



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:56 PM UTC

PDB ID : 9I5T / pdb_00009i5t
EMDB ID : EMD-52635
Title : 50S subunit of P. gingivalis ribosome with Lefamulin
Authors : Hiregange, D.G.; Bashan, A.; Yonath, A.
Deposited on : 2025-01-28
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

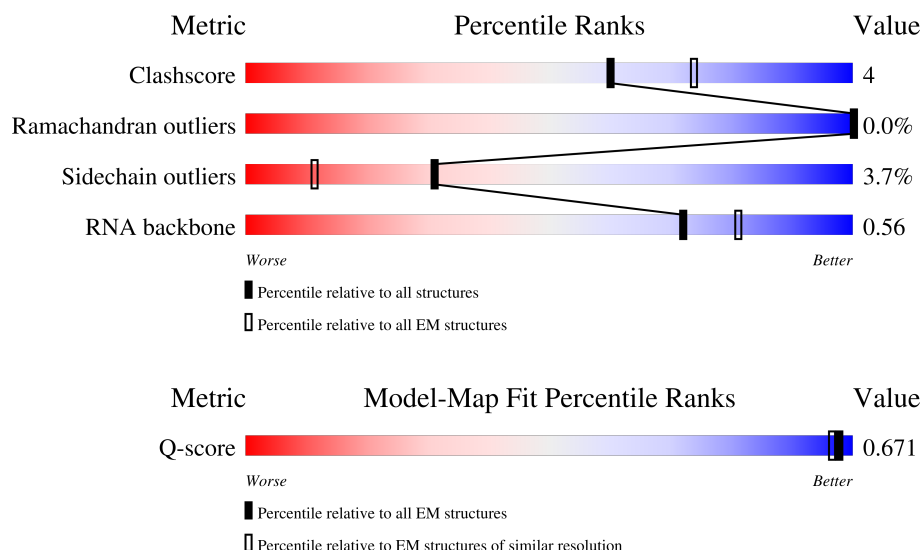
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.60 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.



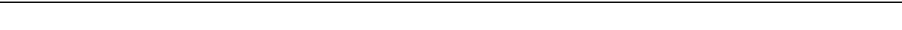
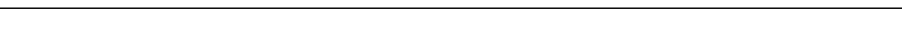
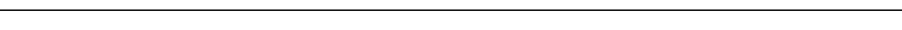
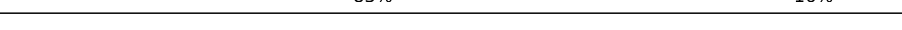
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	0	79	
2	1	64	
3	11	186	

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Mol	Chain	Length	Quality of chain
4	12	85	
5	2	58	
6	4	61	
7	6	50	
8	7	65	
9	8	38	
10	A	2882	
11	B	109	
12	D	274	
13	E	205	
14	F	209	
15	M	151	
16	O	148	
17	P	144	
18	Q	160	
19	R	114	
20	S	121	
21	T	115	
22	U	105	
23	V	134	
24	W	97	
25	X	106	
26	Y	192	
27	Z	85	
28	h	179	

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Mol	Chain	Length	Quality of chain
29	15	49	
30	13	183	
31	N	121	
32	5	62	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 82341 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			600	387	117	93	3		

- Molecule 2 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	63	Total	C	N	O	S	0	0
			466	292	93	78	3		

- Molecule 3 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	11	166	Total	C	N	O	S	0	0
			1033	645	188	198	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	12	52	Total	C	N	O	0	0
			267	159	52	56		

- Molecule 5 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	56	Total	C	N	O	S	0	0
			434	275	89	68	2		

- Molecule 6 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	57	Total	C	N	O	S	0	0
			436	272	91	72	1		

- Molecule 7 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	48	Total	C	N	O	S	0	0
			382	230	89	61	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	64	Total	C	N	O	S	0	0
			508	325	98	84	1		

- Molecule 9 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	38	Total	C	N	O	S	0	0
			297	185	63	47	2		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2529	Total	C	N	O	P	0	0
			54304	24248	10018	17509	2529		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	102	Total	C	N	O	P	0	0
			2187	975	400	710	102		

- Molecule 12 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	272	Total	C	N	O	S	0	0
			2036	1270	396	362	8		

- Molecule 13 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	204	Total	C	N	O	S	0	0
			1497	955	273	262	7		

- Molecule 14 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	208	Total	C	N	O	S	0	0
			1520	966	282	271	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	149	Total	C	N	O	S	0	0
			1136	726	212	193	5		

- Molecule 16 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	146	Total	C	N	O	S	0	0
			1021	641	195	184	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	142	Total	C	N	O	S	0	0
			1095	704	206	182	3		

- Molecule 18 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	123	Total	C	N	O	S	0	0
			968	618	183	161	6		

- Molecule 19 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	110	Total	C	N	O	S	0	0
			751	467	149	135			

- Molecule 20 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	113	Total	C	N	O	S	0	0
			854	548	161	145			

- Molecule 21 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	113	Total	C	N	O	S	0	0
			916	580	188	145	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	104	Total	C	N	O	S	0	0
			782	503	145	131	3		

- Molecule 23 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	127	Total	C	N	O	S	0	0
			1013	627	204	177	5		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	92	Total	C	N	O	S	0	0
			682	439	119	120	4		

- Molecule 25 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	97	Total	C	N	O	S	0	0
			693	434	136	121	2		

- Molecule 26 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	176	Total	C	N	O		0	0
			1166	757	206	203			

- Molecule 27 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	77	Total	C	N	O	S	0	0
			574	354	113	106	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	52	Total	C	N	O	S	0	0
			349	226	61	61	1		

- Molecule 29 is a protein called DUF4295 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	15	35	Total	C	N	O	S	0	0
			256	164	41	49	2		

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	13	177	Total	C	N	O	S	0	0
			1309	828	240	237	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	N	121	Total	C	N	O	S	0	0
			875	547	168	156	4		

- Molecule 32 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	45	Total	C	N	O	S	0	0
			346	216	65	63	2		

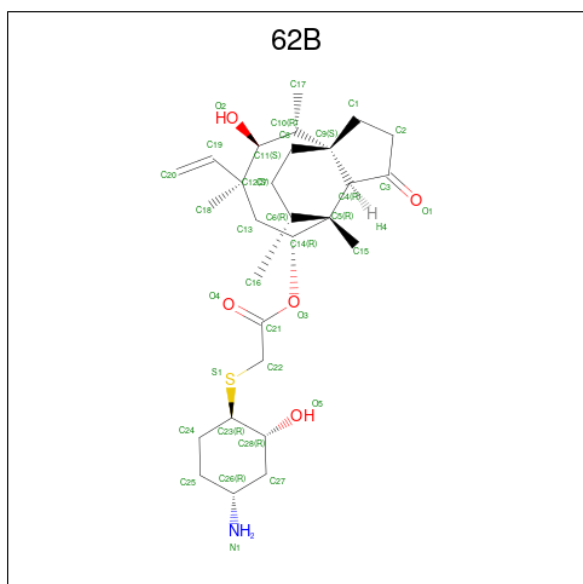
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	4	1	Total	Mg	0
			1	1	
33	A	134	Total	Mg	0
			134	134	
33	B	1	Total	Mg	0
			1	1	
33	F	1	Total	Mg	0
			1	1	
33	V	2	Total	Mg	0
			2	2	

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	4	1	Total	Zn	0
			1	1	

- Molecule 35 is Lefamulin (CCD ID: 62B) (formula: $C_{28}H_{45}NO_5S$).



Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	S	0
			35	28	1	5	1	

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
36	A	18	Total	K	0
			18	18	

- Molecule 37 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
37	A	13	Total	Na	0
			13	13	
37	B	2	Total	Na	0
			2	2	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	0	1	Total 1	O 1	0
38	4	6	Total 6	O 6	0
38	6	12	Total 12	O 12	0
38	7	1	Total 1	O 1	0
38	A	1225	Total 1225	O 1225	0
38	B	4	Total 4	O 4	0
38	D	26	Total 26	O 26	0
38	E	16	Total 16	O 16	0
38	F	19	Total 19	O 19	0
38	O	16	Total 16	O 16	0
38	Q	8	Total 8	O 8	0
38	S	1	Total 1	O 1	0
38	T	15	Total 15	O 15	0
38	U	8	Total 8	O 8	0
38	V	15	Total 15	O 15	0
38	W	2	Total 2	O 2	0
38	Z	5	Total 5	O 5	0

3 Residue-property plots [i](#)

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

- Molecule 1: Large ribosomal subunit protein bL28

Chain 0: 



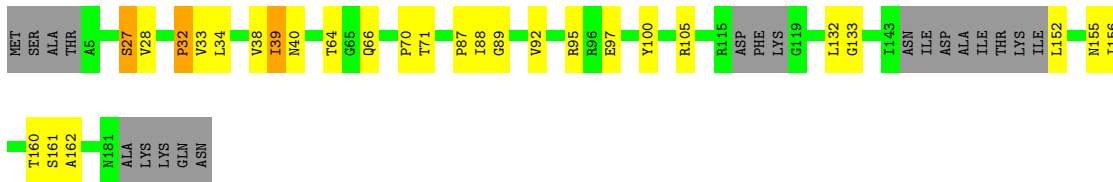
- Molecule 2: Large ribosomal subunit protein uL29

Chain 1: 



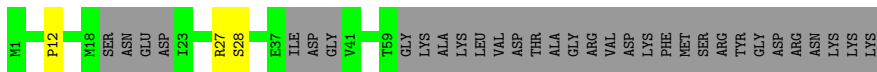
- Molecule 3: Large ribosomal subunit protein uL5

Chain 11: 



- Molecule 4: Large ribosomal subunit protein bL31B

Chain 12: 

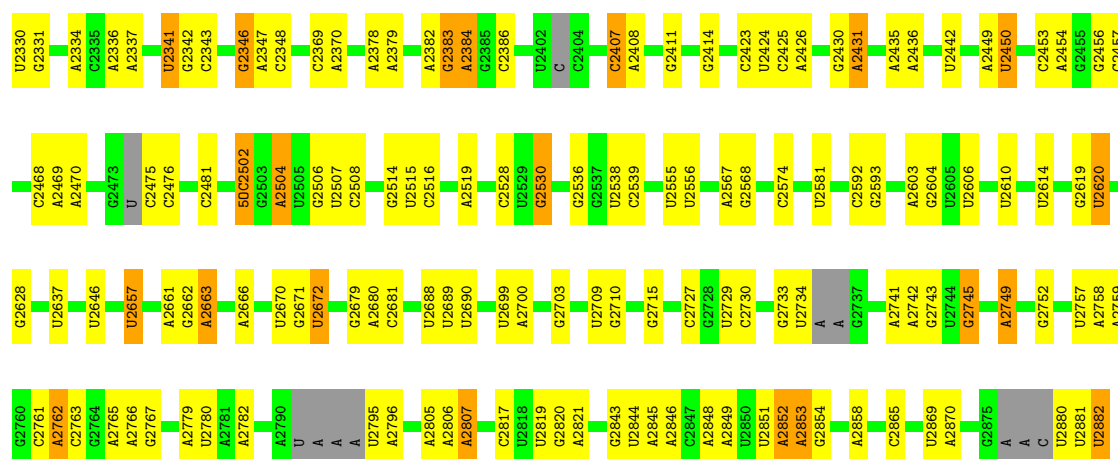


- Molecule 5: Large ribosomal subunit protein uL30

Chain 2: 

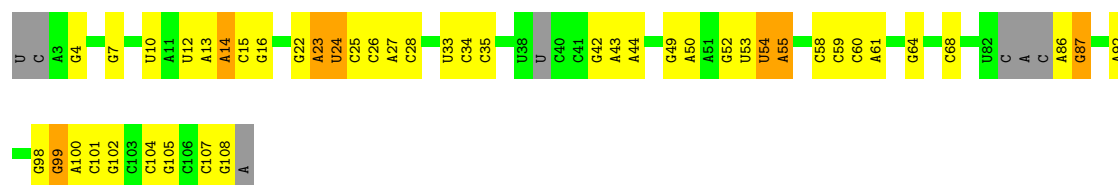






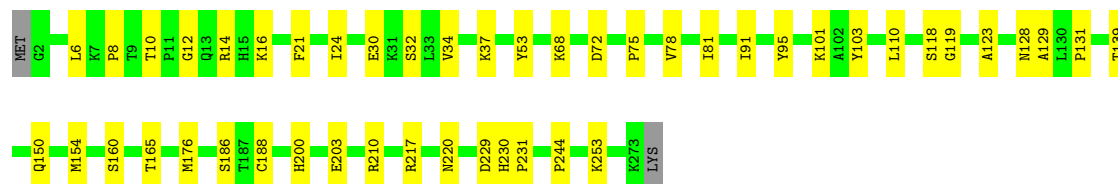
- Molecule 11: 5S rRNA

Chain B: 52% 35% 6% 6%



- Molecule 12: Large ribosomal subunit protein uL2

Chain D: 82% 17%



- Molecule 13: Large ribosomal subunit protein uL3

Chain E: 90% 10%



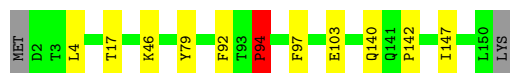
- Molecule 14: Large ribosomal subunit protein uL4

Chain F: 93% 5%



- Molecule 15: Large ribosomal subunit protein uL13

Chain M:  91% 7% ..



- Molecule 16: Large ribosomal subunit protein uL15

Chain O:  85% 12% ..



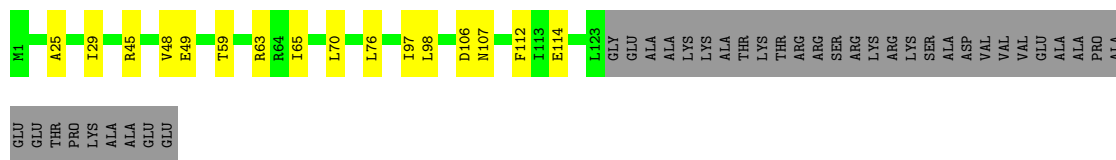
- Molecule 17: Large ribosomal subunit protein uL16

Chain P:  83% 16% .



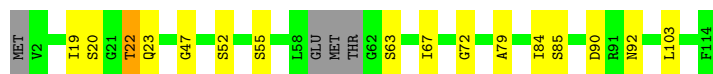
- Molecule 18: Large ribosomal subunit protein bL17

Chain Q:  67% 10% 23%



- Molecule 19: Large ribosomal subunit protein uL18

Chain R:  82% 13% . .



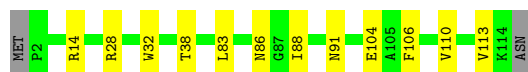
- Molecule 20: Large ribosomal subunit protein bL19

Chain S:  82% 11% 7%



- Molecule 21: Large ribosomal subunit protein bL20

Chain T:  88% 10% .



- Molecule 22: Large ribosomal subunit protein bL21

Chain U:  80% 18% ..



- Molecule 23: Large ribosomal subunit protein uL22

Chain V:  81% 13% 5%



- Molecule 24: Large ribosomal subunit protein uL23

Chain W:  82% 11% 5%



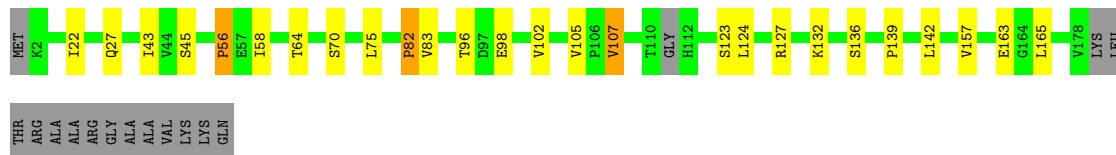
- Molecule 25: Large ribosomal subunit protein uL24

Chain X:  70% 22% 8%



- Molecule 26: Large ribosomal subunit protein bL25

Chain Y:  78% 12% 8%



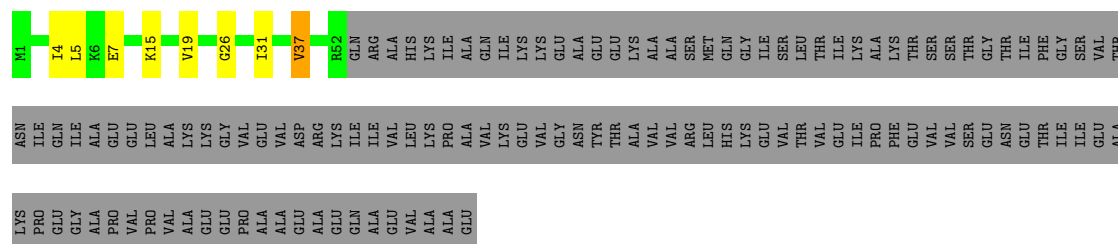
- Molecule 27: Large ribosomal subunit protein bL27

Chain Z:  84% 7% 9%



- Molecule 28: Large ribosomal subunit protein bL9

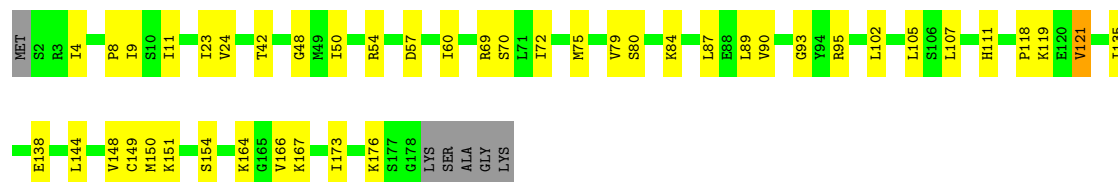
Chain h:  25% 71%



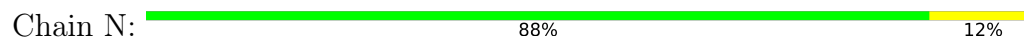
- Molecule 29: DUF4295 domain-containing protein



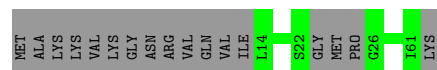
- Molecule 30: Large ribosomal subunit protein uL6



- Molecule 31: Large ribosomal subunit protein uL14



- Molecule 32: Large ribosomal subunit protein bL33



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	223396	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.294	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	370.48, 370.48, 370.48	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 62B, K, 6MA, NA, PSU, OMG, 2MG, OMU, H2U, ZN, 5MC, 2MA, MG, 5OC, 5MU

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	0	0.17	0/609	0.31	0/815
2	1	0.14	0/470	0.28	0/633
3	11	0.70	4/1042 (0.4%)	1.13	9/1425 (0.6%)
4	12	0.11	0/265	0.39	0/366
5	2	0.23	0/437	0.55	1/587 (0.2%)
6	4	0.18	0/447	0.34	0/604
7	6	0.17	0/385	0.34	0/508
8	7	0.18	0/515	0.41	0/683
9	8	0.20	0/299	0.43	0/395
10	A	0.23	0/60371	0.36	0/94092
11	B	0.17	0/2445	0.30	0/3807
12	D	0.20	0/2075	0.45	2/2788 (0.1%)
13	E	0.18	0/1525	0.40	0/2050
14	F	0.16	0/1543	0.30	0/2097
15	M	0.40	1/1161 (0.1%)	0.70	5/1571 (0.3%)
16	O	0.17	0/1032	0.39	0/1387
17	P	0.17	0/1118	0.35	0/1503
18	Q	0.19	0/985	0.37	0/1321
19	R	0.12	0/755	0.30	0/1015
20	S	0.16	0/869	0.33	0/1170
21	T	0.17	0/933	0.32	0/1248
22	U	0.16	0/792	0.37	0/1068
23	V	0.20	0/1026	0.46	2/1370 (0.1%)
24	W	0.16	0/690	0.33	0/924
25	X	0.16	0/698	0.40	0/937
26	Y	0.46	2/1184 (0.2%)	0.95	7/1622 (0.4%)
27	Z	0.16	0/581	0.35	0/777
28	h	0.18	0/351	0.45	0/477
29	15	0.25	0/260	0.78	2/349 (0.6%)
30	13	0.23	1/1327 (0.1%)	0.53	4/1792 (0.2%)
31	N	0.22	0/882	0.49	3/1190 (0.3%)
32	5	0.14	0/348	0.33	0/468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.24	8/87420 (0.0%)	0.40	35/131039 (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
13	E	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	11	32	PRO	CG-CD	-11.94	1.10	1.50
3	11	87	PRO	CG-CD	-11.39	1.12	1.50
3	11	70	PRO	CG-CD	-11.27	1.12	1.50
15	M	142	PRO	CG-CD	-11.14	1.12	1.50
26	Y	139	PRO	CG-CD	-10.69	1.14	1.50
26	Y	139	PRO	CB-CG	-9.24	1.03	1.49
3	11	32	PRO	CB-CG	-6.64	1.16	1.49
30	13	118	PRO	CG-CD	-5.10	1.33	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	11	32	PRO	N-CD-CG	-18.81	74.98	103.20
26	Y	139	PRO	CB-CG-CD	18.29	164.63	106.10
26	Y	139	PRO	N-CD-CG	-17.78	76.53	103.20
3	11	87	PRO	N-CD-CG	-16.76	78.06	103.20
15	M	142	PRO	N-CD-CG	-16.06	79.11	103.20
3	11	32	PRO	CA-CB-CG	-15.22	75.59	104.50
26	Y	139	PRO	CA-CB-CG	-14.27	77.39	104.50
3	11	70	PRO	N-CD-CG	-14.18	81.93	103.20
3	11	32	PRO	CB-CG-CD	13.46	149.16	106.10
3	11	87	PRO	CA-CB-CG	-11.58	82.51	104.50
15	M	142	PRO	CA-CB-CG	-10.38	84.79	104.50
3	11	70	PRO	CA-N-CD	-9.34	98.93	112.00
30	13	118	PRO	N-CD-CG	-8.98	89.74	103.20
31	N	72	PRO	N-CD-CG	-8.56	90.36	103.20
3	11	70	PRO	CA-CB-CG	-8.00	89.30	104.50
23	V	108	PRO	N-CD-CG	-7.22	92.36	103.20
26	Y	56	PRO	N-CD-CG	-7.09	92.57	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	41	PRO	N-CD-CG	-7.06	92.61	103.20
15	M	94	PRO	N-CD-CG	-7.01	92.69	103.20
12	D	75	PRO	N-CD-CG	-6.95	92.77	103.20
29	15	40	PRO	N-CD-CG	-6.86	92.90	103.20
26	Y	82	PRO	N-CD-CG	-6.76	93.06	103.20
26	Y	56	PRO	CA-CB-CG	-6.48	92.19	104.50
15	M	94	PRO	CA-CB-CG	-5.89	93.31	104.50
12	D	75	PRO	CA-CB-CG	-5.75	93.58	104.50
15	M	142	PRO	CA-N-CD	-5.71	104.01	112.00
3	11	87	PRO	CA-N-CD	-5.68	104.04	112.00
31	N	72	PRO	CA-CB-CG	-5.61	93.84	104.50
30	13	8	PRO	CA-N-CD	-5.55	104.23	112.00
30	13	118	PRO	N-CA-CB	-5.50	97.60	103.38
26	Y	82	PRO	CA-CB-CG	-5.46	94.13	104.50
30	13	118	PRO	CA-CB-CG	-5.41	94.22	104.50
29	15	40	PRO	CA-CB-CG	-5.35	94.33	104.50
23	V	108	PRO	CA-N-CD	-5.27	104.62	112.00
31	N	72	PRO	CA-N-CD	-5.02	104.97	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	E	151	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	600	0	632	4	0
2	1	466	0	475	5	0
3	11	1033	0	801	16	0
4	12	267	0	126	2	0
5	2	434	0	482	6	0
6	4	436	0	419	5	0
7	6	382	0	409	4	0
8	7	508	0	557	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	8	297	0	315	6	0
10	A	54304	0	27363	346	0
11	B	2187	0	1105	22	0
12	D	2036	0	2092	22	0
13	E	1497	0	1527	11	0
14	F	1520	0	1504	5	0
15	M	1136	0	1133	8	0
16	O	1021	0	1035	11	0
17	P	1095	0	1124	13	0
18	Q	968	0	1003	10	0
19	R	751	0	711	6	0
20	S	854	0	831	10	0
21	T	916	0	969	7	0
22	U	782	0	804	12	0
23	V	1013	0	1058	10	0
24	W	682	0	685	8	0
25	X	693	0	701	11	0
26	Y	1166	0	1057	10	0
27	Z	574	0	578	3	0
28	h	349	0	344	4	0
29	15	256	0	243	9	0
30	13	1309	0	1300	24	0
31	N	875	0	906	10	0
32	5	346	0	338	0	0
33	4	1	0	0	0	0
33	A	134	0	0	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	V	2	0	0	0	0
34	4	1	0	0	0	0
35	A	35	0	0	0	0
36	A	18	0	0	0	0
37	A	13	0	0	0	0
37	B	2	0	0	0	0
38	0	1	0	0	0	0
38	4	6	0	0	0	0
38	6	12	0	0	1	0
38	7	1	0	0	0	0
38	A	1225	0	0	6	0
38	B	4	0	0	0	0
38	D	26	0	0	0	0
38	E	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	19	0	0	0	0
38	O	16	0	0	0	0
38	Q	8	0	0	1	0
38	S	1	0	0	0	0
38	T	15	0	0	0	0
38	U	8	0	0	0	0
38	V	15	0	0	0	0
38	W	2	0	0	0	0
38	Z	5	0	0	0	0
All	All	82341	0	52627	582	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 4.

All (582) 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)
10:A:1521:G:OP2	12:D:101:LYS:NZ	2.16	0.75
10:A:2671:G:C4	10:A:2672:H2U:H51	2.22	0.74
10:A:2820:G:OP2	13:E:56:LYS:NZ	2.21	0.73
10:A:1862:A:H2'	10:A:1863:A:C8	2.24	0.72
7:6:45:SER:OG	10:A:114:A:OP1	2.08	0.72
30:13:9:ILE:HG12	30:13:69:ARG:HH11	1.56	0.71
3:11:34:LEU:HA	3:11:160:THR:HA	1.72	0.71
10:A:1556:G:H22	10:A:1580:A:H2	1.38	0.71
10:A:1075:A:H2'	10:A:1076:A:C8	2.26	0.70
10:A:140:U:H3	10:A:154:G:H1	1.38	0.69
10:A:1520:G:H4'	10:A:1521:G:OP1	1.92	0.69
13:E:13:SER:O	20:S:56:LYS:NZ	2.26	0.69
7:6:35:ARG:NH2	38:6:101:HOH:O	2.26	0.69
10:A:200:A:H62	10:A:210:G:H8	1.41	0.67
10:A:1509:G:H1	10:A:1542:A:H2	1.40	0.67
10:A:974:A:N7	38:A:3107:HOH:O	2.28	0.67
10:A:1507:U:H3	10:A:1544:U:H5	1.40	0.67
10:A:2024:A:H2'	10:A:2025:A:C8	2.30	0.66
17:P:66:VAL:HG22	17:P:104:PHE:HE2	1.60	0.65
10:A:1077:G:N2	10:A:1149:G:H1	1.94	0.65
10:A:1749:C:H5	10:A:1754:G:H1	1.43	0.65
12:D:68:LYS:NZ	12:D:150:GLN:O	2.30	0.65
10:A:2312:A:HO2'	10:A:2313:C:H6	1.42	0.65
3:11:88:ILE:HD11	10:A:2313:C:H5'	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1685:G:O2'	18:Q:106:ASP:OD2	2.12	0.65
10:A:318:A:OP2	25:X:83:ARG:NH2	2.30	0.65
10:A:143:A:H61	10:A:151:C:H42	1.45	0.64
10:A:1376:G:N7	38:A:3117:HOH:O	2.30	0.64
16:O:82:LEU:HD11	16:O:113:ILE:HD12	1.79	0.64
10:A:2202:G:H2'	10:A:2203:A:H8	1.63	0.64
10:A:1464:A:H2'	10:A:1465:G:C8	2.32	0.64
10:A:1529:A:O2'	10:A:1530:A:N7	2.31	0.63
24:W:74:LYS:NZ	24:W:75:GLU:O	2.31	0.63
10:A:881:U:HO2'	10:A:882:G:H8	1.46	0.63
10:A:2107:U:O2	10:A:2202:G:N2	2.30	0.63
10:A:2662:G:H2'	10:A:2663:A:C8	2.33	0.62
10:A:151:C:H2'	10:A:152:A:C8	2.34	0.62
10:A:1558:A:H2	10:A:1578:G:H1	1.46	0.62
10:A:1002:U:H2'	10:A:1003:C:C6	2.34	0.62
10:A:2202:G:H2'	10:A:2203:A:C8	2.34	0.62
3:11:27:SER:OG	3:11:28:VAL:N	2.32	0.61
12:D:230:HIS:ND1	12:D:231:PRO:HD2	2.15	0.61
17:P:51:ARG:HH11	17:P:51:ARG:HG2	1.64	0.61
10:A:890:G:H2'	10:A:891:A:C8	2.34	0.61
10:A:2035:C:H2'	10:A:2036:G:C8	2.36	0.61
10:A:306:A:H1'	10:A:307:G:C8	2.36	0.60
10:A:2201:G:H2'	10:A:2202:G:C8	2.36	0.60
23:V:98:ALA:HB3	23:V:119:SER:HB2	1.83	0.60
10:A:1463:A:H2'	10:A:1464:A:H8	1.65	0.60
10:A:618:U:H2'	10:A:619:G:C8	2.36	0.60
10:A:1532:C:H4'	10:A:1533:C:OP1	2.01	0.60
10:A:848:U:H2'	10:A:849:C:C6	2.36	0.60
5:2:43:ILE:HD13	5:2:46:MET:HE3	1.83	0.60
8:7:19:THR:HG23	10:A:682:G:H5'	1.84	0.59
10:A:1900:A:H8	10:A:2235:G:H21	1.48	0.59
10:A:2247:G:H2'	10:A:2248:A:C8	2.37	0.59
8:7:23:LYS:NZ	10:A:662:A:OP2	2.35	0.59
10:A:1463:A:H2'	10:A:1464:A:C8	2.37	0.59
23:V:69:ARG:HH11	23:V:69:ARG:HG2	1.67	0.59
10:A:1075:A:H2'	10:A:1076:A:H8	1.67	0.59
22:U:68:LEU:HD11	22:U:94:GLN:HG2	1.84	0.59
16:O:135:GLU:O	16:O:139:VAL:HG23	2.03	0.58
10:A:1540:A:H3'	10:A:1541:G:H21	1.66	0.58
10:A:506:A:H5''	25:X:49:LYS:HG2	1.86	0.58
10:A:1497:U:H5''	10:A:1553:A:H61	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:130:LYS:NZ	26:Y:83:VAL:O	2.37	0.58
10:A:307:G:H2'	10:A:308:A:C8	2.39	0.58
10:A:1502:G:H1	10:A:1548:A:H2	1.51	0.58
10:A:2081:A:H2'	10:A:2082:C:C6	2.39	0.58
18:Q:25:ALA:O	18:Q:29:ILE:HG13	2.04	0.58
20:S:71:GLU:OE1	31:N:78:ARG:NH1	2.36	0.58
16:O:79:LEU:HG	16:O:119:VAL:HB	1.86	0.58
10:A:1077:G:H21	10:A:1149:G:H1	1.52	0.57
10:A:200:A:N6	10:A:210:G:H1'	2.19	0.57
10:A:258:U:H2'	10:A:259:G:C8	2.40	0.57
10:A:1439:A:H2'	10:A:1440:C:C6	2.39	0.57
1:O:70:ARG:NH1	10:A:395:G:OP1	2.37	0.57
10:A:2671:G:C5	10:A:2672:H2U:H51	2.38	0.57
12:D:95:TYR:CE1	12:D:101:LYS:HE2	2.40	0.57
22:U:44:ASN:O	22:U:44:ASN:ND2	2.35	0.57
3:11:40:ASN:O	3:11:155:ASN:N	2.32	0.57
11:B:60:C:H2'	11:B:61:A:H8	1.69	0.57
10:A:2369:C:H2'	10:A:2370:A:H8	1.70	0.57
10:A:307:G:H2'	10:A:308:A:H8	1.67	0.57
18:Q:107:ASN:ND2	38:Q:201:HOH:O	2.38	0.57
17:P:118:LEU:HD12	17:P:131:PHE:HE2	1.69	0.57
10:A:1557:U:H3	10:A:1579:G:H22	1.52	0.56
10:A:2795:U:H2'	10:A:2880:U:H5''	1.87	0.56
10:A:169:A:H2'	10:A:170:C:C6	2.41	0.56
10:A:1875:A:N6	10:A:1885:G:O2'	2.38	0.56
10:A:2646:U:H4'	10:A:2733:G:O2'	2.05	0.56
3:11:32:PRO:HB3	3:11:162:ALA:HB2	1.88	0.56
9:8:36:ARG:NH1	10:A:2743:G:OP1	2.38	0.56
10:A:572:G:O2'	10:A:573:G:OP2	2.22	0.56
23:V:29:THR:O	23:V:120:ASN:ND2	2.36	0.56
8:7:52:LYS:HA	8:7:55:GLU:HG3	1.87	0.56
10:A:1033:A:H2'	10:A:1034:A:C8	2.41	0.56
10:A:1382:A:H2'	10:A:1383:A:C8	2.41	0.56
28:h:4:ILE:HB	28:h:37:VAL:HG12	1.87	0.56
29:15:21:ILE:HG12	29:15:36:GLU:HG3	1.88	0.56
10:A:2107:U:H3	10:A:2202:G:H1	1.53	0.56
25:X:84:ILE:HD13	25:X:96:ARG:HG2	1.86	0.56
3:11:71:THR:N	3:11:89:GLY:O	2.35	0.56
10:A:1883:G:H2'	10:A:1884:A:C8	2.41	0.56
26:Y:96:THR:HG23	26:Y:98:GLU:H	1.68	0.56
10:A:305:U:H2'	10:A:306:A:C4	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:396:U:H5	10:A:424:A:N7	2.03	0.56
10:A:1520:G:H1	10:A:1533:C:H42	1.54	0.56
10:A:1538:U:H5''	10:A:1539:C:H5'	1.89	0.55
10:A:883:U:H2'	10:A:884:U:C6	2.42	0.55
17:P:51:ARG:HG2	17:P:51:ARG:NH1	2.22	0.55
10:A:1811:A:H2'	10:A:1812:A:C8	2.40	0.55
10:A:2328:A:H2'	10:A:2329:A:C8	2.41	0.55
10:A:2329:A:H2'	10:A:2330:U:C6	2.41	0.55
29:15:48:PHE:CE2	30:13:102:LEU:HD21	2.41	0.55
10:A:1901:G:HO2'	10:A:2236:G:HO2'	1.54	0.55
10:A:328:A:O2'	10:A:330:G:N7	2.34	0.55
10:A:553:G:H2'	10:A:553:G:N3	2.21	0.55
10:A:2074:C:H2'	10:A:2075:C:C6	2.41	0.55
9:8:7:VAL:HG22	9:8:38:GLY:HA2	1.88	0.55
15:M:140:GLN:N	15:M:140:GLN:OE1	2.40	0.55
31:N:12:ASP:OD1	31:N:12:ASP:N	2.38	0.55
10:A:2292:U:H2'	10:A:2293:A:C8	2.41	0.55
10:A:2347:A:H4'	10:A:2384:A:OP2	2.07	0.55
14:F:196:THR:HG22	14:F:198:ARG:H	1.72	0.55
8:7:59:LYS:O	8:7:64:LEU:N	2.35	0.55
22:U:1:MET:HE2	22:U:44:ASN:HB3	1.90	0.54
10:A:1483:G:N2	10:A:1483:G:OP2	2.39	0.54
10:A:2431:A:N3	10:A:2431:A:H2'	2.22	0.54
10:A:2657:U:H5	10:A:2666:A:N7	2.06	0.54
3:11:33:VAL:H	3:11:161:SER:HB3	1.72	0.54
10:A:1438:U:H2'	10:A:1439:A:C8	2.42	0.54
10:A:1310:G:H2'	10:A:1311:C:C6	2.43	0.54
10:A:603:C:H2'	10:A:604:U:C6	2.42	0.54
9:8:4:ARG:O	9:8:37:GLN:HG2	2.08	0.54
10:A:311:U:H3	10:A:365:A:H62	1.55	0.54
10:A:352:C:OP1	38:A:3101:HOH:O	2.17	0.54
12:D:6:LEU:HD13	12:D:16:LYS:HD3	1.89	0.54
10:A:1464:A:H61	10:A:1595:C:H5	1.55	0.54
10:A:2234:U:H2'	10:A:2235:G:C8	2.42	0.54
30:13:93:GLY:HA2	30:13:95:ARG:HH12	1.71	0.54
15:M:79:TYR:CE2	15:M:94:PRO:HG3	2.42	0.54
31:N:98:ILE:HG12	31:N:116:LEU:HD12	1.89	0.54
10:A:2096:U:H2'	10:A:2097:U:C6	2.43	0.53
26:Y:107:VAL:HA	26:Y:142:LEU:HB2	1.90	0.53
3:11:64:THR:HG23	3:11:66:GLN:H	1.73	0.53
15:M:103:GLU:H	15:M:103:GLU:CD	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:267:A:H2'	10:A:268:A:C8	2.42	0.53
10:A:1416:C:H2'	10:A:1417:C:C6	2.44	0.53
10:A:2450:OMU:HM21	10:A:2502:5OC:HN4A	1.74	0.53
23:V:30:SER:OG	23:V:33:LYS:HD2	2.08	0.53
26:Y:102:VAL:HG22	26:Y:132:LYS:HB3	1.91	0.53
10:A:267:A:H2'	10:A:268:A:H8	1.72	0.53
10:A:1176:U:H4'	10:A:1177:A:O4'	2.08	0.53
30:13:105:LEU:HB3	30:13:107:LEU:HD13	1.91	0.53
9:8:31:PRO:HB2	10:A:2528:C:H5''	1.90	0.53
11:B:34:C:H2'	11:B:35:C:H6	1.74	0.53
10:A:611:U:H2'	10:A:612:A:H8	1.72	0.52
10:A:831:U:H2'	10:A:832:U:C6	2.44	0.52
10:A:2287:A:H4'	10:A:2288:A:O4'	2.09	0.52
12:D:8:PRO:HB3	12:D:14:ARG:HG3	1.90	0.52
30:13:87:LEU:HB2	30:13:135:ILE:HB	1.90	0.52
10:A:630:A:H2'	10:A:631:A:C8	2.44	0.52
10:A:2843:G:N2	10:A:2846:A:OP2	2.36	0.52
30:13:84:LYS:HE2	30:13:138:GLU:HG3	1.91	0.52
10:A:1544:U:H3'	10:A:1545:G:H8	1.73	0.52
10:A:676:A:H2'	10:A:677:A:C8	2.44	0.52
10:A:1055:G:N2	10:A:1056:U:O4	2.42	0.52
29:15:15:ARG:HA	29:15:41:ASN:HD21	1.75	0.52
19:R:79:ALA:HB1	19:R:84:ILE:HB	1.91	0.52
10:A:2062:G:H4'	13:E:148:ALA:O	2.10	0.52
17:P:30:GLY:HA2	17:P:107:GLU:HB2	1.91	0.52
10:A:1063:A:H2'	10:A:1064:A:C8	2.44	0.51
31:N:22:ILE:HD11	31:N:42:SER:HB2	1.91	0.51
8:7:26:HIS:CE1	8:7:48:SER:HB2	2.45	0.51
10:A:1388:A:H2'	10:A:1389:A:C8	2.46	0.51
10:A:1424:U:H2'	10:A:1425:A:O4'	2.10	0.51
31:N:68:GLU:OE1	31:N:78:ARG:NH2	2.38	0.51
11:B:58:C:H2'	11:B:59:C:C6	2.46	0.51
10:A:320:C:H2'	10:A:321:U:C6	2.46	0.51
10:A:545:G:H2'	10:A:546:C:C6	2.46	0.51
10:A:602:C:H2'	10:A:603:C:C6	2.46	0.51
10:A:610:U:H2'	10:A:611:U:C6	2.46	0.51
14:F:17:VAL:HG21	14:F:125:VAL:HG11	1.93	0.51
10:A:1462:G:H2'	10:A:1463:A:C8	2.46	0.51
10:A:1500:A:H2'	10:A:1501:A:C8	2.46	0.51
25:X:43:MET:SD	25:X:63:GLU:HG3	2.51	0.51
10:A:1799:C:H2'	10:A:1800:A:C5	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2681:C:H5'	13:E:194:PRO:HA	1.93	0.51
26:Y:124:LEU:HD21	26:Y:127:ARG:HA	1.93	0.51
11:B:27:A:H2'	11:B:28:C:C6	2.46	0.50
12:D:91:ILE:HD12	12:D:103:TYR:CD1	2.46	0.50
10:A:385:G:H2'	10:A:386:A:C8	2.46	0.50
10:A:53:A:H62	10:A:79:A:H61	1.59	0.50
10:A:1554:C:H42	10:A:1583:A:H61	1.58	0.50
10:A:2244:U:H2'	10:A:2245:U:C6	2.45	0.50
22:U:25:ILE:HD12	22:U:96:THR:HG21	1.93	0.50
10:A:537:A:H2'	10:A:538:C:C6	2.47	0.50
10:A:2293:A:N1	10:A:2341:U:H5	2.10	0.50
10:A:2330:U:H2'	10:A:2331:G:C8	2.47	0.50
21:T:106:PHE:O	21:T:110:VAL:HG23	2.12	0.50
10:A:1554:C:N4	10:A:1583:A:H61	2.10	0.50
3:11:71:THR:HG21	10:A:2313:C:O3'	2.12	0.50
10:A:611:U:H2'	10:A:612:A:C8	2.46	0.50
10:A:819:G:H5'	10:A:820:G:OP1	2.12	0.50
10:A:1403:U:H2'	10:A:1404:C:C6	2.47	0.50
15:M:17:THR:OG1	15:M:46:LYS:NZ	2.44	0.50
10:A:308:A:H2'	10:A:309:U:C6	2.46	0.50
11:B:23:A:H3'	11:B:24:U:C6	2.47	0.50
17:P:66:VAL:HG22	17:P:104:PHE:CE2	2.45	0.50
29:15:17:TYR:HA	29:15:40:PRO:HA	1.94	0.50
3:11:95:ARG:NH1	11:B:43:A:O4'	2.45	0.49
10:A:258:U:H2'	10:A:259:G:H8	1.74	0.49
10:A:1746:U:H4'	10:A:2844:U:H3	1.77	0.49
12:D:30:GLU:O	12:D:34:VAL:HG22	2.12	0.49
10:A:1184:U:H2'	10:A:1185:U:C6	2.48	0.49
25:X:73:VAL:HG11	25:X:105:ILE:HD13	1.93	0.49
10:A:1392:C:O2'	10:A:1818:A:N3	2.42	0.49
10:A:2247:G:H2'	10:A:2248:A:H8	1.75	0.49
15:M:92:PHE:HE2	15:M:97:PHE:CZ	2.30	0.49
22:U:14:VAL:HG13	22:U:100:VAL:HG21	1.94	0.49
27:Z:26:TYR:O	27:Z:29:GLU:HG3	2.13	0.49
10:A:2762:A:OP1	29:15:31:ALA:HB3	2.11	0.49
10:A:314:G:OP1	25:X:3:LYS:NZ	2.31	0.49
10:A:464:A:H2'	10:A:465:G:C8	2.47	0.49
11:B:49:G:H2'	11:B:50:A:C8	2.48	0.49
18:Q:112:PHE:HE2	18:Q:114:GLU:HG2	1.77	0.49
10:A:437:C:H2'	10:A:438:A:H8	1.77	0.49
10:A:2383:G:H4'	10:A:2384:A:OP2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1480:U:H2'	10:A:1481:C:C6	2.48	0.49
10:A:715:A:H2'	10:A:716:A:C8	2.48	0.49
10:A:1210:A:H2'	10:A:1211:U:C6	2.48	0.49
10:A:1149:G:H2'	10:A:1150:A:C8	2.48	0.49
10:A:255:C:H2'	10:A:256:U:C6	2.47	0.48
10:A:1511:U:H3	10:A:1540:A:H61	1.61	0.48
10:A:1696:G:N7	38:A:3132:HOH:O	2.35	0.48
10:A:2515:U:H2'	10:A:2516:C:C6	2.48	0.48
12:D:154:MET:HB3	12:D:176:MET:HE1	1.95	0.48
10:A:250:A:N1	10:A:283:G:O2'	2.44	0.48
10:A:1518:C:H4'	10:A:1519:G:OP1	2.12	0.48
12:D:210:ARG:HG2	12:D:210:ARG:HH11	1.78	0.48
23:V:10:GLU:O	23:V:14:GLU:HG2	2.13	0.48
10:A:2307:U:H3'	10:A:2308:G:H5'	1.96	0.48
10:A:1509:G:H22	10:A:1542:A:H2	1.60	0.48
12:D:21:PHE:HB3	12:D:24:ILE:HD12	1.95	0.48
31:N:106:LEU:HD22	31:N:113:ILE:HG21	1.94	0.48
12:D:244:PRO:HG2	12:D:253:LYS:HD3	1.95	0.48
25:X:82:THR:HG21	25:X:98:ALA:HB1	1.95	0.48
30:13:11:ILE:HD12	30:13:48:GLY:C	2.38	0.48
6:4:2:ALA:HB3	10:A:2066:G:N2	2.29	0.48
10:A:143:A:H61	10:A:151:C:N4	2.11	0.48
10:A:2453:C:H2'	10:A:2454:A:C8	2.49	0.48
19:R:22:THR:HG22	19:R:23:GLN:H	1.79	0.48
10:A:2592:C:H2'	10:A:2593:G:C8	2.48	0.48
10:A:2011:G:H2'	10:A:2012:C:C6	2.49	0.48
24:W:23:ARG:HG2	24:W:23:ARG:HH11	1.79	0.48
10:A:592:G:H2'	10:A:2040:A:N7	2.29	0.47
10:A:616:U:H2'	10:A:617:U:C6	2.49	0.47
10:A:875:G:C4	10:A:876:H2U:H62	2.49	0.47
10:A:2313:C:H2'	10:A:2314:C:H6	1.80	0.47
20:S:82:GLU:OE2	20:S:82:GLU:HA	2.14	0.47
10:A:1557:U:H3	10:A:1579:G:H1	1.60	0.47
10:A:2201:G:H2'	10:A:2202:G:N7	2.29	0.47
10:A:2450:OMU:HM21	10:A:2502:5OC:O5	2.15	0.47
18:Q:112:PHE:CE2	18:Q:114:GLU:HG2	2.49	0.47
15:M:92:PHE:CE2	15:M:97:PHE:CZ	3.03	0.47
10:A:204:A:O2'	10:A:207:A:N1	2.42	0.47
10:A:324:U:H2'	10:A:325:G:O4'	2.15	0.47
10:A:437:C:H2'	10:A:438:A:C8	2.50	0.47
11:B:26:C:H2'	11:B:27:A:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:45:ARG:O	18:Q:49:GLU:HG3	2.15	0.47
22:U:7:ILE:HG21	22:U:22:VAL:HG11	1.97	0.47
10:A:2084:U:H2'	10:A:2085:U:C6	2.49	0.47
10:A:2318:C:H2'	10:A:2319:G:O4'	2.15	0.47
26:Y:22:ILE:HG23	26:Y:27:GLN:HB2	1.96	0.47
28:h:7:GLU:C	28:h:15:LYS:HB2	2.39	0.47
6:4:11:THR:HG22	6:4:15:LYS:HD2	1.96	0.47
10:A:2039:G:N1	10:A:2043:A:OP2	2.28	0.47
19:R:72:GLY:HA2	19:R:103:LEU:HD23	1.97	0.47
24:W:6:LYS:HG3	24:W:7:PRO:O	2.15	0.47
1:0:13:MET:HG2	1:0:29:PHE:HB2	1.97	0.47
10:A:308:A:H2'	10:A:309:U:H6	1.79	0.47
10:A:738:U:H2'	10:A:739:G:O4'	2.15	0.47
10:A:1388:A:H2'	10:A:1389:A:H8	1.80	0.47
17:P:4:PRO:HD3	17:P:69:PHE:CE2	2.49	0.47
26:Y:64:THR:HG22	26:Y:70:SER:OG	2.14	0.47
8:7:32:ILE:HG22	8:7:35:LYS:HD2	1.97	0.47
10:A:141:G:H2'	10:A:142:A:C8	2.50	0.47
10:A:961:A:H2'	10:A:962:A:C8	2.50	0.46
29:15:22:LYS:HG2	29:15:47:PHE:CE2	2.50	0.46
7:6:41:LYS:NZ	7:6:47:GLU:OE1	2.48	0.46
10:A:255:C:H2'	10:A:256:U:H6	1.79	0.46
10:A:876:H2U:H52	10:A:877:U:C5	2.49	0.46
1:0:4:ILE:CD1	1:0:11:LYS:HB3	2.45	0.46
5:2:10:ARG:HD3	5:2:10:ARG:HA	1.80	0.46
10:A:414:A:H1'	10:A:434:G:O4'	2.16	0.46
10:A:1153:U:H2'	10:A:1154:U:C6	2.49	0.46
10:A:1617:A:H2'	10:A:1618:G:O4'	2.15	0.46
10:A:2242:A:H2'	10:A:2243:G:C8	2.50	0.46
10:A:2749:A:OP1	30:13:70:SER:OG	2.21	0.46
14:F:157:LEU:HD11	14:F:164:VAL:HG11	1.96	0.46
10:A:160:A:H2'	10:A:161:C:C6	2.50	0.46
10:A:618:U:H2'	10:A:619:G:H8	1.80	0.46
10:A:670:U:H2'	10:A:671:C:C6	2.51	0.46
20:S:113:ARG:HG3	20:S:113:ARG:HH11	1.81	0.46
1:0:40:TRP:CE2	1:0:43:GLN:HG2	2.50	0.46
6:4:10:LYS:NZ	10:A:540:C:OP2	2.37	0.46
6:4:24:MET:HG3	6:4:25:PRO:HD2	1.96	0.46
10:A:57:G:H2'	10:A:58:C:O4'	2.15	0.46
11:B:12:U:OP2	11:B:68:C:O2'	2.33	0.46
4:12:12:PRO:HA	4:12:27:ARG:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:116:C:H2'	10:A:117:C:C6	2.50	0.46
13:E:53:VAL:O	13:E:77:ARG:N	2.47	0.46
22:U:65:LEU:HD11	22:U:99:LEU:HB2	1.98	0.46
10:A:1518:C:H42	10:A:1535:C:N4	2.14	0.46
10:A:2308:G:OP2	10:A:2308:G:H3'	2.15	0.46
20:S:86:VAL:HG11	20:S:89:TYR:CE1	2.50	0.46
25:X:8:LYS:HA	25:X:26:VAL:HG12	1.98	0.46
27:Z:30:MET:HE3	27:Z:30:MET:HB3	1.76	0.46
2:1:3:ILE:HD13	10:A:66:U:H5''	1.97	0.46
10:A:1412:A:H4'	10:A:1413:G:O5'	2.16	0.45
10:A:1508:A:H2'	10:A:1509:G:O4'	2.16	0.45
23:V:75:TRP:CE2	23:V:88:LEU:HD21	2.52	0.45
23:V:93:ILE:HG13	23:V:124:ILE:HG13	1.98	0.45
25:X:35:ARG:HB3	25:X:65:PRO:HB2	1.97	0.45
7:6:39:ARG:NH2	10:A:491:G:N7	2.52	0.45
8:7:8:SER:O	8:7:12:LYS:HG3	2.16	0.45
10:A:958:G:H2'	10:A:959:A:C8	2.51	0.45
10:A:1271:C:H2'	10:A:1272:U:C6	2.52	0.45
10:A:1345:U:H2'	10:A:1346:G:H8	1.81	0.45
10:A:1518:C:H42	10:A:1535:C:H42	1.64	0.45
11:B:54:U:H4'	11:B:55:A:O5'	2.16	0.45
12:D:72:ASP:OD1	12:D:118:SER:OG	2.32	0.45
25:X:59:ILE:H	25:X:59:ILE:HD12	1.81	0.45
10:A:38:A:H4'	10:A:39:A:H5''	1.98	0.45
10:A:322:A:H2'	10:A:323:C:C6	2.52	0.45
10:A:1185:U:H2'	10:A:1186:A:C8	2.52	0.45
10:A:1608:A:H2'	10:A:1609:A:C8	2.52	0.45
29:15:19:LYS:HB2	30:13:111:HIS:CD2	2.51	0.45
6:4:48:TYR:CE2	6:4:53:LEU:HD13	2.52	0.45
10:A:612:A:H2'	10:A:613:C:C6	2.51	0.45
10:A:1345:U:H2'	10:A:1346:G:C8	2.51	0.45
10:A:1437:A:N1	10:A:1631:U:H5	2.15	0.45
10:A:2456:G:H2'	10:A:2457:C:C6	2.52	0.45
18:Q:97:ILE:O	18:Q:98:LEU:HD23	2.16	0.45
30:13:121:VAL:HA	30:13:138:GLU:O	2.17	0.45
11:B:86:A:O2'	11:B:87:G:H8	1.99	0.45
12:D:123:ALA:O	12:D:128:ASN:ND2	2.44	0.45
21:T:83:LEU:HD23	21:T:113:VAL:HG11	1.98	0.45
24:W:37:ILE:O	24:W:41:VAL:HG23	2.17	0.45
31:N:98:ILE:HG12	31:N:116:LEU:CD1	2.47	0.45
10:A:516:G:H2'	10:A:517:A:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:703:A:H2'	10:A:705:A:H62	1.81	0.45
10:A:1834:U:H2'	10:A:1835:C:C6	2.52	0.45
11:B:23:A:H5''	11:B:24:U:H5	1.82	0.45
20:S:65:SER:OG	31:N:101:PRO:HG3	2.17	0.45
30:13:24:VAL:HG11	30:13:72:ILE:HD13	1.99	0.45
10:A:562:G:O6	10:A:576:U:H5	1.99	0.45
10:A:629:U:C5	10:A:651:G:C5	3.04	0.45
26:Y:75:LEU:HD23	26:Y:75:LEU:HA	1.74	0.45
10:A:143:A:N6	10:A:151:C:H42	2.10	0.45
10:A:700:A:H2'	10:A:701:G:C8	2.51	0.45
10:A:2628:G:O2'	10:A:2782:A:N1	2.39	0.45
12:D:78:VAL:HG21	12:D:110:LEU:HD21	1.98	0.45
23:V:72:VAL:O	23:V:76:GLU:HG3	2.16	0.45
3:11:105:ARG:HD3	4:12:28:SER:HB2	1.99	0.45
10:A:343:G:H2'	10:A:344:C:C6	2.52	0.45
10:A:2407:C:H6	10:A:2407:C:H5'	1.81	0.45
10:A:2741:A:H2'	10:A:2742:A:C8	2.52	0.45
12:D:53:TYR:HA	12:D:217:ARG:HB2	1.99	0.45
5:2:21:ARG:HD3	10:A:883:U:O2'	2.17	0.44
10:A:636:U:H2'	10:A:637:A:C8	2.52	0.44
10:A:1711:C:O2	13:E:133:THR:HB	2.17	0.44
10:A:1883:G:H2'	10:A:1884:A:H8	1.82	0.44
11:B:24:U:H2'	11:B:25:C:H6	1.82	0.44
10:A:116:C:H2'	10:A:117:C:H6	1.82	0.44
10:A:2047:C:H2'	10:A:2048:G:C8	2.52	0.44
10:A:2745:G:O3'	30:13:150:MET:HE3	2.17	0.44
2:1:30:ILE:HD11	24:W:4:ILE:HG22	1.99	0.44
10:A:1459:G:H2'	10:A:1460:G:H8	1.82	0.44
10:A:1534:G:O2'	10:A:1535:C:OP2	2.34	0.44
10:A:2530:G:OP2	30:13:176:LYS:NZ	2.40	0.44
9:8:23:LEU:HD12	9:8:38:GLY:HA3	1.98	0.44
10:A:795:A:H2'	10:A:796:A:O4'	2.17	0.44
10:A:1502:G:N1	10:A:1548:A:H2	2.15	0.44
8:7:42:ARG:O	8:7:45:THR:HG22	2.17	0.44
10:A:32:G:H2'	10:A:33:A:O4'	2.18	0.44
10:A:125:C:H42	10:A:132:C:H42	1.64	0.44
10:A:1425:A:O2'	10:A:1426:U:O5'	2.33	0.44
17:P:65:TRP:HB2	17:P:105:GLU:HB2	1.99	0.44
22:U:65:LEU:HD12	22:U:97:GLU:HG2	2.00	0.44
30:13:90:VAL:HG12	30:13:164:LYS:HA	1.98	0.44
10:A:2671:G:H2'	10:A:2672:H2U:H62	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:19:ILE:HG21	19:R:90:ASP:HB3	1.99	0.44
5:2:31:LEU:HD12	5:2:31:LEU:HA	1.76	0.44
11:B:60:C:H2'	11:B:61:A:C8	2.51	0.44
11:B:107:C:H2'	11:B:108:G:H8	1.82	0.44
22:U:3:VAL:HG12	22:U:42:VAL:HG22	2.00	0.44
10:A:2729:U:H2'	10:A:2730:C:C6	2.53	0.44
9:8:23:LEU:HB2	9:8:38:GLY:HA3	1.99	0.43
10:A:2805:A:H2'	10:A:2807:A:N7	2.32	0.43
12:D:118:SER:HB2	12:D:129:ALA:HB3	2.00	0.43
23:V:92:ARG:HB2	23:V:125:TYR:HB2	2.00	0.43
28:h:5:LEU:HD11	28:h:19:VAL:HG11	2.00	0.43
30:13:75:MET:O	30:13:79:VAL:HG22	2.18	0.43
30:13:89:LEU:HD23	30:13:166:VAL:HG13	1.99	0.43
2:1:7:LYS:HZ3	2:1:56:VAL:HG22	1.83	0.43
10:A:778:G:O2'	10:A:1695:C:OP1	2.32	0.43
10:A:1599:U:H2'	10:A:1600:C:C6	2.54	0.43
10:A:2752:G:H4'	30:13:4:ILE:HG12	1.99	0.43
11:B:34:C:H2'	11:B:35:C:C6	2.52	0.43
19:R:63:SER:O	19:R:67:ILE:HG13	2.18	0.43
21:T:28:ARG:NH1	21:T:38:THR:OG1	2.50	0.43
3:11:132:LEU:HD12	3:11:133:GLY:N	2.33	0.43
10:A:1956:U:H2'	10:A:1957:C:C6	2.53	0.43
10:A:2003:U:H4'	13:E:133:THR:OG1	2.18	0.43
10:A:2456:G:H2'	10:A:2457:C:H6	1.83	0.43
16:O:86:SER:HB2	16:O:94:ILE:HD11	2.00	0.43
18:Q:70:LEU:HD12	18:Q:76:LEU:HD22	2.00	0.43
21:T:104:GLU:CD	21:T:104:GLU:H	2.26	0.43
10:A:663:A:OP1	16:O:67:LYS:NZ	2.51	0.43
10:A:694:A:H2'	10:A:695:C:C6	2.53	0.43
10:A:2848:A:H2'	10:A:2849:A:C8	2.53	0.43
10:A:185:A:H2'	10:A:186:C:O4'	2.18	0.43
10:A:669:G:H2'	10:A:670:U:C6	2.53	0.43
10:A:1677:A:H2'	10:A:1678:G:O4'	2.18	0.43
10:A:2342:G:H2'	10:A:2343:C:O4'	2.18	0.43
10:A:228:G:H2'	10:A:229:A:C8	2.53	0.43
10:A:1459:G:H2'	10:A:1460:G:C8	2.53	0.43
10:A:1740:G:H2'	10:A:1741:A:C8	2.54	0.43
11:B:13:A:H3'	11:B:14:A:H8	1.82	0.43
20:S:27:THR:HB	20:S:85:THR:HG22	2.00	0.43
30:13:151:LYS:HB2	30:13:151:LYS:HE2	1.76	0.43
31:N:1:MET:HE3	31:N:1:MET:HB2	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:542:U:H2'	10:A:543:C:C6	2.53	0.43
10:A:771:U:H2'	10:A:772:C:C6	2.54	0.43
10:A:1942:A:H2'	10:A:1943:G:O4'	2.19	0.43
10:A:2378:A:H2'	10:A:2379:A:C8	2.54	0.43
12:D:95:TYR:CZ	12:D:101:LYS:HE2	2.54	0.43
10:A:656:G:H2'	10:A:657:A:O4'	2.19	0.43
10:A:1609:A:H2'	10:A:1610:C:O2	2.19	0.43
10:A:2203:A:H2'	10:A:2204:U:C6	2.54	0.43
30:13:54:ARG:NH2	30:13:57:ASP:OD2	2.50	0.43
26:Y:22:ILE:HD13	26:Y:43:ILE:HG12	2.01	0.43
29:15:19:LYS:HB2	30:13:111:HIS:HD2	1.84	0.43
10:A:537:A:H2'	10:A:538:C:H6	1.83	0.43
10:A:1726:A:H2'	10:A:1727:C:O4'	2.19	0.43
10:A:2098:A:H2'	10:A:2099:C:C6	2.54	0.43
10:A:2709:U:H2'	10:A:2710:G:H8	1.84	0.43
10:A:2852:A:H3'	10:A:2853:A:H4'	2.01	0.43
29:15:45:LYS:HD2	29:15:45:LYS:N	2.34	0.43
10:A:141:G:H1	10:A:153:U:H3	1.67	0.42
10:A:2688:U:H2'	10:A:2689:U:O4'	2.19	0.42
11:B:15:C:H2'	11:B:16:G:O4'	2.18	0.42
20:S:94:ARG:HB3	20:S:94:ARG:NH1	2.34	0.42
24:W:4:ILE:HD11	24:W:41:VAL:HG22	2.01	0.42
27:Z:15:GLU:OE2	27:Z:15:GLU:HA	2.19	0.42
10:A:1344:C:H3'	38:A:3206:HOH:O	2.19	0.42
20:S:47:VAL:HG22	20:S:61:VAL:HG22	2.01	0.42
10:A:1860:U:H2'	10:A:1861:U:O4'	2.20	0.42
16:O:71:ARG:HG3	16:O:72:VAL:N	2.34	0.42
16:O:125:VAL:HG21	16:O:138:ILE:HD13	2.01	0.42
10:A:619:G:O2'	16:O:11:GLY:O	2.26	0.42
10:A:1627:U:H2'	10:A:1628:G:H8	1.84	0.42
10:A:2034:U:H2'	10:A:2035:C:C6	2.54	0.42
10:A:2057:C:H2'	10:A:2058:A:H8	1.85	0.42
12:D:72:ASP:OD2	12:D:119:GLY:HA2	2.19	0.42
10:A:790:U:H2'	10:A:791:U:C6	2.55	0.42
10:A:886:U:H2'	10:A:887:C:C6	2.55	0.42
10:A:1632:U:H2'	10:A:1633:A:C8	2.55	0.42
12:D:131:PRO:HA	12:D:188:CYS:O	2.19	0.42
13:E:150:SER:O	13:E:153:ALA:HB2	2.19	0.42
10:A:867:U:H2'	10:A:868:G:C8	2.55	0.42
28:h:26:GLY:O	28:h:31:ILE:HG13	2.19	0.42
10:A:997:C:O2'	10:A:2274:A:N3	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:186:LEU:HD11	20:S:3:PHE:HB3	2.02	0.42
21:T:91:ASN:OD1	21:T:91:ASN:C	2.62	0.42
2:1:27:GLN:HG3	2:1:31:ASN:ND2	2.35	0.42
10:A:207:A:H2'	10:A:208:G:O4'	2.20	0.42
10:A:2679:G:H2'	10:A:2680:A:C8	2.55	0.42
18:Q:65:ILE:HD13	18:Q:65:ILE:HA	1.87	0.42
21:T:14:ARG:HG2	21:T:32:TRP:CE2	2.54	0.42
30:13:144:LEU:O	30:13:148:VAL:HG23	2.19	0.42
10:A:1216:G:H5'	22:U:85:TYR:CE1	2.54	0.42
10:A:2346:G:N3	10:A:2382:A:H2'	2.34	0.42
11:B:86:A:O2'	11:B:87:G:P	2.78	0.42
10:A:121:C:H2'	10:A:122:A:C8	2.55	0.42
10:A:553:G:N2	38:A:3248:HOH:O	2.53	0.42
10:A:637:A:H2	10:A:644:A:N7	2.18	0.42
10:A:884:U:H2'	10:A:885:A:H8	1.83	0.42
10:A:2555:U:H2'	10:A:2556:U:C6	2.54	0.42
12:D:10:THR:HG22	12:D:12:GLY:H	1.85	0.42
30:13:11:ILE:HD11	30:13:50:ILE:HG12	2.02	0.42
10:A:363:A:N3	10:A:364:C:N4	2.57	0.41
10:A:1438:U:H2'	10:A:1439:A:H8	1.84	0.41
10:A:1607:A:H2'	10:A:1608:A:C8	2.54	0.41
10:A:1757:A:H2'	10:A:1758:G:C8	2.55	0.41
10:A:2234:U:H2'	10:A:2235:G:H8	1.82	0.41
10:A:250:A:H8	10:A:251:C:C6	2.38	0.41
10:A:268:A:H2'	10:A:269:A:C8	2.54	0.41
10:A:1522:G:N7	10:A:1529:A:C6	2.88	0.41
10:A:1614:C:H2'	10:A:1615:U:C6	2.55	0.41
10:A:1718:G:H2'	10:A:1719:U:C6	2.55	0.41
16:O:49:GLY:HA3	16:O:58:GLN:HE22	1.84	0.41
10:A:72:A:H2	10:A:91:A:H2	1.68	0.41
10:A:884:U:H2'	10:A:885:A:C8	2.55	0.41
10:A:898:G:H2'	10:A:899:C:C6	2.56	0.41
10:A:964:U:O4	10:A:1211:U:O2'	2.34	0.41
10:A:1555:A:H2'	10:A:1556:G:C8	2.55	0.41
10:A:1589:G:H2'	10:A:1590:U:O4'	2.20	0.41
10:A:2657:U:H6	10:A:2657:U:H2'	1.71	0.41
10:A:2817:C:H2'	10:A:2882:U:O2'	2.20	0.41
11:B:105:G:N2	19:R:47:GLY:O	2.44	0.41
5:2:5:LYS:HB2	5:2:57:VAL:O	2.21	0.41
10:A:387:G:H2'	10:A:388:C:O4'	2.20	0.41
10:A:1040:C:H2'	10:A:1041:G:N2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1719:U:H2'	10:A:1720:C:C6	2.55	0.41
17:P:54:VAL:HG22	17:P:58:MET:HE2	2.02	0.41
10:A:601:A:H2'	10:A:602:C:C6	2.56	0.41
10:A:2330:U:H2'	10:A:2331:G:H8	1.83	0.41
10:A:2514:G:H2'	10:A:2515:U:C6	2.55	0.41
10:A:2637:U:H4'	13:E:81:GLU:OE1	2.21	0.41
17:P:12:GLN:HE21	17:P:72:LYS:HE2	1.86	0.41
17:P:35:LYS:HD3	17:P:100:GLY:HA2	2.02	0.41
17:P:109:VAL:HG23	17:P:114:ALA:HB2	2.03	0.41
30:13:167:LYS:HE2	30:13:173:ILE:HG13	2.03	0.41
3:11:39:ILE:HB	3:11:92:VAL:HG12	2.02	0.41
10:A:88:U:O2	10:A:90:G:N1	2.53	0.41
10:A:1863:A:H2'	10:A:1864:G:O4'	2.20	0.41
14:F:206:LEU:HD12	14:F:206:LEU:HA	1.90	0.41
21:T:88:ILE:HD13	22:U:52:SER:HA	2.03	0.41
26:Y:163:GLU:C	26:Y:165:LEU:H	2.28	0.41
30:13:164:LYS:HB3	30:13:164:LYS:HE3	1.86	0.41
31:N:112:LYS:O	31:N:116:LEU:HG	2.21	0.41
10:A:160:A:H2'	10:A:161:C:H6	1.86	0.41
10:A:134:G:H3'	10:A:135:A:C8	2.56	0.41
3:11:97:GLU:HA	3:11:100:TYR:HB2	2.03	0.41
10:A:186:C:H2'	10:A:187:C:C6	2.56	0.41
10:A:511:G:N2	10:A:513:A:H3'	2.36	0.41
10:A:553:G:C8	10:A:2045:G:H4'	2.55	0.41
10:A:881:U:C2	10:A:882:G:C8	3.09	0.41
10:A:1151:U:H2'	10:A:1152:U:O4'	2.21	0.41
10:A:1509:G:N1	10:A:1542:A:H2	2.13	0.41
10:A:2538:U:H2'	10:A:2539:C:C6	2.56	0.41
12:D:200:HIS:O	12:D:203:GLU:HG2	2.21	0.41
14:F:156:VAL:C	14:F:157:LEU:HD23	2.46	0.41
15:M:79:TYR:HE2	15:M:94:PRO:HG3	1.85	0.41
16:O:48:ILE:HD13	16:O:48:ILE:HA	1.89	0.41
24:W:62:LYS:HD3	24:W:62:LYS:HA	1.73	0.41
8:7:19:THR:OG1	10:A:682:G:OP1	2.28	0.41
10:A:428:G:OP1	10:A:428:G:H8	2.04	0.41
10:A:603:C:H2'	10:A:604:U:H6	1.86	0.41
10:A:1519:G:H4'	10:A:1520:G:OP1	2.18	0.41
11:B:23:A:N3	11:B:23:A:H2'	2.35	0.41
15:M:92:PHE:HE2	15:M:97:PHE:HZ	1.68	0.41
18:Q:59:THR:O	18:Q:63:ARG:HG3	2.21	0.41
22:U:18:ARG:HD2	22:U:18:ARG:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:4:ILE:HD11	5:2:56:ILE:HD12	2.02	0.40
10:A:28:C:H2'	10:A:29:U:H6	1.86	0.40
10:A:1480:U:H2'	10:A:1481:C:H6	1.86	0.40
10:A:2066:G:O6	10:A:2067:6MA:H13	2.21	0.40
10:A:2299:A:H2'	10:A:2300:G:O4'	2.21	0.40
10:A:2468:C:H2'	10:A:2469:A:O4'	2.21	0.40
24:W:23:ARG:HG2	24:W:23:ARG:NH1	2.36	0.40
2:1:18:LEU:O	2:1:22:VAL:HG23	2.20	0.40
3:11:155:ASN:C	3:11:156:ILE:HD12	2.46	0.40
10:A:1034:A:H2'	10:A:1035:G:O4'	2.21	0.40
10:A:2469:A:HO2'	10:A:2470:A:H8	1.69	0.40
23:V:69:ARG:HG2	23:V:69:ARG:NH1	2.33	0.40
3:11:64:THR:HG21	3:11:92:VAL:HG21	2.02	0.40
10:A:248:A:C2	10:A:392:U:H4'	2.57	0.40
10:A:1690:A:O2'	13:E:117:PHE:O	2.32	0.40
10:A:1952:C:OP2	10:A:1953:U:O2'	2.34	0.40
10:A:253:G:H2'	10:A:254:G:H8	1.87	0.40
10:A:2619:G:C4	10:A:2620:H2U:H62	2.57	0.40
10:A:2699:U:H2'	10:A:2700:A:C8	2.56	0.40
11:B:99:G:H2'	11:B:100:A:C8	2.57	0.40
25:X:87:ARG:NH2	25:X:102:GLY:O	2.47	0.40
10:A:119:G:H2'	10:A:120:U:C6	2.55	0.40
10:A:897:A:H2'	10:A:898:G:C8	2.57	0.40
10:A:2515:U:H2'	10:A:2516:C:H6	1.85	0.40
16:O:75:LYS:HA	16:O:76:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	75/79 (95%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
3	11	160/186 (86%)	145 (91%)	15 (9%)	0	100	100
4	12	46/85 (54%)	34 (74%)	12 (26%)	0	100	100
5	2	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
6	4	55/61 (90%)	52 (94%)	3 (6%)	0	100	100
7	6	46/50 (92%)	46 (100%)	0	0	100	100
8	7	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
9	8	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
12	D	270/274 (98%)	264 (98%)	6 (2%)	0	100	100
13	E	202/205 (98%)	190 (94%)	11 (5%)	1 (0%)	24	46
14	F	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
15	M	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
16	O	142/148 (96%)	137 (96%)	5 (4%)	0	100	100
17	P	140/144 (97%)	135 (96%)	5 (4%)	0	100	100
18	Q	121/160 (76%)	119 (98%)	2 (2%)	0	100	100
19	R	106/114 (93%)	102 (96%)	4 (4%)	0	100	100
20	S	111/121 (92%)	109 (98%)	2 (2%)	0	100	100
21	T	111/115 (96%)	111 (100%)	0	0	100	100
22	U	102/105 (97%)	89 (87%)	13 (13%)	0	100	100
23	V	125/134 (93%)	123 (98%)	2 (2%)	0	100	100
24	W	88/97 (91%)	86 (98%)	2 (2%)	0	100	100
25	X	91/106 (86%)	89 (98%)	2 (2%)	0	100	100
26	Y	172/192 (90%)	158 (92%)	14 (8%)	0	100	100
27	Z	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
28	h	50/179 (28%)	44 (88%)	6 (12%)	0	100	100
29	15	33/49 (67%)	30 (91%)	3 (9%)	0	100	100
30	13	175/183 (96%)	170 (97%)	5 (3%)	0	100	100
31	N	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
32	5	41/62 (66%)	41 (100%)	0	0	100	100
All	All	3222/3640 (88%)	3081 (96%)	140 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	E	152	PRO

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	
1	0	59/66 (89%)	59 (100%)	0	100	100
2	1	43/56 (77%)	42 (98%)	1 (2%)	44	71
3	11	66/161 (41%)	62 (94%)	4 (6%)	17	37
4	12	5/77 (6%)	5 (100%)	0	100	100
5	2	47/53 (89%)	45 (96%)	2 (4%)	26	51
6	4	39/50 (78%)	39 (100%)	0	100	100
7	6	37/40 (92%)	36 (97%)	1 (3%)	39	67
8	7	55/58 (95%)	55 (100%)	0	100	100
9	8	29/35 (83%)	28 (97%)	1 (3%)	32	60
12	D	208/218 (95%)	199 (96%)	9 (4%)	26	51
13	E	152/163 (93%)	146 (96%)	6 (4%)	28	55
14	F	147/177 (83%)	140 (95%)	7 (5%)	23	47
15	M	113/128 (88%)	110 (97%)	3 (3%)	39	67
16	O	97/117 (83%)	94 (97%)	3 (3%)	35	63
17	P	107/118 (91%)	104 (97%)	3 (3%)	38	66
18	Q	96/129 (74%)	95 (99%)	1 (1%)	68	86
19	R	59/90 (66%)	53 (90%)	6 (10%)	7	15
20	S	79/107 (74%)	77 (98%)	2 (2%)	42	69
21	T	90/93 (97%)	89 (99%)	1 (1%)	65	84
22	U	80/92 (87%)	77 (96%)	3 (4%)	29	56
23	V	105/113 (93%)	105 (100%)	0	100	100
24	W	66/85 (78%)	62 (94%)	4 (6%)	17	37
25	X	67/89 (75%)	62 (92%)	5 (8%)	12	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Y	91/159 (57%)	82 (90%)	9 (10%)	7	16
27	Z	59/69 (86%)	57 (97%)	2 (3%)	32	60
28	h	30/146 (20%)	29 (97%)	1 (3%)	33	61
29	15	26/42 (62%)	25 (96%)	1 (4%)	29	56
30	13	133/159 (84%)	125 (94%)	8 (6%)	17	37
31	N	88/100 (88%)	86 (98%)	2 (2%)	44	71
32	5	35/58 (60%)	35 (100%)	0	100	100
All	All	2308/3048 (76%)	2223 (96%)	85 (4%)	31	57

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	57	LEU
3	11	27	SER
3	11	38	VAL
3	11	39	ILE
3	11	152	LEU
5	2	42	SER
5	2	55	LEU
7	6	1	MET
9	8	4	ARG
12	D	32	SER
12	D	37	LYS
12	D	81	ILE
12	D	139	THR
12	D	160	SER
12	D	165	THR
12	D	186	SER
12	D	220	ASN
12	D	229	ASP
13	E	7	LYS
13	E	46	SER
13	E	97	VAL
13	E	104	ASP
13	E	197	LYS
13	E	199	SER
14	F	13	THR
14	F	17	VAL
14	F	60	SER
14	F	100	LYS

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Mol	Chain	Res	Type
14	F	115	SER
14	F	140	LYS
14	F	164	VAL
15	M	4	LEU
15	M	94	PRO
15	M	147	ILE
16	O	94	ILE
16	O	105	VAL
16	O	125	VAL
17	P	28	SER
17	P	31	SER
17	P	132	VAL
18	Q	48	VAL
19	R	20	SER
19	R	22	THR
19	R	52	SER
19	R	55	SER
19	R	85	SER
19	R	92	ASN
20	S	56	LYS
20	S	78	SER
21	T	86	ASN
22	U	34	VAL
22	U	61	VAL
22	U	96	THR
24	W	44	MET
24	W	48	LYS
24	W	75	GLU
24	W	77	SER
25	X	7	LYS
25	X	10	ASP
25	X	23	SER
25	X	94	LEU
25	X	101	SER
26	Y	45	SER
26	Y	56	PRO
26	Y	58	ILE
26	Y	82	PRO
26	Y	105	VAL
26	Y	107	VAL
26	Y	123	SER
26	Y	136	SER

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Mol	Chain	Res	Type
26	Y	157	VAL
27	Z	9	SER
27	Z	18	SER
28	h	37	VAL
29	15	26	SER
30	13	23	ILE
30	13	42	THR
30	13	60	ILE
30	13	80	SER
30	13	119	LYS
30	13	121	VAL
30	13	149	CYS
30	13	154	SER
31	N	20	LEU
31	N	28	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	6	GLN
2	1	45	HIS
5	2	19	GLN
6	4	37	HIS
8	7	31	HIS
9	8	35	GLN
12	D	134	ASN
12	D	239	GLN
12	D	243	HIS
13	E	36	GLN
15	M	72	ASN
15	M	89	GLN
16	O	35	HIS
17	P	141	ASN
18	Q	16	HIS
19	R	97	HIS
20	S	17	HIS
21	T	7	HIS
22	U	78	HIS
22	U	89	ASN
23	V	18	GLN
23	V	120	ASN
26	Y	27	GLN

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Mol	Chain	Res	Type
27	Z	12	ASN
29	15	35	GLN
32	5	49	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2492/2882 (86%)	322 (12%)	21 (0%)
11	B	99/109 (90%)	21 (21%)	1 (1%)
All	All	2591/2991 (86%)	343 (13%)	22 (0%)

All (343) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	23	A
10	A	52	A
10	A	60	A
10	A	63	A
10	A	64	G
10	A	80	C
10	A	90	G
10	A	106	A
10	A	107	A
10	A	108	U
10	A	113	C
10	A	122	A
10	A	123	G
10	A	142	A
10	A	174	A
10	A	177	A
10	A	183	U
10	A	184	U
10	A	193	G
10	A	194	A
10	A	200	A
10	A	206	A
10	A	226	G
10	A	272	C
10	A	278	A
10	A	279	A
10	A	280	U

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Mol	Chain	Res	Type
10	A	281	A
10	A	306	A
10	A	307	G
10	A	329	A
10	A	347	G
10	A	348	A
10	A	356	G
10	A	365	A
10	A	386	A
10	A	387	G
10	A	389	A
10	A	396	U
10	A	409	G
10	A	427	U
10	A	428	G
10	A	429	G
10	A	434	G
10	A	435	C
10	A	450	U
10	A	480	A
10	A	504	G
10	A	513	A
10	A	519	G
10	A	528	A
10	A	531	C
10	A	552	A
10	A	554	C
10	A	555	G
10	A	561	A
10	A	572	G
10	A	585	G
10	A	595	U
10	A	596	A
10	A	597	A
10	A	609	G
10	A	625	A
10	A	658	A
10	A	665	G
10	A	668	A
10	A	669	G
10	A	676	A
10	A	721	U

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Mol	Chain	Res	Type
10	A	765	A
10	A	773	G
10	A	781	H2U
10	A	782	U
10	A	783	G
10	A	799	A
10	A	810	G
10	A	811	G
10	A	817	A
10	A	819	G
10	A	820	G
10	A	840	G
10	A	847	C
10	A	862	U
10	A	863	U
10	A	880	A
10	A	881	U
10	A	882	G
10	A	891	A
10	A	893	G
10	A	901	A
10	A	911	U
10	A	944	A
10	A	946	C
10	A	974	A
10	A	978	A
10	A	979	G
10	A	986	G
10	A	994	G
10	A	1007	G
10	A	1029	G
10	A	1045	U
10	A	1046	A
10	A	1068	A
10	A	1069	G
10	A	1074	G
10	A	1158	A
10	A	1163	U
10	A	1164	A
10	A	1168	C
10	A	1177	A
10	A	1203	U

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Mol	Chain	Res	Type
10	A	1204	A
10	A	1205	G
10	A	1210	A
10	A	1234	G
10	A	1251	G
10	A	1252	G
10	A	1253	C
10	A	1267	G
10	A	1285	G
10	A	1300	G
10	A	1301	A
10	A	1305	A
10	A	1329	A
10	A	1330	A
10	A	1387	U
10	A	1394	A
10	A	1402	U
10	A	1403	U
10	A	1408	U
10	A	1412	A
10	A	1413	G
10	A	1414	A
10	A	1416	C
10	A	1420	U
10	A	1422	A
10	A	1425	A
10	A	1426	U
10	A	1447	C
10	A	1448	G
10	A	1449	A
10	A	1458	C
10	A	1483	G
10	A	1484	A
10	A	1491	A
10	A	1519	G
10	A	1520	G
10	A	1521	G
10	A	1522	G
10	A	1523	U
10	A	1524	A
10	A	1525	G
10	A	1527	C

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Mol	Chain	Res	Type
10	A	1530	A
10	A	1531	U
10	A	1532	C
10	A	1533	C
10	A	1534	G
10	A	1535	C
10	A	1536	C
10	A	1537	C
10	A	1538	U
10	A	1539	C
10	A	1540	A
10	A	1544	U
10	A	1552	G
10	A	1581	U
10	A	1584	A
10	A	1586	G
10	A	1588	C
10	A	1591	A
10	A	1592	A
10	A	1603	A
10	A	1606	A
10	A	1613	G
10	A	1615	U
10	A	1618	G
10	A	1629	U
10	A	1630	G
10	A	1643	U
10	A	1644	A
10	A	1646	A
10	A	1654	A
10	A	1668	A
10	A	1670	U
10	A	1683	U
10	A	1684	C
10	A	1710	G
10	A	1767	A
10	A	1773	G
10	A	1782	A
10	A	1791	C
10	A	1800	A
10	A	1809	C
10	A	1810	A

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Mol	Chain	Res	Type
10	A	1811	A
10	A	1826	G
10	A	1838	A
10	A	1856	A
10	A	1859	G
10	A	1867	G
10	A	1886	A
10	A	1887	A
10	A	1895	A
10	A	1916	G
10	A	1937	A
10	A	1939	G
10	A	1940	G
10	A	1947	A
10	A	1948	A
10	A	1951	C
10	A	1965	U
10	A	1973	U
10	A	1975	C
10	A	1977	C
10	A	1980	A
10	A	1981	U
10	A	1982	G
10	A	2001	U
10	A	2002	G
10	A	2003	U
10	A	2041	A
10	A	2042	G
10	A	2043	A
10	A	2053	C
10	A	2065	C
10	A	2066	G
10	A	2071	G
10	A	2072	A
10	A	2079	G
10	A	2202	G
10	A	2208	A
10	A	2223	A
10	A	2226	A
10	A	2227	C
10	A	2239	G
10	A	2240	G

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Mol	Chain	Res	Type
10	A	2269	A
10	A	2280	G
10	A	2284	U
10	A	2288	A
10	A	2306	U
10	A	2308	G
10	A	2318	C
10	A	2322	G
10	A	2323	A
10	A	2326	G
10	A	2334	A
10	A	2336	A
10	A	2337	A
10	A	2341	U
10	A	2346	G
10	A	2348	C
10	A	2383	G
10	A	2384	A
10	A	2386	C
10	A	2407	C
10	A	2408	A
10	A	2411	G
10	A	2414	G
10	A	2423	C
10	A	2424	U
10	A	2425	C
10	A	2426	A
10	A	2430	G
10	A	2431	A
10	A	2435	A
10	A	2436	A
10	A	2442	U
10	A	2449	A
10	A	2476	C
10	A	2481	C
10	A	2504	2MA
10	A	2506	G
10	A	2507	U
10	A	2508	C
10	A	2519	A
10	A	2530	G
10	A	2536	G

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Mol	Chain	Res	Type
10	A	2567	A
10	A	2568	G
10	A	2574	C
10	A	2603	A
10	A	2604	G
10	A	2610	U
10	A	2614	U
10	A	2657	U
10	A	2661	A
10	A	2663	A
10	A	2670	U
10	A	2690	U
10	A	2703	G
10	A	2715	G
10	A	2727	C
10	A	2734	U
10	A	2745	G
10	A	2749	A
10	A	2758	A
10	A	2759	A
10	A	2762	A
10	A	2763	C
10	A	2765	A
10	A	2766	A
10	A	2767	G
10	A	2779	A
10	A	2780	U
10	A	2796	A
10	A	2806	A
10	A	2807	A
10	A	2819	U
10	A	2821	A
10	A	2845	A
10	A	2851	U
10	A	2852	A
10	A	2853	A
10	A	2854	G
10	A	2858	A
10	A	2865	C
10	A	2869	U
10	A	2870	A
10	A	2881	U

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Mol	Chain	Res	Type
10	A	2882	U
11	B	4	G
11	B	7	G
11	B	10	U
11	B	14	A
11	B	22	G
11	B	23	A
11	B	24	U
11	B	33	U
11	B	42	G
11	B	44	A
11	B	52	G
11	B	53	U
11	B	55	A
11	B	64	G
11	B	87	G
11	B	92	A
11	B	98	G
11	B	99	G
11	B	101	C
11	B	102	G
11	B	104	C

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	385	G
10	A	781	H2U
10	A	819	G
10	A	862	U
10	A	1412	A
10	A	1425	A
10	A	1482	U
10	A	1519	G
10	A	1520	G
10	A	1521	G
10	A	1522	G
10	A	1523	U
10	A	1526	G
10	A	1529	A
10	A	1530	A
10	A	1532	C

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Mol	Chain	Res	Type
10	A	2407	C
10	A	2431	A
10	A	2475	C
10	A	2757	U
10	A	2761	C
11	B	54	U

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

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$
10	2MA	A	2504	36,10	22,25,26	4.04	9 (40%)	32,37,40	2.72	10 (31%)
10	OMG	A	2252	10	23,26,27	0.52	0	32,38,41	0.47	0
10	H2U	A	876	10	18,21,22	0.55	0	19,30,33	0.83	1 (5%)
10	OMU	A	2450	10	19,22,23	3.06	8 (42%)	25,31,34	1.93	6 (24%)
10	H2U	A	2672	10	18,21,22	0.51	0	19,30,33	0.89	1 (5%)
10	6MA	A	2069	10	21,24,25	0.20	0	27,34,37	0.44	0
10	5MC	A	1935	10	19,22,23	0.49	0	26,32,35	0.59	0
10	OMG	A	2554	10	23,26,27	0.52	0	32,38,41	0.48	0
10	5OC	A	2502	36,10	18,21,22	4.73	14 (77%)	24,30,33	1.33	3 (12%)
10	PSU	A	2606	10	18,21,22	1.13	1 (5%)	21,30,33	1.94	3 (14%)
10	5MU	A	1949	10	19,22,23	0.48	0	27,32,35	0.48	0
10	MA6	A	2068	10	23,26,27	1.42	4 (17%)	33,38,41	3.72	12 (36%)
10	6MA	A	2067	33,10	21,24,25	0.11	0	27,34,37	0.32	0
10	PSU	A	2581	10	18,21,22	1.12	1 (5%)	21,30,33	1.93	4 (19%)
10	5MC	A	1972	10	19,22,23	0.59	0	26,32,35	0.59	0
10	2MG	A	2446	10	23,26,27	0.59	0	33,38,41	0.52	0
10	H2U	A	2620	10	18,21,22	0.63	0	19,30,33	1.04	1 (5%)
10	H2U	A	781	10	18,21,22	0.48	0	19,30,33	1.29	2 (10%)

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
10	2MA	A	2504	36,10	-	3/7/25/26	0/3/3/3
10	OMG	A	2252	10	-	1/9/27/28	0/3/3/3
10	H2U	A	876	10	-	0/7/38/39	0/2/2/2
10	OMU	A	2450	10	-	0/9/27/28	0/2/2/2
10	H2U	A	2672	10	-	0/7/38/39	0/2/2/2
10	6MA	A	2069	10	-	1/9/23/24	0/3/3/3
10	5MC	A	1935	10	-	0/7/25/26	0/2/2/2
10	OMG	A	2554	10	-	0/9/27/28	0/3/3/3
10	5OC	A	2502	36,10	-	5/7/21/22	0/2/2/2
10	PSU	A	2606	10	-	0/7/25/26	0/2/2/2
10	5MU	A	1949	10	-	0/7/25/26	0/2/2/2
10	MA6	A	2068	10	-	0/11/29/30	0/3/3/3
10	6MA	A	2067	33,10	-	2/9/23/24	0/3/3/3
10	PSU	A	2581	10	-	0/7/25/26	0/2/2/2
10	5MC	A	1972	10	-	1/7/25/26	0/2/2/2
10	2MG	A	2446	10	-	2/9/27/28	0/3/3/3
10	H2U	A	2620	10	-	0/7/38/39	0/2/2/2
10	H2U	A	781	10	-	0/7/38/39	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2504	2MA	C4-N3	12.30	1.50	1.34
10	A	2502	5OC	C6-C5	9.15	1.49	1.35
10	A	2502	5OC	C2'-C3'	-8.60	1.31	1.52
10	A	2504	2MA	C2-N3	8.10	1.47	1.34
10	A	2450	OMU	C2-N1	7.21	1.49	1.38
10	A	2504	2MA	C6-N1	6.92	1.44	1.35
10	A	2450	OMU	C2-N3	6.73	1.49	1.38
10	A	2502	5OC	O4'-C1'	-5.94	1.29	1.42
10	A	2502	5OC	C2-N3	5.91	1.48	1.36
10	A	2504	2MA	C2-N1	5.75	1.43	1.34
10	A	2502	5OC	C4-N3	5.69	1.43	1.34
10	A	2450	OMU	C6-C5	5.61	1.48	1.35
10	A	2502	5OC	O4'-C4'	4.86	1.55	1.45
10	A	2504	2MA	C5-C6	4.83	1.54	1.41
10	A	2502	5OC	C4-N4	4.67	1.46	1.34
10	A	2502	5OC	C2'-C1'	4.36	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2502	5OC	C6-N1	4.27	1.45	1.38
10	A	2502	5OC	C2-N1	4.22	1.48	1.40
10	A	2450	OMU	C4-N3	4.05	1.45	1.38
10	A	2068	MA6	C6-N6	3.78	1.47	1.36
10	A	2606	PSU	C6-C5	3.66	1.39	1.35
10	A	2581	PSU	C6-C5	3.50	1.39	1.35
10	A	2504	2MA	CM2-C2	3.48	1.59	1.49
10	A	2504	2MA	C5-N7	-3.48	1.32	1.39
10	A	2502	5OC	C5-C4	3.47	1.49	1.42
10	A	2502	5OC	C5'-C4'	-3.32	1.41	1.51
10	A	2450	OMU	O4-C4	-3.17	1.18	1.24
10	A	2502	5OC	O3'-C3'	3.03	1.49	1.43
10	A	2068	MA6	C5-C4	-2.99	1.33	1.39
10	A	2450	OMU	O2-C2	-2.94	1.17	1.23
10	A	2450	OMU	C6-N1	2.76	1.44	1.38
10	A	2068	MA6	C5-N7	-2.69	1.34	1.39
10	A	2504	2MA	C6-N6	-2.40	1.28	1.34
10	A	2068	MA6	C8-N9	-2.25	1.33	1.37
10	A	2450	OMU	C5-C4	2.24	1.48	1.43
10	A	2502	5OC	O5-C5	2.11	1.39	1.33
10	A	2504	2MA	C8-N7	2.06	1.35	1.31

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2068	MA6	N1-C6-N6	-14.52	99.17	116.86
10	A	2068	MA6	C5-C6-N6	9.94	141.07	125.33
10	A	2504	2MA	C5-C4-N3	-8.81	117.90	127.18
10	A	2068	MA6	N1-C2-N3	-5.80	119.80	128.58
10	A	2504	2MA	N3-C4-N9	5.78	134.33	126.99
10	A	2450	OMU	C4-N3-C2	-5.78	119.44	126.61
10	A	2504	2MA	C1'-N9-C8	5.11	138.44	127.09
10	A	2504	2MA	C4-N9-C1'	-5.10	114.71	126.63
10	A	2606	PSU	N1-C2-N3	5.02	120.47	115.17
10	A	2581	PSU	C4-N3-C2	-4.93	119.58	126.37
10	A	2606	PSU	C4-N3-C2	-4.91	119.61	126.37
10	A	2068	MA6	C5-C4-N3	-4.67	120.29	126.72
10	A	2581	PSU	N1-C2-N3	4.66	120.08	115.17
10	A	2450	OMU	N3-C2-N1	4.33	120.53	114.89
10	A	2068	MA6	N9-C8-N7	-4.24	107.93	113.94
10	A	2068	MA6	C4-C5-C6	3.73	119.77	115.91
10	A	2068	MA6	C2-N1-C6	3.52	120.42	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2450	OMU	C5-C4-N3	3.50	119.70	114.80
10	A	2504	2MA	N9-C8-N7	-3.47	109.01	113.94
10	A	2068	MA6	C2-N3-C4	3.33	119.97	111.83
10	A	2620	H2U	C5-C4-N3	-3.19	113.30	116.69
10	A	2504	2MA	N3-C2-N1	-3.16	120.20	125.77
10	A	2504	2MA	C6-C5-C4	3.08	121.39	117.18
10	A	781	H2U	C5-C4-N3	-3.06	113.44	116.69
10	A	2504	2MA	C5-N7-C8	2.97	108.12	103.45
10	A	2068	MA6	N3-C4-N9	2.93	132.16	127.17
10	A	2068	MA6	C5-N7-C8	2.85	107.93	103.45
10	A	2672	H2U	C5-C4-N3	-2.82	113.68	116.69
10	A	2450	OMU	O4-C4-C5	-2.82	120.30	125.16
10	A	2502	5OC	C4'-O4'-C1'	-2.80	102.86	109.51
10	A	2502	5OC	O5-C5-C4	2.78	120.60	114.82
10	A	2581	PSU	O2-C2-N1	-2.77	119.93	122.79
10	A	2068	MA6	C4-N9-C8	2.46	108.32	105.74
10	A	2581	PSU	O4'-C1'-C2'	2.42	108.50	105.15
10	A	781	H2U	O2-C2-N1	2.35	125.93	123.10
10	A	876	H2U	C5-C4-N3	-2.29	114.25	116.69
10	A	2606	PSU	C6-N1-C2	-2.26	120.59	122.69
10	A	2504	2MA	N6-C6-N1	2.16	119.94	117.03
10	A	2450	OMU	CM2-O2'-C2'	-2.12	109.03	114.47
10	A	2502	5OC	C6-C5-C4	2.10	120.55	117.24
10	A	2450	OMU	O2-C2-N1	-2.07	120.10	122.80
10	A	2068	MA6	C4-C5-N7	-2.03	108.27	110.58
10	A	2504	2MA	C4-C5-N7	-2.00	108.29	110.58

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2067	6MA	N1-C6-N6-C1
10	A	2502	5OC	O4'-C4'-C5'-O5'
10	A	2502	5OC	C3'-C4'-C5'-O5'
10	A	2446	2MG	C3'-C4'-C5'-O5'
10	A	2504	2MA	O4'-C4'-C5'-O5'
10	A	2252	OMG	C1'-C2'-O2'-CM2
10	A	2067	6MA	C5-C6-N6-C1
10	A	2504	2MA	C3'-C4'-C5'-O5'
10	A	2446	2MG	O4'-C4'-C5'-O5'
10	A	1972	5MC	O4'-C4'-C5'-O5'
10	A	2504	2MA	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
10	A	2502	5OC	C2'-C1'-N1-C6
10	A	2502	5OC	O4'-C1'-N1-C6
10	A	2069	6MA	C5-C6-N6-C1
10	A	2502	5OC	O4'-C1'-N1-C2

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	876	H2U	2	0
10	A	2450	OMU	2	0
10	A	2672	H2U	3	0
10	A	2502	5OC	2	0
10	A	2067	6MA	1	0
10	A	2620	H2U	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 173 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
35	62B	A	2901	-	37,38,38	0.51	0	56,60,60	1.35	7 (12%)

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
35	62B	A	2901	-	-	0/12/86/86	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	2901	62B	C18-C12-C13	-4.35	102.27	105.51
35	A	2901	62B	O1-C3-C2	-3.53	120.47	125.52
35	A	2901	62B	C15-C5-C14	-3.34	105.41	108.81
35	A	2901	62B	C28-C23-S1	-3.05	106.04	111.27
35	A	2901	62B	C12-C11-C10	2.45	117.14	114.75
35	A	2901	62B	C1-C9-C10	-2.25	107.94	110.55
35	A	2901	62B	C16-C6-C5	2.07	118.73	115.15

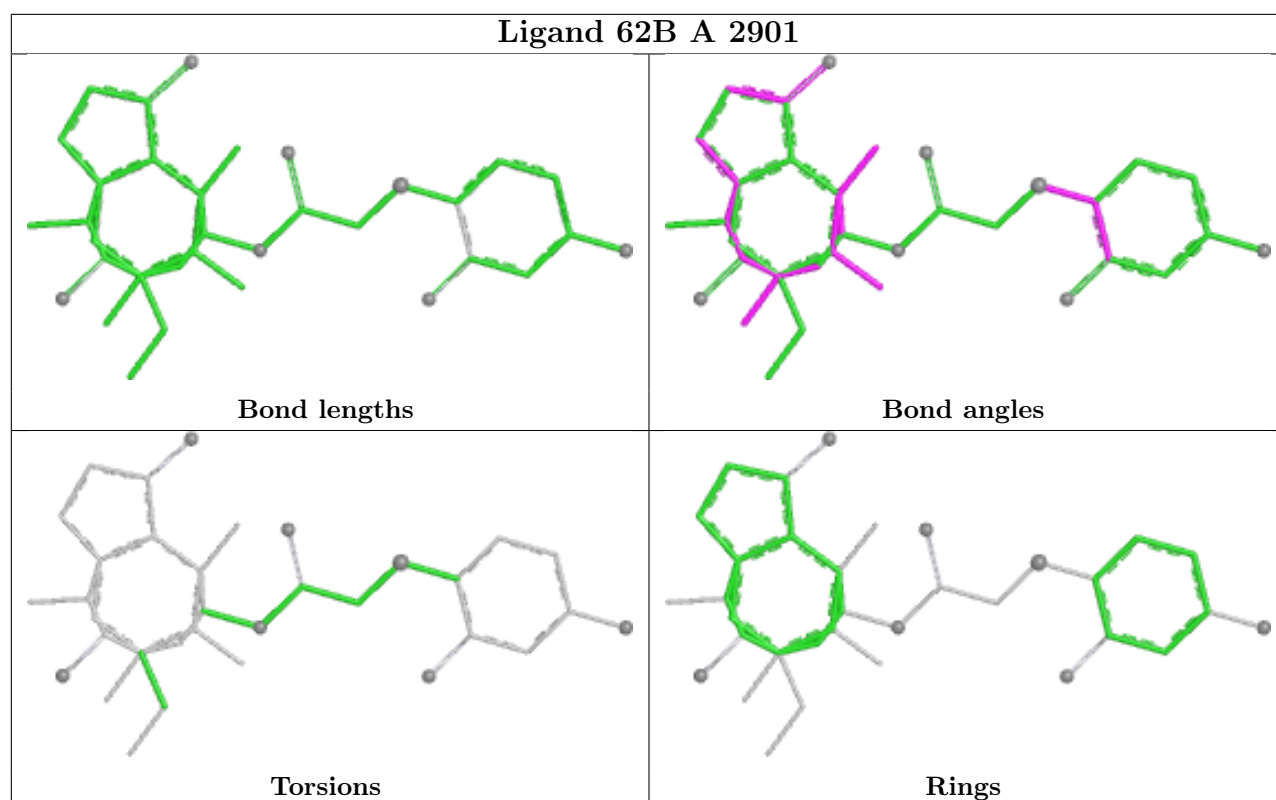
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

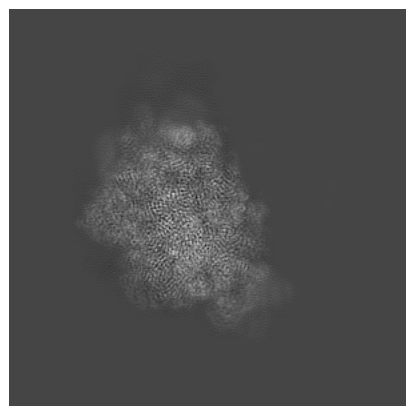
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52635. These allow visual inspection of the internal detail of the map and identification of artifacts.

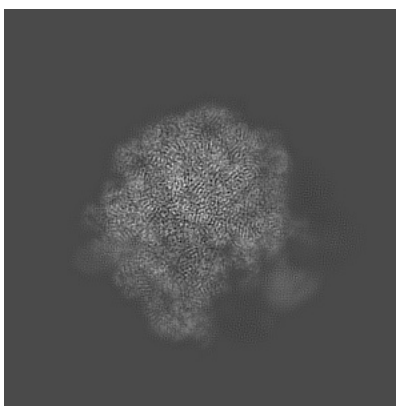
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

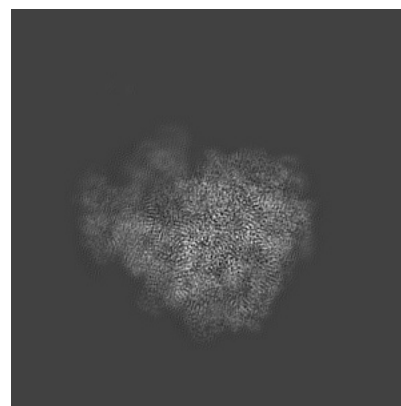
6.1.1 Primary map



X

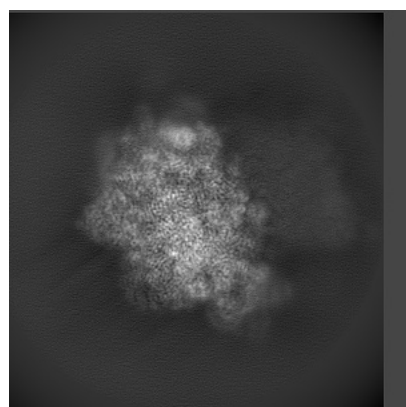


Y

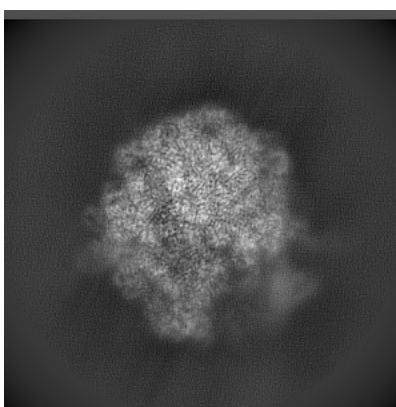


Z

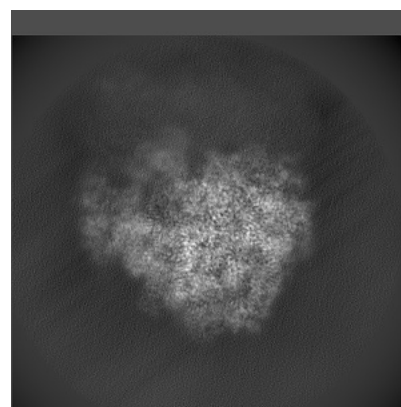
6.1.2 Raw map



X



Y

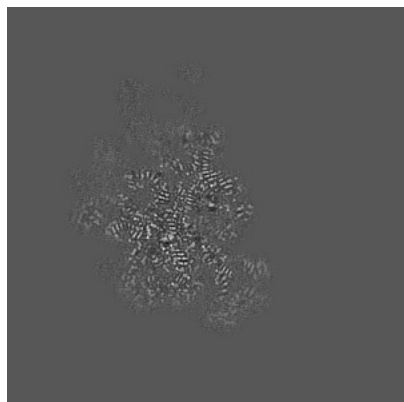


Z

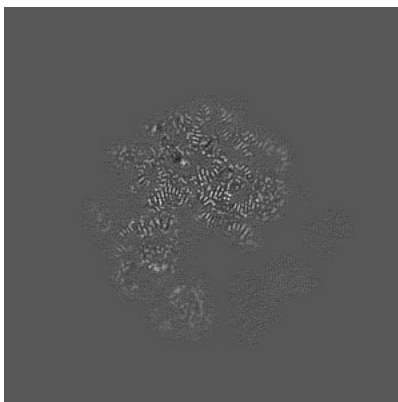
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

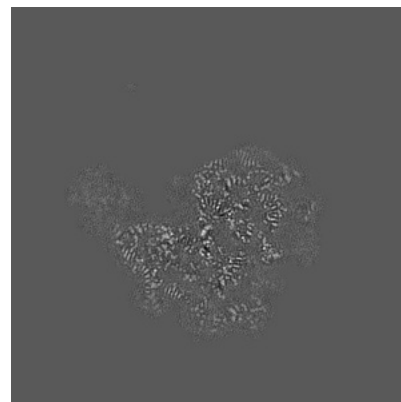
6.2.1 Primary map



X Index: 220

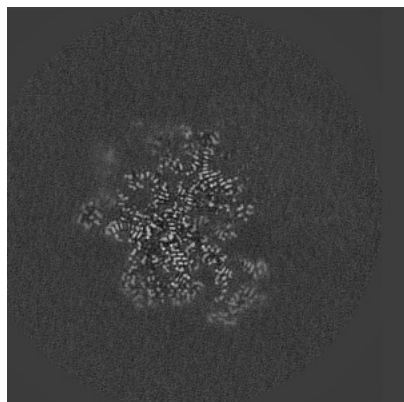


Y Index: 220

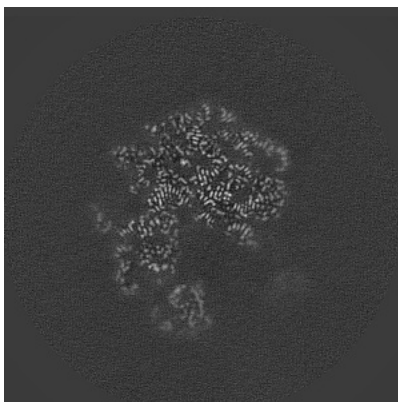


Z Index: 220

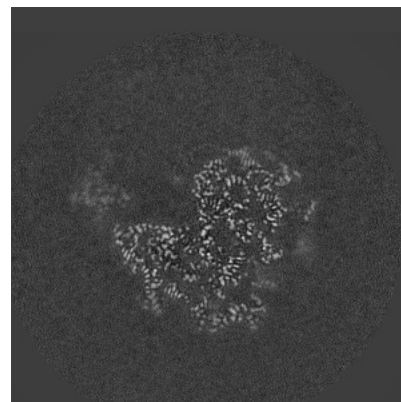
6.2.2 Raw map



X Index: 220



Y Index: 220

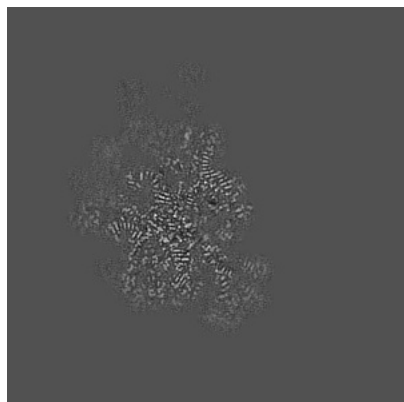


Z Index: 220

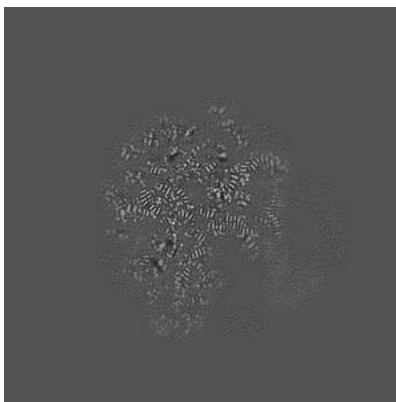
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

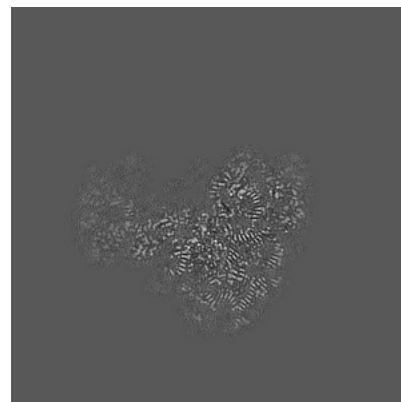
6.3.1 Primary map



X Index: 219

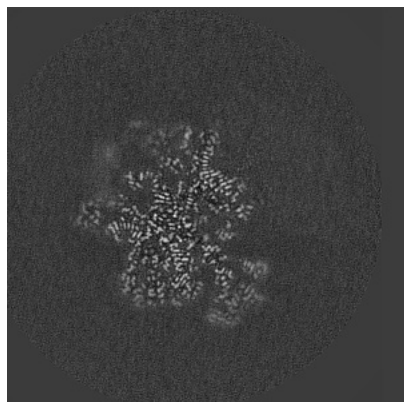


Y Index: 194

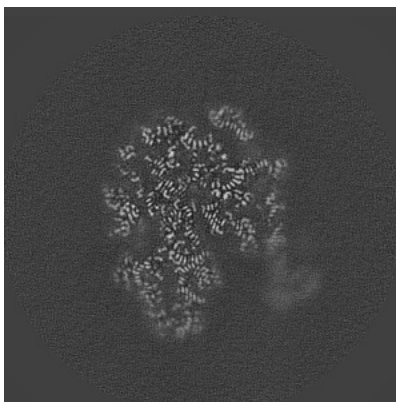


Z Index: 192

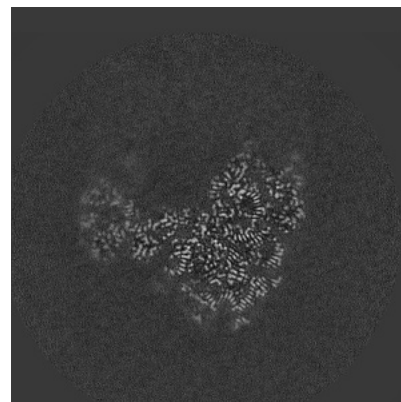
6.3.2 Raw map



X Index: 219



Y Index: 199

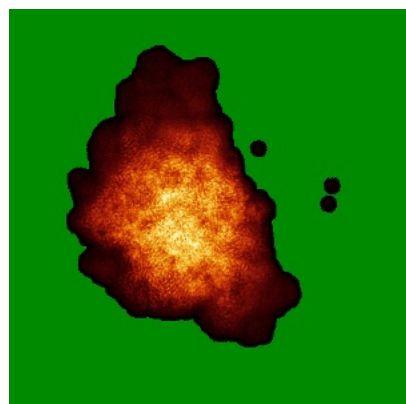


Z Index: 192

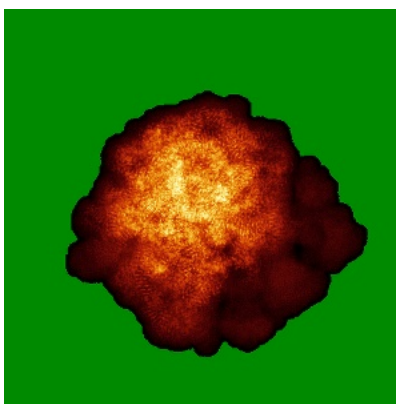
The images above show the largest variance slices of the map in three orthogonal directions.

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

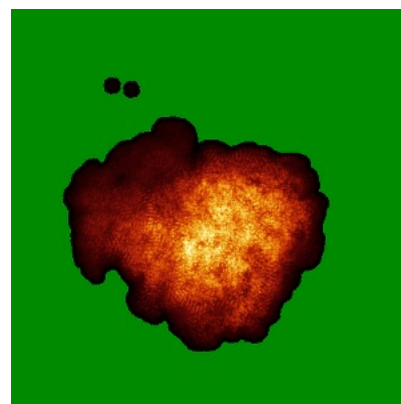
6.4.1 Primary map



X

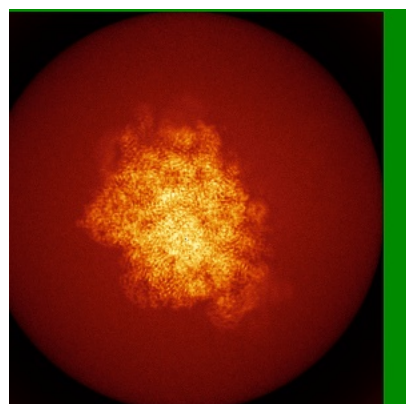


Y

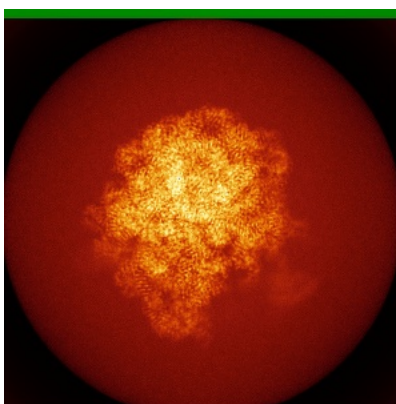


Z

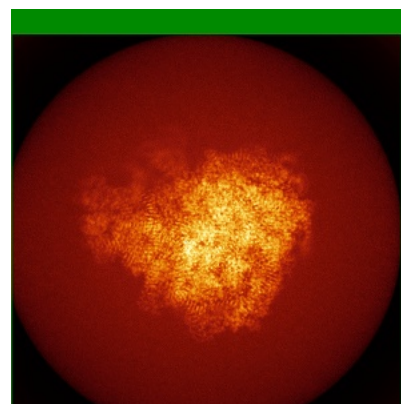
6.4.2 Raw map



X



Y

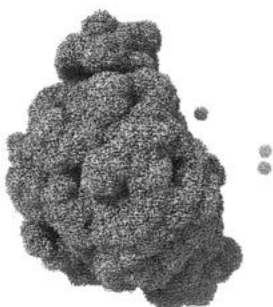


Z

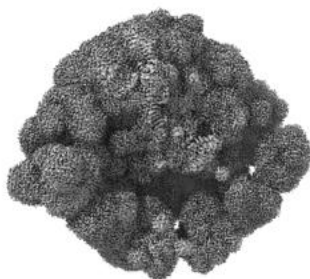
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

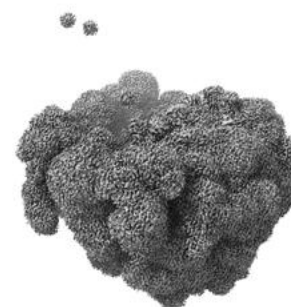
6.5.1 Primary map



X



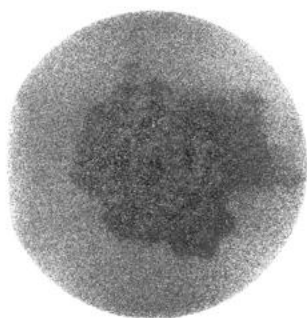
Y



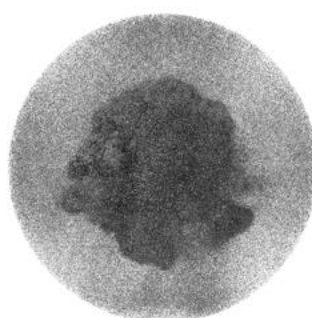
Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

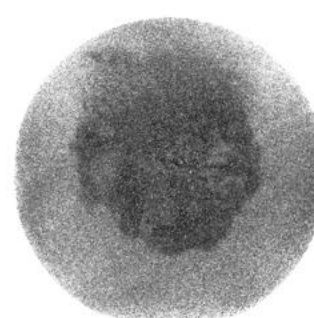
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

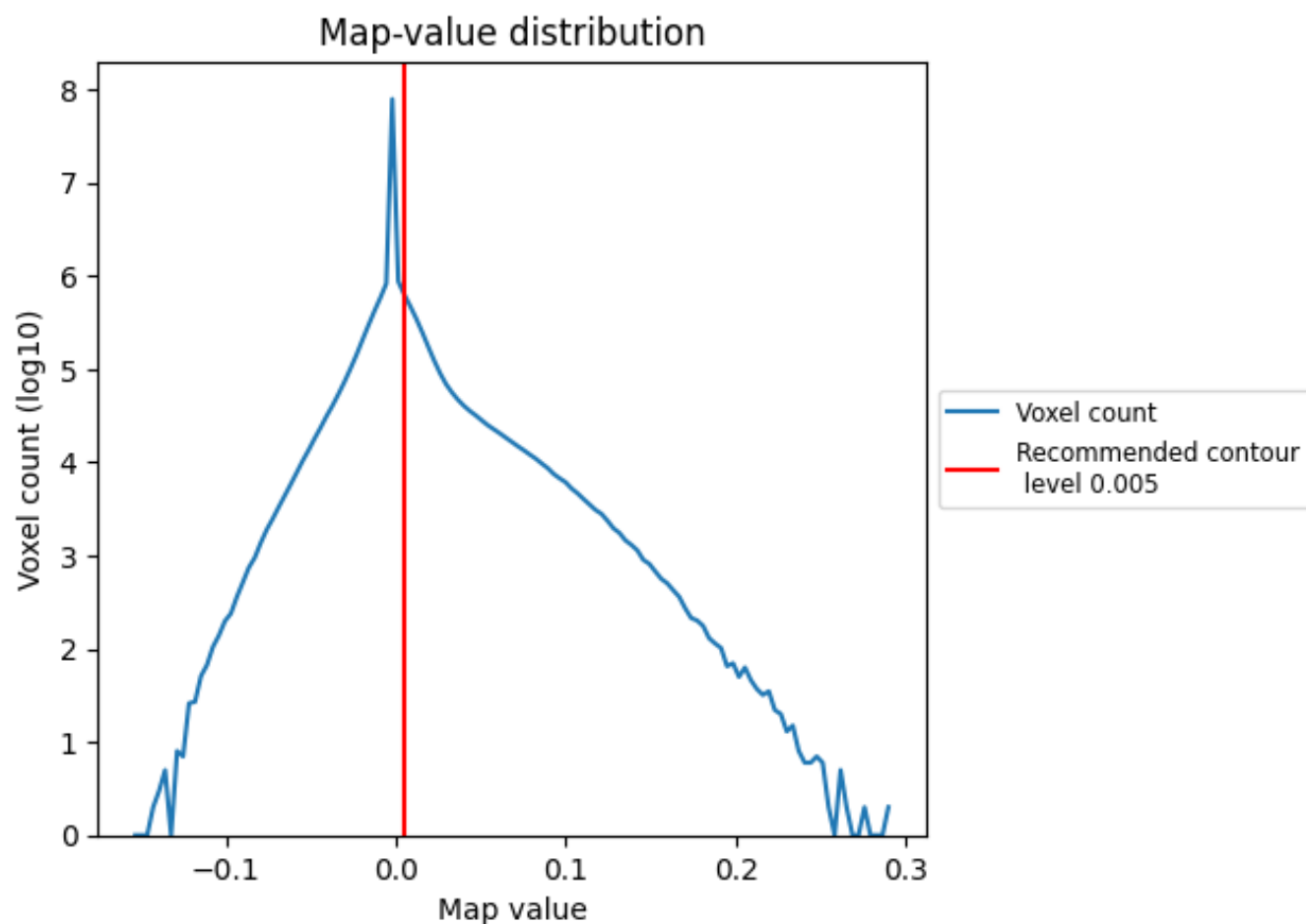
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

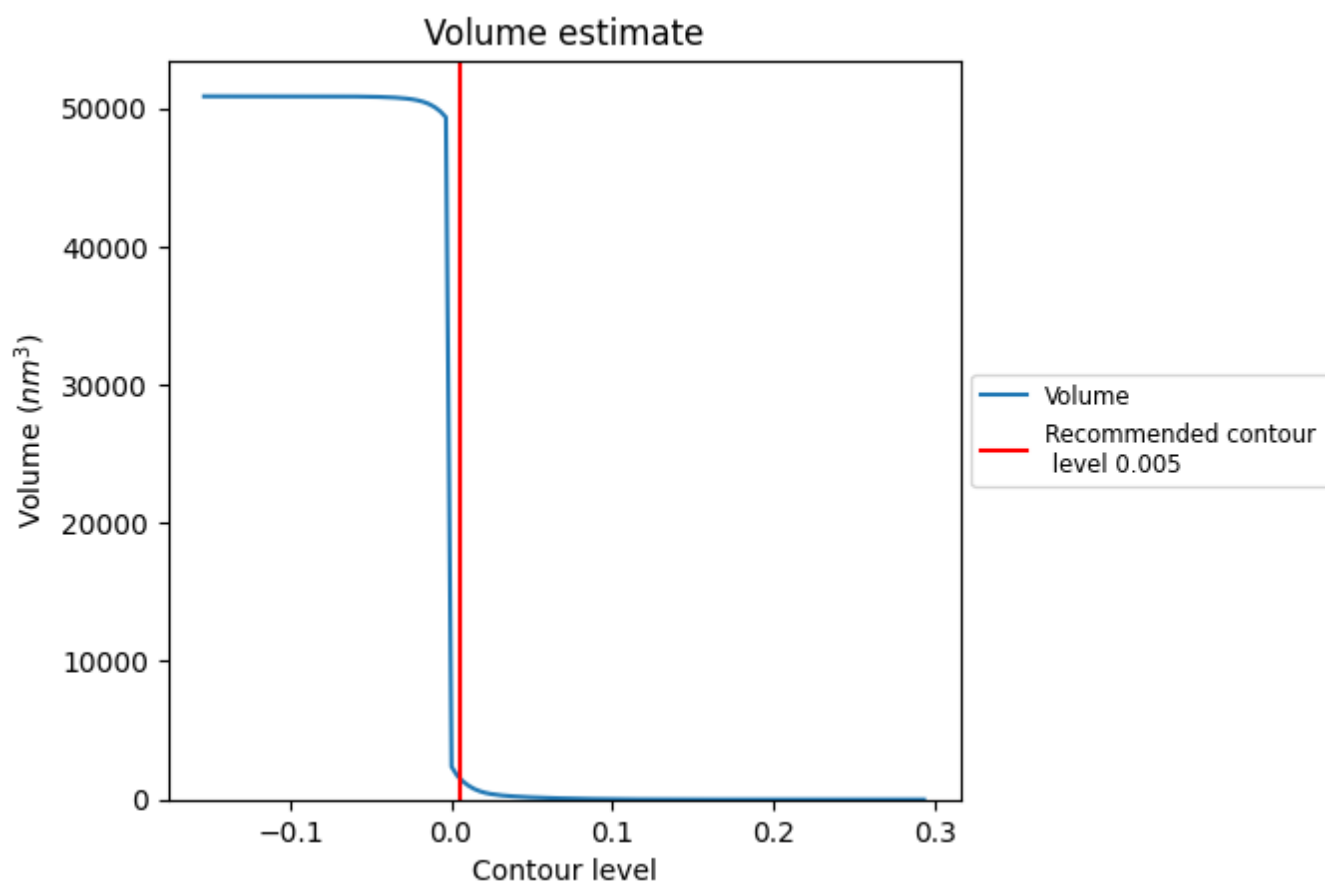
This section contains the results of statistical analysis of the map.

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.

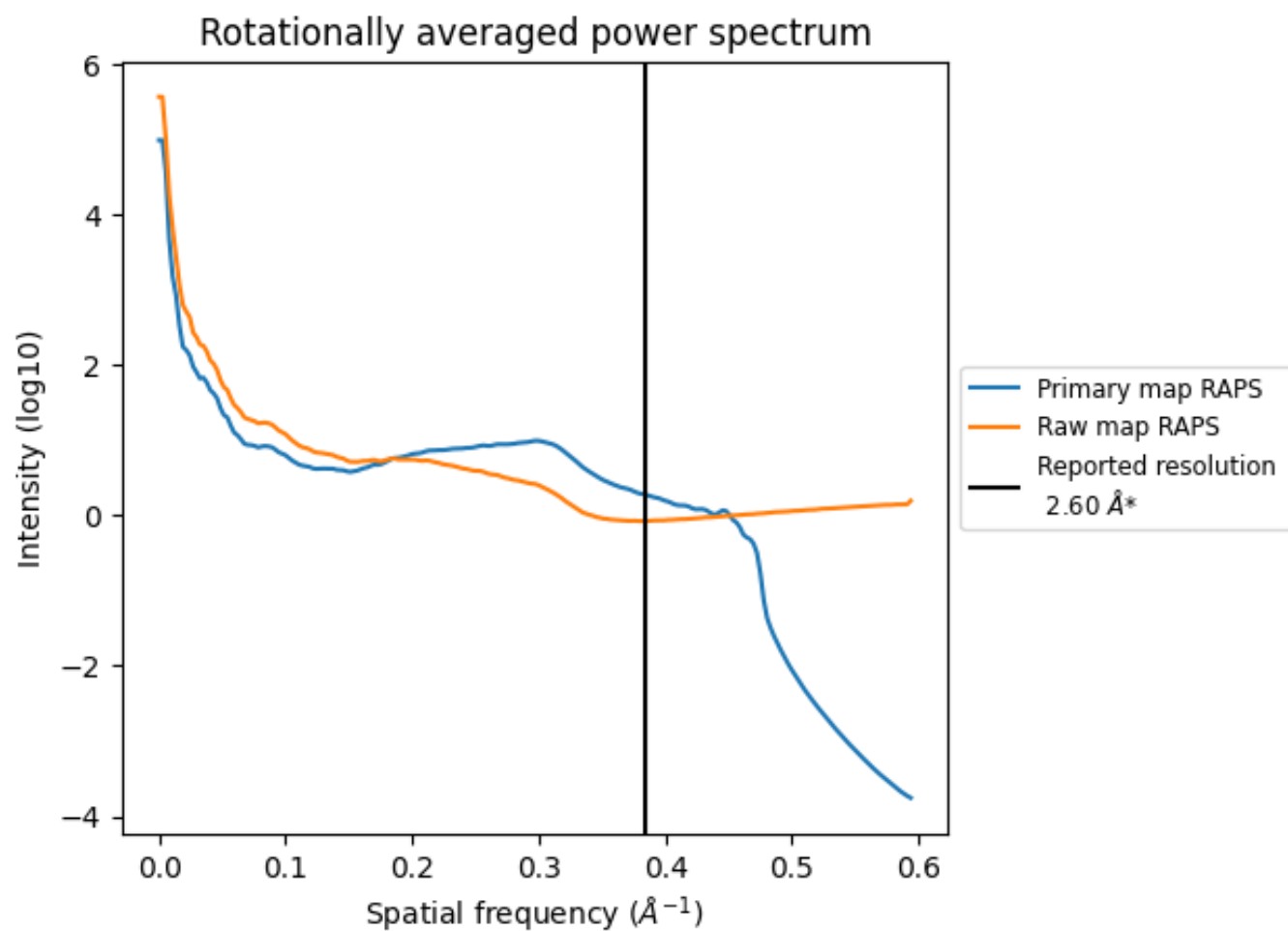
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1587 nm^3 ; this corresponds to an approximate mass of 1434 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 ⓘ

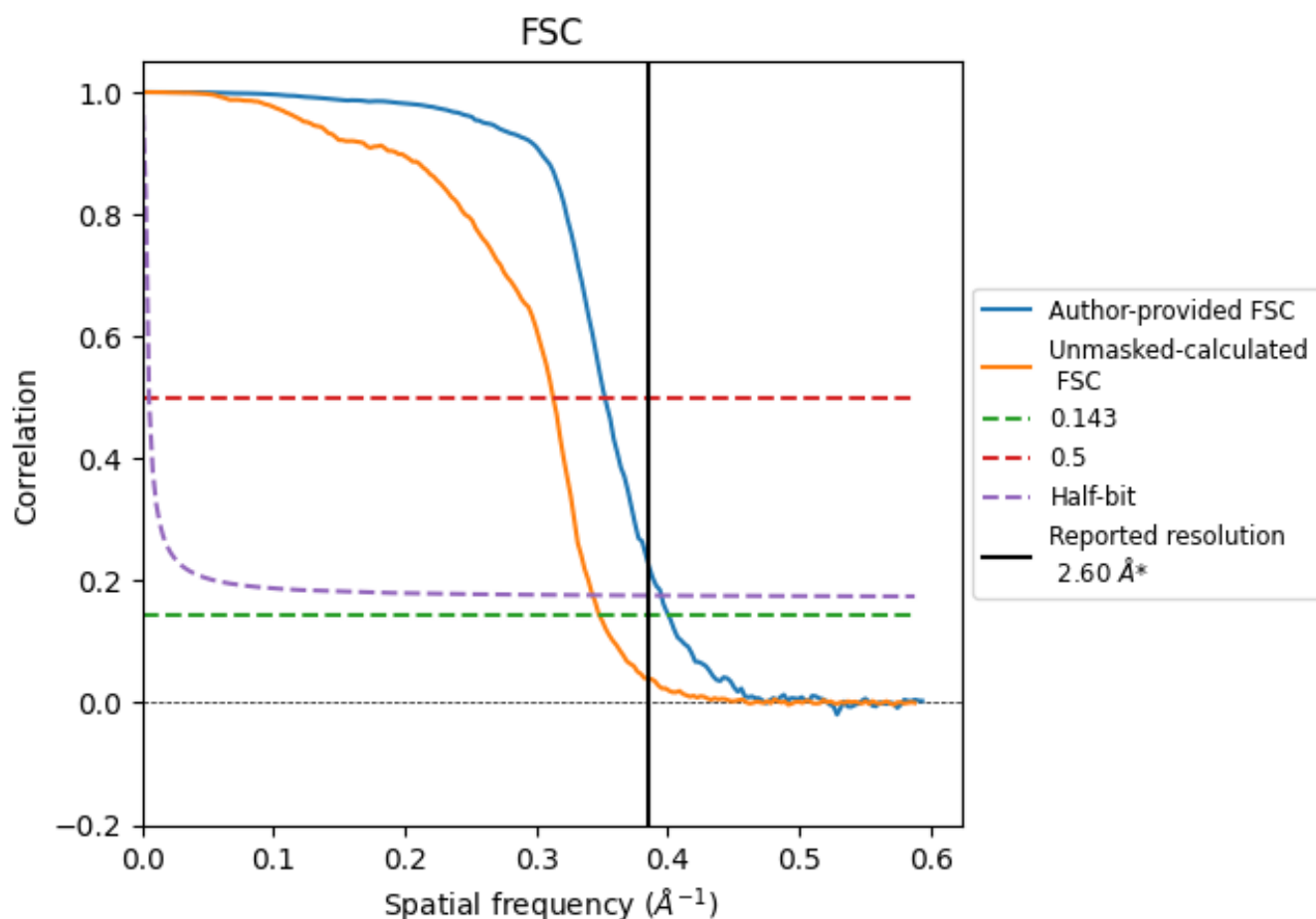


*Reported resolution corresponds to spatial frequency of $0.385 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.50	2.84	2.53
Unmasked-calculated*	2.87	3.20	2.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.87 differs from the reported value 2.6 by more than 10 %

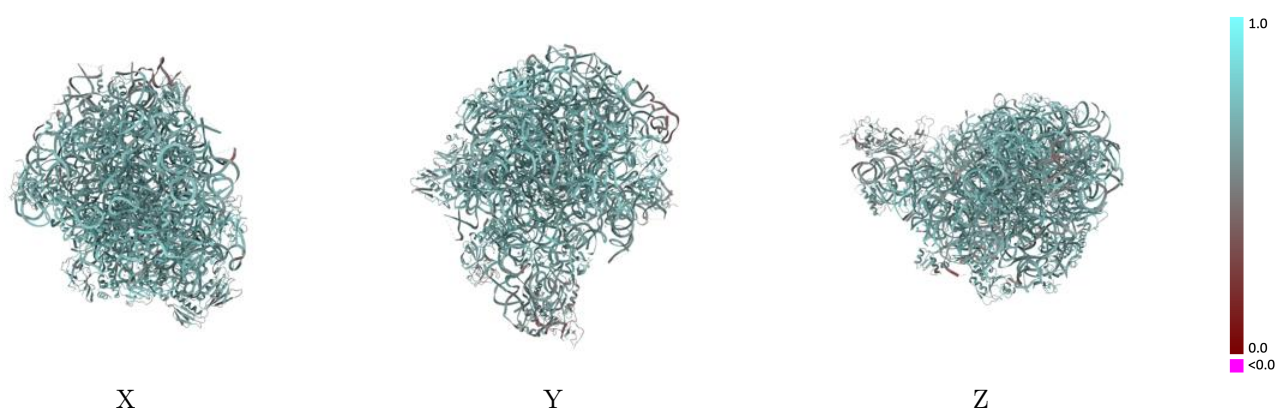
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-52635 and PDB model 9I5T. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

This section was not generated.

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

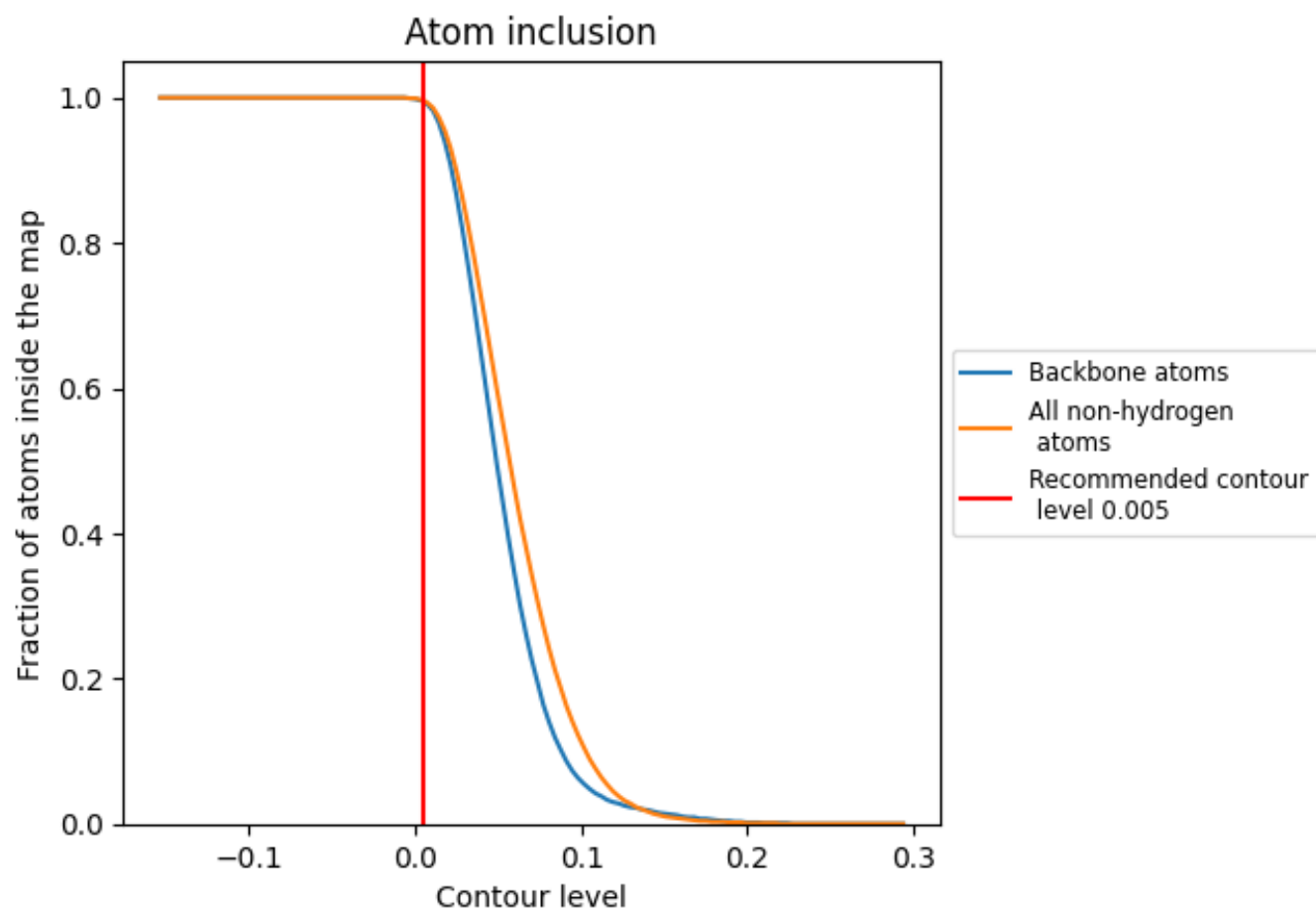


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9960	 0.6710
0	 0.9980	 0.6930
1	 0.9980	 0.6520
11	 0.9900	 0.5420
12	 0.9850	 0.4620
13	 0.9910	 0.5970
15	 0.9920	 0.5930
2	 0.9980	 0.6910
4	 1.0000	 0.7030
5	 0.9940	 0.6780
6	 1.0000	 0.7370
7	 0.9960	 0.7060
8	 0.9930	 0.6790
A	 0.9960	 0.6760
B	 0.9950	 0.5950
D	 0.9990	 0.7050
E	 0.9970	 0.6960
F	 0.9990	 0.6840
M	 0.9940	 0.6890
N	 0.9980	 0.6860
O	 0.9950	 0.6660
P	 0.9970	 0.6840
Q	 0.9990	 0.7150
R	 0.9990	 0.6260
S	 0.9950	 0.6770
T	 0.9980	 0.7210
U	 0.9920	 0.6620
V	 1.0000	 0.7040
W	 0.9930	 0.6600
X	 0.9970	 0.6540
Y	 0.9900	 0.5960
Z	 0.9980	 0.7090
h	 0.9910	 0.6090

