



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 09:56 pm GMT

PDB ID : 7OPE
EMDB ID : EMD-13017
Title : RqcH DR variant bound to 50S-peptidyl-tRNA-RqcP RQC complex (rigid body refinement)
Authors : Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on : 2021-05-31
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.dev113
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) : 2.39

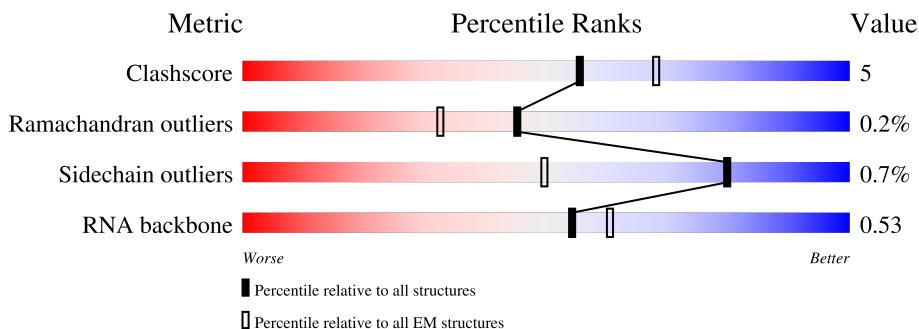
1 Overall quality at a glance

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2926	
2	B	119	
3	E	277	
4	F	209	
5	G	207	
6	H	179	
7	I	179	

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Mol	Chain	Length	Quality of chain
8	K	141	
9	L	166	
10	N	145	
11	O	122	
12	P	146	
13	Q	144	
14	R	120	
15	S	120	
16	T	115	
17	U	119	
18	V	102	
19	W	113	
20	X	95	
21	Y	103	
22	2	76	
23	a	94	
24	b	62	
25	c	66	
26	d	59	
27	f	59	
28	g	49	
29	h	44	
30	i	66	
31	j	37	
32	1	86	

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Mol	Chain	Length	Quality of chain
33	0	599	<div><div></div><div>50%</div><div></div><div>75%</div><div></div><div>12%</div><div></div><div>11%</div></div>

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 93862 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2814	Total	C	N	O	P	0	0
			60436	26962	11170	19491	2813		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	176	Total	C	N	O	S	0	0
			1387	883	241	256	7		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	132	Total	C	N	O	S	0	0
			974	612	172	184	6		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	113	Total	C	N	O	S	0	0
			886	559	152	174	1		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	142	Total	C	N	O	S	0	0
			1124	710	206	203	5		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	115	Total	C	N	O	S	0	0
			945	600	185	159	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	100	Total	C	N	O	0	0
			781	498	138	145		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 22 is a RNA chain called tRNA-Ala-UGC.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	70	Total	C	N	O	P	0	0
			1496	666	271	489	70		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	81	Total	C	N	O		0	0
			624	387	122	115			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 28 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 32 is a protein called Uncharacterized protein YabO.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	83	Total	C	N	O	S	0	0
			659	410	121	126	2		

- Molecule 33 is a protein called Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	0	532	Total	C	N	O	S	0	0
			3962	2504	705	743	10		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	97	ALA	ASP	conflict	UNP A0A6M4JI41
0	98	ALA	ARG	conflict	UNP A0A6M4JI41
0	571	GLY	-	expression tag	UNP A0A6M4JI41
0	572	SER	-	expression tag	UNP A0A6M4JI41
0	573	GLY	-	expression tag	UNP A0A6M4JI41
0	574	GLY	-	expression tag	UNP A0A6M4JI41

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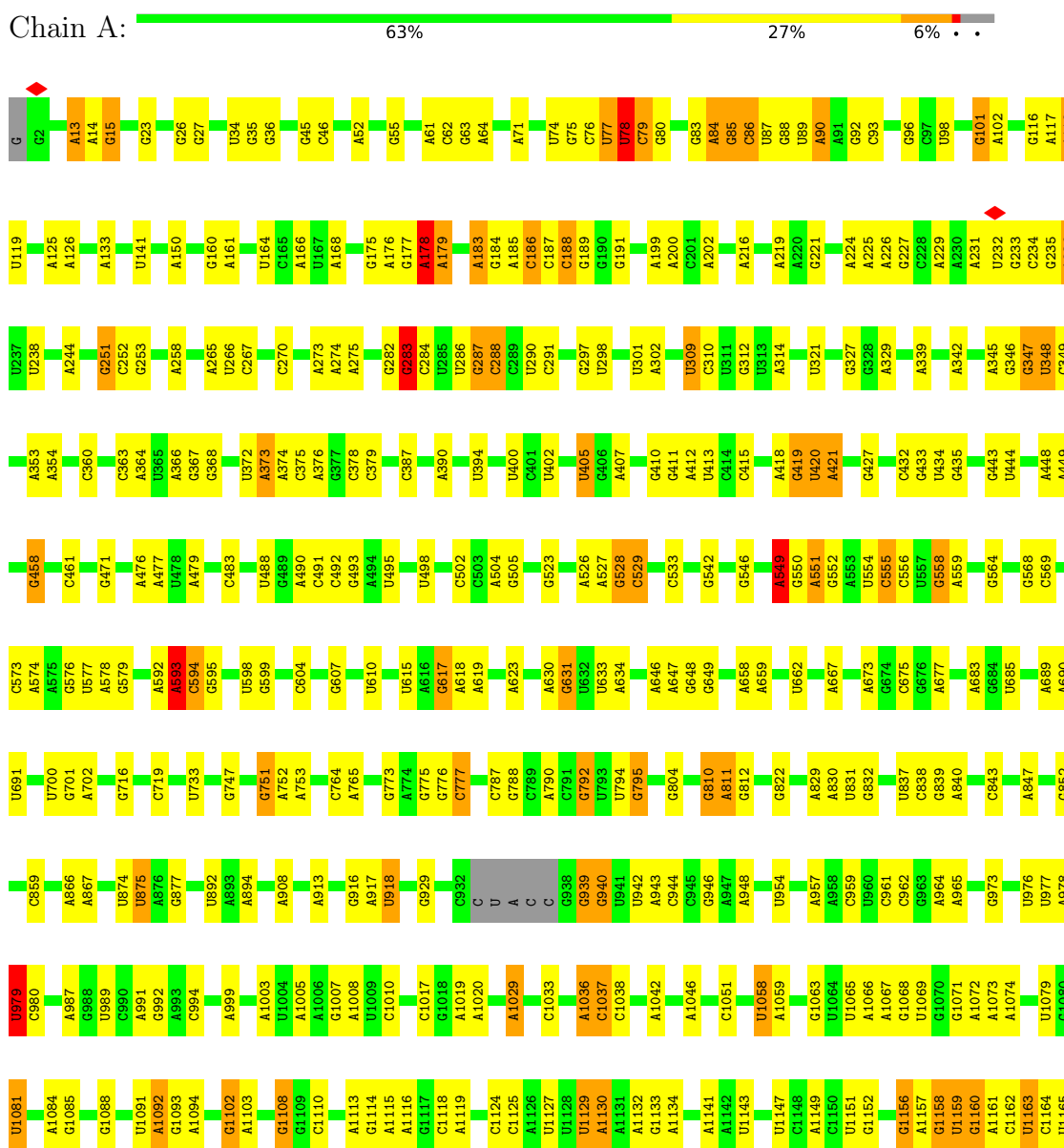
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Chain	Residue	Modelled	Actual	Comment	Reference
0	575	ASP	-	expression tag	UNP A0A6M4JI41
0	576	TYR	-	expression tag	UNP A0A6M4JI41
0	577	LYS	-	expression tag	UNP A0A6M4JI41
0	578	ASP	-	expression tag	UNP A0A6M4JI41
0	579	HIS	-	expression tag	UNP A0A6M4JI41
0	580	ASP	-	expression tag	UNP A0A6M4JI41
0	581	GLY	-	expression tag	UNP A0A6M4JI41
0	582	ASP	-	expression tag	UNP A0A6M4JI41
0	583	TYR	-	expression tag	UNP A0A6M4JI41
0	584	LYS	-	expression tag	UNP A0A6M4JI41
0	585	ASP	-	expression tag	UNP A0A6M4JI41
0	586	HIS	-	expression tag	UNP A0A6M4JI41
0	587	ASP	-	expression tag	UNP A0A6M4JI41
0	588	ILE	-	expression tag	UNP A0A6M4JI41
0	589	ASP	-	expression tag	UNP A0A6M4JI41
0	590	TYR	-	expression tag	UNP A0A6M4JI41
0	591	LYS	-	expression tag	UNP A0A6M4JI41
0	592	ASP	-	expression tag	UNP A0A6M4JI41
0	593	ASP	-	expression tag	UNP A0A6M4JI41
0	594	ASP	-	expression tag	UNP A0A6M4JI41
0	595	ASP	-	expression tag	UNP A0A6M4JI41
0	596	LYS	-	expression tag	UNP A0A6M4JI41
0	597	GLY	-	expression tag	UNP A0A6M4JI41

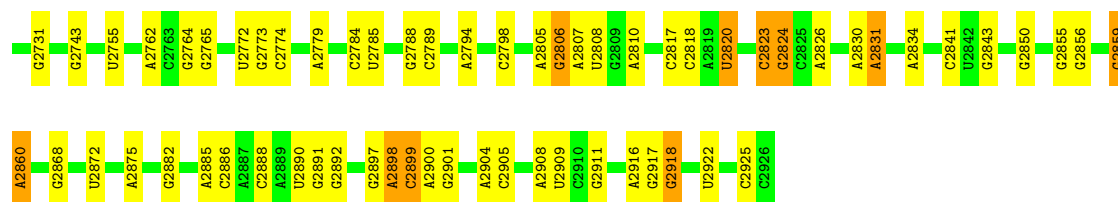
3 Residue-property plots

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

• Molecule 1: 23S rRNA

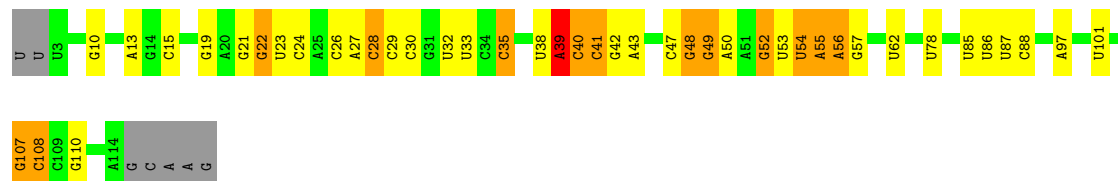






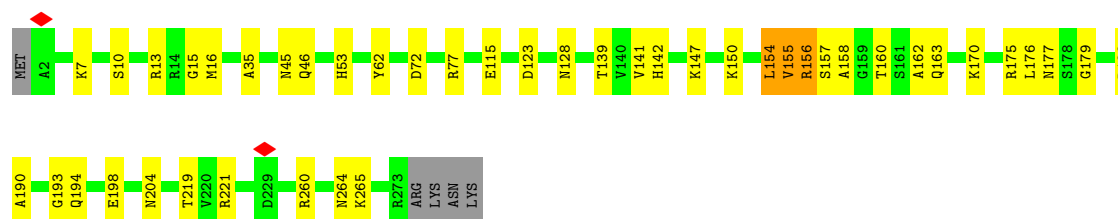
• Molecule 2: 5S rRNA

Chain B: 58% 24% 11% • 6%



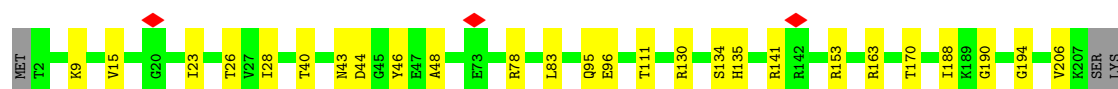
• Molecule 3: 50S ribosomal protein L2

Chain E: 82% 15% • •



• Molecule 4: 50S ribosomal protein L3

Chain F: 86% 12% •



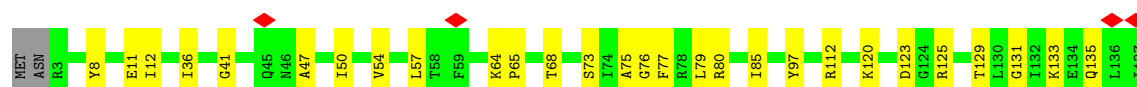
• Molecule 5: 50S ribosomal protein L4

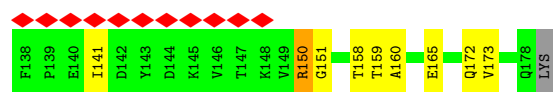
Chain G: 90% 9% •



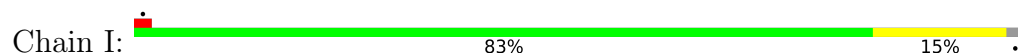
• Molecule 6: 50S ribosomal protein L5

Chain H: 8% 78% 20% • •

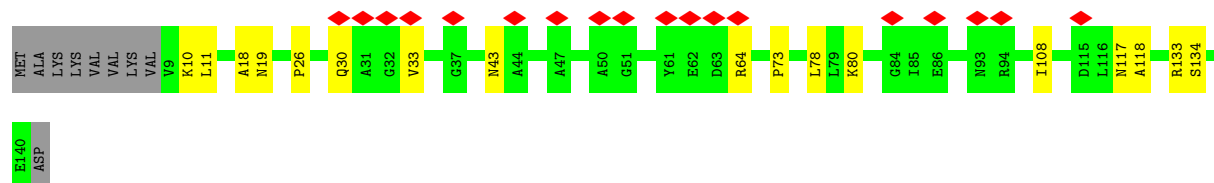
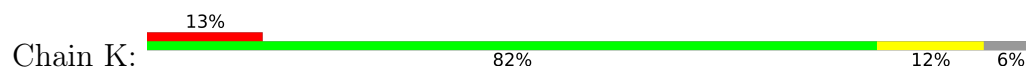




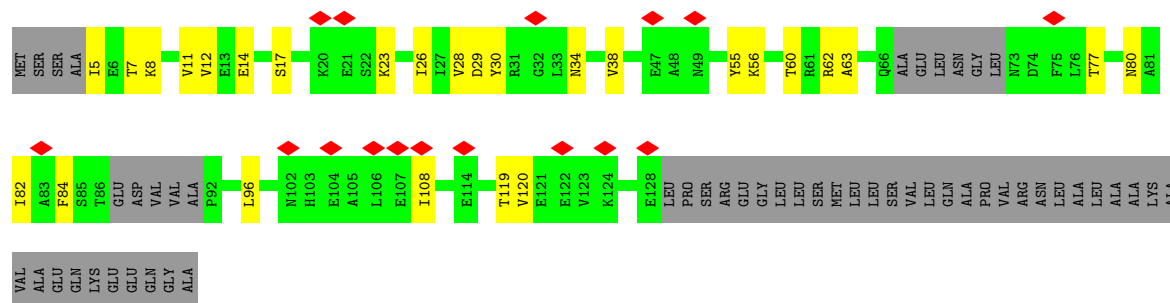
• Molecule 7: 50S ribosomal protein L6



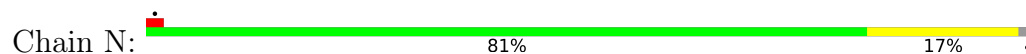
• Molecule 8: 50S ribosomal protein L11



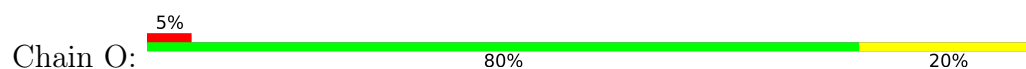
• Molecule 9: 50S ribosomal protein L10



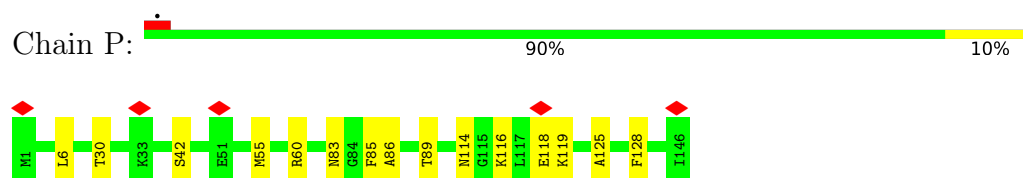
• Molecule 10: 50S ribosomal protein L13



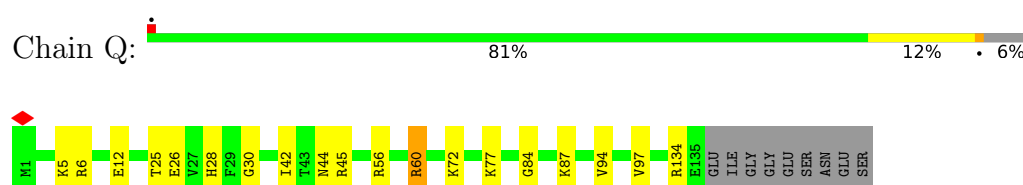
• Molecule 11: 50S ribosomal protein L14



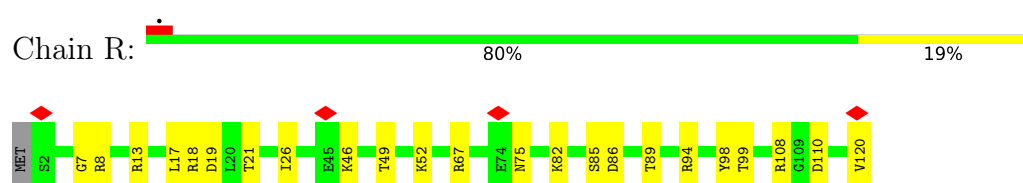
- Molecule 12: 50S ribosomal protein L15



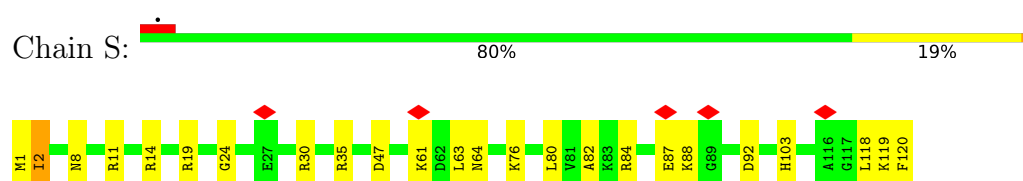
- Molecule 13: 50S ribosomal protein L16



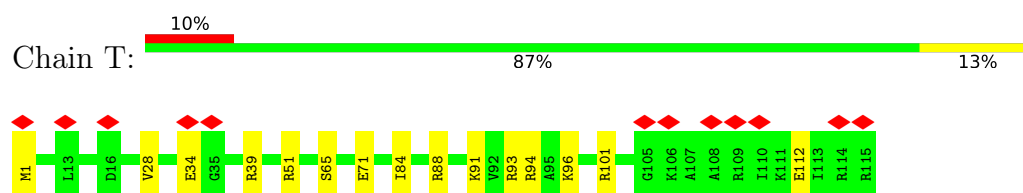
- Molecule 14: 50S ribosomal protein L17



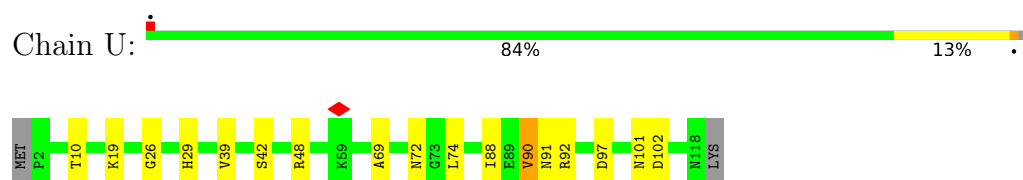
- Molecule 15: 50S ribosomal protein L18



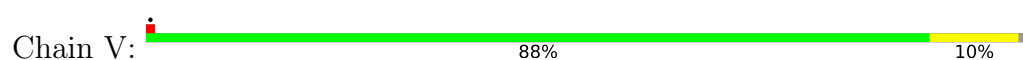
- Molecule 16: 50S ribosomal protein L19



- Molecule 17: 50S ribosomal protein L20



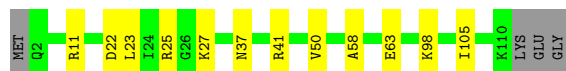
- Molecule 18: 50S ribosomal protein L21





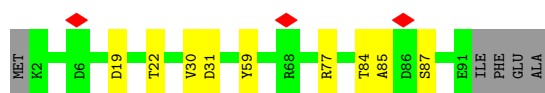
- Molecule 19: 50S ribosomal protein L22

Chain W:
86% 11% .



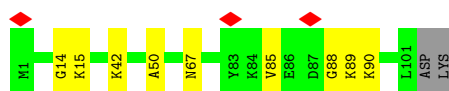
- Molecule 20: 50S ribosomal protein L23

Chain X:
85% 9% 5%



- Molecule 21: 50S ribosomal protein L24

Chain Y:
89% 9% .



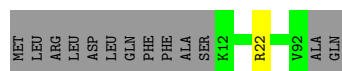
- Molecule 22: tRNA-Ala-UGC

Chain 2:
37% 37% 14% . 8%



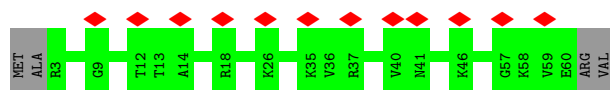
- Molecule 23: 50S ribosomal protein L27

Chain a:
85% . 14%



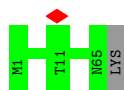
- Molecule 24: 50S ribosomal protein L28

Chain b:
19% 94% 6%



- Molecule 25: 50S ribosomal protein L29

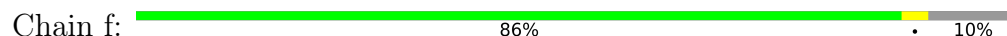
Chain c:
98% .



- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L32



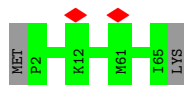
- Molecule 28: 50S ribosomal protein L33 1



- Molecule 29: 50S ribosomal protein L34



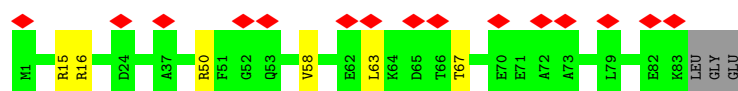
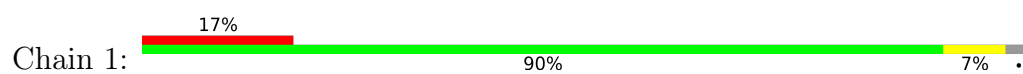
- Molecule 30: 50S ribosomal protein L35



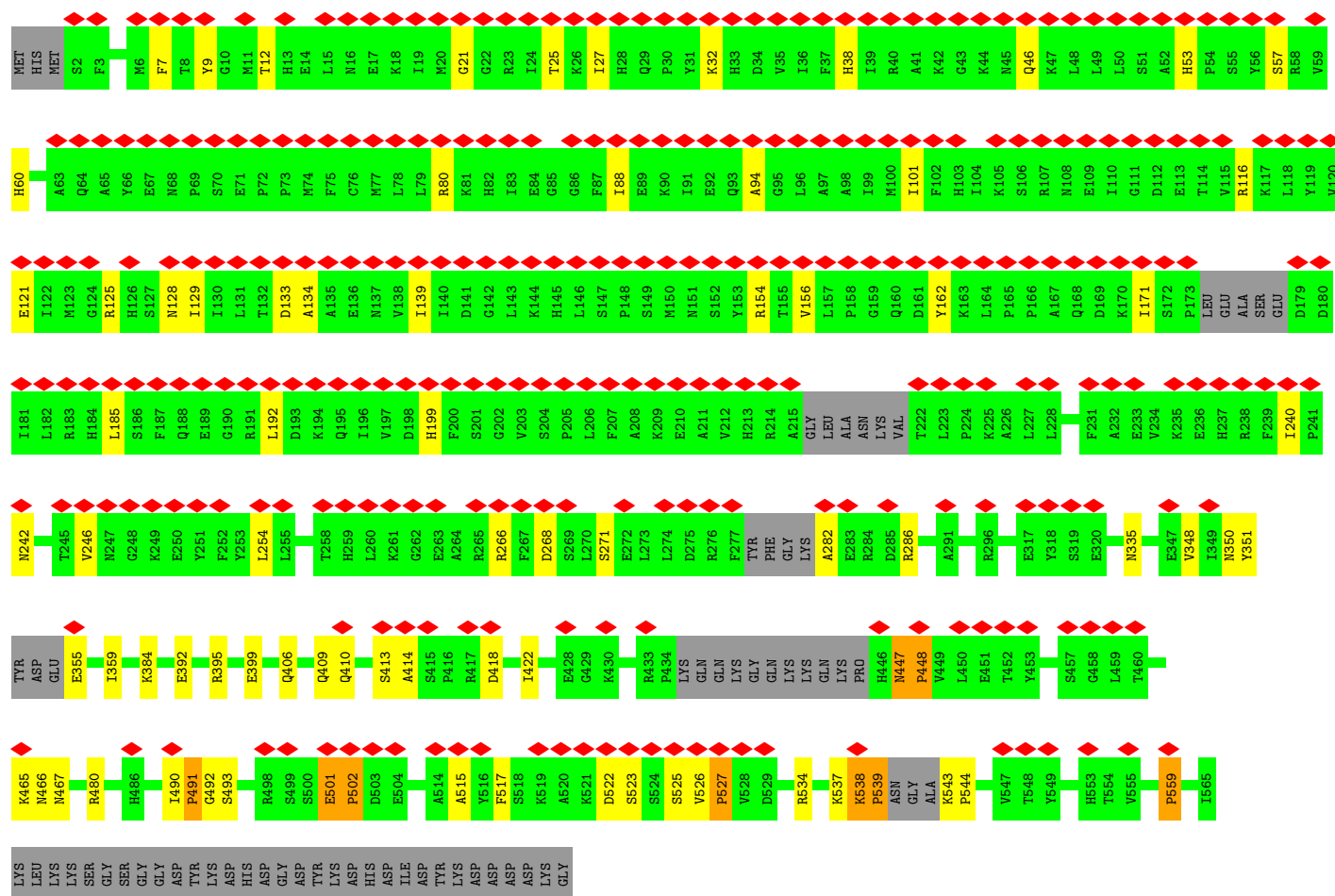
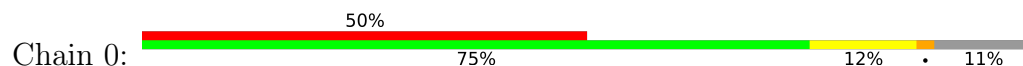
- Molecule 31: 50S ribosomal protein L36



- Molecule 32: Uncharacterized protein YabO



• Molecule 33: Rqc2 homolog RqcH



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (\AA)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.20	8/67693 (0.0%)	1.15	164/105598 (0.2%)
2	B	1.03	1/2675 (0.0%)	1.31	36/4170 (0.9%)
3	E	0.70	0/2120	0.68	0/2845
4	F	0.71	0/1591	0.65	0/2132
5	G	0.68	0/1580	0.62	0/2132
6	H	0.77	0/1406	1.10	2/1888 (0.1%)
7	I	0.51	0/1360	0.63	0/1832
8	K	0.32	0/988	0.57	0/1336
9	L	0.34	0/892	0.58	0/1196
10	N	0.70	0/1147	0.62	0/1542
11	O	0.65	0/928	0.75	0/1245
12	P	0.64	0/1094	0.66	0/1457
13	Q	0.71	0/1099	0.70	0/1468
14	R	0.65	0/961	0.70	0/1284
15	S	0.56	0/922	0.71	0/1236
16	T	0.67	0/958	0.77	0/1279
17	U	0.74	0/952	0.70	0/1266
18	V	0.76	0/792	0.68	0/1063
19	W	0.64	0/851	0.72	0/1146
20	X	0.65	0/731	0.69	0/974
21	Y	0.62	0/772	0.67	1/1032 (0.1%)
22	2	0.97	1/1669 (0.1%)	1.63	37/2596 (1.4%)
23	a	0.76	0/632	0.72	0/839
24	b	0.46	0/448	0.70	0/596
25	c	0.54	0/531	0.71	0/707
26	d	0.63	0/458	0.69	0/613
27	f	0.68	0/425	0.71	1/563 (0.2%)
28	g	0.64	0/406	0.63	0/540
29	h	0.72	0/371	0.78	1/483 (0.2%)
30	i	0.66	0/519	0.68	0/680
31	j	0.75	0/300	0.63	0/393
32	1	0.68	1/662 (0.2%)	1.07	3/882 (0.3%)
33	0	0.39	4/4031 (0.1%)	0.75	18/5456 (0.3%)
All	All	1.05	15/101964 (0.0%)	1.07	263/152469 (0.2%)

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	A	0	15
2	B	0	4
3	E	0	1
6	H	0	1
8	K	0	1
13	Q	0	1
18	V	0	1
22	2	0	7
All	All	0	31

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1220	G	P-OP2	7.36	1.61	1.49
1	A	1220	G	P-OP1	7.35	1.61	1.49
1	A	1939	G	O3'-P	-7.11	1.52	1.61
1	A	1940	U	C1'-N1	6.92	1.59	1.48
33	0	491	PRO	CG-CD	5.91	1.70	1.50
1	A	1867	C	C4-N4	-5.63	1.28	1.33
1	A	574	A	N9-C4	-5.63	1.34	1.37
32	1	58	VAL	C-N	5.31	1.46	1.34
22	2	25	C	C4-N4	-5.17	1.29	1.33
33	0	527	PRO	CG-CD	5.16	1.67	1.50
33	0	448	PRO	CG-CD	5.08	1.67	1.50
1	A	1467	G	C8-N7	-5.05	1.27	1.30
1	A	2333	G	C2-N2	-5.04	1.29	1.34
33	0	544	PRO	CG-CD	5.04	1.67	1.50
2	B	56	A	C5-C4	-5.04	1.35	1.38

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	490	ILE	C-N-CD	-29.05	56.69	120.60
22	2	49	A	O5'-P-OP2	-27.30	77.94	110.70
22	2	49	A	O5'-P-OP1	-24.78	80.96	110.70
22	2	49	A	OP1-P-OP2	18.24	146.97	119.60
1	A	2334	U	O4'-C1'-N1	15.33	120.47	108.20
22	2	48	C	OP1-P-O3'	-12.49	77.72	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2335	U	O4'-C1'-N1	11.76	117.61	108.20
2	B	43	A	N1-C6-N6	-10.44	112.33	118.60
2	B	55	A	N1-C6-N6	-10.20	112.48	118.60
1	A	1939	G	O3'-P-O5'	-10.14	84.73	104.00
22	2	48	C	OP2-P-O3'	-9.67	83.93	105.20
1	A	1757	G	O4'-C1'-N9	9.09	115.47	108.20
1	A	1956	A	N1-C6-N6	-9.04	113.18	118.60
33	0	526	VAL	C-N-CD	-8.85	101.13	120.60
32	1	16	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	1220	G	P-O5'-C5'	-8.77	106.87	120.90
1	A	2338	A	N1-C6-N6	-8.72	113.37	118.60
1	A	2343	A	C5'-C4'-O4'	8.71	119.56	109.10
6	H	150	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	2898	A	N1-C6-N6	-8.66	113.41	118.60
1	A	1957	A	N1-C6-N6	-8.61	113.43	118.60
1	A	2340	A	N1-C6-N6	-8.53	113.48	118.60
1	A	2331	U	O4'-C1'-N1	8.33	114.86	108.20
2	B	27	A	N1-C6-N6	-8.28	113.63	118.60
2	B	56	A	C5-C6-N1	8.16	121.78	117.70
1	A	593	A	N1-C6-N6	-8.07	113.76	118.60
1	A	2503	C	C6-N1-C2	-7.87	117.15	120.30
2	B	42	G	O4'-C1'-N9	7.84	114.47	108.20
22	2	1	G	OP1-P-OP2	-7.84	107.84	119.60
1	A	2340	A	O4'-C1'-N9	7.83	114.47	108.20
1	A	555	C	C6-N1-C2	-7.83	117.17	120.30
22	2	40	C	O4'-C1'-N1	7.76	114.41	108.20
2	B	39	A	C5-C6-N1	7.69	121.55	117.70
1	A	2343	A	N1-C6-N6	-7.69	113.99	118.60
1	A	2338	A	C5-C6-N1	7.68	121.54	117.70
6	H	150	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	2340	A	C5-C6-N1	7.62	121.51	117.70
2	B	39	A	N1-C6-N6	-7.62	114.03	118.60
1	A	1370	C	C6-N1-C2	-7.62	117.25	120.30
1	A	555	C	N1-C2-O2	7.62	123.47	118.90
2	B	52	G	O4'-C1'-N9	7.61	114.29	108.20
2	B	30	C	N3-C2-O2	-7.60	116.58	121.90
2	B	29	C	N3-C2-O2	-7.52	116.64	121.90
1	A	2341	U	O4'-C1'-N1	7.52	114.22	108.20
22	2	25	C	O4'-C1'-N1	7.51	114.21	108.20
1	A	2695	C	N1-C2-O2	7.36	123.31	118.90
1	A	2342	C	N3-C2-O2	-7.34	116.76	121.90
1	A	2327	A	N1-C6-N6	-7.29	114.22	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	A	C5-C6-N1	7.28	121.34	117.70
1	A	2503	C	N3-C2-O2	-7.16	116.89	121.90
1	A	716	G	C4-N9-C1'	7.13	135.77	126.50
1	A	2332	G	C4'-C3'-C2'	-7.12	95.48	102.60
1	A	1956	A	C5-C6-N1	7.12	121.26	117.70
22	2	23	A	N1-C6-N6	-7.12	114.33	118.60
22	2	23	A	C4-C5-C6	-7.09	113.45	117.00
2	B	43	A	C5-C6-N1	7.08	121.24	117.70
1	A	2918	G	C4-N9-C1'	7.07	135.69	126.50
2	B	39	A	O4'-C1'-N9	7.05	113.84	108.20
1	A	1947	A	C2'-C3'-O3'	7.02	124.95	109.50
1	A	1828	G	C8-N9-C4	-7.01	103.60	106.40
32	1	15	ARG	NE-CZ-NH1	6.99	123.80	120.30
2	B	56	A	N1-C6-N6	-6.94	114.44	118.60
22	2	41	A	C4-C5-C6	-6.93	113.53	117.00
1	A	1370	C	C5-C6-N1	6.92	124.46	121.00
1	A	179	A	N1-C6-N6	6.92	122.75	118.60
1	A	2343	A	C5-C6-N1	6.88	121.14	117.70
2	B	56	A	C4-C5-C6	-6.88	113.56	117.00
1	A	1866	C	N3-C2-O2	-6.86	117.10	121.90
1	A	2330	A	C5-C6-N1	6.82	121.11	117.70
1	A	1220	G	OP1-P-OP2	-6.76	109.46	119.60
1	A	1353	C	C6-N1-C2	-6.75	117.60	120.30
2	B	55	A	C4-C5-C6	-6.75	113.63	117.00
1	A	1527	C	C2-N1-C1'	6.73	126.20	118.80
22	2	23	A	C5-C6-N1	6.67	121.04	117.70
1	A	1939	G	OP2-P-O3'	6.67	119.87	105.20
2	B	30	C	N1-C2-O2	6.65	122.89	118.90
1	A	1203	G	C6-C5-N7	-6.65	126.41	130.40
1	A	1804	U	C5-C4-O4	-6.65	121.91	125.90
2	B	27	A	C5-C6-N1	6.62	121.01	117.70
1	A	555	C	N3-C2-O2	-6.56	117.31	121.90
1	A	1352	U	C2-N1-C1'	6.55	125.56	117.70
1	A	1425	C	C6-N1-C2	-6.53	117.69	120.30
1	A	1353	C	C2-N1-C1'	6.52	125.97	118.80
1	A	716	G	C8-N9-C1'	-6.51	118.54	127.00
1	A	2339	A	N1-C6-N6	-6.51	114.70	118.60
1	A	631	G	N3-C4-C5	6.48	131.84	128.60
33	0	491	PRO	N-CA-CB	6.43	111.02	103.30
1	A	2695	C	N3-C2-O2	-6.43	117.40	121.90
1	A	875	U	C2-N1-C1'	6.42	125.41	117.70
1	A	2503	C	N1-C2-O2	6.42	122.75	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1981	A	N1-C6-N6	6.42	122.45	118.60
1	A	1957	A	C4-C5-C6	-6.41	113.80	117.00
22	2	25	C	C6-N1-C2	-6.41	117.74	120.30
1	A	1370	C	C2-N1-C1'	6.39	125.83	118.80
1	A	2304	C	N1-C2-O2	6.39	122.73	118.90
22	2	14	A	N1-C6-N6	-6.38	114.77	118.60
22	2	25	C	N3-C2-O2	-6.37	117.44	121.90
1	A	2273	U	C5-C4-O4	-6.31	122.12	125.90
1	A	1957	A	C5-C6-N1	6.29	120.84	117.70
2	B	41	C	O4'-C1'-N1	6.28	113.23	108.20
22	2	57	G	N1-C6-O6	-6.28	116.13	119.90
1	A	568	G	C6-C5-N7	-6.22	126.67	130.40
29	h	34	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	B	28	C	N1-C2-O2	6.16	122.60	118.90
2	B	28	C	N3-C2-O2	-6.15	117.59	121.90
1	A	2273	U	N3-C4-O4	6.13	123.69	119.40
1	A	2343	A	C5'-C4'-C3'	-6.13	106.19	116.00
22	2	24	G	N1-C6-O6	-6.12	116.23	119.90
22	2	48	C	P-O3'-C3'	6.11	127.03	119.70
1	A	2342	C	O4'-C1'-N1	6.11	113.09	108.20
1	A	2339	A	C5-C6-N1	6.10	120.75	117.70
2	B	41	C	N3-C2-O2	-6.09	117.64	121.90
2	B	28	C	N3-C4-N4	-6.08	113.74	118.00
1	A	1952	U	O4'-C1'-N1	6.06	113.05	108.20
33	0	501	GLU	C-N-CD	-6.05	107.30	120.60
33	0	527	PRO	N-CA-CB	6.04	110.54	103.30
1	A	2918	G	C8-N9-C1'	-6.02	119.17	127.00
1	A	2327	A	C5-C6-N1	6.01	120.71	117.70
1	A	1958	G	N1-C6-O6	-6.00	116.30	119.90
1	A	2343	A	C4-C5-C6	-6.00	114.00	117.00
2	B	27	A	C4-C5-C6	-5.99	114.00	117.00
1	A	1990	C	N1-C2-O2	5.98	122.49	118.90
2	B	43	A	C4-C5-C6	-5.98	114.01	117.00
33	0	544	PRO	N-CA-CB	5.97	110.46	103.30
1	A	1804	U	N3-C4-O4	5.95	123.56	119.40
2	B	39	A	C4-C5-C6	-5.94	114.03	117.00
1	A	1370	C	N3-C4-N4	5.93	122.15	118.00
1	A	1370	C	N1-C2-O2	5.90	122.44	118.90
1	A	2330	A	O4'-C1'-N9	5.89	112.91	108.20
1	A	179	A	C5-N7-C8	-5.89	100.95	103.90
1	A	2277	C	C6-N1-C2	-5.89	117.94	120.30
2	B	28	C	N1-C1'-C2'	-5.87	105.54	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2330	A	C4-C5-C6	-5.86	114.07	117.00
1	A	2345	U	C4'-C3'-C2'	-5.86	96.74	102.60
1	A	1203	G	C4-C5-N7	5.86	113.14	110.80
1	A	186	C	C6-N1-C2	-5.85	117.96	120.30
1	A	2340	A	C4-C5-C6	-5.85	114.08	117.00
1	A	78	U	O4'-C1'-N1	5.83	112.87	108.20
1	A	1773	G	O4'-C1'-N9	5.83	112.86	108.20
33	0	448	PRO	N-CA-CB	5.83	110.30	103.30
1	A	2342	C	N1-C2-O2	5.82	122.39	118.90
22	2	13	C	N3-C2-O2	-5.81	117.83	121.90
22	2	26	G	C4'-C3'-C2'	-5.81	96.79	102.60
1	A	631	G	N3-C4-N9	-5.80	122.52	126.00
33	0	539	PRO	N-CA-CB	5.80	110.26	103.30
22	2	56	C	N3-C2-O2	-5.78	117.85	121.90
22	2	39	G	C8-N9-C4	-5.76	104.10	106.40
22	2	42	G	OP1-P-O3'	5.75	117.86	105.20
1	A	1866	C	C5'-C4'-C3'	-5.75	106.80	116.00
1	A	2330	A	N1-C6-N6	-5.75	115.15	118.60
1	A	1867	C	N3-C4-C5	5.75	124.20	121.90
1	A	1339	A	P-O3'-C3'	5.75	126.60	119.70
22	2	14	A	C5-C6-N1	5.72	120.56	117.70
1	A	179	A	N7-C8-N9	5.72	116.66	113.80
22	2	39	G	N3-C2-N2	-5.71	115.90	119.90
1	A	1953	C	N3-C2-O2	-5.70	117.91	121.90
33	0	559	PRO	N-CA-CB	5.70	110.14	103.30
1	A	86	C	C6-N1-C2	-5.69	118.02	120.30
1	A	2331	U	C5'-C4'-O4'	5.69	115.93	109.10
1	A	1467	G	C6-C5-N7	-5.68	126.99	130.40
22	2	41	A	N1-C6-N6	-5.67	115.20	118.60
1	A	1981	A	C5-C6-N6	-5.67	119.17	123.70
1	A	1828	G	N7-C8-N9	5.66	115.93	113.10
2	B	42	G	N3-C4-C5	-5.66	125.77	128.60
21	Y	50	ALA	C-N-CA	5.64	135.79	121.70
1	A	1558	G	N3-C4-N9	5.63	129.38	126.00
2	B	30	C	N3-C4-C5	5.63	124.15	121.90
1	A	1990	C	N3-C2-O2	-5.62	117.97	121.90
1	A	1957	A	O4'-C1'-N9	5.60	112.68	108.20
1	A	1370	C	C5-C4-N4	-5.59	116.28	120.20
1	A	549	A	C8-N9-C4	-5.59	103.56	105.80
1	A	1527	C	N1-C2-O2	5.59	122.26	118.90
1	A	1631	A	OP1-P-O3'	5.59	117.50	105.20
1	A	309	U	C2-N1-C1'	5.59	124.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1954	C	N3-C2-O2	-5.58	118.00	121.90
1	A	1956	A	C4-C5-C6	-5.57	114.22	117.00
1	A	179	A	C5-C6-N6	-5.56	119.25	123.70
22	2	15	G	N3-C2-N2	-5.55	116.01	119.90
33	0	502	PRO	N-CA-CB	5.54	109.95	103.30
1	A	2335	U	C5'-C4'-C3'	-5.53	107.14	116.00
2	B	42	G	N1-C6-O6	-5.52	116.59	119.90
1	A	1382	G	C4-N9-C1'	5.50	133.65	126.50
1	A	2336	G	N1-C6-O6	-5.47	116.62	119.90
32	1	50	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	979	U	O4'-C1'-N1	5.44	112.55	108.20
1	A	1558	G	N9-C4-C5	-5.43	103.23	105.40
1	A	178	A	N7-C8-N9	5.42	116.51	113.80
1	A	1527	C	C6-N1-C2	-5.42	118.13	120.30
1	A	1203	G	C4-N9-C1'	5.40	133.52	126.50
22	2	40	C	N3-C2-O2	-5.40	118.12	121.90
1	A	2338	A	C4-C5-C6	-5.40	114.30	117.00
1	A	2820	U	C5-C4-O4	-5.39	122.67	125.90
2	B	54	U	C5-C6-N1	-5.38	120.01	122.70
1	A	2695	C	C2-N1-C1'	5.37	124.71	118.80
1	A	2421	A	N1-C6-N6	5.37	121.82	118.60
2	B	43	A	C4'-C3'-C2'	-5.37	97.23	102.60
22	2	24	G	C4'-C3'-C2'	-5.37	97.23	102.60
1	A	1696	G	O4'-C1'-N9	5.35	112.48	108.20
1	A	2345	U	C5-C6-N1	-5.35	120.03	122.70
1	A	2313	C	N1-C2-O2	5.35	122.11	118.90
2	B	40	C	N3-C2-O2	-5.35	118.16	121.90
1	A	1886	G	C4-N9-C1'	5.33	133.42	126.50
1	A	1759	U	O4'-C1'-N1	5.29	112.43	108.20
1	A	1981	A	C5-N7-C8	-5.28	101.26	103.90
1	A	1467	G	N3-C4-N9	5.26	129.16	126.00
1	A	86	C	C5-C6-N1	5.26	123.63	121.00
1	A	283	G	C8-N9-C1'	5.25	133.83	127.00
2	B	42	G	C2-N3-C4	5.25	114.52	111.90
1	A	2314	C	C2-N1-C1'	5.24	124.57	118.80
1	A	2334	U	N1-C1'-C2'	-5.24	106.24	112.00
33	0	539	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	634	A	N7-C8-N9	5.22	116.41	113.80
33	0	491	PRO	CA-N-CD	-5.22	104.19	111.50
33	0	502	PRO	CA-N-CD	-5.22	104.19	111.50
33	0	448	PRO	CA-N-CD	-5.22	104.19	111.50
33	0	527	PRO	CA-N-CD	-5.21	104.20	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1448	U	C5-C4-O4	-5.21	122.77	125.90
33	0	544	PRO	CA-N-CD	-5.21	104.20	111.50
33	0	559	PRO	CA-N-CD	-5.21	104.20	111.50
1	A	1958	G	N9-C4-C5	5.20	107.48	105.40
22	2	41	A	N1-C2-N3	-5.20	126.70	129.30
1	A	2717	G	C2-N3-C4	-5.19	109.31	111.90
22	2	42	G	P-O3'-C3'	5.18	125.91	119.70
22	2	57	G	C6-C5-N7	5.17	133.50	130.40
1	A	1957	A	N9-C1'-C2'	-5.17	106.31	112.00
1	A	2536	C	N1-C2-O2	5.17	122.00	118.90
1	A	2621	G	C6-C5-N7	-5.17	127.30	130.40
1	A	1831	A	N7-C8-N9	5.17	116.38	113.80
1	A	1480	A	O4'-C1'-N9	5.16	112.33	108.20
1	A	1831	A	C5-N7-C8	-5.16	101.32	103.90
1	A	1951	G	N1-C6-O6	-5.15	116.81	119.90
22	2	57	G	C3'-C2'-C1'	-5.15	97.38	101.50
33	0	268	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	2277	C	N1-C2-O2	5.13	121.98	118.90
2	B	54	U	O4'-C1'-N1	5.13	112.30	108.20
1	A	1954	C	O4'-C1'-N1	5.13	112.30	108.20
27	f	16	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	1362	G	C6-C5-N7	-5.13	127.32	130.40
1	A	1425	C	C5-C6-N1	5.12	123.56	121.00
1	A	186	C	C2-N1-C1'	5.12	124.43	118.80
1	A	2342	C	N3-C4-N4	-5.12	114.42	118.00
1	A	1384	C	C6-N1-C2	-5.11	118.26	120.30
1	A	555	C	C5-C6-N1	5.11	123.55	121.00
1	A	1558	G	C6-C5-N7	-5.11	127.34	130.40
1	A	1671	G	P-O3'-C3'	5.10	125.82	119.70
22	2	41	A	C5-C6-N1	5.09	120.24	117.70
1	A	1203	G	C8-N9-C1'	-5.08	120.39	127.00
1	A	2340	A	C4'-C3'-C2'	-5.08	97.52	102.60
2	B	55	A	C5'-C4'-C3'	-5.08	107.88	116.00
1	A	2341	U	N1-C2-N3	5.06	117.94	114.90
1	A	1507	U	P-O3'-C3'	5.05	125.76	119.70
1	A	568	G	C4-C5-N7	5.04	112.82	110.80
1	A	1947	A	C3'-C2'-O2'	-5.04	98.69	113.30
1	A	2330	A	O3'-P-O5'	-5.03	94.45	104.00
22	2	24	G	N3-C4-C5	-5.02	126.09	128.60
1	A	1558	G	C8-N9-C1'	-5.02	120.47	127.00
1	A	2025	C	N1-C2-O2	5.01	121.91	118.90
1	A	634	A	C5-N7-C8	-5.01	101.39	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	39	G	N9-C4-C5	5.01	107.41	105.40
22	2	24	G	C5-C6-N1	5.01	114.00	111.50
1	A	2331	U	N3-C2-O2	-5.00	118.70	122.20
1	A	994	C	C5-C4-N4	-5.00	116.70	120.20
1	A	2481	C	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	2	23	A	Sidechain
22	2	24	G	Sidechain
22	2	39	G	Sidechain
22	2	40	C	Sidechain
22	2	41	A	Sidechain
22	2	42	G	Sidechain
22	2	57	G	Sidechain
1	A	1866	C	Sidechain
1	A	1952	U	Sidechain
1	A	1953	C	Sidechain
1	A	1955	U	Sidechain
1	A	1957	A	Sidechain
1	A	1958	G	Sidechain
1	A	2328	G	Sidechain
1	A	2331	U	Sidechain
1	A	2333	G	Sidechain
1	A	2334	U	Sidechain
1	A	2335	U	Sidechain
1	A	2336	G	Sidechain
1	A	2338	A	Sidechain
1	A	2344	U	Sidechain
1	A	2345	U	Sidechain
2	B	28	C	Sidechain
2	B	39	A	Sidechain
2	B	41	C	Sidechain
2	B	52	G	Sidechain
3	E	154	LEU	Peptide
6	H	97	TYR	Sidechain
8	K	19	ASN	Peptide
13	Q	60	ARG	Peptide
18	V	50	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60436	0	30414	330	0
2	B	2392	0	1213	7	0
3	E	2083	0	2168	29	0
4	F	1569	0	1637	19	0
5	G	1561	0	1647	13	0
6	H	1387	0	1448	74	0
7	I	1342	0	1388	19	0
8	K	974	0	1011	14	0
9	L	886	0	920	16	0
10	N	1124	0	1162	18	0
11	O	921	0	977	21	0
12	P	1082	0	1132	10	0
13	Q	1076	0	1145	13	0
14	R	954	0	983	19	0
15	S	913	0	947	26	0
16	T	945	0	1020	10	0
17	U	940	0	1005	14	0
18	V	781	0	821	9	0
19	W	842	0	899	6	0
20	X	725	0	770	7	0
21	Y	762	0	821	6	0
22	2	1496	0	759	43	0
23	a	624	0	639	0	0
24	b	444	0	487	0	0
25	c	530	0	568	0	0
26	d	456	0	491	0	0
27	f	418	0	435	0	0
28	g	401	0	413	0	0
29	h	368	0	410	0	0
30	i	512	0	564	0	0
31	j	297	0	342	0	0
32	1	659	0	705	1	0
33	0	3962	0	3687	94	0
All	All	93862	0	63028	641	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 5.

All (641) 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:A:2340:A:C2	6:H:79:LEU:HD11	1.55	1.39
1:A:2334:U:O4	6:H:151:GLY:HA3	1.38	1.22
1:A:2334:U:C4	6:H:151:GLY:HA3	1.76	1.19
33:0:537:LYS:C	33:0:539:PRO:HD2	1.65	1.15
6:H:125:ARG:HG3	15:S:1:MET:HB2	1.27	1.14
1:A:2340:A:N3	6:H:79:LEU:HD11	1.64	1.10
22:2:44:A:OP1	33:0:286:ARG:NH2	1.86	1.08
1:A:2334:U:O4	6:H:151:GLY:CA	1.99	1.08
22:2:31:C:C2	33:0:125:ARG:CZ	2.36	1.08
1:A:2340:A:C2	6:H:79:LEU:CD1	2.38	1.05
33:0:414:ALA:HA	33:0:465:LYS:CB	1.87	1.05
33:0:523:SER:O	33:0:559:PRO:HD2	1.55	1.04
33:0:410:GLN:HB3	33:0:465:LYS:O	1.58	1.03
33:0:501:GLU:N	33:0:502:PRO:HD2	1.75	1.02
1:A:2340:A:N3	6:H:79:LEU:CD1	2.24	1.00
6:H:160:ALA:O	15:S:1:MET:HA	1.62	1.00
22:2:44:A:C5'	33:0:286:ARG:HH21	1.76	0.97
1:A:312:G:N2	1:A:405:U:C5	2.33	0.95
11:O:103:ALA:HA	11:O:122:ILE:OXT	1.66	0.95
6:H:125:ARG:HG3	15:S:1:MET:CB	1.95	0.95
1:A:2337:G:C2	6:H:77:PHE:CE1	2.56	0.94
33:0:501:GLU:H	33:0:502:PRO:HD2	1.31	0.93
33:0:413:SER:HB2	33:0:517:PHE:CB	1.99	0.93
22:2:31:C:O2	33:0:125:ARG:NH1	2.03	0.92
1:A:327:G:H1	1:A:400:U:H3	1.18	0.92
33:0:515:ALA:HB1	33:0:559:PRO:HD3	1.49	0.91
33:0:53:HIS:CD2	33:0:282:ALA:HA	2.04	0.91
6:H:159:THR:HG22	15:S:2:ILE:HG21	1.50	0.91
22:2:44:A:H5''	33:0:286:ARG:HH21	1.34	0.90
1:A:2340:A:H2	6:H:79:LEU:HD11	1.28	0.89
1:A:1152:G:HO2'	9:L:30:TYR:HH	1.16	0.89
22:2:36:C:OP1	22:2:37:A:N6	2.06	0.89
33:0:501:GLU:H	33:0:502:PRO:CD	1.86	0.88
1:A:1159:U:OP1	7:I:2:SER:OG	1.90	0.87
6:H:160:ALA:O	15:S:1:MET:CA	2.23	0.87
33:0:501:GLU:N	33:0:502:PRO:CD	2.36	0.87
1:A:2337:G:C5	6:H:77:PHE:CZ	2.65	0.84
1:A:810:G:O2'	1:A:811:A:O5'	1.95	0.83
1:A:2339:A:H2	6:H:76:GLY:HA3	1.43	0.83
33:0:447:ASN:H	33:0:448:PRO:HD2	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:C:O2	1:A:1220:G:N2	2.12	0.82
6:H:160:ALA:O	15:S:1:MET:N	2.12	0.82
1:A:2341:U:H5'	6:H:85:ILE:HD11	1.60	0.82
1:A:1790:U:O2'	1:A:1791:A:O4'	1.98	0.80
22:2:31:C:C2	33:0:125:ARG:NH2	2.49	0.80
6:H:73:SER:HB3	22:2:56:C:C1'	2.12	0.80
1:A:2341:U:H5'	6:H:85:ILE:CD1	2.13	0.79
33:0:409:GLN:CD	33:0:492:GLY:HA2	2.02	0.79
33:0:413:SER:CB	33:0:517:PHE:CB	2.61	0.79
6:H:73:SER:HB2	22:2:56:C:O4'	1.81	0.79
1:A:2009:G:O2'	1:A:2011:U:OP2	2.02	0.78
22:2:31:C:C2	33:0:125:ARG:NH1	2.50	0.77
1:A:1263:G:OP2	18:V:89:ARG:NH1	2.17	0.77
33:0:537:LYS:C	33:0:539:PRO:CD	2.50	0.77
6:H:125:ARG:CG	15:S:1:MET:HB2	2.12	0.77
1:A:84:A:N6	1:A:101:G:O2'	2.18	0.77
6:H:73:SER:CB	22:2:56:C:O4'	2.32	0.77
1:A:2337:G:C6	6:H:77:PHE:CZ	2.73	0.77
1:A:2806:G:OP2	1:A:2810:A:O2'	2.02	0.77
22:2:31:C:H1'	33:0:125:ARG:HD2	1.65	0.76
1:A:363:C:OP2	5:G:137:LYS:NZ	2.18	0.76
1:A:917:A:OP1	13:Q:6:ARG:NH2	2.18	0.76
22:2:44:A:P	33:0:286:ARG:NH2	2.59	0.76
6:H:125:ARG:CG	15:S:1:MET:CB	2.63	0.76
22:2:36:C:OP1	22:2:37:A:C6	2.39	0.76
18:V:68:ALA:O	18:V:89:ARG:NE	2.17	0.76
10:N:88:ARG:NH1	10:N:97:TYR:OH	2.19	0.75
14:R:94:ARG:NH1	14:R:120:VAL:O	2.19	0.75
1:A:364:A:N3	5:G:169:ASN:ND2	2.34	0.75
6:H:75:ALA:HB2	22:2:56:C:O2'	1.87	0.75
6:H:159:THR:HG22	15:S:2:ILE:CG2	2.15	0.75
1:A:840:A:OP2	1:A:2100:A:O2'	2.04	0.75
1:A:2339:A:C2	6:H:76:GLY:HA3	2.23	0.74
4:F:26:THR:OG1	4:F:190:GLY:O	2.06	0.74
22:2:44:A:C5'	33:0:286:ARG:NH2	2.50	0.74
33:0:538:LYS:N	33:0:539:PRO:CD	2.49	0.74
33:0:537:LYS:O	33:0:539:PRO:HD2	1.87	0.74
1:A:2127:U:O2'	1:A:2128:U:OP1	2.06	0.74
10:N:15:LYS:N	10:N:53:ASP:OD1	2.21	0.74
14:R:99:THR:C	14:R:120:VAL:OXT	2.26	0.74
1:A:2372:U:HO2'	1:A:2402:A:HO2'	1.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:46:LYS:O	14:R:49:THR:OG1	2.05	0.73
1:A:1114:G:N2	1:A:1141:A:O2'	2.21	0.73
33:0:523:SER:O	33:0:559:PRO:CD	2.35	0.73
1:A:2532:A:O2'	1:A:2534:G:OP2	2.06	0.73
20:X:19:ASP:O	20:X:22:THR:OG1	2.07	0.73
13:Q:25:THR:OG1	13:Q:26:GLU:OE1	2.05	0.73
33:0:53:HIS:O	33:0:57:SER:N	2.22	0.73
1:A:458:G:OP2	1:A:2435:C:O2'	2.06	0.73
1:A:2498:A:O2'	13:Q:56:ARG:NH1	2.22	0.72
1:A:2025:C:OP1	11:O:31:LYS:NZ	2.22	0.72
1:A:2339:A:H2'	6:H:77:PHE:CE2	2.25	0.72
1:A:1542:A:O2'	1:A:1544:C:N4	2.23	0.72
1:A:1694:G:O2'	14:R:110:ASP:OD1	2.07	0.72
33:0:53:HIS:NE2	33:0:282:ALA:HA	2.03	0.72
1:A:1695:A:HO2'	1:A:1696:G:P	2.12	0.71
1:A:1983:G:O2'	1:A:1985:U:O4	2.08	0.71
1:A:918:U:OP1	13:Q:5:LYS:N	2.22	0.71
1:A:1784:A:O2'	1:A:1785:G:OP1	2.06	0.71
1:A:1876:A:O2'	1:A:1877:A:N7	2.23	0.71
22:2:31:C:H1'	33:0:125:ARG:CD	2.20	0.71
4:F:95:GLN:NE2	4:F:96:GLU:O	2.23	0.71
33:0:538:LYS:N	33:0:539:PRO:HD2	2.06	0.71
1:A:79:C:O2'	1:A:390:A:N3	2.18	0.71
33:0:25:THR:OG1	33:0:38:HIS:O	2.05	0.71
14:R:19:ASP:OD1	14:R:67:ARG:NH1	2.24	0.70
1:A:282:G:O2'	1:A:283:G:O4'	2.09	0.70
1:A:1088:G:H1	1:A:1159:U:H3	1.36	0.70
22:2:31:C:N3	33:0:125:ARG:NH2	2.40	0.70
33:0:27:ILE:O	33:0:80:ARG:NH2	2.25	0.70
1:A:1259:G:OP2	17:U:19:LYS:NZ	2.18	0.70
1:A:1362:G:OP1	19:W:98:LYS:NZ	2.24	0.70
15:S:92:ASP:OD1	15:S:119:LYS:NZ	2.25	0.70
33:0:480:ARG:O	33:0:534:ARG:N	2.25	0.69
1:A:177:G:O2'	1:A:178:A:O5'	2.10	0.69
1:A:2922:U:O2'	10:N:137:LYS:NZ	2.25	0.69
1:A:419:G:N2	1:A:448:A:OP2	2.16	0.69
1:A:2595:A:N1	11:O:28:SER:OG	2.24	0.69
1:A:1036:A:O2'	1:A:1037:C:OP1	2.07	0.69
1:A:1828:G:OP1	3:E:260:ARG:NH1	2.26	0.69
1:A:2772:U:OP2	1:A:2784:C:N4	2.25	0.69
1:A:2339:A:H2'	6:H:77:PHE:HE2	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:85:PHE:O	12:P:119:LYS:NZ	2.17	0.69
1:A:1265:A:OP1	18:V:70:LYS:NZ	2.25	0.69
22:2:58:A:O2'	22:2:60:C:OP2	2.07	0.68
33:0:399:GLU:OE2	33:0:543:LYS:N	2.27	0.68
20:X:84:THR:OG1	20:X:87:SER:OG	2.05	0.68
33:0:410:GLN:HE22	33:0:467:ASN:HA	1.59	0.68
1:A:312:G:N2	1:A:405:U:C4	2.62	0.68
1:A:790:A:O2'	1:A:1704:U:OP1	2.12	0.68
1:A:1130:A:N3	1:A:1151:U:O2'	2.21	0.68
1:A:1365:U:O2'	1:A:1366:C:O4'	2.12	0.68
1:A:1315:G:OP2	1:A:1690:G:O2'	2.04	0.68
1:A:160:G:N2	1:A:168:A:OP2	2.27	0.68
1:A:2287:C:O2'	1:A:2456:C:OP2	2.11	0.67
1:A:2340:A:H2	6:H:79:LEU:CD1	1.92	0.67
7:I:57:SER:OG	7:I:59:GLN:OE1	2.04	0.67
1:A:2294:U:OP2	1:A:2295:A:O2'	2.10	0.67
14:R:52:LYS:NZ	14:R:94:ARG:O	2.27	0.67
33:0:410:GLN:CB	33:0:465:LYS:O	2.41	0.67
1:A:1403:G:N2	1:A:1406:A:OP2	2.25	0.67
1:A:1094:A:OP2	1:A:1156:G:N2	2.25	0.67
22:2:3:G:H1	22:2:70:U:H3	1.43	0.67
1:A:719:C:OP2	12:P:42:SER:OG	2.12	0.66
3:E:72:ASP:OD2	3:E:189:ARG:NH2	2.28	0.66
33:0:410:GLN:HE22	33:0:467:ASN:CA	2.08	0.66
16:T:88:ARG:NH1	16:T:112:GLU:OE1	2.29	0.66
1:A:52:A:OP2	1:A:118:A:N6	2.28	0.66
1:A:1886:G:O2'	1:A:1887:G:O4'	2.03	0.66
1:A:1530:G:O2'	1:A:1531:G:OP1	2.14	0.66
1:A:2340:A:C6	6:H:41:GLY:HA3	2.30	0.66
1:A:2513:G:OP1	13:Q:45:ARG:NH1	2.30	0.65
3:E:13:ARG:NH1	3:E:16:MET:SD	2.69	0.65
8:K:26:PRO:O	8:K:30:GLN:NE2	2.29	0.65
1:A:1991:C:O2'	1:A:1993:G:OP2	2.14	0.65
1:A:2340:A:N3	6:H:79:LEU:HD12	2.11	0.65
1:A:1216:C:N3	1:A:1220:G:N1	2.44	0.65
1:A:2121:U:N3	1:A:2255:C:OP2	2.29	0.65
1:A:161:A:OP2	1:A:166:A:N6	2.30	0.65
1:A:1364:C:OP1	1:A:1692:U:O2'	2.15	0.65
15:S:61:LYS:O	15:S:64:ASN:ND2	2.29	0.65
1:A:353:A:N3	1:A:373:A:O2'	2.31	0.64
10:N:78:HIS:ND1	10:N:79:THR:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:A:OP2	1:A:1180:C:O2'	2.14	0.64
1:A:2341:U:C5'	6:H:85:ILE:HD11	2.26	0.64
33:0:409:GLN:CG	33:0:492:GLY:HA2	2.27	0.64
14:R:99:THR:N	14:R:120:VAL:OXT	2.31	0.64
17:U:90:VAL:O	18:V:11:GLN:NE2	2.30	0.64
1:A:604:C:O2	17:U:48:ARG:NH2	2.31	0.64
1:A:2337:G:C4	6:H:77:PHE:CZ	2.86	0.64
2:B:47:C:OP2	15:S:35:ARG:NH2	2.30	0.64
1:A:312:G:C2	1:A:405:U:C4	2.85	0.64
1:A:186:C:O2'	1:A:479:A:N3	2.25	0.64
1:A:2060:A:N3	1:A:2484:G:O2'	2.28	0.64
3:E:194:GLN:NE2	3:E:198:GLU:OE1	2.31	0.64
1:A:2605:G:O2'	1:A:2608:C:OP2	2.16	0.64
1:A:867:A:N3	1:A:989:U:O2'	2.31	0.64
1:A:77:U:O2'	1:A:78:U:O5'	2.16	0.63
1:A:1291:A:OP1	17:U:10:THR:OG1	2.10	0.63
33:0:121:GLU:OE2	33:0:162:TYR:OH	2.15	0.63
6:H:54:VAL:HG13	6:H:65:PRO:HG2	1.79	0.63
10:N:59:ASN:N	10:N:128:GLY:O	2.32	0.63
1:A:2872:U:OP1	16:T:96:LYS:NZ	2.28	0.63
1:A:633:U:O3'	5:G:95:ARG:NH1	2.31	0.63
1:A:1108:G:N3	8:K:134:SER:OG	2.32	0.63
1:A:2364:A:O2'	1:A:2365:A:O5'	2.14	0.63
33:0:422:ILE:HD11	33:0:466:ASN:HA	1.80	0.63
1:A:1509:C:HO2'	1:A:2731:G:HO2'	1.47	0.62
1:A:1313:A:O2'	1:A:1314:A:OP1	2.17	0.62
1:A:1856:U:OP2	3:E:221:ARG:NH1	2.32	0.62
22:2:44:A:H5'	33:0:286:ARG:HH21	1.61	0.62
1:A:1757:G:O2'	1:A:1758:U:O3'	2.16	0.62
1:A:1843:G:OP2	1:A:1844:A:O2'	2.13	0.62
1:A:2027:A:OP2	4:F:141:ARG:NH1	2.32	0.62
1:A:2337:G:N3	6:H:77:PHE:CE1	2.66	0.62
1:A:2334:U:C6	6:H:133:LYS:HA	2.35	0.62
1:A:2548:U:O4'	1:A:2571:A:N6	2.33	0.62
1:A:2890:U:OP2	1:A:2891:G:O2'	2.13	0.62
1:A:1231:G:OP1	12:P:30:THR:OG1	2.10	0.62
12:P:55:MET:O	12:P:60:ARG:NH2	2.33	0.62
4:F:9:LYS:NZ	4:F:194:GLY:O	2.20	0.62
1:A:372:U:O2'	21:Y:67:ASN:ND2	2.33	0.62
11:O:13:ASN:ND2	11:O:96:THR:OG1	2.32	0.62
1:A:2497:A:O2'	1:A:2498:A:O4'	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:G:OP2	1:A:1172:A:O2'	2.09	0.61
33:0:409:GLN:CD	33:0:492:GLY:CA	2.68	0.61
1:A:1264:G:OP2	18:V:67:ARG:NH2	2.33	0.61
1:A:1379:U:OP2	20:X:59:TYR:OH	2.17	0.61
1:A:1124:C:OP1	8:K:133:ARG:NH2	2.33	0.61
1:A:2841:C:O2	1:A:2908:A:O2'	2.15	0.61
6:H:80:ARG:CZ	22:2:56:C:C5	2.84	0.61
1:A:1695:A:O2'	1:A:1696:G:O5'	2.13	0.61
1:A:2468:A:O2'	1:A:2629:A:OP1	2.13	0.61
1:A:2080:A:O2'	1:A:2643:A:N6	2.34	0.60
1:A:1065:U:OP1	1:A:1081:U:O2'	2.17	0.60
1:A:2665:U:O2'	4:F:46:TYR:OH	2.19	0.60
1:A:2337:G:C5	6:H:77:PHE:HZ	2.19	0.60
1:A:2856:G:N2	1:A:2909:U:OP2	2.34	0.60
14:R:52:LYS:NZ	14:R:98:TYR:OH	2.25	0.60
6:H:73:SER:HB3	22:2:56:C:H1'	1.83	0.60
1:A:2054:C:OP1	4:F:153:ARG:NH2	2.35	0.60
1:A:1036:A:O2'	1:A:1038:C:OP2	2.20	0.60
1:A:2026:A:O5'	4:F:130:ARG:NH1	2.33	0.60
6:H:80:ARG:CZ	22:2:56:C:C4	2.85	0.60
33:0:410:GLN:HE22	33:0:467:ASN:CB	2.15	0.60
1:A:1199:C:OP1	17:U:92:ARG:NH2	2.35	0.60
2:B:26:C:O2	2:B:57:G:N2	2.33	0.60
17:U:39:VAL:O	17:U:42:SER:OG	2.11	0.60
22:2:31:C:C4	33:0:125:ARG:NH2	2.69	0.60
33:0:60:HIS:NE2	33:0:271:SER:O	2.34	0.59
1:A:2341:U:C5'	6:H:85:ILE:CD1	2.79	0.59
11:O:13:ASN:OD1	11:O:96:THR:N	2.35	0.59
1:A:1811:C:O2	1:A:2637:G:O2'	2.04	0.59
1:A:2130:G:N2	1:A:2218:U:O2	2.30	0.59
1:A:2688:G:N2	1:A:2691:A:OP2	2.35	0.59
5:G:101:LEU:O	5:G:106:ARG:NH2	2.35	0.59
14:R:99:THR:CA	14:R:120:VAL:OXT	2.50	0.59
1:A:347:G:O2'	1:A:348:U:OP1	2.19	0.59
33:0:409:GLN:HG3	33:0:492:GLY:HA2	1.83	0.59
1:A:2333:G:O2'	6:H:129:THR:HG21	2.03	0.59
1:A:2882:G:N2	1:A:2885:A:OP2	2.29	0.59
7:I:8:LEU:HD22	7:I:52:THR:HG22	1.83	0.59
1:A:546:G:N1	1:A:549:A:OP2	2.35	0.59
1:A:2333:G:O2'	6:H:129:THR:CG2	2.51	0.59
1:A:753:A:OP1	3:E:7:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:G:O2'	1:A:1149:A:N6	2.36	0.58
33:0:525:SER:O	33:0:527:PRO:HD2	2.03	0.58
1:A:1820:A:N6	1:A:1857:G:O2'	2.35	0.58
33:0:418:ASP:HB3	33:0:466:ASN:CB	2.33	0.58
1:A:251:G:O2'	1:A:2461:A:OP1	2.11	0.58
11:O:87:ILE:HD13	11:O:90:ASP:O	2.04	0.58
1:A:1125:C:O4'	8:K:133:ARG:NH1	2.36	0.58
10:N:14:ARG:NH2	10:N:50:ASP:O	2.36	0.58
33:0:392:GLU:OE1	33:0:395:ARG:NH2	2.37	0.58
1:A:420:U:O2'	1:A:421:A:O5'	2.22	0.57
1:A:843:C:O3'	5:G:62:ARG:NH2	2.37	0.57
5:G:109:ALA:O	5:G:112:SER:OG	2.17	0.57
13:Q:77:LYS:NZ	13:Q:84:GLY:O	2.32	0.57
1:A:2334:U:C5	6:H:133:LYS:HA	2.39	0.57
1:A:1501:U:O2'	1:A:1502:G:N7	2.37	0.57
1:A:2665:U:HO2'	4:F:46:TYR:HH	1.52	0.57
1:A:448:A:O2'	1:A:449:A:O4'	2.11	0.57
3:E:77:ARG:NH2	3:E:115:GLU:OE2	2.38	0.57
1:A:2106:A:OP1	1:A:2267:G:N2	2.33	0.57
1:A:1830:G:OP2	3:E:150:LYS:NZ	2.38	0.57
9:L:29:ASP:OD1	9:L:30:TYR:N	2.38	0.57
1:A:2830:A:O2'	1:A:2831:A:OP2	2.22	0.57
1:A:1757:G:O2'	1:A:1758:U:O5'	2.23	0.56
16:T:28:VAL:HG12	16:T:84:ILE:HG22	1.87	0.56
1:A:2054:C:OP2	4:F:153:ARG:NE	2.38	0.56
1:A:83:G:N2	1:A:102:A:OP2	2.22	0.56
1:A:1010:C:O2'	1:A:2302:A:N3	2.37	0.56
3:E:45:ASN:OD1	3:E:46:GLN:N	2.38	0.56
1:A:2332:G:H4'	6:H:123:ASP:HA	1.87	0.56
1:A:1127:U:O2	8:K:117:ASN:ND2	2.37	0.56
1:A:1782:G:OP1	16:T:93:ARG:NH1	2.38	0.56
1:A:2324:C:OP2	15:S:14:ARG:NE	2.37	0.55
14:R:99:THR:O	14:R:120:VAL:OXT	2.23	0.55
11:O:33:ALA:HB1	11:O:37:ASP:CB	2.36	0.55
33:0:410:GLN:NE2	33:0:467:ASN:HA	2.20	0.55
1:A:2038:G:OP1	19:W:41:ARG:NH1	2.40	0.55
1:A:675:C:O2	1:A:685:U:O2'	2.24	0.55
1:A:623:A:O2'	1:A:2048:U:OP1	2.24	0.55
1:A:2712:C:O2	11:O:76:TYR:OH	2.24	0.55
1:A:1883:A:O2'	1:A:1884:G:OP1	2.23	0.55
1:A:2684:G:O2'	1:A:2693:G:O6	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:83:ASN:O	12:P:119:LYS:NZ	2.24	0.55
33:O:409:GLN:NE2	33:O:492:GLY:HA2	2.21	0.55
1:A:777:C:OP1	1:A:1804:U:O2'	2.20	0.55
1:A:2406:A:O2'	15:S:120:PHE:OXT	2.24	0.55
12:P:116:LYS:NZ	12:P:118:GLU:OE2	2.41	0.54
1:A:1972:U:O2'	1:A:1973:U:OP2	2.26	0.54
7:I:89:GLU:OE1	7:I:89:GLU:N	2.40	0.54
33:O:410:GLN:OE1	33:O:467:ASN:N	2.40	0.54
1:A:339:A:O3'	21:Y:90:LYS:NZ	2.41	0.54
9:L:5:ILE:N	9:L:8:LYS:HZ3	2.05	0.54
1:A:593:A:O2'	1:A:594:C:O5'	2.26	0.54
1:A:2859:G:O2'	1:A:2860:A:O5'	2.24	0.54
1:A:1058:U:O4	10:N:31:SER:OG	2.24	0.54
3:E:142:HIS:ND1	3:E:193:GLY:O	2.40	0.54
6:H:158:THR:HG22	6:H:160:ALA:H	1.73	0.54
33:O:522:ASP:C	33:O:559:PRO:HG2	2.28	0.54
1:A:116:G:OP2	1:A:118:A:O2'	2.26	0.54
1:A:1110:C:OP1	8:K:80:LYS:NZ	2.41	0.54
3:E:154:LEU:O	3:E:156:ARG:N	2.41	0.54
22:2:44:A:H5'	33:O:286:ARG:NH2	2.20	0.54
1:A:373:A:N1	21:Y:15:LYS:NZ	2.56	0.53
1:A:2334:U:O4	6:H:151:GLY:C	2.46	0.53
33:O:185:LEU:HD11	33:O:192:LEU:HD13	1.91	0.53
6:H:75:ALA:CB	22:2:56:C:O2'	2.57	0.53
11:O:22:ILE:HD11	11:O:42:THR:HG23	1.89	0.53
11:O:120:GLU:OE1	16:T:65:SER:OG	2.25	0.53
4:F:43:ASN:OD1	4:F:44:ASP:N	2.41	0.53
1:A:490:A:OP1	5:G:46:GLN:N	2.42	0.53
7:I:158:TYR:O	7:I:172:ARG:NH1	2.39	0.53
10:N:30:SER:HA	10:N:33:VAL:HG22	1.91	0.53
15:S:24:GLY:O	15:S:47:ASP:N	2.42	0.53
1:A:1498:U:O2'	1:A:1499:A:N7	2.42	0.53
1:A:1981:A:OP1	11:O:44:LYS:NZ	2.31	0.53
13:Q:30:GLY:O	13:Q:134:ARG:NH2	2.41	0.53
10:N:50:ASP:OD1	10:N:122:LYS:NZ	2.42	0.53
13:Q:42:ILE:HD12	13:Q:97:VAL:HG21	1.92	0.52
1:A:287:G:N3	1:A:288:C:N4	2.58	0.52
1:A:488:U:O2	5:G:46:GLN:NE2	2.41	0.52
1:A:2233:C:OP1	3:E:147:LYS:NZ	2.42	0.52
1:A:236:A:H61	1:A:476:A:H61	1.57	0.52
1:A:1033:C:O2'	1:A:1046:A:N3	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2364:A:HO2'	1:A:2365:A:P	2.33	0.52
8:K:117:ASN:OD1	8:K:118:ALA:N	2.42	0.52
1:A:1113:A:OP1	33:0:384:LYS:NZ	2.43	0.52
1:A:1462:G:HO2'	1:A:1633:G:HO2'	1.58	0.52
15:S:30:ARG:NH2	15:S:47:ASP:OD1	2.43	0.52
22:2:31:C:H1'	33:0:125:ARG:NE	2.25	0.52
3:E:155:VAL:O	3:E:160:THR:OG1	2.19	0.52
1:A:2344:U:O2'	6:H:125:ARG:HG2	2.10	0.52
1:A:792:G:O2'	1:A:795:G:O2'	2.16	0.51
2:B:21:G:O2'	2:B:22:G:O5'	2.15	0.51
6:H:159:THR:HA	15:S:2:ILE:HG22	1.91	0.51
7:I:108:VAL:HG13	7:I:109:GLY:H	1.76	0.51
33:0:409:GLN:CD	33:0:492:GLY:C	2.69	0.51
1:A:2104:U:OP2	1:A:2267:G:O2'	2.16	0.51
1:A:2404:G:N2	1:A:2407:A:OP2	2.31	0.51
11:O:48:PRO:O	11:O:50:GLY:N	2.43	0.51
15:S:87:GLU:OE2	15:S:88:LYS:NZ	2.43	0.51
1:A:1759:U:HO2'	1:A:1760:A:P	2.34	0.51
14:R:8:ARG:O	14:R:13:ARG:NH2	2.43	0.51
1:A:274:A:HO2'	1:A:415:C:HO2'	1.41	0.51
1:A:2334:U:O4	6:H:151:GLY:N	2.44	0.51
1:A:2850:G:O6	4:F:163:ARG:NH1	2.44	0.51
33:0:447:ASN:H	33:0:448:PRO:CD	2.19	0.51
1:A:52:A:OP2	1:A:116:G:N1	2.43	0.51
1:A:1008:A:HO2'	1:A:2525:C:HO2'	1.59	0.51
33:0:523:SER:N	33:0:559:PRO:HG2	2.26	0.51
1:A:1452:C:H2'	1:A:1453:A:C8	2.46	0.51
1:A:1129:U:N3	1:A:1132:A:OP2	2.41	0.50
1:A:1993:G:O2'	1:A:1996:C:OP2	2.18	0.50
1:A:2337:G:C4	6:H:77:PHE:CE1	2.99	0.50
15:S:19:ARG:NH1	15:S:47:ASP:OD2	2.43	0.50
1:A:1460:G:O2'	1:A:1631:A:N6	2.44	0.50
1:A:1970:C:N4	1:A:1994:C:O4'	2.45	0.50
22:2:31:C:N1	33:0:125:ARG:CZ	2.73	0.50
7:I:59:GLN:OE1	7:I:62:HIS:ND1	2.44	0.50
1:A:2278:U:N3	1:A:2282:G:OP2	2.41	0.50
1:A:2279:G:N2	1:A:2305:G:OP1	2.45	0.50
33:0:128:ASN:OD1	33:0:129:ILE:N	2.45	0.50
9:L:7:THR:O	9:L:11:VAL:HG23	2.12	0.50
9:L:77:THR:O	9:L:80:ASN:ND2	2.44	0.50
1:A:1956:A:H2'	1:A:1957:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:8:LEU:CD2	7:I:52:THR:HG22	2.42	0.50
9:L:56:LYS:O	9:L:60:THR:OG1	2.18	0.50
33:0:94:ALA:HB2	33:0:101:ILE:HD11	1.94	0.49
1:A:274:A:O2'	1:A:415:C:O2'	2.15	0.49
1:A:420:U:HO2'	1:A:421:A:P	2.34	0.49
15:S:8:ASN:OD1	15:S:11:ARG:NH2	2.45	0.49
3:E:53:HIS:CE1	3:E:219:THR:HG23	2.48	0.49
33:0:409:GLN:NE2	33:0:493:SER:N	2.59	0.49
33:0:409:GLN:OE1	33:0:492:GLY:C	2.50	0.49
1:A:347:G:HO2'	1:A:348:U:P	2.35	0.49
1:A:1831:A:H2	1:A:1844:A:H62	1.61	0.49
1:A:2420:G:O2'	1:A:2421:A:O5'	2.30	0.49
3:E:176:LEU:O	3:E:179:GLY:N	2.40	0.49
17:U:90:VAL:HG12	18:V:39:LEU:HD13	1.94	0.49
33:0:9:TYR:O	33:0:12:THR:OG1	2.27	0.49
1:A:528:G:HO2'	1:A:529:C:P	2.36	0.49
1:A:2922:U:O3'	10:N:137:LYS:NZ	2.46	0.49
1:A:1189:A:OP1	10:N:28:ARG:NH1	2.43	0.49
8:K:33:VAL:HG12	8:K:64:ARG:HG2	1.94	0.49
1:A:13:A:O2'	1:A:15:G:N7	2.45	0.49
1:A:265:A:N3	1:A:477:A:O2'	2.39	0.49
1:A:1263:G:N2	1:A:1266:A:OP2	2.38	0.49
1:A:1462:G:O2'	1:A:1633:G:O2'	2.28	0.49
33:0:53:HIS:CD2	33:0:282:ALA:CA	2.89	0.49
1:A:1158:G:O2'	1:A:1159:U:O5'	2.31	0.49
1:A:630:A:H5'	5:G:89:VAL:HG21	1.93	0.48
1:A:1734:A:OP2	1:A:1743:A:N6	2.32	0.48
10:N:63:ILE:O	10:N:94:ARG:NH2	2.46	0.48
3:E:123:ASP:OD1	3:E:128:ASN:ND2	2.45	0.48
1:A:45:G:H21	1:A:183:A:H61	1.61	0.48
1:A:85:G:N1	1:A:98:U:C2	2.82	0.48
1:A:776:G:OP1	3:E:10:SER:OG	2.32	0.48
1:A:1339:A:H4'	1:A:1340:A:H5'	1.95	0.48
33:0:410:GLN:NE2	33:0:467:ASN:CA	2.74	0.48
1:A:2320:U:O2'	1:A:2403:C:O2	2.30	0.48
1:A:2333:G:HO2'	6:H:129:THR:CG2	2.27	0.48
1:A:2340:A:H2	6:H:79:LEU:CG	2.25	0.48
8:K:10:LYS:C	8:K:11:LEU:HD12	2.34	0.48
1:A:1759:U:H3	1:A:1774:A:H62	1.61	0.48
33:0:406:GLN:NE2	33:0:492:GLY:O	2.32	0.48
33:0:522:ASP:CA	33:0:559:PRO:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:A:N3	1:A:2515:G:O2'	2.42	0.48
12:P:125:ALA:HB3	12:P:128:PHE:HE1	1.79	0.48
1:A:1853:G:OP2	3:E:53:HIS:ND1	2.46	0.48
3:E:141:VAL:CG1	3:E:190:ALA:HB1	2.44	0.48
1:A:527:A:O2'	21:Y:42:LYS:O	2.32	0.48
1:A:2688:G:O2'	1:A:2690:G:N7	2.35	0.48
5:G:112:SER:O	5:G:115:SER:OG	2.23	0.48
8:K:18:ALA:HB3	8:K:43:ASN:ND2	2.28	0.48
1:A:965:A:N3	2:B:78:U:O2'	2.46	0.47
3:E:15:GLY:O	3:E:204:ASN:ND2	2.46	0.47
33:O:133:ASP:OD1	33:O:134:ALA:N	2.47	0.47
1:A:1516:A:N7	1:A:1569:A:N1	2.62	0.47
1:A:64:A:H61	1:A:90:A:H61	1.62	0.47
1:A:1475:G:HO2'	1:A:1476:C:H6	1.60	0.47
1:A:27:G:N2	1:A:558:G:O2'	2.47	0.47
1:A:2898:A:O2'	1:A:2899:C:OP1	2.28	0.47
15:S:63:LEU:O	15:S:76:LYS:NZ	2.37	0.47
17:U:90:VAL:HG23	17:U:91:ASN:H	1.79	0.47
7:I:64:ALA:O	7:I:68:THR:HG23	2.15	0.47
1:A:461:C:O2	1:A:1893:U:O2'	2.30	0.47
1:A:1417:A:O2'	1:A:1418:U:OP2	2.25	0.47
1:A:1574:G:N1	1:A:1592:A:OP2	2.43	0.47
1:A:2333:G:HO2'	6:H:129:THR:HG22	1.80	0.47
1:A:2335:U:H2'	1:A:2336:G:C4	2.49	0.47
6:H:135:GLN:HG2	6:H:141:ILE:HG21	1.96	0.47
10:N:108:GLY:O	10:N:112:LYS:NZ	2.48	0.47
16:T:34:GLU:OE2	16:T:39:ARG:NH2	2.48	0.47
1:A:177:G:HO2'	1:A:178:A:P	2.36	0.47
1:A:1846:G:OP2	3:E:156:ARG:NH2	2.44	0.47
1:A:2593:A:OP1	1:A:2677:G:O2'	2.29	0.47
9:L:14:GLU:O	9:L:17:SER:OG	2.21	0.47
1:A:1092:A:N3	9:L:62:ARG:NH1	2.63	0.47
1:A:1252:G:O2'	1:A:1253:A:OP2	2.33	0.47
14:R:18:ARG:O	14:R:21:THR:OG1	2.30	0.47
1:A:1645:C:OP1	20:X:77:ARG:NH1	2.48	0.46
32:1:67:THR:O	32:1:67:THR:HG23	2.16	0.46
1:A:2340:A:C2	6:H:77:PHE:HB3	2.51	0.46
1:A:2823:C:O2'	1:A:2824:G:O4'	2.25	0.46
17:U:97:ASP:OD1	17:U:101:ASN:ND2	2.49	0.46
1:A:312:G:C2	1:A:405:U:O4	2.68	0.46
19:W:58:ALA:O	19:W:63:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2063:U:HO2'	1:A:2064:G:P	2.39	0.46
1:A:2334:U:C4	6:H:151:GLY:CA	2.66	0.46
11:O:113:LYS:O	11:O:117:LEU:HD23	2.16	0.46
17:U:102:ASP:OD2	18:V:2:TYR:OH	2.28	0.46
22:2:44:A:H5''	33:0:286:ARG:NH2	2.17	0.46
1:A:1698:G:O6	14:R:7:GLY:N	2.44	0.46
11:O:87:ILE:HD13	11:O:90:ASP:H	1.81	0.46
21:Y:85:VAL:HG13	21:Y:88:GLY:O	2.15	0.46
33:0:240:ILE:HG23	33:0:240:ILE:O	2.16	0.46
1:A:523:G:N1	1:A:526:A:OP2	2.45	0.46
1:A:2334:U:OP2	6:H:131:GLY:N	2.49	0.46
4:F:15:VAL:O	4:F:23:ILE:N	2.49	0.46
14:R:17:LEU:O	14:R:21:THR:HG23	2.15	0.46
33:0:21:GLY:N	33:0:88:ILE:O	2.44	0.46
8:K:78:LEU:HD13	8:K:108:ILE:HG23	1.98	0.46
1:A:1036:A:HO2'	1:A:1037:C:P	2.33	0.46
17:U:88:ILE:HG22	17:U:88:ILE:O	2.15	0.46
1:A:273:A:OP2	1:A:297:G:N2	2.42	0.45
1:A:2080:A:N6	1:A:2643:A:O2'	2.45	0.45
4:F:111:THR:OG1	4:F:170:THR:HG22	2.16	0.45
6:H:80:ARG:NE	22:2:56:C:C4	2.84	0.45
9:L:34:ASN:O	9:L:38:VAL:HG23	2.16	0.45
33:0:246:VAL:O	33:0:246:VAL:HG13	2.16	0.45
9:L:82:ILE:HD12	9:L:84:PHE:CE2	2.51	0.45
12:P:86:ALA:O	12:P:89:THR:HG22	2.16	0.45
22:2:56:C:H2'	22:2:57:G:O4'	2.17	0.45
1:A:610:U:OP1	18:V:81:ASN:ND2	2.47	0.45
8:K:73:PRO:CG	8:K:78:LEU:HD21	2.46	0.45
22:2:7:U:H3'	22:2:8:U:H5'	1.98	0.45
22:2:42:G:O3'	33:0:32:LYS:NZ	2.50	0.45
1:A:287:G:H21	1:A:288:C:H42	1.63	0.45
1:A:1542:A:N3	1:A:1625:C:O2'	2.49	0.45
4:F:28:ILE:HD12	4:F:188:ILE:HD12	1.99	0.45
1:A:187:C:HO2'	1:A:188:C:H6	1.64	0.45
1:A:1485:A:H2	1:A:1600:G:H21	1.65	0.45
1:A:2703:G:H4'	11:O:30:ARG:HE	1.81	0.45
4:F:40:THR:OG1	4:F:43:ASN:OD1	2.31	0.45
6:H:12:ILE:HD11	6:H:173:VAL:HG12	1.98	0.45
19:W:50:VAL:HG13	19:W:105:ILE:HD12	1.98	0.45
33:0:348:VAL:O	33:0:359:ILE:N	2.41	0.45
1:A:747:G:O2'	1:A:1677:A:N3	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1895:A:N6	1:A:1904:G:O2'	2.49	0.45
3:E:162:ALA:HB1	3:E:175:ARG:O	2.17	0.45
19:W:22:ASP:OD1	19:W:25:ARG:NH1	2.46	0.45
1:A:64:A:H61	1:A:90:A:N6	2.14	0.45
1:A:2341:U:H5'	6:H:85:ILE:HD12	1.94	0.45
6:H:125:ARG:HG3	15:S:1:MET:CG	2.44	0.45
1:A:2053:C:O2'	1:A:2054:C:O5'	2.34	0.45
4:F:48:ALA:HB1	4:F:83:LEU:O	2.17	0.45
8:K:73:PRO:HG2	8:K:78:LEU:HD21	1.99	0.45
1:A:569:C:O2	1:A:598:U:O2'	2.34	0.44
4:F:206:VAL:O	4:F:206:VAL:HG13	2.16	0.44
9:L:28:VAL:HG12	9:L:108:ILE:HA	1.98	0.44
11:O:24:VAL:HG11	11:O:33:ALA:HB2	1.99	0.44
33:O:171:ILE:N	33:O:199:HIS:O	2.50	0.44
1:A:2063:U:O2'	1:A:2064:G:O5'	2.33	0.44
1:A:2252:A:OP1	3:E:170:LYS:NZ	2.45	0.44
1:A:2344:U:H4'	1:A:2345:U:OP1	2.17	0.44
13:Q:44:ASN:OD1	13:Q:45:ARG:N	2.50	0.44
33:O:525:SER:O	33:O:527:PRO:CD	2.64	0.44
1:A:1968:U:OP1	1:A:2633:U:O2'	2.33	0.44
3:E:35:ALA:O	3:E:62:TYR:N	2.51	0.44
4:F:134:SER:OG	4:F:135:HIS:N	2.50	0.44
7:I:166:GLU:OE1	7:I:166:GLU:N	2.42	0.44
22:2:47:U:O2'	22:2:50:G:OP1	2.33	0.44
1:A:1849:U:OP1	3:E:177:ASN:ND2	2.50	0.44
1:A:2344:U:H2'	1:A:2345:U:C6	2.52	0.44
22:2:38:C:H2'	22:2:39:G:C8	2.52	0.44
1:A:1699:A:N6	1:A:2035:C:O4'	2.48	0.44
9:L:108:ILE:HG22	9:L:108:ILE:O	2.18	0.44
33:O:7:PHE:HA	33:O:254:LEU:HD11	1.99	0.44
7:I:108:VAL:HG13	7:I:109:GLY:N	2.32	0.44
13:Q:72:LYS:O	13:Q:94:VAL:N	2.48	0.44
1:A:492:C:H2'	1:A:493:G:O4'	2.18	0.43
1:A:617:G:N2	1:A:2060:A:OP1	2.48	0.43
1:A:751:G:H2'	1:A:773:G:H22	1.82	0.43
1:A:2817:C:O2'	1:A:2834:A:N3	2.45	0.43
18:V:36:GLU:OE1	18:V:36:GLU:N	2.51	0.43
19:W:23:LEU:O	19:W:27:LYS:NZ	2.45	0.43
1:A:1163:U:H2'	1:A:1164:C:C6	2.53	0.43
1:A:2630:C:H5''	22:2:75:C:OP1	2.17	0.43
17:U:88:ILE:O	17:U:90:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:A:H62	1:A:979:U:H3	1.67	0.43
1:A:1783:C:OP1	16:T:94:ARG:NE	2.51	0.43
2:B:107:G:HO2'	2:B:108:C:H6	1.65	0.43
22:2:31:C:O2	33:0:125:ARG:CZ	2.50	0.43
1:A:1158:G:HO2'	1:A:1159:U:P	2.40	0.43
1:A:85:G:C6	1:A:98:U:N3	2.86	0.43
1:A:2688:G:OP2	7:I:159:LYS:NZ	2.47	0.43
16:T:71:GLU:OE1	16:T:101:ARG:NH1	2.51	0.43
14:R:26:ILE:O	14:R:82:LYS:NZ	2.51	0.43
12:P:125:ALA:HB3	12:P:128:PHE:CE1	2.54	0.43
14:R:85:SER:OG	14:R:86:ASP:N	2.52	0.43
22:2:57:G:C2'	22:2:58:A:H5'	2.48	0.43
3:E:157:SER:OG	3:E:158:ALA:N	2.52	0.43
10:N:96:ASN:O	10:N:127:ARG:NH2	2.47	0.43
33:0:242:ASN:HB3	33:0:266:ARG:HG2	2.00	0.43
1:A:2670:A:OP1	10:N:77:ARG:NH1	2.48	0.43
7:I:21:ASP:OD1	7:I:24:THR:OG1	2.31	0.43
22:2:69:C:H2'	22:2:70:U:C6	2.54	0.42
1:A:273:A:OP2	1:A:297:G:N1	2.49	0.42
1:A:1464:A:H2	1:A:1627:A:H62	1.67	0.42
1:A:2316:A:O2'	1:A:2317:A:O5'	2.34	0.42
3:E:264:ASN:OD1	3:E:265:LYS:N	2.51	0.42
1:A:354:A:OP1	21:Y:14:GLY:N	2.52	0.42
1:A:1058:U:O2	10:N:28:ARG:NH1	2.52	0.42
7:I:55:ARG:NH2	7:I:58:ASP:OD1	2.51	0.42
1:A:2337:G:C6	6:H:77:PHE:CE2	3.07	0.42
6:H:125:ARG:O	15:S:1:MET:HB2	2.20	0.42
33:0:409:GLN:HE22	33:0:493:SER:N	2.18	0.42
1:A:342:A:N1	1:A:366:A:O2'	2.47	0.42
1:A:2337:G:N3	6:H:77:PHE:HE1	2.14	0.42
7:I:38:PHE:CE2	7:I:73:LEU:HD21	2.55	0.42
10:N:6:MET:SD	10:N:6:MET:N	2.93	0.42
15:S:82:ALA:HA	15:S:118:LEU:HD11	2.02	0.42
1:A:1159:U:O2'	1:A:1160:G:OP2	2.30	0.42
1:A:2089:A:O2'	1:A:2090:G:OP2	2.37	0.42
11:O:24:VAL:CG1	11:O:33:ALA:HB2	2.49	0.42
1:A:1283:U:O2'	12:P:6:LEU:O	2.35	0.42
6:H:73:SER:CB	22:2:56:C:C1'	2.87	0.42
13:Q:28:HIS:O	13:Q:134:ARG:NH2	2.53	0.42
20:X:30:VAL:HG12	20:X:31:ASP:N	2.35	0.42
1:A:1046:A:OP2	1:A:1200:G:N1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1765:G:N2	1:A:1768:A:OP2	2.52	0.41
9:L:55:TYR:CE2	9:L:82:ILE:HD11	2.55	0.41
11:O:34:ASN:O	11:O:62:ILE:HG21	2.20	0.41
11:O:105:GLU:OE1	11:O:105:GLU:N	2.52	0.41
33:O:335:ASN:ND2	33:O:348:VAL:HG13	2.35	0.41
1:A:2888:C:P	16:T:91:LYS:HZ1	2.43	0.41
6:H:36:ILE:CG2	6:H:57:LEU:HD11	2.50	0.41
1:A:2343:A:H2'	1:A:2344:U:C6	2.55	0.41
5:G:167:ALA:HA	5:G:170:ILE:HD13	2.02	0.41
1:A:376:A:O2'	1:A:378:C:OP2	2.29	0.41
1:A:1452:C:H2'	1:A:1453:A:H8	1.84	0.41
1:A:2577:G:O2'	11:O:4:GLN:NE2	2.50	0.41
2:B:48:G:HO2'	2:B:49:G:P	2.42	0.41
17:U:26:GLY:O	17:U:29:HIS:ND1	2.53	0.41
20:X:84:THR:OG1	20:X:85:ALA:O	2.38	0.41
22:2:37:A:H2'	22:2:38:C:C6	2.56	0.41
1:A:1017:C:O2'	1:A:1029:A:N3	2.49	0.41
1:A:2341:U:H4'	6:H:68:THR:OG1	2.21	0.41
1:A:2466:C:HO2'	1:A:2628:G:HO2'	1.65	0.41
22:2:43:G:P	33:O:32:LYS:HZ2	2.43	0.41
1:A:939:G:O2'	1:A:940:G:O5'	2.38	0.41
1:A:1322:G:N1	1:A:1325:A:OP2	2.54	0.41
6:H:47:ALA:O	6:H:50:ILE:HG22	2.20	0.41
13:Q:12:GLU:O	13:Q:87:LYS:NZ	2.54	0.41
17:U:69:ALA:O	17:U:74:LEU:N	2.48	0.41
33:O:515:ALA:HB1	33:O:559:PRO:CD	2.35	0.41
1:A:221:G:H22	1:A:238:U:H4'	1.86	0.41
1:A:1681:U:O2'	1:A:1789:A:N3	2.48	0.41
1:A:2233:C:OP2	3:E:150:LYS:NZ	2.53	0.41
33:O:350:ASN:OD1	33:O:351:TYR:N	2.54	0.41
1:A:1366:C:O2'	14:R:108:ARG:NH1	2.45	0.41
1:A:1965:A:OP2	1:A:1991:C:N4	2.47	0.41
6:H:12:ILE:HG12	6:H:172:GLN:HB3	2.03	0.41
1:A:551:A:O2'	1:A:552:G:O5'	2.38	0.41
1:A:2875:A:OP2	1:A:2891:G:N1	2.49	0.41
2:B:35:C:O2	15:S:103:HIS:NE2	2.44	0.41
7:I:163:ILE:HD12	7:I:163:ILE:H	1.86	0.41
9:L:12:VAL:HG23	9:L:63:ALA:HB2	2.03	0.41
14:R:86:ASP:O	14:R:89:THR:OG1	2.34	0.41
33:O:46:GLN:N	33:O:46:GLN:OE1	2.53	0.41
33:O:139:ILE:HD13	33:O:156:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:0:522:ASP:HA	33:0:559:PRO:HG2	2.03	0.41
1:A:283:G:O6	1:A:287:G:N2	2.53	0.41
1:A:775:G:H3'	1:A:776:G:H5'	2.03	0.41
1:A:2774:C:H42	1:A:2788:G:H1	1.69	0.41
5:G:53:ASN:OD1	5:G:54:ARG:N	2.52	0.41
1:A:2667:G:HO2'	1:A:2668:A:H8	1.69	0.40
3:E:139:THR:N	3:E:163:GLN:OE1	2.54	0.40
7:I:81:SER:OG	7:I:82:LYS:N	2.54	0.40
1:A:1773:G:HO2'	1:A:1774:A:P	2.44	0.40
5:G:146:LEU:O	5:G:147:SER:OG	2.33	0.40
10:N:139:GLU:OE1	10:N:139:GLU:N	2.55	0.40
33:0:350:ASN:ND2	33:0:355:GLU:OE2	2.54	0.40
1:A:1164:C:H2'	1:A:1165:U:O4'	2.21	0.40
1:A:1691:A:O2'	1:A:1692:U:OP2	2.24	0.40
1:A:2713:U:OP2	16:T:51:ARG:NH1	2.54	0.40
7:I:51:LEU:HD13	7:I:52:THR:N	2.36	0.40
7:I:102:ASN:OD1	7:I:103:LYS:N	2.55	0.40
8:K:33:VAL:HG12	8:K:64:ARG:CG	2.52	0.40
9:L:26:ILE:HG21	9:L:96:LEU:HD13	2.03	0.40
11:O:103:ALA:HB1	11:O:105:GLU:OE1	2.20	0.40
13:Q:26:GLU:OE1	13:Q:26:GLU:N	2.55	0.40
14:R:85:SER:O	14:R:89:THR:HG23	2.22	0.40
15:S:80:LEU:HD21	15:S:84:ARG:CZ	2.51	0.40
9:L:119:THR:HG22	9:L:120:VAL:N	2.36	0.40
20:X:30:VAL:HG12	20:X:31:ASP:OD1	2.22	0.40
1:A:2855:G:OP1	4:F:78:ARG:NH2	2.55	0.40
6:H:8:TYR:HA	6:H:12:ILE:HD12	2.01	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	
3	E	270/277 (98%)	256 (95%)	12 (4%)	2 (1%)	19	54
4	F	204/209 (98%)	187 (92%)	17 (8%)	0	100	100
5	G	203/207 (98%)	184 (91%)	19 (9%)	0	100	100
6	H	174/179 (97%)	166 (95%)	8 (5%)	0	100	100
7	I	173/179 (97%)	153 (88%)	20 (12%)	0	100	100
8	K	130/141 (92%)	115 (88%)	15 (12%)	0	100	100
9	L	107/166 (64%)	106 (99%)	1 (1%)	0	100	100
10	N	140/145 (97%)	127 (91%)	13 (9%)	0	100	100
11	O	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
12	P	144/146 (99%)	136 (94%)	8 (6%)	0	100	100
13	Q	133/144 (92%)	117 (88%)	16 (12%)	0	100	100
14	R	117/120 (98%)	106 (91%)	11 (9%)	0	100	100
15	S	118/120 (98%)	105 (89%)	12 (10%)	1 (1%)	16	51
16	T	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
17	U	115/119 (97%)	106 (92%)	8 (7%)	1 (1%)	14	49
18	V	98/102 (96%)	80 (82%)	18 (18%)	0	100	100
19	W	107/113 (95%)	94 (88%)	13 (12%)	0	100	100
20	X	88/95 (93%)	83 (94%)	5 (6%)	0	100	100
21	Y	99/103 (96%)	84 (85%)	15 (15%)	0	100	100
23	a	79/94 (84%)	71 (90%)	8 (10%)	0	100	100
24	b	56/62 (90%)	50 (89%)	6 (11%)	0	100	100
25	c	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
26	d	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
27	f	51/59 (86%)	47 (92%)	4 (8%)	0	100	100
28	g	46/49 (94%)	41 (89%)	5 (11%)	0	100	100
29	h	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
30	i	62/66 (94%)	59 (95%)	3 (5%)	0	100	100
31	j	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
32	l	81/86 (94%)	79 (98%)	2 (2%)	0	100	100
33	o	518/599 (86%)	476 (92%)	39 (8%)	3 (1%)	22	57
All	All	3742/4023 (93%)	3428 (92%)	307 (8%)	7 (0%)	45	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	156	ARG
15	S	2	ILE
33	0	491	PRO
3	E	155	VAL
33	0	447	ASN
33	0	538	LYS
17	U	90	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	220/225 (98%)	220 (100%)	0	100	100
4	F	167/170 (98%)	167 (100%)	0	100	100
5	G	169/170 (99%)	168 (99%)	1 (1%)	84	92
6	H	151/154 (98%)	145 (96%)	6 (4%)	27	59
7	I	148/151 (98%)	148 (100%)	0	100	100
8	K	102/110 (93%)	102 (100%)	0	100	100
9	L	98/138 (71%)	97 (99%)	1 (1%)	73	87
10	N	120/123 (98%)	120 (100%)	0	100	100
11	O	101/101 (100%)	101 (100%)	0	100	100
12	P	110/110 (100%)	109 (99%)	1 (1%)	75	89
13	Q	109/116 (94%)	108 (99%)	1 (1%)	75	89
14	R	99/100 (99%)	98 (99%)	1 (1%)	73	87
15	S	93/93 (100%)	93 (100%)	0	100	100
16	T	100/100 (100%)	99 (99%)	1 (1%)	73	87
17	U	96/98 (98%)	95 (99%)	1 (1%)	73	87
18	V	83/84 (99%)	83 (100%)	0	100	100
19	W	90/93 (97%)	88 (98%)	2 (2%)	47	73
20	X	81/85 (95%)	81 (100%)	0	100	100
21	Y	85/87 (98%)	84 (99%)	1 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	a	63/74 (85%)	62 (98%)	1 (2%)	58	79
24	b	47/50 (94%)	47 (100%)	0	100	100
25	c	56/57 (98%)	56 (100%)	0	100	100
26	d	52/53 (98%)	52 (100%)	0	100	100
27	f	47/53 (89%)	46 (98%)	1 (2%)	48	74
28	g	46/47 (98%)	46 (100%)	0	100	100
29	h	39/39 (100%)	38 (97%)	1 (3%)	41	70
30	i	54/56 (96%)	54 (100%)	0	100	100
31	j	35/35 (100%)	35 (100%)	0	100	100
32	l	73/75 (97%)	72 (99%)	1 (1%)	62	82
33	o	374/527 (71%)	372 (100%)	2 (0%)	86	93
All	All	3108/3374 (92%)	3086 (99%)	22 (1%)	80	92

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	G	10	ASN
6	H	11	GLU
6	H	64	LYS
6	H	112	ARG
6	H	120	LYS
6	H	150	ARG
6	H	165	GLU
9	L	23	LYS
12	P	114	ASN
13	Q	60	ARG
14	R	75	ASN
16	T	1	MET
17	U	72	ASN
19	W	11	ARG
19	W	37	ASN
21	Y	89	LYS
23	a	22	ARG
27	f	7	ARG
29	h	28	ARG
32	l	63	LEU
33	o	116	ARG
33	o	154	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
17	U	101	ASN
21	Y	67	ASN
30	i	60	GLN
32	1	61	ASN
33	0	326	GLN
33	0	335	ASN
33	0	385	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2808/2926 (95%)	667 (23%)	61 (2%)
2	B	111/119 (93%)	30 (27%)	3 (2%)
22	2	67/76 (88%)	15 (22%)	3 (4%)
All	All	2986/3121 (95%)	712 (23%)	67 (2%)

All (712) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	23	G
1	A	26	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	46	C
1	A	55	G
1	A	61	A
1	A	62	C
1	A	63	G
1	A	71	A
1	A	74	U
1	A	75	G
1	A	76	C
1	A	77	U
1	A	78	U
1	A	79	C
1	A	80	G

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Mol	Chain	Res	Type
1	A	84	A
1	A	85	G
1	A	86	C
1	A	87	U
1	A	89	U
1	A	90	A
1	A	92	G
1	A	93	C
1	A	96	G
1	A	101	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	125	A
1	A	126	A
1	A	133	A
1	A	141	U
1	A	150	A
1	A	164	U
1	A	175	G
1	A	176	A
1	A	178	A
1	A	179	A
1	A	183	A
1	A	184	G
1	A	185	A
1	A	188	C
1	A	189	G
1	A	191	G
1	A	199	A
1	A	200	A
1	A	202	A
1	A	216	A
1	A	219	A
1	A	224	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	229	A
1	A	231	A
1	A	232	U
1	A	233	G

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Mol	Chain	Res	Type
1	A	234	C
1	A	235	G
1	A	236	A
1	A	244	A
1	A	251	G
1	A	252	C
1	A	253	G
1	A	258	A
1	A	266	U
1	A	267	C
1	A	270	C
1	A	275	A
1	A	283	G
1	A	284	C
1	A	286	U
1	A	287	G
1	A	288	C
1	A	290	U
1	A	291	C
1	A	298	U
1	A	301	U
1	A	302	A
1	A	309	U
1	A	310	C
1	A	314	A
1	A	321	U
1	A	329	A
1	A	345	A
1	A	346	G
1	A	348	U
1	A	349	C
1	A	360	C
1	A	367	G
1	A	368	G
1	A	373	A
1	A	374	A
1	A	375	C
1	A	379	C
1	A	387	C
1	A	394	U
1	A	402	U
1	A	405	U

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Mol	Chain	Res	Type
1	A	407	A
1	A	410	G
1	A	411	G
1	A	412	A
1	A	413	U
1	A	418	A
1	A	419	G
1	A	420	U
1	A	421	A
1	A	427	G
1	A	432	C
1	A	433	G
1	A	434	U
1	A	435	G
1	A	444	U
1	A	458	G
1	A	471	G
1	A	483	C
1	A	491	C
1	A	495	U
1	A	498	U
1	A	502	C
1	A	504	A
1	A	505	G
1	A	528	G
1	A	529	C
1	A	533	C
1	A	542	G
1	A	550	G
1	A	551	A
1	A	554	U
1	A	555	C
1	A	556	C
1	A	559	A
1	A	564	G
1	A	573	C
1	A	576	G
1	A	577	U
1	A	578	A
1	A	579	G
1	A	592	A
1	A	593	A

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Mol	Chain	Res	Type
1	A	594	C
1	A	595	G
1	A	599	G
1	A	607	G
1	A	615	U
1	A	617	G
1	A	618	A
1	A	619	A
1	A	631	G
1	A	646	A
1	A	647	A
1	A	648	G
1	A	649	G
1	A	658	A
1	A	659	A
1	A	662	U
1	A	667	A
1	A	673	A
1	A	677	A
1	A	683	A
1	A	690	A
1	A	691	U
1	A	700	U
1	A	701	G
1	A	702	A
1	A	733	U
1	A	752	A
1	A	764	C
1	A	765	A
1	A	777	C
1	A	787	C
1	A	788	G
1	A	792	G
1	A	794	U
1	A	795	G
1	A	804	G
1	A	810	G
1	A	811	A
1	A	812	G
1	A	822	G
1	A	829	A
1	A	830	A

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Mol	Chain	Res	Type
1	A	831	U
1	A	832	G
1	A	837	U
1	A	838	C
1	A	839	G
1	A	847	A
1	A	852	G
1	A	859	C
1	A	866	A
1	A	874	U
1	A	875	U
1	A	877	G
1	A	892	U
1	A	908	A
1	A	913	A
1	A	916	G
1	A	918	U
1	A	929	G
1	A	939	G
1	A	940	G
1	A	942	U
1	A	943	A
1	A	944	C
1	A	946	G
1	A	948	A
1	A	954	U
1	A	957	A
1	A	959	C
1	A	961	C
1	A	962	C
1	A	964	A
1	A	973	G
1	A	977	U
1	A	978	A
1	A	979	U
1	A	980	C
1	A	987	A
1	A	991	A
1	A	992	G
1	A	999	A
1	A	1003	A
1	A	1005	A

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Mol	Chain	Res	Type
1	A	1007	G
1	A	1019	A
1	A	1020	A
1	A	1029	A
1	A	1036	A
1	A	1037	C
1	A	1042	A
1	A	1051	C
1	A	1058	U
1	A	1059	A
1	A	1063	G
1	A	1067	A
1	A	1068	G
1	A	1069	U
1	A	1071	G
1	A	1073	A
1	A	1079	U
1	A	1081	U
1	A	1084	A
1	A	1085	G
1	A	1091	U
1	A	1092	A
1	A	1093	G
1	A	1102	G
1	A	1103	A
1	A	1108	G
1	A	1115	A
1	A	1116	A
1	A	1118	C
1	A	1119	A
1	A	1129	U
1	A	1130	A
1	A	1133	G
1	A	1134	A
1	A	1143	U
1	A	1147	U
1	A	1156	G
1	A	1157	A
1	A	1158	G
1	A	1159	U
1	A	1160	G
1	A	1161	A

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Mol	Chain	Res	Type
1	A	1162	C
1	A	1163	U
1	A	1173	A
1	A	1174	A
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1179	A
1	A	1181	C
1	A	1182	G
1	A	1185	G
1	A	1188	A
1	A	1189	A
1	A	1197	A
1	A	1201	A
1	A	1203	G
1	A	1209	G
1	A	1236	G
1	A	1251	U
1	A	1252	G
1	A	1259	G
1	A	1260	A
1	A	1278	G
1	A	1284	A
1	A	1293	A
1	A	1295	U
1	A	1296	G
1	A	1305	A
1	A	1306	G
1	A	1307	U
1	A	1311	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G
1	A	1319	G
1	A	1323	A
1	A	1333	C
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1343	C

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Mol	Chain	Res	Type
1	A	1346	A
1	A	1351	U
1	A	1352	U
1	A	1363	G
1	A	1364	C
1	A	1365	U
1	A	1366	C
1	A	1368	U
1	A	1370	C
1	A	1371	G
1	A	1372	C
1	A	1375	A
1	A	1376	G
1	A	1380	U
1	A	1384	C
1	A	1385	G
1	A	1388	A
1	A	1389	C
1	A	1391	U
1	A	1404	A
1	A	1417	A
1	A	1418	U
1	A	1424	A
1	A	1425	C
1	A	1426	A
1	A	1427	G
1	A	1428	G
1	A	1431	G
1	A	1434	A
1	A	1435	U
1	A	1436	U
1	A	1442	A
1	A	1448	U
1	A	1449	C
1	A	1451	U
1	A	1459	U
1	A	1460	G
1	A	1465	A
1	A	1466	U
1	A	1472	G
1	A	1473	A
1	A	1474	C

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Mol	Chain	Res	Type
1	A	1476	C
1	A	1481	G
1	A	1489	U
1	A	1490	A
1	A	1499	A
1	A	1500	U
1	A	1501	U
1	A	1502	G
1	A	1506	A
1	A	1507	U
1	A	1508	C
1	A	1516	A
1	A	1525	G
1	A	1526	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	G
1	A	1532	A
1	A	1533	A
1	A	1536	A
1	A	1539	C
1	A	1540	A
1	A	1542	A
1	A	1543	U
1	A	1545	C
1	A	1550	C
1	A	1551	C
1	A	1553	A
1	A	1556	A
1	A	1558	G
1	A	1559	C
1	A	1560	U
1	A	1561	G
1	A	1566	G
1	A	1568	G
1	A	1569	A
1	A	1570	U
1	A	1571	G
1	A	1576	G
1	A	1577	C

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Mol	Chain	Res	Type
1	A	1595	U
1	A	1602	U
1	A	1608	A
1	A	1614	A
1	A	1615	A
1	A	1617	A
1	A	1626	U
1	A	1632	G
1	A	1652	C
1	A	1653	A
1	A	1655	A
1	A	1661	A
1	A	1672	A
1	A	1684	U
1	A	1685	A
1	A	1692	U
1	A	1693	C
1	A	1696	G
1	A	1697	A
1	A	1699	A
1	A	1700	A
1	A	1705	C
1	A	1708	U
1	A	1710	A
1	A	1712	G
1	A	1713	A
1	A	1719	G
1	A	1738	U
1	A	1743	A
1	A	1745	A
1	A	1748	G
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1761	G
1	A	1762	G
1	A	1766	C
1	A	1767	A
1	A	1768	A
1	A	1771	C
1	A	1776	A

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Mol	Chain	Res	Type
1	A	1778	A
1	A	1779	G
1	A	1782	G
1	A	1785	G
1	A	1793	G
1	A	1802	A
1	A	1811	C
1	A	1812	A
1	A	1814	A
1	A	1820	A
1	A	1829	C
1	A	1830	G
1	A	1839	A
1	A	1841	G
1	A	1845	A
1	A	1846	G
1	A	1864	G
1	A	1865	C
1	A	1867	C
1	A	1872	C
1	A	1877	A
1	A	1882	A
1	A	1883	A
1	A	1884	G
1	A	1885	A
1	A	1887	G
1	A	1891	G
1	A	1898	G
1	A	1899	U
1	A	1904	G
1	A	1935	G
1	A	1948	A
1	A	1958	G
1	A	1959	G
1	A	1960	U
1	A	1967	A
1	A	1968	U
1	A	1969	U
1	A	1972	U
1	A	1973	U
1	A	1984	U
1	A	1989	A

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Mol	Chain	Res	Type
1	A	1993	G
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2020	U
1	A	2022	U
1	A	2025	C
1	A	2026	A
1	A	2049	A
1	A	2051	U
1	A	2052	A
1	A	2054	C
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2064	G
1	A	2072	C
1	A	2078	A
1	A	2081	G
1	A	2084	C
1	A	2085	G
1	A	2089	A
1	A	2090	G
1	A	2098	G
1	A	2109	G
1	A	2121	U
1	A	2123	A
1	A	2125	U
1	A	2128	U
1	A	2129	G
1	A	2219	G
1	A	2227	A
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2240	U
1	A	2245	G
1	A	2246	G
1	A	2249	G
1	A	2252	A
1	A	2254	A

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Mol	Chain	Res	Type
1	A	2255	C
1	A	2267	G
1	A	2268	G
1	A	2280	G
1	A	2296	A
1	A	2308	G
1	A	2312	C
1	A	2315	A
1	A	2316	A
1	A	2317	A
1	A	2323	C
1	A	2325	U
1	A	2331	U
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2338	A
1	A	2339	A
1	A	2340	A
1	A	2341	U
1	A	2343	A
1	A	2345	U
1	A	2347	G
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2351	A
1	A	2354	G
1	A	2356	A
1	A	2363	C
1	A	2364	A
1	A	2374	G
1	A	2376	C
1	A	2379	C
1	A	2390	A
1	A	2401	G
1	A	2412	G
1	A	2414	C
1	A	2415	U
1	A	2417	A
1	A	2420	G

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Mol	Chain	Res	Type
1	A	2421	A
1	A	2425	G
1	A	2430	U
1	A	2431	U
1	A	2435	C
1	A	2451	C
1	A	2452	U
1	A	2453	C
1	A	2454	A
1	A	2455	A
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2474	G
1	A	2476	G
1	A	2477	A
1	A	2488	A
1	A	2505	A
1	A	2507	A
1	A	2509	C
1	A	2511	A
1	A	2520	U
1	A	2523	G
1	A	2527	C
1	A	2531	G
1	A	2532	A
1	A	2533	U
1	A	2534	G
1	A	2542	A
1	A	2547	A
1	A	2548	U
1	A	2549	C
1	A	2564	G
1	A	2583	U
1	A	2591	U
1	A	2595	A
1	A	2596	G
1	A	2598	G

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Mol	Chain	Res	Type
1	A	2601	A
1	A	2602	C
1	A	2607	G
1	A	2611	G
1	A	2613	U
1	A	2631	A
1	A	2632	G
1	A	2638	U
1	A	2639	C
1	A	2642	U
1	A	2644	U
1	A	2652	G
1	A	2659	G
1	A	2665	U
1	A	2674	G
1	A	2689	A
1	A	2690	G
1	A	2696	C
1	A	2711	G
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2743	G
1	A	2755	U
1	A	2762	A
1	A	2764	G
1	A	2765	G
1	A	2773	G
1	A	2779	A
1	A	2785	U
1	A	2789	C
1	A	2794	A
1	A	2798	C
1	A	2806	G
1	A	2807	A
1	A	2808	U
1	A	2818	C
1	A	2820	U
1	A	2823	C
1	A	2824	G
1	A	2826	A
1	A	2831	A

Continued on next page...

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Mol	Chain	Res	Type
1	A	2843	G
1	A	2859	G
1	A	2860	A
1	A	2868	G
1	A	2886	C
1	A	2892	G
1	A	2897	G
1	A	2899	C
1	A	2900	A
1	A	2901	G
1	A	2905	C
1	A	2911	G
1	A	2916	A
1	A	2917	G
1	A	2918	G
1	A	2925	C
2	B	10	G
2	B	13	A
2	B	15	C
2	B	19	G
2	B	22	G
2	B	23	U
2	B	24	C
2	B	32	U
2	B	33	U
2	B	35	C
2	B	38	U
2	B	39	A
2	B	40	C
2	B	48	G
2	B	49	G
2	B	50	A
2	B	53	U
2	B	54	U
2	B	55	A
2	B	56	A
2	B	62	U
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	97	A

Continued on next page...

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Mol	Chain	Res	Type
2	B	101	U
2	B	107	G
2	B	108	C
2	B	110	G
22	2	8	U
22	2	20	G
22	2	21	A
22	2	22	G
22	2	29	U
22	2	30	G
22	2	32	U
22	2	37	A
22	2	48	C
22	2	49	A
22	2	58	A
22	2	59	U
22	2	61	C
22	2	75	C
22	2	76	A

All (67) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	88	G
1	A	92	G
1	A	175	G
1	A	224	A
1	A	252	C
1	A	347	G
1	A	411	G
1	A	443	G
1	A	528	G
1	A	549	A
1	A	554	U
1	A	558	G
1	A	631	G
1	A	689	A
1	A	751	G
1	A	831	U
1	A	976	U
1	A	1036	A
1	A	1066	A

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Mol	Chain	Res	Type
1	A	1172	A
1	A	1250	G
1	A	1294	A
1	A	1305	A
1	A	1313	A
1	A	1339	A
1	A	1351	U
1	A	1435	U
1	A	1448	U
1	A	1507	U
1	A	1525	G
1	A	1530	G
1	A	1565	U
1	A	1567	U
1	A	1570	U
1	A	1631	A
1	A	1671	G
1	A	1691	A
1	A	1758	U
1	A	1784	A
1	A	1813	A
1	A	1828	G
1	A	1882	A
1	A	1883	A
1	A	1886	G
1	A	1947	A
1	A	2127	U
1	A	2254	A
1	A	2295	A
1	A	2316	A
1	A	2335	U
1	A	2336	G
1	A	2338	A
1	A	2344	U
1	A	2420	G
1	A	2452	U
1	A	2454	A
1	A	2468	A
1	A	2510	G
1	A	2631	A
1	A	2805	A
1	A	2904	A

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Mol	Chain	Res	Type
2	B	48	G
2	B	49	G
2	B	55	A
22	2	48	C
22	2	58	A
22	2	74	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

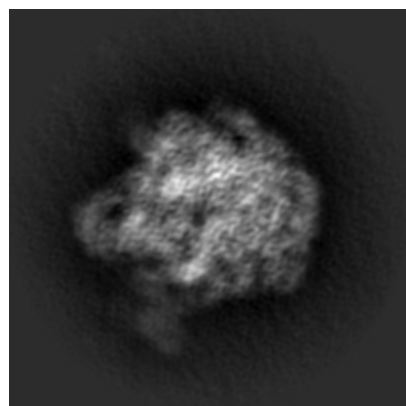
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13017. These allow visual inspection of the internal detail of the map and identification of artifacts.

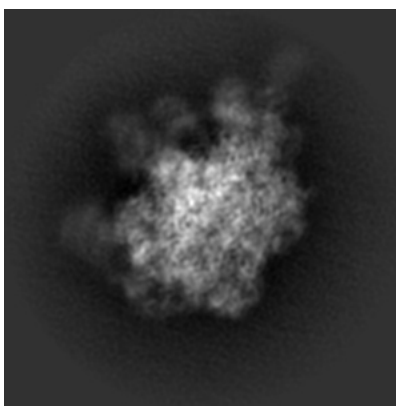
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

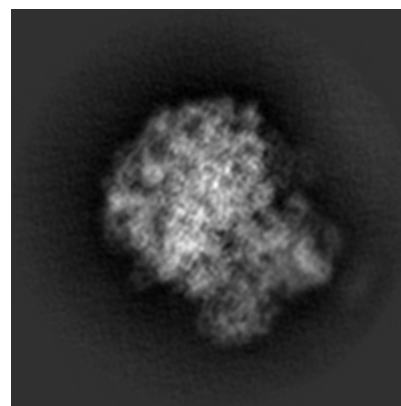
6.1.1 Primary map



X

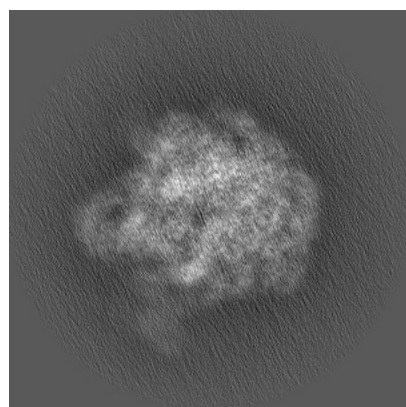


Y

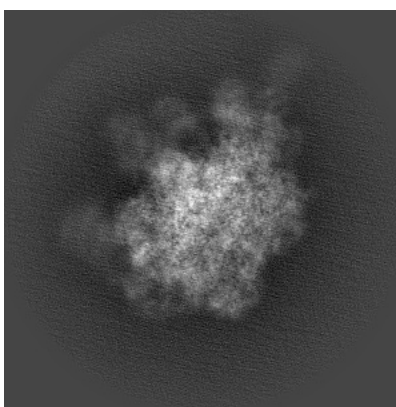


Z

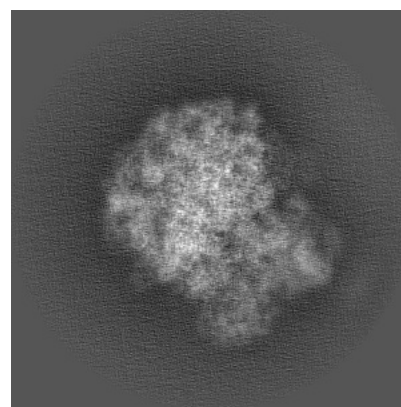
6.1.2 Raw map



X



Y

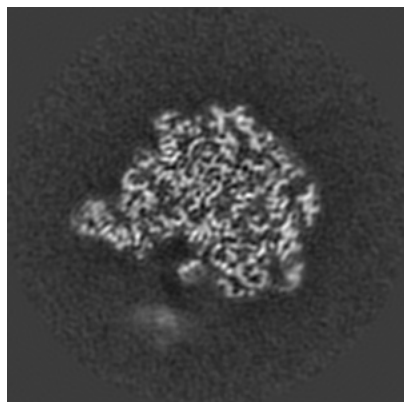


Z

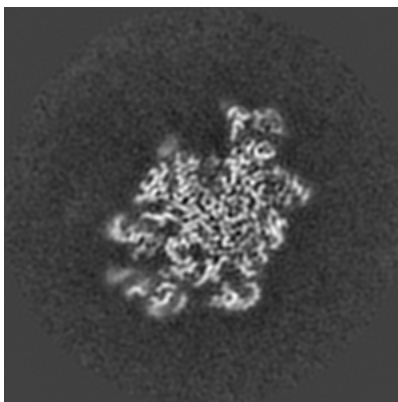
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

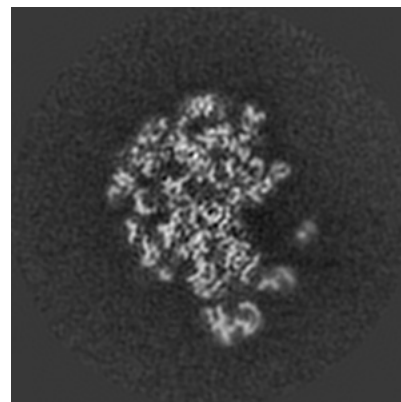
6.2.1 Primary map



X Index: 210

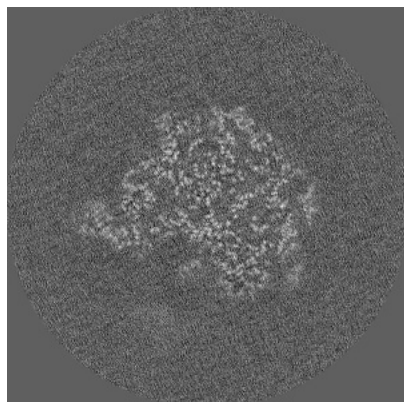


Y Index: 210

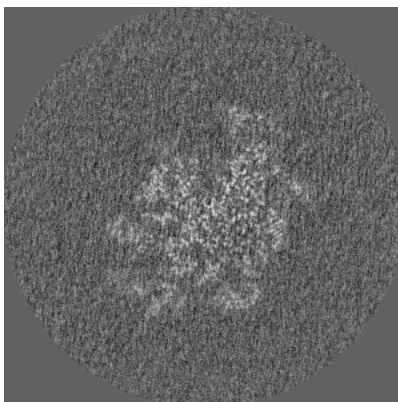


Z Index: 210

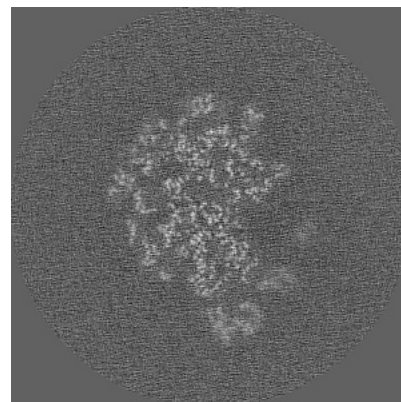
6.2.2 Raw map



X Index: 210



Y Index: 210

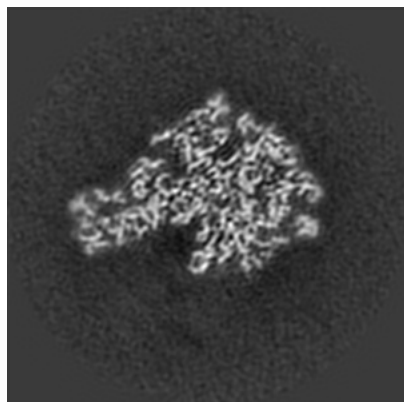


Z Index: 210

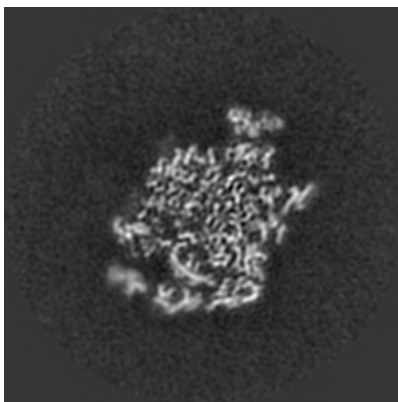
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

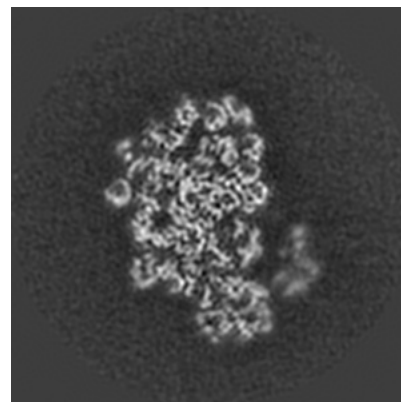
6.3.1 Primary map



X Index: 227

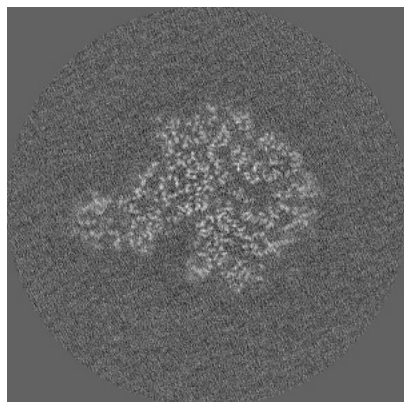


Y Index: 217

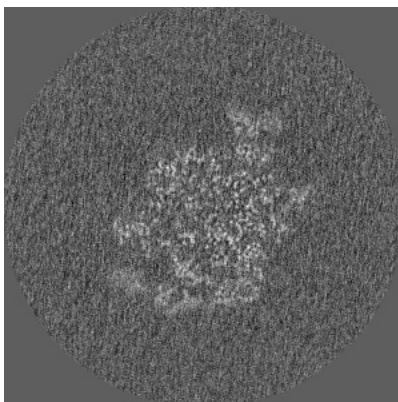


Z Index: 191

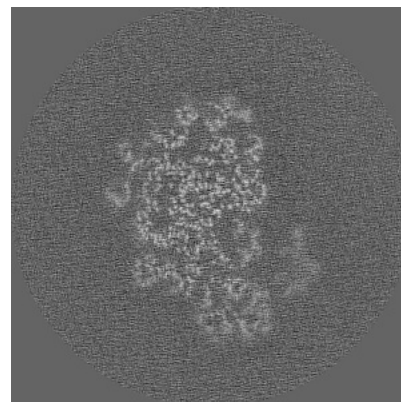
6.3.2 Raw map



X Index: 219



Y Index: 216

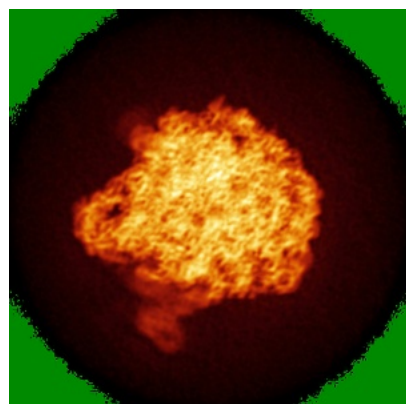


Z Index: 190

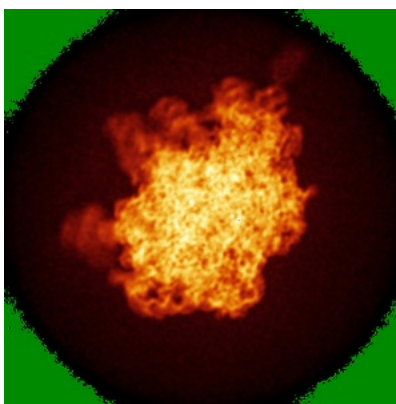
The images above show the largest variance slices of the map in three orthogonal directions.

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

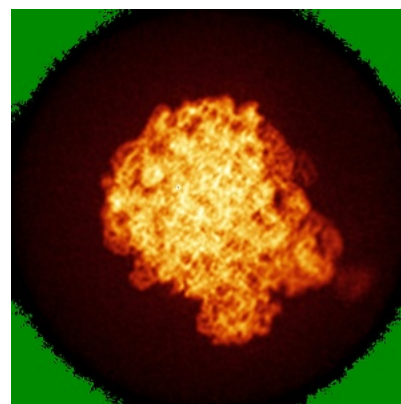
6.4.1 Primary map



X

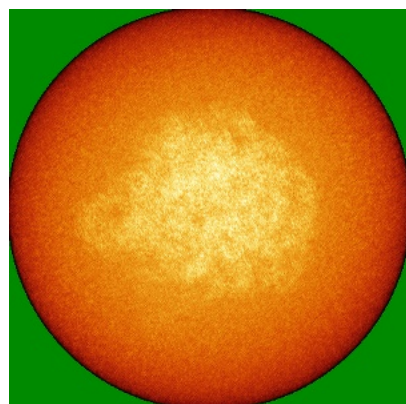


Y

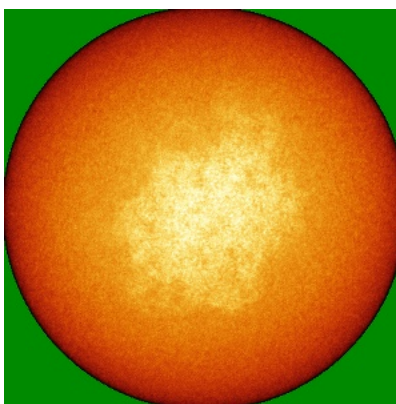


Z

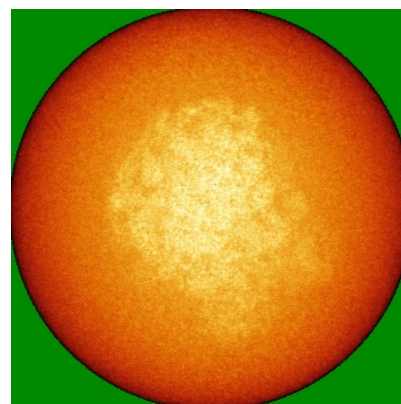
6.4.2 Raw map



X



Y

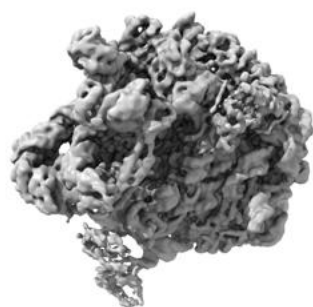


Z

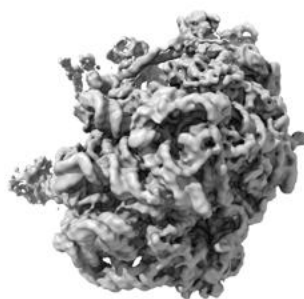
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



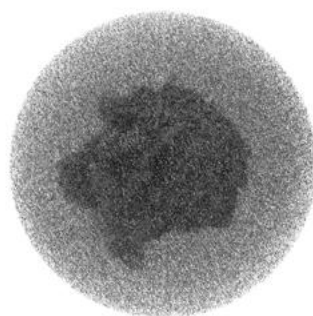
Y



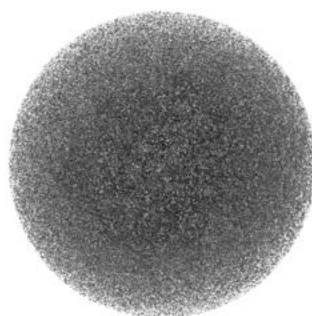
Z

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

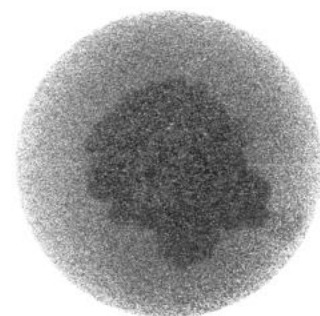
6.5.2 Raw map



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.

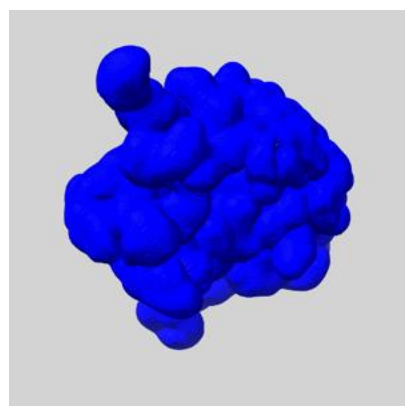
6.6 Mask visualisation [i](#)

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

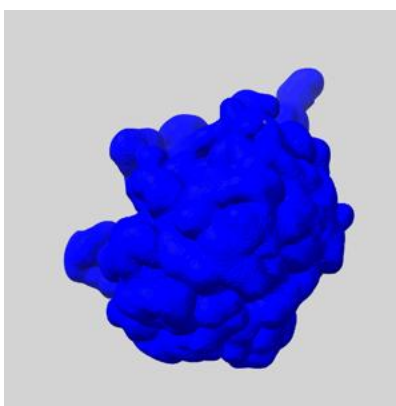
A mask typically either:

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

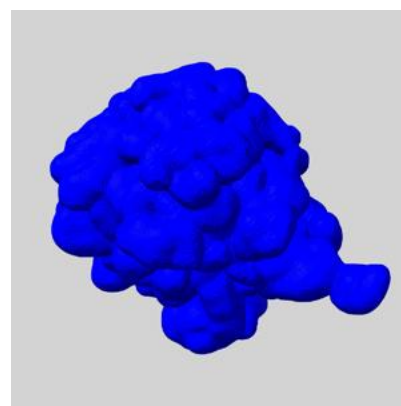
6.6.1 emd_13017_msk_1.map [i](#)



X



Y

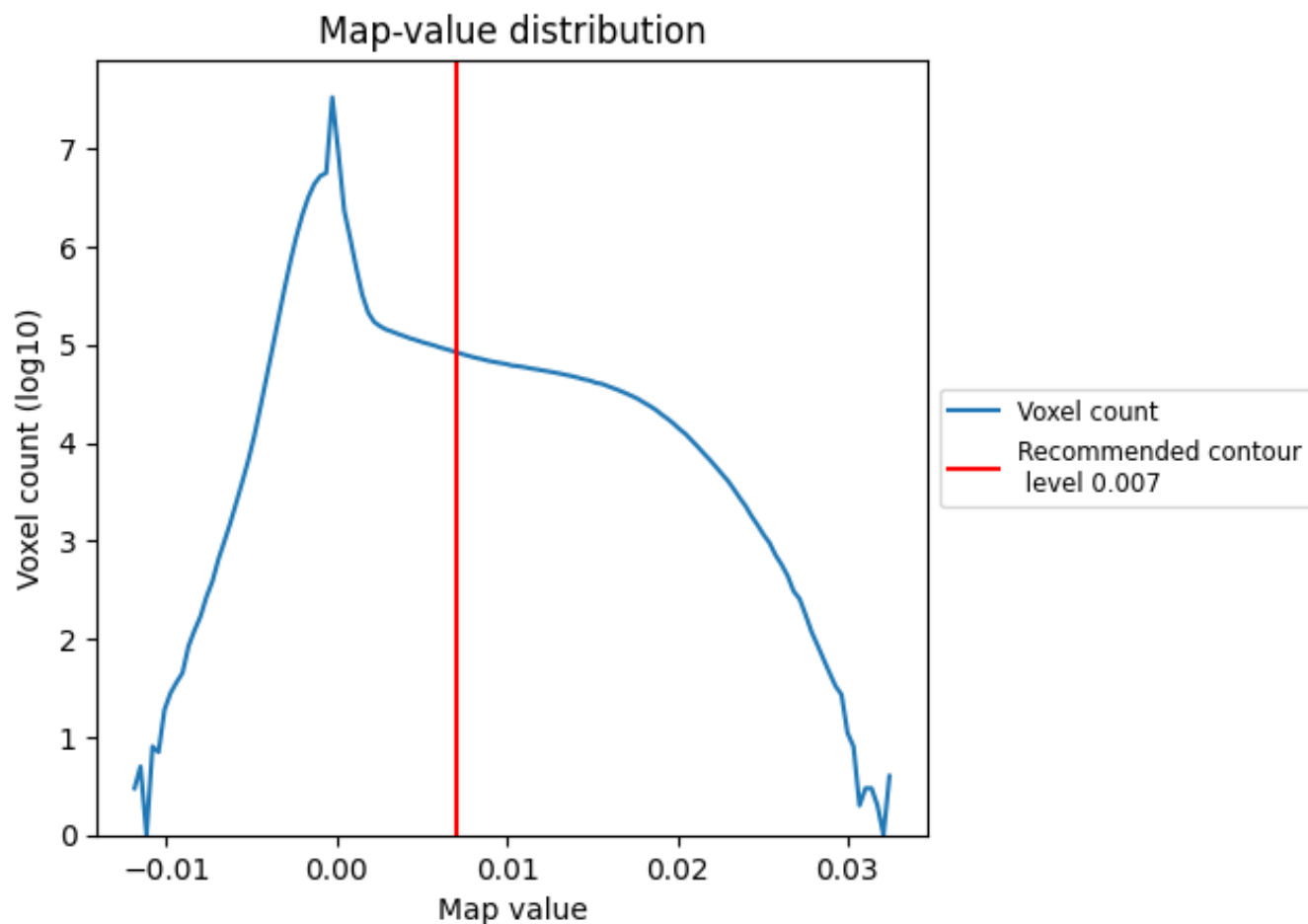


Z

7 Map analysis [i](#)

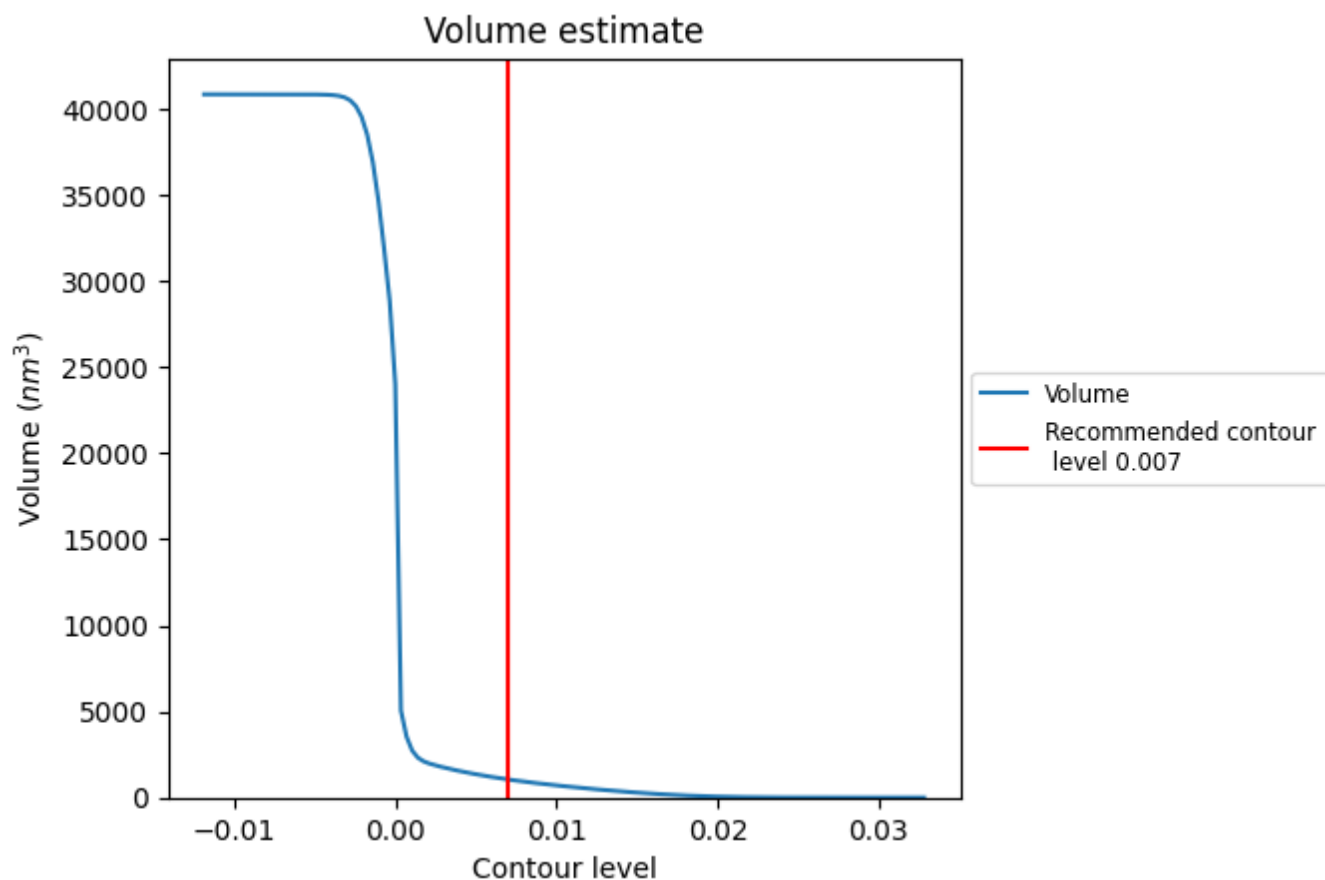
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

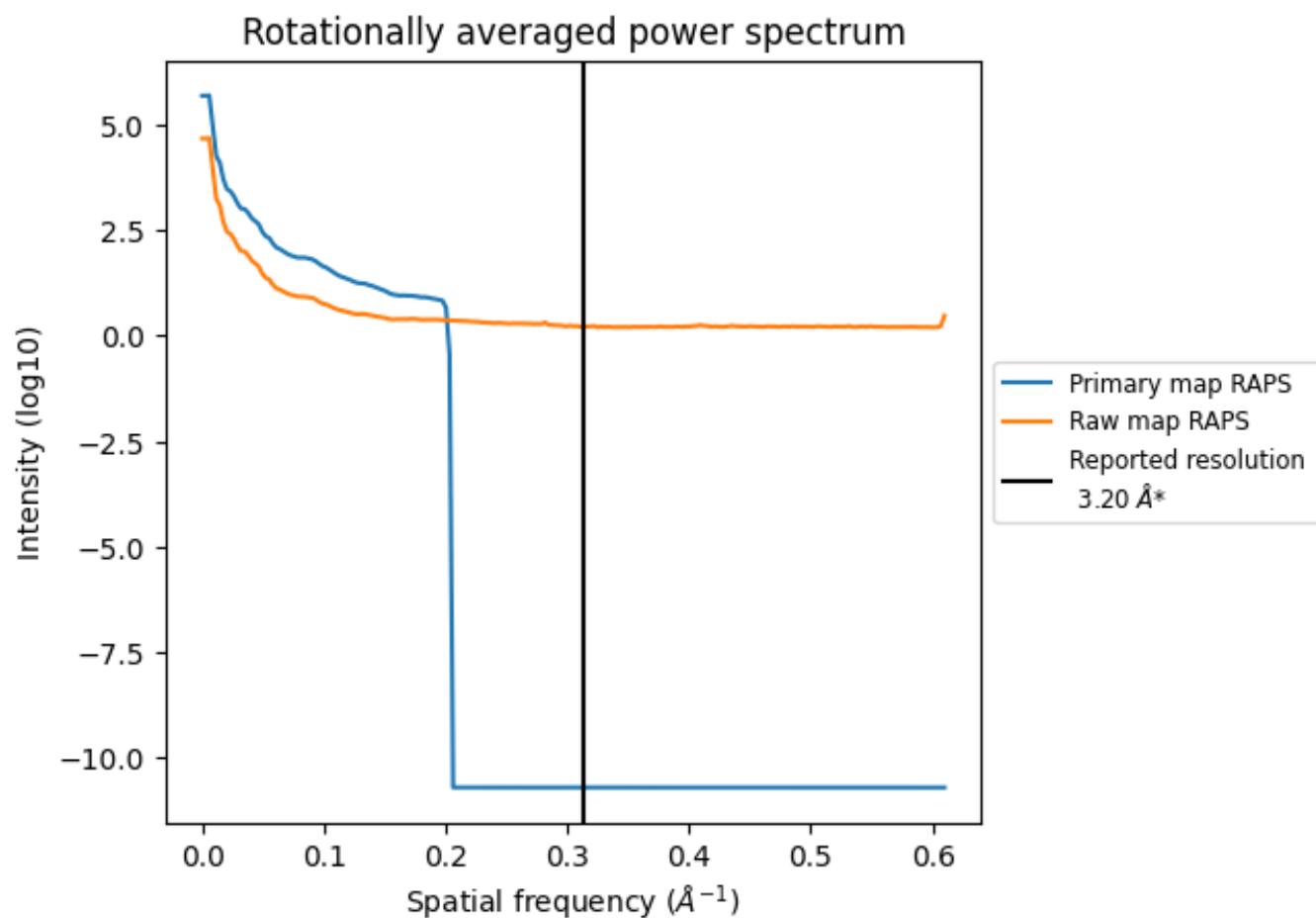
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1052 nm³; this corresponds to an approximate mass of 950 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

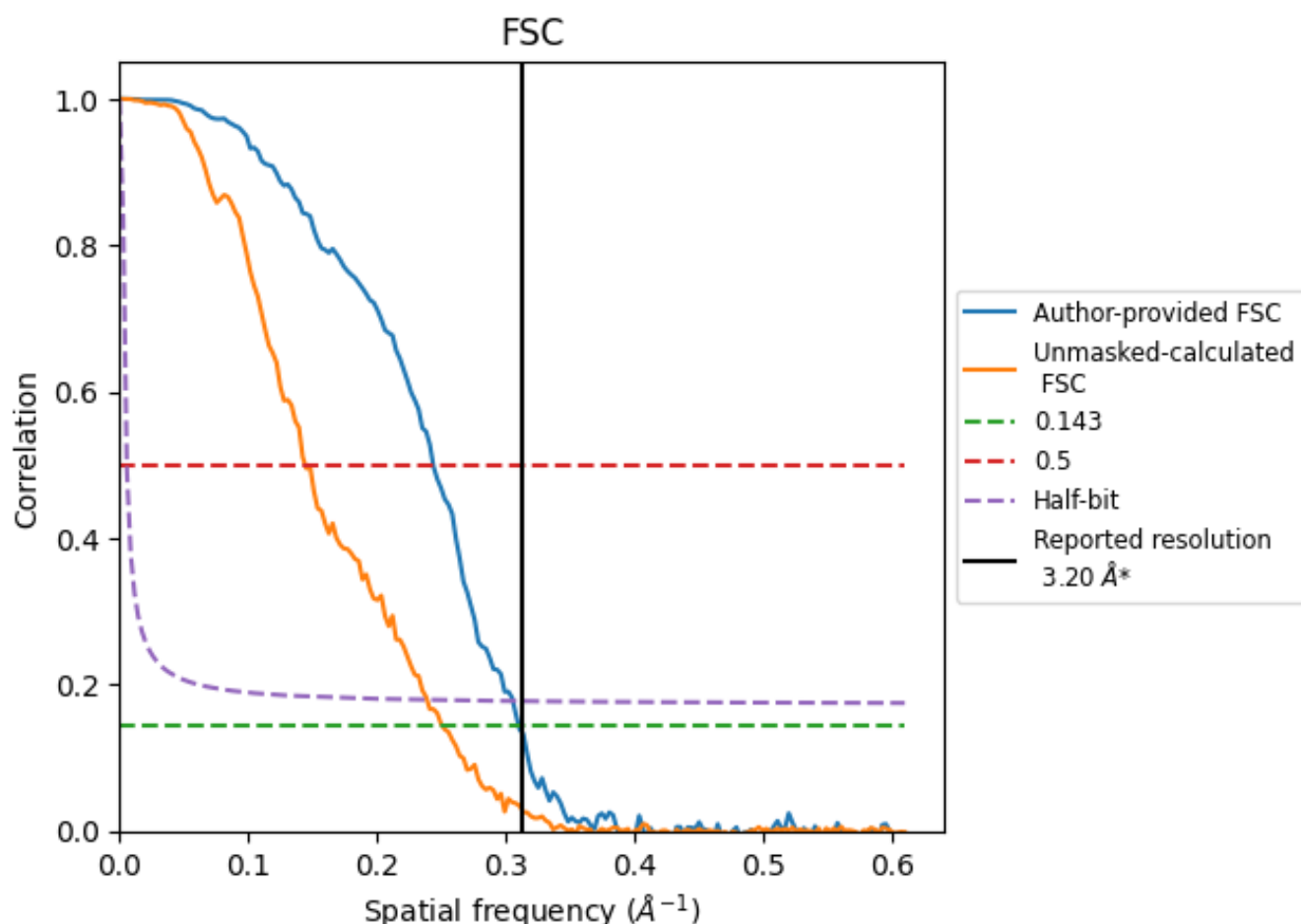


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

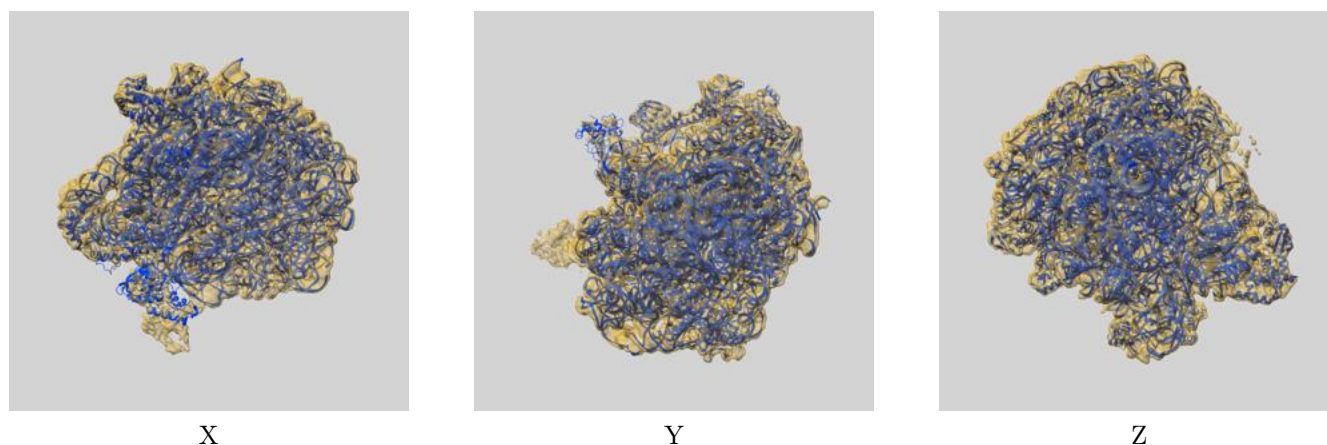
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	4.11	3.27
Unmasked-calculated*	3.99	6.93	4.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

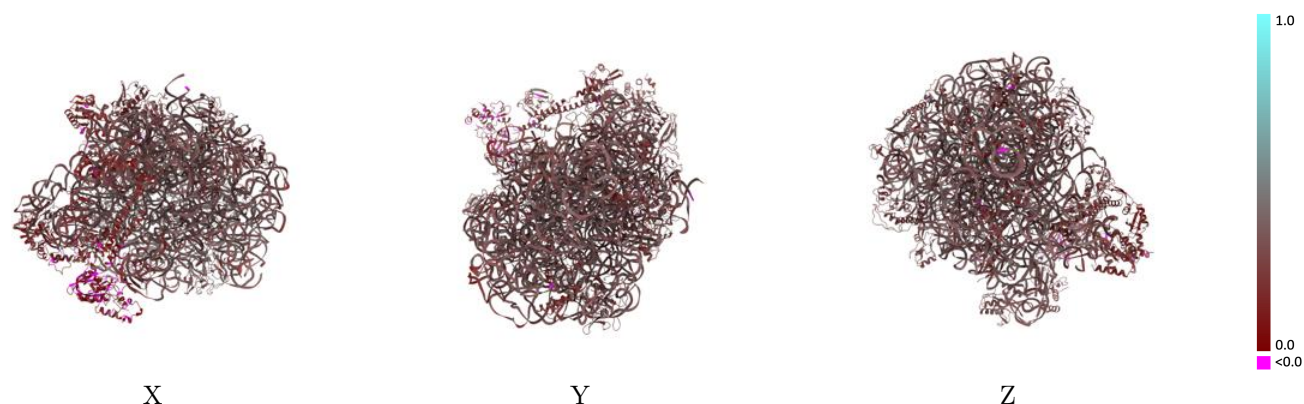
This section contains information regarding the fit between EMDB map EMD-13017 and PDB model 7OPE. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



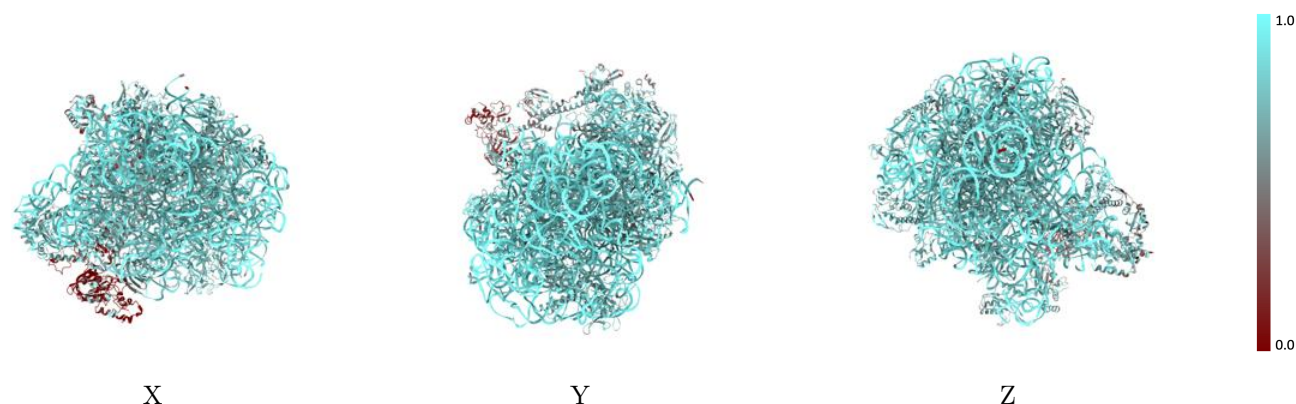
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



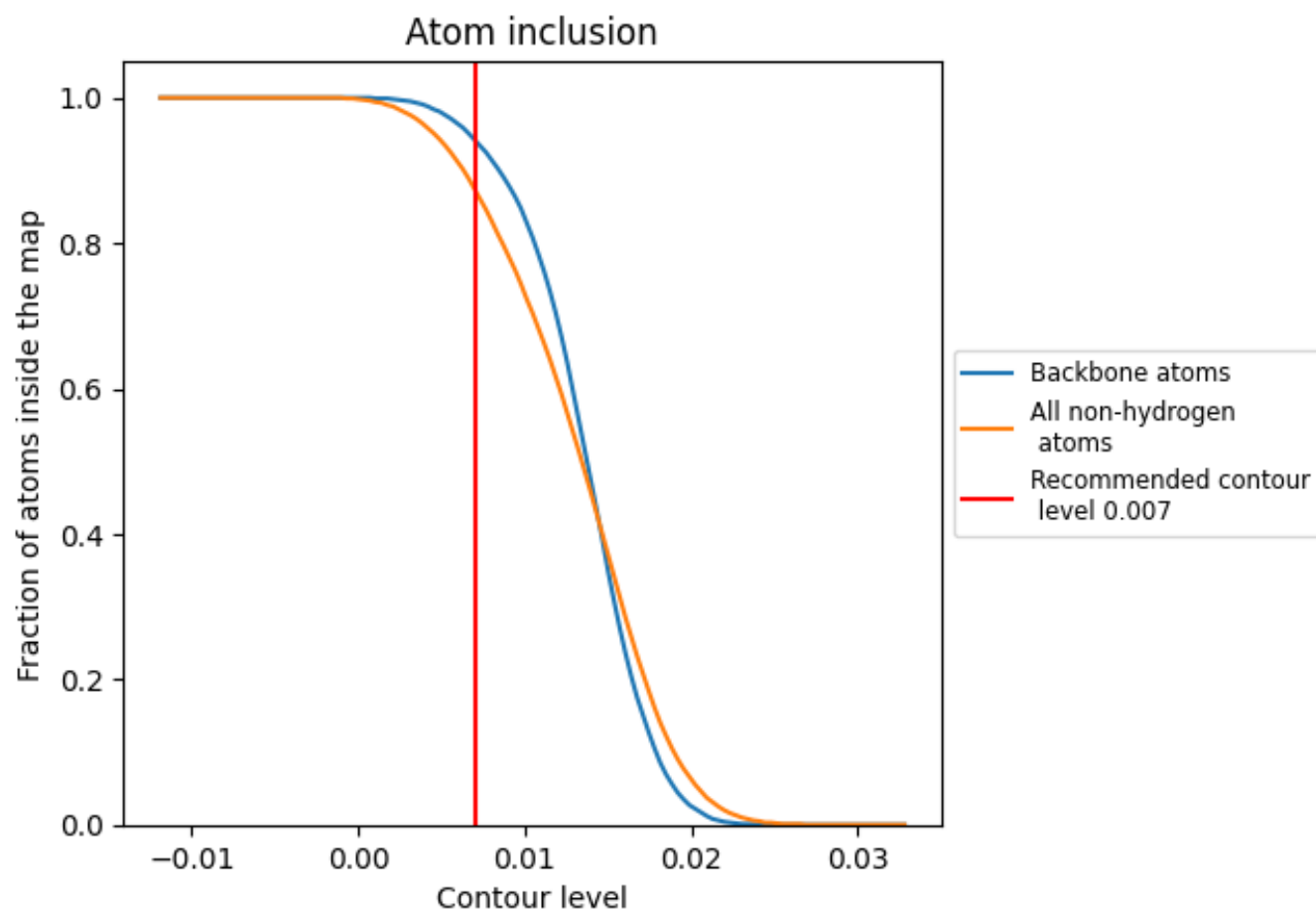
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.3090
0	 0.3380	 0.1470
1	 0.5730	 0.2490
2	 0.9180	 0.3030
A	 0.9630	 0.3310
B	 0.9770	 0.3290
E	 0.7650	 0.2990
F	 0.7350	 0.2990
G	 0.7550	 0.2890
H	 0.6420	 0.2020
I	 0.7560	 0.2910
K	 0.6790	 0.1940
L	 0.6440	 0.2150
N	 0.7420	 0.2950
O	 0.7020	 0.2860
P	 0.7450	 0.2870
Q	 0.7620	 0.3130
R	 0.7240	 0.2620
S	 0.7470	 0.2640
T	 0.6880	 0.2960
U	 0.7630	 0.2580
V	 0.7900	 0.3270
W	 0.7630	 0.3020
X	 0.7440	 0.3020
Y	 0.7590	 0.3050
a	 0.7530	 0.2880
b	 0.5440	 0.2640
c	 0.7410	 0.2410
d	 0.7470	 0.2760
f	 0.7800	 0.3020
g	 0.7910	 0.2860
h	 0.7510	 0.2770
i	 0.7460	 0.3070
j	 0.7530	 0.2990

