Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 03:16 pm GMT

PDB ID	:	9HC4
EMDB ID	:	EMD-52036
Title	:	Cryo-EM structure of P. urativorans 70S ribosome with 2 copies of bS20.
Authors	:	Helena-Bueno, K.; Hill, C.H.; Melnikov, S.V.
Deposited on	:	2024-11-08
Resolution	:	3.20 Å(reported)

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

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

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

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

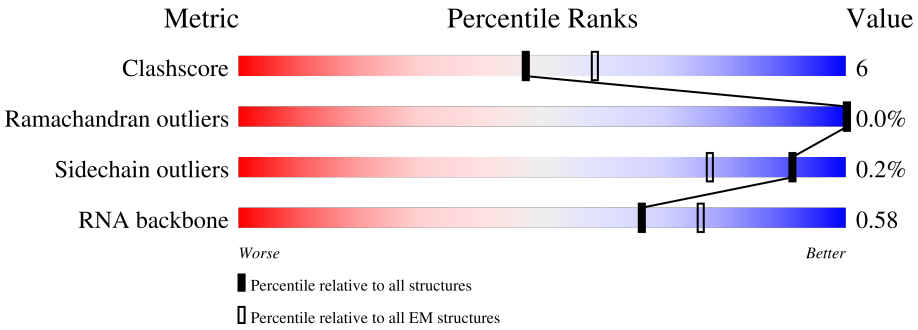
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	F	128	80% 18%
2	C1	166	23% 6% 70%
3	R3	76	62% 12% 26%
4	A4	269	71% 16% 13%
5	E5	171	74% 17% 9%
6	L6	124	92% 6%
7	F7	178	83% 16%

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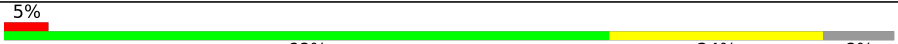
Mol	Chain	Length	Quality of chain
8	E9	200	
9	aA	60	
10	MB	119	
11	UC	219	
12	WD	78	
13	XE	65	
14	RF	109	
15	FG	134	
16	VH	85	
17	TI	105	
18	fJ	93	
19	HK	101	
20	OL	88	
21	MM	118	
22	PO	118	
23	SP	91	
24	BQ	132	
25	GR	177	
26	GS	157	
27	CT	241	
28	KU	129	
29	NV	71	
30	YW	59	
31	IX	142	
32	JY	103	

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Mol	Chain	Length	Quality of chain
33	QZ	91	69% 18% 13%
34	Ba	44	100%
35	Qb	103	100%
36	Nc	116	97%
37	Kd	146	98%
38	Je	122	100%
39	Af	212	100%
40	Lg	137	99%
41	dh	65	94% 5%
42	Oi	130	88% 12%
43	Pj	89	91% 9%
44	bk	51	96%
45	Cl	274	99%
46	Dm	213	100%
47	Sn	116	75% 25%
48	A	88	13% 63% 11% 26%
48	To	88	98%
49	ep	38	100%
50	D8	115	77% 23%
51	iN	1589	76% 18% 5%
52	Z2	2882	68% 24% 6%

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 136434 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 uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	125	948	592	179	176	1	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C1	49	374	244	64	65	1	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	R3	56	457	290	80	87	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A4	233	1807	1138	327	335	7	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E5	156	1151	716	218	211	6	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L6	122	946	583	193	165	5	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F7	177	Total	C	N	O	S	0	0
			1356	870	234	246	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E9	199	Total	C	N	O	S	0	0
			1537	966	282	284	5		

- Molecule 9 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aA	53	Total	C	N	O	S	0	0
			446	267	101	75	3		

- Molecule 10 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	MB	119	Total	C	N	O	S	0	0
			947	587	188	164	8		

- Molecule 11 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UC	96	Total	C	N	O	S	0	0
			750	479	135	135	1		

- Molecule 12 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	WD	76	Total	C	N	O	S	0	0
			618	383	131	101	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	XE	62	Total	C	N	O	S	0	0
			502	307	99	95	1		

- Molecule 14 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	RF	109	Total	C	N	O	S	0	0
			834	521	159	151	3		

- Molecule 15 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	FG	102	Total	C	N	O	S	0	0
			849	535	154	158	2		

- Molecule 16 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	VH	78	Total	C	N	O	S	0	0
			587	365	115	104	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	TI	102	Total	C	N	O	0	0
			784	487	149	148		

- Molecule 18 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	fJ	55	Total	C	N	O	S	0	0
			443	282	74	86	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	HK	100	Total	C	N	O	S	0	0
			811	498	162	144	7		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	OL	86	Total	C	N	O	S	0	0
			694	427	137	128	2		

- Molecule 21 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	MM	110	Total	C	N	O	S	0	0
			858	528	172	155	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	PO	116	Total	C	N	O	S	0	0
			935	586	199	148	2		

- Molecule 23 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SP	80	Total	C	N	O	S	0	0
			637	405	121	108	3		

- Molecule 24 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BQ	131	Total	C	N	O	S	0	0
			974	602	179	187	6		

- Molecule 25 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	GR	173	Total	C	N	O	S	0	0
			1339	836	244	257	2		

- Molecule 26 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	GS	152	Total	C	N	O	S	0	0
			1190	738	230	215	7		

- Molecule 27 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CT	204	Total	C	N	O	S	0	0
			1606	1009	301	290	6		

- Molecule 28 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	KU	114	Total	C	N	O	S	0	0
			836	518	162	155	1		

- Molecule 29 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	NV	57	Total	C	N	O	S	0	0
			472	299	95	77	1		

- Molecule 30 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	YW	56	Total	C	N	O	S	0	0
			438	272	88	76	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	IX	142	Total	C	N	O	S	0	0
			1108	710	198	197	3		

- Molecule 32 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	JY	95	Total	C	N	O	S	0	0
			760	472	145	141	2		

- Molecule 33 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	QZ	79	Total	C	N	O	S	0	0
			632	395	119	116	2		

- Molecule 34 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ba	44	Total	C	N	O	S	0	0
			369	227	89	51	2		

- Molecule 35 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Qb	103	Total	C	N	O	S	0	0
			827	524	153	148	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Nc	113	Total	C	N	O	0	0
			852	530	170	152		

- Molecule 37 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Kd	143	Total	C	N	O	S	1	0
			1053	651	205	194	3		

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Je	122	Total	C	N	O	S	0	0
			937	585	181	166	5		

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Af	211	Total	C	N	O	S	0	0
			1548	954	292	296	6		

- Molecule 40 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lg	137	Total	C	N	O	S	0	0
			1093	697	210	179	7		

- Molecule 41 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	dh	64	Total	C	N	O	S	0	0
			519	326	107	82	4		

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Oi	115	Total 917	C 572	N 184	O 161	0	0

- Molecule 43 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Pj	81	Total 648	C 409	N 126	O 111	S 2	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	bk	49	Total 394	C 254	N 68	O 69	S 3	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Cl	272	Total 2103	C 1302	N 431	O 364	S 6	0	0

- Molecule 46 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Dm	212	Total 1688	C 1058	N 318	O 309	S 3	0	0

- Molecule 47 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Sn	87	Total 690	C 442	N 124	O 122	S 2	0	0

- Molecule 48 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	To	86	Total 675	C 410	N 144	O 119	S 2	0	0
48	A	65	Total 462	C 285	N 93	O 82	S 2	0	0

- Molecule 49 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	ep	38	Total	C	N	O	S	0	0
			298	182	66	46	4		

- Molecule 50 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	D8	115	Total	C	N	O	P	0	0
			2446	1093	436	802	115		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D8	85	U	-	insertion	GB 930356181
D8	88	A	C	variant	GB 930356181

- Molecule 51 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	iN	1503	Total	C	N	O	P	0	0
			32246	14388	5917	10438	1503		

- Molecule 52 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Z2	2705	Total	C	N	O	P	0	0
			58043	25910	10660	18768	2705		

There is a discrepancy between the modelled and reference sequences:

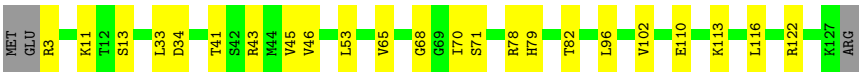
Chain	Residue	Modelled	Actual	Comment	Reference
Z2	1717	U	G	conflict	GB 930356181

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.

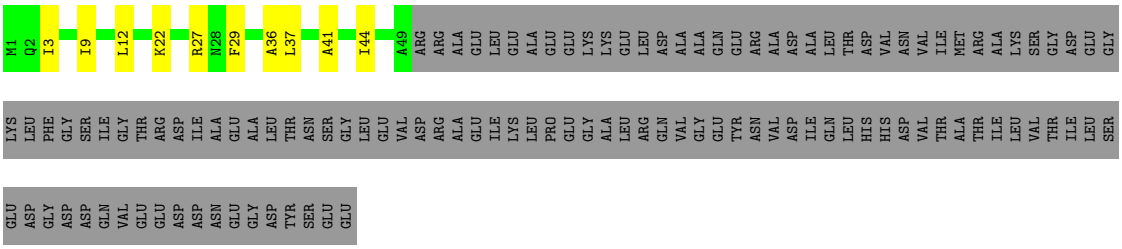
• Molecule 1: Small ribosomal subunit protein uS9

Chain F:



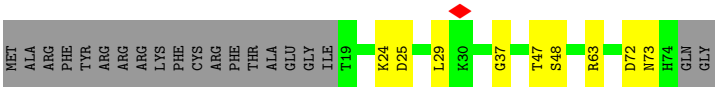
• Molecule 2: Large ribosomal subunit protein bL9

Chain C1:



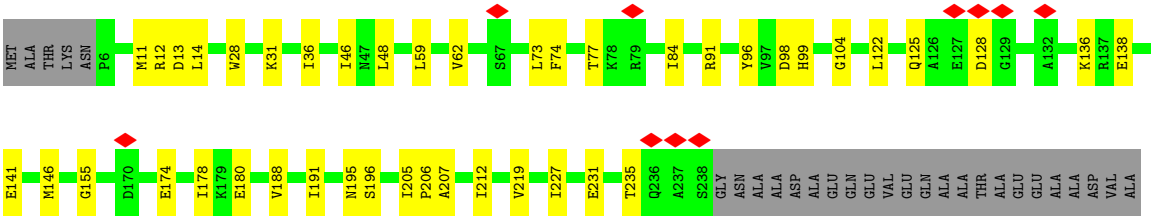
• Molecule 3: Small ribosomal subunit protein bS18

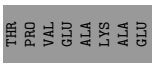
Chain R3:



• Molecule 4: Small ribosomal subunit protein uS2

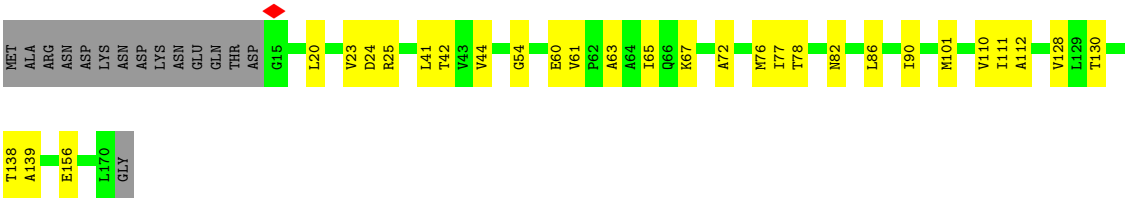
Chain A4:





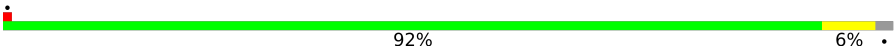
• Molecule 5: Small ribosomal subunit protein uS5

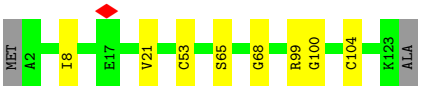
Chain E5:



• Molecule 6: Small ribosomal subunit protein uS12

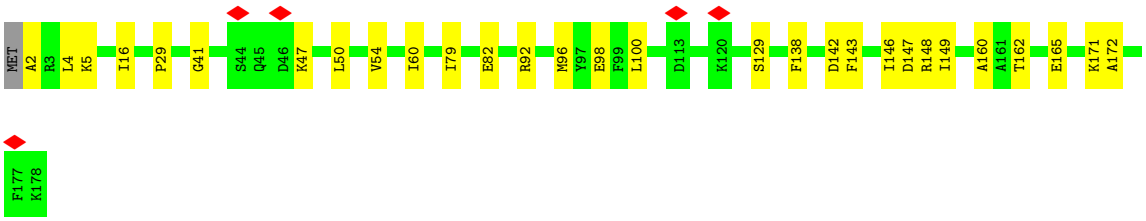
Chain L6:





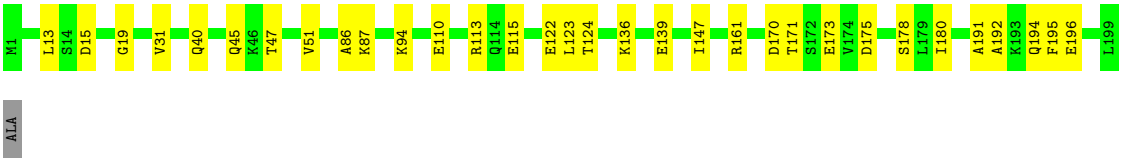
• Molecule 7: Large ribosomal subunit protein uL5

Chain F7:



• Molecule 8: Large ribosomal subunit protein uL4

Chain E9:

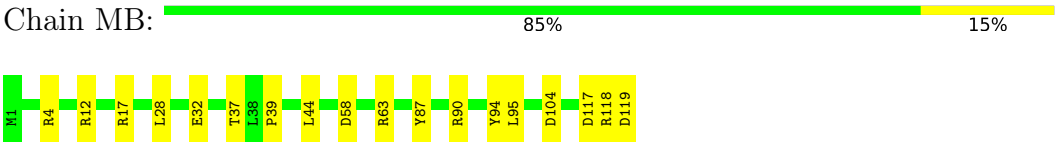


• Molecule 9: Large ribosomal subunit protein bL32

Chain aA:

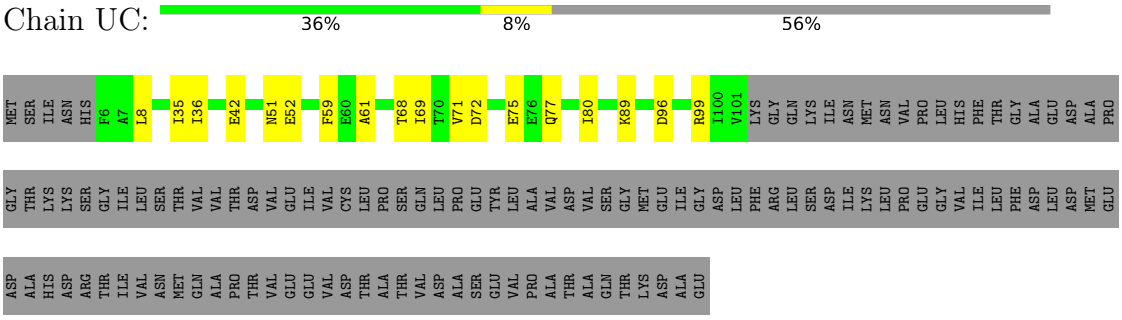
• Molecule 10: Large ribosomal subunit protein bL17

Chain MB:



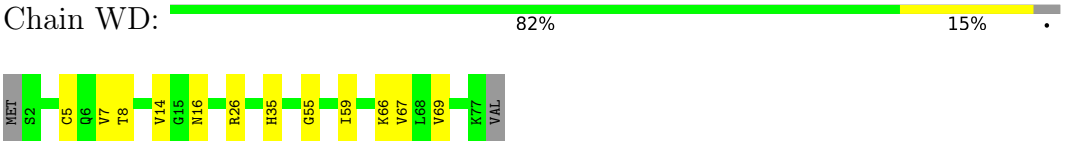
• Molecule 11: Large ribosomal subunit protein bL25

Chain UC:



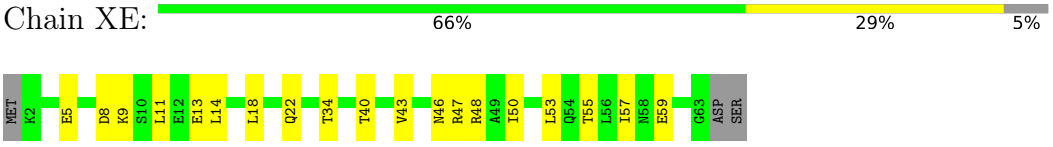
• Molecule 12: Large ribosomal subunit protein bL28

Chain WD:



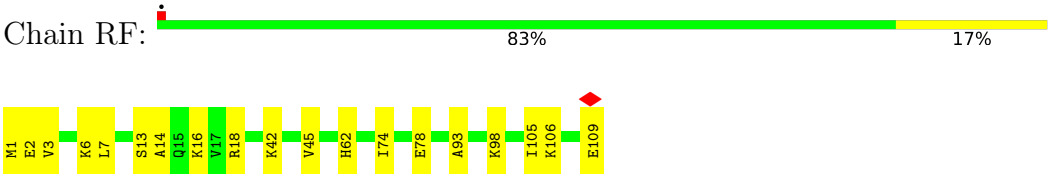
• Molecule 13: Large ribosomal subunit protein uL29

Chain XE:



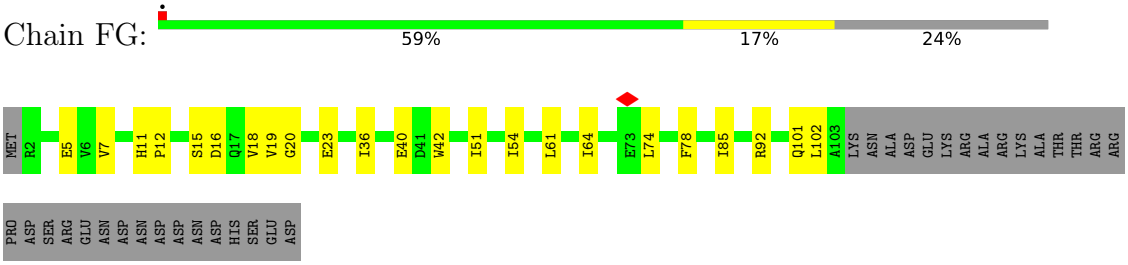
• Molecule 14: Large ribosomal subunit protein uL22

Chain RF:



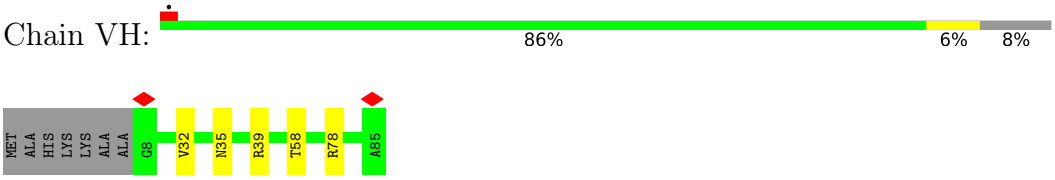
• Molecule 15: Small ribosomal subunit protein bS6

Chain FG:



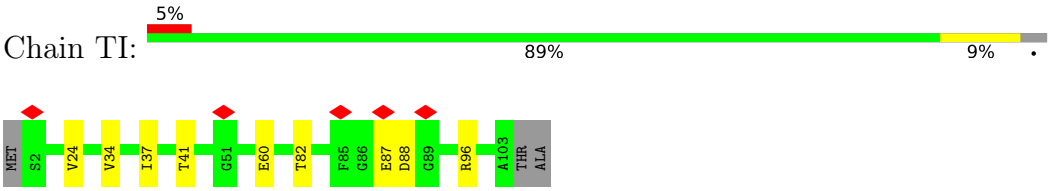
• Molecule 16: Large ribosomal subunit protein bL27

Chain VH:



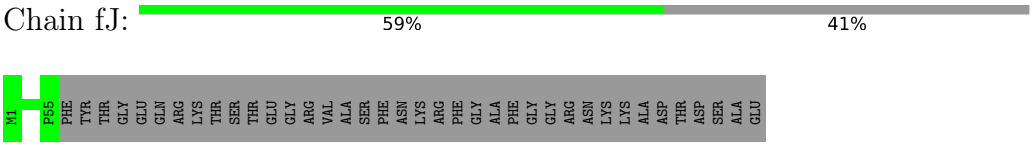
• Molecule 17: Large ribosomal subunit protein uL24

Chain TI:



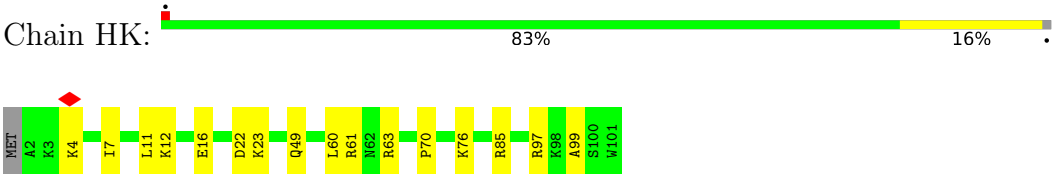
• Molecule 18: Large ribosomal subunit protein bL31B

Chain fJ:



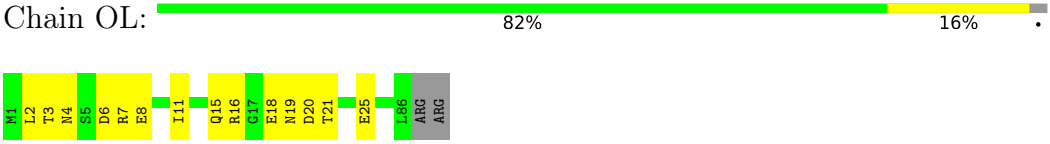
• Molecule 19: Small ribosomal subunit protein uS14

Chain HK:



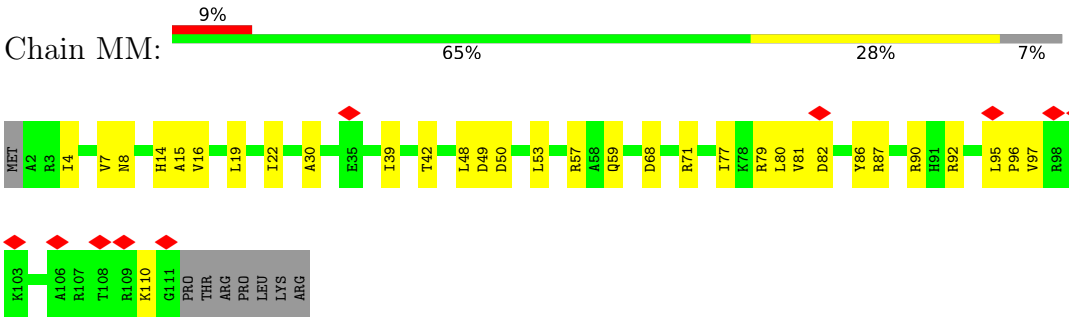
• Molecule 20: Small ribosomal subunit protein uS15

Chain OL:



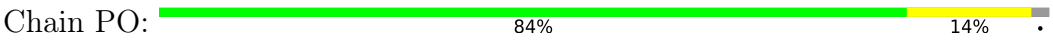
• Molecule 21: Small ribosomal subunit protein uS13

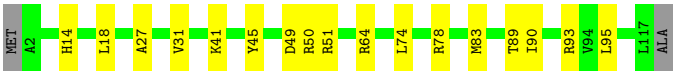
Chain MM:



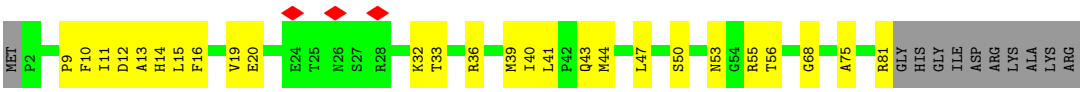
• Molecule 22: Large ribosomal subunit protein bL20

Chain PO:

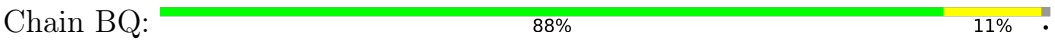


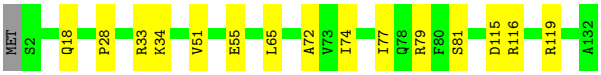


• Molecule 23: Small ribosomal subunit protein uS19

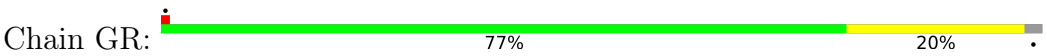


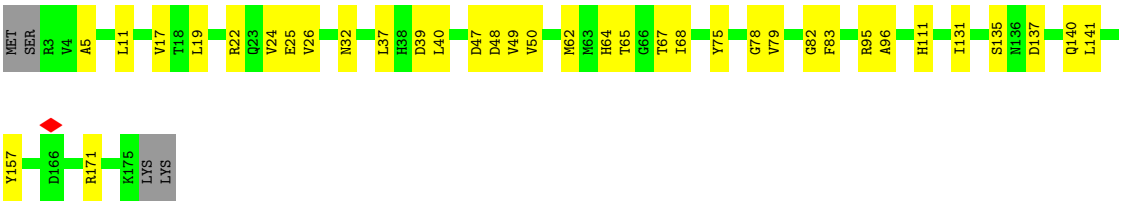
• Molecule 24: Small ribosomal subunit protein uS8



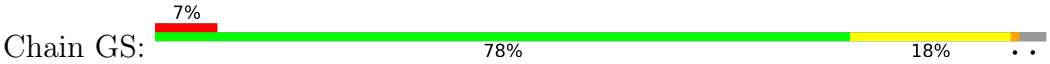


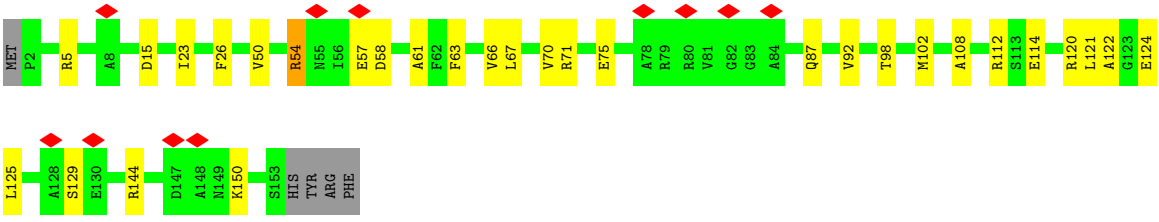
• Molecule 25: Large ribosomal subunit protein uL6



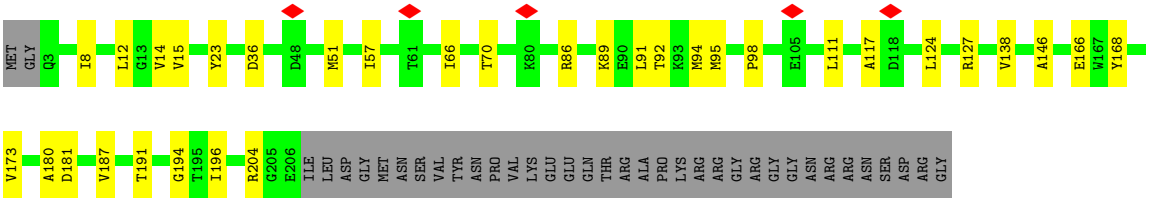


• Molecule 26: Small ribosomal subunit protein uS7



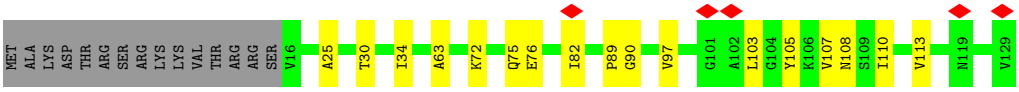


• Molecule 27: Small ribosomal subunit protein uS3



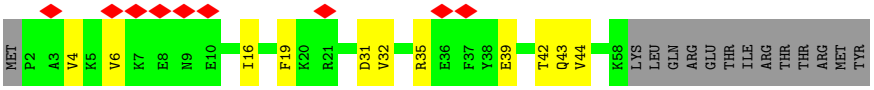
• Molecule 28: Small ribosomal subunit protein uS11

Chain KU:



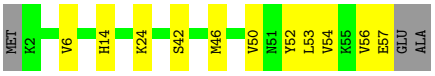
• Molecule 29: Small ribosomal subunit protein bS21

Chain NV:



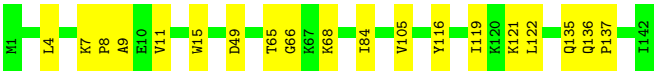
• Molecule 30: Large ribosomal subunit protein uL30

Chain YW:



• Molecule 31: Large ribosomal subunit protein uL13

Chain IX:

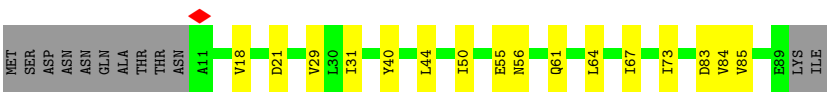


• Molecule 32: Small ribosomal subunit protein uS10

Chain JY:

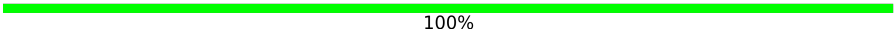
• Molecule 33: Small ribosomal subunit protein uS17

Chain QZ:



• Molecule 34: Large ribosomal subunit protein bL34

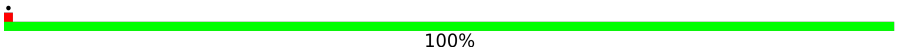
Chain Ba:



There are no outlier residues recorded for this chain.

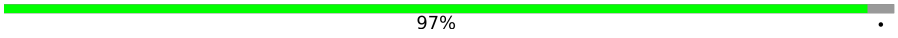
• Molecule 35: Large ribosomal subunit protein bL21

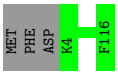
Chain Qb:



• Molecule 36: Large ribosomal subunit protein uL18

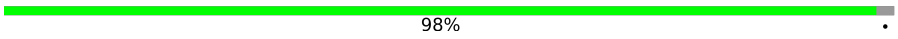
Chain Nc:

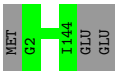




• Molecule 37: Large ribosomal subunit protein uL15

Chain Kd:





• Molecule 38: Large ribosomal subunit protein uL14

Chain Je:

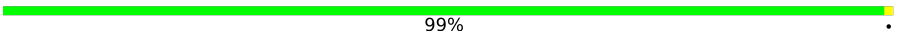
There are no outlier residues recorded for this chain.

• Molecule 39: Large ribosomal subunit protein uL3

Chain Af:

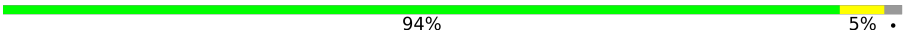
• Molecule 40: Large ribosomal subunit protein uL16

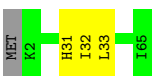
Chain Lg:



• Molecule 41: Large ribosomal subunit protein bL35

Chain dh:



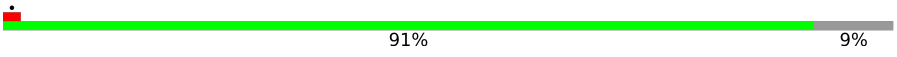


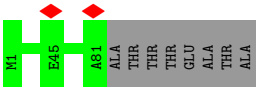
• Molecule 42: Large ribosomal subunit protein bL19

Chain Oi:

• Molecule 43: Small ribosomal subunit protein bS16

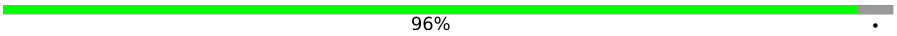
Chain Pj:





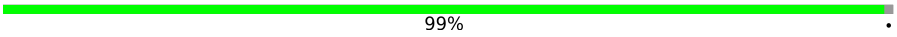
• Molecule 44: Large ribosomal subunit protein bL33

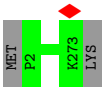
Chain bk:



• Molecule 45: Large ribosomal subunit protein uL2

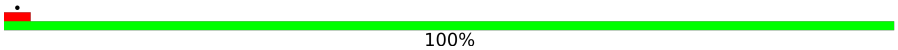
Chain Cl:

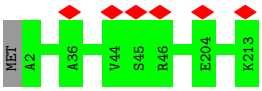




• Molecule 46: Small ribosomal subunit protein uS4

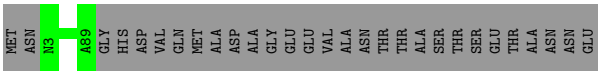
Chain Dm:





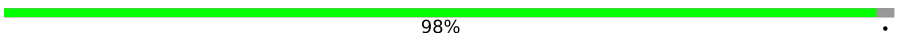
• Molecule 47: Large ribosomal subunit protein uL23

Chain Sn:



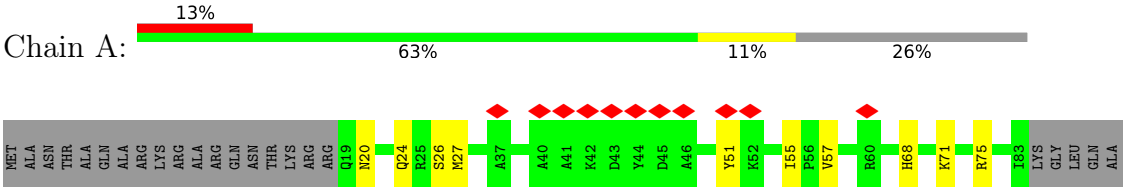
• Molecule 48: Small ribosomal subunit protein bS20

Chain To:



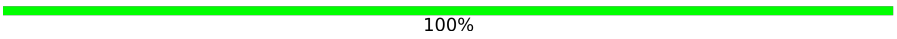
• Molecule 48: Small ribosomal subunit protein bS20

Chain A:



• Molecule 49: Large ribosomal subunit protein bL36

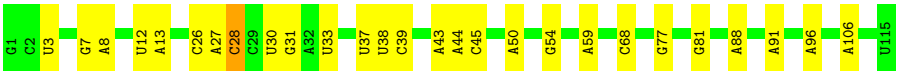
Chain ep:



There are no outlier residues recorded for this chain.

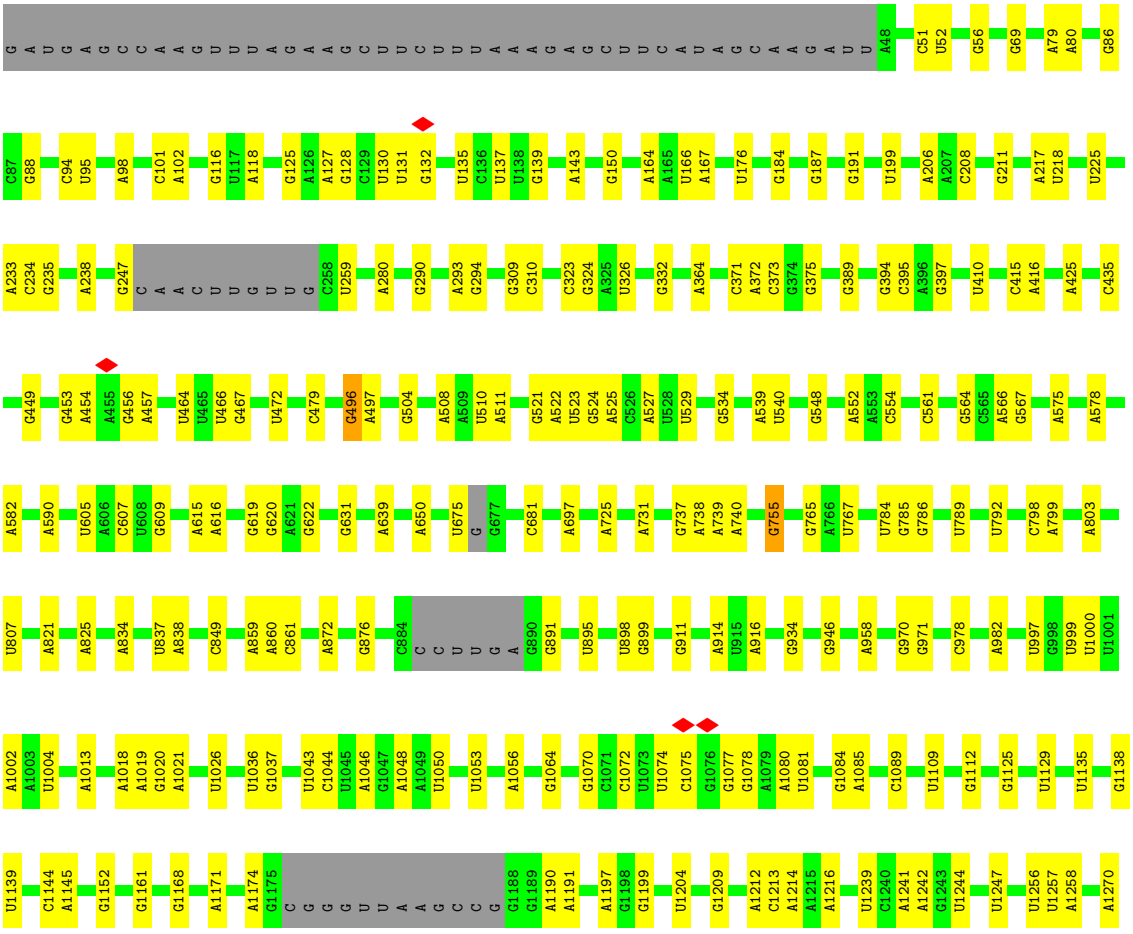
• Molecule 50: 5S rRNA

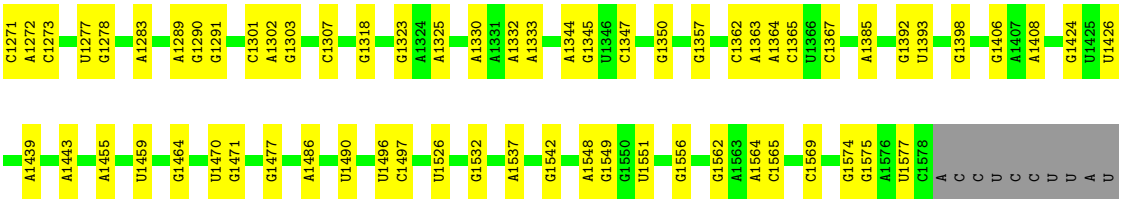
Chain D8:



• Molecule 51: 16S rRNA

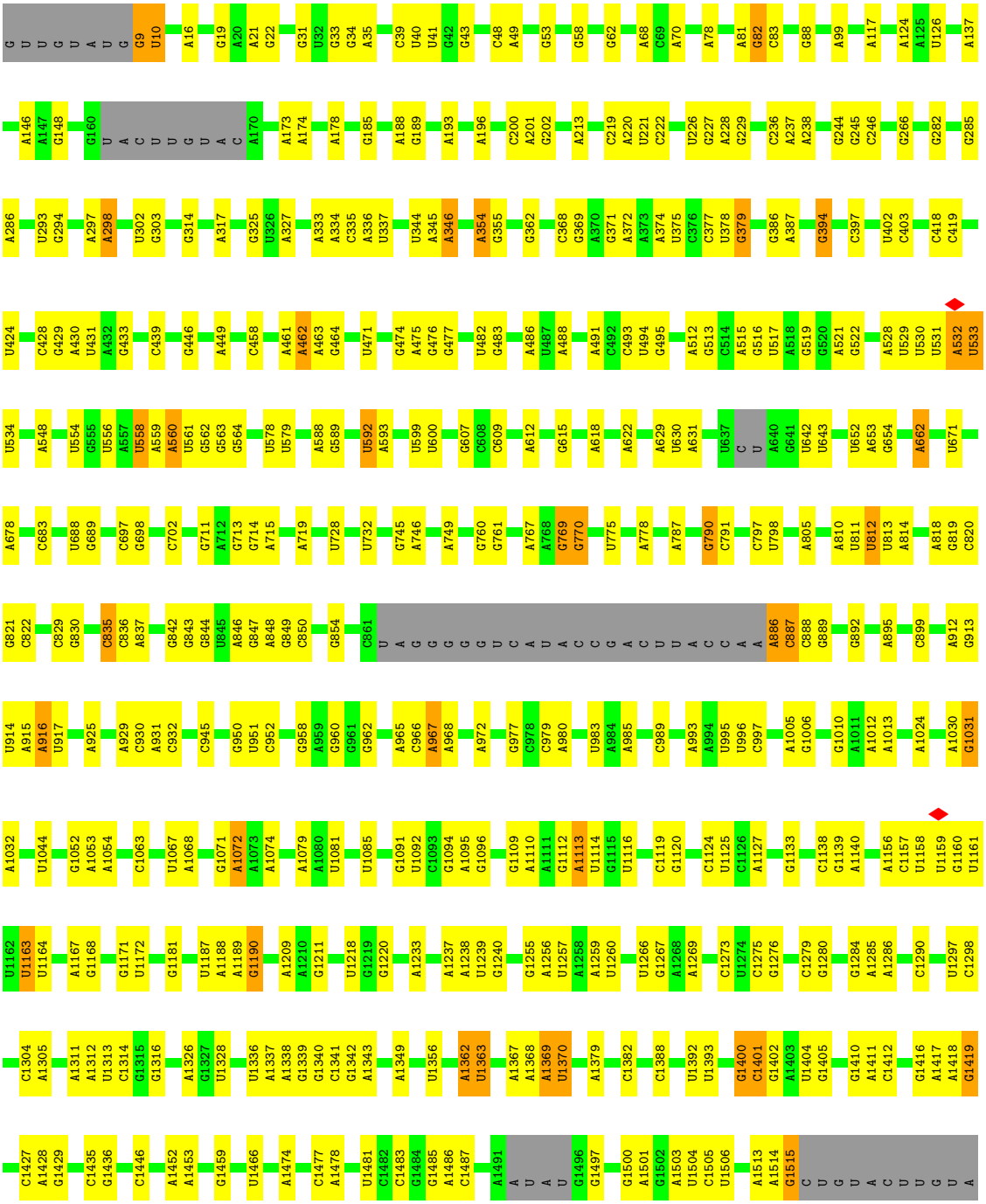
Chain iN:

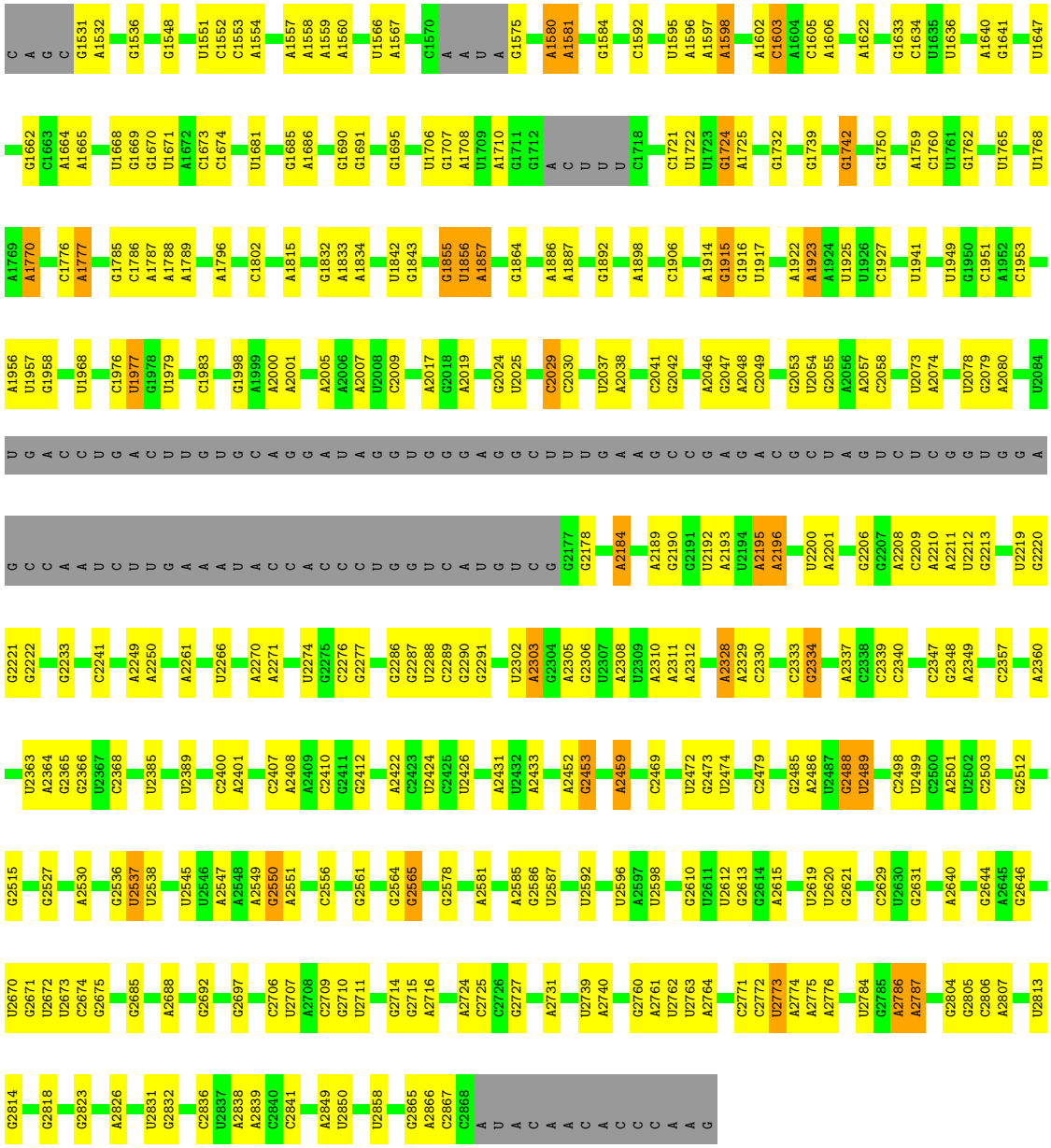




• Molecule 52: 23S rRNA

Chain Z2:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	420.30002, 420.30002, 420.30002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.934, 0.934, 0.934	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	F	0.27	0/961	0.52	0/1293
2	C1	0.28	0/379	0.50	0/511
3	R3	0.24	0/465	0.42	0/629
4	A4	0.27	0/1838	0.46	0/2481
5	E5	0.27	0/1163	0.50	0/1564
6	L6	0.26	0/959	0.50	0/1282
7	F7	0.28	0/1377	0.49	0/1851
8	E9	0.27	0/1559	0.47	0/2103
9	aA	0.25	0/454	0.52	0/600
10	MB	0.26	0/961	0.48	0/1282
11	UC	0.27	0/763	0.46	0/1028
12	WD	0.25	0/628	0.48	0/841
13	XE	0.27	0/503	0.47	0/670
14	RF	0.26	0/840	0.51	0/1125
15	FG	0.25	0/864	0.47	0/1169
16	VH	0.27	0/595	0.48	0/793
17	TI	0.25	0/790	0.47	0/1057
18	fJ	0.28	0/458	0.59	0/626
19	HK	0.27	0/821	0.50	0/1091
20	OL	0.25	0/702	0.42	0/941
21	MM	0.32	0/866	0.57	0/1166
22	PO	0.26	0/947	0.51	0/1261
23	SP	0.27	0/652	0.51	0/879
24	BQ	0.25	0/982	0.46	0/1318
25	GR	0.26	0/1359	0.49	0/1839
26	GS	0.27	0/1208	0.50	1/1619 (0.1%)
27	CT	0.27	0/1630	0.51	0/2192
28	KU	0.27	0/851	0.48	0/1150
29	NV	0.26	0/478	0.41	0/632
30	YW	0.28	0/442	0.51	0/590
31	IX	0.26	0/1134	0.46	0/1529
32	JY	0.28	0/768	0.54	0/1033
33	QZ	0.24	0/638	0.46	0/858
34	Ba	0.29	0/373	0.54	0/489

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	Qb	0.26	0/839	0.50	0/1127
36	Nc	0.26	0/863	0.50	0/1158
37	Kd	0.25	0/1064	0.49	0/1417
38	Je	0.26	0/946	0.48	0/1271
39	Af	0.26	0/1566	0.49	0/2103
40	Lg	0.26	0/1112	0.50	1/1483 (0.1%)
41	dh	0.26	0/524	0.57	0/686
42	Oi	0.26	0/927	0.49	0/1239
43	Pj	0.27	0/660	0.48	0/887
44	bk	0.26	0/401	0.43	0/534
45	Cl	0.26	0/2143	0.49	0/2879
46	Dm	0.27	0/1712	0.50	0/2296
47	Sn	0.27	0/697	0.47	0/928
48	A	0.25	0/465	0.39	0/626
48	To	0.27	0/679	0.45	0/904
49	ep	0.27	0/300	0.47	0/395
50	D8	0.18	0/2733	0.72	0/4256
51	iN	0.20	0/36108	0.76	5/56315 (0.0%)
52	Z2	0.22	0/65009	0.75	3/101385 (0.0%)
All	All	0.23	0/148156	0.69	10/221381 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
5	E5	0	1
41	dh	0	1
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	iN	997	U	C5-C6-N1	6.03	125.71	122.70
52	Z2	1297	U	C2-N1-C1'	5.83	124.70	117.70
51	iN	496	G	O4'-C1'-N9	5.67	112.74	108.20
40	Lg	51	ARG	NE-CZ-NH1	5.39	123.00	120.30
26	GS	54	ARG	NE-CZ-NH1	5.38	122.99	120.30
52	Z2	835	C	N3-C2-O2	-5.29	118.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	iN	755	G	C4-N9-C1'	5.29	133.38	126.50
51	iN	997	U	C2-N1-C1'	5.14	123.87	117.70
52	Z2	775	U	C2-N1-C1'	5.13	123.86	117.70
51	iN	479	C	C2-N1-C1'	5.00	124.31	118.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E5	82	ASN	Peptide
1	F	11	LYS	Peptide
41	dh	31	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	948	0	967	15	0
2	C1	374	0	406	9	0
3	R3	457	0	466	6	0
4	A4	1807	0	1827	25	0
5	E5	1151	0	1205	21	0
6	L6	946	0	1008	8	0
7	F7	1356	0	1391	23	0
8	E9	1537	0	1590	21	0
9	aA	446	0	443	0	0
10	MB	947	0	988	13	0
11	UC	750	0	767	12	0
12	WD	618	0	637	8	0
13	XE	502	0	527	13	0
14	RF	834	0	898	12	0
15	FG	849	0	838	18	0
16	VH	587	0	592	3	0
17	TI	784	0	820	10	0
18	fJ	443	0	391	0	0
19	HK	811	0	845	11	0
20	OL	694	0	710	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	MM	858	0	897	21	0
22	PO	935	0	999	15	0
23	SP	637	0	665	20	0
24	BQ	974	0	1009	10	0
25	GR	1339	0	1371	23	0
26	GS	1190	0	1224	23	0
27	CT	1606	0	1667	19	0
28	KU	836	0	845	19	0
29	NV	472	0	520	13	0
30	YW	438	0	476	10	0
31	IX	1108	0	1145	14	0
32	JY	760	0	789	25	0
33	QZ	632	0	676	13	0
34	Ba	369	0	418	0	0
35	Qb	827	0	862	0	0
36	Nc	852	0	880	0	0
37	Kd	1053	0	1117	0	0
38	Je	937	0	1003	0	0
39	Af	1548	0	1574	0	0
40	Lg	1093	0	1188	0	0
41	dh	519	0	581	0	0
42	Oi	917	0	969	0	0
43	Pj	648	0	661	0	0
44	bk	394	0	412	0	0
45	Cl	2103	0	2184	0	0
46	Dm	1688	0	1745	0	0
47	Sn	690	0	744	0	0
48	A	462	0	453	8	0
48	To	675	0	716	0	0
49	ep	298	0	334	0	0
50	D8	2446	0	1241	14	0
51	iN	32246	0	16224	0	0
52	Z2	58043	0	29179	308	0
All	All	136434	0	92084	735	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 6.

All (735) 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)
1:F:33:LEU:HD11	1:F:46:VAL:HG11	1.47	0.93
52:Z2:2786:A:O2'	52:Z2:2787:A:OP1	1.89	0.89
22:PO:49:ASP:OD2	52:Z2:517:U:O2'	1.92	0.88
52:Z2:1109:G:OP2	52:Z2:1110:A:O2'	1.92	0.87
4:A4:77:THR:OG1	4:A4:174:GLU:OE2	1.94	0.85
21:MM:68:ASP:OD1	21:MM:71:ARG:NH2	2.09	0.83
7:F7:147:ASP:OD2	7:F7:148:ARG:N	2.11	0.83
32:JY:28:THR:HG21	32:JY:90:LEU:HD21	1.61	0.83
52:Z2:2195:A:O2'	52:Z2:2196:A:OP1	1.97	0.82
31:IX:68:LYS:NZ	52:Z2:1124:C:OP2	2.12	0.81
52:Z2:2823:G:N2	52:Z2:2826:A:OP2	2.13	0.80
15:FG:36:ILE:HG13	15:FG:64:ILE:HG22	1.64	0.80
14:RF:1:MET:N	14:RF:109:GLU:OE1	2.15	0.79
32:JY:34:ALA:HB2	32:JY:83:THR:HG21	1.62	0.79
1:F:110:GLU:OE2	1:F:113:LYS:NZ	2.15	0.79
11:UC:42:GLU:O	11:UC:99:ARG:NH2	2.16	0.79
4:A4:98:ASP:OD1	4:A4:99:HIS:N	2.16	0.78
10:MB:90:ARG:O	10:MB:94:TYR:OH	2.01	0.78
7:F7:16:ILE:HD11	7:F7:172:ALA:HB2	1.65	0.77
52:Z2:189:G:O2'	52:Z2:662:A:N1	2.17	0.77
10:MB:12:ARG:O	10:MB:17:ARG:NH2	2.18	0.76
52:Z2:9:G:O2'	52:Z2:10:U:OP1	2.03	0.75
52:Z2:394:G:OP2	52:Z2:2389:U:O2'	2.04	0.75
27:CT:191:THR:OG1	27:CT:194:GLY:O	2.05	0.74
32:JY:102:LEU:O	32:JY:102:LEU:HD23	1.87	0.74
52:Z2:554:U:O2'	52:Z2:967:A:N1	2.22	0.73
52:Z2:1356:U:O2'	52:Z2:2196:A:N3	2.19	0.72
32:JY:32:THR:OG1	32:JY:83:THR:HG22	1.90	0.71
6:L6:53:CYS:SG	6:L6:65:SER:OG	2.49	0.71
52:Z2:236:C:HO2'	52:Z2:607:G:HO2'	1.36	0.71
11:UC:75:GLU:OE2	11:UC:77:GLN:NE2	2.24	0.70
27:CT:14:VAL:HG13	27:CT:15:VAL:HG13	1.73	0.70
52:Z2:886:A:O2'	52:Z2:887:C:OP1	2.07	0.70
2:C1:27:ARG:NH1	52:Z2:2078:U:OP2	2.25	0.70
7:F7:92:ARG:NH1	50:D8:43:A:O4'	2.22	0.70
8:E9:110:GLU:OE1	8:E9:113:ARG:NH1	2.24	0.70
23:SP:12:ASP:OD2	23:SP:14:HIS:NE2	2.24	0.70
5:E5:111:ILE:O	5:E5:130:THR:OG1	2.08	0.70
52:Z2:1580:A:O2'	52:Z2:1581:A:OP1	2.09	0.70
17:TI:87:GLU:N	17:TI:87:GLU:OE1	2.24	0.69
52:Z2:2195:A:HO2'	52:Z2:2196:A:P	2.14	0.69
10:MB:28:LEU:HD21	10:MB:95:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E5:20:LEU:HD13	5:E5:65:ILE:HD12	1.75	0.68
26:GS:114:GLU:O	26:GS:120:ARG:NH1	2.25	0.68
2:C1:3:ILE:CG2	2:C1:36:ALA:HB1	2.24	0.68
50:D8:37:U:O2'	50:D8:44:A:N1	2.27	0.68
52:Z2:34:G:O2'	52:Z2:35:A:OP2	2.12	0.67
52:Z2:1401:C:O2'	52:Z2:1575:G:O2'	2.11	0.67
7:F7:2:ALA:N	7:F7:98:GLU:OE2	2.27	0.67
52:Z2:960:G:HO2'	52:Z2:1140:A:HO2'	1.43	0.66
52:Z2:1765:U:OP2	52:Z2:1770:A:N6	2.27	0.66
8:E9:170:ASP:OD1	8:E9:171:THR:N	2.29	0.65
13:XE:8:ASP:OD2	13:XE:9:LYS:N	2.28	0.65
16:VH:39:ARG:HD2	16:VH:58:THR:HG23	1.79	0.65
52:Z2:2688:A:O2'	52:Z2:2818:G:OP1	2.14	0.65
3:R3:72:ASP:OD1	3:R3:73:ASN:N	2.30	0.65
52:Z2:564:G:O2'	52:Z2:2005:A:OP1	2.15	0.64
28:KU:75:GLN:NE2	28:KU:103:LEU:HD21	2.10	0.64
30:YW:53:LEU:HD12	30:YW:54:VAL:HG13	1.78	0.64
22:PO:93:ARG:NH1	52:Z2:979:C:O2'	2.31	0.63
25:GR:78:GLY:O	25:GR:82:GLY:N	2.32	0.63
52:Z2:1856:U:O2'	52:Z2:1857:A:OP1	2.13	0.63
2:C1:22:LYS:HD2	52:Z2:2080:A:OP1	1.99	0.63
1:F:41:THR:O	1:F:45:VAL:HG23	1.99	0.63
15:FG:15:SER:O	15:FG:18:VAL:HG12	1.99	0.62
25:GR:157:TYR:O	25:GR:171:ARG:NH2	2.32	0.62
52:Z2:244:G:OP2	52:Z2:246:C:N4	2.33	0.62
6:L6:100:GLY:N	6:L6:104:CYS:O	2.29	0.62
17:TI:34:VAL:HG11	17:TI:37:ILE:HD12	1.81	0.62
52:Z2:1280:G:OP1	52:Z2:2692:G:O2'	2.09	0.61
52:Z2:1459:G:O2'	52:Z2:1500:G:O6	2.18	0.61
7:F7:171:LYS:HE3	7:F7:171:LYS:HA	1.83	0.61
30:YW:24:LYS:HE3	30:YW:24:LYS:HA	1.83	0.61
22:PO:89:THR:HG22	22:PO:89:THR:O	1.99	0.61
32:JY:28:THR:HG21	32:JY:90:LEU:CD2	2.30	0.61
14:RF:14:ALA:O	14:RF:18:ARG:HG3	2.01	0.61
28:KU:97:VAL:HG12	29:NV:16:ILE:HD11	1.82	0.61
21:MM:102:THR:HG23	21:MM:102:THR:O	2.01	0.60
7:F7:129:SER:OG	52:Z2:2286:G:O2'	2.19	0.60
21:MM:49:ASP:OD1	21:MM:50:ASP:N	2.32	0.60
27:CT:180:ALA:O	27:CT:181:ASP:OD1	2.19	0.60
10:MB:28:LEU:HD22	10:MB:44:LEU:HD21	1.84	0.60
19:HK:49:GLN:NE2	23:SP:10:PHE:CE1	2.70	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:KU:89:PRO:HG3	29:NV:32:VAL:HG11	1.83	0.60
32:JY:57:VAL:HG12	32:JY:58:ASN:H	1.66	0.60
32:JY:57:VAL:HG12	32:JY:58:ASN:N	2.17	0.59
52:Z2:563:G:OP1	52:Z2:1239:U:O2'	2.20	0.59
28:KU:103:LEU:HD22	28:KU:105:TYR:HD2	1.67	0.59
8:E9:45:GLN:O	8:E9:87:LYS:NZ	2.35	0.59
52:Z2:1286:A:OP2	52:Z2:1595:U:O2'	2.20	0.59
19:HK:7:ILE:O	19:HK:11:LEU:HD23	2.02	0.59
27:CT:92:THR:HG23	27:CT:98:PRO:HA	1.85	0.59
28:KU:72:LYS:O	28:KU:76:GLU:OE1	2.21	0.59
4:A4:227:ILE:O	4:A4:231:GLU:OE1	2.21	0.58
10:MB:117:ASP:O	10:MB:118:ARG:HG2	2.03	0.58
26:GS:66:VAL:HG23	26:GS:129:SER:HA	1.84	0.58
11:UC:59:PHE:CE2	11:UC:61:ALA:HB3	2.39	0.58
24:BQ:115:ASP:OD1	24:BQ:116:ARG:N	2.36	0.58
52:Z2:458:C:O2	52:Z2:462:A:N6	2.36	0.58
52:Z2:2564:G:OP2	52:Z2:2564:G:N2	2.33	0.58
52:Z2:1914:A:H2'	52:Z2:1915:G:O4'	2.04	0.58
52:Z2:495:G:OP1	52:Z2:1218:U:O2'	2.20	0.58
7:F7:29:PRO:HB3	7:F7:160:ALA:HB2	1.84	0.58
21:MM:15:ALA:O	21:MM:19:LEU:HD23	2.02	0.58
24:BQ:18:GLN:OE1	24:BQ:72:ALA:HB1	2.04	0.58
22:PO:51:ARG:NH2	52:Z2:977:G:OP2	2.36	0.57
33:QZ:21:ASP:OD2	33:QZ:61:GLN:N	2.36	0.57
12:WD:59:ILE:HD13	12:WD:67:VAL:HG21	1.86	0.57
52:Z2:2547:A:OP1	52:Z2:2631:G:O2'	2.15	0.57
20:OL:11:ILE:HG21	20:OL:21:THR:HG22	1.86	0.57
52:Z2:1603:C:OP2	52:Z2:1605:C:N4	2.38	0.57
27:CT:111:LEU:HD13	27:CT:146:ALA:HB2	1.85	0.57
31:IX:65:THR:HG21	52:Z2:1125:U:H2'	1.85	0.57
52:Z2:1400:G:O2'	52:Z2:1401:C:OP2	2.18	0.57
7:F7:16:ILE:HD11	7:F7:172:ALA:CB	2.32	0.57
5:E5:156:GLU:OE1	5:E5:156:GLU:N	2.37	0.57
2:C1:3:ILE:HG22	2:C1:36:ALA:HB1	1.86	0.56
32:JY:10:LEU:HD22	32:JY:98:VAL:HG12	1.87	0.56
32:JY:5:ARG:NH1	32:JY:76:ILE:O	2.38	0.56
52:Z2:1316:G:HO2'	52:Z2:1597:A:H2	1.53	0.56
10:MB:37:THR:HG22	10:MB:39:PRO:HD2	1.86	0.56
52:Z2:2675:G:OP1	52:Z2:2836:C:O2'	2.24	0.56
52:Z2:728:U:O2'	52:Z2:1647:U:OP1	2.23	0.56
52:Z2:1707:G:O2'	52:Z2:1725:A:N6	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E5:44:VAL:HG13	5:E5:76:MET:HE2	1.88	0.56
52:Z2:1446:C:O2'	52:Z2:2685:G:O2'	2.09	0.56
4:A4:195:ASN:OD1	4:A4:196:SER:N	2.38	0.56
27:CT:86:ARG:O	27:CT:89:LYS:HG2	2.05	0.56
20:OL:20:ASP:OD1	20:OL:21:THR:N	2.38	0.55
4:A4:13:ASP:OD1	4:A4:14:LEU:N	2.39	0.55
48:A:20:ASN:O	48:A:24:GLN:HG3	2.06	0.55
52:Z2:483:G:N1	52:Z2:486:A:OP2	2.35	0.55
52:Z2:2831:U:OP2	52:Z2:2832:G:O2'	2.06	0.55
33:QZ:83:ASP:OD1	33:QZ:84:VAL:N	2.39	0.55
15:FG:5:GLU:OE1	15:FG:61:LEU:HD21	2.06	0.55
19:HK:76:LYS:NZ	32:JY:47:GLU:OE2	2.33	0.55
5:E5:76:MET:O	5:E5:77:ILE:HD13	2.06	0.55
26:GS:54:ARG:HG3	26:GS:54:ARG:HH11	1.72	0.55
52:Z2:609:C:O2'	52:Z2:642:U:OP1	2.25	0.55
52:Z2:965:A:OP2	52:Z2:966:C:N4	2.35	0.55
52:Z2:1886:A:O2'	52:Z2:1887:A:OP1	2.24	0.55
52:Z2:1760:C:H2'	52:Z2:1760:C:O2	2.05	0.55
27:CT:166:GLU:HA	27:CT:166:GLU:OE1	2.06	0.54
15:FG:12:PRO:HA	15:FG:15:SER:OG	2.07	0.54
25:GR:137:ASP:OD1	25:GR:140:GLN:HB2	2.08	0.54
28:KU:34:ILE:HD12	28:KU:82:ILE:CD1	2.37	0.54
52:Z2:2453:G:O6	52:Z2:2459:A:O2'	2.25	0.54
26:GS:121:LEU:O	26:GS:125:LEU:HD23	2.07	0.54
17:TI:82:THR:OG1	52:Z2:285:G:OP1	2.24	0.54
52:Z2:9:G:HO2'	52:Z2:10:U:P	2.30	0.54
11:UC:36:ILE:HD11	11:UC:69:ILE:HD13	1.90	0.54
15:FG:74:LEU:HG	15:FG:78:PHE:CE2	2.43	0.54
8:E9:123:LEU:HD23	8:E9:147:ILE:HG21	1.89	0.54
2:C1:29:PHE:CD2	52:Z2:2184:A:C8	2.95	0.53
23:SP:12:ASP:OD1	23:SP:13:ALA:N	2.41	0.53
20:OL:11:ILE:O	20:OL:15:GLN:HG2	2.08	0.53
32:JY:10:LEU:HD11	32:JY:25:ILE:HD12	1.91	0.53
48:A:68:HIS:CE1	52:Z2:48:C:H5"	2.43	0.53
50:D8:7:G:C2	50:D8:8:A:C8	2.96	0.53
52:Z2:2274:U:OP1	52:Z2:2363:U:O2'	2.24	0.53
4:A4:84:ILE:HD11	4:A4:212:ILE:HD11	1.89	0.53
32:JY:85:ASP:HB2	32:JY:89:LYS:HZ3	1.73	0.53
52:Z2:82:G:H22	52:Z2:117:A:H2	1.56	0.53
52:Z2:2536:G:O4'	52:Z2:2565:G:O2'	2.21	0.53
24:BQ:34:LYS:HD3	24:BQ:51:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:GS:87:GLN:N	26:GS:87:GLN:OE1	2.40	0.53
5:E5:77:ILE:HG22	5:E5:78:THR:N	2.24	0.53
7:F7:143:PHE:O	7:F7:146:ILE:HG22	2.08	0.53
52:Z2:769:G:H5'	52:Z2:770:G:OP1	2.09	0.53
13:XE:47:ARG:NH2	52:Z2:68:A:OP2	2.42	0.53
52:Z2:9:G:O2'	52:Z2:10:U:P	2.67	0.53
52:Z2:1304:C:H2'	52:Z2:1313:U:OP1	2.09	0.53
5:E5:110:VAL:HG22	5:E5:128:VAL:HG12	1.91	0.53
7:F7:60:ILE:HG23	7:F7:138:PHE:CD2	2.44	0.53
52:Z2:200:C:OP2	52:Z2:201:A:O2'	2.16	0.52
27:CT:173:VAL:HG12	27:CT:173:VAL:O	2.08	0.52
28:KU:103:LEU:HD22	28:KU:105:TYR:CD2	2.44	0.52
13:XE:46:ASN:O	13:XE:50:ILE:HG13	2.10	0.52
27:CT:111:LEU:HD12	27:CT:204:ARG:HG2	1.92	0.52
52:Z2:778:A:OP2	52:Z2:2057:A:O2'	2.24	0.52
1:F:65:VAL:O	1:F:65:VAL:HG13	2.08	0.52
32:JY:57:VAL:CG1	32:JY:58:ASN:H	2.22	0.52
52:Z2:1580:A:O2'	52:Z2:1581:A:P	2.68	0.52
5:E5:20:LEU:HD21	5:E5:23:VAL:HG23	1.92	0.52
5:E5:24:ASP:OD1	5:E5:25:ARG:N	2.43	0.52
8:E9:45:GLN:OE1	8:E9:86:ALA:HB3	2.09	0.52
26:GS:57:GLU:N	26:GS:57:GLU:OE1	2.41	0.52
7:F7:92:ARG:CA	7:F7:96:MET:HB2	2.39	0.52
8:E9:40:GLN:OE1	52:Z2:424:U:O2'	2.24	0.52
14:RF:2:GLU:OE1	14:RF:106:LYS:HE2	2.10	0.52
15:FG:11:HIS:CG	15:FG:12:PRO:HD2	2.45	0.52
52:Z2:188:A:H3'	52:Z2:189:G:H21	1.74	0.52
8:E9:15:ASP:O	8:E9:19:GLY:N	2.40	0.52
8:E9:175:ASP:OD2	8:E9:178:SER:N	2.38	0.52
52:Z2:916:A:N6	52:Z2:1167:A:N3	2.58	0.52
52:Z2:1368:A:O2'	52:Z2:1388:C:O2'	2.11	0.52
1:F:102:VAL:HG22	1:F:102:VAL:O	2.10	0.52
7:F7:16:ILE:CD1	7:F7:172:ALA:HB2	2.37	0.52
23:SP:43:GLN:OE1	23:SP:43:GLN:N	2.42	0.52
27:CT:8:ILE:O	27:CT:12:LEU:HG	2.09	0.52
52:Z2:1187:U:OP2	52:Z2:1188:A:O2'	2.19	0.52
52:Z2:1580:A:HO2'	52:Z2:1581:A:P	2.33	0.52
3:R3:24:LYS:O	15:FG:102:LEU:HD11	2.10	0.51
11:UC:68:THR:HG23	11:UC:75:GLU:OE2	2.10	0.51
52:Z2:2037:U:O2	52:Z2:2038:A:N6	2.36	0.51
8:E9:122:GLU:HG3	8:E9:124:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:KU:103:LEU:HD23	28:KU:103:LEU:O	2.10	0.51
30:YW:50:VAL:O	30:YW:54:VAL:HG22	2.11	0.51
8:E9:115:GLU:O	8:E9:115:GLU:HG3	2.10	0.51
21:MM:90:ARG:HD3	21:MM:95:LEU:HB2	1.93	0.51
22:PO:83:MET:HE2	22:PO:83:MET:HA	1.93	0.51
7:F7:2:ALA:HB1	7:F7:5:LYS:HB3	1.93	0.50
48:A:27:MET:CE	48:A:57:VAL:HG11	2.40	0.50
52:Z2:335:C:H2'	52:Z2:336:A:N3	2.26	0.50
23:SP:14:HIS:ND1	23:SP:15:LEU:HD12	2.25	0.50
52:Z2:2212:U:H2'	52:Z2:2213:G:H8	1.75	0.50
21:MM:7:VAL:HG22	21:MM:8:ASN:N	2.27	0.50
28:KU:30:THR:HG21	28:KU:63:ALA:HB2	1.92	0.50
6:L6:68:GLY:O	6:L6:99:ARG:NH1	2.44	0.50
17:TI:34:VAL:CG1	17:TI:37:ILE:HD12	2.41	0.50
52:Z2:805:A:H4'	52:Z2:821:G:H22	1.76	0.50
13:XE:48:ARG:NH1	52:Z2:83:C:OP1	2.45	0.50
23:SP:36:ARG:NH2	23:SP:75:ALA:O	2.45	0.50
25:GR:64:HIS:O	25:GR:67:THR:HG22	2.11	0.50
26:GS:67:LEU:O	26:GS:71:ARG:HG3	2.12	0.50
33:QZ:29:VAL:HG21	33:QZ:67:ILE:HD13	1.94	0.50
52:Z2:822:C:N3	52:Z2:925:A:N6	2.59	0.50
2:C1:3:ILE:HG23	2:C1:37:LEU:O	2.11	0.50
14:RF:7:LEU:HD23	14:RF:7:LEU:O	2.11	0.50
52:Z2:2714:G:H2'	52:Z2:2715:G:C8	2.47	0.50
52:Z2:562:G:O2'	52:Z2:1238:A:OP1	2.30	0.50
52:Z2:1113:A:O2'	52:Z2:2498:C:O2	2.28	0.50
52:Z2:236:C:O2'	52:Z2:607:G:O2'	2.16	0.49
52:Z2:1417:A:H2'	52:Z2:1418:A:C8	2.47	0.49
52:Z2:2274:U:O2'	52:Z2:2357:C:O2	2.30	0.49
52:Z2:2311:A:H2'	52:Z2:2312:A:C8	2.47	0.49
8:E9:171:THR:HG21	8:E9:194:GLN:OE1	2.11	0.49
27:CT:36:ASP:OD1	27:CT:57:ILE:HG21	2.11	0.49
28:KU:110:ILE:HG22	29:NV:19:PHE:CD1	2.46	0.49
4:A4:104:GLY:N	4:A4:180:GLU:OE2	2.43	0.49
14:RF:6:LYS:HB2	52:Z2:477:G:H4'	1.95	0.49
15:FG:51:ILE:O	15:FG:54:ILE:HG22	2.12	0.49
24:BQ:55:GLU:OE1	24:BQ:55:GLU:N	2.44	0.49
25:GR:17:VAL:HG23	25:GR:26:VAL:HG22	1.94	0.49
27:CT:51:MET:O	27:CT:70:THR:OG1	2.26	0.49
33:QZ:31:ILE:HG13	33:QZ:50:ILE:HD12	1.94	0.49
52:Z2:1427:C:H2'	52:Z2:1428:A:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L6:21:VAL:HG23	6:L6:21:VAL:O	2.12	0.49
24:BQ:77:ILE:HG23	24:BQ:77:ILE:O	2.12	0.49
52:Z2:615:G:N2	52:Z2:618:A:OP2	2.36	0.49
52:Z2:2192:U:O4	52:Z2:2193:A:N6	2.45	0.49
4:A4:28:TRP:HE1	4:A4:36:ILE:HD13	1.77	0.49
52:Z2:678:A:O2'	52:Z2:1337:A:N3	2.42	0.49
52:Z2:886:A:HO2'	52:Z2:887:C:P	2.33	0.49
4:A4:191:ILE:HG23	4:A4:207:ALA:HB3	1.94	0.49
7:F7:41:GLY:N	52:Z2:2290:G:O6	2.43	0.49
52:Z2:1362:A:O2'	52:Z2:1363:U:OP2	2.18	0.49
22:PO:27:ALA:HB1	22:PO:31:VAL:CG2	2.43	0.49
22:PO:41:LYS:HE2	22:PO:45:TYR:CZ	2.48	0.49
27:CT:94:MET:SD	27:CT:95:MET:N	2.85	0.49
4:A4:84:ILE:HG22	4:A4:219:VAL:HG21	1.95	0.49
4:A4:231:GLU:O	4:A4:235:THR:HG23	2.13	0.49
12:WD:14:VAL:HG11	52:Z2:185:G:H5'	1.95	0.49
21:MM:16:VAL:HG23	21:MM:30:ALA:HB3	1.94	0.49
30:YW:6:VAL:HG12	30:YW:56:VAL:HG22	1.93	0.49
52:Z2:2334:G:O2'	52:Z2:2349:A:N6	2.36	0.49
10:MB:118:ARG:O	10:MB:118:ARG:HG3	2.13	0.48
17:TI:24:VAL:HG12	17:TI:34:VAL:HG22	1.95	0.48
25:GR:47:ASP:O	25:GR:48:ASP:HB3	2.13	0.48
26:GS:15:ASP:OD2	26:GS:23:ILE:HG21	2.13	0.48
4:A4:48:LEU:H	4:A4:48:LEU:HD23	1.78	0.48
25:GR:19:LEU:HD13	25:GR:24:VAL:HG22	1.95	0.48
1:F:33:LEU:HD11	1:F:46:VAL:CG1	2.32	0.48
52:Z2:293:U:H2'	52:Z2:294:G:O4'	2.14	0.48
52:Z2:482:U:H2'	52:Z2:483:G:O4'	2.13	0.48
3:R3:25:ASP:O	3:R3:29:LEU:HD13	2.14	0.48
28:KU:107:VAL:O	29:NV:6:VAL:CG1	2.61	0.48
5:E5:44:VAL:HG13	5:E5:76:MET:CE	2.43	0.48
24:BQ:18:GLN:HG2	24:BQ:65:LEU:HD13	1.94	0.48
31:IX:136:GLN:HA	31:IX:136:GLN:OE1	2.14	0.48
52:Z2:1012:A:N3	52:Z2:2469:C:O2'	2.41	0.48
52:Z2:2786:A:HO2'	52:Z2:2787:A:P	2.29	0.48
14:RF:78:GLU:O	52:Z2:31:G:O2'	2.31	0.48
19:HK:12:LYS:O	19:HK:16:GLU:OE1	2.32	0.48
52:Z2:428:C:H2'	52:Z2:429:G:O4'	2.14	0.48
5:E5:41:LEU:HD12	5:E5:54:GLY:O	2.14	0.48
13:XE:55:THR:O	13:XE:59:GLU:HG3	2.14	0.48
19:HK:85:ARG:HB2	32:JY:51:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:HK:99:ALA:N	32:JY:64:GLN:O	2.43	0.48
25:GR:111:HIS:O	25:GR:111:HIS:ND1	2.46	0.48
50:D8:12:U:OP2	50:D8:68:C:O2'	2.29	0.48
52:Z2:688:U:H2'	52:Z2:689:G:O4'	2.13	0.48
2:C1:9:ILE:HD11	2:C1:12:LEU:HD23	1.95	0.47
22:PO:50:ARG:NH1	52:Z2:977:G:OP1	2.47	0.47
52:Z2:2195:A:C2	52:Z2:2196:A:C8	3.02	0.47
1:F:34:ASP:O	1:F:43:ARG:NH2	2.47	0.47
52:Z2:812:U:O2'	52:Z2:2054:U:C2	2.67	0.47
22:PO:78:ARG:HG2	22:PO:78:ARG:HH11	1.79	0.47
27:CT:117:ALA:HB1	27:CT:187:VAL:HG22	1.96	0.47
52:Z2:1776:C:H2'	52:Z2:1777:A:C8	2.49	0.47
20:OL:3:THR:N	20:OL:6:ASP:OD2	2.48	0.47
23:SP:81:ARG:NE	23:SP:81:ARG:HA	2.30	0.47
30:YW:57:GLU:OE1	30:YW:57:GLU:N	2.47	0.47
50:D8:43:A:C4	50:D8:44:A:C8	3.03	0.47
28:KU:89:PRO:HG3	29:NV:32:VAL:CG1	2.44	0.47
13:XE:34:THR:O	13:XE:34:THR:HG22	2.13	0.47
14:RF:42:LYS:O	14:RF:45:VAL:HG12	2.14	0.47
26:GS:108:ALA:HB1	26:GS:124:GLU:OE2	2.14	0.47
6:L6:99:ARG:HG3	6:L6:99:ARG:HH11	1.79	0.47
11:UC:51:ASN:ND2	11:UC:52:GLU:OE1	2.48	0.47
13:XE:11:LEU:HA	13:XE:14:LEU:HD13	1.95	0.47
15:FG:19:VAL:HG23	15:FG:20:GLY:N	2.30	0.47
23:SP:47:LEU:H	23:SP:47:LEU:HD23	1.80	0.47
26:GS:112:ARG:HG3	26:GS:124:GLU:HG2	1.97	0.47
52:Z2:2000:A:H2'	52:Z2:2001:A:C8	2.50	0.47
52:Z2:2710:G:H2'	52:Z2:2711:U:H6	1.79	0.47
22:PO:64:ARG:NH2	31:IX:4:LEU:O	2.43	0.47
52:Z2:221:U:O4	52:Z2:402:U:O2'	2.32	0.47
52:Z2:336:A:C8	52:Z2:337:U:C6	3.03	0.47
52:Z2:1401:C:O5'	52:Z2:1575:G:N2	2.47	0.47
4:A4:46:ILE:HG21	4:A4:206:PRO:O	2.15	0.47
5:E5:86:LEU:HD23	5:E5:90:ILE:HD12	1.96	0.47
25:GR:25:GLU:OE1	25:GR:32:ASN:ND2	2.48	0.47
52:Z2:1275:C:C2	52:Z2:1276:G:C8	3.03	0.47
52:Z2:1922:A:H4'	52:Z2:1923:A:O5'	2.15	0.47
21:MM:39:ILE:H	21:MM:39:ILE:HD12	1.80	0.47
52:Z2:294:G:N1	52:Z2:297:A:OP2	2.39	0.47
52:Z2:1739:G:N1	52:Z2:1742:G:OP2	2.47	0.47
52:Z2:2057:A:H2'	52:Z2:2058:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:CT:66:ILE:CD1	27:CT:91:LEU:HD11	2.45	0.46
52:Z2:521:A:H2'	52:Z2:522:G:O4'	2.16	0.46
21:MM:49:ASP:O	21:MM:53:LEU:HD23	2.15	0.46
30:YW:14:HIS:NE2	52:Z2:972:A:N7	2.62	0.46
10:MB:28:LEU:HD21	10:MB:95:LEU:CD2	2.41	0.46
25:GR:64:HIS:O	25:GR:68:ILE:HG12	2.16	0.46
26:GS:66:VAL:HG23	26:GS:129:SER:CA	2.44	0.46
4:A4:31:LYS:H	4:A4:31:LYS:HD2	1.81	0.46
10:MB:104:ASP:OD2	52:Z2:1269:A:O2'	2.23	0.46
12:WD:16:ASN:OD1	12:WD:26:ARG:NH1	2.44	0.46
52:Z2:1855:G:H3'	52:Z2:1856:U:H5"	1.98	0.46
8:E9:161:ARG:NH2	52:Z2:327:A:O2'	2.48	0.46
12:WD:66:LYS:O	12:WD:69:VAL:HG12	2.15	0.46
25:GR:5:ALA:CB	25:GR:65:THR:HG23	2.45	0.46
52:Z2:1706:U:H2'	52:Z2:1707:G:O4'	2.15	0.46
8:E9:170:ASP:HB2	48:A:26:SER:OG	2.16	0.46
25:GR:22:ARG:NH1	25:GR:37:LEU:O	2.49	0.46
32:JY:57:VAL:CG1	32:JY:58:ASN:N	2.78	0.46
52:Z2:820:C:C2	52:Z2:821:G:C8	3.04	0.46
52:Z2:2515:G:N2	52:Z2:2646:G:O2'	2.49	0.46
5:E5:61:VAL:O	5:E5:65:ILE:HG12	2.16	0.46
5:E5:63:ALA:O	5:E5:67:LYS:HG3	2.15	0.46
7:F7:82:GLU:O	7:F7:82:GLU:HG2	2.16	0.46
11:UC:59:PHE:HE2	11:UC:61:ALA:HB3	1.80	0.46
13:XE:53:LEU:O	13:XE:57:ILE:HG13	2.16	0.46
26:GS:66:VAL:O	26:GS:70:VAL:HG23	2.16	0.46
28:KU:89:PRO:CG	29:NV:32:VAL:HG11	2.46	0.46
52:Z2:88:G:HO2'	52:Z2:282:G:HO2'	1.62	0.46
4:A4:91:ARG:HG2	4:A4:227:ILE:HD11	1.98	0.46
14:RF:98:LYS:HA	52:Z2:1998:G:OP1	2.15	0.46
26:GS:50:VAL:HG13	26:GS:122:ALA:HB1	1.97	0.46
28:KU:89:PRO:HD3	29:NV:32:VAL:HG11	1.98	0.46
52:Z2:476:G:H2'	52:Z2:477:G:O4'	2.16	0.46
52:Z2:592:U:O2	52:Z2:593:A:C8	2.68	0.46
52:Z2:2233:G:O2'	52:Z2:2479:C:OP1	2.19	0.46
13:XE:9:LYS:HB2	13:XE:13:GLU:OE2	2.16	0.46
26:GS:112:ARG:CG	26:GS:124:GLU:HG2	2.46	0.46
31:IX:49:ASP:OD1	31:IX:121:LYS:NZ	2.47	0.46
52:Z2:931:A:H2'	52:Z2:932:C:C6	2.51	0.46
52:Z2:1668:U:H2'	52:Z2:1669:G:O4'	2.16	0.46
3:R3:37:GLY:O	3:R3:63:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E9:31:VAL:HG21	8:E9:180:ILE:HD12	1.96	0.46
52:Z2:532:A:HO2'	52:Z2:533:U:P	2.39	0.46
52:Z2:2472:U:H2'	52:Z2:2473:G:O4'	2.16	0.46
52:Z2:2550:G:H2'	52:Z2:2551:A:C8	2.51	0.46
23:SP:9:PRO:HB3	23:SP:39:MET:HG2	1.96	0.45
30:YW:42:SER:O	52:Z2:836:C:O2'	2.34	0.45
52:Z2:1402:G:N2	52:Z2:1567:A:N7	2.63	0.45
15:FG:7:VAL:HG22	15:FG:61:LEU:HD12	1.97	0.45
48:A:27:MET:HE1	48:A:57:VAL:HG11	1.97	0.45
48:A:51:TYR:O	48:A:55:ILE:HG13	2.17	0.45
52:Z2:2866:A:H2'	52:Z2:2867:C:O4'	2.16	0.45
23:SP:39:MET:HE2	23:SP:68:GLY:H	1.81	0.45
52:Z2:493:C:H2'	52:Z2:493:C:O2	2.15	0.45
52:Z2:950:G:C1'	52:Z2:2250:A:H62	2.30	0.45
52:Z2:2515:G:O2'	52:Z2:2640:A:N1	2.45	0.45
25:GR:39:ASP:OD1	25:GR:40:LEU:N	2.49	0.45
52:Z2:1052:G:N2	52:Z2:1079:A:O2'	2.44	0.45
52:Z2:1410:G:H1'	52:Z2:1560:A:N6	2.32	0.45
52:Z2:1504:U:C2	52:Z2:1505:C:C5	3.05	0.45
52:Z2:2241:C:O2'	52:Z2:2410:C:OP2	2.30	0.45
8:E9:191:ALA:O	8:E9:195:PHE:CD2	2.70	0.45
32:JY:80:THR:OG1	32:JY:83:THR:HG23	2.16	0.45
52:Z2:1664:A:H2'	52:Z2:1665:A:O4'	2.16	0.45
52:Z2:2289:C:OP2	52:Z2:2290:G:O2'	2.20	0.45
50:D8:27:A:H2'	50:D8:28:C:O4'	2.17	0.45
31:IX:84:ILE:HG23	31:IX:84:ILE:O	2.16	0.45
8:E9:13:LEU:HA	8:E9:196:GLU:OE2	2.17	0.45
22:PO:14:HIS:O	22:PO:18:LEU:HD23	2.17	0.45
25:GR:95:ARG:HH11	25:GR:95:ARG:HG3	1.82	0.45
48:A:71:LYS:O	48:A:75:ARG:HG2	2.16	0.45
50:D8:81:G:O6	50:D8:91:A:N6	2.50	0.45
52:Z2:344:U:O2'	52:Z2:345:A:H5'	2.17	0.45
52:Z2:950:G:H1'	52:Z2:2250:A:H62	1.82	0.45
52:Z2:2073:U:H2'	52:Z2:2074:A:H8	1.81	0.45
52:Z2:1515:G:N2	52:Z2:1531:G:O4'	2.49	0.45
52:Z2:1721:C:C2	52:Z2:1722:U:C5	3.04	0.45
5:E5:20:LEU:CD1	5:E5:65:ILE:HD12	2.45	0.45
11:UC:8:LEU:HD11	11:UC:69:ILE:HG12	1.98	0.45
15:FG:40:GLU:OE1	15:FG:40:GLU:HA	2.17	0.45
31:IX:8:PRO:O	31:IX:11:VAL:HG22	2.17	0.45
52:Z2:1592:C:O2'	52:Z2:1598:A:N1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Z2:2024:G:H2'	52:Z2:2025:U:O4'	2.17	0.45
1:F:70:ILE:HG13	1:F:71:SER:N	2.32	0.44
25:GR:62:MET:O	25:GR:65:THR:HG22	2.17	0.44
33:QZ:64:LEU:HD23	33:QZ:85:VAL:CG2	2.47	0.44
52:Z2:578:U:H2'	52:Z2:579:U:C6	2.52	0.44
52:Z2:1776:C:H5"	52:Z2:1777:A:OP1	2.17	0.44
52:Z2:2813:U:H2'	52:Z2:2814:G:O4'	2.17	0.44
15:FG:36:ILE:CG1	15:FG:64:ILE:HG22	2.42	0.44
52:Z2:818:A:H2'	52:Z2:819:G:H8	1.81	0.44
28:KU:103:LEU:HD23	28:KU:103:LEU:C	2.38	0.44
52:Z2:43:G:N3	52:Z2:433:G:O2'	2.48	0.44
52:Z2:1125:U:H4'	52:Z2:1127:A:O4'	2.18	0.44
21:MM:86:TYR:OH	21:MM:90:ARG:NH1	2.51	0.44
28:KU:113:VAL:HG22	28:KU:113:VAL:O	2.16	0.44
52:Z2:368:C:O2'	52:Z2:371:G:N2	2.50	0.44
52:Z2:2249:A:H4'	52:Z2:2250:A:N3	2.33	0.44
6:L6:8:ILE:HG12	33:QZ:40:TYR:CD2	2.52	0.44
21:MM:7:VAL:HG22	21:MM:8:ASN:H	1.81	0.44
25:GR:135:SER:HB3	25:GR:141:LEU:HB2	1.99	0.44
52:Z2:533:U:C2	52:Z2:534:U:C5	3.06	0.44
52:Z2:813:U:H2'	52:Z2:814:A:C8	2.53	0.44
52:Z2:1486:A:C6	52:Z2:1487:C:C4	3.06	0.44
1:F:78:ARG:O	1:F:82:THR:HG23	2.16	0.44
13:XE:9:LYS:O	13:XE:14:LEU:HD11	2.17	0.44
15:FG:19:VAL:O	15:FG:23:GLU:OE1	2.36	0.44
25:GR:11:LEU:HD11	25:GR:50:VAL:HG23	2.00	0.44
25:GR:96:ALA:CB	25:GR:131:ILE:HD11	2.48	0.44
27:CT:124:LEU:HD13	27:CT:196:ILE:HG21	1.99	0.44
52:Z2:237:A:OP2	52:Z2:238:A:O2'	2.28	0.44
52:Z2:532:A:O2'	52:Z2:533:U:P	2.76	0.44
52:Z2:1163:U:O2	52:Z2:1163:U:O4'	2.35	0.44
1:F:53:LEU:O	1:F:53:LEU:HD12	2.18	0.44
11:UC:80:ILE:HG23	11:UC:80:ILE:O	2.16	0.44
52:Z2:798:U:O2'	52:Z2:1209:A:H1'	2.18	0.44
52:Z2:1072:A:H2'	52:Z2:1072:A:N3	2.33	0.44
12:WD:8:THR:HG22	12:WD:8:THR:O	2.17	0.44
24:BQ:79:ARG:NH2	24:BQ:81:SER:O	2.51	0.44
28:KU:107:VAL:O	29:NV:6:VAL:HG11	2.18	0.44
52:Z2:471:U:O2'	52:Z2:474:G:O6	2.35	0.44
52:Z2:836:C:H2'	52:Z2:837:A:H8	1.82	0.44
4:A4:11:MET:SD	4:A4:48:LEU:HD12	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:MB:87:TYR:HB3	10:MB:94:TYR:CE1	2.52	0.44
13:XE:5:GLU:HA	13:XE:8:ASP:OD1	2.18	0.44
19:HK:97:ARG:O	32:JY:65:TYR:HA	2.18	0.44
20:OL:18:GLU:O	20:OL:19:ASN:OD1	2.35	0.44
32:JY:53:THR:HG22	32:JY:63:ASP:OD2	2.18	0.44
52:Z2:683:C:O2'	52:Z2:719:A:N6	2.51	0.44
52:Z2:1341:C:H2'	52:Z2:1342:G:O4'	2.17	0.44
5:E5:112:ALA:HA	5:E5:130:THR:OG1	2.17	0.43
16:VH:32:VAL:HG22	16:VH:35:ASN:OD1	2.18	0.43
52:Z2:713:G:H3'	52:Z2:714:G:H5'	2.00	0.43
2:C1:29:PHE:CE2	52:Z2:2184:A:C8	3.06	0.43
21:MM:97:VAL:HG22	21:MM:97:VAL:O	2.17	0.43
32:JY:85:ASP:HB2	32:JY:89:LYS:NZ	2.32	0.43
52:Z2:2610:G:N2	52:Z2:2760:G:OP2	2.51	0.43
8:E9:173:GLU:O	8:E9:173:GLU:HG3	2.18	0.43
26:GS:75:GLU:HB3	26:GS:92:VAL:HG22	2.00	0.43
52:Z2:1138:C:H2'	52:Z2:1139:G:O4'	2.19	0.43
52:Z2:2739:U:H4'	52:Z2:2740:A:OP1	2.19	0.43
7:F7:4:LEU:HD13	7:F7:100:LEU:HD22	2.01	0.43
25:GR:83:PHE:HB3	25:GR:141:LEU:HD22	2.01	0.43
27:CT:138:VAL:HG11	27:CT:168:TYR:HE2	1.83	0.43
33:QZ:73:ILE:HD12	33:QZ:73:ILE:H	1.82	0.43
21:MM:48:LEU:HD23	21:MM:53:LEU:HD22	2.01	0.43
25:GR:11:LEU:HD11	25:GR:50:VAL:CG2	2.49	0.43
52:Z2:697:C:H2'	52:Z2:698:G:O4'	2.17	0.43
1:F:113:LYS:HB2	1:F:116:LEU:HD12	2.00	0.43
5:E5:20:LEU:HD12	5:E5:42:THR:HG22	2.00	0.43
20:OL:4:ASN:O	20:OL:8:GLU:HG3	2.18	0.43
50:D8:77:G:O2'	52:Z2:846:A:N3	2.50	0.43
52:Z2:1690:G:C6	52:Z2:1691:G:N7	2.86	0.43
52:Z2:1708:A:C6	52:Z2:1725:A:C8	3.06	0.43
50:D8:3:U:OP1	50:D8:59:A:O2'	2.30	0.43
4:A4:96:TYR:O	4:A4:155:GLY:HA3	2.18	0.43
21:MM:77:ILE:O	21:MM:81:VAL:HG23	2.19	0.43
52:Z2:829:C:O2'	52:Z2:830:G:H5'	2.19	0.43
52:Z2:842:G:H2'	52:Z2:843:G:O4'	2.19	0.43
52:Z2:968:A:H2'	52:Z2:968:A:N3	2.34	0.43
3:R3:25:ASP:OD1	15:FG:101:GLN:HG2	2.18	0.43
7:F7:142:ASP:OD1	7:F7:142:ASP:O	2.36	0.43
22:PO:74:LEU:HD11	22:PO:78:ARG:HB2	2.01	0.43
23:SP:15:LEU:HG	23:SP:33:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Z2:561:U:H2'	52:Z2:562:G:C8	2.53	0.43
12:WD:5:CYS:SG	12:WD:7:VAL:HG22	2.59	0.43
21:MM:79:ARG:O	21:MM:82:ASP:OD1	2.37	0.43
26:GS:26:PHE:HA	26:GS:102:MET:SD	2.59	0.43
52:Z2:1266:U:H2'	52:Z2:1267:G:O4'	2.19	0.43
2:C1:41:ALA:HA	2:C1:44:ILE:HG12	2.01	0.42
6:L6:8:ILE:HG21	33:QZ:44:LEU:HD11	2.00	0.42
52:Z2:493:C:N3	52:Z2:494:U:C5	2.87	0.42
52:Z2:1369:A:H4'	52:Z2:1370:U:OP1	2.19	0.42
32:JY:34:ALA:CB	32:JY:83:THR:HG21	2.41	0.42
50:D8:37:U:N3	50:D8:38:U:O4	2.51	0.42
52:Z2:302:U:H2'	52:Z2:303:G:O4'	2.19	0.42
52:Z2:790:G:OP2	52:Z2:791:C:N4	2.50	0.42
52:Z2:1976:C:H2'	52:Z2:1977:U:C1'	2.49	0.42
52:Z2:2578:G:N2	52:Z2:2581:A:OP2	2.36	0.42
5:E5:44:VAL:HG12	5:E5:72:ALA:CB	2.49	0.42
15:FG:101:GLN:OE1	15:FG:101:GLN:N	2.44	0.42
52:Z2:629:A:H2'	52:Z2:631:A:N7	2.33	0.42
52:Z2:1181:G:N2	52:Z2:1233:A:O2'	2.49	0.42
22:PO:89:THR:O	22:PO:89:THR:CG2	2.66	0.42
24:BQ:74:ILE:O	24:BQ:74:ILE:HG22	2.18	0.42
25:GR:49:VAL:HG22	25:GR:50:VAL:N	2.34	0.42
28:KU:108:ASN:O	29:NV:6:VAL:HG12	2.20	0.42
52:Z2:354:A:OP2	52:Z2:386:G:N2	2.52	0.42
52:Z2:2674:C:O2'	52:Z2:2675:G:H5'	2.19	0.42
1:F:82:THR:HB	1:F:96:LEU:HD21	2.00	0.42
5:E5:101:MET:HG2	5:E5:130:THR:HG22	2.00	0.42
11:UC:35:ILE:HG22	11:UC:96:ASP:OD1	2.19	0.42
20:OL:3:THR:O	20:OL:6:ASP:OD2	2.36	0.42
26:GS:150:LYS:O	26:GS:150:LYS:HG2	2.18	0.42
52:Z2:345:A:O2'	52:Z2:346:A:H8	2.03	0.42
52:Z2:810:A:H2'	52:Z2:811:U:O4'	2.19	0.42
52:Z2:1012:A:H2'	52:Z2:1013:A:C8	2.54	0.42
52:Z2:1418:A:H2'	52:Z2:1419:G:O4'	2.20	0.42
52:Z2:1514:A:H3'	52:Z2:1515:G:H5"	2.01	0.42
52:Z2:1673:C:N3	52:Z2:1674:C:C5	2.87	0.42
52:Z2:1842:U:H2'	52:Z2:1843:G:O4'	2.19	0.42
52:Z2:2219:U:H2'	52:Z2:2220:G:O4'	2.19	0.42
52:Z2:2773:U:OP2	52:Z2:2858:U:O2'	2.37	0.42
23:SP:32:LYS:HA	23:SP:50:SER:HB2	2.01	0.42
29:NV:39:GLU:HG2	29:NV:44:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:QZ:55:GLU:OE1	33:QZ:56:ASN:OD1	2.37	0.42
52:Z2:446:G:N2	52:Z2:449:A:OP2	2.37	0.42
52:Z2:1392:U:H2'	52:Z2:1393:U:C6	2.54	0.42
52:Z2:1927:C:N4	52:Z2:1951:C:O4'	2.52	0.42
52:Z2:2286:G:HO2'	52:Z2:2287:G:H5'	1.84	0.42
52:Z2:2339:C:H2'	52:Z2:2340:C:O4'	2.19	0.42
20:OL:2:LEU:O	20:OL:7:ARG:NH1	2.53	0.42
21:MM:80:LEU:HD22	21:MM:87:ARG:HB2	2.01	0.42
22:PO:27:ALA:HB1	22:PO:31:VAL:HG22	2.00	0.42
24:BQ:119:ARG:NH1	24:BQ:119:ARG:HB2	2.35	0.42
30:YW:52:TYR:CE2	30:YW:53:LEU:HD23	2.54	0.42
52:Z2:40:U:O4	52:Z2:429:G:O2'	2.33	0.42
52:Z2:951:U:H2'	52:Z2:952:C:C6	2.54	0.42
52:Z2:1005:A:H3'	52:Z2:1005:A:N3	2.35	0.42
52:Z2:1505:C:H2'	52:Z2:1506:U:C6	2.54	0.42
1:F:13:SER:OG	1:F:68:GLY:HA3	2.19	0.42
21:MM:4:ILE:HB	21:MM:22:ILE:HD11	2.01	0.42
23:SP:39:MET:HE3	23:SP:40:ILE:H	1.84	0.42
52:Z2:362:G:N1	52:Z2:379:G:C6	2.88	0.42
52:Z2:849:G:H2'	52:Z2:850:C:C6	2.55	0.42
52:Z2:1259:A:O2'	52:Z2:1633:G:N3	2.53	0.42
52:Z2:2029:C:C2	52:Z2:2030:C:C5	3.08	0.42
52:Z2:2706:C:H2'	52:Z2:2707:U:O4'	2.19	0.42
4:A4:12:ARG:HA	4:A4:12:ARG:NE	2.35	0.42
7:F7:47:LYS:O	7:F7:47:LYS:HG3	2.19	0.42
7:F7:162:THR:HB	7:F7:165:GLU:OE1	2.20	0.42
27:CT:23:TYR:CD2	32:JY:97:ASP:HB2	2.54	0.42
33:QZ:64:LEU:HD23	33:QZ:85:VAL:HG21	2.01	0.42
48:A:75:ARG:HG3	48:A:75:ARG:HH11	1.84	0.42
52:Z2:228:A:H2'	52:Z2:229:G:O4'	2.19	0.42
52:Z2:334:A:H2'	52:Z2:335:C:C6	2.55	0.42
52:Z2:2620:U:H2'	52:Z2:2621:G:O4'	2.20	0.42
4:A4:205:ILE:HD12	4:A4:205:ILE:N	2.35	0.42
5:E5:60:GLU:OE1	5:E5:60:GLU:HA	2.20	0.42
31:IX:7:LYS:O	31:IX:9:ALA:N	2.53	0.42
52:Z2:220:A:O2'	52:Z2:403:C:O2	2.32	0.42
52:Z2:1109:G:P	52:Z2:1110:A:HO2'	2.33	0.42
52:Z2:1273:C:O2'	52:Z2:1314:C:H4'	2.20	0.42
52:Z2:1416:G:H2'	52:Z2:1417:A:C8	2.54	0.42
52:Z2:2200:U:H2'	52:Z2:2201:A:H8	1.84	0.42
52:Z2:2670:U:H2'	52:Z2:2671:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:MB:4:ARG:NH2	52:Z2:2841:C:OP1	2.50	0.41
14:RF:13:SER:HB3	14:RF:16:LYS:HD2	2.02	0.41
17:TI:96:ARG:HH12	52:Z2:286:A:P	2.43	0.41
20:OL:16:ARG:HD2	20:OL:25:GLU:OE1	2.20	0.41
25:GR:75:TYR:O	25:GR:79:VAL:HG22	2.20	0.41
31:IX:135:GLN:OE1	31:IX:135:GLN:HA	2.20	0.41
33:QZ:18:VAL:HG13	33:QZ:18:VAL:O	2.20	0.41
52:Z2:297:A:O2'	52:Z2:298:A:OP2	2.24	0.41
52:Z2:818:A:H2'	52:Z2:819:G:C8	2.54	0.41
52:Z2:1279:C:C2	52:Z2:1280:G:C8	3.08	0.41
52:Z2:1452:A:H2'	52:Z2:1453:A:C8	2.55	0.41
11:UC:71:VAL:O	11:UC:72:ASP:C	2.59	0.41
31:IX:15:TRP:HB3	31:IX:137:PRO:HB3	2.02	0.41
32:JY:24:GLU:O	32:JY:28:THR:HG23	2.20	0.41
50:D8:28:C:O2	50:D8:28:C:H2'	2.19	0.41
52:Z2:1640:A:H2'	52:Z2:1641:G:O4'	2.20	0.41
52:Z2:2786:A:H2'	52:Z2:2786:A:N3	2.35	0.41
52:Z2:2804:G:C4	52:Z2:2805:G:C8	3.08	0.41
52:Z2:2806:C:H2'	52:Z2:2807:A:H8	1.86	0.41
7:F7:79:ILE:O	7:F7:79:ILE:HG13	2.20	0.41
15:FG:16:ASP:OD1	15:FG:16:ASP:N	2.53	0.41
17:TI:82:THR:HB	17:TI:96:ARG:NE	2.33	0.41
23:SP:44:MET:HB2	23:SP:47:LEU:HD21	2.02	0.41
23:SP:53:ASN:OD1	23:SP:53:ASN:C	2.58	0.41
31:IX:65:THR:HG22	31:IX:66:GLY:N	2.34	0.41
52:Z2:82:G:H2'	52:Z2:82:G:N3	2.35	0.41
52:Z2:713:G:H3'	52:Z2:714:G:C5'	2.50	0.41
52:Z2:1707:G:C6	52:Z2:1724:G:C6	3.09	0.41
7:F7:50:LEU:O	7:F7:54:VAL:HG23	2.21	0.41
17:TI:41:THR:OG1	52:Z2:482:U:H4'	2.21	0.41
19:HK:63:ARG:HG2	19:HK:70:PRO:HA	2.02	0.41
26:GS:112:ARG:HB2	26:GS:120:ARG:HB3	2.02	0.41
30:YW:46:MET:CE	52:Z2:835:C:O2	2.68	0.41
31:IX:116:TYR:O	31:IX:119:ILE:HG22	2.21	0.41
52:Z2:39:C:N4	52:Z2:430:A:OP2	2.54	0.41
52:Z2:462:A:H4'	52:Z2:463:A:OP1	2.20	0.41
52:Z2:1188:A:O4'	52:Z2:1190:G:C8	2.74	0.41
52:Z2:1326:A:HO2'	52:Z2:1328:U:P	2.44	0.41
52:Z2:2049:C:O2	52:Z2:2433:A:N1	2.53	0.41
52:Z2:2053:G:H1	52:Z2:2426:U:H3	1.68	0.41
4:A4:138:GLU:O	4:A4:141:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E9:192:ALA:O	8:E9:196:GLU:HG3	2.20	0.41
17:TI:60:GLU:OE1	17:TI:60:GLU:N	2.49	0.41
22:PO:90:ILE:HG22	22:PO:95:LEU:HG	2.02	0.41
23:SP:15:LEU:O	23:SP:19:VAL:HG13	2.21	0.41
32:JY:23:GLN:HA	32:JY:23:GLN:OE1	2.20	0.41
52:Z2:397:C:O3'	52:Z2:1864:G:N2	2.53	0.41
52:Z2:1338:A:H2'	52:Z2:1339:G:O4'	2.21	0.41
52:Z2:1552:C:H2'	52:Z2:1553:C:C6	2.56	0.41
52:Z2:1788:A:H2'	52:Z2:1789:A:C8	2.56	0.41
52:Z2:2488:G:O2'	52:Z2:2489:U:H5'	2.19	0.41
52:Z2:2615:A:O4'	52:Z2:2776:A:H2	2.03	0.41
4:A4:178:ILE:HD13	4:A4:188:VAL:HG21	2.03	0.41
7:F7:146:ILE:HD13	7:F7:149:ILE:HD13	2.02	0.41
12:WD:55:GLY:O	12:WD:59:ILE:HG12	2.21	0.41
16:VH:78:ARG:NH1	52:Z2:843:G:OP1	2.52	0.41
19:HK:22:ASP:OD1	19:HK:23:LYS:N	2.54	0.41
21:MM:14:HIS:ND1	21:MM:42:THR:O	2.51	0.41
21:MM:19:LEU:HD13	21:MM:22:ILE:HD12	2.01	0.41
21:MM:53:LEU:HB3	21:MM:57:ARG:NH1	2.36	0.41
23:SP:55:ARG:HG2	23:SP:56:THR:HG23	2.02	0.41
27:CT:138:VAL:HG11	27:CT:168:TYR:CE2	2.56	0.41
29:NV:42:THR:HG23	29:NV:43:GLN:N	2.35	0.41
52:Z2:2302:U:O2	52:Z2:2302:U:O4'	2.37	0.41
52:Z2:2328:A:N3	52:Z2:2364:A:H2'	2.36	0.41
52:Z2:2865:G:H2'	52:Z2:2866:A:C8	2.55	0.41
11:UC:89:LYS:HA	11:UC:89:LYS:HD2	1.96	0.41
29:NV:31:ASP:O	29:NV:35:ARG:HG2	2.20	0.41
50:D8:44:A:C5	50:D8:45:C:C5	3.08	0.41
52:Z2:374:A:C5	52:Z2:375:U:C5	3.09	0.41
52:Z2:2610:G:O2'	52:Z2:2764:A:N1	2.42	0.41
52:Z2:2724:A:H2'	52:Z2:2725:C:O4'	2.20	0.41
4:A4:122:LEU:O	4:A4:146:MET:HE2	2.20	0.41
19:HK:4:LYS:HA	19:HK:7:ILE:HD12	2.03	0.41
24:BQ:28:PRO:O	24:BQ:33:ARG:NH1	2.48	0.41
33:QZ:29:VAL:HG22	33:QZ:50:ILE:O	2.21	0.41
52:Z2:377:C:O2'	52:Z2:378:U:H5'	2.21	0.41
52:Z2:962:G:O4'	52:Z2:985:A:H2	2.04	0.41
4:A4:59:LEU:HA	4:A4:62:VAL:HG12	2.03	0.41
4:A4:73:LEU:HD12	4:A4:74:PHE:H	1.85	0.41
8:E9:136:LYS:O	8:E9:139:GLU:HG2	2.20	0.41
10:MB:58:ASP:OD1	10:MB:63:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XE:18:LEU:O	13:XE:22:GLN:HG3	2.20	0.41
19:HK:60:LEU:HD23	19:HK:61:ARG:N	2.35	0.41
21:MM:90:ARG:HD2	21:MM:96:PRO:O	2.21	0.41
23:SP:16:PHE:CE1	23:SP:20:GLU:OE2	2.74	0.41
26:GS:5:ARG:HG3	26:GS:5:ARG:HH11	1.85	0.41
26:GS:63:PHE:O	26:GS:66:VAL:HG12	2.21	0.41
26:GS:71:ARG:NH1	26:GS:98:THR:OG1	2.54	0.41
26:GS:144:ARG:HB2	26:GS:144:ARG:NH1	2.35	0.41
50:D8:30:U:N3	50:D8:31:G:N7	2.68	0.41
52:Z2:173:A:O2'	52:Z2:174:A:H5'	2.21	0.41
52:Z2:178:A:H1'	52:Z2:418:C:O4'	2.21	0.41
52:Z2:189:G:H8	52:Z2:787:A:O2'	2.04	0.41
52:Z2:374:A:H1'	52:Z2:394:G:O4'	2.21	0.41
52:Z2:558:U:O2'	52:Z2:560:A:OP1	2.29	0.41
52:Z2:847:G:H2'	52:Z2:848:A:O4'	2.20	0.41
52:Z2:1031:G:HO2'	52:Z2:1032:A:P	2.44	0.41
52:Z2:1311:A:C4	52:Z2:1312:A:C8	3.08	0.41
52:Z2:2303:A:N3	52:Z2:2303:A:H2'	2.36	0.41
52:Z2:2586:G:C5	52:Z2:2587:U:C5	3.09	0.41
52:Z2:2771:C:O2'	52:Z2:2775:A:N3	2.45	0.41
8:E9:94:LYS:NZ	52:Z2:643:U:O2'	2.53	0.41
13:XE:40:THR:O	13:XE:43:VAL:HG12	2.21	0.41
14:RF:93:ALA:HB2	52:Z2:1602:A:C2	2.56	0.41
29:NV:4:VAL:HG21	29:NV:19:PHE:HA	2.02	0.41
31:IX:65:THR:CG2	31:IX:66:GLY:N	2.84	0.41
52:Z2:1513:A:C4	52:Z2:1532:A:N6	2.88	0.41
52:Z2:1776:C:C3'	52:Z2:1777:A:C8	3.04	0.41
52:Z2:1832:G:O2'	52:Z2:1833:A:H5'	2.20	0.41
52:Z2:2276:C:C2	52:Z2:2277:G:C8	3.09	0.41
26:GS:58:ASP:OD2	26:GS:61:ALA:HB2	2.21	0.40
32:JY:102:LEU:O	32:JY:102:LEU:CD2	2.64	0.40
52:Z2:993:A:N3	52:Z2:1138:C:O2'	2.52	0.40
52:Z2:1171:G:O2'	52:Z2:1172:U:O5'	2.39	0.40
52:Z2:1485:G:H2'	52:Z2:1486:A:H8	1.86	0.40
52:Z2:1503:A:C5	52:Z2:1504:U:C5	3.08	0.40
52:Z2:1695:G:C8	52:Z2:1742:G:C5	3.09	0.40
52:Z2:2400:C:C2	52:Z2:2401:A:C8	3.08	0.40
1:F:116:LEU:HD22	1:F:122:ARG:HG2	2.02	0.40
3:R3:47:THR:HG22	3:R3:48:SER:N	2.36	0.40
7:F7:146:ILE:CD1	7:F7:149:ILE:HD13	2.51	0.40
8:E9:47:THR:O	8:E9:51:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Z2:475:A:H2'	52:Z2:476:G:O4'	2.21	0.40
52:Z2:652:U:H2'	52:Z2:653:A:O4'	2.21	0.40
52:Z2:1428:A:C4	52:Z2:1429:G:C8	3.09	0.40
52:Z2:1670:G:H2'	52:Z2:1671:U:C6	2.56	0.40
4:A4:125:GLN:HA	4:A4:128:ASP:OD1	2.21	0.40
6:L6:8:ILE:CG2	33:QZ:44:LEU:HD11	2.51	0.40
10:MB:32:GLU:HB3	10:MB:119:ASP:CB	2.51	0.40
12:WD:7:VAL:HG23	12:WD:8:THR:N	2.37	0.40
52:Z2:33:G:H2'	52:Z2:34:G:O4'	2.22	0.40
52:Z2:745:G:H2'	52:Z2:746:A:O4'	2.21	0.40
52:Z2:1369:A:H1'	52:Z2:1370:U:C6	2.56	0.40
52:Z2:1685:G:OP2	52:Z2:1686:A:O2'	2.34	0.40
1:F:3:ARG:HE	1:F:3:ARG:HA	1.86	0.40
5:E5:138:THR:HG23	5:E5:139:ALA:N	2.37	0.40
14:RF:74:ILE:HD12	14:RF:105:ILE:HG12	2.03	0.40
17:TI:88:ASP:OD1	17:TI:88:ASP:N	2.52	0.40
23:SP:11:ILE:HG21	23:SP:41:LEU:HD11	2.04	0.40
23:SP:11:ILE:HG22	23:SP:39:MET:HB3	2.04	0.40
28:KU:25:ALA:HB1	28:KU:90:GLY:HA3	2.02	0.40
31:IX:105:VAL:HG11	31:IX:122:LEU:HD22	2.04	0.40
52:Z2:493:C:C2	52:Z2:494:U:C6	3.09	0.40
52:Z2:888:C:O2'	52:Z2:889:G:H5'	2.22	0.40
52:Z2:1091:G:C2	52:Z2:1092:U:C6	3.10	0.40
52:Z2:2209:C:C2	52:Z2:2210:A:C8	3.09	0.40
52:Z2:2347:C:H2'	52:Z2:2348:G:O4'	2.22	0.40
52:Z2:2488:G:O2'	52:Z2:2489:U:C5'	2.70	0.40
14:RF:3:VAL:HG22	14:RF:62:HIS:ND1	2.36	0.40
15:FG:42:TRP:HZ2	15:FG:61:LEU:HD13	1.85	0.40
15:FG:51:ILE:HG21	15:FG:85:ILE:HD12	2.04	0.40
25:GR:140:GLN:HA	25:GR:140:GLN:OE1	2.21	0.40
30:YW:46:MET:HE1	52:Z2:913:G:N2	2.37	0.40
50:D8:26:C:H2'	50:D8:27:A:O4'	2.21	0.40
52:Z2:914:U:O2'	52:Z2:915:A:H5'	2.22	0.40
52:Z2:1112:G:O4'	52:Z2:2499:U:O2'	2.40	0.40
52:Z2:1558:A:H2'	52:Z2:1559:A:C8	2.57	0.40
52:Z2:2211:A:H2'	52:Z2:2212:U:C6	2.57	0.40
52:Z2:2537:U:H2'	52:Z2:2538:U:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	123/128 (96%)	118 (96%)	5 (4%)	0	100	100
2	C1	47/166 (28%)	47 (100%)	0	0	100	100
3	R3	54/76 (71%)	54 (100%)	0	0	100	100
4	A4	231/269 (86%)	228 (99%)	3 (1%)	0	100	100
5	E5	154/171 (90%)	152 (99%)	2 (1%)	0	100	100
6	L6	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
7	F7	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
8	E9	197/200 (98%)	193 (98%)	4 (2%)	0	100	100
9	aA	51/60 (85%)	51 (100%)	0	0	100	100
10	MB	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
11	UC	94/219 (43%)	88 (94%)	6 (6%)	0	100	100
12	WD	74/78 (95%)	73 (99%)	1 (1%)	0	100	100
13	XE	60/65 (92%)	60 (100%)	0	0	100	100
14	RF	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
15	FG	100/134 (75%)	97 (97%)	3 (3%)	0	100	100
16	VH	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
17	TI	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
18	fJ	53/93 (57%)	52 (98%)	1 (2%)	0	100	100
19	HK	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
20	OL	84/88 (96%)	79 (94%)	5 (6%)	0	100	100
21	MM	108/118 (92%)	104 (96%)	4 (4%)	0	100	100
22	PO	114/118 (97%)	114 (100%)	0	0	100	100
23	SP	78/91 (86%)	74 (95%)	4 (5%)	0	100	100
24	BQ	129/132 (98%)	128 (99%)	1 (1%)	0	100	100
25	GR	171/177 (97%)	170 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	GS	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
27	CT	202/241 (84%)	199 (98%)	3 (2%)	0	100	100
28	KU	112/129 (87%)	110 (98%)	2 (2%)	0	100	100
29	NV	55/71 (78%)	55 (100%)	0	0	100	100
30	YW	54/59 (92%)	53 (98%)	1 (2%)	0	100	100
31	IX	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
32	JY	91/103 (88%)	86 (94%)	5 (6%)	0	100	100
33	QZ	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
34	Ba	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
35	Qb	101/103 (98%)	101 (100%)	0	0	100	100
36	Nc	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
37	Kd	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
38	Je	120/122 (98%)	120 (100%)	0	0	100	100
39	Af	209/212 (99%)	202 (97%)	7 (3%)	0	100	100
40	Lg	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
41	dh	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	3	22
42	Oi	113/130 (87%)	112 (99%)	1 (1%)	0	100	100
43	Pj	79/89 (89%)	79 (100%)	0	0	100	100
44	bk	47/51 (92%)	47 (100%)	0	0	100	100
45	Cl	270/274 (98%)	265 (98%)	5 (2%)	0	100	100
46	Dm	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
47	Sn	85/116 (73%)	85 (100%)	0	0	100	100
48	A	63/88 (72%)	61 (97%)	2 (3%)	0	100	100
48	To	84/88 (96%)	83 (99%)	1 (1%)	0	100	100
49	ep	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	5505/6229 (88%)	5391 (98%)	112 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	dh	32	ILE
41	dh	33	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	97/105 (92%)	96 (99%)	1 (1%)	73 87
2	C1	39/135 (29%)	39 (100%)	0	100 100
3	R3	51/67 (76%)	51 (100%)	0	100 100
4	A4	186/211 (88%)	185 (100%)	1 (0%)	86 93
5	E5	118/131 (90%)	118 (100%)	0	100 100
6	L6	102/103 (99%)	102 (100%)	0	100 100
7	F7	138/146 (94%)	138 (100%)	0	100 100
8	E9	159/159 (100%)	159 (100%)	0	100 100
9	aA	47/53 (89%)	47 (100%)	0	100 100
10	MB	101/102 (99%)	101 (100%)	0	100 100
11	UC	78/184 (42%)	78 (100%)	0	100 100
12	WD	67/71 (94%)	66 (98%)	1 (2%)	60 81
13	XE	54/57 (95%)	54 (100%)	0	100 100
14	RF	88/88 (100%)	88 (100%)	0	100 100
15	FG	92/121 (76%)	91 (99%)	1 (1%)	70 86
16	VH	58/62 (94%)	58 (100%)	0	100 100
17	TI	83/85 (98%)	83 (100%)	0	100 100
18	fJ	47/81 (58%)	47 (100%)	0	100 100
19	HK	87/88 (99%)	87 (100%)	0	100 100
20	OL	75/77 (97%)	75 (100%)	0	100 100
21	MM	91/99 (92%)	88 (97%)	3 (3%)	33 64
22	PO	88/90 (98%)	88 (100%)	0	100 100
23	SP	71/79 (90%)	71 (100%)	0	100 100
24	BQ	103/104 (99%)	103 (100%)	0	100 100
25	GR	147/151 (97%)	147 (100%)	0	100 100
26	GS	123/128 (96%)	123 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	CT	167/198 (84%)	166 (99%)	1 (1%)	84	92
28	KU	84/98 (86%)	84 (100%)	0	100	100
29	NV	49/63 (78%)	49 (100%)	0	100	100
30	YW	50/52 (96%)	50 (100%)	0	100	100
31	IX	116/117 (99%)	116 (100%)	0	100	100
32	JY	84/90 (93%)	84 (100%)	0	100	100
33	QZ	73/84 (87%)	73 (100%)	0	100	100
34	Ba	37/37 (100%)	37 (100%)	0	100	100
35	Qb	89/89 (100%)	89 (100%)	0	100	100
36	Nc	81/85 (95%)	81 (100%)	0	100	100
37	Kd	107/110 (97%)	107 (100%)	0	100	100
38	Je	102/102 (100%)	102 (100%)	0	100	100
39	Af	161/162 (99%)	161 (100%)	0	100	100
40	Lg	114/114 (100%)	114 (100%)	0	100	100
41	dh	55/56 (98%)	55 (100%)	0	100	100
42	Oi	97/108 (90%)	97 (100%)	0	100	100
43	Pj	63/68 (93%)	63 (100%)	0	100	100
44	bk	42/46 (91%)	42 (100%)	0	100	100
45	Cl	218/221 (99%)	218 (100%)	0	100	100
46	Dm	177/181 (98%)	177 (100%)	0	100	100
47	Sn	75/97 (77%)	75 (100%)	0	100	100
48	A	39/69 (56%)	39 (100%)	0	100	100
48	To	66/69 (96%)	66 (100%)	0	100	100
49	ep	33/33 (100%)	33 (100%)	0	100	100
All	All	4569/5126 (89%)	4561 (100%)	8 (0%)	91	97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	79	HIS
4	A4	136	LYS
12	WD	35	HIS
15	FG	92	ARG
21	MM	59	GLN

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Mol	Chain	Res	Type
21	MM	92	ARG
21	MM	110	LYS
27	CT	127	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
9	aA	4	GLN
28	KU	118	HIS
39	Af	47	GLN
47	Sn	73	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	D8	114/115 (99%)	9 (7%)	0
51	iN	1498/1589 (94%)	291 (19%)	0
52	Z2	2698/2882 (93%)	344 (12%)	8 (0%)
All	All	4310/4586 (93%)	644 (14%)	8 (0%)

All (644) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	D8	13	A
50	D8	28	C
50	D8	33	U
50	D8	39	C
50	D8	50	A
50	D8	54	G
50	D8	88	A
50	D8	96	A
50	D8	106	A
51	iN	51	C
51	iN	52	U
51	iN	56	G
51	iN	69	G
51	iN	79	A
51	iN	80	A
51	iN	86	G
51	iN	88	G

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Mol	Chain	Res	Type
51	iN	94	C
51	iN	95	U
51	iN	98	A
51	iN	101	C
51	iN	102	A
51	iN	116	G
51	iN	118	A
51	iN	125	G
51	iN	127	A
51	iN	128	G
51	iN	130	U
51	iN	131	U
51	iN	132	G
51	iN	135	U
51	iN	137	U
51	iN	139	G
51	iN	143	A
51	iN	150	G
51	iN	164	A
51	iN	166	U
51	iN	167	A
51	iN	176	U
51	iN	184	G
51	iN	187	G
51	iN	191	G
51	iN	199	U
51	iN	206	A
51	iN	208	C
51	iN	211	G
51	iN	217	A
51	iN	218	U
51	iN	225	U
51	iN	233	A
51	iN	234	C
51	iN	235	G
51	iN	238	A
51	iN	247	G
51	iN	259	U
51	iN	280	A
51	iN	290	G
51	iN	293	A
51	iN	294	G

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Mol	Chain	Res	Type
51	iN	309	G
51	iN	310	C
51	iN	323	C
51	iN	324	G
51	iN	326	U
51	iN	332	G
51	iN	364	A
51	iN	371	C
51	iN	372	A
51	iN	373	C
51	iN	375	G
51	iN	389	G
51	iN	394	G
51	iN	395	C
51	iN	397	G
51	iN	410	U
51	iN	415	C
51	iN	416	A
51	iN	425	A
51	iN	435	C
51	iN	449	G
51	iN	453	G
51	iN	454	A
51	iN	456	G
51	iN	457	A
51	iN	464	U
51	iN	466	U
51	iN	467	G
51	iN	472	U
51	iN	496	G
51	iN	497	A
51	iN	504	G
51	iN	508	A
51	iN	510	U
51	iN	511	A
51	iN	521	G
51	iN	522	A
51	iN	523	U
51	iN	524	G
51	iN	525	A
51	iN	527	A
51	iN	529	U

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Mol	Chain	Res	Type
51	iN	534	G
51	iN	539	A
51	iN	540	U
51	iN	548	G
51	iN	552	A
51	iN	554	C
51	iN	561	C
51	iN	564	G
51	iN	566	A
51	iN	567	G
51	iN	575	A
51	iN	578	A
51	iN	582	A
51	iN	590	A
51	iN	605	U
51	iN	607	C
51	iN	609	G
51	iN	615	A
51	iN	616	A
51	iN	619	G
51	iN	620	G
51	iN	622	G
51	iN	631	G
51	iN	639	A
51	iN	650	A
51	iN	675	U
51	iN	681	C
51	iN	697	A
51	iN	725	A
51	iN	731	A
51	iN	737	G
51	iN	738	A
51	iN	739	A
51	iN	740	A
51	iN	755	G
51	iN	765	G
51	iN	767	U
51	iN	784	U
51	iN	785	G
51	iN	786	G
51	iN	789	U
51	iN	792	U

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Mol	Chain	Res	Type
51	iN	798	C
51	iN	799	A
51	iN	803	A
51	iN	807	U
51	iN	821	A
51	iN	825	A
51	iN	834	A
51	iN	837	U
51	iN	838	A
51	iN	849	C
51	iN	859	A
51	iN	860	A
51	iN	861	C
51	iN	872	A
51	iN	876	G
51	iN	891	G
51	iN	895	U
51	iN	898	U
51	iN	899	G
51	iN	911	G
51	iN	914	A
51	iN	916	A
51	iN	934	G
51	iN	946	G
51	iN	958	A
51	iN	970	G
51	iN	971	G
51	iN	978	C
51	iN	982	A
51	iN	999	U
51	iN	1000	U
51	iN	1002	A
51	iN	1004	U
51	iN	1013	A
51	iN	1018	A
51	iN	1019	A
51	iN	1020	G
51	iN	1021	A
51	iN	1026	U
51	iN	1036	U
51	iN	1037	G
51	iN	1043	U

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Mol	Chain	Res	Type
51	iN	1044	C
51	iN	1046	A
51	iN	1048	A
51	iN	1050	U
51	iN	1053	U
51	iN	1056	A
51	iN	1064	G
51	iN	1070	G
51	iN	1072	C
51	iN	1074	U
51	iN	1075	C
51	iN	1077	G
51	iN	1078	G
51	iN	1080	A
51	iN	1081	U
51	iN	1084	G
51	iN	1085	A
51	iN	1089	C
51	iN	1109	U
51	iN	1112	G
51	iN	1125	G
51	iN	1129	U
51	iN	1135	U
51	iN	1138	G
51	iN	1139	U
51	iN	1144	C
51	iN	1145	A
51	iN	1152	G
51	iN	1161	G
51	iN	1168	G
51	iN	1171	A
51	iN	1174	A
51	iN	1190	A
51	iN	1191	A
51	iN	1197	A
51	iN	1199	G
51	iN	1204	U
51	iN	1209	G
51	iN	1212	A
51	iN	1213	C
51	iN	1214	A
51	iN	1216	A

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Mol	Chain	Res	Type
51	iN	1239	U
51	iN	1241	A
51	iN	1242	A
51	iN	1244	U
51	iN	1247	U
51	iN	1256	U
51	iN	1257	U
51	iN	1258	A
51	iN	1270	A
51	iN	1271	C
51	iN	1272	A
51	iN	1273	C
51	iN	1277	U
51	iN	1278	G
51	iN	1283	A
51	iN	1289	A
51	iN	1290	G
51	iN	1291	G
51	iN	1301	C
51	iN	1302	A
51	iN	1303	G
51	iN	1307	C
51	iN	1318	G
51	iN	1323	G
51	iN	1325	A
51	iN	1330	A
51	iN	1332	A
51	iN	1333	A
51	iN	1344	A
51	iN	1345	G
51	iN	1347	C
51	iN	1350	G
51	iN	1357	G
51	iN	1362	C
51	iN	1363	A
51	iN	1364	A
51	iN	1365	C
51	iN	1367	C
51	iN	1385	A
51	iN	1392	G
51	iN	1393	U
51	iN	1398	G

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Mol	Chain	Res	Type
51	iN	1406	G
51	iN	1408	A
51	iN	1424	G
51	iN	1426	U
51	iN	1439	A
51	iN	1443	A
51	iN	1455	A
51	iN	1459	U
51	iN	1464	G
51	iN	1470	U
51	iN	1471	G
51	iN	1477	G
51	iN	1486	A
51	iN	1490	U
51	iN	1496	U
51	iN	1497	C
51	iN	1526	U
51	iN	1532	G
51	iN	1537	A
51	iN	1542	G
51	iN	1548	A
51	iN	1549	G
51	iN	1551	U
51	iN	1556	G
51	iN	1562	G
51	iN	1564	A
51	iN	1565	C
51	iN	1569	C
51	iN	1574	G
51	iN	1575	G
51	iN	1577	U
52	Z2	10	U
52	Z2	16	A
52	Z2	19	G
52	Z2	21	A
52	Z2	22	G
52	Z2	41	U
52	Z2	49	A
52	Z2	53	G
52	Z2	58	G
52	Z2	62	G
52	Z2	70	A

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Mol	Chain	Res	Type
52	Z2	78	A
52	Z2	81	A
52	Z2	82	G
52	Z2	99	A
52	Z2	124	A
52	Z2	126	U
52	Z2	137	A
52	Z2	146	A
52	Z2	148	G
52	Z2	193	A
52	Z2	196	A
52	Z2	202	G
52	Z2	213	A
52	Z2	219	C
52	Z2	222	C
52	Z2	226	U
52	Z2	227	G
52	Z2	245	G
52	Z2	266	G
52	Z2	298	A
52	Z2	314	G
52	Z2	317	A
52	Z2	325	G
52	Z2	333	A
52	Z2	346	A
52	Z2	354	A
52	Z2	355	G
52	Z2	369	G
52	Z2	372	A
52	Z2	379	G
52	Z2	387	A
52	Z2	394	G
52	Z2	419	C
52	Z2	431	U
52	Z2	439	C
52	Z2	461	A
52	Z2	462	A
52	Z2	464	G
52	Z2	488	A
52	Z2	491	A
52	Z2	512	A
52	Z2	513	G

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Mol	Chain	Res	Type
52	Z2	515	A
52	Z2	516	G
52	Z2	519	G
52	Z2	528	A
52	Z2	529	U
52	Z2	530	U
52	Z2	531	U
52	Z2	532	A
52	Z2	533	U
52	Z2	548	A
52	Z2	556	U
52	Z2	558	U
52	Z2	559	A
52	Z2	560	A
52	Z2	588	A
52	Z2	589	G
52	Z2	592	U
52	Z2	599	U
52	Z2	600	U
52	Z2	612	A
52	Z2	622	A
52	Z2	630	U
52	Z2	654	G
52	Z2	662	A
52	Z2	671	U
52	Z2	702	C
52	Z2	711	G
52	Z2	715	A
52	Z2	732	U
52	Z2	749	A
52	Z2	760	G
52	Z2	761	G
52	Z2	767	A
52	Z2	769	G
52	Z2	770	G
52	Z2	790	G
52	Z2	797	C
52	Z2	812	U
52	Z2	844	G
52	Z2	854	G
52	Z2	887	C
52	Z2	892	G

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Mol	Chain	Res	Type
52	Z2	895	A
52	Z2	899	C
52	Z2	912	A
52	Z2	916	A
52	Z2	917	U
52	Z2	929	A
52	Z2	930	C
52	Z2	945	C
52	Z2	958	G
52	Z2	967	A
52	Z2	980	A
52	Z2	983	U
52	Z2	989	C
52	Z2	995	U
52	Z2	996	U
52	Z2	997	C
52	Z2	1006	G
52	Z2	1010	G
52	Z2	1024	A
52	Z2	1030	A
52	Z2	1031	G
52	Z2	1044	U
52	Z2	1053	A
52	Z2	1054	A
52	Z2	1063	C
52	Z2	1067	U
52	Z2	1068	A
52	Z2	1071	G
52	Z2	1072	A
52	Z2	1074	A
52	Z2	1081	U
52	Z2	1085	U
52	Z2	1094	G
52	Z2	1095	A
52	Z2	1096	G
52	Z2	1113	A
52	Z2	1114	U
52	Z2	1116	U
52	Z2	1119	C
52	Z2	1120	G
52	Z2	1133	G
52	Z2	1156	A

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Mol	Chain	Res	Type
52	Z2	1157	C
52	Z2	1158	U
52	Z2	1159	U
52	Z2	1160	G
52	Z2	1161	U
52	Z2	1163	U
52	Z2	1164	U
52	Z2	1168	G
52	Z2	1189	A
52	Z2	1190	G
52	Z2	1211	G
52	Z2	1220	G
52	Z2	1237	A
52	Z2	1240	G
52	Z2	1255	G
52	Z2	1256	A
52	Z2	1257	U
52	Z2	1260	U
52	Z2	1284	G
52	Z2	1285	A
52	Z2	1290	C
52	Z2	1298	C
52	Z2	1305	A
52	Z2	1336	U
52	Z2	1340	G
52	Z2	1343	A
52	Z2	1349	A
52	Z2	1362	A
52	Z2	1363	U
52	Z2	1367	A
52	Z2	1369	A
52	Z2	1370	U
52	Z2	1379	A
52	Z2	1382	C
52	Z2	1400	G
52	Z2	1401	C
52	Z2	1404	U
52	Z2	1405	G
52	Z2	1411	A
52	Z2	1412	C
52	Z2	1419	G
52	Z2	1435	C

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Mol	Chain	Res	Type
52	Z2	1436	G
52	Z2	1466	U
52	Z2	1474	A
52	Z2	1477	C
52	Z2	1478	A
52	Z2	1481	U
52	Z2	1483	C
52	Z2	1497	G
52	Z2	1501	A
52	Z2	1515	G
52	Z2	1536	G
52	Z2	1548	G
52	Z2	1551	U
52	Z2	1554	A
52	Z2	1557	A
52	Z2	1566	U
52	Z2	1580	A
52	Z2	1581	A
52	Z2	1584	G
52	Z2	1596	A
52	Z2	1598	A
52	Z2	1603	C
52	Z2	1606	A
52	Z2	1622	A
52	Z2	1634	C
52	Z2	1636	U
52	Z2	1662	G
52	Z2	1681	U
52	Z2	1710	A
52	Z2	1724	G
52	Z2	1732	G
52	Z2	1742	G
52	Z2	1750	G
52	Z2	1759	A
52	Z2	1762	G
52	Z2	1768	U
52	Z2	1770	A
52	Z2	1777	A
52	Z2	1785	G
52	Z2	1786	C
52	Z2	1787	A
52	Z2	1796	A

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Mol	Chain	Res	Type
52	Z2	1802	C
52	Z2	1815	A
52	Z2	1834	A
52	Z2	1855	G
52	Z2	1856	U
52	Z2	1857	A
52	Z2	1892	G
52	Z2	1898	A
52	Z2	1906	C
52	Z2	1915	G
52	Z2	1916	G
52	Z2	1917	U
52	Z2	1923	A
52	Z2	1925	U
52	Z2	1941	U
52	Z2	1949	U
52	Z2	1953	C
52	Z2	1956	A
52	Z2	1957	U
52	Z2	1958	G
52	Z2	1968	U
52	Z2	1977	U
52	Z2	1979	U
52	Z2	1983	C
52	Z2	2007	A
52	Z2	2009	C
52	Z2	2017	A
52	Z2	2019	A
52	Z2	2029	C
52	Z2	2041	C
52	Z2	2042	G
52	Z2	2046	A
52	Z2	2047	G
52	Z2	2048	A
52	Z2	2055	G
52	Z2	2079	G
52	Z2	2178	G
52	Z2	2184	A
52	Z2	2189	A
52	Z2	2190	G
52	Z2	2195	A
52	Z2	2196	A

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Mol	Chain	Res	Type
52	Z2	2206	G
52	Z2	2208	A
52	Z2	2221	G
52	Z2	2222	G
52	Z2	2261	A
52	Z2	2266	U
52	Z2	2270	A
52	Z2	2271	A
52	Z2	2288	U
52	Z2	2291	G
52	Z2	2303	A
52	Z2	2305	A
52	Z2	2306	G
52	Z2	2308	A
52	Z2	2310	A
52	Z2	2328	A
52	Z2	2329	A
52	Z2	2330	C
52	Z2	2333	C
52	Z2	2334	G
52	Z2	2337	A
52	Z2	2360	A
52	Z2	2365	G
52	Z2	2366	G
52	Z2	2368	C
52	Z2	2385	U
52	Z2	2407	C
52	Z2	2408	A
52	Z2	2412	G
52	Z2	2422	A
52	Z2	2424	U
52	Z2	2431	A
52	Z2	2452	A
52	Z2	2453	G
52	Z2	2459	A
52	Z2	2474	U
52	Z2	2485	G
52	Z2	2486	A
52	Z2	2488	G
52	Z2	2489	U
52	Z2	2501	A
52	Z2	2503	C

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Mol	Chain	Res	Type
52	Z2	2512	G
52	Z2	2527	G
52	Z2	2530	A
52	Z2	2537	U
52	Z2	2545	U
52	Z2	2549	A
52	Z2	2550	G
52	Z2	2556	C
52	Z2	2561	G
52	Z2	2565	G
52	Z2	2585	A
52	Z2	2592	U
52	Z2	2596	U
52	Z2	2598	U
52	Z2	2612	U
52	Z2	2613	G
52	Z2	2619	U
52	Z2	2629	C
52	Z2	2644	G
52	Z2	2672	U
52	Z2	2673	U
52	Z2	2697	G
52	Z2	2709	C
52	Z2	2716	A
52	Z2	2727	G
52	Z2	2731	A
52	Z2	2761	A
52	Z2	2762	U
52	Z2	2763	U
52	Z2	2772	C
52	Z2	2773	U
52	Z2	2774	A
52	Z2	2784	U
52	Z2	2786	A
52	Z2	2787	A
52	Z2	2838	A
52	Z2	2839	A
52	Z2	2849	A
52	Z2	2850	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	Z2	9	G
52	Z2	532	A
52	Z2	769	G
52	Z2	886	A
52	Z2	1053	A
52	Z2	1580	A
52	Z2	1856	U
52	Z2	2195	A

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

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

5.5 Carbohydrates (i)

There are no 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.

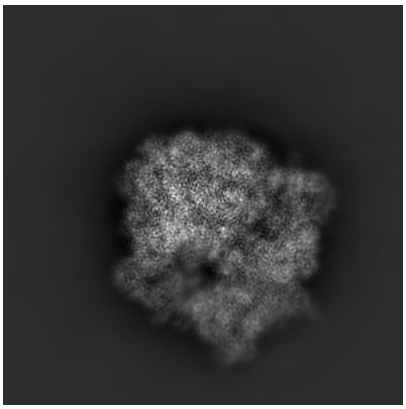
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52036. These allow visual inspection of the internal detail of the map and identification of artifacts.

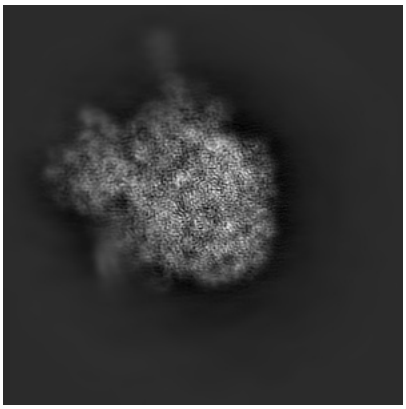
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

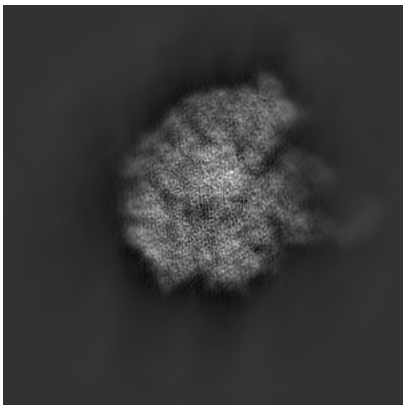
6.1.1 Primary map



X

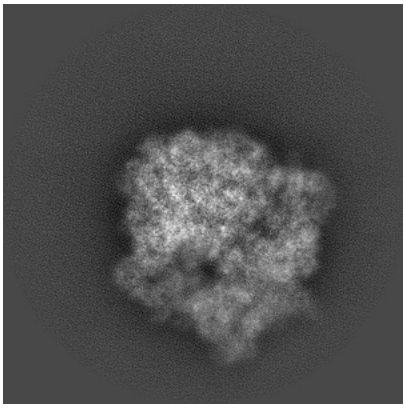


Y

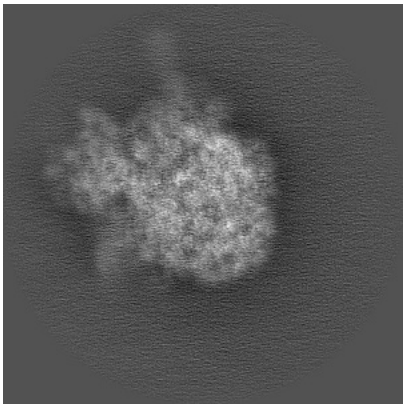


Z

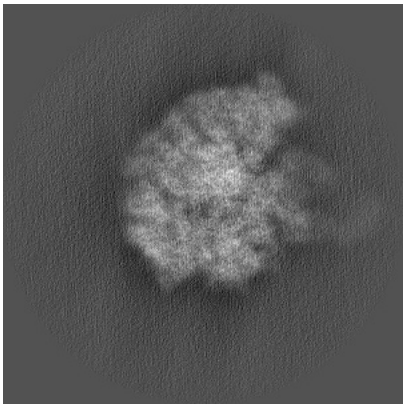
6.1.2 Raw map



X



Y

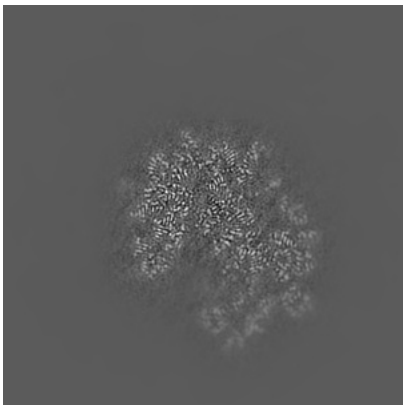


Z

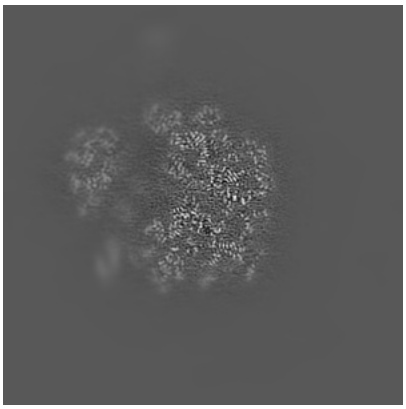
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

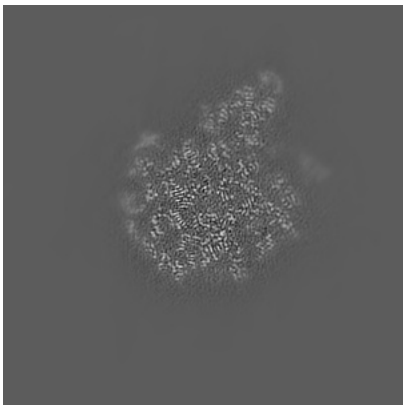
6.2.1 Primary map



X Index: 225

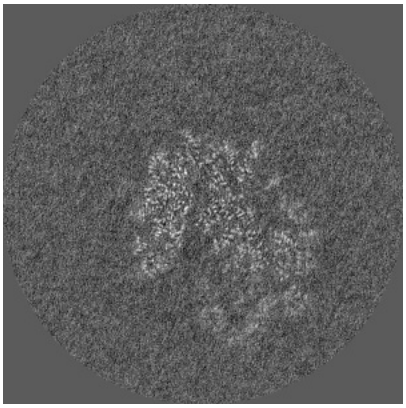


Y Index: 225

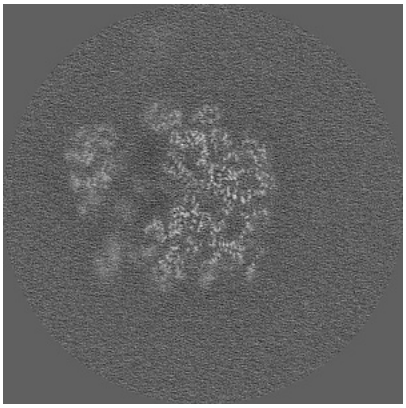


Z Index: 225

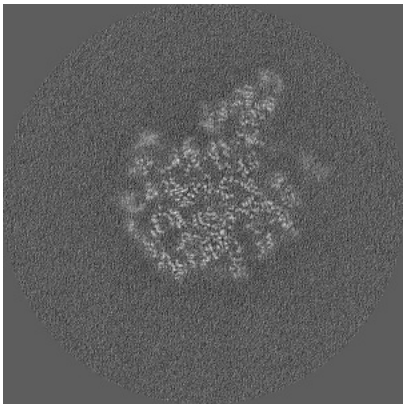
6.2.2 Raw map



X Index: 225



Y Index: 225

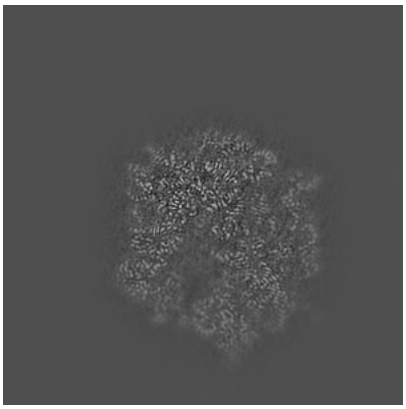


Z Index: 225

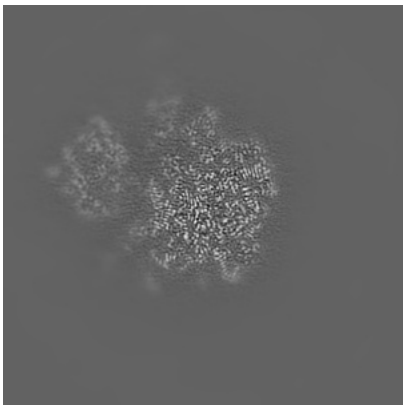
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

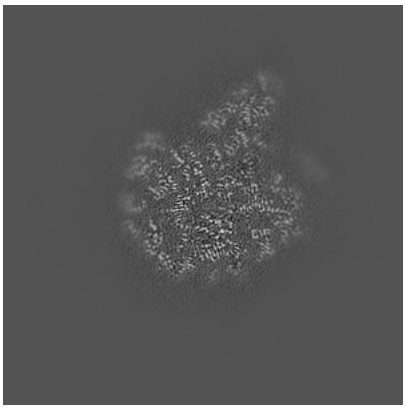
6.3.1 Primary map



X Index: 246

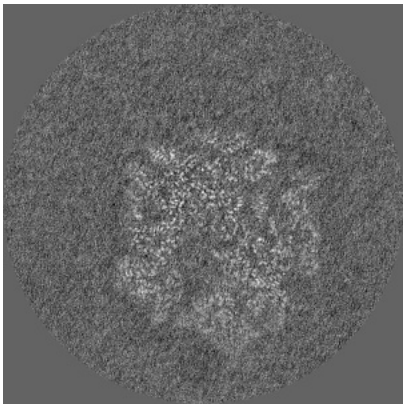


Y Index: 238

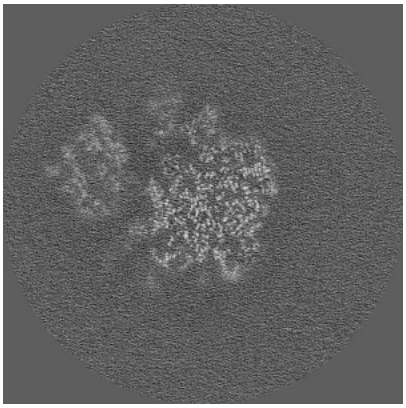


Z Index: 228

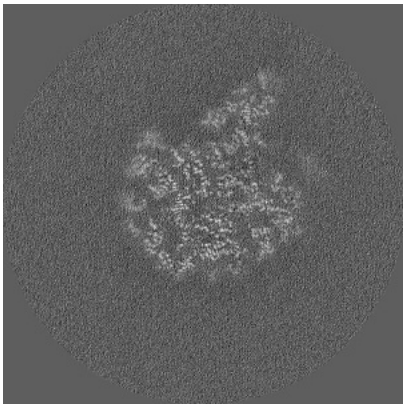
6.3.2 Raw map



X Index: 247



Y Index: 238

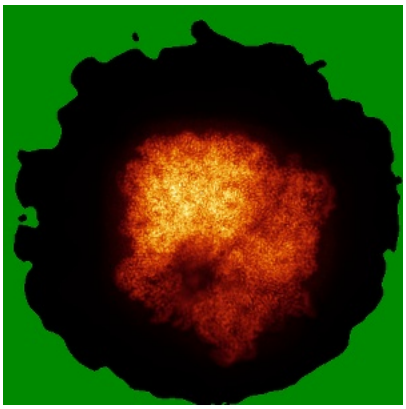


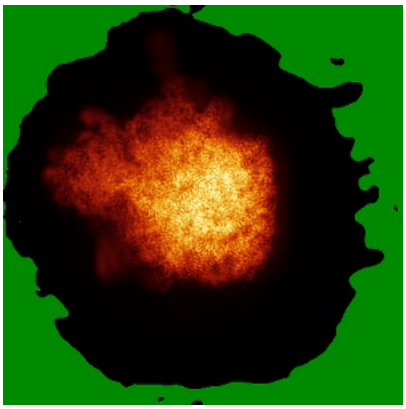
Z Index: 228

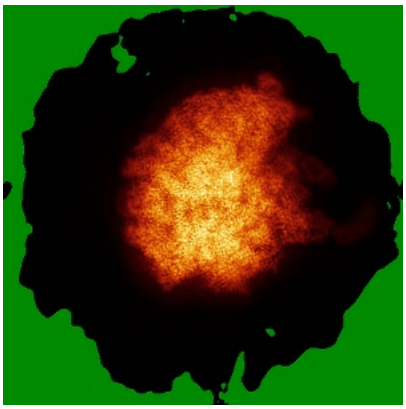
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

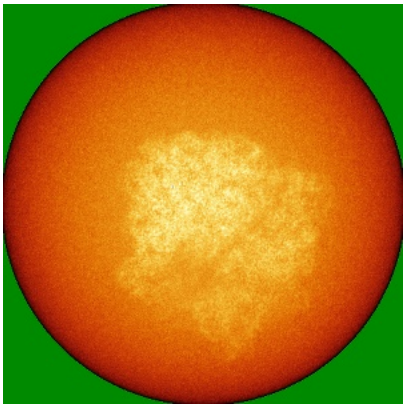
6.4.1 Primary map

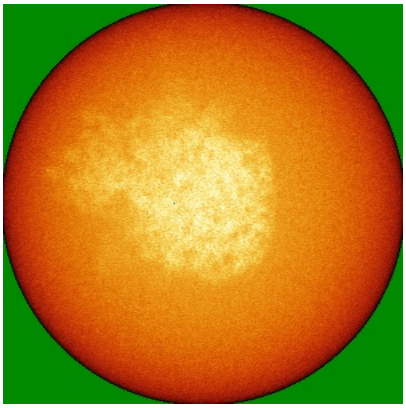

X

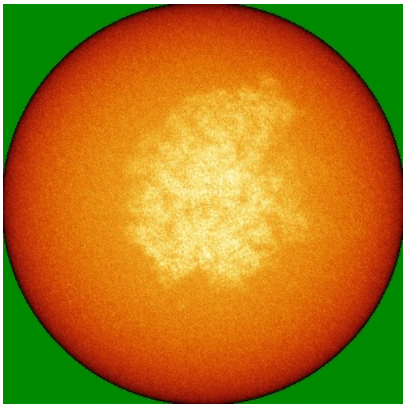

Y


Z

6.4.2 Raw map


X

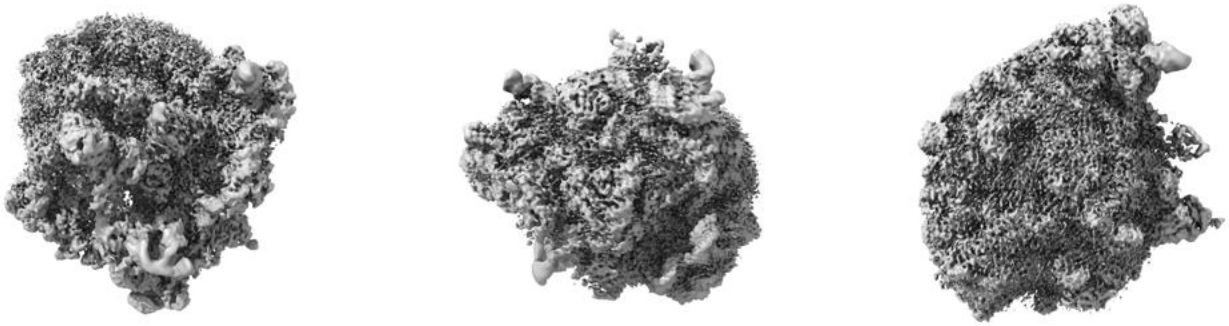

Y


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)

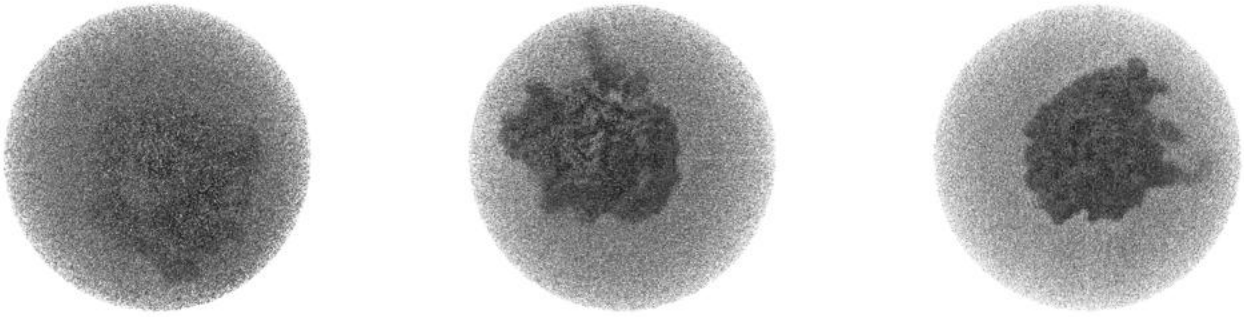
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. 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



X Y Z

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.

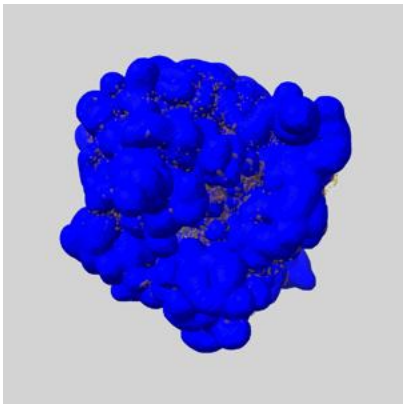
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

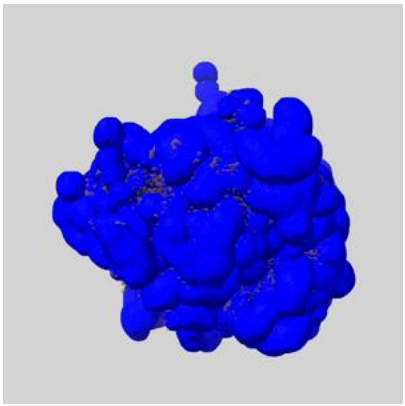
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

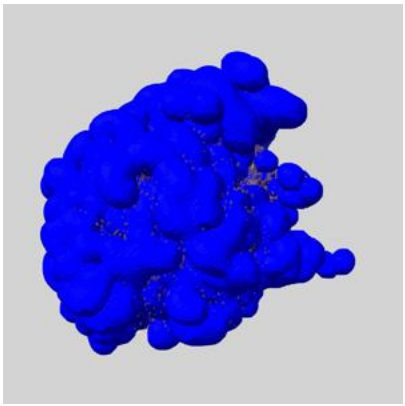
6.6.1 emd_52036_msk_1.map (i)



X



Y

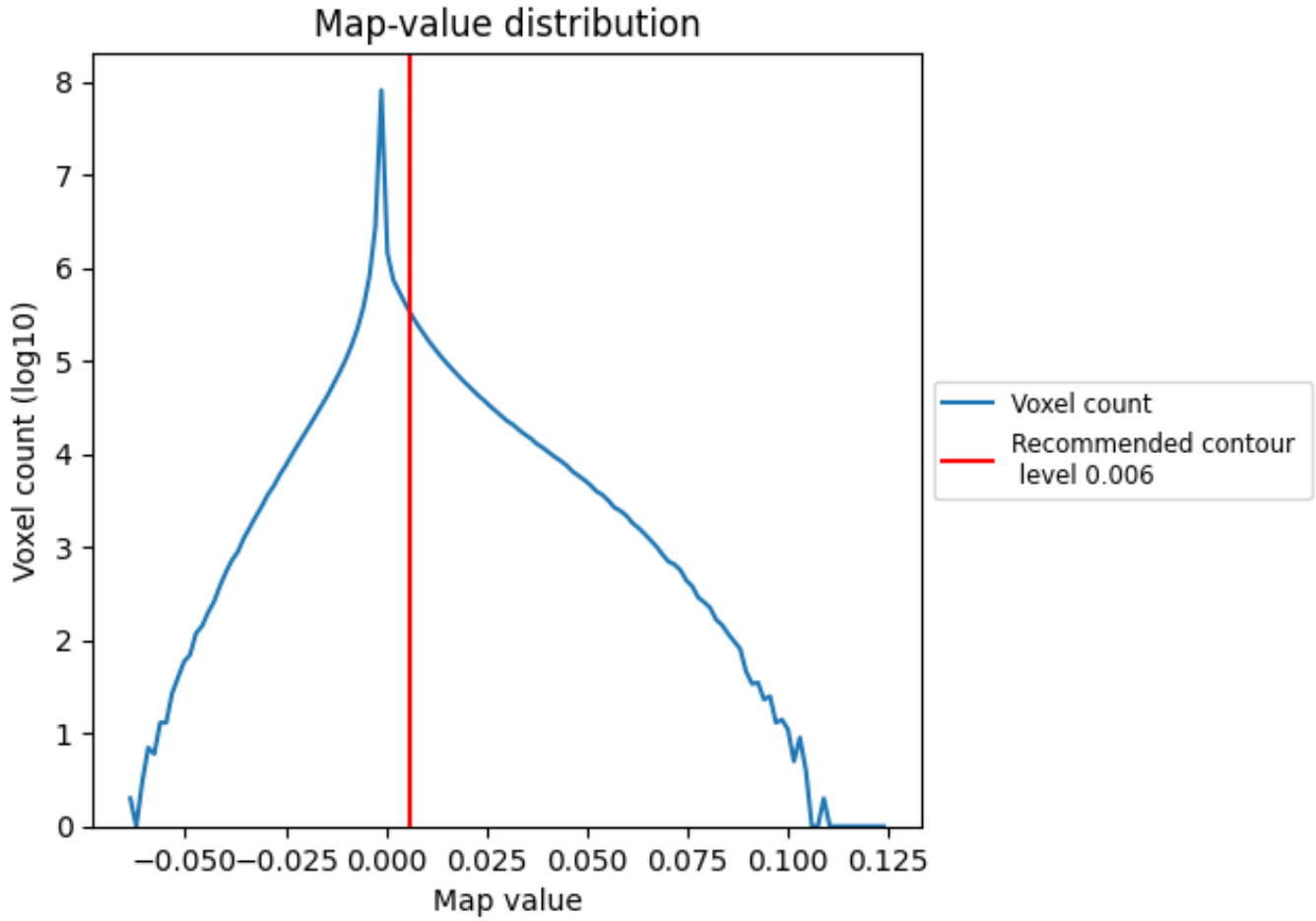


Z

7 Map analysis

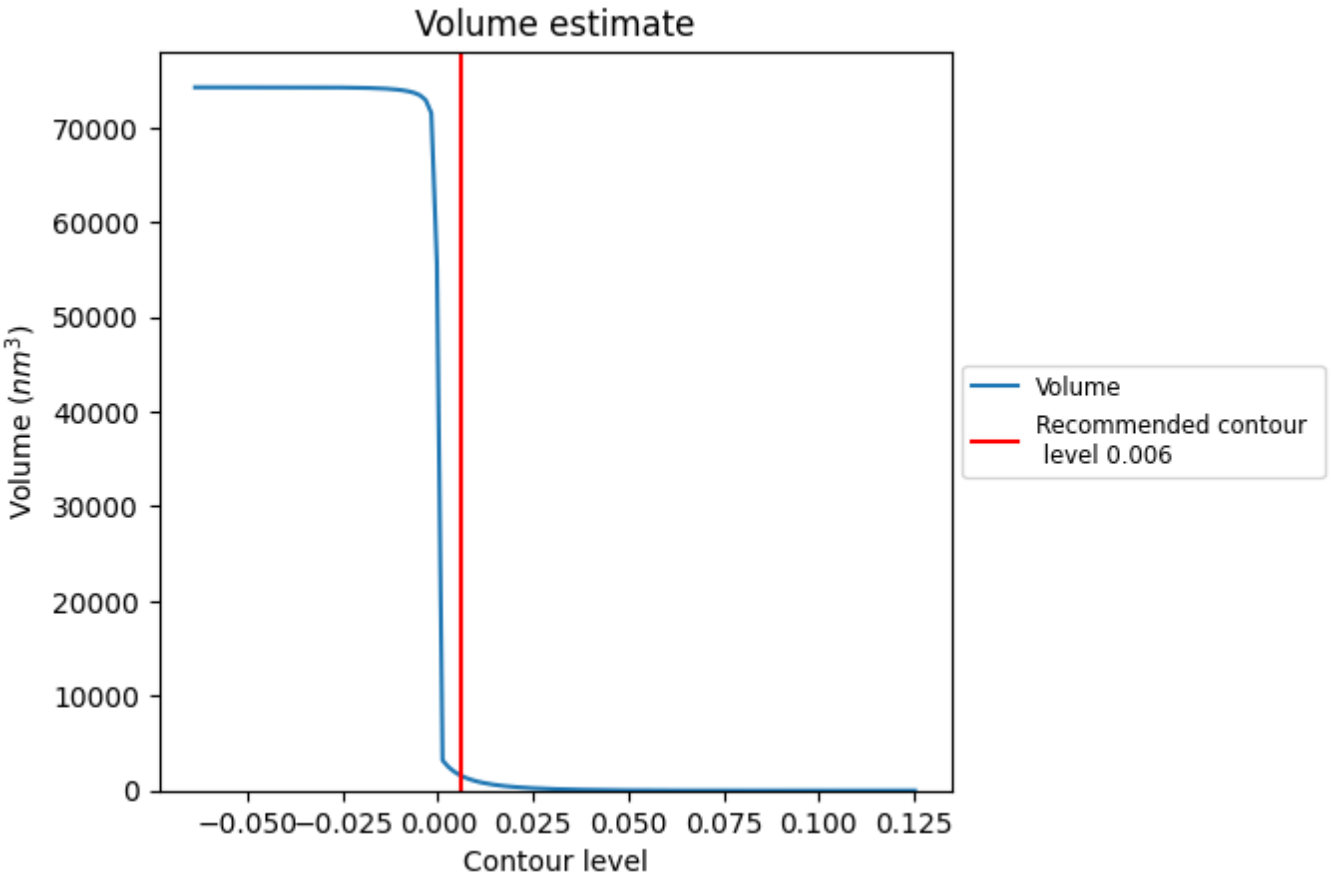
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

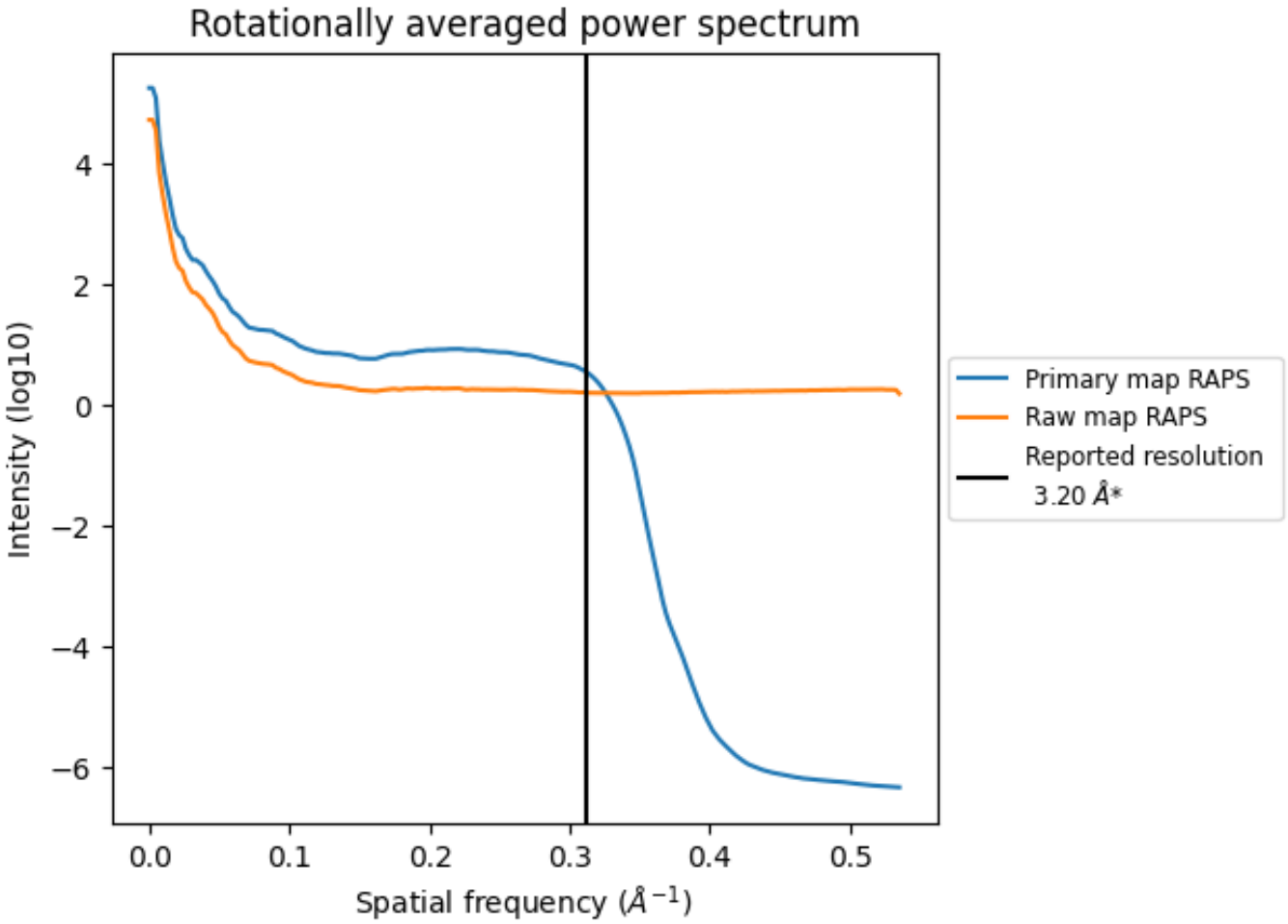
7.2 Volume estimate



The volume at the recommended contour level is 1603 nm^3; this corresponds to an approximate mass of 1448 kDa.

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

7.3 Rotationally averaged power spectrum (i)

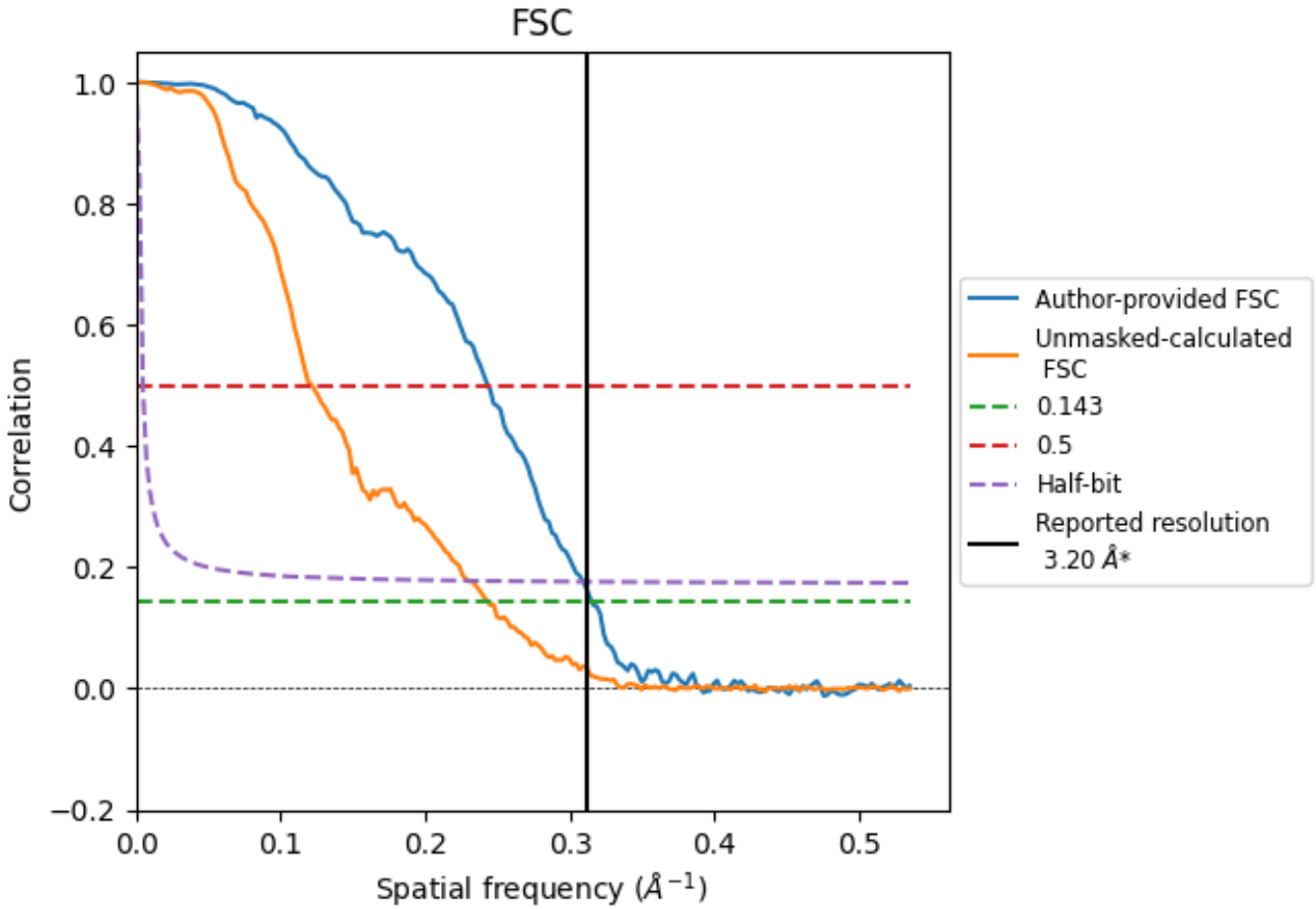


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

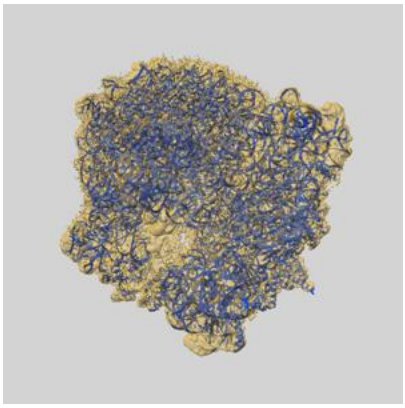
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	4.11	3.23
Unmasked-calculated*	4.11	8.22	4.35

*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 4.11 differs from the reported value 3.2 by more than 10 %

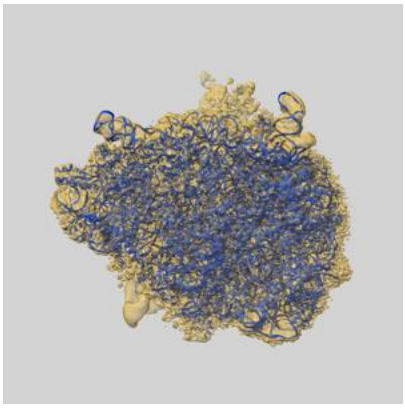
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52036 and PDB model 9HC4. Per-residue inclusion information can be found in section 3 on page 13.

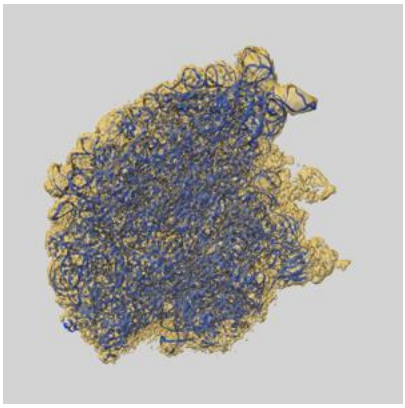
9.1 Map-model overlay



X



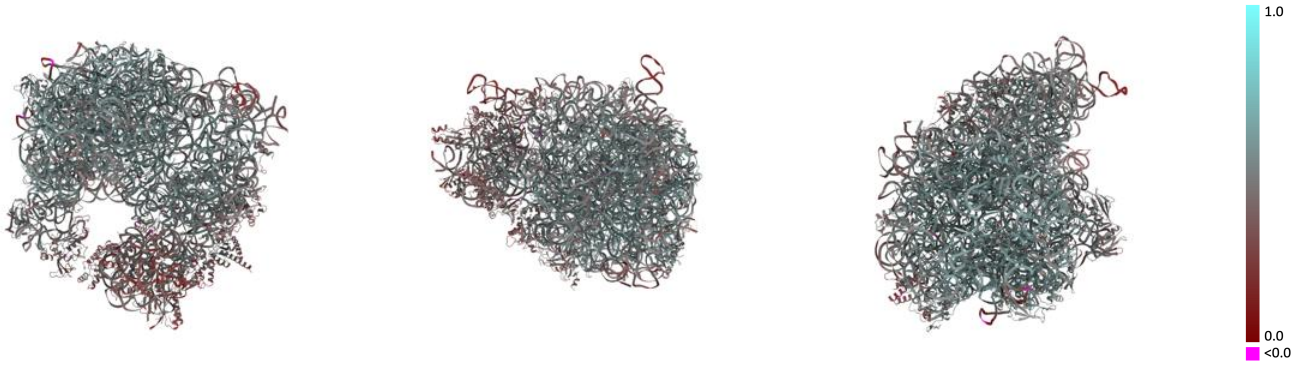
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

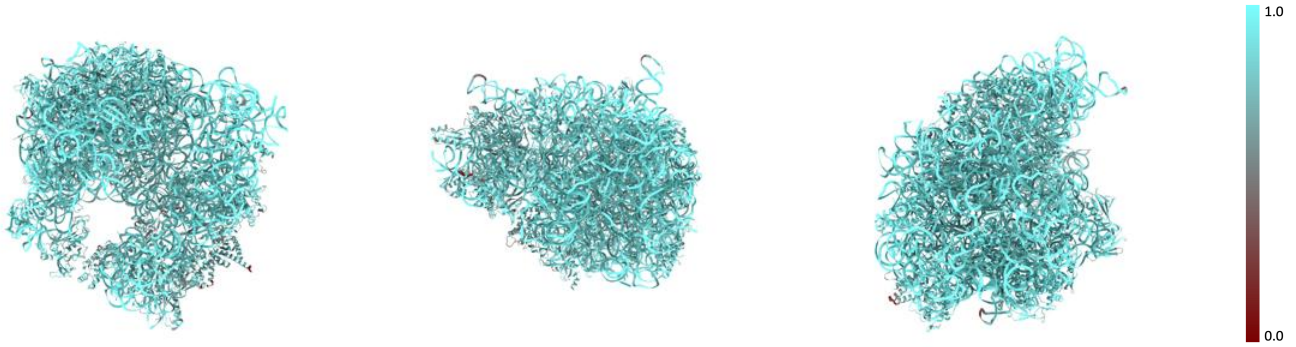
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

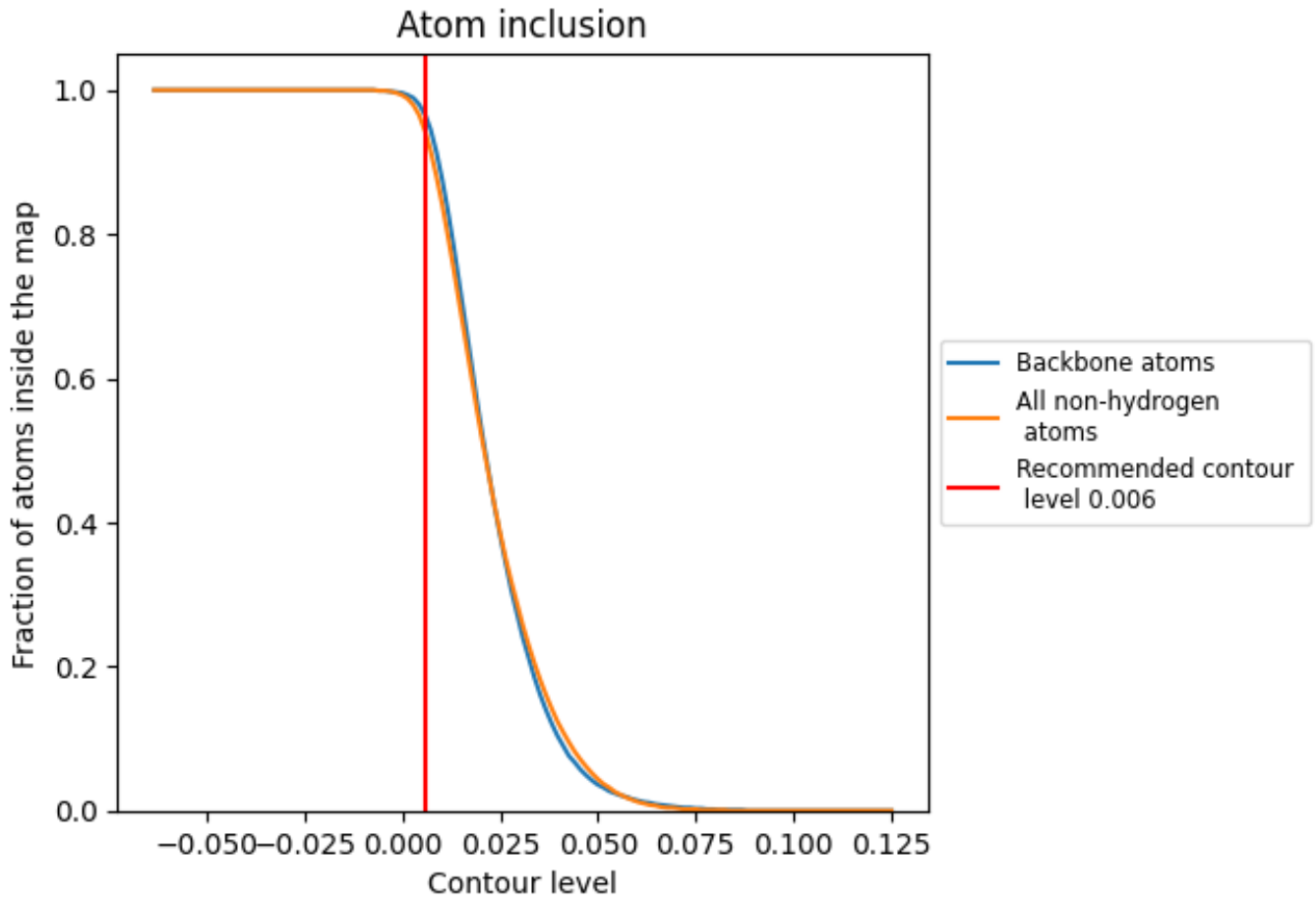
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 96% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.5020
A	0.6920	0.3280
A4	0.7700	0.3910
Af	0.9350	0.5330
BQ	0.9070	0.5050
Ba	0.9370	0.5390
C1	0.8730	0.4280
CT	0.7810	0.4000
Cl	0.9240	0.5250
D8	0.9760	0.4910
Dm	0.8230	0.4180
E5	0.8620	0.4570
E9	0.9070	0.5060
F	0.8440	0.3900
F7	0.8270	0.4080
FG	0.8150	0.4120
GR	0.8750	0.4530
GS	0.7680	0.3670
HK	0.8270	0.3970
IX	0.9430	0.5400
JY	0.7660	0.3800
Je	0.8980	0.5370
KU	0.7800	0.3960
Kd	0.9260	0.5280
L6	0.8610	0.5080
Lg	0.8880	0.5060
MB	0.9610	0.5480
MM	0.7420	0.3400
NV	0.6300	0.3370
Nc	0.9240	0.4890
OL	0.8720	0.4710
Oi	0.8880	0.4970
PO	0.9600	0.5520
Pj	0.8840	0.4650
QZ	0.8700	0.4660

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Chain	Atom inclusion	Q-score
Qb	0.9140	0.5170
R3	0.8050	0.4390
RF	0.9410	0.5400
SP	0.7810	0.3500
Sn	0.9130	0.5090
TI	0.8810	0.4480
To	0.9040	0.4700
UC	0.9120	0.5040
VH	0.9350	0.5520
WD	0.9230	0.5240
XE	0.9180	0.4640
YW	0.9090	0.5250
Z2	0.9760	0.5430
aA	0.9220	0.5040
bk	0.9430	0.5080
dh	0.9260	0.5120
ep	0.9240	0.5040
fJ	0.8450	0.3650
iN	0.9640	0.4800