



Full wwPDB EM Validation Report ⓘ

Jun 9, 2026 – 03:07 pm BST

PDB ID : 9SS6 / pdb_00009ss6
EMDB ID : EMD-55178
Title : 70S ribosome from RimM-KO
Authors : Hassan, A.H.; Demo, G.
Deposited on : 2025-09-25
Resolution : 2.60 Å (reported)
Based on initial model : 6WDE

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:

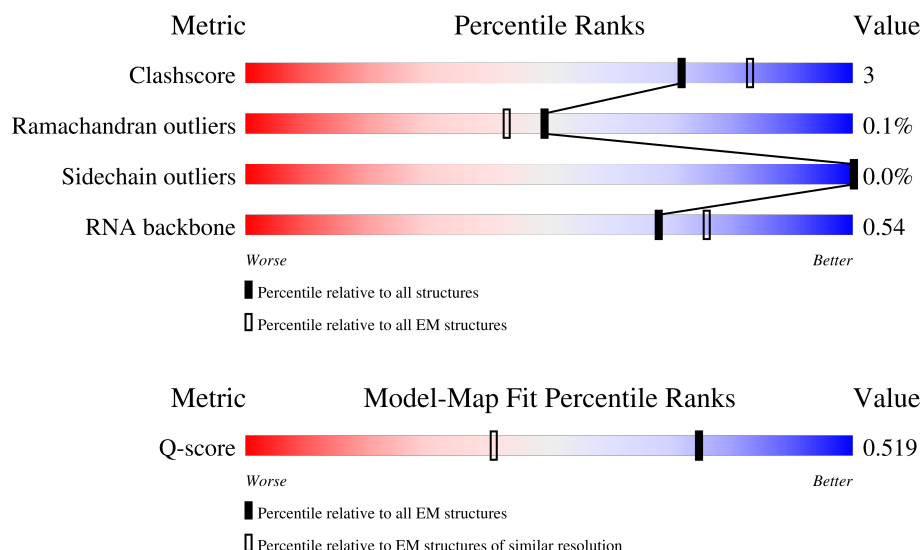
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.60 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.



























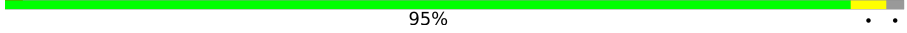
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	AA	241	
2	AB	233	
3	AC	206	



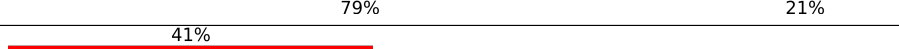
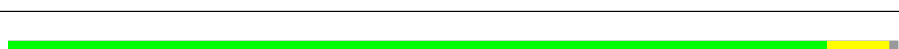
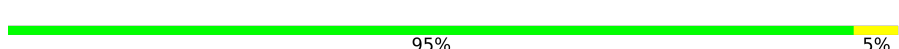


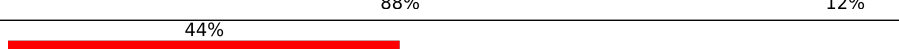



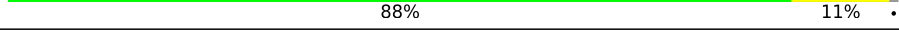



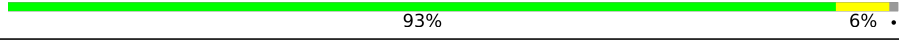
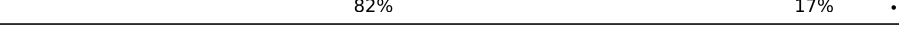







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Mol	Chain	Length	Quality of chain
4	AD	167	
5	AE	135	
6	AF	179	
7	AG	130	
8	AH	130	
9	AI	103	
10	AJ	129	
11	AK	124	
12	AL	118	
13	AM	101	
14	AN	89	
15	AO	82	
16	AP	84	
17	AQ	75	
18	AR	92	
19	AS	87	
19	BG	87	
20	AT	71	
21	B0	85	
22	B1	78	
23	B2	63	
24	B3	59	
25	B4	70	
26	B5	57	
27	B6	55	

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Mol	Chain	Length	Quality of chain
28	B7	46	
29	B8	65	
30	B9	38	
31	BA	234	
32	BB	273	
33	BC	209	
34	BD	201	
35	BE	179	
36	BF	177	
37	BI	149	
38	BK	142	
39	BM	142	
40	BN	123	
41	BO	144	
42	BP	136	
43	BQ	127	
44	BR	117	
45	BS	115	
46	BT	118	
47	BU	103	
48	BV	110	
49	BW	100	
50	BX	104	
51	BY	94	
52	D1	1540	

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Mol	Chain	Length	Quality of chain
53	D2	2903	<div><div></div><div>77%</div><div>20%</div><div></div></div>
54	D3	120	<div><div></div><div>78%</div><div>17%</div><div>6%</div></div>

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 144877 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 Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	225	Total	C	N	O	S	0	0
			1756	1111	315	322	8		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	210	Total	C	N	O	S	0	0
			1648	1043	309	292	4		

- Molecule 3 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 5 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 7 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 15 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 19 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	85	Total	C	N	O	S	0	0
			665	411	137	114	3		
19	BG	69	Total	C	N	O	S	0	0
			543	337	112	91	3		

- Molecule 20 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B0	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 25 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 27 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	B6	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BA	117	Total	C	N	O	S	0	0
			902	570	162	168	2		

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BC	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 34 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 38 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BK	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 39 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BN	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 41 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BO	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BP	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 43 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BQ	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 44 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BX	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 51 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 52 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	D1	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 53 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	D2	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D2	747	C	U	conflict	GB CP194060.1

- Molecule 54 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	D3	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

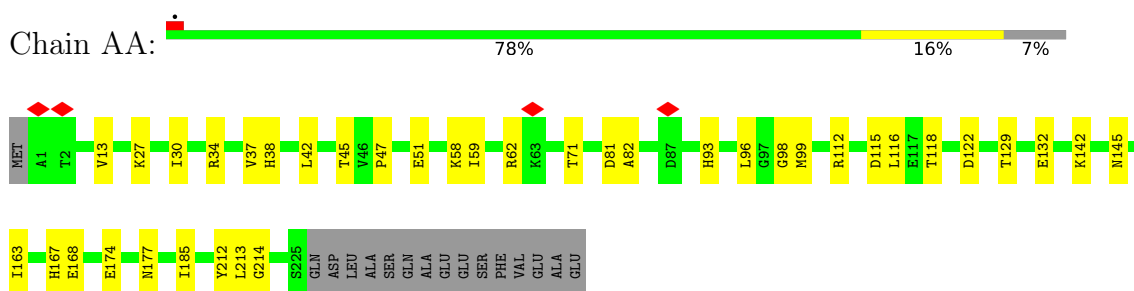
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	120	A	U	conflict	GB CP076697.1

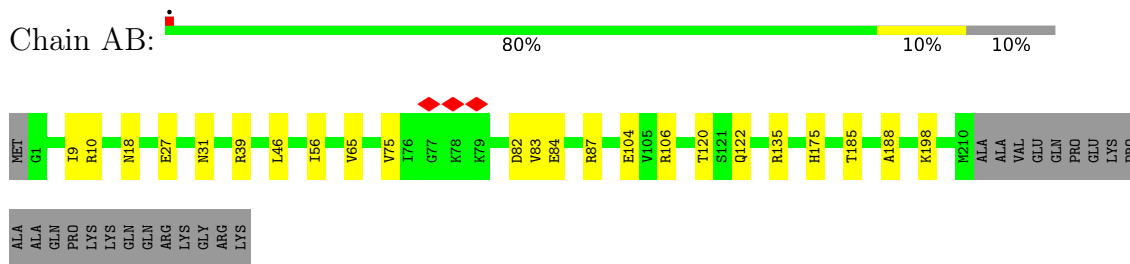
3 Residue-property plots [i](#)

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.

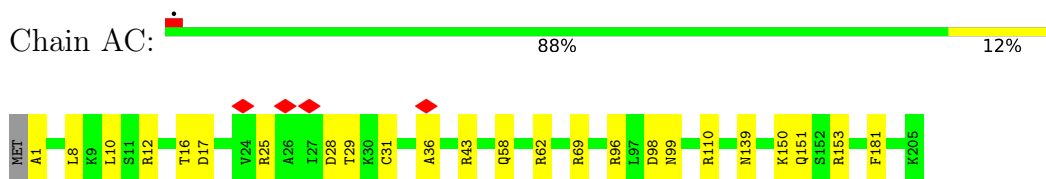
- Molecule 1: Small ribosomal subunit protein uS2



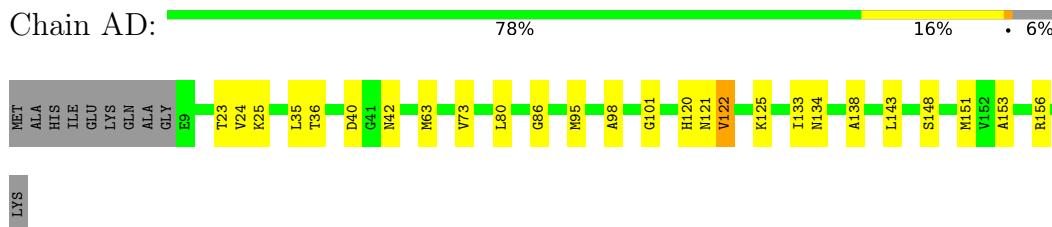
- Molecule 2: Small ribosomal subunit protein uS3



- Molecule 3: Small ribosomal subunit protein uS4

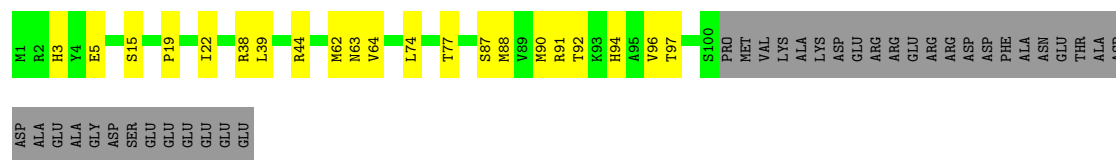


- Molecule 4: Small ribosomal subunit protein uS5



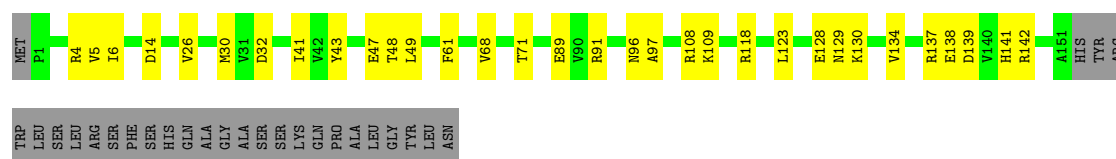
- Molecule 5: Small ribosomal subunit protein bS6, fully modified isoform

Chain AE: 




- Molecule 6: Small ribosomal subunit protein uS7

Chain AF: 




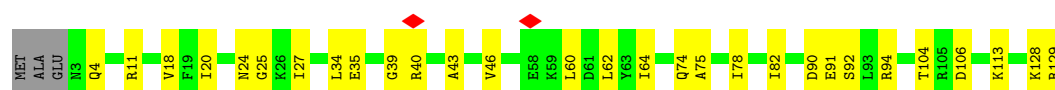
- Molecule 7: Small ribosomal subunit protein uS8

Chain AG: 




- Molecule 8: Small ribosomal subunit protein uS9

Chain AH: 




- Molecule 9: Small ribosomal subunit protein uS10

Chain AI: 

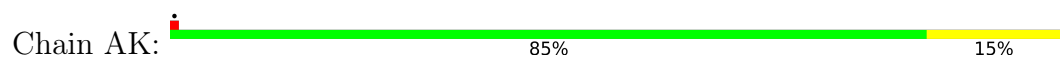


- Molecule 10: Small ribosomal subunit protein uS11

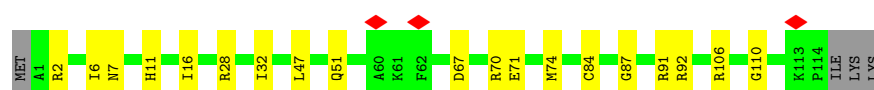
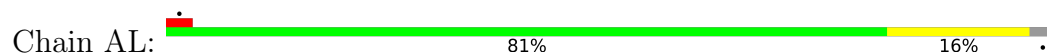
Chain AJ: 



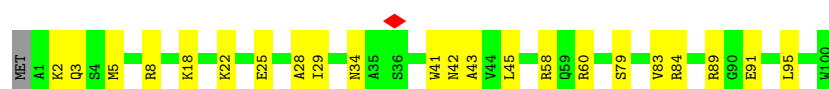
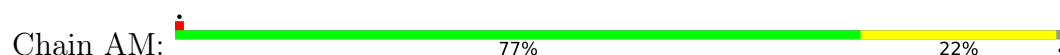
- Molecule 11: Small ribosomal subunit protein uS12



- Molecule 12: Small ribosomal subunit protein uS13



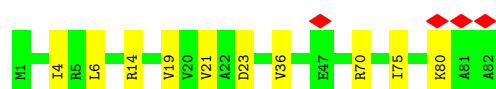
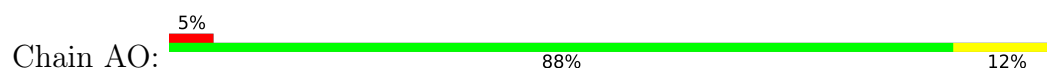
- Molecule 13: Small ribosomal subunit protein uS14



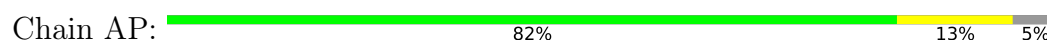
- Molecule 14: Small ribosomal subunit protein uS15



- Molecule 15: Small ribosomal subunit protein bS16



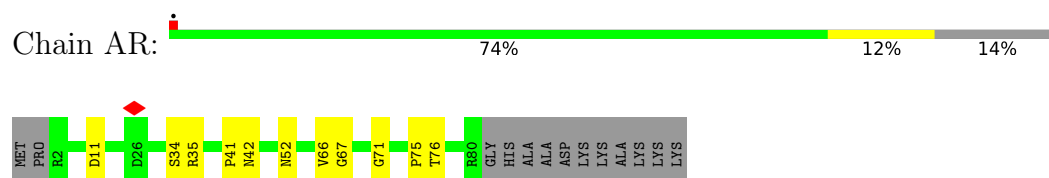
- Molecule 16: Small ribosomal subunit protein uS17



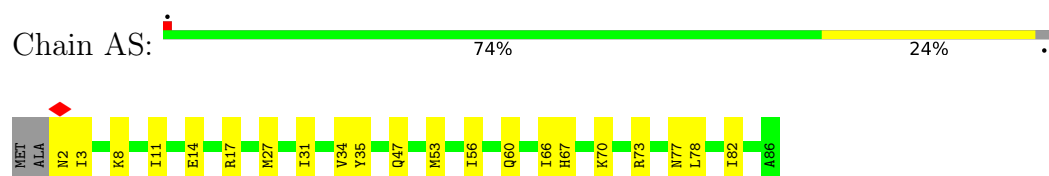
- Molecule 17: Small ribosomal subunit protein bS18



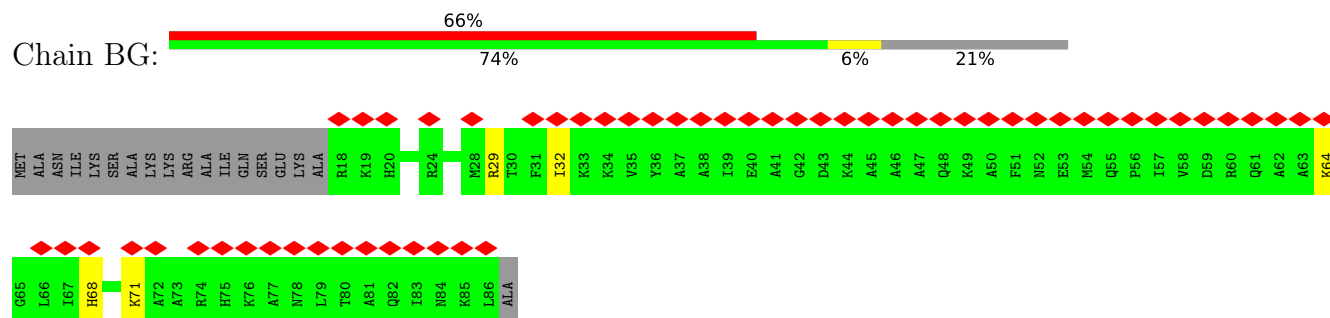
- Molecule 18: Small ribosomal subunit protein uS19



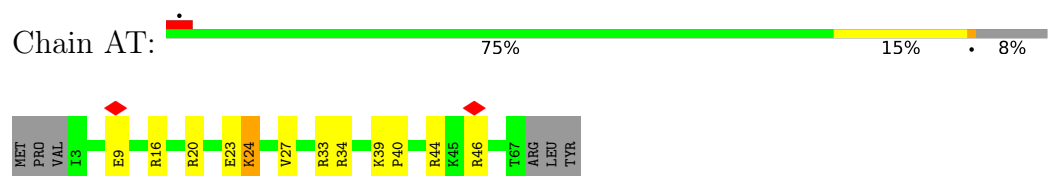
- Molecule 19: Small ribosomal subunit protein bS20



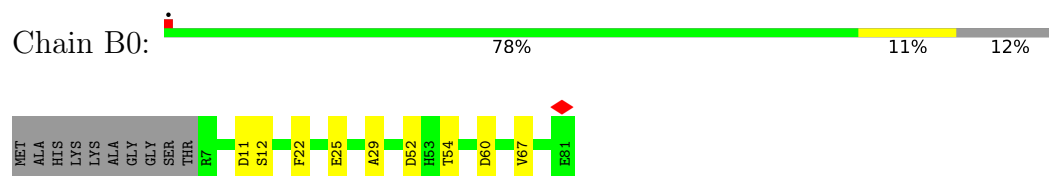
- Molecule 19: Small ribosomal subunit protein bS20



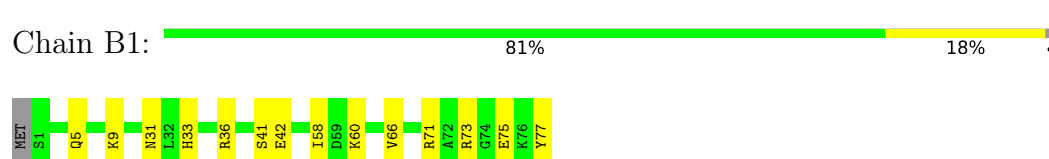
- Molecule 20: Small ribosomal subunit protein bS21



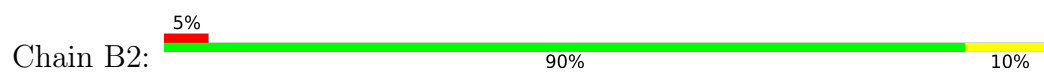
- Molecule 21: Large ribosomal subunit protein bL27



- Molecule 22: Large ribosomal subunit protein bL28



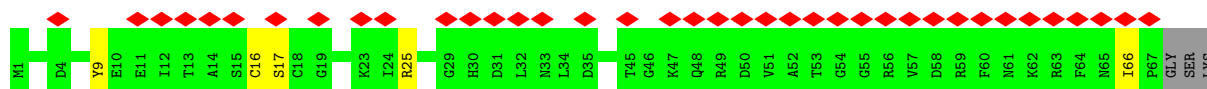
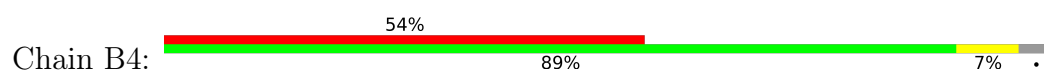
- Molecule 23: Large ribosomal subunit protein uL29



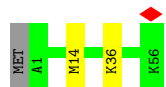
- Molecule 24: Large ribosomal subunit protein uL30



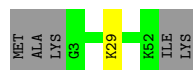
- Molecule 25: Large ribosomal subunit protein bL31A



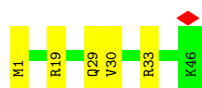
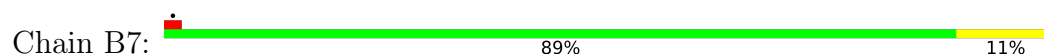
- Molecule 26: Large ribosomal subunit protein bL32



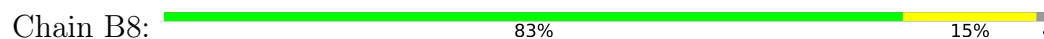
- Molecule 27: Large ribosomal subunit protein bL33




- Molecule 28: Large ribosomal subunit protein bL34



- Molecule 29: Large ribosomal subunit protein bL35

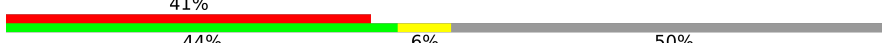


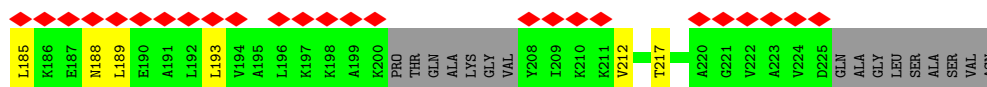
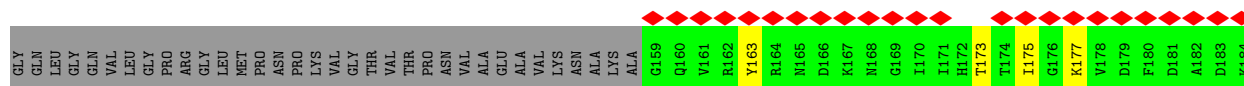
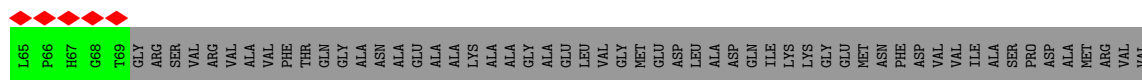
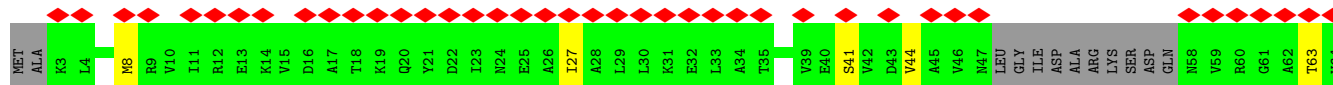
- Molecule 30: Large ribosomal subunit protein bL36A

Chain B9:  79% 21%



- Molecule 31: Large ribosomal subunit protein uL1

Chain BA:  41% 44% 6% 50%



- Molecule 32: Large ribosomal subunit protein uL2

Chain BB:  92% 7%



- Molecule 33: 50S ribosomal protein L3

Chain BC:  95% 5%



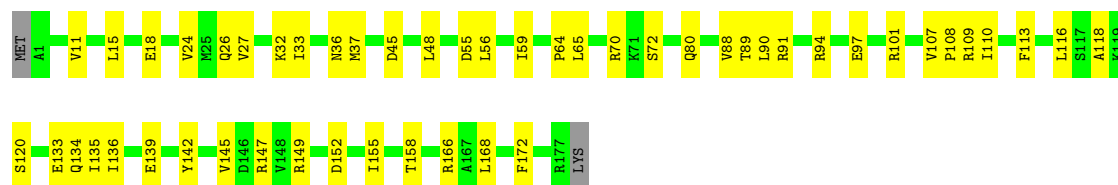
- Molecule 34: Large ribosomal subunit protein uL4

Chain BD:  88% 12%



- Molecule 35: Large ribosomal subunit protein uL5

Chain BE:  71% 28%



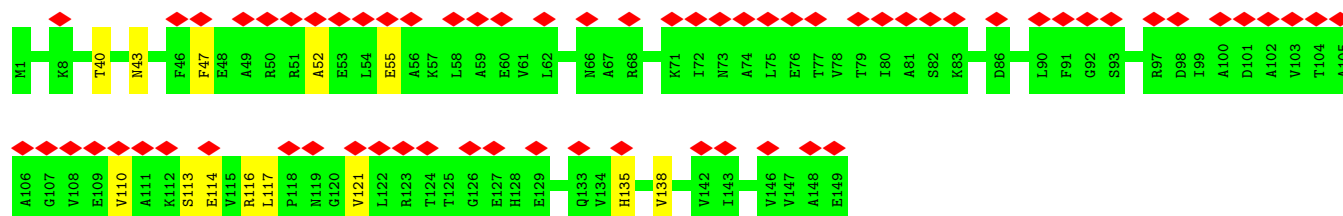
- Molecule 36: Large ribosomal subunit protein uL6

Chain BF: 88% 12%



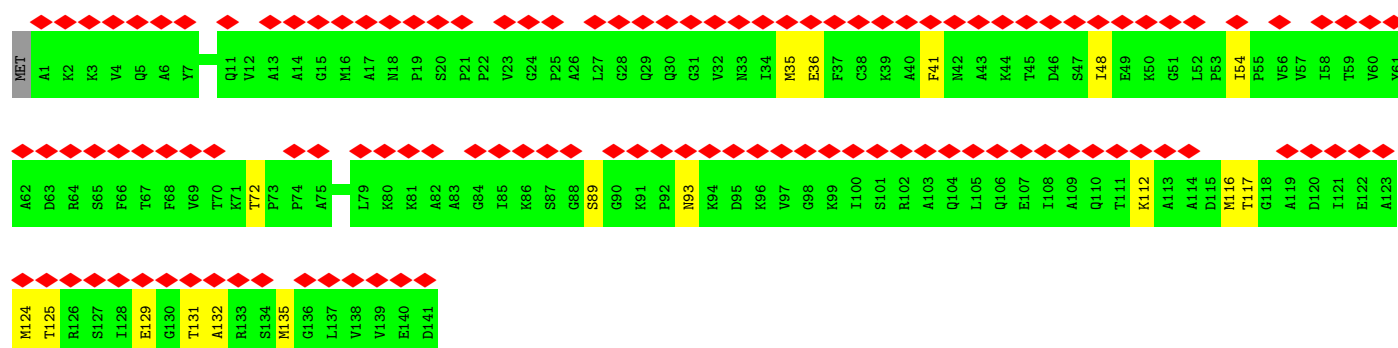
- Molecule 37: Large ribosomal subunit protein bL9

Chain BI: 44% 91% 9%



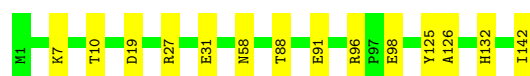
- Molecule 38: 50S ribosomal protein L11

Chain BK: 84% 87% 12%



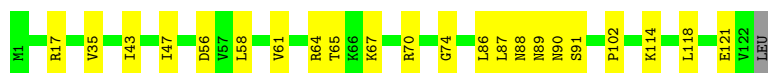
- Molecule 39: Large ribosomal subunit protein uL13

Chain BM: 90% 10%



- Molecule 40: Large ribosomal subunit protein uL14

Chain BN: 81% 18%



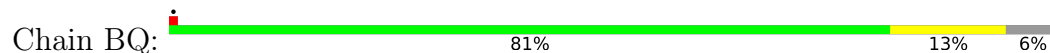
- Molecule 41: Large ribosomal subunit protein uL15



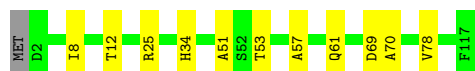
- Molecule 42: 50S ribosomal protein L16



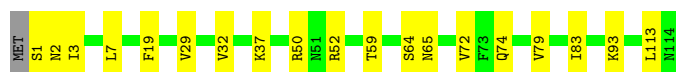
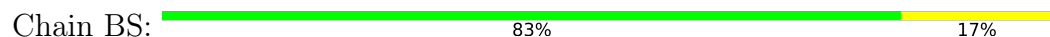
- Molecule 43: Large ribosomal subunit protein bL17



- Molecule 44: Large ribosomal subunit protein uL18



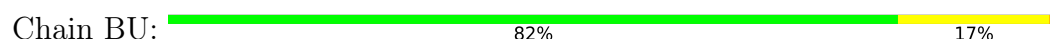
- Molecule 45: Large ribosomal subunit protein bL19

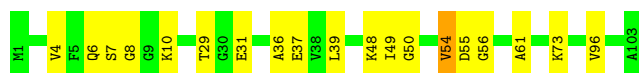


- Molecule 46: Large ribosomal subunit protein bL20



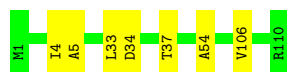
- Molecule 47: Large ribosomal subunit protein bL21





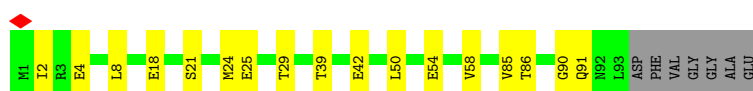
- Molecule 48: Large ribosomal subunit protein uL22

Chain BV: 94% 6%



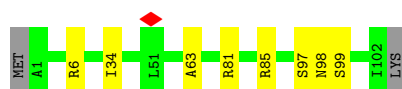
- Molecule 49: Large ribosomal subunit protein uL23

Chain BW: 76% 17% 7%



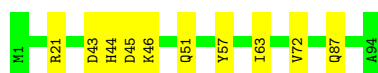
- Molecule 50: Large ribosomal subunit protein uL24

Chain BX: 90% 8% .



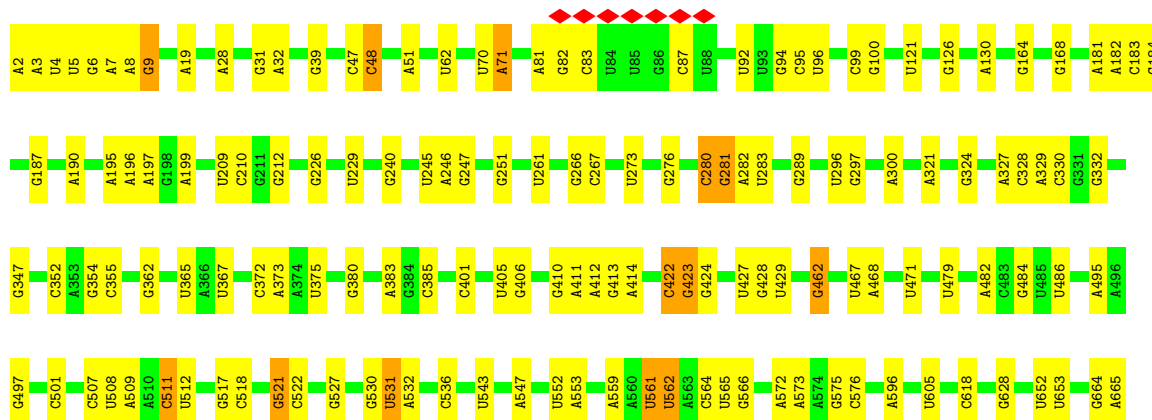
- Molecule 51: Large ribosomal subunit protein bL25

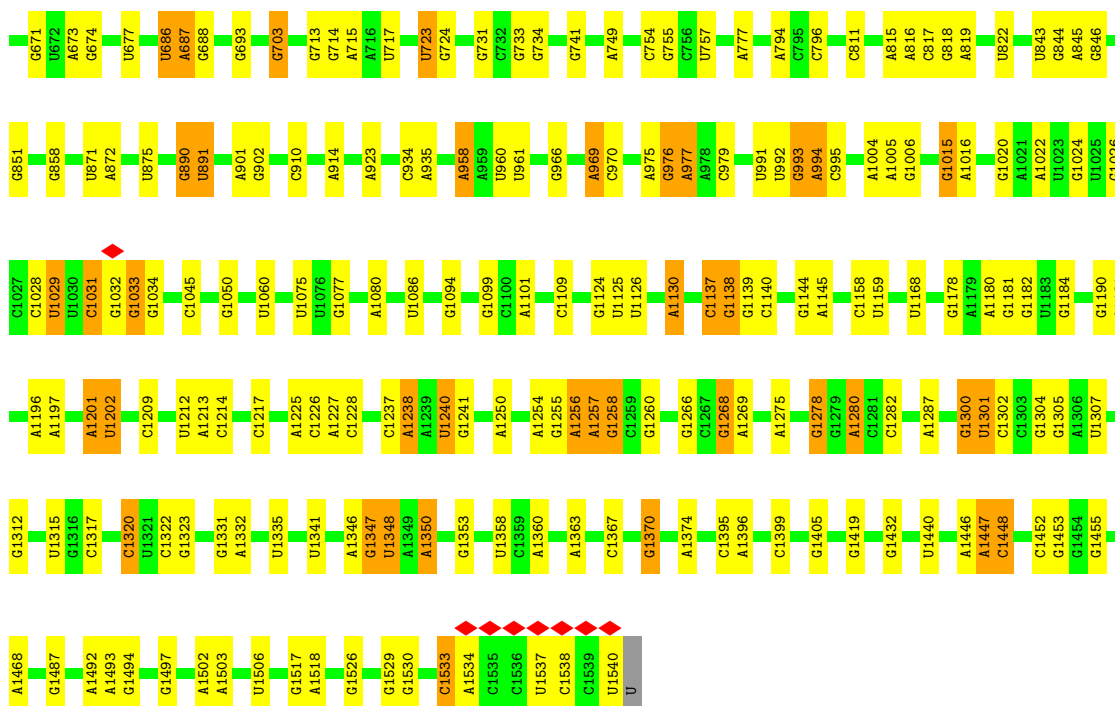
Chain BY: 89% 11%



- Molecule 52: 16S Ribosomal RNA

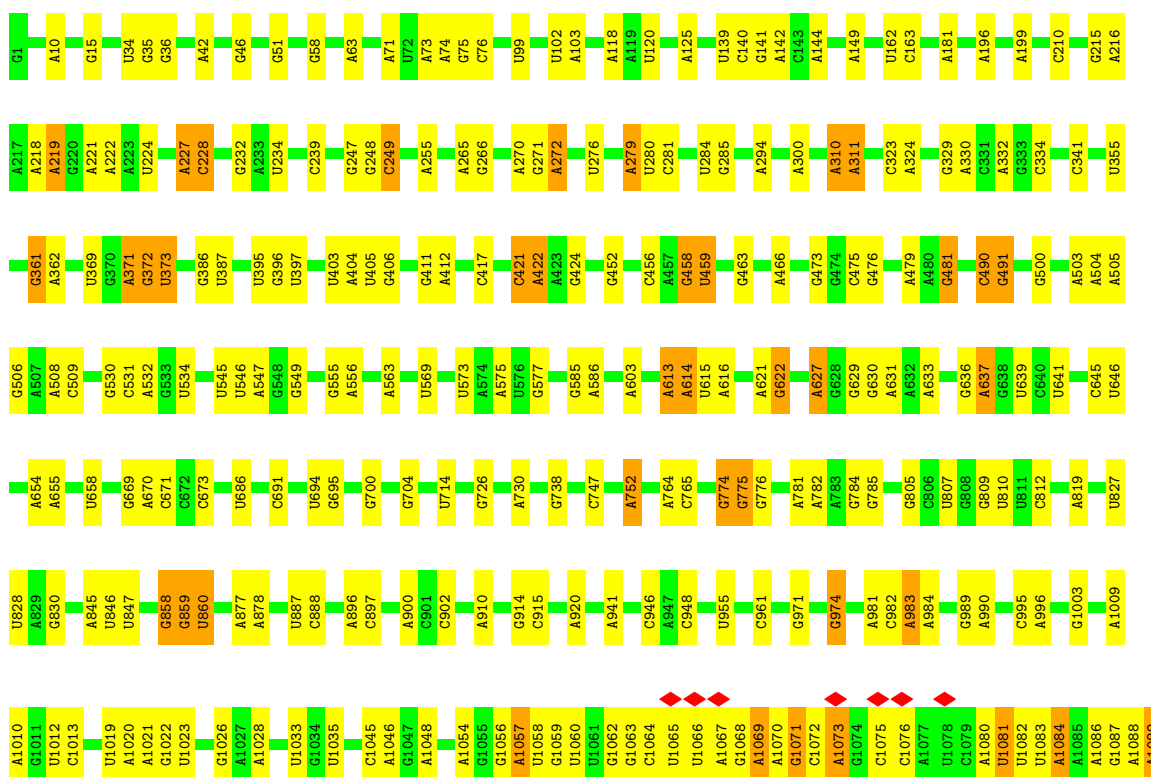
Chain D1: 77% 19% .

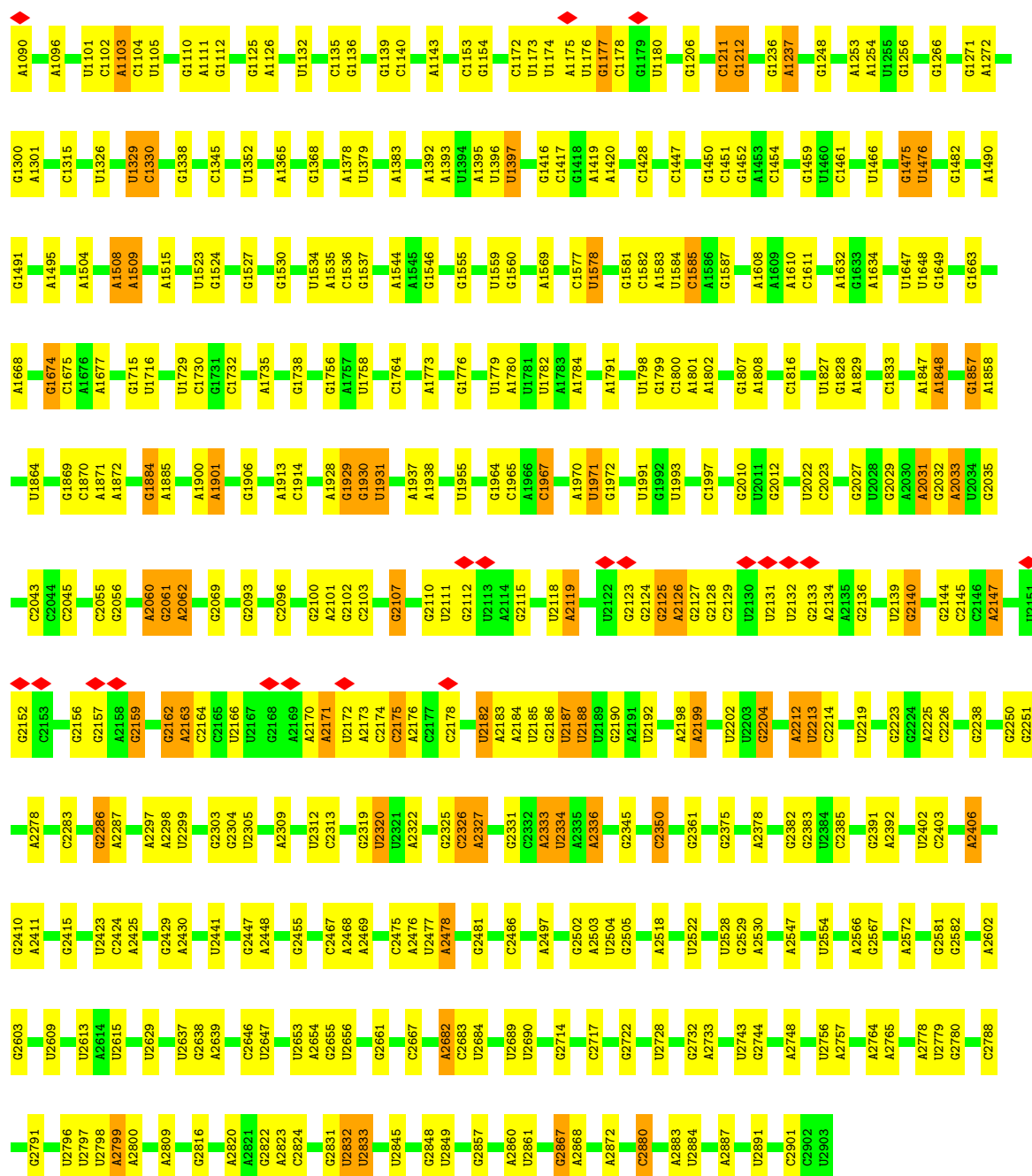




• Molecule 53: 23S Ribosomal RNA

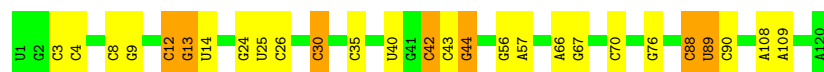
Chain D2: 77% 20%





● Molecule 54: 5S Ribosomal RNA

Chain D3: 78% 17% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	23.559	Depositor
Minimum map value	-6.999	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.068	Depositor
Recommended contour level	2.3	Depositor
Map size (\AA)	400.32, 400.32, 400.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.834, 0.834, 0.834	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	AA	0.16	0/1787	0.37	0/2408
2	AB	0.18	0/1675	0.38	0/2256
3	AC	0.17	0/1665	0.43	2/2227 (0.1%)
4	AD	0.20	0/1169	0.44	0/1573
5	AE	0.20	0/835	0.45	0/1128
6	AF	0.16	0/1195	0.37	0/1602
7	AG	0.18	0/989	0.36	0/1326
8	AH	0.17	0/1034	0.43	0/1375
9	AI	0.30	0/796	0.56	0/1077
10	AJ	0.17	0/885	0.40	0/1195
11	AK	0.20	0/969	0.40	0/1300
12	AL	0.19	0/892	0.46	0/1193
13	AM	0.17	0/817	0.37	0/1088
14	AN	0.17	0/722	0.37	0/964
15	AO	0.17	0/659	0.35	0/884
16	AP	0.19	0/657	0.42	0/881
17	AQ	0.19	0/544	0.37	0/731
18	AR	0.19	0/652	0.39	0/877
19	AS	0.19	0/671	0.47	0/888
19	BG	0.13	0/549	0.31	0/729
20	AT	0.21	0/550	0.56	0/728
21	B0	0.16	0/582	0.29	0/769
22	B1	0.21	0/635	0.35	0/848
23	B2	0.21	0/510	0.49	0/677
24	B3	0.18	0/453	0.33	0/605
25	B4	0.16	0/539	0.32	0/721
26	B5	0.20	0/450	0.40	0/599
27	B6	0.17	0/416	0.40	0/554
28	B7	0.21	0/380	0.29	0/498
29	B8	0.19	0/513	0.36	0/676
30	B9	0.37	0/303	0.53	0/397
31	BA	0.12	0/906	0.32	0/1213
32	BB	0.21	0/2121	0.36	0/2852
33	BC	0.19	0/1586	0.33	0/2134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BD	0.17	0/1571	0.32	0/2113
35	BE	0.17	0/1434	0.39	0/1926
36	BF	0.17	0/1343	0.37	0/1816
37	BI	0.16	0/1122	0.38	0/1515
38	BK	0.17	0/1046	0.36	0/1410
39	BM	0.18	0/1152	0.28	0/1551
40	BN	0.20	0/947	0.37	0/1268
41	BO	0.18	0/1054	0.37	0/1403
42	BP	0.20	0/1093	0.40	0/1460
43	BQ	0.21	0/973	0.42	0/1301
44	BR	0.16	0/902	0.37	0/1209
45	BS	0.19	0/929	0.32	0/1242
46	BT	0.19	0/960	0.31	0/1278
47	BU	0.20	0/829	0.42	0/1107
48	BV	0.20	0/864	0.36	0/1156
49	BW	0.19	0/744	0.42	0/994
50	BX	0.19	0/787	0.43	0/1051
51	BY	0.20	0/766	0.44	0/1025
52	D1	0.17	0/36963	0.27	0/57662
53	D2	0.21	0/69796	0.30	0/108888
54	D3	0.16	0/2872	0.26	0/4479
All	All	0.20	0/157253	0.32	2/234827 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	43	ARG	CA-C-N	6.53	129.76	120.49
3	AC	43	ARG	C-N-CA	6.53	129.76	120.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1756	0	1787	25	0
2	AB	1648	0	1725	13	0
3	AC	1643	0	1710	15	0
4	AD	1156	0	1199	20	0
5	AE	817	0	808	17	0
6	AF	1181	0	1240	20	0
7	AG	979	0	1034	12	0
8	AH	1022	0	1070	22	0
9	AI	786	0	828	17	0
10	AJ	869	0	878	8	0
11	AK	955	0	1019	12	0
12	AL	883	0	944	16	0
13	AM	805	0	847	14	0
14	AN	714	0	737	4	0
15	AO	649	0	666	9	0
16	AP	648	0	691	7	0
17	AQ	535	0	552	12	0
18	AR	637	0	665	9	0
19	AS	665	0	714	17	0
19	BG	543	0	577	6	0
20	AT	544	0	579	9	0
21	B0	575	0	592	5	0
22	B1	625	0	655	9	0
23	B2	509	0	543	5	0
24	B3	449	0	491	4	0
25	B4	529	0	531	5	0
26	B5	444	0	461	2	0
27	B6	409	0	440	1	0
28	B7	377	0	418	5	0
29	B8	504	0	574	6	0
30	B9	302	0	343	6	0
31	BA	902	0	961	12	0
32	BB	2082	0	2157	18	0
33	BC	1565	0	1616	7	0
34	BD	1552	0	1619	17	0
35	BE	1410	0	1447	39	0
36	BF	1323	0	1374	15	0
37	BI	1111	0	1148	8	0
38	BK	1032	0	1088	15	0
39	BM	1129	0	1162	9	0
40	BN	938	0	1012	14	0
41	BO	1045	0	1117	12	0
42	BP	1074	0	1157	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BQ	960	0	1000	10	0
44	BR	892	0	923	6	0
45	BS	917	0	965	15	0
46	BT	947	0	1022	7	0
47	BU	816	0	839	14	0
48	BV	857	0	922	4	0
49	BW	738	0	807	12	0
50	BX	779	0	834	6	0
51	BY	753	0	780	7	0
52	D1	33012	0	16618	133	0
53	D2	62317	0	31346	221	0
54	D3	2568	0	1303	12	0
All	All	144877	0	98535	806	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (806) 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)
53:D2:2848:G:O2'	53:D2:2867:G:N2	2.08	0.85
7:AG:25:THR:OG1	7:AG:57:GLU:OE2	1.95	0.84
24:B3:18:LYS:NZ	53:D2:920:A:OP1	2.12	0.82
25:B4:25:ARG:O	35:BE:101:ARG:NH2	2.12	0.82
39:BM:88:THR:OG1	39:BM:91:GLU:OE1	1.97	0.81
53:D2:372:G:O2'	53:D2:373:U:OP2	1.97	0.81
53:D2:877:A:O2'	53:D2:900:A:N6	2.14	0.81
4:AD:121:ASN:O	4:AD:122:VAL:HG12	1.81	0.81
52:D1:1015:G:O2'	52:D1:1016:A:O4'	1.98	0.81
45:BS:59:THR:HG22	45:BS:72:VAL:HG12	1.62	0.80
51:BY:51:GLN:NE2	51:BY:57:TYR:OH	2.14	0.80
52:D1:1300:G:O2'	52:D1:1301:U:O5'	1.98	0.80
16:AP:6:THR:OG1	16:AP:59:GLU:OE2	1.99	0.80
53:D2:270:A:N1	53:D2:369:U:O2'	2.14	0.80
53:D2:1048:A:OP2	53:D2:1110:G:N2	2.15	0.80
53:D2:481:G:O2'	53:D2:506:G:N2	2.14	0.79
52:D1:1405:G:O2'	52:D1:1518:A:O2'	2.00	0.79
45:BS:50:ARG:NH2	53:D2:2683:C:OP1	2.16	0.79
53:D2:2326:C:O2'	53:D2:2327:A:OP1	2.01	0.79
15:AO:23:ASP:OD2	52:D1:229:U:O2'	2.01	0.78
19:AS:2:ASN:N	52:D1:332:G:OP2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BK:117:THR:OG1	53:D2:1058:U:O2	2.00	0.78
53:D2:1858:A:N6	53:D2:1884:G:O2'	2.16	0.78
4:AD:156:ARG:NH1	7:AG:42:GLU:OE2	2.16	0.78
45:BS:93:LYS:NZ	53:D2:2717:C:O2'	2.17	0.77
7:AG:46:GLU:O	7:AG:61:THR:OG1	2.03	0.77
35:BE:33:ILE:HD12	35:BE:155:ILE:HG22	1.67	0.77
46:BT:48:ASP:OD2	53:D2:534:U:O2'	2.03	0.77
17:AQ:13:THR:OG1	17:AQ:16:GLY:O	2.03	0.76
13:AM:58:ARG:NH1	52:D1:979:C:O2	2.19	0.76
53:D2:1508:A:O2'	53:D2:1509:A:O4'	2.00	0.76
52:D1:1005:A:OP2	52:D1:1024:G:N2	2.18	0.76
35:BE:70:ARG:NH2	53:D2:2299:U:OP2	2.19	0.76
53:D2:219:A:N3	53:D2:234:U:O2'	2.18	0.75
1:AA:58:LYS:O	1:AA:62:ARG:NH1	2.20	0.75
35:BE:55:ASP:OD2	35:BE:149:ARG:NH2	2.20	0.75
52:D1:1432:G:O2'	52:D1:1468:A:N6	2.20	0.75
53:D2:1086:A:O2'	53:D2:1087:G:N7	2.20	0.75
32:BB:250:GLN:NE2	32:BB:251:THR:O	2.19	0.75
29:B8:31:ILE:O	29:B8:35:LYS:NZ	2.20	0.74
42:BP:30:SER:N	42:BP:106:ASP:OD1	2.20	0.74
41:BO:29:LYS:O	41:BO:30:THR:OG1	2.04	0.74
18:AR:11:ASP:OD2	18:AR:34:SER:OG	2.05	0.74
34:BD:6:LYS:O	34:BD:9:GLN:NE2	2.20	0.74
15:AO:75:ILE:O	15:AO:80:LYS:NZ	2.20	0.73
44:BR:34:HIS:ND1	44:BR:53:THR:OG1	2.20	0.73
30:B9:4:ARG:NH2	53:D2:2477:U:O2	2.22	0.73
46:BT:86:SER:OG	47:BU:50:GLY:O	2.05	0.73
53:D2:310:A:O2'	53:D2:311:A:O5'	2.05	0.73
53:D2:858:G:O2'	53:D2:859:G:OP1	2.05	0.73
8:AH:129:ARG:NH2	52:D1:969:A:N7	2.36	0.73
14:AN:12:SER:OG	14:AN:13:GLU:OE1	2.05	0.73
52:D1:1238:A:OP1	52:D1:1335:U:O2'	2.07	0.73
53:D2:227:A:O2'	53:D2:228:C:O5'	2.06	0.73
27:B6:29:LYS:NZ	53:D2:2286:G:OP1	2.21	0.73
26:B5:36:LYS:NZ	48:BV:34:ASP:OD1	2.20	0.72
53:D2:2107:G:N2	53:D2:2182:U:O2	2.17	0.72
14:AN:19:ASN:OD1	52:D1:749:A:O2'	2.06	0.72
53:D2:1069:A:N7	53:D2:1073:A:N6	2.38	0.72
53:D2:475:C:O2	53:D2:479:A:N6	2.23	0.72
11:AK:45:ASN:ND2	11:AK:88:ASP:OD2	2.24	0.71
41:BO:99:ASN:ND2	53:D2:621:A:OP2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D2:1125:G:OP2	53:D2:1126:A:O2'	2.06	0.71
53:D2:2857:G:N2	53:D2:2860:A:OP2	2.19	0.71
52:D1:977:A:O2'	52:D1:979:C:OP2	2.08	0.71
29:B8:28:LEU:O	29:B8:28:LEU:HD12	1.92	0.70
35:BE:134:GLN:NE2	35:BE:147:ARG:O	2.25	0.70
52:D1:1137:C:O2'	52:D1:1138:G:N2	2.25	0.70
40:BN:70:ARG:NH1	53:D2:2684:U:O4'	2.24	0.70
9:AI:29:ALA:O	9:AI:33:GLY:N	2.26	0.69
13:AM:84:ARG:NH2	52:D1:1060:U:OP1	2.26	0.69
25:B4:16:CYS:SG	25:B4:17:SER:N	2.65	0.69
49:BW:90:GLY:O	49:BW:91:GLN:NE2	2.25	0.69
53:D2:1466:U:HO2'	53:D2:1546:G:HO2'	1.31	0.69
52:D1:1255:G:O2'	52:D1:1258:G:N3	2.22	0.69
53:D2:948:C:O2	53:D2:984:A:O2'	2.10	0.69
6:AF:139:ASP:OD1	6:AF:142:ARG:NH2	2.25	0.69
8:AH:46:VAL:HG11	8:AH:75:ALA:HB1	1.74	0.69
42:BP:81:ARG:NH1	53:D2:2251:G:OP1	2.26	0.69
53:D2:2144:G:O2'	53:D2:2147:A:N1	2.25	0.69
42:BP:17:ASN:OD1	42:BP:97:GLN:NE2	2.26	0.68
46:BT:49:ARG:NH2	47:BU:73:LYS:O	2.26	0.68
2:AB:27:GLU:O	2:AB:31:ASN:ND2	2.27	0.68
15:AO:4:ILE:HD12	15:AO:21:VAL:HG22	1.76	0.68
51:BY:43:ASP:OD2	51:BY:46:LYS:NZ	2.27	0.68
4:AD:125:LYS:NZ	52:D1:9:G:OP2	2.25	0.68
53:D2:2134:A:O2'	53:D2:2159:G:N3	2.27	0.68
6:AF:89:GLU:OE2	6:AF:91:ARG:NH1	2.26	0.67
34:BD:95:LYS:NZ	53:D2:658:U:O2'	2.22	0.67
11:AK:109:ARG:NH1	11:AK:111:GLN:O	2.27	0.67
23:B2:49:ASP:OD1	23:B2:52:ARG:NH1	2.27	0.67
53:D2:1019:U:OP1	53:D2:1035:U:O2'	2.11	0.67
8:AH:74:GLN:O	8:AH:78:ILE:HD12	1.95	0.67
53:D2:1057:A:O2'	53:D2:1058:U:O4'	2.11	0.66
53:D2:1315:C:O2'	53:D2:1392:A:N3	2.27	0.66
32:BB:216:ARG:NH1	53:D2:691:C:OP1	2.28	0.66
52:D1:1315:U:O2'	52:D1:1360:A:N3	2.27	0.66
2:AB:104:GLU:OE2	2:AB:106:ARG:NH1	2.29	0.66
52:D1:414:A:OP2	52:D1:428:G:N2	2.27	0.66
32:BB:216:ARG:NH2	53:D2:781:A:OP1	2.28	0.66
52:D1:561:U:O2'	52:D1:562:U:OP2	2.10	0.66
52:D1:1300:G:HO2'	52:D1:1301:U:P	2.19	0.66
52:D1:1178:G:N2	52:D1:1181:G:OP2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D1:530:G:O2'	52:D1:531:U:OP1	2.12	0.65
35:BE:72:SER:N	35:BE:80:GLN:OE1	2.28	0.65
17:AQ:54:LEU:O	17:AQ:58:ILE:HD12	1.96	0.65
30:B9:19:ARG:NE	53:D2:2756:U:OP2	2.28	0.65
53:D2:641:U:O2'	53:D2:2350:C:OP1	2.14	0.65
53:D2:285:G:O6	53:D2:355:U:O2	2.15	0.65
53:D2:1869:G:N2	53:D2:1872:A:OP2	2.28	0.65
35:BE:91:ARG:NH1	54:D3:43:C:O2	2.29	0.65
52:D1:687:A:N6	52:D1:703:G:O2'	2.30	0.65
38:BK:89:SER:N	53:D2:1063:G:O2'	2.30	0.65
52:D1:993:G:O2'	52:D1:994:A:N7	2.30	0.65
41:BO:95:LEU:HD22	41:BO:100:ILE:HD11	1.78	0.65
16:AP:6:THR:OG1	16:AP:60:ILE:O	2.15	0.64
38:BK:131:THR:OG1	53:D2:1060:U:O4	2.11	0.64
4:AD:156:ARG:NH2	7:AG:98:LEU:O	2.30	0.64
6:AF:137:ARG:NH2	6:AF:138:GLU:OE2	2.31	0.64
53:D2:1847:A:O2'	53:D2:1848:A:N7	2.24	0.64
53:D2:2139:U:O2	53:D2:2152:G:O6	2.16	0.64
19:AS:2:ASN:OD1	19:AS:3:ILE:N	2.31	0.64
39:BM:125:TYR:OH	39:BM:132:HIS:NE2	2.31	0.64
53:D2:2581:G:N2	53:D2:2581:G:OP2	2.31	0.64
7:AG:95:MET:HE3	7:AG:129:ALA:HB1	1.80	0.64
49:BW:18:GLU:OE2	53:D2:1392:A:N6	2.29	0.64
35:BE:56:LEU:HD22	35:BE:64:PRO:HB3	1.79	0.64
22:B1:31:ASN:OD1	22:B1:33:HIS:NE2	2.30	0.64
34:BD:171:ASP:OD1	34:BD:172:ALA:N	2.31	0.64
33:BC:151:THR:OG1	53:D2:2032:G:N2	2.31	0.63
46:BT:57:ARG:NH1	53:D2:1154:G:OP2	2.31	0.63
52:D1:187:G:N2	52:D1:190:A:OP2	2.31	0.63
53:D2:1857:G:O2'	53:D2:1885:A:N6	2.31	0.63
13:AM:2:LYS:O	13:AM:5:MET:N	2.30	0.63
36:BF:136:ASP:OD1	36:BF:139:VAL:HG22	1.97	0.63
53:D2:2331:G:O2'	53:D2:2336:A:N1	2.32	0.63
40:BN:88:ASN:OD1	40:BN:89:ASN:N	2.32	0.63
54:D3:24:G:N7	54:D3:56:G:O2'	2.26	0.63
47:BU:31:GLU:N	47:BU:31:GLU:OE1	2.31	0.62
35:BE:45:ASP:OD2	35:BE:48:LEU:N	2.32	0.62
53:D2:2832:U:O2'	53:D2:2833:U:OP2	2.12	0.62
1:AA:82:ALA:HB2	1:AA:213:LEU:HD13	1.81	0.62
52:D1:71:A:N6	52:D1:99:C:O2'	2.32	0.62
53:D2:700:G:O2'	53:D2:1632:A:N3	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BP:66:ARG:NH1	42:BP:104:GLU:OE2	2.33	0.62
43:BQ:114:GLU:OE1	43:BQ:118:ARG:NH1	2.33	0.62
52:D1:686:U:O2'	52:D1:687:A:O5'	2.17	0.62
10:AJ:126:ARG:NH2	52:D1:693:G:OP1	2.32	0.62
35:BE:18:GLU:N	35:BE:18:GLU:OE1	2.33	0.62
46:BT:5:ARG:NH2	53:D2:585:G:N7	2.47	0.62
52:D1:1256:A:O2'	52:D1:1257:A:O5'	2.18	0.62
53:D2:1827:U:OP1	53:D2:1971:U:O2'	2.17	0.61
5:AE:15:SER:OG	5:AE:44:ARG:NH2	2.33	0.61
6:AF:32:ASP:OD1	52:D1:1350:A:O2'	2.17	0.61
17:AQ:36:GLY:O	17:AQ:62:ARG:NH2	2.33	0.61
19:BG:32:ILE:HD11	53:D2:613:A:N7	2.16	0.61
11:AK:38:THR:OG1	11:AK:49:ARG:O	2.07	0.61
52:D1:521:G:HO2'	52:D1:536:C:HO2'	1.49	0.61
2:AB:120:THR:HG23	2:AB:188:ALA:HB2	1.83	0.61
53:D2:1447:C:O2'	53:D2:1544:A:N3	2.33	0.61
52:D1:1307:U:O4	52:D1:1331:G:N2	2.33	0.61
5:AE:91:ARG:HE	5:AE:92:THR:H	1.49	0.60
19:AS:73:ARG:NH1	52:D1:261:U:OP2	2.34	0.60
20:AT:23:GLU:OE1	20:AT:23:GLU:N	2.34	0.60
52:D1:427:U:OP2	52:D1:428:G:O2'	2.13	0.60
54:D3:88:C:O2'	54:D3:89:U:O5'	2.18	0.60
15:AO:36:VAL:HG23	15:AO:36:VAL:O	2.02	0.60
43:BQ:106:ASP:OD2	53:D2:1649:G:O2'	2.14	0.60
1:AA:112:ARG:HH12	1:AA:116:LEU:HD13	1.67	0.60
6:AF:4:ARG:HG3	6:AF:6:ILE:HG23	1.83	0.60
18:AR:76:THR:O	52:D1:958:A:N6	2.34	0.60
4:AD:36:THR:HG21	4:AD:63:MET:HE2	1.83	0.60
13:AM:89:ARG:NH1	13:AM:91:GLU:OE2	2.34	0.60
32:BB:106:PRO:HD2	32:BB:109:LEU:HD22	1.82	0.60
18:AR:35:ARG:NH1	52:D1:1320:C:N3	2.50	0.60
52:D1:757:U:OP1	52:D1:822:U:O2'	2.19	0.60
53:D2:2522:U:O2'	53:D2:2647:U:OP1	2.17	0.60
54:D3:12:C:O2'	54:D3:13:G:O5'	2.19	0.60
16:AP:14:ASP:HA	16:AP:20:ILE:HD12	1.82	0.60
21:B0:52:ASP:OD1	21:B0:54:THR:OG1	2.19	0.60
34:BD:53:THR:HG21	53:D2:452:G:H8	1.66	0.60
36:BF:88:LEU:HD21	36:BF:93:TYR:HB3	1.83	0.60
40:BN:65:THR:HG22	40:BN:67:LYS:H	1.67	0.60
52:D1:518:C:O2'	52:D1:530:G:N2	2.34	0.60
14:AN:45:HIS:O	14:AN:47:LYS:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D1:1238:A:N7	52:D1:1301:U:O4	2.35	0.59
52:D1:3:A:N1	52:D1:628:G:O2'	2.35	0.59
8:AH:91:GLU:OE2	8:AH:94:ARG:NH1	2.35	0.59
22:B1:58:ILE:HG12	22:B1:66:VAL:HG21	1.84	0.59
34:BD:44:ARG:NH2	53:D2:1248:G:OP1	2.35	0.59
49:BW:29:THR:HG22	49:BW:86:THR:HB	1.84	0.59
53:D2:2646:C:OP2	53:D2:2732:G:O2'	2.18	0.59
1:AA:129:THR:N	1:AA:132:GLU:OE2	2.35	0.59
6:AF:4:ARG:CG	6:AF:6:ILE:HG23	2.33	0.59
9:AI:45:ARG:NH2	52:D1:1254:A:OP1	2.36	0.59
53:D2:1084:A:N3	53:D2:1105:U:O2'	2.28	0.59
17:AQ:14:ALA:O	17:AQ:47:ARG:NH1	2.36	0.59
31:BA:217:THR:HG22	53:D2:2124:G:H21	1.67	0.59
13:AM:41:TRP:O	13:AM:45:LEU:HD23	2.02	0.59
1:AA:163:ILE:HD13	1:AA:185:ILE:HD12	1.84	0.59
53:D2:2212:A:O2'	53:D2:2213:U:O5'	2.14	0.59
33:BC:59:ARG:NH2	53:D2:2831:G:OP2	2.36	0.59
5:AE:63:ASN:ND2	5:AE:96:VAL:O	2.36	0.58
7:AG:102:VAL:HG23	7:AG:125:ILE:HB	1.85	0.58
29:B8:51:LYS:HA	29:B8:54:LEU:HD23	1.85	0.58
31:BA:217:THR:HG22	53:D2:2124:G:N2	2.18	0.58
48:BV:4:ILE:HG22	48:BV:106:VAL:HG22	1.85	0.58
8:AH:78:ILE:O	8:AH:82:ILE:HD12	2.03	0.58
1:AA:27:LYS:O	1:AA:30:ILE:HG22	2.03	0.58
22:B1:9:LYS:NZ	53:D2:397:U:OP2	2.36	0.58
52:D1:362:G:N2	52:D1:365:U:OP2	2.36	0.58
12:AL:91:ARG:NH2	53:D2:888:C:OP1	2.35	0.58
12:AL:106:ARG:NH1	52:D1:1228:C:OP1	2.37	0.58
19:AS:47:GLN:OE1	19:AS:82:ILE:HG21	2.04	0.58
32:BB:270:ARG:NH2	53:D2:1798:U:OP2	2.37	0.58
53:D2:247:G:OP2	53:D2:249:C:N4	2.36	0.58
53:D2:271:G:O2'	53:D2:272:A:OP2	2.19	0.58
53:D2:2102:G:N1	53:D2:2188:U:O4	2.36	0.58
53:D2:2162:G:OP1	53:D2:2171:A:N6	2.36	0.58
4:AD:134:ASN:ND2	52:D1:19:A:OP1	2.35	0.58
45:BS:83:ILE:HG22	45:BS:83:ILE:O	2.04	0.58
52:D1:1533:C:O2'	52:D1:1534:A:N7	2.35	0.58
53:D2:500:G:N1	53:D2:503:A:OP2	2.37	0.58
6:AF:96:ASN:OD1	6:AF:97:ALA:N	2.37	0.57
8:AH:39:GLY:O	8:AH:40:ARG:NH1	2.37	0.57
31:BA:175:ILE:HD13	31:BA:189:LEU:HD21	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D2:1900:A:O2'	53:D2:1901:A:OP2	2.22	0.57
38:BK:131:THR:HG22	38:BK:135:MET:HE1	1.86	0.57
52:D1:1029:U:O2'	52:D1:1033:G:N2	2.37	0.57
37:BI:121:VAL:HG12	37:BI:121:VAL:O	2.05	0.57
35:BE:56:LEU:HD23	35:BE:56:LEU:O	2.05	0.57
52:D1:126:G:OP1	52:D1:605:U:O2'	2.17	0.57
53:D2:2653:U:OP2	53:D2:2654:A:O2'	2.14	0.57
8:AH:20:ILE:HD11	8:AH:60:LEU:HB3	1.86	0.57
21:B0:22:PHE:N	21:B0:25:GLU:OE2	2.38	0.57
52:D1:31:G:O2'	52:D1:48:C:N4	2.37	0.57
53:D2:458:G:O2'	53:D2:459:U:OP2	2.21	0.57
53:D2:1056:G:O2'	53:D2:1103:A:N6	2.38	0.57
3:AC:8:LEU:HD13	3:AC:31:CYS:HB3	1.87	0.57
11:AK:113:ARG:NH2	52:D1:501:C:OP1	2.38	0.57
53:D2:1582:C:O2'	53:D2:1585:C:N3	2.36	0.56
53:D2:279:A:N6	53:D2:361:G:O2'	2.36	0.56
13:AM:18:LYS:O	13:AM:22:LYS:NZ	2.36	0.56
15:AO:6:LEU:HD23	15:AO:19:VAL:HG12	1.87	0.56
41:BO:111:ILE:HD11	53:D2:636:G:C5	2.40	0.56
52:D1:422:C:O2'	52:D1:423:G:N2	2.38	0.56
53:D2:774:G:O2'	53:D2:775:G:O5'	2.22	0.56
9:AI:36:VAL:HG23	9:AI:76:ILE:HD13	1.88	0.56
49:BW:39:THR:OG1	49:BW:42:GLU:OE1	2.23	0.56
53:D2:1028:A:N3	53:D2:2486:C:O2'	2.30	0.56
40:BN:61:VAL:CG2	40:BN:87:LEU:HD11	2.34	0.56
6:AF:49:LEU:HD22	6:AF:123:LEU:HD23	1.88	0.56
52:D1:280:C:O2'	52:D1:281:G:OP2	2.24	0.56
52:D1:1124:G:O2'	52:D1:1145:A:N1	2.31	0.56
2:AB:18:ASN:O	2:AB:39:ARG:NH2	2.38	0.56
5:AE:38:ARG:O	5:AE:39:LEU:HD22	2.05	0.56
32:BB:145:MET:CE	32:BB:153:LEU:HD21	2.35	0.56
6:AF:109:LYS:O	6:AF:118:ARG:NE	2.33	0.55
19:AS:67:HIS:O	19:AS:67:HIS:ND1	2.39	0.55
37:BI:113:SER:O	37:BI:116:ARG:NH2	2.38	0.55
52:D1:462:G:C2	52:D1:471:U:O2	2.60	0.55
35:BE:89:THR:OG1	54:D3:42:C:N3	2.37	0.55
36:BF:109:SER:OG	53:D2:2667:C:N3	2.30	0.55
53:D2:332:A:O2'	53:D2:334:C:OP2	2.20	0.55
53:D2:2129:C:H2'	53:D2:2159:G:H22	1.71	0.55
9:AI:8:ILE:HG22	9:AI:100:ILE:HG13	1.88	0.55
43:BQ:103:ARG:HD3	43:BQ:110:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BE:152:ASP:OD1	53:D2:2304:G:O2'	2.21	0.55
53:D2:1266:G:O2'	53:D2:2012:G:O6	2.22	0.55
8:AH:129:ARG:O	52:D1:970:C:N4	2.39	0.55
12:AL:67:ASP:OD1	12:AL:70:ARG:NH1	2.40	0.55
18:AR:35:ARG:NH2	18:AR:71:GLY:O	2.39	0.55
22:B1:60:LYS:NZ	53:D2:371:A:O3'	2.40	0.55
25:B4:9:TYR:OH	35:BE:97:GLU:OE1	2.23	0.55
19:BG:68:HIS:NE2	53:D2:42:A:OP1	2.40	0.55
11:AK:32:VAL:HA	11:AK:78:VAL:HG12	1.88	0.55
38:BK:48:ILE:HD11	38:BK:54:ILE:HD13	1.89	0.55
3:AC:139:ASN:N	3:AC:181:PHE:O	2.39	0.55
12:AL:106:ARG:O	12:AL:110:GLY:N	2.40	0.55
3:AC:25:ARG:NH2	52:D1:410:G:OP1	2.40	0.54
44:BR:8:ILE:O	44:BR:12:THR:HG23	2.07	0.54
53:D2:1527:G:N1	53:D2:1544:A:OP2	2.40	0.54
53:D2:2788:C:O2'	53:D2:2809:A:N3	2.38	0.54
4:AD:120:HIS:O	4:AD:121:ASN:ND2	2.39	0.54
9:AI:9:ARG:NH2	52:D1:1280:A:OP1	2.41	0.54
1:AA:13:VAL:HG23	1:AA:212:TYR:OH	2.07	0.54
24:B3:11:SER:OG	53:D2:989:G:OP2	2.21	0.54
38:BK:35:MET:SD	38:BK:36:GLU:N	2.81	0.54
53:D2:476:G:N1	53:D2:479:A:OP2	2.37	0.54
5:AE:5:GLU:OE2	17:AQ:23:LYS:NZ	2.39	0.54
52:D1:664:G:H22	52:D1:741:G:H1	1.54	0.54
53:D2:2469:A:N6	53:D2:2481:G:O2'	2.37	0.54
2:AB:175:HIS:ND1	52:D1:1109:C:OP2	2.40	0.54
5:AE:87:SER:OG	5:AE:88:MET:N	2.40	0.54
7:AG:14:ARG:NH1	52:D1:875:U:O2'	2.40	0.54
4:AD:153:ALA:HB2	4:AD:163:ILE:HD11	1.89	0.54
11:AK:2:THR:O	11:AK:5:GLN:N	2.40	0.54
17:AQ:32:ILE:HD11	17:AQ:36:GLY:O	2.07	0.54
22:B1:5:GLN:O	22:B1:73:ARG:NH2	2.38	0.54
35:BE:120:SER:O	53:D2:2303:G:O2'	2.24	0.54
39:BM:31:GLU:HG2	39:BM:142:ILE:HG21	1.89	0.54
52:D1:28:A:O2'	52:D1:296:U:OP1	2.24	0.54
26:B5:14:MET:HE2	53:D2:2045:C:H5''	1.89	0.54
15:AO:19:VAL:HG23	15:AO:36:VAL:O	2.08	0.54
45:BS:32:VAL:HG22	45:BS:37:LYS:HG2	1.89	0.54
1:AA:42:LEU:HA	1:AA:45:THR:HG22	1.91	0.53
15:AO:4:ILE:CD1	15:AO:21:VAL:HG22	2.37	0.53
24:B3:36:GLU:O	24:B3:37:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:8:MET:HE2	53:D2:2175:C:H5'	1.90	0.53
31:BA:177:LYS:NZ	53:D2:2126:A:O5'	2.40	0.53
39:BM:96:ARG:NH1	53:D2:2639:A:O2'	2.41	0.53
45:BS:52:ARG:NH1	53:D2:2845:U:O3'	2.42	0.53
4:AD:86:GLY:O	4:AD:138:ALA:HB1	2.09	0.53
20:AT:44:ARG:NH1	52:D1:723:U:OP2	2.42	0.53
36:BF:176:LYS:NZ	53:D2:2661:G:O6	2.42	0.53
3:AC:28:ASP:OD1	3:AC:29:THR:N	2.36	0.53
21:B0:67:VAL:HG12	21:B0:67:VAL:O	2.09	0.53
53:D2:1466:U:O2'	53:D2:1546:G:O2'	2.08	0.53
53:D2:2202:U:O2'	53:D2:2204:G:OP1	2.26	0.53
31:BA:41:SER:O	31:BA:217:THR:HG23	2.09	0.53
34:BD:53:THR:HG22	53:D2:452:G:OP1	2.09	0.53
53:D2:1329:U:O2'	53:D2:1330:C:OP1	2.20	0.53
53:D2:1668:A:O2'	53:D2:1674:G:N7	2.32	0.53
53:D2:858:G:HO2'	53:D2:859:G:P	2.30	0.53
17:AQ:33:THR:OG1	17:AQ:34:GLU:OE1	2.26	0.53
52:D1:1304:G:N1	52:D1:1332:A:OP2	2.40	0.53
1:AA:132:GLU:OE1	1:AA:132:GLU:N	2.36	0.52
22:B1:41:SER:OG	22:B1:42:GLU:OE1	2.26	0.52
29:B8:39:ARG:O	29:B8:43:LEU:HD13	2.08	0.52
32:BB:145:MET:HE1	32:BB:153:LEU:HD21	1.91	0.52
11:AK:49:ARG:NH2	52:D1:522:C:H41	2.07	0.52
52:D1:1305:G:H22	52:D1:1331:G:H2'	1.73	0.52
53:D2:310:A:HO2'	53:D2:311:A:P	2.32	0.52
37:BI:117:LEU:HD23	37:BI:121:VAL:HA	1.91	0.52
52:D1:1124:G:N2	52:D1:1125:U:O4	2.32	0.52
47:BU:61:ALA:HB1	47:BU:96:VAL:HG22	1.91	0.52
51:BY:21:ARG:NH1	51:BY:87:GLN:O	2.43	0.52
4:AD:163:ILE:O	7:AG:113:ARG:NH2	2.42	0.52
52:D1:380:G:N2	52:D1:383:A:OP2	2.36	0.52
45:BS:1:SER:OG	45:BS:2:ASN:N	2.42	0.52
47:BU:49:ILE:HG22	47:BU:54:VAL:H	1.74	0.52
53:D2:2187:U:O2'	53:D2:2188:U:O5'	2.26	0.52
45:BS:3:ILE:O	45:BS:7:LEU:HD23	2.10	0.52
3:AC:12:ARG:NH2	3:AC:36:ALA:O	2.43	0.52
51:BY:43:ASP:OD1	51:BY:44:HIS:N	2.43	0.52
3:AC:1:ALA:N	52:D1:405:U:O4	2.42	0.51
43:BQ:69:ARG:O	43:BQ:70:THR:HG22	2.11	0.51
53:D2:2115:G:N2	53:D2:2119:A:N1	2.57	0.51
1:AA:115:ASP:HA	1:AA:118:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D1:1268:G:O2'	52:D1:1269:A:O4'	2.23	0.51
10:AJ:63:GLN:HB2	10:AJ:98:ALA:HB2	1.92	0.51
34:BD:148:ILE:HD13	34:BD:187:VAL:HG22	1.92	0.51
53:D2:704:G:H2'	53:D2:726:G:H22	1.75	0.51
53:D2:2682:A:H61	53:D2:2728:U:H1'	1.76	0.51
34:BD:49:ARG:NH1	53:D2:673:C:OP1	2.39	0.51
35:BE:26:GLN:NE2	54:D3:57:A:O4'	2.43	0.51
46:BT:104:ALA:O	46:BT:108:LEU:HD23	2.10	0.51
51:BY:21:ARG:NH2	54:D3:76:G:O3'	2.43	0.51
2:AB:122:GLN:OE1	2:AB:135:ARG:NH2	2.44	0.51
4:AD:73:VAL:HG11	4:AD:143:LEU:HB3	1.92	0.51
8:AH:128:LYS:NZ	52:D1:1341:U:O3'	2.44	0.51
19:AS:34:VAL:HG21	19:AS:53:MET:SD	2.50	0.51
19:AS:35:TYR:CZ	19:AS:78:LEU:HD21	2.46	0.51
52:D1:324:G:N1	52:D1:327:A:OP2	2.41	0.51
53:D2:2156:G:O6	53:D2:2157:G:N2	2.43	0.51
35:BE:139:GLU:OE1	35:BE:139:GLU:N	2.44	0.51
36:BF:42:VAL:HG23	36:BF:51:PHE:HE1	1.76	0.51
49:BW:4:GLU:O	49:BW:8:LEU:HD13	2.11	0.51
1:AA:71:THR:OG1	1:AA:168:GLU:OE2	2.28	0.51
5:AE:92:THR:HG22	5:AE:94:HIS:H	1.75	0.51
53:D2:981:A:OP2	53:D2:982:C:N4	2.38	0.51
4:AD:35:LEU:HD22	4:AD:133:ILE:HG13	1.94	0.50
12:AL:28:ARG:NH2	12:AL:32:ILE:HD11	2.26	0.50
19:BG:64:LYS:NZ	53:D2:341:C:OP2	2.31	0.50
9:AI:42:LEU:HD22	9:AI:71:LEU:HD11	1.93	0.50
38:BK:131:THR:HG22	38:BK:135:MET:SD	2.51	0.50
2:AB:185:THR:HG22	2:AB:198:LYS:HG2	1.93	0.50
5:AE:3:HIS:HB2	5:AE:92:THR:HG23	1.92	0.50
8:AH:104:THR:HG22	52:D1:1180:A:OP1	2.11	0.50
9:AI:12:ALA:HB2	9:AI:96:VAL:HG22	1.94	0.50
11:AK:17:LYS:NZ	52:D1:910:C:OP2	2.44	0.50
39:BM:19:ASP:OD1	39:BM:58:ASN:ND2	2.41	0.50
44:BR:57:ALA:O	44:BR:61:GLN:NE2	2.45	0.50
52:D1:462:G:C2	52:D1:471:U:C2	3.00	0.50
52:D1:1250:A:N3	52:D1:1370:G:O2'	2.38	0.50
13:AM:60:ARG:NH2	52:D1:977:A:OP1	2.44	0.50
52:D1:1256:A:N6	52:D1:1278:G:N3	2.59	0.50
15:AO:14:ARG:NH1	52:D1:618:C:O2'	2.43	0.50
9:AI:40:ILE:HD13	52:D1:1125:U:C6	2.47	0.50
12:AL:84:CYS:SG	12:AL:87:GLY:N	2.83	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B0:29:ALA:N	21:B0:60:ASP:OD1	2.45	0.50
30:B9:34:LYS:NZ	53:D2:2743:U:OP1	2.42	0.50
31:BA:177:LYS:NZ	53:D2:2125:G:O2'	2.44	0.50
53:D2:2060:A:O2'	53:D2:2061:G:OP2	2.29	0.50
12:AL:92:ARG:NH2	53:D2:888:C:O4'	2.45	0.50
38:BK:93:ASN:ND2	53:D2:1076:C:O3'	2.45	0.50
51:BY:63:ILE:HD12	51:BY:72:VAL:HG21	1.94	0.50
52:D1:507:C:OP2	52:D1:508:U:O2'	2.17	0.50
1:AA:177:ASN:ND2	52:D1:1075:U:OP1	2.45	0.50
5:AE:74:LEU:O	5:AE:77:THR:OG1	2.30	0.50
10:AJ:41:LEU:HD12	10:AJ:73:VAL:HG12	1.93	0.49
20:AT:23:GLU:HG3	20:AT:27:VAL:HG22	1.94	0.49
35:BE:36:ASN:ND2	53:D2:2313:C:O4'	2.45	0.49
53:D2:1003:G:O2'	53:D2:1010:A:N1	2.35	0.49
42:BP:86:LYS:NZ	53:D2:955:U:OP1	2.34	0.49
35:BE:56:LEU:HD21	35:BE:88:VAL:HG22	1.94	0.49
35:BE:110:ILE:HG22	35:BE:136:ILE:HG21	1.92	0.49
53:D2:58:G:O2'	53:D2:73:A:N1	2.36	0.49
2:AB:56:ILE:HD12	2:AB:65:VAL:HG12	1.93	0.49
30:B9:16:ILE:HD13	30:B9:25:VAL:HG22	1.94	0.49
6:AF:128:GLU:OE1	6:AF:130:LYS:NZ	2.41	0.49
34:BD:173:THR:HG21	19:BG:29:ARG:CZ	2.42	0.49
35:BE:36:ASN:OD1	35:BE:37:MET:N	2.45	0.49
53:D2:569:U:O2'	53:D2:983:A:N1	2.44	0.49
1:AA:98:GLY:N	1:AA:174:GLU:OE2	2.44	0.49
4:AD:148:SER:N	4:AD:151:MET:SD	2.85	0.49
5:AE:19:PRO:HA	5:AE:22:ILE:HG22	1.95	0.49
5:AE:62:MET:HB3	5:AE:64:VAL:HG23	1.95	0.49
35:BE:110:ILE:HD11	35:BE:113:PHE:HD1	1.78	0.49
53:D2:630:G:N2	53:D2:633:A:OP2	2.32	0.49
18:AR:41:PRO:HD2	25:B4:66:ILE:HD11	1.95	0.49
50:BX:85:ARG:NH2	50:BX:99:SER:OG	2.42	0.49
53:D2:2144:G:H1'	53:D2:2147:A:H61	1.77	0.49
17:AQ:33:THR:HG22	17:AQ:37:LYS:O	2.12	0.49
6:AF:108:ARG:O	6:AF:118:ARG:NH2	2.46	0.49
19:AS:53:MET:HE1	19:AS:78:LEU:HD12	1.95	0.49
34:BD:127:GLU:O	34:BD:156:ASN:ND2	2.40	0.49
36:BF:1:SER:OG	36:BF:2:ARG:N	2.46	0.49
52:D1:652:U:O2'	52:D1:653:U:O5'	2.25	0.49
52:D1:993:G:H2'	52:D1:995:C:H41	1.77	0.49
52:D1:1238:A:H62	52:D1:1301:U:H3	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D1:1447:A:O2'	52:D1:1448:C:OP1	2.22	0.49
1:AA:34:ARG:O	1:AA:37:VAL:HG22	2.12	0.49
8:AH:11:ARG:NH1	8:AH:106:ASP:OD2	2.46	0.49
40:BN:61:VAL:HG23	40:BN:87:LEU:HD11	1.94	0.49
42:BP:26:VAL:HG23	42:BP:104:GLU:HG2	1.94	0.49
53:D2:227:A:HO2'	53:D2:228:C:P	2.36	0.49
53:D2:463:G:N2	53:D2:466:A:OP2	2.38	0.49
4:AD:24:VAL:HG22	4:AD:25:LYS:H	1.78	0.48
12:AL:47:LEU:HD12	12:AL:51:GLN:NE2	2.27	0.48
17:AQ:54:LEU:HD23	17:AQ:58:ILE:HD13	1.95	0.48
52:D1:1256:A:HO2'	52:D1:1257:A:P	2.36	0.48
53:D2:490:C:O2'	53:D2:491:G:OP2	2.24	0.48
8:AH:46:VAL:CG1	8:AH:75:ALA:HB1	2.42	0.48
10:AJ:126:ARG:NH1	52:D1:796:C:O3'	2.47	0.48
52:D1:1237:C:O2'	52:D1:1300:G:N2	2.43	0.48
13:AM:3:GLN:NE2	52:D1:995:C:O2	2.38	0.48
23:B2:26:PHE:CZ	49:BW:50:LEU:HD23	2.49	0.48
33:BC:136:ASN:ND2	33:BC:139:SER:O	2.45	0.48
53:D2:2174:C:H2'	53:D2:2175:C:O4'	2.14	0.48
32:BB:131:MET:HA	32:BB:134:ILE:HD13	1.95	0.48
37:BI:40:THR:N	37:BI:43:ASN:OD1	2.47	0.48
50:BX:34:ILE:HD13	50:BX:63:ALA:HA	1.96	0.48
52:D1:1209:C:O2'	52:D1:1214:C:N4	2.46	0.48
10:AJ:45:THR:OG1	10:AJ:48:GLY:N	2.47	0.48
36:BF:46:ASP:OD1	36:BF:47:ASN:N	2.46	0.48
21:B0:11:ASP:OD1	21:B0:12:SER:N	2.45	0.48
36:BF:42:VAL:HG23	36:BF:51:PHE:CE1	2.49	0.48
19:BG:32:ILE:HD11	53:D2:613:A:C8	2.49	0.48
53:D2:372:G:HO2'	53:D2:373:U:P	2.31	0.48
53:D2:629:G:N3	53:D2:639:U:O2'	2.47	0.48
3:AC:150:LYS:HD2	3:AC:150:LYS:O	2.14	0.48
40:BN:43:ILE:HD12	40:BN:56:ASP:HB2	1.95	0.48
36:BF:104:LEU:HB3	36:BF:106:LEU:HD13	1.96	0.48
52:D1:1201:A:O2'	52:D1:1202:U:OP2	2.22	0.48
53:D2:586:A:N1	53:D2:809:G:O2'	2.39	0.48
53:D2:1450:G:H21	53:D2:1452:G:H1	1.62	0.48
41:BO:26:GLY:C	41:BO:27:LEU:HD22	2.38	0.47
50:BX:97:SER:O	50:BX:97:SER:OG	2.32	0.47
14:AN:22:GLY:O	14:AN:27:GLN:NE2	2.47	0.47
53:D2:2123:G:H2'	53:D2:2124:G:C8	2.49	0.47
6:AF:129:ASN:HB2	6:AF:134:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:44:VAL:O	31:BA:173:THR:N	2.43	0.47
52:D1:329:A:O2'	52:D1:332:G:N7	2.42	0.47
53:D2:1779:U:OP2	53:D2:1784:A:N6	2.38	0.47
53:D2:774:G:HO2'	53:D2:775:G:P	2.37	0.47
53:D2:1070:A:N7	53:D2:1096:A:O2'	2.47	0.47
16:AP:16:MET:HE1	52:D1:276:G:H5'	1.95	0.47
34:BD:170:ARG:NH1	34:BD:179:SER:OG	2.48	0.47
36:BF:88:LEU:O	36:BF:88:LEU:HD23	2.15	0.47
38:BK:116:MET:HB3	38:BK:124:MET:HE1	1.96	0.47
53:D2:2816:G:N3	53:D2:2883:A:O2'	2.44	0.47
34:BD:53:THR:HG21	53:D2:452:G:C8	2.48	0.47
34:BD:119:ILE:HB	34:BD:187:VAL:HG12	1.97	0.47
34:BD:149:ILE:HD11	34:BD:188:MET:SD	2.54	0.47
41:BO:128:THR:HG21	53:D2:637:A:OP2	2.15	0.47
53:D2:1009:A:N3	53:D2:1153:C:O2'	2.47	0.47
8:AH:18:VAL:HG23	8:AH:64:ILE:CD1	2.45	0.47
8:AH:43:ALA:O	8:AH:46:VAL:HG12	2.15	0.47
33:BC:49:GLN:NE2	33:BC:79:LEU:HD13	2.30	0.47
43:BQ:90:ARG:NH2	53:D2:2880:C:O3'	2.48	0.47
3:AC:151:GLN:O	3:AC:153:ARG:N	2.48	0.47
32:BB:220:ARG:NH1	53:D2:1827:U:OP2	2.47	0.47
40:BN:17:ARG:HE	40:BN:47:ILE:HD11	1.79	0.47
52:D1:462:G:N1	52:D1:471:U:C2	2.83	0.47
35:BE:158:THR:O	35:BE:158:THR:HG22	2.15	0.46
7:AG:10:LEU:HD22	7:AG:74:ILE:HD11	1.97	0.46
35:BE:118:ALA:HB1	35:BE:166:ARG:HE	1.80	0.46
53:D2:2162:G:OP2	53:D2:2164:C:N4	2.48	0.46
19:AS:8:LYS:O	19:AS:11:ILE:HG12	2.15	0.46
22:B1:73:ARG:NH2	22:B1:75:GLU:OE2	2.46	0.46
32:BB:170:TYR:OH	53:D2:2223:G:OP1	2.28	0.46
33:BC:16:THR:OG1	33:BC:18:ASP:OD1	2.26	0.46
53:D2:2304:G:H22	53:D2:2312:U:H3	1.63	0.46
18:AR:52:ASN:HB2	18:AR:76:THR:HG22	1.98	0.46
43:BQ:73:ASN:HA	43:BQ:76:VAL:HG12	1.97	0.46
53:D2:2637:U:H2'	53:D2:2638:G:O4'	2.16	0.46
3:AC:12:ARG:NH2	52:D1:427:U:OP1	2.42	0.46
9:AI:40:ILE:HD13	52:D1:1125:U:H6	1.81	0.46
32:BB:163:ILE:HD13	32:BB:173:LEU:HD22	1.98	0.46
34:BD:3:LEU:HD13	34:BD:120:VAL:HG21	1.98	0.46
53:D2:1174:U:O2'	53:D2:1176:U:N3	2.46	0.46
7:AG:112:ASP:OD1	7:AG:113:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:40:ILE:HD11	52:D1:1124:G:H4'	1.97	0.46
16:AP:63:CYS:SG	16:AP:73:THR:HG23	2.56	0.46
45:BS:19:PHE:CE2	45:BS:83:ILE:HG21	2.51	0.46
50:BX:81:ARG:NH2	53:D2:300:A:O5'	2.49	0.46
52:D1:565:U:OP2	52:D1:566:G:O2'	2.32	0.46
52:D1:1347:G:N2	52:D1:1374:A:OP2	2.48	0.46
3:AC:10:LEU:HD23	3:AC:62:ARG:HD2	1.98	0.46
8:AH:4:GLN:OE1	52:D1:1130:A:O2'	2.30	0.46
35:BE:33:ILE:HG23	35:BE:155:ILE:HG22	1.98	0.46
53:D2:2061:G:O2'	53:D2:2062:A:OP2	2.33	0.46
53:D2:2467:C:H2'	53:D2:2468:A:O4'	2.15	0.46
8:AH:34:LEU:O	8:AH:39:GLY:N	2.41	0.46
13:AM:29:ILE:O	13:AM:34:ASN:ND2	2.43	0.46
30:B9:19:ARG:O	30:B9:22:VAL:HG22	2.16	0.46
38:BK:125:THR:O	38:BK:129:GLU:OE1	2.34	0.46
50:BX:6:ARG:NH2	53:D2:99:U:O2	2.48	0.46
53:D2:1495:A:N3	53:D2:1578:U:O2'	2.41	0.46
54:D3:14:U:OP2	54:D3:70:C:O2'	2.33	0.46
54:D3:40:U:N3	54:D3:44:G:OP2	2.48	0.46
1:AA:213:LEU:HD12	1:AA:214:GLY:N	2.31	0.45
2:AB:82:ASP:OD1	2:AB:83:VAL:N	2.49	0.45
28:B7:30:VAL:HG22	28:B7:33:ARG:HH22	1.81	0.45
32:BB:76:VAL:HG12	32:BB:114:GLN:OE1	2.16	0.45
54:D3:30:C:H1'	54:D3:57:A:H61	1.81	0.45
13:AM:8:ARG:NH2	52:D1:1217:C:OP1	2.49	0.45
35:BE:142:TYR:HA	35:BE:145:VAL:HG12	1.99	0.45
40:BN:114:LYS:O	40:BN:118:LEU:HD12	2.16	0.45
47:BU:4:VAL:O	47:BU:39:LEU:N	2.49	0.45
8:AH:35:GLU:OE1	8:AH:35:GLU:N	2.47	0.45
49:BW:21:SER:O	49:BW:24:MET:N	2.44	0.45
53:D2:971:G:OP2	53:D2:974:G:N2	2.49	0.45
32:BB:259:ASN:C	32:BB:259:ASN:HD22	2.24	0.45
45:BS:29:VAL:HG13	45:BS:79:VAL:HG12	1.99	0.45
53:D2:2319:G:HO2'	53:D2:2320:U:H6	1.63	0.45
2:AB:84:GLU:OE2	2:AB:87:ARG:NH1	2.50	0.45
3:AC:96:ARG:NH2	3:AC:98:ASP:OD2	2.49	0.45
28:B7:19:ARG:NE	53:D2:125:A:OP2	2.43	0.45
52:D1:297:G:N2	52:D1:300:A:OP2	2.46	0.45
53:D2:974:G:H8	53:D2:990:A:H62	1.63	0.45
53:D2:1475:G:O2'	53:D2:1476:U:P	2.75	0.45
8:AH:113:LYS:HZ1	52:D1:1367:C:P	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D2:1071:G:N2	53:D2:1089:A:HO2'	2.15	0.45
9:AI:92:LEU:HD23	9:AI:92:LEU:H	1.81	0.45
12:AL:92:ARG:NH2	53:D2:888:C:O5'	2.50	0.45
20:AT:23:GLU:O	20:AT:24:LYS:HG2	2.17	0.45
22:B1:36:ARG:NH2	53:D2:2199:A:OP1	2.50	0.45
31:BA:188:ASN:OD1	31:BA:189:LEU:N	2.49	0.45
32:BB:257:ARG:NH1	53:D2:1799:G:OP1	2.47	0.45
35:BE:15:LEU:HD21	35:BE:168:LEU:HB3	1.98	0.45
35:BE:133:GLU:HG3	35:BE:135:ILE:HG22	1.99	0.45
1:AA:81:ASP:OD2	1:AA:82:ALA:N	2.49	0.45
3:AC:69:ARG:NH1	52:D1:401:C:OP2	2.49	0.45
45:BS:59:THR:CG2	45:BS:72:VAL:HG12	2.39	0.45
47:BU:36:ALA:N	47:BU:37:GLU:OE1	2.49	0.45
53:D2:1417:C:HO2'	53:D2:1587:G:HO2'	1.65	0.45
53:D2:1864:U:OP1	53:D2:2410:G:O2'	2.33	0.45
31:BA:27:ILE:HD11	31:BA:185:LEU:HD23	1.99	0.45
36:BF:32:LEU:HB3	36:BF:74:MET:HE3	1.98	0.45
49:BW:29:THR:HG22	49:BW:86:THR:CB	2.46	0.45
52:D1:890:G:O2'	52:D1:891:U:P	2.75	0.45
11:AK:74:GLN:O	11:AK:74:GLN:HG2	2.17	0.45
18:AR:66:VAL:HG23	18:AR:67:GLY:N	2.32	0.45
28:B7:30:VAL:HG22	28:B7:33:ARG:NH2	2.32	0.45
32:BB:244:VAL:HG12	32:BB:250:GLN:HA	1.99	0.45
52:D1:62:U:OP1	52:D1:385:C:O2'	2.35	0.45
52:D1:195:A:O2'	52:D1:196:A:O4'	2.19	0.45
52:D1:811:C:O2'	52:D1:901:A:N1	2.50	0.45
53:D2:2406:A:OP2	53:D2:2411:A:N6	2.46	0.45
2:AB:9:ILE:HG23	2:AB:10:ARG:HG3	1.98	0.44
16:AP:17:GLU:OE2	52:D1:273:U:O2'	2.22	0.44
53:D2:1928:A:H2'	53:D2:1929:G:O4'	2.18	0.44
5:AE:38:ARG:C	5:AE:39:LEU:HD22	2.43	0.44
7:AG:63:LYS:HB3	7:AG:70:VAL:HG21	1.99	0.44
11:AK:67:GLY:O	11:AK:98:ARG:NH1	2.49	0.44
19:AS:3:ILE:O	19:AS:3:ILE:HG13	2.17	0.44
39:BM:27:ARG:NH1	53:D2:1140:C:O3'	2.50	0.44
48:BV:33:LEU:O	48:BV:37:THR:OG1	2.33	0.44
12:AL:6:ILE:HG23	12:AL:7:ASN:N	2.32	0.44
9:AI:65:TYR:HB3	13:AM:95:LEU:HD21	1.98	0.44
10:AJ:41:LEU:CD1	10:AJ:73:VAL:HG12	2.47	0.44
47:BU:37:GLU:OE1	47:BU:37:GLU:N	2.50	0.44
52:D1:1077:G:N2	52:D1:1080:A:OP2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D2:2126:A:H61	53:D2:2163:A:H1'	1.82	0.44
53:D2:2528:U:O2'	53:D2:2530:A:OP1	2.21	0.44
31:BA:193:LEU:HD21	31:BA:212:VAL:HG21	1.99	0.44
47:BU:55:ASP:OD1	47:BU:56:GLY:N	2.49	0.44
52:D1:1029:U:O2	52:D1:1031:C:O2'	2.32	0.44
8:AH:24:ASN:OD1	8:AH:25:GLY:N	2.45	0.44
9:AI:32:THR:O	9:AI:32:THR:HG23	2.18	0.44
17:AQ:32:ILE:HD11	17:AQ:36:GLY:C	2.42	0.44
23:B2:58:ASN:C	23:B2:58:ASN:HD22	2.26	0.44
37:BI:55:GLU:OE1	37:BI:55:GLU:N	2.47	0.44
41:BO:30:THR:HG22	53:D2:810:U:O4	2.17	0.44
52:D1:1086:U:H3	52:D1:1099:G:H22	1.66	0.44
1:AA:167:HIS:ND1	1:AA:168:GLU:OE2	2.51	0.44
4:AD:133:ILE:H	4:AD:133:ILE:HD12	1.82	0.44
8:AH:34:LEU:N	8:AH:34:LEU:HD12	2.33	0.44
9:AI:15:HIS:HA	9:AI:18:ILE:HG22	1.98	0.44
40:BN:121:GLU:OE2	45:BS:64:SER:OG	2.30	0.44
52:D1:976:G:OP2	52:D1:1358:U:O2'	2.35	0.44
3:AC:58:GLN:O	3:AC:62:ARG:HG2	2.17	0.44
38:BK:132:ALA:HA	38:BK:135:MET:HE2	1.98	0.44
46:BT:108:LEU:HA	47:BU:48:LYS:HZ3	1.83	0.44
52:D1:2:A:N6	52:D1:3:A:N1	2.66	0.44
53:D2:239:C:O2'	53:D2:622:G:O2'	2.36	0.44
20:AT:39:LYS:N	20:AT:40:PRO:HD2	2.33	0.44
34:BD:154:ASP:OD2	34:BD:155:GLU:N	2.51	0.44
40:BN:90:ASN:OD1	40:BN:91:SER:N	2.51	0.44
41:BO:43:GLY:N	53:D2:671:C:OP1	2.47	0.44
35:BE:11:VAL:HG21	35:BE:172:PHE:CE1	2.53	0.43
52:D1:509:A:N3	52:D1:543:U:O2'	2.37	0.43
52:D1:652:U:HO2'	52:D1:653:U:P	2.41	0.43
53:D2:2033:A:O2'	53:D2:2035:G:OP2	2.23	0.43
8:AH:27:ILE:HG23	8:AH:62:LEU:HD21	2.00	0.43
8:AH:90:ASP:OD1	8:AH:92:SER:OG	2.28	0.43
44:BR:25:ARG:NH2	54:D3:8:C:O3'	2.47	0.43
47:BU:48:LYS:HG2	47:BU:49:ILE:H	1.82	0.43
53:D2:859:G:O2'	53:D2:860:U:P	2.75	0.43
53:D2:1930:G:O2'	53:D2:1931:U:P	2.76	0.43
41:BO:2:ARG:O	41:BO:5:THR:OG1	2.36	0.43
53:D2:577:G:O2'	53:D2:1254:A:OP1	2.37	0.43
53:D2:1173:U:O2	53:D2:1177:G:C6	2.72	0.43
53:D2:1211:C:HO2'	53:D2:1212:G:P	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:80:LEU:HD11	4:AD:95:MET:HE2	2.00	0.43
38:BK:112:LYS:O	38:BK:124:MET:HE3	2.17	0.43
43:BQ:22:ARG:HG3	43:BQ:70:THR:HA	1.99	0.43
6:AF:47:GLU:OE2	6:AF:48:THR:OG1	2.32	0.43
13:AM:42:ASN:OD1	13:AM:43:ALA:N	2.51	0.43
19:AS:66:ILE:HD12	19:AS:70:LYS:HD3	2.01	0.43
37:BI:47:PHE:O	37:BI:52:ALA:N	2.44	0.43
42:BP:33:LEU:HD13	42:BP:117:PHE:HB3	2.01	0.43
42:BP:57:VAL:O	42:BP:58:LYS:HG2	2.18	0.43
52:D1:1266:G:N2	52:D1:1269:A:OP2	2.43	0.43
1:AA:93:HIS:ND1	1:AA:145:ASN:O	2.48	0.43
19:AS:27:MET:O	19:AS:31:ILE:HD12	2.19	0.43
42:BP:53:MET:HE2	42:BP:117:PHE:CD1	2.53	0.43
47:BU:6:GLN:OE1	47:BU:10:LYS:N	2.52	0.43
19:BG:71:LYS:NZ	53:D2:614:A:N7	2.63	0.43
51:BY:45:ASP:OD2	51:BY:45:ASP:N	2.51	0.43
52:D1:677:U:H3	52:D1:713:G:H22	1.66	0.43
53:D2:1964:G:O2'	53:D2:1967:C:OP2	2.31	0.43
53:D2:2031:A:N3	53:D2:2455:G:O2'	2.43	0.43
20:AT:16:ARG:O	20:AT:20:ARG:NH1	2.52	0.43
42:BP:26:VAL:HG13	42:BP:26:VAL:O	2.19	0.43
49:BW:2:ILE:HG21	53:D2:144:A:H4'	2.01	0.43
19:AS:31:ILE:HD12	19:AS:31:ILE:H	1.84	0.43
32:BB:251:THR:OG1	32:BB:252:LYS:N	2.52	0.43
35:BE:135:ILE:HD11	35:BE:142:TYR:N	2.34	0.43
36:BF:16:VAL:HG12	36:BF:25:ILE:HG12	2.01	0.43
43:BQ:57:THR:HG23	43:BQ:62:ASN:ND2	2.34	0.43
1:AA:122:ASP:OD1	1:AA:122:ASP:N	2.51	0.42
52:D1:1347:G:HO2'	52:D1:1348:U:P	2.42	0.42
5:AE:5:GLU:HA	5:AE:63:ASN:HA	2.01	0.42
12:AL:6:ILE:HG23	12:AL:7:ASN:H	1.84	0.42
15:AO:70:ARG:NH1	52:D1:375:U:OP1	2.49	0.42
20:AT:33:ARG:HG3	20:AT:34:ARG:HG2	2.01	0.42
31:BA:63:THR:HG23	31:BA:163:TYR:HE2	1.84	0.42
35:BE:90:LEU:HD12	35:BE:94:ARG:HB3	2.01	0.42
53:D2:1056:G:N1	53:D2:1102:C:OP2	2.40	0.42
4:AD:98:ALA:O	4:AD:101:GLY:N	2.51	0.42
38:BK:131:THR:HG22	38:BK:135:MET:CE	2.49	0.42
52:D1:673:A:H2'	52:D1:674:G:C8	2.53	0.42
20:AT:46:ARG:HH11	52:D1:1533:C:H42	1.66	0.42
35:BE:70:ARG:NE	53:D2:2298:A:OP1	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BQ:32:GLU:HG2	43:BQ:115:LEU:HD12	2.00	0.42
53:D2:1395:A:O2'	53:D2:1397:U:OP2	2.25	0.42
53:D2:2140:G:N1	53:D2:2152:G:N7	2.68	0.42
53:D2:2375:G:N2	53:D2:2378:A:OP2	2.45	0.42
10:AJ:22:ILE:HD13	10:AJ:31:VAL:HG13	2.01	0.42
18:AR:42:ASN:OD1	25:B4:66:ILE:HD13	2.19	0.42
23:B2:55:THR:HG21	53:D2:76:C:O2'	2.19	0.42
32:BB:153:LEU:HD23	53:D2:1799:G:N2	2.34	0.42
52:D1:1347:G:O2'	52:D1:1348:U:P	2.77	0.42
6:AF:14:ASP:OD1	6:AF:43:TYR:OH	2.30	0.42
9:AI:88:MET:HE3	9:AI:89:ARG:H	1.84	0.42
17:AQ:24:ASP:OD2	17:AQ:27:THR:OG1	2.15	0.42
45:BS:113:LEU:HD12	45:BS:113:LEU:O	2.20	0.42
53:D2:1326:U:O2'	53:D2:2010:G:O2'	2.35	0.42
2:AB:56:ILE:CD1	2:AB:65:VAL:HG12	2.50	0.42
19:AS:14:GLU:OE2	19:AS:17:ARG:NH2	2.45	0.42
1:AA:30:ILE:HD11	1:AA:38:HIS:ND1	2.35	0.42
36:BF:44:HIS:NE2	36:BF:46:ASP:O	2.52	0.42
52:D1:717:U:O2'	52:D1:734:G:O4'	2.32	0.42
53:D2:372:G:O2'	53:D2:373:U:P	2.76	0.42
3:AC:99:ASN:OD1	3:AC:110:ARG:NH1	2.52	0.42
4:AD:40:ASP:OD1	4:AD:42:ASN:N	2.53	0.42
6:AF:61:PHE:CD1	6:AF:123:LEU:HD21	2.54	0.42
13:AM:25:GLU:HA	13:AM:28:ALA:HB3	2.02	0.42
38:BK:72:THR:HG21	38:BK:112:LYS:HG2	2.02	0.42
53:D2:1329:U:OP2	53:D2:1330:C:N4	2.49	0.42
53:D2:2182:U:H2'	53:D2:2183:A:N9	2.35	0.42
1:AA:142:LYS:O	1:AA:145:ASN:OD1	2.38	0.42
40:BN:58:LEU:HD11	40:BN:86:LEU:HD23	2.01	0.42
5:AE:94:HIS:O	5:AE:94:HIS:ND1	2.53	0.41
6:AF:4:ARG:HE	6:AF:5:VAL:H	1.69	0.41
33:BC:151:THR:HB	33:BC:152:PRO:HD3	2.01	0.41
38:BK:41:PHE:HZ	38:BK:54:ILE:HD11	1.84	0.41
39:BM:7:LYS:HB2	39:BM:10:THR:HG22	2.03	0.41
52:D1:246:A:C2	52:D1:282:A:C5	3.07	0.41
53:D2:458:G:O2'	53:D2:459:U:P	2.78	0.41
53:D2:1338:G:O2'	53:D2:1393:A:N1	2.47	0.41
53:D2:2029:G:N1	53:D2:2033:A:OP2	2.49	0.41
53:D2:2175:C:H2'	53:D2:2176:A:C8	2.55	0.41
40:BN:74:GLY:O	45:BS:74:GLN:NE2	2.52	0.41
47:BU:7:SER:OG	47:BU:8:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BE:32:LYS:O	35:BE:33:ILE:HD13	2.20	0.41
35:BE:65:LEU:HD13	54:D3:42:C:C5	2.55	0.41
45:BS:64:SER:OG	45:BS:65:ASN:N	2.52	0.41
53:D2:421:C:O2'	53:D2:422:A:P	2.78	0.41
5:AE:97:THR:HG23	5:AE:97:THR:O	2.21	0.41
23:B2:5:GLU:OE1	23:B2:5:GLU:N	2.42	0.41
24:B3:6:ILE:HD13	24:B3:56:VAL:HG23	2.02	0.41
34:BD:146:VAL:HG12	34:BD:167:VAL:HG12	2.03	0.41
37:BI:135:HIS:HB3	37:BI:138:VAL:HG22	2.01	0.41
39:BM:125:TYR:HH	39:BM:132:HIS:CD2	2.36	0.41
49:BW:58:VAL:HG22	49:BW:85:VAL:HG23	2.02	0.41
5:AE:90:MET:HE1	17:AQ:60:ARG:NH1	2.35	0.41
12:AL:11:HIS:O	12:AL:11:HIS:ND1	2.54	0.41
19:AS:77:ASN:OD1	19:AS:78:LEU:N	2.54	0.41
29:B8:30:HIS:ND1	29:B8:31:ILE:HD12	2.36	0.41
1:AA:96:LEU:H	1:AA:99:MET:HE3	1.85	0.41
9:AI:88:MET:O	9:AI:89:ARG:HD3	2.21	0.41
35:BE:56:LEU:HA	35:BE:59:ILE:HG22	2.03	0.41
41:BO:78:ARG:NH2	53:D2:627:A:OP1	2.54	0.41
50:BX:98:ASN:OD1	50:BX:98:ASN:O	2.38	0.41
52:D1:1125:U:H2'	52:D1:1126:U:H2'	2.02	0.41
52:D1:1130:A:H61	52:D1:1144:G:H1'	1.86	0.41
53:D2:2822:G:O2'	53:D2:2824:C:OP2	2.29	0.41
11:AK:20:VAL:HG23	11:AK:20:VAL:O	2.21	0.41
11:AK:77:SER:O	11:AK:77:SER:OG	2.39	0.41
16:AP:28:VAL:HG22	16:AP:29:LYS:H	1.84	0.41
44:BR:51:ALA:HB3	44:BR:78:VAL:HB	2.03	0.41
6:AF:26:VAL:O	6:AF:30:MET:N	2.53	0.41
7:AG:17:GLN:OE1	7:AG:71:VAL:HG22	2.21	0.41
9:AI:56:HIS:CD2	9:AI:57:VAL:HG13	2.56	0.41
10:AJ:105:ARG:NH2	20:AT:9:GLU:OE1	2.51	0.41
19:AS:56:ILE:O	19:AS:60:GLN:HG2	2.21	0.41
28:B7:1:MET:HE2	53:D2:752:A:OP2	2.21	0.41
33:BC:74:GLU:N	33:BC:74:GLU:OE1	2.54	0.41
35:BE:24:VAL:O	35:BE:27:VAL:HG12	2.21	0.41
35:BE:107:VAL:HG12	35:BE:108:PRO:HD3	2.03	0.41
37:BI:110:VAL:HG22	37:BI:114:GLU:OE2	2.20	0.41
42:BP:82:MET:HE2	42:BP:82:MET:HA	2.02	0.41
52:D1:511:C:O2'	52:D1:512:U:O5'	2.35	0.41
52:D1:552:U:C2	52:D1:553:A:C8	3.09	0.41
52:D1:923:A:O2'	52:D1:1399:C:OP2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D2:421:C:HO2'	53:D2:422:A:P	2.44	0.41
53:D2:631:A:N3	53:D2:2415:G:O2'	2.51	0.41
53:D2:1577:C:H2'	53:D2:1578:U:O4'	2.21	0.41
53:D2:2333:A:H4'	53:D2:2334:U:O5'	2.21	0.41
1:AA:47:PRO:O	1:AA:51:GLU:OE1	2.39	0.41
1:AA:59:ILE:HD12	1:AA:62:ARG:NH2	2.36	0.41
6:AF:68:VAL:O	6:AF:68:VAL:HG12	2.21	0.41
12:AL:71:GLU:HA	12:AL:74:MET:HG2	2.03	0.41
32:BB:145:MET:HE2	32:BB:153:LEU:HD21	2.03	0.41
39:BM:98:GLU:OE2	39:BM:126:ALA:N	2.54	0.41
47:BU:29:THR:O	47:BU:29:THR:HG22	2.20	0.41
3:AC:16:THR:OG1	3:AC:17:ASP:N	2.54	0.40
19:AS:67:HIS:O	19:AS:67:HIS:CG	2.74	0.40
29:B8:8:GLY:O	29:B8:12:ARG:NH1	2.53	0.40
35:BE:116:LEU:H	35:BE:116:LEU:HD23	1.86	0.40
48:BV:5:ALA:HB3	48:BV:54:ALA:HB2	2.03	0.40
53:D2:1081:U:N3	53:D2:1082:U:O4	2.54	0.40
53:D2:1236:G:O2'	53:D2:1237:A:O5'	2.29	0.40
53:D2:2796:U:H3	53:D2:2799:A:H61	1.69	0.40
2:AB:46:LEU:HD12	2:AB:75:VAL:HG12	2.02	0.40
4:AD:24:VAL:HG22	4:AD:25:LYS:N	2.36	0.40
5:AE:3:HIS:ND1	5:AE:92:THR:HG23	2.37	0.40
18:AR:52:ASN:ND2	18:AR:75:PRO:O	2.52	0.40
22:B1:71:ARG:NH1	22:B1:77:TYR:OH	2.51	0.40
28:B7:29:GLN:NE2	53:D2:210:C:OP1	2.54	0.40
30:B9:2:LYS:NZ	53:D2:2478:A:OP2	2.44	0.40
36:BF:63:GLN:HA	36:BF:66:THR:HG22	2.03	0.40
40:BN:35:VAL:O	40:BN:35:VAL:HG22	2.21	0.40
43:BQ:50:PRO:HA	43:BQ:53:THR:HG22	2.03	0.40
44:BR:69:ASP:OD1	44:BR:70:ALA:N	2.54	0.40
1:AA:185:ILE:HD13	1:AA:212:TYR:CD2	2.56	0.40
6:AF:41:ILE:HD11	52:D1:1240:U:O4'	2.22	0.40
6:AF:71:THR:HG1	6:AF:141:HIS:CD2	2.28	0.40
36:BF:1:SER:HG	36:BF:2:ARG:H	1.65	0.40
41:BO:41:ARG:NH2	53:D2:807:U:OP2	2.51	0.40
4:AD:23:THR:HG21	52:D1:1396:A:H2	1.87	0.40
12:AL:16:ILE:HD12	12:AL:16:ILE:H	1.85	0.40
40:BN:64:ARG:NH1	40:BN:102:PRO:O	2.46	0.40
12:AL:2:ARG:HE	35:BE:109:ARG:HH21	1.69	0.40
12:AL:67:ASP:O	12:AL:71:GLU:OE1	2.39	0.40
13:AM:79:SER:O	13:AM:83:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BO:85:VAL:HG13	41:BO:94:THR:O	2.21	0.40
49:BW:21:SER:O	49:BW:25:GLU:OE1	2.40	0.40
49:BW:54:GLU:OE2	49:BW:91:GLN:NE2	2.55	0.40
52:D1:714:G:H2'	52:D1:715:A:C8	2.56	0.40
52:D1:816:A:OP1	52:D1:1526:G:O2'	2.34	0.40
53:D2:2756:U:H4'	53:D2:2757:A:OP1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	223/241 (92%)	207 (93%)	16 (7%)	0	100	100
2	AB	208/233 (89%)	200 (96%)	8 (4%)	0	100	100
3	AC	203/206 (98%)	183 (90%)	20 (10%)	0	100	100
4	AD	155/167 (93%)	134 (86%)	20 (13%)	1 (1%)	21	42
5	AE	98/135 (73%)	83 (85%)	15 (15%)	0	100	100
6	AF	149/179 (83%)	137 (92%)	12 (8%)	0	100	100
7	AG	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AH	125/130 (96%)	110 (88%)	15 (12%)	0	100	100
9	AI	96/103 (93%)	79 (82%)	16 (17%)	1 (1%)	12	28
10	AJ	114/129 (88%)	98 (86%)	16 (14%)	0	100	100
11	AK	121/124 (98%)	102 (84%)	19 (16%)	0	100	100
12	AL	112/118 (95%)	102 (91%)	10 (9%)	0	100	100
13	AM	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
14	AN	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	23
15	AO	80/82 (98%)	72 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	AP	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
17	AQ	63/75 (84%)	61 (97%)	2 (3%)	0	100	100
18	AR	77/92 (84%)	67 (87%)	10 (13%)	0	100	100
19	AS	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
19	BG	67/87 (77%)	66 (98%)	1 (2%)	0	100	100
20	AT	63/71 (89%)	45 (71%)	17 (27%)	1 (2%)	7	16
21	B0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
22	B1	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
23	B2	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
24	B3	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
25	B4	65/70 (93%)	58 (89%)	7 (11%)	0	100	100
26	B5	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
27	B6	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
28	B7	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
29	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	B9	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
31	BA	109/234 (47%)	107 (98%)	2 (2%)	0	100	100
32	BB	269/273 (98%)	249 (93%)	20 (7%)	0	100	100
33	BC	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
34	BD	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	24	46
35	BE	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
36	BF	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
37	BI	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
38	BK	139/142 (98%)	125 (90%)	14 (10%)	0	100	100
39	BM	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
40	BN	120/123 (98%)	108 (90%)	12 (10%)	0	100	100
41	BO	141/144 (98%)	123 (87%)	18 (13%)	0	100	100
42	BP	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
43	BQ	118/127 (93%)	109 (92%)	9 (8%)	0	100	100
44	BR	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
45	BS	112/115 (97%)	105 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	BT	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
47	BU	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	12	28
48	BV	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
49	BW	91/100 (91%)	83 (91%)	8 (9%)	0	100	100
50	BX	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
51	BY	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
All	All	5905/6376 (93%)	5445 (92%)	454 (8%)	6 (0%)	49	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AD	122	VAL
14	AN	46	LYS
47	BU	54	VAL
20	AT	24	LYS
34	BD	83	VAL
9	AI	57	VAL

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	AA	186/199 (94%)	186 (100%)	0	100	100
2	AB	172/190 (90%)	172 (100%)	0	100	100
3	AC	172/173 (99%)	172 (100%)	0	100	100
4	AD	119/126 (94%)	119 (100%)	0	100	100
5	AE	87/116 (75%)	87 (100%)	0	100	100
6	AF	124/147 (84%)	124 (100%)	0	100	100
7	AG	104/105 (99%)	104 (100%)	0	100	100
8	AH	105/107 (98%)	105 (100%)	0	100	100
9	AI	86/90 (96%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	89/99 (90%)	89 (100%)	0	100	100
11	AK	103/104 (99%)	102 (99%)	1 (1%)	68	86
12	AL	92/96 (96%)	92 (100%)	0	100	100
13	AM	83/84 (99%)	83 (100%)	0	100	100
14	AN	76/77 (99%)	76 (100%)	0	100	100
15	AO	65/65 (100%)	65 (100%)	0	100	100
16	AP	74/78 (95%)	74 (100%)	0	100	100
17	AQ	56/65 (86%)	56 (100%)	0	100	100
18	AR	70/79 (89%)	70 (100%)	0	100	100
19	AS	65/66 (98%)	65 (100%)	0	100	100
19	BG	53/66 (80%)	53 (100%)	0	100	100
20	AT	55/61 (90%)	55 (100%)	0	100	100
21	B0	57/63 (90%)	57 (100%)	0	100	100
22	B1	67/68 (98%)	67 (100%)	0	100	100
23	B2	55/55 (100%)	55 (100%)	0	100	100
24	B3	48/49 (98%)	48 (100%)	0	100	100
25	B4	60/62 (97%)	60 (100%)	0	100	100
26	B5	47/48 (98%)	47 (100%)	0	100	100
27	B6	45/49 (92%)	45 (100%)	0	100	100
28	B7	38/38 (100%)	38 (100%)	0	100	100
29	B8	51/52 (98%)	51 (100%)	0	100	100
30	B9	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	BA	97/181 (54%)	97 (100%)	0	100	100
32	BB	216/218 (99%)	216 (100%)	0	100	100
33	BC	164/164 (100%)	164 (100%)	0	100	100
34	BD	165/165 (100%)	165 (100%)	0	100	100
35	BE	148/150 (99%)	148 (100%)	0	100	100
36	BF	137/138 (99%)	137 (100%)	0	100	100
37	BI	114/114 (100%)	114 (100%)	0	100	100
38	BK	109/110 (99%)	109 (100%)	0	100	100
39	BM	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BN	103/104 (99%)	103 (100%)	0	100	100
41	BO	102/103 (99%)	102 (100%)	0	100	100
42	BP	109/109 (100%)	109 (100%)	0	100	100
43	BQ	100/103 (97%)	100 (100%)	0	100	100
44	BR	86/87 (99%)	86 (100%)	0	100	100
45	BS	99/100 (99%)	99 (100%)	0	100	100
46	BT	89/90 (99%)	89 (100%)	0	100	100
47	BU	84/84 (100%)	84 (100%)	0	100	100
48	BV	93/93 (100%)	93 (100%)	0	100	100
49	BW	80/84 (95%)	80 (100%)	0	100	100
50	BX	83/85 (98%)	83 (100%)	0	100	100
51	BY	78/78 (100%)	78 (100%)	0	100	100
All	All	4910/5187 (95%)	4908 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	AK	19	ASN
30	B9	37	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	31	ASN
3	AC	73	ASN
3	AC	125	ASN
3	AC	130	ASN
4	AD	60	GLN
4	AD	131	ASN
8	AH	3	ASN
9	AI	56	HIS
9	AI	99	GLN
11	AK	95	HIS
13	AM	48	GLN
13	AM	70	HIS
14	AN	34	GLN
15	AO	29	ASN

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Mol	Chain	Res	Type
16	AP	44	HIS
19	AS	69	ASN
25	B4	30	HIS
30	B9	13	ASN
32	BB	89	ASN
32	BB	225	ASN
32	BB	250	GLN
33	BC	140	HIS
34	BD	92	HIS
35	BE	51	ASN
36	BF	110	HIS
19	BG	48	GLN
19	BG	61	GLN
38	BK	11	GLN
39	BM	47	HIS
41	BO	54	GLN
42	BP	60	GLN
44	BR	104	GLN
45	BS	40	GLN
46	BT	70	GLN
47	BU	89	HIS
51	BY	51	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	D1	1538/1540 (99%)	215 (13%)	13 (0%)
53	D2	2902/2903 (99%)	447 (15%)	22 (0%)
54	D3	119/120 (99%)	16 (13%)	3 (2%)
All	All	4559/4563 (99%)	678 (14%)	38 (0%)

All (678) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	D1	4	U
52	D1	5	U
52	D1	6	G
52	D1	7	A
52	D1	8	A
52	D1	9	G
52	D1	32	A

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Mol	Chain	Res	Type
52	D1	39	G
52	D1	47	C
52	D1	48	C
52	D1	51	A
52	D1	71	A
52	D1	81	A
52	D1	82	G
52	D1	83	C
52	D1	87	C
52	D1	92	U
52	D1	94	G
52	D1	95	C
52	D1	96	U
52	D1	100	G
52	D1	121	U
52	D1	130	A
52	D1	164	G
52	D1	168	G
52	D1	181	A
52	D1	182	A
52	D1	183	C
52	D1	184	G
52	D1	197	A
52	D1	199	A
52	D1	209	U
52	D1	210	C
52	D1	212	G
52	D1	226	G
52	D1	240	G
52	D1	245	U
52	D1	247	G
52	D1	251	G
52	D1	266	G
52	D1	267	C
52	D1	281	G
52	D1	283	U
52	D1	289	G
52	D1	321	A
52	D1	328	C
52	D1	330	C
52	D1	347	G
52	D1	352	C

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Mol	Chain	Res	Type
52	D1	354	G
52	D1	355	C
52	D1	367	U
52	D1	372	C
52	D1	373	A
52	D1	406	G
52	D1	411	A
52	D1	412	A
52	D1	413	G
52	D1	422	C
52	D1	423	G
52	D1	424	G
52	D1	429	U
52	D1	462	G
52	D1	467	U
52	D1	468	A
52	D1	479	U
52	D1	482	A
52	D1	484	G
52	D1	486	U
52	D1	495	A
52	D1	497	G
52	D1	511	C
52	D1	517	G
52	D1	521	G
52	D1	527	G
52	D1	531	U
52	D1	532	A
52	D1	547	A
52	D1	559	A
52	D1	562	U
52	D1	564	C
52	D1	572	A
52	D1	573	A
52	D1	575	G
52	D1	576	C
52	D1	596	A
52	D1	665	A
52	D1	671	G
52	D1	687	A
52	D1	688	G
52	D1	703	G

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Mol	Chain	Res	Type
52	D1	723	U
52	D1	724	G
52	D1	731	G
52	D1	733	G
52	D1	754	C
52	D1	755	G
52	D1	777	A
52	D1	794	A
52	D1	815	A
52	D1	817	C
52	D1	818	G
52	D1	819	A
52	D1	843	U
52	D1	844	G
52	D1	845	A
52	D1	846	G
52	D1	851	G
52	D1	858	G
52	D1	871	U
52	D1	872	A
52	D1	890	G
52	D1	891	U
52	D1	902	G
52	D1	914	A
52	D1	934	C
52	D1	935	A
52	D1	958	A
52	D1	960	U
52	D1	961	U
52	D1	966	G
52	D1	969	A
52	D1	975	A
52	D1	976	G
52	D1	977	A
52	D1	991	U
52	D1	992	U
52	D1	993	G
52	D1	994	A
52	D1	1004	A
52	D1	1006	G
52	D1	1015	G
52	D1	1020	G

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Mol	Chain	Res	Type
52	D1	1022	A
52	D1	1026	G
52	D1	1028	C
52	D1	1029	U
52	D1	1031	C
52	D1	1032	G
52	D1	1033	G
52	D1	1034	G
52	D1	1045	C
52	D1	1050	G
52	D1	1094	G
52	D1	1101	A
52	D1	1130	A
52	D1	1137	C
52	D1	1138	G
52	D1	1139	G
52	D1	1140	C
52	D1	1158	C
52	D1	1159	U
52	D1	1168	U
52	D1	1182	G
52	D1	1184	G
52	D1	1191	A
52	D1	1196	A
52	D1	1197	A
52	D1	1201	A
52	D1	1202	U
52	D1	1212	U
52	D1	1213	A
52	D1	1225	A
52	D1	1226	C
52	D1	1227	A
52	D1	1238	A
52	D1	1240	U
52	D1	1241	G
52	D1	1257	A
52	D1	1258	G
52	D1	1260	G
52	D1	1268	G
52	D1	1275	A
52	D1	1278	G
52	D1	1280	A

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Mol	Chain	Res	Type
52	D1	1282	C
52	D1	1287	A
52	D1	1300	G
52	D1	1301	U
52	D1	1302	C
52	D1	1312	G
52	D1	1317	C
52	D1	1320	C
52	D1	1322	C
52	D1	1323	G
52	D1	1346	A
52	D1	1347	G
52	D1	1348	U
52	D1	1350	A
52	D1	1353	G
52	D1	1363	A
52	D1	1370	G
52	D1	1395	C
52	D1	1419	G
52	D1	1440	U
52	D1	1446	A
52	D1	1448	C
52	D1	1452	C
52	D1	1453	G
52	D1	1455	G
52	D1	1487	G
52	D1	1492	A
52	D1	1493	A
52	D1	1494	G
52	D1	1497	G
52	D1	1502	A
52	D1	1503	A
52	D1	1506	U
52	D1	1517	G
52	D1	1529	G
52	D1	1530	G
52	D1	1533	C
52	D1	1537	U
52	D1	1538	C
52	D1	1540	U
53	D2	10	A
53	D2	15	G

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Mol	Chain	Res	Type
53	D2	34	U
53	D2	35	G
53	D2	36	G
53	D2	46	G
53	D2	51	G
53	D2	63	A
53	D2	71	A
53	D2	74	A
53	D2	75	G
53	D2	102	U
53	D2	103	A
53	D2	118	A
53	D2	120	U
53	D2	139	U
53	D2	140	C
53	D2	141	G
53	D2	142	A
53	D2	149	A
53	D2	162	U
53	D2	163	C
53	D2	181	A
53	D2	196	A
53	D2	199	A
53	D2	215	G
53	D2	216	A
53	D2	218	A
53	D2	219	A
53	D2	221	A
53	D2	222	A
53	D2	224	U
53	D2	228	C
53	D2	232	G
53	D2	248	G
53	D2	249	C
53	D2	255	A
53	D2	265	A
53	D2	266	G
53	D2	272	A
53	D2	276	U
53	D2	279	A
53	D2	280	U
53	D2	281	C

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Mol	Chain	Res	Type
53	D2	284	U
53	D2	294	A
53	D2	311	A
53	D2	323	C
53	D2	324	A
53	D2	329	G
53	D2	330	A
53	D2	361	G
53	D2	362	A
53	D2	371	A
53	D2	373	U
53	D2	386	G
53	D2	387	U
53	D2	395	U
53	D2	396	G
53	D2	403	U
53	D2	404	A
53	D2	405	U
53	D2	406	G
53	D2	411	G
53	D2	412	A
53	D2	417	C
53	D2	422	A
53	D2	424	G
53	D2	456	C
53	D2	459	U
53	D2	473	G
53	D2	481	G
53	D2	491	G
53	D2	504	A
53	D2	505	A
53	D2	508	A
53	D2	509	C
53	D2	530	G
53	D2	531	C
53	D2	532	A
53	D2	545	U
53	D2	546	U
53	D2	547	A
53	D2	549	G
53	D2	556	A
53	D2	563	A

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Mol	Chain	Res	Type
53	D2	573	U
53	D2	575	A
53	D2	603	A
53	D2	613	A
53	D2	614	A
53	D2	615	U
53	D2	616	A
53	D2	622	G
53	D2	627	A
53	D2	637	A
53	D2	645	C
53	D2	646	U
53	D2	654	A
53	D2	655	A
53	D2	669	G
53	D2	670	A
53	D2	686	U
53	D2	694	U
53	D2	695	G
53	D2	714	U
53	D2	730	A
53	D2	738	G
53	D2	747	C
53	D2	752	A
53	D2	764	A
53	D2	765	C
53	D2	775	G
53	D2	776	G
53	D2	782	A
53	D2	784	G
53	D2	785	G
53	D2	805	G
53	D2	812	C
53	D2	819	A
53	D2	827	U
53	D2	828	U
53	D2	830	G
53	D2	845	A
53	D2	846	U
53	D2	847	U
53	D2	858	G
53	D2	859	G

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Mol	Chain	Res	Type
53	D2	860	U
53	D2	878	A
53	D2	887	U
53	D2	896	A
53	D2	897	C
53	D2	902	C
53	D2	910	A
53	D2	914	G
53	D2	915	C
53	D2	941	A
53	D2	946	C
53	D2	961	C
53	D2	974	G
53	D2	983	A
53	D2	995	C
53	D2	996	A
53	D2	1012	U
53	D2	1013	C
53	D2	1021	A
53	D2	1022	G
53	D2	1023	U
53	D2	1026	G
53	D2	1033	U
53	D2	1045	C
53	D2	1046	A
53	D2	1054	A
53	D2	1057	A
53	D2	1059	G
53	D2	1062	G
53	D2	1064	C
53	D2	1065	U
53	D2	1066	U
53	D2	1067	A
53	D2	1068	G
53	D2	1069	A
53	D2	1071	G
53	D2	1072	C
53	D2	1073	A
53	D2	1075	C
53	D2	1080	A
53	D2	1081	U
53	D2	1083	U

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Mol	Chain	Res	Type
53	D2	1084	A
53	D2	1088	A
53	D2	1089	A
53	D2	1090	A
53	D2	1101	U
53	D2	1103	A
53	D2	1104	C
53	D2	1111	A
53	D2	1112	G
53	D2	1132	U
53	D2	1135	C
53	D2	1136	G
53	D2	1139	G
53	D2	1143	A
53	D2	1172	C
53	D2	1175	A
53	D2	1177	G
53	D2	1178	C
53	D2	1180	U
53	D2	1206	G
53	D2	1212	G
53	D2	1237	A
53	D2	1253	A
53	D2	1256	G
53	D2	1271	G
53	D2	1272	A
53	D2	1300	G
53	D2	1301	A
53	D2	1329	U
53	D2	1330	C
53	D2	1345	C
53	D2	1352	U
53	D2	1365	A
53	D2	1368	G
53	D2	1378	A
53	D2	1379	U
53	D2	1383	A
53	D2	1396	U
53	D2	1397	U
53	D2	1416	G
53	D2	1419	A
53	D2	1420	A

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Mol	Chain	Res	Type
53	D2	1428	C
53	D2	1451	C
53	D2	1454	C
53	D2	1459	G
53	D2	1461	C
53	D2	1476	U
53	D2	1482	G
53	D2	1490	A
53	D2	1491	G
53	D2	1504	A
53	D2	1508	A
53	D2	1509	A
53	D2	1515	A
53	D2	1523	U
53	D2	1524	G
53	D2	1530	G
53	D2	1534	U
53	D2	1535	A
53	D2	1536	C
53	D2	1537	G
53	D2	1555	G
53	D2	1559	U
53	D2	1560	G
53	D2	1569	A
53	D2	1578	U
53	D2	1581	G
53	D2	1583	A
53	D2	1584	U
53	D2	1585	C
53	D2	1608	A
53	D2	1610	A
53	D2	1611	C
53	D2	1634	A
53	D2	1647	U
53	D2	1648	U
53	D2	1663	G
53	D2	1674	G
53	D2	1675	C
53	D2	1677	A
53	D2	1715	G
53	D2	1716	U
53	D2	1729	U

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Mol	Chain	Res	Type
53	D2	1730	C
53	D2	1732	C
53	D2	1735	A
53	D2	1738	G
53	D2	1756	G
53	D2	1758	U
53	D2	1764	C
53	D2	1773	A
53	D2	1776	G
53	D2	1780	A
53	D2	1782	U
53	D2	1791	A
53	D2	1800	C
53	D2	1801	A
53	D2	1802	A
53	D2	1807	G
53	D2	1808	A
53	D2	1816	C
53	D2	1828	G
53	D2	1829	A
53	D2	1833	C
53	D2	1848	A
53	D2	1857	G
53	D2	1870	C
53	D2	1871	A
53	D2	1884	G
53	D2	1901	A
53	D2	1906	G
53	D2	1913	A
53	D2	1914	C
53	D2	1929	G
53	D2	1930	G
53	D2	1931	U
53	D2	1937	A
53	D2	1938	A
53	D2	1955	U
53	D2	1965	C
53	D2	1967	C
53	D2	1970	A
53	D2	1971	U
53	D2	1972	G
53	D2	1991	U

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Mol	Chain	Res	Type
53	D2	1993	U
53	D2	1997	C
53	D2	2022	U
53	D2	2023	C
53	D2	2027	G
53	D2	2031	A
53	D2	2033	A
53	D2	2043	C
53	D2	2055	C
53	D2	2056	G
53	D2	2060	A
53	D2	2061	G
53	D2	2062	A
53	D2	2069	G
53	D2	2093	G
53	D2	2096	C
53	D2	2100	G
53	D2	2101	A
53	D2	2103	C
53	D2	2107	G
53	D2	2110	G
53	D2	2111	U
53	D2	2112	G
53	D2	2118	U
53	D2	2119	A
53	D2	2125	G
53	D2	2126	A
53	D2	2127	G
53	D2	2128	G
53	D2	2131	U
53	D2	2132	U
53	D2	2133	G
53	D2	2136	G
53	D2	2140	G
53	D2	2145	C
53	D2	2147	A
53	D2	2159	G
53	D2	2162	G
53	D2	2163	A
53	D2	2166	U
53	D2	2170	A
53	D2	2171	A

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Mol	Chain	Res	Type
53	D2	2172	U
53	D2	2173	A
53	D2	2175	C
53	D2	2178	C
53	D2	2182	U
53	D2	2184	A
53	D2	2185	U
53	D2	2186	G
53	D2	2187	U
53	D2	2188	U
53	D2	2190	G
53	D2	2192	U
53	D2	2198	A
53	D2	2199	A
53	D2	2204	G
53	D2	2212	A
53	D2	2213	U
53	D2	2214	C
53	D2	2219	U
53	D2	2225	A
53	D2	2226	C
53	D2	2238	G
53	D2	2250	G
53	D2	2278	A
53	D2	2283	C
53	D2	2286	G
53	D2	2287	A
53	D2	2297	A
53	D2	2305	U
53	D2	2309	A
53	D2	2320	U
53	D2	2322	A
53	D2	2325	G
53	D2	2327	A
53	D2	2334	U
53	D2	2336	A
53	D2	2345	G
53	D2	2350	C
53	D2	2361	G
53	D2	2382	G
53	D2	2383	G
53	D2	2385	C

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Mol	Chain	Res	Type
53	D2	2392	A
53	D2	2402	U
53	D2	2403	C
53	D2	2406	A
53	D2	2423	U
53	D2	2424	C
53	D2	2425	A
53	D2	2429	G
53	D2	2430	A
53	D2	2441	U
53	D2	2447	G
53	D2	2448	A
53	D2	2475	C
53	D2	2476	A
53	D2	2478	A
53	D2	2497	A
53	D2	2502	G
53	D2	2503	A
53	D2	2504	U
53	D2	2505	G
53	D2	2518	A
53	D2	2529	G
53	D2	2547	A
53	D2	2554	U
53	D2	2566	A
53	D2	2567	G
53	D2	2572	A
53	D2	2582	G
53	D2	2602	A
53	D2	2603	G
53	D2	2609	U
53	D2	2613	U
53	D2	2615	U
53	D2	2629	U
53	D2	2655	G
53	D2	2656	U
53	D2	2682	A
53	D2	2689	U
53	D2	2690	U
53	D2	2714	G
53	D2	2722	G
53	D2	2733	A

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Mol	Chain	Res	Type
53	D2	2744	G
53	D2	2748	A
53	D2	2764	A
53	D2	2765	A
53	D2	2778	A
53	D2	2779	U
53	D2	2780	G
53	D2	2791	G
53	D2	2797	U
53	D2	2798	U
53	D2	2799	A
53	D2	2800	A
53	D2	2820	A
53	D2	2823	A
53	D2	2833	U
53	D2	2849	U
53	D2	2861	U
53	D2	2867	G
53	D2	2868	A
53	D2	2872	A
53	D2	2880	C
53	D2	2884	U
53	D2	2887	A
53	D2	2891	U
53	D2	2901	C
54	D3	4	C
54	D3	9	G
54	D3	12	C
54	D3	13	G
54	D3	25	U
54	D3	26	C
54	D3	30	C
54	D3	35	C
54	D3	42	C
54	D3	44	G
54	D3	67	G
54	D3	88	C
54	D3	89	U
54	D3	90	C
54	D3	108	A
54	D3	109	A

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	D1	70	U
52	D1	94	G
52	D1	280	C
52	D1	561	U
52	D1	686	U
52	D1	871	U
52	D1	890	G
52	D1	1190	G
52	D1	1201	A
52	D1	1256	A
52	D1	1300	G
52	D1	1347	G
52	D1	1447	A
53	D2	227	A
53	D2	310	A
53	D2	372	G
53	D2	421	C
53	D2	458	G
53	D2	490	C
53	D2	555	G
53	D2	774	G
53	D2	784	G
53	D2	858	G
53	D2	859	G
53	D2	1020	A
53	D2	1211	C
53	D2	1475	G
53	D2	1715	G
53	D2	1930	G
53	D2	2212	A
53	D2	2326	C
53	D2	2333	A
53	D2	2391	G
53	D2	2655	G
53	D2	2832	U
54	D3	3	C
54	D3	66	A
54	D3	88	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

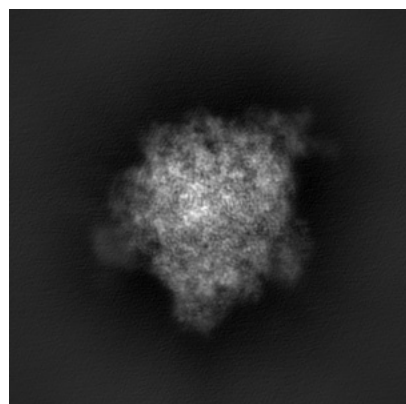
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55178. These allow visual inspection of the internal detail of the map and identification of artifacts.

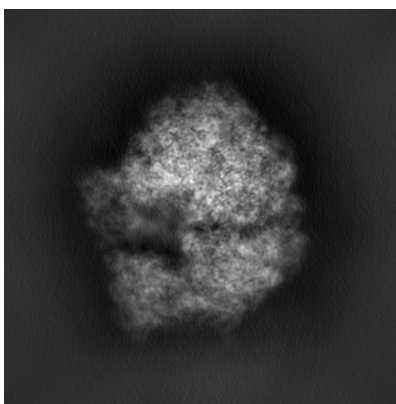
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

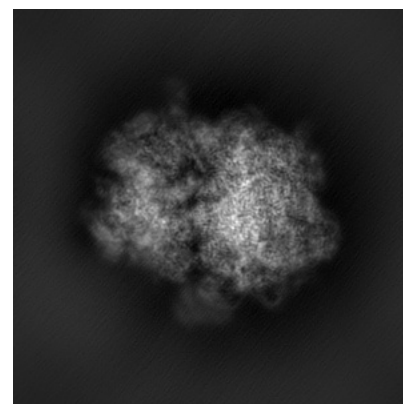
6.1.1 Primary map



X

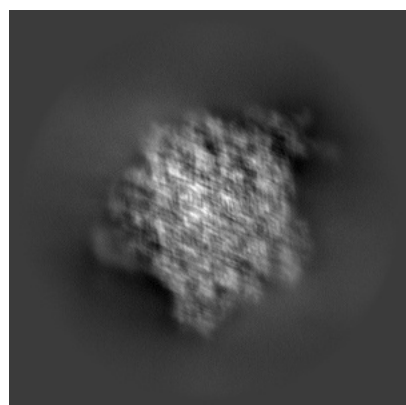


Y

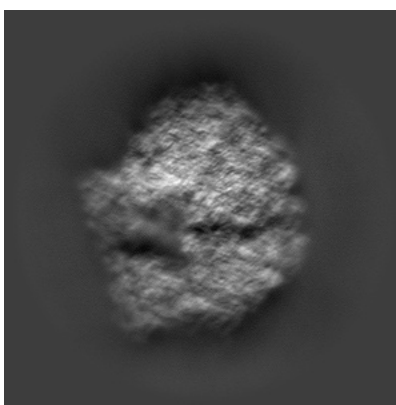


Z

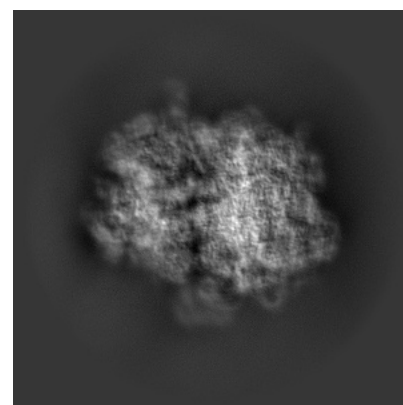
6.1.2 Raw map



X



Y

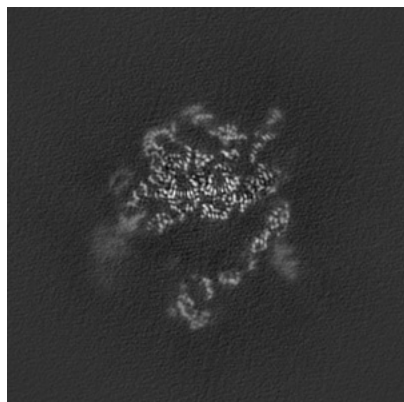


Z

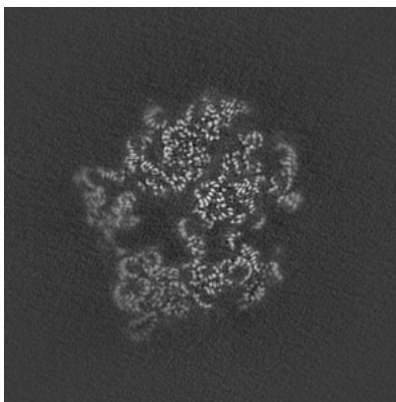
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

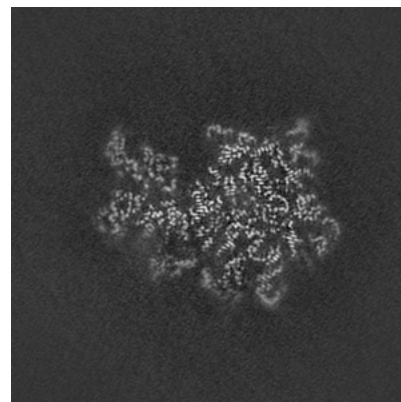
6.2.1 Primary map



X Index: 240

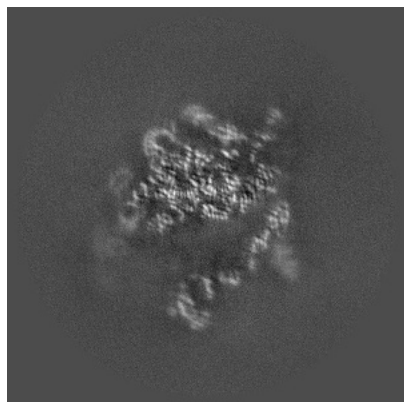


Y Index: 240

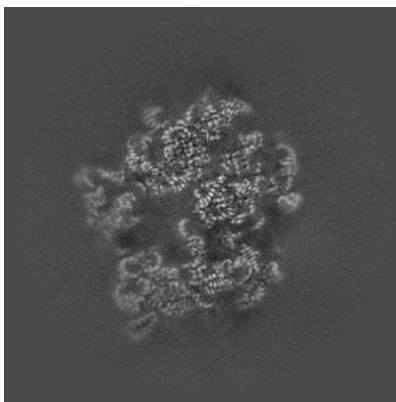


Z Index: 240

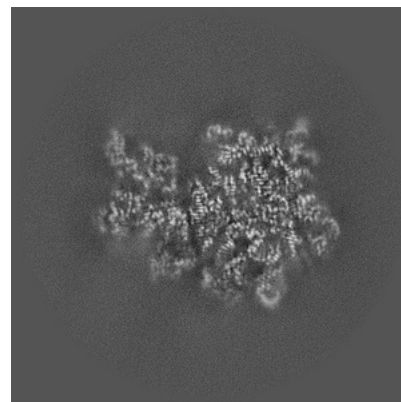
6.2.2 Raw map



X Index: 240



Y Index: 240

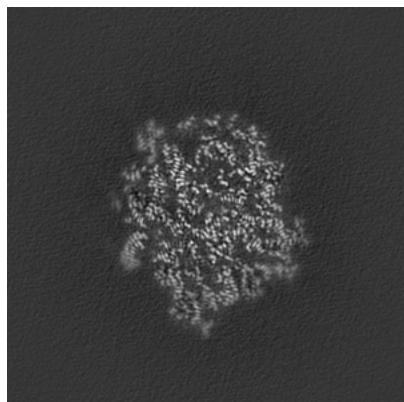


Z Index: 240

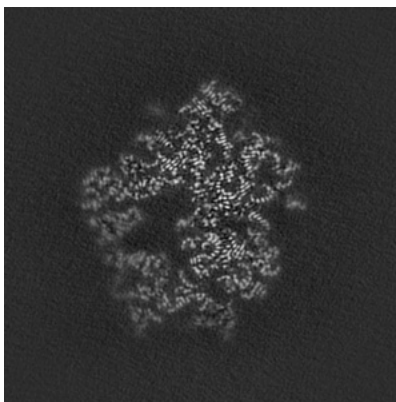
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

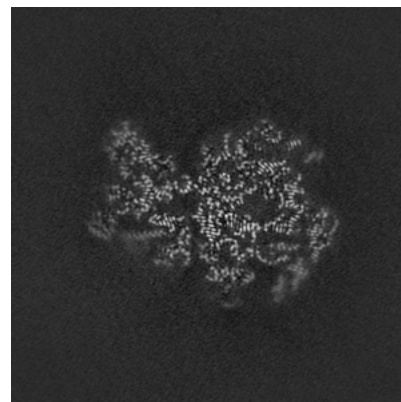
6.3.1 Primary map



X Index: 274

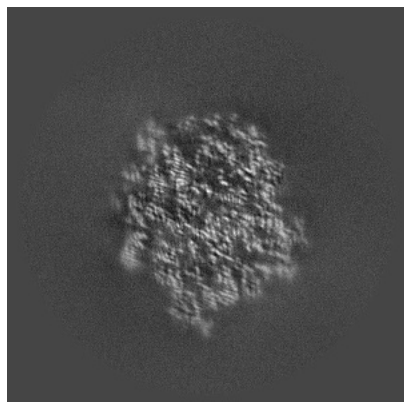


Y Index: 225

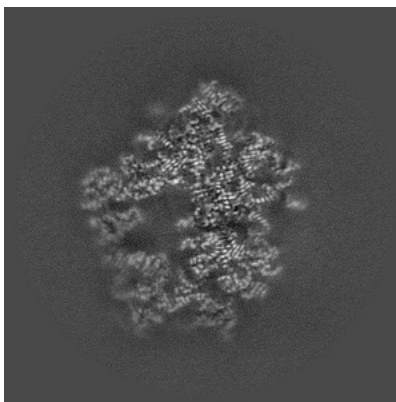


Z Index: 255

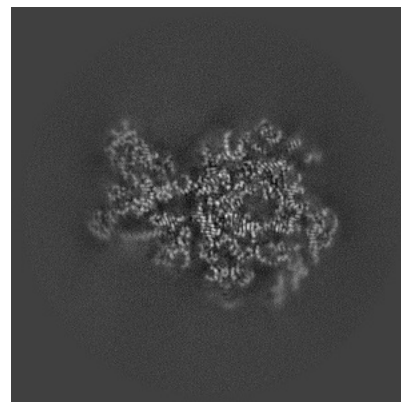
6.3.2 Raw map



X Index: 274



Y Index: 225

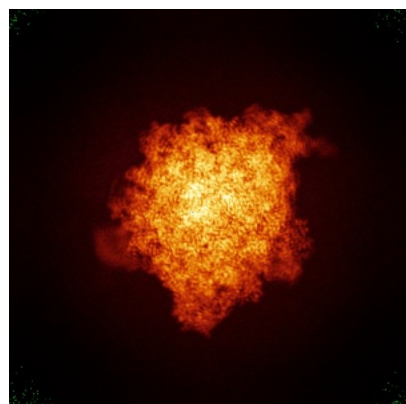


Z Index: 254

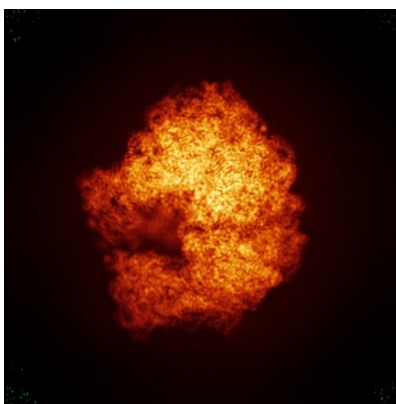
The images above show the largest variance slices of the map in three orthogonal directions.

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

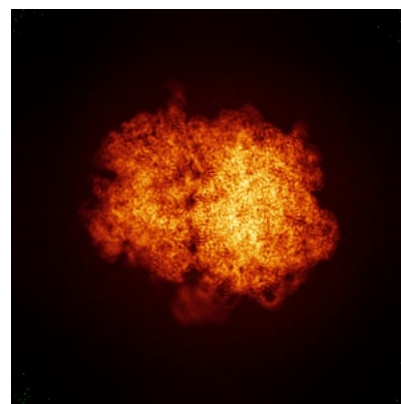
6.4.1 Primary map



X

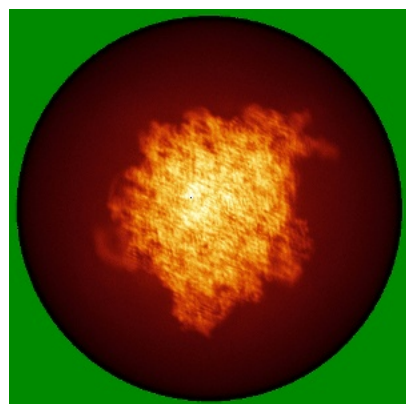


Y

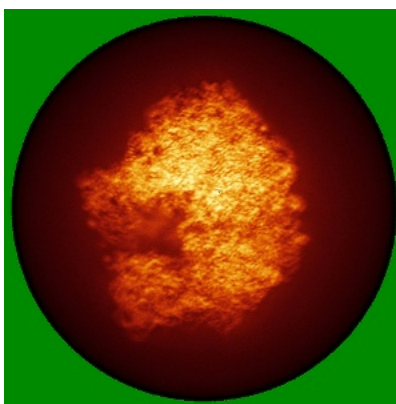


Z

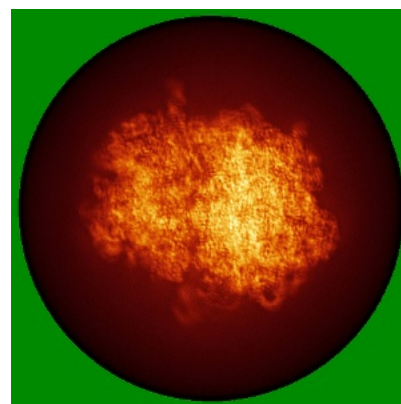
6.4.2 Raw map



X



Y

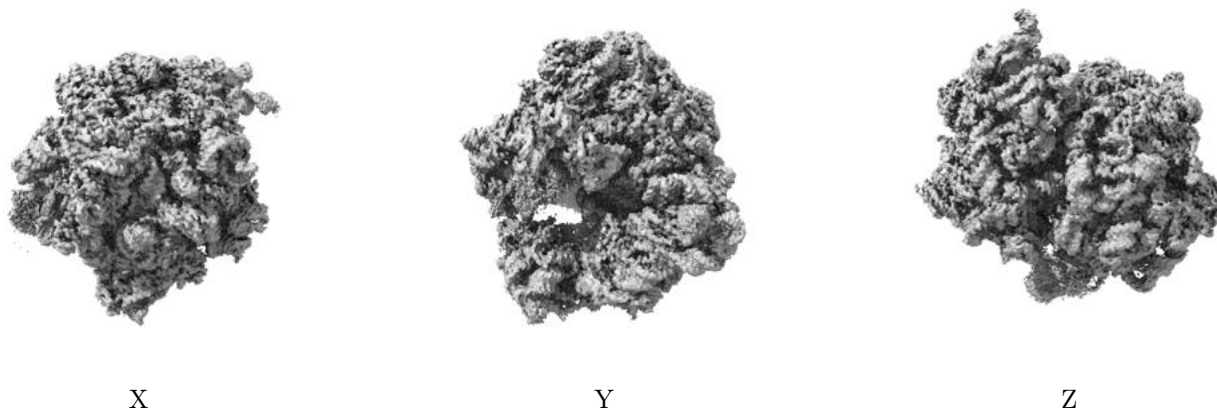


Z

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.

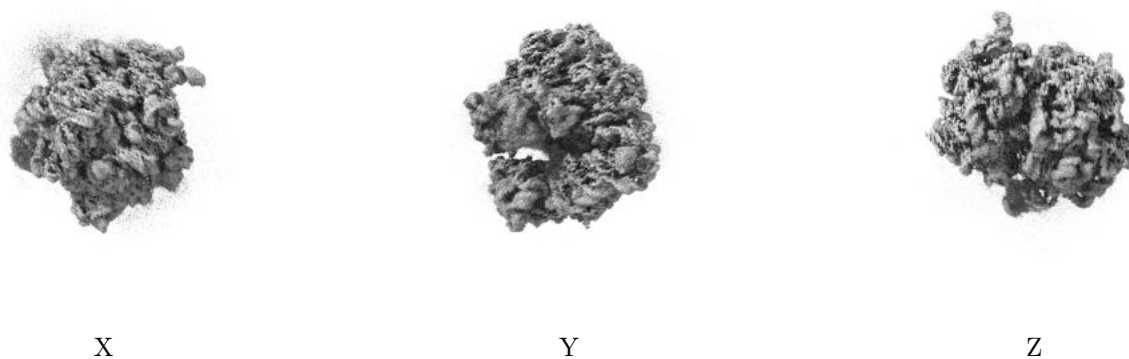
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.3. 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.

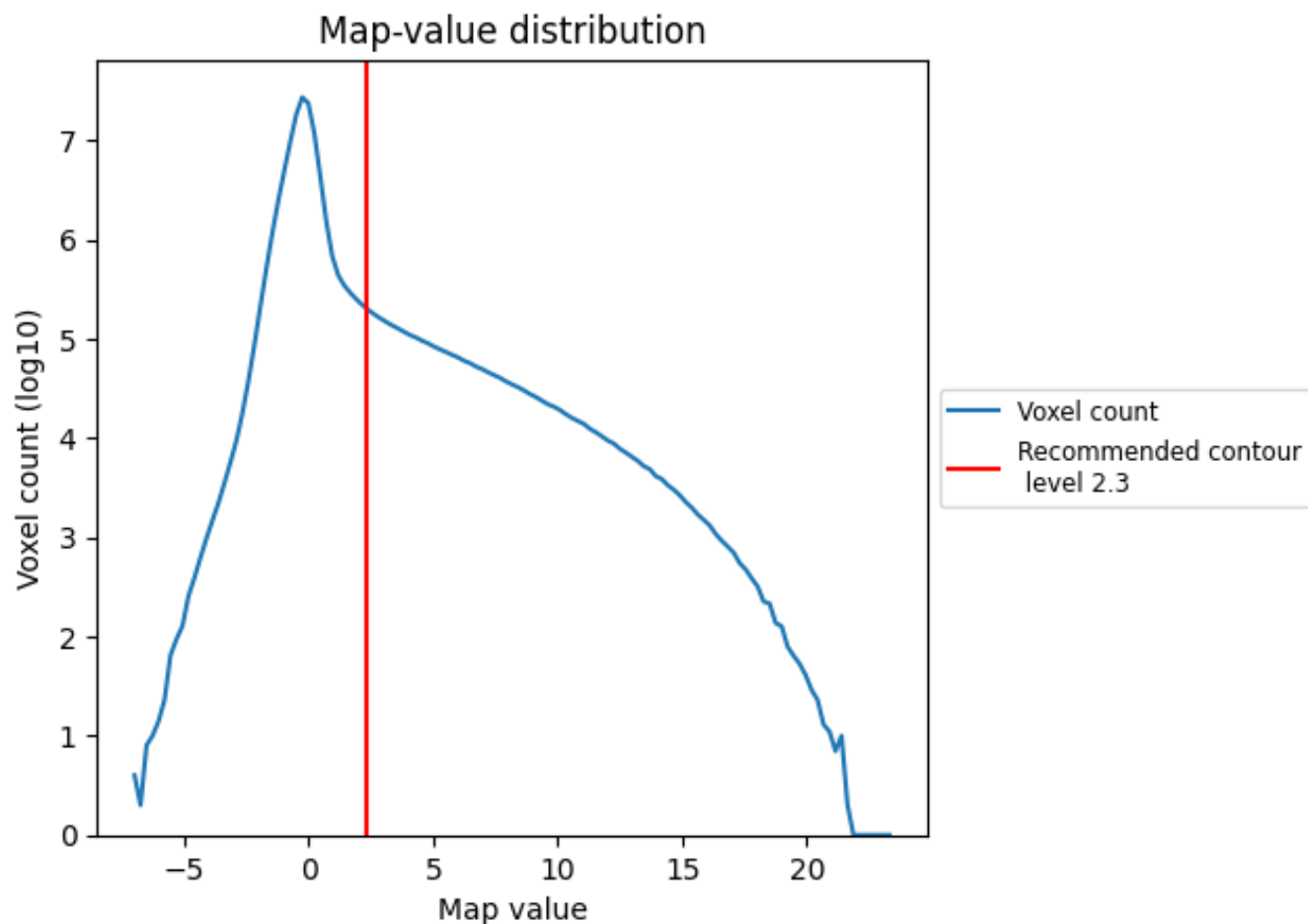
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

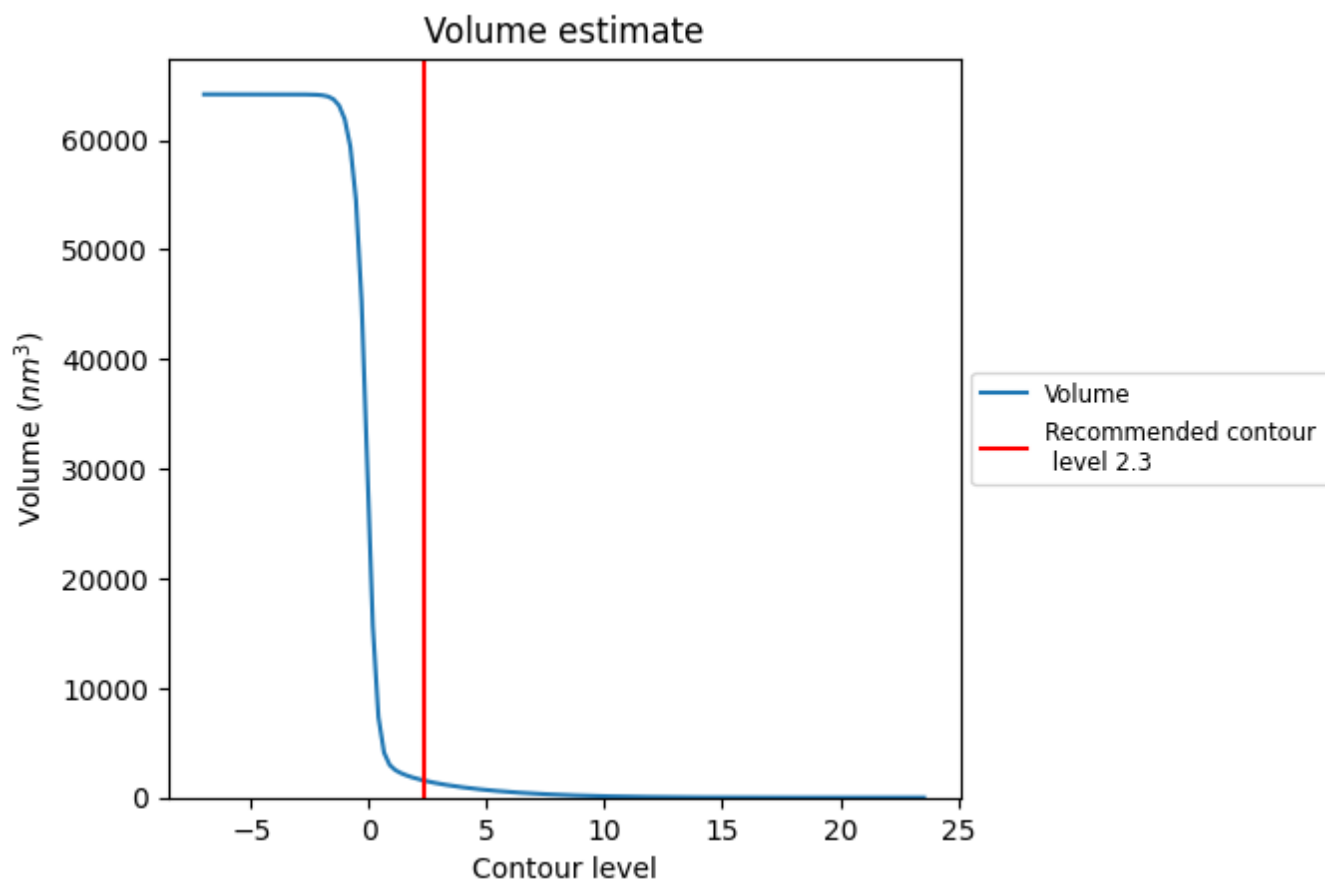
This section contains the results of statistical analysis of the map.

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.

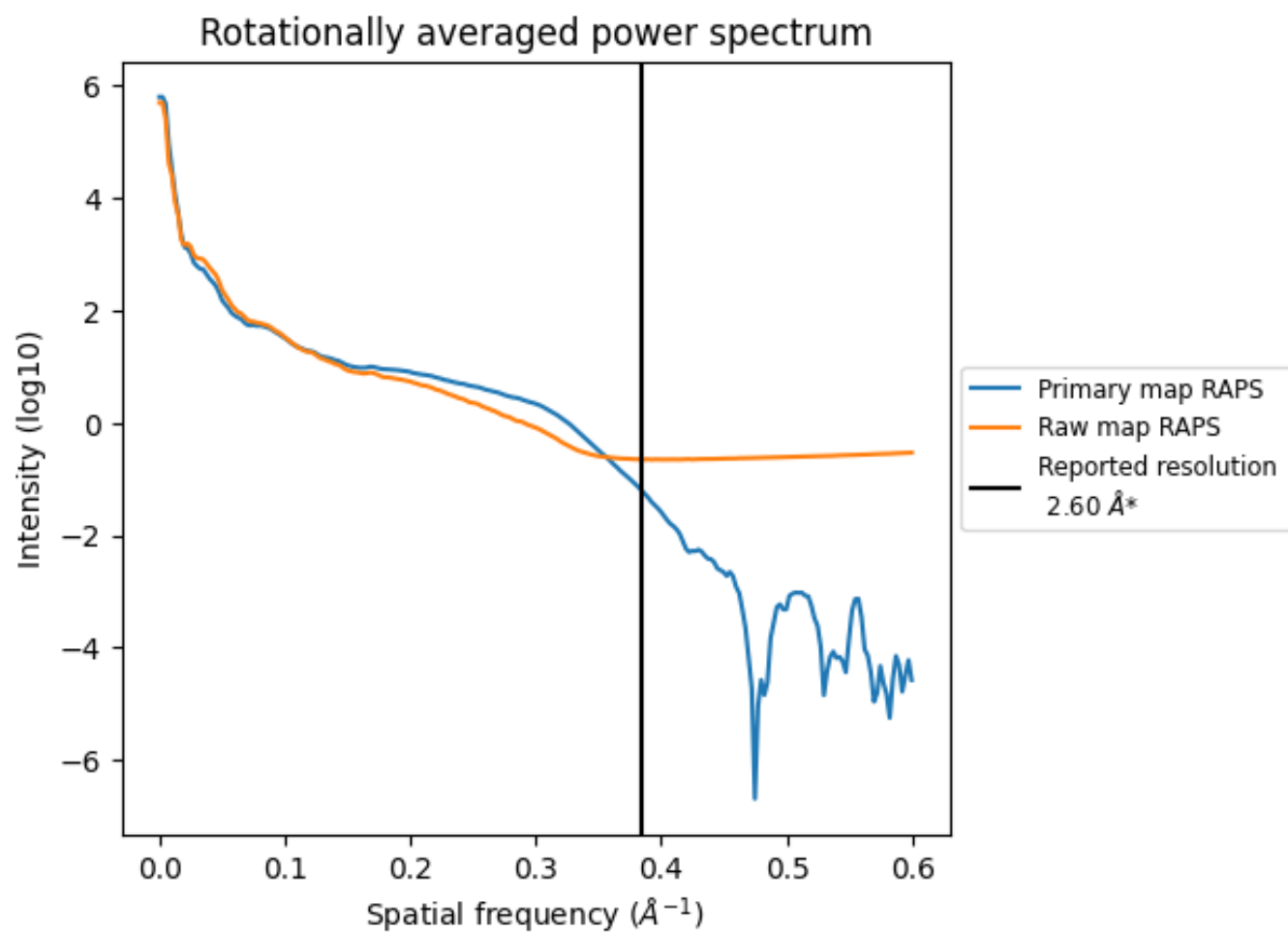
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1570 nm^3 ; this corresponds to an approximate mass of 1418 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 ⓘ

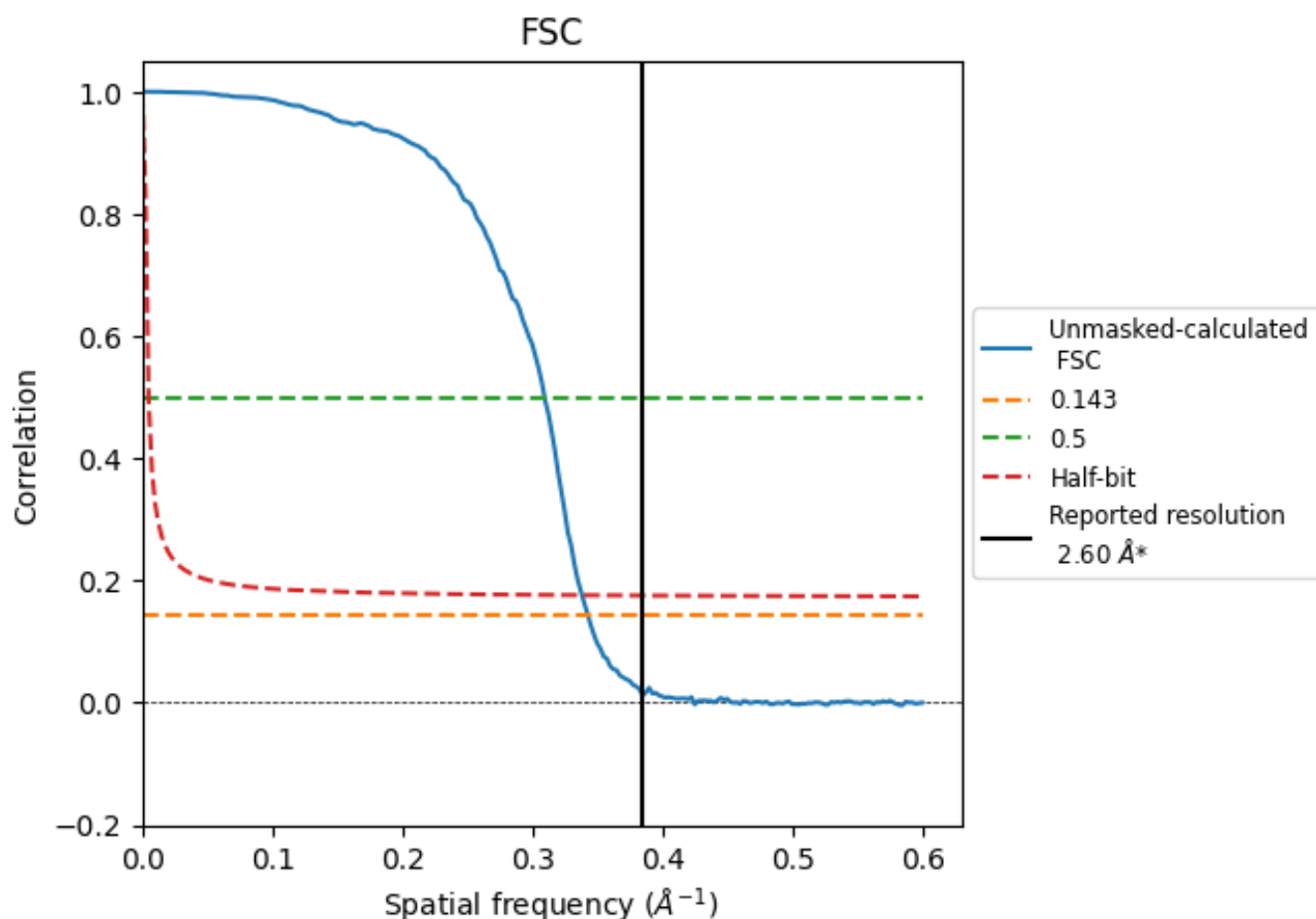


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

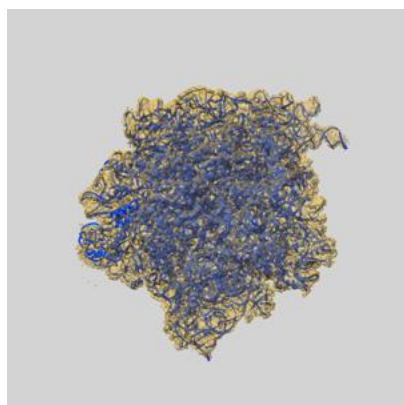
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.92	3.23	2.96

*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 2.92 differs from the reported value 2.6 by more than 10 %

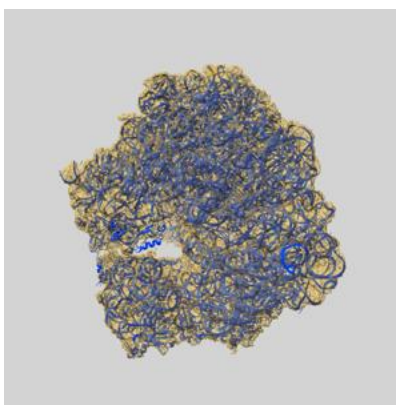
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55178 and PDB model 9SS6. Per-residue inclusion information can be found in section 3 on page 14.

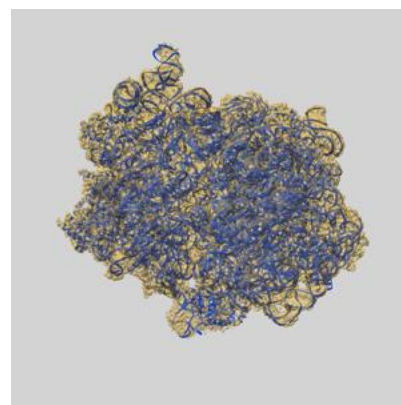
9.1 Map-model overlay [i](#)



X



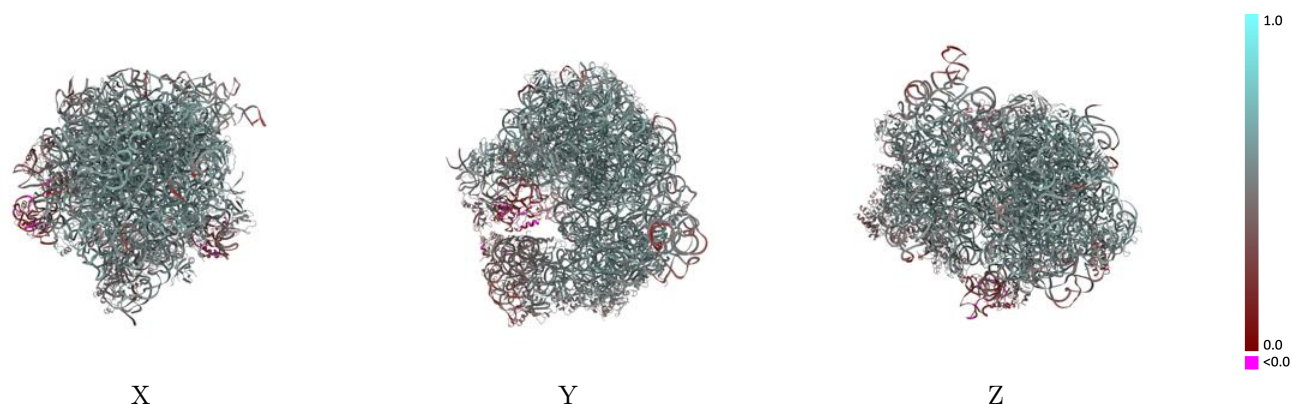
Y



Z

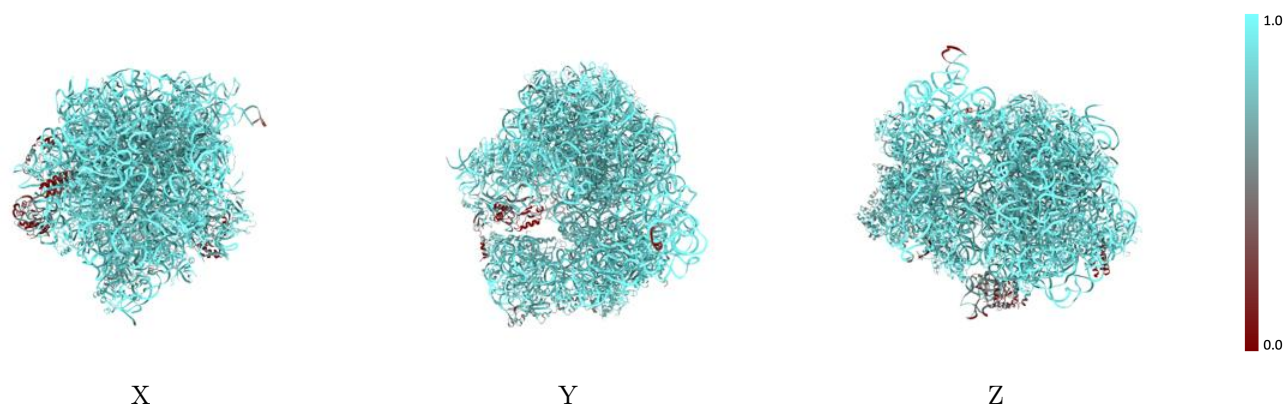
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



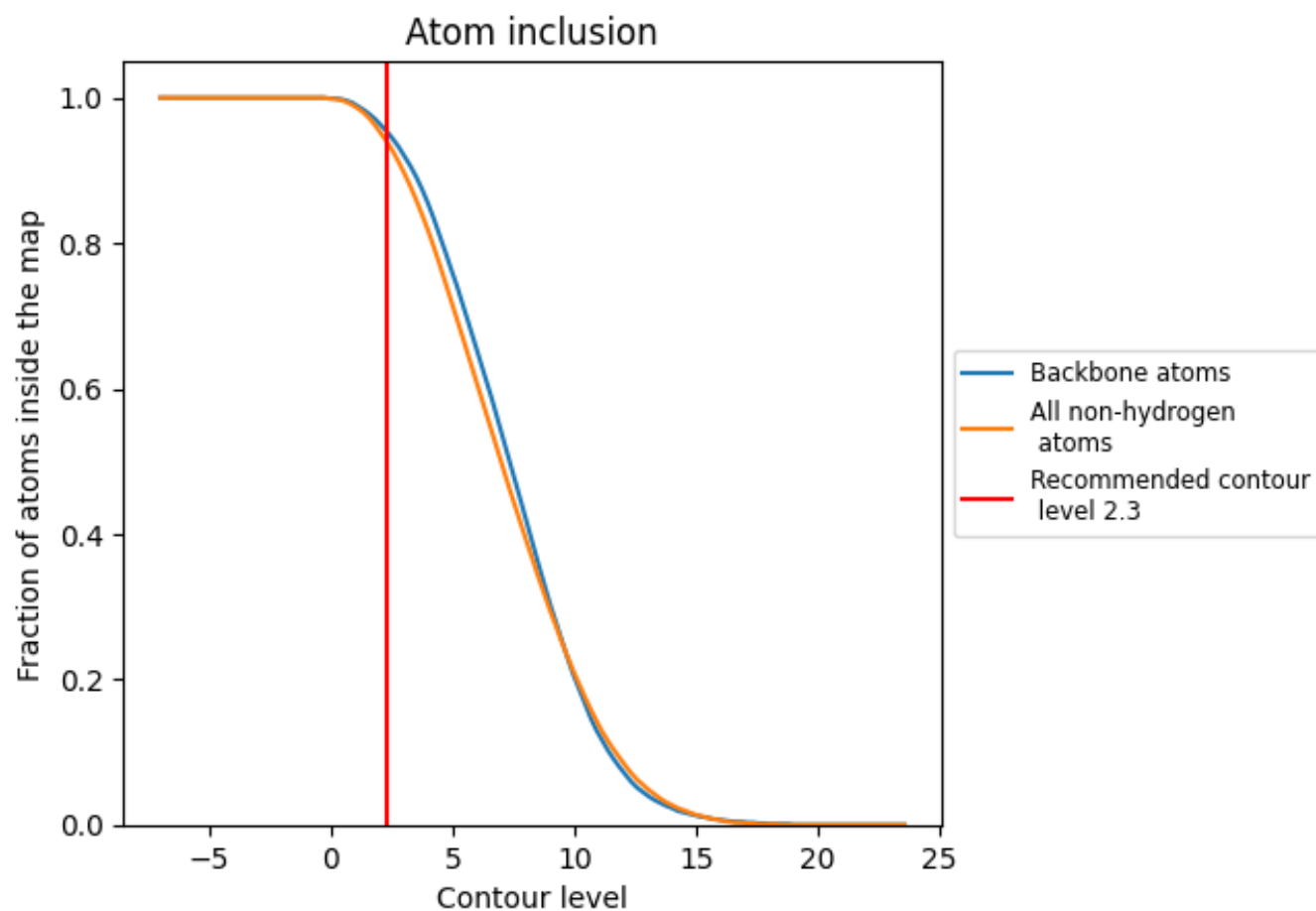
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 94% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.5190
AA	0.7630	0.4520
AB	0.8610	0.5040
AC	0.8880	0.4940
AD	0.9390	0.5270
AE	0.9010	0.4560
AF	0.8690	0.4000
AG	0.9560	0.5440
AH	0.8570	0.3950
AI	0.7310	0.4350
AJ	0.9470	0.5060
AK	0.9360	0.5380
AL	0.8520	0.3790
AM	0.8510	0.4480
AN	0.9450	0.4950
AO	0.9110	0.5250
AP	0.9490	0.5200
AQ	0.8720	0.4820
AR	0.8250	0.3840
AS	0.9080	0.5030
AT	0.7720	0.3680
B0	0.9700	0.5770
B1	0.9570	0.5570
B2	0.8930	0.4650
B3	0.9360	0.5550
B4	0.3550	0.3080
B5	0.9560	0.5650
B6	0.9430	0.5280
B7	0.9750	0.5950
B8	0.9880	0.5950
B9	0.9730	0.5380
BA	0.1710	0.2010
BB	0.9780	0.5770
BC	0.9730	0.5760
BD	0.9140	0.5430



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Chain	Atom inclusion	Q-score
BE	 0.8700	 0.3950
BF	 0.9090	 0.4900
BG	 0.2410	 0.3320
BI	 0.4660	 0.3860
BK	 0.1420	 0.1600
BM	 0.9710	 0.5680
BN	 0.9720	 0.5780
BO	 0.9550	 0.5530
BP	 0.9710	 0.5640
BQ	 0.9780	 0.5730
BR	 0.9200	 0.4880
BS	 0.9540	 0.5720
BT	 0.9680	 0.5790
BU	 0.9300	 0.5410
BV	 0.9610	 0.5710
BW	 0.9130	 0.5240
BX	 0.9230	 0.5240
BY	 0.9320	 0.5170
D1	 0.9780	 0.5130
D2	 0.9770	 0.5440
D3	 0.9900	 0.5040