



## Full wwPDB EM Validation Report ⓘ

Mar 18, 2026 – 12:14 AM UTC

PDB ID : 9I5V / pdb\_00009i5v  
EMDB ID : EMD-52640  
Title : 70S P. gingivalis ribosome erm-delta-porN strain  
Authors : Hiregange, D.G.; Bashan, A.; Yonath, A.  
Deposited on : 2025-01-28  
Resolution : 2.70 Å(reported)

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

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

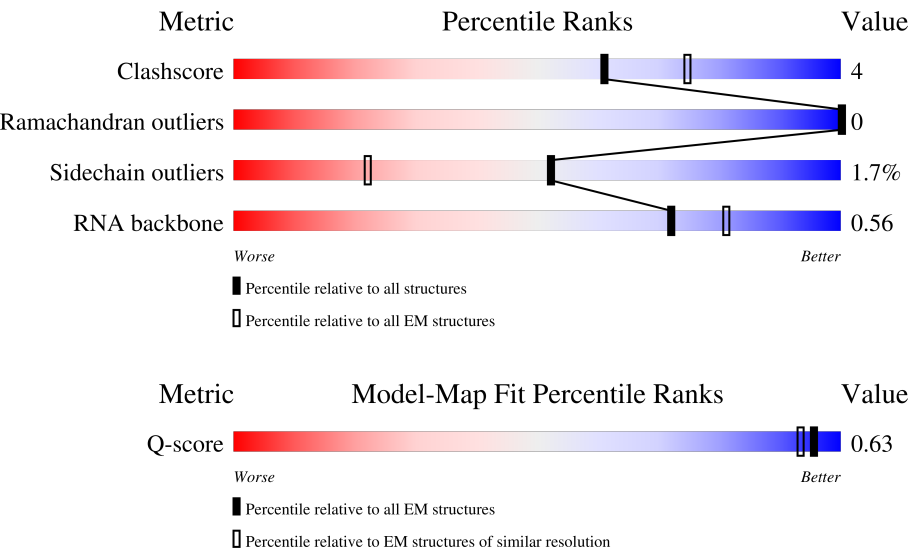
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

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

The reported resolution of this entry is 2.70 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.




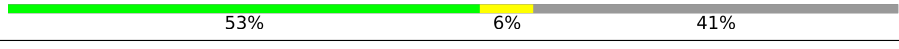
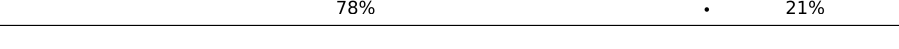
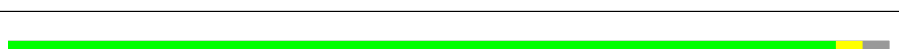



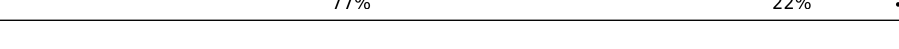



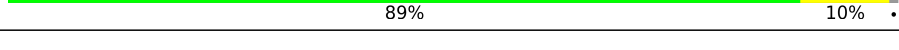

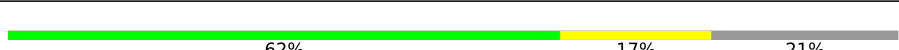

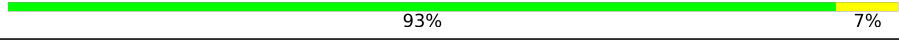
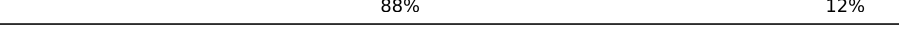







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 ( 2.20 - 3.20 )

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	I	90	
2	1	64	
3	0	79	


























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Mol	Chain	Length	Quality of chain
4	11	186	
5	12	85	
6	13	183	
7	14	401	
8	2	58	
9	4	61	
10	5	62	
11	6	50	
12	7	65	
13	8	38	
14	9	63	
15	A	2889	
16	B	109	
17	D	274	
18	E	205	
19	F	209	
20	K	101	
21	L	128	
22	M	151	
23	N	121	
24	O	148	
25	P	144	
26	Q	160	
27	R	114	
28	S	121	

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Mol	Chain	Length	Quality of chain
29	T	115	
30	U	105	
31	V	134	
32	W	97	
33	X	106	
34	Y	192	
35	Z	85	
36	a	1534	
37	b	117	
38	c	192	
39	d	84	
40	e	84	
41	f	89	
42	g	89	
43	h	179	
44	i	126	
45	j	134	
46	k	246	
47	l	201	
48	m	158	
49	n	172	
50	o	131	
51	15	49	
52	10	30	
53	p	89	

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Mol	Chain	Length	Quality of chain
54	J	128	<div><div></div><div>85%</div><div>12%.</div></div>

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 121970 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 Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	I	52	Total	C	N	O	0	0
			400	262	76	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	63	Total	C	N	O	S	0	0
			490	305	97	85	3		

- Molecule 3 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	77	Total	C	N	O	S	0	0
			608	390	118	97	3		

- Molecule 4 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	11	154	Total	C	N	O	0	0
			758	450	154	154		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	12	50	Total	C	N	O	S	0	0
			299	183	57	58	1		

- Molecule 6 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	13	144	Total	C	N	O	S	0	0
			746	448	149	148	1		

- Molecule 7 is a protein called Ribosome-associated translation inhibitor RaiA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	14	35	Total	C	N	O	S	0	0
			225	136	41	47	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
14	43	TYR	HIS	conflict	UNP A0AAE9X5J6

- Molecule 8 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	56	Total	C	N	O	S	0	0
			431	273	86	70	2		

- Molecule 9 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4	57	Total	C	N	O	S	0	0
			429	267	89	69	4		

- Molecule 10 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	47	Total	C	N	O	S	0	0
			375	232	74	67	2		

- Molecule 11 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	6	48	Total	C	N	O	S	0	0
			391	237	89	63	2		

- Molecule 12 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	7	64	Total	C	N	O	S	0	0
			486	311	93	81	1		

- Molecule 13 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	8	38	Total	C	N	O	S	0	0
			303	190	64	47	2		

- Molecule 14 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	9	46	Total	C	N	O	0	0
			281	178	54	49		

- Molecule 15 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A	2363	Total	C	N	O	P	0	0
			50715	22650	9348	16354	2363		

- Molecule 16 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	104	Total	C	N	O	P	0	0
			2229	994	409	722	104		

- Molecule 17 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	272	Total	C	N	O	S	0	0
			2062	1285	404	365	8		

- Molecule 18 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	204	Total	C	N	O	S	0	0
			1520	968	274	271	7		

- Molecule 19 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	209	Total	C	N	O	S	0	0
			1624	1029	295	298	2		

- Molecule 20 is a protein called Small ribosomal subunit protein uS10.



Mol	Chain	Residues	Atoms				AltConf	Trace
20	K	80	Total	C	N	O	0	0
			567	361	107	99		

- Molecule 21 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	117	Total	C	N	O	S	0	0
			766	479	144	141	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	151	Total	C	N	O	S	0	0
			1173	748	217	203	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	121	Total	C	N	O	S	0	0
			907	566	173	164	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	141	Total	C	N	O	S	0	0
			966	600	185	179	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	141	Total	C	N	O	S	0	0
			1098	707	202	185	4		

- Molecule 26 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	123	Total	C	N	O	S	0	0
			989	630	184	169	6		

- Molecule 27 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	R	113	Total	C	N	O	0	0
			832	521	160	151		

- Molecule 28 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	114	Total	C	N	O	S	0	0
			919	585	171	162	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	114	Total	C	N	O	S	0	0
			925	585	189	148	3		

- Molecule 30 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	104	Total	C	N	O	S	0	0
			811	521	149	138	3		

- Molecule 31 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	128	Total	C	N	O	S	0	0
			1006	625	204	172	5		

- Molecule 32 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	95	Total	C	N	O	S	0	0
			675	429	122	121	3		

- Molecule 33 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	X	103	Total	C	N	O	S	0	0
			740	462	145	131	2		

- Molecule 34 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Y	128	Total	C	N	O	S	0	0
			857	552	154	150	1		

- Molecule 35 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Z	77	Total	C	N	O	S	0	0
			574	355	114	104	1		

- Molecule 36 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	1357	Total	C	N	O	P	0	0
			29121	12998	5348	9418	1357		

- Molecule 37 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	107	Total	C	N	O	S	0	0
			787	510	140	135	2		

- Molecule 38 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	118	Total	C	N	O	S	0	0
			857	532	163	160	2		

- Molecule 39 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	77	Total	C	N	O	S	0	0
			619	384	131	103	1		

- Molecule 40 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	81	Total	C	N	O	S	0	0
			621	393	126	99	3		

- Molecule 41 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	89	Total	C	N	O	S	0	0
			691	440	129	120	2		

- Molecule 42 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	85	Total	C	N	O	S	0	0
			646	405	130	106	5		

- Molecule 43 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	55	Total	C	N	O	S	0	0
			411	261	76	73	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	105	Total	C	N	O	S	0	0
			750	472	139	138	1		

- Molecule 45 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	122	Total	C	N	O	S	0	0
			908	559	187	160	2		

- Molecule 46 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	k	106	Total	C	N	O	S	0	0
			699	446	124	127	2		

- Molecule 47 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	l	200	Total	C	N	O	S	0	0
			1494	948	276	269	1		

- Molecule 48 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m	135	Total	C	N	O	S	0	0
			974	623	176	172	3		

- Molecule 49 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	n	167	Total	C	N	O	S	0	0
			1123	709	211	200	3		

- Molecule 50 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	o	131	Total	C	N	O	S	0	0
			1028	657	183	183	5		

- Molecule 51 is a protein called DUF4295 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	15	34	Total	C	N	O	0	0
			169	101	34	34		

- Molecule 52 is a protein called AURKAIP1/COX24 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	10	27	Total	C	N	O	S	0	0
			235	144	60	30	1		

- Molecule 53 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	p	80	Total	C	N	O	S	0	0
			609	394	109	103	3		

- Molecule 54 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	J	125	Total	C	N	O	0	0
			868	555	168	145		

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	4	1	Total 1	Mg 1	0
55	A	114	Total 114	Mg 114	0
55	B	1	Total 1	Mg 1	0
55	F	1	Total 1	Mg 1	0
55	V	2	Total 2	Mg 2	0
55	a	9	Total 9	Mg 9	0
55	10	1	Total 1	Mg 1	0

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	A	25	Total 25	K 25	0
56	B	1	Total 1	K 1	0
56	a	5	Total 5	K 5	0

- Molecule 57 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
57	A	15	Total 15	Na 15	0
57	B	2	Total 2	Na 2	0
57	a	1	Total 1	Na 1	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	4	2	Total 2	O 2	0
58	9	1	Total 1	O 1	0

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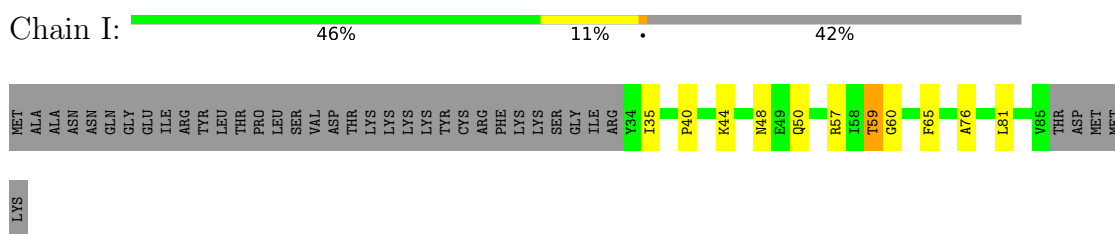
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Mol	Chain	Residues	Atoms		AltConf
58	A	849	Total 849	O 849	0
58	B	11	Total 11	O 11	0
58	D	4	Total 4	O 4	0
58	E	14	Total 14	O 14	0
58	F	5	Total 5	O 5	0
58	M	1	Total 1	O 1	0
58	O	16	Total 16	O 16	0
58	Q	8	Total 8	O 8	0
58	T	10	Total 10	O 10	0
58	U	7	Total 7	O 7	0
58	V	8	Total 8	O 8	0
58	Z	2	Total 2	O 2	0
58	a	66	Total 66	O 66	0
58	p	1	Total 1	O 1	0

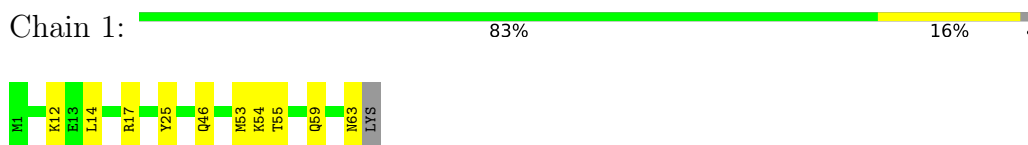
### 3 Residue-property plots [i](#)

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

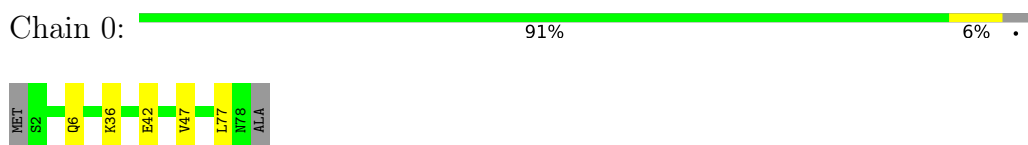
- Molecule 1: Small ribosomal subunit protein bS18



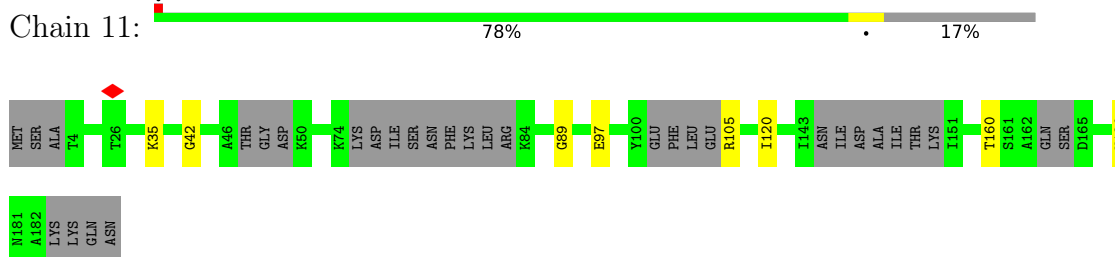
- Molecule 2: Large ribosomal subunit protein uL29



- Molecule 3: Large ribosomal subunit protein bL28



- Molecule 4: Large ribosomal subunit protein uL5



- Molecule 5: Large ribosomal subunit protein bL31B

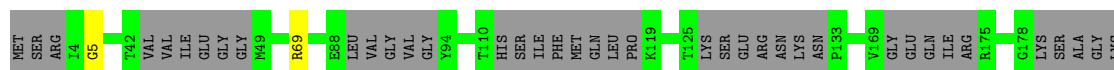






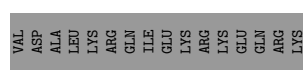
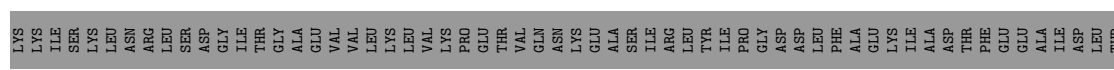
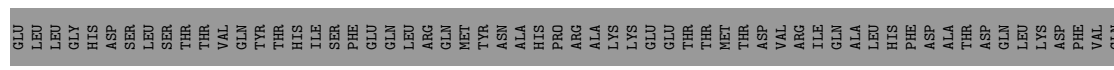
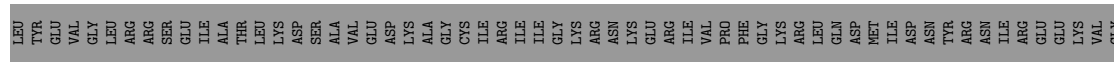
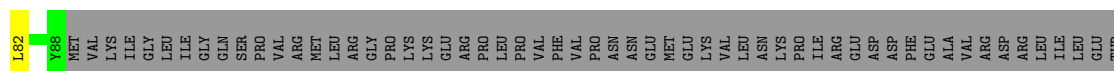
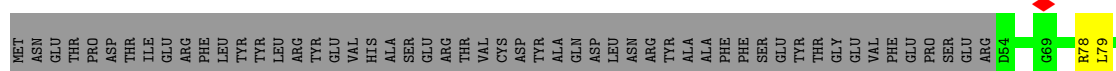
- Molecule 6: Large ribosomal subunit protein uL6

Chain 13: 78% 21%



- Molecule 7: Ribosome-associated translation inhibitor RaiA

Chain 14: 8% 91%



- Molecule 8: Large ribosomal subunit protein uL30

Chain 2: 93% 7%



- Molecule 9: Large ribosomal subunit protein bL32

Chain 4: 90% 7%




- Molecule 10: Large ribosomal subunit protein bL33

Chain 5: 68% 8% 24%





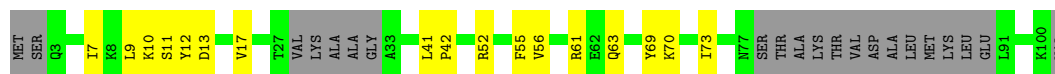


Chain F:  90% 10%



- Molecule 20: Small ribosomal subunit protein uS10

Chain K:  62% 17% 21%



- Molecule 21: Small ribosomal subunit protein uS11

Chain L:  87% 5% 9%




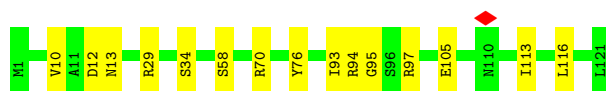
- Molecule 22: Large ribosomal subunit protein uL13

Chain M:  93% 7%




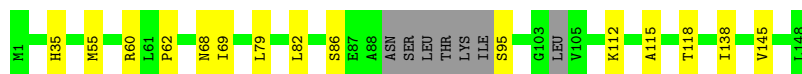
- Molecule 23: Large ribosomal subunit protein uL14

Chain N:  88% 12%




- Molecule 24: Large ribosomal subunit protein uL15

Chain O:  85% 10% 5%



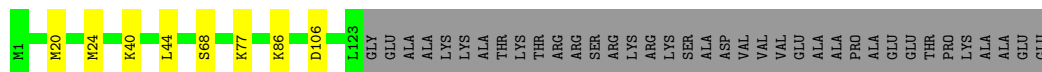
- Molecule 25: Large ribosomal subunit protein uL16

Chain P:  89% 9%




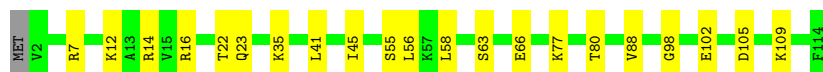
- Molecule 26: Large ribosomal subunit protein bL17

Chain Q:  72% 5% 23%




- Molecule 27: Large ribosomal subunit protein uL18

Chain R:  81% 18% .



- Molecule 28: Large ribosomal subunit protein bL19

Chain S:  86% 8% 6%




- Molecule 29: Large ribosomal subunit protein bL20

Chain T:  94% 5% .




- Molecule 30: Large ribosomal subunit protein bL21

Chain U:  88% 11% .



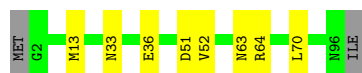
- Molecule 31: Large ribosomal subunit protein uL22

Chain V:  87% 9% .



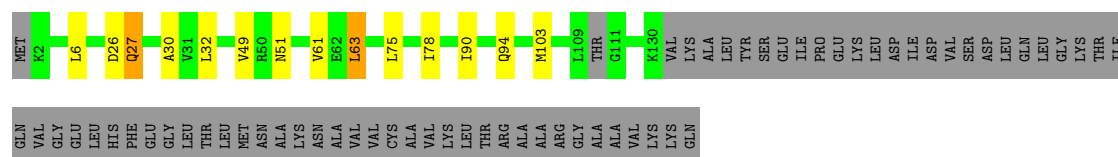
- Molecule 32: Large ribosomal subunit protein uL23

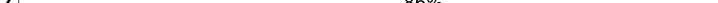
Chain W:  90% 8% .



- Molecule 33: Large ribosomal subunit protein uL24

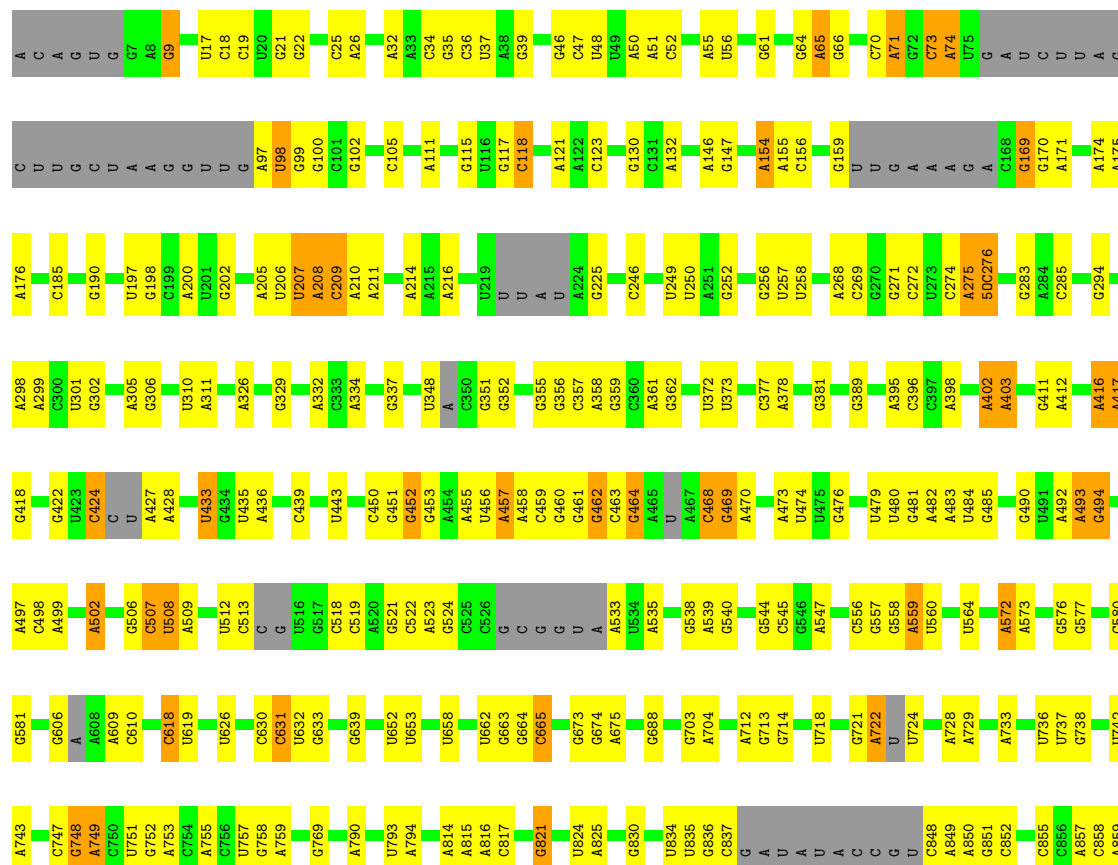
- Chain Y:  59% 6% 33%

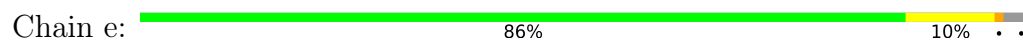


- Chain Z:  86% 9%



- Chain a:  58% 26% . 12%









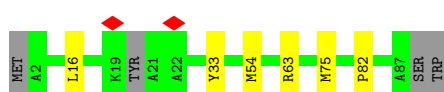
- Molecule 41: Small ribosomal subunit protein uS15

Chain f: 82% 18%



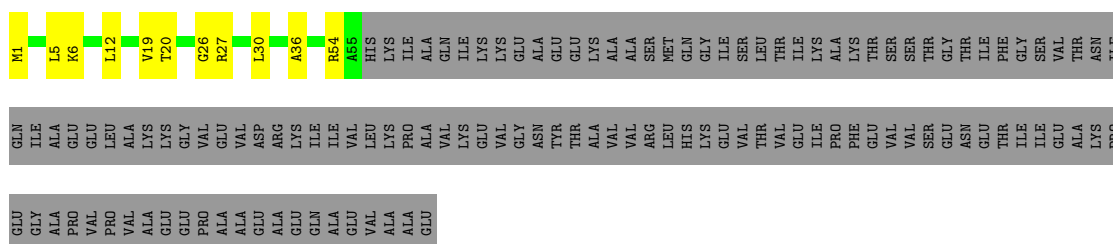
- Molecule 42: Small ribosomal subunit protein uS14

Chain g: 89% 7%



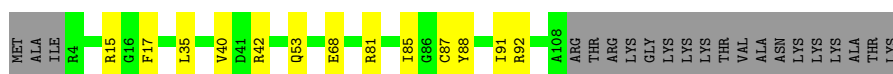
- Molecule 43: Large ribosomal subunit protein bL9

Chain h: 25% 6% 69%



- Molecule 44: Small ribosomal subunit protein uS13

Chain i: 73% 10% 17%



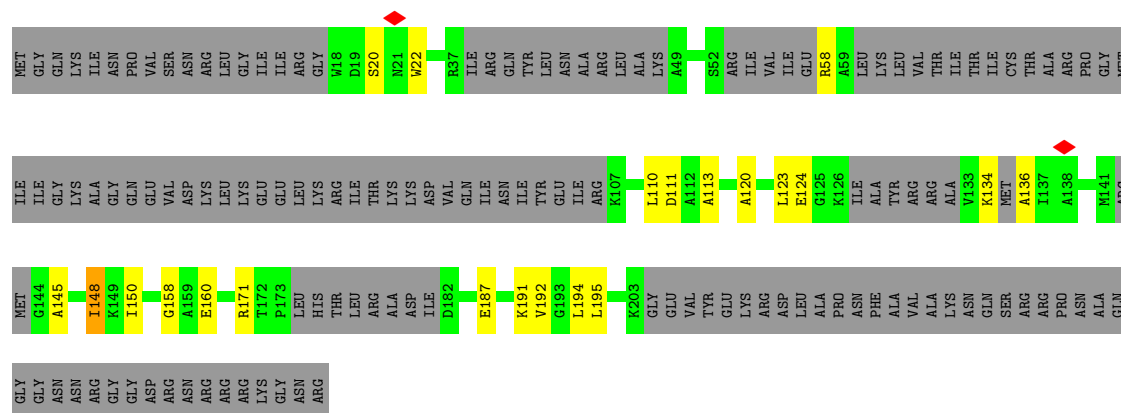
- Molecule 45: Small ribosomal subunit protein uS12

Chain j: 77% 14% 9%

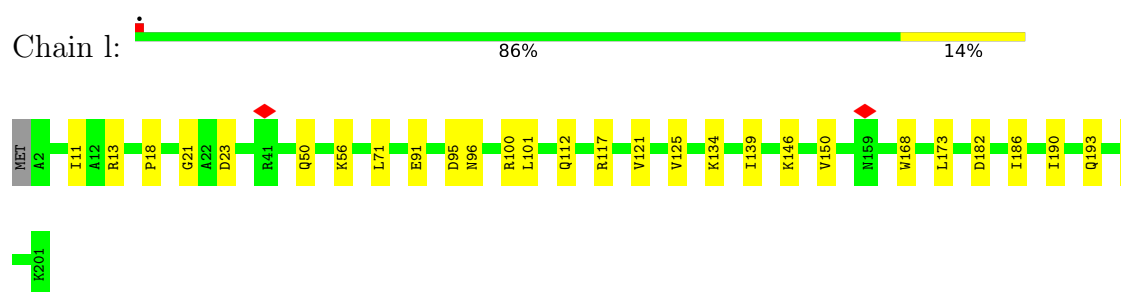


- Molecule 46: Small ribosomal subunit protein uS3

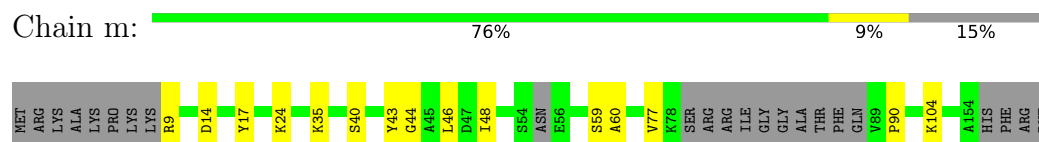
Chain k: 34% 9% 57%



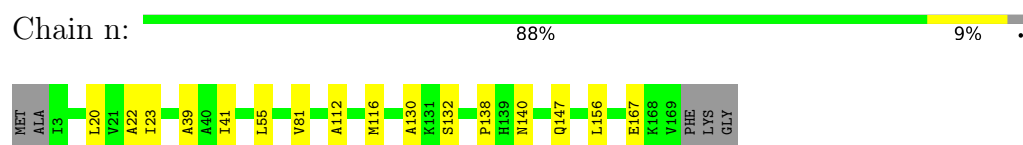
- Molecule 47: Small ribosomal subunit protein uS4



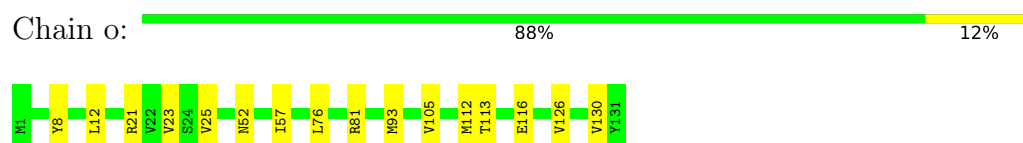
- Molecule 48: Small ribosomal subunit protein uS7



- Molecule 49: Small ribosomal subunit protein uS5

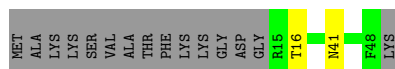


- Molecule 50: Small ribosomal subunit protein uS8

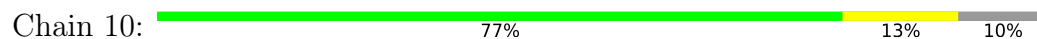


- Molecule 51: DUF4295 domain-containing protein

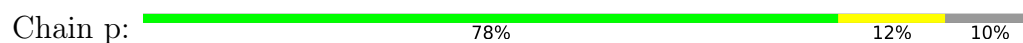




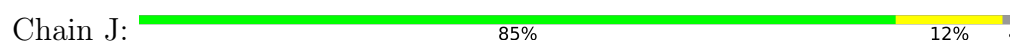
- Molecule 52: AURKAIP1/COX24 domain-containing protein



- Molecule 53: Small ribosomal subunit protein uS19



- Molecule 54: Small ribosomal subunit protein uS9



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155090	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.191	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	370.48, 370.48, 370.48	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, MA6, 2MA, NA, 7MG, 2MG, MG, 4OC, 5MU, 6MA, H2U, OMG, UR3, K, PSU, 5OC, OMU

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	I	0.20	0/408	0.39	0/551
2	1	0.20	0/494	0.32	0/663
3	0	0.25	0/617	0.31	0/825
4	11	0.12	0/752	0.35	0/1036
5	12	0.11	0/299	0.22	0/405
6	13	0.11	0/742	0.27	0/1017
7	14	0.15	0/225	0.36	0/303
8	2	0.27	0/434	0.38	0/584
9	4	0.26	0/440	0.40	0/595
10	5	0.18	0/378	0.32	0/505
11	6	0.26	0/395	0.37	0/521
12	7	0.24	0/493	0.45	0/657
13	8	0.23	0/306	0.45	1/404 (0.2%)
14	9	0.10	0/281	0.20	0/383
15	A	0.35	0/56393	0.36	0/87872
16	B	0.21	0/2492	0.31	0/3880
17	D	0.27	0/2101	0.33	0/2818
18	E	0.26	0/1549	0.38	0/2080
19	F	0.25	0/1647	0.33	0/2219
20	K	0.14	0/574	0.26	0/776
21	L	0.13	0/781	0.33	0/1070
22	M	0.27	0/1198	0.36	0/1618
23	N	0.26	0/914	0.40	0/1229
24	O	0.24	0/976	0.40	0/1313
25	P	0.22	0/1121	0.36	0/1505
26	Q	0.27	0/1006	0.41	0/1347
27	R	0.17	0/839	0.34	0/1122
28	S	0.22	0/934	0.30	0/1247
29	T	0.28	0/942	0.42	0/1260
30	U	0.27	0/822	0.40	0/1104
31	V	0.27	0/1019	0.38	0/1364

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	W	0.23	0/683	0.31	0/922
33	X	0.22	0/746	0.29	0/999
34	Y	0.20	0/870	0.38	0/1186
35	Z	0.24	0/581	0.35	0/776
36	a	0.22	0/32335	0.30	0/50381
37	b	0.17	0/802	0.33	0/1093
38	c	0.19	0/870	0.33	0/1178
39	d	0.19	0/625	0.27	0/835
40	e	0.19	0/632	0.33	0/851
41	f	0.21	0/700	0.40	0/937
42	g	0.16	0/653	0.29	0/867
43	h	0.22	0/413	0.46	0/554
44	i	0.19	0/757	0.32	1/1024 (0.1%)
45	j	0.16	0/923	0.31	0/1250
46	k	0.14	0/702	0.32	0/947
47	l	0.15	0/1525	0.29	0/2066
48	m	0.20	0/988	0.37	0/1339
49	n	0.17	0/1136	0.32	0/1546
50	o	0.19	0/1043	0.33	0/1402
51	15	0.10	0/168	0.23	0/233
52	10	0.20	0/238	0.31	0/305
53	p	0.20	0/623	0.28	0/840
54	J	0.16	0/882	0.31	0/1198
All	All	0.28	0/130467	0.34	2/195002 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	8	12	PRO	CA-N-CD	-5.53	104.26	112.00
44	i	68	GLU	CB-CA-C	-5.40	110.37	116.63

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	400	0	406	7	0
2	1	490	0	511	6	0
3	0	608	0	643	3	0
4	11	758	0	337	4	0
5	12	299	0	200	3	0
6	13	746	0	376	1	0
7	14	225	0	191	1	0
8	2	431	0	473	1	0
9	4	429	0	411	1	0
10	5	375	0	379	2	0
11	6	391	0	418	4	0
12	7	486	0	502	10	0
13	8	303	0	332	3	0
14	9	281	0	233	4	0
15	A	50715	0	25571	286	0
16	B	2229	0	1128	24	0
17	D	2062	0	2145	19	0
18	E	1520	0	1563	15	0
19	F	1624	0	1692	12	0
20	K	567	0	530	13	0
21	L	766	0	661	3	0
22	M	1173	0	1190	6	0
23	N	907	0	971	9	0
24	O	966	0	936	10	0
25	P	1098	0	1132	7	0
26	Q	989	0	1035	4	0
27	R	832	0	843	14	0
28	S	919	0	939	7	0
29	T	925	0	975	4	0
30	U	811	0	859	7	0
31	V	1006	0	1045	8	0
32	W	675	0	643	5	0
33	X	740	0	761	4	0
34	Y	857	0	786	7	0
35	Z	574	0	585	3	0
36	a	29121	0	14700	237	0
37	b	787	0	739	10	0
38	c	857	0	803	9	0
39	d	619	0	659	8	0
40	e	621	0	618	6	0
41	f	691	0	697	9	0
42	g	646	0	690	5	0
43	h	411	0	439	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	i	750	0	719	7	0
45	j	908	0	909	13	0
46	k	699	0	614	14	0
47	l	1494	0	1437	19	0
48	m	974	0	924	11	0
49	n	1123	0	1108	8	0
50	o	1028	0	1082	11	0
51	15	169	0	72	1	0
52	10	235	0	272	3	0
53	p	609	0	621	7	0
54	J	868	0	816	10	0
55	10	1	0	0	0	0
55	4	1	0	0	0	0
55	A	114	0	0	0	0
55	B	1	0	0	0	0
55	F	1	0	0	0	0
55	V	2	0	0	0	0
55	a	9	0	0	0	0
56	A	25	0	0	0	0
56	B	1	0	0	0	0
56	a	5	0	0	0	0
57	A	15	0	0	0	0
57	B	2	0	0	0	0
57	a	1	0	0	0	0
58	4	2	0	0	0	0
58	9	1	0	0	0	0
58	A	849	0	0	21	0
58	B	11	0	0	1	0
58	D	4	0	0	0	0
58	E	14	0	0	0	0
58	F	5	0	0	0	0
58	M	1	0	0	0	0
58	O	16	0	0	1	0
58	Q	8	0	0	0	0
58	T	10	0	0	0	0
58	U	7	0	0	0	0
58	V	8	0	0	1	0
58	Z	2	0	0	0	0
58	a	66	0	0	3	0
58	p	1	0	0	2	0
All	All	121970	0	79321	831	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). The all-atom clashscore for this structure is 4.

All (831) 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)
15:A:1071:C:H5	15:A:1155:G:H1	1.15	0.93
15:A:911:U:H3	15:A:935:G:H1	1.21	0.87
36:a:502:A:H61	36:a:523:A:H62	1.24	0.84
15:A:748:G:H21	15:A:753:A:H2	1.26	0.83
15:A:2353:A:H2	15:A:2366:G:H21	1.27	0.82
36:a:470:A:H1'	38:c:82:MET:HE1	1.62	0.80
15:A:2348:C:H5	15:A:2371:G:H1	1.28	0.80
36:a:508:U:H3	36:a:540:G:H1	1.30	0.79
15:A:1463:A:N1	15:A:1597:G:O6	2.17	0.78
15:A:2406:G:O6	15:A:2413:A:N6	2.17	0.78
36:a:37:U:H3	36:a:402:A:H2	1.33	0.77
12:7:27:ALA:HB2	24:O:62:PRO:HD3	1.66	0.76
20:K:11:SER:HB3	20:K:17:VAL:HG22	1.68	0.76
36:a:497:A:H61	36:a:545:C:H42	1.32	0.76
36:a:834:U:H3	36:a:851:G:H1	1.34	0.76
15:A:1221:G:N7	58:A:3102:HOH:O	2.20	0.74
15:A:1860:U:O2	15:A:2234:U:O2'	2.06	0.74
36:a:1423:G:H3'	36:a:1424:G:H21	1.51	0.73
36:a:73:C:N3	36:a:98:U:O4	2.22	0.73
15:A:820:G:N7	58:A:3103:HOH:O	2.21	0.73
15:A:1376:G:N7	58:A:3104:HOH:O	2.21	0.72
15:A:1827:U:O2'	17:D:154:MET:O	2.07	0.72
15:A:2524:G:H1	15:A:2541:C:H5	1.38	0.71
17:D:124:PRO:HG2	37:b:81:ARG:HD3	1.73	0.71
36:a:1009:U:H3	36:a:1020:G:H1	1.39	0.71
15:A:434:G:H4'	15:A:435:C:H5'	1.73	0.71
14:9:46:ARG:NH1	36:a:1519:G:N7	2.36	0.70
36:a:1063:C:H5	36:a:1189:A:H62	1.40	0.70
1:I:40:PRO:O	1:I:44:LYS:HD2	1.93	0.68
15:A:2550:G:N7	58:A:3111:HOH:O	2.26	0.68
15:A:2254:G:N7	58:A:3113:HOH:O	2.26	0.68
50:o:93:MET:HE1	50:o:105:VAL:HG11	1.75	0.68
36:a:457:A:H62	36:a:476:G:H1	1.41	0.68
36:a:459:C:H41	36:a:474:U:H3	1.41	0.68
36:a:1303:A:N6	36:a:1328:G:O2'	2.26	0.68
36:a:460:G:O6	36:a:473:A:N1	2.26	0.68
15:A:1224:G:N7	58:A:3112:HOH:O	2.26	0.68
15:A:898:G:N7	58:A:3119:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:934:A:H2'	15:A:935:G:C8	2.28	0.67
16:B:98:G:N7	58:B:302:HOH:O	2.27	0.67
15:A:1375:G:N7	58:A:3114:HOH:O	2.27	0.67
15:A:1779:G:N7	58:A:3116:HOH:O	2.27	0.67
15:A:2438:G:N7	58:A:3117:HOH:O	2.27	0.67
36:a:581:G:N7	58:a:1705:HOH:O	2.27	0.67
4:11:97:GLU:O	4:11:105:ARG:N	2.29	0.66
36:a:146:A:N1	36:a:225:G:O6	2.28	0.66
15:A:2392:G:O2'	15:A:2425:C:N4	2.29	0.66
36:a:398:A:OP2	38:c:13:LYS:NZ	2.27	0.66
15:A:1455:U:H3	15:A:1610:C:H42	1.43	0.66
36:a:468:C:O2'	36:a:469:G:N3	2.29	0.66
36:a:673:G:H2'	36:a:674:G:C8	2.31	0.66
36:a:146:A:H2	36:a:225:G:H1	1.39	0.66
15:A:1995:G:N7	58:A:3115:HOH:O	2.27	0.66
15:A:834:G:N7	58:A:3123:HOH:O	2.29	0.66
15:A:1656:G:N7	58:A:3122:HOH:O	2.29	0.66
36:a:70:C:H2'	36:a:97:A:H62	1.60	0.65
18:E:181:MET:HE2	18:E:186:LEU:HD12	1.78	0.65
27:R:66:GLU:OE1	27:R:66:GLU:N	2.28	0.65
15:A:140:U:H3	15:A:154:G:H1	1.44	0.64
48:m:44:GLY:O	48:m:48:ILE:HD12	1.97	0.64
14:9:46:ARG:NH2	36:a:1519:G:O6	2.31	0.64
23:N:105:GLU:OE2	23:N:105:GLU:N	2.30	0.64
15:A:2549:G:N7	58:A:3126:HOH:O	2.30	0.64
31:V:3:ALA:N	58:V:301:HOH:O	2.31	0.64
33:X:87:ARG:NH2	33:X:102:GLY:O	2.30	0.64
15:A:980:G:H21	15:A:1017:A:H8	1.46	0.63
36:a:945:A:H2'	36:a:946:A:C8	2.33	0.63
3:0:42:GLU:N	3:0:42:GLU:OE1	2.28	0.63
15:A:603:C:H2'	15:A:604:U:C6	2.34	0.63
36:a:1144:A:OP1	54:J:9:ARG:NH1	2.32	0.62
15:A:143:A:H61	15:A:151:C:H42	1.48	0.62
15:A:1077:G:H21	15:A:1149:G:H22	1.46	0.62
46:k:120:ALA:O	46:k:124:GLU:HG2	2.00	0.62
36:a:1372:A:OP1	48:m:35:LYS:NZ	2.32	0.62
52:10:22:LYS:HE2	52:10:23:LYS:HE2	1.80	0.62
15:A:2296:C:OP1	27:R:7:ARG:NE	2.29	0.61
46:k:134:LYS:O	46:k:136:ALA:N	2.33	0.61
36:a:424:C:H41	36:a:427:A:H62	1.48	0.61
15:A:124:G:H22	15:A:133:U:H3	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:38:U:H1'	16:B:43:A:H61	1.64	0.61
36:a:1043:A:H62	36:a:1209:U:H3	1.47	0.61
45:j:40:THR:HG21	45:j:90:LEU:HD21	1.82	0.61
15:A:260:U:O3'	43:h:54:ARG:NH2	2.33	0.61
15:A:1980:A:OP2	58:A:3101:HOH:O	2.16	0.61
15:A:2035:C:H2'	15:A:2036:G:C8	2.36	0.60
36:a:835:U:H3	36:a:850:A:H62	1.48	0.60
36:a:1068:C:H2'	36:a:1069:G:H8	1.66	0.60
36:a:1353:C:H2'	36:a:1354:A:H8	1.64	0.60
15:A:848:U:H2'	15:A:849:C:C6	2.36	0.60
15:A:2321:A:N1	15:A:2334:A:N6	2.50	0.60
36:a:1374:U:O4	48:m:9:ARG:NH1	2.32	0.60
20:K:42:PRO:O	20:K:70:LYS:NZ	2.34	0.60
36:a:1353:C:H2'	36:a:1354:A:C8	2.37	0.60
15:A:1811:A:H2'	15:A:1812:A:C8	2.37	0.60
15:A:1077:G:H22	15:A:1149:G:H1	1.47	0.60
17:D:146:LEU:HD13	17:D:154:MET:HE1	1.82	0.60
37:b:72:ILE:O	37:b:76:GLU:HG2	2.02	0.60
15:A:474:U:H4'	19:F:52:LYS:HE2	1.83	0.60
15:A:125:C:H42	15:A:132:C:H42	1.50	0.59
45:j:74:LEU:HD21	45:j:104:THR:HB	1.84	0.59
20:K:10:LYS:HG2	20:K:70:LYS:HG2	1.82	0.59
36:a:301:U:O2'	36:a:556:C:O2'	2.21	0.59
46:k:123:LEU:HD13	46:k:195:LEU:HD23	1.85	0.59
12:7:48:SER:OG	12:7:49:THR:N	2.34	0.59
15:A:890:G:H2'	15:A:891:A:C8	2.38	0.59
47:l:91:GLU:OE2	47:l:100:ARG:NH2	2.35	0.59
49:n:167:GLU:OE2	49:n:167:GLU:N	2.36	0.59
53:p:64:GLU:OE1	53:p:64:GLU:N	2.33	0.59
15:A:811:G:N2	15:A:812:G:O6	2.36	0.59
36:a:722:A:O2'	36:a:724:U:OP1	2.20	0.58
36:a:618:C:H5'	36:a:619:U:H5''	1.85	0.58
36:a:1425:U:H2'	36:a:1426:A:C8	2.38	0.58
36:a:105:C:OP1	39:d:12:ARG:NH1	2.36	0.58
36:a:302:G:N2	36:a:305:A:OP2	2.32	0.58
18:E:181:MET:HB2	18:E:186:LEU:HB2	1.85	0.58
36:a:508:U:O2	36:a:540:G:N2	2.29	0.58
15:A:1672:U:H2'	15:A:1673:A:C8	2.39	0.58
15:A:151:C:H2'	15:A:152:A:C8	2.37	0.58
15:A:1996:G:N7	58:A:3134:HOH:O	2.31	0.58
18:E:13:SER:O	28:S:56:LYS:NZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:674:G:H2'	36:a:675:A:H8	1.67	0.57
37:b:14:LEU:HD23	37:b:14:LEU:H	1.69	0.57
2:1:59:GLN:O	2:1:63:ASN:HB2	2.04	0.57
15:A:2295:C:OP2	27:R:14:ARG:NH1	2.35	0.57
34:Y:51:ASN:HD22	34:Y:75:LEU:HD11	1.68	0.57
36:a:992:G:OP1	36:a:992:G:N2	2.32	0.57
31:V:76:GLU:HG2	31:V:82:LYS:HA	1.86	0.57
49:n:112:ALA:HB2	49:n:130:ALA:HB3	1.85	0.57
15:A:1002:U:H2'	15:A:1003:C:C6	2.39	0.57
15:A:2407:C:N4	15:A:2410:G:OP2	2.24	0.57
12:7:23:LYS:NZ	15:A:662:A:OP2	2.38	0.57
15:A:910:A:H62	15:A:936:U:H3	1.53	0.57
54:J:7:ILE:O	54:J:83:ARG:NH1	2.38	0.57
15:A:2201:G:OP2	15:A:2202:G:N2	2.38	0.57
31:V:99:SER:O	31:V:119:SER:OG	2.23	0.57
15:A:908:G:H2'	15:A:909:G:H1'	1.86	0.57
15:A:1826:G:OP2	17:D:156:ARG:NH2	2.38	0.57
47:l:56:LYS:HE2	47:l:190:ILE:HG13	1.87	0.57
36:a:1178:A:OP2	54:J:97:ARG:NH2	2.38	0.57
15:A:159:A:H2'	15:A:160:A:C8	2.40	0.56
38:c:7:LEU:HB3	38:c:18:TYR:HB3	1.86	0.56
15:A:437:C:H2'	15:A:438:A:C8	2.40	0.56
36:a:538:G:H5''	45:j:111:THR:HB	1.87	0.56
49:n:20:LEU:HD21	49:n:23:ILE:HD11	1.87	0.56
15:A:338:G:N7	19:F:137:LYS:NZ	2.52	0.56
15:A:553:G:H1'	15:A:2045:G:H4'	1.86	0.56
15:A:935:G:H2'	15:A:936:U:H6	1.70	0.56
17:D:34:VAL:HG12	17:D:63:ARG:HG3	1.87	0.56
36:a:1009:U:H3	36:a:1020:G:H22	1.53	0.56
38:c:82:MET:HB2	38:c:85:LEU:HB3	1.87	0.56
47:l:50:GLN:NE2	47:l:197:GLU:OE2	2.38	0.56
36:a:1060:C:H3'	36:a:1061:G:H2'	1.88	0.56
36:a:742:U:H2'	36:a:743:A:H8	1.70	0.56
21:L:58:THR:HG22	21:L:60:TYR:H	1.70	0.56
36:a:1248:A:H2'	36:a:1249:A:C8	2.41	0.56
15:A:883:U:H2'	15:A:884:U:C6	2.41	0.56
36:a:559:A:H4'	36:a:560:U:H3'	1.87	0.56
41:f:4:ASP:N	41:f:4:ASP:OD2	2.37	0.56
36:a:361:A:N3	36:a:373:U:O2'	2.34	0.56
36:a:1121:G:N2	36:a:1122:U:O4	2.32	0.56
49:n:116:MET:HE2	49:n:132:SER:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:2074:C:H2'	15:A:2075:C:C6	2.40	0.55
34:Y:32:LEU:HD11	34:Y:94:GLN:HB2	1.88	0.55
54:J:22:GLY:HA3	54:J:60:ASP:OD2	2.07	0.55
36:a:1425:U:H2'	36:a:1426:A:H8	1.71	0.55
12:7:29:LYS:HG3	12:7:33:LEU:HD21	1.88	0.55
25:P:35:LYS:HD2	25:P:132:VAL:HG11	1.89	0.55
13:8:22:ARG:NH2	15:A:2742:A:OP1	2.39	0.55
15:A:2234:U:H2'	15:A:2235:G:C8	2.42	0.55
15:A:2395:C:H42	15:A:2433:A:H61	1.53	0.55
27:R:105:ASP:O	27:R:109:LYS:HG2	2.07	0.55
36:a:412:A:H61	36:a:439:C:H42	1.54	0.55
36:a:1173:G:H2'	36:a:1174:A:C8	2.41	0.55
15:A:517:A:H4'	31:V:23:LYS:HB2	1.88	0.55
15:A:935:G:H2'	15:A:936:U:C6	2.42	0.55
15:A:2329:A:H2'	15:A:2330:U:C6	2.41	0.55
43:h:26:GLY:HA2	43:h:30:LEU:HB2	1.89	0.55
15:A:1295:G:O6	31:V:30:SER:OG	2.20	0.55
15:A:2287:A:H4'	15:A:2288:A:O4'	2.07	0.54
36:a:146:A:C2	36:a:225:G:N1	2.72	0.54
36:a:728:A:H2'	36:a:729:A:C8	2.42	0.54
15:A:1075:A:H2'	15:A:1076:A:C8	2.42	0.54
15:A:2533:G:O2'	15:A:2658:A:N1	2.41	0.54
1:I:57:ARG:HG3	1:I:57:ARG:HH11	1.71	0.54
16:B:25:C:H5''	27:R:56:LEU:HD11	1.89	0.54
15:A:253:G:H1	15:A:275:G:H1	1.54	0.54
15:A:1778:G:N7	58:A:3140:HOH:O	2.33	0.54
20:K:13:ASP:O	20:K:17:VAL:HG23	2.08	0.54
45:j:68:PRO:O	45:j:99:ARG:NH1	2.37	0.54
30:U:7:ILE:HG21	30:U:22:VAL:HG11	1.89	0.54
12:7:33:LEU:HB2	15:A:2420:U:H5''	1.90	0.54
19:F:155:TYR:HB2	19:F:176:LEU:HD22	1.90	0.54
36:a:658:U:H3	36:a:747:C:H5	1.55	0.54
39:d:58:LEU:HG	39:d:63:ILE:HB	1.90	0.54
40:e:69:SER:O	40:e:73:ARG:NH1	2.39	0.54
36:a:19:C:OP1	49:n:140:ASN:ND2	2.40	0.54
36:a:1064:A:H4'	36:a:1065:G:H5'	1.90	0.54
15:A:719:G:N7	58:A:3143:HOH:O	2.33	0.54
46:k:22:TRP:HB3	46:k:58:ARG:HB2	1.90	0.54
47:l:91:GLU:OE1	47:l:96:ASN:ND2	2.34	0.54
36:a:348:U:O2'	36:a:351:G:O6	2.26	0.53
46:k:158:GLY:HA2	46:k:192:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:2422:G:H2'	15:A:2423:C:C6	2.43	0.53
20:K:61:ARG:NH2	36:a:1364:G:O2'	2.41	0.53
46:k:111:ASP:O	46:k:113:ALA:N	2.42	0.53
17:D:243:HIS:HB3	17:D:251:TYR:HE1	1.73	0.53
25:P:35:LYS:HG2	25:P:102:ILE:HG12	1.90	0.53
36:a:154:A:H3'	36:a:155:A:H8	1.74	0.53
36:a:355:G:H2'	36:a:356:G:C8	2.43	0.53
26:Q:24:MET:HE1	26:Q:40:LYS:HD3	1.91	0.53
15:A:677:A:H4'	15:A:678:G:O5'	2.08	0.53
15:A:898:G:H21	15:A:901:A:H62	1.56	0.53
36:a:674:G:H2'	36:a:675:A:C8	2.43	0.53
15:A:618:U:H2'	15:A:619:G:C8	2.43	0.53
36:a:974:G:H4'	36:a:975:G:H5''	1.91	0.53
53:p:50:ALA:HB1	53:p:57:PHE:HB3	1.91	0.53
15:A:1808:G:OP2	17:D:273:LYS:NZ	2.29	0.53
36:a:402:A:H1'	36:a:403:A:H2'	1.90	0.53
15:A:285:C:H4'	15:A:286:U:O5'	2.09	0.52
54:J:104:ARG:NH1	54:J:105:ASP:O	2.42	0.52
12:7:56:ASN:HA	12:7:59:LYS:HB2	1.91	0.52
36:a:455:A:H4'	36:a:456:U:H5'	1.92	0.52
17:D:269:ILE:HG22	17:D:270:GLU:HG3	1.91	0.52
36:a:835:U:H3	36:a:850:A:N6	2.08	0.52
47:l:121:VAL:HG22	47:l:139:ILE:HG13	1.91	0.52
36:a:1320:G:H2'	36:a:1321:A:C8	2.44	0.52
45:j:50:ARG:NH2	45:j:89:ASP:OD2	2.40	0.52
15:A:2302:C:N3	15:A:2317:G:N2	2.54	0.52
36:a:945:A:H2'	36:a:946:A:H8	1.72	0.52
15:A:54:G:H5'	32:W:64:ARG:HG3	1.92	0.52
15:A:134:G:O2'	15:A:135:A:H8	1.92	0.52
15:A:169:A:H2'	15:A:170:C:C6	2.45	0.52
36:a:174:A:H2'	36:a:175:A:C8	2.45	0.52
15:A:2293:A:N1	15:A:2341:U:H5	2.07	0.52
30:U:3:VAL:HG12	30:U:42:VAL:HG22	1.92	0.52
48:m:59:SER:OG	48:m:60:ALA:N	2.40	0.52
12:7:38:LYS:HE2	15:A:2349:U:OP1	2.10	0.52
15:A:72:A:H2	15:A:91:A:H2	1.58	0.52
15:A:1382:A:H2'	15:A:1383:A:C8	2.45	0.52
15:A:2292:U:H2'	15:A:2293:A:C8	2.45	0.52
36:a:1103:G:H4'	46:k:171:ARG:HD3	1.92	0.52
43:h:1:MET:HE1	43:h:27:ARG:HB2	1.92	0.52
18:E:2:PRO:HB2	18:E:99:PHE:HZ	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:1502:A:H2'	36:a:1503:C:C6	2.45	0.51
15:A:1063:A:H2'	15:A:1064:A:C8	2.45	0.51
28:S:33:LYS:NZ	28:S:35:GLY:O	2.30	0.51
53:p:16:GLU:O	53:p:20:LEU:HG	2.10	0.51
15:A:150:U:H2'	15:A:151:C:C6	2.46	0.51
15:A:317:A:N3	15:A:337:C:O2'	2.41	0.51
15:A:958:G:H2'	15:A:959:A:C8	2.46	0.51
15:A:1387:U:H5	15:A:1401:A:N7	2.07	0.51
43:h:12:LEU:HD12	43:h:19:VAL:HG21	1.92	0.51
18:E:33:VAL:HG12	18:E:94:VAL:HG22	1.92	0.51
47:l:95:ASP:N	47:l:95:ASP:OD1	2.41	0.51
15:A:2440:A:O2'	15:A:2588:A:OP1	2.25	0.51
50:o:116:GLU:H	50:o:116:GLU:CD	2.19	0.51
17:D:123:ALA:O	17:D:128:ASN:ND2	2.30	0.51
36:a:169:G:H2'	36:a:170:G:H8	1.76	0.51
36:a:17:U:H2'	36:a:18:C:C6	2.45	0.51
36:a:1120:A:H61	36:a:1145:C:H42	1.57	0.51
36:a:626:U:OP1	38:c:36:ARG:NH2	2.44	0.51
47:l:193:GLN:O	47:l:197:GLU:HG2	2.11	0.51
36:a:953:G:H21	36:a:1225:A:H62	1.59	0.50
36:a:1136:C:H2'	36:a:1137:G:C8	2.46	0.50
36:a:197:U:H2'	36:a:198:G:H8	1.76	0.50
36:a:509:A:N6	36:a:539:A:H61	2.09	0.50
30:U:52:SER:OG	30:U:53:PRO:HD3	2.12	0.50
50:o:105:VAL:HG22	50:o:126:VAL:HA	1.94	0.50
15:A:2741:A:H2'	15:A:2742:A:C8	2.46	0.50
41:f:14:LYS:NZ	41:f:14:LYS:HB3	2.25	0.50
15:A:2619:G:C4	15:A:2620:H2U:H62	2.47	0.50
17:D:165:THR:HG21	36:a:712:A:H5''	1.93	0.50
36:a:848:C:H2'	36:a:849:A:C8	2.46	0.50
36:a:1102:A:O3'	46:k:171:ARG:NH1	2.44	0.50
14:9:4:VAL:HG21	14:9:19:PHE:HA	1.94	0.50
15:A:610:U:H2'	15:A:611:U:C6	2.47	0.50
15:A:1034:A:H2'	15:A:1035:G:O4'	2.12	0.50
17:D:142:HIS:ND1	17:D:193:GLY:O	2.41	0.50
18:E:8:LYS:HB2	18:E:201:LEU:HD11	1.93	0.50
34:Y:75:LEU:HD22	34:Y:78:ILE:HD11	1.93	0.50
15:A:700:A:H2'	15:A:701:G:C8	2.47	0.50
20:K:7:ILE:HB	20:K:73:ILE:HB	1.93	0.50
41:f:1:MET:HA	41:f:38:HIS:HB3	1.93	0.50
1:I:59:THR:OG1	1:I:60:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1964:G:N2	58:A:3181:HOH:O	2.43	0.50
36:a:814:A:H2'	36:a:816:A:H5''	1.93	0.50
15:A:1075:A:H2'	15:A:1076:A:H8	1.77	0.49
50:o:76:LEU:HD23	50:o:130:VAL:HG22	1.94	0.49
15:A:437:C:H2'	15:A:438:A:H8	1.76	0.49
15:A:670:U:H2'	15:A:671:C:C6	2.47	0.49
15:A:1033:A:H2'	15:A:1034:A:C8	2.47	0.49
20:K:17:VAL:HG21	20:K:69:TYR:HB2	1.93	0.49
36:a:470:A:C1'	38:c:82:MET:HE1	2.37	0.49
36:a:1121:G:H1	36:a:1144:A:H2	1.51	0.49
15:A:1834:U:H2'	15:A:1835:C:C6	2.47	0.49
16:B:27:A:H2'	16:B:28:C:C6	2.47	0.49
20:K:41:LEU:HB2	20:K:70:LYS:HB2	1.95	0.49
21:L:95:ALA:O	21:L:99:ILE:HG23	2.13	0.49
36:a:424:C:H41	36:a:427:A:N6	2.09	0.49
37:b:11:THR:HG22	37:b:55:LYS:HE2	1.94	0.49
15:A:23:A:H8	15:A:24:G:N7	2.10	0.49
15:A:279:A:O2'	15:A:280:U:O5'	2.30	0.49
15:A:592:G:H2'	15:A:2040:A:N7	2.28	0.49
47:l:182:ASP:O	47:l:186:ILE:HG13	2.12	0.49
15:A:1462:G:H2'	15:A:1463:A:C8	2.48	0.49
19:F:2:GLU:HG2	19:F:16:LYS:HG2	1.95	0.49
22:M:97:PHE:HB3	22:M:105:LEU:HB2	1.95	0.49
36:a:190:G:OP1	39:d:74:SER:OG	2.29	0.49
15:A:1028:C:OP2	29:T:54:LYS:NZ	2.45	0.49
32:W:33:ASN:ND2	32:W:36:GLU:OE2	2.45	0.49
15:A:1209:U:H2'	15:A:1210:A:C8	2.47	0.49
24:O:138:ILE:HD11	24:O:145:VAL:HG13	1.95	0.49
36:a:1121:G:H22	36:a:1144:A:H2	1.61	0.49
2:l:25:TYR:HB2	2:l:46:GLN:HG2	1.95	0.49
36:a:975:G:OP2	36:a:1355:U:O2'	2.30	0.49
45:j:49:MET:O	45:j:51:LYS:NZ	2.38	0.49
15:A:1077:G:N2	15:A:1149:G:H1	2.11	0.49
15:A:2332:G:O2'	15:A:2337:A:N1	2.43	0.49
36:a:572:A:OP1	52:10:6:LYS:NZ	2.42	0.49
36:a:722:A:H2	36:a:733:A:H61	1.61	0.49
36:a:1357:A:OP2	42:g:63:ARG:NH2	2.46	0.49
39:d:51:LEU:HD21	39:d:76:LEU:HD13	1.94	0.49
15:A:602:C:H2'	15:A:603:C:C6	2.47	0.48
15:A:1413:G:O2'	15:A:1414:A:O5'	2.29	0.48
36:a:1216:C:H2'	36:a:1217:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:2468:C:H2'	15:A:2469:A:O4'	2.13	0.48
16:B:60:C:H2'	16:B:61:A:H8	1.79	0.48
33:X:35:ARG:HB3	33:X:65:PRO:HB2	1.95	0.48
36:a:558:G:OP2	36:a:559:A:O2'	2.29	0.48
36:a:1068:C:H2'	36:a:1069:G:C8	2.46	0.48
15:A:121:C:H42	15:A:136:C:N4	2.11	0.48
19:F:156:VAL:HB	19:F:195:LEU:HD23	1.94	0.48
30:U:38:LYS:HA	30:U:54:LEU:HD13	1.95	0.48
36:a:864:A:H2'	36:a:865:A:C8	2.49	0.48
47:l:117:ARG:HE	47:l:125:VAL:HG11	1.78	0.48
53:p:69:HIS:NE2	58:p:101:HOH:O	2.35	0.48
15:A:537:A:H2'	15:A:538:C:C6	2.48	0.48
36:a:665:C:H1'	36:a:733:A:H5'	1.95	0.48
3:0:6:GLN:NE2	3:0:77:LEU:O	2.44	0.48
15:A:2066:G:O6	15:A:2067:6MA:H13	2.12	0.48
15:A:2081:A:H2'	15:A:2082:C:C6	2.48	0.48
16:B:28:C:H2'	16:B:29:C:O4'	2.13	0.48
36:a:922:A:O2'	36:a:1397:C:OP2	2.31	0.48
10:5:21:GLU:CG	10:5:22:SER:H	2.26	0.48
15:A:1452:U:H2'	15:A:1453:G:H8	1.78	0.48
15:A:2698:G:N7	58:A:3153:HOH:O	2.35	0.48
36:a:1456:U:H2'	36:a:1457:A:C8	2.49	0.48
42:g:54:MET:HE1	42:g:75:MET:HE1	1.95	0.48
15:A:141:G:H2'	15:A:142:A:C8	2.49	0.48
15:A:1438:U:H2'	15:A:1439:A:C8	2.48	0.48
15:A:2383:G:H3'	15:A:2384:A:H5'	1.96	0.48
31:V:92:ARG:HB2	31:V:125:TYR:HB2	1.96	0.48
37:b:3:ASN:HB2	37:b:93:GLN:HG3	1.95	0.48
15:A:253:G:H22	15:A:275:G:N2	2.12	0.48
22:M:147:ILE:HD12	22:M:150:LEU:HD12	1.96	0.48
23:N:10:VAL:HG12	23:N:12:ASP:OD1	2.14	0.48
23:N:13:ASN:HB3	23:N:97:ARG:HB2	1.96	0.48
36:a:737:U:H2'	36:a:738:G:H8	1.79	0.48
44:i:35:LEU:HD13	44:i:42:ARG:HA	1.96	0.48
15:A:667:G:N7	24:O:112:LYS:NZ	2.51	0.48
36:a:146:A:H2	36:a:225:G:N1	2.09	0.48
15:A:1261:U:H2'	15:A:1262:C:C6	2.48	0.48
15:A:2069:6MA:H5'	19:F:71:GLY:HA2	1.96	0.48
15:A:2638:U:H2'	15:A:2639:G:O4'	2.14	0.48
34:Y:103:MET:HE2	34:Y:103:MET:HB3	1.73	0.48
36:a:433:U:OP1	47:l:13:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:858:C:OP2	36:a:868:G:N1	2.35	0.48
15:A:328:A:O2'	15:A:330:G:N7	2.38	0.47
15:A:636:U:HO2'	15:A:637:A:H8	1.57	0.47
36:a:1139:U:H2'	36:a:1140:G:C4	2.48	0.47
46:k:187:GLU:HG2	46:k:194:LEU:HD22	1.96	0.47
36:a:464:G:O6	36:a:470:A:N6	2.47	0.47
36:a:965:2MG:H2'	36:a:966:A:C8	2.49	0.47
36:a:1076:G:H2'	36:a:1077:A:C8	2.49	0.47
36:a:1507:MA6:H8	36:a:1507:MA6:OP2	2.14	0.47
39:d:43:GLU:O	39:d:47:LYS:HG2	2.14	0.47
15:A:343:G:H2'	15:A:344:C:C6	2.49	0.47
36:a:416:A:O2'	36:a:417:A:O5'	2.32	0.47
15:A:2592:C:H2'	15:A:2593:G:C8	2.50	0.47
27:R:22:THR:HG22	27:R:23:GLN:H	1.79	0.47
32:W:63:ASN:HB3	32:W:70:LEU:HD21	1.96	0.47
33:X:51:SER:OG	33:X:52:ALA:N	2.46	0.47
54:J:86:VAL:HG23	54:J:96:LEU:HD12	1.96	0.47
36:a:9:G:H1	36:a:25:C:H5	1.62	0.47
36:a:1352:G:H2'	36:a:1353:C:C6	2.50	0.47
36:a:1421:G:H2'	36:a:1422:G:C8	2.50	0.47
8:2:47:VAL:HG12	8:2:51:ARG:HH21	1.78	0.47
15:A:464:A:H2'	15:A:465:G:C8	2.49	0.47
15:A:2450:OMU:HM21	15:A:2502:5OC:HN4A	1.79	0.47
16:B:81:G:OP1	16:B:85:C:N4	2.47	0.47
36:a:35:G:H2'	36:a:36:C:C6	2.50	0.47
15:A:160:A:H2'	15:A:161:C:C6	2.50	0.47
15:A:735:G:O2'	15:A:1668:A:N3	2.40	0.47
15:A:1042:A:N3	15:A:1188:C:O2'	2.45	0.47
15:A:2328:A:H2'	15:A:2329:A:C8	2.49	0.47
36:a:452:G:H3'	36:a:453:G:C8	2.50	0.47
15:A:2440:A:N3	15:A:2440:A:H2'	2.30	0.47
36:a:395:A:H2'	36:a:396:C:C6	2.49	0.47
37:b:3:ASN:OD1	37:b:66:GLN:NE2	2.37	0.47
2:1:17:ARG:HH11	2:1:17:ARG:HG2	1.80	0.47
15:A:599:G:H2'	15:A:600:A:C8	2.50	0.47
15:A:901:A:H2'	15:A:902:C:H6	1.79	0.47
15:A:1463:A:N1	15:A:1597:G:C6	2.82	0.47
15:A:2688:U:H2'	15:A:2689:U:O4'	2.15	0.47
19:F:159:GLU:OE2	19:F:198:ARG:NH2	2.48	0.47
32:W:51:ASP:OD1	32:W:52:VAL:N	2.48	0.47
36:a:117:G:H4'	36:a:118:C:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:427:A:H2'	36:a:428:A:C8	2.50	0.47
36:a:1352:G:H2'	36:a:1353:C:H6	1.80	0.47
44:i:87:CYS:O	44:i:91:ILE:HG23	2.15	0.47
15:A:2347:A:H4'	15:A:2384:A:OP2	2.14	0.47
16:B:47:G:H2'	16:B:48:A:C8	2.50	0.47
17:D:22:ASP:OD1	17:D:22:ASP:N	2.41	0.47
36:a:1284:A:H2'	36:a:1285:A:C8	2.50	0.47
44:i:17:PHE:HB3	44:i:42:ARG:HB2	1.97	0.47
48:m:14:ASP:OD2	48:m:17:TYR:N	2.33	0.47
15:A:1942:A:H2'	15:A:1943:G:O4'	2.16	0.46
48:m:14:ASP:OD1	48:m:43:TYR:OH	2.25	0.46
15:A:2105:A:H2'	15:A:2106:U:C6	2.50	0.46
36:a:208:A:O2'	36:a:209:C:OP1	2.30	0.46
15:A:41:A:H2'	15:A:42:A:C8	2.50	0.46
36:a:206:U:H3'	36:a:207:U:H5''	1.97	0.46
36:a:747:C:OP1	36:a:748:G:N1	2.49	0.46
36:a:835:U:H2'	36:a:836:G:C8	2.50	0.46
4:11:35:LYS:H	4:11:160:THR:HA	1.80	0.46
15:A:2272:G:OP1	35:Z:18:SER:HB3	2.16	0.46
11:6:24:THR:HG22	11:6:26:ASN:H	1.80	0.46
18:E:183:GLU:H	18:E:183:GLU:CD	2.23	0.46
36:a:606:G:N2	36:a:631:C:H2'	2.30	0.46
15:A:311:U:H3	15:A:365:A:N6	2.14	0.46
23:N:58:SER:OG	23:N:94:ARG:NH1	2.48	0.46
36:a:170:G:H2'	36:a:171:A:H8	1.80	0.46
36:a:269:C:O2'	40:e:67:PRO:O	2.30	0.46
36:a:934:A:H2'	36:a:935:C:C6	2.51	0.46
15:A:2330:U:H2'	15:A:2331:G:C8	2.50	0.46
15:A:2706:A:O2'	15:A:2838:G:OP1	2.29	0.46
20:K:52:ARG:NH2	36:a:1187:U:OP1	2.49	0.46
15:A:396:U:H5	15:A:424:A:N7	2.14	0.46
15:A:612:A:H2'	15:A:613:C:C6	2.51	0.46
17:D:272:ARG:HD2	17:D:272:ARG:HA	1.72	0.46
25:P:27:LEU:HD23	25:P:102:ILE:HD13	1.96	0.46
36:a:26:A:H62	36:a:557:G:H1	1.63	0.46
36:a:276:5OC:O5'	36:a:276:5OC:H6	2.16	0.46
36:a:480:U:H2'	36:a:481:G:C2	2.50	0.46
36:a:557:G:H2'	36:a:558:G:C8	2.51	0.46
36:a:890:U:H2'	36:a:891:A:H8	1.80	0.46
15:A:2383:G:H4'	15:A:2384:A:OP2	2.16	0.46
36:a:507:C:H5'	36:a:508:U:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:611:U:H2'	15:A:612:A:H8	1.81	0.45
15:A:831:U:H2'	15:A:832:U:C6	2.51	0.45
15:A:1452:U:H2'	15:A:1453:G:C8	2.51	0.45
15:A:1703:G:O2'	15:A:2001:U:O4	2.27	0.45
24:O:86:SER:O	24:O:95:SER:N	2.49	0.45
36:a:130:G:H5''	40:e:4:ASN:HB3	1.98	0.45
38:c:115:ASN:OD1	38:c:115:ASN:N	2.45	0.45
15:A:285:C:H1'	15:A:286:U:OP2	2.17	0.45
15:A:307:G:H2'	15:A:308:A:C8	2.50	0.45
15:A:933:A:H3'	15:A:934:A:C2	2.51	0.45
23:N:93:ILE:HG22	23:N:95:GLY:H	1.81	0.45
30:U:80:LYS:HG3	30:U:85:TYR:CD2	2.52	0.45
36:a:457:A:N6	36:a:476:G:H22	2.14	0.45
15:A:2784:A:H2'	15:A:2785:U:C6	2.51	0.45
28:S:31:ARG:NH1	28:S:82:GLU:OE1	2.46	0.45
36:a:64:G:H5''	36:a:65:A:H5'	1.99	0.45
36:a:268:A:H2'	36:a:269:C:C5	2.51	0.45
36:a:513:C:N3	36:a:533:A:H2	2.14	0.45
36:a:1008:A:H2'	36:a:1009:U:C6	2.51	0.45
4:11:42:GLY:HA2	4:11:89:GLY:HA2	1.98	0.45
15:A:1:U:H2'	15:A:2:A:O4'	2.15	0.45
36:a:1122:U:H5	36:a:1278:A:N7	2.15	0.45
15:A:228:G:H2'	15:A:229:A:C8	2.52	0.45
15:A:875:G:C4	15:A:876:H2U:H62	2.51	0.45
15:A:1227:U:H2'	15:A:1228:U:C6	2.52	0.45
15:A:2084:U:H2'	15:A:2085:U:C6	2.51	0.45
15:A:2820:G:H2'	15:A:2864:A:H61	1.81	0.45
36:a:299:A:OP1	36:a:610:C:O2'	2.26	0.45
36:a:435:U:C2	36:a:436:A:C8	3.04	0.45
2:1:12:LYS:HB3	2:1:12:LYS:HE3	1.69	0.45
15:A:2647:C:H2'	15:A:2648:U:O4'	2.17	0.45
36:a:1313:G:H22	36:a:1316:A:H5'	1.81	0.45
15:A:225:G:H4'	15:A:409:G:C5	2.52	0.45
15:A:2011:G:H2'	15:A:2012:C:C6	2.52	0.45
20:K:10:LYS:HE3	20:K:70:LYS:HD3	1.96	0.45
36:a:1403:G:O2'	36:a:1507:MA6:O2'	2.23	0.45
41:f:41:GLU:OE2	41:f:44:ARG:NH1	2.50	0.45
15:A:2047:C:H2'	15:A:2048:G:C8	2.51	0.45
15:A:150:U:H2'	15:A:151:C:H6	1.81	0.45
15:A:542:U:H2'	15:A:543:C:C6	2.52	0.45
34:Y:61:VAL:HG12	34:Y:63:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:268:A:H2'	36:a:269:C:C6	2.52	0.45
36:a:737:U:H2'	36:a:738:G:C8	2.52	0.45
36:a:1302:G:N2	36:a:1328:G:H2'	2.32	0.45
50:o:12:LEU:HD23	50:o:23:VAL:HG11	1.99	0.45
15:A:562:G:O6	15:A:576:U:H5	2.00	0.45
15:A:1685:G:O2'	26:Q:106:ASP:OD2	2.20	0.45
15:A:2547:U:OP1	23:N:29:ARG:NH1	2.42	0.45
19:F:5:VAL:O	19:F:13:THR:OG1	2.31	0.45
24:O:55:MET:O	24:O:60:ARG:NH1	2.50	0.45
36:a:484:U:H2'	36:a:485:G:O4'	2.16	0.45
36:a:824:U:H2'	36:a:825:A:C8	2.51	0.45
36:a:953:G:N2	36:a:1225:A:H62	2.15	0.45
41:f:3:LEU:HD21	41:f:31:LEU:HD11	1.98	0.45
51:15:16:THR:O	51:15:41:ASN:N	2.50	0.45
7:14:78:ARG:O	7:14:82:LEU:HD12	2.16	0.44
20:K:55:PHE:CD2	20:K:56:VAL:HG22	2.52	0.44
36:a:74:A:C6	36:a:98:U:C4	3.05	0.44
36:a:156:C:N4	36:a:171:A:H61	2.14	0.44
36:a:736:U:H2'	36:a:737:U:C6	2.52	0.44
45:j:89:ASP:OD1	45:j:90:LEU:N	2.50	0.44
15:A:784:A:H4'	15:A:1300:G:N3	2.33	0.44
15:A:1818:A:H2'	15:A:1819:A:C8	2.52	0.44
15:A:2581:PSU:O2'	15:A:2582:G:H5'	2.17	0.44
16:B:61:A:H2'	16:B:62:A:C8	2.53	0.44
28:S:33:LYS:HB3	28:S:33:LYS:HE3	1.70	0.44
31:V:89:PHE:CD1	31:V:129:LEU:HG	2.52	0.44
36:a:757:U:H2'	36:a:758:G:O4'	2.17	0.44
47:l:101:LEU:HD22	47:l:168:TRP:HE3	1.82	0.44
15:A:2300:G:H2'	15:A:2301:G:H8	1.81	0.44
30:U:80:LYS:HG3	30:U:85:TYR:HD2	1.82	0.44
33:X:4:LEU:HD11	33:X:31:VAL:HG22	1.99	0.44
36:a:580:C:H2'	36:a:581:G:O4'	2.16	0.44
36:a:1264:G:N2	36:a:1267:A:OP2	2.38	0.44
15:A:1261:U:H2'	15:A:1262:C:H6	1.83	0.44
19:F:177:ILE:HD12	19:F:186:THR:HG21	2.00	0.44
36:a:508:U:H2'	36:a:509:A:N3	2.32	0.44
36:a:663:G:H2'	36:a:664:G:C8	2.53	0.44
10:5:55:MET:HE3	10:5:55:MET:HB3	1.84	0.44
11:6:39:ARG:NH2	15:A:491:G:N7	2.53	0.44
15:A:611:U:H2'	15:A:612:A:C8	2.52	0.44
15:A:1860:U:H2'	15:A:1861:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:2292:U:OP1	15:A:2381:U:O2'	2.34	0.44
50:o:52:ASN:HD21	50:o:57:ILE:HG12	1.83	0.44
15:A:133:U:H3'	15:A:134:G:H21	1.83	0.44
34:Y:30:ALA:HA	34:Y:90:ILE:O	2.17	0.44
36:a:498:C:H2'	36:a:499:A:C8	2.53	0.44
36:a:1236:A:N7	36:a:1298:U:H5	2.16	0.44
54:J:117:PRO:HG2	54:J:121:LYS:HG2	1.99	0.44
15:A:756:A:H2'	15:A:757:A:C8	2.52	0.44
15:A:771:U:H2'	15:A:772:C:C6	2.52	0.44
15:A:934:A:H2'	15:A:935:G:H8	1.80	0.44
15:A:1718:G:H2'	15:A:1719:U:C6	2.52	0.44
15:A:1830:A:H2'	15:A:1831:U:C6	2.52	0.44
15:A:2406:G:OP2	15:A:2406:G:N2	2.40	0.44
19:F:135:LYS:HE2	19:F:135:LYS:HB2	1.75	0.44
36:a:146:A:N1	36:a:225:G:C6	2.85	0.44
13:8:29:LYS:HA	13:8:29:LYS:HD3	1.61	0.44
15:A:783:G:C8	31:V:108:PRO:HB3	2.52	0.44
15:A:2252:OMG:HM23	15:A:2252:OMG:H1'	1.74	0.44
18:E:90:LYS:NZ	18:E:90:LYS:HB2	2.33	0.44
29:T:14:ARG:HG2	29:T:32:TRP:CZ2	2.53	0.44
32:W:70:LEU:HA	32:W:70:LEU:HD23	1.74	0.44
36:a:65:A:OP2	36:a:65:A:H4'	2.18	0.44
44:i:88:TYR:O	44:i:92:ARG:HG2	2.18	0.44
48:m:77:VAL:HA	48:m:90:PRO:HA	2.00	0.44
2:1:14:LEU:HD11	2:1:53:MET:HG2	1.98	0.44
15:A:186:C:H2'	15:A:187:C:C6	2.53	0.44
15:A:618:U:H2'	15:A:619:G:H8	1.83	0.44
15:A:668:A:H8	15:A:682:G:H21	1.66	0.44
15:A:1070:U:H2'	15:A:1071:C:O2	2.18	0.44
18:E:82:PHE:HB2	18:E:85:PHE:HE2	1.82	0.44
36:a:469:G:H2'	36:a:470:A:O4'	2.18	0.44
36:a:519:C:OP2	45:j:66:TYR:OH	2.32	0.44
36:a:907:A:H2'	36:a:908:A:C8	2.53	0.44
36:a:1143:G:H4'	54:J:7:ILE:HD13	2.00	0.44
1:I:48:ASN:OD1	1:I:50:GLN:N	2.51	0.43
1:I:76:ALA:HB1	1:I:81:LEU:HB2	2.00	0.43
15:A:502:A:N3	15:A:504:G:H5''	2.33	0.43
16:B:4:G:OP1	16:B:58:C:O2'	2.36	0.43
25:P:32:PHE:HB2	25:P:106:VAL:HG22	2.00	0.43
26:Q:20:MET:HE2	26:Q:20:MET:HB3	1.85	0.43
34:Y:26:ASP:O	34:Y:27:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:751:U:H2'	36:a:752:G:O4'	2.17	0.43
44:i:40:VAL:HG22	44:i:53:GLN:HG2	2.00	0.43
46:k:148:ILE:HD11	46:k:150:ILE:HD11	1.99	0.43
15:A:141:G:H1	15:A:153:U:H3	1.66	0.43
15:A:961:A:H2'	15:A:962:A:C8	2.54	0.43
15:A:324:U:H2'	15:A:325:G:O4'	2.17	0.43
15:A:1949:5MU:OP1	15:A:2605:U:O2'	2.34	0.43
15:A:2450:OMU:HM23	58:A:3247:HOH:O	2.18	0.43
15:A:2592:C:H2'	15:A:2593:G:H8	1.83	0.43
18:E:91:LEU:HD12	18:E:91:LEU:HA	1.86	0.43
29:T:104:GLU:CD	29:T:104:GLU:H	2.25	0.43
36:a:298:A:H4'	36:a:609:A:C2	2.53	0.43
36:a:880:A:P	45:j:9:ARG:HH22	2.41	0.43
12:7:29:LYS:HG3	12:7:33:LEU:CD2	2.48	0.43
15:A:307:G:H2'	15:A:308:A:H8	1.83	0.43
15:A:715:A:H2'	15:A:716:A:C8	2.54	0.43
15:A:2105:A:H2'	15:A:2106:U:H6	1.83	0.43
15:A:2380:C:H2'	15:A:2381:U:C6	2.54	0.43
15:A:2822:U:H2'	15:A:2823:A:C8	2.53	0.43
17:D:155:VAL:HG21	17:D:162:ALA:HB2	1.99	0.43
18:E:107:ASP:OD2	18:E:173:GLN:HG3	2.18	0.43
24:O:79:LEU:HG	24:O:115:ALA:HA	2.01	0.43
36:a:919:U:H2'	36:a:920:U:C6	2.54	0.43
36:a:1074:G:N2	36:a:1077:A:OP2	2.37	0.43
36:a:1410:C:H2'	36:a:1411:A:C8	2.53	0.43
36:a:1426:A:H2'	36:a:1427:C:H6	1.83	0.43
37:b:16:ASP:O	37:b:19:MET:HB2	2.19	0.43
46:k:110:LEU:HD21	46:k:145:ALA:HB2	1.99	0.43
15:A:185:A:H2'	15:A:186:C:O4'	2.18	0.43
15:A:2835:U:H4'	15:A:2836:A:H5'	1.99	0.43
20:K:11:SER:OG	20:K:12:TYR:N	2.52	0.43
25:P:134:ARG:HG3	25:P:137:TYR:HB2	2.00	0.43
36:a:34:C:H2'	36:a:35:G:H8	1.83	0.43
36:a:1482:A:O2'	36:a:1483:G:H8	2.02	0.43
36:a:1520:A:H3'	36:a:1521:A:N3	2.33	0.43
15:A:85:G:H2'	15:A:86:A:H8	1.83	0.43
15:A:1210:A:H2'	15:A:1211:U:C6	2.54	0.43
24:O:35:HIS:O	58:O:201:HOH:O	2.21	0.43
28:S:27:THR:OG1	28:S:87:GLU:OE2	2.29	0.43
36:a:497:A:N6	36:a:545:C:H42	2.07	0.43
45:j:30:ARG:NH1	45:j:58:THR:OG1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:35:ILE:HD11	1:I:65:PHE:CE1	2.54	0.43
20:K:9:LEU:O	20:K:70:LYS:HA	2.19	0.43
23:N:12:ASP:OD1	23:N:12:ASP:N	2.52	0.43
27:R:98:GLY:O	27:R:102:GLU:HG2	2.18	0.43
36:a:460:G:H1	36:a:473:A:H2	1.66	0.43
36:a:748:G:H4'	36:a:749:A:O5'	2.18	0.43
36:a:1014:A:C2	36:a:1217:G:H1'	2.54	0.43
36:a:1249:A:H2'	36:a:1250:A:C8	2.54	0.43
50:o:81:ARG:H	50:o:81:ARG:HG2	1.62	0.43
9:4:50:ARG:HD3	15:A:2869:U:O4'	2.19	0.43
15:A:1459:G:H2'	15:A:1460:G:C8	2.53	0.43
15:A:1814:A:H2'	15:A:1815:A:H5''	1.99	0.43
15:A:1939:G:N3	15:A:1939:G:H2'	2.33	0.43
35:Z:66:VAL:HG23	35:Z:82:LYS:HB3	1.99	0.43
36:a:97:A:N1	36:a:100:G:N2	2.67	0.43
36:a:210:A:H2'	36:a:211:A:C8	2.54	0.43
36:a:274:C:H2'	36:a:275:A:C8	2.54	0.43
1:I:57:ARG:HG3	1:I:57:ARG:NH1	2.33	0.43
5:12:77:ARG:NH1	36:a:1309:G:OP2	2.51	0.43
15:A:53:A:H8	15:A:54:G:N7	2.17	0.43
15:A:597:A:OP2	15:A:2500:C:O2'	2.36	0.43
15:A:2096:U:H2'	15:A:2097:U:C6	2.53	0.43
36:a:46:G:N7	58:a:1710:HOH:O	2.37	0.43
36:a:938:G:O3'	48:m:104:LYS:NZ	2.52	0.43
41:f:78:TYR:O	41:f:82:ILE:HG23	2.18	0.43
42:g:82:PRO:HG3	46:k:20:SER:HB2	2.01	0.43
43:h:5:LEU:HD23	43:h:36:ALA:HB2	2.01	0.43
53:p:32:LYS:NZ	53:p:32:LYS:HB2	2.34	0.43
15:A:144:U:H2'	15:A:145:U:C6	2.54	0.43
15:A:1799:C:H2'	15:A:1800:A:C5	2.54	0.43
15:A:2729:U:H2'	15:A:2730:C:C6	2.54	0.43
18:E:77:ARG:HD2	18:E:77:ARG:HA	1.78	0.43
22:M:135:HIS:CE1	22:M:137:HIS:HB2	2.54	0.43
27:R:35:LYS:HB3	27:R:35:LYS:HE2	1.70	0.43
36:a:205:A:H2'	36:a:206:U:H6	1.84	0.43
16:B:7:G:OP1	27:R:16:ARG:NH1	2.47	0.42
16:B:85:C:H4'	16:B:86:A:H4'	2.01	0.42
27:R:77:LYS:HE3	27:R:77:LYS:HB2	1.79	0.42
36:a:1519:G:H2'	36:a:1520:A:N3	2.34	0.42
54:J:37:PHE:O	54:J:43:GLN:NE2	2.51	0.42
15:A:1077:G:N2	15:A:1149:G:H22	2.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:6:U:OP1	27:R:12:LYS:NZ	2.49	0.42
16:B:60:C:H2'	16:B:61:A:C8	2.54	0.42
38:c:5:ILE:HG12	38:c:22:VAL:HG22	2.01	0.42
15:A:882:G:H2'	15:A:883:U:H6	1.84	0.42
15:A:2387:A:H2'	15:A:2388:U:C6	2.53	0.42
16:B:2:C:H2'	16:B:3:A:C8	2.54	0.42
36:a:1373:A:OP1	48:m:24:LYS:NZ	2.51	0.42
47:l:193:GLN:H	47:l:193:GLN:CD	2.27	0.42
4:11:120:ILE:O	4:11:180:LYS:N	2.43	0.42
15:A:2851:U:H2'	15:A:2852:A:C4	2.55	0.42
16:B:24:U:O2'	16:B:25:C:O5'	2.36	0.42
36:a:452:G:H3'	36:a:453:G:H8	1.83	0.42
15:A:121:C:H42	15:A:136:C:H42	1.67	0.42
18:E:188:LEU:HD21	28:S:7:VAL:HG13	2.01	0.42
19:F:19:LEU:HB3	19:F:24:PHE:CD2	2.55	0.42
27:R:41:LEU:HD12	27:R:41:LEU:HA	1.80	0.42
36:a:21:G:H2'	36:a:22:G:C8	2.54	0.42
36:a:1052:A:O2'	46:k:160:GLU:O	2.28	0.42
36:a:1457:A:H2'	36:a:1458:G:O4'	2.20	0.42
36:a:1500:G:N7	58:a:1709:HOH:O	2.36	0.42
47:l:11:ILE:H	47:l:11:ILE:HG12	1.69	0.42
15:A:143:A:H61	15:A:151:C:N4	2.15	0.42
15:A:636:U:O2'	15:A:637:A:H8	2.02	0.42
15:A:757:A:H2'	15:A:758:C:C6	2.55	0.42
15:A:258:U:H2'	15:A:259:G:C8	2.55	0.42
15:A:795:A:H2'	15:A:796:A:O4'	2.19	0.42
16:B:24:U:HO2'	16:B:25:C:C5'	2.33	0.42
36:a:837:C:N4	36:a:848:C:H42	2.17	0.42
36:a:907:A:H2'	36:a:908:A:H8	1.84	0.42
49:n:41:ILE:HD13	49:n:138:PRO:HB2	2.02	0.42
36:a:1513:C:H2'	36:a:1514:G:C8	2.54	0.42
46:k:191:LYS:HA	46:k:191:LYS:HD2	1.92	0.42
15:A:1459:G:H2'	15:A:1460:G:H8	1.85	0.42
15:A:2223:A:H4'	17:D:185:LEU:HD11	2.02	0.42
36:a:521:G:H2'	36:a:522:C:C6	2.54	0.42
40:e:31:LYS:HA	40:e:38:PHE:HA	2.02	0.42
47:l:134:LYS:HE2	47:l:134:LYS:HB3	1.82	0.42
50:o:8:TYR:HD2	50:o:25:VAL:HG11	1.85	0.42
15:A:440:C:H2'	15:A:441:C:C6	2.55	0.42
15:A:898:G:H2'	15:A:899:C:C6	2.55	0.42
15:A:1270:U:H2'	15:A:1271:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:46:A:H2'	16:B:47:G:C8	2.55	0.42
23:N:70:ARG:HB2	23:N:76:TYR:CE2	2.55	0.42
36:a:859:A:H2'	36:a:860:G:O4'	2.20	0.42
36:a:1345:U:H4'	54:J:120:ARG:HG3	2.02	0.42
36:a:1424:G:H2'	36:a:1425:U:H6	1.85	0.42
36:a:1424:G:H2'	36:a:1425:U:C6	2.54	0.42
41:f:31:LEU:O	41:f:35:ARG:HG2	2.20	0.42
5:12:12:PRO:HA	5:12:27:ARG:HA	2.02	0.41
15:A:2247:G:H2'	15:A:2248:A:C8	2.55	0.41
17:D:119:GLY:O	17:D:130:LEU:HD23	2.19	0.41
23:N:113:ILE:O	23:N:116:LEU:HG	2.19	0.41
36:a:257:U:H2'	36:a:258:U:C6	2.54	0.41
36:a:329:G:N1	36:a:332:A:OP2	2.49	0.41
36:a:381:G:H5''	38:c:6:ARG:HB2	2.02	0.41
36:a:863:A:H2'	36:a:864:A:C8	2.55	0.41
36:a:1293:C:OP1	44:i:15:ARG:NH2	2.45	0.41
36:a:1349:C:H2'	36:a:1350:G:C8	2.54	0.41
15:A:1174:C:H5'	22:M:109:VAL:HG13	2.02	0.41
36:a:1431:A:H2'	36:a:1432:A:C8	2.54	0.41
36:a:1518:G:O6	52:10:7:ARG:NH2	2.53	0.41
39:d:63:ILE:H	39:d:63:ILE:HG12	1.71	0.41
42:g:33:TYR:CZ	53:p:7:LYS:HG2	2.55	0.41
47:l:18:PRO:HB2	47:l:21:GLY:O	2.20	0.41
47:l:23:ASP:OD1	47:l:23:ASP:N	2.53	0.41
47:l:173:LEU:HD12	47:l:173:LEU:HA	1.75	0.41
11:6:45:SER:OG	15:A:114:A:OP1	2.35	0.41
12:7:8:SER:HA	12:7:11:LYS:HE2	2.02	0.41
15:A:256:U:H2'	15:A:257:U:C6	2.55	0.41
15:A:1463:A:C6	15:A:1597:G:O6	2.74	0.41
15:A:2513:C:H2'	15:A:2514:G:O4'	2.21	0.41
24:O:82:LEU:HD23	24:O:82:LEU:HA	1.90	0.41
35:Z:71:ARG:NH1	35:Z:71:ARG:HG3	2.35	0.41
39:d:40:ASP:HB3	39:d:43:GLU:HB3	2.02	0.41
15:A:27:U:H2'	15:A:28:C:O4'	2.21	0.41
15:A:882:G:H2'	15:A:883:U:C6	2.55	0.41
15:A:1166:U:C4	18:E:152:PRO:HA	2.56	0.41
16:B:16:G:H2'	16:B:17:U:C6	2.55	0.41
16:B:54:U:H4'	16:B:55:A:O5'	2.20	0.41
36:a:662:U:H3	36:a:743:A:H61	1.68	0.41
37:b:71:VAL:HA	37:b:74:LYS:HD2	2.01	0.41
41:f:12:PHE:CD1	41:f:27:SER:HB3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:f:70:LEU:HB3	41:f:78:TYR:HB2	2.03	0.41
5:12:10:TYR:HA	5:12:29:THR:HG23	2.02	0.41
15:A:516:G:H2'	15:A:517:A:O4'	2.20	0.41
15:A:811:G:O2'	15:A:812:G:OP2	2.32	0.41
15:A:1216:G:H5'	30:U:85:TYR:CE1	2.55	0.41
15:A:2062:G:H4'	18:E:148:ALA:O	2.20	0.41
29:T:58:ARG:HA	29:T:61:TRP:CE3	2.56	0.41
36:a:1403:G:H2'	36:a:1404:U:H6	1.85	0.41
37:b:1:MET:HE3	37:b:1:MET:HB2	1.94	0.41
50:o:112:MET:HE2	50:o:112:MET:HB3	1.94	0.41
15:A:2292:U:H2'	15:A:2293:A:H8	1.84	0.41
16:B:30:U:H2'	16:B:31:C:C6	2.56	0.41
36:a:742:U:H2'	36:a:743:A:C8	2.54	0.41
36:a:1014:A:H2'	36:a:1015:A:C8	2.56	0.41
45:j:56:ARG:HG3	45:j:56:ARG:HH11	1.85	0.41
47:l:146:LYS:HG2	47:l:173:LEU:HD23	2.03	0.41
15:A:738:U:H2'	15:A:739:G:O4'	2.21	0.41
15:A:885:A:H2'	15:A:886:U:C6	2.56	0.41
24:O:68:ASN:OD1	24:O:69:ILE:N	2.54	0.41
36:a:55:A:H2'	36:a:56:U:C6	2.55	0.41
36:a:71:A:N6	36:a:102:G:N7	2.69	0.41
43:h:6:LYS:H	43:h:36:ALA:H	1.68	0.41
11:6:7:PRO:HB2	15:A:1338:G:H4'	2.02	0.41
36:a:462:G:O2'	36:a:463:C:O5'	2.38	0.41
36:a:769:G:H4'	36:a:1502:A:H4'	2.01	0.41
36:a:1485:C:H2'	36:a:1486:G:O4'	2.21	0.41
37:b:12:PRO:HD2	37:b:55:LYS:NZ	2.36	0.41
15:A:630:A:H2'	15:A:631:A:C8	2.56	0.41
15:A:852:C:O2'	15:A:874:U:H5''	2.21	0.41
15:A:1904:C:H2'	15:A:1905:C:C6	2.56	0.41
16:B:46:A:H2'	16:B:47:G:H8	1.86	0.41
17:D:243:HIS:HB3	17:D:251:TYR:CE1	2.54	0.41
25:P:76:LYS:HB2	25:P:91:GLU:HG3	2.02	0.41
36:a:97:A:H1'	36:a:98:U:C5	2.55	0.41
36:a:450:C:H2'	36:a:451:G:O4'	2.20	0.41
36:a:933:C:H5	36:a:1375:A:N1	2.19	0.41
36:a:1389:U:H2'	36:a:1390:G:C8	2.55	0.41
40:e:63:MET:SD	40:e:75:ARG:NH2	2.94	0.41
45:j:34:CYS:SG	45:j:78:SER:OG	2.73	0.41
15:A:616:U:H2'	15:A:617:U:C6	2.55	0.41
15:A:2242:A:H2'	15:A:2243:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:2430:G:N7	24:O:55:MET:HE3	2.36	0.41
16:B:15:C:H2'	16:B:16:G:O4'	2.21	0.41
17:D:23:LYS:HD3	17:D:23:LYS:HA	1.87	0.41
22:M:18:LYS:NZ	22:M:56:GLY:O	2.35	0.41
12:7:22:ILE:HG21	12:7:58:VAL:HG11	2.03	0.40
14:9:28:ALA:O	14:9:31:GLU:HG3	2.21	0.40
15:A:944:A:H2'	15:A:945:A:C8	2.56	0.40
15:A:2302:C:H2'	15:A:2303:C:H6	1.85	0.40
15:A:2342:G:H2'	15:A:2343:C:C6	2.56	0.40
17:D:154:MET:HB2	17:D:154:MET:HE2	1.75	0.40
21:L:118:ASN:HB2	36:a:718:U:H5'	2.02	0.40
22:M:67:ILE:HD13	22:M:106:PHE:HZ	1.86	0.40
27:R:55:SER:HA	27:R:58:LEU:HB3	2.03	0.40
36:a:285:C:C5	40:e:41:LYS:HA	2.56	0.40
36:a:493:A:H3'	36:a:494:G:H5''	2.03	0.40
36:a:1121:G:N1	36:a:1144:A:C2	2.73	0.40
45:j:34:CYS:HG	45:j:78:SER:HG	1.63	0.40
48:m:48:ILE:HD12	48:m:48:ILE:H	1.86	0.40
2:1:54:LYS:HD3	15:A:61:A:C8	2.56	0.40
6:13:5:GLY:HA2	6:13:69:ARG:HD2	2.02	0.40
15:A:251:C:H2'	15:A:252:C:H6	1.87	0.40
15:A:274:G:OP2	15:A:274:G:N2	2.42	0.40
15:A:1040:C:H2'	15:A:1041:G:N2	2.36	0.40
15:A:2300:G:H2'	15:A:2301:G:C8	2.56	0.40
36:a:1423:G:H22	36:a:1464:A:H2	1.69	0.40
49:n:39:ALA:HB1	49:n:55:LEU:HD11	2.03	0.40
53:p:12:ASN:HB3	53:p:15:LEU:HB3	2.04	0.40
26:Q:24:MET:HB3	26:Q:44:LEU:HD13	2.04	0.40
36:a:581:G:N1	36:a:759:A:OP2	2.34	0.40
36:a:713:G:H2'	36:a:714:G:C8	2.56	0.40
42:g:16:LEU:HD23	42:g:16:LEU:HA	1.84	0.40
47:l:71:LEU:HA	47:l:71:LEU:HD23	1.87	0.40
3:0:36:LYS:NZ	15:A:2102:U:OP2	2.54	0.40
13:8:7:VAL:HG22	13:8:38:GLY:HA2	2.02	0.40
15:A:659:G:H2'	15:A:660:C:C6	2.56	0.40
15:A:692:U:H2'	15:A:693:C:C6	2.56	0.40
15:A:2412:A:H2'	15:A:2413:A:C8	2.57	0.40
16:B:37:A:H2'	16:B:38:U:C6	2.57	0.40
19:F:3:LEU:HD23	19:F:3:LEU:HA	1.90	0.40
25:P:34:ILE:HB	25:P:129:THR:CG2	2.52	0.40
27:R:63:SER:HB3	27:R:66:GLU:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:115:G:H1'	36:a:359:G:H5'	2.04	0.40
36:a:652:U:H5	36:a:753:A:N7	2.20	0.40
36:a:1410:C:H2'	36:a:1411:A:H8	1.87	0.40
44:i:81:ARG:NH1	58:p:101:HOH:O	2.55	0.40
50:o:113:THR:HB	50:o:116:GLU:OE1	2.22	0.40
15:A:253:G:H1	15:A:275:G:H22	1.69	0.40
15:A:1297:A:H2'	15:A:1298:A:O4'	2.21	0.40
15:A:2032:U:O2'	15:A:2618:U:H5'	2.22	0.40
15:A:2263:U:H2'	15:A:2264:C:H6	1.86	0.40
28:S:63:LYS:HB2	28:S:63:LYS:HE3	1.92	0.40
39:d:35:PHE:HZ	39:d:80:ILE:HD12	1.87	0.40
48:m:46:LEU:HD23	48:m:46:LEU:HA	1.87	0.40
49:n:22:ALA:O	49:n:23:ILE:HD13	2.21	0.40
50:o:21:ARG:HA	50:o:21:ARG:HD2	1.80	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	50/90 (56%)	47 (94%)	3 (6%)	0	100	100
2	1	61/64 (95%)	61 (100%)	0	0	100	100
3	0	75/79 (95%)	74 (99%)	1 (1%)	0	100	100
4	11	142/186 (76%)	125 (88%)	17 (12%)	0	100	100
5	12	44/85 (52%)	42 (96%)	2 (4%)	0	100	100
6	13	132/183 (72%)	118 (89%)	14 (11%)	0	100	100
7	14	33/401 (8%)	29 (88%)	4 (12%)	0	100	100
8	2	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
9	4	55/61 (90%)	50 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	5	43/62 (69%)	39 (91%)	4 (9%)	0	100	100
11	6	46/50 (92%)	46 (100%)	0	0	100	100
12	7	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
13	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
14	9	42/63 (67%)	42 (100%)	0	0	100	100
17	D	270/274 (98%)	266 (98%)	4 (2%)	0	100	100
18	E	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
19	F	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
20	K	74/101 (73%)	69 (93%)	5 (7%)	0	100	100
21	L	115/128 (90%)	102 (89%)	13 (11%)	0	100	100
22	M	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
23	N	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
24	O	135/148 (91%)	126 (93%)	9 (7%)	0	100	100
25	P	139/144 (96%)	133 (96%)	6 (4%)	0	100	100
26	Q	121/160 (76%)	120 (99%)	1 (1%)	0	100	100
27	R	111/114 (97%)	101 (91%)	10 (9%)	0	100	100
28	S	112/121 (93%)	111 (99%)	1 (1%)	0	100	100
29	T	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
30	U	102/105 (97%)	92 (90%)	10 (10%)	0	100	100
31	V	126/134 (94%)	123 (98%)	3 (2%)	0	100	100
32	W	93/97 (96%)	90 (97%)	3 (3%)	0	100	100
33	X	99/106 (93%)	94 (95%)	5 (5%)	0	100	100
34	Y	124/192 (65%)	107 (86%)	17 (14%)	0	100	100
35	Z	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
37	b	105/117 (90%)	101 (96%)	4 (4%)	0	100	100
38	c	116/192 (60%)	108 (93%)	8 (7%)	0	100	100
39	d	75/84 (89%)	73 (97%)	2 (3%)	0	100	100
40	e	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
41	f	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
42	g	81/89 (91%)	77 (95%)	4 (5%)	0	100	100
43	h	53/179 (30%)	48 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	i	103/126 (82%)	96 (93%)	7 (7%)	0	100	100
45	j	120/134 (90%)	113 (94%)	7 (6%)	0	100	100
46	k	90/246 (37%)	83 (92%)	7 (8%)	0	100	100
47	l	198/201 (98%)	189 (96%)	9 (4%)	0	100	100
48	m	129/158 (82%)	126 (98%)	3 (2%)	0	100	100
49	n	165/172 (96%)	155 (94%)	10 (6%)	0	100	100
50	o	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
51	15	32/49 (65%)	30 (94%)	2 (6%)	0	100	100
52	10	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
53	p	78/89 (88%)	75 (96%)	3 (4%)	0	100	100
54	J	123/128 (96%)	118 (96%)	5 (4%)	0	100	100
All	All	5148/6493 (79%)	4891 (95%)	257 (5%)	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	I	37/80 (46%)	36 (97%)	1 (3%)	39	69
2	1	49/56 (88%)	48 (98%)	1 (2%)	48	76
3	0	62/66 (94%)	61 (98%)	1 (2%)	55	80
5	12	15/77 (20%)	15 (100%)	0	100	100
6	13	11/159 (7%)	11 (100%)	0	100	100
7	14	18/358 (5%)	17 (94%)	1 (6%)	19	44
8	2	47/53 (89%)	47 (100%)	0	100	100
9	4	39/50 (78%)	38 (97%)	1 (3%)	40	70
10	5	40/58 (69%)	38 (95%)	2 (5%)	22	48
11	6	39/40 (98%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	7	48/58 (83%)	47 (98%)	1 (2%)	47	75
13	8	31/35 (89%)	31 (100%)	0	100	100
14	9	16/54 (30%)	16 (100%)	0	100	100
17	D	214/218 (98%)	211 (99%)	3 (1%)	59	82
18	E	159/163 (98%)	154 (97%)	5 (3%)	35	65
19	F	174/177 (98%)	172 (99%)	2 (1%)	65	85
20	K	52/92 (56%)	51 (98%)	1 (2%)	50	77
21	L	59/102 (58%)	58 (98%)	1 (2%)	53	79
22	M	121/128 (94%)	121 (100%)	0	100	100
23	N	98/100 (98%)	97 (99%)	1 (1%)	68	86
24	O	87/117 (74%)	86 (99%)	1 (1%)	65	85
25	P	109/118 (92%)	108 (99%)	1 (1%)	70	87
26	Q	102/129 (79%)	99 (97%)	3 (3%)	37	67
27	R	76/90 (84%)	73 (96%)	3 (4%)	28	57
28	S	95/107 (89%)	94 (99%)	1 (1%)	65	85
29	T	91/93 (98%)	91 (100%)	0	100	100
30	U	88/92 (96%)	86 (98%)	2 (2%)	44	73
31	V	102/113 (90%)	102 (100%)	0	100	100
32	W	60/85 (71%)	59 (98%)	1 (2%)	53	79
33	X	73/89 (82%)	72 (99%)	1 (1%)	59	82
34	Y	69/159 (43%)	65 (94%)	4 (6%)	18	42
35	Z	59/69 (86%)	58 (98%)	1 (2%)	53	79
37	b	69/101 (68%)	68 (99%)	1 (1%)	59	82
38	c	75/137 (55%)	73 (97%)	2 (3%)	39	69
39	d	61/69 (88%)	59 (97%)	2 (3%)	33	63
40	e	59/77 (77%)	58 (98%)	1 (2%)	53	79
41	f	67/79 (85%)	65 (97%)	2 (3%)	36	66
42	g	62/69 (90%)	62 (100%)	0	100	100
43	h	42/146 (29%)	41 (98%)	1 (2%)	43	72
44	i	66/102 (65%)	65 (98%)	1 (2%)	57	81
45	j	92/111 (83%)	91 (99%)	1 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	k	49/197 (25%)	48 (98%)	1 (2%)	48	76
47	l	144/174 (83%)	142 (99%)	2 (1%)	59	82
48	m	85/132 (64%)	84 (99%)	1 (1%)	63	84
49	n	99/130 (76%)	96 (97%)	3 (3%)	36	66
50	o	109/112 (97%)	109 (100%)	0	100	100
52	10	24/28 (86%)	24 (100%)	0	100	100
53	p	64/75 (85%)	63 (98%)	1 (2%)	55	80
54	J	68/106 (64%)	67 (98%)	1 (2%)	57	81
All	All	3575/5230 (68%)	3516 (98%)	59 (2%)	52	79

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	59	THR
2	1	55	THR
3	0	47	VAL
7	14	79	LEU
9	4	46	CYS
10	5	27	ILE
10	5	28	SER
12	7	35	LYS
17	D	120	SER
17	D	157	SER
17	D	220	ASN
18	E	24	CYS
18	E	46	SER
18	E	86	GLU
18	E	107	ASP
18	E	150	SER
19	F	26	ILE
19	F	206	LEU
20	K	63	GLN
21	L	29	ILE
23	N	34	SER
24	O	118	THR
25	P	40	LYS
26	Q	68	SER
26	Q	77	LYS
26	Q	86	LYS

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Mol	Chain	Res	Type
27	R	45	ILE
27	R	80	THR
27	R	88	VAL
28	S	110	ILE
30	U	28	VAL
30	U	34	VAL
32	W	13	MET
33	X	23	SER
34	Y	6	LEU
34	Y	27	GLN
34	Y	49	VAL
34	Y	63	LEU
35	Z	66	VAL
37	b	36	VAL
38	c	3	THR
38	c	96	GLN
39	d	46	LYS
39	d	80	ILE
40	e	41	LYS
41	f	18	SER
41	f	54	ARG
43	h	20	THR
44	i	85	ILE
45	j	87	VAL
46	k	148	ILE
47	l	112	GLN
47	l	150	VAL
48	m	40	SER
49	n	81	VAL
49	n	147	GLN
49	n	156	LEU
53	p	41	SER
54	J	17	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	63	ASN
8	2	8	GLN
9	4	37	HIS
10	5	49	ASN
13	8	35	GLN

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Mol	Chain	Res	Type
13	8	37	GLN
18	E	124	HIS
21	L	21	HIS
22	M	52	HIS
22	M	58	ASN
25	P	61	GLN
26	Q	71	GLN
29	T	86	ASN
30	U	8	GLN
30	U	10	GLN
30	U	78	HIS
31	V	120	ASN
34	Y	27	GLN
45	j	25	ASN
47	l	50	GLN
47	l	67	GLN
48	m	131	ASN
49	n	6	ASN
50	o	52	ASN
52	10	3	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	A	2321/2889 (80%)	302 (13%)	15 (0%)
16	B	101/109 (92%)	23 (22%)	3 (2%)
36	a	1333/1534 (86%)	217 (16%)	0
All	All	3755/4532 (82%)	542 (14%)	18 (0%)

All (542) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	A	2	A
15	A	3	A
15	A	23	A
15	A	24	G
15	A	28	C
15	A	40	G
15	A	52	A
15	A	53	A
15	A	54	G

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Mol	Chain	Res	Type
15	A	60	A
15	A	63	A
15	A	64	G
15	A	80	C
15	A	81	A
15	A	106	A
15	A	107	A
15	A	108	U
15	A	119	G
15	A	132	C
15	A	134	G
15	A	135	A
15	A	136	C
15	A	142	A
15	A	144	U
15	A	159	A
15	A	174	A
15	A	177	A
15	A	183	U
15	A	184	U
15	A	193	G
15	A	194	A
15	A	200	A
15	A	211	A
15	A	226	G
15	A	253	G
15	A	270	G
15	A	275	G
15	A	279	A
15	A	280	U
15	A	281	A
15	A	282	G
15	A	286	U
15	A	307	G
15	A	329	A
15	A	333	U
15	A	347	G
15	A	348	A
15	A	364	C
15	A	365	A
15	A	396	U
15	A	409	G

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Mol	Chain	Res	Type
15	A	419	G
15	A	434	G
15	A	474	U
15	A	480	A
15	A	504	G
15	A	513	A
15	A	514	C
15	A	528	A
15	A	531	C
15	A	554	C
15	A	555	G
15	A	556	G
15	A	561	A
15	A	572	G
15	A	573	G
15	A	585	G
15	A	595	U
15	A	596	A
15	A	597	A
15	A	609	G
15	A	625	A
15	A	637	A
15	A	649	A
15	A	658	A
15	A	665	G
15	A	668	A
15	A	669	G
15	A	677	A
15	A	678	G
15	A	679	G
15	A	721	U
15	A	753	A
15	A	754	C
15	A	755	U
15	A	765	A
15	A	781	H2U
15	A	782	U
15	A	783	G
15	A	799	A
15	A	810	G
15	A	811	G
15	A	817	A

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Mol	Chain	Res	Type
15	A	819	G
15	A	820	G
15	A	827	A
15	A	840	G
15	A	847	C
15	A	862	U
15	A	863	U
15	A	880	A
15	A	881	U
15	A	882	G
15	A	893	G
15	A	900	G
15	A	901	A
15	A	904	G
15	A	907	U
15	A	909	G
15	A	910	A
15	A	911	U
15	A	944	A
15	A	946	C
15	A	964	U
15	A	967	C
15	A	974	A
15	A	978	A
15	A	979	G
15	A	994	G
15	A	1007	G
15	A	1013	A
15	A	1029	G
15	A	1045	U
15	A	1046	A
15	A	1068	A
15	A	1069	G
15	A	1072	A
15	A	1074	G
15	A	1076	A
15	A	1163	U
15	A	1164	A
15	A	1170	C
15	A	1177	A
15	A	1204	A
15	A	1235	A

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Mol	Chain	Res	Type
15	A	1239	A
15	A	1252	G
15	A	1253	C
15	A	1267	G
15	A	1282	A
15	A	1285	G
15	A	1300	G
15	A	1301	A
15	A	1305	A
15	A	1329	A
15	A	1330	A
15	A	1381	U
15	A	1394	A
15	A	1408	U
15	A	1412	A
15	A	1414	A
15	A	1433	A
15	A	1458	C
15	A	1463	A
15	A	1598	C
15	A	1603	A
15	A	1606	A
15	A	1643	U
15	A	1644	A
15	A	1646	A
15	A	1654	A
15	A	1668	A
15	A	1670	U
15	A	1683	U
15	A	1684	C
15	A	1710	G
15	A	1757	A
15	A	1767	A
15	A	1768	A
15	A	1773	G
15	A	1782	A
15	A	1791	C
15	A	1800	A
15	A	1808	G
15	A	1809	C
15	A	1810	A
15	A	1811	A

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Mol	Chain	Res	Type
15	A	1815	A
15	A	1826	G
15	A	1838	A
15	A	1842	C
15	A	1916	G
15	A	1936	U
15	A	1940	G
15	A	1947	A
15	A	1948	A
15	A	1965	U
15	A	1973	U
15	A	1974	G
15	A	1977	C
15	A	1980	A
15	A	1981	U
15	A	1982	G
15	A	2001	U
15	A	2002	G
15	A	2003	U
15	A	2030	A
15	A	2041	A
15	A	2042	G
15	A	2043	A
15	A	2053	C
15	A	2065	C
15	A	2066	G
15	A	2071	G
15	A	2072	A
15	A	2079	G
15	A	2202	G
15	A	2203	A
15	A	2208	A
15	A	2222	G
15	A	2226	A
15	A	2239	G
15	A	2240	G
15	A	2279	A
15	A	2280	G
15	A	2284	U
15	A	2288	A
15	A	2289	A
15	A	2298	C

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Mol	Chain	Res	Type
15	A	2319	C
15	A	2322	G
15	A	2324	G
15	A	2326	G
15	A	2334	A
15	A	2336	A
15	A	2337	A
15	A	2341	U
15	A	2348	C
15	A	2383	G
15	A	2384	A
15	A	2386	C
15	A	2391	U
15	A	2392	G
15	A	2426	A
15	A	2430	G
15	A	2431	A
15	A	2434	A
15	A	2435	A
15	A	2436	A
15	A	2440	A
15	A	2442	U
15	A	2446	2MG
15	A	2449	A
15	A	2492	U
15	A	2506	G
15	A	2509	G
15	A	2519	A
15	A	2530	G
15	A	2536	G
15	A	2548	U
15	A	2552	C
15	A	2567	A
15	A	2568	G
15	A	2574	C
15	A	2582	G
15	A	2586	U
15	A	2603	A
15	A	2604	G
15	A	2610	U
15	A	2614	U
15	A	2631	G

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Mol	Chain	Res	Type
15	A	2646	U
15	A	2657	U
15	A	2671	G
15	A	2683	C
15	A	2690	U
15	A	2703	G
15	A	2715	G
15	A	2727	C
15	A	2730	C
15	A	2734	U
15	A	2735	A
15	A	2737	G
15	A	2745	G
15	A	2749	A
15	A	2753	C
15	A	2759	A
15	A	2763	C
15	A	2765	A
15	A	2766	A
15	A	2767	G
15	A	2779	A
15	A	2780	U
15	A	2781	A
15	A	2790	A
15	A	2791	U
15	A	2798	G
15	A	2806	A
15	A	2807	A
15	A	2819	U
15	A	2821	A
15	A	2822	U
15	A	2842	G
15	A	2845	A
15	A	2852	A
15	A	2853	A
15	A	2858	A
15	A	2865	C
15	A	2868	A
15	A	2869	U
15	A	2870	A
15	A	2871	G
16	B	3	A

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Mol	Chain	Res	Type
16	B	7	G
16	B	9	U
16	B	10	U
16	B	11	A
16	B	12	U
16	B	22	G
16	B	23	A
16	B	25	C
16	B	33	U
16	B	49	G
16	B	50	A
16	B	55	A
16	B	62	A
16	B	64	G
16	B	81	G
16	B	86	A
16	B	92	A
16	B	98	G
16	B	99	G
16	B	100	A
16	B	101	C
16	B	102	G
36	a	9	G
36	a	32	A
36	a	39	G
36	a	47	C
36	a	48	U
36	a	50	A
36	a	51	A
36	a	52	C
36	a	61	G
36	a	65	A
36	a	66	G
36	a	71	A
36	a	73	C
36	a	74	A
36	a	98	U
36	a	99	G
36	a	111	A
36	a	118	C
36	a	121	A
36	a	123	C

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Mol	Chain	Res	Type
36	a	132	A
36	a	147	G
36	a	154	A
36	a	159	G
36	a	169	G
36	a	176	A
36	a	185	C
36	a	200	A
36	a	202	G
36	a	207	U
36	a	208	A
36	a	209	C
36	a	214	A
36	a	216	A
36	a	246	C
36	a	249	U
36	a	250	U
36	a	252	G
36	a	256	G
36	a	271	G
36	a	272	C
36	a	275	A
36	a	283	G
36	a	294	G
36	a	306	G
36	a	310	U
36	a	311	A
36	a	326	A
36	a	334	A
36	a	337	G
36	a	352	G
36	a	357	C
36	a	358	A
36	a	362	G
36	a	372	U
36	a	377	C
36	a	378	A
36	a	389	G
36	a	402	A
36	a	403	A
36	a	411	G
36	a	416	A

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Mol	Chain	Res	Type
36	a	417	A
36	a	418	G
36	a	422	G
36	a	424	C
36	a	433	U
36	a	443	U
36	a	452	G
36	a	457	A
36	a	458	A
36	a	461	G
36	a	462	G
36	a	464	G
36	a	468	C
36	a	469	G
36	a	479	U
36	a	482	A
36	a	483	A
36	a	490	G
36	a	492	A
36	a	493	A
36	a	494	G
36	a	502	A
36	a	506	G
36	a	507	C
36	a	508	U
36	a	512	U
36	a	518	C
36	a	524	G
36	a	535	A
36	a	544	G
36	a	547	A
36	a	559	A
36	a	564	U
36	a	572	A
36	a	573	A
36	a	576	G
36	a	577	G
36	a	618	C
36	a	630	C
36	a	631	C
36	a	632	U
36	a	633	G

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Mol	Chain	Res	Type
36	a	639	G
36	a	653	U
36	a	665	C
36	a	688	G
36	a	703	G
36	a	704	A
36	a	721	G
36	a	722	A
36	a	748	G
36	a	749	A
36	a	755	A
36	a	790	A
36	a	793	U
36	a	794	A
36	a	815	A
36	a	817	C
36	a	821	7MG
36	a	830	G
36	a	852	C
36	a	855	C
36	a	857	A
36	a	901	C
36	a	913	A
36	a	925	G
36	a	926	G
36	a	930	C
36	a	933	C
36	a	934	A
36	a	935	C
36	a	941	G
36	a	959	U
36	a	965	2MG
36	a	968	A
36	a	970	G
36	a	974	G
36	a	975	G
36	a	976	A
36	a	992	G
36	a	1051	C
36	a	1061	G
36	a	1064	A
36	a	1065	G

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Mol	Chain	Res	Type
36	a	1066	C
36	a	1103	G
36	a	1126	U
36	a	1138	C
36	a	1139	U
36	a	1140	G
36	a	1142	G
36	a	1144	A
36	a	1147	C
36	a	1148	U
36	a	1150	C
36	a	1151	C
36	a	1152	G
36	a	1153	A
36	a	1154	G
36	a	1175	G
36	a	1176	G
36	a	1194	A
36	a	1195	A
36	a	1209	U
36	a	1210	U
36	a	1211	A
36	a	1212	C
36	a	1226	C
36	a	1234	A
36	a	1236	A
36	a	1238	U
36	a	1245	G
36	a	1248	A
36	a	1250	A
36	a	1256	G
36	a	1276	G
36	a	1278	A
36	a	1293	C
36	a	1296	A
36	a	1299	U
36	a	1302	G
36	a	1319	C
36	a	1320	G
36	a	1328	G
36	a	1329	A
36	a	1344	G

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Mol	Chain	Res	Type
36	a	1350	G
36	a	1362	U
36	a	1368	G
36	a	1377	G
36	a	1384	G
36	a	1395	C
36	a	1396	A
36	a	1402	5MC
36	a	1409	C
36	a	1417	G
36	a	1422	G
36	a	1423	G
36	a	1436	C
36	a	1452	G
36	a	1453	C
36	a	1460	G
36	a	1461	U
36	a	1462	A
36	a	1463	A
36	a	1468	G
36	a	1488	A
36	a	1493	G
36	a	1495	U
36	a	1505	G
36	a	1506	G
36	a	1507	MA6
36	a	1518	G
36	a	1519	G
36	a	1520	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	A	133	U
15	A	285	C
15	A	677	A
15	A	748	G
15	A	781	H2U
15	A	819	G
15	A	906	U
15	A	1244	G
15	A	1255	A

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Mol	Chain	Res	Type
15	A	1282	A
15	A	1319	C
15	A	2045	G
15	A	2221	C
15	A	2581	PSU
15	A	2670	U
16	B	49	G
16	B	54	U
16	B	61	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	2MA	A	2504	55,56,15	22,25,26	3.98	8 (36%)	32,37,40	2.81	10 (31%)
15	OMG	A	2252	15	23,26,27	0.57	0	32,38,41	0.46	0
15	OMU	A	2450	15	19,22,23	2.96	8 (42%)	25,31,34	1.82	4 (16%)
15	PSU	A	2606	15	18,21,22	1.06	1 (5%)	21,30,33	2.02	4 (19%)
36	5MC	a	1402	36	19,22,23	0.61	0	26,32,35	0.83	0
36	MA6	a	1508	36	23,26,27	1.44	4 (17%)	33,38,41	3.76	12 (36%)
36	UR3	a	1487	36	19,22,23	2.89	5 (26%)	26,32,35	1.66	4 (15%)
15	H2U	A	2620	15	18,21,22	0.76	0	19,30,33	0.93	1 (5%)
15	6MA	A	2067	55,15	21,24,25	0.14	0	27,34,37	0.33	0
15	H2U	A	876	15	18,21,22	0.56	0	19,30,33	0.81	1 (5%)
15	5MC	A	1972	15	19,22,23	0.62	0	26,32,35	0.65	0
36	4OC	a	1400	36	20,23,24	3.08	8 (40%)	25,32,35	0.96	1 (4%)
15	H2U	A	781	15	18,21,22	0.54	0	19,30,33	0.94	1 (5%)
36	2MG	a	1408	36	23,26,27	0.46	0	33,38,41	0.48	0
15	5OC	A	2502	56,15	18,21,22	4.60	13 (72%)	24,30,33	1.20	3 (12%)
15	5MU	A	1949	15	19,22,23	0.60	0	27,32,35	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	5OC	a	276	36	18,21,22	4.79	14 (77%)	24,30,33	1.08	1 (4%)
36	PSU	a	954	36	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
15	5MC	A	1935	15	19,22,23	0.53	0	26,32,35	0.59	0
15	PSU	A	2581	15	18,21,22	1.06	1 (5%)	21,30,33	2.17	7 (33%)
15	MA6	A	2068	15	23,26,27	1.49	4 (17%)	33,38,41	3.65	11 (33%)
15	6MA	A	2069	15	21,24,25	0.32	0	27,34,37	0.40	0
36	2MG	a	965	36	23,26,27	0.48	0	33,38,41	0.61	0
36	MA6	a	1507	36	23,26,27	1.44	4 (17%)	33,38,41	3.59	11 (33%)
36	7MG	a	821	36	23,26,27	1.10	1 (4%)	27,39,42	0.91	2 (7%)
15	2MG	A	2446	15	23,26,27	0.63	0	33,38,41	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	2MA	A	2504	55,56,15	-	1/7/25/26	0/3/3/3
15	OMG	A	2252	15	-	1/9/27/28	0/3/3/3
15	OMU	A	2450	15	-	0/9/27/28	0/2/2/2
15	PSU	A	2606	15	-	0/7/25/26	0/2/2/2
36	5MC	a	1402	36	-	2/7/25/26	0/2/2/2
36	MA6	a	1508	36	-	2/11/29/30	0/3/3/3
36	UR3	a	1487	36	-	0/7/25/26	0/2/2/2
15	H2U	A	2620	15	-	0/7/38/39	0/2/2/2
15	6MA	A	2067	55,15	-	2/9/23/24	0/3/3/3
15	H2U	A	876	15	-	0/7/38/39	0/2/2/2
15	5MC	A	1972	15	-	0/7/25/26	0/2/2/2
36	4OC	a	1400	36	-	2/9/29/30	0/2/2/2
15	H2U	A	781	15	-	0/7/38/39	0/2/2/2
36	2MG	a	1408	36	-	0/9/27/28	0/3/3/3
15	5OC	A	2502	56,15	-	0/7/21/22	0/2/2/2
15	5MU	A	1949	15	-	0/7/25/26	0/2/2/2
36	5OC	a	276	36	-	0/7/21/22	0/2/2/2
36	PSU	a	954	36	-	2/7/25/26	0/2/2/2
15	5MC	A	1935	15	-	2/7/25/26	0/2/2/2
15	PSU	A	2581	15	-	0/7/25/26	0/2/2/2
15	MA6	A	2068	15	-	0/11/29/30	0/3/3/3
15	6MA	A	2069	15	-	2/9/23/24	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	2MG	a	965	36	-	2/9/27/28	0/3/3/3
36	MA6	a	1507	36	-	2/11/29/30	0/3/3/3
36	7MG	a	821	36	-	0/7/37/38	0/3/3/3
15	2MG	A	2446	15	-	2/9/27/28	0/3/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	2504	2MA	C4-N3	12.26	1.50	1.34
15	A	2502	5OC	C2'-C3'	-8.96	1.30	1.52
36	a	276	5OC	C2'-C3'	-8.92	1.30	1.52
36	a	276	5OC	C6-C5	8.81	1.48	1.35
15	A	2502	5OC	C6-C5	8.69	1.48	1.35
36	a	1487	UR3	C2-N1	8.03	1.49	1.38
15	A	2504	2MA	C2-N3	7.92	1.47	1.34
36	a	1400	4OC	C4-N3	7.00	1.44	1.32
15	A	2450	OMU	C2-N1	6.87	1.49	1.38
36	a	1487	UR3	C6-C5	6.74	1.50	1.35
15	A	2504	2MA	C6-N1	6.41	1.43	1.35
15	A	2450	OMU	C2-N3	6.40	1.49	1.38
36	a	276	5OC	C2-N3	6.25	1.48	1.36
15	A	2502	5OC	O4'-C1'	-6.21	1.28	1.42
36	a	276	5OC	C4-N3	6.20	1.44	1.34
36	a	276	5OC	O4'-C1'	-5.77	1.29	1.42
36	a	1400	4OC	C4-N4	5.75	1.47	1.36
36	a	1400	4OC	C6-C5	5.62	1.48	1.35
15	A	2450	OMU	C6-C5	5.54	1.47	1.35
15	A	2504	2MA	C2-N1	5.53	1.43	1.34
36	a	1400	4OC	C2-N3	5.51	1.47	1.36
36	a	1487	UR3	C2-N3	5.50	1.49	1.39
15	A	2502	5OC	C2-N3	5.46	1.47	1.36
15	A	2502	5OC	C4-N3	5.32	1.42	1.34
36	a	276	5OC	C4-N4	4.95	1.46	1.34
36	a	276	5OC	O4'-C4'	4.94	1.56	1.45
15	A	2502	5OC	C4-N4	4.64	1.46	1.34
36	a	821	7MG	C5-N7	4.53	1.41	1.35
15	A	2504	2MA	C5-C6	4.50	1.53	1.41
36	a	1400	4OC	C2-N1	4.48	1.49	1.40
36	a	276	5OC	C2-N1	4.39	1.49	1.40
15	A	2502	5OC	O4'-C4'	4.25	1.54	1.45
36	a	276	5OC	C2'-C1'	4.18	1.63	1.52
15	A	2502	5OC	C2'-C1'	4.13	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	276	5OC	C6-N1	4.11	1.45	1.38
15	A	2502	5OC	C5'-C4'	-4.08	1.39	1.51
36	a	1507	MA6	C6-N6	3.98	1.47	1.36
36	a	1508	MA6	C6-N6	3.97	1.47	1.36
15	A	2502	5OC	C2-N1	3.82	1.48	1.40
15	A	2068	MA6	C6-N6	3.81	1.47	1.36
15	A	2504	2MA	C5-N7	-3.81	1.32	1.39
15	A	2450	OMU	C4-N3	3.79	1.45	1.38
15	A	2502	5OC	C6-N1	3.75	1.44	1.38
36	a	276	5OC	C5'-C4'	-3.65	1.40	1.51
15	A	2504	2MA	CM2-C2	3.48	1.59	1.49
15	A	2450	OMU	O4-C4	-3.39	1.17	1.24
36	a	954	PSU	C6-C5	3.30	1.38	1.35
36	a	276	5OC	C5-C4	3.30	1.49	1.42
36	a	1400	4OC	C5-C4	3.20	1.48	1.41
15	A	2502	5OC	C5-C4	3.18	1.49	1.42
15	A	2606	PSU	C6-C5	3.14	1.38	1.35
15	A	2581	PSU	C6-C5	3.09	1.38	1.35
15	A	2068	MA6	C5-C4	-3.07	1.33	1.39
36	a	1400	4OC	C6-N1	3.02	1.45	1.38
36	a	1508	MA6	C5-C4	-2.98	1.33	1.39
36	a	276	5OC	O3'-C3'	2.95	1.49	1.43
15	A	2450	OMU	O2-C2	-2.94	1.17	1.23
15	A	2068	MA6	C5-N7	-2.94	1.33	1.39
36	a	1507	MA6	C5-C4	-2.85	1.34	1.39
36	a	1507	MA6	C5-N7	-2.79	1.34	1.39
15	A	2502	5OC	O3'-C3'	2.72	1.49	1.43
15	A	2450	OMU	C6-N1	2.66	1.44	1.38
15	A	2504	2MA	C6-N6	-2.60	1.27	1.34
36	a	1508	MA6	C5-N7	-2.60	1.34	1.39
15	A	2068	MA6	C8-N9	-2.49	1.33	1.37
36	a	1487	UR3	C6-N1	2.41	1.43	1.38
36	a	276	5OC	O5-C5	2.40	1.40	1.33
36	a	1507	MA6	C8-N9	-2.35	1.33	1.37
36	a	1508	MA6	C8-N9	-2.33	1.33	1.37
36	a	1487	UR3	C4-N3	2.27	1.45	1.40
36	a	1400	4OC	O2-C2	-2.12	1.19	1.23
15	A	2450	OMU	C5-C4	2.09	1.48	1.43

All (77) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	1508	MA6	N1-C6-N6	-14.51	99.17	116.86
15	A	2068	MA6	N1-C6-N6	-13.84	100.00	116.86
36	a	1507	MA6	N1-C6-N6	-13.52	100.38	116.86
36	a	1508	MA6	C5-C6-N6	10.04	141.22	125.33
15	A	2068	MA6	C5-C6-N6	9.44	140.27	125.33
36	a	1507	MA6	C5-C6-N6	9.21	139.91	125.33
15	A	2504	2MA	C5-C4-N3	-9.09	117.60	127.18
15	A	2504	2MA	N3-C4-N9	6.30	134.99	126.99
36	a	1487	UR3	C4-N3-C2	-5.78	119.93	124.58
36	a	1508	MA6	N1-C2-N3	-5.73	119.91	128.58
36	a	1507	MA6	N1-C2-N3	-5.58	120.13	128.58
15	A	2450	OMU	C4-N3-C2	-5.56	119.71	126.61
15	A	2504	2MA	C4-N9-C1'	-5.44	113.91	126.63
15	A	2504	2MA	C1'-N9-C8	5.37	139.02	127.09
36	a	1507	MA6	C5-C4-N3	-5.36	119.34	126.72
15	A	2068	MA6	C5-C4-N3	-5.30	119.42	126.72
15	A	2068	MA6	N1-C2-N3	-5.26	120.63	128.58
15	A	2606	PSU	C4-N3-C2	-5.25	119.14	126.37
15	A	2581	PSU	C4-N3-C2	-5.17	119.24	126.37
15	A	2581	PSU	N1-C2-N3	5.16	120.61	115.17
15	A	2606	PSU	N1-C2-N3	5.11	120.56	115.17
36	a	954	PSU	N1-C2-N3	5.00	120.44	115.17
36	a	1508	MA6	C5-C4-N3	-4.81	120.09	126.72
36	a	954	PSU	C4-N3-C2	-4.74	119.85	126.37
15	A	2068	MA6	C4-C5-C6	4.65	120.72	115.91
36	a	1507	MA6	C4-C5-C6	4.62	120.69	115.91
36	a	1508	MA6	N9-C8-N7	-4.38	107.72	113.94
15	A	2450	OMU	N3-C2-N1	4.07	120.19	114.89
15	A	2068	MA6	N9-C8-N7	-4.05	108.20	113.94
36	a	1507	MA6	N9-C8-N7	-3.97	108.31	113.94
36	a	1508	MA6	C4-C5-C6	3.87	119.91	115.91
36	a	1487	UR3	C5-C4-N3	3.73	119.95	115.04
15	A	2450	OMU	C5-C4-N3	3.60	119.84	114.80
36	a	1507	MA6	N3-C4-N9	3.59	133.27	127.17
36	a	1508	MA6	C2-N1-C6	3.53	120.44	111.83
15	A	2068	MA6	N3-C4-N9	3.52	133.16	127.17
15	A	2504	2MA	N9-C8-N7	-3.48	108.99	113.94
36	a	1507	MA6	C2-N3-C4	3.43	120.20	111.83
15	A	2504	2MA	N3-C2-N1	-3.38	119.81	125.77
36	a	1508	MA6	C2-N3-C4	3.36	120.04	111.83
36	a	1507	MA6	C2-N1-C6	3.32	119.94	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	2068	MA6	C2-N1-C6	3.24	119.75	111.83
15	A	2068	MA6	C2-N3-C4	3.24	119.74	111.83
36	a	954	PSU	O2-C2-N1	-3.18	119.51	122.79
15	A	2504	2MA	C6-C5-C4	3.03	121.32	117.18
36	a	1508	MA6	C5-N7-C8	2.94	108.08	103.45
36	a	1508	MA6	N3-C4-N9	2.92	132.14	127.17
36	a	276	5OC	O5-C5-C4	2.89	120.84	114.82
15	A	2068	MA6	C5-N7-C8	2.85	107.92	103.45
36	a	1507	MA6	C5-N7-C8	2.83	107.90	103.45
36	a	954	PSU	C6-N1-C2	-2.80	120.09	122.69
15	A	2581	PSU	O2-C2-N1	-2.79	119.91	122.79
15	A	2504	2MA	C5-N7-C8	2.74	107.75	103.45
15	A	2502	5OC	O5-C5-C4	2.71	120.47	114.82
15	A	2606	PSU	O2-C2-N1	-2.71	120.00	122.79
15	A	2450	OMU	O4-C4-C5	-2.70	120.50	125.16
15	A	2502	5OC	C2'-C3'-C4'	2.70	108.28	102.80
36	a	1508	MA6	C4-N9-C8	2.54	108.40	105.74
36	a	1487	UR3	C6-N1-C2	-2.52	119.74	121.80
15	A	2620	H2U	C5-C4-N3	-2.48	114.05	116.69
36	a	1400	4OC	C6-C5-C4	2.40	119.89	117.00
15	A	2504	2MA	CM2-C2-N3	2.37	120.67	117.13
36	a	821	7MG	C5-C4-N9	2.36	109.36	106.33
15	A	2581	PSU	C6-N1-C2	-2.35	120.51	122.69
15	A	781	H2U	C5-C4-N3	-2.33	114.21	116.69
15	A	2581	PSU	O3'-C3'-C2'	2.29	119.15	111.82
15	A	876	H2U	C5-C4-N3	-2.27	114.27	116.69
15	A	2068	MA6	C4-N9-C8	2.27	108.12	105.74
36	a	821	7MG	C4-C5-N7	2.27	108.06	105.38
15	A	2581	PSU	O3'-C3'-C4'	2.26	117.58	111.08
36	a	1508	MA6	C4-C5-N7	-2.22	108.04	110.58
36	a	1507	MA6	C4-N9-C8	2.18	108.03	105.74
15	A	2581	PSU	O2'-C2'-C1'	-2.15	106.11	111.21
15	A	2504	2MA	N6-C6-N1	2.12	119.89	117.03
36	a	1487	UR3	C1'-N1-C2	2.12	120.51	117.04
15	A	2606	PSU	C6-N1-C2	-2.09	120.75	122.69
15	A	2502	5OC	C3'-C2'-C1'	2.01	107.53	102.60

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	2067	6MA	N1-C6-N6-C1

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Mol	Chain	Res	Type	Atoms
15	A	2252	OMG	C1'-C2'-O2'-CM2
36	a	1507	MA6	O4'-C4'-C5'-O5'
36	a	1507	MA6	C3'-C4'-C5'-O5'
15	A	1935	5MC	O4'-C4'-C5'-O5'
15	A	2446	2MG	C3'-C4'-C5'-O5'
36	a	954	PSU	O4'-C4'-C5'-O5'
36	a	1400	4OC	O4'-C4'-C5'-O5'
36	a	954	PSU	C3'-C4'-C5'-O5'
36	a	1400	4OC	C3'-C4'-C5'-O5'
36	a	1402	5MC	C3'-C4'-C5'-O5'
36	a	1508	MA6	O4'-C4'-C5'-O5'
15	A	1935	5MC	C3'-C4'-C5'-O5'
36	a	965	2MG	O4'-C4'-C5'-O5'
36	a	1402	5MC	O4'-C4'-C5'-O5'
15	A	2446	2MG	O4'-C4'-C5'-O5'
36	a	965	2MG	C3'-C4'-C5'-O5'
15	A	2069	6MA	C2'-C1'-N9-C4
15	A	2069	6MA	O4'-C1'-N9-C4
15	A	2067	6MA	C5-C6-N6-C1
36	a	1508	MA6	C3'-C4'-C5'-O5'
15	A	2504	2MA	C4'-C5'-O5'-P

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	2252	OMG	1	0
15	A	2450	OMU	2	0
15	A	2620	H2U	1	0
15	A	2067	6MA	1	0
15	A	876	H2U	1	0
15	A	2502	5OC	1	0
15	A	1949	5MU	1	0
36	a	276	5OC	1	0
15	A	2581	PSU	1	0
15	A	2069	6MA	1	0
36	a	965	2MG	1	0
36	a	1507	MA6	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 178 ligands modelled in this entry, 178 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



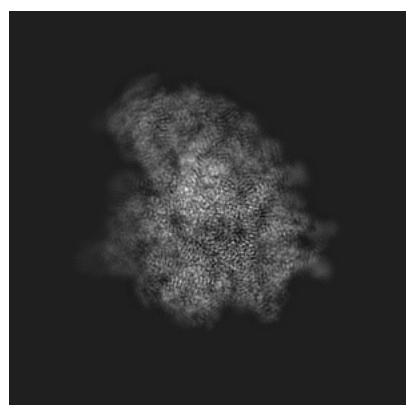
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52640. These allow visual inspection of the internal detail of the map and identification of artifacts.

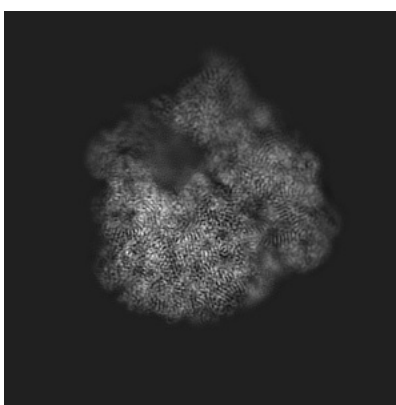
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

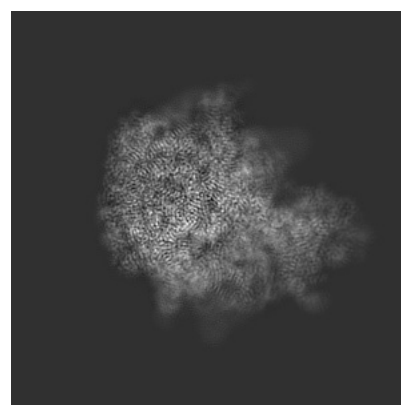
#### 6.1.1 Primary map



X



Y

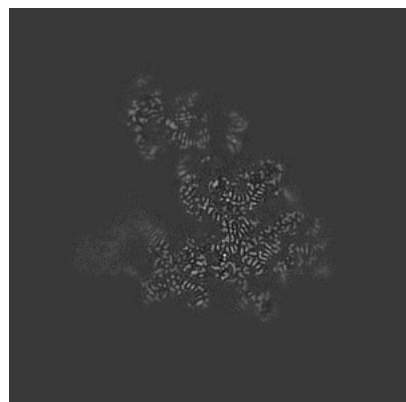


Z

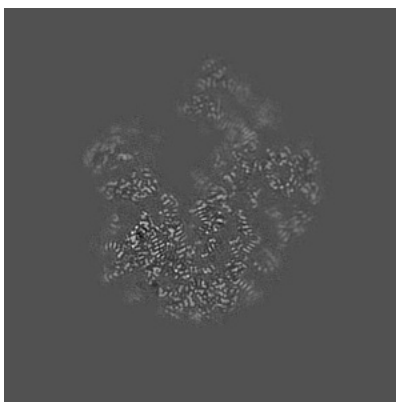
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

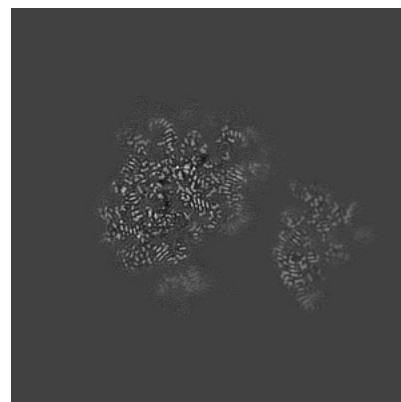
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

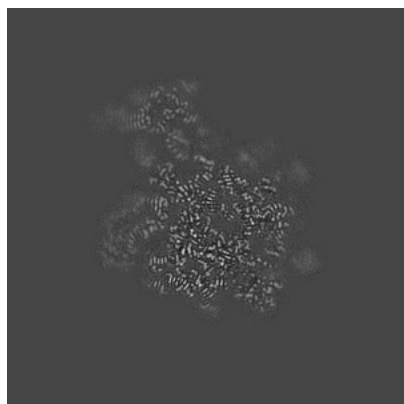


Z Index: 220

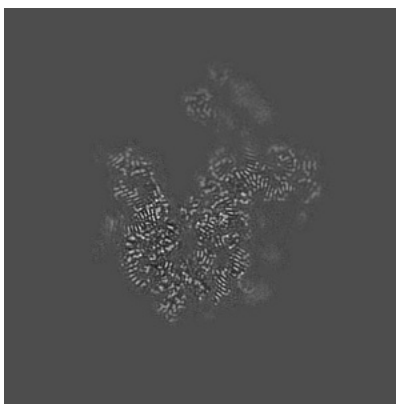
The images above show central slices of the map in three orthogonal directions.

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

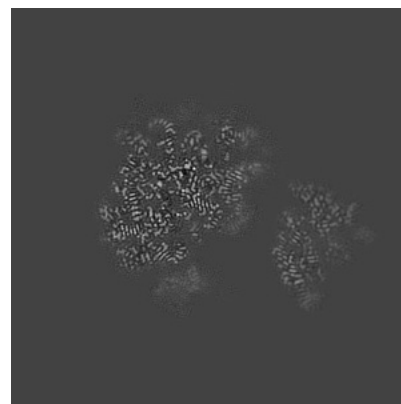
### 6.3.1 Primary map



X Index: 175



Y Index: 233

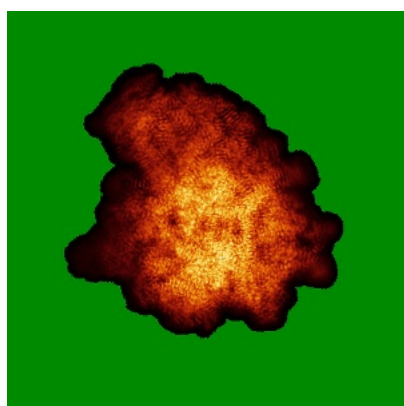


Z Index: 219

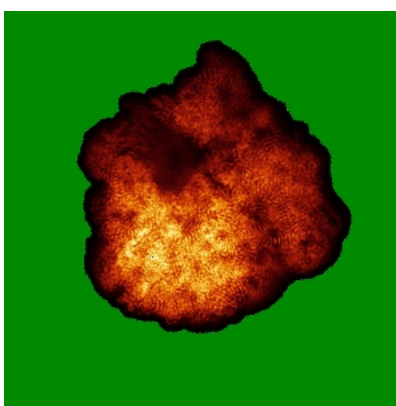
The images above show the largest variance slices of the map in three orthogonal directions.

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

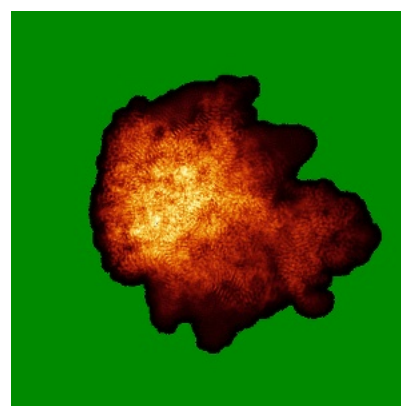
### 6.4.1 Primary map



X



Y



Z

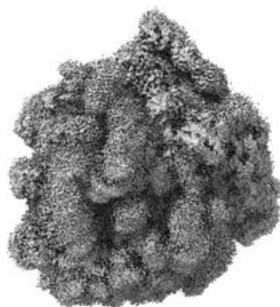
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



Z

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

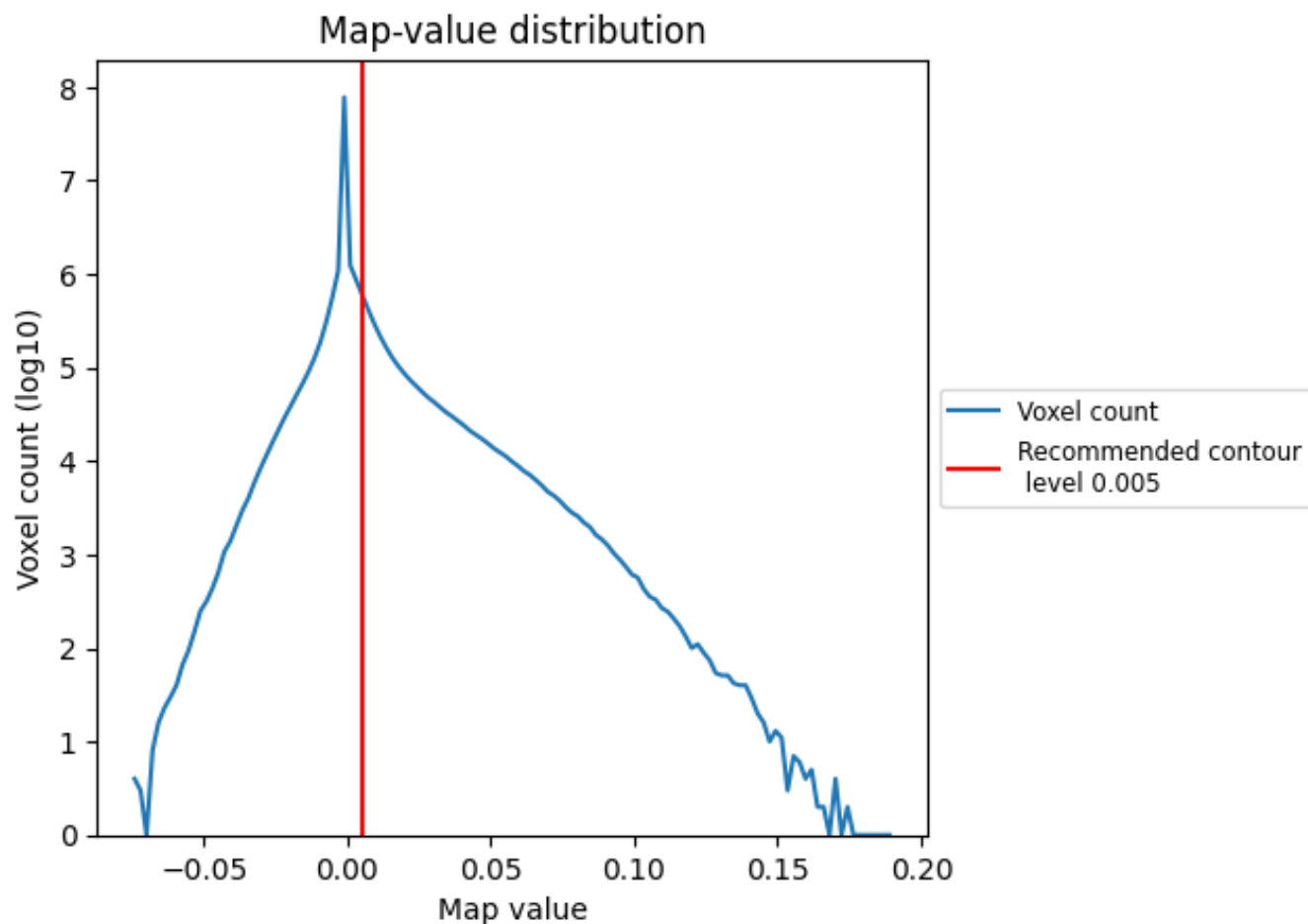
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

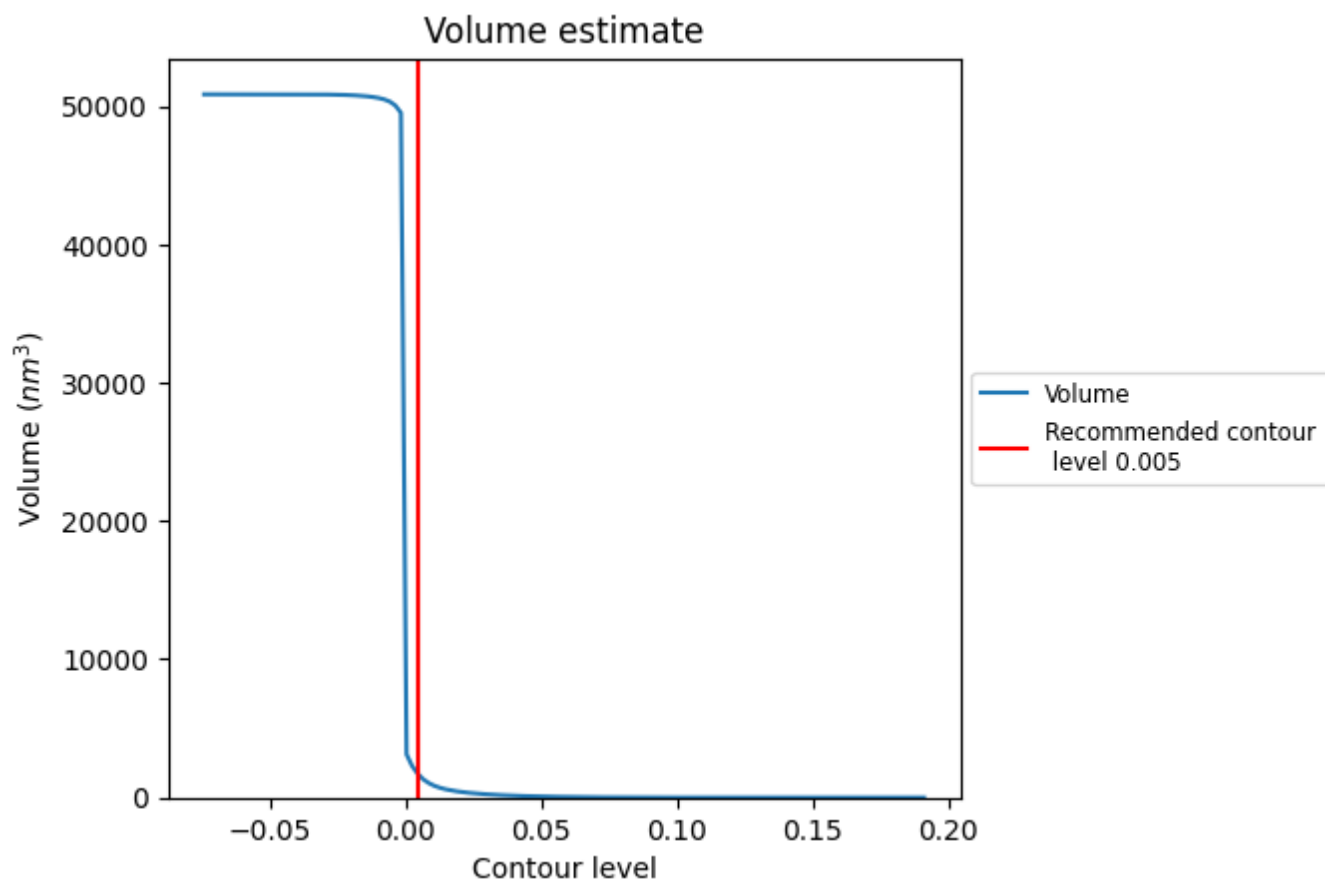
This section contains the results of statistical analysis of the map.

### 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.

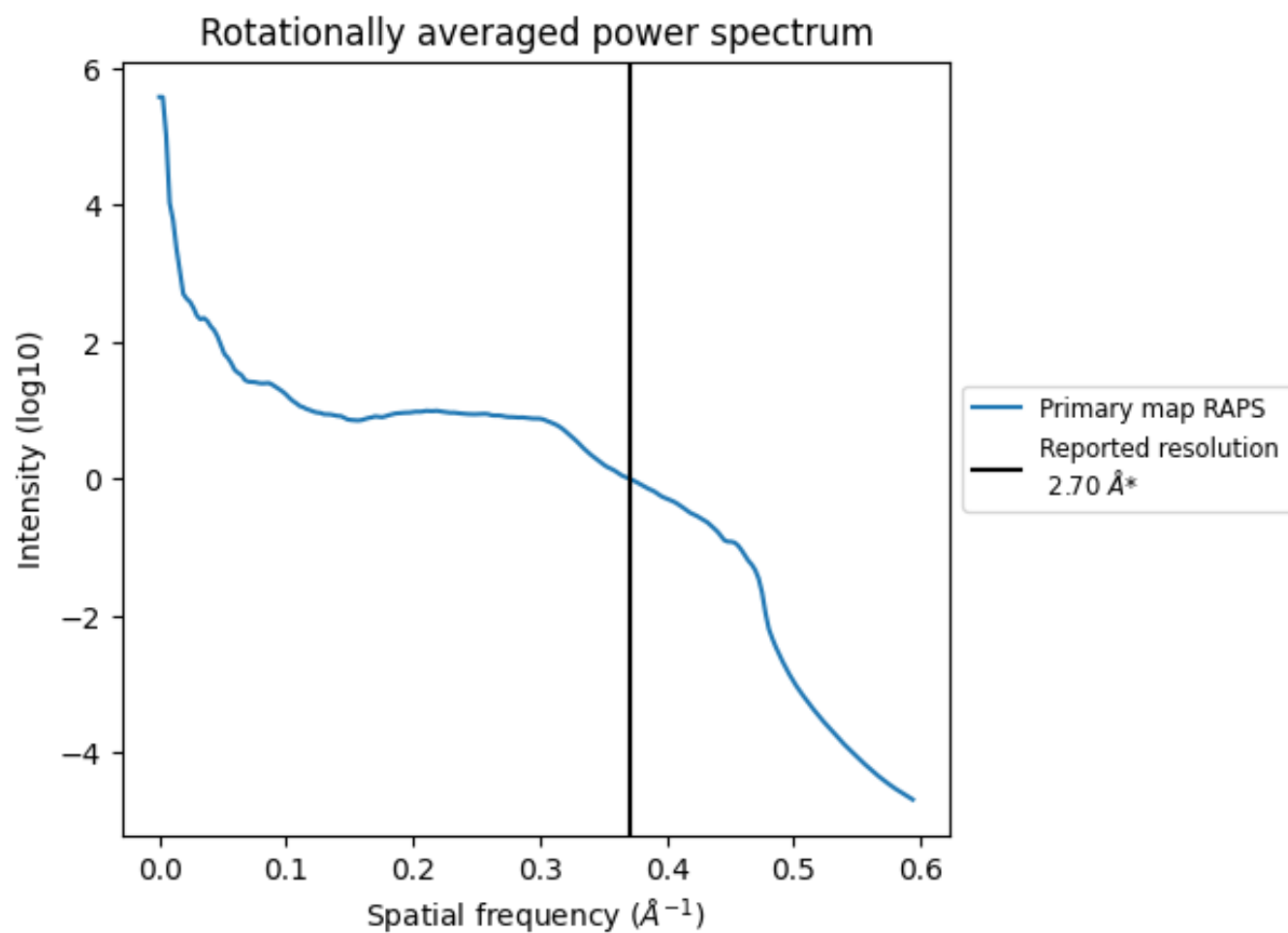
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1632  $\text{nm}^3$ ; this corresponds to an approximate mass of 1474 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 0.370 Å<sup>-1</sup>

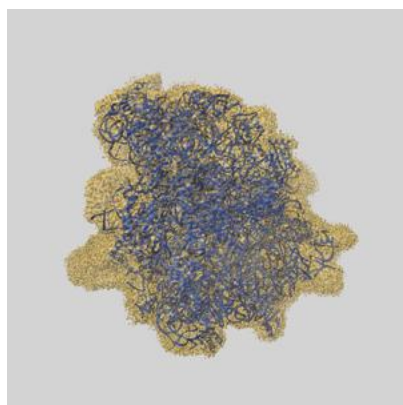
## 8 Fourier-Shell correlation

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

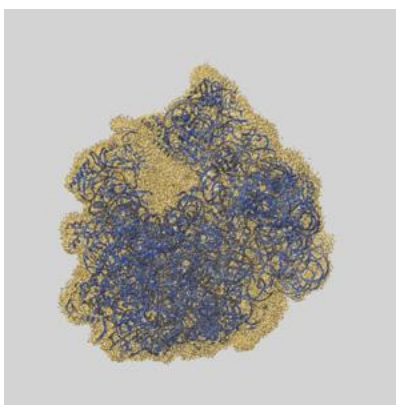
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52640 and PDB model 9I5V. Per-residue inclusion information can be found in section 3 on page 16.

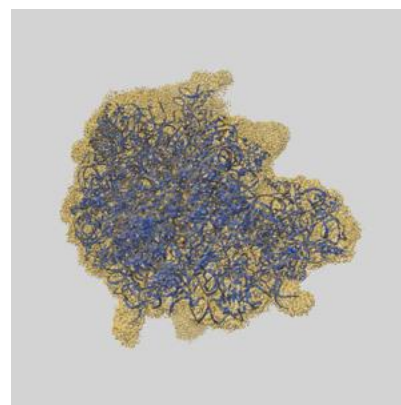
### 9.1 Map-model overlay [i](#)



X



Y

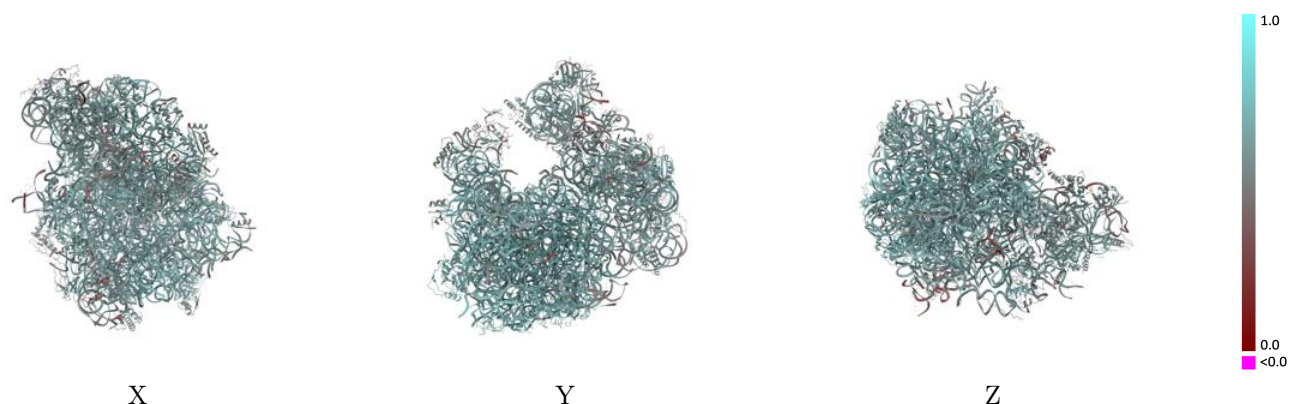


Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

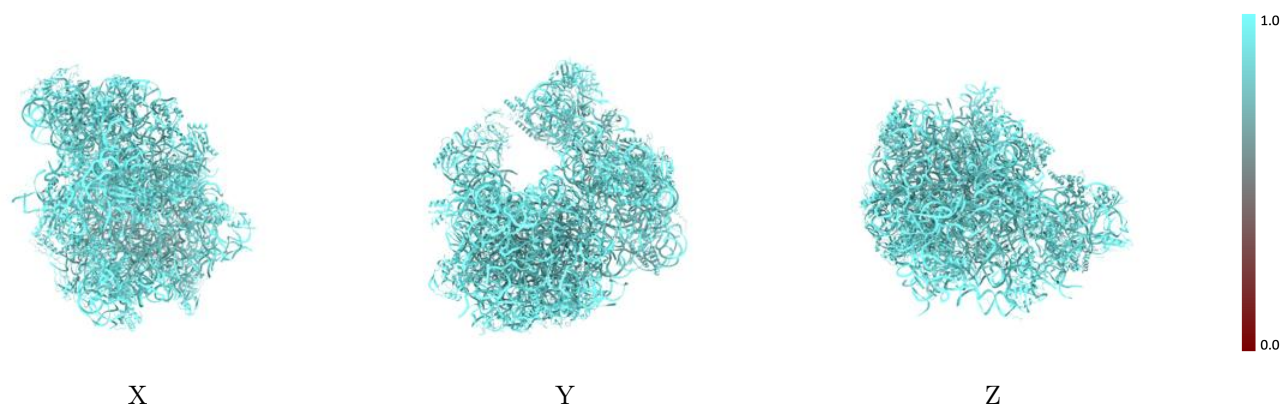


## 9.2 Q-score mapped to coordinate model [i](#)



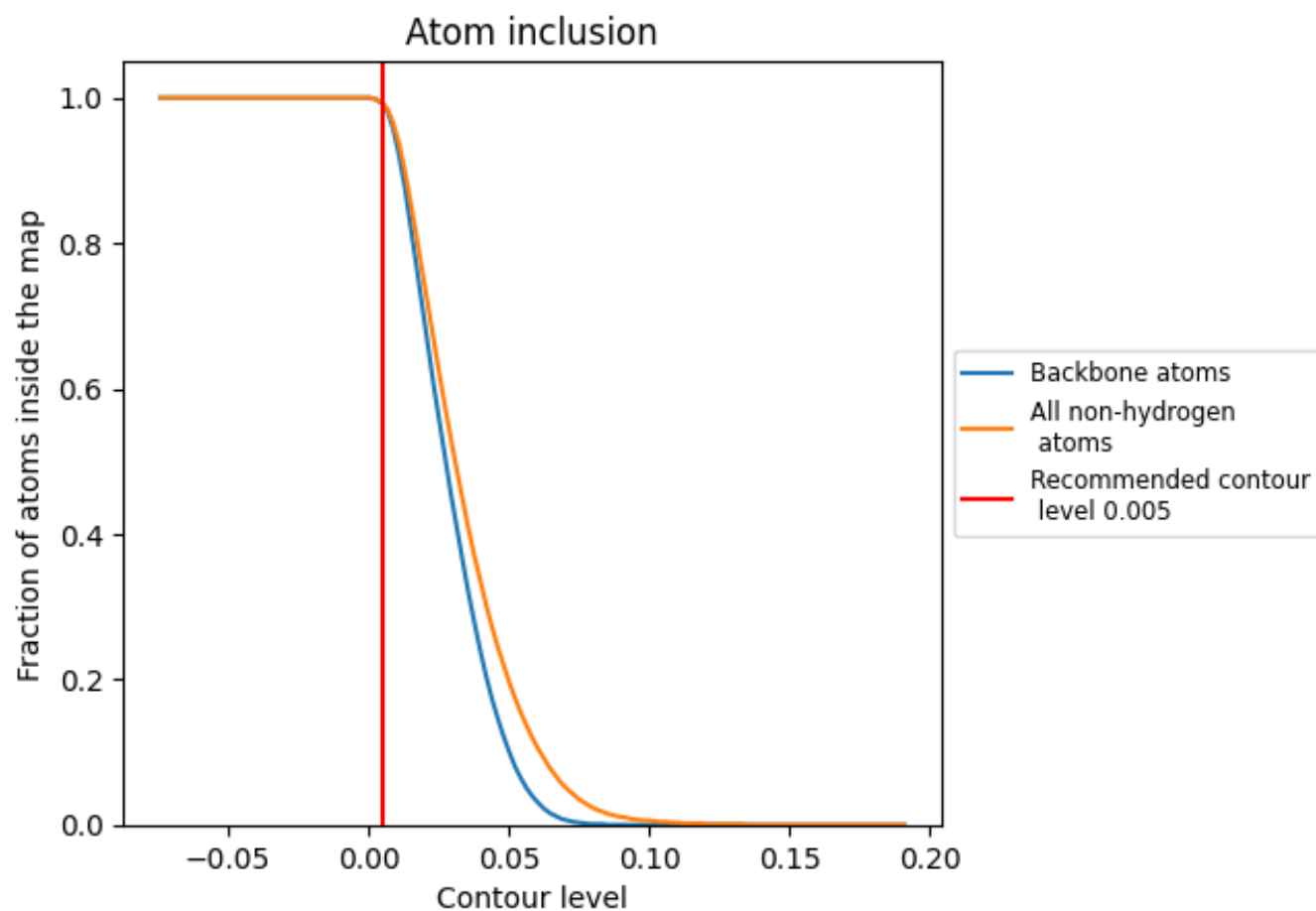
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ









































The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9930	 0.6300
0	 0.9980	 0.6730
1	 0.9980	 0.6240
10	 0.9870	 0.6250
11	 0.9860	 0.4730
12	 0.9860	 0.4790
13	 0.9840	 0.4970
14	 0.9280	 0.5040
15	 0.9880	 0.4960
2	 1.0000	 0.6860
4	 1.0000	 0.6800
5	 0.9920	 0.6430
6	 0.9970	 0.7080
7	 0.9880	 0.6500
8	 1.0000	 0.6380
9	 0.9390	 0.5430
A	 0.9980	 0.6600
B	 0.9950	 0.5740
D	 0.9960	 0.6850
E	 0.9930	 0.6900
F	 0.9960	 0.6720
I	 0.9900	 0.5850
J	 0.9880	 0.5920
K	 0.9820	 0.5830
L	 0.9790	 0.5420
M	 0.9960	 0.6880
N	 0.9900	 0.6710
O	 0.9910	 0.6340
P	 0.9920	 0.6560
Q	 0.9960	 0.6940
R	 0.9850	 0.5770
S	 0.9940	 0.6700
T	 0.9980	 0.7070
U	 0.9930	 0.6730
V	 0.9990	 0.6980



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Chain	Atom inclusion	Q-score
W	 0.9940	 0.6450
X	 0.9960	 0.6460
Y	 0.9930	 0.6000
Z	 0.9960	 0.6870
a	 0.9920	 0.5880
b	 0.9870	 0.5500
c	 0.9880	 0.5780
d	 0.9880	 0.6020
e	 0.9880	 0.6030
f	 0.9930	 0.5970
g	 0.9460	 0.6130
h	 0.9950	 0.5960
i	 0.9890	 0.5870
j	 0.9840	 0.6140
k	 0.9420	 0.5660
l	 0.9800	 0.5640
m	 0.9790	 0.5520
n	 0.9840	 0.5830
o	 0.9890	 0.6220
p	 0.9920	 0.6160