



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:13 AM UTC

PDB ID : 9I88 / pdb\_00009i88  
EMDB ID : EMD-52711  
Title : Structure of the wild-type Staphylococcus aureus 70S ribosome complexed with clincelin  
Authors : Novotna, M.; Boissier, F.; Balikova Novotna, G.; Innis, C.A.  
Deposited on : 2025-02-04  
Resolution : 2.98 Å(reported)  
Based on initial model : 7NHM

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

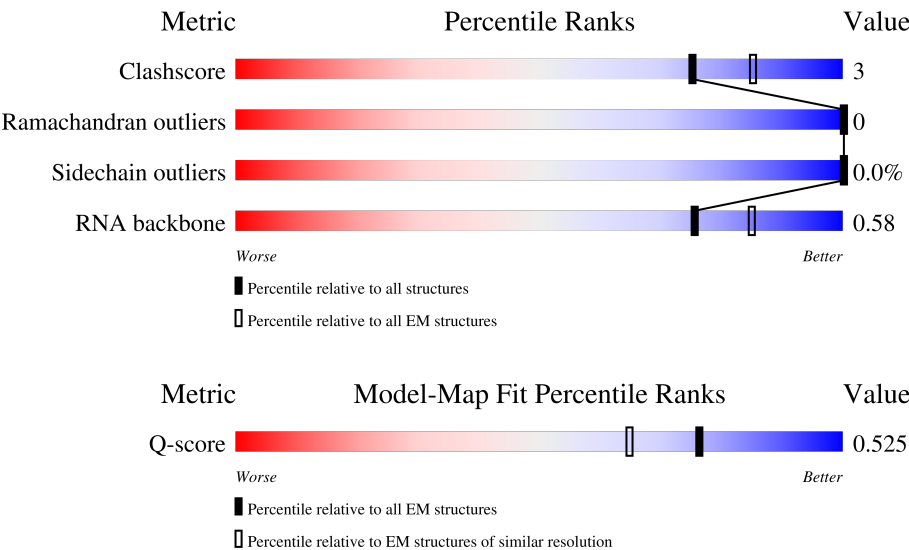
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 2.98 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.









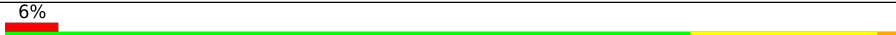
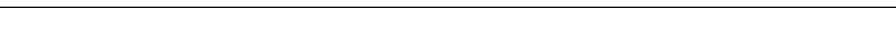
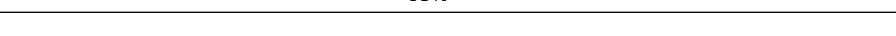
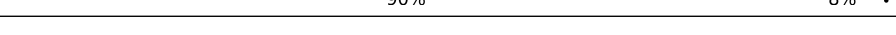
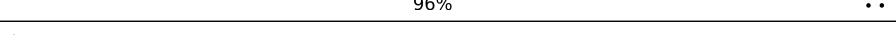
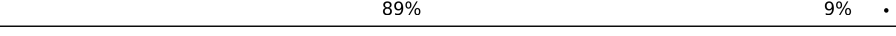



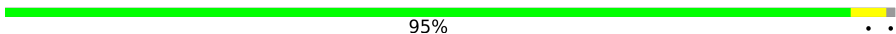









Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 ( 2.48 - 3.48 )

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  $\geq 3$ , 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	1	62	
2	2	69	
3	3	59	



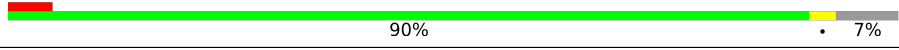
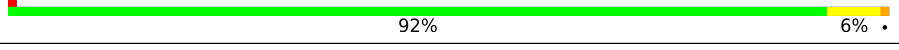


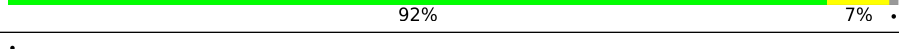
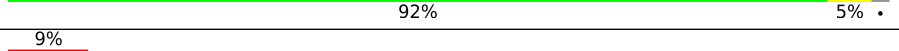
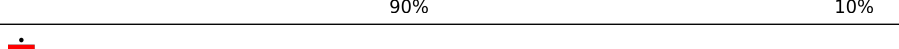
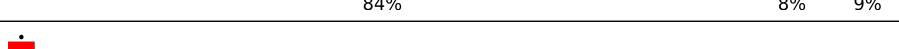
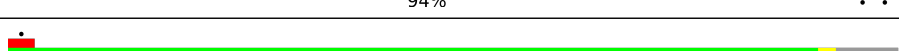
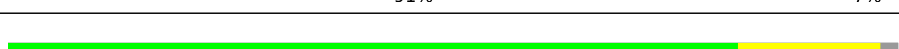

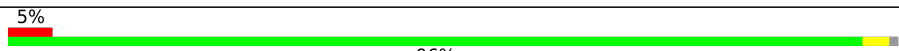
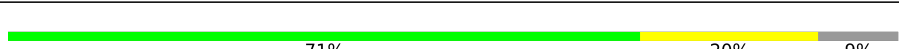





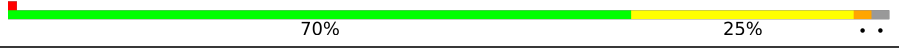


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Mol	Chain	Length	Quality of chain
4	5	57	 82% 9% 7%
5	6	49	 71% 24%
6	7	45	 91% 7%
7	8	66	 85% 12%
8	9	37	 97%
9	B	115	 83% 11%
10	D	77	 6% 77% 21%
11	G	277	 95%
12	H	220	 90% 8%
13	I	207	 96%
14	J	179	 89% 9%
15	K	178	 87% 6% 8%
16	M	145	 90% 8%
17	N	122	 92% 8%
18	O	146	 95%
19	P	144	 87% 7% 6%
20	Q	122	 93% 6%
21	R	119	 89% 9%
22	S	116	 88% 10%
23	T	118	 88% 10%
24	U	102	 95%
25	V	117	 83% 12% 5%
26	W	91	 90% 8%
27	X	105	 89% 6% 6%
28	Y	217	 42% 57%

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Mol	Chain	Length	Quality of chain
29	Z	94	
30	c	255	
31	d	217	
32	e	200	
33	f	166	
34	g	98	
35	i	132	
36	j	130	
37	k	102	
38	l	129	
39	m	137	
40	n	121	
41	o	61	
42	p	89	
43	q	91	
44	r	87	
45	s	80	
46	t	92	
47	u	83	
48	4	84	
49	A	2923	
50	a	1552	
51	h	156	

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 139505 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	1	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	64	Total	C	N	O	0	0
			527	324	99	104		

- Molecule 3 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 4 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

- Molecule 5 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	47	Total	C	N	O	S	0	0
			394	240	78	72	4		

- Molecule 6 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	42	Total	C	N	O	S	0	0
			360	220	88	51	1		

- Molecule 7 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	36	Total	C	N	O	S	0	0
			292	184	59	44	5		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 10 is a RNA chain called fMet-P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	77	Total	C	N	O	P	0	0
			1642	732	295	538	77		

- Molecule 11 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 12 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 13 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	175	Total	C	N	O	S	0	0
			1381	876	237	261	7		

- Molecule 15 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	164	Total	C	N	O	S	0	0
			1284	799	232	250	3		

- Molecule 16 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	142	Total	C	N	O	S	0	0
			1127	704	205	216	2		

- Molecule 17 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

- Molecule 19 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	135	Total	C	N	O	S	0	0
			1081	693	205	180	3		

- Molecule 20 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	R	118	Total	C	N	O	0	0
			914	569	173	172		

- Molecule 22 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	114	Total	C	N	O	0	0
			922	580	185	157		

- Molecule 23 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 24 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 25 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	99	Total	C	N	O	S	0	0
			761	480	140	139	2		

- Molecule 28 is a protein called 50S ribosomal protein L25.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	78	Total	C	N	O	S	0	0
			597	367	116	114			

- Molecule 30 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 31 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 32 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 33 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 34 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 35 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	127	Total	C	N	O	S	0	0
			1008	624	201	182	1		

- Molecule 37 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	102	Total	C	N	O	S	0	0
			814	513	149	150	2		

- Molecule 38 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	118	Total	C	N	O	S	0	0
			877	542	166	166	3		

- Molecule 39 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 40 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 42 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 43 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 44 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	79	Total	C	N	O	S	0	0
			651	413	116	121	1		

- Molecule 45 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 46 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	79	Total	C	N	O	S	0	0
			646	416	116	112	2		

- Molecule 47 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	59	Total	C	N	O	S	0	0
			486	310	88	87	1		

- Molecule 49 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	A	2806	Total	C	N	O	P	0	0
			60163	26863	11008	19486	2806		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	U	C	conflict	GB CP020619.1

- Molecule 50 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	a	1514	Total	C	N	O	P	0	0
			32434	14481	5924	10515	1514		

- Molecule 51 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	h	148	Total	C	N	O	S	0	0
			1180	734	226	216	4		

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	5	1	Total	Zn	0
			1	1	
52	6	1	Total	Zn	0
			1	1	
52	9	1	Total	Zn	0
			1	1	
52	o	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
53	5	1	Total	Mg	0
			1	1	
53	7	1	Total	Mg	0
			1	1	
53	B	5	Total	Mg	0
			5	5	
53	D	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
53	G	2	Total 2	Mg 2	0
53	R	1	Total 1	Mg 1	0
53	S	1	Total 1	Mg 1	0
53	j	1	Total 1	Mg 1	0
53	u	2	Total 2	Mg 2	0
53	A	280	Total 280	Mg 280	0
53	a	88	Total 88	Mg 88	0

- FME
- 
- The chemical structure of FME (Farnesyl pyrophosphate) is shown. It consists of a farnesyl chain (a branched hydrocarbon chain) and a pyrophosphate group. The farnesyl chain is represented by a central carbon atom (C) bonded to a hydroxyl group (HO), a carboxylate group (O), and a pyrophosphate group (N). The pyrophosphate group is represented by a nitrogen atom (N) bonded to a carboxylate group (O1) and a pyrophosphate group (O). The farnesyl chain is further detailed with labels: CE (ethyl), SD (sulfide), CG (gamma-carbon), CB (beta-carbon), and CA(S) (alpha-carbon). The structure is shown in a 3D representation with a wedge bond indicating stereochemistry.

Mol	Chain	Residues	Atoms		AltConf
55	A	2	Total 2	K 2	0

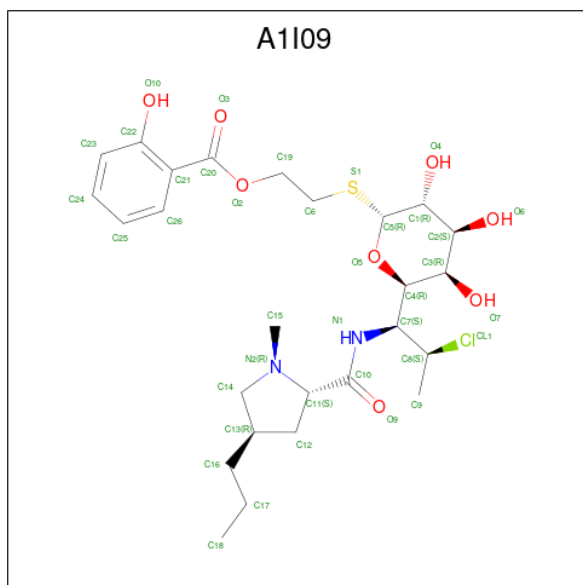


WORLD WIDE  
PDB  
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		AltConf
55	a	1	Total	K	0
			1	1	

- Molecule 56 is Clincelin (CCD ID: A1I09) (formula:  $C_{26}H_{39}ClN_2O_8S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
56	A	1	Total	C	Cl	N	O	S	0
			38	26	1	2	8	1	

### 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 1:  90% 5%




- Molecule 2: Large ribosomal subunit protein uL29

Chain 2:  84% 9% 7%




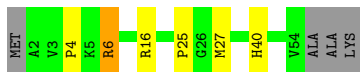
- Molecule 3: Large ribosomal subunit protein uL30

Chain 3:  83% 12% 5%



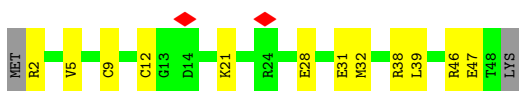
- Molecule 4: Large ribosomal subunit protein bL32

Chain 5:  82% 9% 7%




- Molecule 5: Large ribosomal subunit protein bL33A

Chain 6:  71% 24%




- Molecule 6: Large ribosomal subunit protein bL34

Chain 7:  91% 7%



- Molecule 7: Large ribosomal subunit protein bL35

Chain 8:  85% 12%




- Molecule 8: Large ribosomal subunit protein bL36

Chain 9:  97%




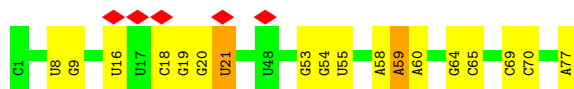
- Molecule 9: 5S ribosomal RNA

Chain B:  83% 11%



- Molecule 10: fMet-P-tRNA

Chain D:  6% 77% 21%




- Molecule 11: Large ribosomal subunit protein uL2

Chain G:  95%



- Molecule 12: Large ribosomal subunit protein uL3

Chain H:  90% 8%



- Molecule 13: Large ribosomal subunit protein uL4

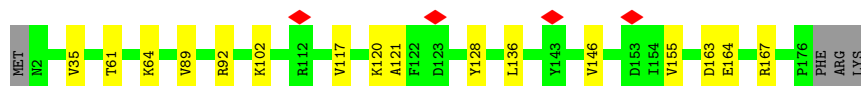


Chain I:  96% ..




- Molecule 14: Large ribosomal subunit protein uL5

Chain J:  89% 9% .




- Molecule 15: Large ribosomal subunit protein uL6

Chain K:  87% 6% 8%



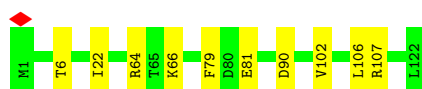
- Molecule 16: Large ribosomal subunit protein uL13

Chain M:  90% 8% .



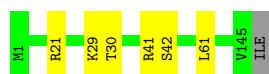
- Molecule 17: Large ribosomal subunit protein uL14

Chain N:  92% 8%




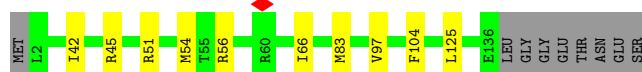
- Molecule 18: Large ribosomal subunit protein uL15

Chain O:  95% ..




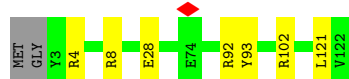
- Molecule 19: Large ribosomal subunit protein uL16

Chain P:  87% 7% 6%




- Molecule 20: Large ribosomal subunit protein bL17

Chain Q:  93% 6% .




- Molecule 21: Large ribosomal subunit protein uL18

Chain R:  89% 9% ..




- Molecule 22: Large ribosomal subunit protein bL19

Chain S:  88% 10% .



- Molecule 23: Large ribosomal subunit protein bL20

Chain T:  88% 10% .




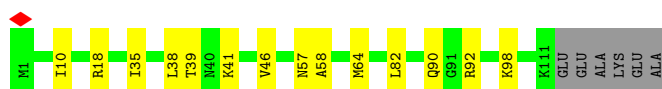
- Molecule 24: Large ribosomal subunit protein bL21

Chain U:  95% ..




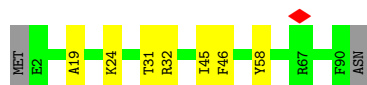
- Molecule 25: Large ribosomal subunit protein uL22

Chain V:  83% 12% 5%



- Molecule 26: Large ribosomal subunit protein uL23

Chain W:  90% 8% .

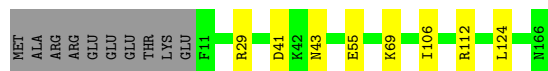


- Chain e:  92% 6%



- Molecule 33: Small ribosomal subunit protein uS5

Chain f: 89% 5% 6%



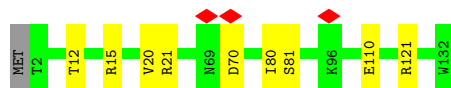
- Molecule 34: Small ribosomal subunit protein bS6

Chain g: 85% 10% 5%



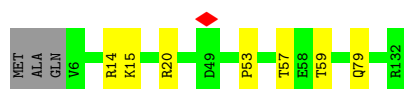
- Molecule 35: Small ribosomal subunit protein uS8

Chain i: 92% 7% .



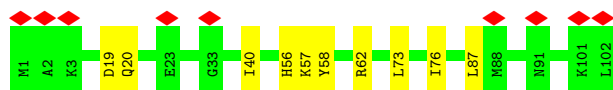
- Molecule 36: Small ribosomal subunit protein uS9

Chain j: 92% 5% .



- Molecule 37: Small ribosomal subunit protein uS10

Chain k: 9% 90% 10%



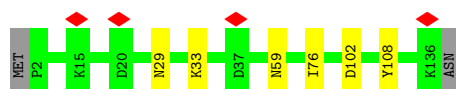
- Molecule 38: Small ribosomal subunit protein uS11

Chain l: 84% 8% 9%




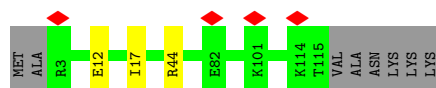
- Molecule 39: Small ribosomal subunit protein uS12

Chain m:  94%




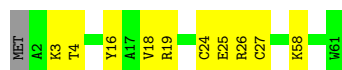
- Molecule 40: Small ribosomal subunit protein uS13

Chain n:  91% 7%




- Molecule 41: Small ribosomal subunit protein uS14B

Chain o:  82% 16%



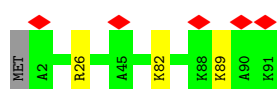
- Molecule 42: Small ribosomal subunit protein uS15

Chain p:  90% 7%



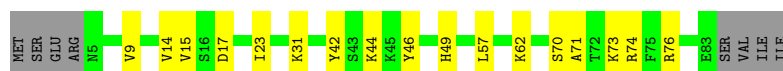
- Molecule 43: Small ribosomal subunit protein bS16

Chain q:  5% 96%



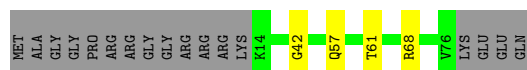
- Molecule 44: Small ribosomal subunit protein uS17

Chain r:  71% 20% 9%



- Molecule 45: Small ribosomal subunit protein bS18

Chain s:  74% 5% 21%



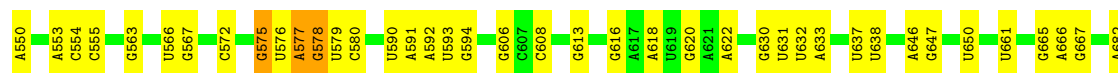
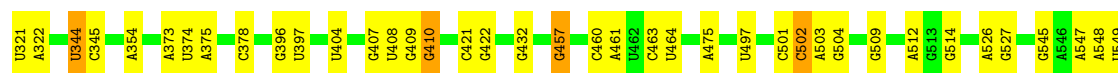
- Molecule 46: Small ribosomal subunit protein uS19

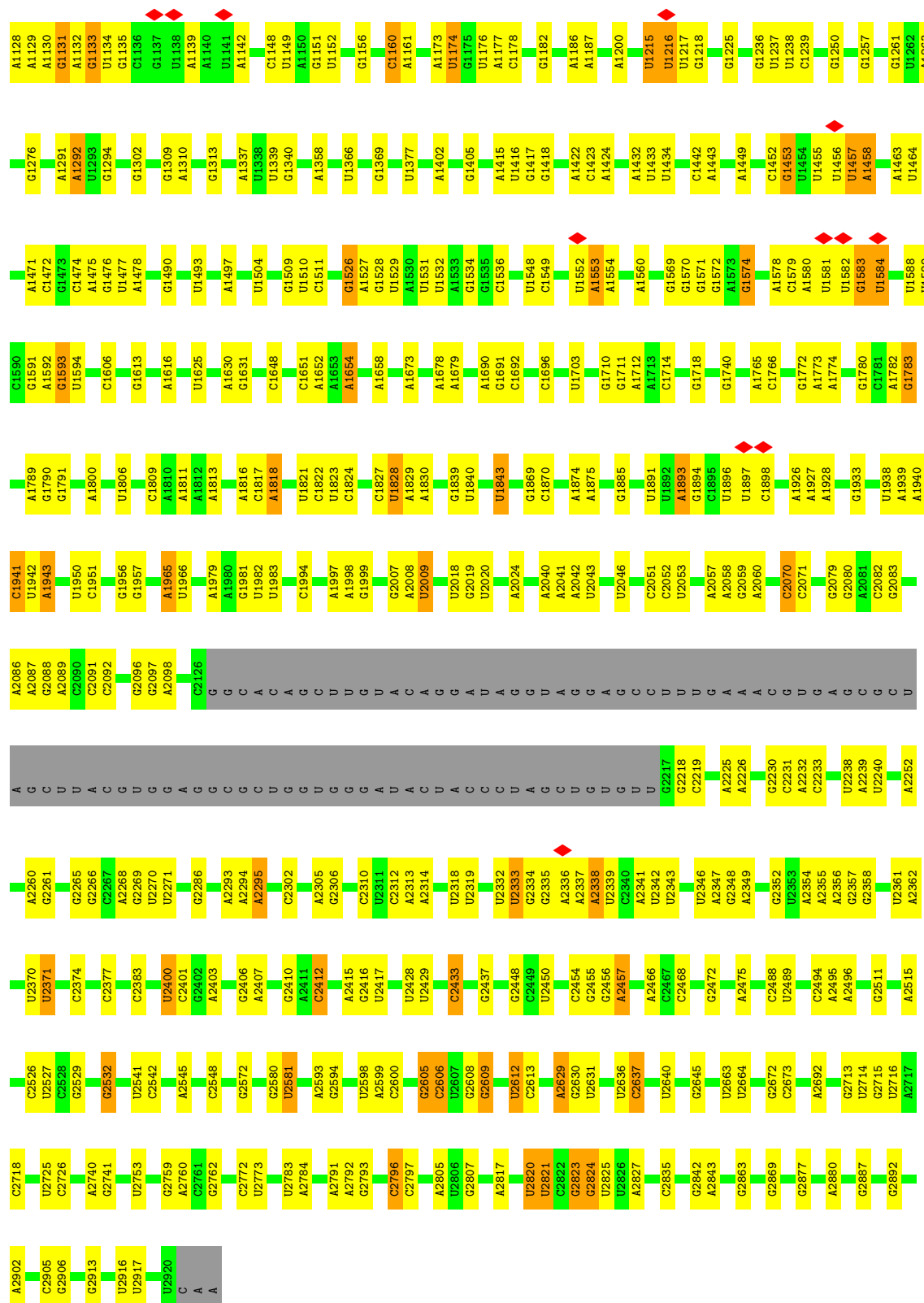


- 

- M1 G26 T30 SER SER GLU GLU MET MET GLU TRP GLU ASP GLY LYS GLU TYR P44 R47 K63 PHE ALA ALA ALA ALA ASP G69 K77 PHE GLY LEU LYS SER ASN ASN

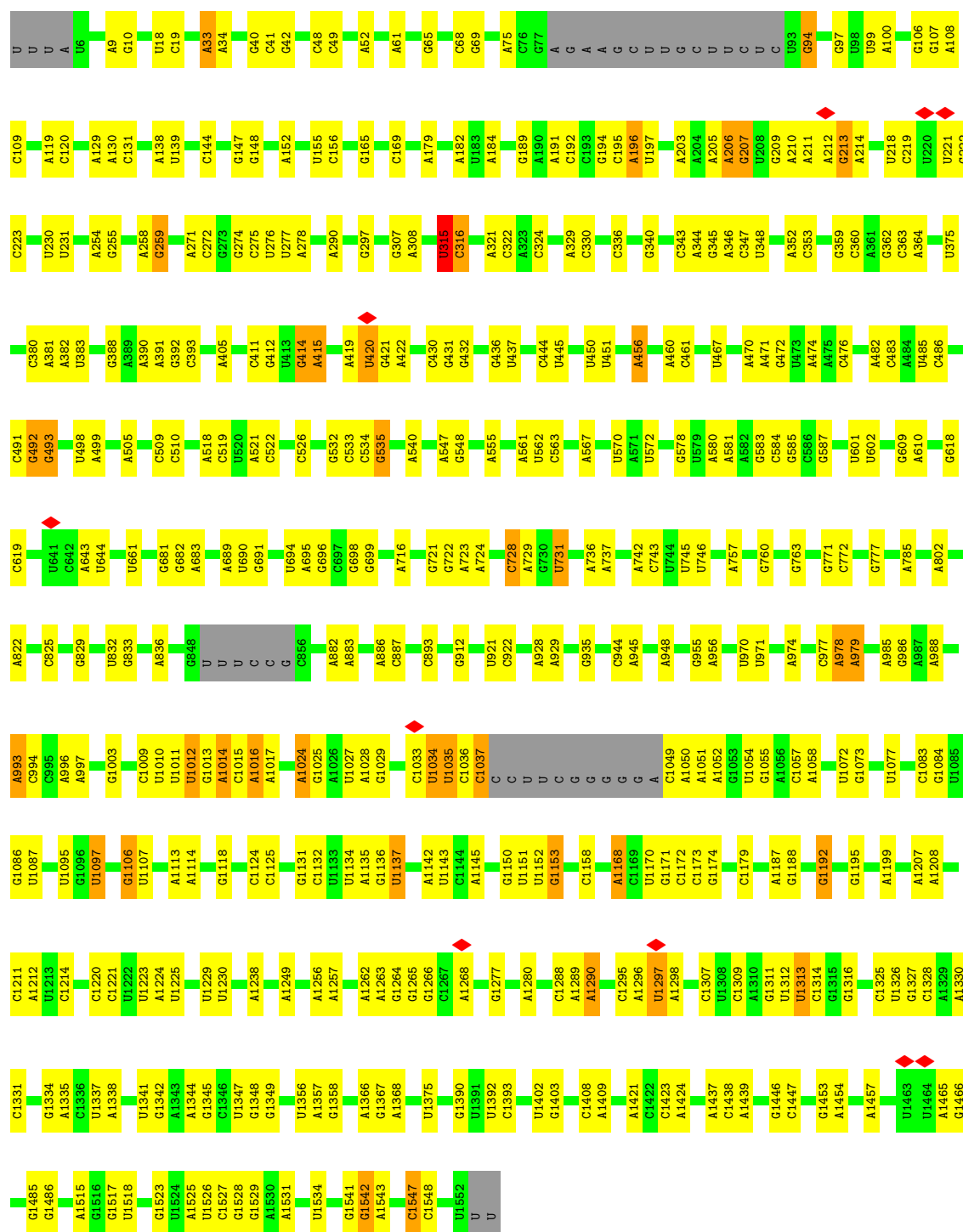
- 
- | Category | Gene Count (approx.) |
|----------|----------------------|
| G        | 100                  |
| U3       | 100                  |
| U12      | 100                  |
| U34      | 100                  |
| U59      | 100                  |
| U63      | 100                  |
| A64      | 100                  |
| A71      | 100                  |
| U74      | 100                  |
| G75      | 100                  |
| G83      | 100                  |
| G92      | 100                  |
| U93      | 100                  |
| A102     | 100                  |
| A117     | 100                  |
| A118     | 100                  |
| U119     | 100                  |
| A150     | 100                  |
| G153     | 100                  |
| A154     | 100                  |
| U155     | 100                  |
| G160     | 100                  |
| A164     | 100                  |
| C165     | 100                  |
| A166     | 100                  |
| U167     | 100                  |
| A168     | 100                  |
| A171     | 100                  |
| U172     | 100                  |
| A176     | 100                  |
| G177     | 100                  |
| G180     | 100                  |
| A183     | 100                  |
| C184     | 1900                 |
| C187     | 100                  |
| C188     | 100                  |
| A194     | 100                  |
| C195     | 100                  |





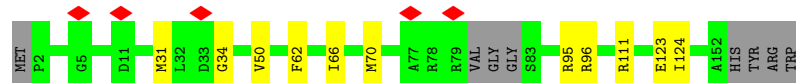
• Molecule 50: 16S ribosomal RNA

Chain a: 70% 25%



• Molecule 51: Small ribosomal subunit protein uS7

Chain h: 88% 7% 5%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61266	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	365.16, 365.16, 365.16	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.895, 0.895, 0.895	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FME, A1I09, ZN, K

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	1	0.33	0/469	0.43	0/625
2	2	0.26	0/528	0.44	0/703
3	3	0.34	0/438	0.53	0/590
4	5	0.34	0/429	0.45	0/571
5	6	0.28	0/399	0.48	0/535
6	7	0.41	0/364	0.53	0/474
7	8	0.34	0/526	0.59	0/690
8	9	0.31	0/295	0.47	0/388
9	B	0.36	0/2692	0.59	0/4193
10	D	0.31	0/1834	0.63	0/2857
11	G	0.35	0/2120	0.47	0/2847
12	H	0.34	0/1661	0.54	2/2227 (0.1%)
13	I	0.32	0/1587	0.50	0/2143
14	J	0.23	0/1398	0.45	0/1877
15	K	0.21	0/1302	0.46	0/1757
16	M	0.33	0/1149	0.50	0/1549
17	N	0.33	0/927	0.46	0/1243
18	O	0.33	0/1104	0.50	0/1471
19	P	0.32	0/1105	0.49	0/1483
20	Q	0.32	0/956	0.48	0/1277
21	R	0.27	0/923	0.48	0/1234
22	S	0.30	0/934	0.43	0/1249
23	T	0.40	0/955	0.52	0/1265
24	U	0.33	0/803	0.46	0/1073
25	V	0.32	0/861	0.49	0/1159
26	W	0.31	0/733	0.44	0/978
27	X	0.24	0/770	0.44	0/1029
28	Y	0.26	0/746	0.51	0/1000
29	Z	0.33	0/603	0.47	0/801
30	c	0.21	0/1808	0.44	0/2426
31	d	0.23	0/1618	0.42	0/2173
32	e	0.25	0/1647	0.46	0/2211

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	f	0.27	0/1174	0.44	0/1583
34	g	0.29	0/784	0.45	0/1052
35	i	0.28	0/1044	0.48	0/1401
36	j	0.21	0/1024	0.43	0/1374
37	k	0.21	0/826	0.42	0/1111
38	l	0.23	0/892	0.44	0/1203
39	m	0.25	0/1075	0.44	0/1439
40	n	0.19	0/909	0.41	0/1218
41	o	0.26	0/512	0.48	0/678
42	p	0.28	0/730	0.46	0/975
43	q	0.26	0/723	0.43	0/971
44	r	0.24	0/659	0.49	0/881
45	s	0.28	0/525	0.40	0/704
46	t	0.17	0/663	0.39	0/889
47	u	0.27	0/606	0.49	0/810
48	4	0.20	0/496	0.43	0/661
49	A	0.45	0/67381	0.62	0/105087
50	a	0.38	0/36313	0.62	1/56623 (0.0%)
51	h	0.22	0/1195	0.48	0/1605
All	All	0.39	0/151215	0.58	3/226363 (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
1	1	0	2
4	5	0	1
11	G	0	1
13	I	0	1
21	R	0	1
32	e	0	2
37	k	0	1
41	o	0	1
48	4	0	1
50	a	0	2
All	All	0	13

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	893	C	N1-C1'-C2'	5.44	120.16	112.00
12	H	159	ASP	CA-C-N	5.12	130.93	121.70
12	H	159	ASP	C-N-CA	5.12	130.93	121.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	27	ARG	Sidechain
1	1	52	ARG	Sidechain
48	4	47	ARG	Sidechain
4	5	6	ARG	Sidechain
11	G	14	ARG	Sidechain
13	I	106	ARG	Sidechain
21	R	35	ARG	Sidechain
50	a	315	U	Sidechain
50	a	61	A	Sidechain
32	e	13	ARG	Sidechain
32	e	3	ARG	Sidechain
37	k	62	ARG	Sidechain
41	o	26	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	463	0	501	1	0
2	2	527	0	554	5	0
3	3	436	0	473	4	0
4	5	422	0	426	8	0
5	6	394	0	398	9	0
6	7	360	0	406	1	0
7	8	521	0	586	7	0
8	9	292	0	336	0	0
9	B	2408	0	1218	10	0
10	D	1642	0	833	7	0
11	G	2085	0	2192	9	0
12	H	1637	0	1680	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	I	1564	0	1611	5	0
14	J	1381	0	1435	10	0
15	K	1284	0	1301	5	0
16	M	1127	0	1117	7	0
17	N	920	0	981	7	0
18	O	1090	0	1131	5	0
19	P	1081	0	1143	7	0
20	Q	952	0	999	6	0
21	R	914	0	956	11	0
22	S	922	0	994	10	0
23	T	943	0	1014	10	0
24	U	793	0	831	4	0
25	V	853	0	914	10	0
26	W	725	0	761	7	0
27	X	761	0	823	3	0
28	Y	738	0	787	2	0
29	Z	597	0	607	4	0
30	c	1781	0	1844	12	0
31	d	1596	0	1659	5	0
32	e	1617	0	1646	14	0
33	f	1160	0	1223	6	0
34	g	773	0	772	6	0
35	i	1032	0	1082	6	0
36	j	1008	0	1031	6	0
37	k	814	0	863	7	0
38	l	877	0	895	7	0
39	m	1058	0	1130	3	0
40	n	902	0	950	2	0
41	o	502	0	523	8	0
42	p	721	0	751	4	0
43	q	712	0	744	3	0
44	r	651	0	689	11	0
45	s	516	0	548	3	0
46	t	646	0	653	2	0
47	u	606	0	650	5	0
48	4	486	0	488	1	0
49	A	60163	0	30241	281	0
50	a	32434	0	16330	222	0
51	h	1180	0	1221	7	0
52	5	1	0	0	0	0
52	6	1	0	0	0	0
52	9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	o	1	0	0	0	0
53	5	1	0	0	0	0
53	7	1	0	0	0	0
53	A	280	0	0	0	0
53	B	5	0	0	0	0
53	D	1	0	0	0	0
53	G	2	0	0	0	0
53	R	1	0	0	0	0
53	S	1	0	0	0	0
53	a	88	0	0	0	0
53	j	1	0	0	0	0
53	u	2	0	0	0	0
54	D	10	0	10	0	0
55	A	2	0	0	0	0
55	a	1	0	0	0	0
56	A	38	0	0	1	0
All	All	139505	0	92951	709	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 (709) 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)
11:G:150:LYS:NZ	49:A:1828:U:OP2	2.13	0.81
49:A:788:A:O2'	49:A:1703:U:OP1	2.03	0.75
32:e:46:GLU:OE2	33:f:112:ARG:NE	2.19	0.75
3:3:5:GLN:NE2	3:3:57:GLU:OE2	2.20	0.74
5:6:2:ARG:NH1	49:A:2312:C:OP2	2.21	0.73
50:a:681:G:H2'	50:a:682:G:C8	2.28	0.69
49:A:2355:A:H2'	49:A:2356:A:C8	2.28	0.68
50:a:1134:U:O4	50:a:1135:A:N6	2.26	0.68
31:d:171:THR:HG22	50:a:1118:G:H5''	1.76	0.68
49:A:1874:A:HO2'	49:A:1875:A:H8	1.41	0.68
51:h:50:VAL:HG21	51:h:124:ILE:HD11	1.78	0.66
4:5:27:MET:HE1	25:V:35:ILE:HA	1.77	0.66
2:2:58:ARG:NH1	2:2:61:GLU:OE1	2.29	0.65
50:a:75:A:OP2	50:a:94:G:N2	2.26	0.64
50:a:324:C:OP2	50:a:359:G:O2'	2.14	0.64
29:Z:22:ARG:NH1	49:A:2306:G:O6	2.31	0.64
5:6:31:GLU:OE2	5:6:46:ARG:NE	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:48:ARG:NH1	23:T:49:ASP:OD1	2.31	0.63
42:p:54:ARG:NH1	50:a:587:G:O2'	2.31	0.63
12:H:159:ASP:OD1	49:A:1174:U:C5	2.52	0.62
18:O:29:LYS:HG3	18:O:30:THR:H	1.64	0.62
36:j:20:ARG:NH1	50:a:1158:C:O2	2.33	0.61
50:a:1024:A:H5'	50:a:1024:A:C8	2.35	0.61
50:a:1229:U:H2'	50:a:1230:U:C6	2.36	0.61
12:H:138:ARG:NH1	49:A:2024:A:OP2	2.31	0.61
22:S:87:GLU:OE2	22:S:89:LYS:NZ	2.24	0.60
50:a:521:A:H2'	50:a:522:C:C6	2.37	0.60
12:H:157:ALA:O	49:A:2080:G:H5'	2.02	0.60
32:e:196:GLU:O	50:a:9:A:N6	2.35	0.60
39:m:59:ASN:ND2	39:m:102:ASP:OD1	2.32	0.59
35:i:12:THR:HG22	35:i:15:ARG:HH12	1.67	0.59
14:J:164:GLU:OE2	14:J:167:ARG:NH1	2.34	0.59
30:c:203:ASN:OD1	30:c:205:ASP:N	2.31	0.59
50:a:33:A:H2'	50:a:34:A:C8	2.38	0.58
25:V:90:GLN:OE1	25:V:92:ARG:NH2	2.36	0.58
27:X:33:VAL:O	27:X:63:ILE:N	2.37	0.58
50:a:152:A:N6	50:a:169:C:C2	2.71	0.58
49:A:2270:U:H2'	49:A:2271:U:C6	2.39	0.58
36:j:14:ARG:NH2	36:j:79:GLN:OE1	2.37	0.58
12:H:158:SER:OG	49:A:2599:A:N7	2.35	0.57
41:o:3:LYS:NZ	50:a:1214:C:OP1	2.37	0.57
4:5:40:HIS:HD1	49:A:2835:C:HO2'	1.52	0.57
17:N:64:ARG:NH2	17:N:81:GLU:OE2	2.35	0.57
23:T:53:ARG:NH2	49:A:1038:C:OP1	2.38	0.57
7:8:12:LYS:NZ	49:A:252:C:O2	2.35	0.57
44:r:70:SER:O	44:r:74:ARG:NH1	2.36	0.57
9:B:41:C:O2	14:J:92:ARG:NH1	2.32	0.56
21:R:35:ARG:HG2	21:R:35:ARG:HH11	1.70	0.56
13:I:74:ARG:HH22	49:A:2472:G:P	2.28	0.56
49:A:1765:A:H2'	49:A:1766:C:C6	2.40	0.56
50:a:532:G:H2'	50:a:533:C:C6	2.40	0.56
50:a:68:C:H2'	50:a:69:G:C8	2.41	0.56
49:A:2341:A:H2'	49:A:2342:U:C6	2.41	0.56
49:A:283:G:H3'	49:A:284:C:H4'	1.88	0.56
49:A:901:G:H2'	49:A:902:A:C8	2.41	0.56
49:A:1874:A:O2'	49:A:1875:A:H8	1.88	0.56
4:5:27:MET:HE2	25:V:38:LEU:HB2	1.88	0.55
3:3:22:THR:HG21	3:3:49:LYS:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:152:A:N6	50:a:169:C:O2	2.39	0.55
11:G:221:ARG:NH1	49:A:1816:A:OP2	2.39	0.55
32:e:95:ASP:OD1	32:e:96:ALA:N	2.39	0.55
25:V:92:ARG:O	49:A:1658:A:N6	2.40	0.55
50:a:1264:G:H2'	50:a:1265:G:H8	1.72	0.55
14:J:61:THR:HG21	14:J:89:VAL:HG11	1.88	0.55
47:u:10:ARG:NE	50:a:106:G:O6	2.34	0.55
49:A:1095:A:H2'	49:A:1096:C:C6	2.42	0.55
49:A:92:G:H2'	49:A:93:U:C6	2.42	0.55
33:f:69:LYS:NZ	50:a:1086:G:OP1	2.37	0.54
35:i:12:THR:HG21	50:a:886:A:H1'	1.89	0.54
49:A:2318:U:H2'	49:A:2319:U:C6	2.42	0.54
21:R:42:ALA:HB3	21:R:80:ILE:HD12	1.88	0.54
37:k:57:LYS:HB3	37:k:58:TYR:CD2	2.42	0.54
49:A:457:G:OP2	49:A:2433:C:O2'	2.23	0.54
50:a:722:G:H2'	50:a:723:A:C8	2.42	0.54
30:c:14:VAL:HG13	30:c:202:ALA:HB1	1.90	0.54
50:a:1367:G:H2'	50:a:1368:A:C8	2.43	0.54
49:A:291:G:H2'	49:A:292:U:C6	2.42	0.54
50:a:955:G:C2	50:a:956:A:C8	2.96	0.54
12:H:159:ASP:O	49:A:2598:U:O2'	2.25	0.54
50:a:948:A:O2'	51:h:95:ARG:NH2	2.40	0.54
49:A:1493:U:HO2'	49:A:1574:G:HO2'	1.54	0.54
50:a:988:A:C2	50:a:1330:A:C4	2.95	0.54
37:k:57:LYS:HE2	50:a:974:A:O2'	2.08	0.53
49:A:1823:U:H2'	49:A:1824:C:C6	2.42	0.53
50:a:721:G:H2'	50:a:722:G:C8	2.43	0.53
50:a:723:A:H2'	50:a:724:A:C8	2.43	0.53
40:n:12:GLU:O	40:n:44:ARG:NH1	2.40	0.53
50:a:521:A:H2'	50:a:522:C:H6	1.71	0.53
50:a:1288:C:H2'	50:a:1289:A:H5''	1.91	0.53
6:7:40:ARG:NH2	49:A:514:G:N7	2.52	0.53
50:a:1083:C:H2'	50:a:1084:G:H8	1.73	0.53
49:A:1100:G:O2'	49:A:1130:A:H1'	2.08	0.53
50:a:1446:G:H2'	50:a:1447:C:C6	2.44	0.53
16:M:78:HIS:CD2	16:M:79:SER:O	2.62	0.53
49:A:153:G:HO2'	49:A:154:A:H8	1.56	0.53
31:d:134:LYS:NZ	33:f:55:GLU:OE1	2.40	0.52
49:A:2606:C:H5'	49:A:2606:C:C6	2.43	0.52
49:A:2606:C:H5'	49:A:2606:C:H6	1.73	0.52
50:a:1049:C:H2'	50:a:1050:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:315:U:H2'	50:a:316:C:C6	2.44	0.52
41:o:16:TYR:OH	50:a:1328:C:N4	2.42	0.52
49:A:2051:C:H2'	49:A:2052:C:C6	2.44	0.52
11:G:100:GLU:OE2	49:A:1534:G:O2'	2.26	0.52
29:Z:26:SER:O	29:Z:28:ARG:NH1	2.41	0.52
49:A:1104:U:N3	49:A:1106:G:O4'	2.41	0.52
50:a:422:A:OP2	50:a:436:G:N2	2.41	0.52
50:a:230:U:H2'	50:a:231:U:C6	2.45	0.52
50:a:1307:C:H4'	50:a:1313:U:O4	2.09	0.52
50:a:822:A:H5'	50:a:1523:G:H4'	1.92	0.52
50:a:1402:U:H2'	50:a:1403:G:C8	2.45	0.52
11:G:154:ILE:HG22	11:G:154:ILE:O	2.08	0.52
49:A:684:U:H2'	49:A:685:C:C6	2.45	0.52
50:a:414:G:H2'	50:a:415:A:H5'	1.91	0.52
49:A:702:U:H2'	49:A:703:A:C8	2.44	0.52
50:a:222:G:H2'	50:a:223:C:C6	2.45	0.52
9:B:49:G:H2'	9:B:50:A:C8	2.45	0.51
21:R:113:ARG:NH1	49:A:2403:A:O2'	2.40	0.51
49:A:12:U:H2'	49:A:12:U:O2	2.10	0.51
49:A:620:G:O2'	49:A:1292:A:OP1	2.25	0.51
50:a:886:A:H2'	50:a:887:C:C6	2.45	0.51
9:B:58:C:H2'	9:B:59:U:C6	2.45	0.51
19:P:54:MET:HE1	19:P:104:PHE:CD1	2.44	0.51
49:A:637:U:H2'	49:A:638:U:C6	2.45	0.51
49:A:1806:U:OP2	49:A:1811:A:N6	2.41	0.51
21:R:56:ALA:HB3	21:R:80:ILE:HG13	1.91	0.51
50:a:213:G:H2'	50:a:214:A:C8	2.45	0.51
50:a:777:G:H4'	50:a:1525:A:H4'	1.91	0.51
50:a:1051:A:H2'	50:a:1052:A:C8	2.46	0.51
50:a:745:U:H2'	50:a:746:U:C6	2.45	0.51
16:M:38:ARG:NH1	49:A:1051:C:OP1	2.42	0.51
5:6:5:VAL:HG13	5:6:47:GLU:HG3	1.92	0.51
49:A:1806:U:H5	49:A:1811:A:N7	2.09	0.51
50:a:277:U:H2'	50:a:278:A:H8	1.76	0.51
50:a:392:G:H2'	50:a:393:C:C6	2.45	0.51
25:V:82:LEU:HB2	25:V:98:LYS:HB2	1.92	0.51
49:A:2526:C:N4	49:A:2527:U:O4	2.44	0.51
50:a:993:A:N3	50:a:993:A:H2'	2.24	0.51
49:A:1095:A:H2'	49:A:1096:C:H6	1.77	0.50
49:A:1782:A:H2'	49:A:1783:G:H5'	1.92	0.50
49:A:2532:G:OP1	56:A:3103:A1I09:O6	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:996:A:H2'	50:a:997:A:C8	2.46	0.50
10:D:53:G:C6	10:D:54:G:N7	2.80	0.50
21:R:113:ARG:NH2	49:A:2403:A:N3	2.59	0.50
50:a:99:U:H2'	50:a:100:A:C8	2.46	0.50
31:d:171:THR:HG22	50:a:1118:G:C5'	2.41	0.50
33:f:41:ASP:OD2	33:f:43:ASN:ND2	2.45	0.50
49:A:153:G:O2'	49:A:154:A:H8	1.94	0.50
4:5:25:PRO:HG2	4:5:27:MET:HE3	1.92	0.50
9:B:39:G:H3'	9:B:40:C:H5'	1.94	0.50
49:A:501:C:H3'	49:A:502:C:H5''	1.94	0.50
11:G:217:ARG:HG3	11:G:217:ARG:HH11	1.75	0.50
31:d:35:ASP:OD1	31:d:58:ARG:NH2	2.37	0.50
49:A:59:U:O2'	49:A:74:U:OP2	2.24	0.50
49:A:1588:U:H2'	49:A:1589:U:C6	2.47	0.50
50:a:1262:A:H2'	50:a:1263:A:C8	2.47	0.50
4:5:16:ARG:NH2	49:A:1302:G:OP1	2.40	0.50
49:A:1823:U:H2'	49:A:1824:C:H6	1.76	0.50
49:A:579:U:H2'	49:A:580:C:C6	2.48	0.49
50:a:689:A:H2'	50:a:690:U:C6	2.47	0.49
32:e:13:ARG:HD3	32:e:31:TYR:O	2.12	0.49
50:a:456:A:OP2	50:a:493:G:N2	2.35	0.49
50:a:1334:G:H2'	50:a:1335:A:C8	2.47	0.49
4:5:40:HIS:ND1	49:A:2835:C:O2'	2.44	0.49
45:s:57:GLN:O	45:s:61:THR:HG23	2.11	0.49
49:A:1839:G:H2'	49:A:1840:U:C6	2.47	0.49
50:a:1277:G:N2	50:a:1280:A:OP2	2.34	0.49
17:N:107:ARG:NH1	22:S:36:GLU:OE2	2.43	0.49
49:A:2007:G:O2'	49:A:2009:U:OP2	2.19	0.49
7:8:26:ARG:HG2	7:8:26:ARG:HH11	1.77	0.49
17:N:6:THR:HG22	49:A:1710:G:H4'	1.94	0.49
19:P:42:ILE:HD12	19:P:97:VAL:HG21	1.94	0.49
49:A:877:G:H2'	49:A:878:C:C6	2.47	0.49
49:A:1238:U:H2'	49:A:1239:C:C6	2.48	0.49
49:A:1528:G:H2'	49:A:1529:U:C6	2.47	0.49
15:K:40:ARG:NH1	15:K:61:ASP:OD1	2.44	0.49
44:r:71:ALA:O	44:r:74:ARG:NH2	2.44	0.49
50:a:771:G:H2'	50:a:772:C:C6	2.48	0.49
22:S:33:ARG:NH1	22:S:84:GLU:OE2	2.44	0.49
46:t:7:LYS:NZ	50:a:1327:G:N7	2.61	0.49
50:a:191:A:H2'	50:a:192:C:C6	2.48	0.49
49:A:2715:G:OP1	49:A:2740:A:N6	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:345:G:H2'	50:a:346:A:C8	2.48	0.48
50:a:363:C:C4	50:a:364:A:N7	2.81	0.48
50:a:1423:C:H2'	50:a:1424:A:C8	2.48	0.48
49:A:1457:U:H2'	49:A:1458:A:N3	2.28	0.48
50:a:1033:C:H2'	50:a:1033:C:O2	2.12	0.48
50:a:1036:C:H5''	50:a:1037:C:O5'	2.13	0.48
7:8:31:HIS:CD2	7:8:32:LEU:HG	2.48	0.48
49:A:2091:C:H2'	49:A:2092:C:C6	2.47	0.48
49:A:2268:A:H2'	49:A:2269:G:C8	2.49	0.48
49:A:2406:G:H2'	49:A:2407:A:C8	2.48	0.48
50:a:485:U:H2'	50:a:486:C:C6	2.49	0.48
49:A:289:U:H2'	49:A:290:U:C6	2.48	0.48
49:A:577:A:H4'	49:A:578:G:C8	2.49	0.48
50:a:155:U:H2'	50:a:156:C:C6	2.49	0.48
11:G:123:ASP:OD1	11:G:124:ILE:N	2.47	0.48
49:A:631:U:H2'	49:A:632:U:C6	2.48	0.48
24:U:70:LYS:NZ	49:A:1263:A:OP1	2.43	0.48
49:A:344:U:C2	49:A:345:C:C5	3.01	0.48
49:A:1531:U:H2'	49:A:1532:U:C6	2.48	0.48
50:a:307:G:H2'	50:a:308:A:C8	2.48	0.48
26:W:31:THR:HG22	26:W:32:ARG:N	2.27	0.48
44:r:14:VAL:HG13	44:r:23:ILE:HG23	1.95	0.48
44:r:76:ARG:NH1	50:a:196:A:O4'	2.46	0.48
49:A:787:U:H2'	49:A:788:A:C8	2.48	0.48
12:H:194:VAL:HG21	22:S:6:LEU:HD21	1.95	0.48
18:O:41:ARG:NH2	49:A:852:U:OP2	2.46	0.48
50:a:347:C:H2'	50:a:348:U:C6	2.49	0.48
20:Q:28:GLU:OE2	20:Q:92:ARG:NH1	2.44	0.47
30:c:110:ARG:HH11	30:c:110:ARG:HG2	1.79	0.47
37:k:19:ASP:OD1	37:k:20:GLN:N	2.45	0.47
38:l:36:ASP:OD2	38:l:40:ASN:ND2	2.38	0.47
49:A:285:U:H4'	49:A:286:U:C5	2.48	0.47
50:a:194:G:N2	50:a:197:U:OP2	2.36	0.47
50:a:1528:G:N2	50:a:1531:A:OP2	2.44	0.47
14:J:120:LYS:HG2	14:J:121:ALA:H	1.79	0.47
26:W:58:TYR:OH	49:A:1377:U:OP2	2.30	0.47
30:c:110:ARG:HD2	30:c:144:LEU:HD21	1.96	0.47
49:A:1115:G:N2	49:A:1135:G:OP2	2.42	0.47
10:D:20:G:H4'	10:D:21:U:OP2	2.13	0.47
32:e:108:ARG:NH2	50:a:415:A:OP1	2.37	0.47
49:A:650:U:C5	49:A:665:G:C5	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:195:C:O3'	50:a:196:A:H2	1.98	0.47
7:8:16:ARG:NH1	7:8:20:GLY:O	2.43	0.47
20:Q:4:ARG:NH1	49:A:1696:C:OP1	2.42	0.47
49:A:2494:C:H2'	49:A:2495:A:O4'	2.14	0.47
12:H:156:MET:O	49:A:2079:G:H4'	2.13	0.47
13:I:106:ARG:HD2	49:A:661:U:OP1	2.13	0.47
42:p:41:GLU:OE2	42:p:44:ARG:NH1	2.43	0.47
49:A:1423:C:H2'	49:A:1424:A:C8	2.49	0.47
50:a:682:G:H2'	50:a:683:A:H8	1.79	0.47
50:a:1173:C:H2'	50:a:1174:G:H8	1.79	0.47
11:G:248:SER:OG	11:G:249:PRO:HD2	2.14	0.47
12:H:196:LEU:HD21	22:S:10:VAL:HG11	1.97	0.47
34:g:43:TRP:HE1	34:g:62:ILE:CD1	2.28	0.47
49:A:153:G:O2'	49:A:154:A:H5'	2.14	0.47
49:A:1442:C:H2'	49:A:1443:A:C8	2.49	0.47
49:A:1457:U:H3'	49:A:1458:A:O4'	2.15	0.47
50:a:189:G:C6	50:a:203:A:C6	3.03	0.47
50:a:1054:U:H2'	50:a:1055:G:C8	2.50	0.47
50:a:1136:G:N2	50:a:1137:U:O4	2.45	0.47
23:T:91:ASN:OD1	23:T:91:ASN:C	2.58	0.47
50:a:1050:A:H2'	50:a:1051:A:C8	2.50	0.47
50:a:1325:C:H2'	50:a:1326:U:C6	2.50	0.47
50:a:1152:U:C2	50:a:1153:G:C8	3.02	0.47
49:A:154:A:O2'	49:A:155:U:OP2	2.29	0.47
49:A:1673:A:O2'	49:A:2725:U:OP1	2.32	0.47
50:a:731:U:O2	50:a:731:U:C2'	2.62	0.47
24:U:67:ARG:NH1	49:A:1261:G:OP1	2.48	0.46
30:c:176:ALA:HB3	30:c:183:ILE:HD11	1.96	0.46
49:A:1476:G:H2'	49:A:1477:U:C6	2.49	0.46
41:o:24:CYS:HB3	41:o:27:CYS:O	2.15	0.46
49:A:1025:A:OP2	49:A:1026:C:N4	2.39	0.46
50:a:18:U:H2'	50:a:19:C:C6	2.50	0.46
50:a:147:G:H2'	50:a:148:G:C8	2.50	0.46
9:B:39:G:O2'	9:B:40:C:OP1	2.32	0.46
49:A:2580:G:H5''	49:A:2581:U:OP2	2.15	0.46
49:A:2609:G:H5'	49:A:2609:G:C8	2.50	0.46
49:A:2725:U:H2'	49:A:2726:C:C6	2.50	0.46
50:a:1296:A:H4'	50:a:1297:U:C5	2.50	0.46
29:Z:39:VAL:CG2	29:Z:43:SER:HB2	2.45	0.46
36:j:53:PRO:O	36:j:57:THR:HG22	2.16	0.46
49:A:566:U:H2'	49:A:567:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A:1124:A:H2'	49:A:1125:U:C6	2.51	0.46
49:A:2406:G:H2'	49:A:2407:A:H8	1.80	0.46
21:R:86:ASP:C	21:R:86:ASP:OD1	2.59	0.46
26:W:19:ALA:HB1	26:W:24:LYS:HB2	1.98	0.46
30:c:73:LYS:NZ	30:c:205:ASP:OD1	2.33	0.46
50:a:75:A:N6	50:a:94:G:O2'	2.48	0.46
50:a:1171:G:C2	50:a:1172:C:C6	3.03	0.46
36:j:14:ARG:NE	36:j:79:GLN:OE1	2.49	0.46
44:r:14:VAL:HG13	44:r:23:ILE:CG2	2.45	0.46
50:a:977:C:H5''	50:a:978:A:OP2	2.15	0.46
50:a:1014:A:H8	50:a:1035:U:O2'	1.99	0.46
49:A:2052:C:H2'	49:A:2053:U:C6	2.51	0.46
49:A:285:U:H4'	49:A:286:U:C6	2.51	0.46
49:A:1780:G:N2	49:A:1783:G:OP2	2.37	0.46
51:h:70:MET:SD	51:h:96:ARG:HB3	2.56	0.46
12:H:22:LEU:C	12:H:22:LEU:HD23	2.41	0.46
46:t:50:ALA:HB1	46:t:57:HIS:HB3	1.96	0.46
49:A:407:G:H2'	49:A:408:U:C6	2.51	0.46
49:A:421:C:H2'	49:A:422:G:H8	1.81	0.46
49:A:2286:G:C8	49:A:2454:C:C4	3.04	0.46
7:8:13:ARG:NH1	18:O:61:LEU:O	2.37	0.46
13:I:39:LEU:C	13:I:39:LEU:HD23	2.41	0.46
25:V:57:ASN:OD1	25:V:57:ASN:C	2.59	0.46
41:o:18:VAL:HG21	50:a:1327:G:H4'	1.98	0.46
49:A:1417:G:C2	49:A:1418:G:C8	3.03	0.46
10:D:64:G:H2'	10:D:65:C:C6	2.51	0.45
38:l:17:GLU:O	38:l:80:LYS:N	2.49	0.45
38:l:128:ARG:NH1	50:a:1534:U:OP1	2.49	0.45
49:A:1966:U:OP1	49:A:2631:U:O2'	2.32	0.45
49:A:2629:A:H4'	49:A:2630:G:C5'	2.46	0.45
50:a:206:A:C2	50:a:207:G:N2	2.84	0.45
50:a:347:C:H2'	50:a:348:U:H6	1.81	0.45
25:V:58:ALA:HB1	25:V:64:MET:HE3	1.98	0.45
49:A:1160:C:H2'	49:A:1161:A:C8	2.52	0.45
49:A:1950:U:H2'	49:A:1951:C:C6	2.51	0.45
50:a:482:A:H2'	50:a:483:C:C6	2.51	0.45
50:a:562:U:H2'	50:a:563:C:C6	2.52	0.45
3:3:6:ILE:HG23	3:3:54:VAL:CG1	2.47	0.45
4:5:6:ARG:NH2	49:A:2046:U:OP2	2.40	0.45
13:I:182:ASN:ND2	13:I:185:ASP:OD2	2.46	0.45
21:R:42:ALA:HB3	21:R:80:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:k:40:ILE:N	37:k:73:LEU:O	2.46	0.45
50:a:682:G:H2'	50:a:683:A:C8	2.51	0.45
50:a:731:U:O2	50:a:731:U:H2'	2.16	0.45
32:e:14:ARG:CD	32:e:33:PRO:HD2	2.47	0.45
49:A:1013:U:H2'	49:A:1014:U:C6	2.52	0.45
49:A:1112:G:N3	49:A:1139:A:O2'	2.50	0.45
50:a:271:A:H2'	50:a:272:C:C6	2.52	0.45
50:a:345:G:H2'	50:a:346:A:H8	1.80	0.45
50:a:736:A:H2'	50:a:737:A:C8	2.51	0.45
51:h:31:MET:CG	51:h:34:GLY:O	2.65	0.45
16:M:136:GLN:C	16:M:137:GLN:HG2	2.41	0.45
42:p:8:LYS:O	42:p:12:ILE:HG23	2.17	0.45
49:A:83:G:H21	49:A:102:A:H2	1.64	0.45
50:a:329:A:H2'	50:a:330:C:C6	2.52	0.45
50:a:643:A:H2'	50:a:644:U:C6	2.52	0.45
25:V:10:ILE:HD13	25:V:46:VAL:CG1	2.46	0.45
32:e:200:ARG:HB3	50:a:9:A:C5	2.51	0.45
42:p:73:LYS:NZ	50:a:760:G:OP1	2.49	0.45
49:A:184:C:OP1	49:A:184:C:H2'	2.16	0.45
50:a:562:U:H2'	50:a:563:C:H6	1.82	0.45
38:l:44:TRP:CH2	50:a:694:U:O4'	2.69	0.45
50:a:189:G:C6	50:a:203:A:N6	2.85	0.45
50:a:1097:U:C2	50:a:1106:G:O6	2.70	0.45
49:A:1028:G:N3	49:A:1028:G:H2'	2.31	0.45
49:A:1806:U:C5	49:A:1811:A:N7	2.85	0.45
49:A:2356:A:H2'	49:A:2357:G:C8	2.52	0.45
50:a:388:G:N2	50:a:391:A:OP2	2.46	0.45
30:c:188:ASP:OD1	30:c:189:THR:N	2.46	0.45
49:A:396:G:H2'	49:A:397:U:C6	2.52	0.45
49:A:613:G:H2'	49:A:2057:A:N7	2.32	0.45
49:A:858:U:H2'	49:A:859:C:C6	2.52	0.45
2:2:26:PHE:CE2	26:W:45:ILE:HD11	2.53	0.44
24:U:79:ARG:N	49:A:608:C:OP2	2.50	0.44
29:Z:28:ARG:HG3	49:A:2383:C:H4'	1.99	0.44
49:A:1553:A:H2'	49:A:1554:A:C8	2.53	0.44
50:a:1187:A:H2'	50:a:1188:G:C8	2.52	0.44
50:a:1220:C:C2	50:a:1221:C:C5	3.05	0.44
30:c:166:PRO:HB3	30:c:173:ILE:CD1	2.47	0.44
32:e:129:PRO:HD2	50:a:411:C:H5''	1.99	0.44
45:s:42:GLY:O	45:s:68:ARG:NH2	2.50	0.44
50:a:392:G:H2'	50:a:393:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:547:A:H2'	50:a:548:G:C8	2.53	0.44
2:2:29:ARG:HG3	2:2:29:ARG:HH11	1.81	0.44
5:6:31:GLU:HG2	5:6:46:ARG:HG2	1.99	0.44
17:N:66:LYS:HA	17:N:79:PHE:O	2.18	0.44
23:T:29:HIS:CD2	23:T:30:THR:HG23	2.52	0.44
44:r:17:ASP:OD2	44:r:57:LEU:N	2.41	0.44
47:u:10:ARG:CD	50:a:107:G:O6	2.65	0.44
49:A:632:U:H2'	49:A:633:A:C8	2.52	0.44
49:A:754:U:H2'	49:A:755:C:C6	2.52	0.44
49:A:1829:A:H2'	49:A:1830:A:C8	2.52	0.44
49:A:1891:U:OP1	49:A:2437:G:O2'	2.28	0.44
49:A:2916:U:H2'	49:A:2917:U:C6	2.51	0.44
50:a:578:G:C6	50:a:883:A:C2	3.04	0.44
50:a:1168:A:C2	50:a:1192:G:C4	3.05	0.44
9:B:58:C:H2'	9:B:59:U:H6	1.82	0.44
12:H:13:THR:CG2	22:S:7:ILE:HG23	2.47	0.44
28:Y:7:ILE:CG2	28:Y:41:VAL:HB	2.48	0.44
49:A:1104:U:C2	49:A:1106:G:O4'	2.71	0.44
49:A:2612:U:O2	49:A:2612:U:H5'	2.17	0.44
50:a:144:C:C2	50:a:179:A:C2	3.05	0.44
19:P:45:ARG:NH1	49:A:2511:G:OP1	2.45	0.44
30:c:187:VAL:HG21	30:c:199:VAL:HG13	1.99	0.44
49:A:291:G:H2'	49:A:292:U:H6	1.82	0.44
49:A:1570:G:H2'	49:A:1571:G:C8	2.52	0.44
49:A:2293:A:H4'	49:A:2294:A:N3	2.32	0.44
49:A:2820:U:H2'	49:A:2821:U:O2	2.17	0.44
50:a:390:A:H2'	50:a:391:A:C8	2.53	0.44
50:a:1316:G:C2	50:a:1342:G:N3	2.86	0.44
5:6:38:ARG:C	5:6:39:LEU:HD12	2.41	0.44
49:A:1148:C:H2'	49:A:1149:U:C6	2.53	0.44
50:a:498:U:H2'	50:a:499:A:H8	1.83	0.44
50:a:1016:A:H2'	50:a:1017:A:O4'	2.17	0.44
5:6:32:MET:HE2	49:A:2371:U:O2'	2.18	0.44
18:O:21:ARG:HA	49:A:856:U:H2'	2.00	0.44
49:A:1509:G:C6	49:A:1510:U:C4	3.05	0.44
49:A:2358:G:N2	49:A:2412:C:C2	2.86	0.44
50:a:209:G:H2'	50:a:210:A:C8	2.52	0.44
50:a:419:A:O4'	50:a:420:U:H2'	2.18	0.44
11:G:154:ILE:O	11:G:154:ILE:CG2	2.64	0.44
21:R:108:LEU:C	21:R:108:LEU:HD23	2.43	0.44
34:g:88:ARG:NH2	50:a:681:G:O3'	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:r:44:LYS:HG2	44:r:46:TYR:CZ	2.52	0.44
49:A:736:C:H2'	49:A:737:C:H6	1.83	0.44
49:A:1648:C:O2'	49:A:1654:A:N1	2.46	0.44
50:a:41:C:H2'	50:a:42:G:H8	1.83	0.44
51:h:31:MET:HG3	51:h:34:GLY:O	2.18	0.44
49:A:194:A:H2'	49:A:195:C:C6	2.53	0.44
49:A:509:G:N2	49:A:512:A:OP2	2.42	0.44
49:A:1981:G:O2'	49:A:1983:U:O4	2.22	0.44
49:A:2877:G:N2	49:A:2880:A:OP2	2.39	0.44
50:a:277:U:H2'	50:a:278:A:C8	2.53	0.44
50:a:1438:C:H2'	50:a:1439:A:C8	2.53	0.44
5:6:21:LYS:NZ	5:6:28:GLU:O	2.50	0.43
9:B:37:A:C2	9:B:42:G:C2	3.06	0.43
11:G:53:HIS:HA	11:G:217:ARG:HB2	2.00	0.43
37:k:57:LYS:NZ	50:a:979:A:OP2	2.50	0.43
44:r:31:LYS:HE3	44:r:42:TYR:CE1	2.53	0.43
49:A:878:C:H2'	49:A:879:U:C6	2.53	0.43
49:A:1101:A:N7	49:A:1130:A:H2'	2.33	0.43
49:A:1711:G:O2'	49:A:2018:U:O4	2.22	0.43
49:A:1893:A:H2'	49:A:1894:G:O4'	2.18	0.43
3:3:39:ASP:OD1	3:3:39:ASP:N	2.39	0.43
7:8:8:ARG:NH2	49:A:247:A:OP2	2.42	0.43
16:M:73:LYS:HE3	16:M:75:TYR:CZ	2.54	0.43
18:O:42:SER:OG	49:A:717:C:OP2	2.34	0.43
31:d:52:SER:HB3	31:d:105:ILE:HD11	1.99	0.43
49:A:164:A:HO2'	49:A:165:C:H6	1.60	0.43
49:A:409:G:H3'	49:A:410:G:C8	2.53	0.43
49:A:1442:C:H2'	49:A:1443:A:H8	1.83	0.43
50:a:1337:U:H2'	50:a:1338:A:C8	2.53	0.43
26:W:31:THR:O	26:W:32:ARG:HG2	2.17	0.43
35:i:21:ARG:NH2	35:i:70:ASP:OD1	2.51	0.43
49:A:171:A:H2'	49:A:172:U:C6	2.54	0.43
49:A:297:G:C2	49:A:298:U:O4	2.71	0.43
49:A:2232:A:H2'	49:A:2233:C:C6	2.52	0.43
49:A:2605:G:C2	49:A:2606:C:C6	3.07	0.43
50:a:230:U:H2'	50:a:231:U:H6	1.81	0.43
14:J:35:VAL:HB	14:J:155:VAL:CG1	2.49	0.43
36:j:59:THR:O	36:j:59:THR:HG22	2.18	0.43
49:A:2820:U:C2'	49:A:2821:U:O2	2.65	0.43
50:a:561:A:H2'	50:a:562:U:C6	2.52	0.43
50:a:1051:A:H2'	50:a:1052:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:11:ARG:HD2	21:R:99:TYR:CZ	2.53	0.43
49:A:224:A:C4	49:A:269:G:N7	2.86	0.43
49:A:575:G:N3	49:A:575:G:H2'	2.34	0.43
49:A:1583:G:OP2	49:A:1583:G:N2	2.39	0.43
49:A:2672:G:H4'	49:A:2759:G:O2'	2.19	0.43
50:a:1438:C:H2'	50:a:1439:A:H8	1.83	0.43
7:8:31:HIS:CE1	49:A:2448:G:N7	2.85	0.43
12:H:6:LEU:H	12:H:33:ASN:ND2	2.17	0.43
49:A:2041:A:H2'	49:A:2042:A:C8	2.54	0.43
49:A:2097:G:H2'	49:A:2098:A:C8	2.54	0.43
49:A:2663:U:H2'	49:A:2664:U:C6	2.53	0.43
50:a:1028:A:C6	50:a:1029:G:N7	2.87	0.43
22:S:23:ARG:NH2	49:A:2869:G:O6	2.49	0.43
23:T:102:ASP:OD1	23:T:102:ASP:N	2.51	0.43
49:A:590:U:C4	49:A:1257:G:C2	3.06	0.43
49:A:1129:A:C5	49:A:1130:A:N6	2.86	0.43
50:a:1337:U:H2'	50:a:1338:A:H8	1.83	0.43
17:N:102:VAL:HG11	17:N:106:LEU:HD12	2.01	0.43
35:i:110:GLU:OE1	35:i:121:ARG:NH2	2.45	0.43
37:k:56:HIS:O	37:k:56:HIS:CG	2.71	0.43
49:A:1712:A:N3	49:A:1714:C:C4	2.87	0.43
49:A:2605:G:C2'	49:A:2606:C:H5''	2.49	0.43
50:a:609:G:H2'	50:a:610:A:H8	1.83	0.43
5:6:9:CYS:HB3	5:6:12:CYS:O	2.19	0.43
16:M:109:MET:HE3	49:A:1182:G:H21	1.84	0.43
49:A:859:C:H2'	49:A:860:U:H6	1.84	0.43
49:A:2772:C:H2'	49:A:2773:U:C6	2.54	0.43
50:a:491:C:H5''	50:a:492:G:OP2	2.19	0.43
50:a:509:C:H2'	50:a:510:C:C6	2.54	0.43
50:a:1072:U:H2'	50:a:1073:G:H8	1.84	0.43
13:I:41:ARG:HG3	13:I:41:ARG:HH11	1.83	0.43
26:W:45:ILE:HG23	26:W:46:PHE:CD2	2.54	0.43
30:c:217:MET:O	30:c:221:ILE:HG12	2.19	0.43
49:A:297:G:N2	49:A:298:U:O4	2.52	0.43
49:A:375:A:C2	49:A:378:C:C5	3.07	0.43
49:A:2348:G:H5''	49:A:2349:A:OP2	2.19	0.43
49:A:2713:G:H2'	49:A:2714:U:C6	2.53	0.43
50:a:1423:C:H2'	50:a:1424:A:H8	1.84	0.43
14:J:117:VAL:CG1	14:J:128:TYR:OH	2.67	0.42
30:c:178:LYS:NZ	50:a:1087:U:OP1	2.45	0.42
49:A:117:A:H5'	49:A:118:A:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A:160:G:H21	49:A:168:A:H2	1.67	0.42
49:A:665:G:N3	49:A:665:G:H5'	2.33	0.42
49:A:724:C:H2'	49:A:725:A:H8	1.84	0.42
49:A:2541:U:H2'	49:A:2542:C:C6	2.54	0.42
50:a:276:U:H2'	50:a:277:U:C6	2.54	0.42
50:a:450:U:H2'	50:a:451:U:H6	1.84	0.42
50:a:1316:G:N2	50:a:1342:G:H1'	2.34	0.42
14:J:102:LYS:HE2	48:4:26:GLY:O	2.19	0.42
22:S:28:LEU:C	22:S:28:LEU:HD12	2.44	0.42
34:g:50:TYR:CE2	34:g:52:ILE:HD11	2.53	0.42
39:m:29:ASN:O	39:m:33:LYS:N	2.52	0.42
41:o:16:TYR:CE2	41:o:19:ARG:HB2	2.54	0.42
45:s:61:THR:CG2	50:a:728:C:O2'	2.67	0.42
49:A:1105:U:H3'	49:A:1106:G:H5''	2.00	0.42
50:a:321:A:H2'	50:a:322:C:C6	2.54	0.42
50:a:1014:A:H5''	50:a:1036:C:C4	2.53	0.42
50:a:1266:G:H2'	50:a:1290:A:H61	1.85	0.42
14:J:163:ASP:OD1	14:J:163:ASP:N	2.53	0.42
16:M:31:SER:HA	16:M:109:MET:CE	2.50	0.42
49:A:730:A:H5'	49:A:819:A:N6	2.35	0.42
49:A:1124:A:H2'	49:A:1125:U:H6	1.84	0.42
49:A:1813:A:H1'	49:A:1965:A:N6	2.34	0.42
50:a:698:G:C6	50:a:699:G:C6	3.07	0.42
50:a:1366:A:H2'	50:a:1367:G:C8	2.54	0.42
19:P:104:PHE:HE2	19:P:125:LEU:HD11	1.85	0.42
49:A:262:G:H21	49:A:666:A:H8	1.67	0.42
49:A:293:U:H2'	49:A:294:G:H8	1.84	0.42
50:a:218:U:H2'	50:a:219:C:O4'	2.20	0.42
50:a:382:A:C6	50:a:383:U:C4	3.08	0.42
50:a:742:A:H2'	50:a:743:C:C6	2.54	0.42
50:a:1015:C:H2'	50:a:1034:U:O2'	2.19	0.42
50:a:1016:A:C8	50:a:1034:U:H1'	2.54	0.42
12:H:70:ASN:OD1	12:H:70:ASN:C	2.63	0.42
12:H:157:ALA:O	49:A:2080:G:C5'	2.67	0.42
44:r:9:VAL:HG21	44:r:62:LYS:HE3	2.01	0.42
49:A:858:U:H2'	49:A:859:C:H6	1.85	0.42
49:A:2091:C:H2'	49:A:2092:C:H6	1.84	0.42
50:a:182:A:N1	50:a:184:A:N1	2.67	0.42
50:a:254:A:C2	50:a:290:A:C5	3.07	0.42
49:A:901:G:H2'	49:A:902:A:H8	1.81	0.42
49:A:1817:C:H2'	49:A:1818:A:C5	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:213:G:H2'	50:a:214:A:H8	1.83	0.42
50:a:1249:A:N7	50:a:1314:C:H1'	2.35	0.42
12:H:163:VAL:HG21	49:A:2645:G:H21	1.84	0.42
41:o:24:CYS:SG	41:o:25:GLU:N	2.93	0.42
43:q:82:LYS:HE3	50:a:482:A:H4'	2.02	0.42
49:A:224:A:C8	49:A:269:G:O6	2.73	0.42
49:A:280:C:H2'	49:A:281:A:C8	2.55	0.42
49:A:622:A:O2'	49:A:2046:U:OP1	2.38	0.42
49:A:830:U:H4'	49:A:1806:U:H4'	2.01	0.42
49:A:1105:U:O4'	49:A:1114:A:H1'	2.19	0.42
49:A:1950:U:H2'	49:A:1951:C:H6	1.84	0.42
49:A:2821:U:N3	49:A:2823:G:OP2	2.49	0.42
50:a:832:U:H2'	50:a:833:G:H8	1.85	0.42
50:a:1011:U:H6	50:a:1011:U:O5'	2.01	0.42
50:a:1256:A:H2'	50:a:1257:A:C8	2.54	0.42
50:a:1485:G:H2'	50:a:1486:G:C8	2.54	0.42
12:H:38:LYS:HE3	12:H:96:VAL:HG12	2.00	0.42
12:H:154:VAL:O	12:H:154:VAL:HG12	2.19	0.42
16:M:50:ASP:CG	16:M:122:LYS:HZ3	2.27	0.42
25:V:39:THR:HG22	25:V:41:LYS:H	1.85	0.42
44:r:49:HIS:HA	44:r:73:LYS:HE3	2.01	0.42
49:A:1942:U:C6	49:A:1943:A:C2	3.07	0.42
49:A:2051:C:H2'	49:A:2052:C:H6	1.84	0.42
49:A:2842:G:H2'	49:A:2843:A:H5''	2.02	0.42
50:a:1341:U:O4	50:a:1342:G:C6	2.73	0.42
50:a:1547:C:C5	50:a:1548:C:C5	3.08	0.42
15:K:57:ASP:O	15:K:62:ARG:NH1	2.38	0.42
20:Q:28:GLU:OE2	20:Q:92:ARG:NH2	2.52	0.42
22:S:6:LEU:C	22:S:6:LEU:HD23	2.45	0.42
49:A:1127:U:O2'	49:A:1128:A:H2'	2.19	0.42
49:A:1869:G:H2'	49:A:1870:C:H6	1.85	0.42
50:a:1009:C:H2'	50:a:1010:U:C6	2.54	0.42
15:K:59:LYS:O	15:K:63:THR:HG23	2.20	0.42
19:P:56:ARG:NH1	49:A:2496:A:O2'	2.44	0.42
25:V:18:ARG:NH1	49:A:563:G:O5'	2.53	0.42
26:W:31:THR:O	26:W:32:ARG:CG	2.68	0.42
30:c:4:ILE:HD11	30:c:216:LYS:HG3	2.02	0.42
34:g:12:PRO:HA	34:g:59:PHE:CE2	2.55	0.42
34:g:76:PHE:CD1	34:g:76:PHE:C	2.97	0.42
49:A:187:C:H2'	49:A:188:C:C6	2.55	0.42
49:A:460:C:H2'	49:A:461:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A:1090:A:H3'	49:A:1091:G:H5'	2.01	0.42
49:A:1422:A:C4	49:A:1423:C:C5	3.08	0.42
50:a:138:A:H2'	50:a:139:U:C6	2.55	0.42
50:a:1392:U:C5	50:a:1393:C:C5	3.08	0.42
1:1:17:ARG:CZ	1:1:27:ARG:HD3	2.50	0.41
43:q:26:ARG:O	50:a:109:C:O2'	2.37	0.41
49:A:730:A:C8	49:A:818:U:C4	3.08	0.41
49:A:1869:G:H2'	49:A:1870:C:C6	2.55	0.41
49:A:2338:A:H2'	49:A:2338:A:N3	2.35	0.41
50:a:470:A:H2'	50:a:471:A:C8	2.55	0.41
50:a:928:A:H2'	50:a:929:A:C8	2.55	0.41
50:a:1095:U:O2'	50:a:1114:A:OP2	2.34	0.41
32:e:14:ARG:HD2	32:e:33:PRO:HD2	2.01	0.41
32:e:41:ARG:NH2	50:a:518:A:OP1	2.50	0.41
32:e:57:LEU:HD12	32:e:194:ILE:CD1	2.50	0.41
38:l:36:ASP:OD1	38:l:36:ASP:C	2.63	0.41
49:A:200:A:N6	49:A:2457:A:O2'	2.49	0.41
49:A:991:A:H2'	49:A:992:A:C8	2.55	0.41
49:A:1843:U:O2	49:A:1843:U:O4'	2.38	0.41
49:A:2636:U:O2'	49:A:2637:C:H5'	2.20	0.41
50:a:189:G:O6	50:a:203:A:N6	2.53	0.41
17:N:90:ASP:OD1	17:N:90:ASP:C	2.63	0.41
32:e:3:ARG:NH2	50:a:412:G:N7	2.67	0.41
49:A:292:U:H2'	49:A:293:U:C6	2.55	0.41
49:A:890:G:O5'	49:A:890:G:H8	2.03	0.41
49:A:1115:G:N1	49:A:1135:G:OP2	2.49	0.41
49:A:1583:G:H1'	49:A:1584:U:OP1	2.20	0.41
49:A:2070:C:C2	49:A:2071:C:C5	3.09	0.41
50:a:155:U:H2'	50:a:156:C:H6	1.84	0.41
50:a:444:C:H2'	50:a:445:U:C6	2.55	0.41
14:J:136:LEU:HD21	14:J:146:VAL:CG2	2.51	0.41
19:P:51:ARG:HG3	19:P:66:ILE:HD11	2.03	0.41
20:Q:8:ARG:NH1	49:A:1313:G:O2'	2.53	0.41
34:g:28:GLY:O	34:g:32:THR:HG23	2.20	0.41
43:q:89:LYS:NZ	50:a:470:A:N3	2.67	0.41
47:u:7:ALA:O	47:u:11:VAL:HG23	2.21	0.41
49:A:304:G:C4	49:A:305:A:C8	3.09	0.41
50:a:381:A:C2	50:a:382:A:C8	3.08	0.41
50:a:618:G:C5	50:a:619:C:C5	3.09	0.41
50:a:691:G:O6	50:a:716:A:C6	2.73	0.41
50:a:988:A:C4	50:a:1330:A:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:1173:C:H2'	50:a:1174:G:C8	2.55	0.41
32:e:200:ARG:NH2	50:a:9:A:OP2	2.50	0.41
49:A:307:A:C6	49:A:409:G:C6	3.09	0.41
49:A:1215:U:H2'	49:A:1216:U:H5''	2.02	0.41
49:A:1572:G:C6	49:A:1591:G:C6	3.08	0.41
49:A:2415:A:N7	49:A:2416:G:C6	2.88	0.41
49:A:2605:G:H2'	49:A:2606:C:H5''	2.02	0.41
50:a:601:U:H2'	50:a:602:U:C6	2.55	0.41
50:a:1526:U:H2'	50:a:1527:C:C6	2.55	0.41
2:2:38:GLU:O	2:2:39:GLU:CG	2.68	0.41
23:T:83:LEU:HD22	23:T:88:ILE:HD11	2.02	0.41
28:Y:7:ILE:HG13	28:Y:63:LEU:CD1	2.51	0.41
49:A:1131:G:O6	49:A:1133:G:N2	2.46	0.41
49:A:1423:C:H2'	49:A:1424:A:H8	1.84	0.41
49:A:1477:U:H2'	49:A:1478:A:C8	2.56	0.41
50:a:534:C:H5''	50:a:535:G:OP2	2.20	0.41
50:a:921:U:H2'	50:a:922:C:C6	2.56	0.41
50:a:1011:U:H5''	50:a:1012:U:OP2	2.21	0.41
50:a:1344:A:H2'	50:a:1345:G:O4'	2.20	0.41
37:k:76:ILE:CD1	37:k:87:LEU:HD11	2.51	0.41
49:A:632:U:H2'	49:A:633:A:H8	1.83	0.41
49:A:1452:C:H3'	49:A:1453:G:H21	1.85	0.41
49:A:2548:C:C2	49:A:2572:G:N2	2.89	0.41
50:a:1151:U:H2'	50:a:1152:U:C6	2.56	0.41
50:a:1330:A:C8	50:a:1334:G:C6	3.09	0.41
10:D:69:C:H2'	10:D:70:C:C6	2.55	0.41
23:T:76:TYR:CZ	23:T:80:MET:HG3	2.56	0.41
38:l:72:LYS:HA	38:l:75:MET:HG2	2.03	0.41
41:o:16:TYR:CZ	50:a:1328:C:C4	3.09	0.41
49:A:666:A:H2'	49:A:667:G:H5'	2.03	0.41
49:A:1115:G:H22	49:A:1135:G:P	2.42	0.41
49:A:1593:G:H8	49:A:1593:G:O5'	2.04	0.41
50:a:1328:C:O2	50:a:1328:C:H2'	2.19	0.41
2:2:38:GLU:O	2:2:39:GLU:HG2	2.21	0.41
5:6:31:GLU:CG	5:6:46:ARG:HG2	2.51	0.41
17:N:22:ILE:HD12	49:A:1979:A:C5	2.56	0.41
20:Q:93:TYR:HH	20:Q:121:LEU:HB3	1.86	0.41
20:Q:102:ARG:NH1	49:A:2902:A:OP1	2.54	0.41
23:T:51:ARG:HD3	49:A:1200:A:C8	2.56	0.41
24:U:92:TYR:CD1	24:U:92:TYR:C	2.99	0.41
33:f:106:ILE:HB	33:f:124:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:o:58:LYS:HE3	50:a:1199:A:O2'	2.21	0.41
47:u:10:ARG:HD3	50:a:107:G:O6	2.21	0.41
49:A:463:C:H2'	49:A:464:U:C6	2.56	0.41
49:A:1071:A:C2	49:A:2515:A:H5'	2.56	0.41
49:A:1089:C:OP1	49:A:1090:A:H5'	2.20	0.41
50:a:450:U:H2'	50:a:451:U:C6	2.55	0.41
50:a:1124:C:H5'	50:a:1125:C:OP2	2.21	0.41
50:a:1262:A:H2'	50:a:1263:A:O4'	2.21	0.41
51:h:111:ARG:NE	51:h:123:GLU:OE1	2.46	0.41
12:H:53:PHE:CG	12:H:54:GLU:N	2.89	0.41
35:i:20:VAL:HG12	35:i:20:VAL:O	2.20	0.41
36:j:15:LYS:HE2	50:a:1358:G:N7	2.35	0.41
47:u:44:ASP:OD1	47:u:45:ASN:N	2.54	0.41
49:A:1474:C:H2'	49:A:1475:A:C8	2.56	0.41
49:A:1941:C:H41	50:a:1421:A:H5'	1.85	0.41
49:A:2332:U:O2'	49:A:2333:U:H5'	2.20	0.41
49:A:2488:C:H2'	49:A:2489:U:C6	2.56	0.41
50:a:352:A:H4'	50:a:353:C:OP2	2.20	0.41
50:a:609:G:H2'	50:a:610:A:C8	2.56	0.41
50:a:689:A:H2'	50:a:690:U:H6	1.85	0.41
9:B:106:G:C6	9:B:107:U:C4	3.09	0.40
10:D:64:G:H2'	10:D:65:C:H6	1.84	0.40
27:X:39:ASN:ND2	27:X:61:ALA:HB3	2.37	0.40
32:e:41:ARG:NH1	50:a:518:A:OP1	2.53	0.40
39:m:76:ILE:HG12	39:m:108:TYR:CE1	2.56	0.40
49:A:749:G:N3	49:A:771:G:C2	2.90	0.40
49:A:1151:G:C6	49:A:1152:U:C4	3.09	0.40
49:A:1526:G:H2'	49:A:1527:A:C8	2.56	0.40
49:A:1548:U:H2'	49:A:1549:C:C6	2.55	0.40
49:A:1773:A:H2'	49:A:1774:A:C8	2.56	0.40
49:A:1821:U:H2'	49:A:1822:C:C6	2.56	0.40
50:a:343:C:H2'	50:a:344:A:H8	1.86	0.40
50:a:414:G:C2'	50:a:415:A:H5'	2.50	0.40
50:a:1027:U:C2	50:a:1028:A:C8	3.09	0.40
15:K:30:LYS:HE2	15:K:82:GLY:HA3	2.03	0.40
19:P:83:MET:HE1	49:A:1000:G:O4'	2.21	0.40
49:A:526:A:N3	49:A:526:A:H2'	2.36	0.40
49:A:903:G:N3	49:A:2295:A:H2'	2.37	0.40
49:A:2260:A:H2'	49:A:2261:G:C8	2.56	0.40
49:A:2400:U:H2'	49:A:2401:C:C6	2.57	0.40
49:A:2824:G:H2'	49:A:2825:U:C6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:258:A:H4'	50:a:259:G:O5'	2.22	0.40
50:a:583:G:O2'	50:a:829:G:OP2	2.29	0.40
50:a:1295:C:OP2	50:a:1296:A:O2'	2.38	0.40
51:h:62:PHE:CZ	51:h:66:ILE:HD11	2.56	0.40
10:D:54:G:C4	10:D:55:U:C5	3.09	0.40
38:l:36:ASP:OD1	38:l:38:PHE:N	2.53	0.40
49:A:407:G:H2'	49:A:408:U:H6	1.86	0.40
49:A:545:G:N2	49:A:547:A:H3'	2.36	0.40
49:A:2673:C:O5'	49:A:2673:C:H6	2.05	0.40
49:A:2796:C:C4	49:A:2797:C:C5	3.10	0.40
4:5:4:PRO:HG2	49:A:2043:U:O2	2.21	0.40
9:B:40:C:OP1	14:J:64:LYS:NZ	2.38	0.40
9:B:42:G:C2	9:B:46:A:C2	3.09	0.40
15:K:19:PHE:HB3	15:K:24:VAL:HA	2.04	0.40
21:R:31:LEU:HD11	21:R:42:ALA:HB1	2.02	0.40
23:T:76:TYR:CD1	23:T:76:TYR:C	2.98	0.40
23:T:83:LEU:CD2	23:T:88:ILE:HD11	2.51	0.40
27:X:47:PRO:HB3	27:X:52:PRO:O	2.21	0.40
33:f:29:ARG:NH2	50:a:1408:C:OP2	2.40	0.40
35:i:80:ILE:HG22	35:i:81:SER:N	2.37	0.40
49:A:1083:G:H2'	49:A:1084:U:C6	2.56	0.40
50:a:1542:G:H2'	50:a:1543:A:C8	2.56	0.40
10:D:58:A:H2'	10:D:59:A:H5''	2.04	0.40
21:R:30:ARG:HA	21:R:93:VAL:O	2.21	0.40
22:S:80:THR:HG22	22:S:82:LYS:H	1.85	0.40
40:n:17:ILE:HG13	50:a:1313:U:C5	2.56	0.40
44:r:15:VAL:O	44:r:15:VAL:CG1	2.68	0.40
49:A:229:A:O2'	49:A:231:A:N1	2.48	0.40
49:A:460:C:H2'	49:A:461:A:H8	1.86	0.40
49:A:849:A:H2'	49:A:851:C:C4	2.57	0.40
49:A:1236:G:H2'	49:A:1237:U:H6	1.86	0.40
49:A:2342:U:H2'	49:A:2343:U:C6	2.57	0.40
49:A:2354:A:H2'	49:A:2355:A:C8	2.57	0.40
50:a:65:G:C6	50:a:99:U:O4	2.74	0.40
50:a:1013:G:N2	50:a:1049:C:O2	2.55	0.40
50:a:1131:G:C6	50:a:1132:C:C4	3.09	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	1	57/62 (92%)	57 (100%)	0	0	100	100
2	2	62/69 (90%)	62 (100%)	0	0	100	100
3	3	54/59 (92%)	53 (98%)	1 (2%)	0	100	100
4	5	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
5	6	45/49 (92%)	45 (100%)	0	0	100	100
6	7	40/45 (89%)	40 (100%)	0	0	100	100
7	8	62/66 (94%)	62 (100%)	0	0	100	100
8	9	34/37 (92%)	34 (100%)	0	0	100	100
11	G	271/277 (98%)	266 (98%)	5 (2%)	0	100	100
12	H	214/220 (97%)	207 (97%)	7 (3%)	0	100	100
13	I	202/207 (98%)	200 (99%)	2 (1%)	0	100	100
14	J	173/179 (97%)	168 (97%)	5 (3%)	0	100	100
15	K	162/178 (91%)	160 (99%)	2 (1%)	0	100	100
16	M	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
17	N	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
18	O	143/146 (98%)	141 (99%)	2 (1%)	0	100	100
19	P	133/144 (92%)	131 (98%)	2 (2%)	0	100	100
20	Q	118/122 (97%)	114 (97%)	4 (3%)	0	100	100
21	R	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
22	S	112/116 (97%)	112 (100%)	0	0	100	100
23	T	114/118 (97%)	114 (100%)	0	0	100	100
24	U	99/102 (97%)	97 (98%)	2 (2%)	0	100	100
25	V	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
26	W	87/91 (96%)	86 (99%)	1 (1%)	0	100	100
27	X	97/105 (92%)	97 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Y	92/217 (42%)	92 (100%)	0	0	100	100
29	Z	76/94 (81%)	74 (97%)	2 (3%)	0	100	100
30	c	219/255 (86%)	216 (99%)	3 (1%)	0	100	100
31	d	200/217 (92%)	197 (98%)	3 (2%)	0	100	100
32	e	197/200 (98%)	193 (98%)	4 (2%)	0	100	100
33	f	154/166 (93%)	153 (99%)	1 (1%)	0	100	100
34	g	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
35	i	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
36	j	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
37	k	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
38	l	116/129 (90%)	113 (97%)	3 (3%)	0	100	100
39	m	133/137 (97%)	130 (98%)	3 (2%)	0	100	100
40	n	111/121 (92%)	111 (100%)	0	0	100	100
41	o	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
42	p	84/89 (94%)	84 (100%)	0	0	100	100
43	q	88/91 (97%)	88 (100%)	0	0	100	100
44	r	77/87 (88%)	75 (97%)	2 (3%)	0	100	100
45	s	61/80 (76%)	60 (98%)	1 (2%)	0	100	100
46	t	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
47	u	78/83 (94%)	78 (100%)	0	0	100	100
48	4	53/84 (63%)	50 (94%)	3 (6%)	0	100	100
51	h	144/156 (92%)	143 (99%)	1 (1%)	0	100	100
All	All	5278/5773 (91%)	5193 (98%)	85 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	49/52 (94%)	49 (100%)	0	100	100
2	2	58/62 (94%)	58 (100%)	0	100	100
3	3	51/53 (96%)	51 (100%)	0	100	100
4	5	48/50 (96%)	48 (100%)	0	100	100
5	6	45/47 (96%)	45 (100%)	0	100	100
6	7	38/40 (95%)	38 (100%)	0	100	100
7	8	55/57 (96%)	55 (100%)	0	100	100
8	9	35/35 (100%)	35 (100%)	0	100	100
11	G	220/224 (98%)	220 (100%)	0	100	100
12	H	174/177 (98%)	174 (100%)	0	100	100
13	I	168/169 (99%)	168 (100%)	0	100	100
14	J	154/158 (98%)	154 (100%)	0	100	100
15	K	144/155 (93%)	144 (100%)	0	100	100
16	M	121/123 (98%)	121 (100%)	0	100	100
17	N	100/100 (100%)	100 (100%)	0	100	100
18	O	111/112 (99%)	111 (100%)	0	100	100
19	P	112/119 (94%)	112 (100%)	0	100	100
20	Q	101/102 (99%)	101 (100%)	0	100	100
21	R	94/95 (99%)	94 (100%)	0	100	100
22	S	100/102 (98%)	100 (100%)	0	100	100
23	T	96/98 (98%)	96 (100%)	0	100	100
24	U	86/86 (100%)	86 (100%)	0	100	100
25	V	90/94 (96%)	90 (100%)	0	100	100
26	W	80/82 (98%)	80 (100%)	0	100	100
27	X	84/90 (93%)	84 (100%)	0	100	100
28	Y	83/190 (44%)	83 (100%)	0	100	100
29	Z	61/75 (81%)	61 (100%)	0	100	100
30	c	192/221 (87%)	192 (100%)	0	100	100
31	d	164/175 (94%)	164 (100%)	0	100	100
32	e	174/175 (99%)	174 (100%)	0	100	100
33	f	122/131 (93%)	122 (100%)	0	100	100
34	g	81/86 (94%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	i	112/113 (99%)	112 (100%)	0	100	100
36	j	105/107 (98%)	105 (100%)	0	100	100
37	k	91/91 (100%)	91 (100%)	0	100	100
38	l	94/104 (90%)	93 (99%)	1 (1%)	65	82
39	m	117/119 (98%)	117 (100%)	0	100	100
40	n	98/104 (94%)	98 (100%)	0	100	100
41	o	52/53 (98%)	51 (98%)	1 (2%)	50	75
42	p	79/81 (98%)	79 (100%)	0	100	100
43	q	76/77 (99%)	76 (100%)	0	100	100
44	r	74/82 (90%)	74 (100%)	0	100	100
45	s	56/68 (82%)	56 (100%)	0	100	100
46	t	70/80 (88%)	70 (100%)	0	100	100
47	u	67/69 (97%)	67 (100%)	0	100	100
48	4	55/75 (73%)	55 (100%)	0	100	100
51	h	126/132 (96%)	126 (100%)	0	100	100
All	All	4563/4890 (93%)	4561 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	l	119	ASN
41	o	4	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	16	ASN
2	2	31	GLN
7	8	31	HIS
12	H	33	ASN
12	H	148	HIS
12	H	200	ASN
14	J	63	GLN
16	M	59	ASN
16	M	78	HIS
17	N	3	GLN

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Mol	Chain	Res	Type
17	N	45	ASN
19	P	123	HIS
22	S	14	GLN
26	W	34	ASN
26	W	54	ASN
26	W	69	GLN
28	Y	88	HIS
30	c	171	ASN
31	d	68	HIS
32	e	35	GLN
32	e	36	HIS
34	g	53	ASN
42	p	46	HIS
42	p	50	HIS
47	u	77	GLN
51	h	40	GLN
51	h	148	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	D	76/77 (98%)	8 (10%)	3 (3%)
49	A	2803/2923 (95%)	330 (11%)	67 (2%)
50	a	1510/1552 (97%)	157 (10%)	0
9	B	112/115 (97%)	9 (8%)	1 (0%)
All	All	4501/4667 (96%)	504 (11%)	71 (1%)

All (504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	B	10	U
9	B	24	C
9	B	39	G
9	B	40	C
9	B	42	G
9	B	55	A
9	B	87	C
9	B	88	G
9	B	106	G
10	D	8	U
10	D	16	U

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Mol	Chain	Res	Type
10	D	18	C
10	D	19	G
10	D	21	U
10	D	59	A
10	D	60	A
10	D	77	A
49	A	34	U
49	A	63	U
49	A	64	A
49	A	71	A
49	A	74	U
49	A	75	G
49	A	117	A
49	A	118	A
49	A	119	U
49	A	150	A
49	A	154	A
49	A	155	U
49	A	164	A
49	A	165	C
49	A	167	U
49	A	177	G
49	A	180	G
49	A	184	C
49	A	199	A
49	A	202	A
49	A	203	U
49	A	218	G
49	A	219	A
49	A	224	A
49	A	225	A
49	A	231	A
49	A	233	U
49	A	251	G
49	A	253	G
49	A	284	C
49	A	285	U
49	A	286	U
49	A	287	G
49	A	289	U
49	A	300	G
49	A	313	U

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Mol	Chain	Res	Type
49	A	314	A
49	A	315	C
49	A	321	U
49	A	322	A
49	A	354	A
49	A	373	A
49	A	374	U
49	A	404	U
49	A	410	G
49	A	432	G
49	A	457	G
49	A	497	U
49	A	502	C
49	A	503	A
49	A	527	G
49	A	548	A
49	A	549	U
49	A	550	A
49	A	553	A
49	A	554	C
49	A	555	C
49	A	572	C
49	A	575	G
49	A	576	U
49	A	577	A
49	A	578	G
49	A	591	A
49	A	592	A
49	A	593	U
49	A	594	G
49	A	606	G
49	A	616	G
49	A	618	A
49	A	630	G
49	A	646	A
49	A	647	G
49	A	682	A
49	A	683	G
49	A	699	U
49	A	731	U
49	A	775	A
49	A	793	G

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Mol	Chain	Res	Type
49	A	794	A
49	A	809	A
49	A	820	G
49	A	827	A
49	A	829	U
49	A	837	G
49	A	850	G
49	A	857	C
49	A	872	U
49	A	873	U
49	A	911	A
49	A	955	A
49	A	970	U
49	A	985	A
49	A	989	A
49	A	990	G
49	A	1005	G
49	A	1018	A
49	A	1027	A
49	A	1040	A
49	A	1049	C
49	A	1056	U
49	A	1057	A
49	A	1070	A
49	A	1077	U
49	A	1089	C
49	A	1090	A
49	A	1106	G
49	A	1107	G
49	A	1114	A
49	A	1115	G
49	A	1123	C
49	A	1131	G
49	A	1132	A
49	A	1133	G
49	A	1134	U
49	A	1156	G
49	A	1160	C
49	A	1173	A
49	A	1174	U
49	A	1176	U
49	A	1177	A

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Mol	Chain	Res	Type
49	A	1178	C
49	A	1186	A
49	A	1187	A
49	A	1215	U
49	A	1216	U
49	A	1217	U
49	A	1218	G
49	A	1225	G
49	A	1250	G
49	A	1276	G
49	A	1291	A
49	A	1292	A
49	A	1294	G
49	A	1309	G
49	A	1310	A
49	A	1337	A
49	A	1339	U
49	A	1340	G
49	A	1358	A
49	A	1366	U
49	A	1402	A
49	A	1405	G
49	A	1415	A
49	A	1416	U
49	A	1432	A
49	A	1433	U
49	A	1434	U
49	A	1449	A
49	A	1455	U
49	A	1456	U
49	A	1457	U
49	A	1458	A
49	A	1463	A
49	A	1464	U
49	A	1471	A
49	A	1472	C
49	A	1490	G
49	A	1497	A
49	A	1504	U
49	A	1511	C
49	A	1526	G
49	A	1536	C

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Mol	Chain	Res	Type
49	A	1552	U
49	A	1553	A
49	A	1560	A
49	A	1569	G
49	A	1574	G
49	A	1578	A
49	A	1579	C
49	A	1580	A
49	A	1581	U
49	A	1582	U
49	A	1583	G
49	A	1584	U
49	A	1592	A
49	A	1593	G
49	A	1594	U
49	A	1606	C
49	A	1613	G
49	A	1616	A
49	A	1625	U
49	A	1630	A
49	A	1631	G
49	A	1651	C
49	A	1652	A
49	A	1654	A
49	A	1678	A
49	A	1679	A
49	A	1690	A
49	A	1691	G
49	A	1692	C
49	A	1718	G
49	A	1740	G
49	A	1772	G
49	A	1783	G
49	A	1789	A
49	A	1790	G
49	A	1791	G
49	A	1800	A
49	A	1809	C
49	A	1818	A
49	A	1827	C
49	A	1828	U
49	A	1843	U

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Mol	Chain	Res	Type
49	A	1885	G
49	A	1893	A
49	A	1896	U
49	A	1897	U
49	A	1898	C
49	A	1926	A
49	A	1927	A
49	A	1928	A
49	A	1933	G
49	A	1939	A
49	A	1940	A
49	A	1941	C
49	A	1943	A
49	A	1956	G
49	A	1957	G
49	A	1965	A
49	A	1982	U
49	A	1994	C
49	A	1997	A
49	A	1998	A
49	A	1999	G
49	A	2008	A
49	A	2009	U
49	A	2019	G
49	A	2020	U
49	A	2040	A
49	A	2058	A
49	A	2059	G
49	A	2060	A
49	A	2070	C
49	A	2082	C
49	A	2083	G
49	A	2086	A
49	A	2087	A
49	A	2088	G
49	A	2089	A
49	A	2096	G
49	A	2218	G
49	A	2219	C
49	A	2225	A
49	A	2226	A
49	A	2230	G

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Mol	Chain	Res	Type
49	A	2231	C
49	A	2238	U
49	A	2239	A
49	A	2240	U
49	A	2252	A
49	A	2265	G
49	A	2266	G
49	A	2295	A
49	A	2305	A
49	A	2310	C
49	A	2313	A
49	A	2314	A
49	A	2333	U
49	A	2334	G
49	A	2335	G
49	A	2336	A
49	A	2337	A
49	A	2338	A
49	A	2339	U
49	A	2346	U
49	A	2347	A
49	A	2352	G
49	A	2361	U
49	A	2362	A
49	A	2370	U
49	A	2371	U
49	A	2374	C
49	A	2377	C
49	A	2400	U
49	A	2410	G
49	A	2412	C
49	A	2417	U
49	A	2428	U
49	A	2429	U
49	A	2433	C
49	A	2450	U
49	A	2455	G
49	A	2456	G
49	A	2457	A
49	A	2466	A
49	A	2468	C
49	A	2475	A

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Mol	Chain	Res	Type
49	A	2529	G
49	A	2532	G
49	A	2545	A
49	A	2581	U
49	A	2593	A
49	A	2594	G
49	A	2600	C
49	A	2605	G
49	A	2606	C
49	A	2608	G
49	A	2609	G
49	A	2612	U
49	A	2613	C
49	A	2629	A
49	A	2637	C
49	A	2640	U
49	A	2692	A
49	A	2716	U
49	A	2718	C
49	A	2741	G
49	A	2753	U
49	A	2760	A
49	A	2762	G
49	A	2784	A
49	A	2791	A
49	A	2792	A
49	A	2793	G
49	A	2796	C
49	A	2805	A
49	A	2807	G
49	A	2817	A
49	A	2820	U
49	A	2821	U
49	A	2823	G
49	A	2824	G
49	A	2827	A
49	A	2863	G
49	A	2887	G
49	A	2892	G
49	A	2905	C
49	A	2906	G
49	A	2913	G

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Mol	Chain	Res	Type
50	a	10	G
50	a	33	A
50	a	40	G
50	a	48	C
50	a	49	C
50	a	52	A
50	a	94	G
50	a	97	G
50	a	108	A
50	a	119	A
50	a	120	C
50	a	129	A
50	a	130	A
50	a	131	C
50	a	165	G
50	a	196	A
50	a	205	A
50	a	206	A
50	a	207	G
50	a	211	A
50	a	212	A
50	a	213	G
50	a	221	U
50	a	255	G
50	a	259	G
50	a	274	G
50	a	275	C
50	a	297	G
50	a	315	U
50	a	316	C
50	a	336	C
50	a	340	G
50	a	360	C
50	a	362	G
50	a	375	U
50	a	380	C
50	a	405	A
50	a	414	G
50	a	415	A
50	a	420	U
50	a	421	G
50	a	430	C

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Mol	Chain	Res	Type
50	a	431	G
50	a	432	G
50	a	437	U
50	a	456	A
50	a	460	A
50	a	461	C
50	a	467	U
50	a	472	G
50	a	474	A
50	a	476	C
50	a	492	G
50	a	493	G
50	a	505	A
50	a	519	C
50	a	526	C
50	a	535	G
50	a	540	A
50	a	555	A
50	a	567	A
50	a	570	U
50	a	572	U
50	a	580	A
50	a	581	A
50	a	584	C
50	a	585	G
50	a	661	U
50	a	695	A
50	a	696	G
50	a	728	C
50	a	729	A
50	a	731	U
50	a	757	A
50	a	763	G
50	a	785	A
50	a	802	A
50	a	825	C
50	a	836	A
50	a	882	A
50	a	912	G
50	a	935	G
50	a	944	C
50	a	945	A

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Mol	Chain	Res	Type
50	a	970	U
50	a	971	U
50	a	978	A
50	a	979	A
50	a	985	A
50	a	986	G
50	a	993	A
50	a	994	C
50	a	1003	G
50	a	1012	U
50	a	1014	A
50	a	1016	A
50	a	1024	A
50	a	1025	G
50	a	1034	U
50	a	1035	U
50	a	1037	C
50	a	1057	C
50	a	1058	A
50	a	1077	U
50	a	1097	U
50	a	1106	G
50	a	1107	U
50	a	1113	A
50	a	1137	U
50	a	1142	A
50	a	1143	U
50	a	1145	A
50	a	1150	G
50	a	1153	G
50	a	1168	A
50	a	1170	U
50	a	1179	C
50	a	1192	G
50	a	1195	G
50	a	1207	A
50	a	1208	A
50	a	1211	C
50	a	1212	A
50	a	1223	U
50	a	1224	A
50	a	1225	U

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Mol	Chain	Res	Type
50	a	1238	A
50	a	1268	A
50	a	1290	A
50	a	1297	U
50	a	1298	A
50	a	1309	C
50	a	1311	G
50	a	1312	U
50	a	1313	U
50	a	1331	C
50	a	1347	U
50	a	1348	G
50	a	1349	G
50	a	1356	U
50	a	1357	A
50	a	1375	U
50	a	1390	G
50	a	1409	A
50	a	1437	A
50	a	1453	G
50	a	1454	A
50	a	1457	A
50	a	1465	A
50	a	1466	G
50	a	1515	A
50	a	1517	G
50	a	1518	U
50	a	1529	G
50	a	1541	G
50	a	1542	G
50	a	1547	C

All (71) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	B	39	G
10	D	9	G
10	D	16	U
10	D	59	A
49	A	63	U
49	A	176	A
49	A	183	A

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Mol	Chain	Res	Type
49	A	202	A
49	A	258	A
49	A	314	A
49	A	344	U
49	A	475	A
49	A	504	G
49	A	548	A
49	A	591	A
49	A	646	A
49	A	756	A
49	A	793	G
49	A	850	G
49	A	988	C
49	A	1024	A
49	A	1089	C
49	A	1106	G
49	A	1113	A
49	A	1114	A
49	A	1133	G
49	A	1142	A
49	A	1177	A
49	A	1186	A
49	A	1216	U
49	A	1291	A
49	A	1339	U
49	A	1369	G
49	A	1432	A
49	A	1433	U
49	A	1453	G
49	A	1578	A
49	A	1580	A
49	A	1583	G
49	A	1592	A
49	A	1654	A
49	A	1678	A
49	A	1691	G
49	A	1789	A
49	A	1897	U
49	A	1927	A
49	A	1938	U
49	A	1939	A
49	A	1965	A

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Mol	Chain	Res	Type
49	A	1982	U
49	A	2008	A
49	A	2059	G
49	A	2086	A
49	A	2218	G
49	A	2238	U
49	A	2302	C
49	A	2335	G
49	A	2338	A
49	A	2346	U
49	A	2370	U
49	A	2417	U
49	A	2428	U
49	A	2457	A
49	A	2606	C
49	A	2608	G
49	A	2629	A
49	A	2637	C
49	A	2716	U
49	A	2783	U
49	A	2820	U
49	A	2887	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 392 ligands modelled in this entry, 390 are monoatomic - leaving 2 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	$\# Z  > 2$
56	A1I09	A	3103	-	39,40,40	3.07	13 (33%)	47,56,56	1.54	7 (14%)
54	FME	D	102	10	8,9,10	0.98	0	8,9,11	1.39	1 (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
56	A1I09	A	3103	-	-	4/30/62/62	0/3/3/3
54	FME	D	102	10	-	0/7/9/11	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A	3103	A1I09	C26-C21	8.89	1.53	1.39
56	A	3103	A1I09	C23-C22	8.29	1.53	1.39
56	A	3103	A1I09	C10-N1	7.12	1.49	1.34
56	A	3103	A1I09	C25-C24	7.00	1.53	1.38
56	A	3103	A1I09	C21-C22	-5.50	1.32	1.40
56	A	3103	A1I09	C24-C23	-3.85	1.32	1.38
56	A	3103	A1I09	C25-C26	-3.63	1.32	1.38
56	A	3103	A1I09	O2-C20	3.09	1.41	1.33
56	A	3103	A1I09	O5-C4	-2.59	1.40	1.44
56	A	3103	A1I09	O9-C10	-2.57	1.18	1.23
56	A	3103	A1I09	C21-C20	2.31	1.55	1.50
56	A	3103	A1I09	O10-C22	2.08	1.40	1.36
56	A	3103	A1I09	C15-N2	-2.01	1.42	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A	3103	A1I09	C9-C8-C7	-4.09	108.79	114.17
56	A	3103	A1I09	C12-C13-C14	3.68	107.64	102.23
56	A	3103	A1I09	C12-C13-C16	-3.59	110.56	114.68
56	A	3103	A1I09	O2-C20-C21	3.35	118.81	112.24
54	D	102	FME	C-CA-N	3.27	115.81	109.50
56	A	3103	A1I09	C6-S1-C5	3.12	107.19	100.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A	3103	A1I09	C7-N1-C10	-2.47	119.45	123.20
56	A	3103	A1I09	C5-O5-C4	2.35	117.25	114.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

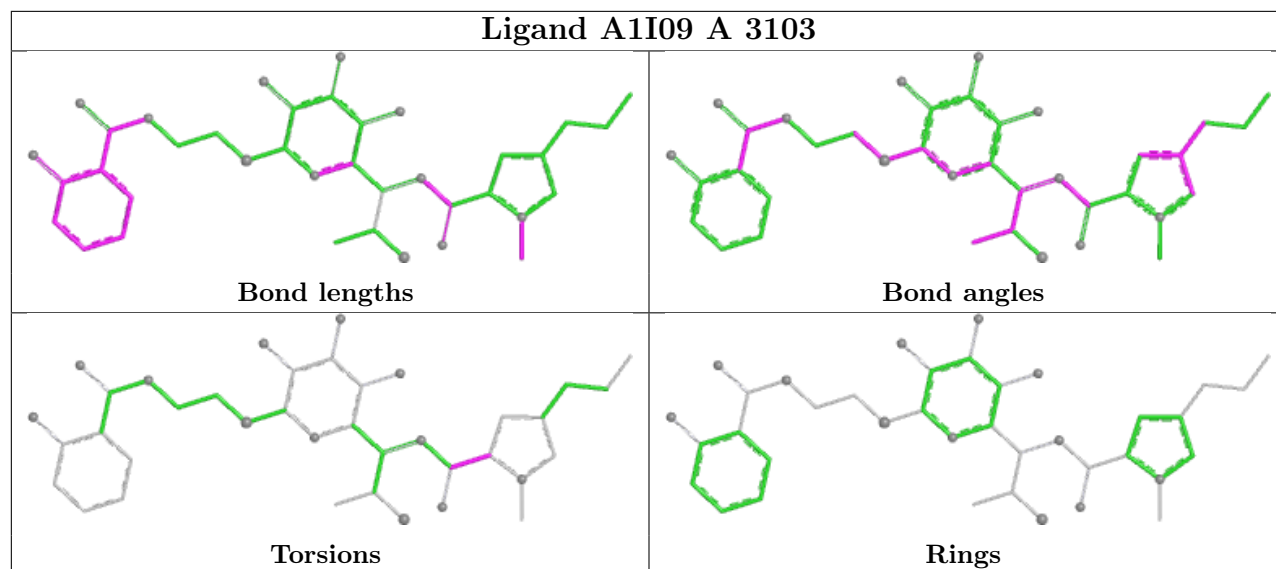
Mol	Chain	Res	Type	Atoms
56	A	3103	A1I09	O9-C10-C11-C12
56	A	3103	A1I09	N1-C10-C11-C12
56	A	3103	A1I09	O9-C10-C11-N2
56	A	3103	A1I09	N1-C10-C11-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	A	3103	A1I09	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 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.

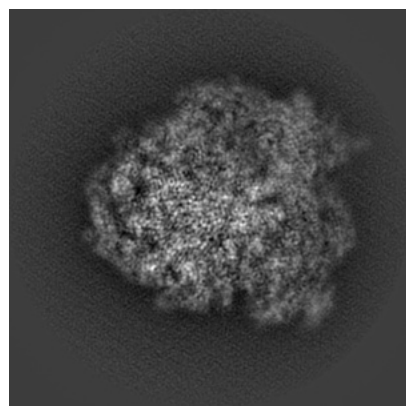
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52711. These allow visual inspection of the internal detail of the map and identification of artifacts.

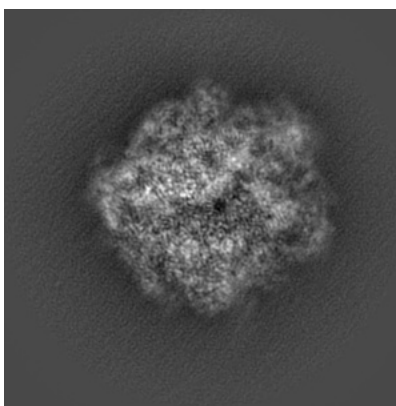
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

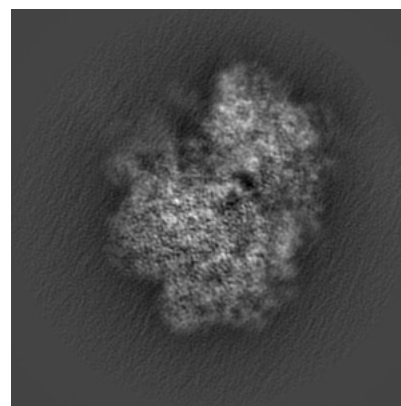
#### 6.1.1 Primary map



X

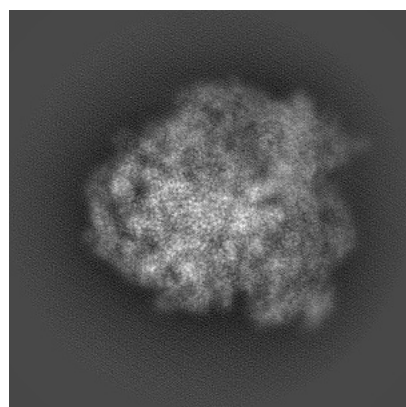


Y

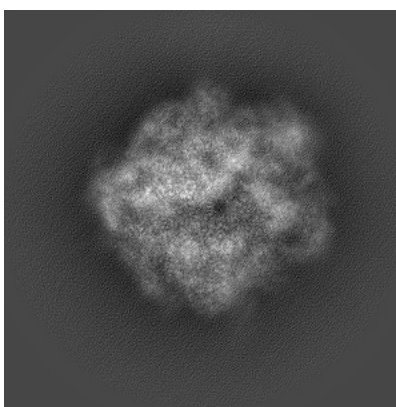


Z

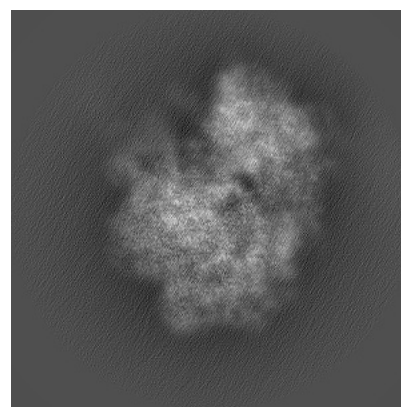
#### 6.1.2 Raw map



X



Y

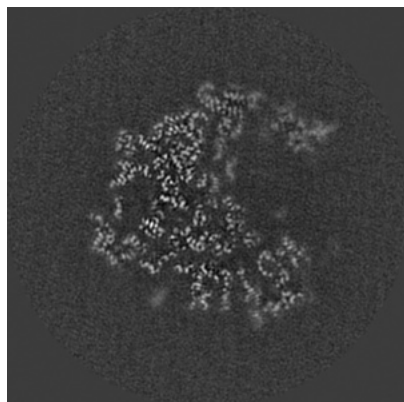


Z

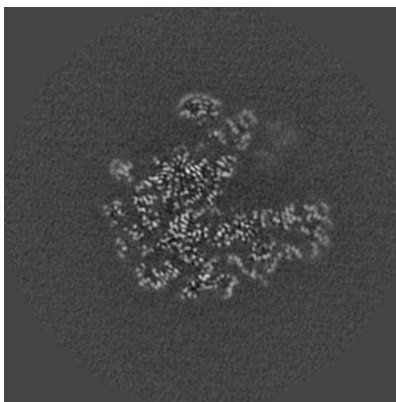
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

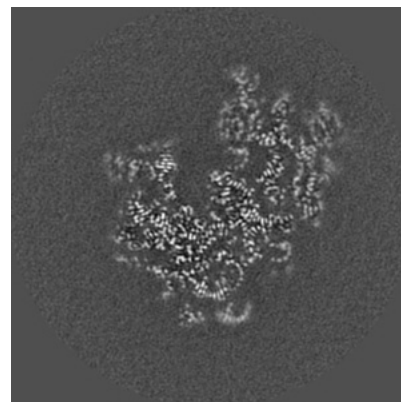
### 6.2.1 Primary map



X Index: 204

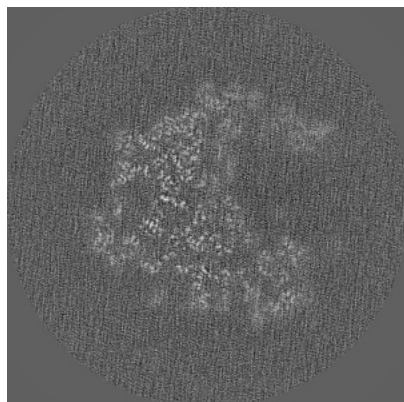


Y Index: 204

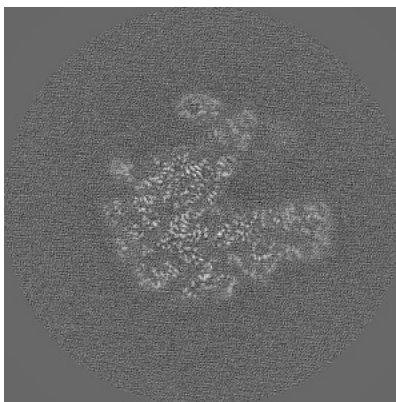


Z Index: 204

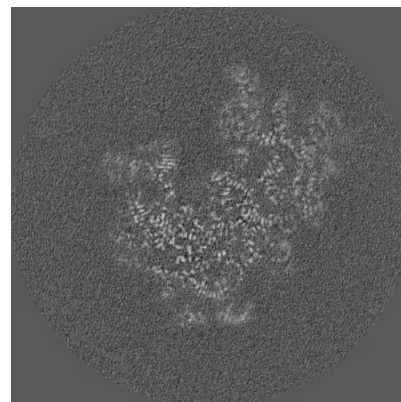
### 6.2.2 Raw map



X Index: 204



Y Index: 204



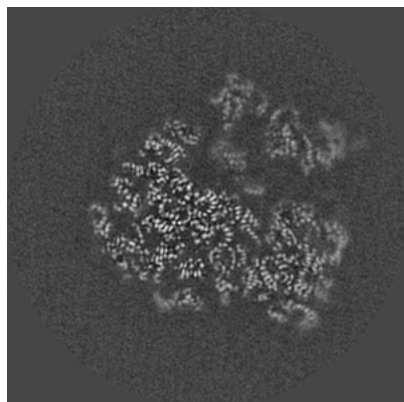
Z Index: 204

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

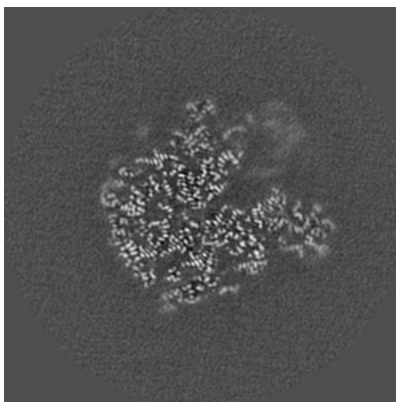


## 6.3 Largest variance slices [i](#)

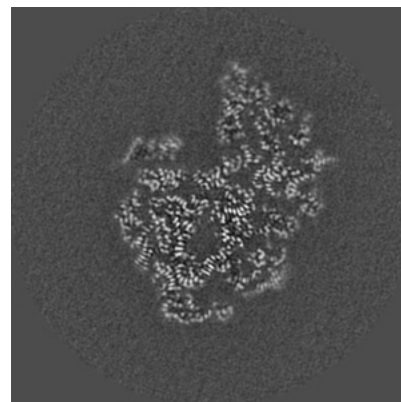
### 6.3.1 Primary map



X Index: 217

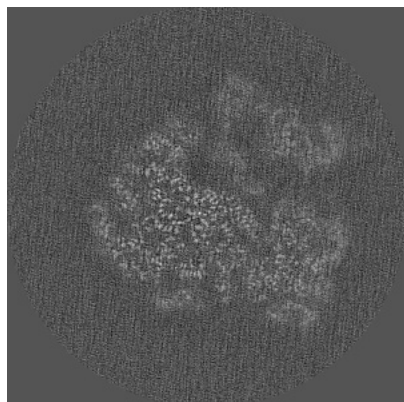


Y Index: 195

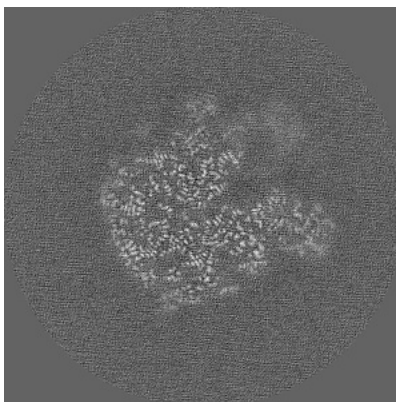


Z Index: 188

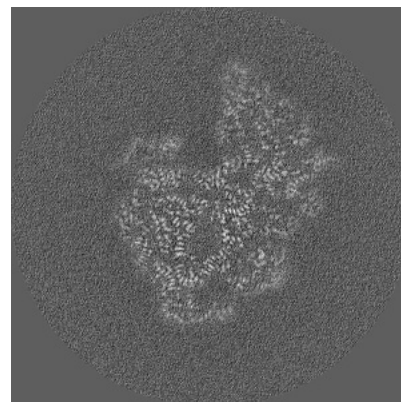
### 6.3.2 Raw map



X Index: 218



Y Index: 195



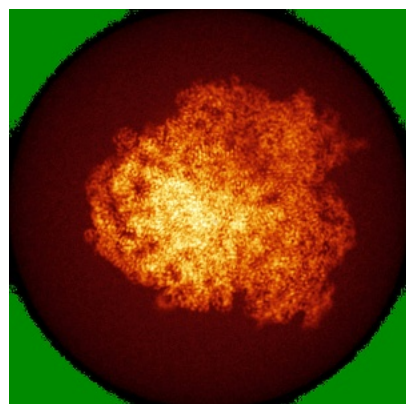
Z Index: 188

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

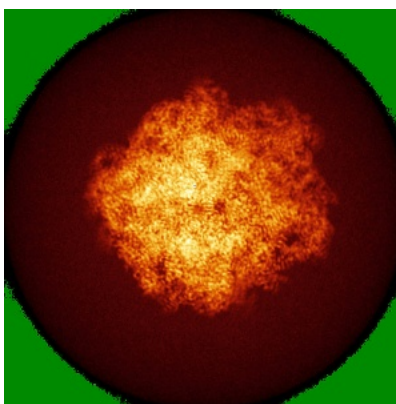


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

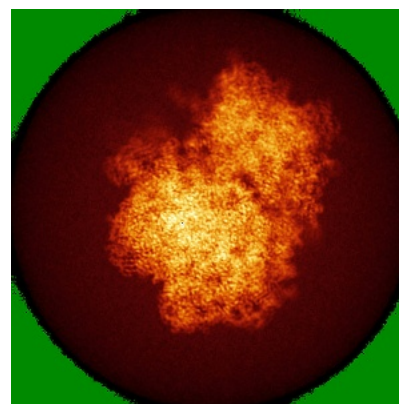
### 6.4.1 Primary map



X

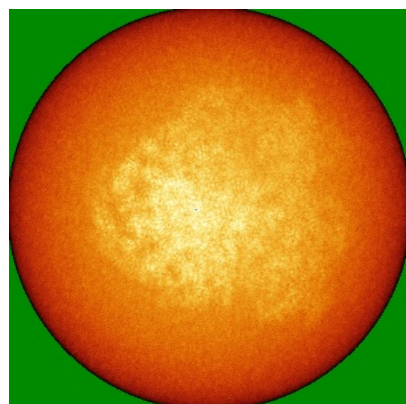


Y

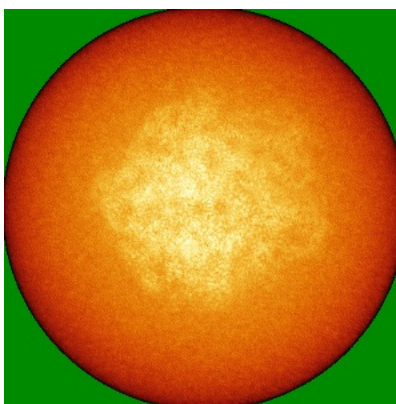


Z

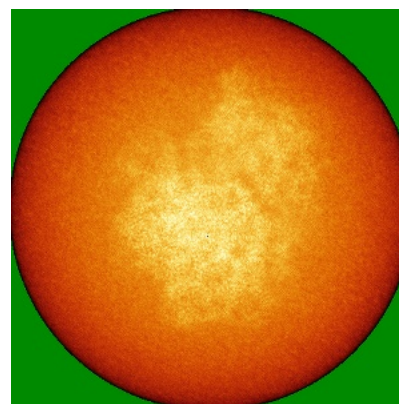
### 6.4.2 Raw map



X



Y

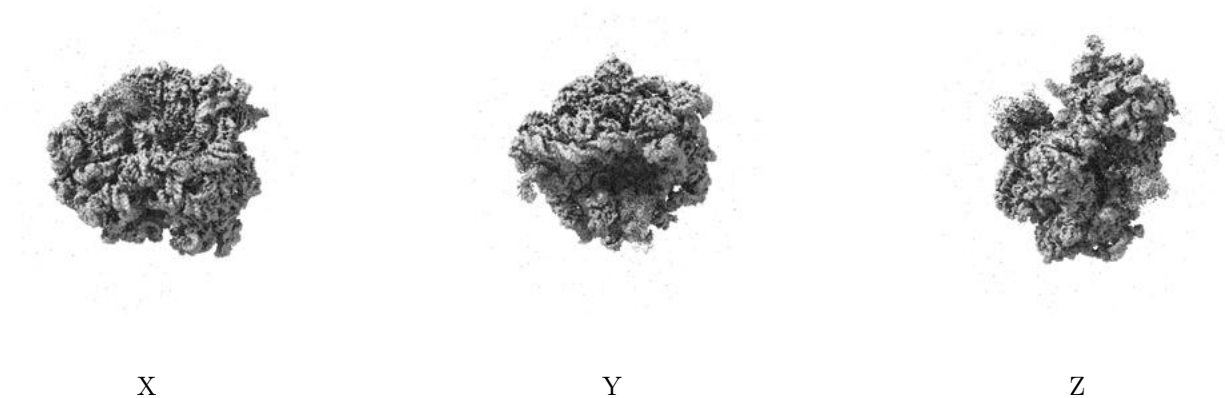


Z

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.

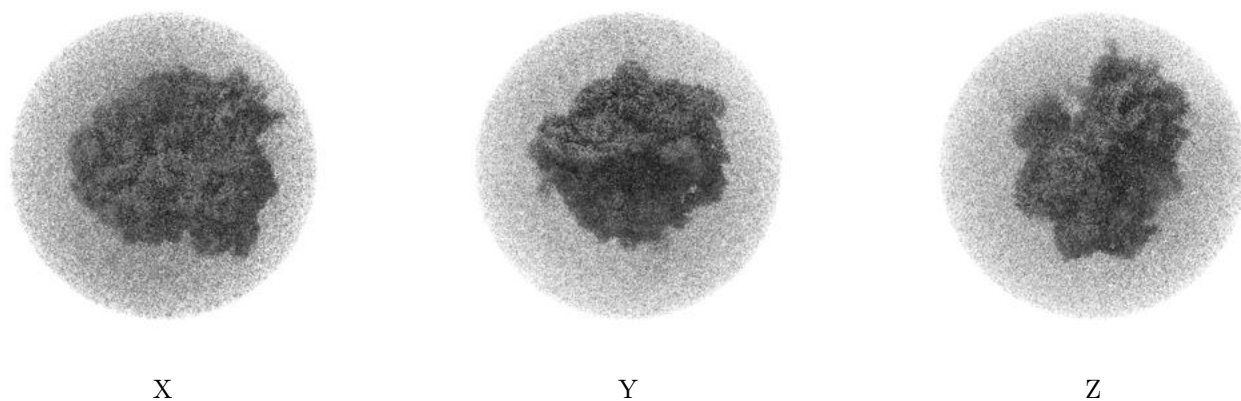
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0035. 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



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.

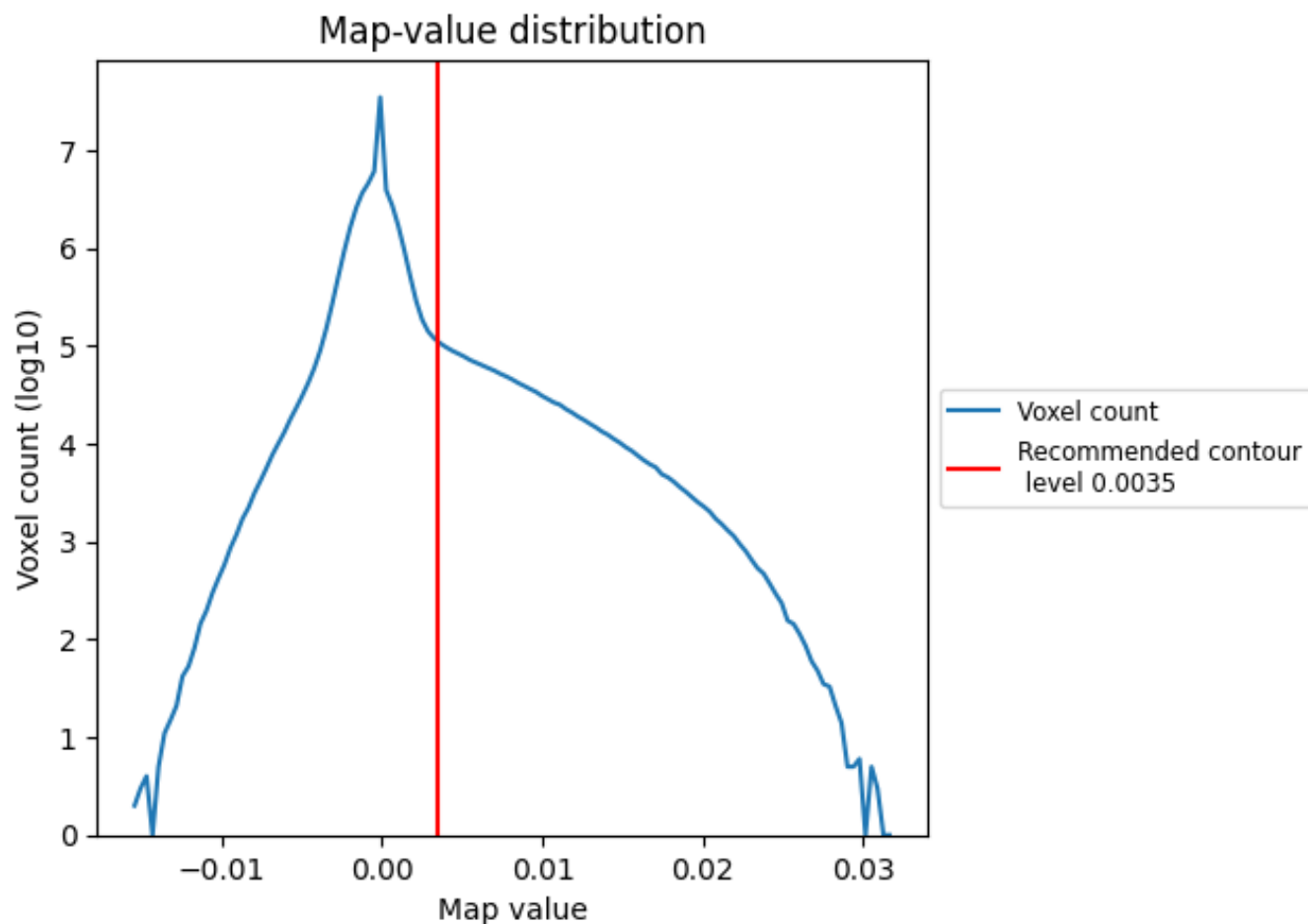
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

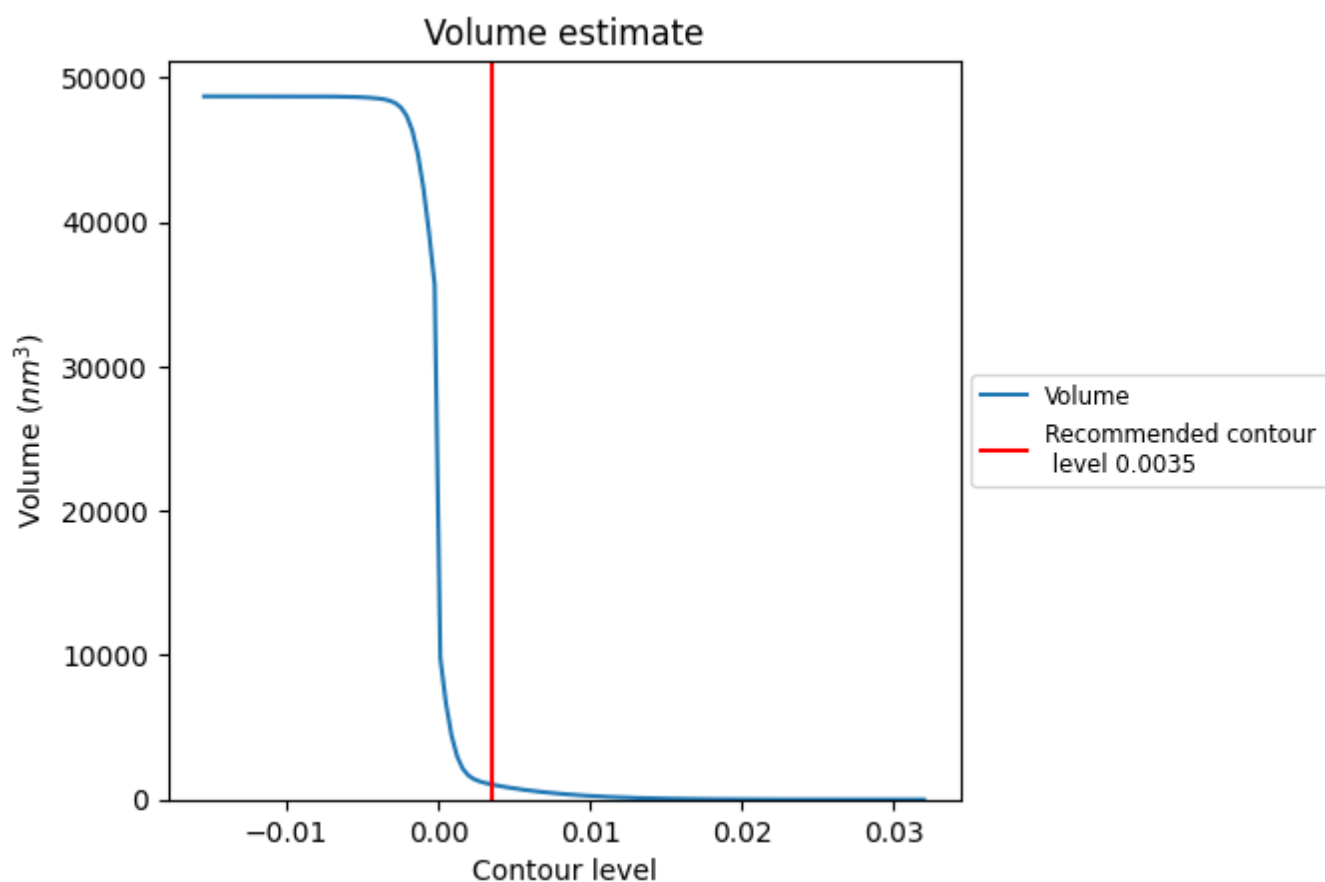
This section contains the results of statistical analysis of the map.

### 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.

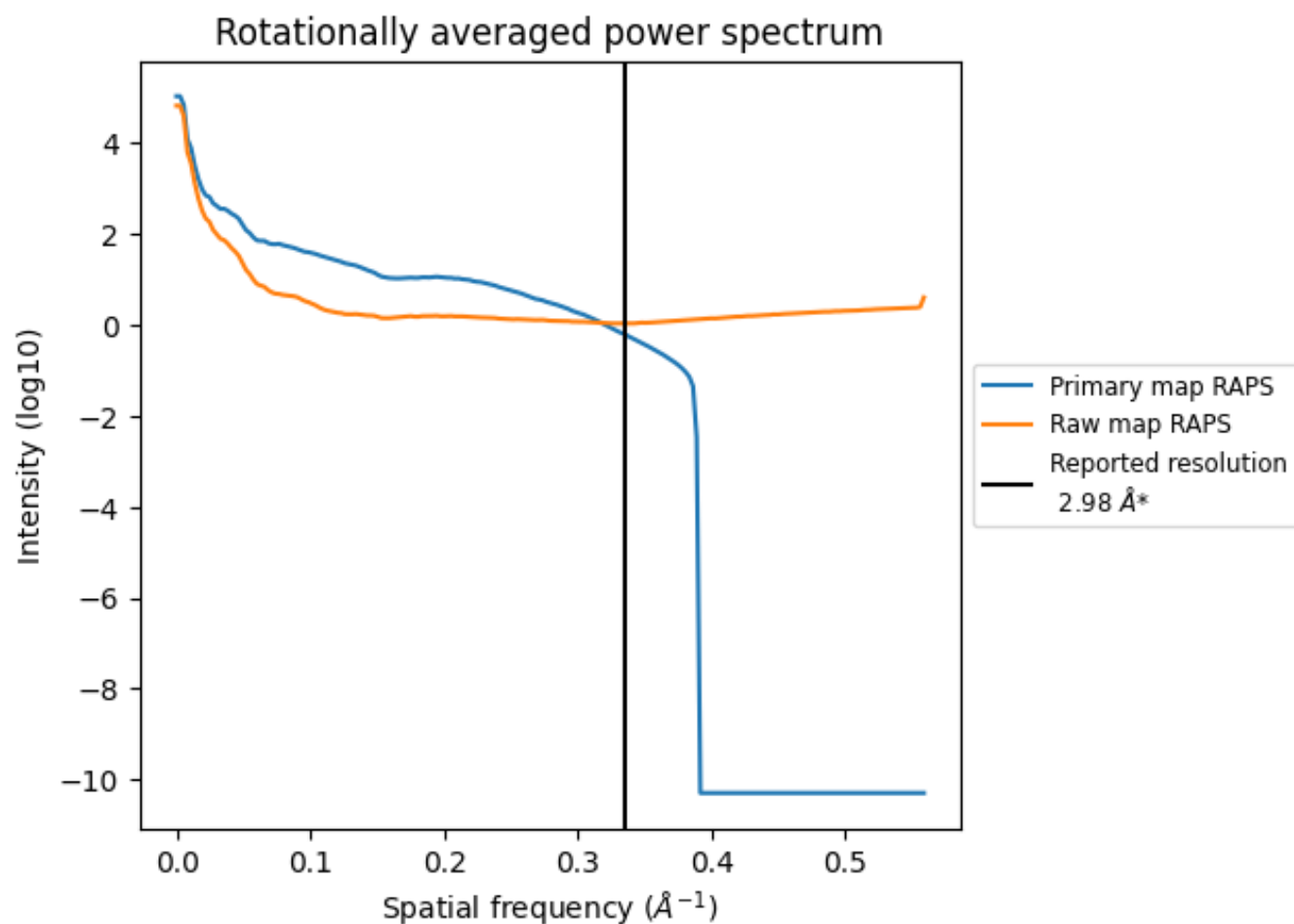
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1052 nm<sup>3</sup>; this corresponds to an approximate mass of 950 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 ⓘ

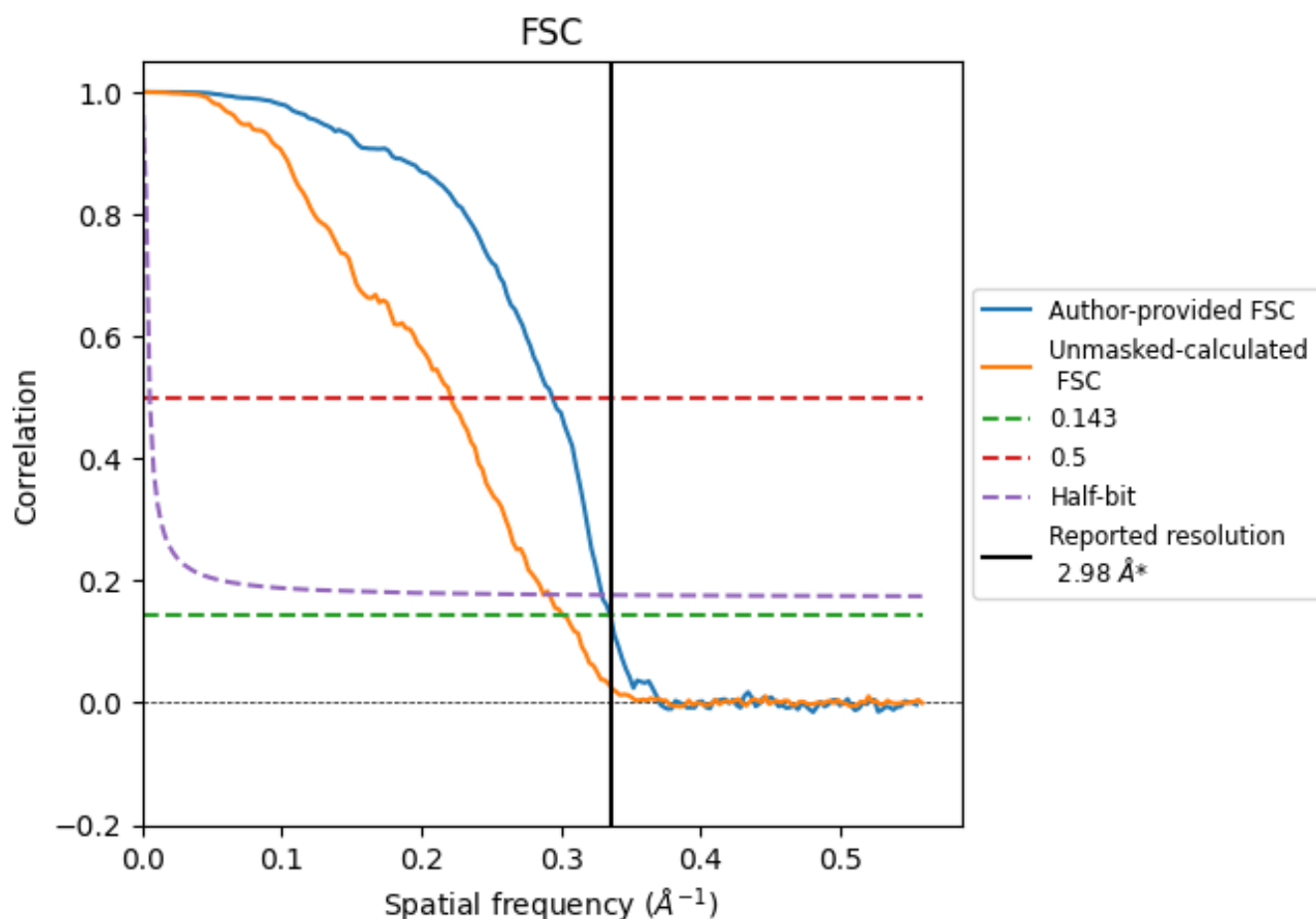


\*Reported resolution corresponds to spatial frequency of 0.336  $\text{\AA}^{-1}$

## 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 0.336  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

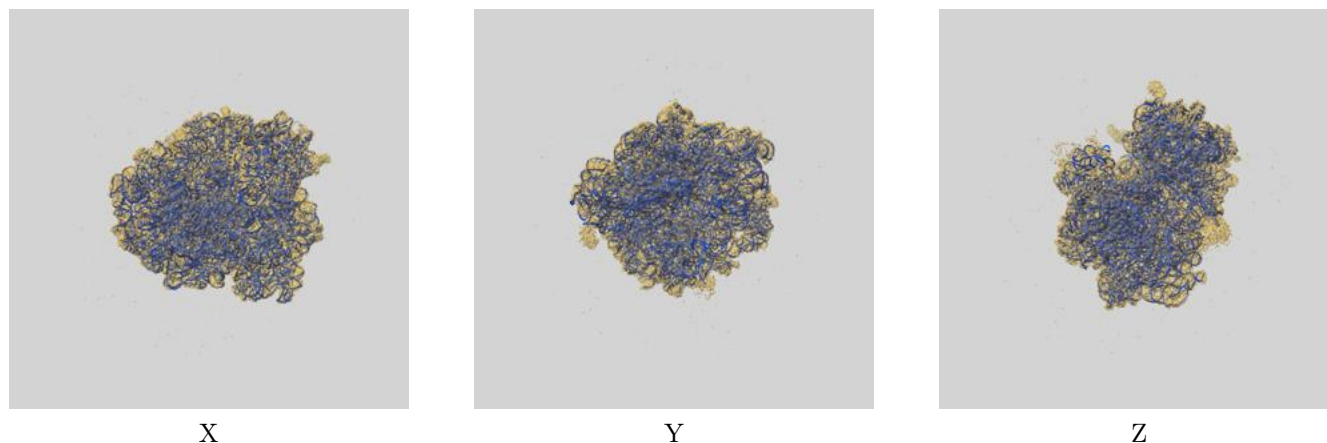
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.40	3.04
Unmasked-calculated*	3.32	4.52	3.48

\*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 3.32 differs from the reported value 2.98 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52711 and PDB model 9I88. Per-residue inclusion information can be found in section [3](#) on page [15](#).

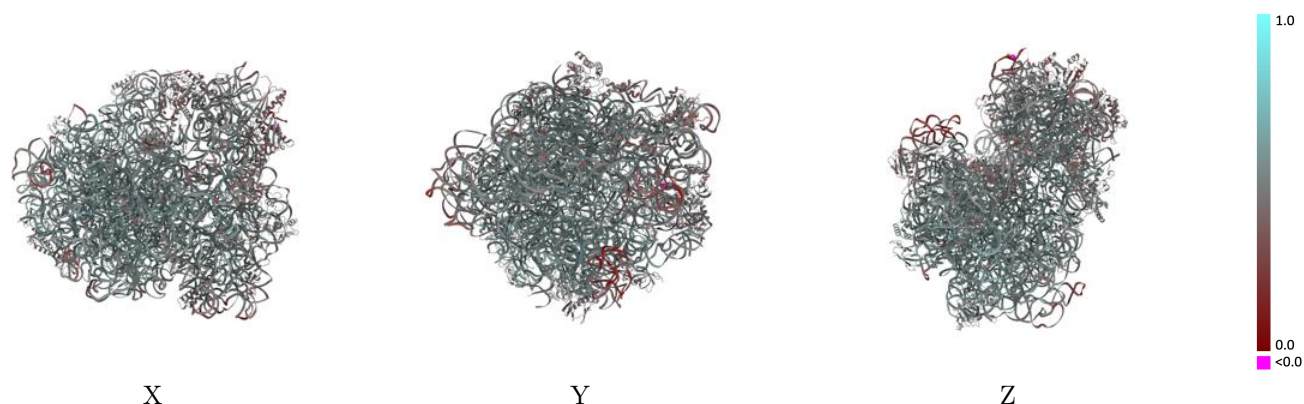
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

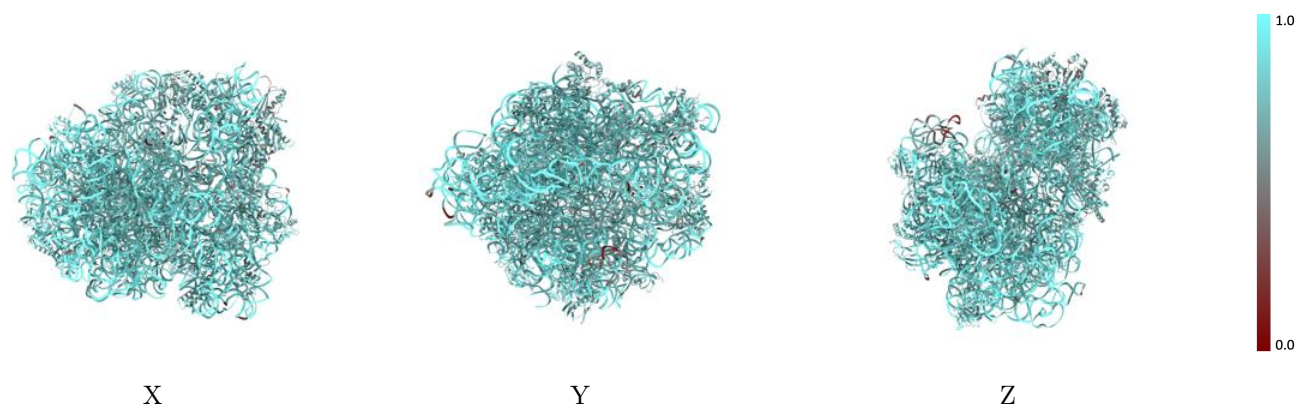


## 9.2 Q-score mapped to coordinate model [i](#)



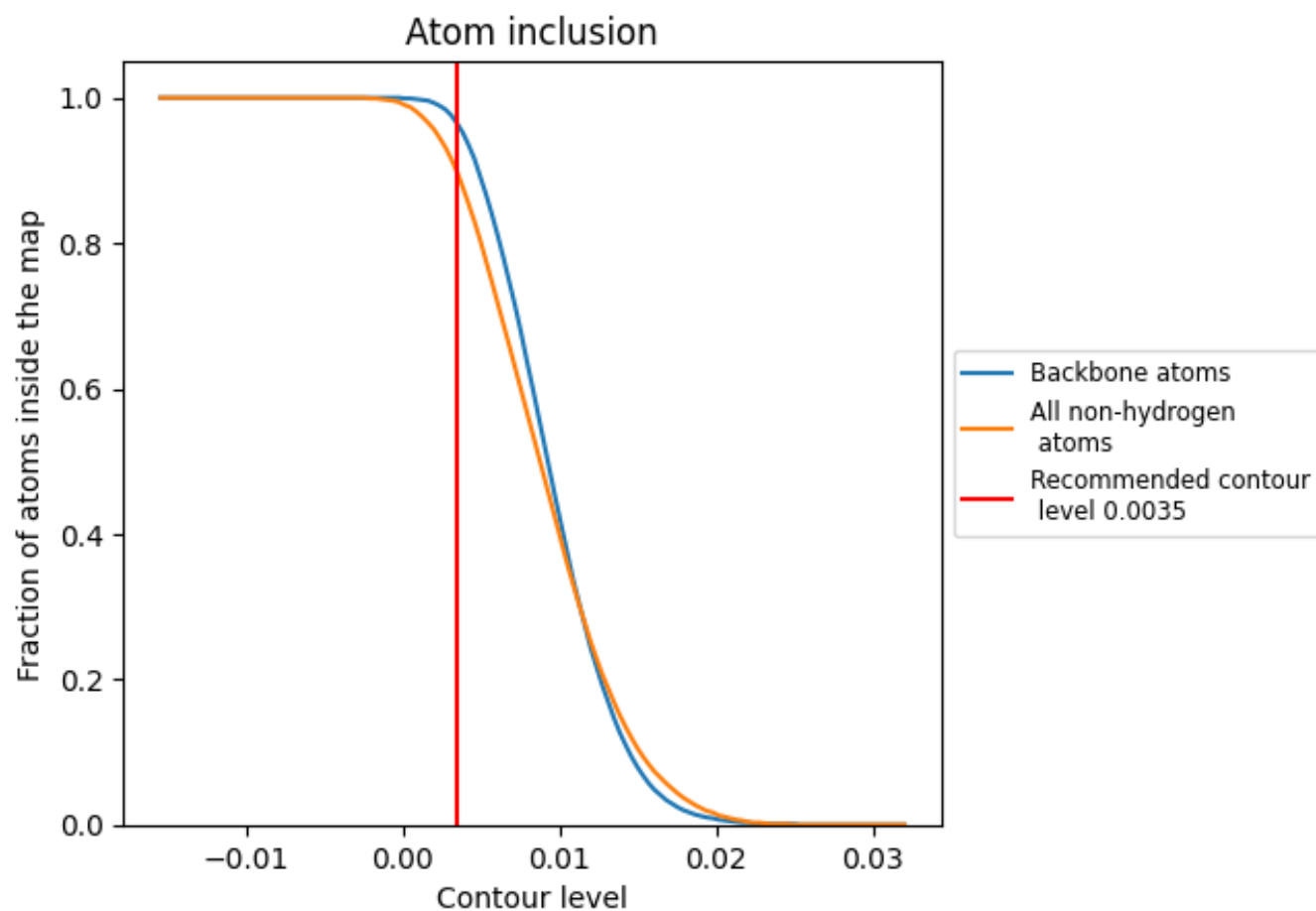
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0035).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.5250
1	 0.8300	 0.5320
2	 0.8000	 0.4780
3	 0.8320	 0.5270
4	 0.7880	 0.4570
5	 0.8290	 0.5460
6	 0.7740	 0.5200
7	 0.9060	 0.5790
8	 0.8610	 0.5590
9	 0.8150	 0.5450
A	 0.9530	 0.5520
B	 0.9550	 0.5100
D	 0.8140	 0.4830
G	 0.8520	 0.5570
H	 0.8490	 0.5440
I	 0.8370	 0.5270
J	 0.7070	 0.4470
K	 0.7720	 0.4500
M	 0.8480	 0.5410
N	 0.7960	 0.5300
O	 0.8290	 0.5340
P	 0.8230	 0.5370
Q	 0.8120	 0.5280
R	 0.7970	 0.4780
S	 0.8250	 0.5250
T	 0.8670	 0.5500
U	 0.8530	 0.5300
V	 0.8170	 0.5390
W	 0.7980	 0.5170
X	 0.7720	 0.4920
Y	 0.7530	 0.4630
Z	 0.8290	 0.5470
a	 0.9370	 0.5160
c	 0.6730	 0.4340
d	 0.6970	 0.4580



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Chain	Atom inclusion	Q-score
e	 0.7610	 0.4750
f	 0.7930	 0.5130
g	 0.7740	 0.4770
h	 0.7260	 0.4410
i	 0.7660	 0.4960
j	 0.7370	 0.4610
k	 0.6550	 0.4200
l	 0.7340	 0.4670
m	 0.7630	 0.5150
n	 0.7170	 0.4250
o	 0.7490	 0.4840
p	 0.7910	 0.4780
q	 0.7510	 0.4910
r	 0.7580	 0.4860
s	 0.8350	 0.5010
t	 0.7090	 0.4410
u	 0.7450	 0.4580