



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:29 AM UTC

PDB ID : 6YEF / pdb_00006yef
EMDB ID : EMD-10791
Title : 70S initiation complex with assigned rRNA modifications from *Staphylococcus aureus*
Authors : Fatkhullin, B.; Golubev, A.; Khusainov, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2020-03-24
Resolution : 3.20 Å(reported)
Based on initial model : 5LI0

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:

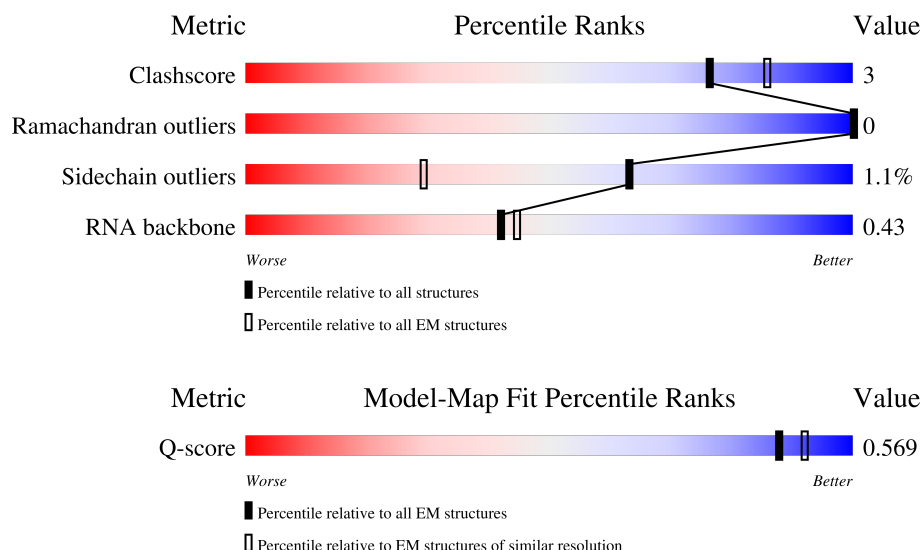
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	15020 (2.70 - 3.70)

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	1556	7% 72% 25% ..
2	b	255	63% 67% 18% 14%
3	c	217	17% 80% 12% 8%

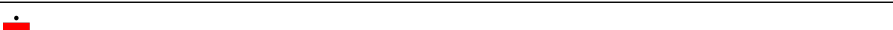
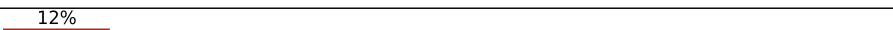
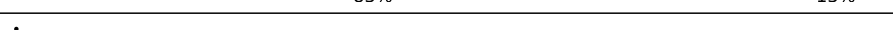
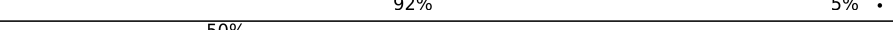
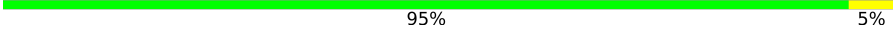
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Mol	Chain	Length	Quality of chain
4	d	200	
5	e	166	
6	f	98	
7	g	156	
8	h	132	
9	i	132	
10	j	102	
11	k	129	
12	l	137	
13	m	121	
14	n	89	
15	o	89	
16	p	91	
17	q	87	
18	r	80	
19	s	92	
20	t	83	
21	v	29	
22	A	2923	
23	B	115	
24	D	277	
25	E	220	
26	F	207	
27	G	179	
28	H	178	

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Mol	Chain	Length	Quality of chain
29	M	145	
30	N	122	
31	O	146	
32	P	144	
33	Q	122	
34	R	119	
35	S	116	
36	T	118	
37	U	102	
38	V	117	
39	W	91	
40	X	105	
41	Y	217	
42	Z	94	
43	0	62	
44	1	69	
45	2	59	
46	3	84	
47	4	58	
48	5	49	
49	6	45	
50	7	66	
51	8	37	
52	x	77	

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 141837 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	1545	Total	C	N	O	P	0	0
			33097	14781	6034	10737	1545		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	219	Total	C	N	O	S	0	0
			1762	1123	307	325	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	200	Total	C	N	O	S	0	0
			1578	993	296	287	2		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	197	Total	C	N	O	S	0	0
			1600	1009	300	289	2		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1169	735	214	218	2		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	96	Total	C	N	O	S	0	0
			798	503	139	153	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	146	Total	C	N	O	S	0	0
			1176	733	225	214	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1008	623	201	183	1		

- Molecule 10 is a protein called ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			783	494	143	145	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	113	Total	C	N	O	S	0	0
			833	514	156	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	117	Total	C	N	O	S	0	0
			927	569	184	173	1		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			481	296	103	80	2		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			738	454	153	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	85	Total	C	N	O	S	0	0
			698	441	125	131	1		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	64	Total	C	N	O	S	0	0
			527	335	97	92	3		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	82	Total	C	N	O	S	0	0
			661	426	118	115	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 21 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	v	21	Total	C	N	O	P	0	0
			462	207	96	138	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	2881	Total	C	N	O	P	0	0
			61802	27593	11324	20004	2881		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	E	216	Total	C	N	O	S	0	0
			1635	1023	301	306	5		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	F	203	Total	C	N	O	S	0	0
			1540	966	284	288	2		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	G	154	Total	C	N	O	S	0	0
			1191	751	206	228	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	160	Total	C	N	O	S	0	0
			1250	781	222	244	3		

- Molecule 29 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	M	145	Total	C	N	O	S	0	0
			1151	717	211	220	3		

- Molecule 30 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 31 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	O	146	Total	C	N	O	S	0	0
			1098	680	215	202	1		

- Molecule 32 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	137	Total	C	N	O	S	0	0
			1097	704	207	182	4		

- Molecule 33 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Q	119	Total	C	N	O	S	0	0
			940	575	181	183	1		

- Molecule 34 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R	118	Total	C	N	O		0	0
			911	568	173	170			

- Molecule 35 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	S	109	Total	C	N	O		
			877	552	176	149	0	0

- Molecule 36 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	T	116	Total	C	N	O	S	
			943	593	189	157	4	0

- Molecule 37 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	U	100	Total	C	N	O	S	
			784	497	140	146	1	0

- Molecule 38 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	V	112	Total	C	N	O	S	
			862	537	164	158	3	0

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	W	89	Total	C	N	O	S	
			725	457	130	134	4	0

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	X	87	Total	C	N	O	S	
			662	420	119	122	1	0

- Molecule 41 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Y	94	Total	C	N	O	S	
			731	465	131	133	2	0

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Z	82	Total	C	N	O	0	0
			626	386	122	118		

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	0	45	Total	C	N	O	0	0
			358	222	78	58		

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	1	65	Total	C	N	O	0	0
			536	330	101	105		

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	2	57	Total	C	N	O	0	0
			441	274	83	84		

- Molecule 46 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	75	Total	C	N	O	S	0	0
			593	371	106	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	52	Total	C	N	O	S	0	0
			411	249	85	72	5		

- Molecule 48 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	44	Total	C	N	O	S	0	0
			371	223	76	68	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	7	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	8	37	Total	C	N	O	S	0	0
			296	186	60	46	4		

- Molecule 52 is a RNA chain called P-site tRNA.

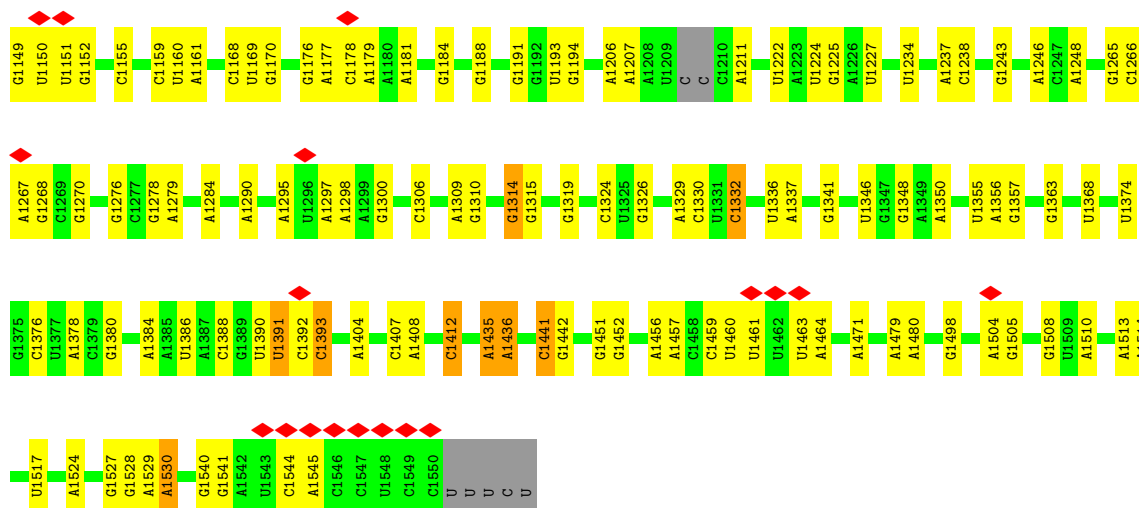
Mol	Chain	Residues	Atoms					AltConf	Trace	
52	x	77	Total	C	N	O	P	S	0	0
			1659	741	299	541	76	2		

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

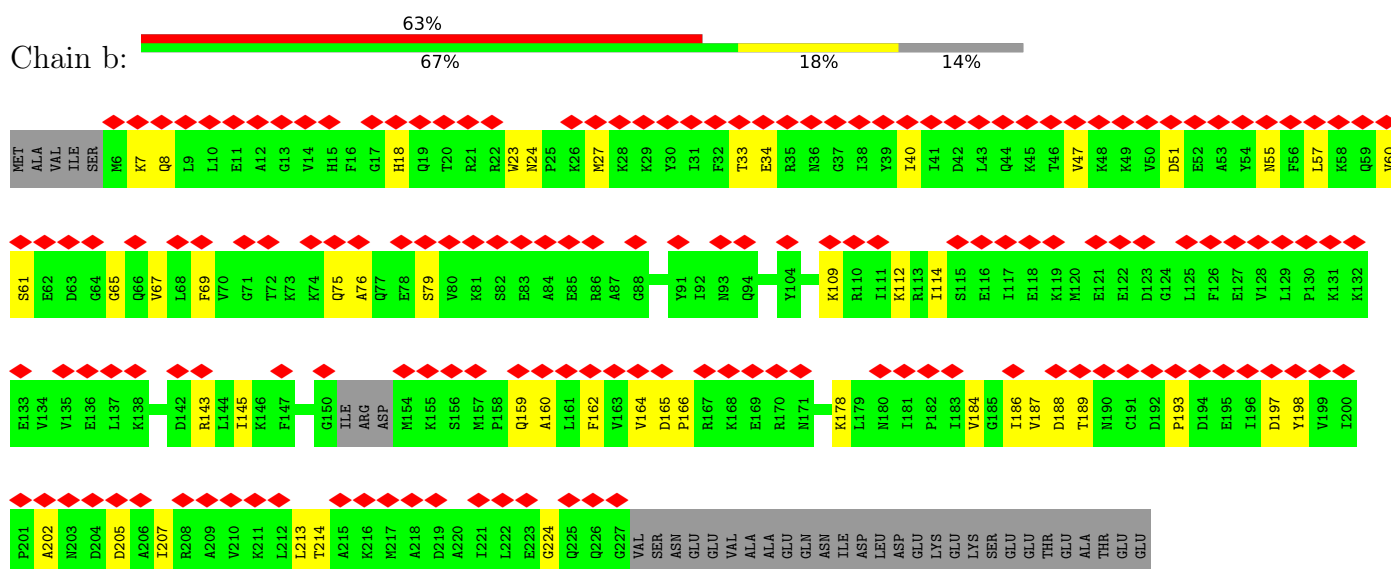
Mol	Chain	Residues	Atoms		AltConf
53	a	54	Total	Mg	0
			54	54	
53	v	1	Total	Mg	0
			1	1	
53	A	207	Total	Mg	0
			207	207	
53	B	2	Total	Mg	0
			2	2	
53	D	1	Total	Mg	0
			1	1	
53	O	1	Total	Mg	0
			1	1	
53	X	1	Total	Mg	0
			1	1	
53	x	1	Total	Mg	0
			1	1	

- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

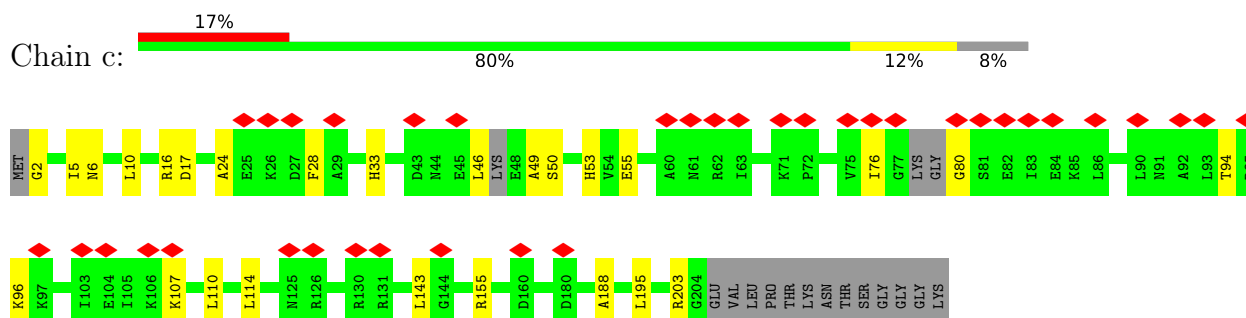
Mol	Chain	Residues	Atoms		AltConf
54	a	2	Total 2	K 2	0
54	A	18	Total 18	K 18	0



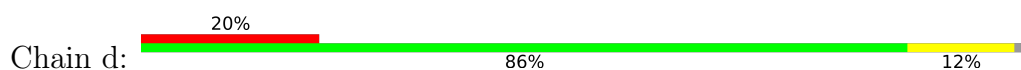
• Molecule 2: 30S ribosomal protein S2

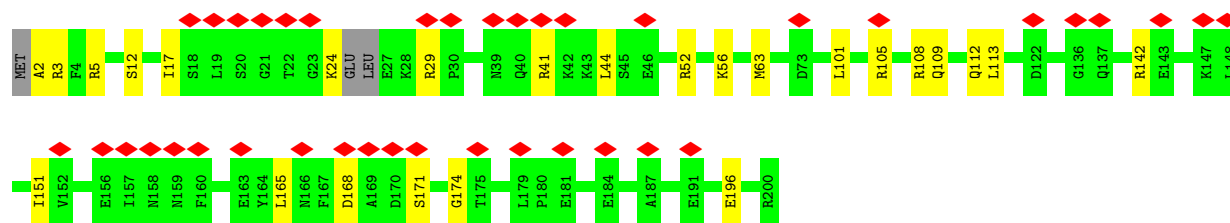


• Molecule 3: 30S ribosomal protein S3

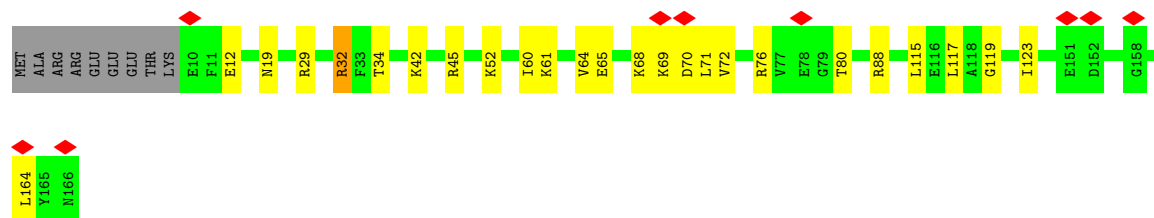
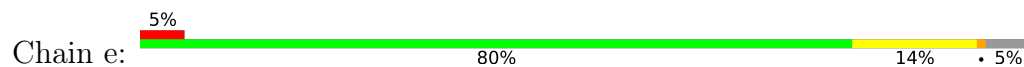


• Molecule 4: 30S ribosomal protein S4

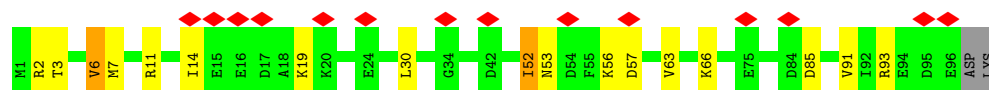
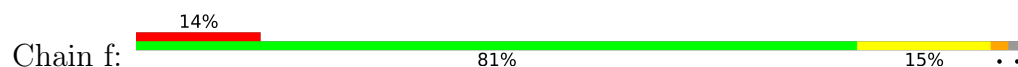




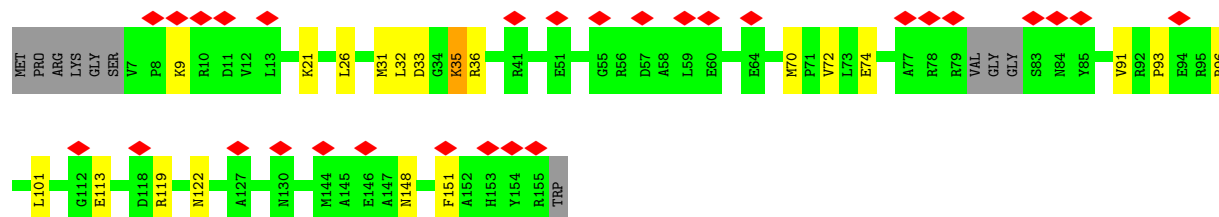
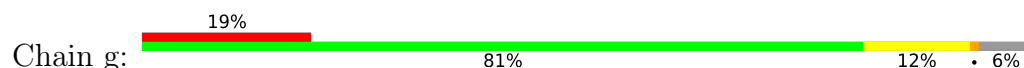
• Molecule 5: 30S ribosomal protein S5



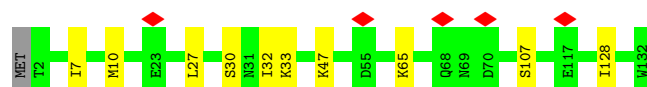
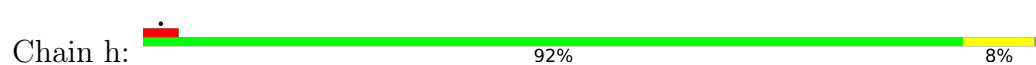
• Molecule 6: 30S ribosomal protein S6



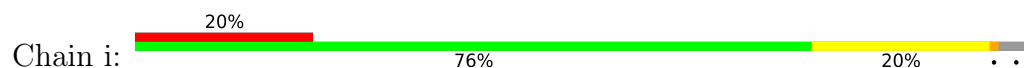
• Molecule 7: 30S ribosomal protein S7

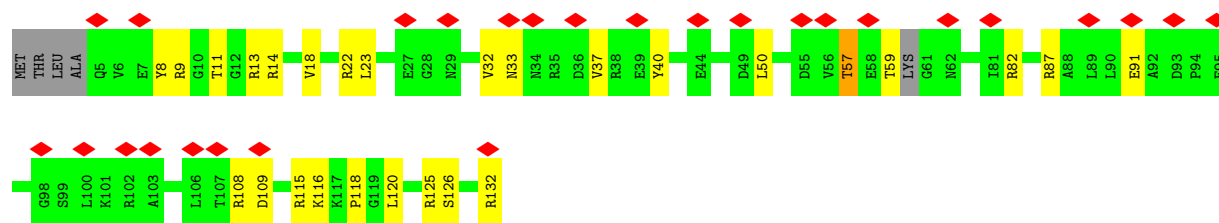


• Molecule 8: 30S ribosomal protein S8

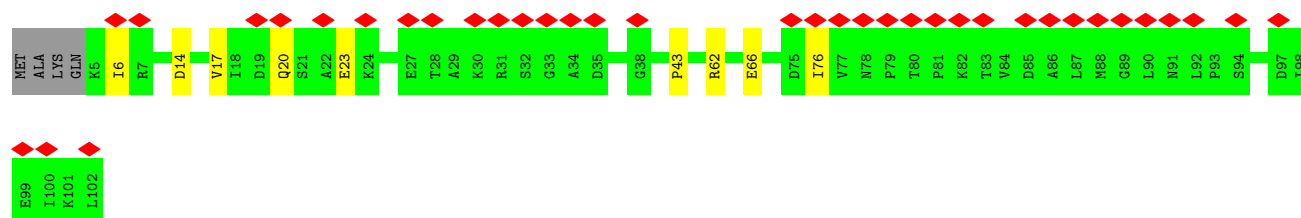
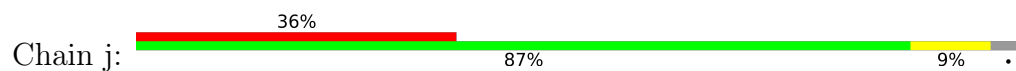


• Molecule 9: 30S ribosomal protein S9

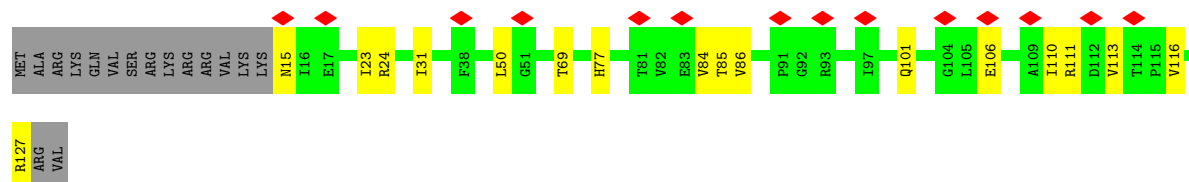
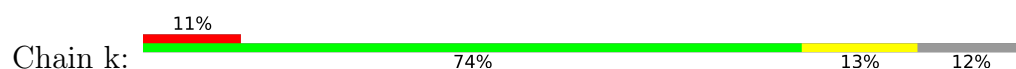




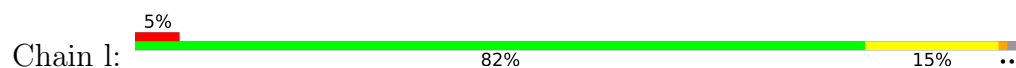
- Molecule 10: ribosomal protein uS10



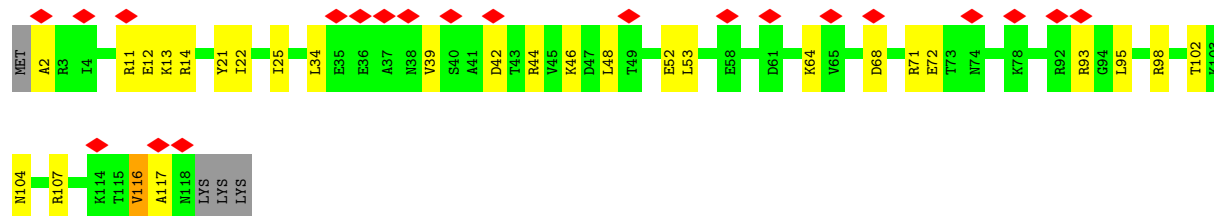
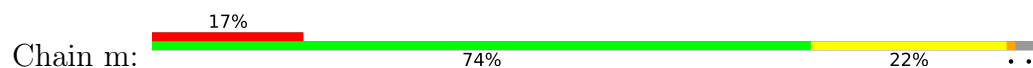
- Molecule 11: 30S ribosomal protein S11



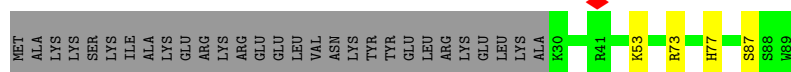
- Molecule 12: 30S ribosomal protein S12



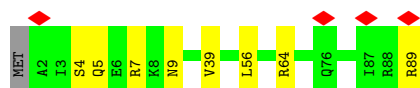
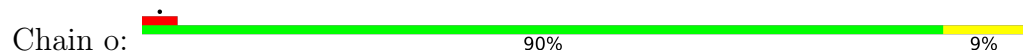
- Molecule 13: 30S ribosomal protein S13



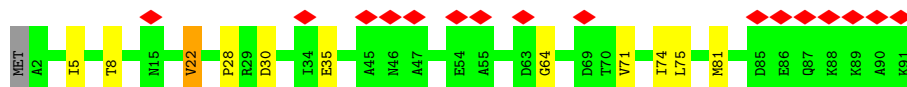
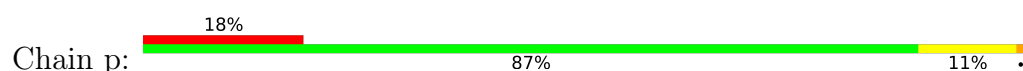
- Molecule 14: 30S ribosomal protein S14



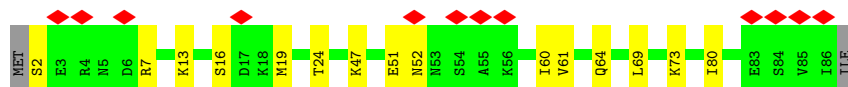
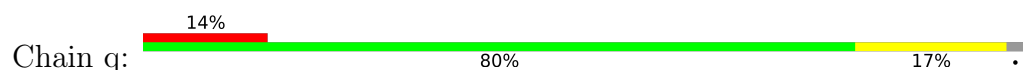
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



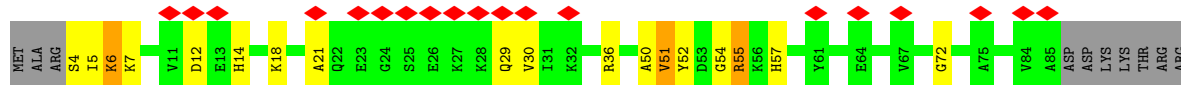
- Molecule 17: 30S ribosomal protein S17



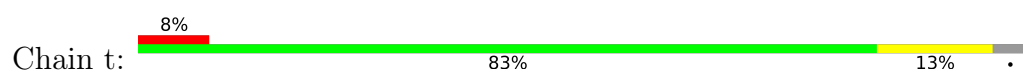
- Molecule 18: 30S ribosomal protein S18

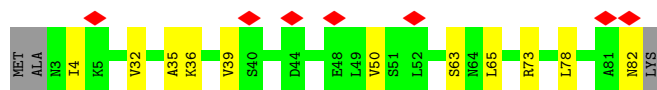


- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

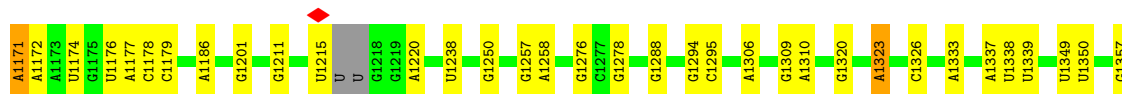
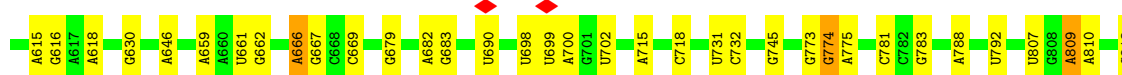
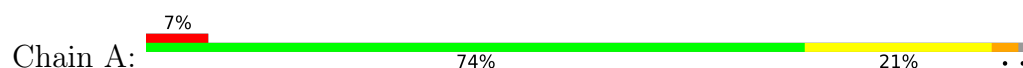


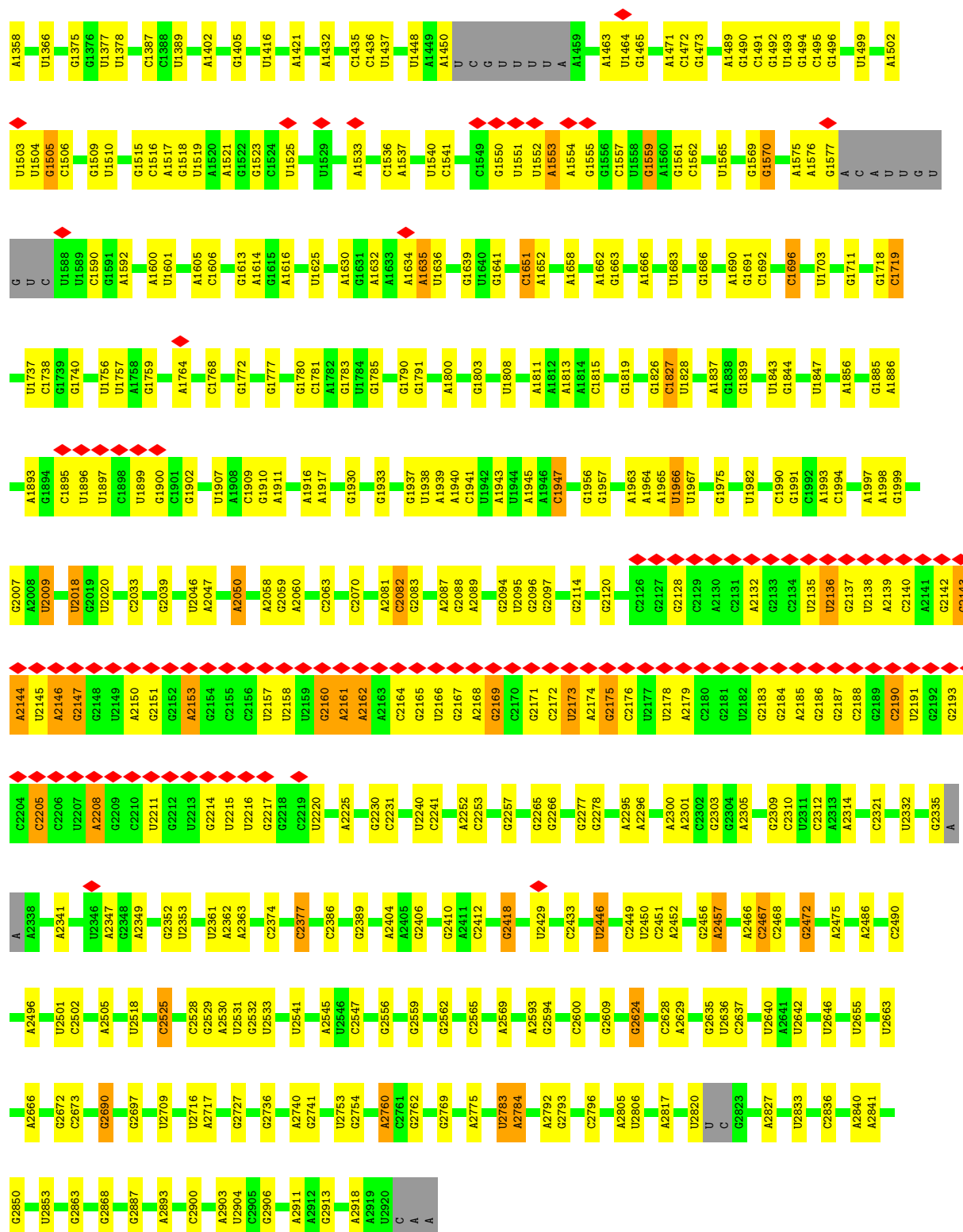


• Molecule 21: mRNA



• Molecule 22: 23S rRNA

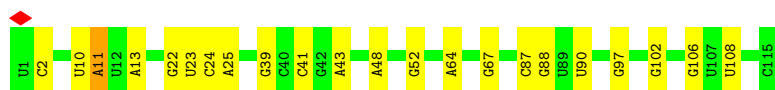




• Molecule 23: 5S rRNA

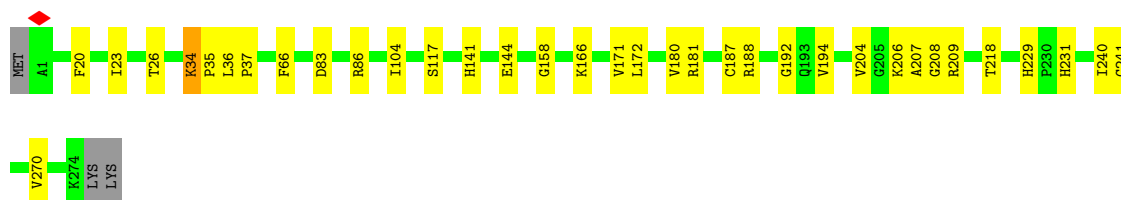
Chain B:





- Molecule 24: 50S ribosomal protein L2

Chain D: 86% 12% .



- Molecule 25: 50S ribosomal protein L3

Chain E: 92% 6% .



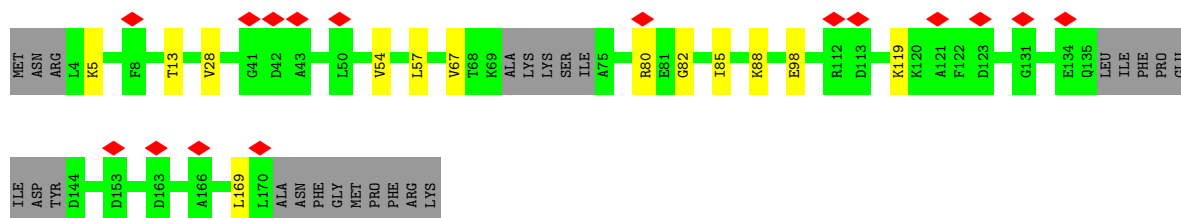
- Molecule 26: 50S ribosomal protein L4

Chain F: 83% 13% . .



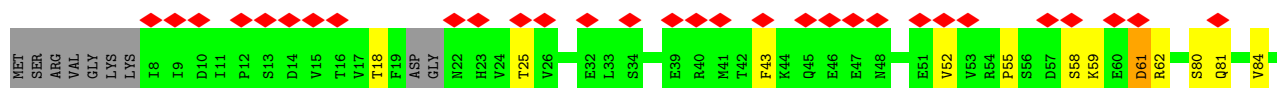
- Molecule 27: 50S ribosomal protein L5

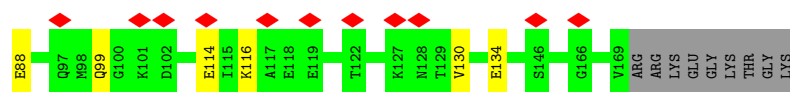
Chain G: 9% 79% 7% 14%



- Molecule 28: 50S ribosomal protein L6

Chain H: 23% 80% 10% 10%





- Molecule 29: 50S ribosomal protein L13

Chain M: 92% 8%



- Molecule 30: 50S ribosomal protein L14

Chain N: 93% 7%



- Molecule 31: 50S ribosomal protein L15

Chain O: 82% 14% 2%



- Molecule 32: 50S ribosomal protein L16

Chain P: 85% 9% 5%



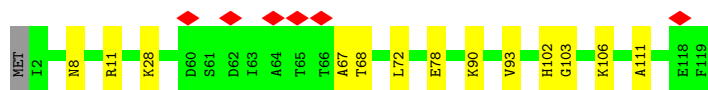
- Molecule 33: 50S ribosomal protein L17

Chain Q: 89% 8%

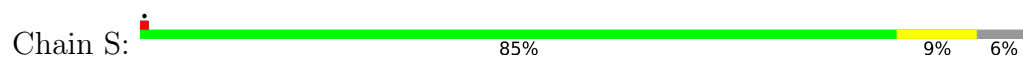


- Molecule 34: 50S ribosomal protein L18

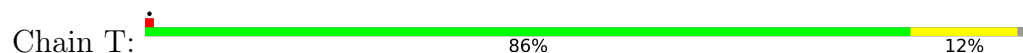
Chain R: 5% 88% 11%



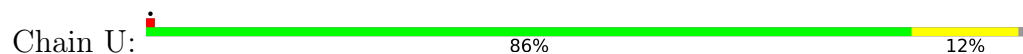
- Molecule 35: 50S ribosomal protein L19



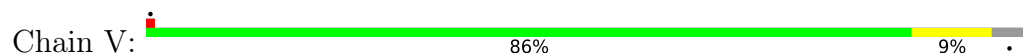
- Molecule 36: 50S ribosomal protein L20



- Molecule 37: 50S ribosomal protein L21



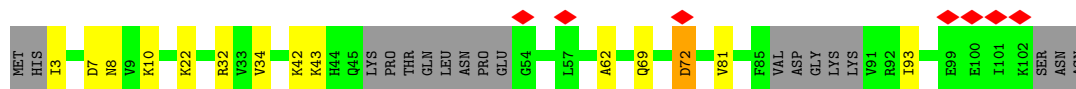
- Molecule 38: 50S ribosomal protein L22



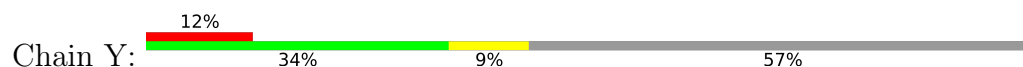
- Molecule 39: 50S ribosomal protein L23



- Molecule 40: 50S ribosomal protein L24

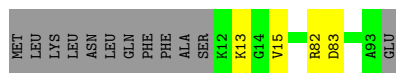
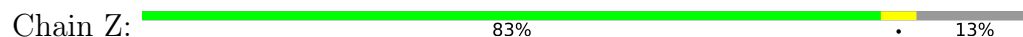


- Molecule 41: 50S ribosomal protein L25





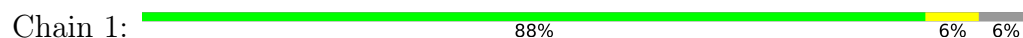
- Molecule 42: 50S ribosomal protein L27



- Molecule 43: 50S ribosomal protein L28



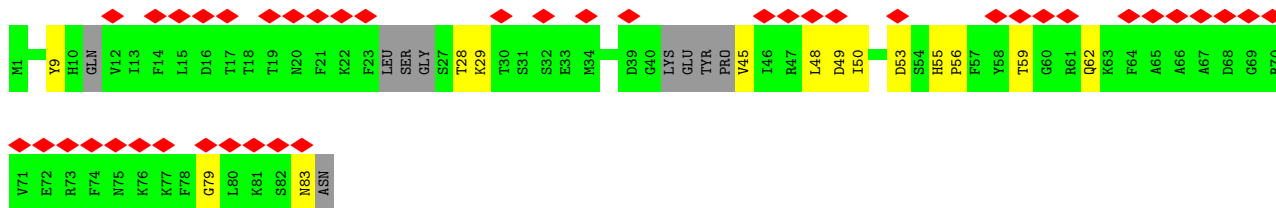
- Molecule 44: 50S ribosomal protein L29



- Molecule 45: 50S ribosomal protein L30



- Molecule 46: 50S ribosomal protein L31 type B



- Molecule 47: 50S ribosomal protein L32

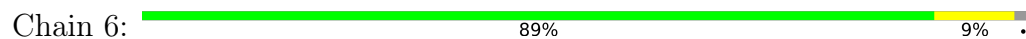




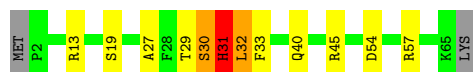
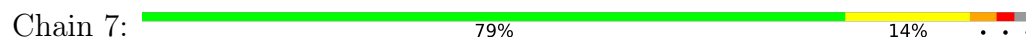
- Molecule 48: 50S ribosomal protein L33 2



- Molecule 49: 50S ribosomal protein L34



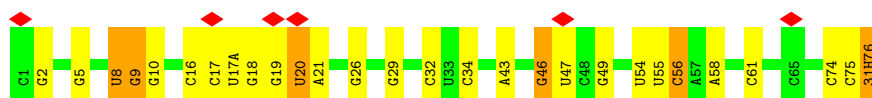
- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36



- Molecule 52: P-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	83000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.682	Depositor
Minimum map value	-0.428	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.0524	Depositor
Map size ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, PSU, MA6, 7MG, 4SU, 5MU, K, 2MG, 4OC, MG, OMG, OMC, 31H, H2U

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	0.22	0/36920	0.34	0/57570
2	b	0.21	0/1788	0.51	0/2397
3	c	0.20	0/1598	0.50	0/2145
4	d	0.23	0/1629	0.55	0/2185
5	e	0.25	0/1183	0.60	2/1595 (0.1%)
6	f	0.22	0/809	0.50	0/1085
7	g	0.23	0/1192	0.49	0/1603
8	h	0.23	0/1044	0.50	0/1401
9	i	0.24	0/1023	0.60	2/1372 (0.1%)
10	j	0.22	0/795	0.52	0/1071
11	k	0.21	0/848	0.46	0/1147
12	l	0.25	0/1075	0.57	0/1439
13	m	0.23	0/934	0.60	0/1253
14	n	0.24	0/490	0.51	0/650
15	o	0.21	0/747	0.43	0/996
16	p	0.25	0/723	0.56	0/971
17	q	0.22	0/706	0.56	0/944
18	r	0.23	0/536	0.53	0/718
19	s	0.22	0/679	0.57	0/912
20	t	0.19	0/606	0.45	0/810
21	v	0.20	0/521	0.45	0/812
22	A	0.36	0/69062	0.40	0/107697
23	B	0.23	0/2733	0.36	0/4257
24	D	0.45	4/2129 (0.2%)	0.69	4/2858 (0.1%)
25	E	0.36	0/1659	0.62	2/2224 (0.1%)
26	F	0.35	0/1563	0.65	1/2113 (0.0%)
27	G	0.22	0/1201	0.51	0/1610
28	H	0.22	0/1267	0.53	0/1710
29	M	0.30	0/1173	0.50	0/1578
30	N	0.33	0/927	0.55	0/1243
31	O	0.44	2/1112 (0.2%)	0.85	8/1482 (0.5%)
32	P	0.33	0/1121	0.75	3/1504 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Q	0.31	0/943	0.59	0/1259
34	R	0.23	0/920	0.52	1/1230 (0.1%)
35	S	0.31	0/889	0.55	0/1189
36	T	0.37	0/955	0.61	1/1265 (0.1%)
37	U	0.30	0/791	0.52	0/1051
38	V	0.33	0/870	0.55	0/1171
39	W	0.31	0/733	0.58	0/978
40	X	0.27	0/666	0.64	0/886
41	Y	0.22	0/738	0.49	0/989
42	Z	0.36	0/632	0.52	0/838
43	0	0.38	0/363	0.73	0/486
44	1	0.22	0/537	0.47	0/714
45	2	0.31	0/443	0.55	0/597
46	3	0.25	0/602	0.62	0/802
47	4	0.51	2/416 (0.5%)	0.74	2/550 (0.4%)
48	5	0.29	0/373	0.79	1/495 (0.2%)
49	6	0.41	0/377	0.57	0/491
50	7	0.37	0/526	0.69	2/690 (0.3%)
51	8	0.31	0/299	0.53	0/392
52	x	0.26	0/1671	0.41	0/2605
All	All	0.31	8/153537 (0.0%)	0.44	29/230030 (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
3	c	0	1
5	e	0	1
26	F	0	1
30	N	0	1
36	T	0	1
44	1	0	2
48	5	0	1
All	All	0	8

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	7	LYS	C-N	6.06	1.41	1.33
24	D	34	LYS	C-N	5.83	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	36	LEU	C-N	5.83	1.41	1.33
31	O	8	PRO	N-CD	5.50	1.55	1.47
24	D	35	PRO	N-CD	5.36	1.55	1.47
24	D	37	PRO	N-CD	5.30	1.55	1.47
47	4	30	CYS	C-N	5.30	1.41	1.34
47	4	31	PRO	N-CD	5.15	1.54	1.47

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	P	84	GLY	N-CA-C	13.21	128.58	112.73
32	P	83	MET	N-CA-C	9.34	121.46	111.28
26	F	189	ALA	N-CA-C	8.54	120.59	111.28
32	P	85	ALA	N-CA-C	8.54	120.21	111.07
36	T	30	THR	N-CA-C	7.55	119.59	111.36
31	O	7	LYS	CA-C-N	-7.24	113.35	120.52
31	O	7	LYS	C-N-CA	-7.24	113.35	120.52
50	7	31	HIS	N-CA-C	7.04	118.60	111.07
25	E	148	HIS	CA-C-N	6.63	134.21	121.54
25	E	148	HIS	C-N-CA	6.63	134.21	121.54
24	D	34	LYS	CA-C-N	-6.51	113.27	119.85
24	D	34	LYS	C-N-CA	-6.51	113.27	119.85
24	D	36	LEU	CA-C-N	-6.44	113.35	119.85
24	D	36	LEU	C-N-CA	-6.44	113.35	119.85
5	e	80	THR	CA-C-N	6.21	139.02	120.69
5	e	80	THR	C-N-CA	6.21	139.02	120.69
31	O	43	GLY	CA-C-N	6.14	125.82	119.92
31	O	43	GLY	C-N-CA	6.14	125.82	119.92
31	O	44	GLY	N-CA-C	6.03	118.41	111.36
34	R	103	GLY	N-CA-C	5.88	119.79	112.73
50	7	30	SER	N-CA-C	5.68	119.73	112.12
31	O	127	LYS	N-CA-C	5.61	119.13	111.39
47	4	30	CYS	CA-C-N	-5.46	112.98	119.05
47	4	30	CYS	C-N-CA	-5.46	112.98	119.05
48	5	26	ASN	N-CA-C	5.36	121.66	109.81
9	i	57	THR	CA-C-N	5.26	131.58	121.54
9	i	57	THR	C-N-CA	5.26	131.58	121.54
31	O	105	GLU	CA-C-N	5.17	127.98	120.79
31	O	105	GLU	C-N-CA	5.17	127.98	120.79

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	1	58	ARG	Sidechain
44	1	7	ARG	Sidechain
48	5	26	ASN	Peptide
26	F	188	ASN	Peptide
30	N	17	ARG	Sidechain
36	T	25	PHE	Peptide
3	c	155	ARG	Sidechain
5	e	32	ARG	Sidechain

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	33097	0	16677	100	0
2	b	1762	0	1818	28	0
3	c	1578	0	1631	15	0
4	d	1600	0	1628	18	0
5	e	1169	0	1229	19	0
6	f	798	0	794	12	0
7	g	1176	0	1208	13	0
8	h	1032	0	1082	5	0
9	i	1008	0	1025	17	0
10	j	783	0	825	6	0
11	k	833	0	838	9	0
12	l	1058	0	1130	15	0
13	m	927	0	975	16	0
14	n	481	0	500	4	0
15	o	738	0	769	5	0
16	p	712	0	744	6	0
17	q	698	0	738	9	0
18	r	527	0	551	4	0
19	s	661	0	664	24	0
20	t	606	0	650	7	0
21	v	462	0	229	2	0
22	A	61802	0	31073	131	0
23	B	2445	0	1240	5	0
24	D	2094	0	2208	20	0
25	E	1635	0	1678	9	0
26	F	1540	0	1577	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	G	1191	0	1223	9	0
28	H	1250	0	1267	18	0
29	M	1151	0	1145	7	0
30	N	920	0	981	7	0
31	O	1098	0	1142	18	0
32	P	1097	0	1166	13	0
33	Q	940	0	990	6	0
34	R	911	0	954	8	0
35	S	877	0	945	8	0
36	T	943	0	1014	9	0
37	U	784	0	823	8	0
38	V	862	0	920	7	0
39	W	725	0	761	5	0
40	X	662	0	714	9	0
41	Y	731	0	780	11	0
42	Z	626	0	645	6	0
43	0	358	0	383	4	0
44	1	536	0	567	1	0
45	2	441	0	478	1	0
46	3	593	0	566	8	0
47	4	411	0	415	26	0
48	5	371	0	378	6	0
49	6	373	0	420	4	0
50	7	521	0	586	12	0
51	8	296	0	337	2	0
52	x	1659	0	856	5	0
53	A	207	0	0	0	0
53	B	2	0	0	0	0
53	D	1	0	0	0	0
53	O	1	0	0	0	0
53	X	1	0	0	0	0
53	a	54	0	0	0	0
53	v	1	0	0	0	0
53	x	1	0	0	0	0
54	A	18	0	0	0	0
54	a	2	0	0	0	0
All	All	141837	0	93937	640	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 (640) 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)
47:4:33:CYS:SG	47:4:44:CYS:HB3	1.60	1.39
19:s:5:ILE:CG1	19:s:7:LYS:HG3	1.46	1.25
19:s:5:ILE:CG1	19:s:7:LYS:CG	2.14	1.17
52:x:76:31H:O4'	52:x:76:31H:C4'	1.66	1.15
19:s:5:ILE:HG12	19:s:7:LYS:CG	1.70	1.14
26:F:57:VAL:HG11	26:F:79:ARG:HD2	1.37	1.07
47:4:30:CYS:HB3	47:4:33:CYS:HB2	1.35	1.07
47:4:33:CYS:SG	47:4:44:CYS:CB	2.48	1.00
26:F:120:GLU:O	26:F:121:ASN:ND2	1.95	0.99
47:4:33:CYS:HG	47:4:44:CYS:CB	1.78	0.97
1:a:194:G:HO2'	17:q:2:SER:N	1.66	0.94
36:T:26:GLY:HA2	36:T:29:HIS:CE1	2.03	0.93
47:4:33:CYS:HG	47:4:44:CYS:HB3	1.29	0.88
19:s:5:ILE:HG21	19:s:7:LYS:HE3	1.58	0.85
47:4:30:CYS:CB	47:4:33:CYS:HB2	2.07	0.85
47:4:30:CYS:SG	47:4:33:CYS:N	2.49	0.85
26:F:57:VAL:CG1	26:F:79:ARG:HD2	2.08	0.83
28:H:59:LYS:HA	28:H:62:ARG:NH1	1.96	0.81
5:e:45:ARG:HG3	5:e:71:LEU:HD13	1.63	0.80
47:4:30:CYS:HB3	47:4:33:CYS:CB	2.13	0.77
26:F:185:ASP:OD2	26:F:186:ILE:N	2.18	0.76
22:A:2095:U:H3	22:A:2457:A:H2	1.33	0.76
19:s:5:ILE:HG12	19:s:7:LYS:HG3	0.77	0.75
31:O:139:LYS:HA	31:O:139:LYS:CE	2.17	0.74
19:s:6:LYS:HD2	19:s:6:LYS:O	1.89	0.73
50:7:32:LEU:N	50:7:32:LEU:HD22	2.05	0.71
5:e:70:ASP:O	5:e:71:LEU:HD23	1.90	0.71
22:A:2167:G:H1	22:A:2178:U:H3	1.39	0.70
36:T:28:LYS:O	36:T:35:ALA:HB2	1.92	0.70
1:a:154:U:H3	1:a:167:A:H61	1.40	0.70
29:M:126:TYR:HH	29:M:133:HIS:HE2	1.38	0.70
22:A:1523:G:H1	22:A:1557:C:H42	1.38	0.69
5:e:65:GLU:O	5:e:69:LYS:HG3	1.92	0.69
22:A:1518:G:H1	22:A:1562:C:H42	1.40	0.69
31:O:119:LYS:O	31:O:139:LYS:HG3	1.93	0.69
1:a:185:U:H3	1:a:205:A:H61	1.42	0.68
22:A:2039:G:OP1	38:V:11:ARG:NH2	2.27	0.68
26:F:149:PRO:HD2	26:F:190:ASP:OD2	1.94	0.68
22:A:2303:G:P	32:P:84:GLY:O	2.51	0.68
26:F:126:VAL:HG12	26:F:127:ASP:O	1.93	0.67
22:A:930:C:H42	22:A:936:G:H1	1.39	0.67
9:i:13:ARG:HB2	9:i:108:ARG:HE	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1663:G:HO2'	49:6:2:VAL:N	1.93	0.67
28:H:62:ARG:HH11	28:H:62:ARG:HB2	1.60	0.66
5:e:64:VAL:O	5:e:68:LYS:HG3	1.96	0.66
28:H:62:ARG:HH11	28:H:62:ARG:CB	2.09	0.66
1:a:216:G:H22	1:a:478:G:H21	1.43	0.65
2:b:65:GLY:HA3	2:b:159:GLN:HE22	1.62	0.65
31:O:139:LYS:HA	31:O:139:LYS:HE2	1.77	0.65
19:s:6:LYS:HD2	19:s:6:LYS:C	2.22	0.65
22:A:262:G:H21	22:A:666:A:H8	1.44	0.65
47:4:33:CYS:HA	47:4:47:CYS:SG	2.37	0.65
52:x:9:G:O2'	52:x:10:G:N7	2.31	0.64
22:A:444:C:OP1	43:0:34:GLN:NE2	2.30	0.64
7:g:32:LEU:O	7:g:33:ASP:HB2	1.97	0.64
3:c:94:THR:HG23	3:c:96:LYS:H	1.62	0.63
47:4:30:CYS:CB	47:4:44:CYS:SG	2.86	0.63
1:a:412:G:N7	4:d:3:ARG:NH1	2.44	0.63
22:A:591:A:H4'	22:A:592:A:H5'	1.81	0.63
9:i:115:ARG:HH12	9:i:118:PRO:HD3	1.64	0.63
27:G:67:VAL:HG22	27:G:82:GLY:H	1.63	0.63
22:A:2153:A:H1'	22:A:2190:C:H42	1.64	0.63
31:O:139:LYS:HE2	31:O:139:LYS:CA	2.28	0.62
26:F:185:ASP:OD2	26:F:186:ILE:HG13	2.00	0.62
5:e:61:LYS:O	5:e:65:GLU:OE2	2.18	0.62
19:s:55:ARG:HG3	19:s:55:ARG:NH1	2.14	0.62
24:D:229:HIS:HD2	24:D:231:HIS:H	1.46	0.62
8:h:107:SER:HB3	8:h:128:ILE:HD11	1.82	0.62
19:s:55:ARG:CG	19:s:55:ARG:HH11	2.13	0.61
2:b:27:MET:HE3	2:b:193:PRO:HB3	1.82	0.61
28:H:55:PRO:HD2	28:H:61:ASP:OD2	2.00	0.61
1:a:1357:G:O6	9:i:14:ARG:NH2	2.33	0.61
9:i:13:ARG:HG2	9:i:18:VAL:HG23	1.81	0.61
50:7:32:LEU:HD22	50:7:32:LEU:H	1.62	0.61
5:e:12:GLU:HB3	5:e:117:LEU:HD11	1.82	0.61
22:A:2312:C:OP2	48:5:3:ARG:NH2	2.34	0.61
1:a:700:U:H5''	11:k:127:ARG:HH12	1.66	0.61
10:j:66:GLU:HB2	14:n:87:SER:HB2	1.81	0.61
12:l:99:ARG:CG	12:l:99:ARG:HH11	2.14	0.61
1:a:837:A:H61	1:a:866:U:H3	1.49	0.60
22:A:150:A:H61	22:A:179:A:H2	1.49	0.60
22:A:2277:G:N2	32:P:84:GLY:HA2	2.17	0.60
47:4:30:CYS:HB2	47:4:44:CYS:SG	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:5:ARG:HA	4:d:108:ARG:HH22	1.65	0.60
22:A:963:A:H62	22:A:2295:A:H2	1.48	0.60
28:H:99:GLN:NE2	28:H:114:GLU:OE2	2.35	0.59
2:b:33:THR:HG23	2:b:40:ILE:HD13	1.84	0.59
3:c:53:HIS:HB3	3:c:55:GLU:HG3	1.84	0.59
19:s:55:ARG:HG3	19:s:55:ARG:HH11	1.67	0.59
6:f:7:MET:HG2	18:r:70:MET:HE2	1.82	0.59
12:l:99:ARG:HG2	12:l:100:VAL:N	2.16	0.59
24:D:158:GLY:H	24:D:194:VAL:HB	1.67	0.59
13:m:104:ASN:O	13:m:107:ARG:NH2	2.35	0.59
24:D:144:GLU:HB2	24:D:187:CYS:HB3	1.83	0.59
19:s:29:GLN:HG2	19:s:30:VAL:HG13	1.84	0.59
22:A:208:G:O6	43:0:28:ARG:NH2	2.36	0.59
13:m:12:GLU:O	13:m:44:ARG:NH1	2.37	0.58
1:a:1391:U:O2'	1:a:1393:C:N4	2.36	0.58
22:A:1101:A:N6	22:A:1131:G:OP2	2.36	0.58
1:a:1306:C:H5'	13:m:14:ARG:HH12	1.69	0.58
1:a:695:A:O2'	1:a:709:C:N4	2.36	0.58
1:a:194:G:O2'	17:q:2:SER:N	2.34	0.58
12:l:99:ARG:HG3	12:l:99:ARG:NH1	2.18	0.58
2:b:51:ASP:O	2:b:55:ASN:ND2	2.36	0.58
1:a:1109:C:OP2	2:b:143:ARG:NH1	2.34	0.58
1:a:1326:G:N1	1:a:1329:A:OP2	2.35	0.58
22:A:1002:U:OP2	32:P:14:ARG:NH1	2.36	0.58
31:O:61:LEU:O	50:7:13:ARG:NH1	2.37	0.57
32:P:85:ALA:HB2	42:Z:15:VAL:HG13	1.86	0.57
8:h:47:LYS:HG3	8:h:65:LYS:HB3	1.86	0.57
22:A:1108:C:H42	22:A:1118:G:H22	1.50	0.57
22:A:2303:G:OP2	32:P:84:GLY:O	2.23	0.57
46:3:56:PRO:HA	46:3:62:GLN:HB2	1.87	0.57
1:a:418:G:H21	1:a:440:A:H62	1.52	0.57
40:X:7:ASP:OD2	40:X:69:GLN:NE2	2.38	0.57
1:a:371:A:OP2	12:l:44:ARG:NH1	2.37	0.57
47:4:30:CYS:SG	47:4:33:CYS:SG	3.02	0.57
19:s:5:ILE:CG2	19:s:7:LYS:HE3	2.24	0.57
6:f:11:ARG:NH1	6:f:85:ASP:OD1	2.37	0.56
35:S:80:THR:HG22	35:S:82:LYS:H	1.70	0.56
38:V:11:ARG:HH21	38:V:98:LYS:HD3	1.70	0.56
22:A:2446:U:H5''	50:7:33:PHE:HB2	1.86	0.56
31:O:110:LYS:HG3	31:O:127:LYS:O	2.06	0.56
22:A:2717:A:N6	33:Q:39:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:4:33:CYS:N	47:4:47:CYS:SG	2.78	0.56
47:4:30:CYS:SG	47:4:33:CYS:CB	2.94	0.56
1:a:519:C:OP1	4:d:41:ARG:NH1	2.39	0.56
6:f:6:VAL:HG13	6:f:63:VAL:HG13	1.87	0.56
30:N:64:ARG:NH2	30:N:99:PHE:O	2.39	0.56
7:g:113:GLU:OE2	7:g:122:ASN:ND2	2.39	0.56
40:X:81:VAL:HG13	40:X:93:ILE:HG22	1.87	0.56
29:M:29:LEU:HD12	29:M:143:LEU:HD11	1.87	0.56
1:a:1319:G:OP2	13:m:98:ARG:NH1	2.39	0.55
19:s:51:VAL:O	19:s:57:HIS:HA	2.07	0.55
1:a:456:A:O2'	1:a:493:G:N7	2.34	0.55
2:b:61:SER:HB2	2:b:224:GLY:HA3	1.89	0.55
28:H:43:PHE:HB3	28:H:52:VAL:HA	1.89	0.55
29:M:20:ASP:OD1	29:M:59:ASN:ND2	2.39	0.55
9:i:11:THR:O	9:i:87:ARG:NH1	2.40	0.55
1:a:1058:G:HO2'	1:a:1225:G:HO2'	1.54	0.55
11:k:85:THR:HG22	11:k:111:ARG:HB3	1.87	0.55
1:a:1441:C:H5	1:a:1480:A:H61	1.55	0.54
22:A:1238:U:H1'	36:T:4:VAL:HG22	1.88	0.54
1:a:157:G:H2'	1:a:158:G:H8	1.72	0.54
28:H:84:VAL:HG12	28:H:134:GLU:HG2	1.88	0.54
22:A:575:G:N2	22:A:2050:A:OP1	2.41	0.54
22:A:2624:G:H5'	24:D:241:GLY:HA3	1.90	0.54
1:a:1265:G:O2'	1:a:1268:G:N3	2.40	0.54
47:4:33:CYS:CA	47:4:47:CYS:SG	2.96	0.54
1:a:1238:C:O2'	13:m:116:VAL:O	2.25	0.54
11:k:50:LEU:HD11	11:k:69:THR:HG21	1.90	0.54
22:A:1141:U:H2'	22:A:1142:A:H8	1.72	0.54
31:O:6:LEU:O	31:O:7:LYS:HD3	2.08	0.54
4:d:24:LYS:HE2	4:d:29:ARG:HH11	1.72	0.54
30:N:17:ARG:NH1	30:N:45:ASN:OD1	2.41	0.54
1:a:1070:U:O3'	14:n:73:ARG:NH2	2.40	0.54
4:d:17:ILE:HD12	4:d:56:LYS:HE3	1.89	0.54
13:m:93:ARG:HB3	13:m:95:LEU:HD23	1.90	0.53
33:Q:24:LEU:HD23	33:Q:44:VAL:HG21	1.89	0.53
3:c:110:LEU:O	3:c:203:ARG:NH2	2.41	0.53
26:F:188:ASN:OD1	26:F:188:ASN:N	2.42	0.53
46:3:29:LYS:HD2	46:3:45:VAL:HG13	1.89	0.53
1:a:1386:U:OP2	7:g:9:LYS:NZ	2.35	0.53
7:g:113:GLU:O	7:g:119:ARG:NH1	2.40	0.53
17:q:7:ARG:HB2	17:q:64:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1384:A:OP1	7:g:36:ARG:NH2	2.42	0.53
35:S:36:GLU:OE2	35:S:41:ARG:NH1	2.42	0.53
6:f:52:ILE:CG2	6:f:53:ASN:H	2.22	0.53
40:X:72:ASP:OD1	40:X:72:ASP:N	2.38	0.53
16:p:8:THR:OG1	16:p:30:ASP:OD1	2.26	0.53
36:T:26:GLY:HA2	36:T:29:HIS:HE1	1.68	0.53
1:a:1012:G:N2	1:a:1013:A:O2'	2.41	0.53
1:a:1097:U:H3	1:a:1110:G:H22	1.57	0.53
18:r:23:ILE:HG13	18:r:24:THR:HG23	1.91	0.53
22:A:2389:G:OP1	50:7:40:GLN:NE2	2.42	0.53
22:A:2918:A:H5'	29:M:137:GLN:HE21	1.74	0.53
43:0:35:LYS:HB3	43:0:48:TRP:HB3	1.90	0.53
50:7:54:ASP:OD1	50:7:57:ARG:NH2	2.41	0.53
22:A:199:A:H62	31:O:38:GLN:HE22	1.56	0.53
32:P:85:ALA:HB2	42:Z:15:VAL:CG1	2.38	0.53
47:4:39:LEU:HB2	47:4:42:ARG:HG3	1.90	0.53
12:l:99:ARG:HH11	12:l:99:ARG:HG3	1.74	0.52
28:H:59:LYS:N	28:H:62:ARG:HH12	2.07	0.52
5:e:42:LYS:HZ3	5:e:117:LEU:HA	1.74	0.52
11:k:15:ASN:ND2	11:k:77:HIS:O	2.43	0.52
40:X:8:ASN:OD1	40:X:22:LYS:NZ	2.41	0.52
10:j:14:ASP:HB3	10:j:17:VAL:HG12	1.90	0.52
3:c:16:ARG:NH1	3:c:17:ASP:O	2.43	0.52
24:D:117:SER:OG	24:D:188:ARG:NH1	2.43	0.52
9:i:8:TYR:HB3	9:i:91:GLU:HB3	1.92	0.52
26:F:159:GLU:HG2	26:F:177:THR:HG21	1.91	0.52
3:c:76:ILE:O	3:c:80:GLY:N	2.43	0.52
22:A:1103:G:O6	22:A:1124:A:N6	2.42	0.52
22:A:2007:G:O2'	22:A:2009:U:OP2	2.27	0.52
50:7:32:LEU:N	50:7:32:LEU:CD2	2.73	0.52
22:A:1658:A:N6	38:V:92:ARG:O	2.42	0.52
34:R:78:GLU:HG3	34:R:111:ALA:HB1	1.91	0.52
13:m:14:ARG:HD2	13:m:42:ASP:HA	1.91	0.52
5:e:115:LEU:HD13	5:e:123:ILE:HG21	1.92	0.52
6:f:52:ILE:HG22	6:f:53:ASN:N	2.25	0.52
22:A:1106:G:N7	22:A:1132:A:O2'	2.42	0.52
10:j:6:ILE:HB	10:j:76:ILE:HB	1.92	0.51
26:F:123:LEU:HD12	26:F:124:THR:N	2.24	0.51
47:4:32:ASN:C	47:4:47:CYS:SG	2.93	0.51
2:b:197:ASP:OD1	2:b:197:ASP:N	2.42	0.51
1:a:509:C:OP1	12:l:127:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:52:ILE:CG2	6:f:53:ASN:N	2.73	0.51
33:Q:29:ARG:NH1	33:Q:120:GLU:OE1	2.43	0.51
38:V:6:VAL:HG22	38:V:104:THR:HG23	1.93	0.51
41:Y:64:GLY:HA2	41:Y:69:THR:HA	1.92	0.51
24:D:141:HIS:ND1	24:D:192:GLY:O	2.40	0.51
2:b:33:THR:OG1	2:b:34:GLU:N	2.44	0.51
22:A:2257:G:H1'	43:O:34:GLN:HB3	1.92	0.51
33:Q:31:GLU:HG2	33:Q:118:ILE:HG22	1.91	0.51
46:3:79:GLY:HA2	46:3:83:ASN:HB2	1.93	0.51
9:i:108:ARG:NH1	9:i:109:ASP:O	2.44	0.51
22:A:459:C:HO2'	22:A:1907:U:HO2'	1.57	0.51
22:A:1106:G:H2'	22:A:1107:G:H8	1.75	0.51
22:A:1320:G:N2	22:A:1323:A:OP2	2.42	0.51
1:a:1276:G:N2	1:a:1279:A:OP2	2.36	0.51
7:g:70:MET:HE3	7:g:96:ARG:HB3	1.93	0.51
28:H:62:ARG:NH1	28:H:62:ARG:CB	2.73	0.51
2:b:109:LYS:HA	2:b:112:LYS:HE2	1.93	0.51
25:E:118:VAL:HG12	25:E:211:ILE:HG12	1.91	0.51
1:a:217:G:HO2'	1:a:477:U:HO2'	1.57	0.51
22:A:788:A:O2'	22:A:1703:U:OP1	2.27	0.51
22:A:2850:G:H5'	25:E:67:LYS:HD3	1.92	0.51
1:a:269:U:OP2	20:t:73:ARG:NH2	2.40	0.51
34:R:8:ASN:HD21	34:R:11:ARG:HH21	1.59	0.51
1:a:838:G:H5'	2:b:23:TRP:HE1	1.74	0.50
4:d:113:LEU:HD11	4:d:151:ILE:HD11	1.93	0.50
22:A:327:G:H1	22:A:399:U:H3	1.59	0.50
47:4:30:CYS:SG	47:4:33:CYS:HB2	2.50	0.50
1:a:1376:C:O2'	10:j:62:ARG:NH2	2.42	0.50
2:b:69:PHE:HB3	2:b:162:PHE:HB3	1.93	0.50
8:h:10:MET:HG3	8:h:27:LEU:HD11	1.93	0.50
22:A:922:G:H22	22:A:945:A:H62	1.59	0.50
22:A:1493:U:H3	22:A:1505:G:H1	1.58	0.50
22:A:1711:G:O2'	22:A:2018:U:O4	2.25	0.50
30:N:73:ASP:OD1	30:N:73:ASP:N	2.42	0.50
40:X:42:LYS:NZ	40:X:43:LYS:O	2.41	0.50
1:a:498:U:OP1	4:d:142:ARG:NH2	2.45	0.50
45:2:10:ARG:HB2	45:2:53:LEU:HB2	1.94	0.50
15:o:5:GLN:O	15:o:9:ASN:ND2	2.45	0.50
39:W:7:LEU:HD12	39:W:45:ILE:HD12	1.93	0.50
1:a:615:A:OP1	1:a:639:G:N2	2.45	0.50
11:k:101:GLN:NE2	11:k:106:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:967:A:C4	19:s:55:ARG:HD3	2.46	0.50
11:k:84:VAL:HB	11:k:110:ILE:HG22	1.93	0.50
39:W:58:TYR:HB2	39:W:75:ARG:HB2	1.94	0.50
46:3:28:THR:HG23	46:3:48:LEU:HD21	1.93	0.50
12:l:80:ILE:HG12	12:l:110:ILE:HD12	1.93	0.50
31:O:130:ALA:O	31:O:134:GLU:HG2	2.11	0.50
1:a:659:C:N4	1:a:761:A:OP2	2.41	0.49
31:O:10:GLU:HG2	31:O:11:GLY:N	2.27	0.49
22:A:2496:A:O2'	32:P:56:ARG:NH1	2.37	0.49
1:a:1092:G:OP2	5:e:52:LYS:NZ	2.40	0.49
3:c:107:LYS:HG3	3:c:143:LEU:HD12	1.94	0.49
22:A:528:C:H4'	40:X:43:LYS:HD2	1.94	0.49
22:A:1696:C:OP1	33:Q:4:ARG:NH1	2.42	0.49
42:Z:83:ASP:OD1	42:Z:83:ASP:N	2.45	0.49
22:A:2146:A:N6	22:A:2197:G:O6	2.44	0.49
15:o:4:SER:HB2	15:o:7:ARG:H	1.78	0.49
37:U:4:ILE:HD12	37:U:40:PHE:HB3	1.94	0.49
22:A:416:G:OP2	22:A:469:A:N6	2.46	0.49
24:D:83:ASP:OD2	24:D:86:ARG:NH1	2.42	0.49
1:a:889:C:H2'	1:a:890:G:H8	1.77	0.49
3:c:50:SER:HB2	3:c:114:LEU:HD22	1.95	0.49
28:H:88:GLU:HG3	28:H:130:VAL:HG22	1.93	0.49
13:m:34:LEU:HD13	13:m:39:VAL:HB	1.95	0.49
39:W:62:LYS:NZ	39:W:71:TYR:OH	2.46	0.48
5:e:76:ARG:NH1	5:e:119:GLY:O	2.43	0.48
22:A:320:U:H5''	22:A:321:U:H5'	1.94	0.48
22:A:1110:U:O2'	22:A:1113:A:N6	2.46	0.48
30:N:64:ARG:NH1	30:N:81:GLU:OE2	2.46	0.48
2:b:186:ILE:HG23	2:b:202:ALA:HB3	1.95	0.48
7:g:31:MET:HG3	7:g:35:LYS:O	2.14	0.48
22:A:2151:G:N2	22:A:2202:U:O2	2.46	0.48
1:a:492:G:N2	1:a:493:G:N7	2.54	0.48
2:b:27:MET:HE1	2:b:187:VAL:HG21	1.95	0.48
12:l:69:ARG:HB3	12:l:75:GLU:HG2	1.95	0.48
48:5:9:ALA:HB2	48:5:15:ARG:HG2	1.95	0.48
22:A:505:U:H5''	49:6:41:LYS:HE3	1.94	0.48
22:A:593:U:OP2	37:U:64:LYS:NZ	2.41	0.48
22:A:1357:G:C2	22:A:1366:U:H5''	2.48	0.48
1:a:112:G:N3	1:a:361:A:O2'	2.46	0.48
2:b:76:ALA:HB2	2:b:164:VAL:HG21	1.95	0.48
22:A:2418:G:O2'	22:A:2451:C:N4	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Y:21:LEU:HG	41:Y:26:LYS:HB2	1.95	0.48
1:a:1006:U:H3	1:a:1054:G:H22	1.61	0.48
1:a:1278:G:N3	1:a:1336:U:O2'	2.46	0.48
22:A:2466:A:H4'	22:A:2467:C:H3'	1.96	0.48
1:a:1159:C:OP2	9:i:13:ARG:NH2	2.46	0.48
22:A:1521:A:H61	22:A:1559:G:H22	1.61	0.48
22:A:1938:U:O2'	22:A:1945:A:N1	2.42	0.48
22:A:2171:G:O2'	22:A:2173:U:OP1	2.31	0.48
23:B:11:A:O2'	23:B:13:A:OP2	2.31	0.48
37:U:19:GLU:OE1	37:U:94:LYS:NZ	2.35	0.48
1:a:1246:A:H4'	1:a:1314:G:H4'	1.96	0.48
1:a:1407:C:OP2	5:e:29:ARG:NH2	2.45	0.48
25:E:118:VAL:HG21	25:E:201:VAL:HG12	1.96	0.48
31:O:139:LYS:CE	31:O:139:LYS:CA	2.88	0.48
38:V:108:SER:OG	38:V:109:ASP:O	2.32	0.48
1:a:1324:C:N4	19:s:4:SER:O	2.41	0.47
4:d:168:ASP:OD2	4:d:171:SER:OG	2.31	0.47
22:A:774:G:H1	24:D:207:ALA:H	1.62	0.47
22:A:2046:U:OP2	47:4:6:ARG:NH2	2.47	0.47
22:A:2377:C:OP2	50:7:45:ARG:NH2	2.47	0.47
25:E:142:SER:OG	25:E:143:HIS:N	2.46	0.47
6:f:3:THR:HG22	6:f:66:LYS:HG2	1.96	0.47
36:T:102:ASP:OD1	36:T:102:ASP:N	2.46	0.47
48:5:10:CYS:HG	48:5:43:THR:HG1	1.60	0.47
1:a:9:A:N6	4:d:196:GLU:O	2.47	0.47
23:B:22:G:H21	23:B:25:A:H62	1.62	0.47
26:F:80:ALA:HB3	26:F:83:TRP:HD1	1.79	0.47
47:4:30:CYS:HG	47:4:44:CYS:HG	0.48	0.47
48:5:26:ASN:O	48:5:28:GLU:N	2.42	0.47
1:a:1012:G:O2'	1:a:1014:C:OP1	2.29	0.47
3:c:6:ASN:HD22	14:n:77:HIS:HB3	1.79	0.47
22:A:1037:A:OP1	36:T:50:ARG:NH1	2.47	0.47
28:H:59:LYS:CA	28:H:62:ARG:HH12	2.28	0.47
31:O:10:GLU:OE1	31:O:10:GLU:N	2.40	0.47
22:A:1651:C:N4	22:A:1666:A:OP2	2.40	0.47
31:O:79:LEU:HG	31:O:113:GLY:HA2	1.96	0.47
33:Q:73:ASN:HB2	33:Q:77:THR:HB	1.96	0.47
41:Y:65:VAL:HG23	41:Y:67:SER:H	1.80	0.47
13:m:13:LYS:NZ	13:m:21:TYR:OH	2.48	0.47
22:A:164:A:O2'	22:A:165:C:O4'	2.29	0.47
22:A:522:G:N1	22:A:525:A:OP2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:X:3:ILE:HG22	40:X:69:GLN:HE21	1.78	0.47
41:Y:8:ILE:HB	41:Y:42:LYS:HE3	1.96	0.47
1:a:136:C:O2'	16:p:64:GLY:O	2.32	0.47
3:c:5:ILE:HD11	3:c:10:LEU:HD12	1.97	0.47
9:i:32:VAL:HG12	9:i:37:VAL:HG22	1.95	0.47
22:A:1641:G:OP1	39:W:39:LYS:NZ	2.42	0.47
22:A:2082:C:H2'	22:A:2531:U:H4'	1.97	0.47
22:A:2147:G:H1	22:A:2205:C:H42	1.62	0.47
23:B:11:A:N1	23:B:67:G:O2'	2.45	0.47
28:H:59:LYS:CA	28:H:62:ARG:NH1	2.73	0.47
34:R:67:ALA:HB3	34:R:72:LEU:HG	1.97	0.47
1:a:122:C:OP1	1:a:319:C:O2'	2.28	0.47
1:a:522:C:H2'	1:a:523:G:H8	1.80	0.47
1:a:800:A:O2'	1:a:802:A:N7	2.43	0.47
1:a:1044:G:H2'	1:a:1045:G:H8	1.79	0.47
5:e:70:ASP:OD1	5:e:70:ASP:N	2.48	0.47
39:W:13:THR:H	39:W:16:SER:HB3	1.80	0.47
4:d:12:SER:OG	4:d:17:ILE:O	2.33	0.47
22:A:2047:A:H5'	47:4:9:SER:HB3	1.97	0.47
38:V:1:MET:HG3	38:V:64:MET:HE2	1.96	0.47
16:p:71:VAL:HA	16:p:74:ILE:HG12	1.96	0.47
22:A:615:A:OP2	37:U:79:ARG:NH1	2.45	0.47
24:D:20:PHE:HB3	24:D:23:ILE:HD12	1.97	0.47
24:D:166:LYS:HG2	24:D:171:VAL:HG22	1.97	0.47
27:G:80:ARG:NH2	52:x:56:C:O2	2.48	0.47
37:U:67:ARG:HA	37:U:91:PRO:HA	1.97	0.47
1:a:665:U:H3	1:a:757:A:H62	1.63	0.46
20:t:63:SER:O	20:t:63:SER:OG	2.32	0.46
22:A:1509:G:OP2	22:A:1509:G:N2	2.42	0.46
26:F:78:ILE:HG13	26:F:79:ARG:HG2	1.97	0.46
40:X:32:ARG:NH2	40:X:62:ALA:O	2.47	0.46
48:5:22:ASN:ND2	48:5:25:ASN:OD1	2.47	0.46
19:s:5:ILE:HD11	19:s:7:LYS:HG2	1.19	0.46
22:A:2449:C:C5	50:7:31:HIS:CE1	3.03	0.46
4:d:101:LEU:HD21	4:d:174:GLY:HA3	1.96	0.46
47:4:43:VAL:HG12	47:4:50:TYR:HB2	1.97	0.46
1:a:777:G:H4'	1:a:1524:A:H4'	1.97	0.46
2:b:57:LEU:HA	2:b:60:VAL:HG12	1.97	0.46
19:s:36:ARG:HB3	19:s:72:GLY:HA3	1.98	0.46
22:A:718:C:OP1	26:F:54:ARG:NH1	2.46	0.46
1:a:899:G:O2'	1:a:915:G:O6	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:526:C:H4'	1:a:527:C:H5''	1.97	0.46
1:a:1025:A:O2'	1:a:1227:U:O2'	2.33	0.46
19:s:5:ILE:HG12	19:s:7:LYS:H	1.80	0.46
22:A:1515:G:H22	22:A:1565:U:H3	1.63	0.46
41:Y:13:GLN:HE21	41:Y:18:LEU:HD13	1.80	0.46
1:a:125:G:OP1	1:a:613:U:O2'	2.29	0.46
18:r:30:ASP:HB3	18:r:33:LEU:HB3	1.97	0.46
50:7:27:ALA:O	50:7:29:THR:N	2.49	0.46
1:a:620:C:H42	1:a:636:G:H1	1.64	0.46
11:k:24:ARG:HB3	11:k:31:ILE:HG23	1.97	0.46
28:H:80:SER:OG	28:H:81:GLN:N	2.49	0.46
22:A:1171:A:N6	22:A:2490:C:O2'	2.49	0.46
31:O:91:VAL:HA	31:O:95:LEU:HD23	1.98	0.46
5:e:19:ASN:HB3	5:e:34:THR:HG22	1.98	0.45
20:t:32:VAL:HG13	20:t:78:LEU:HD11	1.97	0.45
22:A:1827:C:OP2	24:D:181:ARG:NH2	2.48	0.45
22:A:669:C:O2'	22:A:702:U:OP1	2.33	0.45
31:O:139:LYS:HE2	31:O:139:LYS:N	2.31	0.45
36:T:80:MET:HE1	36:T:95:LEU:HD13	1.96	0.45
1:a:1234:U:O2'	1:a:1332:C:OP1	2.33	0.45
1:a:1451:G:O2'	1:a:1471:A:N6	2.47	0.45
7:g:72:VAL:HG12	7:g:96:ARG:NH1	2.30	0.45
26:F:80:ALA:HB3	26:F:83:TRP:CD1	2.52	0.45
1:a:414:G:H21	4:d:112:GLN:HE22	1.65	0.45
2:b:186:ILE:HG12	2:b:213:LEU:HD13	1.98	0.45
4:d:105:ARG:H	4:d:109:GLN:HE21	1.65	0.45
5:e:60:ILE:O	5:e:64:VAL:HG23	2.16	0.45
9:i:33:ASN:ND2	9:i:40:TYR:OH	2.49	0.45
13:m:11:ARG:HE	13:m:46:LYS:HA	1.81	0.45
17:q:13:LYS:HG2	17:q:60:ILE:HG12	1.97	0.45
22:A:1000:G:H2'	22:A:1001:A:H2'	1.99	0.45
22:A:1040:A:H4'	36:T:91:ASN:HD22	1.81	0.45
28:H:18:THR:HB	28:H:25:THR:HB	1.97	0.45
26:F:126:VAL:HG12	26:F:127:ASP:N	2.31	0.45
26:F:182:ASN:O	26:F:185:ASP:OD2	2.35	0.45
37:U:19:GLU:HG2	37:U:96:THR:HB	1.99	0.45
8:h:30:SER:HB3	8:h:33:LYS:HG3	1.98	0.45
15:o:39:VAL:HB	15:o:56:LEU:HD12	1.99	0.45
19:s:12:ASP:OD2	19:s:14:HIS:NE2	2.49	0.45
35:S:4:HIS:HD2	35:S:6:LEU:H	1.64	0.45
2:b:24:ASN:H	2:b:189:THR:HB	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:66:PHE:HE1	24:D:104:ILE:HD11	1.81	0.45
27:G:13:THR:HG23	27:G:28:VAL:HG21	1.98	0.45
1:a:1086:U:OP1	2:b:178:LYS:NZ	2.40	0.45
28:H:62:ARG:NH1	28:H:62:ARG:HB3	2.32	0.45
32:P:85:ALA:CB	42:Z:15:VAL:HG13	2.45	0.45
1:a:1188:G:N2	1:a:1191:G:OP2	2.47	0.45
22:A:1780:G:N2	22:A:1783:G:OP2	2.39	0.45
41:Y:13:GLN:HB2	41:Y:17:ASP:HB2	1.98	0.45
1:a:1442:G:O2'	1:a:1479:A:N6	2.51	0.44
19:s:52:TYR:CE1	19:s:54:GLY:O	2.70	0.44
22:A:2646:U:OP1	25:E:165:LYS:NZ	2.38	0.44
32:P:77:LYS:NZ	32:P:86:GLY:O	2.50	0.44
1:a:790:A:H62	1:a:808:G:H21	1.64	0.44
1:a:1033:U:N3	1:a:1034:U:O2	2.44	0.44
7:g:148:ASN:HB2	7:g:151:PHE:HE1	1.81	0.44
1:a:416:G:O2'	4:d:105:ARG:NH2	2.47	0.44
13:m:48:LEU:HD23	13:m:52:GLU:HG3	1.99	0.44
22:A:10:A:N6	22:A:2655:U:OP1	2.50	0.44
22:A:275:A:HO2'	22:A:413:C:HO2'	1.65	0.44
22:A:2836:C:OP1	47:4:42:ARG:NH2	2.47	0.44
28:H:116:LYS:HD2	28:H:116:LYS:HA	1.76	0.44
1:a:480:G:O6	1:a:481:C:N4	2.51	0.44
4:d:44:LEU:HD22	4:d:52:ARG:HH11	1.83	0.44
4:d:101:LEU:HD13	4:d:165:LEU:HD22	1.99	0.44
1:a:1176:G:N1	1:a:1179:A:OP2	2.42	0.44
7:g:93:PRO:HA	7:g:96:ARG:HD3	2.00	0.44
11:k:23:ILE:HB	11:k:86:VAL:HG12	1.98	0.44
15:o:89:ARG:HA	15:o:89:ARG:HD3	1.86	0.44
22:A:809:A:H5'	24:D:208:GLY:HA3	1.99	0.44
27:G:54:VAL:HA	27:G:57:LEU:HD12	1.99	0.44
8:h:7:ILE:HD11	8:h:32:ILE:HG23	1.98	0.44
19:s:52:TYR:CZ	19:s:54:GLY:O	2.70	0.44
27:G:119:LYS:HE3	27:G:169:LEU:HB3	2.00	0.44
41:Y:55:VAL:HG12	41:Y:59:GLY:HA3	1.99	0.44
1:a:1160:U:H4'	10:j:43:PRO:HG3	1.99	0.44
6:f:57:ASP:OD1	6:f:57:ASP:N	2.50	0.44
22:A:1089:C:O2	22:A:1091:G:N2	2.34	0.44
34:R:90:LYS:HE3	34:R:90:LYS:HB2	1.90	0.44
51:8:1:MET:HE3	51:8:1:MET:HB2	1.86	0.44
1:a:851:U:O2'	1:a:852:C:O4'	2.36	0.44
1:a:1022:G:N2	1:a:1025:A:OP2	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:18:HIS:HD2	2:b:205:ASP:HB2	1.83	0.44
5:e:72:VAL:O	5:e:72:VAL:HG23	2.17	0.44
6:f:14:ILE:HD12	6:f:19:LYS:HA	1.99	0.44
22:A:2143:G:N3	22:A:2144:A:N6	2.57	0.44
50:7:30:SER:O	50:7:33:PHE:CE2	2.70	0.44
13:m:2:ALA:HB3	13:m:53:LEU:HD21	1.98	0.43
29:M:3:GLN:HE22	37:U:13:LYS:H	1.65	0.43
12:l:2:PRO:HD2	12:l:12:ARG:HH22	1.83	0.43
22:A:820:G:OP1	22:A:822:G:O2'	2.34	0.43
22:A:922:G:H1	22:A:945:A:H62	1.64	0.43
22:A:1781:C:H5	35:S:96:ARG:HH21	1.66	0.43
22:A:1885:G:H1'	22:A:1911:A:H61	1.83	0.43
24:D:204:VAL:HG13	24:D:209:ARG:HD3	1.99	0.43
28:H:59:LYS:HA	28:H:62:ARG:HH12	1.76	0.43
32:P:11:ARG:HD3	32:P:87:LYS:HG2	2.00	0.43
41:Y:7:ILE:HD12	41:Y:41:VAL:HG11	1.99	0.43
1:a:642:C:H2'	1:a:643:A:C8	2.53	0.43
1:a:683:A:O2'	11:k:116:VAL:O	2.37	0.43
3:c:24:ALA:HB3	3:c:28:PHE:HD2	1.83	0.43
31:O:20:GLY:HA2	31:O:28:GLY:HA2	1.99	0.43
49:6:44:SER:O	49:6:44:SER:OG	2.33	0.43
1:a:217:G:O2'	1:a:477:U:O2'	2.31	0.43
3:c:188:ALA:HB3	3:c:195:LEU:HB3	2.01	0.43
22:A:590:U:OP1	22:A:1257:G:O2'	2.33	0.43
9:i:9:ARG:HG2	9:i:22:ARG:HD3	1.99	0.43
22:A:1448:U:H3	22:A:1635:A:H62	1.65	0.43
24:D:34:LYS:HA	24:D:34:LYS:HD2	1.86	0.43
38:V:65:ASN:ND2	38:V:68:GLU:OE2	2.51	0.43
46:3:59:THR:HB	46:3:62:GLN:HG3	1.99	0.43
17:q:61:VAL:HG12	17:q:80:ILE:HG12	2.01	0.43
13:m:22:ILE:HD12	13:m:25:ILE:HD12	2.01	0.43
22:A:2193:G:H8	22:A:2198:A:H62	1.67	0.43
41:Y:72:VAL:HG13	41:Y:91:PHE:HB3	2.01	0.43
2:b:7:LYS:HB3	2:b:47:VAL:HG23	2.00	0.43
12:l:87:LEU:HD21	12:l:117:THR:HG23	2.00	0.43
13:m:117:ALA:HB3	52:x:29:G:H5''	2.01	0.43
1:a:1017:C:H42	1:a:1030:G:H1	1.67	0.43
4:d:63:MET:HE3	4:d:63:MET:HB2	1.91	0.43
22:A:2169:G:H1	22:A:2175:G:H22	1.67	0.43
1:a:682:G:H2'	1:a:683:A:C8	2.53	0.43
22:A:1569:G:H5''	22:A:1570:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:28:LEU:HD21	44:1:42:ARG:HE	1.84	0.43
2:b:184:VAL:HG22	2:b:198:TYR:HD2	1.84	0.42
19:s:18:LYS:HA	19:s:21:ALA:HB3	2.00	0.42
22:A:89:U:H3'	22:A:90:A:H2'	2.01	0.42
29:M:25:THR:HB	29:M:28:ARG:HG3	2.01	0.42
46:3:50:ILE:HD11	46:3:55:HIS:HD2	1.84	0.42
3:c:46:LEU:HD12	3:c:49:ALA:HB3	2.00	0.42
9:i:125:ARG:NH1	9:i:126:SER:O	2.52	0.42
16:p:22:VAL:HG22	16:p:35:GLU:HB3	2.01	0.42
22:A:1097:U:H3	22:A:1151:G:H21	1.67	0.42
24:D:229:HIS:CD2	24:D:231:HIS:H	2.33	0.42
26:F:194:ILE:HG13	26:F:197:ALA:H	1.83	0.42
29:M:60:ALA:HB3	29:M:127:GLY:HA2	2.00	0.42
1:a:731:U:O2	1:a:864:G:O2'	2.37	0.42
22:A:1138:U:H2'	22:A:1140:A:H5'	2.01	0.42
22:A:1916:A:H2'	22:A:1917:A:C8	2.54	0.42
22:A:2136:U:H5'	22:A:2169:G:H21	1.85	0.42
34:R:28:LYS:HD3	34:R:93:VAL:HG13	2.00	0.42
1:a:589:G:H4'	15:o:64:ARG:HH22	1.83	0.42
1:a:695:A:N1	1:a:708:G:O2'	2.45	0.42
2:b:165:ASP:HA	2:b:166:PRO:HD3	1.89	0.42
4:d:2:ALA:HB3	4:d:108:ARG:HH21	1.84	0.42
31:O:6:LEU:C	31:O:7:LYS:HD3	2.45	0.42
1:a:68:C:H2'	1:a:69:G:C8	2.55	0.42
1:a:225:G:O2'	1:a:479:U:O2	2.25	0.42
1:a:642:C:H2'	1:a:643:A:H8	1.84	0.42
7:g:26:LEU:HD13	7:g:101:LEU:HB2	2.02	0.42
7:g:74:GLU:HG2	7:g:91:VAL:HG22	2.01	0.42
19:s:5:ILE:CG1	19:s:7:LYS:HG2	2.23	0.42
22:A:342:A:N3	22:A:362:C:O2'	2.50	0.42
22:A:1493:U:H3	22:A:1505:G:H22	1.67	0.42
5:e:45:ARG:CG	5:e:71:LEU:HD13	2.42	0.42
21:v:6:G:H2'	21:v:7:G:H8	1.85	0.42
22:A:2312:C:H5	48:5:3:ARG:HH12	1.68	0.42
47:4:30:CYS:HB3	47:4:33:CYS:SG	2.59	0.42
1:a:645:U:H2'	1:a:646:G:H8	1.85	0.42
6:f:6:VAL:HB	6:f:91:VAL:HG12	2.01	0.42
13:m:68:ASP:OD1	13:m:71:ARG:NH2	2.52	0.42
22:A:330:C:H42	22:A:396:G:H1	1.66	0.42
22:A:2136:U:OP1	22:A:2169:G:N2	2.52	0.42
9:i:8:TYR:HD2	9:i:23:LEU:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1886:A:N6	22:A:1910:G:O2'	2.52	0.42
22:A:2162:A:H5'	22:A:2187:G:H4'	2.01	0.42
22:A:2341:A:OP1	27:G:88:LYS:NZ	2.49	0.42
12:l:52:THR:OG1	12:l:53:MET:N	2.53	0.42
17:q:16:SER:HB2	17:q:24:THR:HB	2.01	0.42
17:q:51:GLU:OE1	17:q:52:ASN:ND2	2.53	0.42
19:s:50:ALA:HB1	19:s:57:HIS:HB3	2.02	0.42
20:t:36:LYS:HB2	20:t:36:LYS:HE3	1.92	0.42
22:A:1117:A:H62	22:A:1118:G:H21	1.67	0.42
23:B:11:A:OP1	42:Z:82:ARG:NH1	2.53	0.42
22:A:275:A:H62	22:A:296:G:H21	1.67	0.42
22:A:1333:A:OP1	22:A:2736:G:O2'	2.30	0.42
12:l:4:ILE:HD13	12:l:4:ILE:HA	1.92	0.41
18:r:41:ARG:HG3	18:r:78:GLU:HB2	2.02	0.41
34:R:102:HIS:O	34:R:106:LYS:HB2	2.20	0.41
1:a:723:A:H2'	1:a:724:A:C8	2.55	0.41
3:c:107:LYS:HB3	3:c:110:LEU:HB2	2.01	0.41
9:i:50:LEU:HA	9:i:82:ARG:HB3	2.02	0.41
22:A:732:C:H1'	49:6:5:THR:HG22	2.02	0.41
22:A:2081:A:H2'	47:4:5:LYS:HE2	2.01	0.41
1:a:985:G:OP2	1:a:1368:U:O2'	2.38	0.41
22:A:2160:G:H4'	22:A:2161:A:H5'	2.02	0.41
28:H:58:SER:C	28:H:62:ARG:HH12	2.28	0.41
1:a:1071:U:H5	3:c:2:GLY:HA2	1.85	0.41
5:e:32:ARG:HD3	5:e:52:LYS:HD3	2.01	0.41
22:A:2760:A:C6	25:E:216:LYS:HD3	2.56	0.41
51:8:6:SER:O	51:8:6:SER:OG	2.34	0.41
9:i:57:THR:HG23	9:i:59:THR:H	1.86	0.41
12:l:120:VAL:HG13	12:l:121:ASP:HB2	2.02	0.41
22:A:1101:A:N6	22:A:1125:U:O4	2.53	0.41
22:A:1719:C:O2	25:E:142:SER:OG	2.39	0.41
26:F:184:LEU:HD12	26:F:184:LEU:HA	1.79	0.41
40:X:10:LYS:HE3	40:X:10:LYS:HB2	1.87	0.41
1:a:1435:A:O2'	1:a:1436:A:O4'	2.38	0.41
2:b:8:GLN:H	2:b:8:GLN:HG2	1.69	0.41
5:e:42:LYS:HD3	5:e:42:LYS:HA	1.74	0.41
16:p:75:LEU:HD23	16:p:81:MET:HB2	2.03	0.41
20:t:35:ALA:HB1	20:t:50:VAL:HG12	2.01	0.41
22:A:774:G:C6	24:D:206:LYS:HB2	2.55	0.41
24:D:240:ILE:HD13	24:D:240:ILE:HG21	1.91	0.41
27:G:67:VAL:HG12	27:G:85:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:O:132:ALA:O	31:O:136:ILE:HD12	2.20	0.41
2:b:67:VAL:HG12	2:b:160:ALA:HB3	2.02	0.41
2:b:114:ILE:HD11	2:b:145:ILE:HD12	2.01	0.41
22:A:1113:A:H4'	22:A:1140:A:H1'	2.02	0.41
22:A:2783:U:H1'	22:A:2784:A:H5''	2.02	0.41
24:D:172:LEU:HD22	24:D:180:VAL:HG12	2.02	0.41
37:U:73:VAL:HB	37:U:86:LYS:HB2	2.01	0.41
47:4:30:CYS:CB	47:4:33:CYS:CB	2.85	0.41
1:a:1011:U:H2'	1:a:1012:G:H8	1.86	0.41
17:q:69:LEU:HB2	17:q:73:LYS:HG2	2.03	0.41
23:B:48:A:H5''	34:R:68:THR:HG23	2.03	0.41
24:D:172:LEU:HD21	24:D:270:VAL:HG21	2.02	0.41
42:Z:13:LYS:HB3	42:Z:15:VAL:HG23	2.03	0.41
1:a:469:U:O4	1:a:481:C:N4	2.54	0.41
2:b:75:GLN:HG3	2:b:207:ILE:HB	2.02	0.41
12:l:18:LYS:HD2	12:l:19:SER:H	1.86	0.41
22:A:117:A:H5'	22:A:118:A:H8	1.85	0.41
22:A:1111:A:H2'	22:A:1112:G:H8	1.86	0.41
22:A:2559:G:N2	22:A:2690:G:O2'	2.54	0.41
26:F:151:LYS:HE2	26:F:188:ASN:HB3	2.03	0.41
27:G:98:GLU:OE1	46:3:9:TYR:OH	2.34	0.41
32:P:35:GLN:HE22	41:Y:81:PRO:HB2	1.86	0.41
1:a:193:C:H2'	1:a:194:G:H8	1.86	0.41
2:b:188:ASP:OD1	2:b:188:ASP:N	2.54	0.41
5:e:164:LEU:HD13	5:e:164:LEU:HA	1.87	0.41
9:i:116:LYS:NZ	9:i:120:LEU:O	2.47	0.41
12:l:26:LYS:HB2	12:l:72:ASN:HD22	1.86	0.41
25:E:6:LEU:HD23	25:E:210:GLU:HB3	2.02	0.41
26:F:66:LYS:HB2	26:F:66:LYS:HE3	1.80	0.41
30:N:101:PRO:HD3	35:S:68:SER:HB2	2.03	0.41
34:R:102:HIS:O	34:R:106:LYS:CB	2.69	0.41
1:a:110:G:H5''	16:p:28:PRO:HG3	2.03	0.40
1:a:534:C:C5	1:a:535:7MG:H1'	2.56	0.40
17:q:19:MET:HE1	17:q:47:LYS:HE3	2.03	0.40
20:t:65:LEU:HA	20:t:65:LEU:HD23	1.85	0.40
21:v:6:G:H2'	21:v:7:G:C8	2.56	0.40
22:A:2300:A:H2'	22:A:2301:A:C8	2.56	0.40
27:G:5:LYS:HE2	27:G:5:LYS:HB2	1.84	0.40
30:N:17:ARG:HH11	30:N:45:ASN:CG	2.29	0.40
30:N:75:SER:HB3	35:S:74:ARG:HH12	1.86	0.40
35:S:108:LYS:HD3	35:S:108:LYS:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Y:33:GLY:HA3	41:Y:93:ALA:HB3	2.03	0.40
1:a:1006:U:H3	1:a:1054:G:H1	1.69	0.40
6:f:2:ARG:HG2	6:f:93:ARG:HH21	1.86	0.40
9:i:132:ARG:NH1	52:x:34:C:OP2	2.55	0.40
10:j:20:GLN:HA	10:j:23:GLU:HG2	2.02	0.40
26:F:143:LEU:HD11	26:F:152:VAL:HG21	2.02	0.40
7:g:21:LYS:HA	7:g:21:LYS:HD3	1.83	0.40
20:t:50:VAL:HG21	20:t:82:ASN:HD21	1.87	0.40
22:A:2136:U:O2'	22:A:2208:A:N6	2.55	0.40
22:A:2868:G:OP1	35:S:96:ARG:NH1	2.50	0.40
2:b:79:SER:HB3	2:b:214:THR:HG21	2.04	0.40
3:c:33:HIS:CE1	14:n:53:LYS:HB2	2.55	0.40
6:f:52:ILE:HG22	6:f:53:ASN:H	1.86	0.40
13:m:64:LYS:HE3	13:m:72:GLU:HG3	2.02	0.40
22:A:1553:A:H2'	22:A:1554:A:C8	2.57	0.40
25:E:26:THR:HG21	25:E:201:VAL:HG13	2.04	0.40
26:F:182:ASN:OD1	26:F:182:ASN:N	2.54	0.40
36:T:15:LYS:HE3	36:T:15:LYS:HB3	1.93	0.40
46:3:53:ASP:OD2	46:3:53:ASP:N	2.52	0.40
1:a:456:A:H4'	1:a:457:A:H5'	2.02	0.40
22:A:329:A:H61	22:A:397:U:H3	1.69	0.40
32:P:59:LYS:HE3	32:P:59:LYS:HB2	1.90	0.40
32:P:104:PHE:HE2	32:P:125:LEU:HD11	1.87	0.40
50:7:19:SER:O	50:7:19:SER:OG	2.32	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	215/255 (84%)	202 (94%)	13 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	194/217 (89%)	186 (96%)	8 (4%)	0	100	100
4	d	193/200 (96%)	187 (97%)	6 (3%)	0	100	100
5	e	155/166 (93%)	151 (97%)	4 (3%)	0	100	100
6	f	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
7	g	142/156 (91%)	137 (96%)	5 (4%)	0	100	100
8	h	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
9	i	123/132 (93%)	117 (95%)	6 (5%)	0	100	100
10	j	96/102 (94%)	90 (94%)	6 (6%)	0	100	100
11	k	111/129 (86%)	105 (95%)	6 (5%)	0	100	100
12	l	133/137 (97%)	126 (95%)	7 (5%)	0	100	100
13	m	115/121 (95%)	113 (98%)	2 (2%)	0	100	100
14	n	58/89 (65%)	58 (100%)	0	0	100	100
15	o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	p	88/91 (97%)	83 (94%)	5 (6%)	0	100	100
17	q	83/87 (95%)	75 (90%)	8 (10%)	0	100	100
18	r	62/80 (78%)	60 (97%)	2 (3%)	0	100	100
19	s	80/92 (87%)	78 (98%)	2 (2%)	0	100	100
20	t	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
24	D	272/277 (98%)	265 (97%)	7 (3%)	0	100	100
25	E	214/220 (97%)	205 (96%)	9 (4%)	0	100	100
26	F	201/207 (97%)	192 (96%)	9 (4%)	0	100	100
27	G	148/179 (83%)	139 (94%)	9 (6%)	0	100	100
28	H	156/178 (88%)	145 (93%)	11 (7%)	0	100	100
29	M	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
30	N	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
31	O	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
32	P	135/144 (94%)	134 (99%)	1 (1%)	0	100	100
33	Q	117/122 (96%)	114 (97%)	3 (3%)	0	100	100
34	R	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
35	S	107/116 (92%)	101 (94%)	6 (6%)	0	100	100
36	T	114/118 (97%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	U	94/102 (92%)	90 (96%)	4 (4%)	0	100	100
38	V	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
39	W	87/91 (96%)	84 (97%)	3 (3%)	0	100	100
40	X	81/105 (77%)	75 (93%)	6 (7%)	0	100	100
41	Y	92/217 (42%)	90 (98%)	2 (2%)	0	100	100
42	Z	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
43	0	43/62 (69%)	38 (88%)	5 (12%)	0	100	100
44	1	63/69 (91%)	62 (98%)	1 (2%)	0	100	100
45	2	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
46	3	67/84 (80%)	62 (92%)	5 (8%)	0	100	100
47	4	47/58 (81%)	45 (96%)	2 (4%)	0	100	100
48	5	40/49 (82%)	36 (90%)	4 (10%)	0	100	100
49	6	42/45 (93%)	40 (95%)	2 (5%)	0	100	100
50	7	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
51	8	35/37 (95%)	35 (100%)	0	0	100	100
All	All	5220/5804 (90%)	5003 (96%)	217 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	189/221 (86%)	189 (100%)	0	100	100
3	c	162/175 (93%)	162 (100%)	0	100	100
4	d	172/175 (98%)	172 (100%)	0	100	100
5	e	123/131 (94%)	122 (99%)	1 (1%)	73	82
6	f	84/86 (98%)	80 (95%)	4 (5%)	23	56
7	g	125/132 (95%)	124 (99%)	1 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	112/113 (99%)	112 (100%)	0	100	100
9	i	105/109 (96%)	105 (100%)	0	100	100
10	j	88/91 (97%)	88 (100%)	0	100	100
11	k	89/104 (86%)	88 (99%)	1 (1%)	65	79
12	l	117/119 (98%)	115 (98%)	2 (2%)	53	75
13	m	100/104 (96%)	98 (98%)	2 (2%)	48	72
14	n	50/78 (64%)	50 (100%)	0	100	100
15	o	80/81 (99%)	80 (100%)	0	100	100
16	p	76/77 (99%)	74 (97%)	2 (3%)	40	69
17	q	80/82 (98%)	80 (100%)	0	100	100
18	r	57/68 (84%)	57 (100%)	0	100	100
19	s	71/80 (89%)	68 (96%)	3 (4%)	26	60
20	t	67/69 (97%)	65 (97%)	2 (3%)	36	66
24	D	221/224 (99%)	219 (99%)	2 (1%)	70	81
25	E	173/177 (98%)	171 (99%)	2 (1%)	63	79
26	F	163/169 (96%)	155 (95%)	8 (5%)	22	55
27	G	131/158 (83%)	131 (100%)	0	100	100
28	H	141/155 (91%)	140 (99%)	1 (1%)	76	83
29	M	123/123 (100%)	123 (100%)	0	100	100
30	N	100/100 (100%)	99 (99%)	1 (1%)	68	80
31	O	112/112 (100%)	106 (95%)	6 (5%)	20	53
32	P	114/119 (96%)	112 (98%)	2 (2%)	51	74
33	Q	100/102 (98%)	100 (100%)	0	100	100
34	R	93/95 (98%)	93 (100%)	0	100	100
35	S	95/102 (93%)	95 (100%)	0	100	100
36	T	96/98 (98%)	95 (99%)	1 (1%)	68	80
37	U	84/86 (98%)	84 (100%)	0	100	100
38	V	91/94 (97%)	91 (100%)	0	100	100
39	W	80/82 (98%)	80 (100%)	0	100	100
40	X	72/90 (80%)	70 (97%)	2 (3%)	38	68
41	Y	82/190 (43%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	Z	64/75 (85%)	64 (100%)	0	100	100
43	0	37/52 (71%)	37 (100%)	0	100	100
44	1	59/62 (95%)	59 (100%)	0	100	100
45	2	51/53 (96%)	50 (98%)	1 (2%)	48	72
46	3	63/75 (84%)	62 (98%)	1 (2%)	55	75
47	4	46/51 (90%)	45 (98%)	1 (2%)	45	71
48	5	43/47 (92%)	43 (100%)	0	100	100
49	6	39/40 (98%)	39 (100%)	0	100	100
50	7	55/57 (96%)	53 (96%)	2 (4%)	31	63
51	8	34/35 (97%)	34 (100%)	0	100	100
All	All	4509/4918 (92%)	4461 (99%)	48 (1%)	63	79

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	88	ARG
6	f	6	VAL
6	f	30	LEU
6	f	52	ILE
6	f	56	LYS
7	g	35	LYS
11	k	113	VAL
12	l	99	ARG
12	l	111	VAL
13	m	102	THR
13	m	116	VAL
16	p	5	ILE
16	p	22	VAL
19	s	6	LYS
19	s	51	VAL
19	s	55	ARG
20	t	4	ILE
20	t	39	VAL
24	D	26	THR
24	D	218	THR
25	E	13	THR
25	E	131	ILE
26	F	117	LYS

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Mol	Chain	Res	Type
26	F	120	GLU
26	F	121	ASN
26	F	125	VAL
26	F	184	LEU
26	F	188	ASN
26	F	190	ASP
26	F	193	VAL
28	H	61	ASP
30	N	10	VAL
31	O	7	LYS
31	O	19	VAL
31	O	91	VAL
31	O	126	HIS
31	O	134	GLU
31	O	139	LYS
32	P	27	VAL
32	P	96	VAL
36	T	27	SER
40	X	34	VAL
40	X	72	ASP
45	2	54	VAL
46	3	49	ASP
47	4	42	ARG
50	7	31	HIS
50	7	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	15	HIS
2	b	55	ASN
2	b	59	GLN
3	c	6	ASN
3	c	64	ASN
3	c	91	ASN
3	c	133	GLN
4	d	8	ASN
4	d	109	GLN
4	d	137	GLN
4	d	192	GLN
5	e	135	ASN
5	e	145	GLN

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Mol	Chain	Res	Type
5	e	166	ASN
6	f	61	ASN
7	g	86	GLN
7	g	106	ASN
7	g	122	ASN
7	g	129	ASN
8	h	122	ASN
9	i	16	ASN
9	i	33	ASN
12	l	25	ASN
12	l	73	ASN
12	l	125	GLN
13	m	74	ASN
15	o	37	ASN
15	o	42	HIS
15	o	65	HIS
15	o	68	ASN
16	p	62	ASN
16	p	72	HIS
17	q	52	ASN
17	q	64	GLN
18	r	57	GLN
19	s	47	HIS
19	s	69	HIS
20	t	3	ASN
20	t	24	GLN
20	t	67	HIS
24	D	85	ASN
24	D	152	GLN
24	D	203	ASN
24	D	225	ASN
24	D	229	HIS
25	E	33	ASN
25	E	143	HIS
26	F	3	ASN
26	F	141	ASN
26	F	148	GLN
26	F	158	ASN
27	G	15	ASN
27	G	21	ASN
27	G	37	ASN
27	G	52	ASN

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Mol	Chain	Res	Type
28	H	48	ASN
28	H	65	HIS
28	H	120	ASN
29	M	3	GLN
29	M	8	ASN
29	M	11	ASN
29	M	81	HIS
30	N	82	ASN
31	O	17	ASN
31	O	38	GLN
31	O	143	HIS
32	P	25	ASN
32	P	35	GLN
33	Q	106	GLN
34	R	8	ASN
34	R	55	GLN
35	S	4	HIS
37	U	11	GLN
38	V	40	ASN
38	V	65	ASN
39	W	37	GLN
39	W	69	GLN
40	X	69	GLN
41	Y	20	GLN
42	Z	58	ASN
43	0	16	ASN
43	0	32	ASN
46	3	55	HIS
46	3	75	ASN
46	3	83	ASN
48	5	26	ASN
49	6	7	GLN
50	7	31	HIS
50	7	40	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1544/1556 (99%)	312 (20%)	0
21	v	20/29 (68%)	8 (40%)	0
22	A	2871/2923 (98%)	585 (20%)	8 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	B	114/115 (99%)	17 (14%)	1 (0%)
52	x	75/77 (97%)	21 (28%)	0
All	All	4624/4700 (98%)	943 (20%)	9 (0%)

All (943) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	G
1	a	8	G
1	a	10	G
1	a	11	A
1	a	31	U
1	a	33	A
1	a	40	G
1	a	45	G
1	a	48	C
1	a	49	C
1	a	50	U
1	a	51	A
1	a	52	A
1	a	55	C
1	a	64	C
1	a	65	G
1	a	78	A
1	a	80	A
1	a	83	C
1	a	84	U
1	a	85	U
1	a	86	G
1	a	88	U
1	a	89	U
1	a	91	U
1	a	93	U
1	a	94	G
1	a	108	A
1	a	115	A
1	a	120	C
1	a	126	G
1	a	128	U
1	a	129	A
1	a	130	A
1	a	132	C

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Mol	Chain	Res	Type
1	a	138	A
1	a	152	A
1	a	156	C
1	a	159	G
1	a	162	A
1	a	173	U
1	a	177	G
1	a	182	A
1	a	183	U
1	a	184	A
1	a	185	U
1	a	192	C
1	a	195	C
1	a	201	U
1	a	203	A
1	a	204	A
1	a	207	G
1	a	211	A
1	a	212	A
1	a	213	G
1	a	216	G
1	a	218	U
1	a	220	U
1	a	221	U
1	a	222	G
1	a	249	G
1	a	253	U
1	a	255	G
1	a	258	A
1	a	259	G
1	a	261	U
1	a	274	G
1	a	275	C
1	a	287	A
1	a	297	G
1	a	310	G
1	a	316	C
1	a	329	A
1	a	336	C
1	a	338	C
1	a	353	C
1	a	355	G

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Mol	Chain	Res	Type
1	a	360	C
1	a	362	G
1	a	375	U
1	a	380	C
1	a	382	A
1	a	392	G
1	a	396	G
1	a	405	A
1	a	406	C
1	a	414	G
1	a	419	A
1	a	420	U
1	a	421	G
1	a	429	U
1	a	432	G
1	a	437	U
1	a	451	U
1	a	454	G
1	a	456	A
1	a	462	A
1	a	465	U
1	a	466	G
1	a	467	U
1	a	468	G
1	a	469	U
1	a	472	G
1	a	476	C
1	a	477	U
1	a	480	G
1	a	481	C
1	a	482	A
1	a	483	C
1	a	485	U
1	a	486	C
1	a	493	G
1	a	503	A
1	a	505	A
1	a	517	A
1	a	519	C
1	a	526	C
1	a	527	C
1	a	532	G

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Mol	Chain	Res	Type
1	a	535	7MG
1	a	536	C
1	a	539	U
1	a	540	A
1	a	546	U
1	a	555	A
1	a	557	C
1	a	567	A
1	a	572	U
1	a	580	A
1	a	581	A
1	a	584	C
1	a	585	G
1	a	595	G
1	a	604	A
1	a	609	G
1	a	626	C
1	a	635	G
1	a	641	U
1	a	646	G
1	a	649	A
1	a	650	A
1	a	659	C
1	a	660	U
1	a	661	U
1	a	662	G
1	a	673	A
1	a	681	G
1	a	693	G
1	a	695	A
1	a	711	G
1	a	715	U
1	a	729	A
1	a	741	G
1	a	742	A
1	a	756	A
1	a	763	G
1	a	769	G
1	a	785	A
1	a	795	A
1	a	801	U
1	a	802	A

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Mol	Chain	Res	Type
1	a	803	C
1	a	807	G
1	a	817	G
1	a	820	G
1	a	823	A
1	a	825	C
1	a	829	G
1	a	836	A
1	a	840	G
1	a	851	U
1	a	852	C
1	a	854	G
1	a	855	C
1	a	862	G
1	a	864	G
1	a	881	A
1	a	911	G
1	a	925	G
1	a	931	G
1	a	935	G
1	a	943	C
1	a	944	A
1	a	969	U
1	a	974	A
1	a	977	A
1	a	978	A
1	a	980	G
1	a	984	A
1	a	985	G
1	a	992	A
1	a	1000	U
1	a	1001	U
1	a	1002	G
1	a	1011	U
1	a	1013	A
1	a	1015	A
1	a	1016	A
1	a	1019	C
1	a	1024	G
1	a	1027	A
1	a	1029	A
1	a	1034	U

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Mol	Chain	Res	Type
1	a	1035	C
1	a	1036	C
1	a	1038	C
1	a	1039	U
1	a	1040	U
1	a	1042	G
1	a	1043	G
1	a	1044	G
1	a	1046	G
1	a	1047	A
1	a	1055	A
1	a	1056	C
1	a	1057	A
1	a	1064	G
1	a	1075	G
1	a	1076	U
1	a	1097	U
1	a	1105	G
1	a	1106	U
1	a	1112	A
1	a	1119	G
1	a	1121	A
1	a	1135	G
1	a	1136	U
1	a	1137	U
1	a	1138	G
1	a	1141	A
1	a	1149	G
1	a	1150	U
1	a	1151	U
1	a	1152	G
1	a	1155	C
1	a	1161	A
1	a	1168	C
1	a	1169	U
1	a	1170	G
1	a	1177	A
1	a	1178	C
1	a	1181	A
1	a	1184	G
1	a	1193	U
1	a	1194	G

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Mol	Chain	Res	Type
1	a	1206	A
1	a	1207	A
1	a	1211	A
1	a	1222	U
1	a	1224	U
1	a	1237	A
1	a	1243	G
1	a	1248	A
1	a	1266	C
1	a	1267	A
1	a	1270	G
1	a	1284	A
1	a	1290	A
1	a	1295	A
1	a	1297	A
1	a	1298	A
1	a	1300	G
1	a	1309	A
1	a	1310	G
1	a	1314	G
1	a	1315	G
1	a	1330	C
1	a	1332	C
1	a	1337	A
1	a	1341	G
1	a	1346	U
1	a	1348	G
1	a	1350	A
1	a	1355	U
1	a	1356	A
1	a	1363	G
1	a	1374	U
1	a	1378	A
1	a	1380	G
1	a	1388	C
1	a	1390	U
1	a	1391	U
1	a	1392	C
1	a	1393	C
1	a	1404	A
1	a	1408	A
1	a	1412	4OC

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Mol	Chain	Res	Type
1	a	1435	A
1	a	1436	A
1	a	1441	C
1	a	1452	G
1	a	1456	A
1	a	1457	A
1	a	1459	C
1	a	1460	U
1	a	1461	U
1	a	1463	U
1	a	1464	A
1	a	1498	G
1	a	1504	A
1	a	1505	G
1	a	1508	G
1	a	1510	A
1	a	1513	A
1	a	1514	A
1	a	1517	U
1	a	1528	G
1	a	1530	MA6
1	a	1540	G
1	a	1541	G
1	a	1544	C
1	a	1545	A
21	v	12	A
21	v	13	A
21	v	14	A
21	v	15	A
21	v	19	G
21	v	23	A
21	v	24	A
21	v	25	A
22	A	13	A
22	A	23	G
22	A	24	G
22	A	34	U
22	A	37	C
22	A	43	A
22	A	64	A
22	A	71	A
22	A	74	U

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Mol	Chain	Res	Type
22	A	75	G
22	A	89	U
22	A	90	A
22	A	95	A
22	A	96	G
22	A	100	U
22	A	101	G
22	A	117	A
22	A	118	A
22	A	119	U
22	A	120	G
22	A	124	A
22	A	129	C
22	A	130	A
22	A	150	A
22	A	154	A
22	A	161	A
22	A	162	A
22	A	164	A
22	A	165	C
22	A	167	U
22	A	168	A
22	A	169	G
22	A	173	A
22	A	176	A
22	A	177	G
22	A	179	A
22	A	180	G
22	A	185	A
22	A	199	A
22	A	200	A
22	A	202	A
22	A	218	G
22	A	219	A
22	A	225	A
22	A	227	G
22	A	231	A
22	A	233	U
22	A	236	A
22	A	251	G
22	A	255	G
22	A	268	A

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Mol	Chain	Res	Type
22	A	280	C
22	A	282	A
22	A	290	U
22	A	294	G
22	A	298	U
22	A	300	G
22	A	301	U
22	A	302	A
22	A	308	C
22	A	321	U
22	A	324	A
22	A	327	G
22	A	328	G
22	A	329	A
22	A	338	G
22	A	354	A
22	A	365	A
22	A	372	A
22	A	373	A
22	A	374	U
22	A	377	U
22	A	386	C
22	A	388	A
22	A	398	C
22	A	401	U
22	A	404	U
22	A	432	G
22	A	435	A
22	A	451	U
22	A	457	G
22	A	458	A
22	A	466	C
22	A	471	G
22	A	481	C
22	A	482	U
22	A	502	C
22	A	510	U
22	A	513	G
22	A	523	A
22	A	527	G
22	A	539	G
22	A	550	A

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Mol	Chain	Res	Type
22	A	553	A
22	A	554	C
22	A	567	G
22	A	572	C
22	A	575	G
22	A	576	U
22	A	577	A
22	A	578	G
22	A	583	A
22	A	592	A
22	A	593	U
22	A	594	G
22	A	606	G
22	A	611	U
22	A	616	G
22	A	618	A
22	A	630	G
22	A	646	A
22	A	659	A
22	A	661	U
22	A	662	G
22	A	666	A
22	A	667	G
22	A	679	G
22	A	682	A
22	A	683	G
22	A	690	U
22	A	698	U
22	A	699	U
22	A	700	A
22	A	715	A
22	A	731	U
22	A	745	G
22	A	773	G
22	A	774	G
22	A	775	A
22	A	781	C
22	A	783	G
22	A	792	U
22	A	807	U
22	A	809	A
22	A	810	A

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Mol	Chain	Res	Type
22	A	813	G
22	A	820	G
22	A	822	G
22	A	824	A
22	A	827	A
22	A	829	U
22	A	830	U
22	A	834	A
22	A	837	G
22	A	839	A
22	A	847	A
22	A	850	G
22	A	851	C
22	A	857	C
22	A	872	U
22	A	873	U
22	A	888	G
22	A	891	A
22	A	904	G
22	A	910	C
22	A	911	A
22	A	919	G
22	A	923	A
22	A	926	G
22	A	929	C
22	A	930	C
22	A	931	C
22	A	932	U
22	A	936	G
22	A	938	G
22	A	955	A
22	A	959	C
22	A	960	C
22	A	971	U
22	A	972	A
22	A	985	A
22	A	989	A
22	A	990	G
22	A	1001	A
22	A	1005	G
22	A	1018	A
22	A	1023	A

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Mol	Chain	Res	Type
22	A	1026	C
22	A	1027	A
22	A	1033	G
22	A	1039	C
22	A	1040	A
22	A	1053	A
22	A	1055	A
22	A	1056	U
22	A	1057	A
22	A	1060	U
22	A	1061	G
22	A	1069	G
22	A	1070	A
22	A	1071	A
22	A	1077	U
22	A	1090	A
22	A	1091	G
22	A	1096	C
22	A	1102	U
22	A	1105	U
22	A	1106	G
22	A	1108	C
22	A	1109	U
22	A	1110	U
22	A	1111	A
22	A	1113	A
22	A	1114	A
22	A	1115	G
22	A	1116	C
22	A	1117	A
22	A	1120	C
22	A	1122	U
22	A	1124	A
22	A	1127	U
22	A	1128	A
22	A	1129	A
22	A	1131	G
22	A	1132	A
22	A	1133	G
22	A	1137	G
22	A	1138	U
22	A	1139	A

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Mol	Chain	Res	Type
22	A	1140	A
22	A	1143	G
22	A	1145	U
22	A	1146	C
22	A	1147	A
22	A	1151	G
22	A	1152	U
22	A	1153	C
22	A	1154	G
22	A	1155	A
22	A	1156	G
22	A	1171	A
22	A	1172	A
22	A	1174	U
22	A	1176	U
22	A	1177	A
22	A	1178	C
22	A	1179	C
22	A	1186	A
22	A	1201	G
22	A	1211	G
22	A	1215	U
22	A	1220	A
22	A	1250	G
22	A	1258	A
22	A	1276	G
22	A	1278	G
22	A	1288	G
22	A	1294	G
22	A	1295	C
22	A	1306	A
22	A	1309	G
22	A	1310	A
22	A	1323	A
22	A	1326	C
22	A	1337	A
22	A	1338	U
22	A	1339	U
22	A	1349	U
22	A	1350	U
22	A	1358	A
22	A	1375	G

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Mol	Chain	Res	Type
22	A	1377	U
22	A	1378	U
22	A	1387	C
22	A	1389	U
22	A	1402	A
22	A	1405	G
22	A	1416	U
22	A	1421	A
22	A	1432	A
22	A	1435	C
22	A	1436	C
22	A	1437	U
22	A	1450	A
22	A	1463	A
22	A	1464	U
22	A	1465	G
22	A	1471	A
22	A	1472	C
22	A	1473	G
22	A	1489	A
22	A	1490	G
22	A	1491	C
22	A	1492	G
22	A	1494	G
22	A	1495	C
22	A	1496	G
22	A	1499	U
22	A	1502	A
22	A	1503	U
22	A	1504	U
22	A	1505	G
22	A	1506	C
22	A	1510	U
22	A	1516	C
22	A	1517	A
22	A	1519	U
22	A	1525	U
22	A	1533	A
22	A	1536	C
22	A	1537	A
22	A	1540	U
22	A	1541	C

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Mol	Chain	Res	Type
22	A	1550	G
22	A	1551	U
22	A	1552	U
22	A	1553	A
22	A	1555	G
22	A	1559	G
22	A	1561	G
22	A	1570	G
22	A	1575	A
22	A	1576	A
22	A	1577	G
22	A	1590	C
22	A	1592	A
22	A	1600	A
22	A	1601	U
22	A	1605	A
22	A	1606	C
22	A	1613	G
22	A	1614	A
22	A	1616	A
22	A	1625	U
22	A	1630	A
22	A	1632	A
22	A	1634	A
22	A	1635	A
22	A	1636	U
22	A	1639	G
22	A	1651	C
22	A	1652	A
22	A	1662	A
22	A	1683	U
22	A	1686	G
22	A	1690	A
22	A	1691	G
22	A	1692	C
22	A	1696	C
22	A	1718	G
22	A	1719	C
22	A	1737	U
22	A	1738	C
22	A	1740	G
22	A	1756	U

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Mol	Chain	Res	Type
22	A	1757	U
22	A	1759	G
22	A	1764	A
22	A	1768	C
22	A	1772	G
22	A	1777	G
22	A	1785	G
22	A	1790	G
22	A	1791	G
22	A	1800	A
22	A	1803	G
22	A	1808	U
22	A	1811	A
22	A	1813	A
22	A	1815	C
22	A	1819	G
22	A	1826	G
22	A	1827	C
22	A	1828	U
22	A	1837	A
22	A	1839	G
22	A	1843	U
22	A	1844	G
22	A	1847	U
22	A	1856	A
22	A	1893	A
22	A	1895	C
22	A	1896	U
22	A	1897	U
22	A	1899	U
22	A	1900	G
22	A	1902	G
22	A	1909	C
22	A	1930	G
22	A	1933	G
22	A	1937	G
22	A	1939	A
22	A	1940	A
22	A	1941	C
22	A	1943	A
22	A	1947	OMC
22	A	1956	G

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Mol	Chain	Res	Type
22	A	1957	G
22	A	1963	A
22	A	1964	A
22	A	1965	A
22	A	1966	5MU
22	A	1967	U
22	A	1975	G
22	A	1982	U
22	A	1990	C
22	A	1991	G
22	A	1993	A
22	A	1994	C
22	A	1997	A
22	A	1998	A
22	A	1999	G
22	A	2009	U
22	A	2018	U
22	A	2020	U
22	A	2033	C
22	A	2050	A
22	A	2058	A
22	A	2059	G
22	A	2060	A
22	A	2063	C
22	A	2070	C
22	A	2082	C
22	A	2083	G
22	A	2087	A
22	A	2088	G
22	A	2089	A
22	A	2094	G
22	A	2096	G
22	A	2097	G
22	A	2114	G
22	A	2120	G
22	A	2128	G
22	A	2132	A
22	A	2135	U
22	A	2136	U
22	A	2137	G
22	A	2138	U
22	A	2139	A

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Mol	Chain	Res	Type
22	A	2140	C
22	A	2142	G
22	A	2143	G
22	A	2144	A
22	A	2145	U
22	A	2146	A
22	A	2147	G
22	A	2150	A
22	A	2153	A
22	A	2157	U
22	A	2158	U
22	A	2160	G
22	A	2161	A
22	A	2162	A
22	A	2164	C
22	A	2165	G
22	A	2166	U
22	A	2168	A
22	A	2169	G
22	A	2172	C
22	A	2173	U
22	A	2174	A
22	A	2175	G
22	A	2176	C
22	A	2179	A
22	A	2183	G
22	A	2184	G
22	A	2185	A
22	A	2186	G
22	A	2188	C
22	A	2190	C
22	A	2191	U
22	A	2194	U
22	A	2195	G
22	A	2196	G
22	A	2198	A
22	A	2200	A
22	A	2201	C
22	A	2205	C
22	A	2208	A
22	A	2211	U
22	A	2214	G

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Mol	Chain	Res	Type
22	A	2215	U
22	A	2217	G
22	A	2220	U
22	A	2225	A
22	A	2230	G
22	A	2231	C
22	A	2240	U
22	A	2241	C
22	A	2252	A
22	A	2253	C
22	A	2265	G
22	A	2266	G
22	A	2296	A
22	A	2305	A
22	A	2309	G
22	A	2310	C
22	A	2314	A
22	A	2321	C
22	A	2332	U
22	A	2335	G
22	A	2347	A
22	A	2349	A
22	A	2352	G
22	A	2353	U
22	A	2361	U
22	A	2362	A
22	A	2363	A
22	A	2374	C
22	A	2377	C
22	A	2386	C
22	A	2404	A
22	A	2406	G
22	A	2410	G
22	A	2412	C
22	A	2418	G
22	A	2429	U
22	A	2433	C
22	A	2446	U
22	A	2450	U
22	A	2452	A
22	A	2456	G
22	A	2457	A

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Mol	Chain	Res	Type
22	A	2467	C
22	A	2468	C
22	A	2472	2MG
22	A	2475	A
22	A	2486	A
22	A	2501	U
22	A	2502	C
22	A	2505	A
22	A	2518	U
22	A	2525	OMC
22	A	2528	C
22	A	2529	G
22	A	2532	G
22	A	2533	U
22	A	2541	U
22	A	2545	A
22	A	2547	C
22	A	2556	G
22	A	2562	G
22	A	2565	C
22	A	2569	A
22	A	2593	A
22	A	2594	G
22	A	2600	C
22	A	2609	G
22	A	2624	G
22	A	2628	C
22	A	2629	A
22	A	2635	G
22	A	2636	U
22	A	2637	C
22	A	2640	U
22	A	2642	U
22	A	2663	U
22	A	2666	A
22	A	2672	G
22	A	2673	C
22	A	2690	G
22	A	2697	G
22	A	2709	U
22	A	2716	U
22	A	2727	G

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Mol	Chain	Res	Type
22	A	2740	A
22	A	2741	G
22	A	2753	U
22	A	2754	G
22	A	2760	A
22	A	2762	G
22	A	2769	G
22	A	2775	A
22	A	2784	A
22	A	2792	A
22	A	2793	G
22	A	2796	C
22	A	2805	A
22	A	2806	U
22	A	2817	A
22	A	2820	U
22	A	2827	A
22	A	2833	U
22	A	2840	A
22	A	2841	A
22	A	2853	U
22	A	2863	G
22	A	2887	G
22	A	2893	A
22	A	2900	C
22	A	2903	A
22	A	2904	U
22	A	2906	G
22	A	2911	A
22	A	2913	G
23	B	2	C
23	B	10	U
23	B	11	A
23	B	23	U
23	B	24	C
23	B	39	G
23	B	41	C
23	B	43	A
23	B	52	G
23	B	64	A
23	B	87	C
23	B	88	G

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Mol	Chain	Res	Type
23	B	90	U
23	B	97	G
23	B	102	G
23	B	106	G
23	B	108	U
52	x	2	G
52	x	5	G
52	x	8	4SU
52	x	9	G
52	x	16	C
52	x	17	C
52	x	17(A)	U
52	x	18	G
52	x	19	G
52	x	20	H2U
52	x	21	A
52	x	26	G
52	x	43	A
52	x	46	7MG
52	x	47	U
52	x	49	G
52	x	56	C
52	x	58	A
52	x	61	C
52	x	74	C
52	x	75	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	179	A
22	A	327	G
22	A	328	G
22	A	971	U
22	A	1503	U
22	A	1550	G
22	A	2216	U
22	A	2783	U
23	B	23	U

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

18 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
22	5MU	A	1966	54,22	19,22,23	4.87	7 (36%)	27,32,35	3.81	9 (33%)
52	31H	x	76	53,52	31,34,35	4.30	15 (48%)	35,47,50	2.62	13 (37%)
52	5MU	x	54	52	23,23,23	4.58	7 (30%)	34,35,35	3.85	15 (44%)
22	OMC	A	1947	22	19,22,23	2.85	8 (42%)	25,31,34	0.90	1 (4%)
22	2MG	A	2472	22	23,26,27	2.64	8 (34%)	33,38,41	2.48	11 (33%)
1	7MG	a	535	1	23,26,27	3.55	11 (47%)	27,39,42	2.21	9 (33%)
22	OMG	A	2278	22,52	23,26,27	2.25	8 (34%)	32,38,41	1.89	8 (25%)
22	OMC	A	2525	22	19,22,23	2.76	7 (36%)	25,31,34	1.02	1 (4%)
52	4SU	x	8	52	22,22,22	1.81	4 (18%)	32,33,33	2.93	13 (40%)
52	OMC	x	32	52	23,23,23	2.75	8 (34%)	32,34,34	2.35	8 (25%)
52	PSU	x	55	52	22,22,22	1.28	3 (13%)	28,33,33	2.87	12 (42%)
1	MA6	a	1530	1	23,26,27	1.46	4 (17%)	33,38,41	3.31	13 (39%)
22	2MA	A	2530	53,22,54	22,25,26	3.87	10 (45%)	32,37,40	2.81	11 (34%)
52	7MG	x	46	52	27,27,27	3.28	11 (40%)	34,42,42	2.87	15 (44%)
52	H2U	x	20	52	22,22,22	0.95	2 (9%)	26,33,33	2.53	5 (19%)
1	4OC	a	1412	1	20,23,24	3.09	8 (40%)	25,32,35	1.07	2 (8%)
1	MA6	a	1529	1	23,26,27	1.44	4 (17%)	33,38,41	3.09	12 (36%)
1	2MG	a	1527	1	23,26,27	2.73	9 (39%)	33,38,41	2.29	12 (36%)

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
22	5MU	A	1966	54,22	-	2/7/25/26	0/2/2/2
52	31H	x	76	53,52	-	13/22/40/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	5MU	x	54	52	-	2/10/26/26	0/2/2/2
22	OMC	A	1947	22	-	2/9/27/28	0/2/2/2
22	2MG	A	2472	22	-	2/9/27/28	0/3/3/3
1	7MG	a	535	1	-	2/7/37/38	0/3/3/3
22	OMG	A	2278	22,52	-	0/9/27/28	0/3/3/3
22	OMC	A	2525	22	-	2/9/27/28	0/2/2/2
52	4SU	x	8	52	-	1/10/26/26	0/2/2/2
52	OMC	x	32	52	-	4/12/28/28	0/2/2/2
52	PSU	x	55	52	-	4/10/26/26	0/2/2/2
1	MA6	a	1530	1	-	2/11/29/30	0/3/3/3
22	2MA	A	2530	53,22,54	-	2/7/25/26	0/3/3/3
52	7MG	x	46	52	-	5/10/38/38	0/3/3/3
52	H2U	x	20	52	-	4/10/39/39	0/2/2/2
1	4OC	a	1412	1	-	2/9/29/30	0/2/2/2
1	MA6	a	1529	1	-	1/11/29/30	0/3/3/3
1	2MG	a	1527	1	-	0/9/27/28	0/3/3/3

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	x	76	31H	C4'-C3'	-13.93	1.28	1.52
22	A	2530	2MA	C4-N3	11.84	1.49	1.34
52	x	54	5MU	C2-N1	11.84	1.57	1.38
52	x	54	5MU	C6-N1	11.17	1.57	1.38
22	A	1966	5MU	C6-N1	10.86	1.56	1.38
22	A	1966	5MU	C2-N1	10.84	1.55	1.38
52	x	54	5MU	C4-C5	10.11	1.61	1.44
52	x	76	31H	O4'-C4'	9.76	1.66	1.45
22	A	1966	5MU	C4-C5	9.47	1.60	1.44
52	x	76	31H	C3'-N3'	8.41	1.58	1.45
52	x	46	7MG	C8-N9	8.11	1.51	1.45
1	a	535	7MG	C8-N9	7.93	1.51	1.45
22	A	1966	5MU	C4-N3	-7.76	1.24	1.38
52	x	54	5MU	C4-N3	-7.37	1.25	1.38
1	a	535	7MG	C5-N7	7.37	1.45	1.35
52	x	46	7MG	C5-N7	7.34	1.44	1.35
22	A	2530	2MA	C6-N1	7.02	1.44	1.35
1	a	1527	2MG	C2-N3	6.97	1.45	1.32
22	A	1966	5MU	C6-C5	6.73	1.45	1.34
22	A	2472	2MG	C2-N3	6.72	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1412	4OC	C4-N3	6.50	1.43	1.32
22	A	2530	2MA	C2-N3	6.47	1.45	1.34
52	x	54	5MU	C6-C5	6.45	1.45	1.34
52	x	32	OMC	C2-N3	6.42	1.49	1.36
52	x	76	31H	C-N3'	6.39	1.47	1.34
1	a	1527	2MG	C4-N3	6.25	1.48	1.34
1	a	1412	4OC	C6-C5	6.23	1.49	1.35
22	A	2472	2MG	C4-N3	6.17	1.48	1.34
22	A	2278	OMG	C4-N3	6.12	1.48	1.34
22	A	1947	OMC	C2-N3	6.11	1.48	1.36
52	x	76	31H	CN-N	6.04	1.53	1.33
22	A	2525	OMC	C2-N3	5.97	1.48	1.36
22	A	1947	OMC	C6-C5	5.94	1.48	1.35
1	a	1412	4OC	C2-N3	5.92	1.48	1.36
52	x	32	OMC	C6-C5	5.87	1.48	1.35
22	A	2530	2MA	C2-N1	5.83	1.44	1.34
52	x	46	7MG	C2-N3	5.82	1.47	1.33
1	a	535	7MG	C2-N3	5.78	1.47	1.33
1	a	535	7MG	C4-N3	5.75	1.47	1.34
52	x	46	7MG	C4-N3	5.62	1.47	1.34
52	x	76	31H	C6-N6	5.55	1.48	1.34
22	A	2525	OMC	C6-C5	5.47	1.47	1.35
1	a	1527	2MG	C2-N2	5.46	1.44	1.33
1	a	535	7MG	C4-N9	5.39	1.44	1.37
52	x	76	31H	O4'-C1'	-5.39	1.29	1.42
52	x	46	7MG	C4-N9	5.14	1.44	1.37
52	x	8	4SU	C4-S4	-5.10	1.59	1.68
52	x	32	OMC	C4-N3	5.08	1.44	1.34
22	A	2278	OMG	C2-N3	5.01	1.45	1.33
22	A	2472	2MG	C2-N2	4.98	1.43	1.33
52	x	32	OMC	C2-N1	4.98	1.50	1.40
52	x	46	7MG	C2-N2	4.95	1.45	1.34
1	a	535	7MG	C2-N2	4.85	1.45	1.34
1	a	1412	4OC	C4-N4	4.78	1.45	1.36
52	x	32	OMC	C4-N4	4.66	1.45	1.33
22	A	1947	OMC	C4-N4	4.57	1.45	1.33
22	A	1947	OMC	C4-N3	4.54	1.43	1.34
1	a	1412	4OC	C2-N1	4.45	1.49	1.40
22	A	2525	OMC	C4-N3	4.45	1.43	1.34
1	a	1527	2MG	C2-N1	4.44	1.43	1.36
22	A	2525	OMC	C4-N4	4.43	1.44	1.33
22	A	2530	2MA	C5-C6	4.42	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	2525	OMC	C2-N1	4.39	1.49	1.40
22	A	1947	OMC	C2-N1	4.31	1.49	1.40
1	a	1530	MA6	C6-N6	4.23	1.48	1.36
1	a	1529	MA6	C6-N6	4.20	1.48	1.36
52	x	76	31H	O2'-C2'	-4.16	1.32	1.43
52	x	8	4SU	C5-C4	-4.10	1.37	1.42
1	a	535	7MG	C5-C6	3.90	1.53	1.43
52	x	46	7MG	C5-C6	3.73	1.52	1.43
1	a	535	7MG	C2-N1	3.69	1.46	1.37
52	x	46	7MG	C2-N1	3.67	1.46	1.37
22	A	2472	2MG	C2-N1	3.63	1.42	1.36
22	A	2530	2MA	C6-N6	-3.57	1.25	1.34
1	a	1412	4OC	C5-C4	3.53	1.48	1.41
22	A	2278	OMG	C2-N2	3.36	1.42	1.34
22	A	2278	OMG	O6-C6	-3.27	1.17	1.23
22	A	2472	2MG	C5-N7	-3.25	1.32	1.39
52	x	8	4SU	C4-N3	-3.25	1.34	1.37
52	x	55	PSU	C6-C5	3.24	1.38	1.35
1	a	1412	4OC	C6-N1	3.24	1.45	1.38
22	A	2278	OMG	C5-N7	-3.22	1.32	1.39
22	A	2472	2MG	O6-C6	-3.20	1.17	1.23
1	a	1530	MA6	C5-C4	-3.17	1.33	1.39
22	A	1966	5MU	O4-C4	-3.14	1.17	1.23
52	x	32	OMC	C6-N1	3.14	1.45	1.38
1	a	1529	MA6	C5-C4	-3.09	1.33	1.39
1	a	1527	2MG	C5-N7	-3.08	1.32	1.39
52	x	46	7MG	C6-N1	3.05	1.44	1.38
1	a	535	7MG	C6-N1	3.02	1.44	1.38
52	x	76	31H	C2'-C3'	3.01	1.59	1.53
22	A	1947	OMC	C6-N1	3.01	1.45	1.38
22	A	1966	5MU	O2-C2	-2.98	1.17	1.23
52	x	54	5MU	O4-C4	-2.98	1.17	1.23
1	a	1412	4OC	O2-C2	-2.88	1.18	1.23
22	A	2525	OMC	O2-C2	-2.85	1.18	1.23
22	A	2530	2MA	C5-N7	-2.85	1.33	1.39
22	A	2525	OMC	C6-N1	2.81	1.44	1.38
52	x	55	PSU	C4-N3	-2.76	1.33	1.38
52	x	20	H2U	C2-N3	-2.76	1.33	1.38
22	A	1947	OMC	O2-C2	-2.75	1.18	1.23
52	x	32	OMC	O2-C2	-2.71	1.18	1.23
52	x	54	5MU	O2-C2	-2.64	1.18	1.23
52	x	46	7MG	O6-C6	-2.62	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	535	7MG	O6-C6	-2.60	1.18	1.23
22	A	2530	2MA	C4-N9	-2.59	1.32	1.37
1	a	1529	MA6	C5-N7	-2.59	1.34	1.39
52	x	76	31H	O-C	-2.52	1.18	1.23
1	a	1527	2MG	O6-C6	-2.52	1.18	1.23
52	x	8	4SU	C2-N1	2.51	1.42	1.38
1	a	1527	2MG	C5-C6	2.41	1.53	1.44
52	x	76	31H	C5-N7	-2.40	1.34	1.39
22	A	2530	2MA	C5-C4	-2.40	1.34	1.39
22	A	2472	2MG	C4-N9	-2.40	1.32	1.38
52	x	76	31H	CB-CG	2.39	1.61	1.51
1	a	1530	MA6	C5-N7	-2.39	1.34	1.39
1	a	1529	MA6	C8-N9	-2.35	1.33	1.37
1	a	1530	MA6	C8-N9	-2.26	1.33	1.37
52	x	55	PSU	C2-N3	-2.25	1.33	1.37
22	A	2530	2MA	C8-N9	-2.24	1.33	1.37
52	x	20	H2U	C4-N3	-2.20	1.33	1.37
52	x	32	OMC	C5-C4	2.17	1.48	1.42
52	x	76	31H	C5-C6	-2.17	1.35	1.41
22	A	2472	2MG	C5-C6	2.16	1.52	1.44
22	A	2278	OMG	C5-C6	2.16	1.52	1.44
1	a	1527	2MG	C4-N9	-2.16	1.32	1.38
1	a	535	7MG	C5-C4	2.16	1.44	1.37
22	A	2278	OMG	C6-N1	2.14	1.42	1.38
22	A	2278	OMG	C4-N9	-2.12	1.32	1.38
52	x	76	31H	C8-N7	2.06	1.35	1.31
22	A	1947	OMC	C5-C4	2.05	1.47	1.42
52	x	46	7MG	C5-C4	2.05	1.44	1.37
52	x	76	31H	C8-N9	-2.04	1.34	1.37
1	a	1527	2MG	C6-N1	2.03	1.42	1.38

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1966	5MU	C5-C4-N3	12.52	126.20	115.32
52	x	54	5MU	C5-C4-N3	12.10	125.84	115.32
1	a	1530	MA6	N1-C6-N6	-11.61	102.72	116.86
52	x	20	H2U	OP3-P-O5'	-10.57	79.11	106.67
22	A	1966	5MU	C5-C6-N1	-10.41	112.00	123.31
1	a	1529	MA6	N1-C6-N6	-10.24	104.38	116.86
52	x	54	5MU	C5-C6-N1	-8.88	113.67	123.31
1	a	1530	MA6	C5-C6-N6	8.07	138.11	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	x	55	PSU	OP3-P-O5'	-7.66	86.69	106.67
22	A	2530	2MA	C1'-N9-C8	-7.38	110.71	127.09
22	A	2472	2MG	C2-N3-C4	7.18	120.99	112.00
1	a	1529	MA6	C5-C6-N6	7.11	136.58	125.33
52	x	8	4SU	OP3-P-O5'	-6.82	88.88	106.67
52	x	32	OMC	OP3-P-OP1	-6.73	84.60	110.83
1	a	1527	2MG	C2-N3-C4	6.46	120.08	112.00
1	a	1530	MA6	N1-C2-N3	-6.41	118.88	128.58
22	A	2530	2MA	N9-C8-N7	-6.36	104.91	113.94
52	x	54	5MU	OP3-P-O5'	-6.22	90.44	106.67
52	x	76	31H	N1-C2-N3	-6.09	119.36	128.58
52	x	46	7MG	OP3-P-OP2	-6.08	85.01	107.80
52	x	54	5MU	OP3-P-OP1	-6.06	87.21	110.83
52	x	55	PSU	N1-C2-N3	6.05	121.55	115.17
52	x	46	7MG	OP3-P-OP1	-6.02	87.39	110.83
1	a	1529	MA6	N1-C2-N3	-5.97	119.54	128.58
52	x	46	7MG	OP3-P-O5'	-5.94	91.17	106.67
52	x	8	4SU	C5-C4-S4	-5.86	117.61	124.31
22	A	1966	5MU	O4-C4-C5	-5.73	118.36	124.92
22	A	2472	2MG	C5-C4-N3	-5.73	119.26	128.39
22	A	2530	2MA	C4-N9-C8	5.72	111.75	105.74
52	x	32	OMC	OP3-P-OP2	-5.65	86.61	107.80
52	x	54	5MU	OP3-P-OP2	-5.62	86.73	107.80
52	x	8	4SU	C4-N3-C2	-5.47	122.07	127.31
22	A	1966	5MU	C4-N3-C2	-5.40	120.26	127.34
52	x	54	5MU	O4-C4-C5	-5.34	118.81	124.92
22	A	2278	OMG	C5-C4-N3	-5.34	119.89	128.39
52	x	32	OMC	OP3-P-O5'	-5.32	92.80	106.67
1	a	1527	2MG	C5-C4-N3	-5.30	119.96	128.39
52	x	8	4SU	C5-C4-N3	5.24	119.63	114.75
1	a	535	7MG	C5-C6-N1	5.21	120.11	110.94
52	x	46	7MG	C5-C6-N1	5.21	120.11	110.94
52	x	76	31H	N9-C8-N7	-5.19	106.57	113.94
52	x	46	7MG	OP2-P-OP1	5.15	130.91	110.83
22	A	1966	5MU	N3-C2-N1	5.12	121.56	114.89
52	x	8	4SU	OP2-P-OP1	5.08	130.63	110.83
22	A	2530	2MA	C5-C4-N3	-5.06	121.84	127.18
1	a	1529	MA6	C5-C4-N3	-4.96	119.89	126.72
22	A	2472	2MG	C2-N1-C6	-4.91	118.61	124.55
52	x	55	PSU	OP2-P-OP1	4.83	129.66	110.83
1	a	535	7MG	C2-N3-C4	4.79	120.55	112.30
52	x	76	31H	N6-C6-N1	-4.77	107.75	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	x	54	5MU	C4-N3-C2	-4.72	121.15	127.34
52	x	54	5MU	OP2-P-OP1	4.70	129.16	110.83
52	x	76	31H	C5-C4-N3	-4.67	120.28	126.72
22	A	2530	2MA	C4-N9-C1'	4.66	137.54	126.63
52	x	46	7MG	C2-N3-C4	4.66	120.32	112.30
22	A	2278	OMG	C2-N3-C4	4.65	120.30	112.30
52	x	32	OMC	OP2-P-OP1	4.64	128.92	110.83
52	x	54	5MU	N3-C2-N1	4.63	120.92	114.89
52	x	8	4SU	OP3-P-OP1	-4.55	93.13	110.83
1	a	1530	MA6	C5-C4-N3	-4.54	120.46	126.72
22	A	2472	2MG	N1-C2-N2	4.48	121.13	116.56
52	x	76	31H	C4-N9-C8	4.43	110.39	105.74
1	a	1530	MA6	N9-C8-N7	-4.42	107.66	113.94
1	a	1527	2MG	C2-N1-C6	-4.37	119.27	124.55
1	a	1529	MA6	C4-C5-C6	4.35	120.41	115.91
1	a	535	7MG	C5-C4-N3	-4.31	120.03	128.13
1	a	1529	MA6	N9-C8-N7	-4.23	107.94	113.94
52	x	55	PSU	OP3-P-OP1	-4.21	94.43	110.83
52	x	54	5MU	C5M-C5-C4	4.21	123.28	118.78
52	x	8	4SU	C1'-N1-C2	4.19	125.12	117.59
1	a	1527	2MG	N1-C2-N2	4.16	120.81	116.56
52	x	76	31H	C4-N9-C1'	-4.10	117.03	126.63
52	x	46	7MG	C5-C4-N3	-4.09	120.46	128.13
22	A	2530	2MA	N3-C4-N9	4.05	132.14	126.99
52	x	55	PSU	C4-N3-C2	-4.03	120.82	126.37
1	a	1530	MA6	C2-N1-C6	3.99	121.59	111.83
52	x	76	31H	N3-C4-N9	3.91	133.82	127.17
52	x	54	5MU	C5M-C5-C6	-3.90	117.58	122.85
22	A	2530	2MA	N3-C2-N1	-3.87	118.95	125.77
52	x	8	4SU	N3-C2-N1	3.74	119.77	114.89
1	a	1529	MA6	C2-N1-C6	3.68	120.81	111.83
52	x	76	31H	C5-C6-N6	3.66	132.35	123.29
22	A	2530	2MA	C5-N7-C8	3.62	109.13	103.45
52	x	8	4SU	O5'-P-OP1	3.59	116.14	106.44
52	x	55	PSU	OP3-P-OP2	-3.57	94.40	107.80
52	x	20	H2U	OP3-P-OP1	3.55	124.67	110.83
1	a	1530	MA6	C2-N3-C4	3.55	120.50	111.83
52	x	46	7MG	C4-C5-N7	3.49	109.49	105.38
1	a	1529	MA6	C2-N3-C4	3.47	120.32	111.83
1	a	535	7MG	C5-C4-N9	3.43	110.73	106.33
52	x	46	7MG	C5-C4-N9	3.39	110.68	106.33
1	a	1530	MA6	C4-C5-C6	3.39	119.41	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	x	32	OMC	O5'-P-OP1	3.37	115.56	106.44
1	a	535	7MG	C4-C5-N7	3.36	109.35	105.38
52	x	76	31H	C2-N3-C4	3.36	120.05	111.83
52	x	8	4SU	C6-N1-C2	-3.33	116.95	121.00
52	x	54	5MU	O5'-P-OP1	3.31	115.38	106.44
22	A	2472	2MG	N9-C4-N3	3.30	132.54	125.95
22	A	2278	OMG	C2-N1-C6	-3.28	119.16	125.11
52	x	55	PSU	OP2-P-O5'	3.27	115.19	106.67
22	A	2472	2MG	CM2-N2-C2	-3.26	116.65	123.65
52	x	54	5MU	OP2-P-O5'	3.23	115.09	106.67
52	x	32	OMC	OP2-P-O5'	3.22	115.06	106.67
1	a	1529	MA6	N3-C4-N9	3.22	132.64	127.17
52	x	55	PSU	O2-C2-N1	-3.16	119.53	122.79
52	x	20	H2U	O5'-P-OP1	-3.15	97.93	106.44
1	a	1530	MA6	C5-N7-C8	3.14	108.38	103.45
52	x	8	4SU	OP3-P-OP2	-3.13	96.06	107.80
22	A	2472	2MG	C5-C6-N1	3.12	121.20	113.25
22	A	2530	2MA	CM2-C2-N1	3.10	121.76	117.13
52	x	76	31H	C5-N7-C8	3.09	108.31	103.45
52	x	55	PSU	O5'-P-OP1	3.07	114.73	106.44
22	A	2278	OMG	N9-C4-N3	3.06	132.06	125.95
52	x	46	7MG	OP2-P-O5'	3.05	114.62	106.67
1	a	1529	MA6	C5-N7-C8	3.02	108.20	103.45
22	A	1966	5MU	O2-C2-N1	-2.99	118.90	122.80
52	x	76	31H	C4'-O4'-C1'	-2.94	102.97	109.47
52	x	55	PSU	C6-C5-C4	-2.91	116.21	118.17
1	a	535	7MG	C2-N1-C6	-2.89	119.87	125.11
22	A	2278	OMG	N9-C8-N7	-2.89	108.04	113.40
22	A	2472	2MG	N9-C8-N7	-2.86	108.10	113.40
52	x	46	7MG	C2-N1-C6	-2.84	119.96	125.11
1	a	1527	2MG	N9-C4-N3	2.84	131.63	125.95
1	a	1527	2MG	N9-C8-N7	-2.82	108.16	113.40
52	x	46	7MG	O5'-P-OP1	2.78	113.96	106.44
1	a	1412	4OC	O2-C2-N3	-2.77	117.97	122.33
52	x	32	OMC	O2-C2-N3	-2.76	117.98	122.33
22	A	2278	OMG	C5-C6-N1	2.76	120.27	113.25
1	a	535	7MG	N9-C8-N7	2.70	107.19	103.37
1	a	1527	2MG	CM2-N2-C2	-2.63	117.99	123.65
52	x	20	H2U	C5-C6-N1	-2.63	103.57	111.52
1	a	1530	MA6	C4-C5-N7	-2.62	107.58	110.58
22	A	2472	2MG	O6-C6-C5	-2.61	119.63	126.53
1	a	535	7MG	N9-C4-N3	2.58	129.24	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1527	2MG	C5-C6-N1	2.57	119.80	113.25
22	A	2525	OMC	O2-C2-N3	-2.54	118.33	122.33
52	x	54	5MU	O4-C4-N3	-2.53	115.35	120.11
52	x	46	7MG	N9-C8-N7	2.51	106.93	103.37
22	A	1966	5MU	O4-C4-N3	-2.49	115.44	120.11
1	a	1530	MA6	N3-C4-N9	2.45	131.34	127.17
52	x	8	4SU	S4-C4-N3	2.45	122.76	120.20
52	x	76	31H	C1'-N9-C8	2.42	132.46	127.09
22	A	2278	OMG	O6-C6-C5	-2.41	120.17	126.53
22	A	2530	2MA	N6-C6-N1	2.40	120.26	117.03
1	a	1527	2MG	C1'-N9-C4	-2.40	119.41	126.49
1	a	1529	MA6	C4-N9-C8	2.39	108.25	105.74
52	x	46	7MG	O6-C6-C5	-2.38	121.78	127.62
1	a	1412	4OC	C6-C5-C4	2.36	119.84	117.00
22	A	1966	5MU	C5M-C5-C6	-2.33	119.70	122.85
52	x	46	7MG	N9-C4-N3	2.32	128.86	125.46
1	a	1530	MA6	C4-N9-C8	2.32	108.17	105.74
52	x	32	OMC	C1'-N1-C2	2.31	123.55	118.44
52	x	76	31H	C2'-C1'-N9	2.29	119.00	113.30
1	a	1527	2MG	O6-C6-C5	-2.27	120.54	126.53
1	a	535	7MG	O6-C6-C5	-2.23	122.15	127.62
52	x	55	PSU	O3'-C3'-C4'	2.22	117.47	111.08
52	x	8	4SU	OP2-P-O5'	2.22	112.45	106.67
22	A	1966	5MU	C6-C5-C4	2.22	119.85	118.02
52	x	20	H2U	OP2-P-OP1	2.21	119.43	110.83
1	a	1530	MA6	C5-C4-N9	2.19	108.20	105.81
22	A	1947	OMC	O2-C2-N3	-2.19	118.88	122.33
1	a	1527	2MG	C1'-N9-C8	2.18	132.93	126.73
22	A	2472	2MG	C1'-N9-C4	-2.16	120.09	126.49
1	a	1529	MA6	C4-C5-N7	-2.13	108.14	110.58
1	a	1527	2MG	C8-N7-C5	2.13	108.06	104.26
22	A	2530	2MA	C4-C5-N7	-2.09	108.19	110.58
22	A	2472	2MG	N1-C2-N3	-2.08	120.17	123.68
22	A	2278	OMG	C8-N7-C5	2.04	107.90	104.26
52	x	54	5MU	C6-N1-C2	-2.04	119.27	121.30
52	x	55	PSU	O3'-C3'-C2'	2.01	118.26	111.82

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1530	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	A	1947	OMC	O4'-C4'-C5'-O5'
52	x	32	OMC	C5'-O5'-P-OP1
52	x	46	7MG	C5'-O5'-P-OP3
52	x	54	5MU	C5'-O5'-P-OP3
52	x	55	PSU	O4'-C1'-C5-C4
52	x	55	PSU	O4'-C1'-C5-C6
52	x	55	PSU	C5'-O5'-P-OP1
52	x	55	PSU	C5'-O5'-P-OP3
52	x	76	31H	C-CA-N-CN
52	x	76	31H	CB-CA-N-CN
52	x	76	31H	C-CA-CB-CG
52	x	76	31H	N-CA-CB-CG
52	x	76	31H	OCN-CN-N-CA
52	x	76	31H	C3'-C4'-C5'-O5'
1	a	1412	4OC	O4'-C4'-C5'-O5'
22	A	1966	5MU	O4'-C4'-C5'-O5'
52	x	76	31H	O4'-C4'-C5'-O5'
1	a	535	7MG	O4'-C4'-C5'-O5'
1	a	535	7MG	C3'-C4'-C5'-O5'
52	x	20	H2U	C2'-C1'-N1-C2
1	a	1530	MA6	C3'-C4'-C5'-O5'
22	A	1947	OMC	C3'-C4'-C5'-O5'
52	x	20	H2U	O4'-C4'-C5'-O5'
22	A	1966	5MU	C3'-C4'-C5'-O5'
22	A	2472	2MG	C3'-C4'-C5'-O5'
22	A	2525	OMC	C3'-C4'-C5'-O5'
52	x	46	7MG	C3'-C4'-C5'-O5'
1	a	1412	4OC	C3'-C4'-C5'-O5'
22	A	2525	OMC	O4'-C4'-C5'-O5'
52	x	46	7MG	O4'-C4'-C5'-O5'
1	a	1529	MA6	C5-C6-N6-C9
52	x	20	H2U	C2'-C1'-N1-C6
52	x	76	31H	CB-CG-SD-CE
52	x	46	7MG	C5'-O5'-P-OP1
52	x	76	31H	O-C-CA-N
52	x	76	31H	N3'-C-CA-N
52	x	76	31H	C4'-C5'-O5'-P
52	x	20	H2U	C3'-C4'-C5'-O5'
52	x	32	OMC	C3'-C4'-C5'-O5'
52	x	76	31H	O-C-CA-CB
22	A	2472	2MG	O4'-C4'-C5'-O5'
52	x	8	4SU	C5'-O5'-P-OP1

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Mol	Chain	Res	Type	Atoms
52	x	76	31H	N3'-C-CA-CB
52	x	46	7MG	C4'-C5'-O5'-P
52	x	32	OMC	O4'-C4'-C5'-O5'
52	x	32	OMC	C5'-O5'-P-OP3
52	x	54	5MU	C5'-O5'-P-OP1
22	A	2530	2MA	O4'-C4'-C5'-O5'
22	A	2530	2MA	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	x	76	31H	1	0
1	a	535	7MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 288 ligands modelled in this entry, 288 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	53:GLU	C	57:GLU	N	9.89

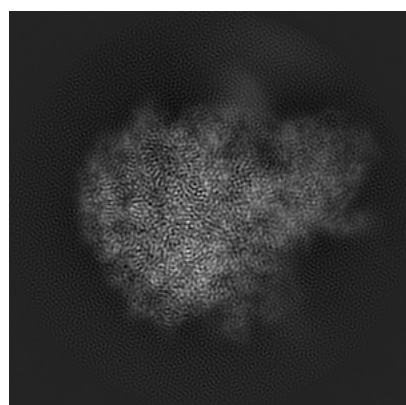
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10791. These allow visual inspection of the internal detail of the map and identification of artifacts.

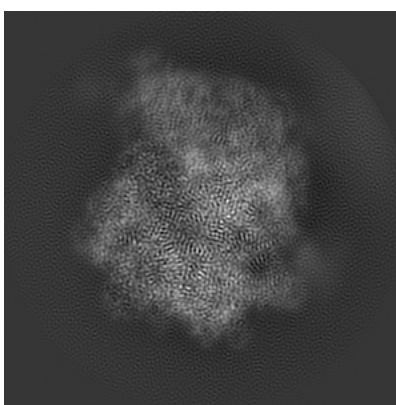
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

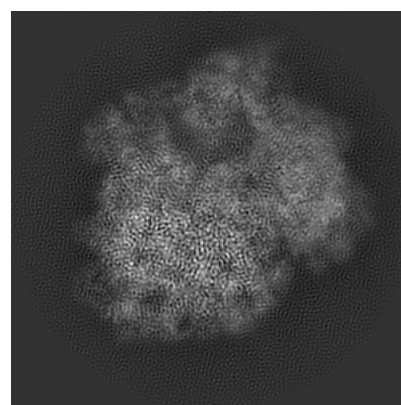
6.1.1 Primary map



X



Y

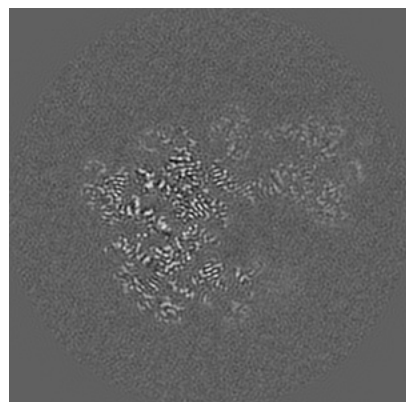


Z

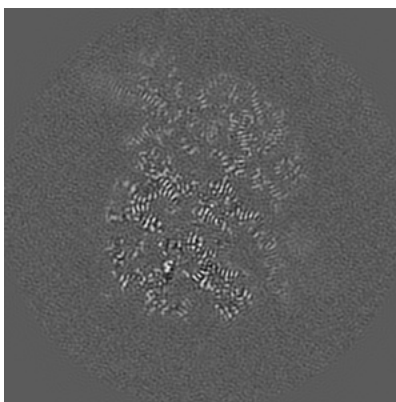
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

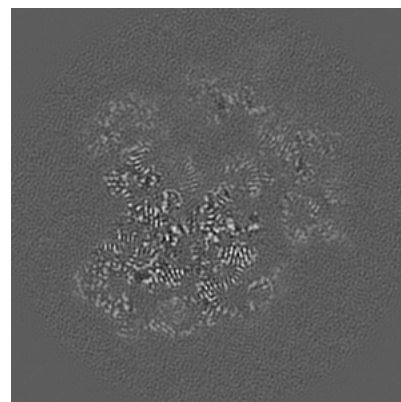
6.2.1 Primary map



X Index: 150



Y Index: 150

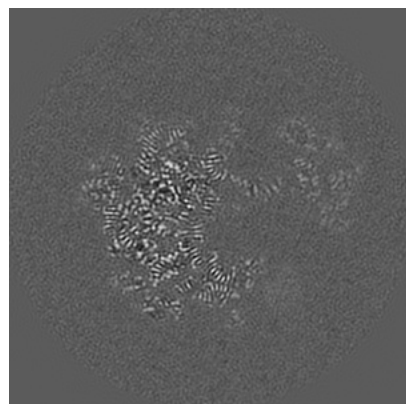


Z Index: 150

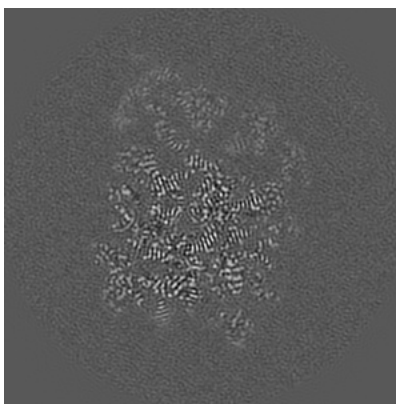
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

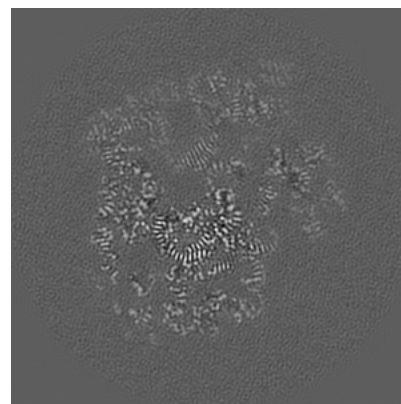
6.3.1 Primary map



X Index: 143



Y Index: 134

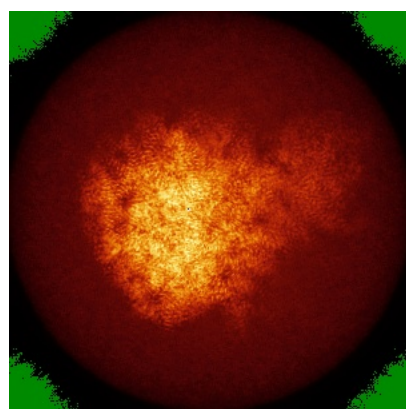


Z Index: 163

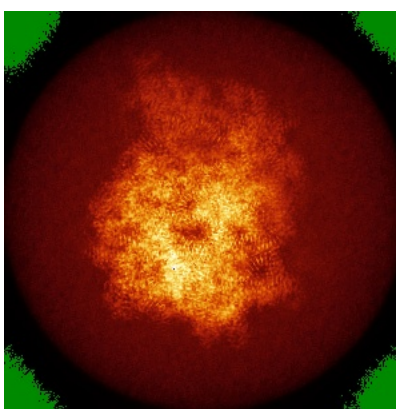
The images above show the largest variance slices of the map in three orthogonal directions.

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

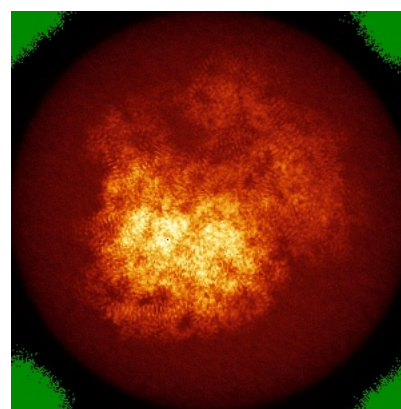
6.4.1 Primary map



X



Y

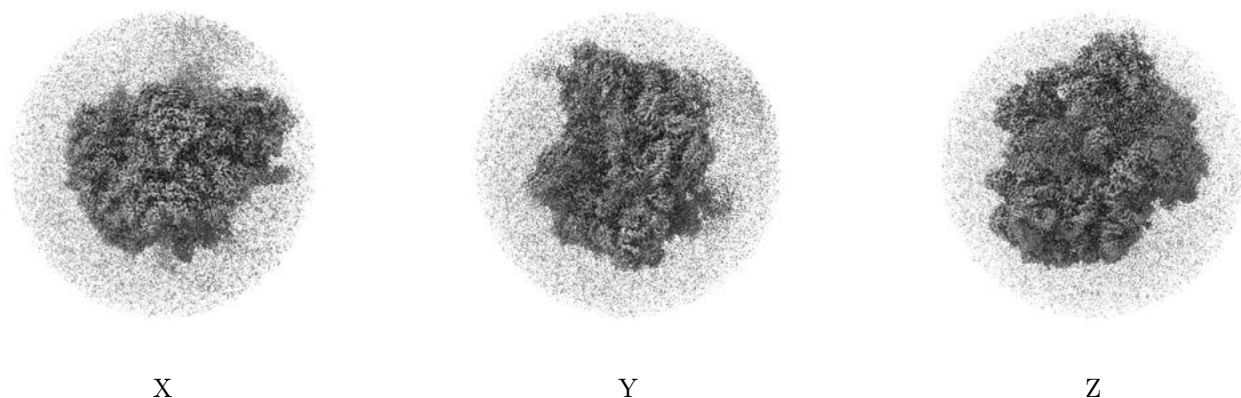


Z

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 0.0524. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

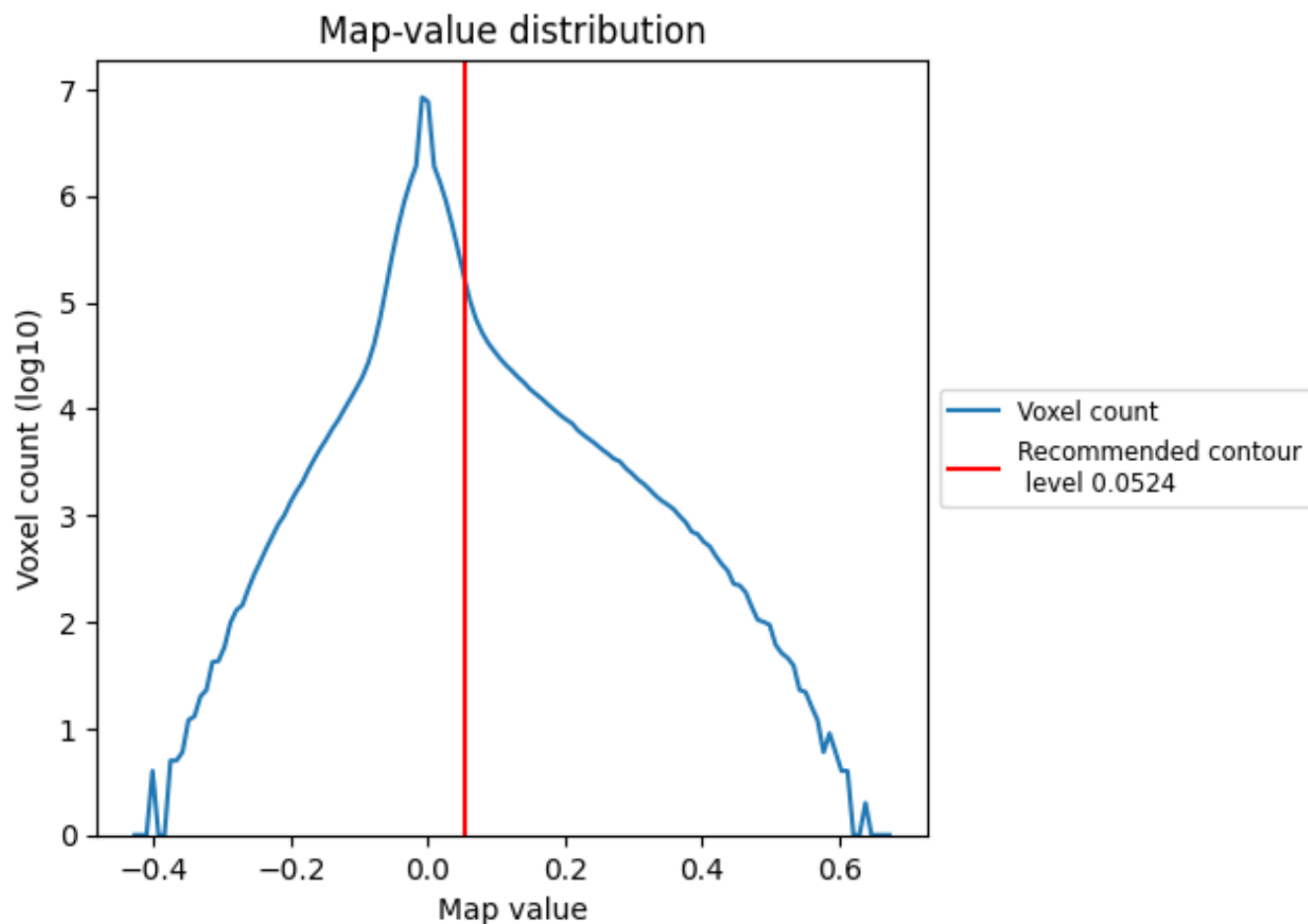
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

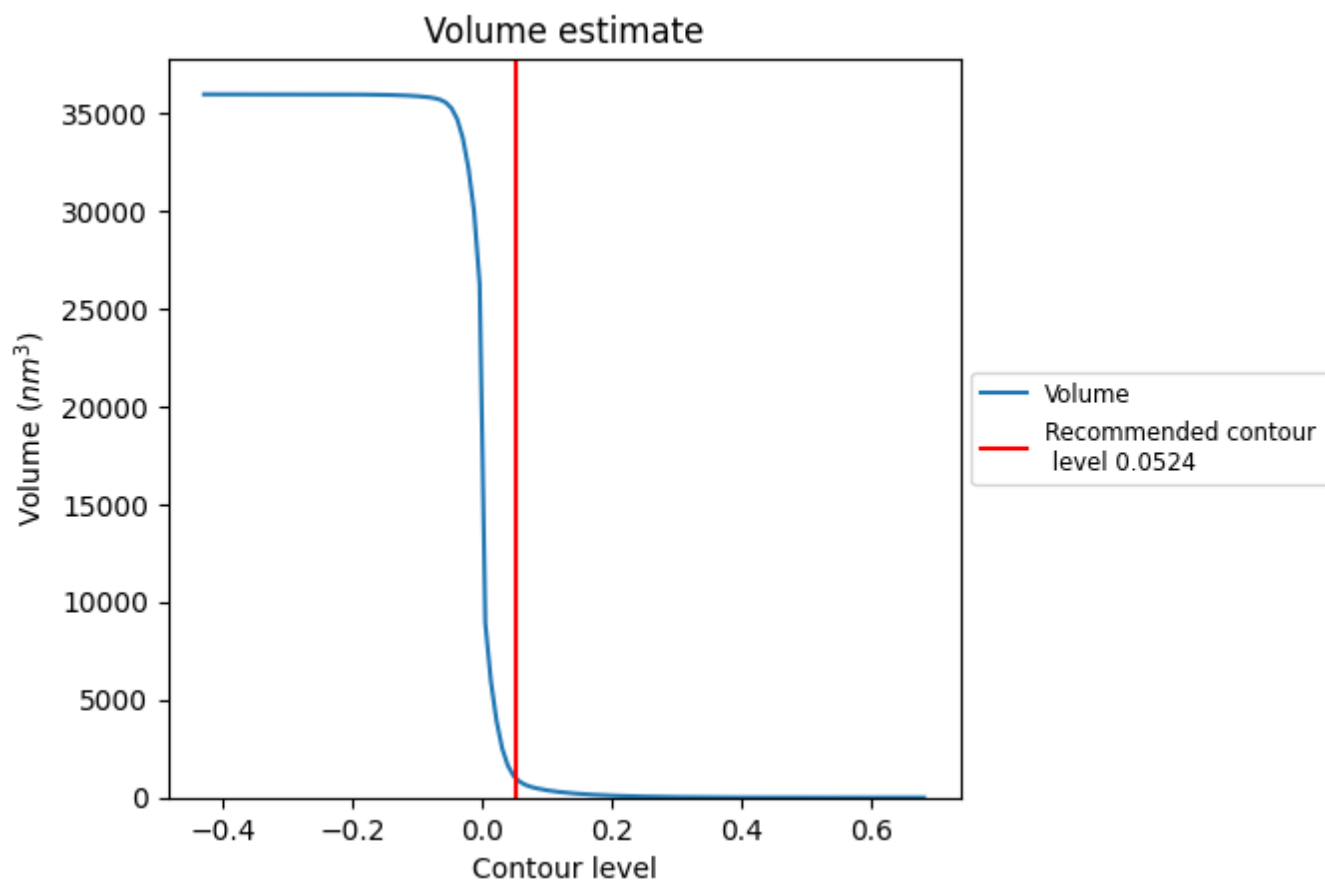
This section contains the results of statistical analysis of the map.

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.

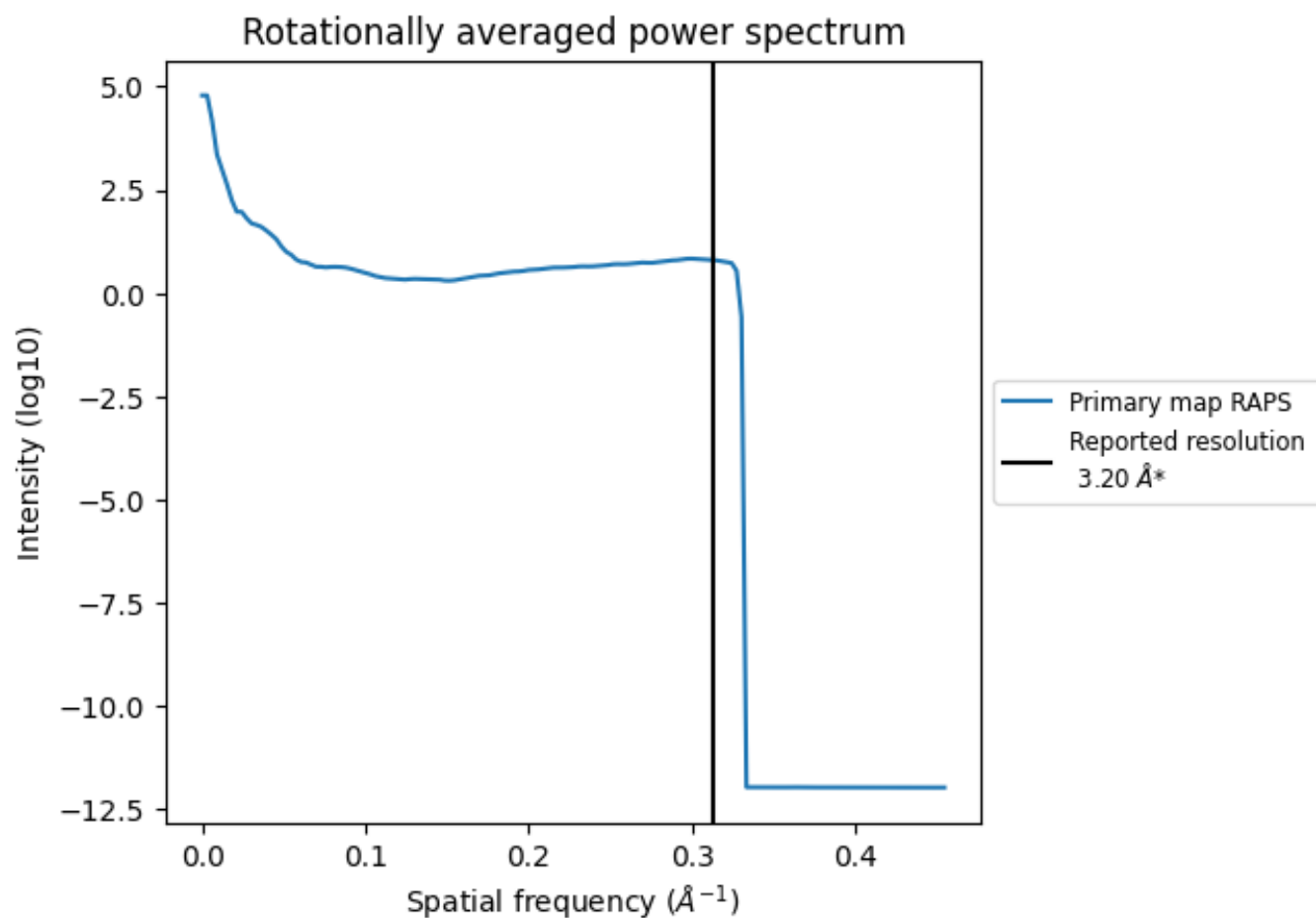
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1006 nm³; this corresponds to an approximate mass of 909 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

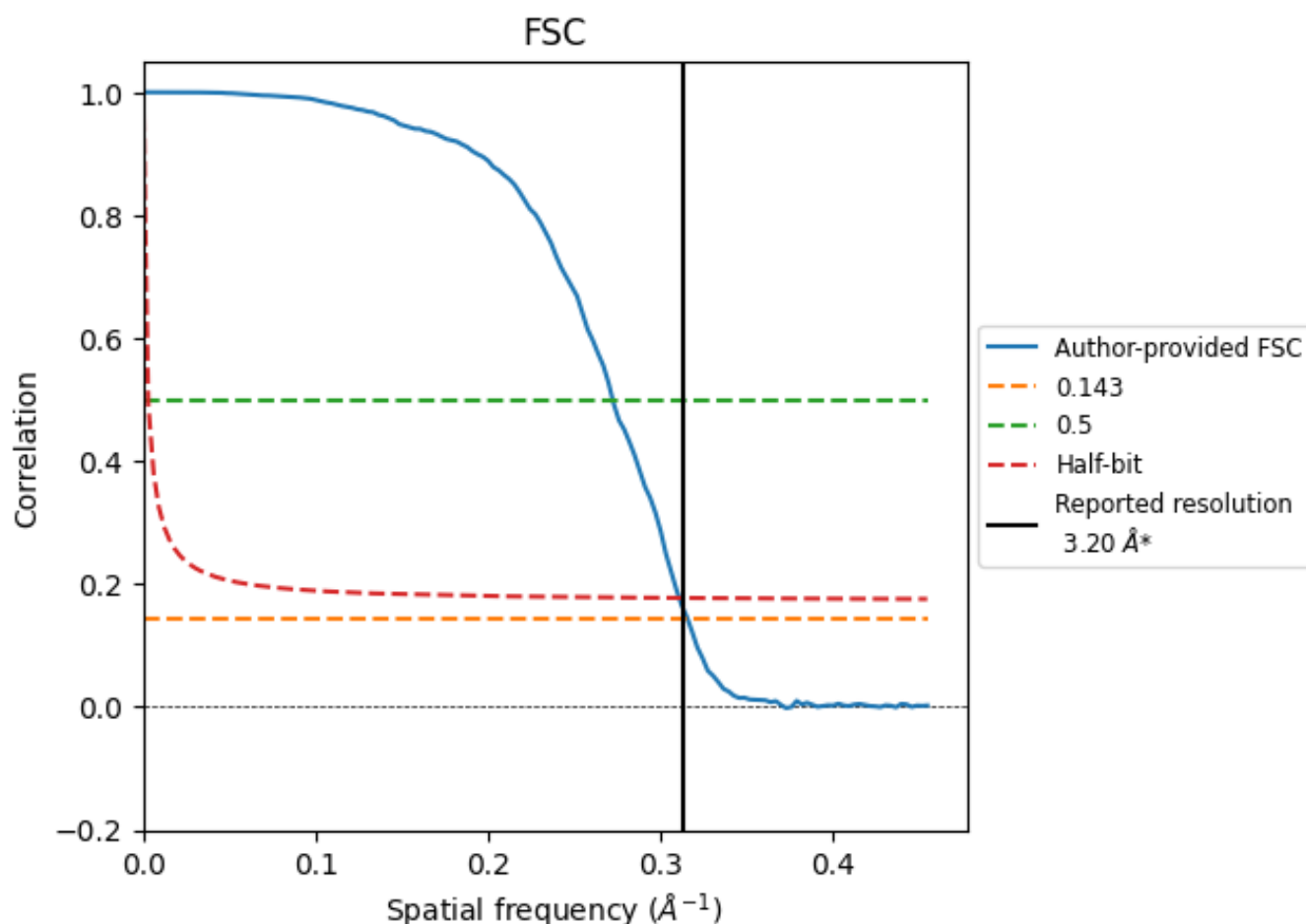


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.68	3.22
Unmasked-calculated*	-	-	-

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

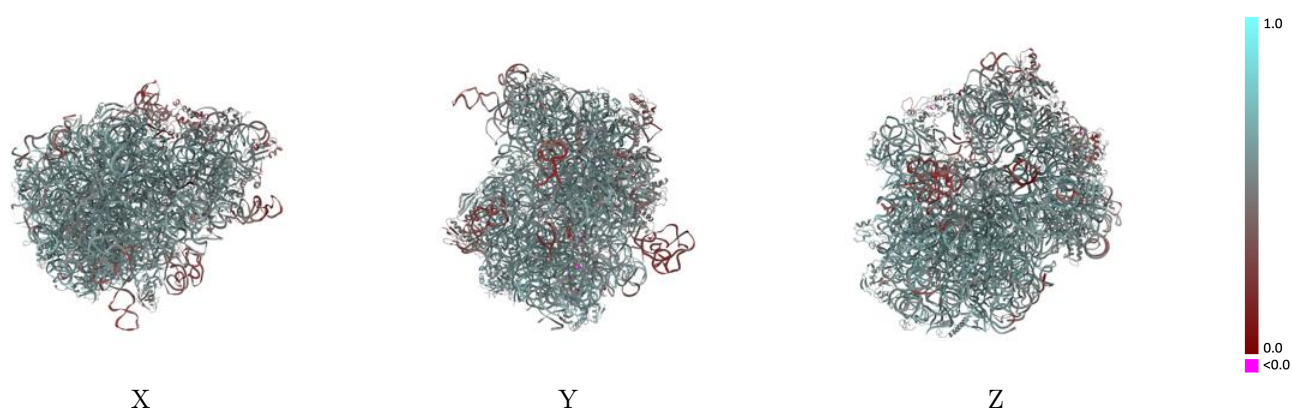
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10791 and PDB model 6YEF. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

This section was not generated.

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

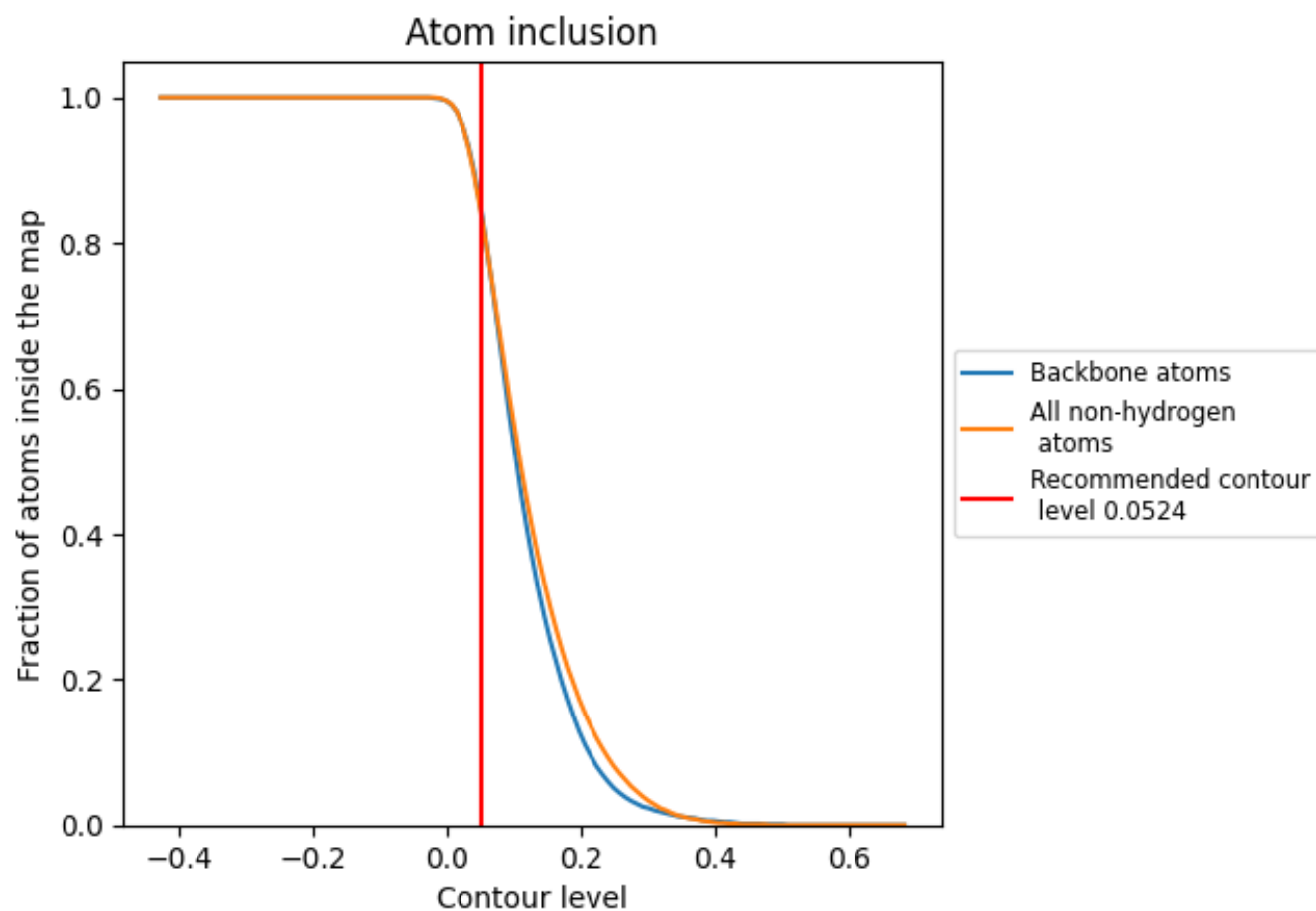


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.0524) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8310	 0.5690
0	 0.7990	 0.5430
1	 0.7940	 0.5600
2	 0.9170	 0.6130
3	 0.3450	 0.3840
4	 0.8390	 0.5780
5	 0.7650	 0.5500
6	 0.9660	 0.6410
7	 0.9500	 0.6220
8	 0.8720	 0.6080
A	 0.8930	 0.5900
B	 0.8970	 0.5720
D	 0.9250	 0.6190
E	 0.9190	 0.6130
F	 0.8750	 0.5950
G	 0.6700	 0.5000
H	 0.5790	 0.4830
M	 0.9180	 0.6220
N	 0.9160	 0.6040
O	 0.8750	 0.5840
P	 0.8940	 0.6050
Q	 0.8930	 0.6070
R	 0.7750	 0.5640
S	 0.8930	 0.6010
T	 0.9300	 0.6220
U	 0.9030	 0.6100
V	 0.9060	 0.6160
W	 0.8390	 0.5930
X	 0.7370	 0.5260
Y	 0.5830	 0.5130
Z	 0.9180	 0.6170
a	 0.8260	 0.5530
b	 0.2880	 0.4170
c	 0.6330	 0.5170
d	 0.6330	 0.5250



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Chain	Atom inclusion	Q-score
e	 0.7870	 0.5680
f	 0.6720	 0.5380
g	 0.5950	 0.5020
h	 0.7740	 0.5650
i	 0.6200	 0.5020
j	 0.5310	 0.4860
k	 0.6480	 0.5210
l	 0.7620	 0.5570
m	 0.5980	 0.5000
n	 0.7700	 0.5520
o	 0.7740	 0.5720
p	 0.6630	 0.5320
q	 0.6800	 0.5430
r	 0.6500	 0.5310
s	 0.5880	 0.4870
t	 0.6710	 0.5430
v	 0.3390	 0.2870
x	 0.7420	 0.5240