Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 08:32 am GMT

PDB ID	:	6S0Z
EMDB ID	:	EMD-10077
Title	:	Erythromycin Resistant Staphylococcus aureus 50S ribosome (delta R88 A89 uL22) in complex with erythromycin.
Authors	:	Halfon, Y.; Matozv, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Kjeldgaard, J.; Ingmer, H.; Yonath, A.
Deposited on	:	2019-06-18
Resolution	:	2.30 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:

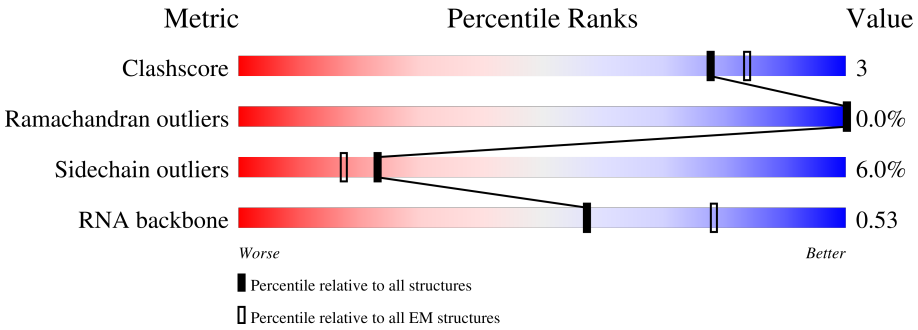
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	2905	14% 68% 26% 6%
2	B	114	76% 19%
3	C	274	90% 9%
4	D	215	87% 13%
5	E	206	86% 13%
6	F	173	68% 81% 18%
7	G	173	42% 86% 13%

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Mol	Chain	Length	Quality of chain
8	H	145	92% 7%
9	I	122	83% 17%
10	J	146	91% 7%
11	K	137	85% 14%
12	L	120	89% 9%
13	M	118	13% 87% 12%
14	N	114	90% 10%
15	O	116	89% 11%
16	P	102	90% 9%
17	Q	110	5% 87% 13%
18	R	89	81% 18%
19	S	103	9% 83% 17%
20	T	94	89% 10%
21	U	77	83% 17%
22	V	49	6% 98%
23	W	67	88% 9%
24	X	58	88% 12%
25	Y	59	97% 86% 14%
26	Z	48	29% 90% 10%
27	1	47	21% 72% 26%
28	2	43	91% 7%
29	3	64	86% 12%
30	4	37	84% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	ERY	A	3001	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 145863 atoms, of which 57285 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	2905	93573	27803	31296	11387	20182	2905	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	B	114	3654	1085	1229	433	794	113	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	274	4291	1301	2201	415	369	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	215	3294	1018	1667	299	305	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	206	3191	986	1619	288	296	2	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	173	2653	831	1338	225	253	6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	173	Total	C	H	N	O	S	0	0
			2454	780	1206	236	229	3		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	145	Total	C	H	N	O	S	0	0
			2293	717	1144	211	218	3		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	122	Total	C	H	N	O	S	0	0
			1899	572	981	174	168	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	146	Total	C	H	N	O	S	0	0
			2211	674	1125	214	197	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	137	Total	C	H	N	O	S	0	0
			2216	694	1137	204	177	4		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	120	Total	C	H	N	O	S	0	0
			1915	576	983	182	173	1		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	118	Total	C	H	N	O	0	0
			1796	552	913	173	158		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	H	N	O	0	0
			1826	563	937	175	151		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	116	Total	C	H	N	O	S	0	0
			1957	593	1014	189	157	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	102	Total	C	H	N	O	S	0	0
			1620	503	830	142	144	1		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	110	Total	C	H	N	O	S	0	0
			1734	525	896	159	151	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	ARG	deletion	UNP A0A077UKF9
Q	?	-	ALA	deletion	UNP A0A077UKF9

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	89	Total	C	H	N	O	S	0	0
			1463	453	748	127	131	4		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	103	Total	C	H	N	O	S	0	0
			1579	486	809	142	141	1		

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	94	Total	C	H	N	O	0	0
			1488	463	766	130	129		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	77	Total	C	H	N	O	0	0
			1187	363	600	115	109		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	49	Total	C	H	N	O	0	0
			779	234	400	82	63		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	67	Total	C	H	N	O	0	0
			1104	333	563	102	106		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	58	Total	C	H	N	O	0	0
			940	280	491	85	84		

- Molecule 25 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	59	Total	C	H	N	O	S	0	0
			613	225	243	68	76	1		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	48	Total	C	H	N	O	S	0	0
			718	222	358	77	59	2		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1	47	Total	C	H	N	O	S	0	0
			773	238	383	78	70	4		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	2	43	Total	C	H	N	O	S	0	0
			782	225	415	89	52	1		

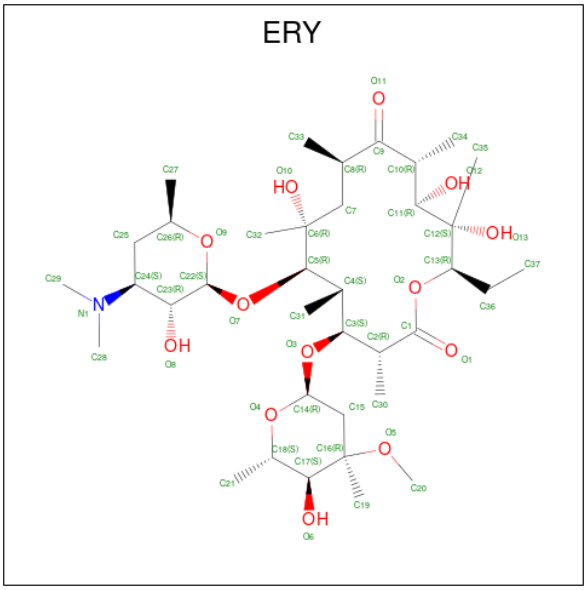
- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	3	64	Total	C	H	N	O	S	0	0
			1107	324	586	113	82	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	4	37	Total	C	H	N	O	S	0	0
			635	186	340	60	44	5		

- Molecule 31 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



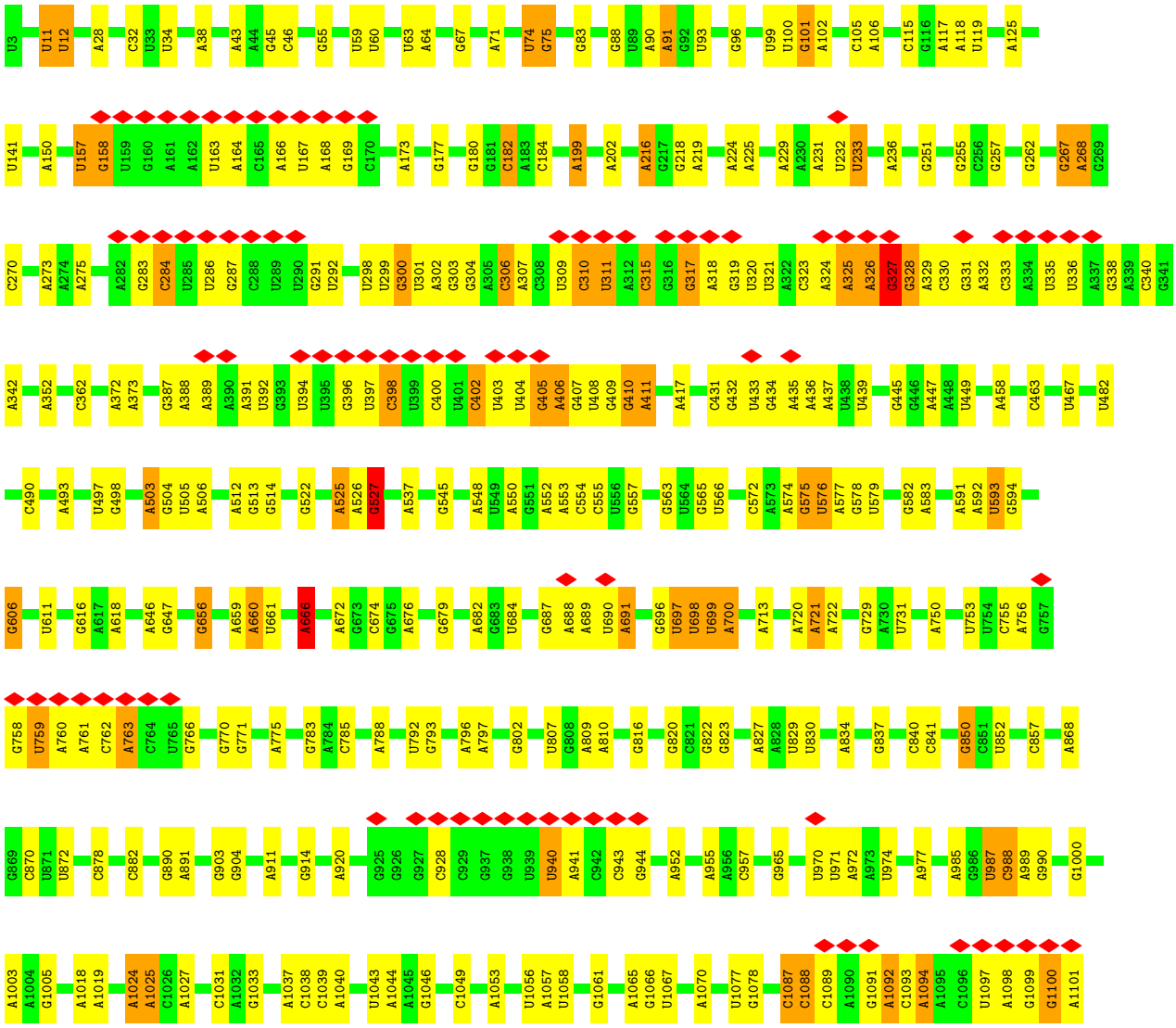
Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	H	N	O	0
			118	37	67	1	13	

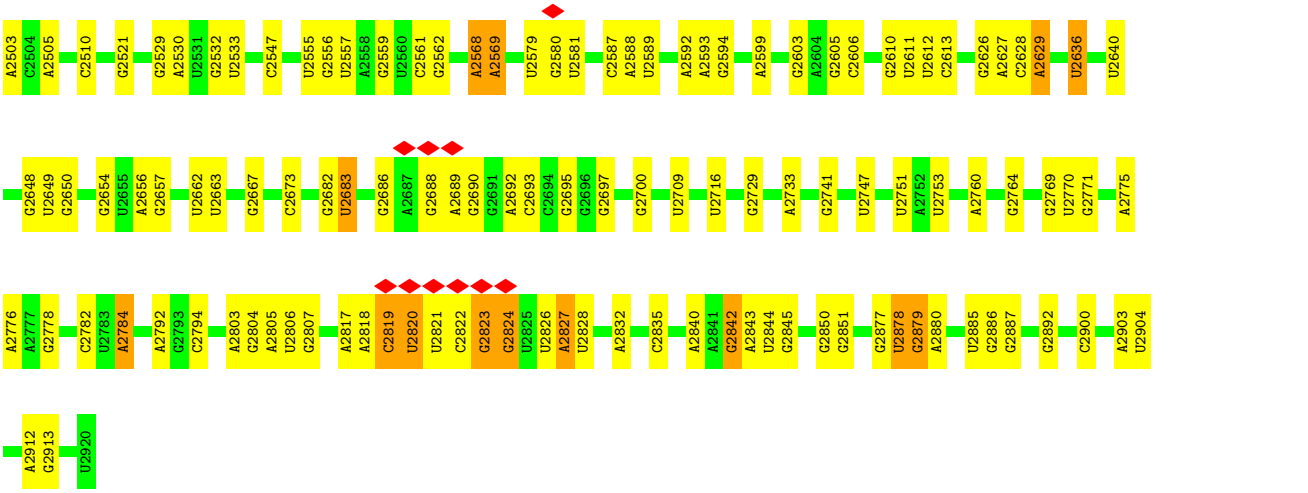
3 Residue-property plots (i)

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: 23S ribosomal RNA

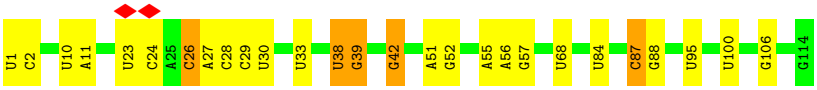
Chain A:





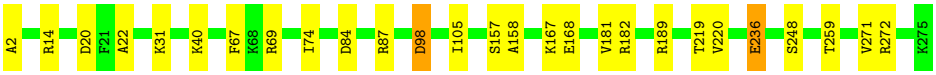
• Molecule 2: 5S ribosomal RNA

Chain B:



• Molecule 3: 50S ribosomal protein L2

Chain C:

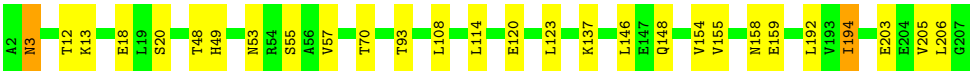


• Molecule 4: 50S ribosomal protein L3

Chain D:

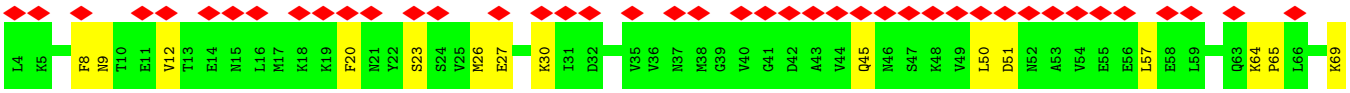
• Molecule 5: 50S ribosomal protein L4

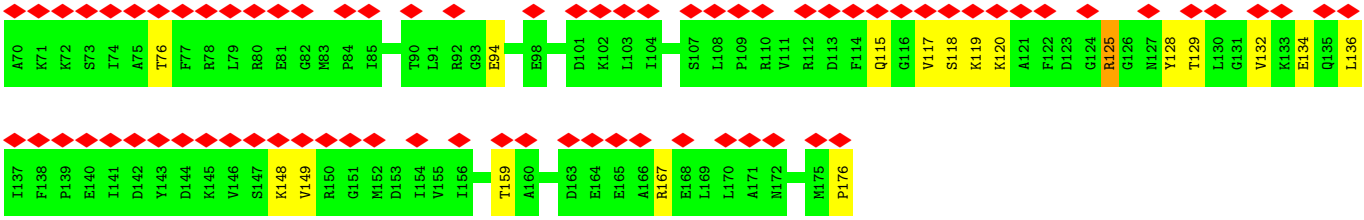
Chain E:



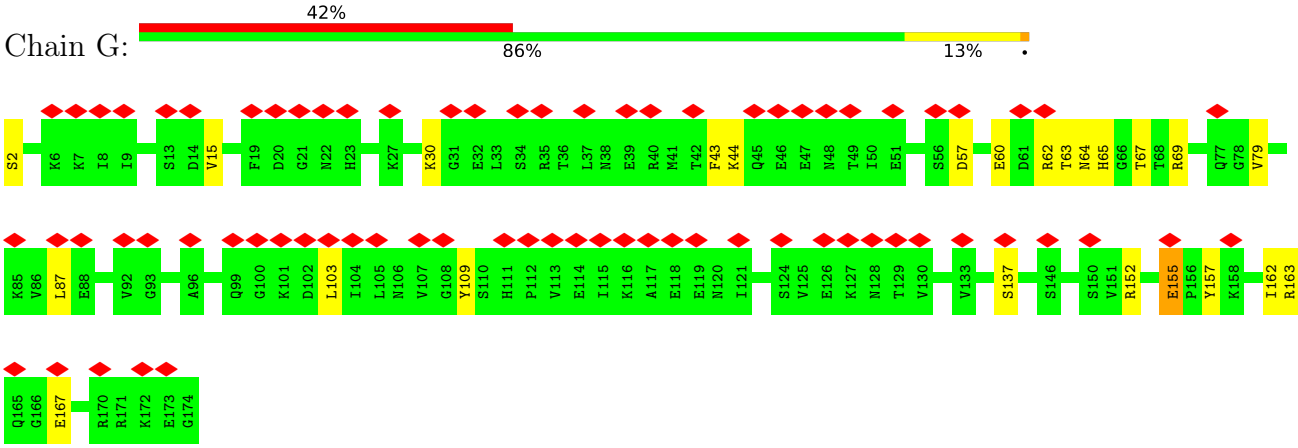
• Molecule 6: 50S ribosomal protein L5

Chain F:

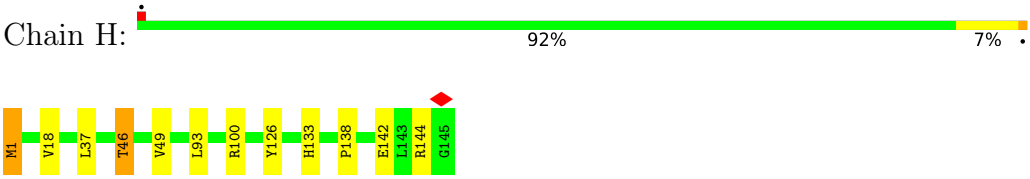




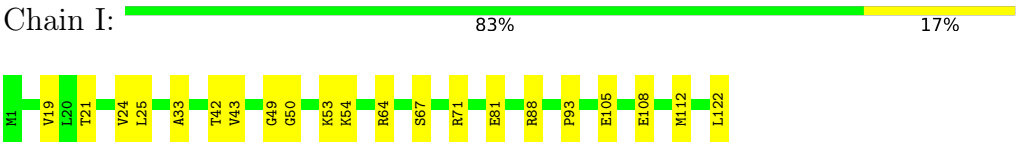
• Molecule 7: 50S ribosomal protein L6



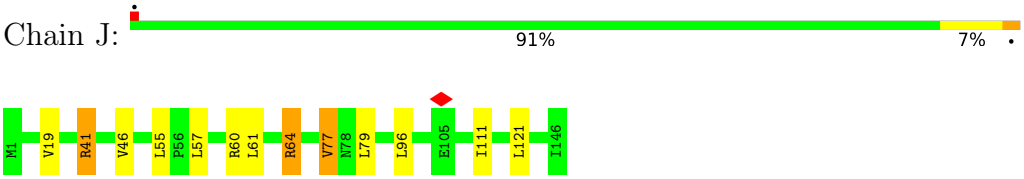
• Molecule 8: 50S ribosomal protein L13



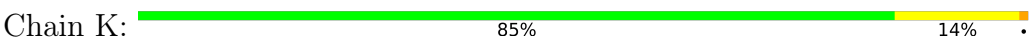
• Molecule 9: 50S ribosomal protein L14



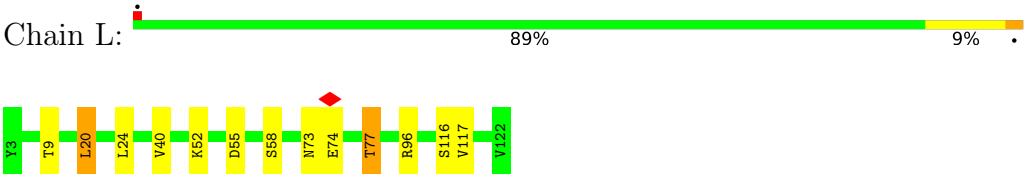
• Molecule 10: 50S ribosomal protein L15



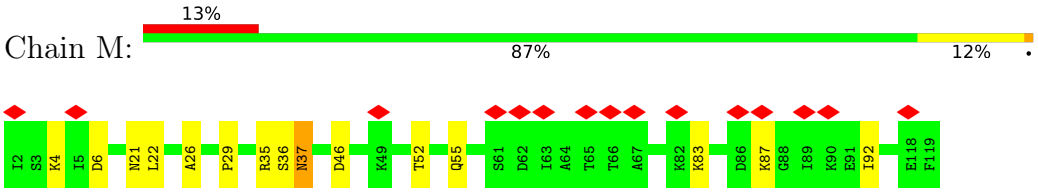
• Molecule 11: 50S ribosomal protein L16



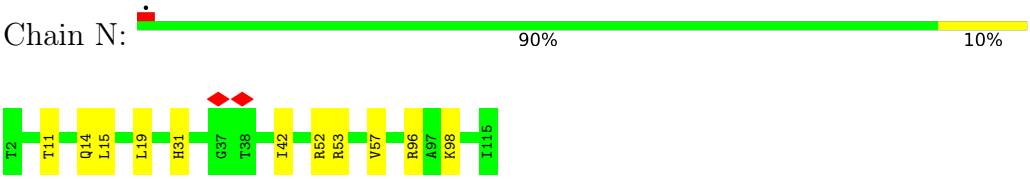
• Molecule 12: 50S ribosomal protein L17



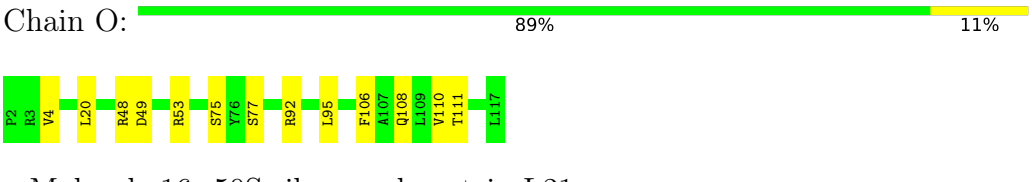
• Molecule 13: 50S ribosomal protein L18



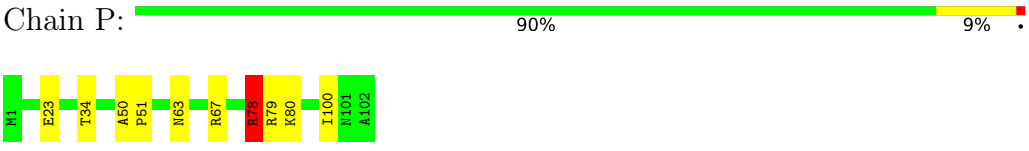
• Molecule 14: 50S ribosomal protein L19



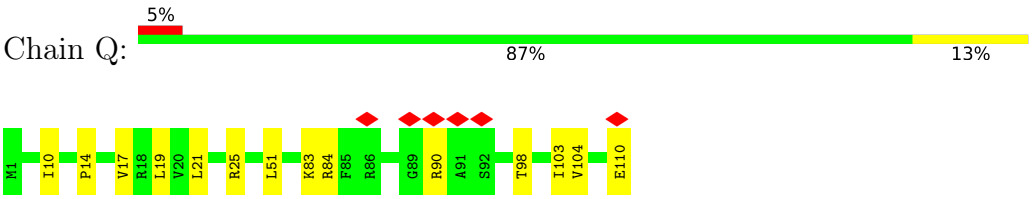
• Molecule 15: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L21

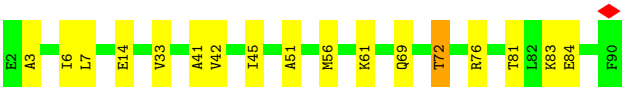


• Molecule 17: 50S ribosomal protein L22



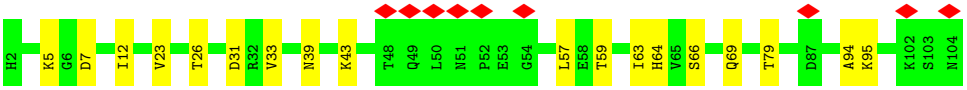
• Molecule 18: 50S ribosomal protein L23

Chain R:



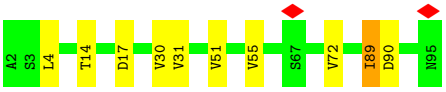
• Molecule 19: 50S ribosomal protein L24

Chain S:



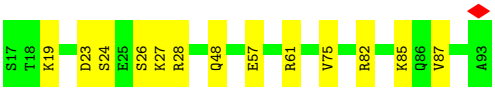
• Molecule 20: 50S ribosomal protein L25

Chain T:



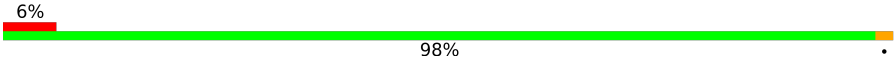
• Molecule 21: 50S ribosomal protein L27

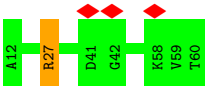
Chain U:



• Molecule 22: 50S ribosomal protein L28

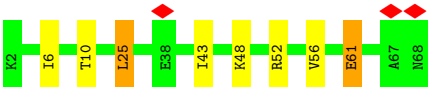
Chain V:





• Molecule 23: 50S ribosomal protein L29

Chain W:

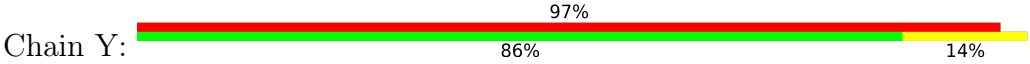


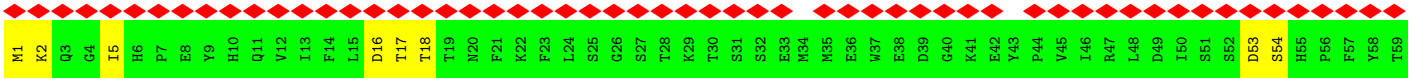
• Molecule 24: 50S ribosomal protein L30

Chain X:

• Molecule 25: 50S ribosomal protein L31 type B

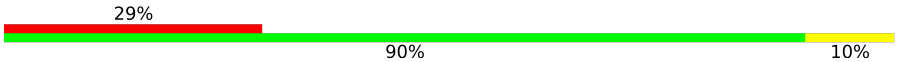
Chain Y:

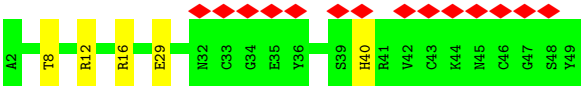




• Molecule 26: 50S ribosomal protein L32

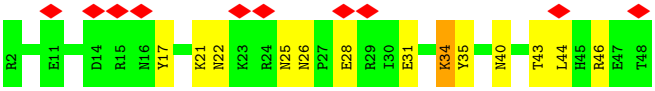
Chain Z:





• Molecule 27: 50S ribosomal protein L33

Chain 1:



• Molecule 28: 50S ribosomal protein L34

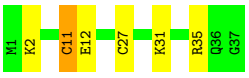
Chain 2:

• Molecule 29: 50S ribosomal protein L35

Chain 3:

• Molecule 30: 50S ribosomal protein L36

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	378309	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.076	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	0.292	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	426.80002, 426.80002, 426.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ERY

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	0.66	1/69739 (0.0%)	0.96	64/108751 (0.1%)
2	B	0.44	0/2711	0.88	2/4223 (0.0%)
3	C	0.45	0/2125	0.64	0/2853
4	D	0.49	0/1651	0.59	0/2215
5	E	0.44	0/1595	0.60	0/2154
6	F	0.27	0/1329	0.53	0/1791
7	G	0.27	0/1266	0.54	0/1717
8	H	0.46	0/1171	0.60	0/1577
9	I	0.47	0/925	0.67	0/1242
10	J	0.41	0/1100	0.68	0/1467
11	K	0.42	0/1103	0.60	0/1481
12	L	0.42	0/936	0.67	0/1253
13	M	0.30	0/892	0.60	0/1195
14	N	0.43	0/901	0.64	0/1209
15	O	0.50	0/955	0.67	0/1265
16	P	0.48	0/800	0.64	1/1070 (0.1%)
17	Q	0.43	0/846	0.64	1/1140 (0.1%)
18	R	0.40	0/723	0.62	0/966
19	S	0.35	0/779	0.54	0/1043
20	T	0.35	0/730	0.60	0/981
21	U	0.47	0/593	0.64	0/788
22	V	0.34	0/384	0.63	0/515
23	W	0.32	0/542	0.60	0/722
24	X	0.42	0/451	0.58	0/606
25	Y	0.26	0/378	0.49	0/521
26	Z	0.43	0/366	0.70	1/489 (0.2%)
27	1	0.29	0/395	0.55	0/530
28	2	0.50	0/371	0.78	1/484 (0.2%)
29	3	0.39	0/526	0.65	0/690
30	4	0.34	0/298	0.58	0/392
All	All	0.60	1/96581 (0.0%)	0.90	70/145330 (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
16	P	0	1
29	3	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	721	A	N9-C4	-5.15	1.34	1.37

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	770	G	OP1-P-O3'	-11.50	79.89	105.20
1	A	2150	A	C5-N7-C8	10.23	109.02	103.90
1	A	1506	C	N3-C2-O2	-8.99	115.61	121.90
1	A	576	U	C2-N1-C1'	8.57	127.99	117.70
1	A	1602	U	C5-C4-O4	-7.91	121.15	125.90
1	A	2636	U	C2-N1-C1'	7.69	126.93	117.70
1	A	2361	U	C2-N1-C1'	7.68	126.92	117.70
1	A	1602	U	N3-C4-O4	7.56	124.69	119.40
1	A	2150	A	N7-C8-N9	7.39	117.50	113.80
1	A	1953	U	C2-N1-C1'	7.02	126.12	117.70
1	A	770	G	OP2-P-O3'	-7.00	89.81	105.20
1	A	1179	C	N1-C2-O2	6.55	122.83	118.90
1	A	1053	A	N7-C8-N9	6.42	117.01	113.80
1	A	576	U	N1-C2-O2	6.25	127.17	122.80
1	A	2636	U	N1-C2-O2	6.19	127.13	122.80
1	A	1804	U	C2-N1-C1'	6.14	125.07	117.70
1	A	1179	C	N3-C2-O2	-6.13	117.61	121.90
1	A	2636	U	N3-C2-O2	-6.13	117.91	122.20
1	A	1351	C	C2-N1-C1'	6.13	125.54	118.80
1	A	1179	C	C6-N1-C2	-6.11	117.86	120.30
1	A	771	G	O5'-P-OP2	6.04	117.95	110.70
1	A	2361	U	N3-C2-O2	-5.99	118.01	122.20
1	A	1351	C	C6-N1-C2	-5.98	117.91	120.30
1	A	576	U	C6-N1-C1'	-5.97	112.84	121.20
1	A	771	G	OP1-P-OP2	5.94	128.51	119.60
1	A	576	U	N3-C2-O2	-5.92	118.06	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2249	G	O4'-C1'-N9	5.91	112.93	108.20
1	A	1994	C	C2-N1-C1'	5.89	125.28	118.80
2	B	87	C	C2-N1-C1'	5.83	125.21	118.80
1	A	1228	A	N1-C6-N6	5.81	122.09	118.60
1	A	2326	G	C6-C5-N7	-5.76	126.94	130.40
1	A	1604	C	OP2-P-O3'	5.72	117.78	105.20
1	A	2361	U	N1-C2-O2	5.70	126.79	122.80
1	A	721	A	C5-N7-C8	-5.62	101.09	103.90
1	A	1179	C	C2-N1-C1'	5.62	124.98	118.80
1	A	575	G	C4-N9-C1'	5.61	133.79	126.50
1	A	1994	C	N1-C2-O2	5.60	122.26	118.90
1	A	2131	C	C6-N1-C2	-5.54	118.08	120.30
1	A	1053	A	C5-N7-C8	-5.54	101.13	103.90
1	A	503	A	N1-C6-N6	5.53	121.92	118.60
1	A	1494	G	O4'-C1'-N9	5.49	112.59	108.20
1	A	1932	C	C2-N1-C1'	5.49	124.84	118.80
26	Z	16	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	1936	C	N3-C2-O2	-5.47	118.07	121.90
1	A	527	G	O4'-C1'-N9	5.46	112.57	108.20
1	A	1604	C	P-O3'-C3'	5.41	126.19	119.70
16	P	78	ARG	NE-CZ-NH1	5.39	122.99	120.30
28	2	34	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	1914	C	N1-C2-O2	5.35	122.11	118.90
1	A	2131	C	N3-C2-O2	-5.34	118.16	121.90
1	A	1227	U	C2-N1-C1'	5.33	124.10	117.70
1	A	1865	C	C6-N1-C2	-5.31	118.18	120.30
1	A	327	G	C4-N9-C1'	5.30	133.40	126.50
17	Q	25	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	2448	G	N3-C4-N9	5.29	129.17	126.00
1	A	666	A	N1-C6-N6	5.27	121.76	118.60
2	B	100	U	C2-N1-C1'	5.27	124.02	117.70
1	A	882	C	C2-N1-C1'	5.24	124.56	118.80
1	A	1481	A	N9-C4-C5	-5.24	103.71	105.80
1	A	2747	U	C2-N1-C1'	5.22	123.96	117.70
1	A	2326	G	C4-N9-C1'	5.21	133.27	126.50
1	A	1227	U	N3-C2-O2	-5.20	118.56	122.20
1	A	1506	C	C6-N1-C2	-5.19	118.22	120.30
1	A	1988	C	N1-C2-O2	5.18	122.01	118.90
1	A	439	U	C2-N1-C1'	5.16	123.89	117.70
1	A	1506	C	N1-C2-N3	5.07	122.75	119.20
1	A	1988	C	N3-C2-O2	-5.06	118.36	121.90
1	A	1767	G	C4-N9-C1'	5.06	133.07	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	557	G	O4'-C1'-N9	5.05	112.24	108.20
1	A	2249	G	C4-N9-C1'	5.01	133.01	126.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	3	31	HIS	Peptide
16	P	50	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	31296	31306	241	0
2	B	2425	1229	1229	10	0
3	C	2090	2201	2201	15	0
4	D	1627	1667	1667	12	0
5	E	1572	1619	1619	12	0
6	F	1315	1338	1338	15	0
7	G	1248	1206	1205	9	0
8	H	1149	1144	1145	7	0
9	I	918	981	981	10	0
10	J	1086	1125	1125	5	0
11	K	1079	1137	1138	12	0
12	L	932	983	983	5	0
13	M	883	913	913	5	0
14	N	889	937	937	3	0
15	O	943	1014	1014	6	0
16	P	790	830	830	2	0
17	Q	838	896	896	4	0
18	R	715	748	748	8	0
19	S	770	809	809	8	0
20	T	722	766	766	3	0
21	U	587	600	600	8	0
22	V	379	400	400	1	0
23	W	541	563	563	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	449	491	491	4	0
25	Y	370	243	243	5	0
26	Z	360	358	358	5	0
27	1	390	383	395	7	0
28	2	367	415	415	2	0
29	3	521	586	586	5	0
30	4	295	340	340	3	0
31	A	51	67	67	1	0
All	All	88578	57285	57308	383	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 (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2649:U:O2'	1:A:2845:G:N2	2.15	0.79
1:A:1226:G:O2'	1:A:1227:U:O2	2.01	0.79
1:A:1465:G:O2'	1:A:1537:A:N6	2.17	0.78
1:A:75:G:O2'	23:W:48:LYS:NZ	2.18	0.77
1:A:1486:C:N3	1:A:1597:U:O4	2.18	0.76
1:A:2361:U:O4	1:A:2363:A:N7	2.18	0.76
1:A:304:G:N7	1:A:410:G:N2	2.33	0.76
2:B:29:C:O2	2:B:51:A:N6	2.19	0.75
1:A:1796:A:O2'	1:A:1985:C:OP1	2.05	0.75
1:A:1038:C:OP1	15:O:53:ARG:NH2	2.20	0.74
1:A:318:A:O2'	1:A:402:C:N3	2.19	0.74
1:A:1423:C:O2'	1:A:1512:U:O2	2.05	0.74
1:A:1762:U:O4	1:A:1765:A:O2'	2.05	0.74
27:1:22:ASN:ND2	27:1:25:ASN:OD1	2.21	0.73
1:A:2421:C:N3	1:A:2459:A:N6	2.36	0.73
1:A:1092:A:N6	1:A:1155:A:O4'	2.22	0.73
1:A:1781:C:OP1	14:N:96:ARG:NH2	2.22	0.73
1:A:273:A:N7	1:A:298:U:O2	2.22	0.72
1:A:2374:C:O2'	27:1:17:TYR:OH	2.07	0.72
3:C:84:ASP:OD2	3:C:87:ARG:NH1	2.22	0.72
1:A:2510:C:N3	11:K:124:LYS:NZ	2.36	0.72
1:A:1737:U:O2'	3:C:14:ARG:NH2	2.22	0.72
1:A:1884:G:N2	1:A:1912:A:H62	1.87	0.72
1:A:1540:U:O2'	1:A:1624:C:O3'	2.04	0.72
2:B:27:A:O2'	2:B:56:A:N1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:33:VAL:O	18:R:76:ARG:NH2	2.22	0.72
1:A:579:U:O2'	15:O:49:ASP:OD2	2.07	0.72
1:A:1758:A:O2'	1:A:1761:G:O6	2.07	0.72
10:J:77:VAL:HG13	10:J:111:ILE:HD13	1.71	0.71
1:A:2177:U:OP1	1:A:2187:G:O2'	2.06	0.71
1:A:690:U:O2'	1:A:691:A:O5'	2.07	0.71
2:B:1:U:O2	2:B:2:C:N4	2.24	0.70
1:A:1536:C:N4	1:A:2238:U:OP2	2.24	0.70
15:O:108:GLN:O	15:O:111:THR:OG1	2.09	0.70
1:A:1490:G:O2'	1:A:1491:C:O5'	2.09	0.70
3:C:2:ALA:N	3:C:20:ASP:OD2	2.24	0.70
1:A:1099:G:N2	1:A:1149:U:O2	2.24	0.70
1:A:329:A:N6	1:A:398:C:O2	2.24	0.70
6:F:148:LYS:NZ	6:F:149:VAL:O	2.22	0.70
1:A:182:C:N4	1:A:216:A:N7	2.40	0.70
1:A:434:G:O2'	1:A:436:A:OP2	2.10	0.69
1:A:2007:G:O2'	1:A:2009:U:OP2	2.09	0.69
1:A:1605:A:O2'	1:A:1607:A:OP1	2.10	0.69
1:A:2885:U:OP2	1:A:2886:G:O2'	2.07	0.69
1:A:315:C:O2'	1:A:317:G:O6	2.08	0.69
1:A:2347:A:N7	1:A:2360:A:N6	2.42	0.68
1:A:1884:G:N2	1:A:1912:A:N6	2.41	0.68
4:D:2:THR:OG1	4:D:3:LYS:N	2.26	0.68
1:A:405:G:O2'	1:A:406:A:O4'	2.11	0.67
1:A:796:A:OP2	17:Q:90:ARG:NH1	2.26	0.67
1:A:157:U:O2'	1:A:158:G:OP1	2.11	0.67
1:A:903:G:OP2	21:U:85:LYS:NZ	2.23	0.67
1:A:1099:G:O2'	1:A:1130:A:N6	2.27	0.67
1:A:788:A:O2'	1:A:1703:U:OP1	2.12	0.67
1:A:2686:G:N2	1:A:2689:A:OP2	2.28	0.67
1:A:1000:G:N7	11:K:14:ARG:NH2	2.43	0.67
1:A:2366:G:O3'	2:B:39:G:N2	2.27	0.67
7:G:163:ARG:NH2	7:G:167:GLU:O	2.28	0.67
1:A:1466:G:O3'	1:A:1535:G:O2'	2.13	0.66
1:A:2769:G:OP1	30:4:35:ARG:NH1	2.28	0.66
1:A:1261:G:OP1	16:P:67:ARG:NH2	2.29	0.66
11:K:48:GLU:OE2	11:K:51:ARG:NH1	2.29	0.66
1:A:1455:U:O2'	1:A:1457:U:O4	2.09	0.66
1:A:59:U:O2'	1:A:74:U:OP2	2.12	0.66
1:A:1452:C:N4	1:A:1633:A:N7	2.44	0.66
1:A:2568:A:O2'	1:A:2569:A:OP1	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:48:ARG:NH2	15:O:49:ASP:OD1	2.29	0.65
1:A:1712:A:O2'	1:A:1718:G:N7	2.27	0.65
1:A:325:A:O2'	1:A:326:A:OP1	2.14	0.65
1:A:2140:C:N3	1:A:2195:G:O2'	2.28	0.65
1:A:2132:A:O2'	1:A:2133:G:O4'	2.12	0.64
1:A:1979:A:N3	1:A:2587:C:O2'	2.30	0.64
1:A:2302:C:O2'	11:K:84:GLY:O	2.15	0.64
1:A:2850:G:OP2	4:D:86:ARG:NH2	2.30	0.64
1:A:545:G:N1	1:A:548:A:OP2	2.30	0.64
5:E:3:ASN:ND2	5:E:18:GLU:OE1	2.31	0.64
1:A:2157:U:O2'	1:A:2185:A:N1	2.31	0.63
1:A:320:U:OP1	1:A:323:C:N4	2.31	0.63
1:A:327:G:O2'	1:A:328:G:OP1	2.12	0.63
1:A:1963:A:OP2	1:A:1989:C:N4	2.32	0.63
9:I:88:ARG:NH1	9:I:93:PRO:O	2.32	0.63
2:B:11:A:N7	21:U:82:ARG:NH2	2.47	0.63
30:4:2:LYS:NZ	30:4:31:LYS:O	2.32	0.63
1:A:342:A:OP1	19:S:95:LYS:NZ	2.27	0.62
1:A:1024:A:O2'	1:A:1025:A:OP1	2.13	0.62
2:B:29:C:OP1	13:M:4:LYS:NZ	2.32	0.62
27:1:35:TYR:OH	27:1:40:ASN:OD1	2.14	0.62
27:1:21:LYS:NZ	27:1:26:ASN:O	2.26	0.62
1:A:1135:G:O2'	1:A:1146:C:N3	2.28	0.62
9:I:108:GLU:OE1	9:I:108:GLU:N	2.33	0.62
1:A:1101:A:N6	1:A:1131:G:OP2	2.33	0.61
29:3:54:ASP:OD1	29:3:57:ARG:NH1	2.34	0.61
1:A:522:G:N1	1:A:525:A:OP2	2.33	0.61
1:A:1884:G:H21	1:A:1912:A:N6	1.99	0.61
1:A:2878:U:O2'	1:A:2879:G:OP1	2.17	0.61
1:A:2851:G:N2	1:A:2904:U:OP2	2.33	0.61
1:A:1215:U:O2'	1:A:1217:U:OP1	2.14	0.60
1:A:163:U:O4	1:A:2244:G:O2'	2.17	0.60
1:A:1490:G:O2'	1:A:1491:C:O4'	2.20	0.60
1:A:2580:G:H21	1:A:2610:G:HO2'	1.48	0.60
7:G:57:ASP:OD1	7:G:62:ARG:NH2	2.35	0.60
1:A:2152:G:N2	1:A:2189:G:O2'	2.35	0.60
1:A:2141:A:O2'	1:A:2193:G:O3'	2.20	0.59
1:A:1122:U:O2'	1:A:1132:A:N3	2.36	0.59
1:A:2627:A:N6	3:C:236:GLU:OE2	2.35	0.59
1:A:2450:U:O2'	1:A:2451:C:O5'	2.12	0.59
1:A:229:A:O2'	1:A:231:A:N1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1938:U:O2'	1:A:1945:A:N7	2.36	0.58
1:A:687:G:N1	1:A:690:U:OP2	2.36	0.58
1:A:1031:C:O2'	1:A:1044:A:N3	2.34	0.58
1:A:1100:G:O2'	1:A:1101:A:O4'	2.22	0.58
1:A:1112:G:OP2	1:A:1113:A:N6	2.32	0.58
25:Y:17:THR:HG23	25:Y:18:THR:HG23	1.85	0.58
1:A:2372:G:OP2	27:1:34:LYS:NZ	2.30	0.57
13:M:36:SER:OG	13:M:37:ASN:N	2.37	0.57
6:F:30:LYS:N	6:F:159:THR:OG1	2.37	0.57
1:A:656:G:H21	1:A:660:A:H2	1.52	0.57
5:E:123:LEU:HD11	5:E:194:ILE:HD11	1.85	0.57
2:B:26:C:O2'	2:B:57:G:N2	2.37	0.57
1:A:431:C:O2	1:A:436:A:N6	2.37	0.57
6:F:23:SER:N	6:F:27:GLU:OE2	2.38	0.57
21:U:48:GLN:N	21:U:48:GLN:OE1	2.38	0.57
1:A:342:A:N3	1:A:362:C:O2'	2.37	0.56
1:A:2667:G:OP1	8:H:100:ARG:NH1	2.39	0.56
1:A:2842:G:O2'	1:A:2844:U:OP2	2.09	0.56
1:A:1115:G:N2	1:A:1135:G:OP2	2.37	0.56
25:Y:18:THR:HG21	25:Y:53:ASP:HB3	1.88	0.56
4:D:18:GLU:OE1	4:D:18:GLU:N	2.39	0.56
9:I:81:GLU:N	9:I:81:GLU:OE1	2.39	0.55
1:A:63:U:O4	1:A:91:A:N6	2.39	0.55
1:A:574:A:N3	1:A:575:G:N2	2.53	0.55
1:A:721:A:H8	1:A:2096:G:H21	1.54	0.55
14:N:11:THR:HB	14:N:57:VAL:HG21	1.88	0.55
13:M:29:PRO:HD2	13:M:92:ILE:HG22	1.89	0.55
1:A:1658:A:OP1	1:A:1661:C:N4	2.38	0.55
1:A:852:U:OP2	10:J:41:ARG:NH2	2.40	0.54
1:A:2049:U:OP2	26:Z:12:ARG:NH2	2.39	0.54
4:D:158:SER:O	4:D:161:SER:OG	2.24	0.54
24:X:58:GLU:N	24:X:58:GLU:OE1	2.41	0.54
1:A:309:U:O2	1:A:406:A:O2'	2.24	0.54
1:A:2388:A:OP2	29:3:24:ARG:NH1	2.38	0.54
1:A:2778:G:N2	1:A:2778:G:OP1	2.40	0.54
27:1:28:GLU:OE1	27:1:28:GLU:N	2.40	0.54
1:A:1111:A:N1	1:A:1139:A:O2'	2.38	0.54
1:A:2580:G:N2	1:A:2610:G:O2'	2.27	0.54
1:A:1094:A:N6	1:A:1153:C:O2'	2.40	0.54
1:A:2465:U:O2'	1:A:2467:C:OP1	2.24	0.54
1:A:2770:U:OP2	1:A:2782:C:N4	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2835:C:O2'	26:Z:40:HIS:ND1	2.31	0.54
1:A:1501:G:H22	1:A:2729:G:H22	1.55	0.54
1:A:1538:A:O2'	1:A:1626:A:O4'	2.22	0.54
1:A:2654:G:N2	1:A:2804:G:OP2	2.41	0.54
5:E:53:ASN:O	5:E:57:VAL:HG23	2.08	0.54
19:S:31:ASP:OD1	19:S:64:HIS:NE2	2.41	0.54
7:G:155:GLU:OE1	7:G:157:TYR:N	2.42	0.53
12:L:55:ASP:OD1	12:L:58:SER:OG	2.23	0.53
6:F:45:GLN:O	6:F:45:GLN:NE2	2.40	0.53
21:U:57:GLU:N	21:U:57:GLU:OE1	2.41	0.53
1:A:1756:U:O4	1:A:1774:A:N6	2.42	0.53
5:E:205:VAL:HG23	5:E:206:LEU:HD22	1.90	0.53
1:A:1632:A:N7	1:A:1633:A:N6	2.57	0.53
17:Q:83:LYS:O	17:Q:84:ARG:NE	2.41	0.53
1:A:2495:A:HO2'	1:A:2496:A:H8	1.55	0.53
1:A:2165:G:N1	1:A:2181:G:O6	2.42	0.52
1:A:2555:U:O2'	1:A:2557:U:OP1	2.18	0.52
21:U:26:SER:O	21:U:28:ARG:NH2	2.41	0.52
6:F:115:GLN:NE2	6:F:176:PRO:O	2.41	0.52
11:K:25:ASN:N	11:K:25:ASN:OD1	2.43	0.52
1:A:2827:A:H62	1:A:2912:A:H61	1.56	0.52
6:F:94:GLU:N	6:F:94:GLU:OE1	2.43	0.52
1:A:32:C:N4	1:A:493:A:OP2	2.43	0.52
1:A:1472:C:O2'	1:A:1616:A:OP2	2.25	0.52
12:L:20:LEU:HB3	12:L:40:VAL:HG21	1.90	0.52
1:A:2628:C:O2'	1:A:2629:A:O4'	2.19	0.52
8:H:1:MET:SD	8:H:1:MET:N	2.66	0.52
1:A:405:G:HO2'	1:A:406:A:P	2.33	0.51
1:A:759:U:HO2'	1:A:763:A:H62	1.57	0.51
17:Q:14:PRO:HA	17:Q:17:VAL:HG12	1.93	0.51
1:A:1934:G:O6	1:A:1950:U:N3	2.43	0.51
12:L:74:GLU:O	12:L:77:THR:OG1	2.28	0.51
17:Q:10:ILE:O	17:Q:98:THR:OG1	2.17	0.51
24:X:39:ASP:OD2	24:X:44:ARG:NH2	2.43	0.51
1:A:262:G:O2'	1:A:666:A:O2'	2.02	0.51
1:A:1767:G:OP2	1:A:1768:C:N4	2.43	0.51
1:A:362:C:OP2	5:E:137:LYS:NZ	2.44	0.51
13:M:26:ALA:N	13:M:46:ASP:OD1	2.43	0.51
5:E:205:VAL:HG23	5:E:206:LEU:CD2	2.40	0.51
1:A:1453:G:N3	1:A:1631:G:N1	2.59	0.51
9:I:50:GLY:O	9:I:53:LYS:NZ	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:119:THR:OG1	4:D:179:THR:HG22	2.12	0.51
7:G:60:GLU:O	7:G:64:ASN:ND2	2.44	0.51
30:4:11:CYS:SG	30:4:12:GLU:N	2.83	0.51
1:A:1699:A:N6	1:A:2032:A:O2'	2.44	0.50
1:A:1827:C:OP2	3:C:182:ARG:NH2	2.42	0.50
1:A:1410:A:O2'	1:A:2238:U:O2	2.28	0.50
9:I:49:GLY:O	9:I:53:LYS:NZ	2.41	0.50
18:R:84:GLU:N	18:R:84:GLU:OE1	2.44	0.50
1:A:38:A:N3	5:E:48:THR:OG1	2.41	0.50
1:A:257:G:N7	29:3:5:LYS:NZ	2.52	0.50
8:H:18:VAL:HG23	8:H:138:PRO:HB2	1.93	0.50
6:F:8:PHE:O	6:F:12:VAL:HG13	2.12	0.50
6:F:132:VAL:HG12	6:F:134:GLU:H	1.77	0.50
1:A:232:U:O2'	1:A:233:U:O5'	2.30	0.50
1:A:943:C:N4	1:A:944:G:O6	2.45	0.49
1:A:987:U:O2'	1:A:988:C:OP1	2.22	0.49
1:A:310:C:O2'	1:A:311:U:O5'	2.30	0.49
9:I:24:VAL:HG13	9:I:33:ALA:HB2	1.93	0.49
1:A:527:G:O2'	1:A:552:A:N6	2.42	0.49
1:A:1470:G:N7	3:C:31:LYS:NZ	2.60	0.49
3:C:20:ASP:OD1	3:C:22:ALA:N	2.44	0.49
8:H:126:TYR:OH	8:H:133:HIS:NE2	2.24	0.49
1:A:514:G:N7	28:2:40:ARG:NH1	2.59	0.49
1:A:1505:G:C4'	1:A:2729:G:H21	2.24	0.49
11:K:81:VAL:HG22	11:K:82:ARG:H	1.78	0.49
1:A:1301:U:O3'	26:Z:8:THR:OG1	2.29	0.48
1:A:575:G:N2	1:A:2050:A:OP1	2.45	0.48
1:A:1000:G:OP2	11:K:87:LYS:NZ	2.46	0.48
11:K:10:ARG:NH1	11:K:90:VAL:HG11	2.29	0.48
1:A:309:U:O2'	1:A:310:C:O5'	2.26	0.48
1:A:2559:G:N2	1:A:2690:G:O2'	2.47	0.48
1:A:2682:G:N2	1:A:2683:U:O4	2.41	0.48
20:T:89:ILE:HD12	20:T:90:ASP:N	2.28	0.48
4:D:156:MET:SD	4:D:156:MET:N	2.86	0.48
9:I:43:VAL:HG23	9:I:54:LYS:HA	1.94	0.48
19:S:5:LYS:O	19:S:23:VAL:HG13	2.14	0.48
9:I:71:ARG:NE	9:I:105:GLU:OE2	2.47	0.48
1:A:1450:A:N6	1:A:1635:A:H62	2.11	0.48
1:A:1969:C:OP2	1:A:1970:U:O2'	2.10	0.48
1:A:2325:A:H62	1:A:2345:A:H8	1.61	0.48
19:S:79:THR:OG1	19:S:94:ALA:O	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:2:ALA:O	24:X:39:ASP:N	2.45	0.48
1:A:1118:G:O2'	1:A:1119:C:O5'	2.31	0.48
11:K:27:VAL:HG23	11:K:134:ARG:CD	2.44	0.48
23:W:25:LEU:HD21	23:W:43:ILE:HG23	1.95	0.48
1:A:1533:A:C5	3:C:74:ILE:HD13	2.49	0.48
1:A:940:U:O4	1:A:941:A:N6	2.47	0.47
1:A:1097:U:O4	1:A:1098:A:N6	2.48	0.47
1:A:2259:C:OP2	22:V:27:ARG:NH2	2.40	0.47
1:A:115:C:HO2'	1:A:125:A:H8	1.61	0.47
1:A:1033:G:N7	24:X:13:ILE:HG21	2.29	0.47
1:A:2212:G:O2'	1:A:2213:U:O4'	2.11	0.47
11:K:40:SER:OG	11:K:41:TRP:N	2.48	0.47
3:C:67:PHE:HE1	3:C:105:ILE:HD11	1.79	0.47
1:A:60:U:O2	1:A:74:U:O2'	2.21	0.47
1:A:697:U:O2'	1:A:698:U:OP1	2.30	0.47
1:A:2663:U:HO2'	4:D:46:TYR:HH	1.62	0.47
1:A:674:C:O2	1:A:684:U:O2'	2.31	0.47
1:A:699:U:HO2'	1:A:700:A:C5'	2.28	0.47
1:A:1395:G:O2'	1:A:1410:A:N6	2.47	0.47
1:A:1824:C:O2'	3:C:259:THR:OG1	2.16	0.47
6:F:119:LYS:O	6:F:167:ARG:NH1	2.47	0.47
18:R:51:ALA:HB3	18:R:81:THR:O	2.15	0.47
4:D:104:GLU:N	4:D:104:GLU:OE1	2.48	0.47
1:A:2603:G:O2'	1:A:2606:C:OP2	2.31	0.46
5:E:20:SER:N	5:E:203:GLU:OE2	2.48	0.46
12:L:52:LYS:NZ	12:L:96:ARG:O	2.48	0.46
1:A:1593:G:OP2	1:A:1593:G:N2	2.48	0.46
18:R:3:ALA:O	18:R:45:ILE:HD11	2.15	0.46
1:A:1533:A:N6	3:C:98:ASP:OD1	2.48	0.46
1:A:2285:C:O2'	1:A:2454:C:OP2	2.30	0.46
1:A:2686:G:O2'	1:A:2688:G:N7	2.46	0.46
6:F:64:LYS:NZ	6:F:65:PRO:O	2.46	0.46
1:A:2784:A:N1	7:G:67:THR:HG21	2.31	0.46
1:A:267:G:HO2'	1:A:268:A:C5'	2.27	0.46
1:A:326:A:O2'	1:A:398:C:N4	2.49	0.46
2:B:38:U:N3	2:B:42:G:OP2	2.47	0.46
1:A:759:U:O2'	1:A:763:A:N6	2.33	0.46
1:A:1466:G:O2'	1:A:1535:G:N3	2.48	0.46
1:A:1101:A:OP2	1:A:1133:G:N2	2.49	0.46
10:J:55:LEU:O	10:J:60:ARG:NH1	2.49	0.45
1:A:405:G:N2	1:A:406:A:O3'	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:C:H1'	1:A:1155:A:H61	1.81	0.45
1:A:878:C:O2'	29:3:57:ARG:NH2	2.47	0.45
1:A:1552:U:O2'	1:A:1553:A:O4'	2.35	0.45
14:N:31:HIS:HB3	14:N:42:ILE:HD11	1.99	0.45
1:A:987:U:HO2'	1:A:988:C:P	2.36	0.45
11:K:27:VAL:HG23	11:K:134:ARG:HD3	1.98	0.45
19:S:57:LEU:CD1	19:S:59:THR:HG23	2.47	0.45
20:T:51:VAL:O	20:T:55:VAL:HG12	2.15	0.45
1:A:83:G:O2'	1:A:101:G:N2	2.45	0.45
1:A:199:A:O2'	1:A:850:G:O6	2.23	0.45
15:O:106:PHE:O	15:O:110:VAL:HG23	2.17	0.45
20:T:14:THR:N	20:T:17:ASP:OD2	2.45	0.45
1:A:1197:C:OP1	15:O:92:ARG:NH2	2.47	0.45
1:A:1491:C:O2'	1:A:1492:G:O4'	2.18	0.45
1:A:1945:A:N7	1:A:1946:A:N6	2.65	0.45
1:A:1952:C:O2'	1:A:1953:U:O4'	2.07	0.45
1:A:2288:C:OP1	21:U:27:LYS:NZ	2.46	0.45
1:A:2819:C:O2'	1:A:2820:U:OP1	2.29	0.45
1:A:1450:A:H61	1:A:1635:A:H62	1.65	0.44
1:A:2126:C:O2'	1:A:2127:G:O5'	2.29	0.44
7:G:2:SER:OG	7:G:65:HIS:ND1	2.35	0.44
2:B:68:U:O3'	21:U:82:ARG:NH1	2.49	0.44
10:J:55:LEU:HD23	10:J:60:ARG:HG2	1.99	0.44
1:A:2650:G:O5'	1:A:2845:G:N2	2.51	0.44
28:2:4:ARG:O	28:2:7:GLN:NE2	2.46	0.44
1:A:1901:C:O2	1:A:1903:A:O2'	2.29	0.44
1:A:11:U:O2'	1:A:12:U:OP1	2.32	0.44
1:A:2153:A:N3	1:A:2190:C:N4	2.66	0.44
1:A:2835:C:HO2'	26:Z:40:HIS:CE1	2.26	0.44
23:W:6:ILE:HG22	23:W:56:VAL:HG21	2.00	0.44
2:B:52:G:H21	6:F:26:MET:CE	2.31	0.44
3:C:69:ARG:O	3:C:189:ARG:NH1	2.51	0.44
1:A:99:U:O2	1:A:101:G:N1	2.50	0.44
18:R:7:LEU:HD21	18:R:42:VAL:HG12	2.00	0.44
25:Y:16:ASP:OD2	25:Y:18:THR:OG1	2.20	0.44
1:A:2377:C:OP2	29:3:45:ARG:NH2	2.45	0.43
1:A:1991:G:O2'	1:A:1994:C:OP2	2.11	0.43
1:A:2877:G:N2	1:A:2880:A:OP2	2.44	0.43
4:D:26:THR:OG1	4:D:199:GLY:O	2.35	0.43
27:1:31:GLU:OE1	27:1:46:ARG:NH2	2.51	0.43
5:E:155:VAL:HB	5:E:194:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1935:C:N4	1:A:1949:G:O6	2.51	0.43
1:A:2129:C:O2	1:A:2213:U:N3	2.51	0.43
1:A:2662:U:O2'	4:D:50:GLN:OE1	2.33	0.43
6:F:9:ASN:O	6:F:12:VAL:HG22	2.17	0.43
18:R:51:ALA:HB2	18:R:83:LYS:HG3	2.00	0.43
1:A:306:C:H42	1:A:409:G:H22	1.65	0.43
1:A:498:G:H21	1:A:503:A:H8	1.66	0.43
6:F:128:TYR:O	6:F:129:THR:OG1	2.34	0.43
26:Z:29:GLU:N	26:Z:29:GLU:OE1	2.47	0.43
1:A:1487:G:N7	1:A:1596:G:N2	2.67	0.43
5:E:12:THR:OG1	5:E:13:LYS:N	2.51	0.43
19:S:12:ILE:HD11	19:S:69:GLN:HB2	2.01	0.43
21:U:23:ASP:OD1	21:U:24:SER:N	2.51	0.43
1:A:914:G:O3'	11:K:6:ARG:NH1	2.53	0.42
1:A:1504:U:O2'	1:A:1505:G:OP2	2.37	0.42
1:A:2776:A:C1'	7:G:63:THR:HG22	2.50	0.42
18:R:61:LYS:O	18:R:72:THR:OG1	2.36	0.42
1:A:1582:U:O2'	1:A:1585:G:O6	2.37	0.42
1:A:1886:A:H61	1:A:1910:G:C2'	2.32	0.42
5:E:146:LEU:O	5:E:148:GLN:N	2.52	0.42
1:A:262:G:H21	1:A:666:A:H8	1.66	0.42
1:A:1515:G:H22	1:A:1565:U:H3	1.66	0.42
3:C:236:GLU:OE1	3:C:236:GLU:N	2.53	0.42
7:G:152:ARG:O	7:G:162:ILE:N	2.50	0.42
1:A:100:U:O2'	1:A:101:G:OP1	2.37	0.42
1:A:606:G:OP2	16:P:78:ARG:NH2	2.49	0.42
1:A:2170:C:O2'	1:A:2171:G:O4'	2.28	0.42
31:A:3001:ERY:H203	31:A:3001:ERY:H192	1.68	0.42
1:A:1087:C:N4	1:A:1088:C:H41	2.18	0.42
8:H:126:TYR:HH	8:H:133:HIS:CD2	2.36	0.42
13:M:55:GLN:O	13:M:83:LYS:NZ	2.40	0.42
25:Y:53:ASP:OD1	25:Y:54:SER:N	2.53	0.42
9:I:67:SER:O	9:I:67:SER:OG	2.34	0.42
1:A:352:A:N3	1:A:372:A:O2'	2.42	0.42
19:S:7:ASP:O	19:S:23:VAL:HG12	2.20	0.42
1:A:267:G:O2'	1:A:268:A:O5'	2.26	0.41
1:A:325:A:H1'	1:A:400:C:H42	1.85	0.41
5:E:158:ASN:OD1	5:E:159:GLU:N	2.46	0.41
9:I:64:ARG:NE	9:I:81:GLU:OE2	2.53	0.41
1:A:2693:C:H42	7:G:109:TYR:HA	1.84	0.41
4:D:180:VAL:HG21	4:D:183:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:A:OP1	10:J:64:ARG:NH1	2.53	0.41
1:A:284:C:HO2'	1:A:287:G:H1	1.67	0.41
1:A:582:G:OP1	1:A:1039:C:N4	2.50	0.41
1:A:1875:A:HO2'	1:A:1876:G:C5'	2.33	0.41
1:A:697:U:HO2'	1:A:698:U:P	2.43	0.41
1:A:1478:A:H2'	1:A:1479:G:O4'	2.21	0.41
1:A:1763:U:N3	1:A:1766:C:OP2	2.46	0.41
6:F:115:GLN:OE1	6:F:118:SER:N	2.53	0.41
8:H:46:THR:OG1	8:H:49:VAL:HG12	2.21	0.41
8:H:142:GLU:O	8:H:144:ARG:NH1	2.51	0.41
18:R:6:ILE:HD11	18:R:41:ALA:HB2	2.01	0.41
1:A:2823:G:O2'	1:A:2824:G:OP1	2.34	0.41
1:A:2342:U:O2	6:F:125:ARG:NH2	2.54	0.41
1:A:2568:A:HO2'	1:A:2569:A:P	2.40	0.41
3:C:157:SER:OG	3:C:158:ALA:N	2.54	0.41
12:L:73:ASN:N	12:L:77:THR:O	2.53	0.41
1:A:1884:G:N2	1:A:1912:A:C6	2.89	0.41
1:A:2433:C:H3'	1:A:2434:A:H5"	2.03	0.41
25:Y:2:LYS:HD2	25:Y:5:ILE:HD11	2.03	0.41
1:A:409:G:N2	1:A:411:A:H62	2.19	0.41
1:A:2126:C:HO2'	1:A:2127:G:P	2.44	0.40
1:A:2128:G:N2	1:A:2214:G:O6	2.54	0.40
3:C:181:VAL:HG22	3:C:272:ARG:HB3	2.04	0.40
1:A:300:G:H1	1:A:467:U:HO2'	1.67	0.40
23:W:61:GLU:N	23:W:61:GLU:OE1	2.54	0.40
1:A:592:A:O2'	1:A:593:U:O5'	2.38	0.40
1:A:1312:A:N1	1:A:1332:C:O2'	2.46	0.40
1:A:1518:G:O2'	1:A:1519:U:OP2	2.30	0.40
4:D:187:GLN:HG2	4:D:196:LEU:HD12	2.03	0.40
19:S:33:VAL:O	19:S:63:ILE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
4	D	213/215 (99%)	194 (91%)	19 (9%)	0	100	100
5	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
6	F	171/173 (99%)	142 (83%)	29 (17%)	0	100	100
7	G	171/173 (99%)	154 (90%)	17 (10%)	0	100	100
8	H	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
9	I	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	J	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
11	K	135/137 (98%)	125 (93%)	10 (7%)	0	100	100
12	L	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
13	M	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	N	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
15	O	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
16	P	100/102 (98%)	91 (91%)	8 (8%)	1 (1%)	15	17
17	Q	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
18	R	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
19	S	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
20	T	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
21	U	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
22	V	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
23	W	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
24	X	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
25	Y	57/59 (97%)	45 (79%)	12 (21%)	0	100	100
26	Z	46/48 (96%)	39 (85%)	7 (15%)	0	100	100
27	1	45/47 (96%)	45 (100%)	0	0	100	100
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
30	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	3050/3106 (98%)	2831 (93%)	218 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	51	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	220/221 (100%)	211 (96%)	9 (4%)	30	43
4	D	173/173 (100%)	162 (94%)	11 (6%)	17	23
5	E	168/168 (100%)	157 (94%)	11 (6%)	17	23
6	F	141/152 (93%)	131 (93%)	10 (7%)	14	19
7	G	122/151 (81%)	112 (92%)	10 (8%)	11	14
8	H	123/123 (100%)	119 (97%)	4 (3%)	38	53
9	I	100/100 (100%)	94 (94%)	6 (6%)	19	26
10	J	109/112 (97%)	99 (91%)	10 (9%)	9	11
11	K	110/114 (96%)	105 (96%)	5 (4%)	27	39
12	L	96/101 (95%)	90 (94%)	6 (6%)	18	24
13	M	85/94 (90%)	78 (92%)	7 (8%)	11	14
14	N	93/100 (93%)	87 (94%)	6 (6%)	17	23
15	O	96/96 (100%)	91 (95%)	5 (5%)	23	32
16	P	84/86 (98%)	77 (92%)	7 (8%)	11	14
17	Q	88/90 (98%)	82 (93%)	6 (7%)	16	21
18	R	78/80 (98%)	74 (95%)	4 (5%)	24	33
19	S	81/88 (92%)	77 (95%)	4 (5%)	25	35
20	T	78/82 (95%)	73 (94%)	5 (6%)	17	23
21	U	59/60 (98%)	55 (93%)	4 (7%)	16	21
22	V	39/41 (95%)	38 (97%)	1 (3%)	46	63
23	W	58/60 (97%)	54 (93%)	4 (7%)	15	20
24	X	52/52 (100%)	50 (96%)	2 (4%)	33	47
25	Y	23/56 (41%)	22 (96%)	1 (4%)	29	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Z	35/44 (80%)	35 (100%)	0	100	100
27	1	44/45 (98%)	41 (93%)	3 (7%)	16	21
28	2	39/39 (100%)	38 (97%)	1 (3%)	46	63
29	3	55/55 (100%)	51 (93%)	4 (7%)	14	18
30	4	35/35 (100%)	33 (94%)	2 (6%)	20	28
All	All	2484/2618 (95%)	2336 (94%)	148 (6%)	23	26

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	40	LYS
3	C	98	ASP
3	C	167	LYS
3	C	168	GLU
3	C	219	THR
3	C	220	VAL
3	C	236	GLU
3	C	248	SER
3	C	271	VAL
4	D	2	THR
4	D	13	THR
4	D	15	VAL
4	D	25	VAL
4	D	27	VAL
4	D	36	LEU
4	D	100	GLU
4	D	125	LYS
4	D	145	SER
4	D	159	ASP
4	D	178	VAL
5	E	3	ASN
5	E	49	HIS
5	E	55	SER
5	E	70	THR
5	E	93	THR
5	E	108	LEU
5	E	114	LEU
5	E	120	GLU
5	E	154	VAL
5	E	192	LEU

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Mol	Chain	Res	Type
5	E	194	ILE
6	F	20	PHE
6	F	50	LEU
6	F	51	ASP
6	F	57	LEU
6	F	69	LYS
6	F	76	THR
6	F	117	VAL
6	F	120	LYS
6	F	125	ARG
6	F	136	LEU
7	G	15	VAL
7	G	30	LYS
7	G	43	PHE
7	G	44	LYS
7	G	69	ARG
7	G	79	VAL
7	G	87	LEU
7	G	103	LEU
7	G	137	SER
7	G	155	GLU
8	H	1	MET
8	H	37	LEU
8	H	46	THR
8	H	93	LEU
9	I	19	VAL
9	I	21	THR
9	I	25	LEU
9	I	42	THR
9	I	112	MET
9	I	122	LEU
10	J	19	VAL
10	J	41	ARG
10	J	46	VAL
10	J	57	LEU
10	J	61	LEU
10	J	64	ARG
10	J	77	VAL
10	J	79	LEU
10	J	96	LEU
10	J	121	LEU
11	K	25	ASN

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Mol	Chain	Res	Type
11	K	37	THR
11	K	109	VAL
11	K	125	LEU
11	K	137	LEU
12	L	9	THR
12	L	20	LEU
12	L	24	LEU
12	L	77	THR
12	L	116	SER
12	L	117	VAL
13	M	6	ASP
13	M	21	ASN
13	M	22	LEU
13	M	35	ARG
13	M	37	ASN
13	M	52	THR
13	M	87	LYS
14	N	14	GLN
14	N	15	LEU
14	N	19	LEU
14	N	52	ARG
14	N	53	ARG
14	N	98	LYS
15	O	4	VAL
15	O	20	LEU
15	O	75	SER
15	O	77	SER
15	O	95	LEU
16	P	23	GLU
16	P	34	THR
16	P	63	ASN
16	P	78	ARG
16	P	79	ARG
16	P	80	LYS
16	P	100	ILE
17	Q	19	LEU
17	Q	21	LEU
17	Q	51	LEU
17	Q	103	ILE
17	Q	104	VAL
17	Q	110	GLU
18	R	14	GLU

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Mol	Chain	Res	Type
18	R	56	MET
18	R	69	GLN
18	R	72	THR
19	S	26	THR
19	S	39	ASN
19	S	43	LYS
19	S	66	SER
20	T	4	LEU
20	T	30	VAL
20	T	31	VAL
20	T	72	VAL
20	T	89	ILE
21	U	19	LYS
21	U	61	ARG
21	U	75	VAL
21	U	87	VAL
22	V	27	ARG
23	W	10	THR
23	W	25	LEU
23	W	52	ARG
23	W	61	GLU
24	X	12	VAL
24	X	18	THR
25	Y	1	MET
27	1	34	LYS
27	1	43	THR
27	1	44	LEU
28	2	40	ARG
29	3	14	VAL
29	3	31	HIS
29	3	32	LEU
29	3	51	SER
30	4	11	CYS
30	4	27	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	86	ASN
5	E	169	ASN
7	G	64	ASN
8	H	11	ASN

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Mol	Chain	Res	Type
20	T	84	ASN
27	1	22	ASN
27	1	25	ASN
28	2	17	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2896/2905 (99%)	685 (23%)	24 (0%)
2	B	113/114 (99%)	15 (13%)	1 (0%)
All	All	3009/3019 (99%)	700 (23%)	25 (0%)

All (700) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	28	A
1	A	34	U
1	A	43	A
1	A	45	G
1	A	46	C
1	A	55	G
1	A	64	A
1	A	67	G
1	A	71	A
1	A	74	U
1	A	75	G
1	A	88	G
1	A	90	A
1	A	91	A
1	A	93	U
1	A	96	G
1	A	101	G
1	A	102	A
1	A	105	C
1	A	106	A
1	A	117	A
1	A	118	A
1	A	119	U
1	A	141	U
1	A	150	A

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Mol	Chain	Res	Type
1	A	158	G
1	A	164	A
1	A	166	A
1	A	167	U
1	A	168	A
1	A	169	G
1	A	173	A
1	A	177	G
1	A	180	G
1	A	182	C
1	A	184	C
1	A	199	A
1	A	202	A
1	A	216	A
1	A	218	G
1	A	219	A
1	A	224	A
1	A	225	A
1	A	233	U
1	A	236	A
1	A	251	G
1	A	255	G
1	A	268	A
1	A	270	C
1	A	275	A
1	A	283	G
1	A	284	C
1	A	286	U
1	A	292	U
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	303	G
1	A	306	C
1	A	307	A
1	A	310	C
1	A	311	U
1	A	315	C
1	A	317	G
1	A	319	G
1	A	321	U

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Mol	Chain	Res	Type
1	A	324	A
1	A	325	A
1	A	326	A
1	A	327	G
1	A	328	G
1	A	330	C
1	A	331	G
1	A	332	A
1	A	333	C
1	A	335	U
1	A	336	U
1	A	338	G
1	A	340	C
1	A	373	A
1	A	387	G
1	A	388	A
1	A	389	A
1	A	391	A
1	A	392	U
1	A	394	U
1	A	396	G
1	A	397	U
1	A	398	C
1	A	402	C
1	A	404	U
1	A	405	G
1	A	406	A
1	A	407	G
1	A	408	U
1	A	410	G
1	A	411	A
1	A	417	A
1	A	432	G
1	A	433	U
1	A	435	A
1	A	437	A
1	A	445	G
1	A	447	A
1	A	449	U
1	A	458	A
1	A	463	C
1	A	482	U

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Mol	Chain	Res	Type
1	A	490	C
1	A	497	U
1	A	504	G
1	A	505	U
1	A	506	A
1	A	512	A
1	A	513	G
1	A	525	A
1	A	526	A
1	A	527	G
1	A	537	A
1	A	550	A
1	A	553	A
1	A	554	C
1	A	555	C
1	A	563	G
1	A	565	G
1	A	566	U
1	A	572	C
1	A	576	U
1	A	577	A
1	A	578	G
1	A	583	A
1	A	591	A
1	A	593	U
1	A	594	G
1	A	606	G
1	A	611	U
1	A	616	G
1	A	618	A
1	A	646	A
1	A	647	G
1	A	656	G
1	A	659	A
1	A	660	A
1	A	661	U
1	A	666	A
1	A	672	A
1	A	679	G
1	A	682	A
1	A	688	A
1	A	689	A

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Mol	Chain	Res	Type
1	A	691	A
1	A	696	G
1	A	698	U
1	A	699	U
1	A	700	A
1	A	713	A
1	A	720	A
1	A	722	A
1	A	729	G
1	A	731	U
1	A	750	A
1	A	753	U
1	A	755	C
1	A	756	A
1	A	758	G
1	A	759	U
1	A	760	A
1	A	761	A
1	A	762	C
1	A	763	A
1	A	766	G
1	A	775	A
1	A	783	G
1	A	785	C
1	A	792	U
1	A	793	G
1	A	797	A
1	A	802	G
1	A	807	U
1	A	809	A
1	A	810	A
1	A	816	G
1	A	820	G
1	A	822	G
1	A	823	G
1	A	827	A
1	A	829	U
1	A	830	U
1	A	834	A
1	A	837	G
1	A	841	C
1	A	850	G

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Mol	Chain	Res	Type
1	A	857	C
1	A	868	A
1	A	870	C
1	A	872	U
1	A	890	G
1	A	891	A
1	A	904	G
1	A	911	A
1	A	920	A
1	A	928	C
1	A	940	U
1	A	952	A
1	A	955	A
1	A	957	C
1	A	965	G
1	A	970	U
1	A	971	U
1	A	972	A
1	A	974	U
1	A	977	A
1	A	985	A
1	A	988	C
1	A	989	A
1	A	990	G
1	A	1003	A
1	A	1005	G
1	A	1018	A
1	A	1019	A
1	A	1024	A
1	A	1025	A
1	A	1027	A
1	A	1037	A
1	A	1040	A
1	A	1043	U
1	A	1046	G
1	A	1049	C
1	A	1056	U
1	A	1057	A
1	A	1058	U
1	A	1061	G
1	A	1065	A
1	A	1066	G

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Mol	Chain	Res	Type
1	A	1067	U
1	A	1070	A
1	A	1077	U
1	A	1078	G
1	A	1087	C
1	A	1088	C
1	A	1089	C
1	A	1091	G
1	A	1092	A
1	A	1093	C
1	A	1094	A
1	A	1100	G
1	A	1103	G
1	A	1105	U
1	A	1106	G
1	A	1109	U
1	A	1111	A
1	A	1113	A
1	A	1114	A
1	A	1115	G
1	A	1117	A
1	A	1118	G
1	A	1119	C
1	A	1120	C
1	A	1121	A
1	A	1122	U
1	A	1127	U
1	A	1130	A
1	A	1132	A
1	A	1133	G
1	A	1137	G
1	A	1138	U
1	A	1139	A
1	A	1140	A
1	A	1143	G
1	A	1146	C
1	A	1147	A
1	A	1150	A
1	A	1155	A
1	A	1156	G
1	A	1158	G
1	A	1159	A

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Mol	Chain	Res	Type
1	A	1160	C
1	A	1161	A
1	A	1162	C
1	A	1163	U
1	A	1166	G
1	A	1172	A
1	A	1176	U
1	A	1178	C
1	A	1186	A
1	A	1192	A
1	A	1201	G
1	A	1208	A
1	A	1214	C
1	A	1215	U
1	A	1216	U
1	A	1217	U
1	A	1218	G
1	A	1219	G
1	A	1220	A
1	A	1253	G
1	A	1265	G
1	A	1275	A
1	A	1276	G
1	A	1285	A
1	A	1288	G
1	A	1290	G
1	A	1291	A
1	A	1294	G
1	A	1298	G
1	A	1300	G
1	A	1304	G
1	A	1309	G
1	A	1310	A
1	A	1311	A
1	A	1312	A
1	A	1321	A
1	A	1337	A
1	A	1338	U
1	A	1354	G
1	A	1370	C
1	A	1389	U
1	A	1397	G

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Mol	Chain	Res	Type
1	A	1402	A
1	A	1405	G
1	A	1416	U
1	A	1421	A
1	A	1424	A
1	A	1447	A
1	A	1450	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1454	U
1	A	1455	U
1	A	1456	U
1	A	1459	A
1	A	1460	U
1	A	1463	A
1	A	1464	U
1	A	1467	G
1	A	1471	A
1	A	1472	C
1	A	1479	G
1	A	1480	G
1	A	1483	A
1	A	1489	A
1	A	1490	G
1	A	1491	C
1	A	1495	C
1	A	1496	G
1	A	1498	U
1	A	1503	U
1	A	1504	U
1	A	1510	U
1	A	1516	C
1	A	1519	U
1	A	1520	A
1	A	1525	U
1	A	1526	G
1	A	1527	A
1	A	1533	A
1	A	1534	G
1	A	1537	A
1	A	1550	G

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Mol	Chain	Res	Type
1	A	1552	U
1	A	1553	A
1	A	1554	A
1	A	1555	G
1	A	1556	G
1	A	1561	G
1	A	1566	G
1	A	1569	G
1	A	1570	G
1	A	1575	A
1	A	1578	A
1	A	1581	U
1	A	1582	U
1	A	1583	G
1	A	1584	U
1	A	1586	U
1	A	1588	U
1	A	1590	C
1	A	1591	G
1	A	1593	G
1	A	1594	U
1	A	1595	C
1	A	1601	U
1	A	1602	U
1	A	1603	U
1	A	1605	A
1	A	1606	C
1	A	1613	G
1	A	1616	A
1	A	1627	G
1	A	1629	U
1	A	1630	A
1	A	1631	G
1	A	1633	A
1	A	1634	A
1	A	1635	A
1	A	1636	U
1	A	1639	G
1	A	1651	C
1	A	1653	A
1	A	1654	A
1	A	1658	A

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Mol	Chain	Res	Type
1	A	1660	A
1	A	1661	C
1	A	1666	A
1	A	1679	A
1	A	1690	A
1	A	1692	C
1	A	1718	G
1	A	1731	G
1	A	1732	U
1	A	1737	U
1	A	1740	G
1	A	1742	A
1	A	1747	G
1	A	1756	U
1	A	1757	U
1	A	1760	G
1	A	1761	G
1	A	1762	U
1	A	1763	U
1	A	1764	A
1	A	1765	A
1	A	1766	C
1	A	1768	C
1	A	1769	C
1	A	1770	C
1	A	1771	A
1	A	1772	G
1	A	1773	A
1	A	1790	G
1	A	1791	G
1	A	1797	G
1	A	1800	A
1	A	1803	G
1	A	1806	U
1	A	1818	A
1	A	1819	G
1	A	1820	G
1	A	1827	C
1	A	1828	U
1	A	1829	A
1	A	1843	U
1	A	1856	A

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Mol	Chain	Res	Type
1	A	1860	C
1	A	1875	A
1	A	1877	G
1	A	1885	G
1	A	1886	A
1	A	1893	A
1	A	1895	C
1	A	1897	U
1	A	1899	U
1	A	1900	G
1	A	1901	C
1	A	1902	G
1	A	1903	A
1	A	1904	A
1	A	1910	G
1	A	1912	A
1	A	1914	C
1	A	1915	G
1	A	1916	A
1	A	1917	A
1	A	1933	G
1	A	1938	U
1	A	1939	A
1	A	1945	A
1	A	1946	A
1	A	1948	G
1	A	1950	U
1	A	1951	C
1	A	1956	G
1	A	1957	G
1	A	1964	A
1	A	1965	A
1	A	1966	U
1	A	1982	U
1	A	1990	C
1	A	1994	C
1	A	1996	A
1	A	1997	A
1	A	1998	A
1	A	1999	G
1	A	2009	U
1	A	2018	U

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Mol	Chain	Res	Type
1	A	2020	U
1	A	2024	A
1	A	2029	G
1	A	2050	A
1	A	2058	A
1	A	2059	G
1	A	2060	A
1	A	2062	G
1	A	2063	C
1	A	2070	C
1	A	2082	C
1	A	2083	G
1	A	2086	A
1	A	2087	A
1	A	2088	G
1	A	2089	A
1	A	2096	G
1	A	2097	G
1	A	2109	A
1	A	2118	U
1	A	2120	G
1	A	2127	G
1	A	2128	G
1	A	2129	C
1	A	2130	A
1	A	2132	A
1	A	2133	G
1	A	2134	C
1	A	2136	U
1	A	2139	A
1	A	2143	G
1	A	2144	A
1	A	2145	U
1	A	2146	A
1	A	2153	A
1	A	2155	C
1	A	2156	C
1	A	2158	U
1	A	2160	G
1	A	2161	A
1	A	2164	C
1	A	2165	G

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Mol	Chain	Res	Type
1	A	2173	U
1	A	2175	G
1	A	2180	C
1	A	2181	G
1	A	2185	A
1	A	2186	G
1	A	2187	G
1	A	2188	C
1	A	2190	C
1	A	2194	U
1	A	2195	G
1	A	2197	G
1	A	2204	C
1	A	2212	G
1	A	2215	U
1	A	2224	U
1	A	2225	A
1	A	2229	C
1	A	2231	C
1	A	2232	A
1	A	2235	A
1	A	2238	U
1	A	2240	U
1	A	2241	C
1	A	2252	A
1	A	2262	G
1	A	2265	G
1	A	2266	G
1	A	2290	C
1	A	2295	A
1	A	2306	G
1	A	2310	C
1	A	2314	A
1	A	2321	C
1	A	2324	C
1	A	2328	A
1	A	2330	G
1	A	2331	G
1	A	2332	U
1	A	2333	U
1	A	2334	G
1	A	2335	G

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Mol	Chain	Res	Type
1	A	2336	A
1	A	2337	A
1	A	2345	A
1	A	2346	U
1	A	2347	A
1	A	2348	G
1	A	2352	G
1	A	2357	G
1	A	2362	A
1	A	2369	C
1	A	2372	G
1	A	2374	C
1	A	2377	C
1	A	2388	A
1	A	2396	A
1	A	2410	G
1	A	2412	C
1	A	2417	U
1	A	2418	G
1	A	2427	G
1	A	2429	U
1	A	2430	C
1	A	2433	C
1	A	2434	A
1	A	2438	A
1	A	2441	G
1	A	2449	C
1	A	2450	U
1	A	2451	C
1	A	2452	A
1	A	2456	G
1	A	2457	A
1	A	2460	A
1	A	2461	A
1	A	2468	C
1	A	2474	G
1	A	2475	A
1	A	2502	C
1	A	2503	A
1	A	2505	A
1	A	2521	G
1	A	2529	G

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Mol	Chain	Res	Type
1	A	2530	A
1	A	2532	G
1	A	2533	U
1	A	2547	C
1	A	2556	G
1	A	2561	C
1	A	2562	G
1	A	2569	A
1	A	2579	U
1	A	2581	U
1	A	2588	A
1	A	2589	U
1	A	2592	A
1	A	2593	A
1	A	2594	G
1	A	2599	A
1	A	2605	G
1	A	2611	U
1	A	2612	U
1	A	2613	C
1	A	2626	G
1	A	2629	A
1	A	2636	U
1	A	2640	U
1	A	2648	G
1	A	2656	A
1	A	2657	G
1	A	2673	C
1	A	2683	U
1	A	2692	A
1	A	2695	G
1	A	2697	G
1	A	2700	G
1	A	2709	U
1	A	2716	U
1	A	2733	A
1	A	2741	G
1	A	2751	U
1	A	2753	U
1	A	2760	A
1	A	2764	G
1	A	2771	G

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Mol	Chain	Res	Type
1	A	2775	A
1	A	2784	A
1	A	2792	A
1	A	2794	C
1	A	2803	A
1	A	2805	A
1	A	2806	U
1	A	2807	G
1	A	2817	A
1	A	2818	A
1	A	2819	C
1	A	2820	U
1	A	2821	U
1	A	2822	C
1	A	2823	G
1	A	2824	G
1	A	2826	U
1	A	2827	A
1	A	2828	U
1	A	2832	A
1	A	2840	A
1	A	2842	G
1	A	2843	A
1	A	2879	G
1	A	2887	G
1	A	2892	G
1	A	2900	C
1	A	2903	A
1	A	2913	G
2	B	10	U
2	B	23	U
2	B	24	C
2	B	26	C
2	B	28	C
2	B	30	U
2	B	33	U
2	B	39	G
2	B	42	G
2	B	55	A
2	B	84	U
2	B	87	C
2	B	88	G

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Mol	Chain	Res	Type
2	B	95	U
2	B	106	G

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	11	U
1	A	157	U
1	A	267	G
1	A	291	G
1	A	325	A
1	A	327	G
1	A	403	U
1	A	576	U
1	A	688	A
1	A	697	U
1	A	840	C
1	A	872	U
1	A	987	U
1	A	1024	A
1	A	1604	C
1	A	1731	G
1	A	2117	A
1	A	2127	G
1	A	2211	U
1	A	2261	G
1	A	2450	U
1	A	2568	A
1	A	2823	G
1	A	2878	U
2	B	38	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
31	ERY	A	3001	-	53,53,53	2.15	12 (22%)	82,82,82	4.55	35 (42%)

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
31	ERY	A	3001	-	3/3/21/21	31/72/107/107	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	3001	ERY	O2-C1	10.61	1.59	1.34
31	A	3001	ERY	C19-C16	3.85	1.60	1.52
31	A	3001	ERY	O2-C13	-3.62	1.40	1.46
31	A	3001	ERY	O4-C14	3.55	1.51	1.42
31	A	3001	ERY	O10-C6	-3.45	1.38	1.44
31	A	3001	ERY	C7-C6	3.03	1.59	1.54
31	A	3001	ERY	O9-C22	2.98	1.49	1.41
31	A	3001	ERY	C12-C13	2.86	1.60	1.54
31	A	3001	ERY	C10-C11	-2.79	1.50	1.54
31	A	3001	ERY	C24-N1	2.14	1.53	1.48
31	A	3001	ERY	C10-C9	2.12	1.56	1.52
31	A	3001	ERY	O13-C12	-2.10	1.40	1.44

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	3001	ERY	O5-C16-C17	-16.60	79.22	103.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	3001	ERY	O13-C12-C13	-12.66	86.93	107.28
31	A	3001	ERY	O5-C16-C15	-11.57	94.42	112.96
31	A	3001	ERY	O5-C16-C19	-11.39	91.93	110.92
31	A	3001	ERY	O13-C12-C35	-11.29	84.46	107.78
31	A	3001	ERY	O13-C12-C11	-10.62	87.48	108.90
31	A	3001	ERY	O10-C6-C7	-9.68	83.44	108.40
31	A	3001	ERY	O10-C6-C5	-9.49	89.58	107.59
31	A	3001	ERY	O10-C6-C32	-9.31	87.01	108.47
31	A	3001	ERY	C15-C16-C17	7.34	120.83	107.67
31	A	3001	ERY	C20-O5-C16	7.03	132.22	117.55
31	A	3001	ERY	C35-C12-C13	6.43	120.36	111.31
31	A	3001	ERY	C32-C6-C7	5.93	121.13	111.09
31	A	3001	ERY	C19-C16-C15	5.08	119.55	110.49
31	A	3001	ERY	C7-C6-C5	4.90	120.05	110.48
31	A	3001	ERY	C35-C12-C11	4.81	121.49	113.05
31	A	3001	ERY	C32-C6-C5	4.37	117.80	110.12
31	A	3001	ERY	C13-C12-C11	4.36	116.89	108.28
31	A	3001	ERY	C19-C16-C17	4.00	119.42	111.24
31	A	3001	ERY	C25-C24-N1	-3.75	105.08	115.67
31	A	3001	ERY	C34-C10-C11	-3.67	109.81	114.38
31	A	3001	ERY	C6-C5-C4	3.58	119.11	114.05
31	A	3001	ERY	C13-O2-C1	-3.51	111.95	118.18
31	A	3001	ERY	C14-O3-C3	3.28	121.30	114.66
31	A	3001	ERY	O12-C11-C12	3.23	112.71	106.68
31	A	3001	ERY	C27-C26-C25	-2.88	108.88	113.40
31	A	3001	ERY	O3-C3-C2	-2.72	106.40	111.14
31	A	3001	ERY	C12-C11-C10	-2.68	113.08	116.43
31	A	3001	ERY	O3-C3-C4	2.62	111.38	108.22
31	A	3001	ERY	C31-C4-C3	-2.42	107.05	111.40
31	A	3001	ERY	O7-C5-C4	-2.38	107.97	111.54
31	A	3001	ERY	C23-C24-N1	2.23	117.27	110.83
31	A	3001	ERY	C16-C17-C18	2.08	114.32	111.14
31	A	3001	ERY	C21-C18-C17	-2.07	109.04	112.57
31	A	3001	ERY	O4-C14-C15	-2.02	108.28	112.12

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	A	3001	ERY	C14
31	A	3001	ERY	C12
31	A	3001	ERY	C6

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	3001	ERY	C34-C10-C11-C12
31	A	3001	ERY	C10-C11-C12-O13
31	A	3001	ERY	O12-C11-C12-C35
31	A	3001	ERY	O12-C11-C12-O13
31	A	3001	ERY	C11-C12-C13-O2
31	A	3001	ERY	C11-C12-C13-C36
31	A	3001	ERY	C35-C12-C13-C36
31	A	3001	ERY	C12-C13-O2-C1
31	A	3001	ERY	C4-C5-C6-C32
31	A	3001	ERY	O7-C5-C6-C7
31	A	3001	ERY	O7-C5-C6-C32
31	A	3001	ERY	C32-C6-C7-C8
31	A	3001	ERY	O4-C14-O3-C3
31	A	3001	ERY	C23-C24-N1-C28
31	A	3001	ERY	C23-C24-N1-C29
31	A	3001	ERY	C25-C24-N1-C28
31	A	3001	ERY	C25-C24-N1-C29
31	A	3001	ERY	C35-C12-C13-O2
31	A	3001	ERY	C36-C13-O2-C1
31	A	3001	ERY	O9-C22-O7-C5
31	A	3001	ERY	O10-C6-C7-C8
31	A	3001	ERY	C4-C5-C6-C7
31	A	3001	ERY	O1-C1-C2-C3
31	A	3001	ERY	O2-C1-C2-C3
31	A	3001	ERY	C9-C10-C11-C12
31	A	3001	ERY	O2-C13-C36-C37
31	A	3001	ERY	C23-C22-O7-C5
31	A	3001	ERY	O3-C3-C4-C31
31	A	3001	ERY	C34-C10-C11-O12
31	A	3001	ERY	C9-C10-C11-O12
31	A	3001	ERY	C2-C3-C4-C31

There are no ring outliers.

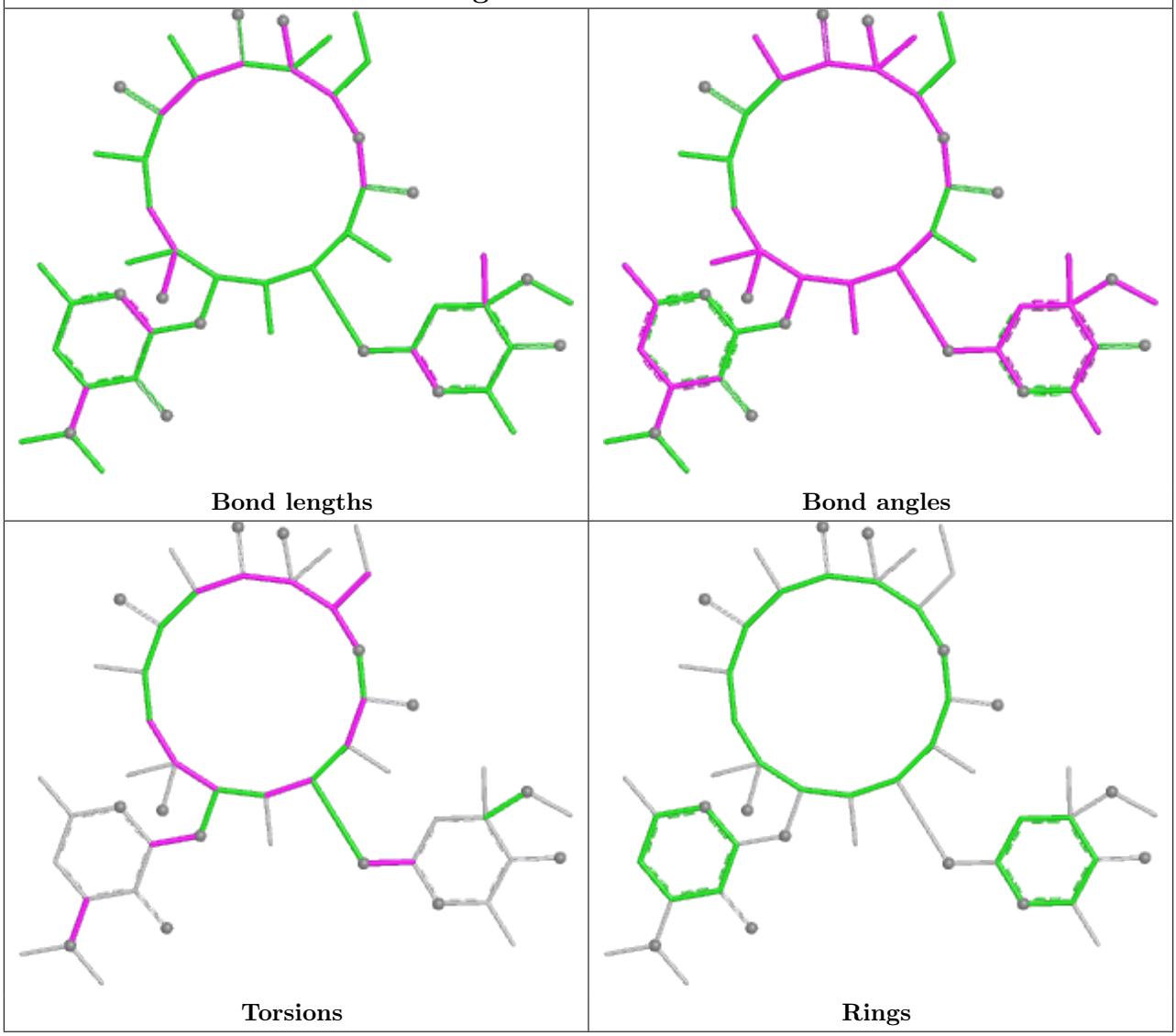
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	3001	ERY	1	0

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 then 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.

Ligand ERY A 3001



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
1	A	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1939:A	O3'	1944:U	P	12.58
1	A	929:C	O3'	937:G	P	11.18
1	A	2207:U	O3'	2208:A	P	9.28
1	A	1096:C	O3'	1097:U	P	6.34
1	A	1153:C	O3'	1154:G	P	5.30
1	A	2217:G	O3'	2218:G	P	3.26
1	A	1448:U	O3'	1449:A	P	3.19
1	A	328:G	O3'	329:A	P	3.09

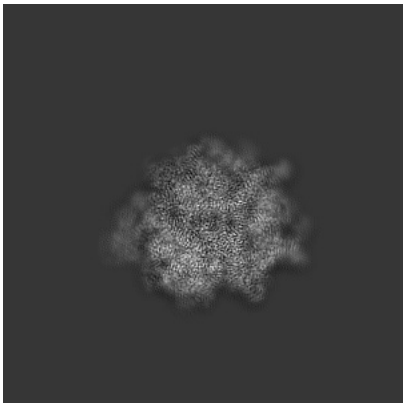
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10077. These allow visual inspection of the internal detail of the map and identification of artifacts.

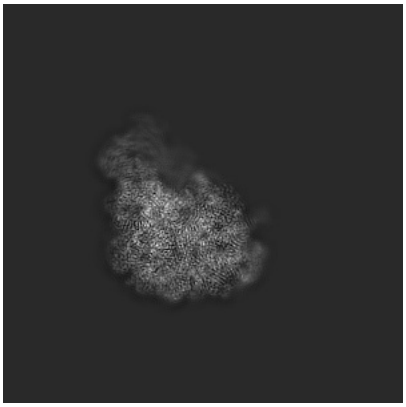
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

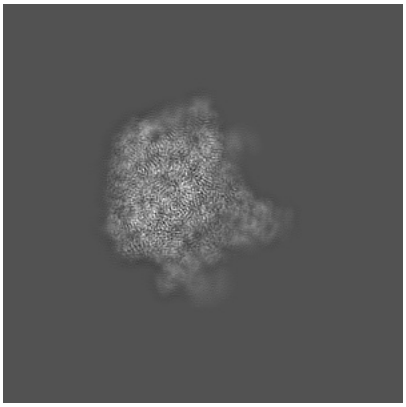
6.1.1 Primary map



X



Y

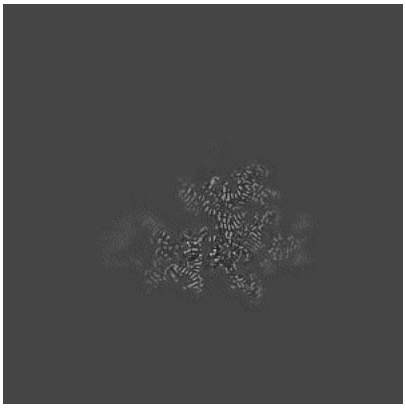


Z

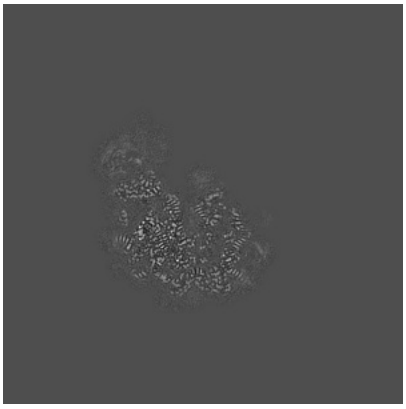
The images above show the map projected in three orthogonal directions.

6.2 Central slices

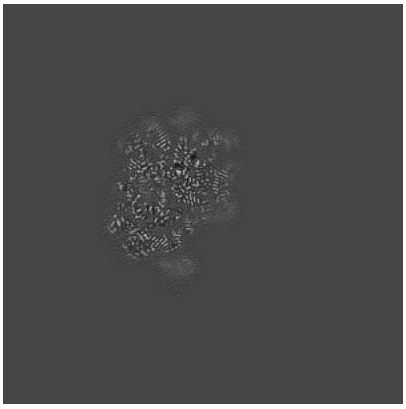
6.2.1 Primary map



X Index: 200



Y Index: 200

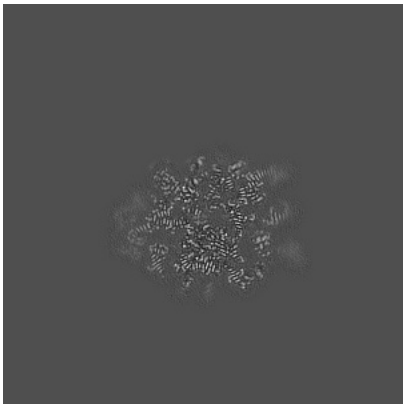


Z Index: 200

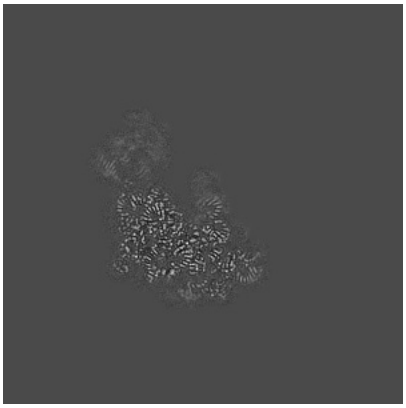
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

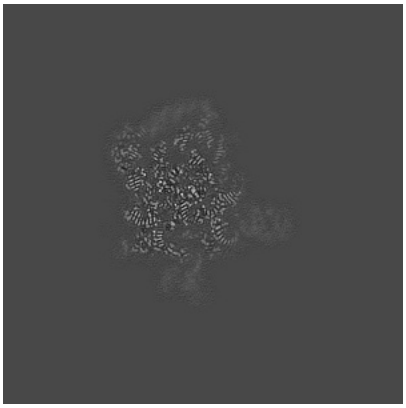
6.3.1 Primary map



X Index: 171



Y Index: 186

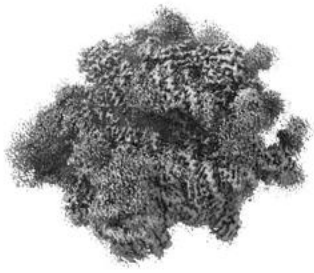


Z Index: 148

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

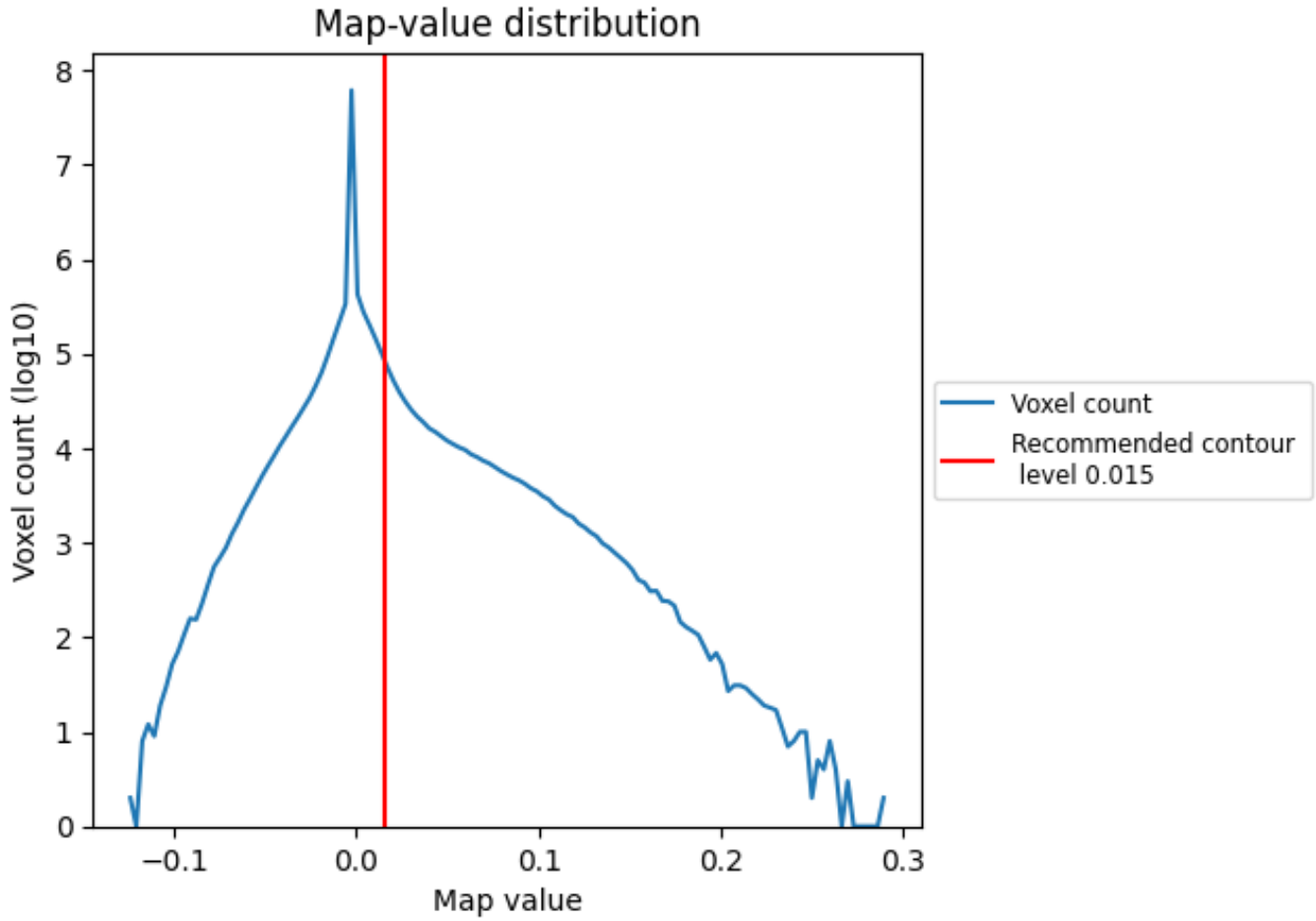
6.5 Mask visualisation (i)

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

7 Map analysis

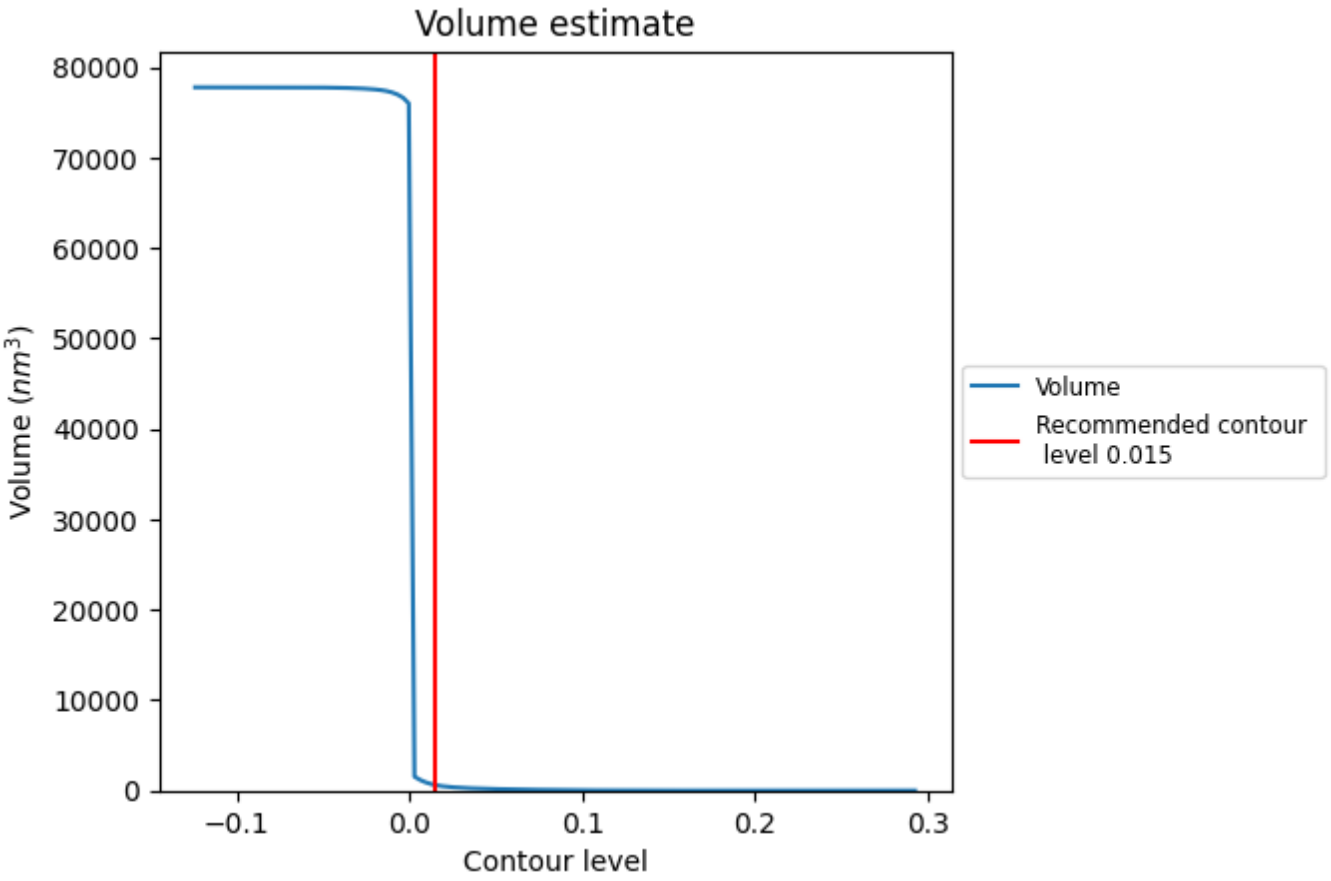
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

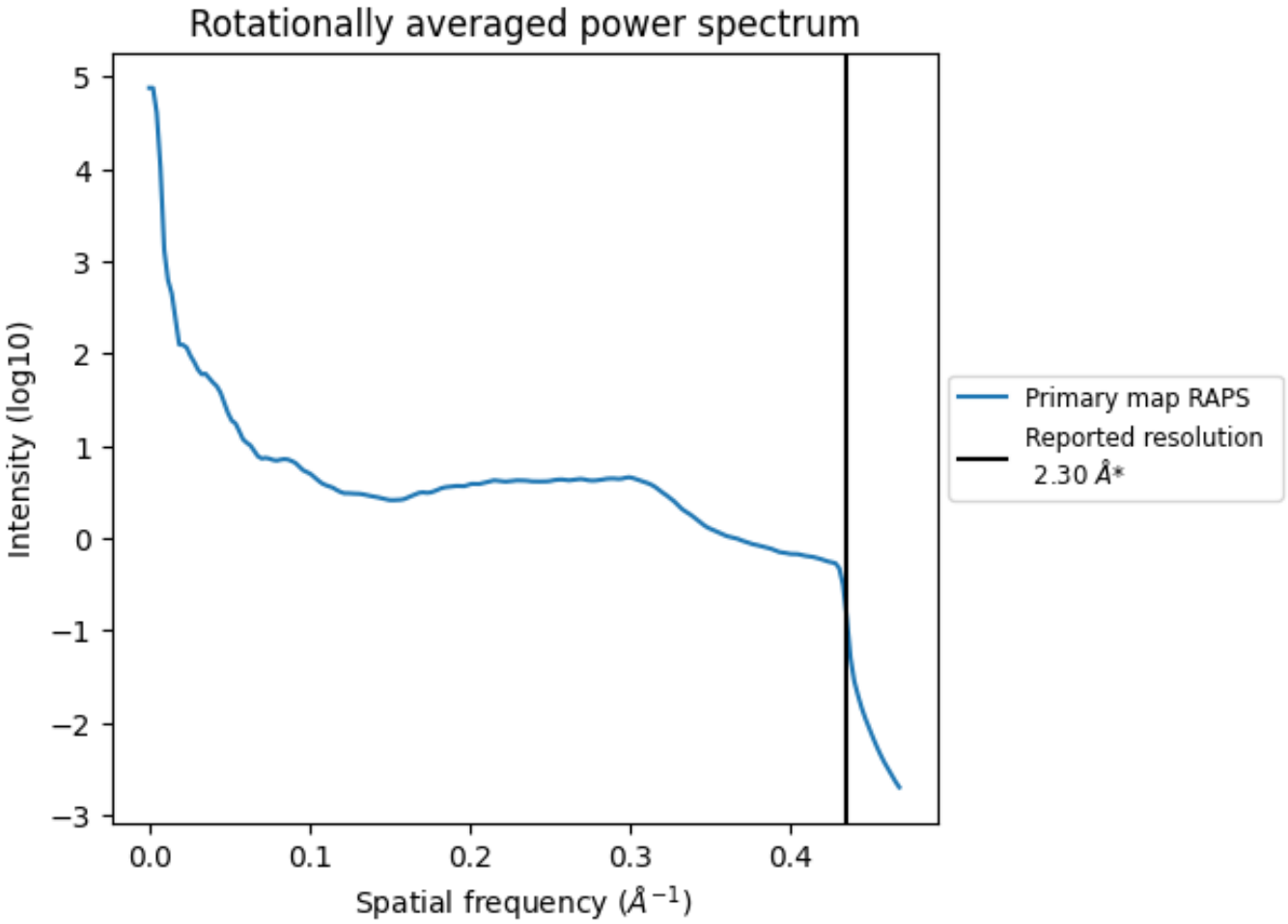
7.2 Volume estimate (i)



The volume at the recommended contour level is 616 nm^3; this corresponds to an approximate mass of 556 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 (i)



*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

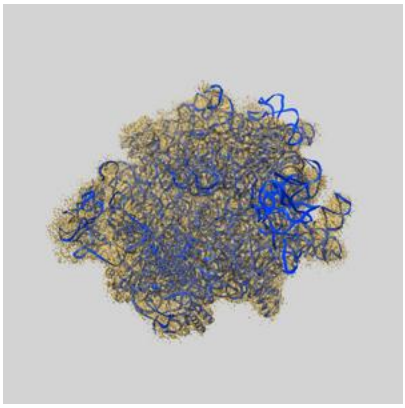
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

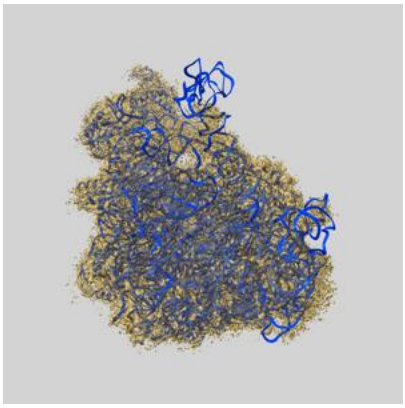
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10077 and PDB model 6S0Z. Per-residue inclusion information can be found in section 3 on page 10.

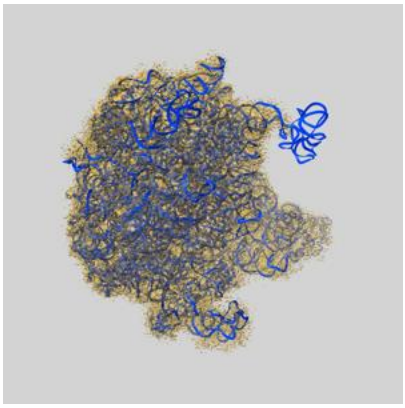
9.1 Map-model overlay



X



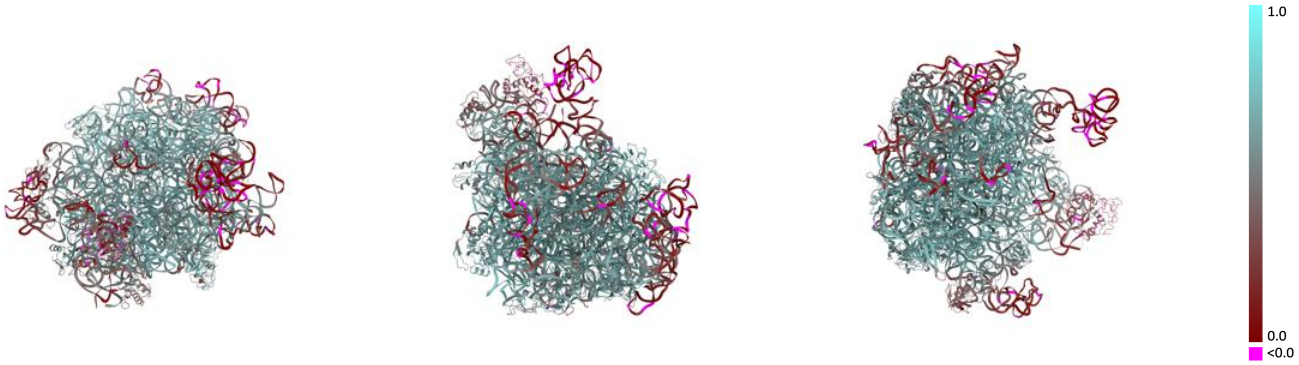
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

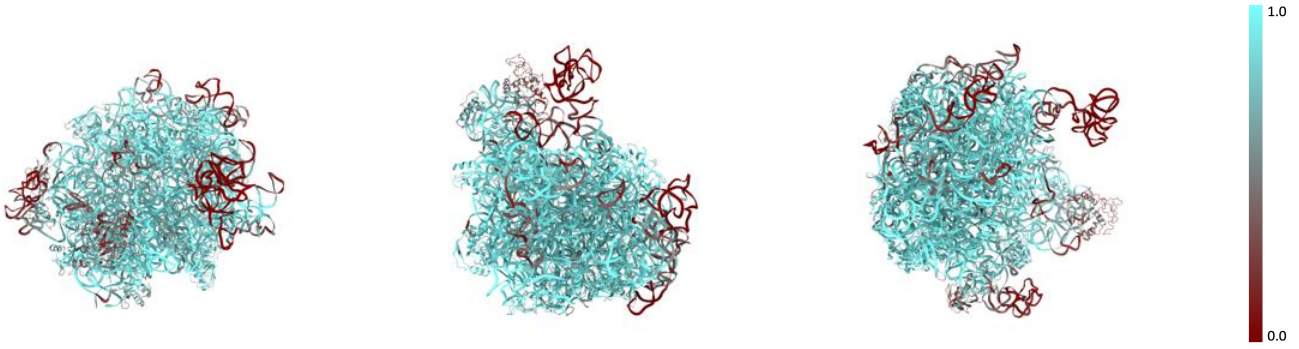
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

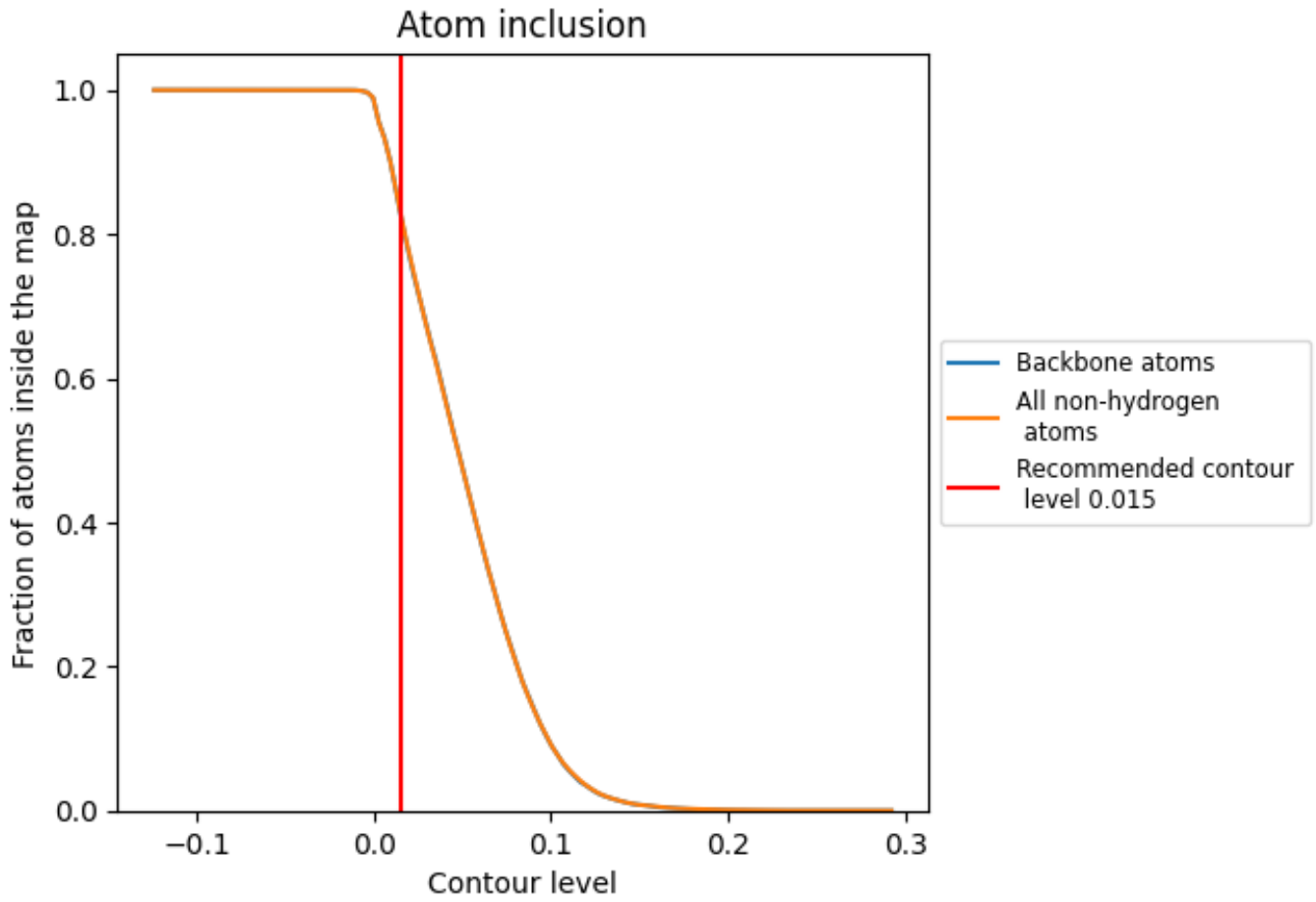
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 83% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8321	0.5540
1	0.5680	0.5260
2	0.9740	0.6820
3	0.9283	0.6510
4	0.8270	0.5730
A	0.8340	0.5490
B	0.8812	0.4930
C	0.9449	0.6620
D	0.9389	0.6500
E	0.9104	0.6420
F	0.3127	0.2050
G	0.4664	0.3480
H	0.9322	0.6510
I	0.9218	0.6450
J	0.9163	0.6270
K	0.9264	0.6350
L	0.9244	0.6500
M	0.7271	0.4690
N	0.8999	0.6280
O	0.9571	0.6770
P	0.9229	0.6410
Q	0.8875	0.6270
R	0.8512	0.5810
S	0.7824	0.5260
T	0.7898	0.5370
U	0.9313	0.6460
V	0.8521	0.5820
W	0.7752	0.5260
X	0.9093	0.6420
Y	0.1304	0.1440
Z	0.7147	0.5180