46	
3	2	65	

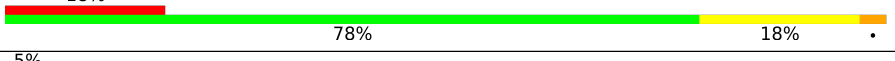
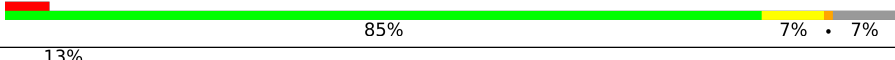
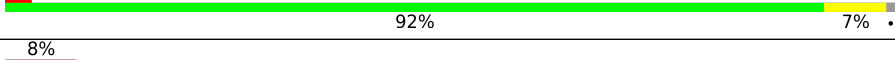
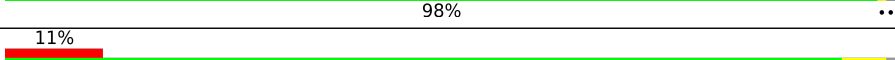
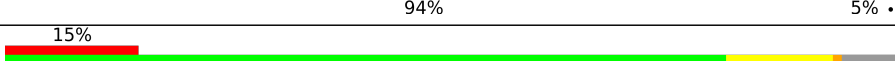
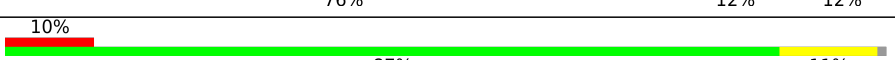
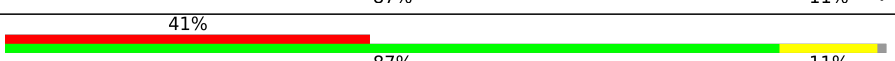
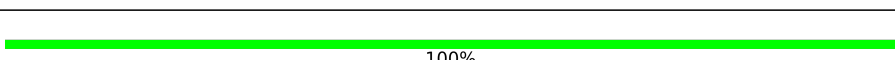
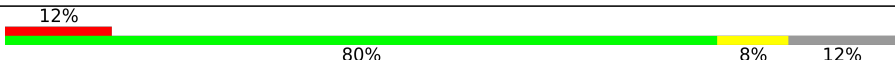
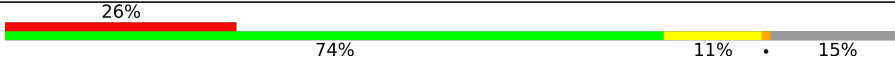
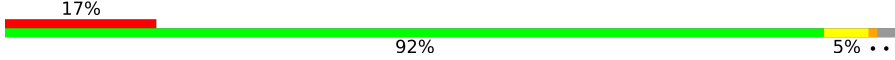
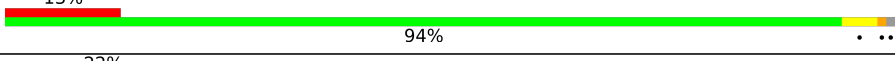
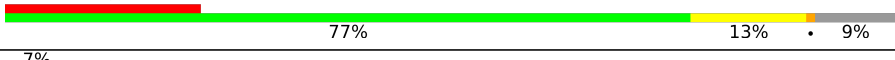
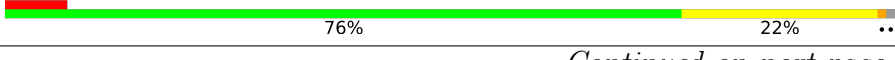
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Mol	Chain	Length	Quality of chain
4	3	38	
5	b	120	
6	c	273	
7	d	209	
8	e	201	
9	f	179	
10	g	177	
11	h	149	
12	i	142	
13	k	144	
14	l	136	
15	m	127	
16	n	117	
17	o	115	
18	p	118	
19	q	103	
20	r	110	
21	s	100	
22	t	104	
23	u	94	
24	v	85	
25	w	78	
26	x	63	
27	y	59	
28	z	57	

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Mol	Chain	Length	Quality of chain
29	4	70	
30	a	2903	
31	j	123	
32	B	241	
33	D	206	
34	E	167	
35	F	135	
36	H	130	
37	K	129	
38	L	124	
39	O	89	
40	P	82	
41	Q	84	
42	R	75	
43	T	87	
44	U	71	
45	X	3	
46	C	233	
47	G	179	
48	I	130	
49	J	103	
50	M	118	
51	N	101	
52	S	92	
53	A	1534	

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Mol	Chain	Length	Quality of chain
54	Z	77	34% 68% 26% • 5%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 140031 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 Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 11 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	variant	UNP P0ADY7

- Molecule 15 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 16 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	n	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 17 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 19 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	83	Total	C	N	O	S	0	0
			629	388	128	112	1		

- Molecule 25 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 28 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	118	Total	C	N	O	S	0	0
			901	567	170	158	6		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 33 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 34 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 35 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 36 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 37 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 38 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 39 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 40 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 42 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 43 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 44 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 45 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 46 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 47 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 48 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 49 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 50 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 51 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 52 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1519	Total	C	N	O	P	0	0
			32608	14548	5986	10555	1519		

- Molecule 54 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Z	73	Total	C	N	O	P	0	0
			1563	696	286	508	73		

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

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	b	5	Total	Mg	0
			5	5	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	k	1	Total	Mg	0
			1	1	
56	p	1	Total	Mg	0
			1	1	
56	z	1	Total	Mg	0
			1	1	
56	a	205	Total	Mg	0
			205	205	
56	A	91	Total	Mg	0
			91	91	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	d	1	Total	K	0
			1	1	
57	a	1	Total	K	0
			1	1	
57	A	1	Total	K	0
			1	1	

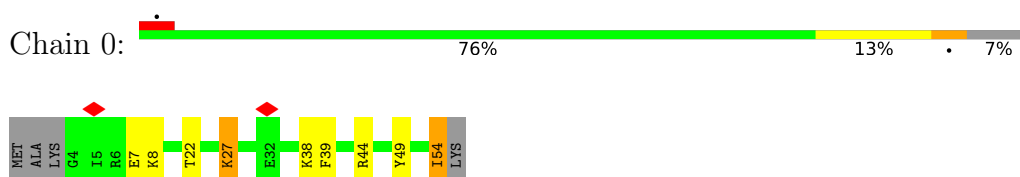
- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	a	1	Total 1	O 1	0
58	X	7	Total 7	O 7	0
58	A	28	Total 28	O 28	0
58	Z	3	Total 3	O 3	0

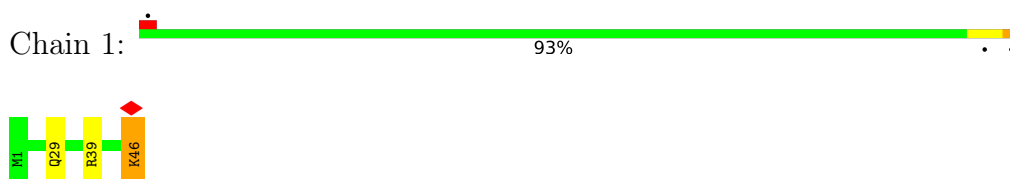
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

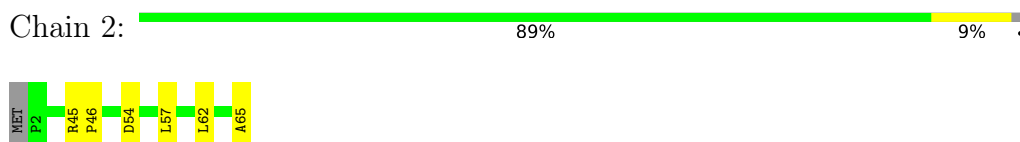
- Molecule 1: Large ribosomal subunit protein bL33



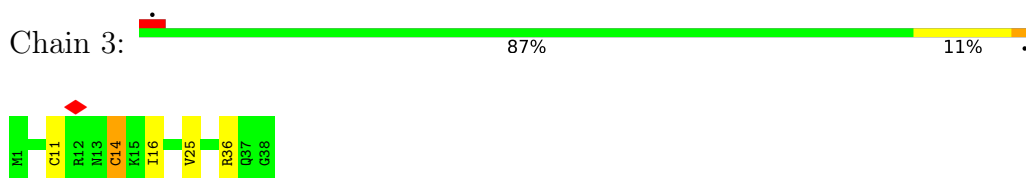
- Molecule 2: Large ribosomal subunit protein bL34



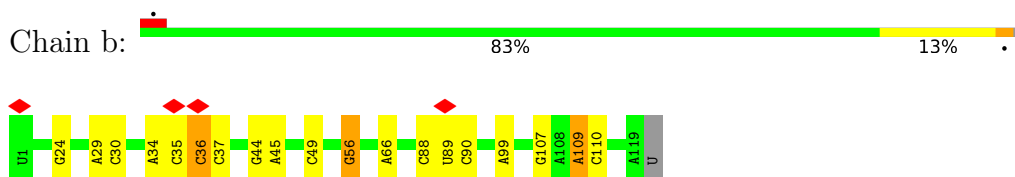
- Molecule 3: Large ribosomal subunit protein bL35



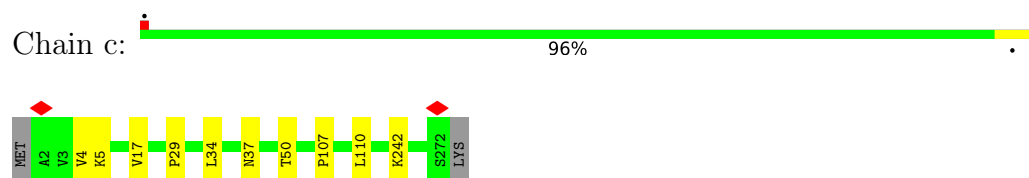
- Molecule 4: Large ribosomal subunit protein bL36A



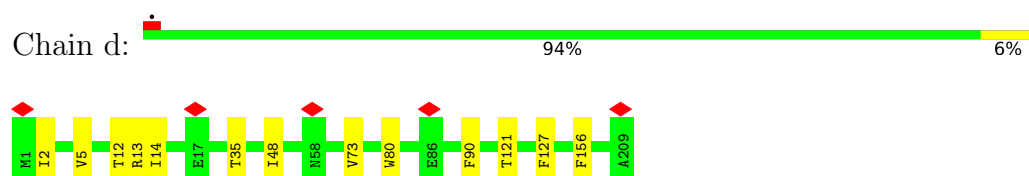
- Molecule 5: 5S ribosomal RNA



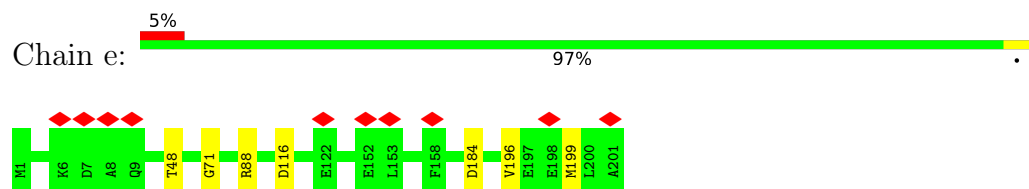
- Molecule 6: Large ribosomal subunit protein uL2



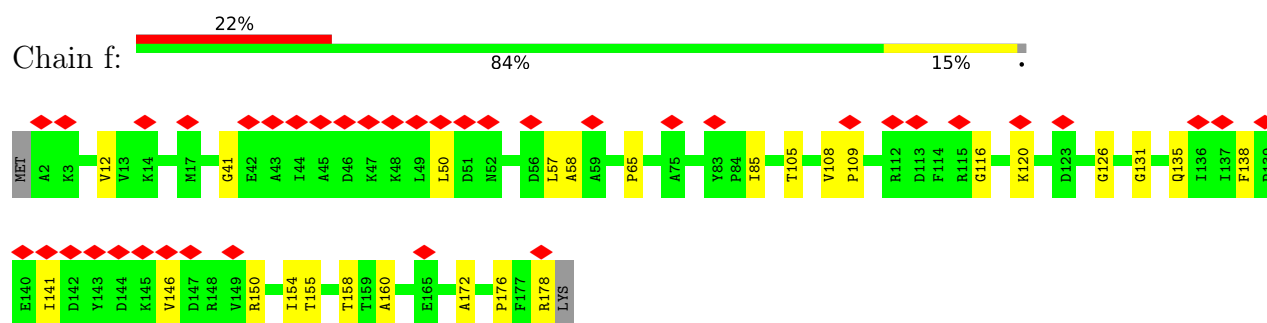
- Molecule 7: Large ribosomal subunit protein uL3



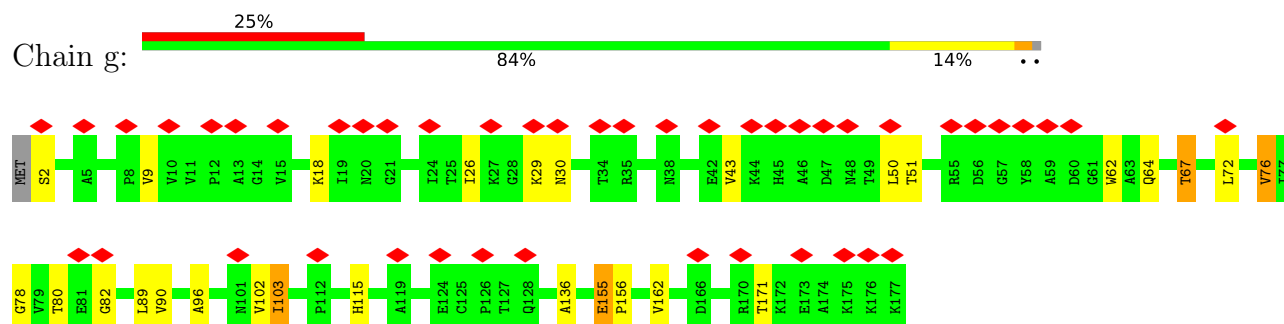
- Molecule 8: Large ribosomal subunit protein uL4



- Molecule 9: Large ribosomal subunit protein uL5

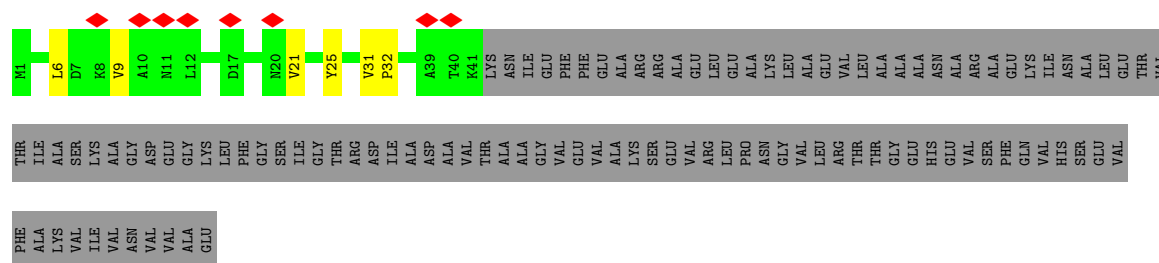


- Molecule 10: Large ribosomal subunit protein uL6

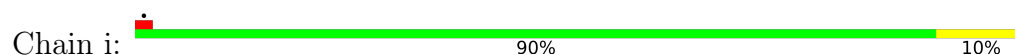


- Molecule 11: Large ribosomal subunit protein bL9





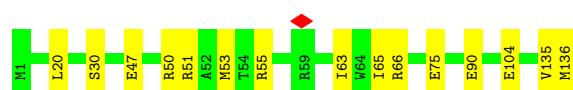
- Molecule 12: Large ribosomal subunit protein uL13



- Molecule 13: 50S ribosomal protein L15



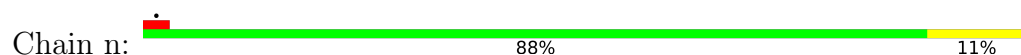
- Molecule 14: Large ribosomal subunit protein uL16



- Molecule 15: Large ribosomal subunit protein bL17

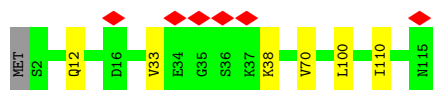


- Molecule 16: Large ribosomal subunit protein uL18



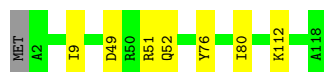
- Molecule 17: Large ribosomal subunit protein bL19





- Molecule 18: Large ribosomal subunit protein bL20

Chain p: 93% 6%



- Molecule 19: Large ribosomal subunit protein bL21

Chain q: 5% 95%



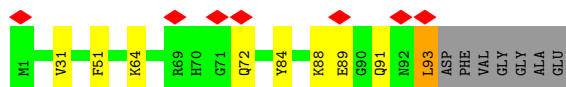
- Molecule 20: Large ribosomal subunit protein uL22

Chain r: 95% 5%



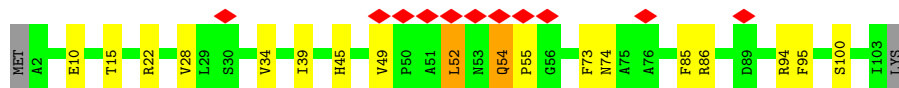
- Molecule 21: Large ribosomal subunit protein uL23

Chain s: 7% 84% 8% 7%



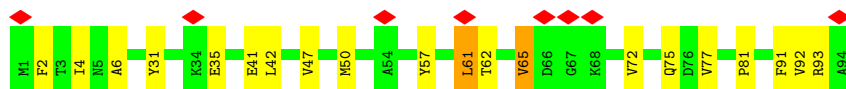
- Molecule 22: Large ribosomal subunit protein uL24

Chain t: 11% 81% 15%

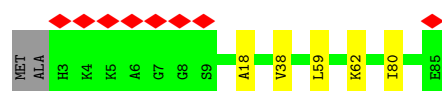
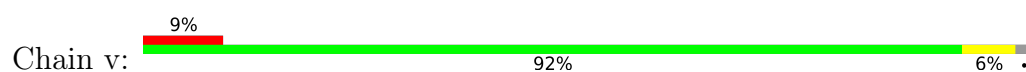


- Molecule 23: 50S ribosomal protein L25

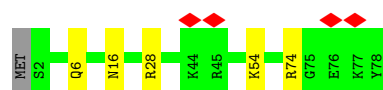
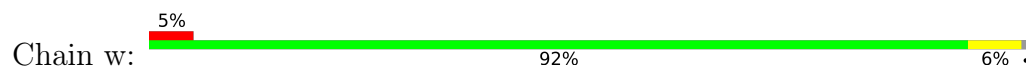
Chain u: 9% 79% 19%



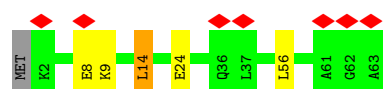
- Molecule 24: Large ribosomal subunit protein bL27



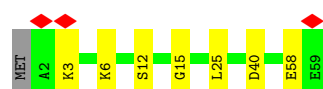
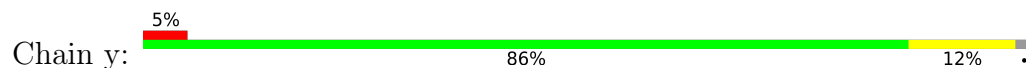
- Molecule 25: Large ribosomal subunit protein bL28



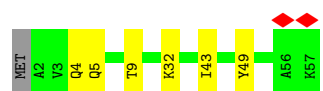
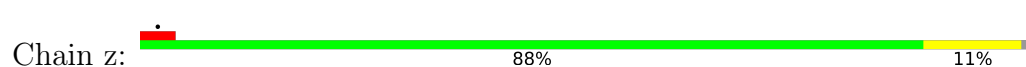
- Molecule 26: Large ribosomal subunit protein uL29



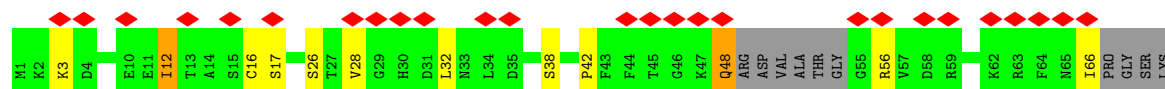
- Molecule 27: Large ribosomal subunit protein uL30



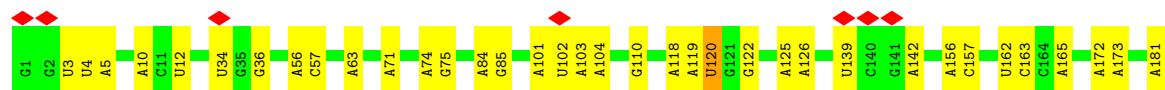
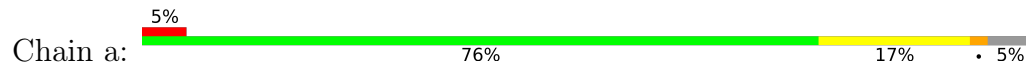
- Molecule 28: Large ribosomal subunit protein bL32



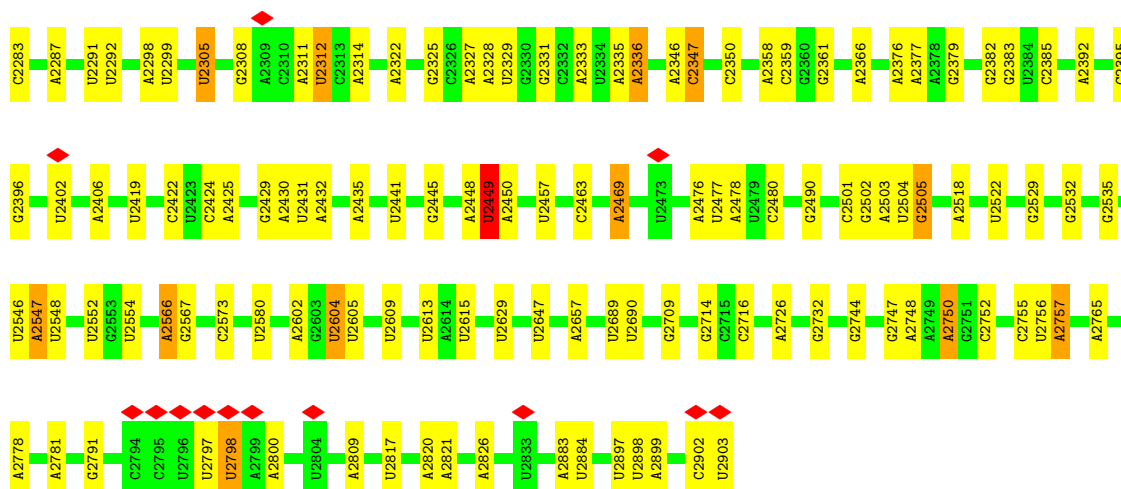
- Molecule 29: Large ribosomal subunit protein bL31A



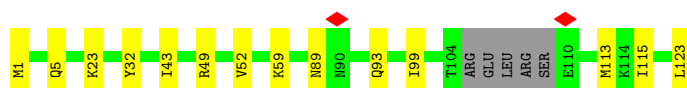
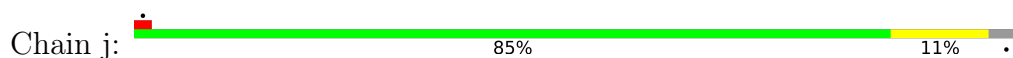
- Molecule 30: 23S ribosomal RNA



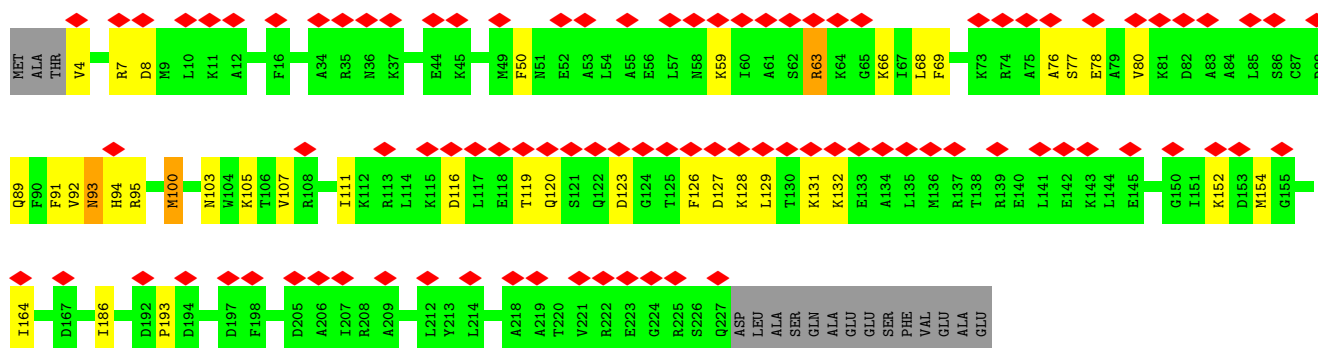
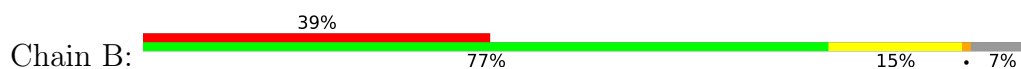




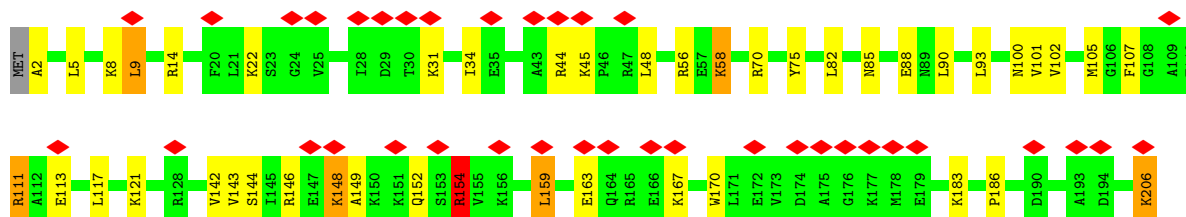
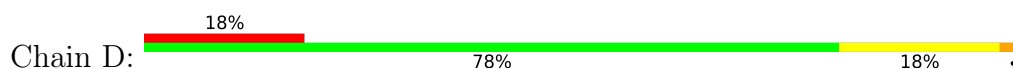
- Molecule 31: Large ribosomal subunit protein uL14



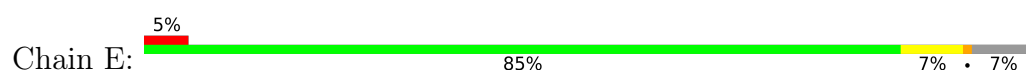
- Molecule 32: 30S ribosomal protein S2



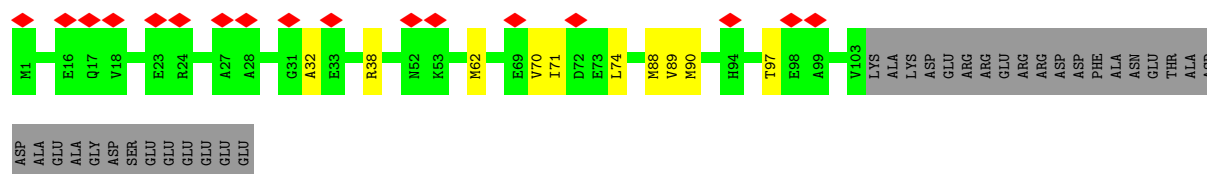
- Molecule 33: Small ribosomal subunit protein uS4



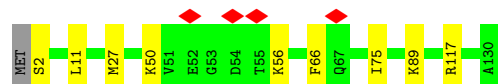
- Molecule 34: Small ribosomal subunit protein uS5



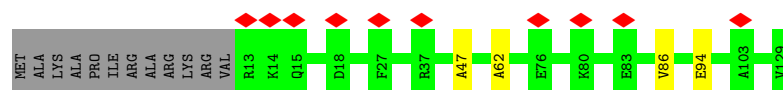
- Molecule 35: 30S ribosomal protein S6, fully modified isoform



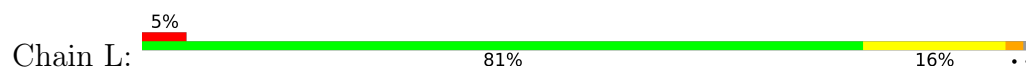
- Molecule 36: Small ribosomal subunit protein uS8



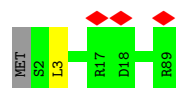
- Molecule 37: Small ribosomal subunit protein uS11



- Molecule 38: Small ribosomal subunit protein uS12

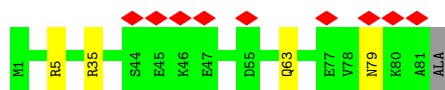


- Molecule 39: Small ribosomal subunit protein uS15

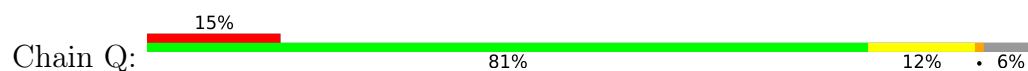


- Molecule 40: 30S ribosomal protein S16

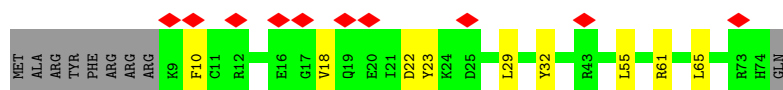
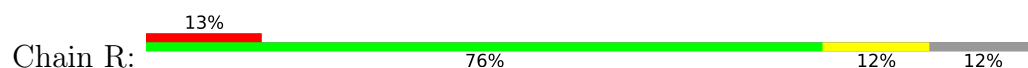




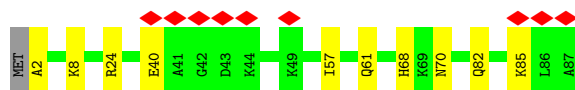
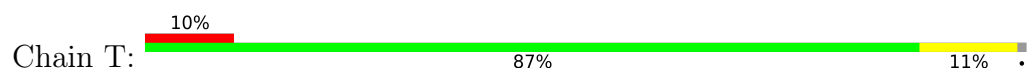
- Molecule 41: Small ribosomal subunit protein uS17



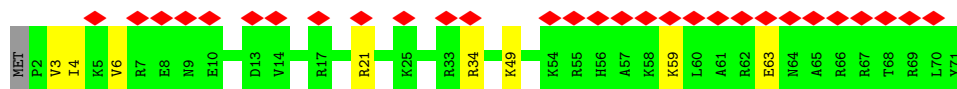
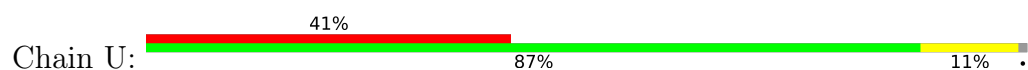
- Molecule 42: Small ribosomal subunit protein bS18



- Molecule 43: 30S ribosomal protein S20



- Molecule 44: Small ribosomal subunit protein bS21

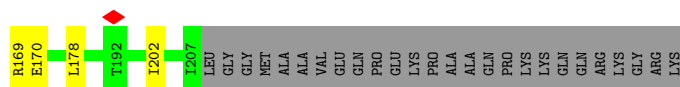
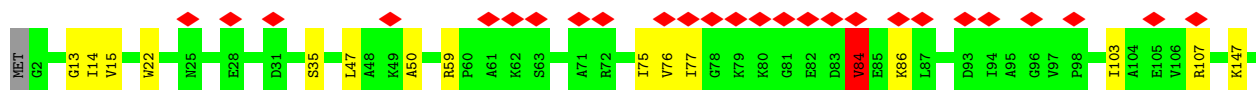
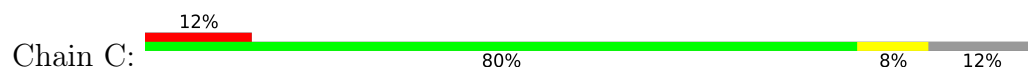


- Molecule 45: messenger RNA

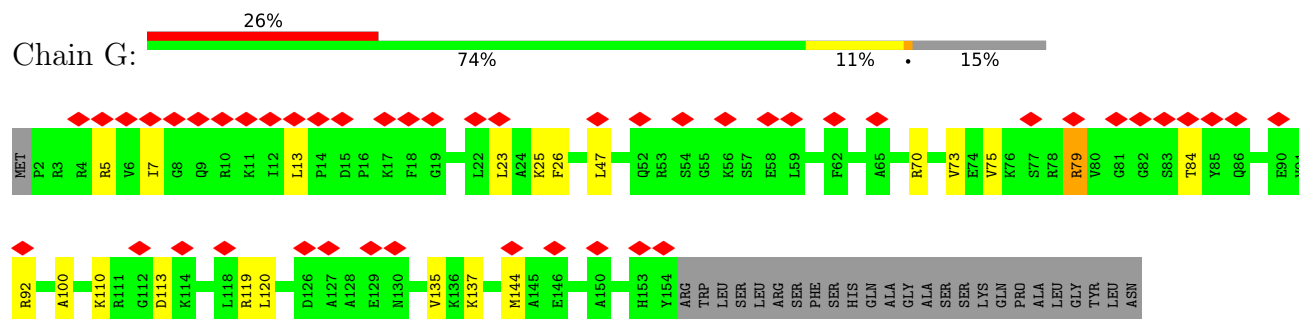


There are no outlier residues recorded for this chain.

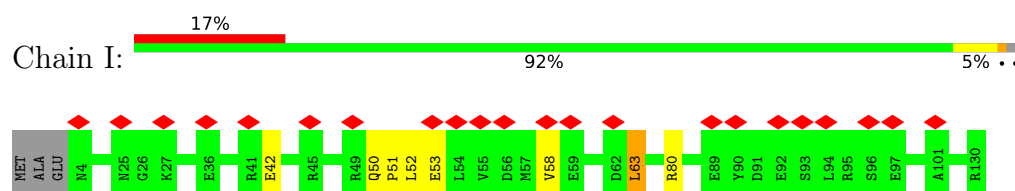
- Molecule 46: Small ribosomal subunit protein uS3



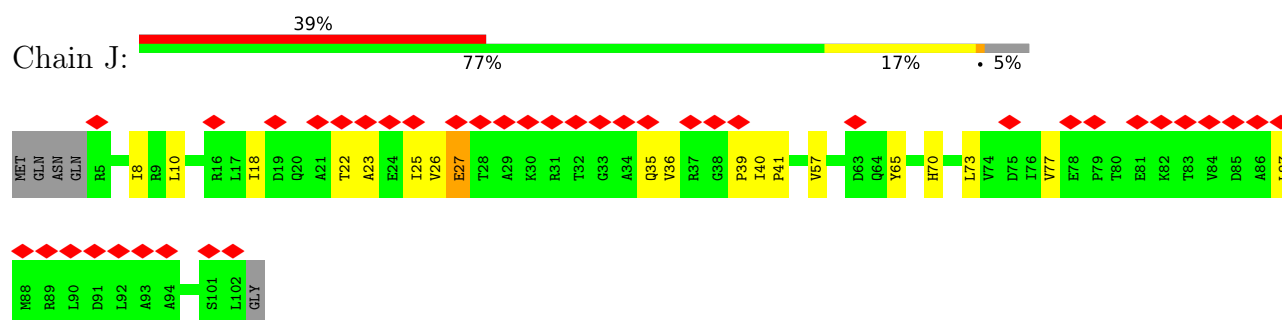
- Molecule 47: 30S ribosomal protein S7



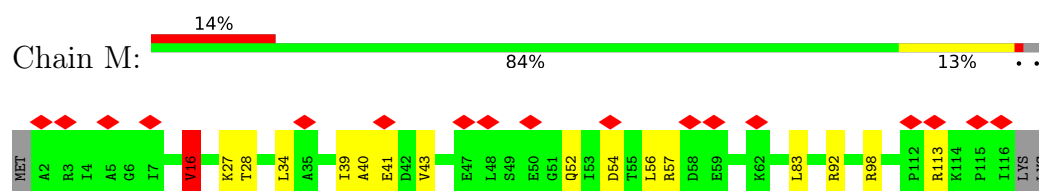
- Molecule 48: Small ribosomal subunit protein uS9



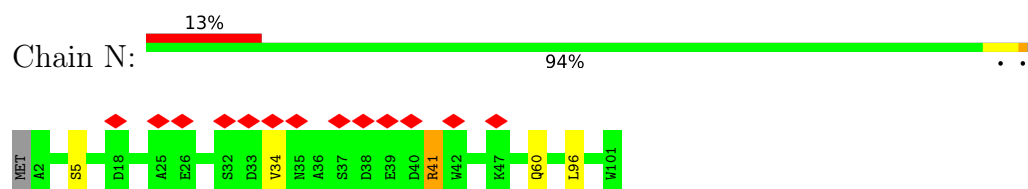
- Molecule 49: Small ribosomal subunit protein uS10



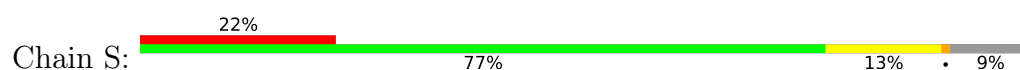
- Molecule 50: Small ribosomal subunit protein uS13

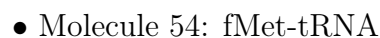


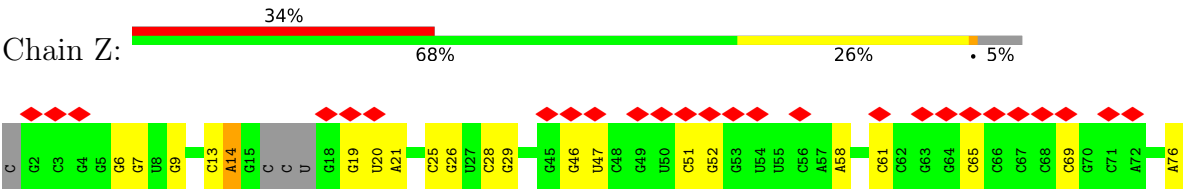
- Molecule 51: Small ribosomal subunit protein uS14



- Molecule 52: Small ribosomal subunit protein uS19







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84771	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 2MA, OMU, IAS, K, ZN, MG, 5MU, OMG, G7M, 3TD, 4OC, 6MZ, 4D4, MEQ, OMC, D2T, 1MG, H2U, PSU, 5MC, 2MG, MS6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.56	0/424	0.88	0/565
2	1	0.65	0/380	0.94	0/498
3	2	0.64	0/513	0.95	0/676
4	3	0.62	0/303	0.85	0/397
5	b	0.53	0/2850	0.83	0/4444
6	c	0.64	0/2121	0.89	0/2852
7	d	0.59	0/1576	0.88	0/2119
8	e	0.58	0/1571	0.92	0/2113
9	f	0.55	0/1434	0.95	0/1926
10	g	0.60	0/1343	0.94	1/1816 (0.1%)
11	h	0.57	0/306	0.93	0/413
12	i	0.58	0/1152	0.89	0/1551
13	k	0.62	0/1062	0.90	0/1413
14	l	0.56	0/1073	0.88	0/1433
15	m	0.63	0/958	0.95	0/1281
16	n	0.58	0/902	0.91	0/1209
17	o	0.59	0/929	0.84	0/1242
18	p	0.62	0/960	0.97	0/1278
19	q	0.58	0/829	0.81	0/1107
20	r	0.60	0/864	0.91	0/1156
21	s	0.58	0/744	0.83	0/994
22	t	0.57	0/787	0.88	0/1051
23	u	0.58	0/766	0.87	0/1025
24	v	0.60	0/637	0.84	0/841
25	w	0.60	0/635	0.91	0/848
26	x	0.52	0/502	0.99	0/667
27	y	0.56	0/453	0.92	0/605
28	z	0.61	0/450	0.94	0/599
29	4	0.59	0/488	0.95	0/649
30	a	0.54	0/65651	0.90	59/102413 (0.1%)
31	j	0.60	0/909	0.85	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	B	0.55	0/1784	0.99	0/2403
33	D	0.56	0/1665	0.99	1/2227 (0.0%)
34	E	0.59	0/1165	0.92	0/1568
35	F	0.56	0/858	0.91	0/1160
36	H	0.56	0/989	0.89	0/1326
37	K	0.61	0/884	0.90	0/1191
38	L	0.65	1/960 (0.1%)	0.89	0/1286
39	O	0.56	0/722	0.97	0/964
40	P	0.55	0/653	0.89	0/877
41	Q	0.56	0/650	0.85	0/871
42	R	0.56	0/553	0.99	0/742
43	T	0.56	0/676	1.02	0/895
44	U	0.57	0/597	1.07	0/792
45	X	0.45	0/72	0.79	0/110
46	C	0.57	0/1651	0.91	1/2225 (0.0%)
47	G	0.57	0/1219	0.97	0/1635
48	I	0.59	0/1034	0.93	0/1375
49	J	0.60	0/796	0.95	0/1077
50	M	0.57	0/900	1.00	1/1204 (0.1%)
51	N	0.56	0/817	0.97	0/1088
52	S	0.60	0/685	0.91	0/922
53	A	0.53	1/36287 (0.0%)	0.85	12/56602 (0.0%)
54	Z	0.60	0/1746	0.80	0/2719
All	All	0.55	2/150935 (0.0%)	0.89	75/225657 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
25	w	0	1
30	a	0	5
32	B	0	1
33	D	0	1
34	E	0	1
36	H	0	1
38	L	0	1
46	C	0	1
51	N	0	1
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	L	87	VAL	C-N	9.10	1.46	1.33
53	A	527	G7M	O3'-P	5.13	1.61	1.56

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1971	U	C4'-C3'-O3'	-8.37	100.44	113.00
53	A	429	U	C2'-C3'-O3'	8.20	121.80	109.50
30	a	204	A	O3'-P-O5'	-7.70	92.44	104.00
30	a	1929	G	O3'-P-O5'	-7.41	92.89	104.00
30	a	569	U	O3'-P-O5'	-7.36	92.95	104.00
30	a	1185	G	O3'-P-O5'	-7.32	93.02	104.00
53	A	429	U	O3'-P-O5'	-7.26	93.11	104.00
30	a	763	G	O3'-P-O5'	-7.15	93.28	104.00
30	a	1131	G	O3'-P-O5'	-6.64	94.03	104.00
30	a	2001	C	O3'-P-O5'	-6.58	94.13	104.00
30	a	2463	C	O3'-P-O5'	-6.53	94.20	104.00
30	a	2826	A	O3'-P-O5'	-6.37	94.44	104.00
30	a	964	C	O3'-P-O5'	-6.36	94.45	104.00
30	a	1643	G	O3'-P-O5'	-6.30	94.56	104.00
30	a	1293	C	O3'-P-O5'	-6.29	94.57	104.00
30	a	385	C	O3'-P-O5'	-6.21	94.68	104.00
53	A	921	U	O3'-P-O5'	-6.11	94.84	104.00
30	a	1025	G	O3'-P-O5'	6.05	113.07	104.00
30	a	310	A	O3'-P-O5'	-6.01	94.99	104.00
30	a	1565	C	O3'-P-O5'	-5.97	95.05	104.00
46	C	84	VAL	N-CA-CB	5.95	117.11	110.51
30	a	2379	G	O3'-P-O5'	-5.93	95.11	104.00
30	a	2477	U	O3'-P-O5'	-5.87	95.20	104.00
30	a	2050	C	O3'-P-O5'	-5.87	95.20	104.00
30	a	818	G	O3'-P-O5'	-5.82	95.27	104.00
30	a	859	G	O3'-P-O5'	-5.81	95.29	104.00
30	a	2051	A	O3'-P-O5'	-5.78	95.33	104.00
53	A	329	A	O3'-P-O5'	-5.76	95.36	104.00
30	a	1847	A	O3'-P-O5'	-5.70	95.45	104.00
30	a	1619	G	C1'-C2'-O2'	5.69	116.93	108.40
10	g	155	GLU	CB-CA-C	5.65	116.53	108.68
30	a	2501	C	O3'-P-O5'	-5.63	95.55	104.00
53	A	872	A	O3'-P-O5'	-5.60	95.59	104.00
30	a	2817	U	O3'-P-O5'	-5.59	95.61	104.00
50	M	16	VAL	N-CA-CB	5.57	116.69	110.51
30	a	1254	A	C4'-C3'-O3'	-5.56	104.66	113.00
30	a	781	A	O3'-P-O5'	-5.56	95.66	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1966	A	O3'-P-O5'	-5.55	95.68	104.00
30	a	2546	U	O3'-P-O5'	-5.54	95.70	104.00
30	a	2382	G	O3'-P-O5'	-5.53	95.71	104.00
30	a	1667	G	O3'-P-O5'	-5.50	95.76	104.00
30	a	193	U	O3'-P-O5'	-5.49	95.76	104.00
30	a	1133	A	O3'-P-O5'	-5.49	95.77	104.00
30	a	784	G	O3'-P-O5'	-5.46	95.80	104.00
30	a	2238	G	O3'-P-O5'	-5.45	95.83	104.00
33	D	154	ARG	CG-CD-NE	5.43	123.95	112.00
30	a	2781	A	O3'-P-O5'	-5.42	95.86	104.00
30	a	2060	A	O3'-P-O5'	-5.41	95.88	104.00
53	A	1269	A	O3'-P-O5'	-5.41	95.88	104.00
53	A	1078	U	O3'-P-O5'	-5.39	95.92	104.00
30	a	2566	A	O3'-P-O5'	-5.38	95.93	104.00
30	a	1825	U	O3'-P-O5'	-5.34	95.98	104.00
30	a	784	G	C2'-C3'-O3'	-5.33	105.70	113.70
30	a	1394	U	O3'-P-O5'	-5.32	96.02	104.00
53	A	652	U	O3'-P-O5'	-5.30	96.04	104.00
30	a	2490	G	O3'-P-O5'	-5.26	96.10	104.00
30	a	747	5MU	O3'-P-O5'	-5.26	96.11	104.00
30	a	1913	A	O3'-P-O5'	-5.25	96.13	104.00
30	a	1832	C	O3'-P-O5'	-5.24	96.15	104.00
53	A	1080	A	O3'-P-O5'	-5.19	96.22	104.00
30	a	952	G	O3'-P-O5'	-5.18	96.23	104.00
30	a	1810	A	O3'-P-O5'	-5.16	96.25	104.00
30	a	2094	A	O3'-P-O5'	-5.12	96.32	104.00
30	a	1816	C	O3'-P-O5'	-5.11	96.34	104.00
53	A	572	A	O3'-P-O5'	-5.11	96.34	104.00
30	a	514	A	O3'-P-O5'	-5.10	96.35	104.00
30	a	1757	A	C4'-C3'-O3'	-5.10	105.35	113.00
30	a	1142	A	O3'-P-O5'	-5.08	96.38	104.00
30	a	2505	G	O3'-P-O5'	-5.07	96.40	104.00
30	a	621	A	O3'-P-O5'	-5.05	96.42	104.00
53	A	1336	C	O3'-P-O5'	-5.04	96.45	104.00
30	a	573	U	O3'-P-O5'	-5.03	96.45	104.00
53	A	645	G	O3'-P-O5'	-5.03	96.45	104.00
30	a	295	G	O3'-P-O5'	-5.01	96.48	104.00
30	a	1238	G	O3'-P-O5'	-5.00	96.50	104.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	B	193	PRO	Peptide
46	C	13	GLY	Peptide
33	D	154	ARG	Sidechain
34	E	108	GLY	Peptide
36	H	27	MET	Peptide
38	L	44	LYS	Peptide
51	N	41	ARG	Sidechain
30	a	1253	A	Sidechain
30	a	2732	G	Sidechain
30	a	395	U	Sidechain
30	a	512	G	Sidechain
30	a	956	G	Sidechain
25	w	16	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	5	0
2	1	377	0	418	3	0
3	2	504	0	572	3	0
4	3	302	0	340	3	0
5	b	2549	0	1291	5	0
6	c	2082	0	2154	5	0
7	d	1566	0	1617	7	0
8	e	1552	0	1619	3	0
9	f	1410	0	1444	15	0
10	g	1323	0	1371	12	0
11	h	303	0	327	2	0
12	i	1129	0	1162	8	0
13	k	1053	0	1129	3	0
14	l	1075	0	1145	8	0
15	m	945	0	989	3	0
16	n	892	0	923	5	0
17	o	917	0	962	4	0
18	p	947	0	1019	5	0
19	q	816	0	839	2	0
20	r	857	0	922	3	0
21	s	738	0	807	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	t	779	0	831	7	0
23	u	753	0	780	11	0
24	v	629	0	648	4	0
25	w	625	0	652	2	0
26	x	501	0	531	1	0
27	y	449	0	488	4	0
28	z	444	0	458	4	0
29	4	480	0	478	6	0
30	a	59130	0	29769	140	0
31	j	901	0	974	8	0
32	B	1753	0	1780	18	0
33	D	1643	0	1707	23	0
34	E	1152	0	1196	6	0
35	F	839	0	833	6	0
36	H	979	0	1031	2	0
37	K	877	0	884	1	0
38	L	957	0	1017	6	0
39	O	714	0	734	0	0
40	P	643	0	661	2	0
41	Q	641	0	682	7	0
42	R	544	0	565	4	0
43	T	670	0	719	5	0
44	U	589	0	629	1	0
45	X	65	0	33	0	0
46	C	1624	0	1696	9	0
47	G	1203	0	1254	8	0
48	I	1022	0	1070	4	0
49	J	786	0	828	10	0
50	M	891	0	952	9	0
51	N	805	0	844	3	0
52	S	668	0	693	6	0
53	A	32608	0	16424	99	0
54	Z	1563	0	794	4	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
56	A	91	0	0	0	0
56	a	205	0	0	0	0
56	b	5	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	k	1	0	0	0	0
56	p	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	z	1	0	0	0	0
57	A	1	0	0	0	0
57	a	1	0	0	0	0
57	d	1	0	0	0	0
58	A	28	0	0	0	0
58	X	7	0	0	0	0
58	Z	3	0	0	0	0
58	a	1	0	0	0	0
All	All	140031	0	94136	460	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 2.

All (460) 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)
38:L:107:VAL:HG12	38:L:117:TYR:HB3	1.69	0.73
33:D:9:LEU:HD11	53:A:429:U:H3'	1.69	0.72
30:a:568:U:H1'	30:a:2030:6MZ:H9C1	1.73	0.70
12:i:58:ASN:HD21	12:i:128:ASN:HD22	1.41	0.69
46:C:35:SER:OG	46:C:59:ARG:NH2	2.26	0.69
49:J:35:GLN:HG2	49:J:77:VAL:HB	1.73	0.68
22:t:49:VAL:HB	22:t:52:LEU:O	1.94	0.67
33:D:154:ARG:HG2	33:D:154:ARG:HH21	1.60	0.65
53:A:664:G:H22	53:A:741:G:H1	1.44	0.65
46:C:50:ALA:HB1	46:C:76:VAL:HG22	1.77	0.65
46:C:77:ILE:HA	46:C:84:VAL:HG13	1.79	0.65
50:M:28:THR:HG21	53:A:1328:C:H5''	1.78	0.65
53:A:946:A:H2'	53:A:947:G:C8	2.33	0.63
30:a:1047:G:HO2'	30:a:1110:G:H1	1.45	0.62
7:d:35:THR:HG22	7:d:73:VAL:HG21	1.82	0.61
30:a:12:U:H2'	30:a:12:U:O2	2.01	0.61
9:f:135:GLN:HG2	9:f:141:ILE:HG21	1.83	0.60
46:C:50:ALA:HA	46:C:75:ILE:HD11	1.83	0.60
36:H:2:SER:N	53:A:823:C:HO2'	1.99	0.60
52:S:50:ALA:HB1	52:S:57:HIS:HB3	1.85	0.59
48:I:51:PRO:HD3	48:I:80:ARG:HG3	1.84	0.59
53:A:769:G:H4'	53:A:1513:A:H4'	1.83	0.58
3:2:54:ASP:HB3	13:k:57:LEU:HD22	1.86	0.58
2:1:39:ARG:NH2	30:a:468:G:N7	2.48	0.58
38:L:4:VAL:HG23	41:Q:34:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:11:CYS:SG	4:3:14:CYS:N	2.77	0.58
10:g:78:GLY:HA2	10:g:82:GLY:HA2	1.86	0.57
33:D:58:LYS:NZ	53:A:545:C:OP1	2.38	0.57
1:0:22:THR:HG21	30:a:2419:U:H4'	1.87	0.57
27:y:25:LEU:HD11	30:a:930:G:H1'	1.87	0.56
41:Q:47:HIS:HB3	41:Q:74:THR:HG22	1.86	0.56
30:a:2797:U:H3'	30:a:2798:U:H5''	1.87	0.56
30:a:644:A:H2'	30:a:645:C:O4'	2.04	0.56
10:g:96:ALA:HB1	10:g:103:ILE:HD11	1.86	0.56
29:4:56:ARG:HG3	52:S:65:GLU:HA	1.87	0.56
5:b:36:C:N4	5:b:49:C:O2	2.39	0.55
20:r:92:ARG:NH1	30:a:2014:A:O2'	2.32	0.55
30:a:1939:5MU:OP1	30:a:2604:PSU:O2'	2.23	0.55
23:u:75:GLN:HB2	23:u:92:VAL:HG23	1.89	0.55
9:f:108:VAL:HG11	9:f:176:PRO:HG3	1.88	0.55
32:B:68:LEU:HD11	32:B:92:VAL:HG23	1.89	0.55
33:D:90:LEU:HD12	33:D:93:LEU:HD11	1.88	0.54
23:u:47:VAL:HA	23:u:50:MET:HE3	1.89	0.54
50:M:34:LEU:HD13	50:M:41:GLU:HA	1.89	0.54
33:D:48:LEU:HD21	33:D:56:ARG:HG3	1.89	0.54
30:a:2243:U:H2'	30:a:2244:U:C6	2.42	0.54
30:a:1026:G:H2'	30:a:1027:A:C8	2.43	0.54
33:D:206:LYS:HB3	53:A:8:A:C6	2.42	0.54
54:Z:25:C:H2'	54:Z:26:G:O4'	2.07	0.53
54:Z:51:C:H2'	54:Z:52:G:C8	2.44	0.53
40:P:5:ARG:HB2	53:A:376:G:H5''	1.90	0.53
30:a:1736:U:H2'	30:a:1737:G:O4'	2.08	0.53
29:4:42:PRO:HB2	29:4:48:GLN:HG3	1.90	0.53
10:g:9:VAL:HG22	10:g:50:LEU:HB2	1.90	0.53
21:s:51:PHE:HB3	21:s:93:LEU:HD21	1.90	0.53
35:F:32:ALA:HB2	35:F:70:VAL:HG11	1.91	0.53
53:A:457:G:H3'	53:A:458:U:H5''	1.91	0.52
53:A:945:G:C2	53:A:946:A:C8	2.97	0.52
30:a:1980:G:O2'	30:a:1982:U:OP2	2.25	0.52
41:Q:64:CYS:SG	41:Q:74:THR:HG23	2.49	0.52
53:A:524:G:H2'	53:A:525:C:C6	2.44	0.52
30:a:2273:A:H2'	30:a:2274:A:C8	2.44	0.52
53:A:382:A:H2'	53:A:383:A:C8	2.45	0.52
9:f:58:ALA:HB2	9:f:65:PRO:HD3	1.91	0.52
6:c:107:PRO:HD2	6:c:110:LEU:HD22	1.91	0.52
30:a:588:U:H2'	30:a:589:U:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:C:22:TRP:HB3	46:C:59:ARG:HB2	1.91	0.52
36:H:11:LEU:HD22	36:H:75:ILE:HD11	1.91	0.52
38:L:110:ARG:HB3	38:L:119:VAL:HG21	1.90	0.52
30:a:2445:2MG:HM21	30:a:2449:H2U:O4	2.10	0.52
10:g:103:ILE:HG23	10:g:115:HIS:HB3	1.92	0.52
53:A:429:U:H1'	53:A:430:A:H5''	1.90	0.52
7:d:12:THR:HG22	7:d:13:ARG:H	1.74	0.51
9:f:158:THR:HG22	9:f:160:ALA:H	1.74	0.51
35:F:88:MET:HB2	42:R:65:LEU:HD21	1.91	0.51
51:N:34:VAL:HA	51:N:41:ARG:NH1	2.25	0.51
30:a:1020:A:C2	30:a:1141:U:C2	2.98	0.51
38:L:40:THR:HG23	38:L:90:LEU:HD11	1.92	0.51
30:a:2233:U:H2'	30:a:2234:G:C8	2.46	0.51
32:B:103:ASN:ND2	53:A:1073:U:O2'	2.44	0.51
54:Z:13:C:H2'	54:Z:14:A:H5''	1.93	0.51
9:f:12:VAL:HG22	9:f:172:ALA:HB1	1.93	0.50
53:A:1053:G:N7	53:A:1200:C:H5'	2.25	0.50
53:A:1273:C:H2'	53:A:1274:A:O4'	2.11	0.50
28:z:43:ILE:HG22	28:z:49:TYR:HB2	1.94	0.50
30:a:476:G:H4'	30:a:502:A:N1	2.26	0.50
30:a:493:G:H2'	30:a:494:G:O4'	2.11	0.50
47:G:79:ARG:HA	47:G:84:THR:HA	1.94	0.50
32:B:100:MET:HA	32:B:107:VAL:HG21	1.93	0.50
33:D:113:GLU:HG3	53:A:408:A:H5'	1.94	0.50
53:A:151:A:H2'	53:A:152:A:O4'	2.12	0.50
9:f:105:THR:HA	29:4:38:SER:HB2	1.94	0.49
46:C:14:ILE:HG22	46:C:15:VAL:HG13	1.94	0.49
53:A:1176:A:H2'	53:A:1177:G:C8	2.47	0.49
10:g:89:LEU:HD22	10:g:162:VAL:HG22	1.94	0.49
38:L:21:VAL:HG21	53:A:553:A:H5''	1.95	0.49
34:E:159:LYS:HB2	34:E:164:ILE:HD13	1.94	0.49
50:M:40:ALA:HB3	50:M:43:VAL:HG23	1.94	0.49
29:4:28:VAL:HG21	29:4:32:LEU:HD21	1.95	0.49
48:I:52:LEU:HD11	48:I:63:LEU:HD11	1.93	0.49
30:a:1183:U:H2'	30:a:1184:U:C6	2.48	0.49
32:B:77:SER:HA	32:B:93:ASN:HB2	1.94	0.49
8:e:184:ASP:HA	13:k:2:ARG:HH12	1.78	0.49
49:J:70:HIS:ND1	53:A:1152:A:OP1	2.44	0.49
27:y:3:LYS:HG3	27:y:40:ASP:HB3	1.94	0.49
3:2:62:LEU:HB3	3:2:65:ALA:HB2	1.95	0.48
8:e:48:THR:HG23	8:e:88:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:C:77:ILE:HG12	46:C:103:ILE:HG13	1.95	0.48
20:r:4:ILE:HG12	20:r:106:VAL:HG22	1.93	0.48
53:A:299:G:H2'	53:A:300:A:C8	2.49	0.48
30:a:1932:A:H2'	30:a:1933:G:O4'	2.14	0.48
31:j:49:ARG:NH1	53:A:1422:G:O3'	2.46	0.48
31:j:99:ILE:HG12	31:j:115:ILE:HG23	1.95	0.48
34:E:76:LEU:HD23	34:E:147:MET:HE1	1.95	0.48
37:K:47:ALA:HB1	37:K:62:ALA:HB1	1.95	0.48
41:Q:25:ILE:HB	41:Q:42:THR:HG23	1.95	0.48
53:A:999:C:N3	53:A:1042:A:N6	2.62	0.48
10:g:26:ILE:HD13	10:g:76:VAL:HG23	1.95	0.48
22:t:28:VAL:HA	22:t:34:VAL:HG12	1.94	0.48
32:B:111:ILE:HD12	32:B:152:LYS:HA	1.95	0.48
30:a:2208:C:H2'	30:a:2209:G:C8	2.49	0.48
23:u:72:VAL:HB	23:u:91:PHE:HB3	1.96	0.48
30:a:546:U:H3'	30:a:547:A:H8	1.79	0.48
30:a:1169:A:H8	30:a:1169:A:H5''	1.78	0.48
30:a:819:A:C4	30:a:1189:A:C2	3.02	0.48
30:a:2392:A:OP2	30:a:2422:C:N4	2.42	0.48
30:a:395:U:O2'	30:a:396:G:N7	2.45	0.48
30:a:890:C:H3'	30:a:891:G:O4'	2.14	0.48
30:a:1870:C:H3'	30:a:1871:A:C8	2.48	0.48
33:D:9:LEU:HD22	33:D:9:LEU:H	1.79	0.48
33:D:75:TYR:CD1	33:D:93:LEU:HD13	2.49	0.48
9:f:85:ILE:HD11	30:a:2312:U:H5'	1.96	0.47
33:D:121:LYS:O	33:D:146:ARG:HD3	2.14	0.47
53:A:532:A:N6	53:A:1206:G:O2'	2.47	0.47
53:A:663:A:H5'	53:A:836:G:OP1	2.13	0.47
30:a:2346:A:H3'	30:a:2347:C:H5''	1.96	0.47
30:a:2902:C:H2'	30:a:2903:U:O4'	2.14	0.47
47:G:7:ILE:HG21	53:A:1377:A:C6	2.49	0.47
8:e:196:VAL:HA	8:e:199:MET:HE2	1.95	0.47
16:n:35:ILE:HG21	16:n:71:ALA:HA	1.96	0.47
30:a:277:G:H1'	30:a:278:A:C5	2.49	0.47
49:J:41:PRO:HB2	53:A:1151:A:O4'	2.15	0.47
53:A:465:A:H2'	53:A:466:A:C8	2.49	0.47
4:3:11:CYS:N	4:3:14:CYS:SG	2.88	0.47
24:v:38:VAL:HG12	24:v:59:LEU:HB2	1.97	0.47
47:G:13:LEU:HD11	48:I:50:GLN:HE22	1.79	0.47
50:M:16:VAL:HG13	50:M:34:LEU:HD12	1.97	0.47
50:M:54:ASP:OD1	50:M:57:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2038:G:H2'	30:a:2039:U:O4'	2.14	0.47
10:g:156:PRO:O	10:g:171:THR:HA	2.14	0.47
17:o:100:LEU:HD11	17:o:110:ILE:HD11	1.97	0.47
33:D:206:LYS:HB3	53:A:8:A:C5	2.49	0.47
53:A:371:A:H2'	53:A:372:C:O4'	2.14	0.47
53:A:410:G:H2'	53:A:429:U:C4	2.50	0.47
13:k:21:ARG:HA	30:a:811:U:H2'	1.97	0.47
25:w:6:GLN:O	25:w:74:ARG:NH1	2.48	0.47
30:a:1853:A:N1	30:a:2087:G:H1'	2.30	0.47
12:i:9:GLU:HG2	12:i:10:THR:HG23	1.95	0.47
12:i:110:PRO:O	12:i:115:GLY:HA3	2.14	0.47
30:a:2291:U:H2'	30:a:2292:U:C6	2.50	0.47
33:D:102:VAL:HG13	33:D:107:PHE:HB2	1.96	0.47
15:m:66:ALA:O	15:m:69:ARG:O	2.33	0.47
30:a:1778:U:H2'	30:a:1784:A:N6	2.31	0.47
30:a:1881:C:H2'	30:a:1882:U:O4'	2.15	0.47
30:a:2547:A:H2'	30:a:2548:U:C6	2.50	0.47
43:T:82:GLN:HA	43:T:85:LYS:HD3	1.97	0.47
53:A:1356:G:H2'	53:A:1357:A:C8	2.50	0.47
49:J:8:ILE:HD11	49:J:87:LEU:HD13	1.97	0.46
53:A:505:G:H5'	53:A:534:U:H2'	1.96	0.46
53:A:1391:U:H2'	53:A:1392:G:C8	2.50	0.46
30:a:888:C:OP1	50:M:92:ARG:HB3	2.16	0.46
32:B:89:GLN:HE21	32:B:89:GLN:HA	1.79	0.46
46:C:47:LEU:HB3	46:C:50:ALA:HB3	1.97	0.46
14:l:136:MET:HE2	23:u:57:TYR:CD1	2.50	0.46
30:a:340:A:H2'	30:a:341:C:O4'	2.16	0.46
34:E:18:VAL:HA	34:E:34:THR:O	2.15	0.46
30:a:2395:C:H2'	30:a:2396:G:O4'	2.15	0.46
33:D:105:MET:HE1	33:D:143:VAL:HB	1.97	0.46
9:f:126:GLY:HA3	9:f:160:ALA:HB3	1.96	0.46
10:g:64:GLN:O	10:g:67:THR:HG22	2.15	0.46
22:t:86:ARG:HG3	22:t:95:PHE:CE1	2.51	0.46
53:A:1086:U:H3	53:A:1099:G:H22	1.62	0.46
14:l:47:GLU:HG3	14:l:51:ARG:HD2	1.97	0.46
29:4:12:ILE:HG12	29:4:26:SER:HB3	1.97	0.46
30:a:1820:U:H4'	30:a:1821:A:OP2	2.16	0.46
29:4:16:CYS:SG	29:4:17:SER:N	2.80	0.46
53:A:502:A:H2'	53:A:503:C:O4'	2.16	0.46
6:c:29:PRO:HG2	6:c:34:LEU:HD21	1.98	0.46
14:l:66:ARG:NH1	14:l:104:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:59:LEU:HD12	24:v:80:ILE:HD12	1.98	0.46
30:a:1182:G:H2'	30:a:1183:U:O4'	2.15	0.46
32:B:94:HIS:O	32:B:95:ARG:C	2.59	0.46
33:D:121:LYS:O	33:D:148:LYS:NZ	2.42	0.46
30:a:2532:G:O2'	30:a:2657:A:N1	2.49	0.46
43:T:57:ILE:O	43:T:61:GLN:HG2	2.15	0.46
2:l:46:LYS:HE2	30:a:56:A:H5''	1.97	0.45
30:a:2014:A:H2'	30:a:2015:A:C8	2.51	0.45
35:F:90:MET:SD	42:R:61:ARG:NH1	2.88	0.45
49:J:26:VAL:HG11	49:J:39:PRO:HD3	1.96	0.45
2:l:29:GLN:NE2	30:a:210:C:OP1	2.48	0.45
14:l:50:ARG:HD3	14:l:65:ILE:HD11	1.98	0.45
30:a:1296:G:OP1	30:a:2709:G:O2'	2.27	0.45
53:A:986:U:H2'	53:A:987:G:O4'	2.16	0.45
14:l:55:ARG:CD	30:a:2469:A:H4'	2.47	0.45
28:z:9:THR:CG2	30:a:2020:A:H5'	2.47	0.45
34:E:56:VAL:HB	34:E:57:PRO:HD3	1.99	0.45
44:U:34:ARG:HH11	44:U:34:ARG:HG2	1.82	0.45
1:0:8:LYS:HB3	1:0:54:ILE:HG13	1.97	0.45
30:a:690:G:H2'	30:a:691:C:O4'	2.16	0.45
53:A:381:C:H2'	53:A:382:A:O4'	2.16	0.45
53:A:1025:U:H4'	53:A:1026:G:C8	2.52	0.45
53:A:1206:G:H2'	53:A:1207:2MG:O4'	2.17	0.45
9:f:57:LEU:HD23	9:f:65:PRO:HB3	1.98	0.45
27:y:15:GLY:HA2	30:a:969:G:O3'	2.17	0.45
23:u:2:PHE:HB2	23:u:61:LEU:HD12	1.99	0.45
30:a:1583:A:H4'	30:a:1585:C:C2	2.51	0.45
32:B:66:LYS:HD2	32:B:154:MET:HG3	1.99	0.45
49:J:40:ILE:HB	49:J:73:LEU:HB3	1.98	0.45
30:a:894:U:H2'	30:a:895:U:O4'	2.17	0.45
32:B:4:VAL:HG11	32:B:50:PHE:CD2	2.52	0.45
9:f:131:GLY:HA3	30:a:2305:U:H5''	1.99	0.45
14:l:75:GLU:HB2	14:l:90:GLU:HG3	1.98	0.45
23:u:31:TYR:CE1	23:u:92:VAL:HG22	2.52	0.45
30:a:901:C:H2'	30:a:902:C:O4'	2.17	0.45
30:a:2522:U:O2'	30:a:2647:U:OP1	2.19	0.45
50:M:39:ILE:HD11	50:M:52:GLN:HB3	1.98	0.45
53:A:649:A:H2'	53:A:650:G:O4'	2.16	0.45
27:y:6:LYS:HB2	27:y:58:GLU:HB2	1.99	0.44
30:a:207:A:H2'	30:a:208:C:O4'	2.17	0.44
30:a:1607:C:H4'	30:a:1608:A:O5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1722:A:H2'	30:a:1723:G:O4'	2.18	0.44
34:E:16:ILE:HD11	34:E:38:VAL:HG13	1.99	0.44
41:Q:7:THR:HG22	41:Q:62:ARG:HB3	2.00	0.44
49:J:65:TYR:HB3	51:N:96:LEU:HD11	1.99	0.44
54:Z:28:C:H2'	54:Z:29:G:C8	2.51	0.44
5:b:24:G:N7	5:b:56:G:H2'	2.33	0.44
17:o:70:VAL:HG11	31:j:123:LEU:HD13	2.00	0.44
50:M:39:ILE:HD12	50:M:56:LEU:HG	2.00	0.44
53:A:1456:A:H2'	53:A:1457:G:O4'	2.17	0.44
16:n:56:LYS:HA	16:n:59:ALA:HB3	1.99	0.44
23:u:35:GLU:HB3	23:u:93:ARG:CZ	2.47	0.44
26:x:9:LYS:HB2	26:x:14:LEU:HD13	1.99	0.44
53:A:1003:G:N2	53:A:1005:A:H5'	2.32	0.44
14:l:20:LEU:HD13	23:u:81:PRO:HG3	1.99	0.44
30:a:1744:A:H3'	30:a:1745:A:H8	1.82	0.44
51:N:5:SER:HB3	53:A:1216:A:H5''	1.99	0.44
7:d:156:PHE:CE1	12:i:81:ILE:HD13	2.52	0.44
53:A:67:C:H2'	53:A:68:G:C8	2.53	0.44
15:m:56:LYS:HE2	15:m:87:PHE:O	2.18	0.44
12:i:114:LEU:HG	12:i:118:MET:HE3	2.00	0.44
21:s:88:LYS:O	21:s:91:GLN:HG2	2.18	0.44
30:a:244:A:C2	30:a:255:A:C4	3.06	0.44
30:a:2063:C:O2	30:a:2450:A:N1	2.50	0.44
40:P:35:ARG:NH2	53:A:626:G:OP1	2.51	0.44
53:A:244:U:O4	53:A:906:A:H1'	2.17	0.44
53:A:1027:C:H2'	53:A:1028:C:C6	2.53	0.44
9:f:108:VAL:HB	9:f:109:PRO:HD3	2.00	0.43
18:p:51:ARG:HG2	30:a:1156:A:C8	2.53	0.43
43:T:2:ALA:HB3	43:T:8:LYS:HG3	1.99	0.43
53:A:831:A:H2'	53:A:832:G:O4'	2.18	0.43
10:g:2:SER:HB3	10:g:62:TRP:HB3	2.00	0.43
30:a:1422:G:H1'	30:a:1496:A:N1	2.34	0.43
5:b:66:A:N6	5:b:107:G:H2'	2.33	0.43
12:i:134:ALA:HB1	30:a:2898:U:O2	2.18	0.43
33:D:22:LYS:NZ	53:A:430:A:OP2	2.51	0.43
42:R:32:TYR:HB3	42:R:55:LEU:HD21	2.00	0.43
47:G:119:ARG:NH2	53:A:1240:U:OP1	2.51	0.43
53:A:87:C:H2'	53:A:88:U:C2	2.53	0.43
53:A:555:U:H2'	53:A:556:C:C6	2.53	0.43
53:A:1252:A:H2'	53:A:1253:G:O4'	2.18	0.43
30:a:460:A:H2'	30:a:461:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1746:A:H2'	30:a:1747:U:C6	2.54	0.43
32:B:119:THR:O	32:B:123:ASP:N	2.52	0.43
32:B:126:PHE:HA	32:B:129:LEU:HD12	2.00	0.43
41:Q:51:ASN:N	41:Q:51:ASN:OD1	2.50	0.43
53:A:660:C:H2'	53:A:661:G:O4'	2.17	0.43
12:i:28:LEU:HD12	12:i:142:ILE:HG21	2.00	0.43
30:a:3:U:H2'	30:a:4:U:C6	2.53	0.43
30:a:36:G:N3	30:a:450:G:O2'	2.51	0.43
30:a:723:C:H2'	30:a:724:U:O4'	2.19	0.43
53:A:975:A:N1	53:A:1366:C:O2'	2.43	0.43
30:a:1046:A:H3'	30:a:1047:G:C5'	2.48	0.43
47:G:70:ARG:HA	47:G:100:ALA:HB2	2.01	0.43
53:A:102:G:N3	53:A:151:A:H2	2.16	0.43
53:A:407:U:H2'	53:A:408:A:C8	2.52	0.43
5:b:109:A:H2'	5:b:110:C:O4'	2.19	0.43
14:l:53:MET:HG3	14:l:63:ILE:HD13	2.01	0.43
30:a:1434:A:H2'	30:a:1435:G:H8	1.84	0.43
33:D:70:ARG:HE	33:D:70:ARG:HA	1.83	0.43
50:M:98:ARG:NH2	53:A:1309:G:N7	2.66	0.43
53:A:320:A:H2'	53:A:321:A:O4'	2.19	0.43
9:f:138:PHE:HZ	9:f:154:ILE:HD11	1.84	0.42
22:t:45:HIS:NE2	30:a:498:G:O2'	2.48	0.42
30:a:2552:OMU:H6	30:a:2552:OMU:O5'	2.19	0.42
35:F:32:ALA:CB	35:F:70:VAL:HG11	2.48	0.42
9:f:41:GLY:HA3	30:a:2311:A:C2	2.55	0.42
23:u:6:ALA:HB3	23:u:65:VAL:HB	2.01	0.42
30:a:478:A:N1	30:a:500:G:H4'	2.34	0.42
30:a:1394:U:H4'	30:a:1603:A:H4'	2.01	0.42
30:a:2331:G:O2'	30:a:2336:A:N1	2.44	0.42
32:B:76:ALA:HB1	32:B:80:VAL:HG23	2.00	0.42
53:A:1414:U:H2'	53:A:1415:G:H8	1.85	0.42
7:d:5:VAL:HG21	7:d:80:TRP:CD2	2.54	0.42
15:m:24:MET:HE1	15:m:40:LYS:HD3	2.01	0.42
30:a:884:U:H2'	30:a:885:C:C6	2.54	0.42
53:A:71:A:N1	53:A:99:C:O2'	2.49	0.42
53:A:519:C:H2'	53:A:520:A:C8	2.54	0.42
5:b:29:A:H2'	5:b:30:C:O4'	2.18	0.42
30:a:414:C:H2'	30:a:415:A:C8	2.54	0.42
47:G:23:LEU:HD11	47:G:47:LEU:HD11	2.01	0.42
1:0:7:GLU:CD	1:0:27:LYS:HD3	2.45	0.42
30:a:2210:U:H4'	30:a:2211:A:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:C:50:ALA:HB1	46:C:76:VAL:CG2	2.48	0.42
52:S:52:HIS:HD2	53:A:1220:G:H1'	1.84	0.42
53:A:337:G:H2'	53:A:338:A:C8	2.55	0.42
53:A:918:A:H2'	53:A:919:A:O4'	2.20	0.42
23:u:42:LEU:HB3	23:u:47:VAL:HG21	2.00	0.42
28:z:4:GLN:HA	30:a:2615:U:C2	2.55	0.42
30:a:565:C:H2'	30:a:566:U:O4'	2.20	0.42
30:a:861:A:C2	30:a:917:A:C4	3.07	0.42
30:a:1326:U:O2'	30:a:2010:G:O2'	2.36	0.42
53:A:31:G:O2'	53:A:48:C:N4	2.52	0.42
53:A:71:A:H2'	53:A:72:A:O4'	2.20	0.42
53:A:780:A:C2	53:A:801:U:C5	3.07	0.42
1:0:38:LYS:HB2	1:0:49:TYR:CD1	2.55	0.42
16:n:27:VAL:HG21	16:n:40:ILE:HD12	2.02	0.42
30:a:1421:G:C2	30:a:1422:G:C8	3.08	0.42
35:F:38:ARG:HB2	35:F:97:THR:HA	2.01	0.42
52:S:49:ILE:HD12	52:S:71:LEU:HD21	2.01	0.42
19:q:83:TYR:CE1	30:a:1187:G:H5''	2.54	0.42
30:a:714:U:O2'	30:a:716:A:N7	2.50	0.42
30:a:1020:A:N1	30:a:1141:U:O2'	2.46	0.42
31:j:43:ILE:CD1	31:j:52:VAL:HB	2.50	0.42
47:G:7:ILE:HG21	53:A:1377:A:C5	2.55	0.42
49:J:8:ILE:HG21	49:J:25:ILE:HD13	2.02	0.42
53:A:1005:A:H5''	53:A:1038:C:H1'	2.01	0.42
18:p:51:ARG:NH2	30:a:993:G:OP2	2.52	0.42
30:a:84:A:N3	30:a:85:G:H1'	2.35	0.42
30:a:547:A:H1'	30:a:548:G:C8	2.55	0.42
30:a:2750:A:H1'	30:a:2752:C:N4	2.34	0.42
33:D:170:TRP:CE2	33:D:186:PRO:HG3	2.55	0.42
35:F:71:ILE:CG2	35:F:89:VAL:HG11	2.49	0.42
43:T:24:ARG:HB3	43:T:61:GLN:HE22	1.85	0.42
52:S:31:LEU:O	52:S:50:ALA:N	2.52	0.42
6:c:242:LYS:O	30:a:1902:C:H4'	2.20	0.42
10:g:9:VAL:CG2	10:g:50:LEU:HB2	2.50	0.42
20:r:82:MET:HB2	20:r:98:LYS:HB2	2.01	0.42
24:v:62:LYS:HE3	30:a:2366:A:H4'	2.02	0.42
30:a:857:G:H2'	30:a:858:G:O4'	2.20	0.42
30:a:1469:A:H2'	30:a:1470:A:C8	2.55	0.42
30:a:2747:G:O6	30:a:2755:C:H5''	2.20	0.42
31:j:59:LYS:HG3	31:j:89:ASN:HD22	1.85	0.42
32:B:89:GLN:HA	32:B:89:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D:14:ARG:HD2	53:A:543:U:OP1	2.19	0.42
16:n:39:VAL:HB	16:n:49:VAL:HG22	2.02	0.41
18:p:76:TYR:CZ	18:p:80:ILE:HG13	2.55	0.41
30:a:351:C:H2'	30:a:352:A:C8	2.54	0.41
30:a:2327:A:H2'	30:a:2328:A:C8	2.55	0.41
31:j:1:MET:HE3	31:j:32:TYR:CZ	2.54	0.41
41:Q:20:SER:OG	41:Q:71:LYS:NZ	2.53	0.41
30:a:162:U:O4	30:a:2218:G:H4'	2.20	0.41
31:j:113:MET:HE2	31:j:113:MET:HA	2.02	0.41
53:A:1288:A:N1	53:A:1371:G:H1'	2.35	0.41
53:A:1428:A:H2'	53:A:1429:A:O4'	2.20	0.41
6:c:5:LYS:HD2	6:c:17:VAL:HG22	2.01	0.41
9:f:116:GLY:HA3	9:f:178:ARG:HB3	2.00	0.41
11:h:31:VAL:HB	11:h:32:PRO:HD3	2.02	0.41
28:z:5:GLN:O	30:a:2017:U:H4'	2.20	0.41
30:a:248:G:O2'	30:a:2432:A:OP1	2.31	0.41
30:a:964:C:O2'	30:a:2273:A:N3	2.52	0.41
53:A:160:A:H2'	53:A:161:A:O4'	2.19	0.41
53:A:1402:4OC:O2	53:A:1500:A:N1	2.54	0.41
18:p:9:ILE:HD11	30:a:1198:U:H5'	2.02	0.41
22:t:85:PHE:CE1	22:t:94:ARG:HG2	2.56	0.41
30:a:2897:U:H2'	30:a:2898:U:C6	2.56	0.41
33:D:2:ALA:HB3	53:A:404:G:N7	2.36	0.41
49:J:10:LEU:HD12	49:J:22:THR:HG22	2.02	0.41
7:d:14:ILE:HA	17:o:12:GLN:HE22	1.85	0.41
22:t:54:GLN:N	22:t:55:PRO:HD2	2.35	0.41
30:a:191:A:H2'	30:a:192:C:C6	2.55	0.41
30:a:2328:A:H2'	30:a:2329:U:C6	2.55	0.41
30:a:2756:U:H1'	30:a:2757:A:H5''	2.02	0.41
32:B:116:ASP:O	32:B:120:GLN:N	2.51	0.41
10:g:78:GLY:HA3	10:g:136:ALA:O	2.21	0.41
25:w:28:ARG:NH2	30:a:1365:A:O5'	2.47	0.41
33:D:101:VAL:HG12	33:D:105:MET:HE2	2.03	0.41
49:J:23:ALA:O	49:J:27:GLU:HB2	2.21	0.41
53:A:1305:G:N2	53:A:1331:G:H1'	2.36	0.41
7:d:121:THR:HB	7:d:127:PHE:CD2	2.55	0.41
30:a:56:A:H2'	30:a:57:C:O4'	2.20	0.41
30:a:172:A:H2'	30:a:173:A:C8	2.55	0.41
32:B:76:ALA:O	32:B:77:SER:C	2.63	0.41
7:d:48:ILE:HG21	7:d:90:PHE:HB2	2.03	0.41
32:B:59:LYS:HG2	32:B:63:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D:149:ALA:O	33:D:152:GLN:HG2	2.21	0.41
53:A:155:A:H2'	53:A:156:C:O4'	2.20	0.41
53:A:1324:A:H2'	53:A:1325:C:O4'	2.19	0.41
53:A:1382:C:H2'	53:A:1383:C:H6	1.85	0.41
1:0:39:PHE:CZ	1:0:44:ARG:HA	2.56	0.41
3:2:45:ARG:N	3:2:46:PRO:HD2	2.35	0.41
6:c:50:THR:HB	30:a:1805:A:N3	2.36	0.41
10:g:30:ASN:HB2	10:g:80:THR:O	2.20	0.41
12:i:37:ARG:NH2	30:a:1007:C:OP1	2.51	0.41
17:o:33:VAL:HG22	17:o:38:LYS:HG3	2.03	0.41
19:q:14:VAL:HG11	19:q:20:VAL:HG21	2.03	0.41
23:u:4:ILE:HG22	23:u:42:LEU:HD22	2.03	0.41
30:a:5:A:C2	30:a:2899:A:C2	3.09	0.41
30:a:103:A:H2'	30:a:104:A:O4'	2.21	0.41
30:a:120:U:H5'	30:a:122:G:OP2	2.20	0.41
30:a:1726:C:H2'	30:a:1727:C:C6	2.56	0.41
30:a:2298:A:H2'	30:a:2299:U:O4'	2.20	0.41
32:B:164:ILE:O	32:B:186:ILE:HB	2.20	0.41
34:E:15:LEU:HD21	34:E:18:VAL:HG23	2.01	0.41
48:I:50:GLN:N	48:I:51:PRO:HD2	2.36	0.41
53:A:51:A:N7	53:A:114:U:O2'	2.50	0.41
53:A:171:A:H2'	53:A:172:A:C8	2.56	0.41
53:A:714:G:H2'	53:A:715:A:C8	2.55	0.41
53:A:1516:2MG:HM21	53:A:1519:A:N7	2.35	0.41
4:3:16:ILE:HD13	4:3:25:VAL:HG22	2.02	0.41
18:p:49:ASP:HA	18:p:52:GLN:HB2	2.03	0.41
30:a:657:U:H2'	30:a:658:U:C6	2.56	0.41
30:a:1720:U:H2'	30:a:1721:G:O4'	2.21	0.41
33:D:100:ASN:HD22	33:D:111:ARG:HD3	1.86	0.41
47:G:26:PHE:HZ	47:G:120:LEU:HD11	1.86	0.41
52:S:55:ARG:HG3	52:S:56:GLN:HG2	2.03	0.41
53:A:451:A:H61	53:A:481:G:H5'	1.86	0.41
53:A:677:U:H3	53:A:713:G:H22	1.67	0.41
16:n:41:ALA:HB2	16:n:48:LEU:HD21	2.02	0.40
30:a:639:U:H2'	30:a:640:C:C6	2.56	0.40
43:T:68:HIS:HD2	43:T:70:ASN:H	1.69	0.40
53:A:1315:U:H2'	53:A:1316:G:O4'	2.21	0.40
30:a:247:G:H4'	30:a:386:G:C5	2.56	0.40
30:a:2251:OMG:HM23	30:a:2251:OMG:H1'	1.83	0.40
30:a:2376:A:H2'	30:a:2377:A:O4'	2.21	0.40
33:D:159:LEU:O	33:D:163:GLU:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A:1148:U:H2'	53:A:1149:C:O4'	2.21	0.40
53:A:1477:U:H2'	53:A:1478:U:C6	2.56	0.40
30:a:1187:G:N2	30:a:1188:U:O4	2.53	0.40
30:a:2026:U:H2'	30:a:2027:G:O4'	2.22	0.40
30:a:2358:A:H2'	30:a:2359:C:O4'	2.21	0.40
30:a:2548:U:O2	31:j:23:LYS:NZ	2.54	0.40
32:B:69:PHE:O	32:B:91:PHE:HA	2.21	0.40
38:L:107:VAL:CG1	38:L:117:TYR:HB3	2.44	0.40
53:A:767:A:H2'	53:A:768:A:O4'	2.22	0.40
11:h:21:VAL:HG22	11:h:25:TYR:HB3	2.03	0.40
22:t:22:ARG:HD3	22:t:73:PHE:CE1	2.57	0.40
30:a:156:A:H2'	30:a:157:C:O4'	2.21	0.40
30:a:987:C:H2'	30:a:988:A:O4'	2.21	0.40
53:A:673:A:H2'	53:A:674:G:C8	2.56	0.40
9:f:155:THR:HG21	30:a:2314:A:H1'	2.04	0.40
21:s:31:VAL:HG22	21:s:84:TYR:CD1	2.57	0.40
24:v:18:ALA:HB1	30:a:2271:G:OP1	2.21	0.40
30:a:586:A:N1	30:a:809:G:O2'	2.51	0.40
30:a:1872:A:H3'	30:a:1873:G:O4'	2.21	0.40
42:R:23:TYR:HA	42:R:29:LEU:HD11	2.02	0.40
53:A:49:U:O2	53:A:362:G:H1'	2.22	0.40
53:A:945:G:H2'	53:A:945:G:N3	2.37	0.40
53:A:994:A:N1	53:A:1047:G:H4'	2.36	0.40
53:A:1218:C:H2'	53:A:1219:A:C8	2.55	0.40
53:A:1424:U:H2'	53:A:1425:U:O4'	2.22	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	0	49/55 (89%)	47 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
6	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
7	d	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
8	e	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	24	37
9	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
10	g	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
11	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
12	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
13	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	18	28
14	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
15	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
16	n	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	14	22
17	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
18	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
19	q	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	20
20	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
21	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
22	t	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	12	20
23	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
24	v	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
25	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
26	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
27	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
28	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
29	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
31	j	114/123 (93%)	108 (95%)	5 (4%)	1 (1%)	14	22
32	B	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
33	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
34	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
36	H	127/130 (98%)	122 (96%)	4 (3%)	1 (1%)	16	25
37	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
38	L	120/124 (97%)	110 (92%)	9 (8%)	1 (1%)	16	25
39	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
40	P	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
41	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
42	R	64/75 (85%)	60 (94%)	3 (5%)	1 (2%)	7	11
43	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
44	U	68/71 (96%)	66 (97%)	1 (2%)	1 (2%)	8	12
46	C	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
47	G	151/179 (84%)	145 (96%)	6 (4%)	0	100	100
48	I	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
49	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	20
50	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
51	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
52	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
All	All	5479/5913 (93%)	5271 (96%)	197 (4%)	11 (0%)	44	58

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	n	88	LYS
49	J	57	VAL
19	q	45	GLU
13	k	29	LYS
36	H	66	PHE
44	U	6	VAL
31	j	5	GLN
42	R	22	ASP
22	t	39	ILE
38	L	45	PRO
8	e	71	GLY

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	0	46/49 (94%)	44 (96%)	2 (4%)	26	44
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	63
3	2	51/52 (98%)	50 (98%)	1 (2%)	48	70
4	3	34/34 (100%)	32 (94%)	2 (6%)	18	31
6	c	216/218 (99%)	214 (99%)	2 (1%)	70	85
7	d	163/163 (100%)	162 (99%)	1 (1%)	78	89
8	e	165/165 (100%)	164 (99%)	1 (1%)	78	89
9	f	148/150 (99%)	144 (97%)	4 (3%)	39	62
10	g	137/138 (99%)	126 (92%)	11 (8%)	11	19
11	h	32/114 (28%)	30 (94%)	2 (6%)	16	29
12	i	116/116 (100%)	115 (99%)	1 (1%)	70	85
13	k	103/103 (100%)	101 (98%)	2 (2%)	50	71
14	l	107/107 (100%)	105 (98%)	2 (2%)	50	71
15	m	98/103 (95%)	97 (99%)	1 (1%)	68	84
16	n	86/87 (99%)	84 (98%)	2 (2%)	44	66
17	o	99/100 (99%)	99 (100%)	0	100	100
18	p	89/90 (99%)	88 (99%)	1 (1%)	65	82
19	q	84/84 (100%)	82 (98%)	2 (2%)	43	65
20	r	93/93 (100%)	93 (100%)	0	100	100
21	s	80/84 (95%)	76 (95%)	4 (5%)	22	38
22	t	83/85 (98%)	77 (93%)	6 (7%)	13	23
23	u	78/78 (100%)	73 (94%)	5 (6%)	16	28
24	v	62/63 (98%)	62 (100%)	0	100	100
25	w	67/68 (98%)	66 (98%)	1 (2%)	57	77
26	x	54/55 (98%)	50 (93%)	4 (7%)	13	22
27	y	48/49 (98%)	47 (98%)	1 (2%)	47	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	z	47/48 (98%)	46 (98%)	1 (2%)	47	69
29	4	55/62 (89%)	51 (93%)	4 (7%)	13	22
31	j	99/104 (95%)	98 (99%)	1 (1%)	68	84
32	B	186/199 (94%)	175 (94%)	11 (6%)	18	31
33	D	172/173 (99%)	151 (88%)	21 (12%)	5	7
34	E	119/126 (94%)	115 (97%)	4 (3%)	32	54
35	F	90/116 (78%)	88 (98%)	2 (2%)	45	67
36	H	104/105 (99%)	100 (96%)	4 (4%)	29	49
37	K	89/98 (91%)	87 (98%)	2 (2%)	45	67
38	L	102/103 (99%)	90 (88%)	12 (12%)	5	7
39	O	76/77 (99%)	75 (99%)	1 (1%)	61	80
40	P	65/65 (100%)	63 (97%)	2 (3%)	35	57
41	Q	73/78 (94%)	72 (99%)	1 (1%)	59	79
42	R	57/65 (88%)	55 (96%)	2 (4%)	32	53
43	T	65/66 (98%)	64 (98%)	1 (2%)	57	77
44	U	60/61 (98%)	54 (90%)	6 (10%)	7	11
46	C	170/190 (90%)	162 (95%)	8 (5%)	23	41
47	G	126/147 (86%)	115 (91%)	11 (9%)	9	16
48	I	105/107 (98%)	101 (96%)	4 (4%)	29	49
49	J	86/90 (96%)	83 (96%)	3 (4%)	32	53
50	M	93/96 (97%)	89 (96%)	4 (4%)	26	44
51	N	83/84 (99%)	82 (99%)	1 (1%)	63	81
52	S	72/79 (91%)	67 (93%)	5 (7%)	14	24
All	All	4571/4825 (95%)	4401 (96%)	170 (4%)	31	51

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	27	LYS
1	0	54	ILE
2	1	46	LYS
3	2	57	LEU
4	3	14	CYS
4	3	36	ARG

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Mol	Chain	Res	Type
6	c	4	VAL
6	c	37	ASN
7	d	2	ILE
8	e	116	ASP
9	f	50	LEU
9	f	120	LYS
9	f	146	VAL
9	f	150	ARG
10	g	18	LYS
10	g	29	LYS
10	g	43	VAL
10	g	51	THR
10	g	67	THR
10	g	72	LEU
10	g	76	VAL
10	g	90	VAL
10	g	102	VAL
10	g	103	ILE
10	g	155	GLU
11	h	6	LEU
11	h	9	VAL
12	i	138	GLN
13	k	112	LEU
13	k	129	LYS
14	l	30	SER
14	l	135	VAL
15	m	51	LEU
16	n	2	ASP
16	n	84	GLU
18	p	112	LYS
19	q	20	VAL
19	q	70	GLU
21	s	64	LYS
21	s	72	GLN
21	s	89	GLU
21	s	93	LEU
22	t	10	GLU
22	t	15	THR
22	t	52	LEU
22	t	54	GLN
22	t	74	ASN
22	t	100	SER

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Mol	Chain	Res	Type
23	u	41	GLU
23	u	61	LEU
23	u	62	THR
23	u	65	VAL
23	u	77	VAL
25	w	54	LYS
26	x	8	GLU
26	x	14	LEU
26	x	24	GLU
26	x	56	LEU
27	y	12	SER
28	z	32	LYS
29	4	3	LYS
29	4	12	ILE
29	4	48	GLN
29	4	66	ILE
31	j	93	GLN
32	B	7	ARG
32	B	8	ASP
32	B	63	ARG
32	B	78	GLU
32	B	93	ASN
32	B	100	MET
32	B	105	LYS
32	B	127	ASP
32	B	128	LYS
32	B	131	LYS
32	B	132	LYS
33	D	5	LEU
33	D	8	LYS
33	D	9	LEU
33	D	31	LYS
33	D	34	ILE
33	D	44	ARG
33	D	45	LYS
33	D	58	LYS
33	D	82	LEU
33	D	85	ASN
33	D	88	GLU
33	D	111	ARG
33	D	117	LEU
33	D	142	VAL

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Mol	Chain	Res	Type
33	D	144	SER
33	D	148	LYS
33	D	154	ARG
33	D	159	LEU
33	D	167	LYS
33	D	183	LYS
33	D	206	LYS
34	E	14	LYS
34	E	38	VAL
34	E	162	GLU
34	E	164	ILE
35	F	62	MET
35	F	74	LEU
36	H	50	LYS
36	H	56	LYS
36	H	89	LYS
36	H	117	ARG
37	K	86	VAL
37	K	94	GLU
38	L	4	VAL
38	L	14	ARG
38	L	15	LYS
38	L	16	VAL
38	L	54	ARG
38	L	55	VAL
38	L	70	GLU
38	L	75	GLN
38	L	87	VAL
38	L	88	LYS
38	L	111	LYS
38	L	123	LYS
39	O	3	LEU
40	P	63	GLN
40	P	79	ASN
41	Q	51	ASN
42	R	10	PHE
42	R	18	VAL
43	T	40	GLU
44	U	3	VAL
44	U	4	ILE
44	U	21	ARG
44	U	49	LYS

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Mol	Chain	Res	Type
44	U	59	LYS
44	U	63	GLU
46	C	84	VAL
46	C	86	LYS
46	C	107	ARG
46	C	147	LYS
46	C	169	ARG
46	C	170	GLU
46	C	178	LEU
46	C	202	ILE
47	G	5	ARG
47	G	25	LYS
47	G	73	VAL
47	G	75	VAL
47	G	79	ARG
47	G	92	ARG
47	G	110	LYS
47	G	113	ASP
47	G	135	VAL
47	G	137	LYS
47	G	144	MET
48	I	42	GLU
48	I	53	GLU
48	I	58	VAL
48	I	63	LEU
49	J	18	ILE
49	J	27	GLU
49	J	36	VAL
50	M	16	VAL
50	M	27	LYS
50	M	83	LEU
50	M	113	ARG
51	N	60	GLN
52	S	15	LEU
52	S	42	PRO
52	S	43	ASN
52	S	55	ARG
52	S	63	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
6	c	25	HIS
6	c	90	ASN
6	c	115	GLN
6	c	153	GLN
6	c	197	ASN
6	c	243	HIS
8	e	94	GLN
8	e	115	GLN
11	h	33	GLN
12	i	47	HIS
12	i	80	HIS
12	i	128	ASN
12	i	138	GLN
14	l	13	HIS
14	l	60	GLN
16	n	19	GLN
16	n	29	HIS
16	n	100	HIS
17	o	12	GLN
19	q	66	HIS
20	r	40	ASN
21	s	28	ASN
21	s	72	GLN
22	t	53	ASN
22	t	74	ASN
23	u	12	GLN
24	v	57	HIS
25	w	6	GLN
26	x	27	ASN
26	x	38	GLN
27	y	9	GLN
28	z	6	ASN
29	4	20	ASN
29	4	30	HIS
29	4	65	ASN
31	j	5	GLN
31	j	89	ASN
32	B	42	ASN
32	B	89	GLN
32	B	103	ASN
33	D	85	ASN
33	D	100	ASN
33	D	116	GLN

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Mol	Chain	Res	Type
33	D	164	GLN
34	E	82	GLN
34	E	89	HIS
34	E	97	GLN
34	E	121	HIS
35	F	55	HIS
36	H	21	ASN
37	K	38	GLN
37	K	118	HIS
39	O	80	GLN
40	P	59	HIS
42	R	54	GLN
43	T	20	HIS
46	C	6	HIS
46	C	100	GLN
46	C	139	GLN
47	G	68	ASN
48	I	31	ASN
48	I	32	GLN
49	J	15	HIS
49	J	58	ASN
50	M	12	HIS
50	M	14	HIS
51	N	4	GLN
51	N	66	GLN
52	S	43	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	a	2749/2903 (94%)	299 (10%)	0
45	X	2/3 (66%)	0	0
5	b	118/120 (98%)	12 (10%)	0
53	A	1516/1534 (98%)	195 (12%)	25 (1%)
54	Z	71/77 (92%)	14 (19%)	3 (4%)
All	All	4456/4637 (96%)	520 (11%)	28 (0%)

All (520) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	b	34	A

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Mol	Chain	Res	Type
5	b	35	C
5	b	36	C
5	b	37	C
5	b	44	G
5	b	45	A
5	b	56	G
5	b	88	C
5	b	89	U
5	b	90	C
5	b	99	A
5	b	109	A
30	a	10	A
30	a	34	U
30	a	63	A
30	a	71	A
30	a	74	A
30	a	75	G
30	a	101	A
30	a	102	U
30	a	110	G
30	a	118	A
30	a	119	A
30	a	120	U
30	a	125	A
30	a	126	A
30	a	139	U
30	a	142	A
30	a	163	C
30	a	165	A
30	a	181	A
30	a	196	A
30	a	199	A
30	a	200	U
30	a	215	G
30	a	216	A
30	a	221	A
30	a	222	A
30	a	233	A
30	a	248	G
30	a	267	C
30	a	272	A
30	a	278	A

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Mol	Chain	Res	Type
30	a	279	A
30	a	289	G
30	a	311	A
30	a	329	G
30	a	330	A
30	a	361	G
30	a	362	A
30	a	386	G
30	a	396	G
30	a	403	U
30	a	404	A
30	a	405	U
30	a	411	G
30	a	451	U
30	a	454	A
30	a	455	C
30	a	481	G
30	a	491	G
30	a	504	A
30	a	505	A
30	a	509	C
30	a	530	G
30	a	531	C
30	a	532	A
30	a	533	G
30	a	545	U
30	a	546	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	563	A
30	a	573	U
30	a	575	A
30	a	586	A
30	a	603	A
30	a	615	U
30	a	627	A
30	a	637	A
30	a	645	C
30	a	647	G
30	a	653	U
30	a	654	A

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Mol	Chain	Res	Type
30	a	655	A
30	a	686	U
30	a	717	C
30	a	730	A
30	a	747	5MU
30	a	764	A
30	a	765	C
30	a	775	G
30	a	776	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	805	G
30	a	812	C
30	a	827	U
30	a	828	U
30	a	846	U
30	a	847	U
30	a	856	G
30	a	859	G
30	a	883	G
30	a	884	U
30	a	888	C
30	a	890	C
30	a	891	G
30	a	895	U
30	a	896	A
30	a	897	C
30	a	910	A
30	a	914	G
30	a	931	U
30	a	934	U
30	a	946	C
30	a	961	C
30	a	962	G
30	a	974	G
30	a	983	A
30	a	984	A
30	a	985	C
30	a	996	A
30	a	1012	U
30	a	1013	C

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Mol	Chain	Res	Type
30	a	1022	G
30	a	1033	U
30	a	1045	C
30	a	1046	A
30	a	1047	G
30	a	1111	A
30	a	1112	G
30	a	1116	G
30	a	1122	G
30	a	1128	G
30	a	1129	A
30	a	1132	U
30	a	1133	A
30	a	1134	A
30	a	1135	C
30	a	1142	A
30	a	1143	A
30	a	1169	A
30	a	1172	C
30	a	1253	A
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1286	A
30	a	1287	A
30	a	1300	G
30	a	1301	A
30	a	1303	G
30	a	1352	U
30	a	1365	A
30	a	1379	U
30	a	1383	A
30	a	1416	G
30	a	1427	A
30	a	1428	C
30	a	1451	C
30	a	1452	G
30	a	1453	A
30	a	1458	U
30	a	1482	G
30	a	1493	C
30	a	1504	A

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Mol	Chain	Res	Type
30	a	1509	A
30	a	1510	G
30	a	1515	A
30	a	1535	A
30	a	1536	C
30	a	1537	G
30	a	1538	G
30	a	1566	A
30	a	1569	A
30	a	1578	U
30	a	1583	A
30	a	1584	U
30	a	1585	C
30	a	1608	A
30	a	1609	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1738	G
30	a	1764	C
30	a	1773	A
30	a	1782	U
30	a	1800	C
30	a	1801	A
30	a	1808	A
30	a	1809	A
30	a	1816	C
30	a	1829	A
30	a	1847	A
30	a	1848	A
30	a	1858	A
30	a	1870	C
30	a	1871	A
30	a	1873	G
30	a	1906	G
30	a	1907	G
30	a	1913	A
30	a	1915	3TD

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Mol	Chain	Res	Type
30	a	1929	G
30	a	1930	G
30	a	1936	A
30	a	1937	A
30	a	1938	A
30	a	1955	U
30	a	1965	C
30	a	1967	C
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1993	U
30	a	2020	A
30	a	2023	C
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M
30	a	2077	A
30	a	2080	A
30	a	2093	G
30	a	2198	A
30	a	2203	U
30	a	2204	G
30	a	2211	A
30	a	2212	A
30	a	2225	A
30	a	2238	G
30	a	2268	A
30	a	2278	A
30	a	2282	G
30	a	2283	C
30	a	2287	A
30	a	2305	U
30	a	2308	G
30	a	2312	U

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Mol	Chain	Res	Type
30	a	2322	A
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2336	A
30	a	2347	C
30	a	2350	C
30	a	2361	G
30	a	2383	G
30	a	2385	C
30	a	2402	U
30	a	2406	A
30	a	2424	C
30	a	2425	A
30	a	2429	G
30	a	2430	A
30	a	2431	U
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2449	H2U
30	a	2469	A
30	a	2476	A
30	a	2478	A
30	a	2480	C
30	a	2502	G
30	a	2505	G
30	a	2518	A
30	a	2529	G
30	a	2535	G
30	a	2547	A
30	a	2554	U
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2689	U
30	a	2690	U
30	a	2714	G

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Mol	Chain	Res	Type
30	a	2716	C
30	a	2726	A
30	a	2744	G
30	a	2748	A
30	a	2750	A
30	a	2757	A
30	a	2765	A
30	a	2778	A
30	a	2791	G
30	a	2798	U
30	a	2800	A
30	a	2809	A
30	a	2820	A
30	a	2821	A
30	a	2883	A
30	a	2884	U
53	A	4	U
53	A	5	U
53	A	6	G
53	A	8	A
53	A	9	G
53	A	32	A
53	A	39	G
53	A	47	C
53	A	48	C
53	A	50	A
53	A	51	A
53	A	70	U
53	A	71	A
53	A	83	C
53	A	84	U
53	A	85	U
53	A	86	G
53	A	87	C
53	A	88	U
53	A	91	U
53	A	94	G
53	A	95	C
53	A	120	A
53	A	122	G
53	A	131	A
53	A	141	G

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Mol	Chain	Res	Type
53	A	143	A
53	A	144	G
53	A	159	G
53	A	164	G
53	A	182	A
53	A	183	C
53	A	197	A
53	A	202	G
53	A	226	G
53	A	240	G
53	A	245	U
53	A	247	G
53	A	251	G
53	A	266	G
53	A	267	C
53	A	289	G
53	A	321	A
53	A	328	C
53	A	348	G
53	A	352	C
53	A	354	G
53	A	367	U
53	A	372	C
53	A	384	G
53	A	406	G
53	A	411	A
53	A	412	A
53	A	413	G
53	A	414	A
53	A	421	U
53	A	422	C
53	A	423	G
53	A	424	G
53	A	429	U
53	A	438	U
53	A	439	U
53	A	453	G
53	A	457	G
53	A	458	U
53	A	467	U
53	A	468	A
53	A	479	U

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Mol	Chain	Res	Type
53	A	484	G
53	A	486	U
53	A	511	C
53	A	518	C
53	A	532	A
53	A	536	C
53	A	547	A
53	A	559	A
53	A	562	U
53	A	572	A
53	A	573	A
53	A	576	C
53	A	577	G
53	A	587	G
53	A	588	G
53	A	596	A
53	A	633	G
53	A	642	A
53	A	650	G
53	A	653	U
53	A	665	A
53	A	723	U
53	A	724	G
53	A	734	G
53	A	748	G
53	A	755	G
53	A	777	A
53	A	793	U
53	A	794	A
53	A	815	A
53	A	817	C
53	A	832	G
53	A	849	G
53	A	874	G
53	A	890	G
53	A	914	A
53	A	926	G
53	A	931	C
53	A	934	C
53	A	935	A
53	A	960	U
53	A	961	U

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Mol	Chain	Res	Type
53	A	966	2MG
53	A	969	A
53	A	971	G
53	A	975	A
53	A	976	G
53	A	977	A
53	A	984	C
53	A	993	G
53	A	994	A
53	A	996	A
53	A	1003	G
53	A	1004	A
53	A	1009	U
53	A	1027	C
53	A	1028	C
53	A	1029	U
53	A	1031	C
53	A	1033	G
53	A	1034	G
53	A	1036	A
53	A	1039	G
53	A	1042	A
53	A	1065	U
53	A	1085	U
53	A	1086	U
53	A	1094	G
53	A	1095	U
53	A	1101	A
53	A	1124	G
53	A	1125	U
53	A	1129	C
53	A	1130	A
53	A	1132	C
53	A	1135	U
53	A	1137	C
53	A	1138	G
53	A	1140	C
53	A	1145	A
53	A	1146	A
53	A	1171	A
53	A	1184	G
53	A	1196	A

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Mol	Chain	Res	Type
53	A	1197	A
53	A	1213	A
53	A	1214	C
53	A	1227	A
53	A	1238	A
53	A	1256	A
53	A	1257	A
53	A	1260	G
53	A	1275	A
53	A	1280	A
53	A	1286	U
53	A	1287	A
53	A	1300	G
53	A	1302	C
53	A	1317	C
53	A	1319	A
53	A	1320	C
53	A	1332	A
53	A	1338	G
53	A	1346	A
53	A	1353	G
53	A	1363	A
53	A	1370	G
53	A	1378	C
53	A	1379	G
53	A	1381	U
53	A	1397	C
53	A	1398	A
53	A	1419	G
53	A	1429	A
53	A	1441	A
53	A	1450	U
53	A	1451	U
53	A	1453	G
53	A	1492	A
53	A	1497	G
53	A	1503	A
53	A	1505	G
53	A	1506	U
53	A	1517	G
53	A	1529	G
53	A	1530	G

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Mol	Chain	Res	Type
53	A	1533	C
54	Z	6	G
54	Z	7	G
54	Z	9	G
54	Z	14	A
54	Z	19	G
54	Z	20	U
54	Z	21	A
54	Z	46	G
54	Z	47	U
54	Z	58	A
54	Z	61	C
54	Z	65	C
54	Z	69	C
54	Z	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	A	7	A
53	A	70	U
53	A	86	G
53	A	94	G
53	A	199	A
53	A	361	G
53	A	438	U
53	A	547	A
53	A	587	G
53	A	733	G
53	A	776	G
53	A	793	U
53	A	858	G
53	A	993	G
53	A	1026	G
53	A	1035	A
53	A	1045	C
53	A	1124	G
53	A	1129	C
53	A	1139	G
53	A	1145	A
53	A	1211	U
53	A	1225	A

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Mol	Chain	Res	Type
53	A	1319	A
53	A	1505	G
54	Z	6	G
54	Z	7	G
54	Z	47	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

38 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	PSU	a	746	56,30	18,21,22	0.93	1 (5%)	22,30,33	0.67	0
53	2MG	A	1516	53	23,26,27	0.35	0	32,38,41	0.54	0
53	4OC	A	1402	53	20,23,24	0.40	0	26,32,35	0.57	0
30	5MU	a	747	30	19,22,23	0.35	0	28,32,35	0.39	0
30	OMU	a	2552	30	19,22,23	0.36	0	26,31,34	0.52	0
53	2MG	A	1207	53	23,26,27	0.41	0	32,38,41	0.41	0
53	5MC	A	1407	53	18,22,23	0.36	0	26,32,35	0.66	0
30	3TD	a	1915	30	18,22,23	1.07	1 (5%)	22,32,35	0.61	0
30	PSU	a	2504	57,30	18,21,22	0.95	1 (5%)	22,30,33	0.71	0
53	PSU	A	516	53,56	18,21,22	0.90	1 (5%)	22,30,33	0.59	0
14	MS6	l	82	14	5,7,8	0.38	0	2,7,9	0.33	0
7	MEQ	d	150	7	8,9,10	0.43	0	5,10,12	0.97	0
30	PSU	a	1911	30	18,21,22	0.91	1 (5%)	22,30,33	0.63	0
30	PSU	a	1917	30	18,21,22	0.96	1 (5%)	22,30,33	0.60	0
30	6MZ	a	2030	30	22,25,26	0.63	0	30,36,39	0.67	0
30	5MU	a	1939	30	19,22,23	0.39	0	28,32,35	0.44	0
30	H2U	a	2449	30	18,21,22	0.59	0	21,30,33	1.10	3 (14%)
30	PSU	a	955	30	18,21,22	0.83	1 (5%)	22,30,33	0.73	0
30	6MZ	a	1618	30	22,25,26	0.55	0	30,36,39	0.63	0
30	2MG	a	1835	30	23,26,27	0.46	0	32,38,41	0.41	0
53	2MG	A	966	53	23,26,27	0.44	0	32,38,41	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	5MC	a	1962	30	18,22,23	0.33	0	26,32,35	0.59	0
30	2MG	a	2445	30	23,26,27	0.57	0	32,38,41	0.41	0
30	2MA	a	2503	56,30	22,25,26	1.15	4 (18%)	33,37,40	1.10	3 (9%)
37	IAS	K	119	37	6,7,8	0.86	0	6,8,10	0.99	0
30	PSU	a	2604	30	18,21,22	0.89	1 (5%)	22,30,33	0.93	1 (4%)
30	OMG	a	2251	54,30	23,26,27	0.35	0	33,38,41	0.45	0
53	UR3	A	1498	53,57	19,22,23	0.41	0	26,32,35	0.75	1 (3%)
38	D2T	L	89	38	7,9,10	0.94	0	6,11,13	1.55	2 (33%)
30	PSU	a	2580	30	18,21,22	0.94	1 (5%)	22,30,33	0.81	1 (4%)
30	OMC	a	2498	56,30	19,22,23	0.50	0	26,31,34	0.54	0
30	1MG	a	745	30	22,26,27	0.91	2 (9%)	33,39,42	0.43	0
14	4D4	l	81	14	9,11,12	0.66	0	8,13,15	0.69	0
53	5MC	A	967	53	18,22,23	0.38	0	26,32,35	0.59	0
53	G7M	A	527	53	23,26,27	0.71	1 (4%)	35,39,42	0.61	0
30	PSU	a	2605	30	18,21,22	0.94	1 (5%)	22,30,33	0.80	1 (4%)
30	G7M	a	2069	30	23,26,27	0.89	1 (4%)	35,39,42	0.71	1 (2%)
30	PSU	a	2457	30	18,21,22	1.05	1 (5%)	22,30,33	0.63	0

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
30	PSU	a	746	56,30	-	1/7/25/26	0/2/2/2
53	2MG	A	1516	53	-	0/9/27/28	0/3/3/3
53	4OC	A	1402	53	-	0/9/29/30	0/2/2/2
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2
30	OMU	a	2552	30	-	0/9/27/28	0/2/2/2
53	2MG	A	1207	53	-	0/9/27/28	0/3/3/3
53	5MC	A	1407	53	-	0/7/25/26	0/2/2/2
30	3TD	a	1915	30	-	2/7/25/26	0/2/2/2
30	PSU	a	2504	57,30	-	0/7/25/26	0/2/2/2
53	PSU	A	516	53,56	-	0/7/25/26	0/2/2/2
14	MS6	l	82	14	-	1/4/6/8	-
7	MEQ	d	150	7	-	2/8/9/11	-
30	PSU	a	1911	30	-	0/7/25/26	0/2/2/2
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
30	6MZ	a	2030	30	-	2/9/27/28	0/3/3/3
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
30	6MZ	a	1618	30	-	0/9/27/28	0/3/3/3
30	2MG	a	1835	30	-	0/9/27/28	0/3/3/3
53	2MG	A	966	53	-	0/9/27/28	0/3/3/3
30	5MC	a	1962	30	-	2/7/25/26	0/2/2/2
30	2MG	a	2445	30	-	1/9/27/28	0/3/3/3
30	2MA	a	2503	56,30	-	2/7/25/26	0/3/3/3
37	IAS	K	119	37	-	0/7/7/8	-
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2251	54,30	-	1/9/27/28	0/3/3/3
53	UR3	A	1498	53,57	-	0/7/25/26	0/2/2/2
38	D2T	L	89	38	-	2/7/12/14	-
30	PSU	a	2580	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	56,30	-	0/9/27/28	0/2/2/2
30	1MG	a	745	30	-	0/7/25/26	0/3/3/3
14	4D4	l	81	14	-	1/11/12/14	-
53	5MC	A	967	53	-	0/7/25/26	0/2/2/2
53	G7M	A	527	53	-	1/7/25/26	0/3/3/3
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	G7M	a	2069	30	-	2/7/25/26	0/3/3/3
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2457	PSU	C6-C5	4.05	1.40	1.35
30	a	1915	3TD	C6-C5	4.01	1.40	1.35
30	a	1911	PSU	C6-C5	3.58	1.39	1.35
30	a	1917	PSU	C6-C5	3.57	1.39	1.35
30	a	2605	PSU	C6-C5	3.43	1.39	1.35
53	A	516	PSU	C6-C5	3.39	1.39	1.35
30	a	746	PSU	C6-C5	3.36	1.39	1.35
30	a	2069	G7M	C8-N7	3.33	1.39	1.33
30	a	2580	PSU	C6-C5	3.32	1.39	1.35
30	a	2503	2MA	C2-N1	3.24	1.39	1.34
30	a	2604	PSU	C6-C5	3.03	1.38	1.35
30	a	2504	PSU	C6-C5	2.96	1.38	1.35
30	a	745	1MG	C1'-N9	-2.85	1.39	1.47
30	a	955	PSU	C6-C5	2.55	1.38	1.35
53	A	527	G7M	C8-N7	2.37	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2503	2MA	C6-N6	-2.26	1.28	1.34
30	a	2503	2MA	C6-N1	2.12	1.38	1.35
30	a	745	1MG	C5-C6	-2.06	1.40	1.45
30	a	2503	2MA	C2-N3	2.01	1.37	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2449	H2U	C4-N3-C2	-2.99	123.31	125.79
30	a	2503	2MA	C5-C4-N3	-2.59	124.28	127.19
30	a	2449	H2U	O2-C2-N1	-2.49	119.98	123.11
30	a	2449	H2U	N3-C2-N1	2.45	119.24	116.65
30	a	2580	PSU	C3'-C2'-C1'	2.41	104.44	101.64
30	a	2604	PSU	C2'-C3'-C4'	-2.35	98.07	102.64
30	a	2503	2MA	N3-C2-N1	-2.30	121.49	125.72
53	A	1498	UR3	C6-N1-C2	-2.18	119.84	121.79
38	L	89	D2T	O-C-CA	-2.14	119.17	124.78
30	a	2503	2MA	CM2-C2-N1	2.13	120.47	117.15
30	a	2069	G7M	N9-C8-N7	-2.12	106.97	112.21
30	a	2605	PSU	C2'-C3'-C4'	-2.11	98.54	102.64
38	L	89	D2T	OD1-CG-CB	-2.08	118.08	122.44

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	L	89	D2T	SB-CB-CG-OD2
30	a	746	PSU	O4'-C1'-C5-C6
30	a	1915	3TD	C3'-C4'-C5'-O5'
30	a	1915	3TD	O4'-C4'-C5'-O5'
30	a	2251	OMG	C1'-C2'-O2'-CM2
30	a	2445	2MG	N3-C2-N2-CM2
7	d	150	MEQ	NE2-CD-CG-CB
7	d	150	MEQ	OE1-CD-CG-CB
30	a	2030	6MZ	O4'-C4'-C5'-O5'
38	L	89	D2T	CG-CB-SB-CB1
30	a	2069	G7M	C4'-C5'-O5'-P
53	A	527	G7M	C3'-C4'-C5'-O5'
30	a	747	5MU	C3'-C4'-C5'-O5'
14	l	82	MS6	CB-CG-SD-CE
30	a	2030	6MZ	C3'-C4'-C5'-O5'
30	a	1962	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
30	a	1962	5MC	O4'-C1'-N1-C6
30	a	2503	2MA	O4'-C1'-N9-C8
30	a	2069	G7M	O4'-C4'-C5'-O5'
30	a	2503	2MA	O4'-C4'-C5'-O5'
14	l	81	4D4	O-C-CA-CB

There are no ring outliers.

10 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	A	1516	2MG	1	0
53	A	1402	4OC	1	0
30	a	2552	OMU	1	0
53	A	1207	2MG	1	0
30	a	2030	6MZ	1	0
30	a	1939	5MU	1	0
30	a	2449	H2U	1	0
30	a	2445	2MG	1	0
30	a	2604	PSU	1	0
30	a	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 311 ligands modelled in this entry, 311 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

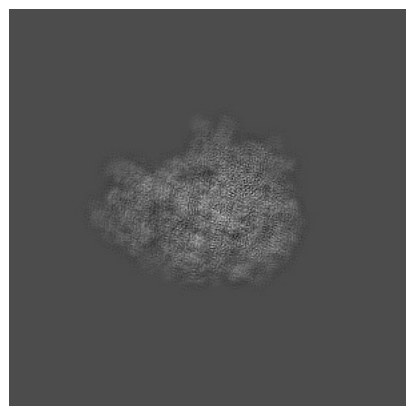
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50296. These allow visual inspection of the internal detail of the map and identification of artifacts.

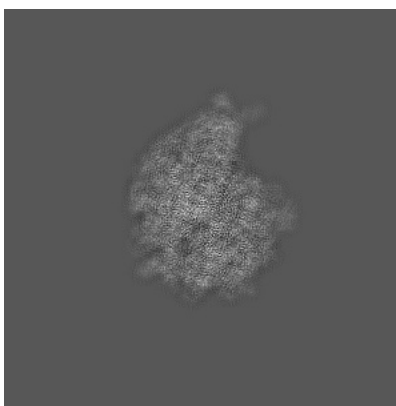
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

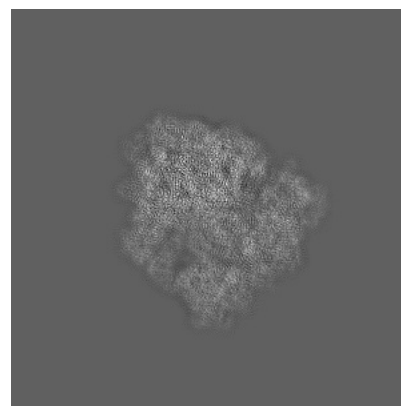
6.1.1 Primary map



X

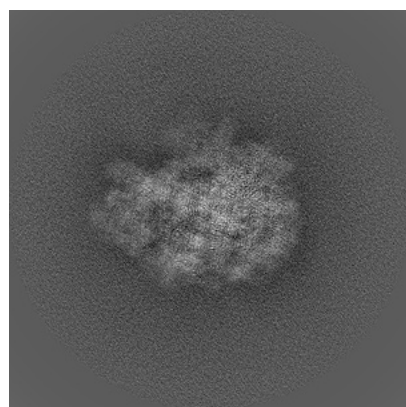


Y

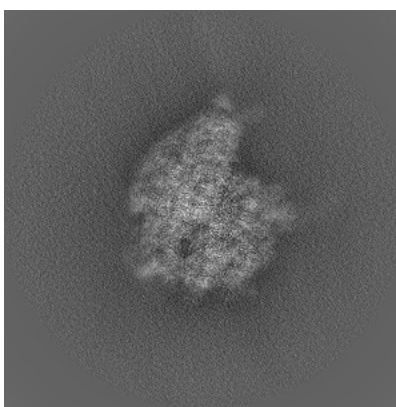


Z

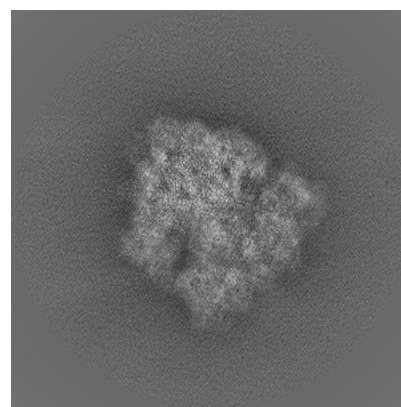
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

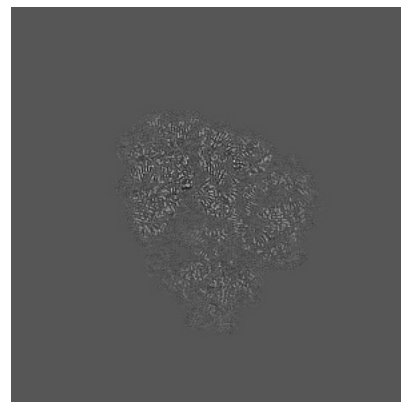
6.2.1 Primary map



X Index: 300

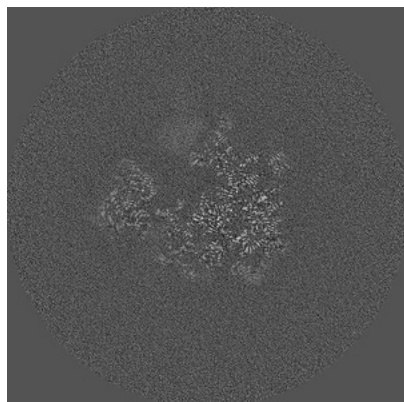


Y Index: 300

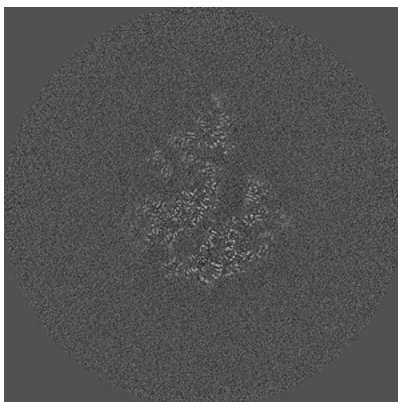


Z Index: 300

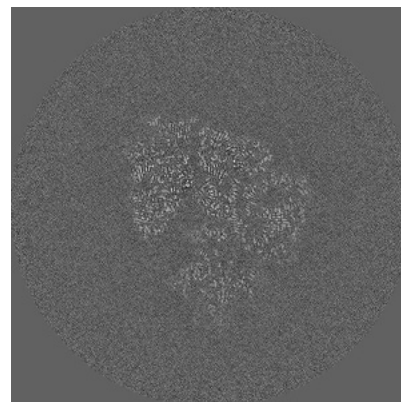
6.2.2 Raw map



X Index: 300



Y Index: 300

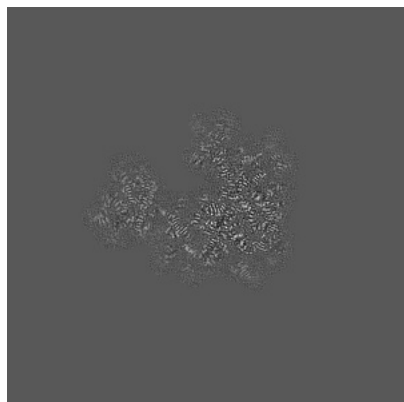


Z Index: 300

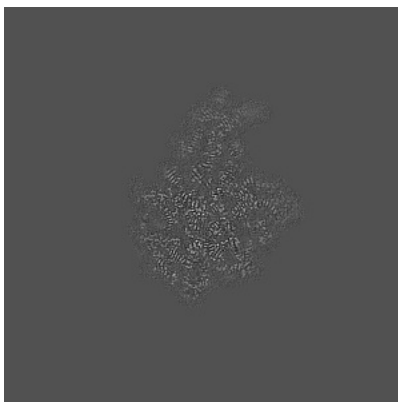
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

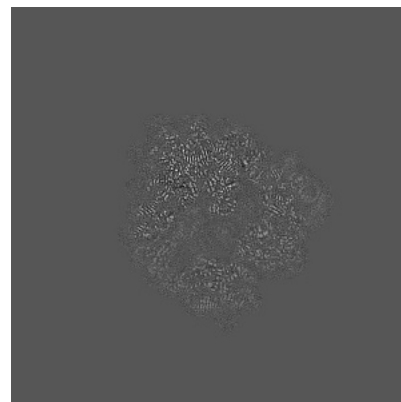
6.3.1 Primary map



X Index: 297

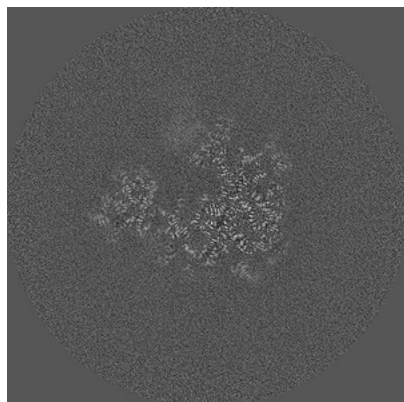


Y Index: 323

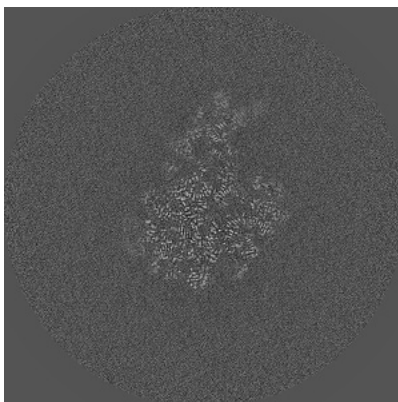


Z Index: 317

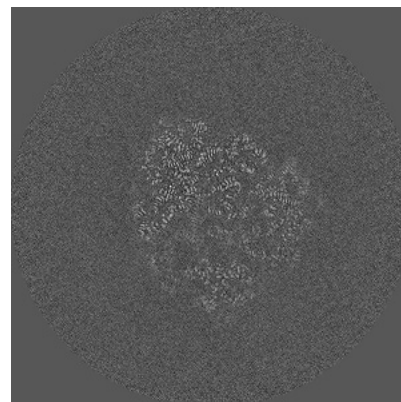
6.3.2 Raw map



X Index: 297



Y Index: 313

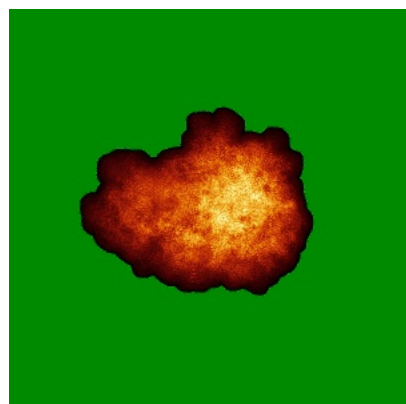


Z Index: 311

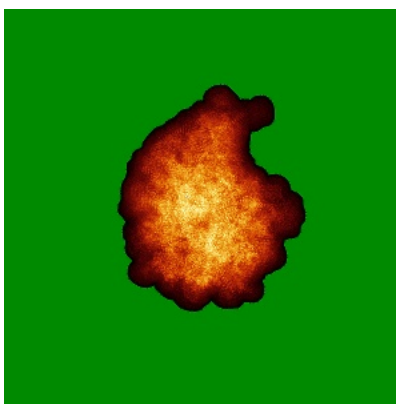
The images above show the largest variance slices of the map in three orthogonal directions.

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

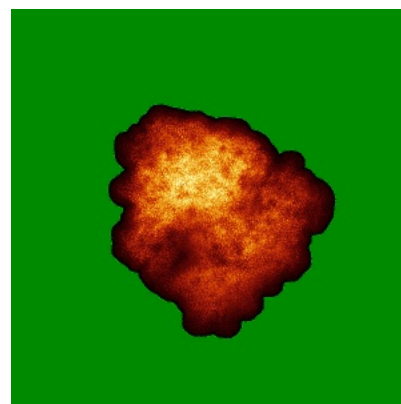
6.4.1 Primary map



X

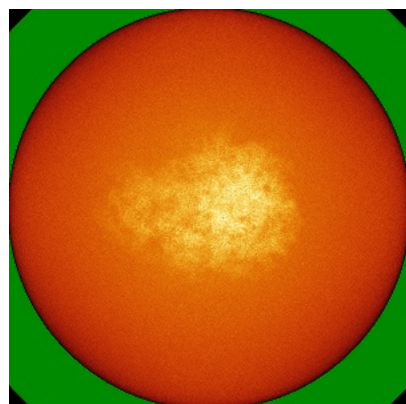


Y

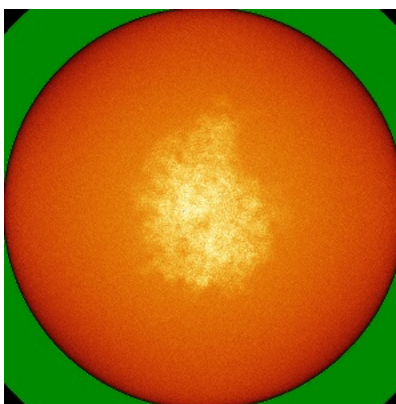


Z

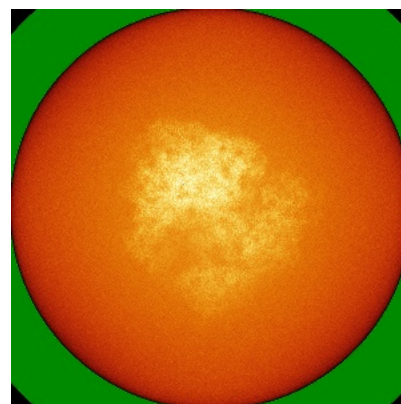
6.4.2 Raw map



X



Y

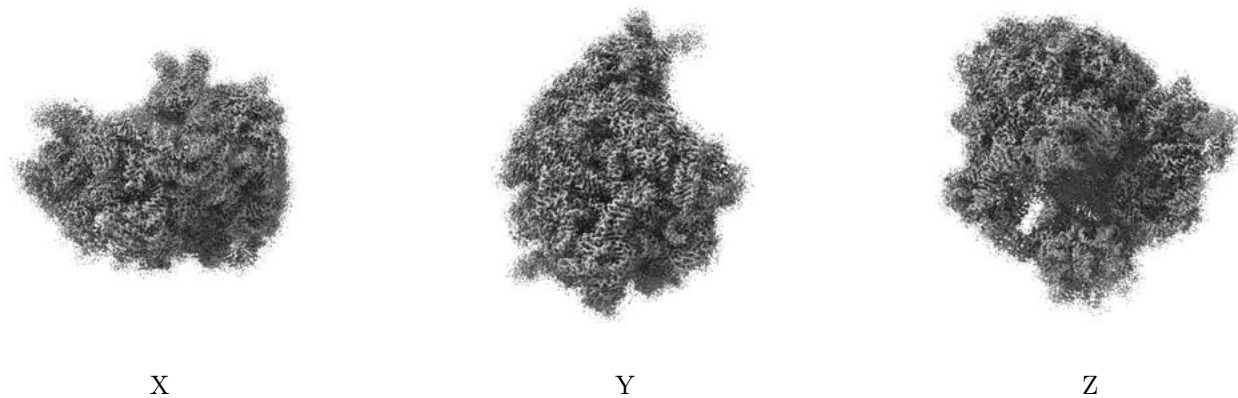


Z

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.

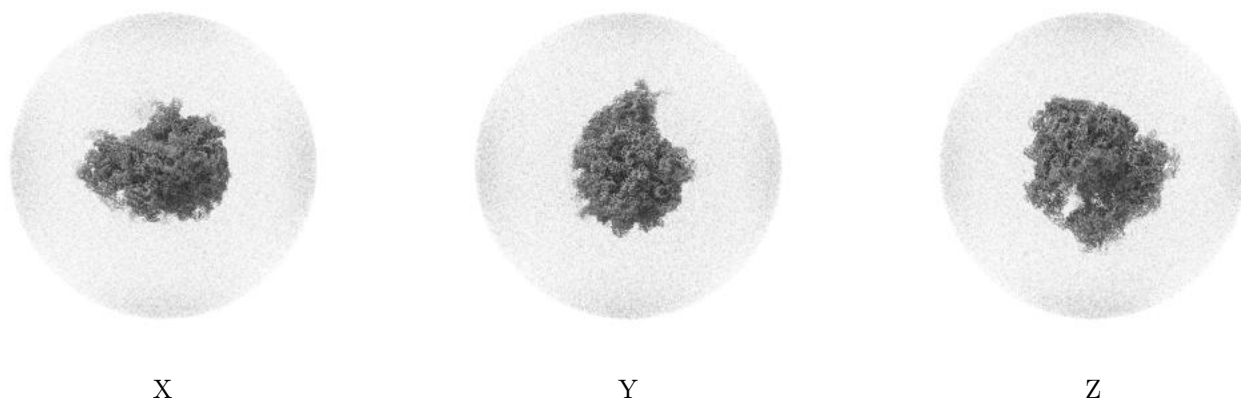
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

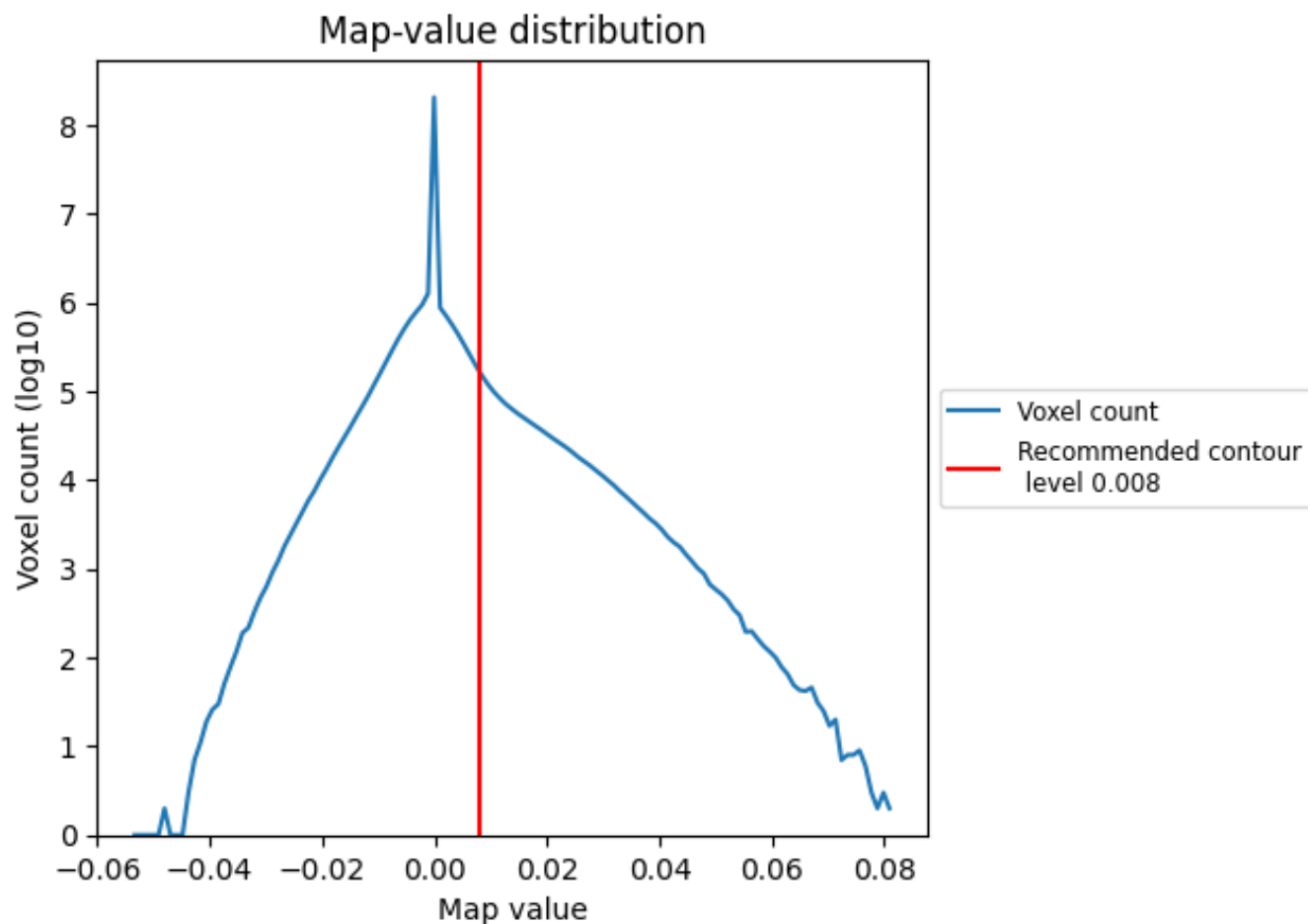
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

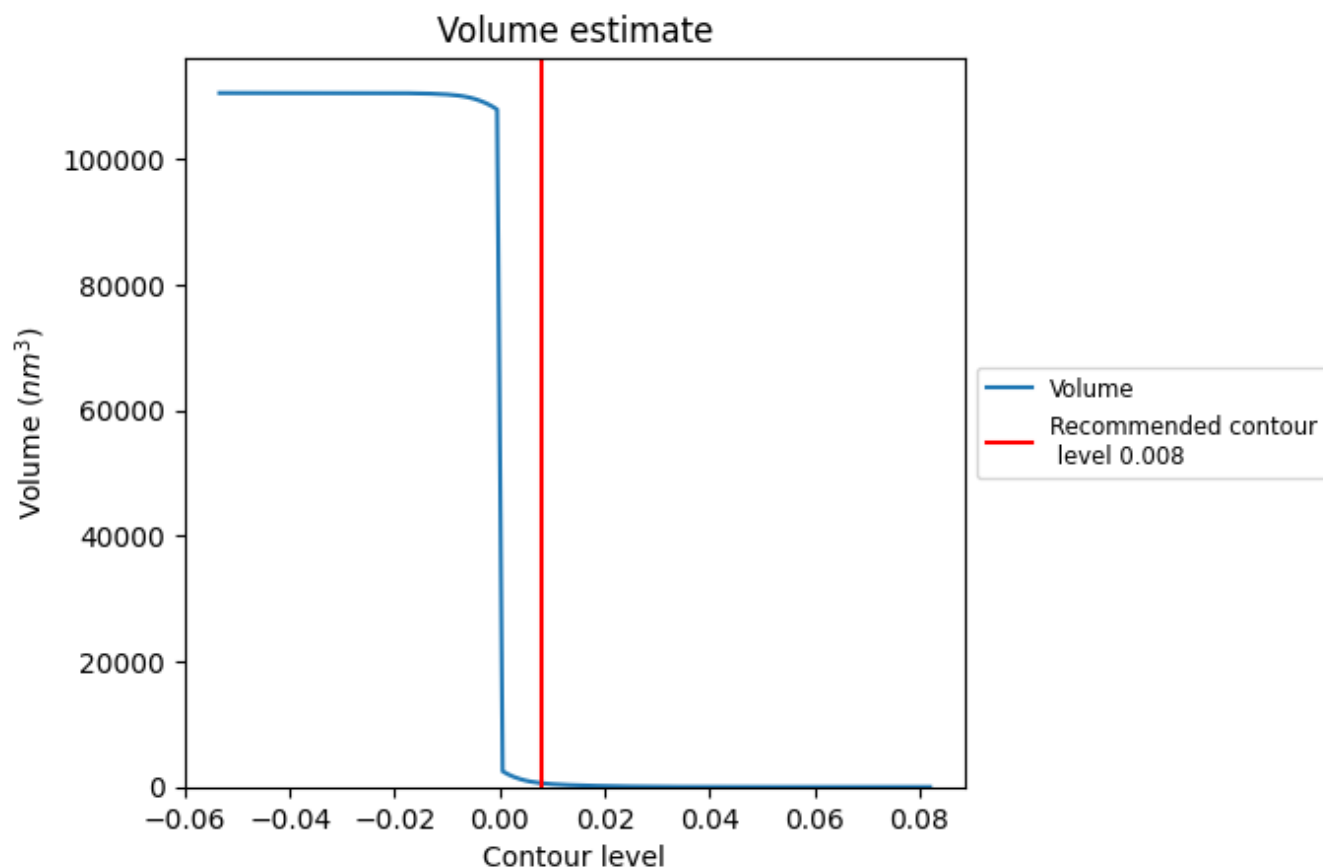
This section contains the results of statistical analysis of the map.

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.

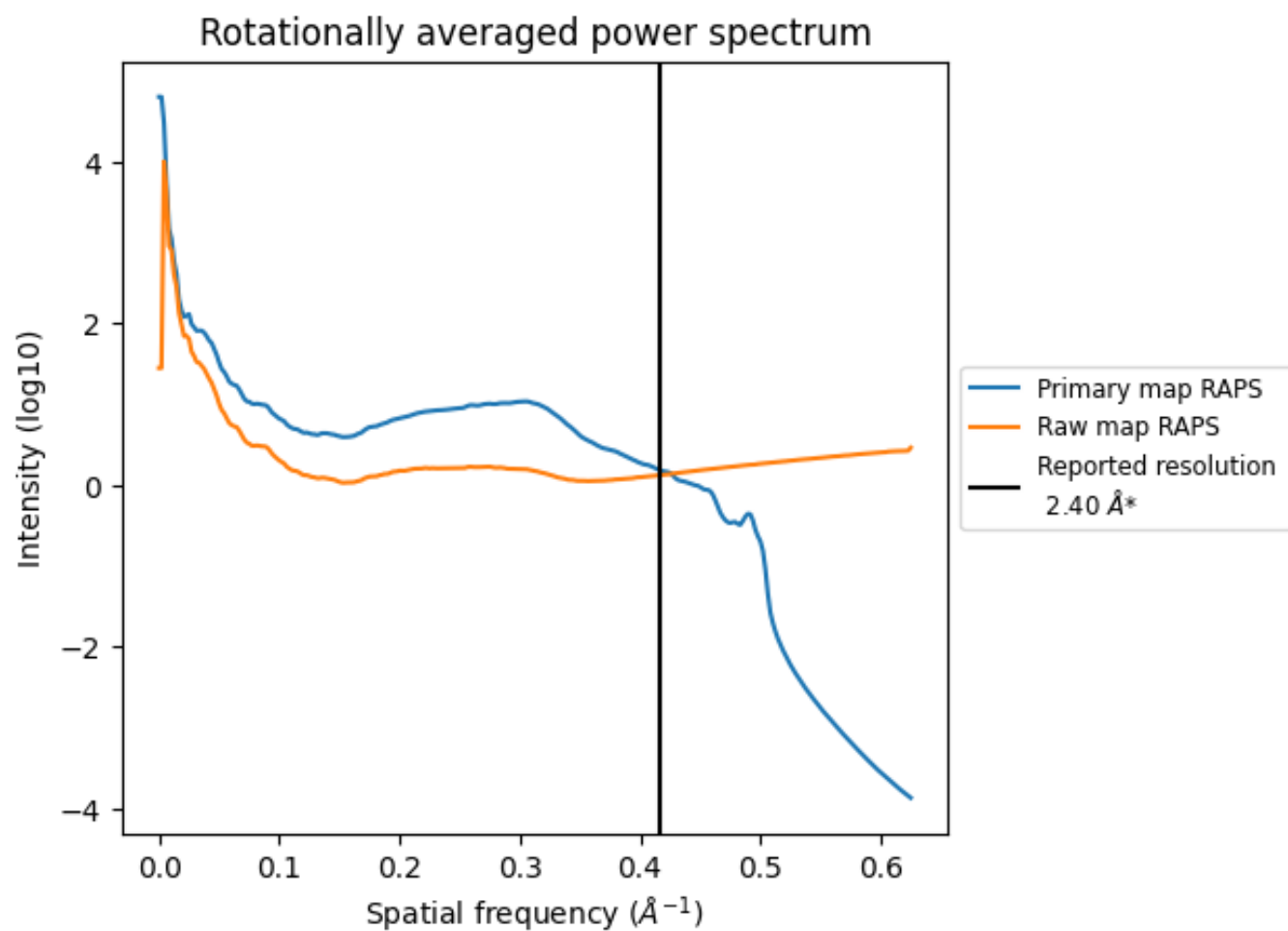
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 596 nm³; this corresponds to an approximate mass of 539 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 ⓘ

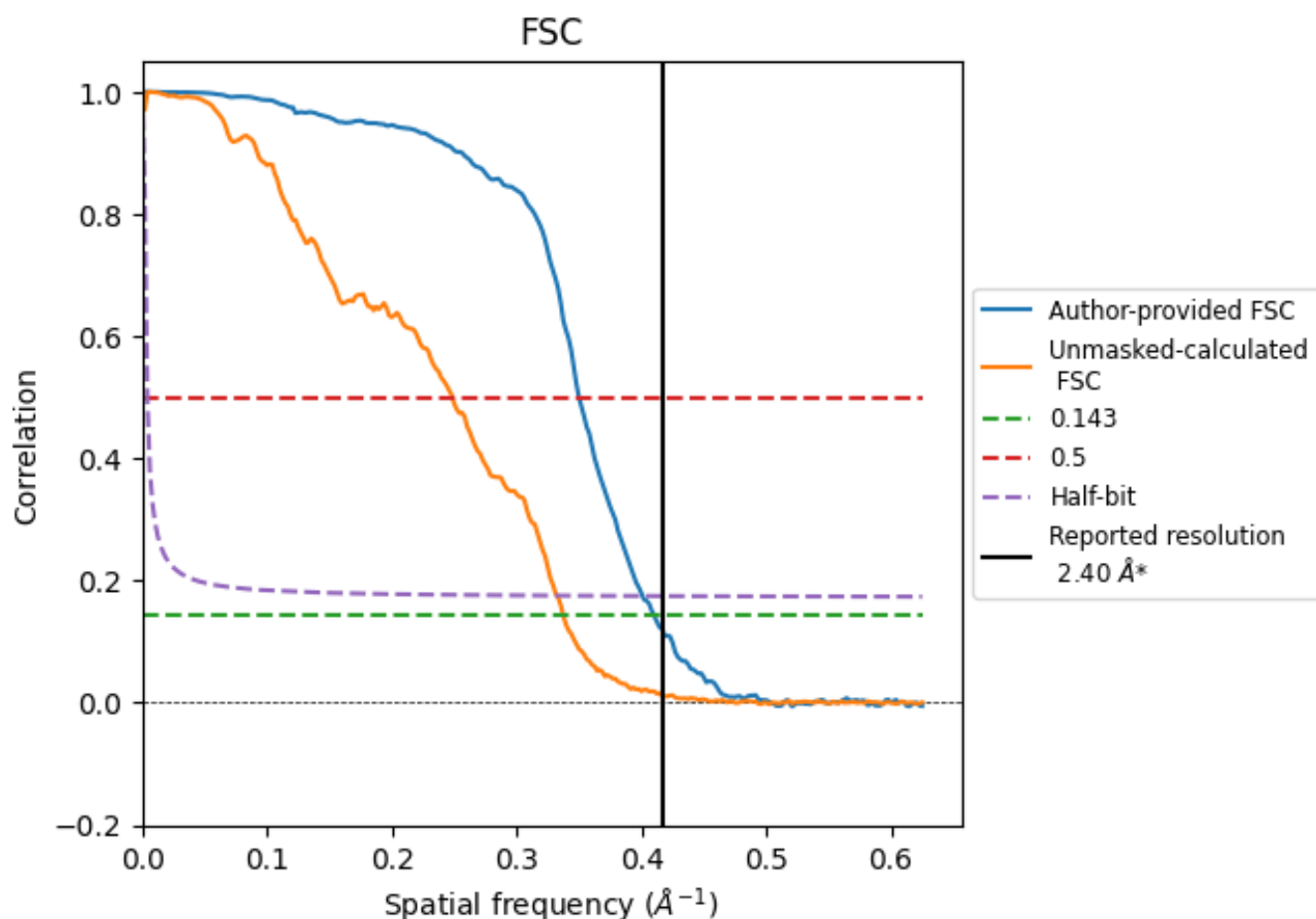


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

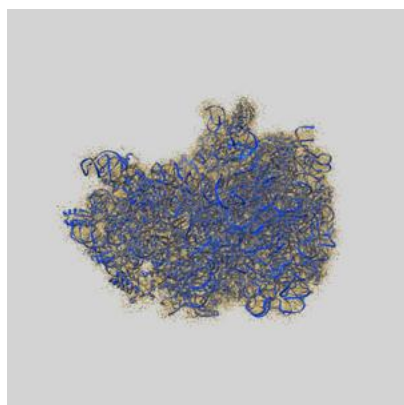
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.86	2.49
Unmasked-calculated*	2.96	4.02	3.01

*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 2.96 differs from the reported value 2.4 by more than 10 %

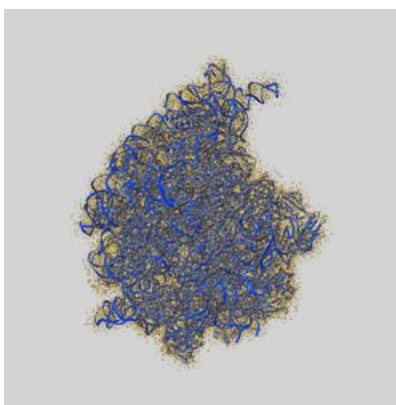
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50296 and PDB model 9FBV. Per-residue inclusion information can be found in section 3 on page 16.

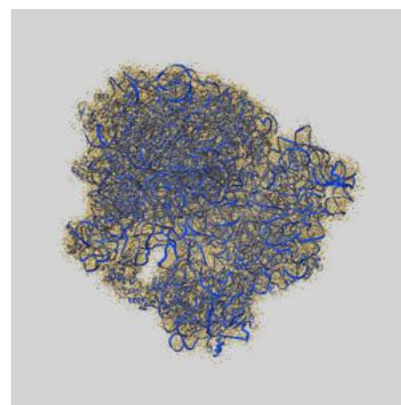
9.1 Map-model overlay [i](#)



X



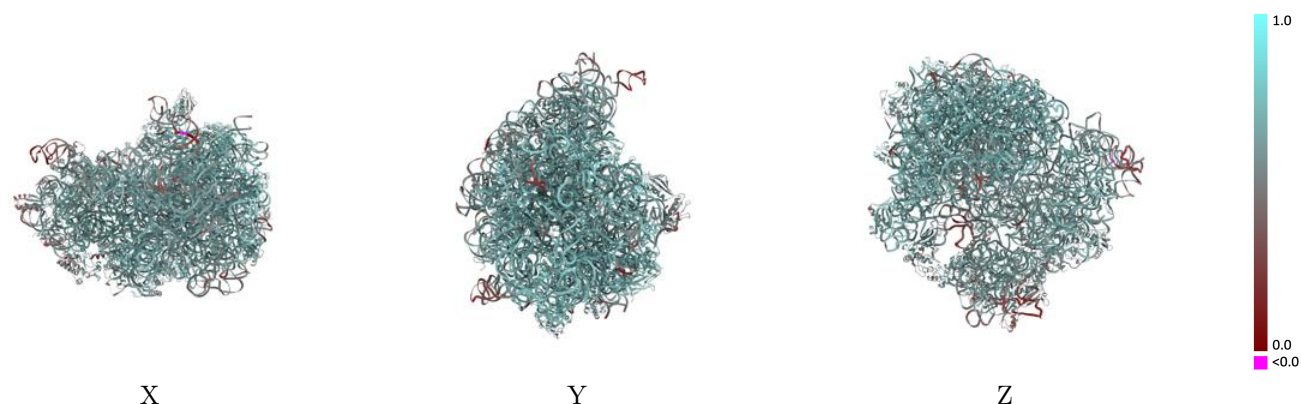
Y



Z

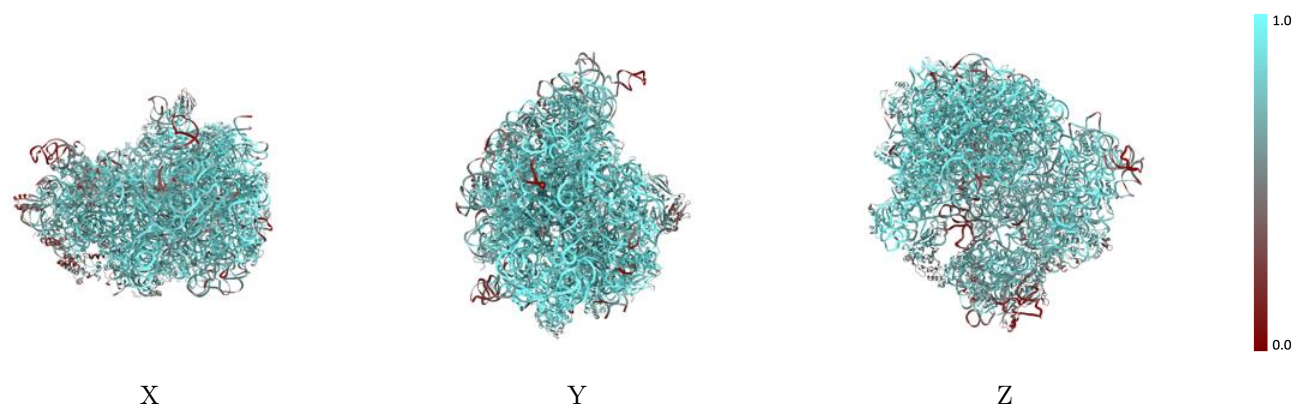
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



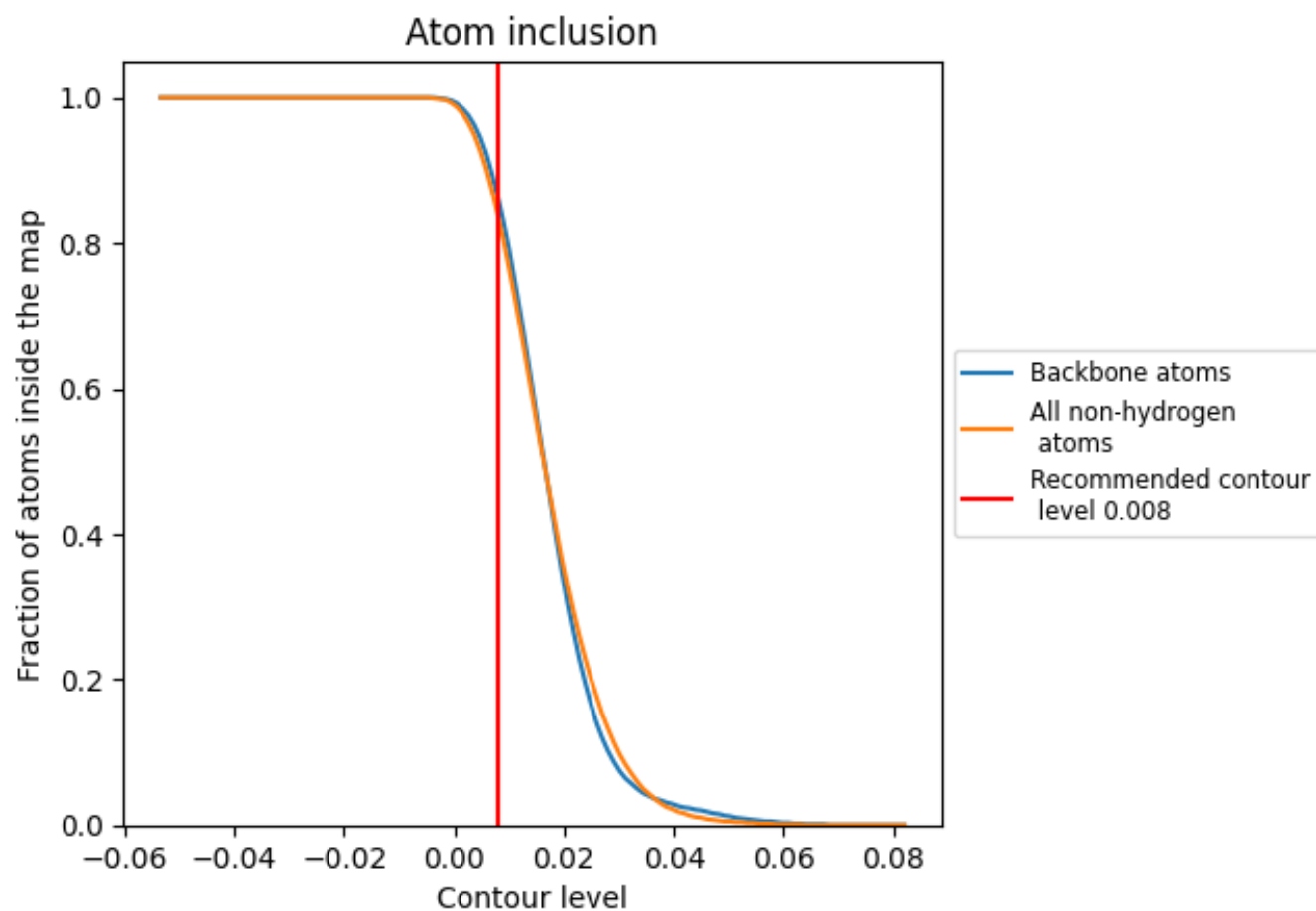
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.6430
0	 0.8190	 0.6550
1	 0.9490	 0.7240
2	 0.9610	 0.7230
3	 0.8870	 0.6680
4	 0.4450	 0.4930
A	 0.8360	 0.6230
B	 0.4850	 0.5140
C	 0.7040	 0.5980
D	 0.6400	 0.5870
E	 0.8270	 0.6530
F	 0.6170	 0.5710
G	 0.5470	 0.5390
H	 0.8250	 0.6450
I	 0.6580	 0.5760
J	 0.5390	 0.5270
K	 0.7470	 0.6190
L	 0.7710	 0.6310
M	 0.6720	 0.5830
N	 0.7380	 0.6020
O	 0.7700	 0.6400
P	 0.7750	 0.6300
Q	 0.6700	 0.5910
R	 0.7190	 0.6030
S	 0.5910	 0.5510
T	 0.7560	 0.6100
U	 0.4940	 0.5050
X	 0.9230	 0.6770
Z	 0.5250	 0.5160
a	 0.9060	 0.6680
b	 0.8640	 0.6340
c	 0.9200	 0.7040
d	 0.9010	 0.6980
e	 0.8240	 0.6620
f	 0.6210	 0.5650



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Chain	Atom inclusion	Q-score
g	 0.5730	 0.5450
h	 0.6470	 0.5760
i	 0.9110	 0.6970
j	 0.8740	 0.6870
k	 0.8980	 0.6860
l	 0.8790	 0.6810
m	 0.9500	 0.7170
n	 0.8240	 0.6400
o	 0.8720	 0.6850
p	 0.9570	 0.7230
q	 0.8410	 0.6710
r	 0.8910	 0.6920
s	 0.8140	 0.6520
t	 0.7600	 0.6200
u	 0.7600	 0.6320
v	 0.8400	 0.6800
w	 0.8520	 0.6740
x	 0.7180	 0.6130
y	 0.8670	 0.6800
z	 0.8650	 0.6770