



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 05:24 PM UTC

PDB ID : 6N8M / pdb_00006n8m
EMDB ID : EMD-0372
Title : Cryo-EM structure of pre-Lsg1 (PL) pre-60S ribosomal subunit
Authors : Zhou, Y.; Musalgaonkar, S.; Johnson, A.W.; Taylor, D.W.
Deposited on : 2018-11-29
Resolution : 3.50 Å(reported)
Based on initial model : 5T62

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

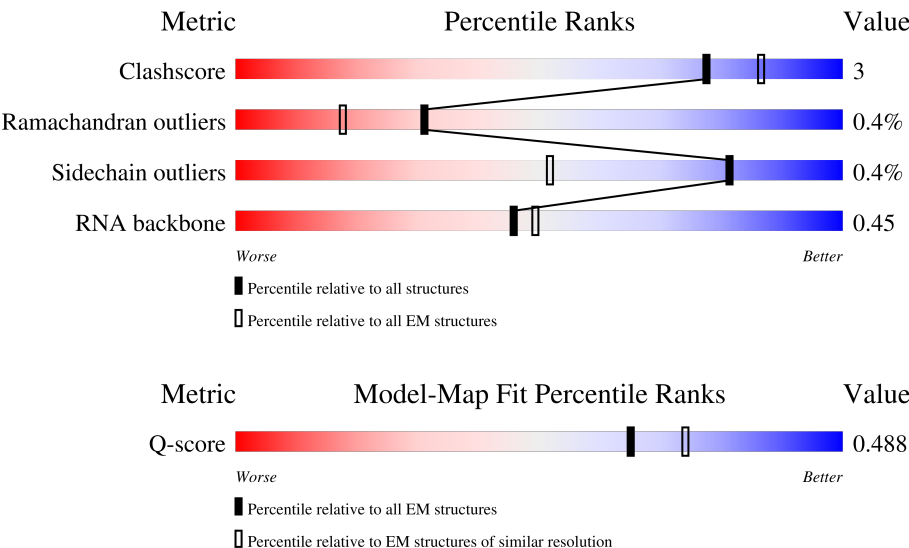
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



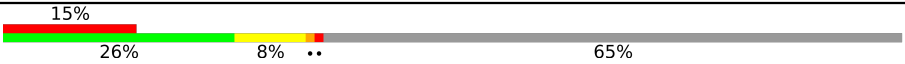
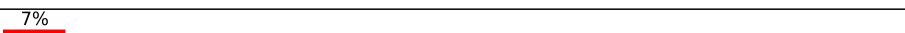
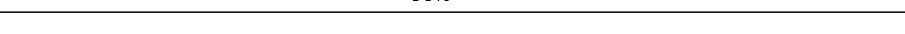
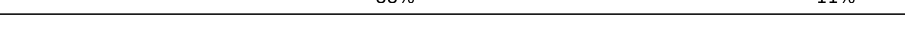
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	3396	
2	B	121	
3	C	158	

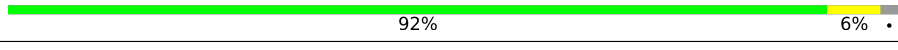
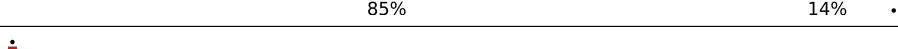
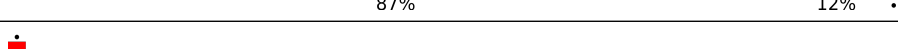
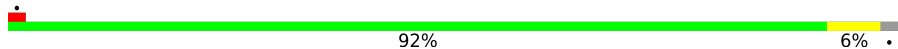
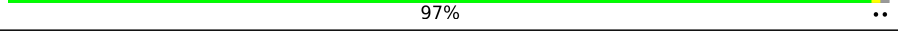
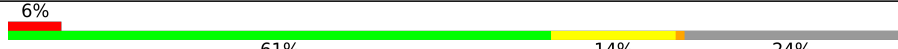
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Mol	Chain	Length	Quality of chain
4	Y	364	
5	D	254	
6	E	387	
7	F	362	
8	G	297	
9	H	176	
10	I	244	
11	J	256	
12	K	191	
13	M	174	
14	N	199	
15	O	138	
16	Q	106	
17	R	92	
18	S	217	
19	a	204	
20	b	199	
21	c	184	
22	d	186	
23	e	189	
24	f	172	
25	g	160	
26	h	121	
27	i	137	
28	j	155	

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Mol	Chain	Length	Quality of chain
29	k	142	
30	l	127	
31	m	136	
32	n	149	
33	o	59	
34	p	105	
35	q	113	
36	r	130	
37	s	107	
38	t	121	
39	u	120	
40	v	100	
41	w	88	
42	x	78	
43	y	51	
44	z	128	
45	V	518	
46	L	165	
47	X	245	

2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 128867 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 *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3203	Total	C	N	O	P	0	0
			68513	30603	12353	22354	3203		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a protein called Tyrosine-protein phosphatase YVH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	128	Total	C	N	O	S	0	0
			991	625	179	179	8		

- Molecule 5 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	246	Total	C	N	O	S	0	0
			1874	1168	380	325	1		

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	384	Total	C	N	O	S	0	0
			3059	1940	582	529	8		

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	282	Total	C	N	O	S	0	0
			2271	1435	395	439	2		

- Molecule 9 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	155	Total	C	N	O	S	0	0
			1217	785	220	211	1		

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	220	Total	C	N	O	S	0	0
			1770	1143	322	304	1		

- Molecule 11 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	227	Total	C	N	O	S	0	0
			1762	1128	315	316	3		

- Molecule 12 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	193	Total	C	N	O	0	0
			1539	959	314	266		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 16 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 17 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	88	Total	C	N	O	S	0	0
			673	416	135	116	6		

- Molecule 18 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 19 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 20 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 21 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 22 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 23 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	e	151	Total	C	N	O	0	0
			1219	757	258	204		

- Molecule 24 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	f	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 25 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	g	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 26 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	h	97	Total	C	N	O	0	0
			766	496	126	144		

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	132	Total	C	N	O	S	0	0
			981	617	184	173	7		

- Molecule 28 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	61	Total	C	N	O	S	0	0
			509	328	100	80	1		

- Molecule 29 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	k	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 30 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	125	Total	C	N	O		0	0
			984	620	191	173			

- Molecule 31 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 33 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 35 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	107	Total	C	N	O	S	0	0
			866	550	165	150	1		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	126	Total	C	N	O	S	0	0
			1012	641	204	166	1		

- Molecule 37 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 38 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 39 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 40 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	98	Total	C	N	O	S	0	0
			753	471	150	130	2		

- Molecule 41 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	x	77	Total	C	N	O	0	0
			608	388	114	106		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 44 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	51	Total	C	N	O	S	0	0
			408	253	84	66	5		

- Molecule 45 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	393	Total	C	N	O	S	0	0
			3065	1947	528	570	20		

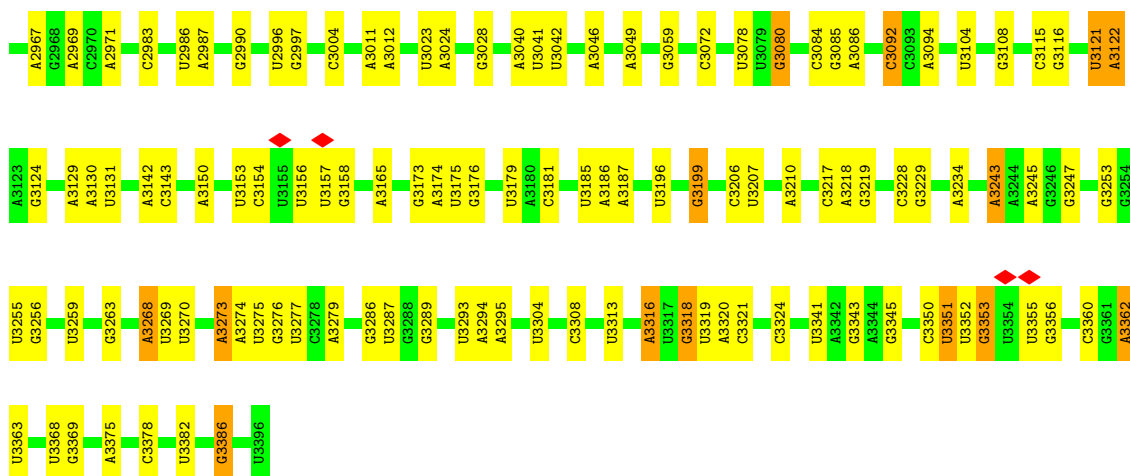
- Molecule 46 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	L	147	Total	C	N	O	0	0
			825	504	160	161		

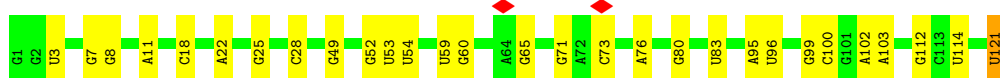
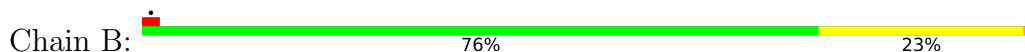
- Molecule 47 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	X	234	Total	C	N	O	S	0	0
			1710	1063	294	346	7		

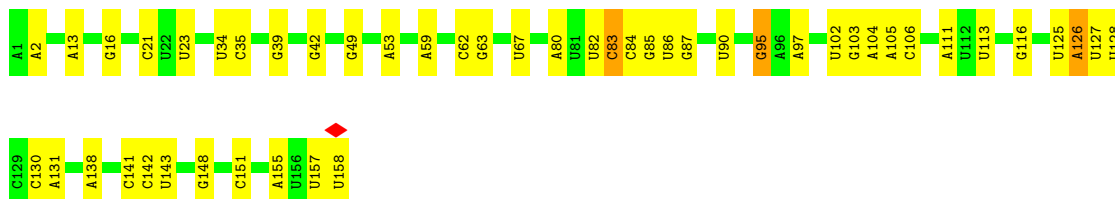




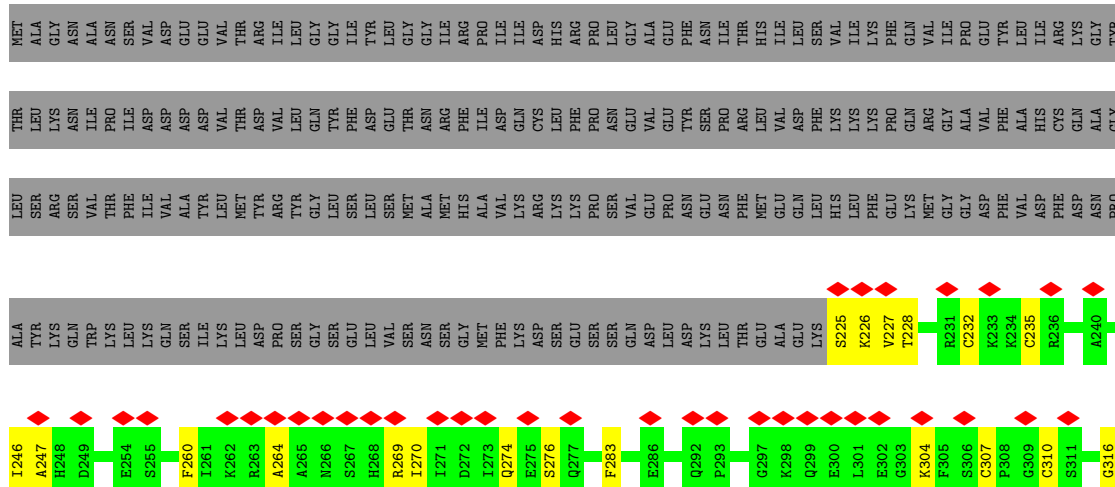
• Molecule 2: 5S rRNA

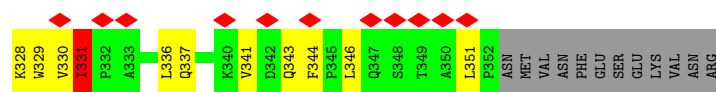


• Molecule 3: 5.8S RNA



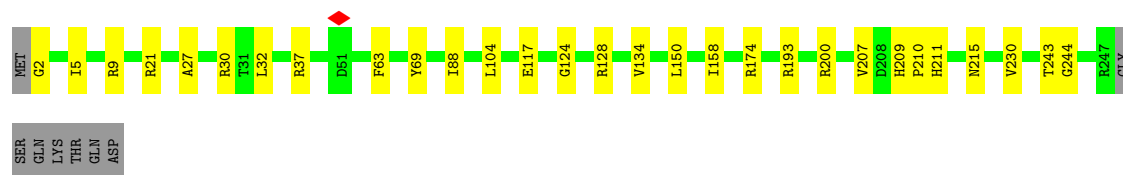
• Molecule 4: Tyrosine-protein phosphatase YVH1





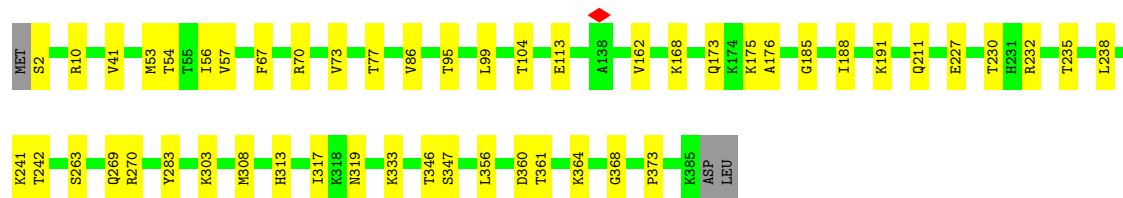
- Molecule 5: 60S ribosomal protein L2-A

Chain D: 85% 11% .



- Molecule 6: 60S ribosomal protein L3

Chain E: 86% 13% .



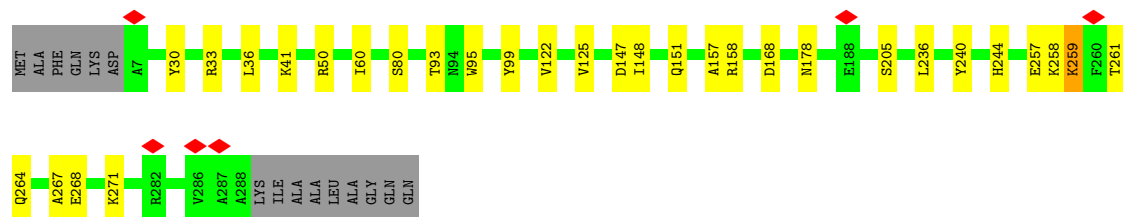
- Molecule 7: 60S ribosomal protein L4-A

Chain F: 88% 11% .



- Molecule 8: 60S ribosomal protein L5

Chain G: 85% 10% 5%



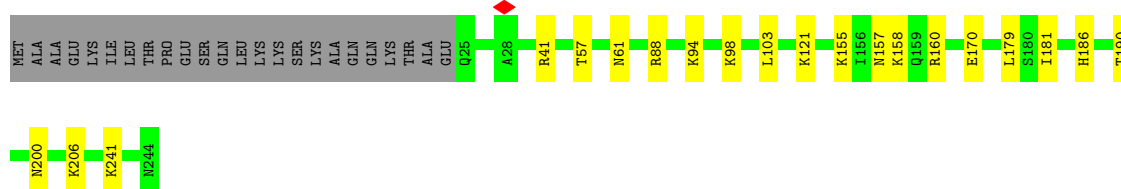
- Molecule 9: 60S ribosomal protein L6-A

Chain H: 78% 10% 12%



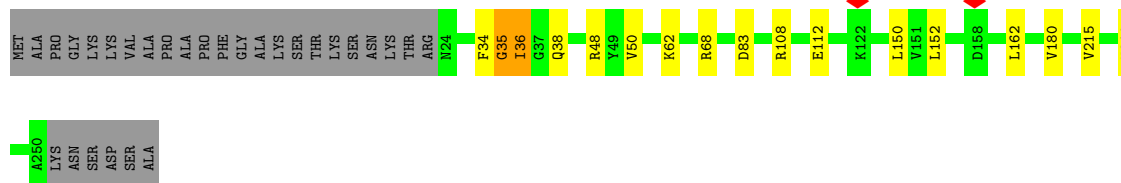
- Molecule 10: 60S ribosomal protein L7-A

Chain I: 82% 8% 10%



- Molecule 11: 60S ribosomal protein L8-A

Chain J: 82% 6% 11%



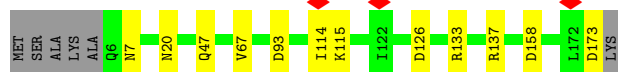
- Molecule 12: 60S ribosomal protein L9-A

Chain K: 88% 10% 2%



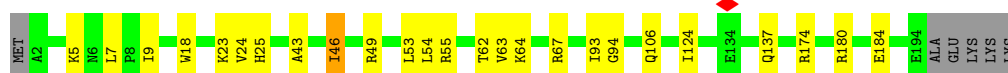
- Molecule 13: 60S ribosomal protein L11-A

Chain M: 90% 7% 3%



- Molecule 14: 60S ribosomal protein L13-A

Chain N: 84% 12% 4%

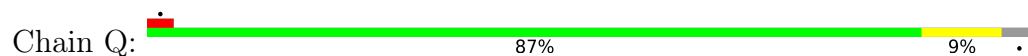


- Molecule 15: 60S ribosomal protein L14-A

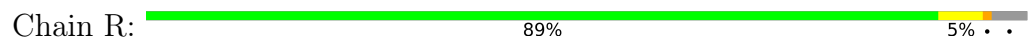
Chain O: 89% 9% 2%



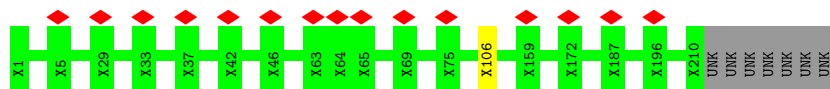
- Molecule 16: 60S ribosomal protein L42-A



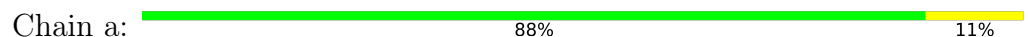
- Molecule 17: 60S ribosomal protein L43-A



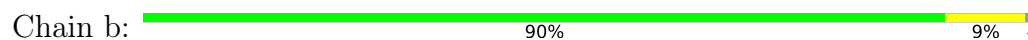
- Molecule 18: Ribosomal Protein uL1



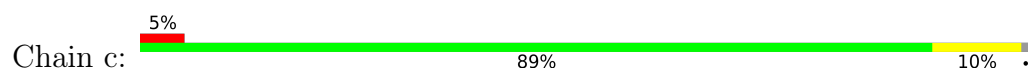
- Molecule 19: 60S ribosomal protein L15-A



- Molecule 20: 60S ribosomal protein L16-A



- Molecule 21: 60S ribosomal protein L17-A



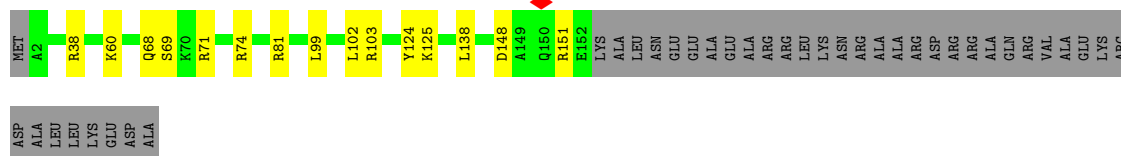
- Molecule 22: 60S ribosomal protein L18-A

Chain d:  89% 10% ..



- Molecule 23: 60S ribosomal protein L19-A

Chain e:  72% 8% 20%



- Molecule 24: 60S ribosomal protein L20-A

Chain f:  87% 9% ...



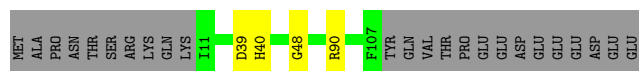
- Molecule 25: 60S ribosomal protein L21-A

Chain g:  84% 15% .



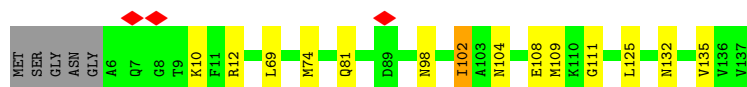
- Molecule 26: 60S ribosomal protein L22-A

Chain h:  77% 20%



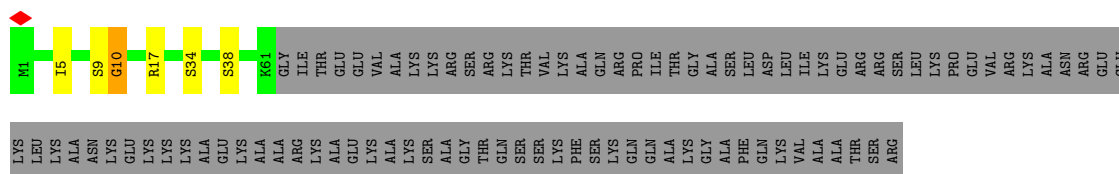
- Molecule 27: 60S ribosomal protein L23-A

Chain i:  86% 9% ..

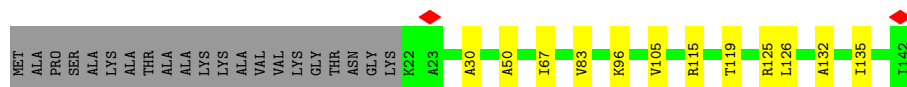
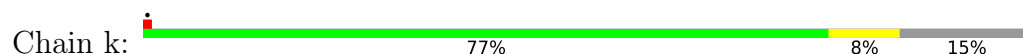


- Molecule 28: 60S ribosomal protein L24-A

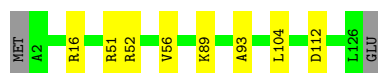
Chain j:  35% 61%



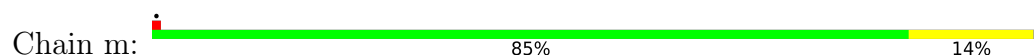
- Molecule 29: 60S ribosomal protein L25



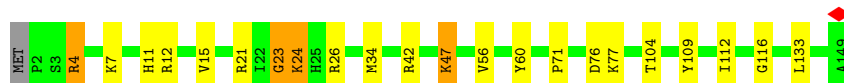
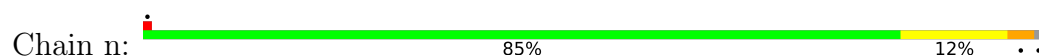
- Molecule 30: 60S ribosomal protein L26-A



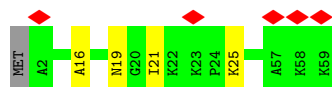
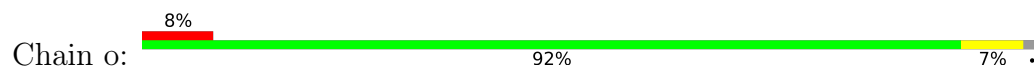
- Molecule 31: 60S ribosomal protein L27-A



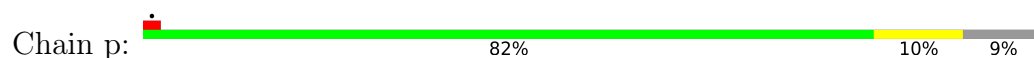
- Molecule 32: 60S ribosomal protein L28



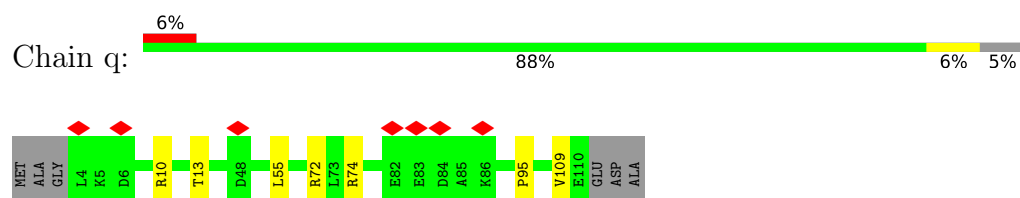
- Molecule 33: 60S ribosomal protein L29



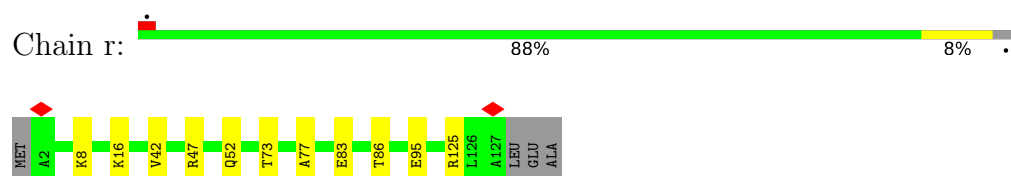
- Molecule 34: 60S ribosomal protein L30



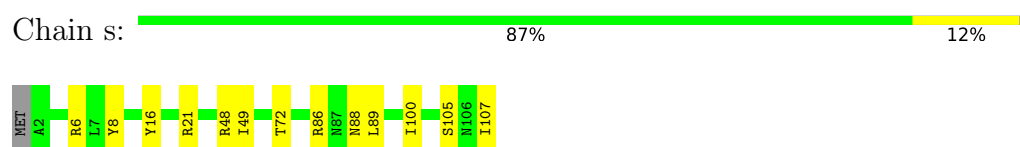
- Molecule 35: 60S ribosomal protein L31-A



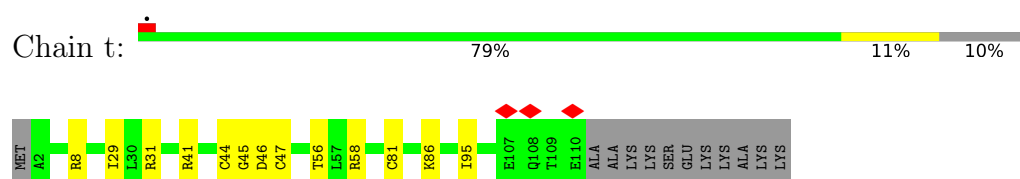
- Molecule 36: 60S ribosomal protein L32



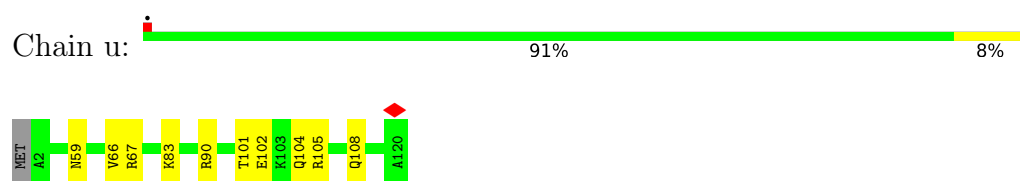
- Molecule 37: 60S ribosomal protein L33-A



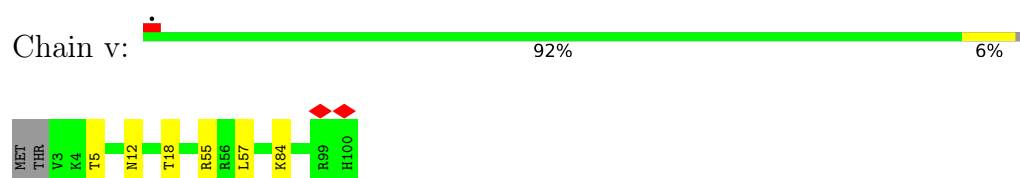
- Molecule 38: 60S ribosomal protein L34-A



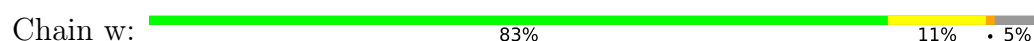
- Molecule 39: 60S ribosomal protein L35-A

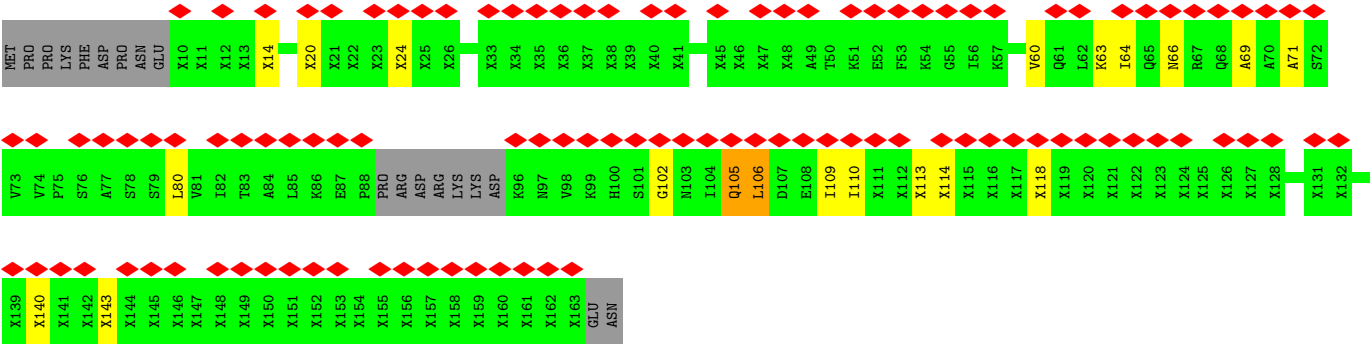


- Molecule 40: 60S ribosomal protein L36-A

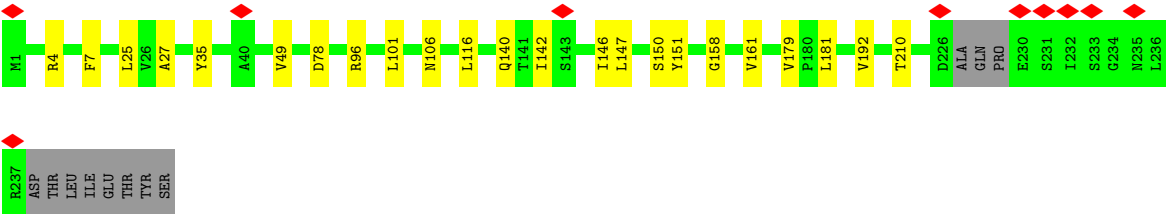
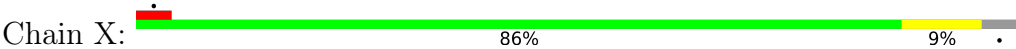


- Molecule 41: 60S ribosomal protein L37-A





● Molecule 47: Eukaryotic translation initiation factor 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98980	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.088	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.31	0/76692	0.34	8/119572 (0.0%)
2	B	0.26	0/2883	0.27	0/4491
3	C	0.32	0/3746	0.32	0/5832
4	Y	0.34	0/1016	1.03	9/1368 (0.7%)
5	D	0.36	0/1908	0.62	0/2564
6	E	0.35	0/3130	0.63	0/4206
7	F	0.33	0/2800	0.70	3/3790 (0.1%)
8	G	0.27	0/2320	0.63	4/3131 (0.1%)
9	H	0.28	0/1236	0.61	0/1661
10	I	0.33	0/1807	0.65	0/2432
11	J	0.29	0/1794	0.63	0/2425
12	K	0.31	0/1514	0.63	0/2039
13	M	0.26	0/1365	0.67	0/1831
14	N	0.31	0/1564	0.72	3/2102 (0.1%)
15	O	0.29	0/1068	0.54	0/1438
16	Q	0.29	0/831	0.59	0/1097
17	R	0.32	0/680	0.66	0/905
19	a	0.37	0/1757	0.61	0/2354
20	b	0.32	0/1585	0.60	0/2128
21	c	0.35	0/1443	0.66	0/1944
22	d	0.33	0/1465	0.65	1/1965 (0.1%)
23	e	0.31	0/1236	0.60	0/1650
24	f	0.32	0/1468	0.64	2/1973 (0.1%)
25	g	0.31	0/1300	0.62	0/1743
26	h	0.28	0/781	0.63	0/1058
27	i	0.32	0/996	0.57	0/1340
28	j	0.28	0/521	0.58	0/691
29	k	0.32	0/979	0.59	0/1321
30	l	0.32	0/995	0.57	0/1329
31	m	0.34	0/1118	0.64	0/1497
32	n	0.34	0/1204	0.81	6/1612 (0.4%)
33	o	0.31	0/473	0.73	0/629
34	p	0.27	0/745	0.51	0/1001
35	q	0.35	0/880	0.60	0/1182

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	r	0.32	0/1033	0.62	0/1383
37	s	0.36	0/868	0.61	0/1168
38	t	0.35	0/871	0.62	1/1164 (0.1%)
39	u	0.30	0/978	0.63	0/1301
40	v	0.29	0/759	0.62	0/1009
41	w	0.37	0/680	0.73	0/901
42	x	0.26	0/614	0.53	0/822
43	y	0.32	0/443	0.64	0/588
44	z	0.25	0/414	0.57	0/551
45	V	0.33	0/3124	0.80	10/4246 (0.2%)
46	L	0.30	0/367	0.85	4/498 (0.8%)
47	X	0.26	0/1729	0.64	4/2355 (0.2%)
All	All	0.31	0/137180	0.48	55/202287 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	Y	0	3
6	E	0	1
7	F	0	1
10	I	0	1
11	J	0	2
12	K	0	1
13	M	0	1
18	S	0	1
24	f	0	2
32	n	0	1
33	o	0	1
39	u	0	1
45	V	0	8
47	X	0	1
All	All	0	25

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	t	81	CYS	CA-CB-SG	7.75	132.23	114.40
7	F	182	LEU	N-CA-C	-6.97	106.68	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	328	LYS	CA-C-N	6.85	134.62	121.54
4	Y	328	LYS	C-N-CA	6.85	134.62	121.54
32	n	47	LYS	CA-C-N	6.62	134.19	121.54
32	n	47	LYS	C-N-CA	6.62	134.19	121.54
47	X	142	ILE	CA-C-N	6.50	130.57	120.82
47	X	142	ILE	C-N-CA	6.50	130.57	120.82
8	G	257	GLU	CA-C-N	6.41	133.78	121.54
8	G	257	GLU	C-N-CA	6.41	133.78	121.54
45	V	32	LEU	CA-C-N	6.33	133.36	121.97
45	V	32	LEU	C-N-CA	6.33	133.36	121.97
4	Y	329	TRP	N-CA-C	-6.24	97.52	110.80
45	V	95	VAL	CA-C-N	6.08	133.16	121.54
45	V	95	VAL	C-N-CA	6.08	133.16	121.54
14	N	93	ILE	N-CA-C	-6.06	105.47	111.77
4	Y	326	CYS	CB-CA-C	-6.05	98.37	110.42
45	V	146	CYS	CA-CB-SG	6.01	128.22	114.40
4	Y	325	SER	CA-C-N	5.88	132.76	121.54
4	Y	325	SER	C-N-CA	5.88	132.76	121.54
46	L	105	GLN	CA-C-N	5.87	129.63	120.82
46	L	105	GLN	C-N-CA	5.87	129.63	120.82
32	n	116	GLY	N-CA-C	5.86	127.07	113.18
1	A	1576	G	P-O3'-C3'	5.82	128.93	120.20
45	V	96	ARG	CA-C-N	5.82	132.65	121.54
45	V	96	ARG	C-N-CA	5.82	132.65	121.54
24	f	23	LYS	CA-C-N	5.77	132.56	121.54
24	f	23	LYS	C-N-CA	5.77	132.56	121.54
32	n	23	GLY	CA-C-N	5.63	132.30	121.54
32	n	23	GLY	C-N-CA	5.63	132.30	121.54
1	A	1029	G	P-O3'-C3'	5.62	128.63	120.20
4	Y	331	ILE	N-CA-C	-5.60	96.78	108.88
45	V	35	CYS	CA-CB-SG	5.58	127.23	114.40
14	N	46	ILE	CA-C-N	5.54	127.90	120.58
14	N	46	ILE	C-N-CA	5.54	127.90	120.58
1	A	1027	A	P-O3'-C3'	5.53	128.49	120.20
32	n	47	LYS	CA-CB-CG	5.51	125.12	114.10
1	A	2541	U	P-O3'-C3'	5.50	128.46	120.20
8	G	258	LYS	CA-C-N	5.46	131.97	121.54
8	G	258	LYS	C-N-CA	5.46	131.97	121.54
1	A	1576	G	C2'-C3'-O3'	5.40	117.60	109.50
47	X	161	VAL	CA-C-N	5.34	127.81	120.39
47	X	161	VAL	C-N-CA	5.34	127.81	120.39
1	A	1815	U	P-O3'-C3'	5.32	128.18	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	V	15	ALA	CA-C-N	5.29	131.65	121.54
45	V	15	ALA	C-N-CA	5.29	131.65	121.54
1	A	979	U	P-O3'-C3'	5.28	128.12	120.20
1	A	1038	C	P-O3'-C3'	5.22	128.03	120.20
7	F	4	PRO	CA-C-N	5.17	131.43	121.54
7	F	4	PRO	C-N-CA	5.17	131.43	121.54
46	L	106	LEU	CA-C-N	5.12	127.86	120.38
46	L	106	LEU	C-N-CA	5.12	127.86	120.38
4	Y	329	TRP	CA-C-N	-5.08	112.82	121.97
4	Y	329	TRP	C-N-CA	-5.08	112.82	121.97
22	d	99	THR	N-CA-C	5.01	117.00	110.43

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	E	346	THR	Peptide
7	F	4	PRO	Peptide
10	I	157	ASN	Peptide
11	J	34	PHE	Peptide
11	J	35	GLY	Peptide
12	K	21	LYS	Peptide
13	M	7	ASN	Peptide
18	S	106	UNK	Peptide
45	V	104	TRP	Peptide
45	V	14	ALA	Peptide
45	V	15	ALA	Peptide
45	V	16	THR	Peptide
45	V	278	LYS	Peptide
45	V	31	GLY	Peptide
45	V	32	LEU	Peptide
45	V	96	ARG	Peptide
47	X	7	PHE	Peptide
4	Y	325	SER	Peptide
4	Y	327	GLY	Peptide
4	Y	331	ILE	Peptide
24	f	12	ARG	Peptide
24	f	23	LYS	Peptide
32	n	23	GLY	Peptide
33	o	25	LYS	Peptide
39	u	83	LYS	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	68513	0	34428	247	0
2	B	2579	0	1304	10	0
3	C	3353	0	1695	13	0
4	Y	991	0	980	18	0
5	D	1874	0	1943	20	0
6	E	3059	0	3127	27	0
7	F	2748	0	2859	32	0
8	G	2271	0	2217	21	0
9	H	1217	0	1308	13	0
10	I	1770	0	1851	14	0
11	J	1762	0	1839	12	0
12	K	1493	0	1566	12	0
13	M	1344	0	1370	6	0
14	N	1539	0	1597	14	0
15	O	1053	0	1149	7	0
16	Q	819	0	890	8	0
17	R	673	0	715	3	0
18	S	1050	0	237	0	0
19	a	1720	0	1779	20	0
20	b	1555	0	1659	12	0
21	c	1420	0	1437	12	0
22	d	1441	0	1543	14	0
23	e	1219	0	1301	11	0
24	f	1432	0	1470	15	0
25	g	1276	0	1323	18	0
26	h	766	0	782	3	0
27	i	981	0	1031	10	0
28	j	509	0	537	5	0
29	k	964	0	1025	8	0
30	l	984	0	1075	5	0
31	m	1092	0	1155	13	0
32	n	1173	0	1215	15	0
33	o	462	0	491	2	0
34	p	737	0	792	5	0
35	q	866	0	908	4	0
36	r	1012	0	1079	9	0
37	s	850	0	880	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	t	861	0	919	8	0
39	u	969	0	1078	7	0
40	v	753	0	826	4	0
41	w	665	0	668	9	0
42	x	608	0	671	2	0
43	y	436	0	475	7	0
44	z	408	0	446	3	0
45	V	3065	0	3047	38	0
46	L	825	0	439	11	0
47	X	1710	0	1667	11	0
All	All	128867	0	92793	589	0

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

All (589) 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)
4:Y:307:CYS:SG	4:Y:310:CYS:N	2.61	0.73
20:b:119:VAL:HG11	24:f:167:ARG:HE	1.57	0.70
45:V:58:CYS:SG	45:V:143:CYS:N	2.65	0.68
20:b:37:ARG:HH21	20:b:160:ARG:HH22	1.39	0.68
2:B:121:U:H3	8:G:264:GLN:HB3	1.57	0.68
1:A:3274:A:H2'	21:c:171:ARG:HH12	1.60	0.67
11:J:35:GLY:HA3	11:J:38:GLN:HE21	1.61	0.66
36:r:42:VAL:HG12	36:r:52:GLN:HE21	1.60	0.66
13:M:47:GLN:HG2	13:M:67:VAL:HG12	1.78	0.66
6:E:10:ARG:NH2	6:E:263:SER:O	2.30	0.65
4:Y:260:PHE:HB2	4:Y:274:GLN:HB2	1.79	0.65
41:w:19:CYS:SG	41:w:22:CYS:N	2.70	0.65
1:A:664:U:H5'	7:F:107:ARG:HA	1.79	0.65
25:g:75:ILE:HG22	25:g:88:ARG:HG2	1.79	0.64
21:c:126:ARG:NH2	21:c:140:GLU:OE2	2.30	0.64
45:V:290:THR:HA	45:V:335:LEU:HD11	1.79	0.63
25:g:136:ARG:HG3	25:g:139:ARG:HH22	1.63	0.63
1:A:2452:G:N2	1:A:2462:A:N7	2.47	0.63
24:f:13:ARG:HD2	24:f:51:VAL:HG22	1.79	0.63
2:B:121:U:OP2	8:G:259:LYS:NZ	2.33	0.62
5:D:117:GLU:HG2	5:D:124:GLY:H	1.65	0.62
21:c:78:VAL:HG12	21:c:80:LYS:H	1.64	0.62
1:A:2137:U:OP2	1:A:2142:A:N6	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:e:103:ARG:NH1	23:e:124:TYR:OH	2.32	0.62
31:m:121:ARG:NH2	31:m:127:ASN:OD1	2.32	0.62
1:A:1571:A:H2'	1:A:1572:U:H4'	1.80	0.62
15:O:72:LEU:HD11	15:O:81:VAL:HG22	1.81	0.62
4:Y:351:LEU:HG	45:V:12:GLN:HE22	1.65	0.61
47:X:4:ARG:NH1	47:X:210:THR:O	2.34	0.61
19:a:47:LYS:HA	19:a:50:ARG:HE	1.66	0.61
23:e:102:LEU:HD22	23:e:138:LEU:HD13	1.81	0.61
11:J:50:VAL:HG12	29:k:30:ALA:HA	1.84	0.60
45:V:156:ARG:HH12	45:V:239:THR:HA	1.67	0.60
45:V:359:LEU:HD22	45:V:362:ILE:HD11	1.84	0.60
1:A:1334:U:H5''	10:I:206:LYS:HB3	1.85	0.59
1:A:1383:G:OP1	7:F:203:ARG:NH2	2.35	0.59
1:A:3343:G:H21	1:A:3362:A:H2	1.50	0.59
1:A:2221:G:N2	1:A:2224:A:OP2	2.34	0.59
1:A:712:G:OP1	14:N:174:ARG:NH1	2.35	0.59
14:N:24:VAL:HG12	19:a:199:LEU:HB2	1.84	0.59
1:A:1057:A:OP1	10:I:98:LYS:NZ	2.35	0.59
10:I:88:ARG:HE	10:I:103:LEU:HD13	1.67	0.59
1:A:499:G:H5''	37:s:48:ARG:HH12	1.67	0.59
1:A:496:C:OP1	36:r:8:LYS:NZ	2.36	0.58
38:t:44:CYS:SG	38:t:45:GLY:N	2.76	0.58
7:F:237:GLN:O	7:F:246:ARG:NH1	2.37	0.58
1:A:597:G:OP1	10:I:41:ARG:NH2	2.35	0.58
6:E:168:LYS:O	6:E:319:ASN:ND2	2.37	0.58
40:v:5:THR:HG23	40:v:12:ASN:HB2	1.86	0.58
45:V:168:LYS:HB3	45:V:171:PHE:HB3	1.85	0.58
14:N:180:ARG:NH2	14:N:184:GLU:OE2	2.37	0.58
1:A:2284:C:O2	45:V:205:ASN:ND2	2.37	0.57
25:g:17:ARG:NH1	25:g:45:ASN:OD1	2.37	0.57
1:A:824:C:H5''	5:D:21:ARG:HD3	1.85	0.57
1:A:1392:G:OP1	36:r:125:ARG:NH2	2.36	0.57
6:E:227:GLU:HG3	6:E:270:ARG:HE	1.69	0.57
30:l:56:VAL:HG11	30:l:104:LEU:HD13	1.87	0.57
1:A:1671:C:OP1	23:e:60:LYS:NZ	2.37	0.57
1:A:813:G:O2'	41:w:45:ARG:NH2	2.37	0.57
24:f:109:ASP:OD1	24:f:113:ARG:NH1	2.38	0.57
1:A:3042:U:OP2	1:A:3092:C:N4	2.37	0.57
1:A:845:G:N2	1:A:848:A:OP2	2.38	0.57
13:M:133:ARG:NH2	13:M:158:ASP:OD2	2.37	0.57
14:N:46:ILE:HG22	14:N:49:ARG:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:i:135:VAL:HG22	47:X:101:LEU:HA	1.87	0.57
35:q:55:LEU:HB2	35:q:95:PRO:HD3	1.87	0.57
1:A:1724:U:O4	23:e:125:LYS:NZ	2.38	0.57
7:F:92:ASN:HD22	7:F:100:PHE:HB2	1.69	0.57
8:G:41:LYS:HE3	25:g:93:VAL:HG11	1.87	0.57
1:A:2462:A:H61	1:A:2493:U:H3	1.52	0.57
20:b:10:ASP:HB2	20:b:117:ARG:HB3	1.87	0.57
1:A:3386:G:H4'	35:q:10:ARG:HH12	1.68	0.56
1:A:371:G:N1	1:A:374:A:OP2	2.38	0.56
1:A:804:C:OP1	7:F:98:ARG:NH2	2.38	0.56
1:A:1845:G:H5''	1:A:1846:C:H5''	1.87	0.56
46:L:60:VAL:HB	46:L:80:LEU:HD11	1.87	0.56
4:Y:304:LYS:HA	4:Y:316:GLY:HA2	1.86	0.56
8:G:240:TYR:O	8:G:244:HIS:ND1	2.38	0.56
47:X:106:ASN:ND2	47:X:150:SER:OG	2.38	0.56
1:A:198:A:N3	1:A:218:G:O2'	2.38	0.56
1:A:1404:G:O6	36:r:16:LYS:NZ	2.37	0.56
1:A:1609:C:OP1	29:k:125:ARG:NH2	2.39	0.56
1:A:216:G:OP1	30:l:16:ARG:NH1	2.38	0.56
1:A:2457:G:H22	1:A:2487:U:H3	1.52	0.56
2:B:3:U:O2'	2:B:25:G:N3	2.39	0.56
6:E:232:ARG:NH1	6:E:269:GLN:O	2.39	0.56
8:G:261:THR:OG1	8:G:264:GLN:NE2	2.38	0.56
1:A:329:U:N3	7:F:54:GLU:OE2	2.38	0.56
3:C:142:C:OP1	19:a:38:ARG:NH1	2.39	0.56
22:d:96:PHE:HE2	22:d:113:LYS:HE3	1.71	0.56
1:A:1028:U:H4'	1:A:1029:G:H3'	1.88	0.56
1:A:3268:A:OP1	9:H:46:ARG:NH1	2.37	0.55
6:E:53:MET:HG2	6:E:77:THR:HG22	1.88	0.55
12:K:20:ILE:HG12	12:K:25:VAL:HG22	1.88	0.55
41:w:25:ARG:HG3	43:y:51:ILE:HD12	1.87	0.55
16:Q:90:HIS:NE2	45:V:314:GLN:OE1	2.39	0.55
1:A:534:U:OP1	24:f:132:THR:OG1	2.25	0.55
1:A:785:G:O6	32:n:77:LYS:NZ	2.38	0.55
1:A:2448:G:N2	1:A:2499:U:O2	2.40	0.55
20:b:22:VAL:HG21	20:b:120:VAL:HG11	1.89	0.55
1:A:2261:G:O2'	1:A:2263:C:N4	2.40	0.55
2:B:7:G:OP1	8:G:33:ARG:NH1	2.40	0.55
3:C:97:A:O2'	39:u:59:ASN:ND2	2.40	0.55
31:m:54:THR:HG23	31:m:56:LYS:H	1.72	0.55
1:A:2964:G:N2	1:A:2967:A:OP2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:334:PHE:HA	7:F:339:LEU:HD12	1.89	0.54
1:A:3277:U:O4	21:c:172:GLN:NE2	2.40	0.54
8:G:60:ILE:HB	8:G:80:SER:HB3	1.89	0.54
1:A:3185:U:HO2'	24:f:170:THR:HG1	1.52	0.54
3:C:21:C:OP1	7:F:193:LYS:NZ	2.36	0.54
8:G:50:ARG:NH1	8:G:147:ASP:OD2	2.41	0.54
9:H:85:ILE:HG23	37:s:107:ILE:HG21	1.90	0.54
11:J:62:LYS:HD3	19:a:29:GLU:HG3	1.90	0.54
31:m:23:VAL:HG12	31:m:45:GLY:HA3	1.90	0.54
1:A:1004:U:H3	1:A:1046:A:H61	1.55	0.54
1:A:1306:G:N2	1:A:1307:G:N7	2.53	0.54
1:A:2631:U:OP2	25:g:4:SER:OG	2.26	0.54
6:E:188:ILE:HG22	6:E:191:LYS:HD2	1.90	0.54
31:m:3:LYS:O	31:m:6:LYS:NZ	2.40	0.54
1:A:805:G:O2'	7:F:73:ARG:NH2	2.40	0.54
1:A:1223:A:N1	1:A:1287:A:O2'	2.38	0.54
1:A:1521:G:O6	43:y:17:LYS:NZ	2.41	0.54
6:E:368:GLY:O	28:j:17:ARG:NH1	2.41	0.54
1:A:89:A:OP1	22:d:170:ARG:NH2	2.40	0.53
1:A:2415:C:OP1	5:D:2:GLY:N	2.41	0.53
1:A:3049:A:O2'	6:E:364:LYS:NZ	2.41	0.53
16:Q:38:GLN:OE1	16:Q:41:ARG:NH2	2.41	0.53
1:A:845:G:O2'	1:A:847:A:N7	2.34	0.53
1:A:1062:A:H5''	1:A:1063:G:H5'	1.90	0.53
1:A:1793:C:O2	5:D:174:ARG:NH1	2.41	0.53
3:C:83:C:N3	30:l:52:ARG:NH2	2.56	0.53
4:Y:232:CYS:HA	4:Y:341:VAL:HG23	1.90	0.53
24:f:42:TRP:HE1	24:f:58:ILE:HD11	1.72	0.53
32:n:7:LYS:O	32:n:11:HIS:ND1	2.33	0.53
4:Y:276:SER:HB3	4:Y:326:CYS:HA	1.90	0.53
24:f:99:ARG:NH1	24:f:126:VAL:O	2.41	0.53
31:m:46:ILE:HA	31:m:70:PRO:HA	1.90	0.53
1:A:1223:A:OP2	1:A:1285:G:N2	2.41	0.53
1:A:1320:C:O2	24:f:115:ARG:NH2	2.41	0.53
6:E:57:VAL:HG22	6:E:73:VAL:HG12	1.90	0.53
1:A:348:A:N3	1:A:352:A:O2'	2.41	0.53
8:G:41:LYS:NZ	25:g:30:TYR:O	2.38	0.53
45:V:33:VAL:HG12	45:V:34:MET:HG2	1.90	0.53
1:A:2953:U:H2'	1:A:2954:U:H2'	1.90	0.53
1:A:1150:A:O2'	37:s:21:ARG:NH2	2.42	0.53
45:V:143:CYS:O	45:V:147:ALA:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:U:H5''	22:d:141:ARG:HH22	1.73	0.53
1:A:2895:G:O2'	44:z:100:TYR:O	2.27	0.53
7:F:40:THR:O	7:F:44:LYS:NZ	2.40	0.53
7:F:327:LEU:HD23	10:I:181:ILE:HG21	1.91	0.53
1:A:358:G:N2	1:A:361:A:OP2	2.42	0.52
6:E:67:PHE:HD1	6:E:70:ARG:HG2	1.74	0.52
8:G:93:THR:OG1	8:G:158:ARG:NH1	2.42	0.52
13:M:114:ILE:HG22	13:M:115:LYS:HG3	1.92	0.52
1:A:2724:U:OP2	1:A:2726:C:N4	2.43	0.52
27:i:109:MET:SD	27:i:132:ASN:ND2	2.80	0.52
1:A:1017:C:O2	1:A:1035:G:N2	2.43	0.52
1:A:1050:U:OP1	25:g:12:ARG:NH2	2.42	0.52
1:A:1192:C:N4	1:A:1302:A:OP2	2.38	0.52
1:A:1385:C:OP1	7:F:141:ARG:NH1	2.43	0.52
1:A:1018:G:N2	1:A:1035:G:N3	2.56	0.52
1:A:1863:G:N1	1:A:1866:C:OP2	2.40	0.52
1:A:2969:A:N7	5:D:215:ASN:ND2	2.58	0.52
4:Y:228:THR:HG21	4:Y:343:GLN:HE21	1.75	0.52
7:F:283:THR:HG22	7:F:285:ASP:H	1.74	0.52
7:F:226:GLU:HB3	7:F:237:GLN:HE21	1.74	0.52
1:A:1103:A:N6	1:A:1363:A:O2'	2.43	0.52
1:A:2584:G:O2'	11:J:240:ASN:ND2	2.42	0.52
46:L:63:LYS:HG2	46:L:71:ALA:HB3	1.92	0.52
1:A:2908:G:O2'	44:z:114:LYS:NZ	2.42	0.52
45:V:63:ARG:HE	45:V:71:TRP:HB3	1.74	0.52
1:A:268:A:OP1	19:a:50:ARG:NH2	2.43	0.52
1:A:1350:A:OP2	7:F:291:ASN:ND2	2.42	0.52
21:c:56:ARG:NH1	21:c:75:GLU:OE2	2.43	0.52
8:G:205:SER:HB3	8:G:236:LEU:HD23	1.92	0.51
1:A:20:A:P	39:u:90:ARG:HH12	2.32	0.51
9:H:31:ARG:NH2	37:s:105:SER:O	2.43	0.51
1:A:1134:G:O2'	1:A:2642:A:N3	2.40	0.51
1:A:2227:C:OP1	16:Q:32:LYS:NZ	2.39	0.51
45:V:280:SER:OG	45:V:281:ASN:N	2.42	0.51
2:B:28:C:OP1	13:M:137:ARG:NH1	2.43	0.51
24:f:23:LYS:O	25:g:146:ASN:ND2	2.31	0.51
46:L:105:GLN:HA	46:L:143:UNK:HA	1.92	0.51
15:O:23:ILE:HA	15:O:63:VAL:HG23	1.93	0.51
1:A:428:A:O2'	37:s:88:ASN:ND2	2.44	0.51
1:A:1914:G:N2	23:e:81:ARG:O	2.41	0.51
1:A:2255:A:N6	1:A:2260:U:O4	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2987:A:H5''	20:b:68:ARG:HH12	1.74	0.51
3:C:13:A:O2'	21:c:121:GLN:O	2.29	0.51
1:A:3040:A:H5''	27:i:12:ARG:HB2	1.93	0.51
16:Q:61:LYS:NZ	45:V:380:ASN:O	2.41	0.51
1:A:1613:A:OP1	42:x:2:ALA:N	2.43	0.51
14:N:9:ILE:HG23	32:n:34:MET:HE3	1.93	0.51
1:A:3243:A:H4'	6:E:95:THR:HG22	1.92	0.50
3:C:126:A:O2'	3:C:128:U:OP2	2.29	0.50
34:p:16:LEU:HB2	34:p:98:SER:HB2	1.93	0.50
1:A:3199:G:H5''	15:O:6:ILE:HG21	1.92	0.50
41:w:35:SER:O	41:w:45:ARG:NH1	2.45	0.50
43:y:27:ILE:O	43:y:33:ASN:ND2	2.42	0.50
1:A:1592:G:OP1	38:t:58:ARG:NH2	2.44	0.50
1:A:2186:U:OP2	5:D:200:ARG:NH2	2.43	0.50
25:g:18:ASP:HB2	25:g:21:LYS:HB2	1.91	0.50
27:i:81:GLN:HA	27:i:98:ASN:HD22	1.76	0.50
1:A:1682:U:O4	26:h:90:ARG:NH1	2.44	0.50
6:E:56:ILE:HD11	6:E:356:LEU:HD13	1.94	0.50
46:L:106:LEU:O	46:L:110:ILE:N	2.34	0.50
1:A:412:G:OP1	21:c:62:ARG:NH1	2.44	0.50
7:F:181:VAL:HG22	7:F:202:ARG:HB2	1.93	0.50
12:K:90:MET:HB2	12:K:144:ILE:HG23	1.94	0.50
20:b:157:GLU:OE1	20:b:160:ARG:NH2	2.42	0.50
32:n:24:LYS:HD2	32:n:26:ARG:HH21	1.77	0.50
9:H:54:TYR:HA	9:H:65:ILE:HG22	1.92	0.50
45:V:326:THR:HG21	45:V:356:ARG:HH22	1.76	0.50
23:e:148:ASP:OD1	23:e:151:ARG:NH2	2.44	0.50
6:E:303:LYS:HD2	6:E:361:THR:HG21	1.94	0.50
7:F:4:PRO:HD2	7:F:22:LEU:HD13	1.93	0.50
12:K:41:ILE:HD11	12:K:67:ALA:HB1	1.93	0.50
4:Y:264:ALA:HB3	4:Y:269:ARG:HB3	1.93	0.49
1:A:497:C:O3'	37:s:86:ARG:NH2	2.45	0.49
1:A:546:C:OP1	1:A:548:G:N2	2.46	0.49
1:A:1506:A:H5''	1:A:1507:G:H5''	1.94	0.49
12:K:3:TYR:HA	24:f:142:GLN:HE22	1.77	0.49
12:K:9:GLN:O	12:K:72:LYS:NZ	2.37	0.49
1:A:1778:G:O2'	1:A:1780:G:OP2	2.27	0.49
1:A:1899:G:O2'	1:A:2334:U:O4	2.30	0.49
1:A:3316:A:OP1	1:A:3318:G:N2	2.45	0.49
47:X:151:TYR:HE1	47:X:192:VAL:HG22	1.78	0.49
1:A:309:U:OP1	40:v:84:LYS:NZ	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:U:OP2	45:V:169:ARG:NH2	2.45	0.49
1:A:2899:C:O2'	1:A:2901:G:OP2	2.30	0.49
10:I:170:GLU:HG3	10:I:179:LEU:HB2	1.94	0.49
31:m:24:VAL:HG11	31:m:87:LEU:HD23	1.93	0.49
45:V:51:ARG:HH22	45:V:132:PHE:HB2	1.77	0.49
1:A:1921:A:OP2	1:A:1930:A:N6	2.46	0.49
27:i:74:MET:HE3	27:i:102:ILE:HG21	1.93	0.49
27:i:109:MET:HG2	27:i:111:GLY:H	1.77	0.49
1:A:172:G:N2	1:A:248:U:O2	2.45	0.49
1:A:1376:C:HO2'	1:A:1408:G:HO2'	1.61	0.49
1:A:2843:U:O4	4:Y:270:ILE:N	2.44	0.49
1:A:3024:A:OP1	4:Y:304:LYS:NZ	2.37	0.49
1:A:3092:C:O2'	1:A:3094:A:OP2	2.28	0.49
1:A:3186:A:N3	12:K:44:THR:OG1	2.46	0.49
19:a:112:ASN:HB2	19:a:138:GLN:HE22	1.78	0.49
1:A:1431:G:OP2	32:n:12:ARG:NH1	2.46	0.49
1:A:2185:G:O2'	1:A:2314:U:OP2	2.27	0.49
1:A:353:G:O6	41:w:52:LYS:NZ	2.39	0.49
16:Q:38:GLN:HA	16:Q:41:ARG:HH21	1.78	0.49
23:e:68:GLN:OE1	23:e:71:ARG:NH2	2.46	0.48
29:k:50:ALA:HB1	39:u:66:VAL:HG11	1.94	0.48
1:A:2940:A:OP2	6:E:2:SER:N	2.45	0.48
30:l:89:LYS:HB2	30:l:93:ALA:HB3	1.94	0.48
9:H:43:LEU:HD11	9:H:85:ILE:HG13	1.95	0.48
10:I:155:LYS:NZ	10:I:200:ASN:O	2.46	0.48
1:A:3351:U:O2'	1:A:3353:G:N2	2.46	0.48
37:s:49:ILE:HG12	37:s:100:ILE:HG13	1.96	0.48
1:A:2415:C:H5'	5:D:207:VAL:HG12	1.95	0.48
1:A:188:U:O2'	1:A:207:U:O2	2.30	0.48
1:A:998:A:O2'	2:B:103:A:N3	2.44	0.48
13:M:20:ASN:HB3	13:M:126:ASP:HB2	1.96	0.48
19:a:99:ARG:NH2	19:a:118:SER:O	2.46	0.48
7:F:338:LYS:O	7:F:340:GLY:N	2.47	0.48
16:Q:65:THR:O	16:Q:87:ARG:NH1	2.47	0.48
1:A:117:U:O2'	1:A:119:U:OP2	2.29	0.48
1:A:905:U:O2	1:A:910:G:O2'	2.32	0.48
19:a:37:HIS:HE1	19:a:63:ARG:HH11	1.60	0.48
21:c:108:ASP:OD2	21:c:111:LYS:NZ	2.46	0.48
22:d:86:THR:HG22	22:d:105:ARG:HB2	1.95	0.48
1:A:975:C:H42	1:A:1106:G:H1	1.62	0.48
1:A:2945:G:O2'	1:A:2948:C:OP2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:C:O2'	37:s:21:ARG:O	2.32	0.47
21:c:109:ALA:HA	21:c:112:LEU:HD13	1.95	0.47
45:V:46:THR:HG23	45:V:49:ILE:HD12	1.96	0.47
1:A:408:A:N3	1:A:655:C:O2'	2.42	0.47
1:A:411:U:H2'	1:A:412:G:H8	1.80	0.47
1:A:969:C:OP1	33:o:19:ASN:ND2	2.45	0.47
1:A:2473:C:H3'	1:A:2474:G:H4'	1.96	0.47
1:A:2799:A:O2'	32:n:42:ARG:NH1	2.48	0.47
1:A:1747:G:H21	42:x:2:ALA:HB1	1.79	0.47
1:A:2305:G:OP2	1:A:2305:G:N2	2.39	0.47
4:Y:225:SER:OG	4:Y:226:LYS:N	2.45	0.47
1:A:1193:A:OP2	20:b:49:ARG:NH1	2.44	0.47
6:E:86:VAL:HG22	6:E:162:VAL:HG12	1.97	0.47
1:A:221:A:O2'	1:A:223:U:OP2	2.31	0.47
1:A:289:A:O2'	19:a:93:LYS:O	2.33	0.47
1:A:298:U:H5''	1:A:299:G:H5'	1.95	0.47
1:A:1034:U:H2'	1:A:1035:G:H4'	1.95	0.47
1:A:1242:G:OP1	1:A:1242:G:N2	2.44	0.47
1:A:1258:U:O2'	1:A:1260:A:N7	2.46	0.47
1:A:1260:A:HO2'	1:A:1279:C:HO2'	1.56	0.47
1:A:1940:G:O2'	1:A:3362:A:O2'	2.31	0.47
20:b:36:VAL:HB	20:b:108:ILE:HG12	1.97	0.47
24:f:80:ARG:HE	25:g:156:TYR:HB2	1.79	0.47
32:n:71:PRO:HG2	32:n:109:TYR:HA	1.95	0.47
45:V:13:ASN:ND2	47:X:181:LEU:O	2.47	0.47
1:A:3028:G:OP1	4:Y:337:GLN:NE2	2.48	0.47
6:E:317:ILE:O	6:E:319:ASN:N	2.45	0.47
11:J:83:ASP:OD1	11:J:83:ASP:N	2.48	0.47
13:M:93:ASP:H	13:M:173:ASP:HB3	1.80	0.47
37:s:6:ARG:NH1	37:s:8:TYR:O	2.48	0.47
45:V:149:SER:HA	45:V:154:THR:HG22	1.96	0.47
1:A:634:C:H4'	36:r:47:ARG:HH12	1.80	0.47
1:A:911:C:OP2	5:D:9:ARG:NE	2.45	0.47
1:A:3023:U:H2'	1:A:3024:A:H8	1.79	0.47
11:J:108:ARG:O	11:J:112:GLU:N	2.45	0.47
46:L:66:ASN:H	46:L:69:ALA:HB3	1.79	0.47
22:d:175:ALA:HB2	32:n:56:VAL:HG13	1.96	0.46
1:A:1293:U:O4	1:A:1294:A:N6	2.48	0.46
6:E:113:GLU:HB3	6:E:176:ALA:HB2	1.96	0.46
1:A:148:G:OP2	19:a:4:TYR:OH	2.25	0.46
1:A:1246:G:O2'	1:A:1264:G:OP2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:267:ALA:O	8:G:271:LYS:NZ	2.47	0.46
27:i:104:ASN:OD1	27:i:108:GLU:N	2.48	0.46
19:a:17:ASP:OD2	40:v:55:ARG:NH2	2.49	0.46
21:c:64:ASN:O	21:c:80:LYS:NZ	2.41	0.46
38:t:41:ARG:HG2	38:t:56:THR:HG21	1.97	0.46
1:A:1156:C:OP2	10:I:94:LYS:NZ	2.49	0.46
12:K:8:GLN:HB3	12:K:72:LYS:HD2	1.97	0.46
46:L:20:UNK:CB	46:L:24:UNK:CB	2.93	0.46
1:A:86:G:O2'	1:A:98:G:O6	2.33	0.46
5:D:243:THR:OG1	5:D:244:GLY:N	2.49	0.46
19:a:42:PRO:HG3	19:a:61:ILE:HG13	1.97	0.46
26:h:39:ASP:OD1	26:h:40:HIS:ND1	2.47	0.46
1:A:1597:C:OP1	38:t:8:ARG:NH2	2.48	0.46
28:j:9:SER:OG	28:j:10:GLY:N	2.49	0.46
1:A:339:C:OP1	1:A:1380:G:O2'	2.34	0.46
1:A:969:C:OP1	25:g:82:ASN:ND2	2.49	0.46
1:A:1354:G:N7	1:A:1357:G:O2'	2.46	0.46
3:C:95:G:OP1	41:w:76:ASN:ND2	2.38	0.46
4:Y:228:THR:OG1	4:Y:344:PHE:O	2.33	0.46
12:K:9:GLN:HG2	12:K:54:LYS:HG2	1.98	0.46
1:A:1602:A:H5''	23:e:38:ARG:HG3	1.97	0.45
2:B:59:U:H2'	2:B:60:G:H8	1.80	0.45
3:C:130:C:H2'	3:C:131:A:H8	1.82	0.45
8:G:99:TYR:OH	8:G:168:ASP:OD2	2.29	0.45
22:d:92:ARG:HG2	32:n:76:ASP:HB3	1.97	0.45
22:d:122:ILE:HG23	22:d:126:GLN:HB2	1.98	0.45
1:A:1363:A:OP1	10:I:160:ARG:NH1	2.44	0.45
1:A:2307:G:O2'	1:A:2310:U:OP2	2.35	0.45
9:H:146:ILE:HD13	9:H:149:ILE:HD12	1.97	0.45
15:O:15:VAL:HG23	15:O:35:ILE:HD13	1.96	0.45
45:V:318:PHE:HE1	45:V:342:ARG:HG2	1.81	0.45
1:A:406:G:O2'	3:C:16:G:N2	2.41	0.45
1:A:1112:A:N3	1:A:1370:G:O2'	2.48	0.45
1:A:2424:A:H61	5:D:230:VAL:HG11	1.82	0.45
7:F:82:THR:HG23	7:F:84:ARG:H	1.82	0.45
7:F:264:SER:OG	7:F:265:GLU:N	2.49	0.45
16:Q:71:ARG:HH21	16:Q:80:ARG:HD3	1.81	0.45
1:A:1025:A:O4'	45:V:333:ARG:NH2	2.49	0.45
2:B:8:G:OP2	8:G:30:TYR:OH	2.25	0.45
2:B:96:U:OP1	24:f:43:TYR:OH	2.29	0.45
6:E:54:THR:OG1	6:E:360:ASP:O	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:V:58:CYS:HB3	45:V:61:CYS:HB2	1.97	0.45
1:A:717:C:OP1	1:A:751:A:O2'	2.35	0.45
1:A:799:G:O2'	14:N:18:TRP:NE1	2.36	0.45
22:d:100:THR:HG23	22:d:122:ILE:HD13	1.99	0.45
45:V:186:ASP:OD2	45:V:206:HIS:ND1	2.49	0.45
6:E:41:VAL:HG22	6:E:185:GLY:HA3	1.98	0.45
15:O:38:ILE:HG22	15:O:44:VAL:HG12	1.97	0.45
1:A:2249:G:H1	1:A:2267:C:H42	1.62	0.45
4:Y:283:PHE:HB2	4:Y:336:LEU:HB3	1.99	0.45
38:t:29:ILE:HD11	38:t:31:ARG:HH21	1.81	0.45
1:A:940:G:OP2	32:n:24:LYS:NZ	2.49	0.45
1:A:1236:G:N2	1:A:1244:A:OP1	2.50	0.45
8:G:93:THR:HG1	8:G:158:ARG:NH1	2.15	0.45
17:R:39:CYS:SG	17:R:40:SER:N	2.89	0.45
23:e:69:SER:HB2	23:e:74:ARG:HG3	1.98	0.45
34:p:57:GLU:OE2	34:p:69:TYR:OH	2.27	0.45
1:A:1231:A:H5''	1:A:1232:C:H5'	1.99	0.45
1:A:1447:G:N7	21:c:25:SER:OG	2.46	0.45
1:A:2424:A:OP1	19:a:90:ASN:ND2	2.50	0.45
4:Y:324:CYS:O	4:Y:327:GLY:N	2.47	0.45
6:E:313:HIS:O	6:E:333:LYS:NZ	2.39	0.45
14:N:43:ALA:HB1	14:N:137:GLN:HE22	1.82	0.45
21:c:23:ARG:HH22	21:c:125:GLN:HG3	1.82	0.45
43:y:21:ARG:HH12	43:y:24:PRO:HG3	1.82	0.45
45:V:142:GLN:HE21	45:V:147:ALA:HB2	1.81	0.45
1:A:993:G:N3	1:A:2637:A:H2'	2.32	0.44
1:A:2661:G:H2'	1:A:2662:G:H8	1.82	0.44
6:E:308:MET:HG2	6:E:373:PRO:HD3	1.98	0.44
11:J:162:LEU:HA	19:a:7:LEU:HD11	1.99	0.44
14:N:53:LEU:HB2	14:N:55:ARG:HH12	1.81	0.44
20:b:3:VAL:HG13	20:b:4:GLU:HG3	1.99	0.44
20:b:54:TYR:HD2	20:b:145:VAL:HG11	1.82	0.44
24:f:57:GLU:OE1	25:g:136:ARG:NH1	2.51	0.44
1:A:2242:A:H5''	5:D:244:GLY:HA3	1.98	0.44
8:G:36:LEU:HB3	8:G:50:ARG:HD3	1.98	0.44
9:H:52:VAL:HG11	9:H:65:ILE:HD13	1.99	0.44
12:K:134:ILE:HG13	12:K:146:LEU:HG	1.99	0.44
12:K:137:SER:HB3	12:K:143:GLU:HB3	2.00	0.44
20:b:113:ASP:O	20:b:117:ARG:NH1	2.50	0.44
46:L:14:UNK:HA	46:L:64:ILE:HG12	1.99	0.44
47:X:78:ASP:OD1	47:X:96:ARG:NH2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:G:H4'	10:I:41:ARG:HH22	1.83	0.44
1:A:2116:G:OP1	1:A:2118:C:N4	2.46	0.44
1:A:2483:G:N2	1:A:2486:A:OP2	2.46	0.44
6:E:238:LEU:HB3	6:E:242:THR:HG21	2.00	0.44
34:p:25:LEU:O	34:p:29:SER:OG	2.30	0.44
1:A:999:G:N3	1:A:1002:A:N6	2.65	0.44
1:A:3041:U:OP1	27:i:12:ARG:NH1	2.51	0.44
20:b:54:TYR:OH	20:b:73:PHE:O	2.34	0.44
39:u:102:GLU:HG2	39:u:105:ARG:HH11	1.82	0.44
47:X:116:LEU:HD22	47:X:140:GLN:HB3	1.98	0.44
1:A:634:C:O2'	36:r:47:ARG:NH1	2.48	0.44
1:A:671:U:H2'	1:A:672:A:H8	1.82	0.44
31:m:57:HIS:HB3	31:m:61:LYS:HB2	2.00	0.44
38:t:8:ARG:HH22	38:t:31:ARG:HH11	1.64	0.44
1:A:2168:A:N6	1:A:2170:U:O2	2.50	0.44
6:E:173:GLN:HG2	6:E:175:LYS:H	1.83	0.44
7:F:190:GLY:O	7:F:193:LYS:NZ	2.50	0.44
19:a:73:ARG:HH21	19:a:92:LEU:HD21	1.82	0.44
1:A:1723:A:OP2	23:e:103:ARG:NH2	2.50	0.44
1:A:2406:C:HO2'	1:A:2619:G:H21	1.63	0.44
1:A:2505:U:O2	1:A:2506:U:N3	2.32	0.44
1:A:2557:A:OP1	5:D:69:TYR:OH	2.29	0.44
22:d:97:PRO:HB2	22:d:99:THR:HG23	1.99	0.44
27:i:69:LEU:HD12	27:i:74:MET:HE1	1.98	0.44
34:p:30:THR:HG22	34:p:91:SER:HB2	2.00	0.44
1:A:563:U:OP1	24:f:71:LYS:NZ	2.51	0.44
31:m:83:THR:HG23	31:m:85:TYR:H	1.82	0.44
37:s:16:TYR:OH	37:s:89:LEU:O	2.32	0.44
46:L:114:UNK:O	46:L:118:UNK:N	2.51	0.44
1:A:1005:G:N2	1:A:1006:A:N1	2.66	0.43
12:K:18:VAL:HG12	12:K:27:VAL:HG22	2.00	0.43
14:N:5:LYS:O	14:N:7:LEU:N	2.51	0.43
14:N:64:LYS:O	14:N:67:ARG:NH1	2.51	0.43
29:k:132:ALA:HA	29:k:135:ILE:HG22	1.99	0.43
1:A:2445:A:H61	1:A:2500:A:H61	1.66	0.43
1:A:2949:U:O3'	6:E:241:LYS:NZ	2.50	0.43
3:C:143:U:OP1	19:a:38:ARG:NH2	2.47	0.43
7:F:206:LEU:HD11	7:F:237:GLN:HG2	2.00	0.43
45:V:84:ILE:HG12	45:V:136:TYR:HE2	1.83	0.43
45:V:325:SER:HA	45:V:336:ALA:HA	1.98	0.43
1:A:674:G:OP1	7:F:31:ARG:NH1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3004:C:O2'	6:E:99:LEU:O	2.31	0.43
6:E:211:GLN:NE2	6:E:283:TYR:O	2.51	0.43
17:R:8:VAL:O	17:R:27:LYS:NZ	2.46	0.43
1:A:1604:G:H4'	1:A:1835:A:H4'	2.01	0.43
10:I:57:THR:O	10:I:61:ASN:ND2	2.51	0.43
24:f:12:ARG:HH21	25:g:139:ARG:HE	1.66	0.43
31:m:54:THR:HG22	31:m:57:HIS:CD2	2.54	0.43
47:X:27:ALA:O	47:X:35:TYR:OH	2.30	0.43
1:A:2727:A:OP2	1:A:2728:G:N2	2.45	0.43
4:Y:323:ARG:HG3	4:Y:324:CYS:H	1.82	0.43
6:E:230:THR:HA	6:E:235:THR:HG22	2.00	0.43
22:d:40:THR:OG1	22:d:45:ASN:ND2	2.50	0.43
1:A:402:A:OP1	43:y:36:ARG:NH2	2.52	0.43
1:A:1386:A:OP2	7:F:141:ARG:NH2	2.52	0.43
1:A:1419:A:H5''	7:F:193:LYS:HE2	2.01	0.43
1:A:2462:A:C6	1:A:2463:G:H1'	2.53	0.43
46:L:102:GLY:H	46:L:140:UNK:HA	1.84	0.43
1:A:1208:U:O2	1:A:3115:C:N4	2.51	0.43
4:Y:324:CYS:SG	4:Y:327:GLY:N	2.92	0.43
25:g:43:LYS:HG3	25:g:58:GLN:HE22	1.83	0.43
29:k:105:VAL:HG11	29:k:126:LEU:HD22	2.01	0.43
1:A:1524:A:O2'	1:A:1526:U:OP2	2.31	0.43
8:G:148:ILE:HG12	8:G:151:GLN:HB3	2.00	0.43
11:J:150:LEU:HD12	11:J:215:VAL:HG22	1.99	0.43
45:V:45:ILE:HD13	45:V:128:ILE:HG23	2.01	0.43
14:N:23:LYS:HE2	14:N:25:HIS:CE1	2.53	0.43
29:k:115:ARG:NH1	29:k:119:THR:OG1	2.52	0.43
39:u:101:THR:HG23	39:u:104:GLN:H	1.83	0.43
16:Q:2:VAL:N	16:Q:90:HIS:O	2.52	0.42
45:V:169:ARG:HH21	45:V:253:LYS:HD3	1.84	0.42
47:X:25:LEU:HD23	47:X:49:VAL:HB	2.01	0.42
1:A:1390:A:N6	1:A:1418:A:O2'	2.51	0.42
1:A:2832:C:H2'	1:A:2833:A:H8	1.83	0.42
7:F:3:ARG:HH12	7:F:24:ALA:HA	1.84	0.42
22:d:158:HIS:H	22:d:186:VAL:HG11	1.82	0.42
39:u:104:GLN:OE1	39:u:108:GLN:NE2	2.52	0.42
1:A:1427:U:OP2	32:n:4:ARG:NH2	2.51	0.42
1:A:2745:G:N2	1:A:2748:A:OP2	2.50	0.42
1:A:89:A:N7	22:d:171:LYS:NZ	2.67	0.42
1:A:903:U:HO2'	1:A:1536:G:HO2'	1.66	0.42
5:D:104:LEU:HD22	5:D:158:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:186:HIS:O	10:I:190:THR:OG1	2.34	0.42
25:g:99:SER:HG	25:g:101:CYS:HG	1.62	0.42
31:m:54:THR:H	31:m:57:HIS:HD2	1.66	0.42
14:N:106:GLN:HB3	40:v:18:THR:HG23	2.00	0.42
1:A:351:A:N6	43:y:37:TYR:O	2.47	0.42
1:A:2514:U:OP1	11:J:68:ARG:NH1	2.53	0.42
7:F:74:ILE:H	7:F:74:ILE:HG13	1.68	0.42
28:j:5:ILE:H	28:j:5:ILE:HG13	1.72	0.42
45:V:210:MET:HE2	45:V:214:LEU:HD11	2.01	0.42
1:A:608:A:O3'	7:F:326:ARG:NH1	2.52	0.42
7:F:99:MET:HE3	7:F:102:PRO:HA	2.02	0.42
46:L:109:ILE:O	46:L:113:UNK:N	2.53	0.42
1:A:709:A:N3	1:A:2787:G:O2'	2.52	0.42
1:A:1494:U:P	43:y:42:ARG:HH22	2.43	0.42
1:A:2746:A:H5'	8:G:178:ASN:HD21	1.85	0.42
1:A:3255:U:H2'	1:A:3256:G:H8	1.85	0.42
45:V:329:SER:HA	45:V:334:VAL:H	1.85	0.42
11:J:36:ILE:H	11:J:36:ILE:HG13	1.67	0.42
29:k:67:ILE:HD12	29:k:83:VAL:HG12	2.01	0.42
1:A:1192:C:OP1	44:z:113:ARG:NH2	2.38	0.42
2:B:121:U:H1'	8:G:268:GLU:HG3	2.02	0.42
8:G:95:TRP:NE1	8:G:157:ALA:O	2.46	0.42
9:H:3:ALA:HB2	36:r:77:ALA:HB2	2.02	0.42
31:m:14:VAL:HG22	38:t:86:LYS:HG2	2.01	0.42
45:V:203:GLN:HB2	45:V:206:HIS:CD2	2.55	0.42
1:A:2117:A:O2'	1:A:3080:G:O2'	2.34	0.41
1:A:2942:C:H5''	1:A:2943:G:H5''	2.01	0.41
5:D:134:VAL:HG12	5:D:150:LEU:HA	2.01	0.41
9:H:40:LEU:HD13	9:H:84:VAL:HG11	2.01	0.41
26:h:39:ASP:O	26:h:48:GLY:N	2.50	0.41
1:A:939:U:OP2	32:n:26:ARG:NH2	2.39	0.41
1:A:3121:U:H1'	1:A:3122:A:H5''	2.03	0.41
3:C:141:C:O3'	19:a:62:TYR:OH	2.39	0.41
33:o:16:ALA:HB1	33:o:21:ILE:HD11	2.02	0.41
35:q:13:THR:HG23	35:q:72:ARG:HH11	1.85	0.41
1:A:815:G:OP2	41:w:31:LYS:NZ	2.42	0.41
1:A:1159:A:O5'	22:d:2:GLY:N	2.54	0.41
5:D:5:ILE:HD13	5:D:210:PRO:HD3	2.02	0.41
30:l:51:ARG:NH1	30:l:112:ASP:OD2	2.53	0.41
1:A:88:A:O2'	32:n:60:TYR:O	2.31	0.41
1:A:181:U:H4'	41:w:75:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:A:H4'	37:s:72:THR:HG22	2.01	0.41
3:C:103:G:OP2	3:C:105:A:O2'	2.37	0.41
9:H:100:LYS:NZ	9:H:137:ASP:OD1	2.47	0.41
10:I:121:LYS:HB2	25:g:133:ALA:HB3	2.03	0.41
25:g:36:VAL:HG13	25:g:65:TYR:HA	2.02	0.41
46:L:106:LEU:O	46:L:109:ILE:N	2.53	0.41
1:A:873:C:H4'	1:A:1908:A:H5'	2.02	0.41
1:A:1563:C:O2	1:A:1577:G:N2	2.53	0.41
1:A:2198:A:H1'	1:A:2270:A:C8	2.55	0.41
1:A:3085:G:OP1	28:j:34:SER:OG	2.36	0.41
27:i:10:LYS:HD3	27:i:125:LEU:HD22	2.03	0.41
36:r:73:THR:OG1	36:r:95:GLU:OE1	2.38	0.41
45:V:17:LEU:HD13	45:V:28:GLY:HA2	2.02	0.41
45:V:267:MET:HB2	45:V:294:ALA:HB1	2.02	0.41
1:A:149:U:P	19:a:49:ARG:HH12	2.43	0.41
1:A:289:A:H2'	1:A:290:G:H8	1.84	0.41
1:A:576:C:OP1	10:I:241:LYS:NZ	2.34	0.41
1:A:584:G:H2'	1:A:585:A:H8	1.86	0.41
1:A:2174:G:P	5:D:193:ARG:HH11	2.43	0.41
1:A:2374:C:OP1	1:A:2823:G:O2'	2.36	0.41
1:A:3273:A:OP2	9:H:77:ARG:NH2	2.44	0.41
8:G:122:VAL:HG23	8:G:125:VAL:HG22	2.03	0.41
38:t:44:CYS:SG	38:t:46:ASP:N	2.84	0.41
1:A:2103:U:OP1	23:e:81:ARG:NH1	2.54	0.41
1:A:2477:G:H5''	1:A:2478:C:H5	1.84	0.41
14:N:53:LEU:HD22	14:N:94:GLY:HA2	2.03	0.41
15:O:19:ARG:HG2	15:O:65:LEU:HD22	2.02	0.41
45:V:119:GLN:NE2	45:V:129:GLN:OE1	2.54	0.41
1:A:411:U:H2'	1:A:412:G:C8	2.56	0.41
1:A:696:C:OP2	7:F:119:ARG:NH2	2.52	0.41
1:A:999:G:N2	1:A:1050:U:O2	2.54	0.41
1:A:1404:G:N2	1:A:1407:A:OP2	2.52	0.41
1:A:1547:G:OP1	19:a:108:ARG:NH2	2.45	0.41
1:A:1638:A:H5'	31:m:15:ARG:HD3	2.02	0.41
1:A:1807:G:H5''	31:m:135:ARG:HH22	1.85	0.41
1:A:3084:C:OP1	28:j:38:SER:OG	2.32	0.41
1:A:3255:U:H2'	1:A:3256:G:C8	2.56	0.41
3:C:97:A:OP1	39:u:67:ARG:NH2	2.54	0.41
4:Y:227:VAL:HG23	4:Y:346:LEU:HB3	2.01	0.41
17:R:42:CYS:HB3	17:R:60:CYS:HB3	1.46	0.41
19:a:112:ASN:OD1	19:a:112:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:79:MET:HB3	25:g:84:TYR:CE1	2.56	0.41
32:n:104:THR:HG21	32:n:112:ILE:HD11	2.02	0.41
41:w:8:PHE:HD1	41:w:11:ARG:HE	1.69	0.41
29:k:96:LYS:HE3	29:k:96:LYS:HB2	1.91	0.41
35:q:74:ARG:HH12	35:q:109:VAL:HG11	1.86	0.41
47:X:158:GLY:HA2	47:X:179:VAL:HB	2.02	0.41
1:A:612:U:H2'	1:A:613:G:C8	2.56	0.40
1:A:3108:G:N3	12:K:163:GLN:NE2	2.57	0.40
7:F:233:LEU:HD23	7:F:233:LEU:HA	1.87	0.40
14:N:62:THR:O	14:N:64:LYS:N	2.54	0.40
34:p:92:ILE:HG21	34:p:100:ILE:HD11	2.03	0.40
1:A:439:C:H4'	1:A:494:G:H8	1.85	0.40
5:D:27:ALA:O	5:D:128:ARG:NH2	2.55	0.40
9:H:76:LEU:H	9:H:138:GLN:HE22	1.68	0.40
5:D:30:ARG:HD2	5:D:63:PHE:CD2	2.57	0.40
36:r:83:GLU:O	36:r:86:THR:OG1	2.33	0.40
45:V:35:CYS:HB2	45:V:38:CYS:HB2	2.02	0.40
45:V:105:THR:HG21	45:V:113:ARG:HD2	2.03	0.40
45:V:220:ILE:HG22	45:V:248:ILE:HD13	2.03	0.40
45:V:350:ASP:OD1	45:V:350:ASP:N	2.53	0.40
1:A:800:G:H22	7:F:101:ALA:HA	1.87	0.40
1:A:2364:G:H22	1:A:2396:G:H1'	1.86	0.40
1:A:2526:C:N3	11:J:48:ARG:NH2	2.69	0.40
5:D:32:LEU:HD21	5:D:37:ARG:HD3	2.03	0.40
5:D:209:HIS:HD2	5:D:211:HIS:HB2	1.87	0.40
9:H:34:LEU:HD23	9:H:34:LEU:HA	1.95	0.40
15:O:20:VAL:O	15:O:66:THR:OG1	2.31	0.40
47:X:146:ILE:HG13	47:X:147:LEU:HD12	2.03	0.40
1:A:640:U:H5''	32:n:21:ARG:HH12	1.86	0.40
1:A:971:G:OP1	22:d:8:LYS:NZ	2.46	0.40
1:A:1814:A:H4'	1:A:1815:U:H5'	2.02	0.40
1:A:2451:G:O2'	1:A:2497:U:O2	2.37	0.40
11:J:152:LEU:HD22	11:J:180:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Y	126/364 (35%)	96 (76%)	26 (21%)	4 (3%)	3	24
5	D	244/254 (96%)	229 (94%)	15 (6%)	0	100	100
6	E	382/387 (99%)	355 (93%)	26 (7%)	1 (0%)	36	67
7	F	359/362 (99%)	328 (91%)	28 (8%)	3 (1%)	16	49
8	G	280/297 (94%)	263 (94%)	16 (6%)	1 (0%)	30	62
9	H	151/176 (86%)	140 (93%)	11 (7%)	0	100	100
10	I	218/244 (89%)	209 (96%)	8 (4%)	1 (0%)	24	57
11	J	225/256 (88%)	217 (96%)	7 (3%)	1 (0%)	30	62
12	K	186/191 (97%)	173 (93%)	13 (7%)	0	100	100
13	M	166/174 (95%)	151 (91%)	15 (9%)	0	100	100
14	N	191/199 (96%)	172 (90%)	18 (9%)	1 (0%)	24	57
15	O	134/138 (97%)	127 (95%)	7 (5%)	0	100	100
16	Q	100/106 (94%)	93 (93%)	7 (7%)	0	100	100
17	R	86/92 (94%)	80 (93%)	6 (7%)	0	100	100
19	a	201/204 (98%)	189 (94%)	12 (6%)	0	100	100
20	b	195/199 (98%)	187 (96%)	8 (4%)	0	100	100
21	c	181/184 (98%)	170 (94%)	11 (6%)	0	100	100
22	d	183/186 (98%)	176 (96%)	7 (4%)	0	100	100
23	e	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
24	f	168/172 (98%)	158 (94%)	8 (5%)	2 (1%)	10	41
25	g	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
26	h	95/121 (78%)	90 (95%)	5 (5%)	0	100	100
27	i	130/137 (95%)	129 (99%)	1 (1%)	0	100	100
28	j	59/155 (38%)	56 (95%)	2 (3%)	1 (2%)	7	35
29	k	119/142 (84%)	112 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	l	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
31	m	133/136 (98%)	117 (88%)	16 (12%)	0	100	100
32	n	146/149 (98%)	127 (87%)	16 (11%)	3 (2%)	5	31
33	o	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
34	p	94/105 (90%)	90 (96%)	4 (4%)	0	100	100
35	q	105/113 (93%)	99 (94%)	6 (6%)	0	100	100
36	r	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
37	s	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
38	t	107/121 (88%)	101 (94%)	6 (6%)	0	100	100
39	u	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
40	v	96/100 (96%)	87 (91%)	9 (9%)	0	100	100
41	w	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
42	x	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
43	y	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
44	z	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
45	V	391/518 (76%)	338 (86%)	46 (12%)	7 (2%)	6	34
46	L	53/165 (32%)	48 (91%)	5 (9%)	0	100	100
47	X	230/245 (94%)	219 (95%)	11 (5%)	0	100	100
All	All	6618/7629 (87%)	6158 (93%)	435 (7%)	25 (0%)	31	62

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	F	339	LEU
4	Y	326	CYS
8	G	259	LYS
11	J	36	ILE
14	N	63	VAL
24	f	13	ARG
32	n	24	LYS
45	V	32	LEU
45	V	97	LEU
4	Y	247	ALA
10	I	158	LYS
24	f	24	LEU
45	V	16	THR

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Mol	Chain	Res	Type
4	Y	323	ARG
7	F	4	PRO
7	F	5	GLN
32	n	47	LYS
45	V	15	ALA
6	E	347	SER
45	V	47	GLN
45	V	68	PRO
32	n	15	VAL
4	Y	246	ILE
45	V	33	VAL
28	j	10	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Y	110/323 (34%)	107 (97%)	3 (3%)	39	62
5	D	189/196 (96%)	188 (100%)	1 (0%)	81	80
6	E	318/323 (98%)	317 (100%)	1 (0%)	86	83
7	F	288/289 (100%)	287 (100%)	1 (0%)	86	83
8	G	235/245 (96%)	235 (100%)	0	100	100
9	H	131/153 (86%)	131 (100%)	0	100	100
10	I	185/205 (90%)	185 (100%)	0	100	100
11	J	182/208 (88%)	182 (100%)	0	100	100
12	K	168/171 (98%)	168 (100%)	0	100	100
13	M	146/150 (97%)	146 (100%)	0	100	100
14	N	153/159 (96%)	151 (99%)	2 (1%)	61	72
15	O	107/109 (98%)	107 (100%)	0	100	100
16	Q	87/91 (96%)	87 (100%)	0	100	100
17	R	69/72 (96%)	68 (99%)	1 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	a	175/176 (99%)	174 (99%)	1 (1%)	78	79
20	b	160/162 (99%)	160 (100%)	0	100	100
21	c	140/146 (96%)	139 (99%)	1 (1%)	76	78
22	d	150/151 (99%)	149 (99%)	1 (1%)	76	78
23	e	125/154 (81%)	124 (99%)	1 (1%)	73	77
24	f	155/156 (99%)	154 (99%)	1 (1%)	78	79
25	g	136/137 (99%)	136 (100%)	0	100	100
26	h	84/107 (78%)	84 (100%)	0	100	100
27	i	102/105 (97%)	101 (99%)	1 (1%)	68	75
28	j	54/129 (42%)	54 (100%)	0	100	100
29	k	104/118 (88%)	104 (100%)	0	100	100
30	l	108/110 (98%)	108 (100%)	0	100	100
31	m	115/116 (99%)	115 (100%)	0	100	100
32	n	118/119 (99%)	116 (98%)	2 (2%)	53	70
33	o	46/47 (98%)	46 (100%)	0	100	100
34	p	81/88 (92%)	81 (100%)	0	100	100
35	q	92/97 (95%)	92 (100%)	0	100	100
36	r	108/111 (97%)	108 (100%)	0	100	100
37	s	90/91 (99%)	90 (100%)	0	100	100
38	t	94/103 (91%)	92 (98%)	2 (2%)	47	66
39	u	104/105 (99%)	104 (100%)	0	100	100
40	v	78/82 (95%)	77 (99%)	1 (1%)	61	72
41	w	69/71 (97%)	68 (99%)	1 (1%)	59	71
42	x	67/69 (97%)	67 (100%)	0	100	100
43	y	45/46 (98%)	45 (100%)	0	100	100
44	z	46/116 (40%)	46 (100%)	0	100	100
45	V	339/467 (73%)	336 (99%)	3 (1%)	70	76
46	L	32/65 (49%)	32 (100%)	0	100	100
47	X	186/211 (88%)	186 (100%)	0	100	100
All	All	5571/6349 (88%)	5547 (100%)	24 (0%)	81	81

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Y	235	CYS
4	Y	330	VAL
4	Y	331	ILE
5	D	88	ILE
6	E	104	THR
7	F	74	ILE
14	N	54	LEU
14	N	124	ILE
17	R	42	CYS
19	a	50	ARG
21	c	114	VAL
22	d	122	ILE
23	e	99	LEU
24	f	24	LEU
27	i	102	ILE
32	n	4	ARG
32	n	133	LEU
38	t	47	CYS
38	t	95	ILE
40	v	57	LEU
41	w	22	CYS
45	V	22	CYS
45	V	89	LEU
45	V	143	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
4	Y	274	GLN
4	Y	343	GLN
5	D	79	ASN
5	D	132	ASN
5	D	209	HIS
5	D	218	HIS
6	E	173	GLN
6	E	224	HIS
7	F	43	ASN
7	F	221	ASN
7	F	237	GLN
7	F	361	HIS
8	G	90	HIS
8	G	151	GLN
8	G	264	GLN

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Mol	Chain	Res	Type
9	H	28	GLN
9	H	138	GLN
9	H	167	ASN
10	I	61	ASN
10	I	64	GLN
10	I	112	ASN
10	I	200	ASN
10	I	244	ASN
11	J	24	ASN
11	J	38	GLN
11	J	61	GLN
11	J	95	ASN
11	J	138	HIS
11	J	221	ASN
11	J	240	ASN
11	J	243	GLN
12	K	9	GLN
12	K	149	ASN
14	N	19	GLN
14	N	25	HIS
14	N	137	GLN
15	O	41	GLN
19	a	37	HIS
19	a	70	ASN
20	b	55	HIS
21	c	133	HIS
22	d	5	HIS
22	d	15	HIS
23	e	58	HIS
24	f	8	GLN
24	f	142	GLN
25	g	22	HIS
25	g	131	GLN
27	i	98	ASN
28	j	32	GLN
31	m	36	HIS
31	m	57	HIS
32	n	14	HIS
32	n	41	HIS
32	n	74	ASN
32	n	120	ASN
34	p	36	GLN

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Mol	Chain	Res	Type
35	q	21	HIS
35	q	57	GLN
36	r	20	HIS
36	r	52	GLN
38	t	69	HIS
39	u	59	ASN
39	u	99	GLN
39	u	108	GLN
41	w	57	HIS
42	x	10	GLN
42	x	67	GLN
43	y	43	ASN
44	z	90	ASN
44	z	109	ASN
45	V	108	HIS
45	V	119	GLN
45	V	142	GLN
45	V	167	HIS
45	V	349	ASN
45	V	351	GLN
45	V	364	HIS
47	X	50	HIS
47	X	106	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3200/3396 (94%)	675 (21%)	32 (1%)
2	B	120/121 (99%)	20 (16%)	0
3	C	157/158 (99%)	35 (22%)	1 (0%)
All	All	3477/3675 (94%)	730 (20%)	33 (0%)

All (730) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	22	G
1	A	26	A
1	A	30	G
1	A	40	A
1	A	43	A
1	A	45	A

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Mol	Chain	Res	Type
1	A	49	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A
1	A	71	A
1	A	74	G
1	A	76	G
1	A	92	G
1	A	99	A
1	A	109	A
1	A	110	G
1	A	116	A
1	A	117	U
1	A	118	U
1	A	122	A
1	A	136	G
1	A	155	G
1	A	156	G
1	A	157	A
1	A	166	C
1	A	168	U
1	A	171	G
1	A	173	G
1	A	176	G
1	A	181	U
1	A	182	U
1	A	187	A
1	A	190	U
1	A	191	U
1	A	200	C
1	A	206	G
1	A	210	U
1	A	211	A
1	A	213	A
1	A	218	G
1	A	219	A
1	A	240	U
1	A	241	G
1	A	243	G
1	A	246	U
1	A	247	C

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Mol	Chain	Res	Type
1	A	249	U
1	A	250	U
1	A	251	G
1	A	252	U
1	A	253	A
1	A	269	G
1	A	270	U
1	A	286	U
1	A	295	A
1	A	298	U
1	A	323	A
1	A	329	U
1	A	338	A
1	A	339	C
1	A	343	U
1	A	349	A
1	A	351	A
1	A	372	A
1	A	375	A
1	A	376	G
1	A	382	U
1	A	398	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	406	G
1	A	420	G
1	A	421	G
1	A	422	A
1	A	429	U
1	A	437	G
1	A	439	C
1	A	520	U
1	A	521	A
1	A	532	A
1	A	534	U
1	A	536	U
1	A	543	C
1	A	545	U
1	A	546	C
1	A	547	G

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Mol	Chain	Res	Type
1	A	548	G
1	A	549	U
1	A	551	A
1	A	552	G
1	A	553	U
1	A	555	U
1	A	557	A
1	A	559	A
1	A	578	A
1	A	579	G
1	A	592	A
1	A	597	G
1	A	598	A
1	A	600	G
1	A	603	A
1	A	604	G
1	A	611	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	637	C
1	A	649	A
1	A	660	A
1	A	677	A
1	A	681	U
1	A	683	U
1	A	689	U
1	A	691	A
1	A	692	A
1	A	705	A
1	A	709	A
1	A	712	G
1	A	715	A
1	A	719	U
1	A	720	A
1	A	725	G
1	A	763	G
1	A	767	U
1	A	771	A
1	A	776	U
1	A	777	U
1	A	780	A

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Mol	Chain	Res	Type
1	A	781	G
1	A	785	G
1	A	801	A
1	A	806	A
1	A	808	A
1	A	817	A
1	A	830	A
1	A	846	A
1	A	848	A
1	A	849	C
1	A	861	C
1	A	869	G
1	A	874	U
1	A	879	U
1	A	880	G
1	A	888	A
1	A	890	C
1	A	896	A
1	A	897	U
1	A	907	G
1	A	908	G
1	A	914	A
1	A	915	A
1	A	916	G
1	A	917	A
1	A	924	G
1	A	933	A
1	A	937	G
1	A	941	G
1	A	944	C
1	A	959	C
1	A	960	U
1	A	961	C
1	A	965	A
1	A	967	A
1	A	974	G
1	A	978	G
1	A	979	U
1	A	980	A
1	A	981	U
1	A	982	C
1	A	984	G

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Mol	Chain	Res	Type
1	A	991	G
1	A	995	U
1	A	1001	G
1	A	1002	A
1	A	1006	A
1	A	1008	U
1	A	1009	A
1	A	1010	G
1	A	1013	G
1	A	1014	U
1	A	1015	U
1	A	1016	C
1	A	1017	C
1	A	1018	G
1	A	1020	G
1	A	1021	G
1	A	1022	U
1	A	1026	A
1	A	1027	A
1	A	1028	U
1	A	1029	G
1	A	1030	A
1	A	1035	G
1	A	1036	A
1	A	1037	C
1	A	1038	C
1	A	1039	U
1	A	1040	A
1	A	1041	U
1	A	1042	U
1	A	1045	C
1	A	1047	A
1	A	1049	C
1	A	1064	A
1	A	1065	A
1	A	1069	C
1	A	1081	U
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1096	U
1	A	1097	G

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Mol	Chain	Res	Type
1	A	1098	A
1	A	1103	A
1	A	1104	G
1	A	1117	G
1	A	1124	U
1	A	1131	G
1	A	1140	G
1	A	1144	U
1	A	1153	A
1	A	1157	G
1	A	1159	A
1	A	1171	G
1	A	1179	A
1	A	1180	A
1	A	1181	U
1	A	1192	C
1	A	1196	C
1	A	1201	C
1	A	1209	G
1	A	1212	A
1	A	1213	G
1	A	1222	G
1	A	1223	A
1	A	1229	G
1	A	1235	U
1	A	1236	G
1	A	1237	G
1	A	1239	C
1	A	1241	U
1	A	1242	G
1	A	1244	A
1	A	1245	A
1	A	1246	G
1	A	1248	C
1	A	1251	A
1	A	1252	A
1	A	1253	U
1	A	1258	U
1	A	1262	G
1	A	1263	A
1	A	1264	G
1	A	1266	G

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Mol	Chain	Res	Type
1	A	1272	C
1	A	1273	A
1	A	1282	G
1	A	1285	G
1	A	1286	A
1	A	1292	C
1	A	1307	G
1	A	1309	U
1	A	1312	C
1	A	1313	G
1	A	1330	A
1	A	1348	U
1	A	1349	G
1	A	1350	A
1	A	1351	U
1	A	1352	A
1	A	1353	U
1	A	1354	G
1	A	1355	A
1	A	1356	U
1	A	1357	G
1	A	1372	C
1	A	1383	G
1	A	1386	A
1	A	1399	A
1	A	1400	G
1	A	1419	A
1	A	1427	U
1	A	1429	G
1	A	1430	U
1	A	1434	G
1	A	1437	C
1	A	1446	A
1	A	1450	G
1	A	1455	U
1	A	1481	A
1	A	1484	U
1	A	1503	A
1	A	1508	C
1	A	1523	U
1	A	1533	U
1	A	1536	G

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Mol	Chain	Res	Type
1	A	1555	U
1	A	1556	C
1	A	1557	A
1	A	1560	G
1	A	1562	C
1	A	1563	C
1	A	1564	U
1	A	1567	U
1	A	1568	U
1	A	1569	U
1	A	1570	U
1	A	1572	U
1	A	1573	G
1	A	1576	G
1	A	1577	G
1	A	1579	C
1	A	1581	C
1	A	1582	C
1	A	1583	A
1	A	1589	A
1	A	1593	A
1	A	1603	A
1	A	1618	G
1	A	1619	A
1	A	1620	U
1	A	1629	U
1	A	1642	A
1	A	1643	A
1	A	1644	C
1	A	1645	U
1	A	1650	G
1	A	1657	C
1	A	1662	G
1	A	1677	G
1	A	1683	A
1	A	1688	U
1	A	1716	U
1	A	1717	U
1	A	1724	U
1	A	1725	C
1	A	1730	G
1	A	1736	G

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Mol	Chain	Res	Type
1	A	1741	A
1	A	1749	A
1	A	1750	A
1	A	1751	G
1	A	1756	C
1	A	1760	A
1	A	1762	C
1	A	1765	U
1	A	1766	G
1	A	1770	G
1	A	1780	G
1	A	1790	G
1	A	1793	C
1	A	1797	A
1	A	1814	A
1	A	1816	A
1	A	1817	G
1	A	1820	U
1	A	1821	U
1	A	1839	A
1	A	1842	A
1	A	1845	G
1	A	1846	C
1	A	1849	C
1	A	1850	A
1	A	1874	A
1	A	1878	G
1	A	1880	U
1	A	1886	A
1	A	1893	A
1	A	1906	G
1	A	1909	A
1	A	1915	A
1	A	1926	C
1	A	1927	G
1	A	1930	A
1	A	1951	C
1	A	1952	G
1	A	1953	G
1	A	1954	G
1	A	2101	C
1	A	2102	U

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Mol	Chain	Res	Type
1	A	2111	G
1	A	2113	A
1	A	2114	C
1	A	2121	G
1	A	2122	G
1	A	2131	A
1	A	2139	A
1	A	2140	U
1	A	2158	A
1	A	2169	G
1	A	2176	U
1	A	2184	U
1	A	2185	G
1	A	2198	A
1	A	2205	U
1	A	2209	U
1	A	2210	G
1	A	2246	G
1	A	2252	A
1	A	2253	G
1	A	2255	A
1	A	2256	A
1	A	2257	C
1	A	2258	U
1	A	2259	A
1	A	2260	U
1	A	2261	G
1	A	2264	U
1	A	2267	C
1	A	2269	U
1	A	2270	A
1	A	2271	A
1	A	2272	G
1	A	2273	G
1	A	2282	U
1	A	2285	C
1	A	2286	U
1	A	2287	C
1	A	2288	G
1	A	2298	U
1	A	2307	G
1	A	2308	C

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Mol	Chain	Res	Type
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2334	U
1	A	2335	G
1	A	2372	A
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2385	G
1	A	2393	G
1	A	2394	G
1	A	2397	A
1	A	2401	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2411	U
1	A	2412	G
1	A	2415	C
1	A	2418	G
1	A	2435	G
1	A	2437	G
1	A	2440	G
1	A	2447	A
1	A	2448	G
1	A	2449	A
1	A	2450	G
1	A	2452	G
1	A	2453	U
1	A	2454	G
1	A	2456	A
1	A	2457	G
1	A	2458	A
1	A	2459	A
1	A	2460	U
1	A	2461	A
1	A	2462	A
1	A	2463	G
1	A	2464	U
1	A	2465	G

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Mol	Chain	Res	Type
1	A	2468	A
1	A	2471	U
1	A	2472	U
1	A	2473	C
1	A	2474	G
1	A	2476	C
1	A	2477	G
1	A	2480	A
1	A	2484	A
1	A	2485	A
1	A	2488	A
1	A	2490	C
1	A	2495	C
1	A	2496	C
1	A	2497	U
1	A	2498	U
1	A	2499	U
1	A	2502	A
1	A	2503	G
1	A	2505	U
1	A	2506	U
1	A	2507	C
1	A	2508	U
1	A	2509	U
1	A	2514	U
1	A	2515	A
1	A	2522	G
1	A	2524	A
1	A	2525	G
1	A	2531	C
1	A	2533	G
1	A	2537	U
1	A	2538	U
1	A	2539	C
1	A	2540	A
1	A	2541	U
1	A	2542	U
1	A	2543	U
1	A	2544	U
1	A	2549	G
1	A	2550	U
1	A	2552	C

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Mol	Chain	Res	Type
1	A	2554	A
1	A	2561	A
1	A	2562	A
1	A	2569	A
1	A	2570	U
1	A	2571	U
1	A	2572	C
1	A	2573	G
1	A	2576	G
1	A	2577	C
1	A	2585	G
1	A	2593	A
1	A	2594	C
1	A	2600	C
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2648	G
1	A	2652	U
1	A	2656	A
1	A	2674	A
1	A	2677	G
1	A	2689	A
1	A	2691	A
1	A	2696	A
1	A	2704	A
1	A	2705	A
1	A	2714	G
1	A	2719	U
1	A	2728	G
1	A	2729	U
1	A	2746	A
1	A	2753	G
1	A	2755	C
1	A	2772	C
1	A	2777	G
1	A	2778	G
1	A	2799	A
1	A	2800	G
1	A	2801	A
1	A	2802	A
1	A	2803	A

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Mol	Chain	Res	Type
1	A	2810	C
1	A	2814	G
1	A	2816	G
1	A	2817	A
1	A	2818	U
1	A	2828	G
1	A	2842	U
1	A	2843	U
1	A	2844	C
1	A	2845	A
1	A	2847	A
1	A	2850	G
1	A	2860	U
1	A	2861	U
1	A	2867	C
1	A	2871	G
1	A	2872	A
1	A	2875	U
1	A	2887	A
1	A	2888	U
1	A	2899	C
1	A	2904	U
1	A	2916	U
1	A	2923	U
1	A	2928	C
1	A	2935	U
1	A	2936	A
1	A	2941	A
1	A	2947	G
1	A	2951	G
1	A	2971	A
1	A	2983	C
1	A	2986	U
1	A	2990	G
1	A	2996	U
1	A	2997	G
1	A	3011	A
1	A	3012	A
1	A	3046	A
1	A	3059	G
1	A	3072	C
1	A	3078	U

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Mol	Chain	Res	Type
1	A	3080	G
1	A	3086	A
1	A	3092	C
1	A	3104	U
1	A	3116	G
1	A	3122	A
1	A	3124	G
1	A	3129	A
1	A	3130	A
1	A	3131	U
1	A	3142	A
1	A	3143	C
1	A	3150	A
1	A	3153	U
1	A	3154	C
1	A	3156	U
1	A	3157	U
1	A	3158	G
1	A	3165	A
1	A	3173	G
1	A	3174	A
1	A	3175	U
1	A	3176	G
1	A	3179	U
1	A	3181	C
1	A	3187	A
1	A	3196	U
1	A	3199	G
1	A	3206	C
1	A	3207	U
1	A	3210	A
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3229	G
1	A	3234	A
1	A	3243	A
1	A	3245	A
1	A	3247	G
1	A	3253	G
1	A	3259	U
1	A	3263	G

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Mol	Chain	Res	Type
1	A	3268	A
1	A	3269	U
1	A	3270	U
1	A	3273	A
1	A	3275	U
1	A	3276	G
1	A	3279	A
1	A	3286	G
1	A	3287	U
1	A	3289	G
1	A	3293	U
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3308	C
1	A	3313	U
1	A	3316	A
1	A	3318	G
1	A	3319	U
1	A	3320	A
1	A	3321	C
1	A	3324	C
1	A	3341	U
1	A	3345	G
1	A	3350	C
1	A	3351	U
1	A	3352	U
1	A	3353	G
1	A	3355	U
1	A	3356	G
1	A	3360	C
1	A	3362	A
1	A	3363	U
1	A	3368	U
1	A	3369	G
1	A	3375	A
1	A	3378	C
1	A	3382	U
1	A	3386	G
2	B	11	A
2	B	18	C
2	B	22	A

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Mol	Chain	Res	Type
2	B	49	G
2	B	52	G
2	B	53	U
2	B	54	U
2	B	65	G
2	B	71	G
2	B	73	C
2	B	76	A
2	B	80	G
2	B	83	U
2	B	95	A
2	B	99	G
2	B	100	C
2	B	102	A
2	B	112	G
2	B	114	U
2	B	121	U
3	C	2	A
3	C	23	U
3	C	34	U
3	C	35	C
3	C	39	G
3	C	42	G
3	C	49	G
3	C	53	A
3	C	59	A
3	C	62	C
3	C	63	G
3	C	67	U
3	C	80	A
3	C	82	U
3	C	83	C
3	C	84	C
3	C	86	U
3	C	87	G
3	C	90	U
3	C	95	G
3	C	102	U
3	C	104	A
3	C	106	C
3	C	111	A
3	C	113	U

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Mol	Chain	Res	Type
3	C	116	G
3	C	125	U
3	C	126	A
3	C	127	U
3	C	138	A
3	C	148	G
3	C	151	C
3	C	155	A
3	C	157	U
3	C	158	U

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	239	G
1	A	547	G
1	A	599	C
1	A	916	G
1	A	979	U
1	A	1027	A
1	A	1029	G
1	A	1038	C
1	A	1064	A
1	A	1097	G
1	A	1103	A
1	A	1222	G
1	A	1241	U
1	A	1352	A
1	A	1355	A
1	A	1554	U
1	A	1576	G
1	A	1716	U
1	A	1815	U
1	A	1816	A
1	A	2101	C
1	A	2112	U
1	A	2209	U
1	A	2255	A
1	A	2453	U
1	A	2495	C
1	A	2501	U
1	A	2541	U

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Mol	Chain	Res	Type
1	A	3121	U
1	A	3218	A
1	A	3228	C
1	A	3269	U
3	C	85	G

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.

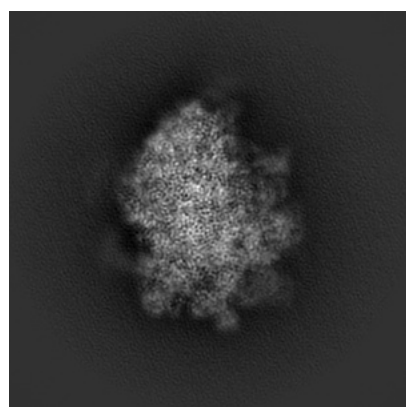
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0372. These allow visual inspection of the internal detail of the map and identification of artifacts.

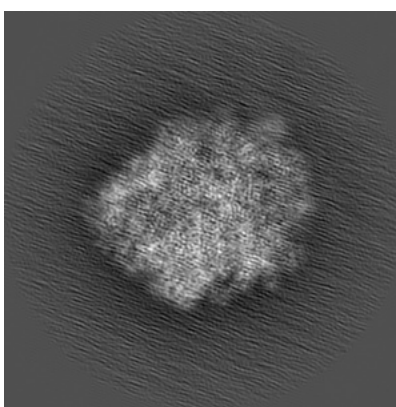
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

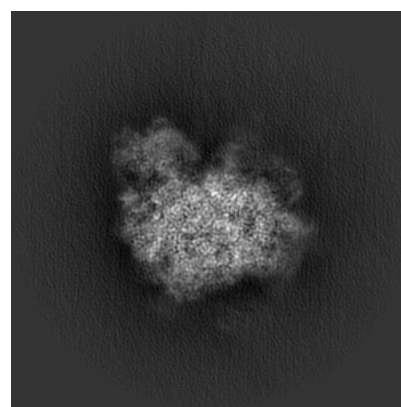
6.1.1 Primary map



X



Y

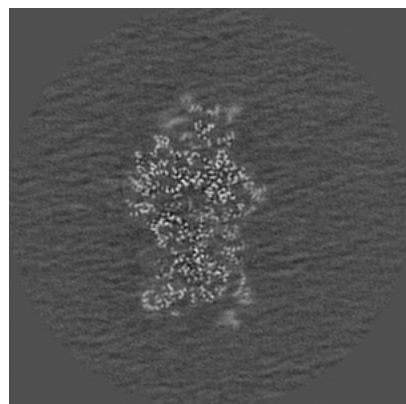


Z

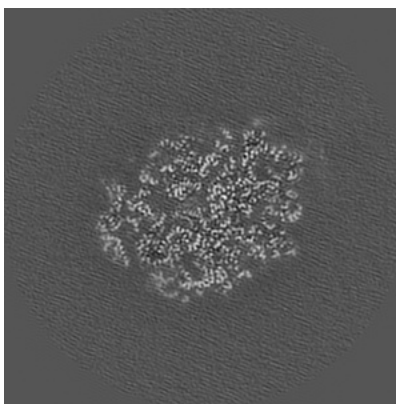
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

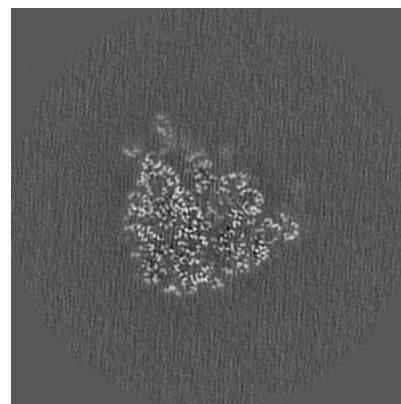
6.2.1 Primary map



X Index: 192



Y Index: 192

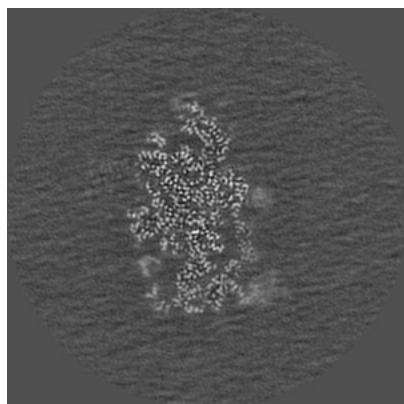


Z Index: 192

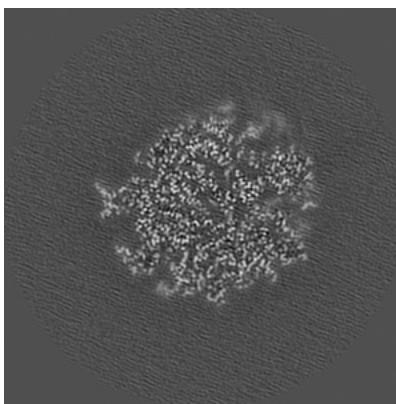
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

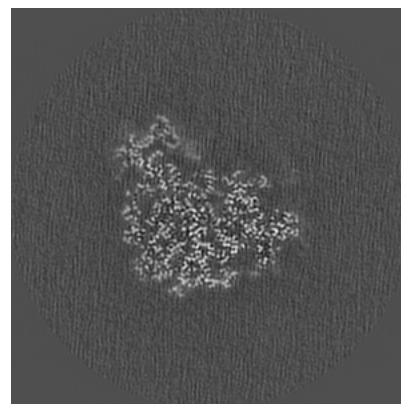
6.3.1 Primary map



X Index: 207



Y Index: 176

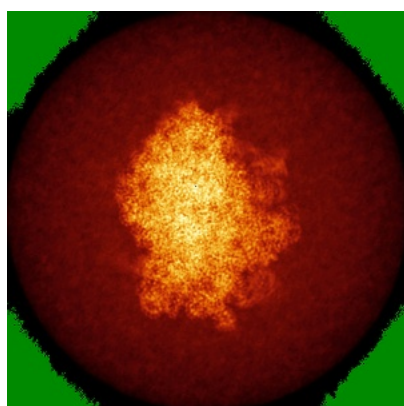


Z Index: 185

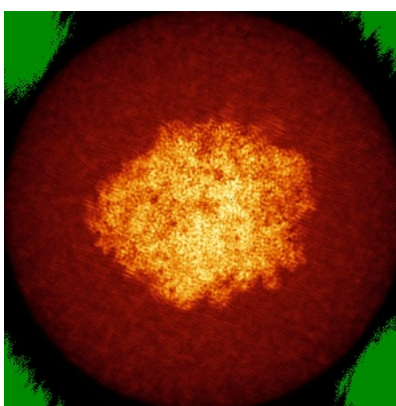
The images above show the largest variance slices of the map in three orthogonal directions.

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

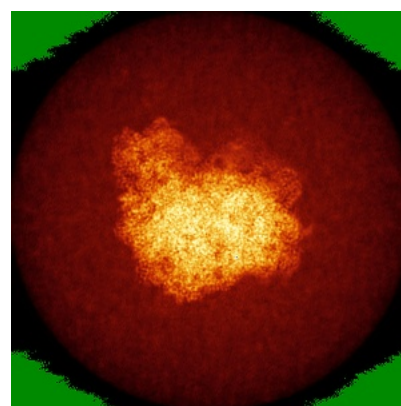
6.4.1 Primary map



X



Y

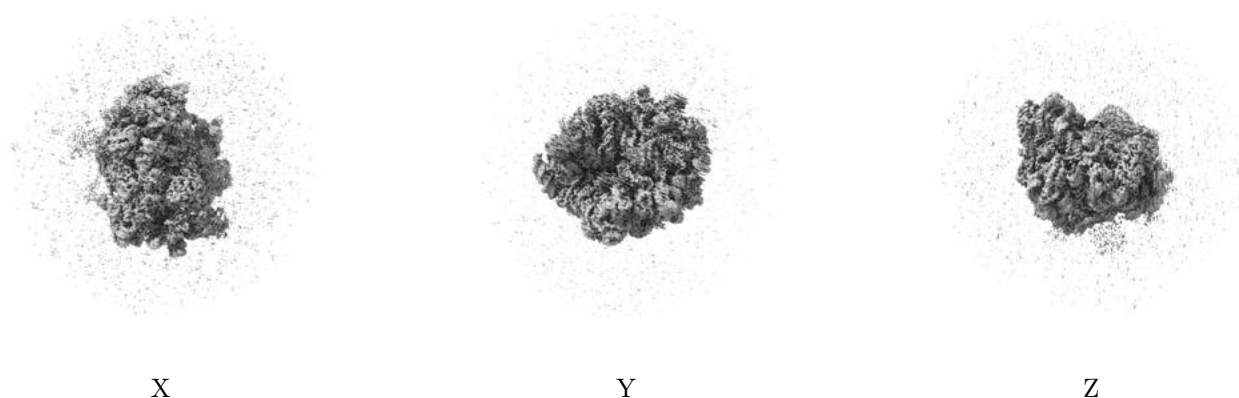


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

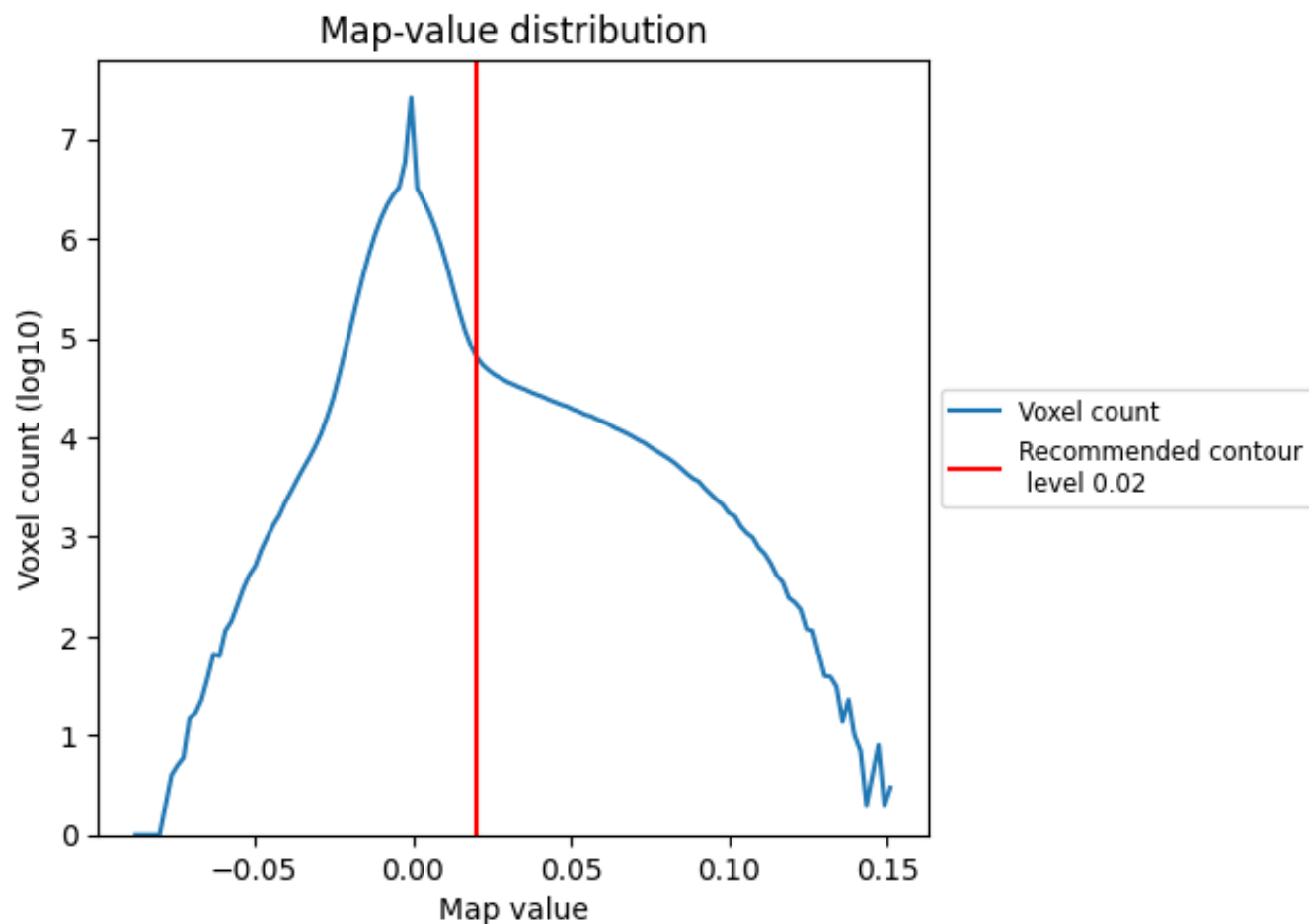
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

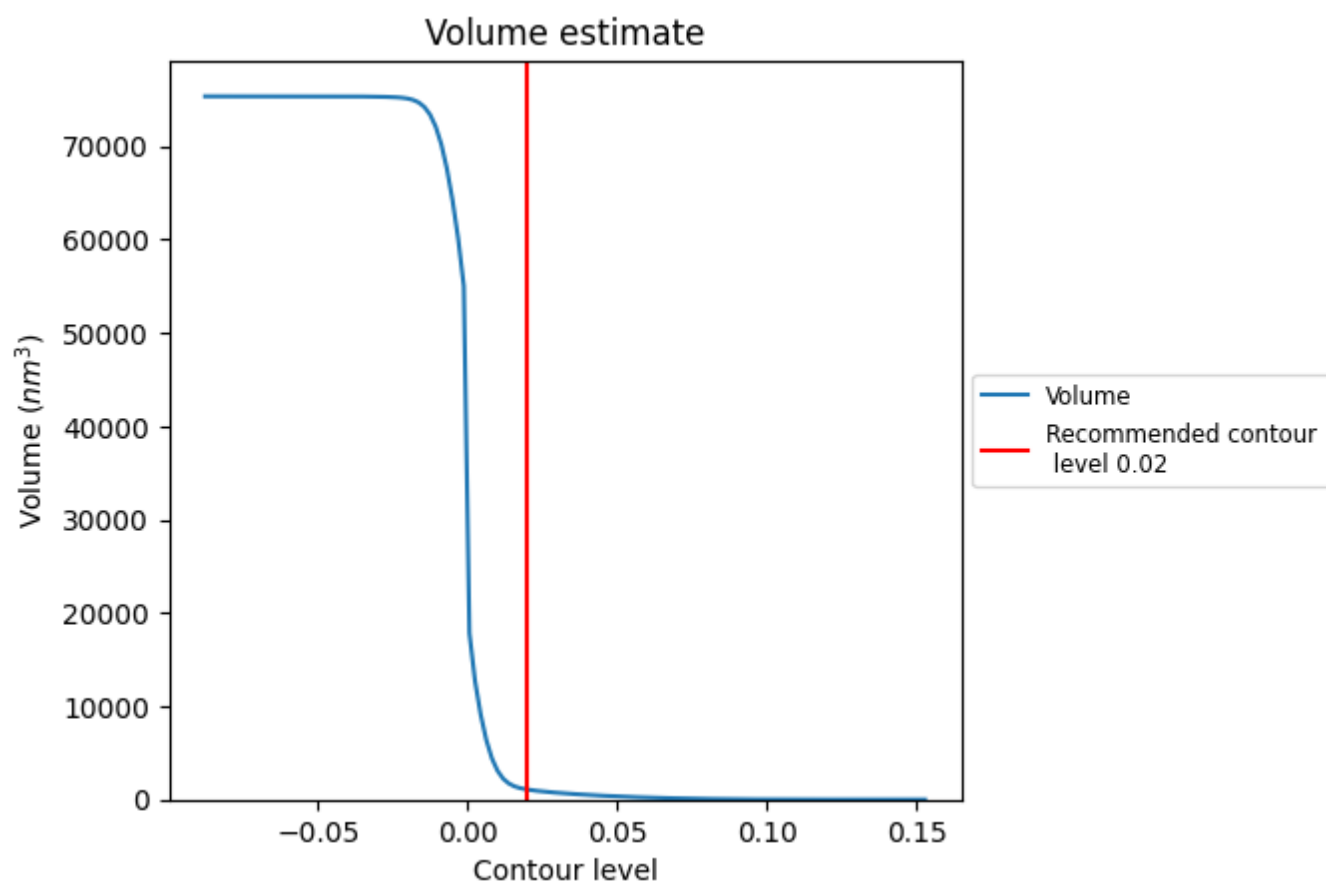
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

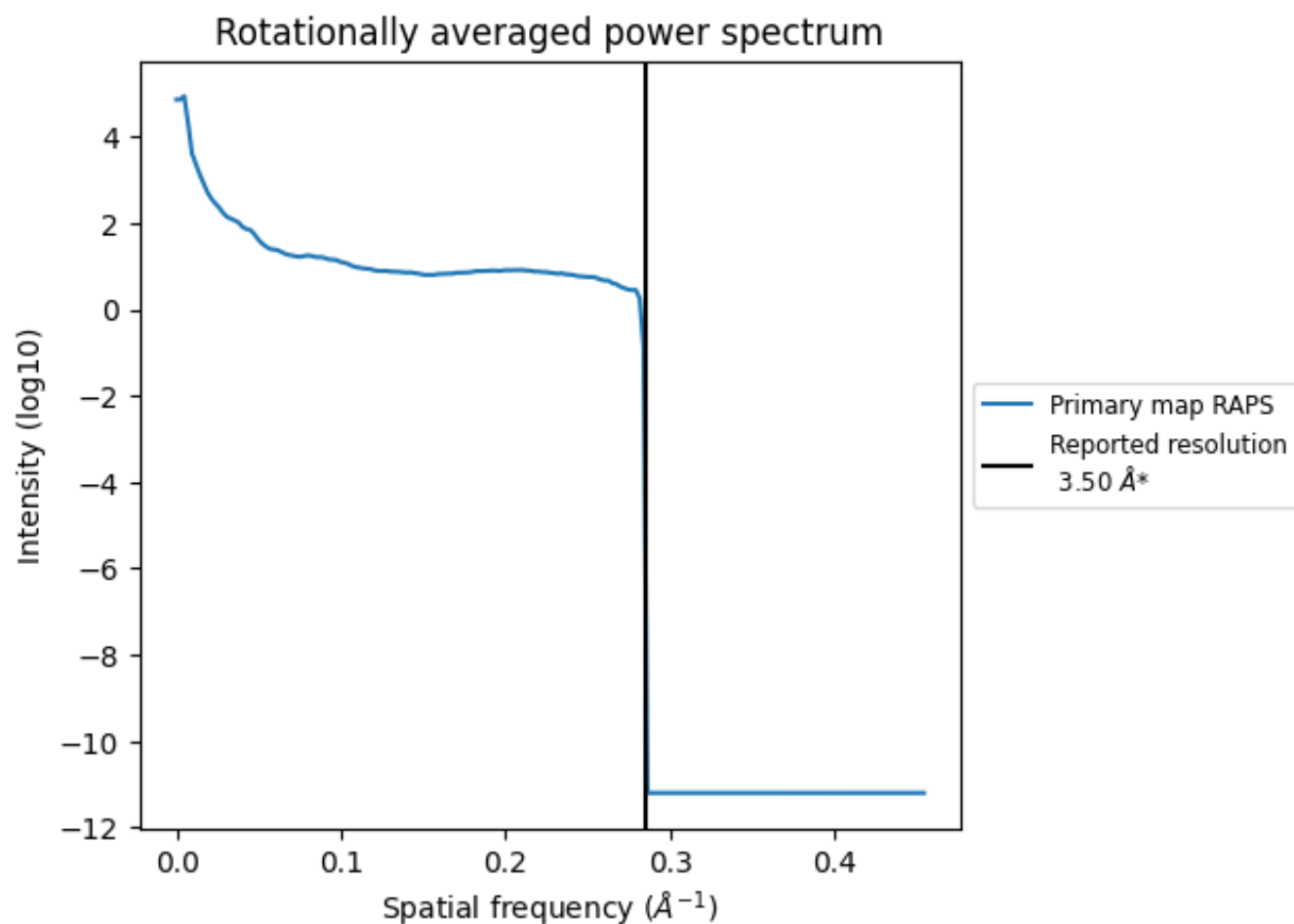
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1078 nm³; this corresponds to an approximate mass of 974 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 ⓘ

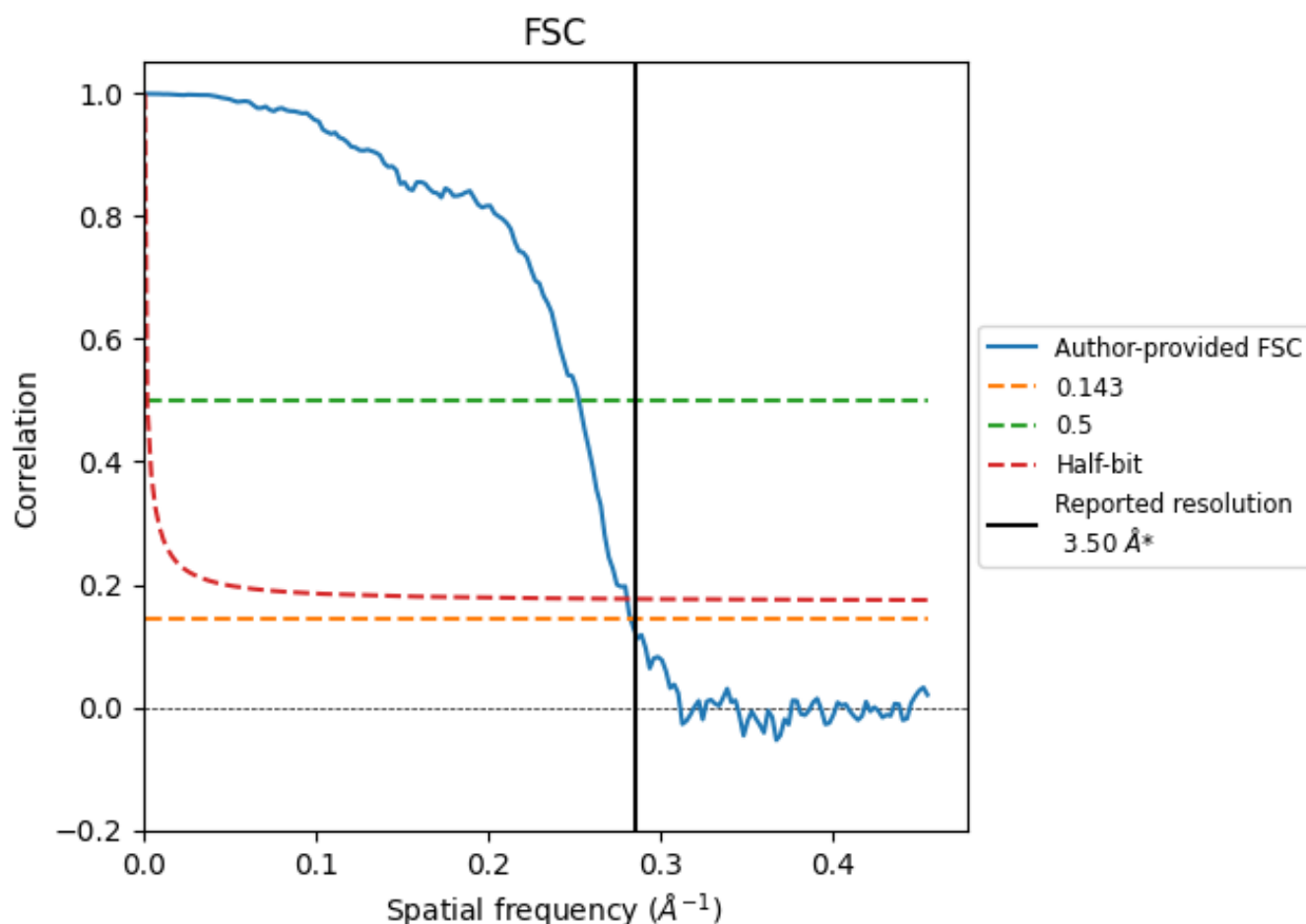


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

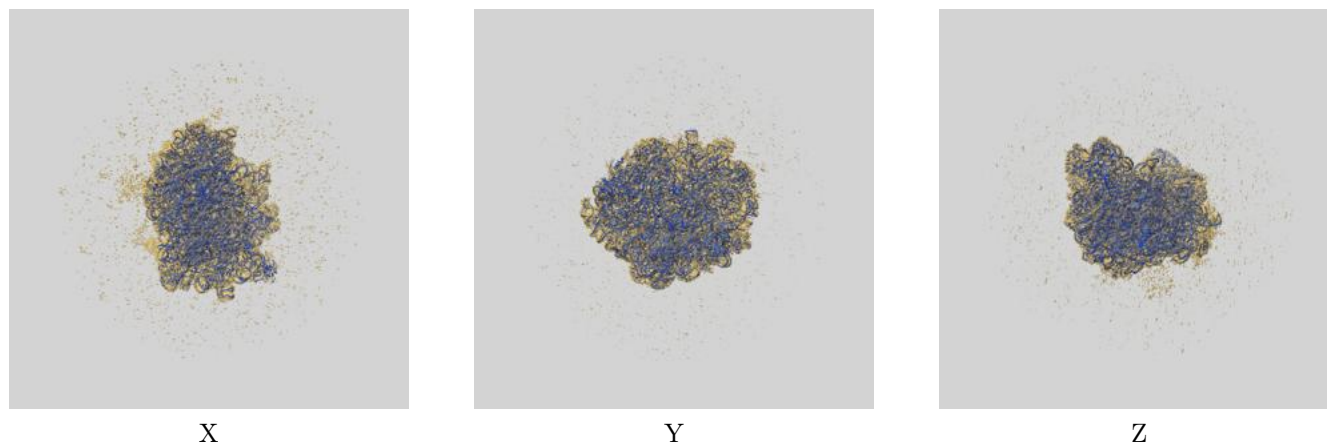
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.54	3.96	3.57
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

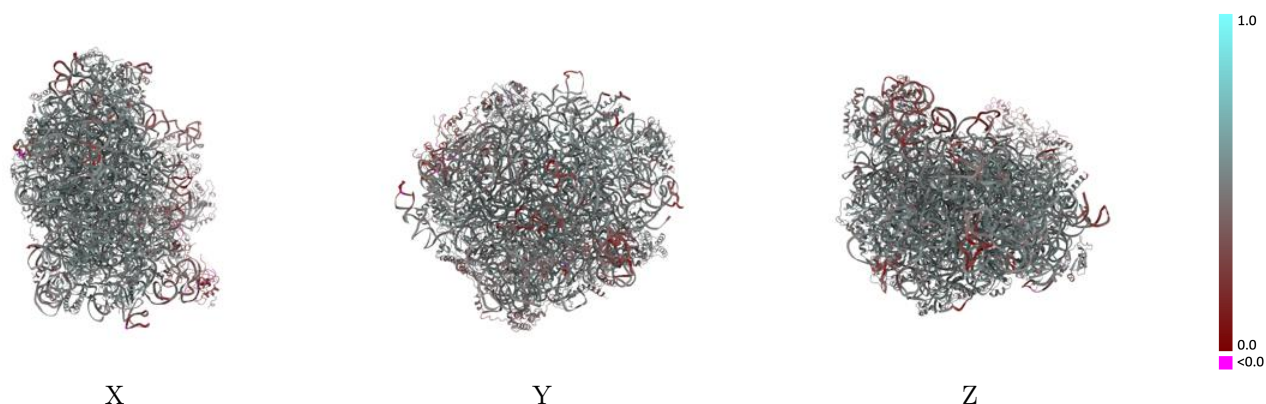
This section contains information regarding the fit between EMDB map EMD-0372 and PDB model 6N8M. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



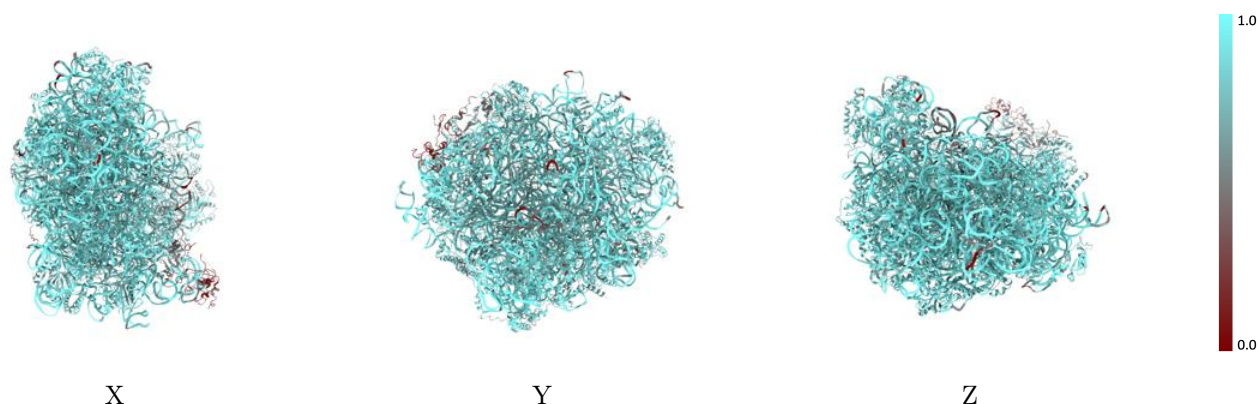
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



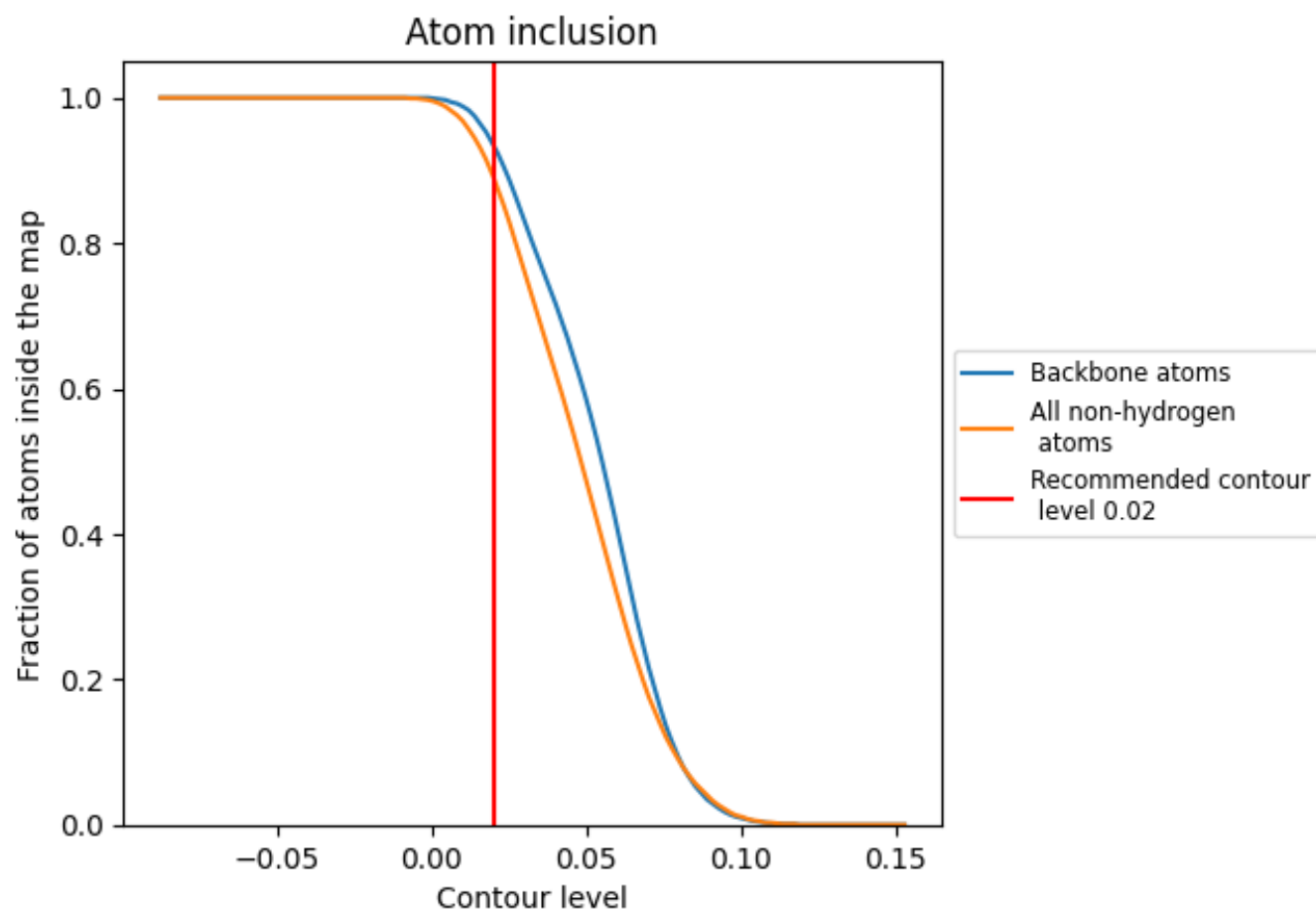
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.4880
A	 0.9380	 0.4870
B	 0.9640	 0.4810
C	 0.9570	 0.5010
D	 0.8710	 0.5280
E	 0.8770	 0.5190
F	 0.8540	 0.5060
G	 0.8240	 0.4460
H	 0.8370	 0.4930
I	 0.8500	 0.4970
J	 0.8610	 0.4860
K	 0.8610	 0.5020
L	 0.2670	 0.2670
M	 0.7810	 0.4210
N	 0.8540	 0.4950
O	 0.8720	 0.5020
Q	 0.8250	 0.5110
R	 0.8740	 0.5210
S	 0.8270	 0.3980
V	 0.7140	 0.4440
X	 0.7670	 0.4660
Y	 0.4550	 0.3580
a	 0.8750	 0.5260
b	 0.8580	 0.5200
c	 0.8370	 0.5000
d	 0.8440	 0.5070
e	 0.8740	 0.5180
f	 0.8500	 0.5060
g	 0.8200	 0.4970
h	 0.8590	 0.4600
i	 0.8220	 0.5190
j	 0.8740	 0.5150
k	 0.8540	 0.5040
l	 0.8510	 0.5060
m	 0.8550	 0.4940



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Chain	Atom inclusion	Q-score
n	 0.8630	 0.5180
o	 0.7990	 0.4670
p	 0.8320	 0.4860
q	 0.8190	 0.4880
r	 0.8450	 0.5220
s	 0.8660	 0.5330
t	 0.8280	 0.5170
u	 0.8590	 0.5010
v	 0.8310	 0.4790
w	 0.9080	 0.5350
x	 0.7850	 0.4760
y	 0.8430	 0.5210
z	 0.7510	 0.4850