



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 07:14 pm BST

PDB ID : 8PVA / pdb_00008pva
EMDB ID : EMD-17959
Title : Structure of bacterial ribosome determined by cryoEM at 100 keV
Authors : McMullan, G.; Naydenova, K.; Mihaylov, D.; Peet, M.J.; Wilson, H.; Yamashita, K.; Dickerson, J.L.; Chen, S.; Cannone, G.; Lee, Y.; Hutchings, K.A.; Gittins, O.; Sobhy, M.; Wells, T.; El-Gomati, M.M.; Dalby, J.; Meffert, M.; Schulze-Briese, C.; Henderson, R.; Russo, C.J.
Deposited on : 2023-07-17
Resolution : 4.50 Å(reported)
Based on initial model : 7k00

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

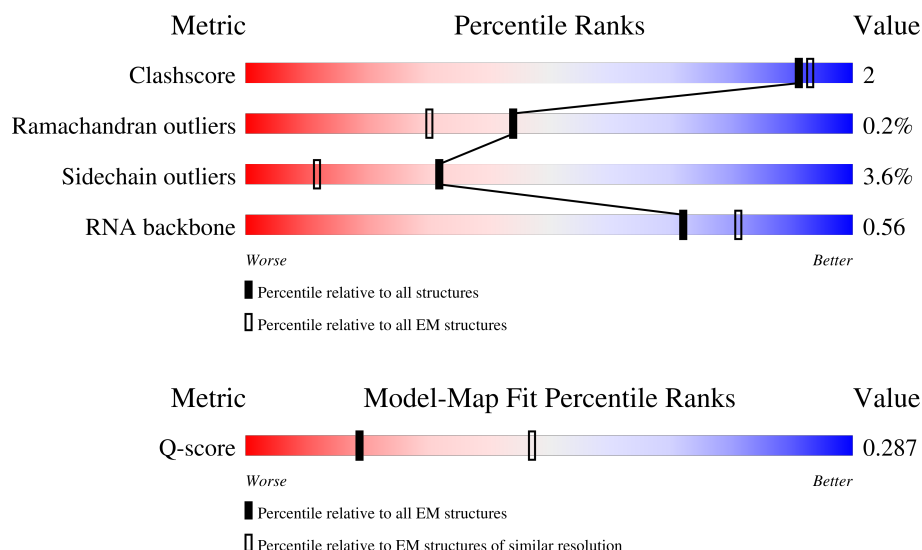
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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	1542	
2	B	241	

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Mol	Chain	Length	Quality of chain
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	

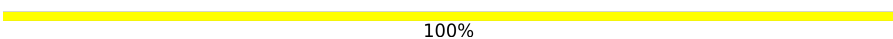
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Mol	Chain	Length	Quality of chain
28	g	177	
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	

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Mol	Chain	Length	Quality of chain
53	X	28	 7% 32% 11% 50%
54	Y	76	 26% 45% 39% 13% 1%
55	Z	76	 11% 53% 39% 8%
56	5	2	 100%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 141565 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

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

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

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 22 is a RNA chain called 23S rRNA.

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

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	12	Total	C	N	O	P	0	0
			260	117	51	80	12		

- Molecule 54 is a RNA chain called A-site tRNA-val.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Y	74	Total	C	N	O	P	0	0
			1579	705	287	514	73		

- Molecule 55 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

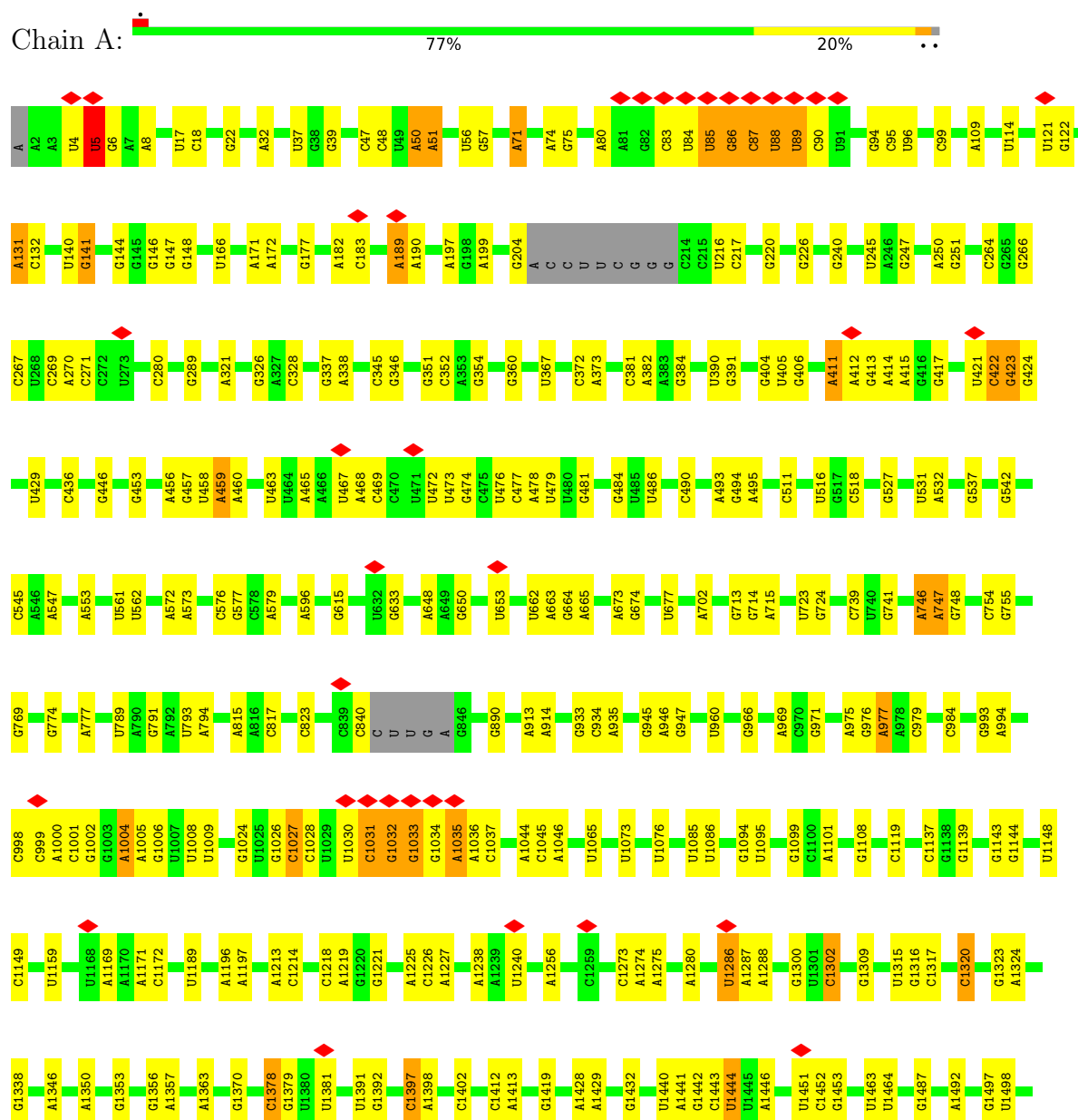
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

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.

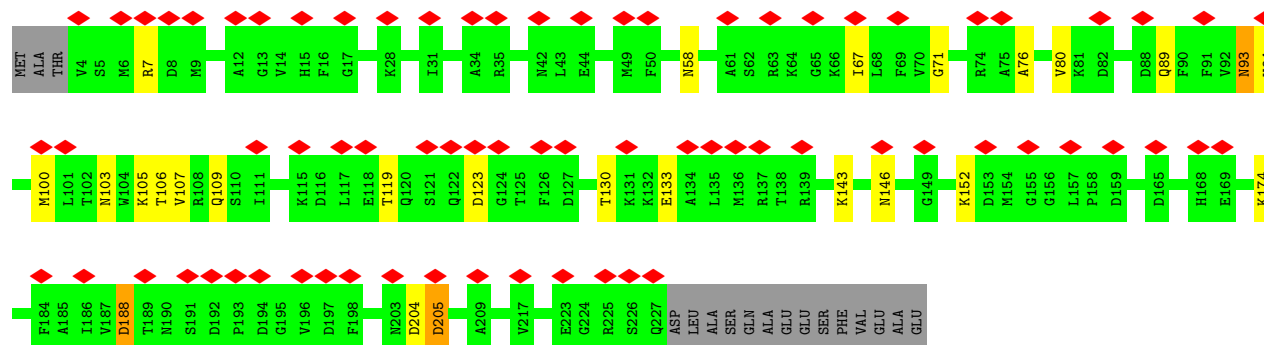
• Molecule 1: 16S rRNA





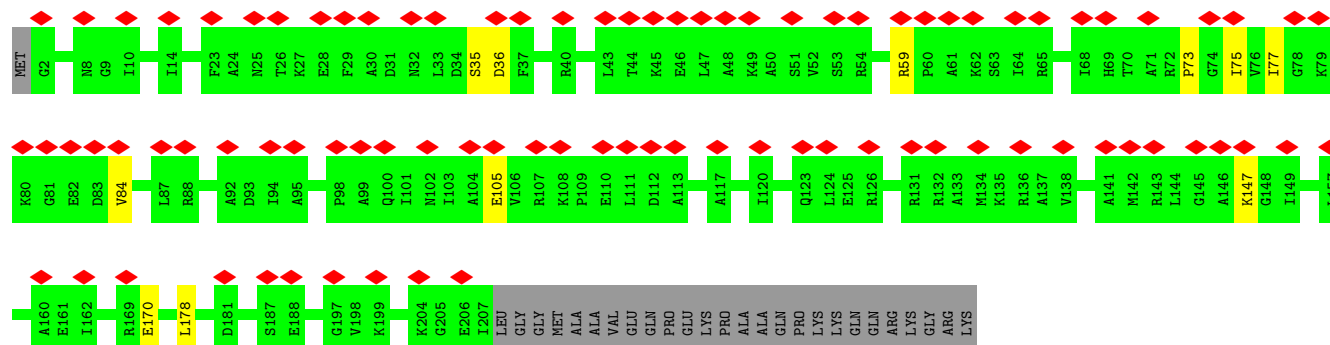
• Molecule 2: Small ribosomal subunit protein uS2

Chain B: 30% 82% 10% 7%



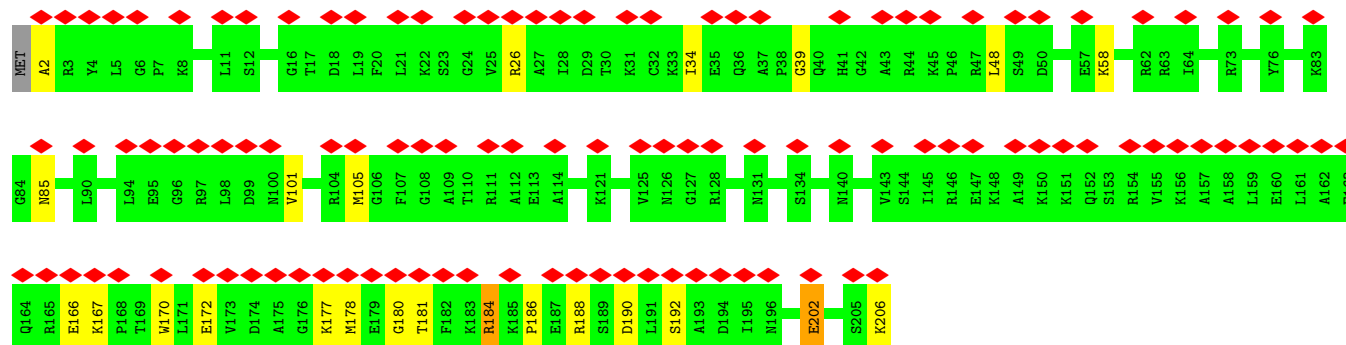
• Molecule 3: Small ribosomal subunit protein uS3

Chain C: 38% 84% 5% 12%

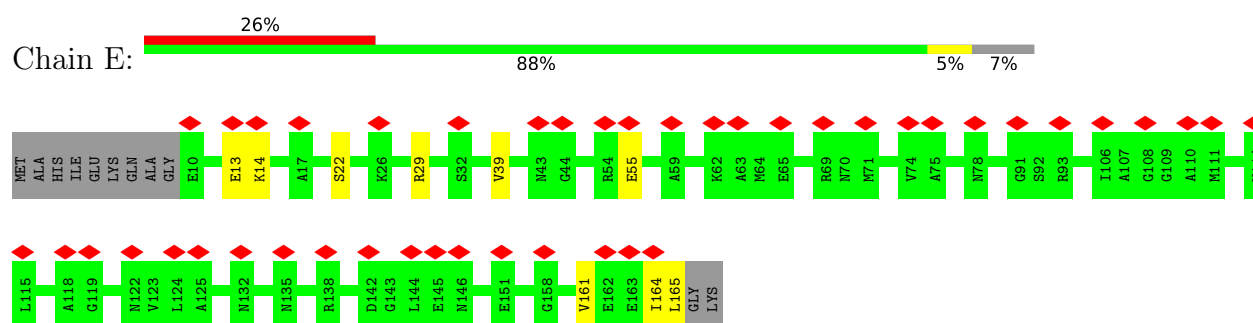


• Molecule 4: Small ribosomal subunit protein uS4

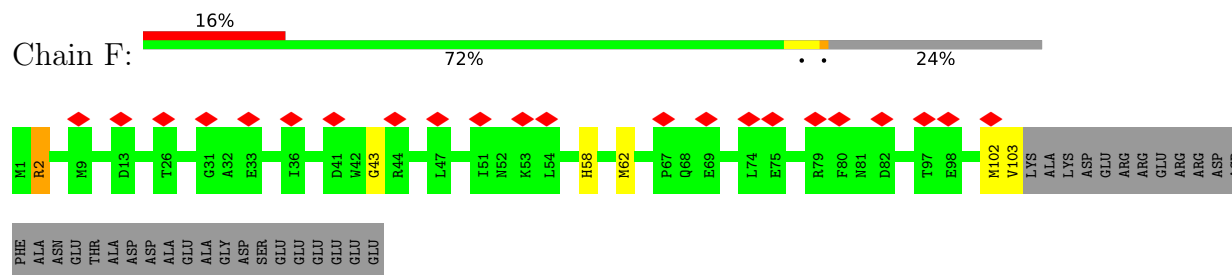
Chain D: 54% 88% 11% 7%



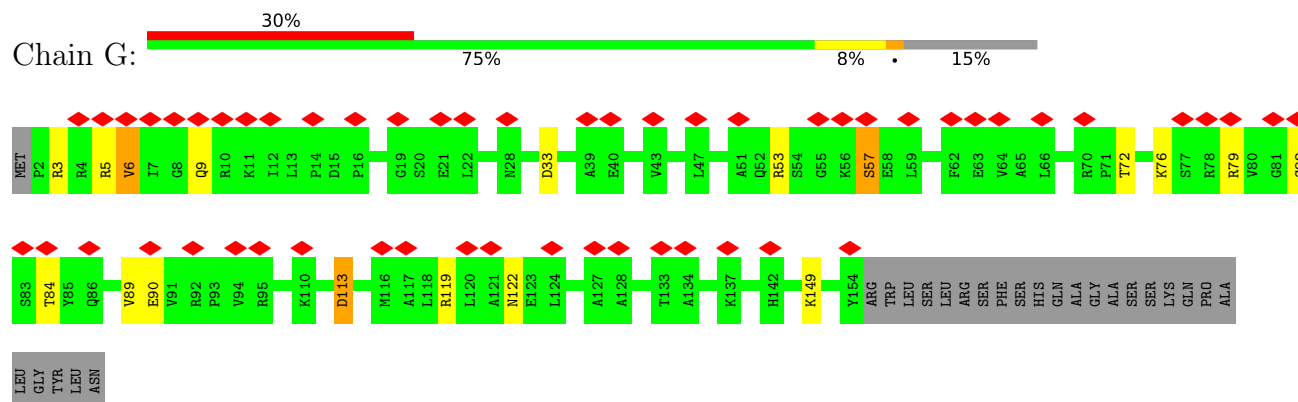
• Molecule 5: Small ribosomal subunit protein uS5



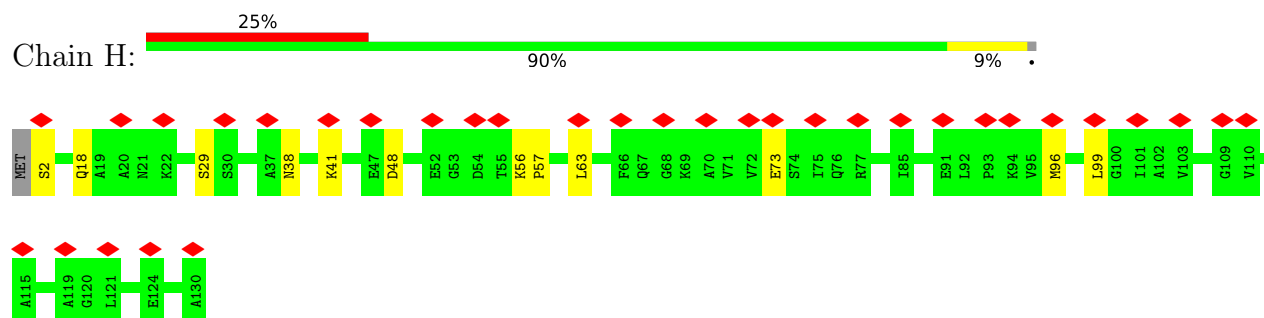
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



- Molecule 7: Small ribosomal subunit protein uS7

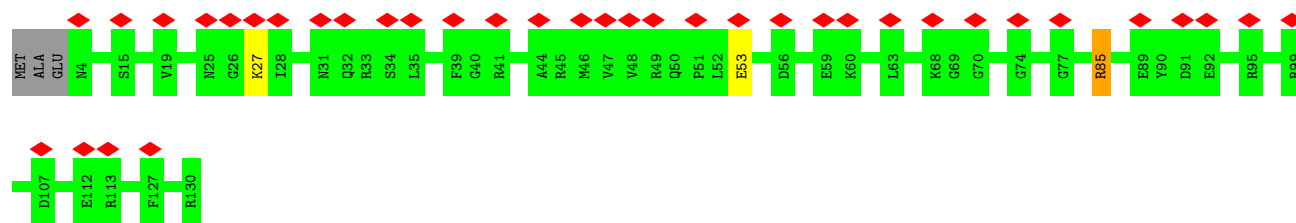


- Molecule 8: Small ribosomal subunit protein uS8

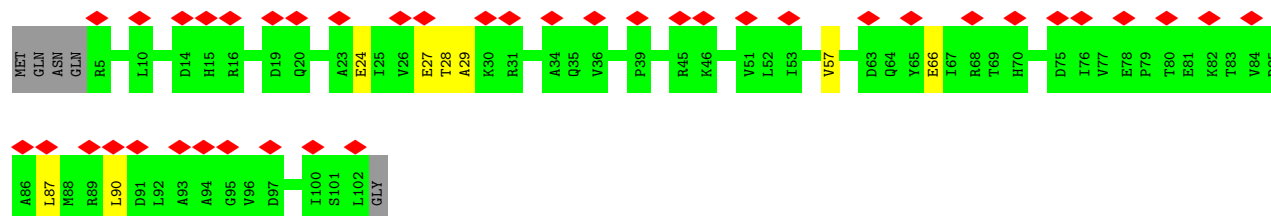
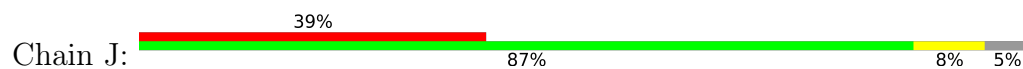


- Molecule 9: Small ribosomal subunit protein uS9

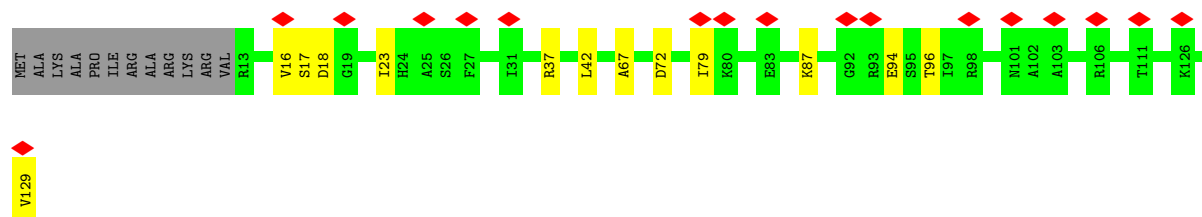
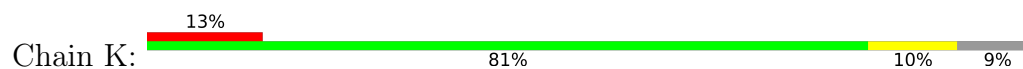




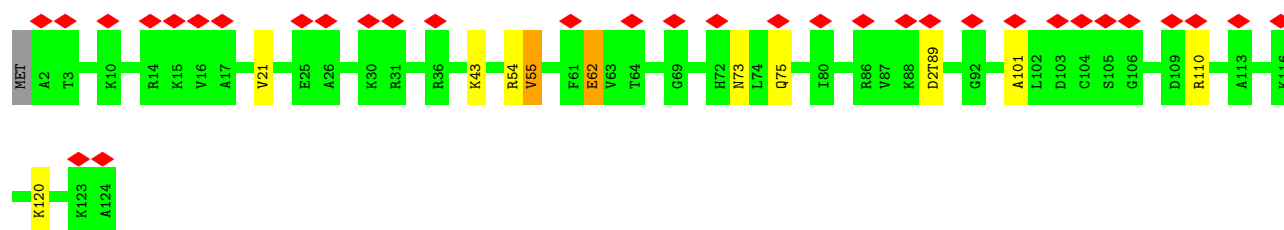
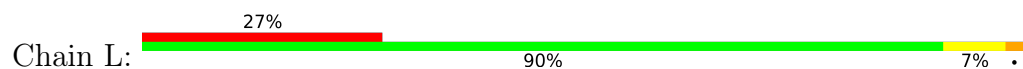
- Molecule 10: Small ribosomal subunit protein uS10



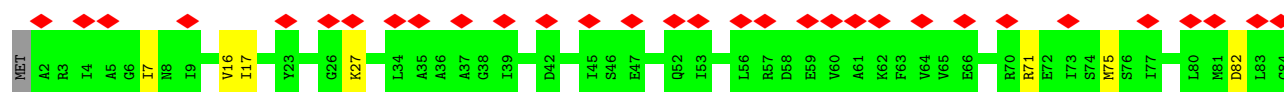
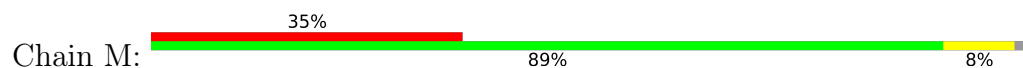
- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein uS12



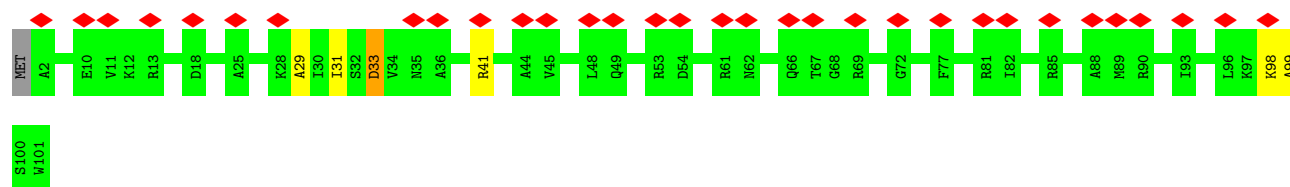
- Molecule 13: Small ribosomal subunit protein uS13





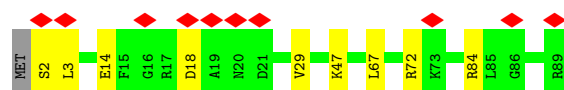
- Molecule 14: Small ribosomal subunit protein uS14

Chain N: 32% 93% 5% ..



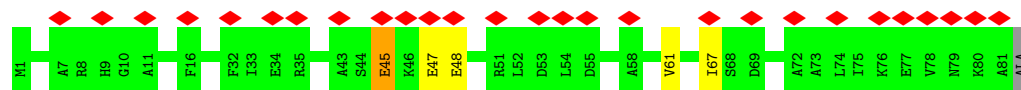
- Molecule 15: Small ribosomal subunit protein uS15

Chain O: 11% 89% 10% .



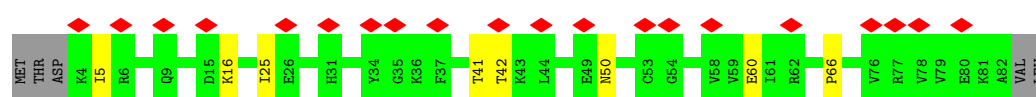
- Molecule 16: Small ribosomal subunit protein bS16

Chain P: 33% 93% 5% ..



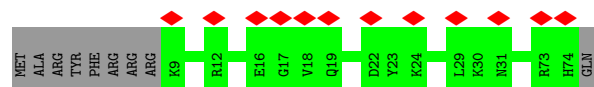
- Molecule 17: Small ribosomal subunit protein uS17

Chain Q: 24% 85% 10% 6%



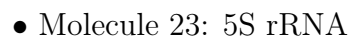
- Molecule 18: Small ribosomal subunit protein bS18

Chain R: 16% 88% 12%



- Molecule 19: Small ribosomal subunit protein uS19

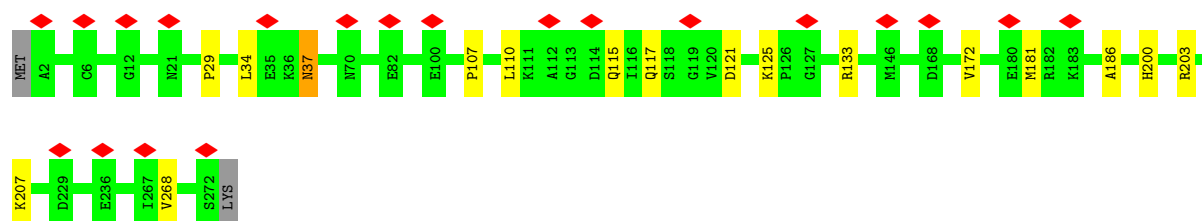
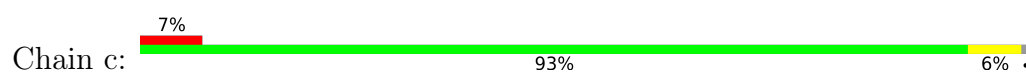
Chain S: 29% 85% 7% 9%



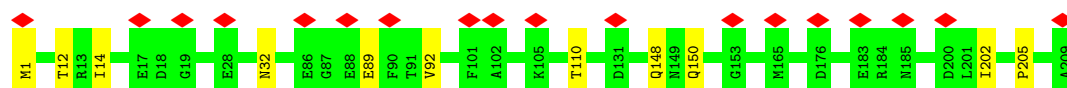
Chain b:



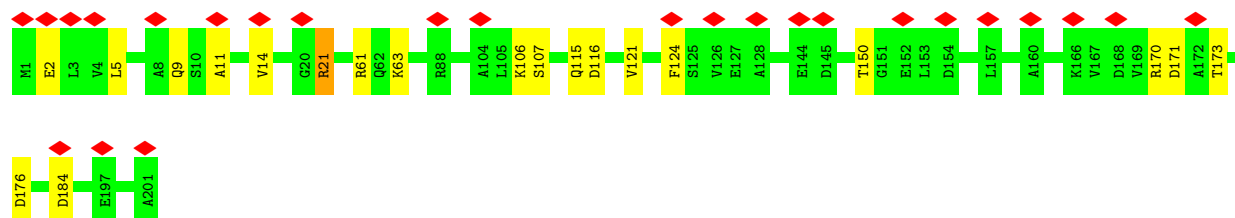
- Molecule 24: Large ribosomal subunit protein uL2



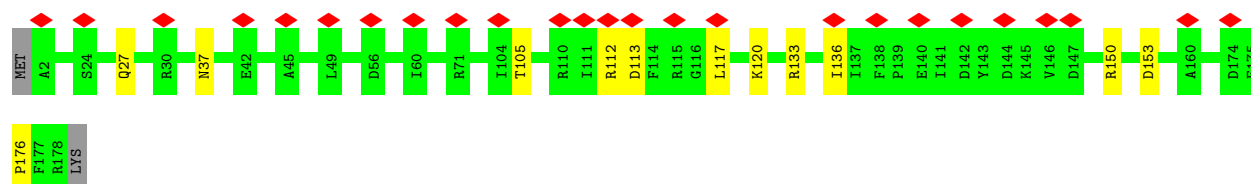
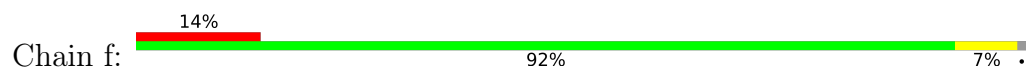
- Molecule 25: Large ribosomal subunit protein uL3



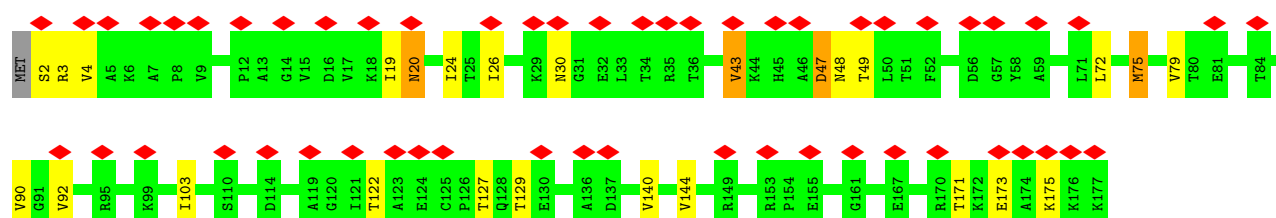
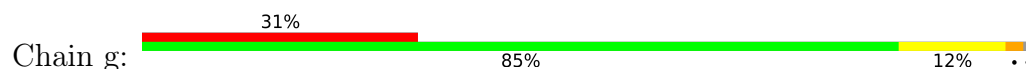
- Molecule 26: Large ribosomal subunit protein uL4



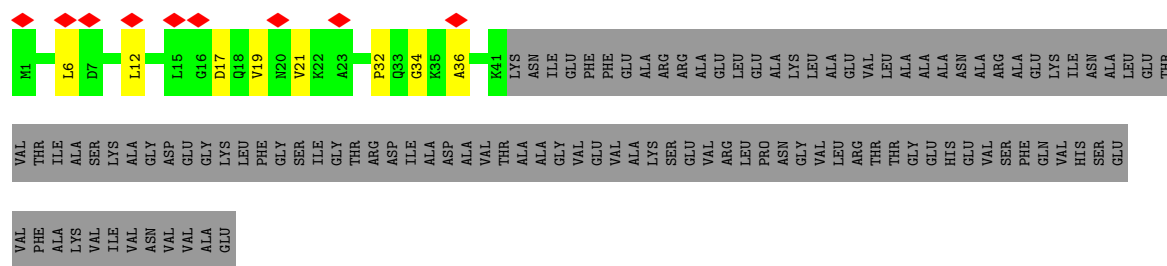
- Molecule 27: Large ribosomal subunit protein uL5



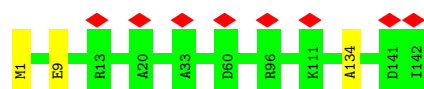
- Molecule 28: Large ribosomal subunit protein uL6



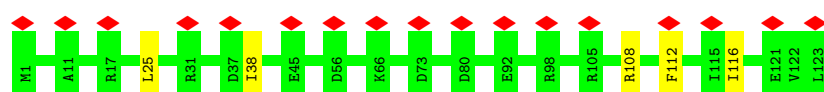
Chain h: 6% 22% 5% 67%



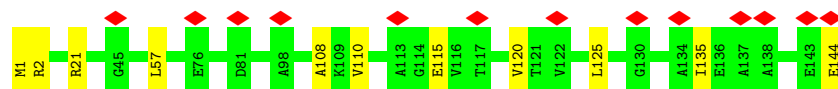
Chain i: 98% 6%



Chain j: 14% 96%



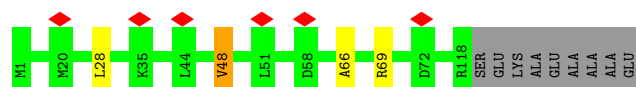
Chain k: 9% 92% 8%



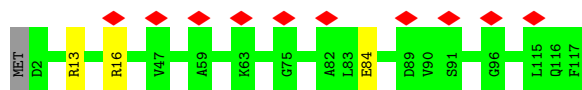
Chain 1: 5% 95% 5%



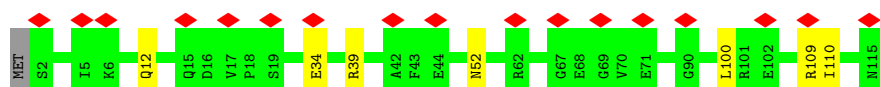
Chain m: 5% 90% .. 7%



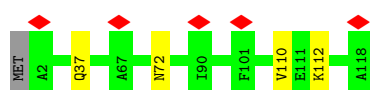
- Molecule 35: 50S ribosomal protein L18



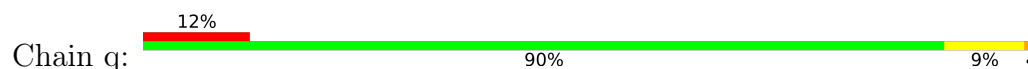
- Molecule 36: 50S ribosomal protein L19



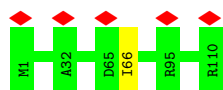
- Molecule 37: 50S ribosomal protein L20



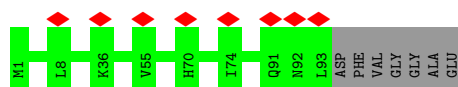
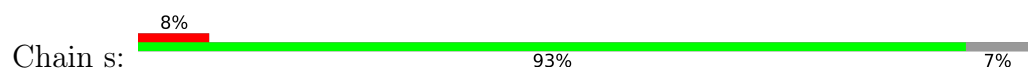
- Molecule 38: 50S ribosomal protein L21



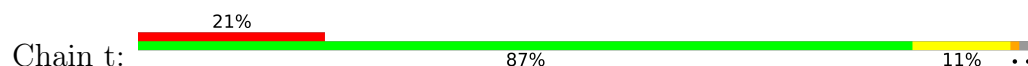
- Molecule 39: 50S ribosomal protein L22

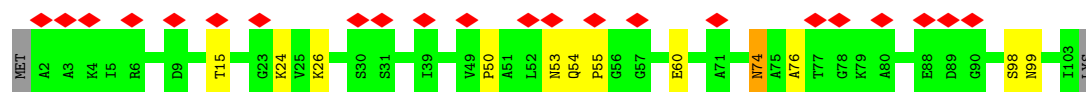


- Molecule 40: 50S ribosomal protein L23

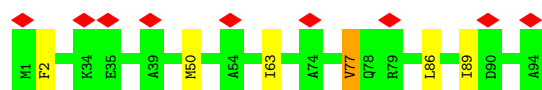
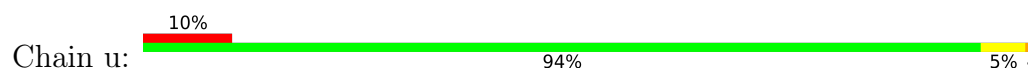


- Molecule 41: 50S ribosomal protein L24

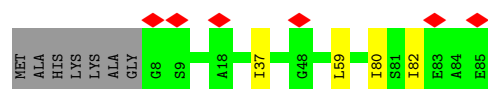
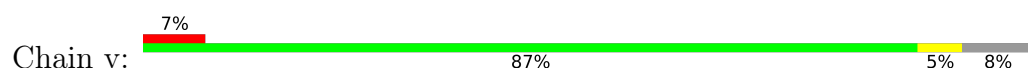




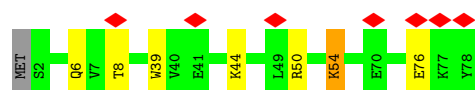
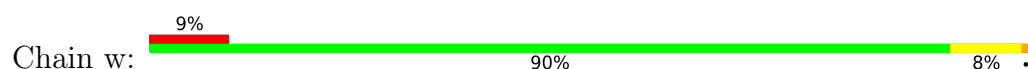
- Molecule 42: 50S ribosomal protein L25



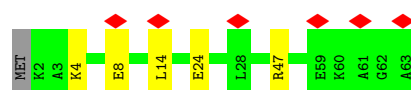
- Molecule 43: 50S ribosomal protein L27



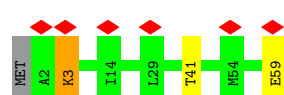
- Molecule 44: 50S ribosomal protein L28



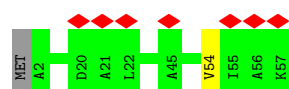
- Molecule 45: 50S ribosomal protein L29



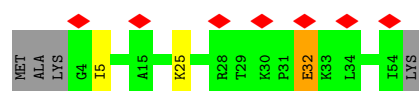
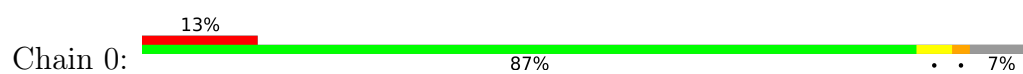
- Molecule 46: 50S ribosomal protein L30



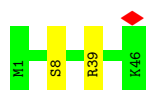
- Molecule 47: 50S ribosomal protein L32



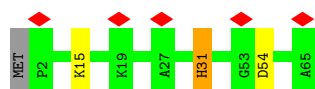
- Molecule 48: 50S ribosomal protein L33



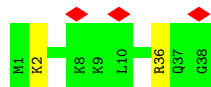
- Molecule 49: 50S ribosomal protein L34



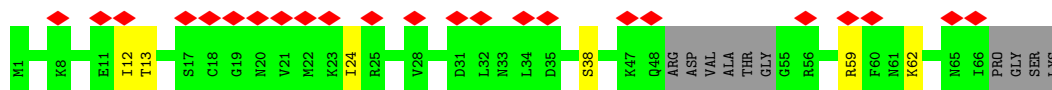
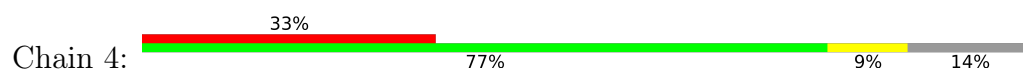
- Molecule 50: 50S ribosomal protein L35



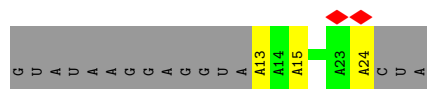
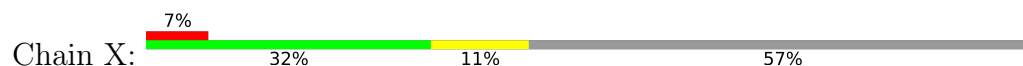
- Molecule 51: 50S ribosomal protein L36



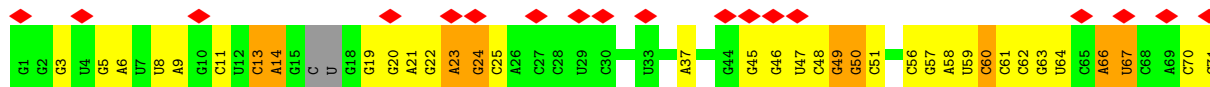
- Molecule 52: Large ribosomal subunit protein bL31A



- Molecule 53: mRNA

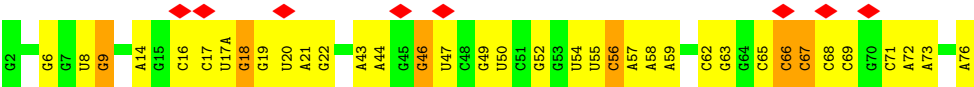


- Molecule 54: A-site tRNA-val





● Molecule 55: P-site tRNA-fMet



● Molecule 56: E-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 1400/HR + YPS FEG	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	DECTRIS SINGLA (1k x 1k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	412.4, 412.4, 412.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.031, 1.031, 1.031	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, D2T, 6MZ, ZN, IAS, MS6, OMG, G7M, 2MG, 4OC, 5MU, 4D4, 3TD, H2U, MA6, UR3, OMC, MEQ, 2MA, 5MC, 1MG, PSU

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	0.64	1/36236 (0.0%)	0.87	9/56520 (0.0%)
2	B	0.69	0/1784	1.23	0/2403
3	C	0.68	0/1651	1.12	0/2225
4	D	0.67	0/1665	1.21	0/2227
5	E	0.67	0/1165	1.17	0/1568
6	F	0.69	0/858	1.14	0/1160
7	G	0.68	0/1219	1.25	0/1635
8	H	0.67	0/989	1.11	0/1326
9	I	0.67	0/1034	1.15	0/1375
10	J	0.67	0/796	1.14	0/1077
11	K	0.70	0/884	1.09	0/1191
12	L	0.66	0/960	1.07	0/1286
13	M	0.72	0/900	1.27	0/1204
14	N	0.67	0/817	1.16	0/1088
15	O	0.64	0/722	1.21	0/964
16	P	0.66	0/653	1.14	1/877 (0.1%)
17	Q	0.64	0/650	1.06	0/871
18	R	0.67	0/553	1.24	0/742
19	S	0.71	0/685	1.13	0/922
20	T	0.67	0/676	1.31	1/895 (0.1%)
21	U	0.64	0/597	1.24	0/792
22	a	0.62	2/65651 (0.0%)	0.90	31/102413 (0.0%)
23	b	0.65	0/2850	0.87	1/4444 (0.0%)
24	c	0.68	0/2121	1.08	1/2852 (0.0%)
25	d	0.63	0/1576	1.05	0/2119
26	e	0.63	0/1571	1.16	1/2113 (0.0%)
27	f	0.66	0/1434	1.14	0/1926
28	g	0.71	0/1343	1.20	0/1816
29	h	0.74	0/306	1.23	0/413
30	i	0.64	0/1152	1.10	0/1551
31	j	0.64	0/955	1.06	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.66	0/1062	1.09	0/1413
33	l	0.62	0/1073	1.13	0/1433
34	m	0.63	0/958	1.14	0/1281
35	n	0.66	0/902	1.18	0/1209
36	o	0.64	0/929	1.05	0/1242
37	p	0.60	0/960	1.18	0/1278
38	q	0.65	0/829	1.04	0/1107
39	r	0.63	0/864	1.14	0/1156
40	s	0.63	0/744	1.13	0/994
41	t	0.66	0/787	1.17	0/1051
42	u	0.65	0/766	1.11	0/1025
43	v	0.62	0/593	1.04	0/785
44	w	0.63	0/635	1.14	0/848
45	x	0.65	0/502	1.31	0/667
46	y	0.66	0/453	1.21	0/605
47	z	0.65	0/450	1.14	0/599
48	0	0.65	0/424	1.14	0/565
49	1	0.60	0/380	1.14	0/498
50	2	0.65	0/513	1.18	0/676
51	3	0.65	0/303	1.04	0/397
52	4	0.66	0/488	1.08	0/649
53	X	0.67	0/292	0.91	0/453
54	Y	0.69	0/1764	1.01	0/2747
55	Z	0.68	0/1813	0.94	1/2825 (0.0%)
56	5	0.89	0/46	0.80	0/69
All	All	0.64	3/152983 (0.0%)	0.96	46/228846 (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
2	B	0	1
12	L	0	1
28	g	0	2
46	y	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2069	G7M	O3'-P	5.46	1.61	1.56
1	A	527	G7M	O3'-P	5.39	1.61	1.56
22	a	2552	OMU	O3'-P	5.00	1.61	1.56

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	U	O3'-P-O5'	-7.36	92.97	104.00
22	a	2519	U	O3'-P-O5'	-7.26	93.10	104.00
1	A	913	A	O3'-P-O5'	-6.39	94.41	104.00
1	A	5	U	C2'-C3'-O3'	-6.38	104.13	113.70
22	a	887	U	O3'-P-O5'	-6.31	94.54	104.00
22	a	1131	G	O3'-P-O5'	-6.24	94.64	104.00
22	a	404	A	C2'-C3'-O3'	6.05	118.57	109.50
22	a	1568	G	O3'-P-O5'	-5.87	95.19	104.00
22	a	1969	A	O3'-P-O5'	-5.76	95.36	104.00
24	c	37	ASN	CB-CA-C	5.69	119.67	111.82
22	a	2050	C	O3'-P-O5'	-5.67	95.50	104.00
23	b	69	G	C1'-C2'-O2'	5.65	116.87	108.40
22	a	2501	C	O3'-P-O5'	-5.61	95.58	104.00
1	A	1108	G	C1'-C2'-O2'	5.59	116.78	108.40
22	a	330	A	O3'-P-O5'	-5.59	95.62	104.00
22	a	1905	C	C4'-C3'-O3'	-5.55	104.67	113.00
22	a	404	A	P-O3'-C3'	5.54	128.51	120.20
22	a	1701	A	C1'-C2'-O2'	5.54	116.70	108.40
22	a	204	A	O3'-P-O5'	-5.53	95.71	104.00
22	a	940	G	C1'-C2'-O2'	5.53	116.69	108.40
22	a	954	G	C1'-C2'-O2'	5.50	116.65	108.40
1	A	351	G	O3'-P-O5'	-5.48	95.78	104.00
22	a	2614	A	O3'-P-O5'	-5.48	95.78	104.00
22	a	2654	A	O3'-P-O5'	-5.44	95.84	104.00
22	a	1452	G	O3'-P-O5'	-5.43	95.86	104.00
22	a	781	A	O3'-P-O5'	-5.40	95.90	104.00
22	a	989	G	O3'-P-O5'	-5.28	96.08	104.00
1	A	5	U	C4'-C3'-O3'	5.28	120.91	113.00
22	a	846	U	N1-C1'-C2'	5.27	119.91	112.00
22	a	1929	G	O3'-P-O5'	-5.19	96.21	104.00
22	a	2490	G	O3'-P-O5'	-5.18	96.23	104.00
22	a	2061	G	O3'-P-O5'	-5.17	96.25	104.00
26	e	116	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	1221	G	C1'-C2'-O2'	5.13	116.10	108.40
22	a	1359	A	O3'-P-O5'	-5.11	96.34	104.00
1	A	1035	A	P-O3'-C3'	5.09	127.84	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	G	C1'-C2'-O2'	5.09	116.04	108.40
55	Z	67	C	O3'-P-O5'	5.08	111.62	104.00
22	a	1667	G	O3'-P-O5'	-5.07	96.40	104.00
22	a	784	G	P-O3'-C3'	5.06	127.80	120.20
22	a	1436	G	C1'-C2'-O2'	5.05	115.98	108.40
22	a	277	G	P-O3'-C3'	5.04	127.77	120.20
22	a	241	A	O3'-P-O5'	-5.04	96.44	104.00
22	a	329	G	O3'-P-O5'	-5.03	96.45	104.00
20	T	24	ARG	CB-CG-CD	5.01	122.83	111.30
16	P	45	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	THR	Peptide
12	L	101	ALA	Peptide
28	g	43	VAL	Peptide
28	g	47	ASP	Peptide
46	y	3	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32612	0	16432	89	0
2	B	1753	0	1780	11	0
3	C	1624	0	1696	4	0
4	D	1643	0	1707	12	0
5	E	1152	0	1196	3	0
6	F	839	0	833	2	0
7	G	1203	0	1254	9	0
8	H	979	0	1031	5	0
9	I	1022	0	1070	1	0
10	J	786	0	828	4	0
11	K	877	0	884	5	0
12	L	957	0	1017	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	891	0	952	8	0
14	N	805	0	844	4	0
15	O	714	0	734	3	0
16	P	643	0	661	1	0
17	Q	641	0	682	2	0
18	R	544	0	565	0	0
19	S	668	0	693	3	0
20	T	670	0	719	3	0
21	U	589	0	629	1	0
22	a	59130	0	29769	135	0
23	b	2549	0	1291	4	0
24	c	2082	0	2154	9	0
25	d	1566	0	1618	4	0
26	e	1552	0	1619	8	0
27	f	1410	0	1444	9	0
28	g	1323	0	1371	9	0
29	h	303	0	327	3	0
30	i	1129	0	1162	1	0
31	j	946	0	1023	4	0
32	k	1053	0	1129	6	0
33	l	1075	0	1145	3	0
34	m	945	0	989	2	0
35	n	892	0	923	0	0
36	o	917	0	962	6	0
37	p	947	0	1019	2	0
38	q	816	0	839	3	0
39	r	857	0	922	0	0
40	s	738	0	807	0	0
41	t	779	0	831	3	0
42	u	753	0	780	3	0
43	v	586	0	596	3	0
44	w	625	0	652	3	0
45	x	501	0	531	1	0
46	y	449	0	488	0	0
47	z	444	0	458	0	0
48	0	417	0	451	1	0
49	1	377	0	418	1	0
50	2	504	0	572	2	0
51	3	302	0	340	1	0
52	4	480	0	478	1	0
53	X	260	0	130	1	0
54	Y	1579	0	804	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	Z	1623	0	825	8	0
56	5	42	0	23	1	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
All	All	141565	0	95097	366	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (366) 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)
13:M:71:ARG:NH2	27:f:113:ASP:OD1	1.94	0.99
13:M:71:ARG:NH2	27:f:113:ASP:CG	2.25	0.95
13:M:71:ARG:NH2	27:f:113:ASP:OD2	2.04	0.91
22:a:1252:G:H1	37:p:37:GLN:HE21	1.32	0.77
22:a:2554:U:O2	54:Y:74:C:N4	2.17	0.77
13:M:71:ARG:HH22	27:f:113:ASP:CG	1.92	0.77
1:A:664:G:H22	1:A:741:G:H1	1.34	0.76
1:A:1073:U:O2'	2:B:103:ASN:ND2	2.20	0.75
55:Z:18:G:N1	55:Z:55:U:O2	2.18	0.74
54:Y:58:A:O2'	54:Y:60:C:OP2	2.06	0.72
54:Y:13:C:O2	54:Y:22:G:N1	2.20	0.70
2:B:119:THR:O	2:B:123:ASP:HB2	1.92	0.70
22:a:1478:G:H1	22:a:1513:U:H3	1.38	0.69
54:Y:23:A:H2'	54:Y:24:G:C8	2.28	0.68
7:G:113:ASP:OD2	7:G:122:ASN:ND2	2.28	0.66
22:a:1582:C:O2'	22:a:1585:C:N3	2.25	0.66
1:A:37:U:OP2	12:L:120:LYS:NZ	2.30	0.65
54:Y:23:A:H2'	54:Y:24:G:H8	1.62	0.65
1:A:1119:C:OP1	9:I:85:ARG:NH2	2.31	0.64
22:a:2478:A:OP2	51:3:2:LYS:NZ	2.25	0.64
22:a:1047:G:HO2'	22:a:1110:G:H1	1.44	0.64
1:A:1086:U:H3	1:A:1099:G:H22	1.45	0.64
55:Z:62:C:H2'	55:Z:63:G:C8	2.32	0.63
1:A:673:A:H2'	1:A:674:G:C8	2.34	0.62
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.81	0.62
31:j:108:ARG:HH21	36:o:34:GLU:HB3	1.64	0.62
10:J:29:ALA:HB2	10:J:87:LEU:HD21	1.81	0.62
22:a:896:A:H2'	54:Y:56:C:O2	2.00	0.61
4:D:101:VAL:HG12	4:D:105:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:U:H3	1:A:713:G:H22	1.49	0.61
1:A:754:C:OP1	15:O:72:ARG:NH2	2.34	0.61
22:a:1434:A:H2'	22:a:1435:G:C8	2.36	0.61
1:A:933:G:O6	7:G:3:ARG:NH2	2.29	0.60
22:a:1720:U:H2'	22:a:1721:G:O4'	2.01	0.60
33:l:66:ARG:NH1	33:l:104:GLU:OE2	2.35	0.60
1:A:823:C:HO2'	8:H:2:SER:N	1.99	0.59
22:a:84:A:N1	22:a:98:G:O2'	2.30	0.59
7:G:113:ASP:OD1	7:G:113:ASP:N	2.36	0.59
22:a:1434:A:H2'	22:a:1435:G:H8	1.67	0.59
1:A:1189:U:OP1	14:N:98:LYS:NZ	2.36	0.59
22:a:878:A:N7	22:a:899:A:H2	2.01	0.59
22:a:172:A:H2'	22:a:173:A:C8	2.38	0.58
22:a:1047:G:O2'	22:a:1109:C:N4	2.36	0.58
2:B:205:ASP:OD1	2:B:205:ASP:N	2.37	0.58
1:A:946:A:H2'	1:A:947:G:C8	2.39	0.58
55:Z:62:C:H2'	55:Z:63:G:H8	1.69	0.58
28:g:2:SER:OG	28:g:3:ARG:N	2.37	0.57
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.85	0.56
11:K:23:ILE:HG12	11:K:96:THR:HG21	1.86	0.56
22:a:5:A:H2'	22:a:6:A:C8	2.41	0.56
1:A:404:G:O6	4:D:2:ALA:N	2.39	0.55
1:A:422:C:O2	1:A:423:G:N1	2.39	0.55
3:C:35:SER:OG	3:C:59:ARG:NH2	2.40	0.55
1:A:1391:U:H2'	1:A:1392:G:C8	2.42	0.55
1:A:1356:G:H2'	1:A:1357:A:C8	2.42	0.55
22:a:1469:A:H2'	22:a:1470:A:C8	2.42	0.55
22:a:2751:G:H4'	28:g:4:VAL:HG23	1.89	0.55
3:C:77:ILE:HA	3:C:84:VAL:HG13	1.88	0.55
22:a:2748:A:H5'	28:g:4:VAL:HG21	1.88	0.55
1:A:405:U:O4	4:D:2:ALA:N	2.40	0.54
25:d:14:ILE:HA	36:o:12:GLN:HE22	1.73	0.54
38:q:1:MET:HE3	38:q:43:ASN:HD21	1.72	0.54
7:G:53:ARG:NH2	7:G:122:ASN:OD1	2.39	0.54
22:a:639:U:H2'	22:a:640:C:C6	2.43	0.54
22:a:549:G:H2'	22:a:550:C:C6	2.43	0.54
36:o:100:LEU:HD11	36:o:110:ILE:HD11	1.89	0.54
28:g:72:LEU:HA	28:g:75:MET:HB2	1.90	0.54
1:A:1004:A:H2'	1:A:1005:A:O4'	2.08	0.54
22:a:1181:U:H2'	22:a:1182:G:C8	2.42	0.54
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:A:N6	4:D:202:GLU:O	2.41	0.53
1:A:216:U:H2'	1:A:217:C:C6	2.42	0.53
10:J:66:GLU:HB2	14:N:99:ALA:HB2	1.91	0.53
22:a:1913:A:N1	54:Y:37:A:O2'	2.40	0.53
41:t:74:ASN:HD22	41:t:76:ALA:H	1.56	0.53
29:h:12:LEU:HD13	29:h:19:VAL:HG21	1.89	0.53
54:Y:14:A:C2	54:Y:22:G:H1'	2.43	0.53
10:J:28:THR:HG23	10:J:87:LEU:HD23	1.91	0.53
24:c:200:HIS:HE1	24:c:203:ARG:HH11	1.56	0.53
1:A:553:A:H5''	12:L:21:VAL:HG21	1.91	0.53
22:a:1115:G:O2'	22:a:1116:G:O5'	2.26	0.52
1:A:662:U:H2'	1:A:663:A:C8	2.44	0.52
22:a:2505:G:N2	22:a:2506:U:O4	2.42	0.52
22:a:2547:A:H2'	22:a:2548:U:C6	2.45	0.52
1:A:493:A:H2'	1:A:494:G:C8	2.45	0.52
3:C:73:PRO:HG3	3:C:105:GLU:HG2	1.91	0.52
22:a:2432:A:H1'	56:5:75:C:O4'	2.09	0.52
1:A:545:C:OP1	4:D:58:LYS:NZ	2.43	0.52
22:a:2327:A:H2'	22:a:2328:A:C8	2.45	0.52
1:A:346:G:OP1	36:o:39:ARG:NH2	2.39	0.51
22:a:851:C:H2'	22:a:852:U:C6	2.46	0.51
22:a:2052:A:H4'	25:d:148:GLN:O	2.10	0.51
1:A:50:A:O2'	1:A:360:G:N2	2.43	0.51
1:A:1031:C:O2'	1:A:1032:G:N2	2.44	0.51
7:G:82:GLY:HA3	53:X:13:A:C8	2.45	0.51
1:A:1526:G:N7	21:U:40:LYS:NZ	2.57	0.51
22:a:2392:A:OP2	50:2:31:HIS:HE1	1.94	0.51
27:f:105:THR:HA	52:4:38:SER:HB2	1.92	0.51
1:A:337:G:H2'	1:A:338:A:C8	2.45	0.50
22:a:2273:A:H2'	22:a:2274:A:C8	2.47	0.50
55:Z:43:A:H2'	55:Z:44:A:C8	2.47	0.50
20:T:39:ILE:HD11	20:T:83:ILE:HG13	1.94	0.49
22:a:1939:5MU:OP1	22:a:2604:PSU:O2'	2.29	0.49
4:D:184:ARG:NH2	4:D:190:ASP:OD2	2.38	0.49
1:A:71:A:N1	1:A:99:C:O2'	2.45	0.49
1:A:147:G:H2'	1:A:148:G:C8	2.48	0.49
1:A:390:U:H2'	1:A:391:G:C8	2.47	0.49
12:L:73:ASN:O	12:L:75:GLN:NE2	2.45	0.49
54:Y:50:G:H2'	54:Y:51:C:O4'	2.11	0.49
1:A:1273:C:H2'	1:A:1274:A:O4'	2.12	0.49
22:a:273:G:H2'	22:a:274:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2243:U:H2'	22:a:2244:U:C6	2.47	0.49
44:w:6:GLN:HE21	44:w:50:ARG:H	1.61	0.49
22:a:1020:A:N1	22:a:1141:U:O2'	2.42	0.49
22:a:1495:A:N3	22:a:1578:U:O2'	2.43	0.49
22:a:172:A:H2'	22:a:173:A:H8	1.77	0.49
25:d:110:THR:HG23	25:d:202:ILE:HB	1.94	0.49
22:a:2291:U:H2'	22:a:2292:U:C6	2.48	0.49
22:a:1048:A:H62	22:a:1110:G:H21	1.61	0.49
1:A:131:A:H2'	1:A:132:C:C6	2.48	0.48
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.95	0.48
1:A:1218:C:H2'	1:A:1219:A:C8	2.48	0.48
31:j:38:ILE:HD11	31:j:112:PHE:HZ	1.77	0.48
54:Y:50:G:H1	54:Y:64:U:H3	1.60	0.48
1:A:171:A:H2'	1:A:172:A:C8	2.49	0.48
1:A:1320:C:O2	19:S:36:ARG:NH2	2.47	0.48
22:a:1405:U:H2'	22:a:1406:U:C6	2.47	0.48
27:f:112:ARG:HH12	27:f:133:ARG:HH22	1.60	0.48
1:A:140:U:H2'	1:A:141:G:O4'	2.13	0.48
22:a:896:A:H2'	54:Y:56:C:C2	2.49	0.48
1:A:51:A:N7	1:A:114:U:O2'	2.46	0.48
31:j:108:ARG:HH11	31:j:116:ILE:HG21	1.79	0.48
1:A:269:C:H2'	1:A:270:A:C8	2.47	0.48
1:A:472:U:H2'	1:A:473:U:C6	2.49	0.48
1:A:542:G:H5'	4:D:39:GLY:HA3	1.96	0.48
1:A:1350:A:O2'	7:G:33:ASP:OD1	2.28	0.48
22:a:2202:U:O2'	22:a:2204:G:OP1	2.28	0.48
22:a:720:U:H2'	22:a:721:A:C8	2.49	0.48
55:Z:56:C:C2	55:Z:57:A:C8	3.02	0.47
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.96	0.47
12:L:55:VAL:O	12:L:62:GLU:HA	2.14	0.47
17:Q:25:ILE:HB	17:Q:42:THR:HG23	1.97	0.47
29:h:32:PRO:HA	44:w:39:TRP:CD1	2.49	0.47
22:a:1494:A:H2'	22:a:1495:A:C8	2.50	0.47
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.97	0.47
26:e:121:VAL:HG21	26:e:124:PHE:HB2	1.96	0.47
22:a:197:A:N6	22:a:2430:A:O2'	2.48	0.47
23:b:48:U:H2'	23:b:49:C:C6	2.50	0.47
8:H:18:GLN:HG2	8:H:63:LEU:HD13	1.97	0.47
22:a:871:U:H2'	22:a:872:U:C6	2.50	0.47
22:a:219:A:N3	22:a:234:U:O2'	2.43	0.47
22:a:2537:U:H2'	22:a:2538:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:200:HIS:CE1	24:c:203:ARG:HH11	2.32	0.47
2:B:188:ASP:HB2	2:B:204:ASP:OD2	2.15	0.47
11:K:67:ALA:HB2	11:K:96:THR:HG23	1.97	0.47
22:a:1182:G:H2'	22:a:1183:U:O4'	2.15	0.47
24:c:181:MET:HB3	24:c:268:VAL:HB	1.97	0.47
22:a:1509:A:HO2'	22:a:1510:G:H8	1.63	0.47
16:P:61:VAL:HG21	16:P:67:ILE:HD11	1.97	0.46
54:Y:62:C:H2'	54:Y:63:G:C8	2.50	0.46
22:a:366:C:H2'	22:a:367:G:O4'	2.15	0.46
1:A:87:C:H2'	1:A:88:U:C6	2.50	0.46
1:A:411:A:P	4:D:26:ARG:HH12	2.39	0.46
22:a:593:U:H2'	22:a:594:U:C6	2.50	0.46
22:a:1378:A:O2'	22:a:1380:G:N7	2.41	0.46
1:A:404:G:N7	4:D:2:ALA:HB3	2.30	0.46
2:B:94:HIS:ND1	2:B:146:ASN:O	2.49	0.46
22:a:305:C:H2'	22:a:306:U:C6	2.50	0.46
48:O:25:LYS:NZ	48:O:32:GLU:O	2.48	0.46
22:a:642:U:O2'	22:a:644:A:N7	2.46	0.46
54:Y:49:G:H2'	54:Y:50:G:H8	1.81	0.46
22:a:299:A:N3	22:a:319:G:O2'	2.46	0.46
22:a:1386:C:H2'	22:a:1387:A:C8	2.50	0.46
22:a:1715:G:O2'	22:a:1743:G:O6	2.31	0.46
38:q:57:GLY:HA2	38:q:102:SER:O	2.15	0.46
42:u:2:PHE:HB3	42:u:50:MET:HE3	1.98	0.46
22:a:493:G:H2'	22:a:494:G:O4'	2.15	0.46
1:A:1027:C:H2'	1:A:1028:C:C6	2.51	0.46
8:H:41:LYS:NZ	8:H:48:ASP:OD1	2.47	0.46
11:K:18:ASP:OD1	11:K:37:ARG:NH1	2.49	0.46
27:f:37:ASN:HB3	27:f:153:ASP:OD1	2.16	0.46
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.97	0.45
22:a:1028:A:N6	22:a:1125:G:H2'	2.31	0.45
1:A:56:U:H2'	1:A:57:G:C8	2.51	0.45
26:e:171:ASP:OD2	26:e:173:THR:OG1	2.34	0.45
14:N:29:ALA:O	14:N:33:ASP:HB2	2.16	0.45
23:b:36:C:N4	23:b:49:C:O2	2.49	0.45
1:A:381:C:H2'	1:A:382:A:O4'	2.16	0.45
1:A:739:C:OP2	6:F:2:ARG:NH2	2.49	0.45
19:S:69:HIS:ND1	19:S:73:GLU:OE1	2.50	0.45
22:a:352:A:H2'	22:a:353:C:O4'	2.17	0.45
22:a:811:U:H2'	32:k:21:ARG:HA	1.99	0.45
2:B:106:THR:HA	2:B:109:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:13:GLU:HG2	5:E:39:VAL:HG12	1.99	0.45
20:T:68:HIS:HD2	20:T:70:ASN:H	1.64	0.45
22:a:290:U:H2'	22:a:291:G:O4'	2.16	0.45
1:A:1309:G:N7	13:M:98:ARG:NH2	2.65	0.45
2:B:76:ALA:O	2:B:80:VAL:HG23	2.16	0.45
24:c:115:GLN:O	24:c:125:LYS:NZ	2.50	0.45
1:A:769:G:H4'	1:A:1513:A:H4'	1.98	0.45
1:A:1076:U:OP1	2:B:174:LYS:NZ	2.37	0.45
8:H:96:MET:HE2	8:H:99:LEU:HB2	1.99	0.45
10:J:24:GLU:HB2	10:J:90:LEU:HD11	1.99	0.45
22:a:851:C:H2'	22:a:852:U:H6	1.81	0.45
1:A:1302:C:C5	13:M:17:ILE:HG13	2.52	0.44
22:a:813:U:H2'	22:a:814:C:C6	2.52	0.44
22:a:1266:G:O2'	22:a:2012:G:O6	2.33	0.44
22:a:1853:A:N1	22:a:2087:G:H1'	2.32	0.44
22:a:543:G:C6	22:a:551:G:C6	3.05	0.44
22:a:2491:U:H5''	22:a:2570:G:H5''	1.99	0.44
26:e:61:ARG:NH2	26:e:63:LYS:O	2.50	0.44
28:g:30:ASN:HB3	28:g:79:VAL:HA	1.99	0.44
42:u:86:LEU:HD13	42:u:89:ILE:HD11	1.98	0.44
22:a:349:U:H2'	22:a:350:G:H8	1.82	0.44
1:A:746:A:H2'	1:A:747:A:C8	2.53	0.44
1:A:1378:C:O2	7:G:76:LYS:NZ	2.46	0.44
22:a:155:A:H2'	22:a:156:A:C8	2.53	0.44
1:A:17:U:H2'	1:A:18:C:C6	2.52	0.44
1:A:189:A:H2'	1:A:190:A:C8	2.52	0.44
1:A:714:G:H2'	1:A:715:A:C8	2.53	0.44
26:e:2:GLU:OE1	26:e:11:ALA:HB1	2.17	0.44
22:a:351:C:H2'	22:a:352:A:C8	2.53	0.44
22:a:414:C:H2'	22:a:415:A:C8	2.53	0.44
22:a:1414:C:H2'	22:a:1415:U:O4'	2.16	0.44
22:a:2687:U:H2'	22:a:2688:G:O4'	2.18	0.44
23:b:2:G:H2'	23:b:3:C:C6	2.53	0.44
22:a:340:A:H2'	22:a:341:C:O4'	2.17	0.44
22:a:1794:A:H2'	22:a:1795:C:C6	2.53	0.44
55:Z:66:C:H2'	55:Z:67:C:C6	2.52	0.44
4:D:184:ARG:HH21	4:D:186:PRO:HA	1.83	0.44
11:K:17:SER:HA	11:K:79:ILE:HA	1.99	0.44
22:a:1179:G:H2'	22:a:1180:U:C6	2.53	0.44
22:a:1485:U:H2'	22:a:1486:U:C6	2.53	0.44
22:a:2532:G:O2'	22:a:2657:A:N1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:t:50:PRO:HA	41:t:54:GLN:HB3	1.99	0.44
1:A:190:A:O5'	1:A:190:A:H8	2.01	0.43
1:A:1412:C:H2'	1:A:1413:A:C8	2.53	0.43
1:A:1443:C:H2'	1:A:1444:U:O4'	2.18	0.43
22:a:1786:A:H1'	22:a:1938:A:N6	2.33	0.43
26:e:170:ARG:NH2	26:e:176:ASP:OD1	2.45	0.43
55:Z:72:A:H2'	55:Z:73:A:O4'	2.19	0.43
26:e:115:GLN:HE22	32:k:1:MET:HB3	1.82	0.43
22:a:1563:U:H2'	22:a:1564:C:C6	2.53	0.43
23:b:66:A:H61	23:b:107:G:H2'	1.84	0.43
1:A:1005:A:O2'	1:A:1037:C:O2'	2.36	0.43
1:A:1032:G:C6	1:A:1033:G:H1'	2.54	0.43
22:a:1180:U:H2'	22:a:1181:U:O4'	2.19	0.43
22:a:1874:C:H2'	22:a:1875:G:O4'	2.19	0.43
22:a:581:C:H2'	22:a:582:A:C8	2.54	0.43
22:a:2788:C:H2'	22:a:2789:C:C6	2.54	0.43
44:w:8:THR:HG21	44:w:54:LYS:HE3	2.01	0.43
20:T:68:HIS:CD2	20:T:70:ASN:H	2.36	0.43
22:a:2329:U:H2'	22:a:2330:G:C8	2.54	0.43
22:a:2902:C:H2'	22:a:2903:U:O4'	2.18	0.43
22:a:856:G:H2'	22:a:857:G:C8	2.54	0.43
29:h:34:GLY:O	29:h:36:ALA:N	2.46	0.43
38:q:33:VAL:HG23	38:q:61:ALA:HB3	2.00	0.43
1:A:89:U:H2'	1:A:90:C:C6	2.54	0.42
22:a:468:G:N7	49:l:39:ARG:NH2	2.57	0.42
22:a:743:A:O2'	22:a:1659:G:OP1	2.35	0.42
22:a:2845:U:H5''	36:o:52:ASN:O	2.19	0.42
25:d:1:MET:HE2	25:d:205:PRO:HG3	2.01	0.42
22:a:547:A:H4'	22:a:548:G:O4'	2.19	0.42
22:a:1904:G:O2'	22:a:1928:A:N1	2.51	0.42
22:a:2482:A:H4'	54:Y:63:G:O2'	2.19	0.42
27:f:117:LEU:HD12	27:f:176:PRO:HD2	2.01	0.42
1:A:1286:U:N3	1:A:1288:A:OP1	2.52	0.42
22:a:2196:C:H2'	22:a:2197:U:C6	2.54	0.42
22:a:890:C:H3'	22:a:891:G:O4'	2.18	0.42
24:c:133:ARG:HB3	24:c:186:ALA:HB1	2.01	0.42
1:A:264:C:O2'	17:Q:66:PRO:O	2.37	0.42
1:A:1323:G:H2'	1:A:1324:A:C8	2.55	0.42
34:m:66:ALA:O	34:m:69:ARG:O	2.38	0.42
2:B:100:MET:HA	2:B:107:VAL:HG21	2.01	0.42
7:G:79:ARG:HA	7:G:84:THR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:e:184:ASP:HA	32:k:2:ARG:HH12	1.84	0.42
1:A:1148:U:H2'	1:A:1149:C:O4'	2.19	0.42
1:A:1428:A:H2'	1:A:1429:A:O4'	2.19	0.42
4:D:170:TRP:CD1	4:D:186:PRO:HD3	2.54	0.42
22:a:1486:U:H2'	22:a:1487:U:H6	1.85	0.42
34:m:28:LEU:HD23	34:m:48:VAL:HG21	2.00	0.42
43:v:37:ILE:HD11	43:v:82:ILE:HD11	2.00	0.42
54:Y:66:A:C6	54:Y:67:U:C4	3.08	0.42
1:A:85:U:H4'	1:A:86:G:N2	2.35	0.42
1:A:1463:U:H2'	1:A:1464:U:C6	2.55	0.42
22:a:2063:C:O2	22:a:2450:A:N1	2.52	0.42
22:a:2901:C:C4	22:a:2902:C:N4	2.87	0.42
22:a:372:G:O2'	22:a:400:G:O6	2.38	0.42
22:a:476:G:H4'	22:a:502:A:N1	2.34	0.42
22:a:1486:U:H2'	22:a:1487:U:C6	2.55	0.42
28:g:19:ILE:HG12	28:g:24:ILE:HD12	2.02	0.42
43:v:37:ILE:HG21	43:v:80:ILE:HG21	2.02	0.42
1:A:945:G:C2	1:A:946:A:C8	3.08	0.41
1:A:1225:A:H2'	1:A:1226:C:C5	2.55	0.41
5:E:161:VAL:O	5:E:165:LEU:N	2.49	0.41
22:a:1009:A:N3	22:a:1153:C:O2'	2.51	0.41
22:a:1416:G:C4	22:a:1417:C:C5	3.08	0.41
22:a:1872:A:C5	22:a:1873:G:H1'	2.54	0.41
22:a:2469:A:N6	22:a:2481:G:O2'	2.53	0.41
28:g:26:ILE:HB	28:g:75:MET:HG2	2.02	0.41
54:Y:49:G:H2'	54:Y:50:G:C8	2.55	0.41
22:a:153:U:H2'	22:a:154:U:C6	2.55	0.41
22:a:1042:G:H1	22:a:1113:U:H3	1.68	0.41
22:a:1141:U:H4'	22:a:1142:A:O4'	2.19	0.41
22:a:2086:U:H2'	22:a:2087:G:C8	2.55	0.41
33:l:136:MET:HG2	42:u:77:VAL:HG12	2.02	0.41
1:A:1001:C:C2	1:A:1002:G:C8	3.08	0.41
22:a:717:C:H3'	22:a:718:A:H8	1.85	0.41
22:a:1723:G:C2	22:a:1724:G:H1'	2.55	0.41
1:A:459:A:H2'	1:A:460:A:C8	2.56	0.41
1:A:537:G:OP1	12:L:110:ARG:NH2	2.54	0.41
1:A:999:C:H2'	1:A:1000:A:C8	2.56	0.41
22:a:358:U:N3	22:a:359:G:N7	2.69	0.41
22:a:729:G:C6	24:c:207:LYS:HB2	2.55	0.41
22:a:1790:C:H2'	22:a:1791:A:C5	2.55	0.41
22:a:2698:U:H2'	22:a:2699:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:110:VAL:HG11	32:k:135:ILE:HD11	2.02	0.41
1:A:109:A:C6	1:A:326:G:C6	3.09	0.41
8:H:29:SER:HB3	8:H:57:PRO:HB2	2.02	0.41
13:M:89:LEU:O	13:M:93:ARG:HD2	2.19	0.41
41:t:53:ASN:ND2	41:t:55:PRO:O	2.54	0.41
1:A:1315:U:H2'	1:A:1316:G:O4'	2.21	0.41
22:a:1482:G:H1'	22:a:1509:A:H61	1.85	0.41
22:a:1580:A:C8	22:a:1581:G:C8	3.09	0.41
22:a:1509:A:O2'	22:a:1510:G:H8	2.04	0.41
28:g:140:VAL:O	28:g:144:VAL:HG23	2.21	0.41
33:l:53:MET:HE1	33:l:103:TYR:CD2	2.55	0.41
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.54	0.41
14:N:31:ILE:O	14:N:41:ARG:HD3	2.21	0.41
22:a:64:A:H2'	22:a:65:U:C6	2.56	0.41
43:v:59:LEU:HD12	43:v:80:ILE:HD12	2.02	0.41
2:B:67:ILE:H	2:B:89:GLN:HE21	1.68	0.41
2:B:71:GLY:O	2:B:93:ASN:HA	2.21	0.41
22:a:747:5MU:O2	22:a:2014:A:H1'	2.21	0.41
22:a:829:A:N7	22:a:2248:C:H5'	2.36	0.41
22:a:849:A:H2'	22:a:850:U:C6	2.55	0.41
22:a:909:A:H2'	22:a:912:C:C5	2.56	0.41
22:a:1370:C:H2'	22:a:1371:G:O4'	2.21	0.41
22:a:1432:G:H2'	22:a:1433:A:C8	2.56	0.41
22:a:2900:A:C6	22:a:2901:C:C4	3.09	0.41
31:j:25:LEU:HD12	31:j:38:ILE:HG22	2.03	0.41
55:Z:9:G:O4'	55:Z:46:G:H1'	2.21	0.41
11:K:42:LEU:HD12	11:K:79:ILE:HD11	2.02	0.41
13:M:71:ARG:HH21	27:f:113:ASP:CG	2.02	0.41
15:O:14:GLU:OE2	15:O:84:ARG:NH2	2.53	0.41
22:a:898:C:H2'	22:a:899:A:O4'	2.21	0.41
1:A:789:U:O2'	1:A:791:G:N7	2.49	0.40
1:A:977:A:O2'	1:A:979:C:OP2	2.36	0.40
1:A:1171:A:H2'	1:A:1172:C:C6	2.57	0.40
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.56	0.40
22:a:2898:U:O2'	30:i:134:ALA:O	2.34	0.40
26:e:21:ARG:HD3	26:e:106:LYS:HB3	2.03	0.40
28:g:20:ASN:OD1	28:g:20:ASN:N	2.54	0.40
37:p:72:ASN:HB3	37:p:110:VAL:HG11	2.04	0.40
3:C:36:ASP:OD1	3:C:59:ARG:NH2	2.38	0.40
22:a:12:U:O2	22:a:2626:C:H4'	2.21	0.40
22:a:61:C:OP2	45:x:47:ARG:NH2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:U:H6	1:A:5:U:OP1	2.03	0.40
1:A:1000:A:H2'	1:A:1001:C:C6	2.57	0.40
22:a:1183:U:H2'	22:a:1184:U:C6	2.56	0.40
1:A:476:U:H2'	1:A:477:C:C6	2.56	0.40
1:A:1464:U:P	36:o:109:ARG:HH22	2.45	0.40
4:D:172:GLU:O	4:D:180:GLY:HA2	2.22	0.40
22:a:2585:U:O4	54:Y:76:A:O2'	2.35	0.40
24:c:117:GLN:NE2	24:c:121:ASP:OD1	2.55	0.40
32:k:108:ALA:HB3	32:k:125:LEU:HD22	2.03	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	
2	B	222/241 (92%)	208 (94%)	14 (6%)	0	100	100
3	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
4	D	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
5	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
6	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
7	G	151/179 (84%)	138 (91%)	10 (7%)	3 (2%)	6	31
8	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	47
11	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
12	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
14	N	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
18	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
19	S	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
24	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
25	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
26	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
28	g	174/177 (98%)	152 (87%)	19 (11%)	3 (2%)	7	35
29	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
30	i	140/142 (99%)	140 (100%)	0	0	100	100
31	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
32	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
33	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
34	m	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
35	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
36	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	99 (98%)	1 (1%)	1 (1%)	12	47
39	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
40	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
41	t	100/104 (96%)	90 (90%)	9 (9%)	1 (1%)	12	47
42	u	92/94 (98%)	92 (100%)	0	0	100	100
43	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
44	w	75/78 (96%)	75 (100%)	0	0	100	100
45	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5481/5913 (93%)	5273 (96%)	198 (4%)	10 (0%)	44	77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	g	47	ASP
28	g	92	VAL
7	G	57	SER
10	J	57	VAL
14	N	33	ASP
41	t	99	ASN
28	g	48	ASN
7	G	6	VAL
7	G	5	ARG
38	q	44	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	
2	B	186/199 (94%)	177 (95%)	9 (5%)	23	45
3	C	170/190 (90%)	166 (98%)	4 (2%)	43	63
4	D	172/173 (99%)	159 (92%)	13 (8%)	12	33
5	E	119/126 (94%)	115 (97%)	4 (3%)	32	54
6	F	90/116 (78%)	86 (96%)	4 (4%)	25	47
7	G	126/147 (86%)	118 (94%)	8 (6%)	16	38
8	H	104/105 (99%)	101 (97%)	3 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	105/107 (98%)	102 (97%)	3 (3%)	37	58
10	J	86/90 (96%)	85 (99%)	1 (1%)	63	73
11	K	89/98 (91%)	84 (94%)	5 (6%)	19	41
12	L	102/103 (99%)	98 (96%)	4 (4%)	28	50
13	M	93/96 (97%)	88 (95%)	5 (5%)	20	42
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	72 (95%)	4 (5%)	20	42
16	P	65/65 (100%)	62 (95%)	3 (5%)	24	46
17	Q	73/78 (94%)	68 (93%)	5 (7%)	14	37
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	71 (99%)	1 (1%)	59	71
20	T	65/66 (98%)	60 (92%)	5 (8%)	12	32
21	U	60/61 (98%)	54 (90%)	6 (10%)	7	24
24	c	216/218 (99%)	214 (99%)	2 (1%)	70	76
25	d	163/163 (100%)	159 (98%)	4 (2%)	42	62
26	e	165/165 (100%)	159 (96%)	6 (4%)	31	52
27	f	148/150 (99%)	144 (97%)	4 (3%)	39	59
28	g	137/138 (99%)	125 (91%)	12 (9%)	9	29
29	h	32/114 (28%)	29 (91%)	3 (9%)	8	26
30	i	116/116 (100%)	114 (98%)	2 (2%)	53	67
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	100 (97%)	3 (3%)	37	58
33	l	107/107 (100%)	105 (98%)	2 (2%)	50	66
34	m	98/103 (95%)	97 (99%)	1 (1%)	68	76
35	n	86/87 (99%)	83 (96%)	3 (4%)	32	53
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	88 (99%)	1 (1%)	65	74
38	q	84/84 (100%)	80 (95%)	4 (5%)	23	45
39	r	93/93 (100%)	92 (99%)	1 (1%)	65	74
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	77 (93%)	6 (7%)	13	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	u	78/78 (100%)	76 (97%)	2 (3%)	40	60
43	v	58/63 (92%)	58 (100%)	0	100	100
44	w	67/68 (98%)	64 (96%)	3 (4%)	24	46
45	x	54/55 (98%)	50 (93%)	4 (7%)	13	34
46	y	48/49 (98%)	45 (94%)	3 (6%)	16	38
47	z	47/48 (98%)	46 (98%)	1 (2%)	47	65
48	0	46/49 (94%)	44 (96%)	2 (4%)	26	48
49	1	38/38 (100%)	37 (97%)	1 (3%)	40	60
50	2	51/52 (98%)	49 (96%)	2 (4%)	28	50
51	3	34/34 (100%)	33 (97%)	1 (3%)	37	58
52	4	55/62 (89%)	50 (91%)	5 (9%)	9	28
All	All	4572/4825 (95%)	4407 (96%)	165 (4%)	32	52

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	ARG
2	B	58	ASN
2	B	93	ASN
2	B	105	LYS
2	B	133	GLU
2	B	143	LYS
2	B	152	LYS
2	B	188	ASP
2	B	205	ASP
3	C	75	ILE
3	C	147	LYS
3	C	170	GLU
3	C	178	LEU
4	D	34	ILE
4	D	48	LEU
4	D	85	ASN
4	D	166	GLU
4	D	167	LYS
4	D	177	LYS
4	D	178	MET
4	D	181	THR
4	D	184	ARG

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Mol	Chain	Res	Type
4	D	188	ARG
4	D	192	SER
4	D	202	GLU
4	D	206	LYS
5	E	14	LYS
5	E	22	SER
5	E	55	GLU
5	E	164	ILE
6	F	2	ARG
6	F	62	MET
6	F	102	MET
6	F	103	VAL
7	G	6	VAL
7	G	9	GLN
7	G	57	SER
7	G	72	THR
7	G	89	VAL
7	G	90	GLU
7	G	113	ASP
7	G	149	LYS
8	H	38	ASN
8	H	56	LYS
8	H	73	GLU
9	I	27	LYS
9	I	53	GLU
9	I	85	ARG
10	J	27	GLU
11	K	16	VAL
11	K	72	ASP
11	K	87	LYS
11	K	94	GLU
11	K	129	VAL
12	L	43	LYS
12	L	54	ARG
12	L	55	VAL
12	L	62	GLU
13	M	7	ILE
13	M	16	VAL
13	M	27	LYS
13	M	75	MET
13	M	82	ASP
15	O	2	SER

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Mol	Chain	Res	Type
15	O	3	LEU
15	O	18	ASP
15	O	47	LYS
16	P	45	GLU
16	P	47	GLU
16	P	48	GLU
17	Q	5	ILE
17	Q	16	LYS
17	Q	41	THR
17	Q	50	ASN
17	Q	60	GLU
19	S	43	ASN
20	T	6	SER
20	T	13	GLN
20	T	44	LYS
20	T	54	MET
20	T	85	LYS
21	U	3	VAL
21	U	8	GLU
21	U	9	ASN
21	U	44	GLU
21	U	60	LEU
21	U	63	GLU
24	c	37	ASN
24	c	172	VAL
25	d	12	THR
25	d	32	ASN
25	d	89	GLU
25	d	92	VAL
26	e	5	LEU
26	e	9	GLN
26	e	14	VAL
26	e	21	ARG
26	e	107	SER
26	e	150	THR
27	f	27	GLN
27	f	120	LYS
27	f	136	ILE
27	f	150	ARG
28	g	20	ASN
28	g	43	VAL
28	g	49	THR

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Mol	Chain	Res	Type
28	g	75	MET
28	g	90	VAL
28	g	103	ILE
28	g	122	THR
28	g	127	THR
28	g	129	THR
28	g	171	THR
28	g	173	GLU
28	g	175	LYS
29	h	6	LEU
29	h	17	ASP
29	h	21	VAL
30	i	1	MET
30	i	9	GLU
32	k	115	GLU
32	k	120	VAL
32	k	144	GLU
33	l	7	THR
33	l	51	ARG
34	m	48	VAL
35	n	13	ARG
35	n	16	ARG
35	n	84	GLU
37	p	112	LYS
38	q	33	VAL
38	q	47	VAL
38	q	48	LYS
38	q	72	VAL
39	r	66	ILE
41	t	15	THR
41	t	24	LYS
41	t	26	LYS
41	t	60	GLU
41	t	74	ASN
41	t	98	SER
42	u	63	ILE
42	u	77	VAL
44	w	44	LYS
44	w	54	LYS
44	w	76	GLU
45	x	4	LYS
45	x	8	GLU

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Mol	Chain	Res	Type
45	x	14	LEU
45	x	24	GLU
46	y	3	LYS
46	y	41	THR
46	y	59	GLU
47	z	54	VAL
48	0	5	ILE
48	0	32	GLU
49	1	8	SER
50	2	15	LYS
50	2	31	HIS
51	3	36	ARG
52	4	12	ILE
52	4	13	THR
52	4	24	ILE
52	4	59	ARG
52	4	62	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	GLN
2	B	58	ASN
2	B	89	GLN
2	B	103	ASN
2	B	109	GLN
3	C	6	HIS
3	C	100	GLN
3	C	123	GLN
3	C	139	GLN
4	D	40	GLN
4	D	100	ASN
5	E	12	GLN
5	E	73	ASN
5	E	82	GLN
5	E	146	ASN
5	E	148	ASN
6	F	37	HIS
6	F	52	ASN
6	F	55	HIS
7	G	86	GLN
8	H	4	GLN

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Mol	Chain	Res	Type
9	I	31	ASN
9	I	110	GLN
10	J	35	GLN
10	J	58	ASN
11	K	38	GLN
11	K	40	ASN
12	L	75	GLN
12	L	112	GLN
13	M	8	ASN
14	N	66	GLN
15	O	50	HIS
17	Q	51	ASN
18	R	52	GLN
19	S	52	HIS
19	S	57	HIS
19	S	83	HIS
20	T	84	ASN
21	U	56	HIS
24	c	90	ASN
24	c	117	GLN
24	c	197	ASN
26	e	94	GLN
26	e	136	GLN
28	g	38	ASN
28	g	48	ASN
28	g	101	ASN
28	g	104	ASN
28	g	115	HIS
30	i	47	HIS
30	i	86	GLN
30	i	128	ASN
31	j	5	GLN
31	j	9	ASN
33	l	13	HIS
35	n	100	HIS
36	o	12	GLN
36	o	41	GLN
37	p	37	GLN
37	p	72	ASN
38	q	6	GLN
38	q	43	ASN
39	r	31	GLN

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Mol	Chain	Res	Type
39	r	40	ASN
40	s	48	GLN
41	t	74	ASN
42	u	49	ASN
44	w	6	GLN
44	w	36	HIS
45	x	15	ASN
46	y	9	GLN
47	z	6	ASN
50	2	31	HIS
52	4	20	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1516/1542 (98%)	207 (13%)	6 (0%)
22	a	2749/2904 (94%)	346 (12%)	0
23	b	118/120 (98%)	13 (11%)	0
53	X	11/28 (39%)	2 (18%)	0
54	Y	72/76 (94%)	31 (43%)	6 (8%)
55	Z	75/76 (98%)	27 (36%)	1 (1%)
56	5	1/2 (50%)	1 (100%)	0
All	All	4542/4748 (95%)	627 (13%)	13 (0%)

All (627) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	80	A

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Mol	Chain	Res	Type
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	89	U
1	A	94	G
1	A	95	C
1	A	96	U
1	A	121	U
1	A	122	G
1	A	131	A
1	A	141	G
1	A	144	G
1	A	146	G
1	A	166	U
1	A	177	G
1	A	182	A
1	A	183	C
1	A	189	A
1	A	197	A
1	A	204	G
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	271	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	345	C
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G

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Mol	Chain	Res	Type
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	417	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	436	C
1	A	446	G
1	A	453	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	459	A
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	474	G
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	490	C
1	A	495	A
1	A	511	C
1	A	518	C
1	A	531	U
1	A	532	A
1	A	547	A
1	A	562	U
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G

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Mol	Chain	Res	Type
1	A	579	A
1	A	596	A
1	A	615	G
1	A	633	G
1	A	648	A
1	A	650	G
1	A	653	U
1	A	665	A
1	A	702	A
1	A	723	U
1	A	724	G
1	A	746	A
1	A	747	A
1	A	748	G
1	A	755	G
1	A	774	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	840	C
1	A	890	G
1	A	914	A
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	993	G
1	A	994	A
1	A	998	C
1	A	1004	A
1	A	1006	G
1	A	1008	U
1	A	1009	U
1	A	1024	G

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Mol	Chain	Res	Type
1	A	1027	C
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1044	A
1	A	1045	C
1	A	1046	A
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1137	C
1	A	1139	G
1	A	1143	G
1	A	1144	G
1	A	1159	U
1	A	1169	A
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1256	A
1	A	1275	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1317	C
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1378	C

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Mol	Chain	Res	Type
1	A	1379	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1419	G
1	A	1432	G
1	A	1440	U
1	A	1441	A
1	A	1442	G
1	A	1444	U
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
22	a	10	A
22	a	15	G
22	a	34	U
22	a	42	A
22	a	45	G
22	a	58	G
22	a	71	A
22	a	74	A
22	a	75	G
22	a	80	G
22	a	84	A
22	a	101	A
22	a	102	U
22	a	110	G
22	a	118	A
22	a	119	A
22	a	120	U

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Mol	Chain	Res	Type
22	a	139	U
22	a	140	C
22	a	142	A
22	a	163	C
22	a	165	A
22	a	181	A
22	a	196	A
22	a	215	G
22	a	216	A
22	a	221	A
22	a	222	A
22	a	248	G
22	a	264	C
22	a	265	A
22	a	272	A
22	a	274	C
22	a	278	A
22	a	279	A
22	a	282	A
22	a	285	G
22	a	286	U
22	a	289	G
22	a	292	U
22	a	294	A
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	357	C
22	a	361	G
22	a	362	A
22	a	386	G
22	a	404	A
22	a	405	U
22	a	411	G
22	a	412	A
22	a	451	U
22	a	481	G
22	a	491	G
22	a	503	A
22	a	504	A
22	a	505	A

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Mol	Chain	Res	Type
22	a	509	C
22	a	528	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	533	G
22	a	543	G
22	a	544	C
22	a	545	U
22	a	546	U
22	a	547	A
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	614	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C
22	a	646	U
22	a	647	G
22	a	653	U
22	a	654	A
22	a	655	A
22	a	685	A
22	a	686	U
22	a	714	U
22	a	717	C
22	a	721	A
22	a	730	A
22	a	747	5MU
22	a	764	A
22	a	765	C
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	789	A
22	a	805	G

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Mol	Chain	Res	Type
22	a	812	C
22	a	827	U
22	a	828	U
22	a	846	U
22	a	847	U
22	a	856	G
22	a	859	G
22	a	869	G
22	a	879	G
22	a	883	G
22	a	884	U
22	a	885	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	898	C
22	a	899	A
22	a	905	A
22	a	910	A
22	a	914	G
22	a	915	C
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	984	A
22	a	985	C
22	a	996	A
22	a	1012	U
22	a	1013	C
22	a	1017	G
22	a	1022	G
22	a	1033	U
22	a	1041	G
22	a	1045	C
22	a	1046	A
22	a	1047	G
22	a	1048	A
22	a	1051	G
22	a	1108	U

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Mol	Chain	Res	Type
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1116	G
22	a	1120	G
22	a	1122	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1171	G
22	a	1227	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1275	A
22	a	1294	U
22	a	1300	G
22	a	1301	A
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1411	U
22	a	1416	G
22	a	1417	C
22	a	1420	A
22	a	1421	G
22	a	1427	A
22	a	1428	C
22	a	1452	G
22	a	1453	A
22	a	1468	U
22	a	1476	U
22	a	1482	G
22	a	1486	U
22	a	1487	U
22	a	1493	C
22	a	1497	U
22	a	1504	A
22	a	1508	A

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Mol	Chain	Res	Type
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1554	U
22	a	1559	U
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1586	A
22	a	1590	A
22	a	1593	A
22	a	1608	A
22	a	1609	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1722	A
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1732	C
22	a	1733	G
22	a	1736	U
22	a	1738	G
22	a	1750	G
22	a	1764	C
22	a	1773	A
22	a	1782	U
22	a	1791	A
22	a	1800	C
22	a	1801	A
22	a	1808	A

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Mol	Chain	Res	Type
22	a	1816	C
22	a	1829	A
22	a	1847	A
22	a	1858	A
22	a	1867	G
22	a	1868	C
22	a	1870	C
22	a	1871	A
22	a	1873	G
22	a	1906	G
22	a	1907	G
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1965	C
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2020	A
22	a	2023	C
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2194	U
22	a	2198	A
22	a	2203	U
22	a	2204	G
22	a	2208	C
22	a	2211	A
22	a	2223	G
22	a	2225	A

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Mol	Chain	Res	Type
22	a	2238	G
22	a	2268	A
22	a	2279	G
22	a	2282	G
22	a	2283	C
22	a	2287	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2335	A
22	a	2347	C
22	a	2350	C
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2424	C
22	a	2425	A
22	a	2429	G
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2470	G
22	a	2476	A
22	a	2478	A
22	a	2491	U
22	a	2502	G
22	a	2505	G
22	a	2518	A
22	a	2529	G
22	a	2535	G
22	a	2547	A
22	a	2554	U
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2586	U

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Mol	Chain	Res	Type
22	a	2602	A
22	a	2603	G
22	a	2609	U
22	a	2613	U
22	a	2629	U
22	a	2670	A
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2716	C
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2751	G
22	a	2752	C
22	a	2757	A
22	a	2765	A
22	a	2778	A
22	a	2790	U
22	a	2792	A
22	a	2795	C
22	a	2798	U
22	a	2799	A
22	a	2802	G
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2873	A
22	a	2883	A
22	a	2884	U
22	a	2891	U
22	a	2899	A
22	a	2901	C
22	a	2902	C
23	b	9	G
23	b	13	G
23	b	34	A
23	b	35	C
23	b	36	C
23	b	45	A
23	b	56	G

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Mol	Chain	Res	Type
23	b	57	A
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	109	A
53	X	15	A
53	X	24	A
54	Y	3	G
54	Y	5	G
54	Y	6	A
54	Y	8	U
54	Y	9	A
54	Y	11	C
54	Y	13	C
54	Y	14	A
54	Y	19	G
54	Y	20	G
54	Y	21	A
54	Y	23	A
54	Y	24	G
54	Y	25	C
54	Y	45	G
54	Y	46	G
54	Y	47	U
54	Y	48	C
54	Y	49	G
54	Y	50	G
54	Y	57	G
54	Y	59	U
54	Y	60	C
54	Y	61	C
54	Y	66	A
54	Y	67	U
54	Y	70	C
54	Y	71	C
54	Y	73	A
54	Y	74	C
54	Y	75	C
55	Z	6	G
55	Z	8	U
55	Z	9	G

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Mol	Chain	Res	Type
55	Z	14	A
55	Z	16	C
55	Z	17	C
55	Z	17(A)	U
55	Z	18	G
55	Z	19	G
55	Z	20	U
55	Z	21	A
55	Z	22	G
55	Z	46	G
55	Z	47	U
55	Z	49	G
55	Z	50	U
55	Z	52	G
55	Z	54	U
55	Z	56	C
55	Z	58	A
55	Z	59	A
55	Z	65	C
55	Z	66	C
55	Z	68	C
55	Z	69	C
55	Z	71	C
55	Z	76	A
56	5	76	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	199	A
1	A	250	A
1	A	993	G
1	A	1026	G
1	A	1035	A
54	Y	13	C
54	Y	19	G
54	Y	45	G
54	Y	46	G
54	Y	48	C
54	Y	60	C
55	Z	58	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	A	527	1	23,26,27	0.70	1 (4%)	35,39,42	0.75	0
1	2MG	A	1516	1	23,26,27	0.43	0	32,38,41	0.59	0
22	G7M	a	2069	22	23,26,27	0.65	1 (4%)	35,39,42	0.75	0
22	OMC	a	2498	22	19,22,23	0.42	0	26,31,34	0.74	0
22	H2U	a	2449	22	18,21,22	0.86	1 (5%)	21,30,33	0.78	1 (4%)
22	5MU	a	1939	22	19,22,23	0.42	0	28,32,35	0.50	0
22	PSU	a	2580	22	18,21,22	1.00	1 (5%)	22,30,33	0.83	1 (4%)
22	5MC	a	1962	22	18,22,23	0.44	0	26,32,35	0.84	1 (3%)
22	PSU	a	955	22	18,21,22	0.99	1 (5%)	22,30,33	0.75	0
22	PSU	a	1917	22	18,21,22	1.01	1 (5%)	22,30,33	0.77	1 (4%)
22	1MG	a	745	22	22,26,27	0.57	0	33,39,42	0.55	0
1	MA6	A	1519	1	23,26,27	0.42	0	34,38,41	1.10	1 (2%)
1	5MC	A	967	1	18,22,23	0.44	0	26,32,35	0.77	0
22	5MU	a	747	22	19,22,23	0.44	0	28,32,35	0.51	0
22	2MA	a	2503	22	22,25,26	1.10	3 (13%)	33,37,40	1.12	4 (12%)
1	UR3	A	1498	1	19,22,23	0.41	0	26,32,35	0.83	2 (7%)
1	MA6	A	1518	1	23,26,27	0.42	0	34,38,41	0.84	1 (2%)
22	6MZ	a	1618	22	22,25,26	0.57	1 (4%)	30,36,39	0.64	0
22	2MG	a	1835	22	23,26,27	0.45	0	32,38,41	0.57	0
1	2MG	A	1207	1	23,26,27	0.48	0	32,38,41	0.62	0
22	6MZ	a	2030	22	22,25,26	0.40	0	30,36,39	0.59	0
22	OMG	a	2251	55,22	23,26,27	0.39	0	33,38,41	0.59	0
33	4D4	l	81	33	9,11,12	0.50	0	8,13,15	0.70	0
33	MS6	l	82	33	5,7,8	0.30	0	2,7,9	0.43	0
22	PSU	a	1911	22	18,21,22	1.02	1 (5%)	22,30,33	0.74	0
1	4OC	A	1402	1	20,23,24	0.49	0	26,32,35	0.82	1 (3%)
22	PSU	a	2605	22	18,21,22	1.03	1 (5%)	22,30,33	0.89	0
1	2MG	A	966	1	23,26,27	0.51	0	32,38,41	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	a	746	22	18,21,22	1.16	1 (5%)	22,30,33	0.84	0
25	MEQ	d	150	25	8,9,10	0.45	0	5,10,12	1.71	2 (40%)
22	PSU	a	2457	22	18,21,22	1.00	1 (5%)	22,30,33	0.75	0
22	3TD	a	1915	22	19,22,23	1.03	1 (5%)	21,32,35	1.00	2 (9%)
12	D2T	L	89	12	7,9,10	1.04	0	6,11,13	1.64	3 (50%)
22	PSU	a	2504	22	18,21,22	0.98	1 (5%)	22,30,33	0.74	0
22	2MG	a	2445	22	23,26,27	0.43	0	32,38,41	0.58	0
22	PSU	a	2604	22	18,21,22	1.03	1 (5%)	22,30,33	0.90	0
1	PSU	A	516	1	18,21,22	1.02	1 (5%)	22,30,33	0.73	0
11	IAS	K	119	11	6,7,8	0.94	0	6,8,10	1.02	0
1	5MC	A	1407	1	18,22,23	0.45	0	26,32,35	0.86	0
22	OMU	a	2552	22	19,22,23	0.36	0	26,31,34	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	A	527	1	-	1/7/25/26	0/3/3/3
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
22	G7M	a	2069	22	-	2/7/25/26	0/3/3/3
22	OMC	a	2498	22	-	0/9/27/28	0/2/2/2
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	2MA	a	2503	22	-	2/7/25/26	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMG	a	2251	55,22	-	0/9/27/28	0/3/3/3
33	4D4	l	81	33	-	1/11/12/14	-
33	MS6	l	82	33	-	0/4/6/8	-
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3
22	PSU	a	746	22	-	1/7/25/26	0/2/2/2
25	MEQ	d	150	25	-	2/8/9/11	-
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	2/7/12/14	-
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	1/9/27/28	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	1/9/27/28	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	746	PSU	C6-C5	4.46	1.40	1.35
22	a	2605	PSU	C6-C5	4.07	1.40	1.35
1	A	516	PSU	C6-C5	4.05	1.40	1.35
22	a	1911	PSU	C6-C5	4.04	1.40	1.35
22	a	2580	PSU	C6-C5	4.01	1.40	1.35
22	a	1917	PSU	C6-C5	4.00	1.40	1.35
22	a	2604	PSU	C6-C5	3.97	1.39	1.35
22	a	2457	PSU	C6-C5	3.96	1.39	1.35
22	a	1915	3TD	C6-C5	3.93	1.39	1.35
22	a	955	PSU	C6-C5	3.91	1.39	1.35
22	a	2504	PSU	C6-C5	3.91	1.39	1.35
22	a	2503	2MA	C6-N1	2.79	1.39	1.35
22	a	2503	2MA	C2-N1	2.43	1.38	1.34
22	a	2069	G7M	C8-N7	2.35	1.37	1.33
1	A	527	G7M	C8-N7	2.35	1.37	1.33
22	a	2449	H2U	C2-N1	2.31	1.38	1.35
22	a	1618	6MZ	C6-N6	2.20	1.36	1.34
22	a	2503	2MA	C6-N6	-2.05	1.29	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	MA6	C2-N1-C6	3.44	119.89	111.75
1	A	1519	MA6	C2-N1-C6	3.30	119.54	111.75
22	a	2503	2MA	CM2-C2-N1	3.24	122.22	117.15
22	a	2503	2MA	C5-C4-N3	-2.61	124.25	127.19
22	a	2503	2MA	C2-N1-C6	2.36	121.75	118.08
25	d	150	MEQ	CG-CD-NE2	2.31	119.50	116.29
25	d	150	MEQ	OE1-CD-CG	-2.30	117.81	122.02
12	L	89	D2T	O-C-CA	-2.29	118.77	124.78
1	A	1498	UR3	C4-N3-C2	-2.29	122.41	124.56
12	L	89	D2T	OD2-CG-CB	2.25	118.01	113.15
1	A	1498	UR3	C6-N1-C2	-2.22	119.80	121.79
12	L	89	D2T	OD1-CG-CB	-2.16	117.91	122.44
22	a	2449	H2U	C4-N3-C2	-2.16	124.00	125.79
22	a	1915	3TD	C4-N3-C2	-2.15	122.28	124.61
1	A	1402	4OC	O2'-C2'-C1'	2.14	113.25	109.08
22	a	1915	3TD	O2'-C2'-C3'	2.12	118.69	111.82
22	a	2503	2MA	N3-C2-N1	-2.12	121.82	125.72
22	a	1917	PSU	O2'-C2'-C3'	2.10	118.63	111.82
22	a	1962	5MC	CM5-C5-C6	-2.08	120.07	122.85
22	a	2580	PSU	C3'-C2'-C1'	2.04	104.02	101.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CG-CB-SB-CB1
22	a	2030	6MZ	O4'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
22	a	2030	6MZ	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	2504	PSU	O4'-C4'-C5'-O5'
22	a	2069	G7M	C4'-C5'-O5'-P
12	L	89	D2T	CA-CB-SB-CB1
22	a	2503	2MA	C4'-C5'-O5'-P
22	a	2445	2MG	C3'-C4'-C5'-O5'
22	a	2504	PSU	C3'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C6
1	A	527	G7M	C4'-C5'-O5'-P
22	a	2552	OMU	C3'-C2'-O2'-CM2
1	A	1519	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	a	2069	G7M	O4'-C4'-C5'-O5'
22	a	2503	2MA	O4'-C4'-C5'-O5'
33	l	81	4D4	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	1939	5MU	1	0
22	a	747	5MU	1	0
22	a	2030	6MZ	1	0
22	a	2604	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

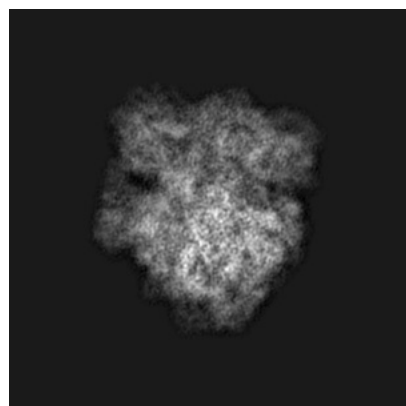
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17959. These allow visual inspection of the internal detail of the map and identification of artifacts.

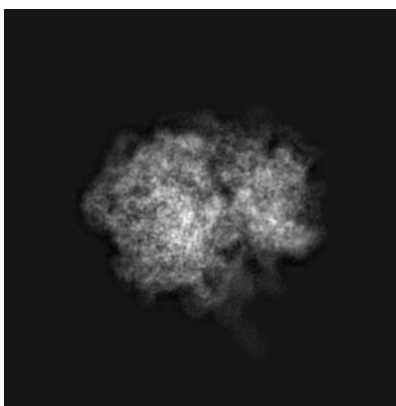
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

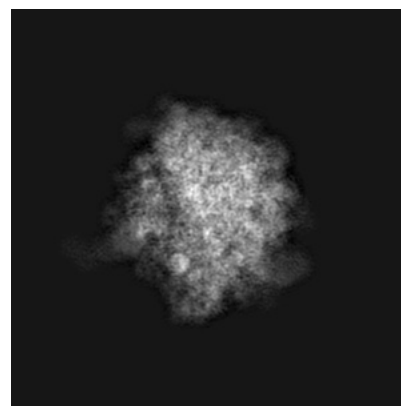
6.1.1 Primary map



X

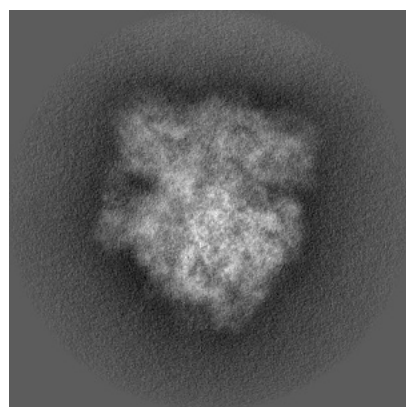


Y

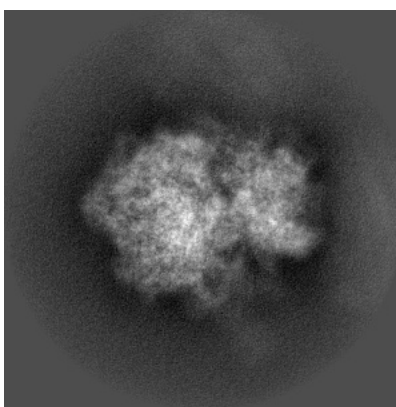


Z

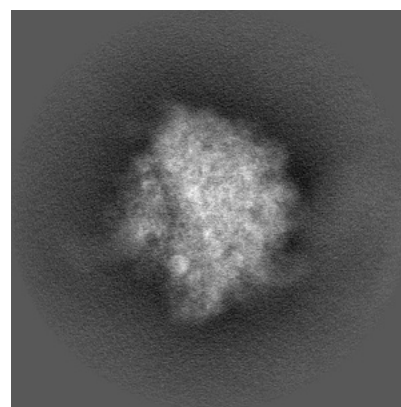
6.1.2 Raw map



X



Y

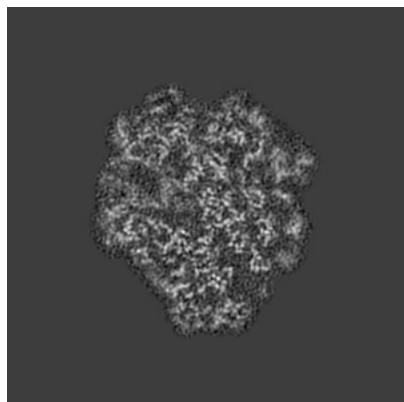


Z

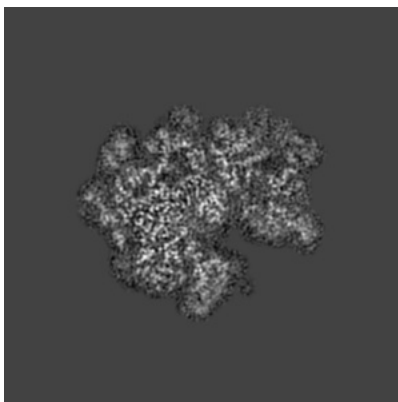
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

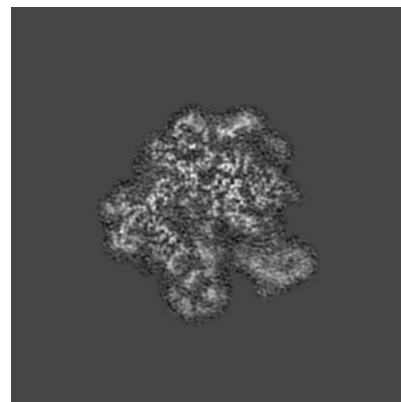
6.2.1 Primary map



X Index: 200

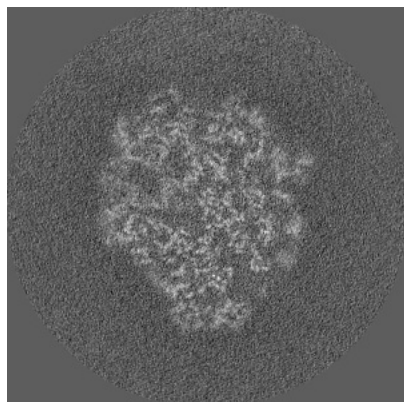


Y Index: 200

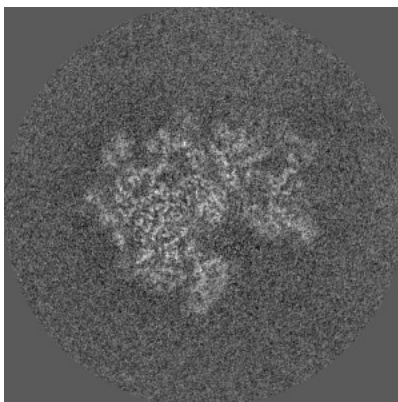


Z Index: 200

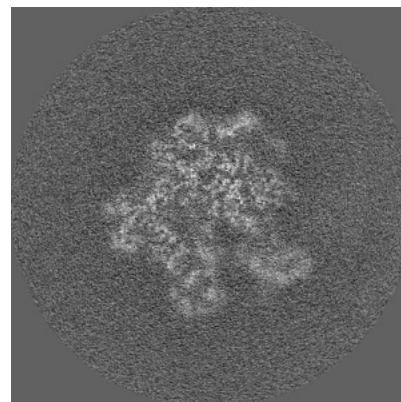
6.2.2 Raw map



X Index: 200



Y Index: 200

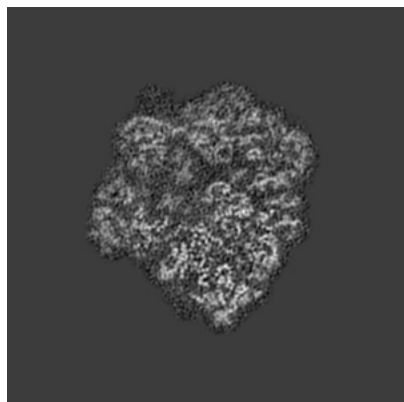


Z Index: 200

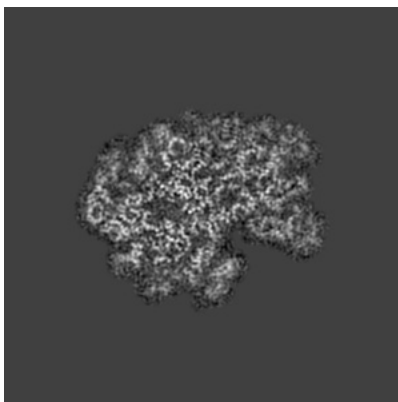
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

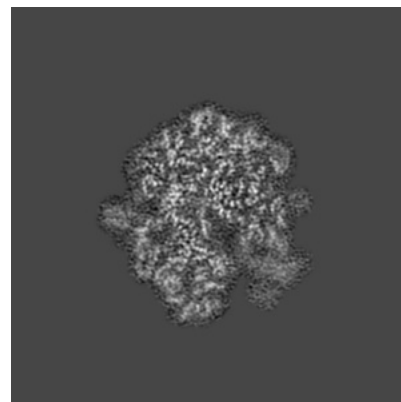
6.3.1 Primary map



X Index: 185

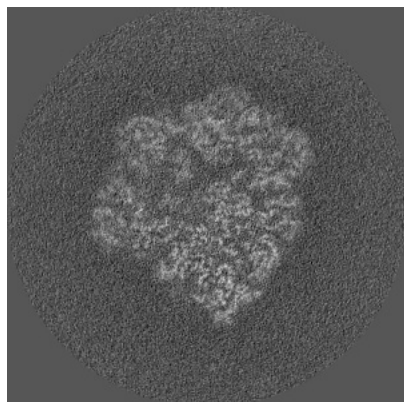


Y Index: 214

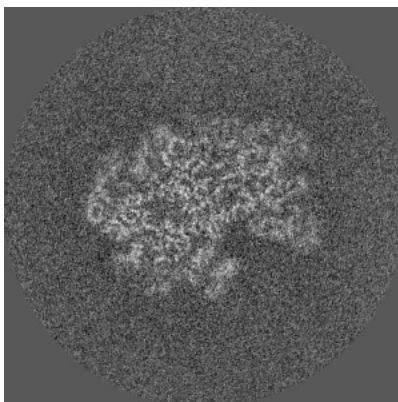


Z Index: 184

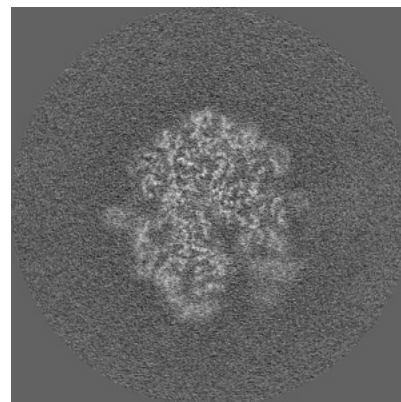
6.3.2 Raw map



X Index: 184



Y Index: 214

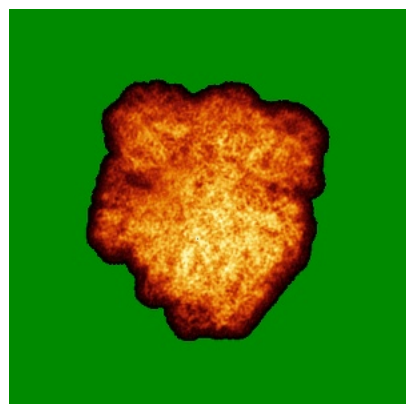


Z Index: 183

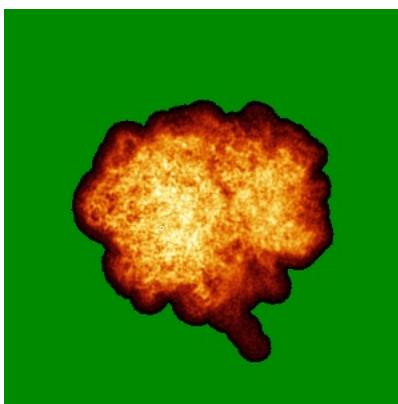
The images above show the largest variance slices of the map in three orthogonal directions.

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

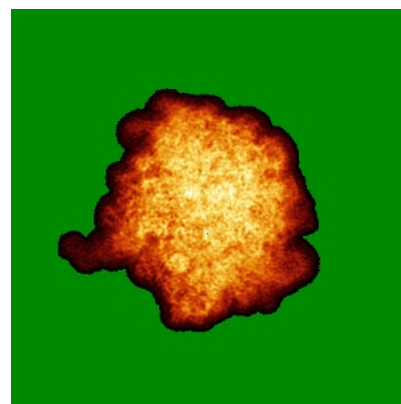
6.4.1 Primary map



X

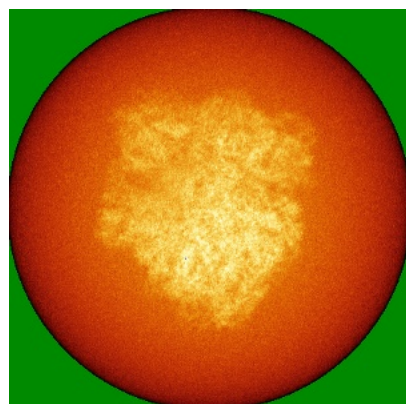


Y

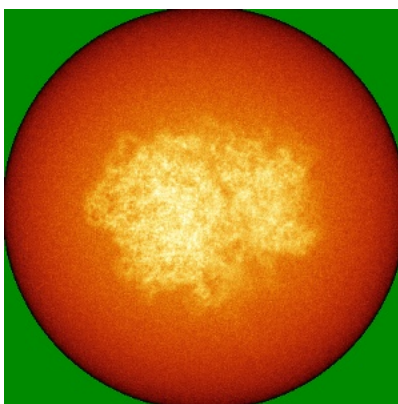


Z

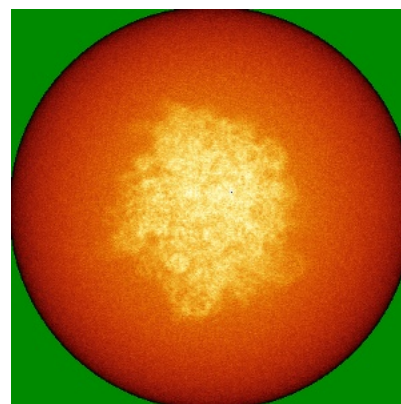
6.4.2 Raw map



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



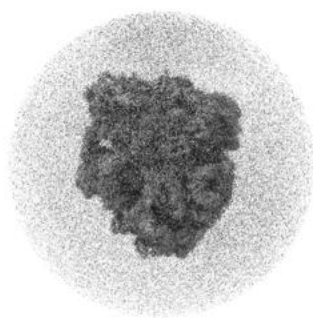
Y



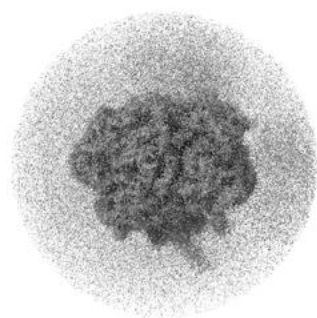
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

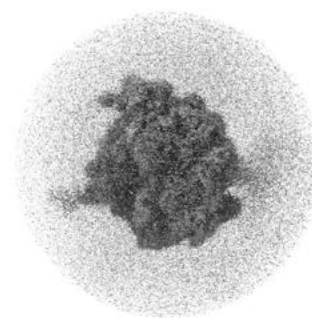
6.5.2 Raw map



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.

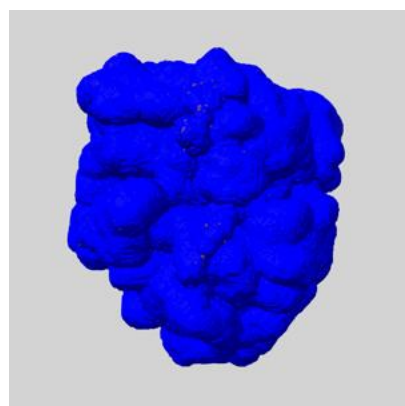
6.6 Mask visualisation [i](#)

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

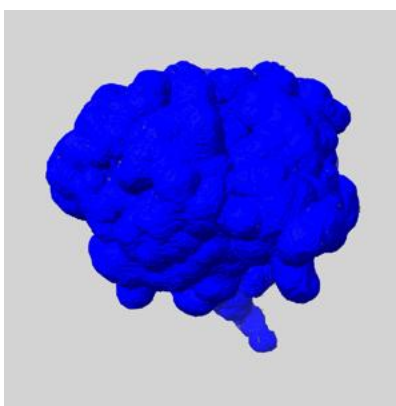
A mask typically either:

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

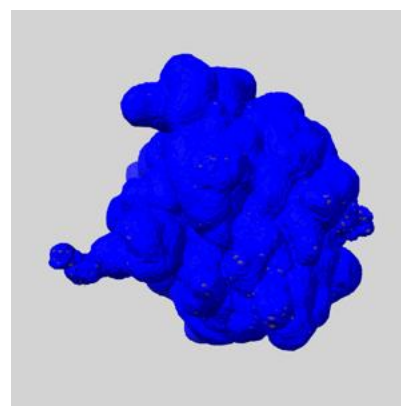
6.6.1 emd_17959_msk_1.map [i](#)



X



Y

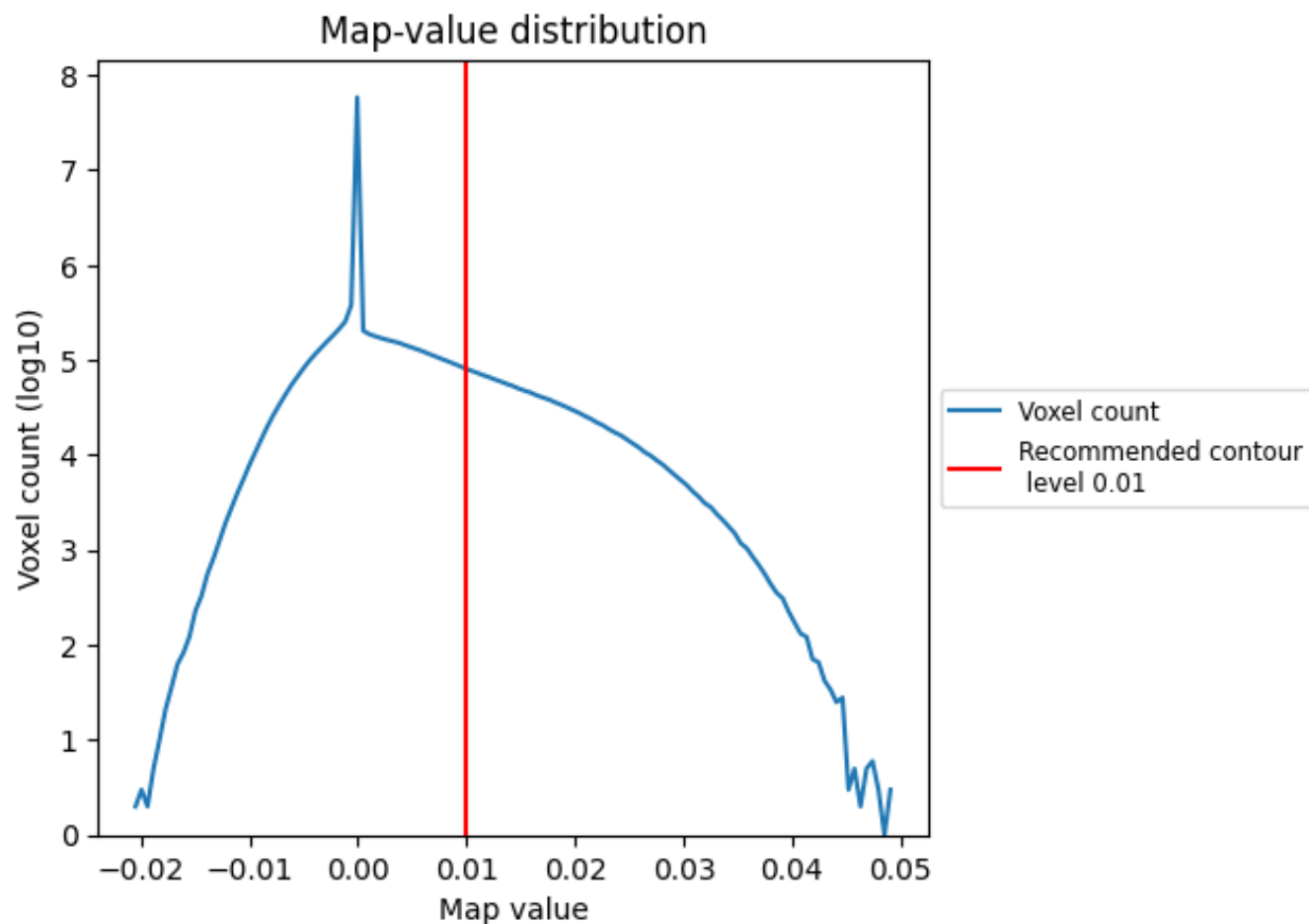


Z

7 Map analysis [i](#)

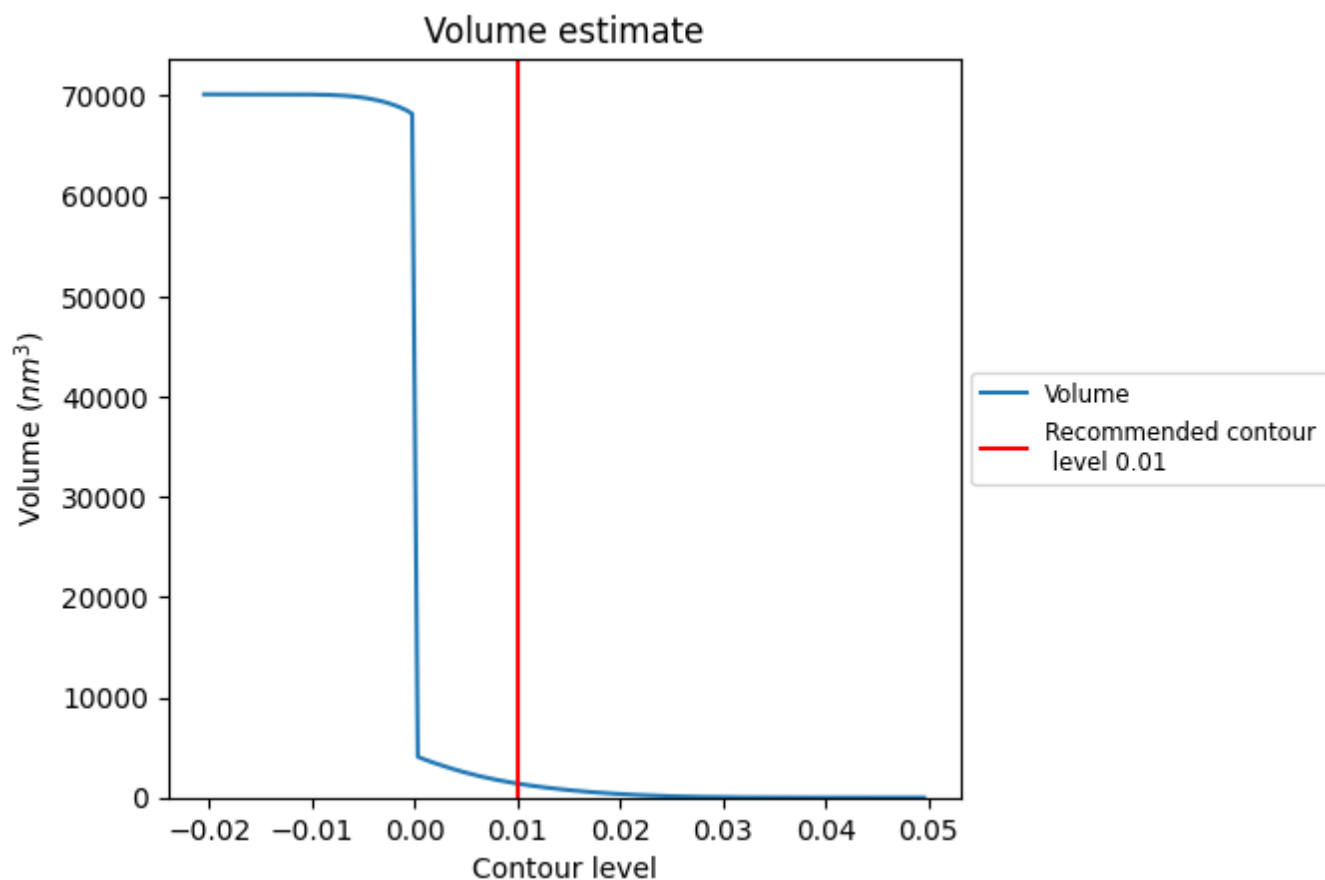
This section contains the results of statistical analysis of the map.

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.

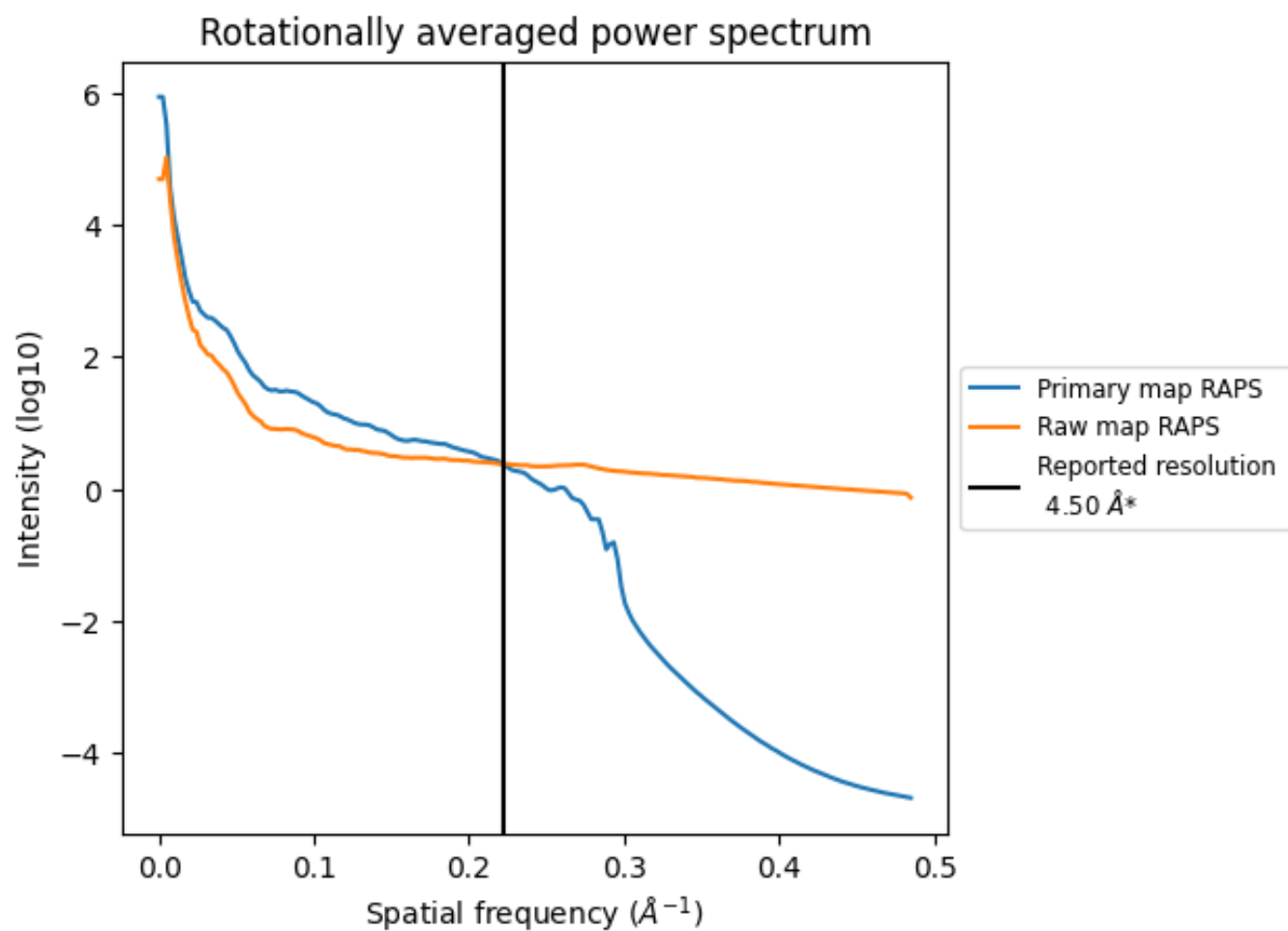
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1400 nm³; this corresponds to an approximate mass of 1264 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 ⓘ

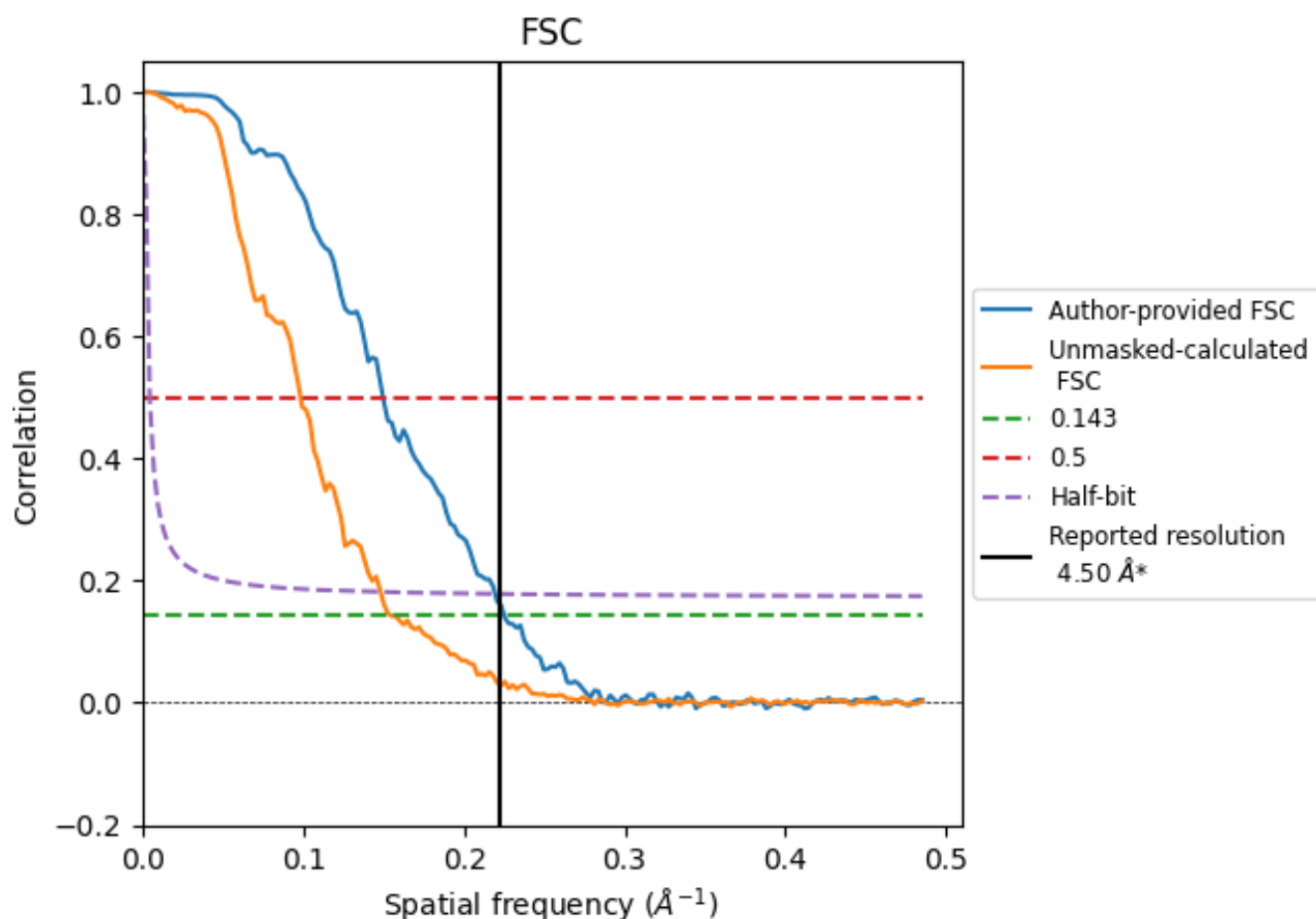


*Reported resolution corresponds to spatial frequency of $0.222 \text{ \AA}^{-1}$

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 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

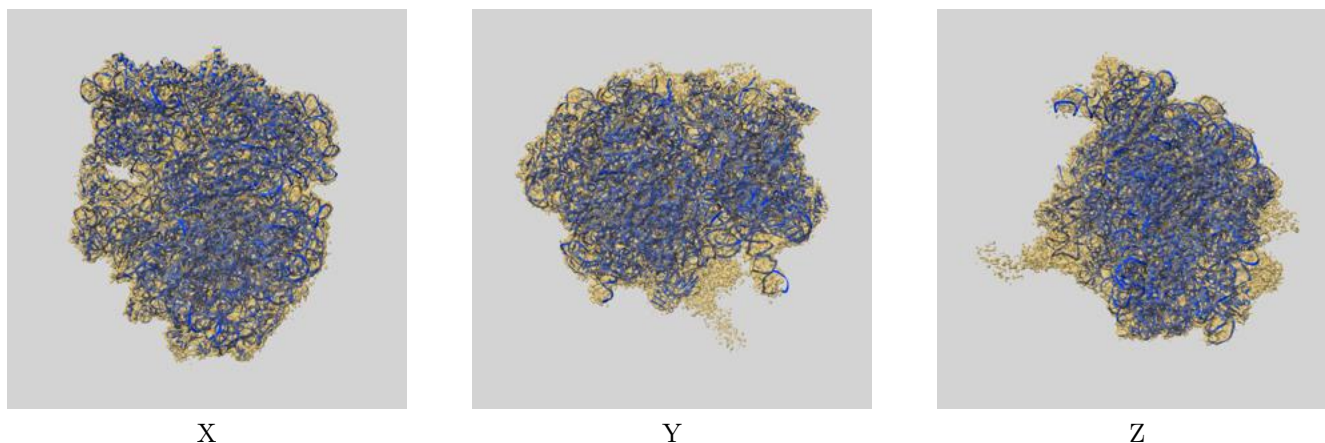
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.44	6.68	4.56
Unmasked-calculated*	6.47	10.16	6.74

*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 6.47 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

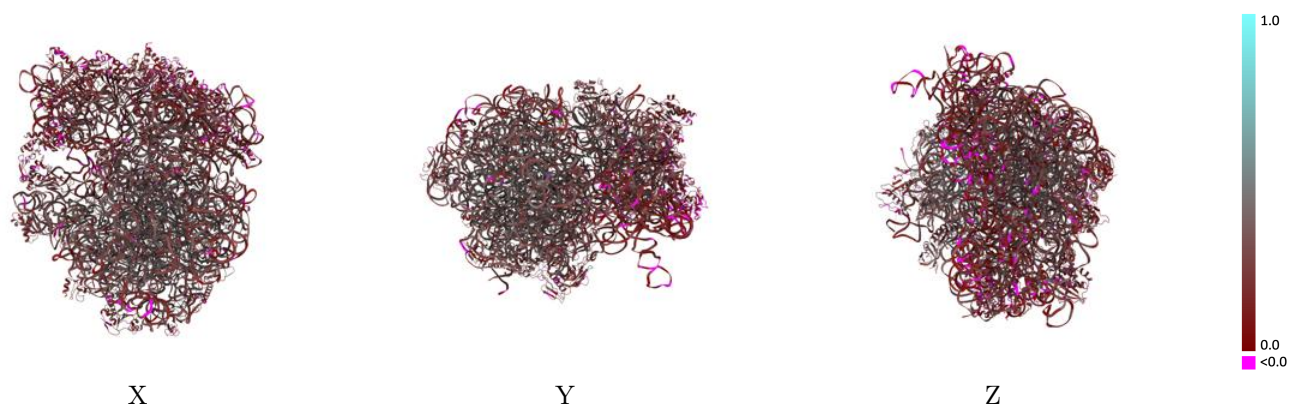
This section contains information regarding the fit between EMDB map EMD-17959 and PDB model 8PVA. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



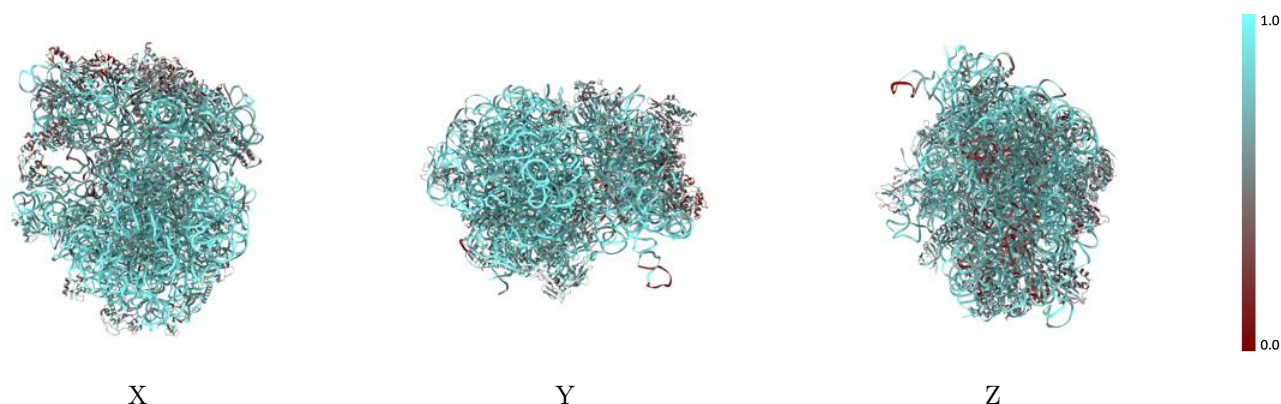
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



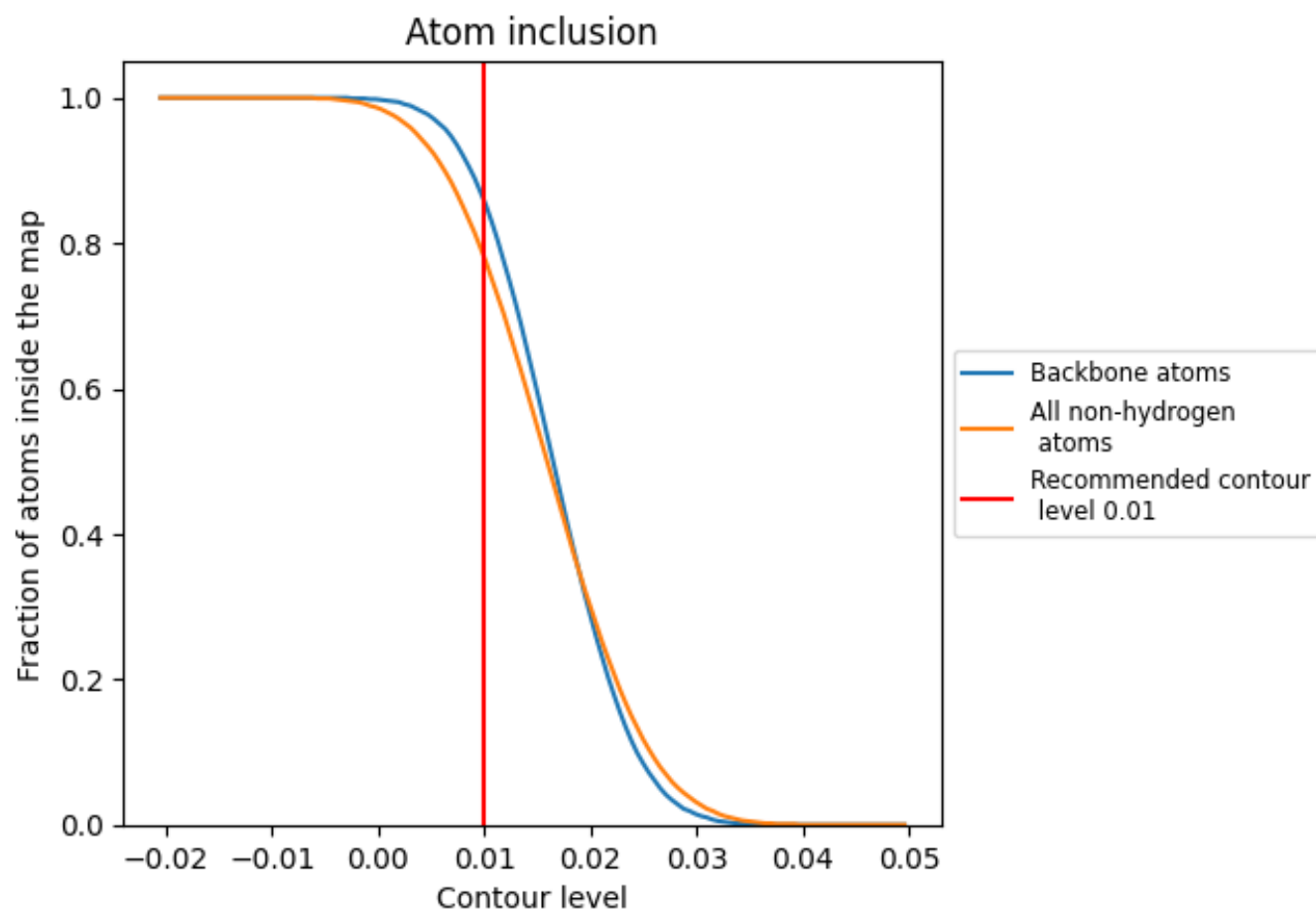
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.2870
0	 0.6240	 0.2300
1	 0.7520	 0.3560
2	 0.6970	 0.3600
3	 0.6890	 0.2800
4	 0.4750	 0.1650
5	 0.7140	 0.3100
A	 0.8230	 0.2540
B	 0.4910	 0.1880
C	 0.4500	 0.1830
D	 0.3740	 0.1230
E	 0.5410	 0.2140
F	 0.5560	 0.2540
G	 0.5080	 0.1960
H	 0.5710	 0.2020
I	 0.5300	 0.2130
J	 0.4440	 0.1720
K	 0.6160	 0.2990
L	 0.5500	 0.1700
M	 0.5060	 0.1700
N	 0.5210	 0.1640
O	 0.6380	 0.2370
P	 0.4890	 0.1670
Q	 0.5440	 0.1790
R	 0.5990	 0.2830
S	 0.5260	 0.1360
T	 0.5510	 0.1550
U	 0.4870	 0.2210
X	 0.6310	 0.2330
Y	 0.5350	 0.1650
Z	 0.6540	 0.1760
a	 0.9000	 0.3420
b	 0.9030	 0.2940
c	 0.6910	 0.3340
d	 0.6800	 0.3160



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Chain	Atom inclusion	Q-score
e	 0.6350	 0.3010
f	 0.5920	 0.2150
g	 0.5580	 0.1870
h	 0.5600	 0.2410
i	 0.6840	 0.3120
j	 0.6240	 0.2950
k	 0.6620	 0.3060
l	 0.6810	 0.3210
m	 0.7120	 0.3350
n	 0.6780	 0.2530
o	 0.6240	 0.2560
p	 0.7070	 0.3250
q	 0.6300	 0.2810
r	 0.6670	 0.3410
s	 0.6370	 0.3190
t	 0.5710	 0.2560
u	 0.6640	 0.2610
v	 0.7010	 0.3210
w	 0.6570	 0.3140
x	 0.6320	 0.2360
y	 0.6290	 0.2930
z	 0.6710	 0.3170