



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 05:57 am BST

PDB ID : 9R3A / pdb_00009r3a
EMDB ID : EMD-53553
Title : Structure of Stalled Beta-Galactosidase 70S Ribosome Nascent Chain
Authors : Jurkeviciute, G.; He, J.Z.; Enchev, R.I.
Deposited on : 2025-05-03
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

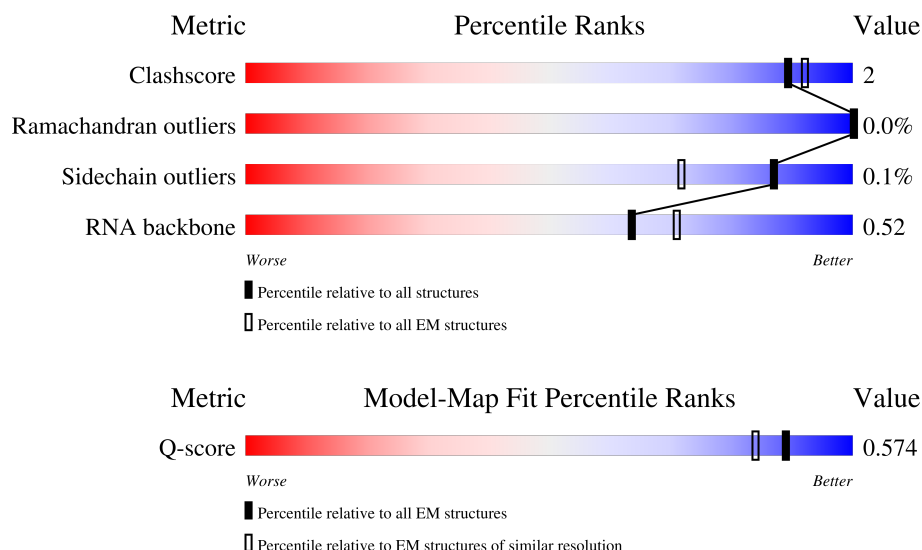
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	 89% 11%
2	1	46	 100%
3	2	65	 91% 8% .

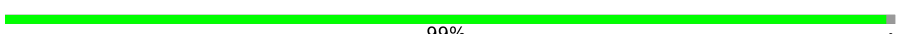
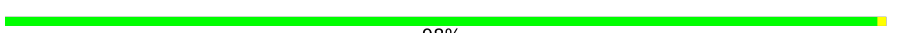
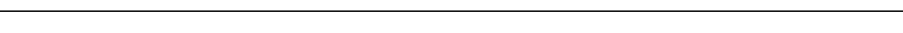
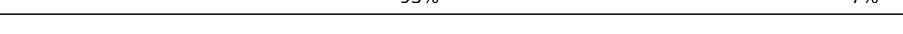
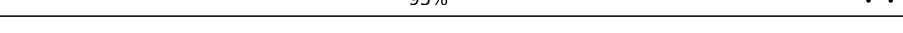
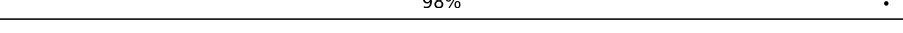
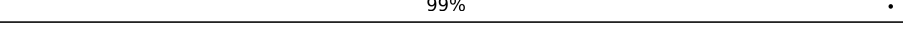
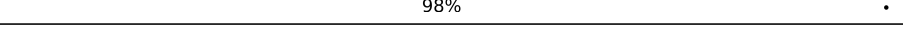
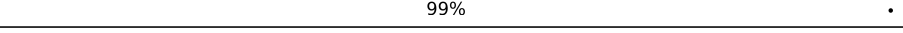
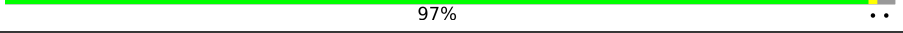
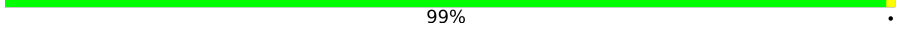
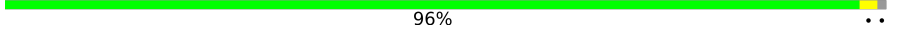
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Mol	Chain	Length	Quality of chain
4	3	38	100%
5	4	70	86% 14%
6	5	2	50% 50%
7	6	56	98% .
8	A	1543	73% 20% 5% .
9	C	233	86% . 12%
10	D	206	97% .
11	E	167	92% . 7%
12	F	135	76% 24%
13	G	179	85% . 15%
14	H	130	98% ..
15	I	130	95% ..
16	J	103	92% .. 5%
17	K	129	86% .. 10%
18	L	124	98% ..
19	M	118	97% ..
20	N	101	91% 8% .
21	O	89	99% .
22	P	82	98% .
23	Q	84	89% . 8%
24	R	75	88% 12%
25	S	92	89% . 9%
26	T	87	98% ..
27	U	71	93% 6% .
28	V	241	92% . 7%

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Mol	Chain	Length	Quality of chain
29	Y	77	 82% 16% .
30	Z	76	 84% 16%
31	a	2904	 81% 13% . 5%
32	b	120	 83% 13% ..
33	c	273	 99% .
34	d	209	 98% .
35	e	201	 98% .
36	f	179	 98% ..
37	g	177	 98% .
38	h	149	 25% . 72%
39	i	142	 99% .
40	j	123	 100%
41	k	144	 81% 19%
42	l	136	 95% . .
43	m	127	 93% 7%
44	n	117	 95% . .
45	o	115	 98% .
46	p	118	 99% .
47	q	103	 98% .
48	r	110	 99% .
49	s	100	 89% 11%
50	t	104	 97% ..
51	u	94	 99% .
52	v	85	 96% ..
53	w	78	 99% .

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Mol	Chain	Length	Quality of chain
54	x	63	97%
55	y	59	93% • 5%
56	z	57	89% • 7%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 141933 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	49	Total	C	N	O	0	0
			405	261	74	70		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 7 is a protein called Beta-Galactosidase Nascent Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	55	Total	C	N	O	S	0	0
			427	271	79	75	2		

- Molecule 8 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	1513	Total	C	N	O	P	0	0
			32469	14484	5958	10514	1513		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 12 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	116	Total	C	N	O	S	0	0
			869	535	172	159	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	80	Total	C	N	O	S	0	0
			635	398	126	111			

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	77	Total	C	N	O	S	0	0
			624	394	117	110	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 28 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 29 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	77	Total	C	N	O	P	0	0
			1644	733	295	540	76		

- Molecule 30 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	76	Total	C	N	O	P	0	0
			1621	722	287	536	76		

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 32 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 33 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	208	Total	C	N	O	S	0	0
			1557	974	287	293	3		

- Molecule 35 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 36 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 37 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 38 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 40 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 41 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 42 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

- Molecule 43 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 44 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 45 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 46 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 47 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 48 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 49 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	89	Total	C	N	O	S	0	0
			709	449	133	125	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 51 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	84	Total	C	N	O	S	0	0
			628	388	126	113	1		

- Molecule 53 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 54 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	61	Total	C	N	O	S	0	0
			492	302	96	93	1		

- Molecule 55 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	56	Total	C	N	O	S	0	0
			435	272	84	77	2		

- Molecule 56 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	53	Total	C	N	O	S	0	0
			421	254	90	76	1		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	A	34	Total	K	0
			34	34	
58	F	1	Total	K	0
			1	1	
58	L	1	Total	K	0
			1	1	
58	a	90	Total	K	0
			90	90	
58	c	4	Total	K	0
			4	4	
58	e	1	Total	K	0
			1	1	

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

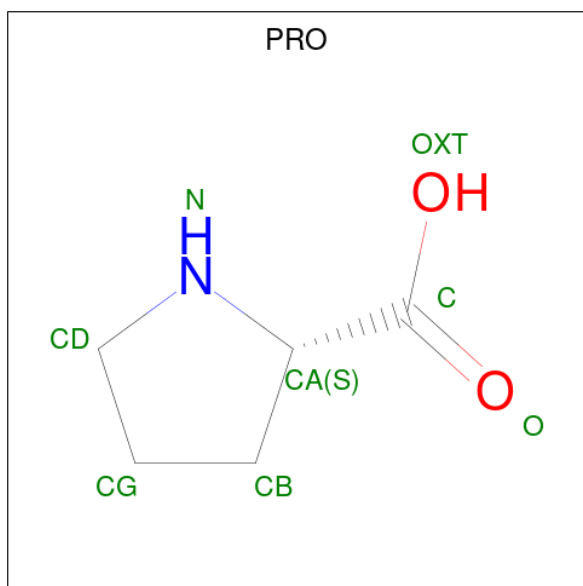
Mol	Chain	Residues	Atoms		AltConf
59	A	58	Total	Mg	0
			58	58	
59	M	1	Total	Mg	0
			1	1	
59	Z	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
59	a	217	Total	Mg	0
			217	217	
59	b	5	Total	Mg	0
			5	5	
59	c	2	Total	Mg	0
			2	2	
59	k	1	Total	Mg	0
			1	1	
59	m	1	Total	Mg	0
			1	1	
59	z	1	Total	Mg	0
			1	1	

- Molecule 60 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



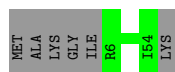
Mol	Chain	Residues	Atoms				AltConf
60	Y	1	Total	C	N	O	0
			7	5	1	1	

3 Residue-property plots [i](#)

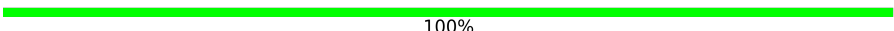
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Large ribosomal subunit protein bL33

Chain 0:  89% 11%



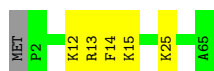
- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  100%

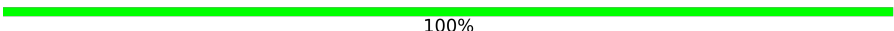
There are no outlier residues recorded for this chain.

- Molecule 3: Large ribosomal subunit protein bL35

Chain 2:  91% 8%



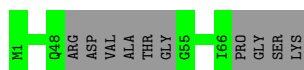
- Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Large ribosomal subunit protein bL31A

Chain 4:  86% 14%

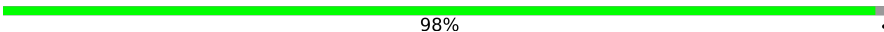


- Molecule 6: E-site tRNA

Chain 5:  50% 50%



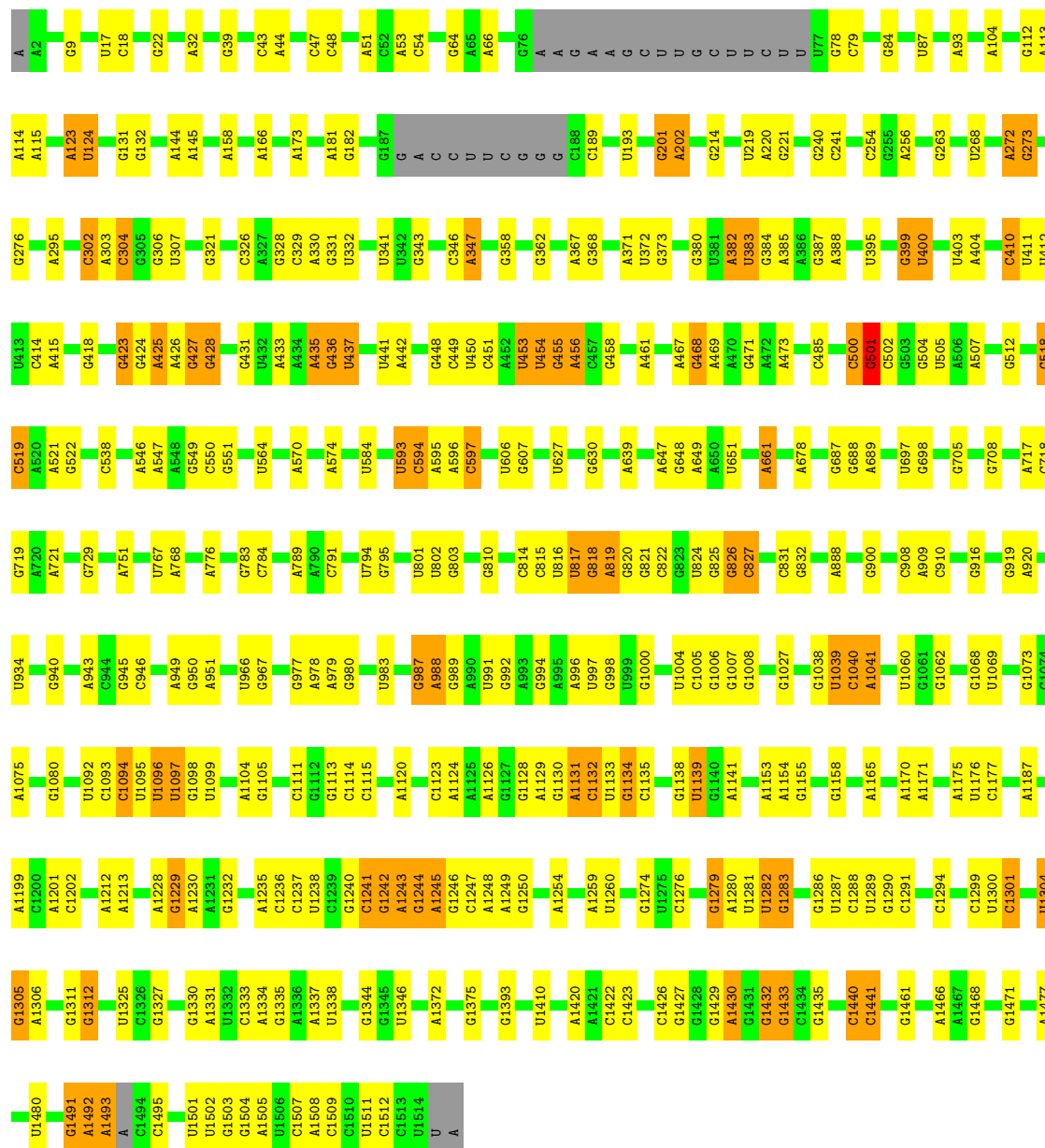
- Molecule 7: Beta-Galactosidase Nascent Chain

Chain 6:  98%



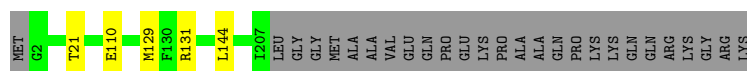
- Molecule 8: 16S rRNA

Chain A:  73% 20% 5%



- Molecule 9: Small ribosomal subunit protein uS3

Chain C:  86% 12%



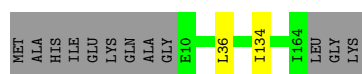
- Molecule 10: Small ribosomal subunit protein uS4

Chain D: 97%



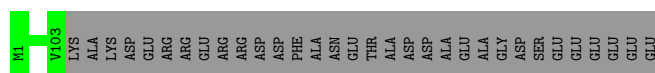
- Molecule 11: Small ribosomal subunit protein uS5

Chain E: 92%



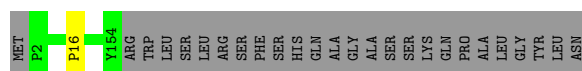
- Molecule 12: Small ribosomal subunit protein bS6, fully modified isoform

Chain F: 76%



- Molecule 13: Small ribosomal subunit protein uS7

Chain G: 85%



- Molecule 14: Small ribosomal subunit protein uS8

Chain H: 98%



- Molecule 15: Small ribosomal subunit protein uS9

Chain I: 95%



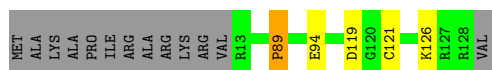
- Molecule 16: Small ribosomal subunit protein uS10

Chain J: 92%



- Molecule 17: Small ribosomal subunit protein uS11

Chain K: 86% .. 10%



- Molecule 18: Small ribosomal subunit protein uS12

Chain L: 98% ..



- Molecule 19: Small ribosomal subunit protein uS13

Chain M: 97% ..



- Molecule 20: Small ribosomal subunit protein uS14

Chain N: 91% 8% .



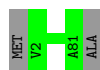
- Molecule 21: Small ribosomal subunit protein uS15

Chain O: 99% .



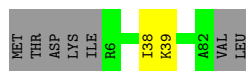
- Molecule 22: Small ribosomal subunit protein bS16

Chain P: 98% .



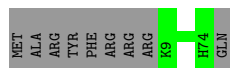
- Molecule 23: Small ribosomal subunit protein uS17

Chain Q: 89% 8%



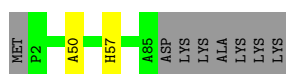
- Molecule 24: Small ribosomal subunit protein bS18

Chain R: 88% 12%



- Molecule 25: Small ribosomal subunit protein uS19

Chain S: 89% 9%



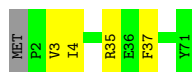
- Molecule 26: Small ribosomal subunit protein bS20

Chain T: 98% ..



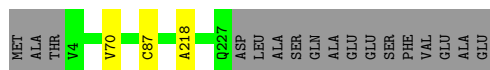
- Molecule 27: Small ribosomal subunit protein bS21

Chain U: 93% 6% .



- Molecule 28: Small ribosomal subunit protein uS2

Chain V: 92% 7%



- Molecule 29: A-site tRNA

Chain Y: 82% 16% .



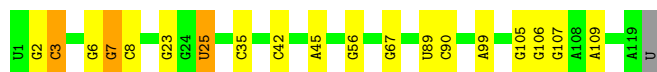
- Molecule 30: P-site tRNA

Chain Z: 84% 16%



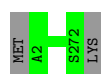
- Molecule 32: 5S rRNA

Chain b: 83% 13% ..



- Molecule 33: Large ribosomal subunit protein uL2

Chain c: 99% .



- Molecule 34: 50S ribosomal protein L3

Chain d: 98% .



- Molecule 35: Large ribosomal subunit protein uL4

Chain e: 98% .



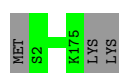
- Molecule 36: Large ribosomal subunit protein uL5

Chain f: 98% ..



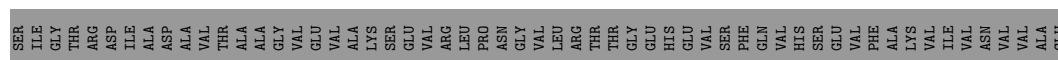
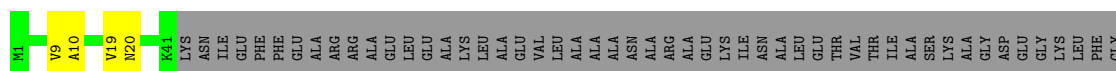
- Molecule 37: Large ribosomal subunit protein uL6

Chain g: 98% .



- Molecule 38: Large ribosomal subunit protein bL9

Chain h: 25% . 72%



- Molecule 39: Large ribosomal subunit protein uL13

Chain i: 99%



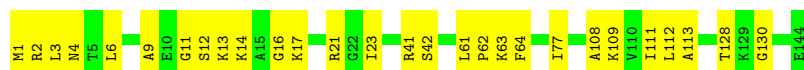
- Molecule 40: Large ribosomal subunit protein uL14

Chain j: 100%

There are no outlier residues recorded for this chain.

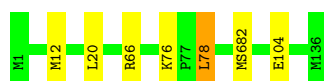
- Molecule 41: Large ribosomal subunit protein uL15

Chain k: 81%



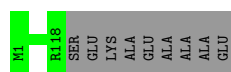
- Molecule 42: Large ribosomal subunit protein uL16

Chain l: 95%



- Molecule 43: Large ribosomal subunit protein bL17

Chain m: 93%



- Molecule 44: Large ribosomal subunit protein uL18

Chain n: 95%

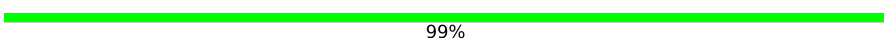


- Molecule 45: Large ribosomal subunit protein bL19

Chain o: 98%

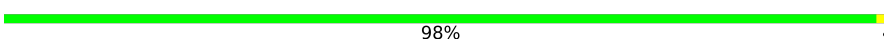


- Molecule 46: Large ribosomal subunit protein bL20

Chain p:  99%

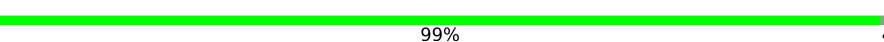


- Molecule 47: Large ribosomal subunit protein bL21

Chain q:  98%



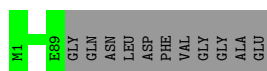
- Molecule 48: Large ribosomal subunit protein uL22

Chain r:  99%

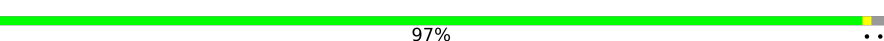


- Molecule 49: Large ribosomal subunit protein uL23

Chain s:  89% 11%

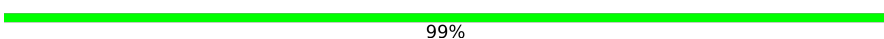


- Molecule 50: Large ribosomal subunit protein uL24

Chain t:  97%

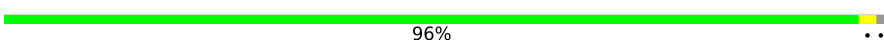


- Molecule 51: Large ribosomal subunit protein bL25

Chain u:  99%



- Molecule 52: Large ribosomal subunit protein bL27

Chain v:  96%



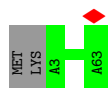
- Molecule 53: Large ribosomal subunit protein bL28

Chain w: 99%



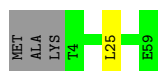
- Molecule 54: Large ribosomal subunit protein uL29

Chain x: 97%



- Molecule 55: Large ribosomal subunit protein uL30

Chain y: 93% 5%



- Molecule 56: Large ribosomal subunit protein bL32

Chain z: 89% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	389472	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 ($e^-/\text{\AA}^2$)	29.8	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.00692	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, MA6, 3TD, H2U, OMG, OMC, PSU, IAS, ZN, 4D4, 6MZ, 2MG, OMU, MG, K, G7M, 5MC, 2MA, MS6, 5MU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.14	0/412	0.36	0/549
2	1	0.22	0/380	0.62	0/498
3	2	0.17	0/513	0.43	0/676
4	3	0.19	0/303	0.45	0/397
5	4	0.14	0/488	0.36	0/649
6	5	0.13	0/46	0.13	0/69
7	6	0.21	0/442	0.45	0/608
8	A	0.20	1/36272 (0.0%)	0.34	5/56577 (0.0%)
9	C	0.15	0/1651	0.42	0/2225
10	D	0.15	0/1665	0.44	0/2227
11	E	0.15	0/1157	0.39	0/1557
12	F	0.16	0/858	0.38	0/1160
13	G	0.15	0/1219	0.44	0/1635
14	H	0.15	0/989	0.37	0/1326
15	I	0.16	0/1034	0.48	0/1375
16	J	0.23	0/796	0.50	0/1077
17	K	0.54	0/876	1.00	1/1181 (0.1%)
18	L	0.15	0/969	0.45	0/1300
19	M	0.16	0/900	0.48	0/1204
20	N	0.17	0/817	0.50	0/1088
21	O	0.17	0/722	0.46	0/964
22	P	0.15	0/645	0.47	0/867
23	Q	0.13	0/633	0.41	0/849
24	R	0.16	0/553	0.46	0/742
25	S	0.14	0/685	0.37	0/922
26	T	0.18	0/676	0.44	0/895
27	U	0.16	0/598	0.54	0/792
28	V	0.14	0/1784	0.39	0/2403
29	Y	0.14	0/1837	0.27	0/2864
30	Z	0.15	0/1810	0.29	0/2820
31	a	0.20	2/65651 (0.0%)	0.33	4/102413 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.16	0/2850	0.27	0/4444
33	c	0.17	0/2121	0.46	0/2852
34	d	0.16	0/1578	0.39	0/2124
35	e	0.16	0/1571	0.39	0/2113
36	f	0.15	0/1434	0.40	0/1926
37	g	0.13	0/1324	0.37	0/1794
38	h	0.15	0/306	0.34	0/413
39	i	0.17	0/1143	0.40	0/1540
40	j	0.17	0/956	0.45	0/1279
41	k	0.51	0/1062	0.87	0/1413
42	l	0.49	0/1073	0.90	0/1433
43	m	0.20	0/958	0.53	0/1281
44	n	0.15	0/902	0.45	0/1209
45	o	0.16	0/920	0.43	0/1231
46	p	0.21	0/960	0.54	0/1278
47	q	0.16	0/829	0.38	0/1107
48	r	0.17	0/852	0.42	0/1142
49	s	0.17	0/715	0.44	0/955
50	t	0.13	0/787	0.36	0/1051
51	u	0.16	0/766	0.36	0/1025
52	v	0.16	0/636	0.41	0/841
53	w	0.17	0/635	0.49	0/848
54	x	0.16	0/493	0.44	0/656
55	y	0.16	0/439	0.42	0/587
56	z	0.17	0/427	0.46	0/570
All	All	0.20	3/153118 (0.0%)	0.38	10/229021 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	501	G7M	O3'-P	9.97	1.66	1.56
31	a	2069	G7M	O3'-P	5.76	1.62	1.56
31	a	2552	OMU	O3'-P	5.74	1.61	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	747	5MU	O3'-P-O5'	-25.31	66.03	104.00
8	A	501	G7M	OP1-P-O3'	-17.16	67.46	105.20
8	A	501	G7M	OP2-P-O3'	-14.82	72.60	105.20
31	a	747	5MU	OP2-P-O3'	-12.80	69.58	108.00
8	A	501	G7M	O3'-P-O5'	-12.55	80.16	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	747	5MU	OP1-P-O3'	-8.62	82.14	108.00
8	A	501	G7M	P-O3'-C3'	8.60	130.02	119.70
31	a	747	5MU	P-O3'-C3'	5.65	128.68	120.20
17	K	89	PRO	N-CA-CB	-5.11	97.89	103.25
8	A	500	C	C2'-C3'-O3'	-5.09	106.07	113.70

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	0	405	0	437	0	0
2	1	377	0	418	0	0
3	2	504	0	572	8	0
4	3	302	0	340	0	0
5	4	480	0	479	0	0
6	5	42	0	23	0	0
7	6	427	0	404	0	0
8	A	32469	0	16348	147	0
9	C	1624	0	1696	3	0
10	D	1643	0	1707	3	0
11	E	1144	0	1185	1	0
12	F	839	0	833	0	0
13	G	1203	0	1254	1	0
14	H	979	0	1031	1	0
15	I	1022	0	1070	2	0
16	J	786	0	828	2	0
17	K	869	0	875	4	0
18	L	955	0	1016	1	0
19	M	891	0	952	1	0
20	N	805	0	844	7	0
21	O	714	0	734	0	0
22	P	635	0	649	0	0
23	Q	624	0	658	1	0
24	R	544	0	565	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	S	668	0	693	1	0
26	T	670	0	719	1	0
27	U	590	0	629	4	0
28	V	1753	0	1780	2	0
29	Y	1644	0	832	4	0
30	Z	1621	0	819	5	0
31	a	59130	0	29763	181	0
32	b	2549	0	1291	7	0
33	c	2082	0	2154	0	0
34	d	1557	0	1604	2	0
35	e	1552	0	1618	21	0
36	f	1410	0	1444	1	0
37	g	1304	0	1345	0	0
38	h	303	0	327	2	0
39	i	1120	0	1151	0	0
40	j	947	0	1023	0	0
41	k	1053	0	1129	66	0
42	l	1075	0	1145	11	0
43	m	945	0	989	0	0
44	n	892	0	923	3	0
45	o	908	0	956	0	0
46	p	947	0	1019	0	0
47	q	816	0	839	3	0
48	r	845	0	909	0	0
49	s	709	0	779	0	0
50	t	779	0	831	1	0
51	u	753	0	780	1	0
52	v	628	0	642	2	0
53	w	625	0	652	0	0
54	x	492	0	518	0	0
55	y	435	0	470	1	0
56	z	421	0	429	1	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
58	A	34	0	0	0	0
58	F	1	0	0	0	0
58	L	1	0	0	0	0
58	a	90	0	0	0	0
58	c	4	0	0	0	0
58	e	1	0	0	0	0
59	A	58	0	0	0	0
59	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	Z	1	0	0	0	0
59	a	217	0	0	0	0
59	b	5	0	0	0	0
59	c	2	0	0	0	0
59	k	1	0	0	0	0
59	m	1	0	0	0	0
59	z	1	0	0	0	0
60	Y	7	0	7	1	0
All	All	141933	0	95127	416	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 2.

All (416) 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)
31:a:662:G:O3'	41:k:16:GLY:HA2	1.61	1.01
3:2:15:LYS:HD3	41:k:64:PHE:CZ	2.02	0.94
35:e:23:PHE:HE1	41:k:1:MET:SD	1.99	0.86
8:A:425:A:N7	8:A:455:G:O6	2.09	0.86
31:a:2374:C:H42	31:a:2379:G:H22	1.20	0.85
31:a:2352:A:H62	31:a:2365:G:H21	1.25	0.85
31:a:663:G:OP1	41:k:17:LYS:N	2.13	0.80
31:a:713:G:H21	31:a:718:A:H62	1.29	0.79
35:e:32:VAL:HG11	41:k:3:LEU:CD2	2.14	0.78
3:2:15:LYS:HD3	41:k:64:PHE:CE2	2.21	0.76
35:e:23:PHE:CE1	41:k:1:MET:SD	2.80	0.74
31:a:713:G:N2	31:a:718:A:H62	1.84	0.74
31:a:1243:C:O2	41:k:4:ASN:HB2	1.86	0.74
17:K:126:LYS:HA	27:U:37:PHE:CD1	2.26	0.71
31:a:2355:G:H21	31:a:2356:U:H1'	1.56	0.71
17:K:119:IAS:O	27:U:35:ARG:NH2	2.24	0.70
31:a:670:A:H5''	41:k:42:SER:OG	1.91	0.70
31:a:637:A:OP1	41:k:130:GLY:HA3	1.92	0.70
35:e:29:HIS:HA	41:k:6:LEU:HD13	1.74	0.69
31:a:598:U:O2'	41:k:9:ALA:HB3	1.93	0.68
31:a:1032:A:C2	31:a:1034:G:C8	2.82	0.68
31:a:663:G:H5''	41:k:17:LYS:HG3	1.76	0.67
8:A:501:G7M:H2'	8:A:502:C:H5'	1.77	0.67
8:A:651:U:H1'	17:K:121:CYS:SG	2.35	0.67
8:A:501:G7M:C2'	8:A:502:C:H5'	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:15:LYS:CD	41:k:64:PHE:CZ	2.76	0.66
31:a:2460:U:C4'	42:l:78:LEU:HD21	2.27	0.65
35:e:29:HIS:HB2	41:k:6:LEU:HB3	1.77	0.65
35:e:29:HIS:HD2	41:k:6:LEU:CB	2.10	0.65
41:k:23:ILE:HG12	47:q:82:HIS:CE1	2.32	0.65
31:a:2535:G:H3'	31:a:2536:G:H5'	1.79	0.64
8:A:810:G:C2	8:A:824:U:O2	2.50	0.64
31:a:2535:G:H3'	31:a:2536:G:C5'	2.25	0.64
35:e:29:HIS:HD2	41:k:6:LEU:HB2	1.61	0.64
31:a:636:G:C8	41:k:128:THR:HG22	2.33	0.63
11:E:36:LEU:HD22	11:E:134:ILE:HD13	1.81	0.63
31:a:663:G:H4'	41:k:17:LYS:HE3	1.80	0.63
31:a:2459:A:O2'	42:l:78:LEU:HD11	1.97	0.62
8:A:1281:U:H3'	8:A:1282:U:H5'	1.81	0.62
3:2:13:ARG:NE	41:k:61:LEU:O	2.32	0.61
35:e:32:VAL:HG11	41:k:3:LEU:HD22	1.82	0.61
31:a:2374:C:N4	31:a:2379:G:H22	1.95	0.61
31:a:957:C:OP1	42:l:76:LYS:HB2	1.99	0.61
8:A:596:A:H3'	8:A:597:C:H5''	1.82	0.61
8:A:647:A:H2'	8:A:648:G:C8	2.36	0.60
20:N:31:ILE:HD12	20:N:45:VAL:HG22	1.81	0.60
3:2:15:LYS:HD3	41:k:64:PHE:HZ	1.66	0.60
31:a:1121:C:H2'	31:a:1122:G:O3'	2.01	0.60
35:e:108:ILE:HG23	41:k:1:MET:HE1	1.83	0.60
15:I:84:THR:HG23	15:I:98:LEU:HD13	1.85	0.59
8:A:1039:U:C2	8:A:1040:C:C5	2.90	0.59
8:A:1177:C:H5'	20:N:67:THR:HG23	1.83	0.59
31:a:636:G:N7	41:k:109:LYS:NZ	2.46	0.59
31:a:2460:U:H4'	42:l:78:LEU:HD21	1.84	0.59
31:a:671:C:OP1	41:k:42:SER:HA	2.03	0.58
8:A:423:G:H21	8:A:424:G:H2'	1.68	0.58
31:a:724:U:O2'	31:a:725:G:H5'	2.03	0.58
35:e:32:VAL:CG1	41:k:3:LEU:CD2	2.82	0.58
35:e:29:HIS:CB	41:k:6:LEU:HB3	2.33	0.58
31:a:707:G:H2'	31:a:708:G:O4'	2.04	0.58
8:A:1130:G:H4'	8:A:1131:A:C8	2.39	0.58
8:A:1281:U:C3'	8:A:1282:U:H5'	2.35	0.57
31:a:597:G:N2	41:k:12:SER:O	2.36	0.57
31:a:2459:A:O2'	42:l:78:LEU:CD1	2.53	0.56
35:e:108:ILE:HG23	41:k:1:MET:CE	2.36	0.56
35:e:29:HIS:CD2	41:k:6:LEU:CB	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:2898:U:O2'	31:a:2899:A:O4'	2.24	0.56
31:a:636:G:N1	41:k:111:ILE:HG21	2.21	0.56
8:A:1282:U:H4'	8:A:1283:G:O5'	2.06	0.56
8:A:810:G:N2	8:A:824:U:O2	2.39	0.55
8:A:987:G:H2'	8:A:988:A:H3'	1.88	0.55
31:a:662:G:H5'	41:k:14:LYS:O	2.06	0.55
31:a:636:G:H3'	41:k:128:THR:HB	1.87	0.55
31:a:2366:A:H4'	52:v:60:PHE:CE1	2.41	0.55
8:A:1062:G:H21	8:A:1141:A:H62	1.53	0.55
10:D:28:ILE:H	10:D:28:ILE:HD12	1.72	0.55
31:a:587:C:P	41:k:21:ARG:HH12	2.29	0.54
8:A:1334:A:H3'	8:A:1335:G:H21	1.70	0.54
8:A:1280:A:C2	8:A:1306:A:C4	2.95	0.54
8:A:1281:U:O5'	8:A:1282:U:H2'	2.08	0.54
9:C:110:GLU:HB2	9:C:144:LEU:HD12	1.88	0.54
31:a:627:A:N7	41:k:113:ALA:HB2	2.23	0.54
31:a:1349:C:C2	31:a:1350:C:C5	2.95	0.54
35:e:32:VAL:CG1	41:k:3:LEU:HD22	2.37	0.54
8:A:596:A:O5'	8:A:597:C:H5''	2.07	0.54
17:K:126:LYS:HA	27:U:37:PHE:CG	2.43	0.54
31:a:725:G:O2'	31:a:726:G:P	2.65	0.54
3:2:14:PHE:CZ	41:k:61:LEU:HD12	2.43	0.53
28:V:70:VAL:O	28:V:70:VAL:HG12	2.07	0.53
31:a:806:C:OP2	41:k:41:ARG:NH1	2.41	0.53
27:U:3:VAL:C	27:U:4:ILE:HD12	2.32	0.53
41:k:77:ILE:HD11	41:k:108:ALA:HB1	1.91	0.53
8:A:1131:A:H1'	8:A:1155:G:N2	2.24	0.53
8:A:594:C:C4	8:A:595:A:N6	2.76	0.53
31:a:707:G:C6	31:a:708:G:C5	2.97	0.53
31:a:636:G:N7	41:k:109:LYS:HD3	2.24	0.53
31:a:1243:C:O2	41:k:4:ASN:CB	2.57	0.52
31:a:2459:A:C2'	42:l:78:LEU:HD11	2.39	0.52
35:e:29:HIS:CD2	41:k:6:LEU:HB3	2.45	0.52
31:a:784:G:H5'	31:a:785:G:OP1	2.09	0.52
31:a:587:C:OP2	41:k:21:ARG:NH2	2.42	0.52
60:Y:101:PRO:HG2	31:a:2451:A:C2	2.45	0.52
31:a:1121:C:O3'	31:a:1122:G:H4'	2.10	0.52
31:a:2308:G:H22	31:a:2311:A:H2	1.58	0.52
31:a:2650:U:O2	31:a:2671:G:N2	2.43	0.52
30:Z:27:C:C2	30:Z:28:G:C8	2.98	0.51
31:a:1048:A:C2	31:a:1049:C:C6	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:117:ARG:NH2	41:k:2:ARG:NH2	2.58	0.51
31:a:1121:C:C3'	31:a:1122:G:H4'	2.41	0.51
3:2:12:LYS:HD3	41:k:63:LYS:HD2	1.91	0.51
35:e:108:ILE:HG12	41:k:1:MET:SD	2.50	0.51
29:Y:26:C:N3	29:Y:27:A:C8	2.79	0.51
31:a:1031:G:N1	31:a:1032:A:C2	2.79	0.51
31:a:1039:A:H2	31:a:1116:G:H22	1.57	0.51
8:A:1501:U:O2'	8:A:1502:U:H5'	2.10	0.51
31:a:637:A:H5''	41:k:112:LEU:HD23	1.92	0.51
31:a:709:U:H3'	31:a:710:U:C6	2.46	0.51
31:a:1141:U:H4'	31:a:1142:A:O4'	2.11	0.50
31:a:2541:A:N3	31:a:2541:A:H2'	2.27	0.50
35:e:117:ARG:CZ	41:k:2:ARG:NH2	2.75	0.50
8:A:425:A:C5	8:A:455:G:O6	2.64	0.50
31:a:2355:G:N2	31:a:2356:U:H1'	2.24	0.50
8:A:414:C:C2	8:A:415:A:C8	3.00	0.50
31:a:1036:G:H1	31:a:1119:U:H3	1.60	0.50
31:a:2364:C:C6	31:a:2365:G:C8	2.99	0.50
31:a:747:5MU:H5''	31:a:748:G:H5'	1.94	0.50
31:a:1508:A:H2'	31:a:1509:A:O4'	2.12	0.50
8:A:435:A:HO2'	8:A:436:G:P	2.34	0.50
8:A:1130:G:O3'	8:A:1131:A:O4'	2.30	0.50
8:A:1281:U:C5	8:A:1282:U:C2	3.00	0.50
31:a:2368:C:H2'	31:a:2369:A:C8	2.47	0.50
31:a:597:G:H21	41:k:12:SER:HA	1.77	0.50
31:a:660:C:O2'	41:k:13:LYS:HE3	2.11	0.50
42:l:66:ARG:NH1	42:l:104:GLU:OE2	2.45	0.50
8:A:201:G:HO2'	8:A:202:A:H8	1.59	0.49
16:J:57:VAL:O	16:J:58:ASN:C	2.54	0.49
31:a:725:G:O2'	31:a:726:G:O5'	2.26	0.49
8:A:1038:G:C5	8:A:1040:C:N4	2.80	0.49
31:a:2459:A:H2'	42:l:78:LEU:HD11	1.93	0.49
31:a:2363:G:H2'	31:a:2364:C:C6	2.48	0.49
32:b:6:G:C2'	32:b:7:G:H5'	2.41	0.49
31:a:708:G:O2'	31:a:709:U:H5'	2.13	0.49
31:a:1023:U:O2'	31:a:1121:C:O3'	2.26	0.49
35:e:29:HIS:CD2	41:k:6:LEU:C	2.91	0.49
8:A:1040:C:H42	8:A:1165:A:H62	1.61	0.48
8:A:826:G:H3'	8:A:827:C:C5'	2.42	0.48
31:a:670:A:C5'	41:k:42:SER:OG	2.60	0.48
8:A:1432:G:H2'	8:A:1433:G:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:548:G:H2'	31:a:549:G:C8	2.48	0.48
8:A:596:A:H3'	8:A:597:C:C5'	2.43	0.48
31:a:856:G:H2'	31:a:857:G:C8	2.47	0.48
8:A:826:G:H3'	8:A:827:C:H5'	1.95	0.48
8:A:1134:G:C2	8:A:1135:C:C6	3.01	0.48
31:a:2535:G:H2'	31:a:2535:G:N3	2.28	0.48
35:e:32:VAL:HG11	41:k:3:LEU:HD23	1.92	0.48
8:A:826:G:H2'	8:A:827:C:H5'	1.96	0.48
31:a:2552:OMU:OP2	31:a:2552:OMU:H6	2.13	0.48
31:a:724:U:OP1	31:a:725:G:OP2	2.32	0.48
35:e:29:HIS:CD2	41:k:6:LEU:O	2.67	0.48
31:a:1915:3TD:H6	31:a:1915:3TD:O5'	2.14	0.47
8:A:1244:G:O2'	8:A:1245:A:O4'	2.32	0.47
8:A:1279:G:H21	8:A:1306:A:H2	1.61	0.47
31:a:1618:6MZ:O3'	31:a:1619:G:P	2.73	0.47
31:a:2366:A:H3'	31:a:2367:G:C8	2.48	0.47
8:A:1039:U:C2	8:A:1040:C:C6	3.02	0.47
31:a:636:G:N7	41:k:109:LYS:CD	2.78	0.47
31:a:2534:A:O2'	31:a:2535:G:H5''	2.14	0.47
8:A:367:A:C2	8:A:368:G:C8	3.03	0.47
8:A:453:U:H3'	8:A:454:U:H3'	1.96	0.47
8:A:593:U:C2	8:A:594:C:O2	2.68	0.47
8:A:825:G:O2'	8:A:826:G:C8	2.62	0.47
31:a:2379:G:C2	31:a:2380:C:N4	2.83	0.47
8:A:1280:A:C2	8:A:1306:A:N3	2.82	0.47
14:H:11:LEU:HD22	14:H:75:ILE:HD11	1.96	0.47
20:N:67:THR:HG22	20:N:67:THR:O	2.14	0.47
31:a:2356:U:O2	31:a:2356:U:H2'	2.15	0.47
31:a:597:G:H21	41:k:12:SER:CA	2.27	0.47
31:a:2259:U:N3	31:a:2260:C:C5	2.83	0.47
9:C:21:THR:O	9:C:21:THR:HG22	2.15	0.46
31:a:747:5MU:H3'	31:a:748:G:H5'	1.96	0.46
13:G:16:PRO:HG3	15:I:43:THR:HG22	1.96	0.46
8:A:1228:A:H1'	8:A:1229:G:H5'	1.97	0.46
32:b:25:U:H2'	32:b:25:U:O2	2.13	0.46
8:A:87:U:O2	8:A:87:U:O4'	2.33	0.46
8:A:1433:G:OP1	8:A:1433:G:O4'	2.34	0.46
29:Y:13:C:O2'	29:Y:14:A:P	2.72	0.46
31:a:2460:U:O4'	42:l:78:LEU:HD21	2.15	0.46
3:2:25:LYS:HB3	41:k:62:PRO:HG2	1.97	0.46
8:A:435:A:C2'	8:A:436:G:O5'	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1244:G:O5'	8:A:1299:C:O2'	2.30	0.46
31:a:723:C:H3'	31:a:724:U:H4'	1.96	0.46
31:a:2519:U:C4	31:a:2541:A:C5	3.04	0.46
8:A:382:A:O2'	8:A:383:U:P	2.74	0.46
31:a:2071:A:H2'	31:a:2072:C:C6	2.51	0.46
31:a:2259:U:C2	31:a:2260:C:C6	3.04	0.46
8:A:717:A:O2'	8:A:826:G:N3	2.43	0.46
10:D:132:ILE:HG23	10:D:135:TYR:HB2	1.98	0.46
31:a:2064:C:H2'	31:a:2065:C:C6	2.51	0.46
8:A:584:U:H2'	8:A:584:U:O2	2.15	0.46
31:a:597:G:O2'	41:k:11:GLY:HA3	2.16	0.46
31:a:725:G:H1'	31:a:726:G:C8	2.51	0.46
31:a:2378:A:C6	31:a:2379:G:O2'	2.69	0.46
31:a:2534:A:O2'	31:a:2535:G:O4'	2.33	0.46
8:A:688:G:H2'	8:A:689:A:C8	2.51	0.45
8:A:1153:A:H2'	8:A:1154:A:O4'	2.16	0.45
23:Q:38:ILE:HG22	23:Q:39:LYS:N	2.30	0.45
31:a:661:A:O4'	41:k:13:LYS:HD3	2.16	0.45
31:a:1120:G:H2'	31:a:1121:C:C6	2.52	0.45
8:A:919:G:C2	8:A:920:A:C8	3.04	0.45
25:S:50:ALA:HB1	25:S:57:HIS:HB3	1.98	0.45
8:A:687:G:H2'	8:A:688:G:C8	2.51	0.45
8:A:501:G7M:H2'	8:A:502:C:C5'	2.43	0.45
8:A:1039:U:O2	8:A:1040:C:C6	2.69	0.45
31:a:706:A:H2'	31:a:707:G:C8	2.51	0.45
31:a:636:G:O6	41:k:109:LYS:HD2	2.16	0.45
31:a:832:U:H2'	31:a:833:A:H8	1.82	0.45
31:a:2352:A:C8	31:a:2366:A:N6	2.84	0.45
8:A:987:G:C2'	8:A:988:A:H3'	2.47	0.45
8:A:1429:G:O2'	8:A:1430:A:O5'	2.28	0.45
8:A:220:A:C2	8:A:256:A:C5	3.04	0.45
31:a:2473:U:O2	31:a:2473:U:H2'	2.16	0.45
8:A:1422:C:O2	8:A:1422:C:O4'	2.34	0.45
31:a:707:G:C6	31:a:708:G:C6	3.05	0.45
31:a:708:G:C6	31:a:709:U:C4	3.05	0.45
31:a:2352:A:C1'	31:a:2366:A:H61	2.29	0.45
31:a:2364:C:H2'	31:a:2365:G:O4'	2.17	0.45
8:A:595:A:C5	8:A:596:A:C6	3.05	0.45
8:A:329:C:C4	8:A:330:A:N7	2.85	0.45
8:A:597:C:H4'	8:A:597:C:OP1	2.17	0.45
8:A:717:A:O2'	8:A:826:G:H1'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1282:U:HO2'	8:A:1282:U:H6	1.65	0.45
8:A:1433:G:OP2	26:T:23:SER:HB3	2.16	0.45
8:A:1491:G:N7	8:A:1492:MA6:H93	2.31	0.45
20:N:66:GLN:O	20:N:67:THR:HB	2.16	0.45
30:Z:26:A:C2	30:Z:27:C:C6	3.05	0.45
30:Z:26:A:C5	30:Z:27:C:C5	3.05	0.45
41:k:23:ILE:CG1	47:q:82:HIS:CE1	3.00	0.45
8:A:821:G:H2'	8:A:822:C:H5'	1.98	0.44
8:A:1432:G:C2'	8:A:1433:G:OP1	2.65	0.44
31:a:948:C:C2	31:a:949:G:C8	3.05	0.44
8:A:123:A:O2'	8:A:124:U:P	2.75	0.44
8:A:1130:G:O2'	8:A:1131:A:H5''	2.16	0.44
8:A:1492:MA6:N6	8:A:1493:MA6:H93	2.32	0.44
31:a:713:G:H21	31:a:718:A:N6	2.06	0.44
31:a:2840:C:C2	31:a:2841:C:C5	3.06	0.44
8:A:427:G:N7	8:A:428:G:C2	2.85	0.44
8:A:661:A:C2	8:A:678:A:C5	3.06	0.44
10:D:177:LYS:O	10:D:178:MET:C	2.61	0.44
8:A:467:A:H2'	8:A:468:G:O4'	2.17	0.44
8:A:1240:G:H3'	8:A:1241:C:C5'	2.47	0.44
31:a:404:A:H1'	31:a:405:U:OP2	2.16	0.44
31:a:548:G:H2'	31:a:549:G:N9	2.32	0.44
8:A:302:C:O2	8:A:302:C:C2'	2.65	0.44
8:A:435:A:H2'	8:A:436:G:O5'	2.18	0.44
8:A:826:G:C3'	8:A:827:C:H5'	2.47	0.44
31:a:593:U:H2'	31:a:594:U:C6	2.53	0.44
31:a:707:G:C4	31:a:708:G:C8	3.06	0.44
31:a:1349:C:N3	31:a:1350:C:C5	2.86	0.44
8:A:144:A:H2'	8:A:145:A:O4'	2.18	0.44
8:A:272:A:HO2'	8:A:273:G:P	2.41	0.44
8:A:1300:U:O2'	8:A:1301:C:H5	2.01	0.44
20:N:28:LYS:HA	20:N:31:ILE:HG22	2.00	0.44
32:b:106:G:H2'	32:b:107:G:O4'	2.18	0.44
8:A:399:G:O2'	8:A:400:U:P	2.75	0.43
8:A:817:U:H5''	8:A:818:G:C2	2.53	0.43
8:A:1228:A:O2'	8:A:1229:G:O5'	2.36	0.43
8:A:1430:A:OP1	8:A:1430:A:H4'	2.18	0.43
31:a:947:A:H2'	31:a:948:C:C6	2.53	0.43
34:d:146:ILE:HG22	34:d:146:ILE:O	2.18	0.43
44:n:26:LEU:HD12	44:n:38:GLN:O	2.18	0.43
31:a:724:U:H3'	31:a:725:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1348:C:C5	31:a:1349:C:C5	3.06	0.43
8:A:518:G:O2'	8:A:519:C:P	2.76	0.43
8:A:1282:U:OP2	19:M:109:ARG:HD2	2.18	0.43
31:a:706:A:C6	31:a:707:G:C6	3.06	0.43
31:a:1830:C:O2	31:a:1831:G:C8	2.71	0.43
38:h:19:VAL:HG22	38:h:20:ASN:N	2.32	0.43
8:A:1139:U:O2	8:A:1139:U:O4'	2.35	0.43
31:a:1433:A:H2'	31:a:1434:A:C8	2.53	0.43
31:a:2534:A:HO2'	31:a:2535:G:H8	1.61	0.43
31:a:2065:C:N3	31:a:2066:C:C5	2.86	0.43
8:A:371:A:C2'	8:A:371:A:N3	2.82	0.43
8:A:1244:G:O2'	8:A:1245:A:P	2.76	0.43
8:A:1282:U:H1'	8:A:1283:G:C8	2.53	0.43
8:A:794:U:H4'	8:A:795:G:OP2	2.19	0.43
8:A:818:G:H21	8:A:819:A:C1'	2.32	0.43
30:Z:26:A:C6	30:Z:27:C:C5	3.07	0.43
31:a:708:G:C2'	31:a:709:U:H5'	2.48	0.43
56:z:3:VAL:HG22	56:z:4:GLN:N	2.34	0.43
31:a:2063:C:C4	31:a:2064:C:C5	3.07	0.43
31:a:2291:U:H2'	31:a:2292:U:C6	2.53	0.43
8:A:648:G:H2'	8:A:649:A:H8	1.84	0.43
8:A:826:G:C2'	8:A:827:C:H5'	2.49	0.43
31:a:1802:A:H2'	31:a:1803:A:C8	2.54	0.43
8:A:347:A:C2	8:A:456:A:N6	2.87	0.42
29:Y:27:A:C2	29:Y:28:A:C8	3.07	0.42
31:a:984:A:N3	31:a:984:A:H2'	2.34	0.42
31:a:2352:A:N9	31:a:2366:A:N6	2.67	0.42
8:A:268:U:O2	8:A:268:U:O4'	2.37	0.42
8:A:427:G:O6	8:A:428:G:N2	2.52	0.42
31:a:1032:A:N3	31:a:1034:G:C8	2.87	0.42
8:A:410:C:O2'	8:A:411:U:H5'	2.19	0.42
8:A:1128:G:N3	8:A:1128:G:H2'	2.35	0.42
8:A:1422:C:H5	8:A:1429:G:H22	1.67	0.42
31:a:663:G:H5''	41:k:17:LYS:CG	2.48	0.42
31:a:835:C:C2	31:a:836:G:C8	3.08	0.42
32:b:2:G:O2'	32:b:3:C:P	2.77	0.42
8:A:825:G:HO2'	8:A:826:G:H8	1.58	0.42
8:A:1282:U:H1'	8:A:1283:G:N7	2.34	0.42
31:a:545:U:H5''	31:a:546:U:OP1	2.18	0.42
31:a:2266:A:H4'	31:a:2267:A:N3	2.35	0.42
31:a:2381:A:N3	31:a:2381:A:H3'	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:2897:U:C3'	31:a:2898:U:O4'	2.68	0.42
9:C:129:MET:HE1	9:C:131:ARG:HB2	2.01	0.42
8:A:1243:A:H4'	8:A:1300:U:O4'	2.19	0.42
8:A:1281:U:H5	8:A:1282:U:C2	2.37	0.42
31:a:645:C:H2'	31:a:647:G:N7	2.35	0.42
31:a:1348:C:C4	31:a:1349:C:C6	3.07	0.42
31:a:2519:U:O2	31:a:2519:U:C2'	2.67	0.42
8:A:131:G:H2'	8:A:132:G:C8	2.54	0.42
8:A:1304:U:OP2	8:A:1305:G:H5'	2.19	0.42
31:a:1114:C:H2'	31:a:1115:G:H8	1.85	0.42
32:b:6:G:O2'	32:b:7:G:H5'	2.19	0.42
8:A:304:C:O2	8:A:304:C:O4'	2.38	0.42
8:A:423:G:H2'	8:A:424:G:C8	2.55	0.42
30:Z:27:C:O2	30:Z:28:G:C8	2.73	0.42
31:a:2757:A:N3	31:a:2757:A:H2'	2.35	0.42
31:a:2812:G:H2'	31:a:2813:A:C8	2.54	0.42
42:l:20:LEU:HD13	51:u:81:PRO:HG3	2.01	0.42
31:a:364:C:H2'	31:a:365:U:C6	2.55	0.42
31:a:710:U:H2'	31:a:711:G:C8	2.55	0.42
31:a:2352:A:H2'	31:a:2353:G:H5'	2.02	0.42
31:a:2366:A:H1'	52:v:34:GLY:HA2	2.02	0.42
31:a:2897:U:H2'	31:a:2898:U:C2	2.55	0.42
32:b:2:G:HO2'	32:b:3:C:P	2.42	0.42
8:A:1281:U:H3'	8:A:1282:U:C3'	2.50	0.41
8:A:1330:G:H2'	8:A:1331:A:C8	2.55	0.41
31:a:639:U:H2'	31:a:640:C:C6	2.55	0.41
36:f:152:LEU:HD12	36:f:152:LEU:C	2.44	0.41
8:A:1242:G:O4'	8:A:1301:C:O5'	2.37	0.41
8:A:1280:A:C2	8:A:1281:U:C4	3.09	0.41
31:a:645:C:H2'	31:a:647:G:C8	2.55	0.41
31:a:956:G:H4'	42:l:82:MS6:SD	2.60	0.41
31:a:2043:C:C2	31:a:2044:C:C5	3.08	0.41
31:a:2065:C:C2	31:a:2066:C:C5	3.08	0.41
31:a:2815:C:C2	31:a:2816:G:C8	3.08	0.41
32:b:2:G:O2'	32:b:3:C:OP1	2.37	0.41
8:A:1039:U:H1'	8:A:1040:C:OP2	2.19	0.41
31:a:1829:A:C8	31:a:1830:C:C5	3.09	0.41
8:A:1104:A:C8	8:A:1105:G:C8	3.08	0.41
8:A:1129:A:H2'	8:A:1130:G:O4'	2.19	0.41
31:a:663:G:C5'	41:k:17:LYS:HG3	2.48	0.41
31:a:723:C:C3'	31:a:724:U:H4'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:831:C:H2'	8:A:832:G:O4'	2.21	0.41
8:A:1440:C:HO2'	8:A:1441:C:P	2.44	0.41
29:Y:27:A:C4	29:Y:28:A:C8	3.08	0.41
31:a:1114:C:H2'	31:a:1115:G:C8	2.54	0.41
31:a:2327:A:H2'	31:a:2328:A:C8	2.56	0.41
20:N:74:LEU:O	20:N:77:PHE:O	2.39	0.41
31:a:78:U:H2'	31:a:79:C:C6	2.55	0.41
8:A:43:C:O2'	8:A:596:A:H2'	2.20	0.41
8:A:1094:C:H2'	8:A:1095:U:C6	2.56	0.41
8:A:1440:C:O2'	8:A:1441:C:P	2.78	0.41
28:V:87:CYS:SG	28:V:218:ALA:HA	2.60	0.41
31:a:636:G:C6	41:k:111:ILE:HG21	2.56	0.41
41:k:23:ILE:HG12	47:q:82:HIS:NE2	2.35	0.41
8:A:123:A:H4'	8:A:123:A:OP1	2.21	0.41
8:A:306:G:C2	8:A:307:U:C6	3.09	0.41
8:A:814:C:N4	8:A:816:U:H4'	2.35	0.41
16:J:52:LEU:O	20:N:81:ARG:HD3	2.21	0.41
31:a:1204:A:O4'	31:a:1206:G:C8	2.74	0.41
31:a:1469:A:H2'	31:a:1470:A:C8	2.55	0.41
31:a:2356:U:O2	31:a:2357:G:H8	2.04	0.41
31:a:2533:U:H2'	31:a:2534:A:H5'	2.03	0.41
34:d:62:LYS:N	34:d:63:PRO:HD2	2.35	0.41
50:t:52:LEU:HD13	50:t:52:LEU:C	2.45	0.41
8:A:436:G:HO2'	8:A:437:U:H6	1.63	0.41
8:A:1040:C:O2'	8:A:1041:A:O5'	2.38	0.41
8:A:1131:A:OP1	8:A:1132:C:H5'	2.21	0.41
8:A:1280:A:N1	8:A:1281:U:C4	2.89	0.41
31:a:933:A:H5'	31:a:934:U:OP2	2.21	0.41
8:A:718:C:H2'	8:A:719:G:H8	1.85	0.40
8:A:1281:U:C2'	8:A:1282:U:H5'	2.51	0.40
31:a:960:A:H5''	31:a:961:C:OP1	2.20	0.40
31:a:2355:G:N3	31:a:2356:U:C6	2.89	0.40
8:A:201:G:O2'	8:A:202:A:H8	2.04	0.40
8:A:330:A:H2'	8:A:331:G:H5'	2.02	0.40
8:A:810:G:N1	8:A:824:U:C2	2.89	0.40
8:A:1104:A:C2	8:A:1120:A:C6	3.09	0.40
31:a:1034:G:O5'	31:a:1035:U:OP2	2.38	0.40
44:n:106:LEU:HD23	44:n:106:LEU:C	2.47	0.40
8:A:1282:U:C1'	8:A:1283:G:C8	3.04	0.40
31:a:1507:C:H2'	31:a:1508:A:O4'	2.22	0.40
31:a:2352:A:H2'	31:a:2353:G:C5'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:n:48:LEU:HD13	44:n:87:ILE:HD11	2.04	0.40
8:A:17:U:H2'	8:A:18:C:C6	2.57	0.40
8:A:272:A:O2'	8:A:273:G:P	2.79	0.40
8:A:425:A:N7	8:A:455:G:C6	2.85	0.40
18:L:16:VAL:HG12	18:L:17:ALA:N	2.37	0.40
31:a:404:A:C1'	31:a:405:U:OP2	2.69	0.40
31:a:2351:G:N3	31:a:2351:G:H2'	2.35	0.40
31:a:2898:U:O2	31:a:2899:A:C8	2.75	0.40
38:h:9:VAL:HG12	38:h:10:ALA:N	2.37	0.40
8:A:825:G:H2'	8:A:826:G:OP2	2.21	0.40
8:A:1060:U:O2	8:A:1060:U:H2'	2.21	0.40
8:A:1096:U:N3	8:A:1097:U:O4	2.55	0.40
8:A:1311:G:H5''	8:A:1312:G:OP1	2.20	0.40
31:a:362:A:C4	31:a:363:G:C8	3.09	0.40
31:a:1110:G:OP2	31:a:1110:G:C8	2.75	0.40
31:a:1349:C:O2	31:a:1350:C:C6	2.75	0.40
31:a:2328:A:H2'	31:a:2329:U:C6	2.56	0.40
31:a:2366:A:H2'	31:a:2367:G:O4'	2.22	0.40
31:a:2519:U:O2	31:a:2519:U:H2'	2.22	0.40
31:a:2803:G:H2'	31:a:2804:U:H6	1.86	0.40
31:a:2898:U:H2'	31:a:2899:A:H5''	2.02	0.40
55:y:25:LEU:HD13	55:y:25:LEU:C	2.46	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	0	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
2	1	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
3	2	62/65 (95%)	57 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
7	6	53/56 (95%)	53 (100%)	0	0	100	100
9	C	204/233 (88%)	200 (98%)	4 (2%)	0	100	100
10	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
11	E	153/167 (92%)	149 (97%)	4 (3%)	0	100	100
12	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
13	G	151/179 (84%)	147 (97%)	4 (3%)	0	100	100
14	H	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
15	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
16	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	25
17	K	112/129 (87%)	103 (92%)	9 (8%)	0	100	100
18	L	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
19	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
20	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
21	O	86/89 (97%)	86 (100%)	0	0	100	100
22	P	78/82 (95%)	77 (99%)	1 (1%)	0	100	100
23	Q	75/84 (89%)	73 (97%)	2 (3%)	0	100	100
24	R	64/75 (85%)	64 (100%)	0	0	100	100
25	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	68/71 (96%)	68 (100%)	0	0	100	100
28	V	222/241 (92%)	219 (99%)	3 (1%)	0	100	100
33	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
34	d	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
35	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
36	f	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
37	g	172/177 (97%)	168 (98%)	4 (2%)	0	100	100
38	h	39/149 (26%)	38 (97%)	1 (3%)	0	100	100
39	i	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
40	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
42	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
43	m	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
44	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
45	o	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
46	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
47	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
48	r	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
49	s	87/100 (87%)	86 (99%)	1 (1%)	0	100	100
50	t	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
51	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
52	v	82/85 (96%)	78 (95%)	4 (5%)	0	100	100
53	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
54	x	59/63 (94%)	59 (100%)	0	0	100	100
55	y	54/59 (92%)	53 (98%)	1 (2%)	0	100	100
56	z	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
All	All	5519/5969 (92%)	5378 (97%)	140 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	J	57	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	45/49 (92%)	45 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	55 (100%)	0	100	100
7	6	39/40 (98%)	39 (100%)	0	100	100
9	C	170/190 (90%)	170 (100%)	0	100	100
10	D	172/173 (99%)	172 (100%)	0	100	100
11	E	118/126 (94%)	118 (100%)	0	100	100
12	F	90/116 (78%)	90 (100%)	0	100	100
13	G	126/147 (86%)	126 (100%)	0	100	100
14	H	104/105 (99%)	104 (100%)	0	100	100
15	I	105/107 (98%)	105 (100%)	0	100	100
16	J	86/90 (96%)	86 (100%)	0	100	100
17	K	88/98 (90%)	86 (98%)	2 (2%)	44	68
18	L	103/104 (99%)	103 (100%)	0	100	100
19	M	93/96 (97%)	93 (100%)	0	100	100
20	N	83/84 (99%)	83 (100%)	0	100	100
21	O	76/77 (99%)	76 (100%)	0	100	100
22	P	64/65 (98%)	64 (100%)	0	100	100
23	Q	71/78 (91%)	71 (100%)	0	100	100
24	R	57/65 (88%)	57 (100%)	0	100	100
25	S	72/79 (91%)	72 (100%)	0	100	100
26	T	65/66 (98%)	65 (100%)	0	100	100
27	U	60/61 (98%)	60 (100%)	0	100	100
28	V	186/199 (94%)	186 (100%)	0	100	100
33	c	216/218 (99%)	216 (100%)	0	100	100
34	d	163/164 (99%)	163 (100%)	0	100	100
35	e	165/165 (100%)	165 (100%)	0	100	100
36	f	148/150 (99%)	148 (100%)	0	100	100
37	g	135/138 (98%)	135 (100%)	0	100	100
38	h	32/114 (28%)	32 (100%)	0	100	100
39	i	115/116 (99%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	104/104 (100%)	104 (100%)	0	100	100
41	k	103/103 (100%)	103 (100%)	0	100	100
42	l	107/107 (100%)	105 (98%)	2 (2%)	50	72
43	m	98/103 (95%)	98 (100%)	0	100	100
44	n	86/87 (99%)	86 (100%)	0	100	100
45	o	98/100 (98%)	98 (100%)	0	100	100
46	p	89/90 (99%)	89 (100%)	0	100	100
47	q	84/84 (100%)	83 (99%)	1 (1%)	63	80
48	r	92/93 (99%)	92 (100%)	0	100	100
49	s	77/84 (92%)	77 (100%)	0	100	100
50	t	83/85 (98%)	83 (100%)	0	100	100
51	u	78/78 (100%)	78 (100%)	0	100	100
52	v	61/63 (97%)	61 (100%)	0	100	100
53	w	67/68 (98%)	67 (100%)	0	100	100
54	x	53/55 (96%)	53 (100%)	0	100	100
55	y	47/49 (96%)	47 (100%)	0	100	100
56	z	45/48 (94%)	45 (100%)	0	100	100
All	All	4597/4867 (94%)	4592 (100%)	5 (0%)	87	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	K	89	PRO
17	K	94	GLU
42	l	12	MET
42	l	78	LEU
47	q	85	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	19	HIS
9	C	176	HIS
9	C	190	HIS
10	D	40	GLN

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Mol	Chain	Res	Type
10	D	41	HIS
10	D	196	ASN
10	D	198	HIS
11	E	89	HIS
15	I	5	GLN
16	J	56	HIS
16	J	58	ASN
18	L	96	HIS
20	N	4	GLN
22	P	79	ASN
24	R	54	GLN
26	T	61	GLN
28	V	39	HIS
34	d	130	GLN
34	d	140	HIS
35	e	29	HIS
35	e	115	GLN
37	g	115	HIS
38	h	11	ASN
38	h	33	GLN
39	i	58	ASN
39	i	128	ASN
41	k	54	GLN
42	l	13	HIS
42	l	60	GLN
44	n	29	HIS
46	p	44	GLN
47	q	12	HIS
50	t	27	ASN
54	x	27	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Y	76/77 (98%)	10 (13%)	1 (1%)
30	Z	75/76 (98%)	9 (12%)	0
31	a	2749/2904 (94%)	264 (9%)	0
32	b	118/120 (98%)	15 (12%)	0
6	5	1/2 (50%)	1 (100%)	0
8	A	1510/1543 (97%)	292 (19%)	19 (1%)
All	All	4529/4722 (95%)	591 (13%)	20 (0%)

All (591) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
8	A	9	G
8	A	22	G
8	A	32	A
8	A	39	G
8	A	44	A
8	A	47	C
8	A	48	C
8	A	51	A
8	A	53	A
8	A	54	C
8	A	64	G
8	A	66	A
8	A	78	G
8	A	79	C
8	A	84	G
8	A	93	A
8	A	104	A
8	A	112	G
8	A	113	A
8	A	114	A
8	A	115	A
8	A	123	A
8	A	124	U
8	A	158	A
8	A	166	A
8	A	173	A
8	A	181	A
8	A	182	G
8	A	189	C
8	A	193	U
8	A	201	G
8	A	202	A
8	A	214	G
8	A	219	U
8	A	221	G
8	A	240	G
8	A	241	C
8	A	254	C
8	A	263	G
8	A	273	G
8	A	276	G

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Mol	Chain	Res	Type
8	A	295	A
8	A	302	C
8	A	303	A
8	A	304	C
8	A	321	G
8	A	326	C
8	A	328	G
8	A	332	U
8	A	341	U
8	A	343	G
8	A	346	C
8	A	347	A
8	A	358	G
8	A	362	G
8	A	372	U
8	A	373	G
8	A	380	G
8	A	383	U
8	A	384	G
8	A	385	A
8	A	387	G
8	A	388	A
8	A	395	U
8	A	399	G
8	A	400	U
8	A	403	U
8	A	410	C
8	A	412	U
8	A	418	G
8	A	423	G
8	A	425	A
8	A	426	A
8	A	428	G
8	A	431	G
8	A	433	A
8	A	436	G
8	A	437	U
8	A	441	U
8	A	442	A
8	A	448	G
8	A	449	C
8	A	450	U

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Mol	Chain	Res	Type
8	A	451	C
8	A	453	U
8	A	454	U
8	A	456	A
8	A	458	G
8	A	461	A
8	A	468	G
8	A	469	A
8	A	471	G
8	A	473	A
8	A	485	C
8	A	500	C
8	A	501	G7M
8	A	504	G
8	A	505	U
8	A	507	A
8	A	512	G
8	A	519	C
8	A	521	A
8	A	522	G
8	A	538	C
8	A	546	A
8	A	547	A
8	A	549	G
8	A	550	C
8	A	551	G
8	A	564	U
8	A	570	A
8	A	574	A
8	A	593	U
8	A	594	C
8	A	597	C
8	A	606	U
8	A	607	G
8	A	627	U
8	A	630	G
8	A	639	A
8	A	661	A
8	A	697	U
8	A	698	G
8	A	705	G
8	A	708	G

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Mol	Chain	Res	Type
8	A	721	A
8	A	729	G
8	A	751	A
8	A	767	U
8	A	768	A
8	A	776	A
8	A	783	G
8	A	784	C
8	A	789	A
8	A	791	C
8	A	801	U
8	A	802	U
8	A	803	G
8	A	815	C
8	A	817	U
8	A	818	G
8	A	819	A
8	A	820	G
8	A	826	G
8	A	827	C
8	A	888	A
8	A	900	G
8	A	908	C
8	A	909	A
8	A	910	C
8	A	916	G
8	A	934	U
8	A	940	G
8	A	943	A
8	A	945	G
8	A	946	C
8	A	949	A
8	A	950	G
8	A	951	A
8	A	966	U
8	A	967	G
8	A	977	G
8	A	978	A
8	A	979	A
8	A	980	G
8	A	983	U
8	A	987	G

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Mol	Chain	Res	Type
8	A	988	A
8	A	989	G
8	A	991	U
8	A	992	G
8	A	994	G
8	A	996	A
8	A	997	U
8	A	998	G
8	A	1000	G
8	A	1004	U
8	A	1005	C
8	A	1006	G
8	A	1007	G
8	A	1008	G
8	A	1027	G
8	A	1039	U
8	A	1040	C
8	A	1041	A
8	A	1068	G
8	A	1069	U
8	A	1073	G
8	A	1075	A
8	A	1080	G
8	A	1092	U
8	A	1093	C
8	A	1094	C
8	A	1096	U
8	A	1097	U
8	A	1098	G
8	A	1099	U
8	A	1111	C
8	A	1113	G
8	A	1114	C
8	A	1115	C
8	A	1123	C
8	A	1124	A
8	A	1126	A
8	A	1131	A
8	A	1132	C
8	A	1133	U
8	A	1134	G
8	A	1138	G

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Mol	Chain	Res	Type
8	A	1139	U
8	A	1158	G
8	A	1170	A
8	A	1171	A
8	A	1176	U
8	A	1187	A
8	A	1199	A
8	A	1201	A
8	A	1202	C
8	A	1212	A
8	A	1213	A
8	A	1229	G
8	A	1230	A
8	A	1232	G
8	A	1235	A
8	A	1236	C
8	A	1237	C
8	A	1238	U
8	A	1241	C
8	A	1242	G
8	A	1243	A
8	A	1244	G
8	A	1245	A
8	A	1246	G
8	A	1247	C
8	A	1248	A
8	A	1249	A
8	A	1250	G
8	A	1254	A
8	A	1259	A
8	A	1260	U
8	A	1274	G
8	A	1276	C
8	A	1279	G
8	A	1282	U
8	A	1283	G
8	A	1286	G
8	A	1287	U
8	A	1288	C
8	A	1289	U
8	A	1290	G
8	A	1291	C

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Mol	Chain	Res	Type
8	A	1294	C
8	A	1301	C
8	A	1304	U
8	A	1305	G
8	A	1312	G
8	A	1325	U
8	A	1327	G
8	A	1333	C
8	A	1337	A
8	A	1338	U
8	A	1344	G
8	A	1346	U
8	A	1372	A
8	A	1375	G
8	A	1393	G
8	A	1410	U
8	A	1420	A
8	A	1423	C
8	A	1426	C
8	A	1427	G
8	A	1430	A
8	A	1432	G
8	A	1433	G
8	A	1435	G
8	A	1441	C
8	A	1461	G
8	A	1466	A
8	A	1468	G
8	A	1471	G
8	A	1477	A
8	A	1480	U
8	A	1491	G
8	A	1495	C
8	A	1503	G
8	A	1504	G
8	A	1505	A
8	A	1507	C
8	A	1508	A
8	A	1509	C
8	A	1511	U
8	A	1512	C
29	Y	9	A

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Mol	Chain	Res	Type
29	Y	14	A
29	Y	20	G
29	Y	21	U
29	Y	22	A
29	Y	23	G
29	Y	46	G
29	Y	47	G
29	Y	74	A
29	Y	75	C
30	Z	17	U
30	Z	18	G
30	Z	20	U
30	Z	21	A
30	Z	29	A
30	Z	46	G
30	Z	47	U
30	Z	58	A
30	Z	76	A
31	a	4	U
31	a	34	U
31	a	63	A
31	a	71	A
31	a	74	A
31	a	75	G
31	a	101	A
31	a	102	U
31	a	118	A
31	a	119	A
31	a	120	U
31	a	139	U
31	a	142	A
31	a	163	C
31	a	181	A
31	a	196	A
31	a	199	A
31	a	215	G
31	a	216	A
31	a	221	A
31	a	222	A
31	a	233	A
31	a	248	G
31	a	272	A

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Mol	Chain	Res	Type
31	a	278	A
31	a	311	A
31	a	329	G
31	a	330	A
31	a	345	A
31	a	361	G
31	a	362	A
31	a	386	G
31	a	396	G
31	a	405	U
31	a	411	G
31	a	412	A
31	a	420	C
31	a	456	C
31	a	481	G
31	a	491	G
31	a	504	A
31	a	505	A
31	a	509	C
31	a	530	G
31	a	532	A
31	a	545	U
31	a	546	U
31	a	547	A
31	a	549	G
31	a	563	A
31	a	573	U
31	a	575	A
31	a	603	A
31	a	615	U
31	a	627	A
31	a	637	A
31	a	645	C
31	a	653	U
31	a	654	A
31	a	686	U
31	a	696	G
31	a	710	U
31	a	714	U
31	a	715	A
31	a	717	C
31	a	724	U

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Mol	Chain	Res	Type
31	a	725	G
31	a	726	G
31	a	730	A
31	a	740	C
31	a	747	5MU
31	a	748	G
31	a	775	G
31	a	776	G
31	a	782	A
31	a	784	G
31	a	785	G
31	a	805	G
31	a	812	C
31	a	827	U
31	a	828	U
31	a	846	U
31	a	858	G
31	a	859	G
31	a	881	G
31	a	890	C
31	a	891	G
31	a	896	A
31	a	910	A
31	a	914	G
31	a	915	C
31	a	931	U
31	a	946	C
31	a	961	C
31	a	974	G
31	a	983	A
31	a	996	A
31	a	1012	U
31	a	1013	C
31	a	1022	G
31	a	1027	A
31	a	1033	U
31	a	1034	G
31	a	1044	C
31	a	1046	A
31	a	1047	G
31	a	1111	A
31	a	1112	G

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Mol	Chain	Res	Type
31	a	1122	G
31	a	1123	C
31	a	1132	U
31	a	1135	C
31	a	1142	A
31	a	1253	A
31	a	1256	G
31	a	1271	G
31	a	1272	A
31	a	1273	U
31	a	1300	G
31	a	1301	A
31	a	1322	A
31	a	1365	A
31	a	1379	U
31	a	1383	A
31	a	1386	C
31	a	1416	G
31	a	1419	A
31	a	1428	C
31	a	1452	G
31	a	1482	G
31	a	1493	C
31	a	1515	A
31	a	1524	G
31	a	1535	A
31	a	1536	C
31	a	1537	G
31	a	1569	A
31	a	1578	U
31	a	1584	U
31	a	1585	C
31	a	1608	A
31	a	1647	U
31	a	1648	U
31	a	1674	G
31	a	1715	G
31	a	1730	C
31	a	1738	G
31	a	1756	G
31	a	1764	C
31	a	1773	A

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Mol	Chain	Res	Type
31	a	1791	A
31	a	1800	C
31	a	1801	A
31	a	1807	G
31	a	1808	A
31	a	1816	C
31	a	1829	A
31	a	1848	A
31	a	1873	G
31	a	1906	G
31	a	1912	A
31	a	1929	G
31	a	1930	G
31	a	1936	A
31	a	1938	A
31	a	1940	U
31	a	1955	U
31	a	1963	U
31	a	1964	G
31	a	1967	C
31	a	1970	A
31	a	1971	U
31	a	1972	G
31	a	1991	U
31	a	1993	U
31	a	2023	C
31	a	2027	G
31	a	2030	6MZ
31	a	2031	A
31	a	2033	A
31	a	2043	C
31	a	2052	A
31	a	2055	C
31	a	2056	G
31	a	2060	A
31	a	2061	G
31	a	2069	G7M
31	a	2198	A
31	a	2204	G
31	a	2225	A
31	a	2238	G
31	a	2239	G

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Mol	Chain	Res	Type
31	a	2283	C
31	a	2287	A
31	a	2288	A
31	a	2305	U
31	a	2306	C
31	a	2307	G
31	a	2308	G
31	a	2322	A
31	a	2325	G
31	a	2333	A
31	a	2345	G
31	a	2347	C
31	a	2353	G
31	a	2354	C
31	a	2361	G
31	a	2375	G
31	a	2376	A
31	a	2377	A
31	a	2379	G
31	a	2380	C
31	a	2383	G
31	a	2385	C
31	a	2396	G
31	a	2402	U
31	a	2403	C
31	a	2406	A
31	a	2425	A
31	a	2429	G
31	a	2441	U
31	a	2448	A
31	a	2474	U
31	a	2491	U
31	a	2502	G
31	a	2505	G
31	a	2518	A
31	a	2520	C
31	a	2525	G
31	a	2529	G
31	a	2531	A
31	a	2532	G
31	a	2533	U
31	a	2535	G

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Mol	Chain	Res	Type
31	a	2536	G
31	a	2547	A
31	a	2552	OMU
31	a	2554	U
31	a	2566	A
31	a	2567	G
31	a	2602	A
31	a	2608	G
31	a	2609	U
31	a	2613	U
31	a	2615	U
31	a	2629	U
31	a	2663	G
31	a	2689	U
31	a	2690	U
31	a	2714	G
31	a	2726	A
31	a	2729	G
31	a	2733	A
31	a	2748	A
31	a	2778	A
31	a	2791	G
31	a	2798	U
31	a	2820	A
31	a	2849	U
31	a	2861	U
31	a	2873	A
31	a	2880	C
31	a	2883	A
31	a	2898	U
32	b	3	C
32	b	7	G
32	b	8	C
32	b	23	G
32	b	25	U
32	b	35	C
32	b	42	C
32	b	45	A
32	b	56	G
32	b	67	G
32	b	89	U
32	b	90	C

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Mol	Chain	Res	Type
32	b	99	A
32	b	105	G
32	b	109	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	123	A
8	A	272	A
8	A	382	A
8	A	399	G
8	A	404	A
8	A	427	G
8	A	435	A
8	A	455	G
8	A	504	G
8	A	518	G
8	A	521	A
8	A	996	A
8	A	1039	U
8	A	1175	A
8	A	1244	G
8	A	1248	A
8	A	1440	C
8	A	1503	G
8	A	1511	U
29	Y	13	C

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

30 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	$\# Z > 2$
31	5MC	a	1962	31	18,22,23	0.35	0	26,32,35	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PSU	a	2580	58,31	18,21,22	4.76	8 (44%)	22,30,33	3.58	8 (36%)
31	PSU	a	955	31	18,21,22	4.79	7 (38%)	22,30,33	3.54	6 (27%)
31	PSU	a	2604	31	18,21,22	4.81	7 (38%)	22,30,33	3.55	7 (31%)
31	PSU	a	2457	31	18,21,22	4.79	8 (44%)	22,30,33	3.58	7 (31%)
31	2MG	a	2445	31	23,26,27	0.37	0	32,38,41	0.34	0
31	H2U	a	2449	31	18,21,22	0.71	1 (5%)	21,30,33	0.84	1 (4%)
31	6MZ	a	1618	31	22,25,26	2.82	5 (22%)	30,36,39	2.35	11 (36%)
17	IAS	K	119	17	6,7,8	0.95	0	6,8,10	0.92	0
42	4D4	l	81	42	9,11,12	0.82	0	8,13,15	1.22	0
31	5MU	a	747	31	19,22,23	0.44	0	28,32,35	0.87	1 (3%)
8	G7M	A	501	8	23,26,27	0.80	1 (4%)	35,39,42	0.92	1 (2%)
31	1MG	a	745	31	22,26,27	0.54	0	33,39,42	0.56	0
31	G7M	a	2069	31	23,26,27	0.69	1 (4%)	35,39,42	0.59	0
31	2MA	a	2503	59,58,31	22,25,26	1.56	5 (22%)	33,37,40	2.54	11 (33%)
8	MA6	A	1492	8	23,26,27	0.27	0	34,38,41	0.64	1 (2%)
31	2MG	a	1835	31	23,26,27	0.37	0	32,38,41	0.42	0
31	5MU	a	1939	58,31	19,22,23	0.29	0	28,32,35	0.42	0
31	OMU	a	2552	59,31	19,22,23	0.20	0	26,31,34	0.61	0
31	6MZ	a	2030	31	22,25,26	0.32	0	30,36,39	0.59	0
31	PSU	a	746	59,31	18,21,22	4.80	8 (44%)	22,30,33	3.52	7 (31%)
31	PSU	a	2504	58,31	18,21,22	4.77	7 (38%)	22,30,33	3.51	7 (31%)
31	OMC	a	2498	31	19,22,23	0.29	0	26,31,34	0.45	0
31	PSU	a	1917	31	18,21,22	4.79	7 (38%)	22,30,33	3.57	7 (31%)
31	PSU	a	2605	31	18,21,22	4.80	7 (38%)	22,30,33	3.54	7 (31%)
31	PSU	a	1911	31	18,21,22	4.82	8 (44%)	22,30,33	3.59	8 (36%)
42	MS6	l	82	42	5,7,8	0.40	0	2,7,9	0.76	0
31	3TD	a	1915	-	18,22,23	0.85	1 (5%)	22,32,35	0.75	0
31	OMG	a	2251	30,58,31	23,26,27	0.31	0	33,38,41	0.37	0
8	MA6	A	1493	8	23,26,27	0.25	0	34,38,41	0.70	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	5MC	a	1962	31	-	3/7/25/26	0/2/2/2
31	PSU	a	2580	58,31	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	a	955	31	-	0/7/25/26	0/2/2/2
31	PSU	a	2604	31	-	0/7/25/26	0/2/2/2
31	PSU	a	2457	31	-	0/7/25/26	0/2/2/2
31	2MG	a	2445	31	-	0/9/27/28	0/3/3/3
31	H2U	a	2449	31	-	0/7/38/39	0/2/2/2
31	6MZ	a	1618	31	-	0/9/27/28	0/3/3/3
17	IAS	K	119	17	-	0/7/7/8	-
42	4D4	l	81	42	-	1/11/12/14	-
31	5MU	a	747	31	-	1/7/25/26	0/2/2/2
8	G7M	A	501	8	-	3/7/25/26	0/3/3/3
31	1MG	a	745	31	-	0/7/25/26	0/3/3/3
31	G7M	a	2069	31	-	2/7/25/26	0/3/3/3
31	2MA	a	2503	59,58,31	-	1/7/25/26	0/3/3/3
8	MA6	A	1492	8	-	3/11/29/30	0/3/3/3
31	2MG	a	1835	31	-	0/9/27/28	0/3/3/3
31	5MU	a	1939	58,31	-	0/7/25/26	0/2/2/2
31	OMU	a	2552	59,31	-	2/9/27/28	0/2/2/2
31	6MZ	a	2030	31	-	1/9/27/28	0/3/3/3
31	PSU	a	746	59,31	-	1/7/25/26	0/2/2/2
31	PSU	a	2504	58,31	-	0/7/25/26	0/2/2/2
31	OMC	a	2498	31	-	0/9/27/28	0/2/2/2
31	PSU	a	1917	31	-	0/7/25/26	0/2/2/2
31	PSU	a	2605	31	-	0/7/25/26	0/2/2/2
31	PSU	a	1911	31	-	2/7/25/26	0/2/2/2
42	MS6	l	82	42	-	1/4/6/8	-
31	3TD	a	1915	-	-	0/7/25/26	0/2/2/2
31	OMG	a	2251	30,58,31	-	0/9/27/28	0/3/3/3
8	MA6	A	1493	8	-	3/11/29/30	0/3/3/3

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1911	PSU	C2-N1	14.04	1.55	1.36
31	a	2604	PSU	C2-N1	14.01	1.55	1.36
31	a	746	PSU	C2-N1	13.97	1.55	1.36
31	a	2457	PSU	C2-N1	13.93	1.55	1.36
31	a	2605	PSU	C2-N1	13.92	1.55	1.36
31	a	955	PSU	C2-N1	13.89	1.55	1.36
31	a	1917	PSU	C2-N1	13.89	1.55	1.36
31	a	2504	PSU	C2-N1	13.80	1.55	1.36
31	a	2580	PSU	C2-N1	13.67	1.55	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1911	PSU	C6-N1	13.16	1.58	1.36
31	a	2605	PSU	C6-N1	13.14	1.58	1.36
31	a	2580	PSU	C6-N1	13.07	1.57	1.36
31	a	2504	PSU	C6-N1	13.04	1.57	1.36
31	a	2604	PSU	C6-N1	13.04	1.57	1.36
31	a	2457	PSU	C6-N1	13.03	1.57	1.36
31	a	1917	PSU	C6-N1	13.02	1.57	1.36
31	a	746	PSU	C6-N1	13.02	1.57	1.36
31	a	955	PSU	C6-N1	13.01	1.57	1.36
31	a	1618	6MZ	C6-N6	12.07	1.47	1.34
31	a	2503	2MA	C6-N6	4.44	1.45	1.34
31	a	2604	PSU	C4-N3	-4.10	1.31	1.38
31	a	2457	PSU	C4-N3	-4.06	1.31	1.38
31	a	2580	PSU	C4-N3	-4.06	1.31	1.38
31	a	2605	PSU	C4-N3	-4.05	1.31	1.38
31	a	955	PSU	C4-N3	-4.01	1.31	1.38
31	a	1917	PSU	C4-N3	-4.01	1.31	1.38
31	a	1911	PSU	C4-N3	-3.91	1.31	1.38
31	a	2504	PSU	C4-N3	-3.88	1.31	1.38
31	a	746	PSU	C4-N3	-3.86	1.31	1.38
31	a	1915	3TD	C6-C5	3.24	1.39	1.35
31	a	746	PSU	C2-N3	3.04	1.42	1.37
31	a	1917	PSU	C2-N3	3.01	1.42	1.37
31	a	1911	PSU	C2-N3	2.99	1.42	1.37
31	a	2504	PSU	C2-N3	2.98	1.42	1.37
31	a	2580	PSU	C2-N3	2.97	1.42	1.37
31	a	2503	2MA	C5-C4	-2.96	1.33	1.39
31	a	955	PSU	C2-N3	2.90	1.42	1.37
31	a	2605	PSU	C2-N3	2.86	1.42	1.37
31	a	955	PSU	C6-C5	-2.84	1.32	1.35
31	a	2457	PSU	C2-N3	2.82	1.42	1.37
31	a	2604	PSU	C6-C5	-2.82	1.32	1.35
31	a	2604	PSU	C2-N3	2.80	1.42	1.37
31	a	1917	PSU	C6-C5	-2.76	1.32	1.35
31	a	2504	PSU	O4-C4	-2.70	1.18	1.23
31	a	2504	PSU	C6-C5	-2.64	1.32	1.35
31	a	1618	6MZ	C5-C4	-2.63	1.34	1.39
31	a	2503	2MA	C5-N7	-2.62	1.34	1.39
31	a	1911	PSU	C6-C5	-2.62	1.32	1.35
31	a	2604	PSU	O4-C4	-2.61	1.18	1.23
31	a	2457	PSU	O4-C4	-2.61	1.18	1.23
31	a	2605	PSU	O4-C4	-2.60	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	746	PSU	O4-C4	-2.58	1.18	1.23
31	a	1917	PSU	O4-C4	-2.58	1.18	1.23
31	a	746	PSU	C6-C5	-2.57	1.32	1.35
31	a	955	PSU	O4-C4	-2.56	1.18	1.23
31	a	2580	PSU	O4-C4	-2.53	1.18	1.23
8	A	501	G7M	C8-N7	2.52	1.37	1.33
31	a	1911	PSU	O4-C4	-2.47	1.18	1.23
31	a	2503	2MA	C6-N1	-2.45	1.31	1.35
31	a	2580	PSU	O4'-C1'	-2.45	1.40	1.43
31	a	2605	PSU	C6-C5	-2.44	1.32	1.35
31	a	2457	PSU	C6-C5	-2.39	1.32	1.35
31	a	2069	G7M	C8-N7	2.35	1.37	1.33
31	a	2580	PSU	O2-C2	-2.35	1.18	1.23
31	a	955	PSU	O2-C2	-2.31	1.18	1.23
31	a	2457	PSU	O2-C2	-2.30	1.18	1.23
31	a	1917	PSU	O2-C2	-2.27	1.18	1.23
31	a	2605	PSU	O2-C2	-2.27	1.18	1.23
31	a	1911	PSU	O2-C2	-2.25	1.18	1.23
31	a	2604	PSU	O2-C2	-2.25	1.18	1.23
31	a	2504	PSU	O2-C2	-2.25	1.18	1.23
31	a	746	PSU	O2-C2	-2.21	1.18	1.23
31	a	2580	PSU	C6-C5	-2.20	1.32	1.35
31	a	2449	H2U	C2-N3	-2.19	1.34	1.38
31	a	1618	6MZ	C5-N7	-2.13	1.35	1.39
31	a	1618	6MZ	C8-N9	-2.12	1.33	1.37
31	a	746	PSU	O4'-C1'	-2.10	1.40	1.43
31	a	1911	PSU	O4'-C1'	-2.05	1.41	1.43
31	a	1618	6MZ	C8-N7	2.04	1.35	1.31
31	a	2503	2MA	C8-N9	-2.02	1.33	1.37
31	a	2457	PSU	O4'-C1'	-2.01	1.41	1.43

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1917	PSU	C6-N1-C2	-13.04	109.34	122.68
31	a	2580	PSU	C6-N1-C2	-13.01	109.38	122.68
31	a	955	PSU	C6-N1-C2	-12.84	109.56	122.68
31	a	1911	PSU	C6-N1-C2	-12.83	109.56	122.68
31	a	2457	PSU	C6-N1-C2	-12.82	109.57	122.68
31	a	2604	PSU	C6-N1-C2	-12.81	109.58	122.68
31	a	746	PSU	C6-N1-C2	-12.77	109.62	122.68
31	a	2605	PSU	C6-N1-C2	-12.69	109.70	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	2504	PSU	C6-N1-C2	-12.67	109.72	122.68
31	a	2503	2MA	CM2-C2-N3	7.00	128.08	117.15
31	a	2457	PSU	C6-C5-C4	6.69	122.87	118.20
31	a	2503	2MA	C5-C4-N3	-6.64	119.72	127.19
31	a	2604	PSU	C6-C5-C4	6.63	122.83	118.20
31	a	1917	PSU	C6-C5-C4	6.63	122.83	118.20
31	a	1911	PSU	C6-C5-C4	6.62	122.82	118.20
31	a	2605	PSU	C6-C5-C4	6.54	122.77	118.20
31	a	955	PSU	C6-C5-C4	6.33	122.63	118.20
31	a	2504	PSU	C6-C5-C4	6.27	122.58	118.20
31	a	2580	PSU	C6-C5-C4	6.14	122.49	118.20
31	a	746	PSU	C6-C5-C4	5.76	122.22	118.20
31	a	1911	PSU	N1-C2-N3	5.56	121.44	115.13
31	a	2457	PSU	N1-C2-N3	5.54	121.40	115.13
31	a	1618	6MZ	C5-C4-N3	-5.53	119.53	126.75
31	a	2580	PSU	N1-C2-N3	5.49	121.35	115.13
31	a	2604	PSU	N1-C2-N3	5.48	121.34	115.13
31	a	2605	PSU	N1-C2-N3	5.47	121.33	115.13
31	a	955	PSU	N1-C2-N3	5.46	121.32	115.13
31	a	2504	PSU	N1-C2-N3	5.45	121.30	115.13
31	a	1618	6MZ	N1-C2-N3	-5.36	120.21	128.60
31	a	746	PSU	N1-C2-N3	5.27	121.10	115.13
31	a	1917	PSU	N1-C2-N3	5.26	121.09	115.13
31	a	1618	6MZ	N9-C8-N7	-4.52	107.73	113.91
31	a	1618	6MZ	C4-C5-C6	4.49	120.29	116.81
31	a	2503	2MA	N9-C8-N7	-4.24	108.11	113.91
31	a	2503	2MA	N6-C6-N1	-4.19	111.12	117.03
31	a	2503	2MA	N3-C4-N9	4.02	132.57	126.99
31	a	1618	6MZ	C2-N3-C4	3.55	120.14	111.75
31	a	1917	PSU	O2-C2-N1	-3.52	118.92	122.79
31	a	1618	6MZ	C5-N7-C8	3.48	108.45	103.51
31	a	2503	2MA	CM2-C2-N1	-3.48	111.72	117.15
31	a	1911	PSU	O2-C2-N1	-3.48	118.96	122.79
31	a	746	PSU	O2-C2-N1	-3.43	119.01	122.79
31	a	2504	PSU	O2-C2-N1	-3.40	119.05	122.79
31	a	2580	PSU	O2-C2-N1	-3.37	119.08	122.79
31	a	955	PSU	O2-C2-N1	-3.36	119.09	122.79
31	a	2504	PSU	C4-N3-C2	-3.36	121.50	126.34
31	a	1911	PSU	C4-N3-C2	-3.31	121.57	126.34
31	a	2449	H2U	C4-N3-C2	-3.24	123.10	125.79
31	a	2605	PSU	C4-N3-C2	-3.23	121.68	126.34
31	a	955	PSU	C4-N3-C2	-3.23	121.69	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	2604	PSU	C4-N3-C2	-3.21	121.71	126.34
31	a	2457	PSU	O2-C2-N1	-3.20	119.27	122.79
31	a	2605	PSU	O2-C2-N1	-3.19	119.27	122.79
31	a	2457	PSU	C4-N3-C2	-3.19	121.74	126.34
31	a	746	PSU	C4-N3-C2	-3.13	121.82	126.34
8	A	501	G7M	C2'-C3'-C4'	-3.13	96.56	102.64
31	a	2604	PSU	O2-C2-N1	-3.08	119.40	122.79
31	a	1618	6MZ	N3-C4-N9	3.08	132.16	127.08
31	a	2503	2MA	C5-N7-C8	3.07	107.88	103.51
31	a	2503	2MA	N3-C2-N1	-3.00	120.20	125.72
31	a	2580	PSU	C4-N3-C2	-2.99	122.03	126.34
8	A	1492	MA6	C2-N1-C6	2.94	118.71	111.75
31	a	1917	PSU	C4-N3-C2	-2.85	122.23	126.34
8	A	1493	MA6	C2-N1-C6	2.78	118.31	111.75
31	a	2504	PSU	C5-C4-N3	2.73	122.76	116.58
31	a	1618	6MZ	C9-N6-C6	-2.71	120.54	122.87
31	a	746	PSU	C5-C4-N3	2.69	122.67	116.58
31	a	2605	PSU	C5-C4-N3	2.68	122.64	116.58
31	a	955	PSU	C5-C4-N3	2.64	122.56	116.58
31	a	1911	PSU	C5-C4-N3	2.64	122.56	116.58
31	a	2604	PSU	C5-C4-N3	2.62	122.52	116.58
31	a	2457	PSU	C5-C4-N3	2.61	122.48	116.58
31	a	746	PSU	C3'-C2'-C1'	2.58	104.64	101.64
31	a	1618	6MZ	C4-C5-N7	-2.57	107.49	110.62
31	a	2580	PSU	C5-C4-N3	2.55	122.35	116.58
31	a	2503	2MA	C4-N9-C1'	-2.55	120.53	126.59
31	a	747	5MU	O3'-C3'-C4'	2.51	118.32	111.05
31	a	2580	PSU	O4'-C1'-C2'	2.43	108.56	105.14
31	a	1917	PSU	C5-C4-N3	2.42	122.05	116.58
31	a	2503	2MA	C5-C6-N6	2.30	128.43	123.43
31	a	2457	PSU	O4'-C1'-C2'	2.21	108.26	105.14
31	a	1618	6MZ	C5-C4-N9	2.17	108.31	105.78
31	a	1911	PSU	O4'-C1'-C2'	2.17	108.20	105.14
31	a	1618	6MZ	C4-N9-C8	2.10	108.01	105.73
31	a	1911	PSU	O4-C4-C5	-2.10	118.56	124.05
31	a	2503	2MA	C4-N9-C8	2.09	107.99	105.73
31	a	2504	PSU	O4-C4-C5	-2.04	118.73	124.05
31	a	1917	PSU	O4-C4-C5	-2.02	118.75	124.05
31	a	2605	PSU	O4'-C1'-C2'	2.01	107.98	105.14
31	a	2580	PSU	O4-C4-C5	-2.01	118.79	124.05
31	a	2604	PSU	O4-C4-C5	-2.00	118.81	124.05

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	501	G7M	O4'-C4'-C5'-O5'
8	A	501	G7M	C3'-C4'-C5'-O5'
8	A	1492	MA6	C5-C6-N6-C10
8	A	1493	MA6	C5-C6-N6-C9
8	A	1493	MA6	C5-C6-N6-C10
31	a	2552	OMU	C3'-C4'-C5'-O5'
31	a	2552	OMU	O4'-C4'-C5'-O5'
8	A	1493	MA6	N1-C6-N6-C10
8	A	1492	MA6	C5-C6-N6-C9
42	l	82	MS6	CB-CG-SD-CE
31	a	747	5MU	C3'-C4'-C5'-O5'
31	a	1911	PSU	O4'-C4'-C5'-O5'
8	A	1492	MA6	N1-C6-N6-C10
8	A	501	G7M	C4'-C5'-O5'-P
31	a	2030	6MZ	O4'-C4'-C5'-O5'
31	a	2580	PSU	O4'-C4'-C5'-O5'
31	a	1962	5MC	C2'-C1'-N1-C6
31	a	1962	5MC	O4'-C1'-N1-C6
31	a	1911	PSU	C3'-C4'-C5'-O5'
31	a	746	PSU	O4'-C1'-C5-C6
31	a	1962	5MC	O4'-C1'-N1-C2
31	a	2069	G7M	C4'-C5'-O5'-P
31	a	2503	2MA	O4'-C4'-C5'-O5'
31	a	2069	G7M	O4'-C4'-C5'-O5'
42	l	81	4D4	O-C-CA-CB

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	1618	6MZ	1	0
17	K	119	IAS	1	0
31	a	747	5MU	2	0
8	A	501	G7M	3	0
8	A	1492	MA6	2	0
31	a	2552	OMU	1	0
42	l	82	MS6	1	0
31	a	1915	3TD	1	0
8	A	1493	MA6	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 421 ligands modelled in this entry, 420 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	PRO	Y	101	29	5,7,8	0.70	0	7,8,10	1.36	1 (14%)

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
60	PRO	Y	101	29	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Y	101	PRO	CB-CA-N	-3.11	96.00	104.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	Y	101	PRO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
31	a	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	2029:G	O3'	2030:6MZ	P	3.08
1	a	1914:C	O3'	1915:3TD	P	3.06
1	a	1915:3TD	O3'	1916:A	P	3.06
1	a	2030:6MZ	O3'	2031:A	P	2.92
1	a	1618:6MZ	O3'	1619:G	P	2.73

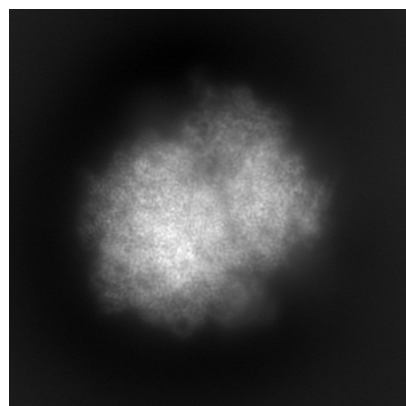
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53553. These allow visual inspection of the internal detail of the map and identification of artifacts.

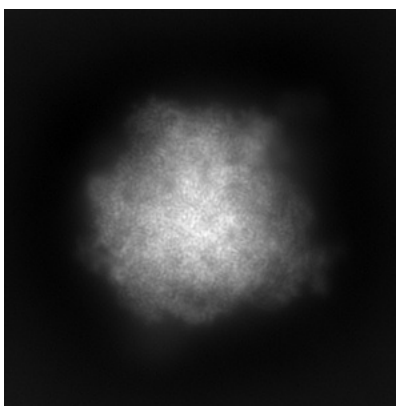
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

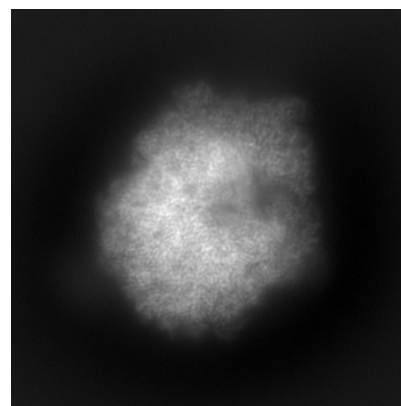
6.1.1 Primary map



X

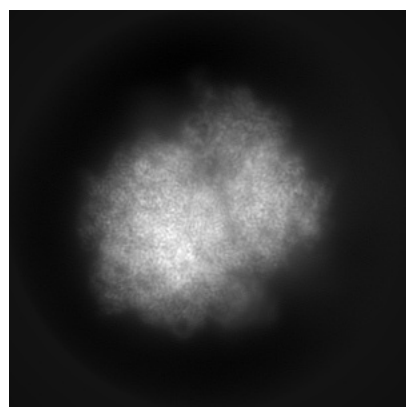


Y

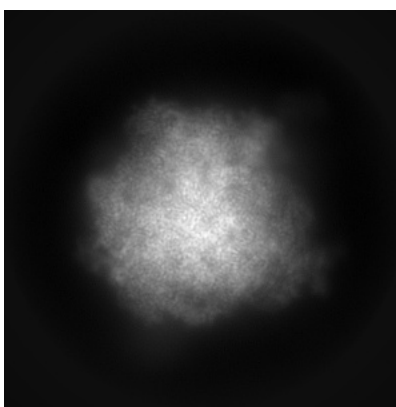


Z

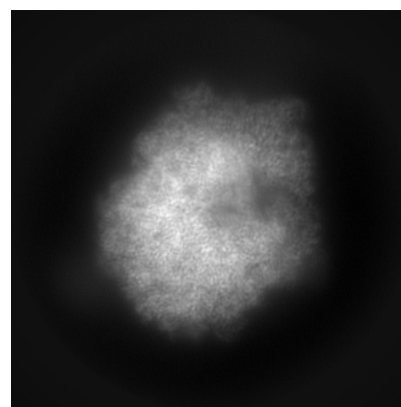
6.1.2 Raw map



X



Y

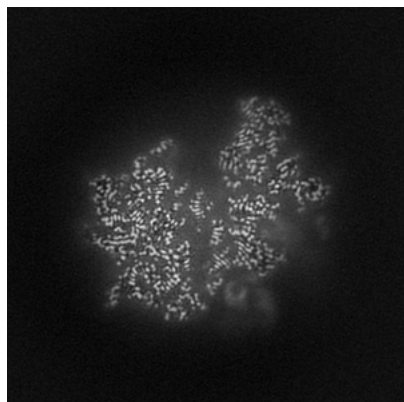


Z

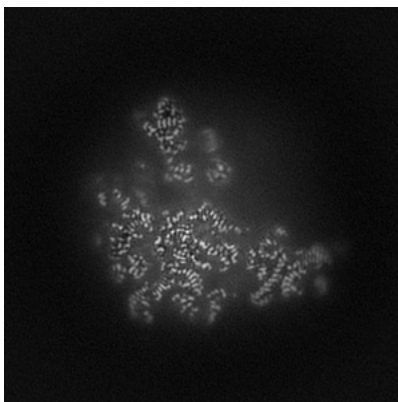
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

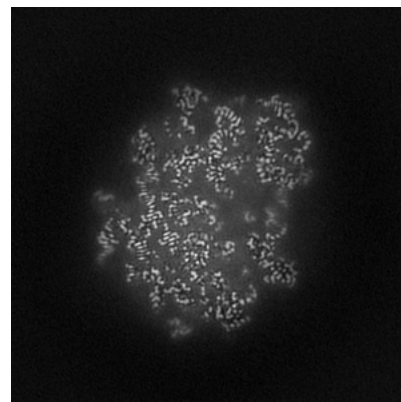
6.2.1 Primary map



X Index: 180

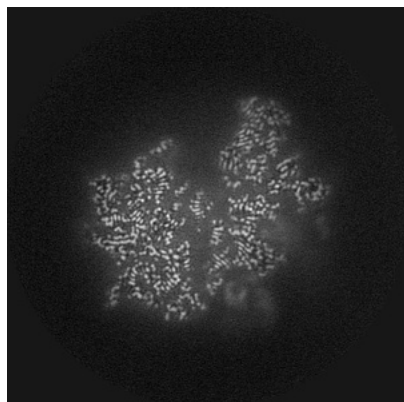


Y Index: 180

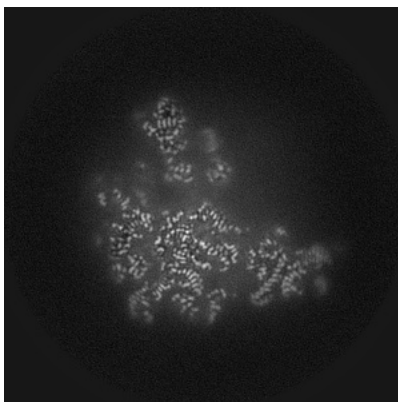


Z Index: 180

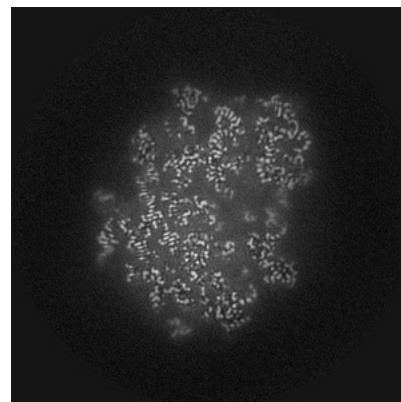
6.2.2 Raw map



X Index: 180



Y Index: 180

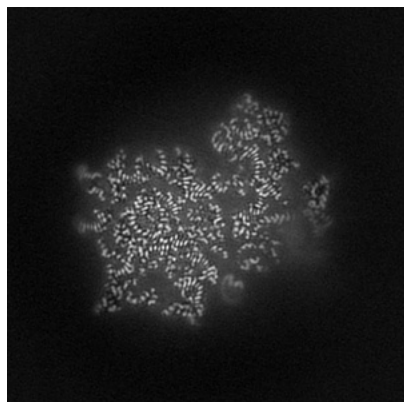


Z Index: 180

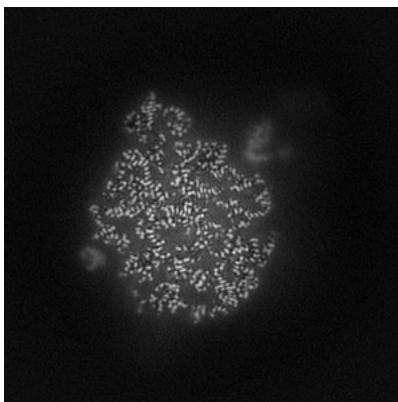
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

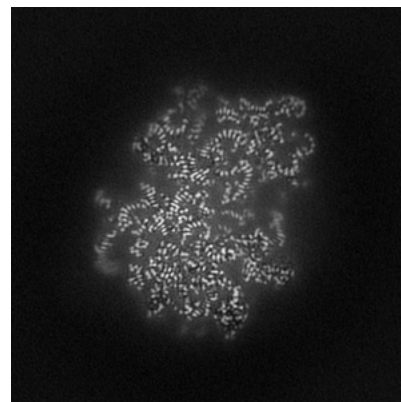
6.3.1 Primary map



X Index: 166

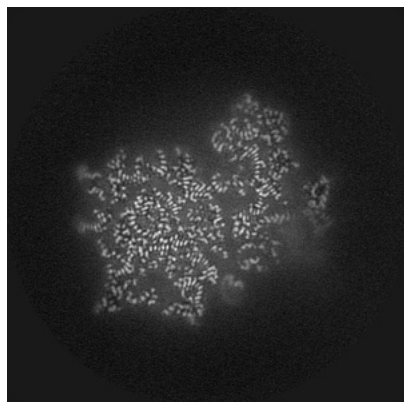


Y Index: 143

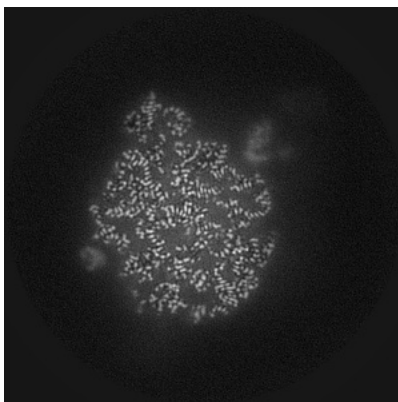


Z Index: 172

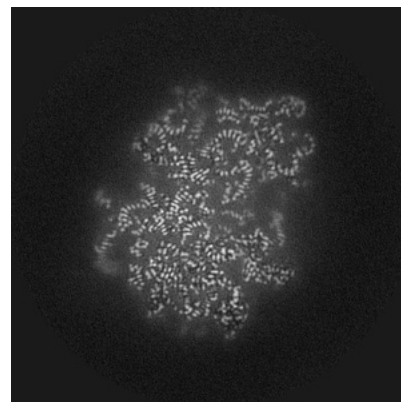
6.3.2 Raw map



X Index: 166



Y Index: 143

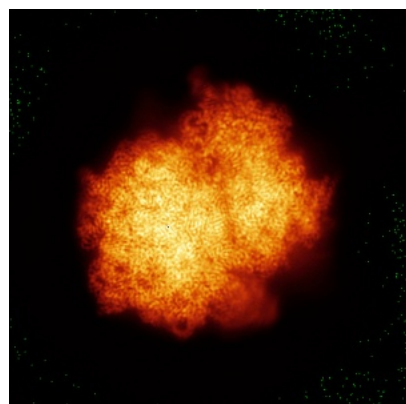


Z Index: 172

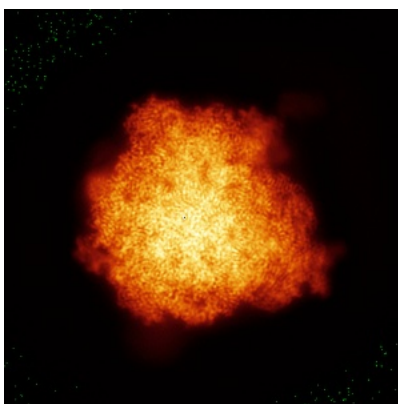
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

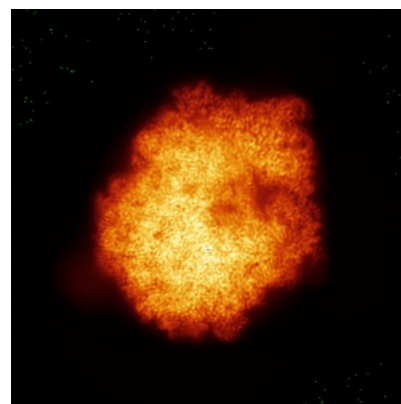
6.4.1 Primary map



X

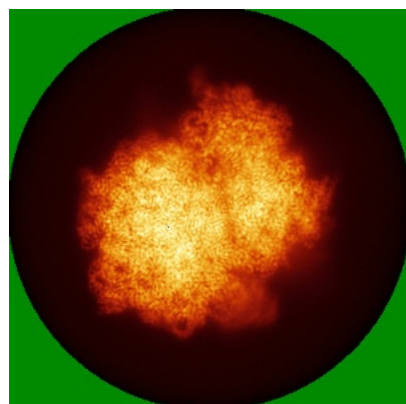


Y

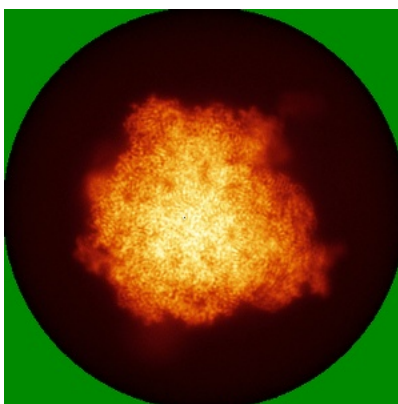


Z

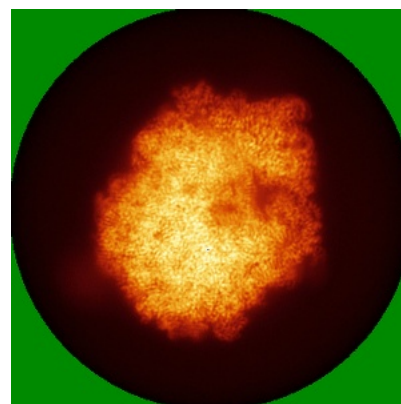
6.4.2 Raw map



X



Y

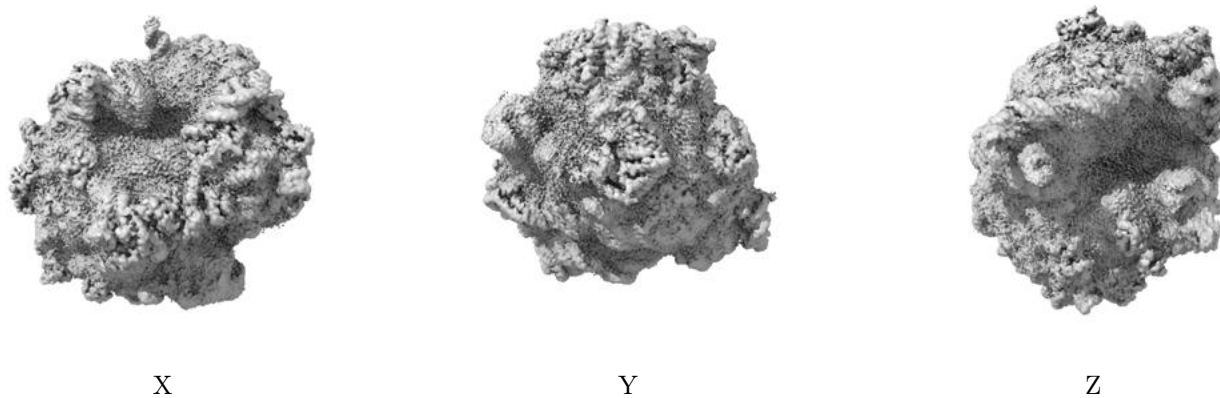


Z

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

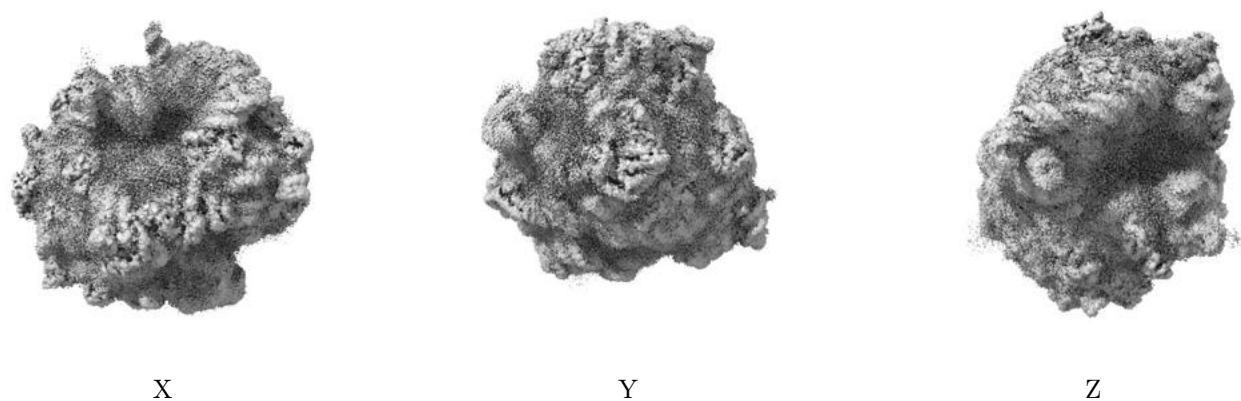
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00692. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

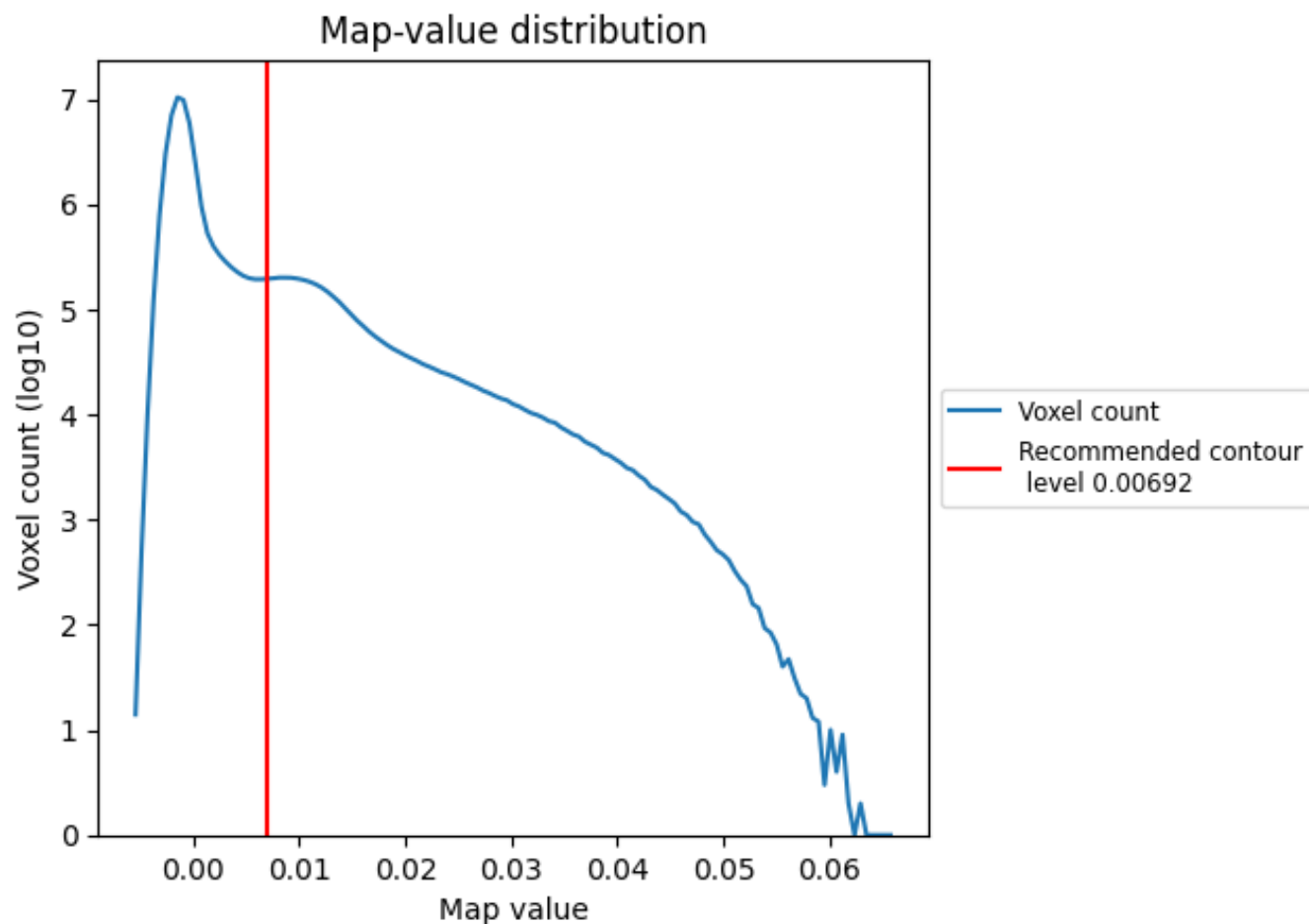
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

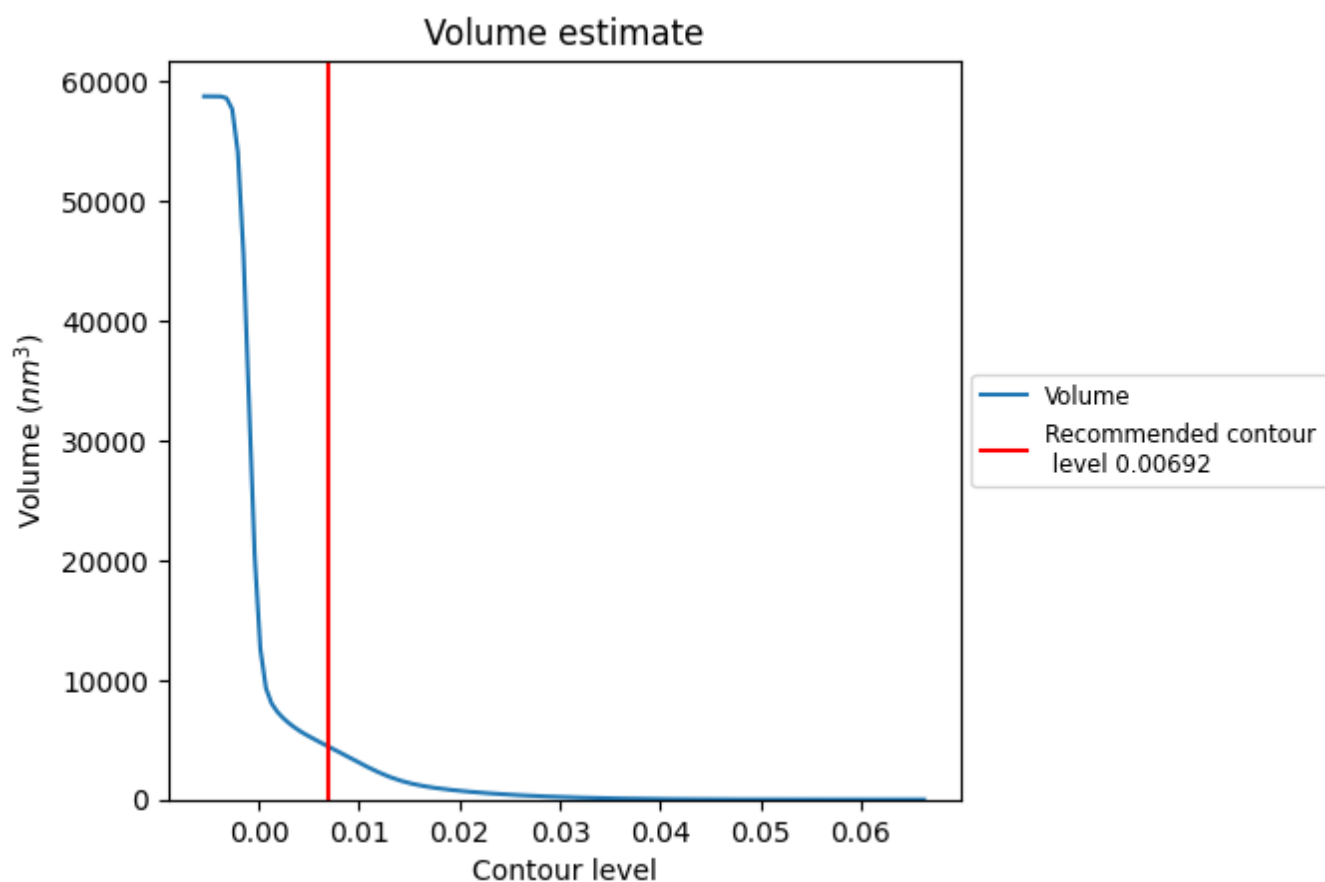
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

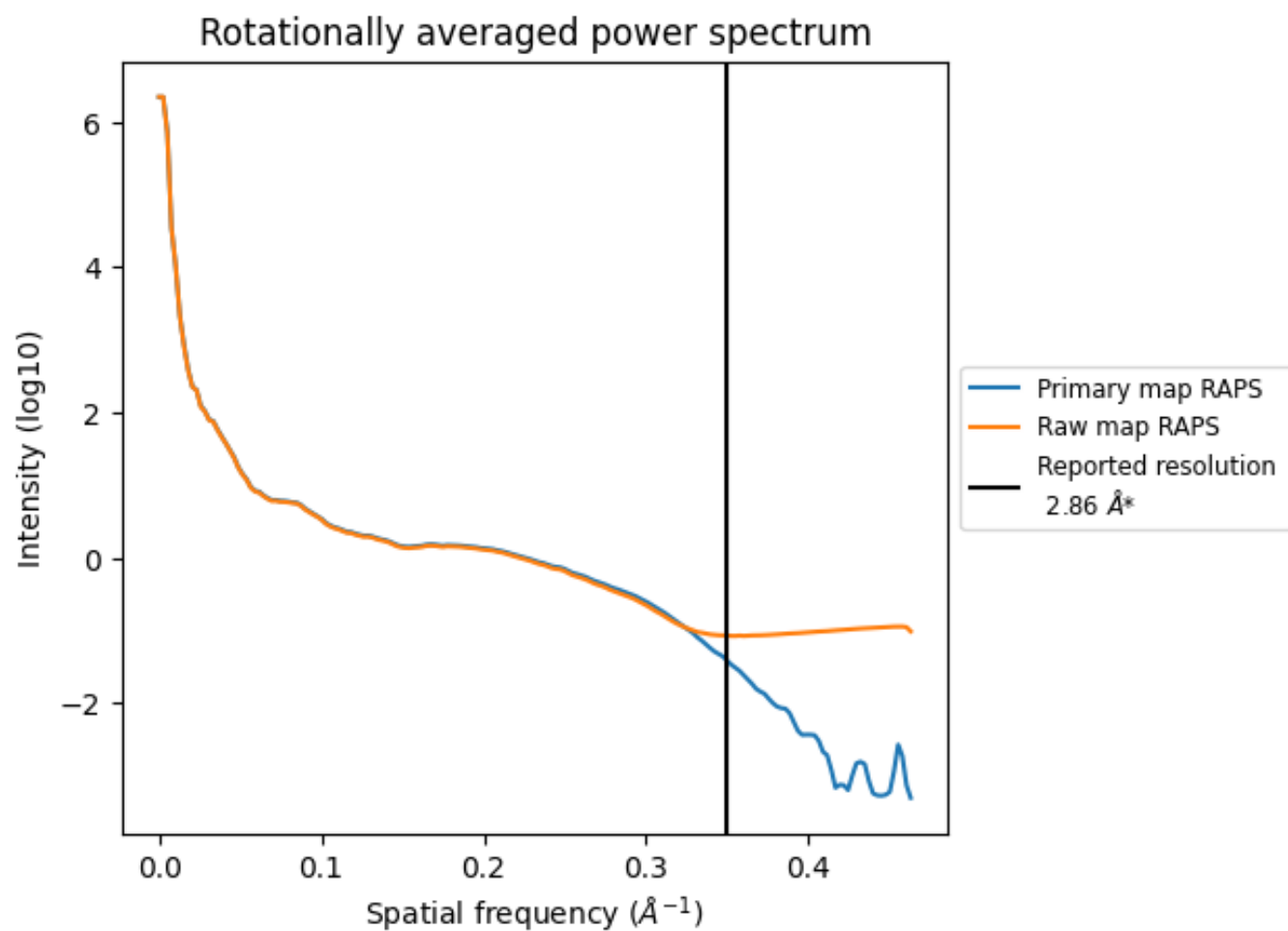
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4461 nm³; this corresponds to an approximate mass of 4030 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 ⓘ

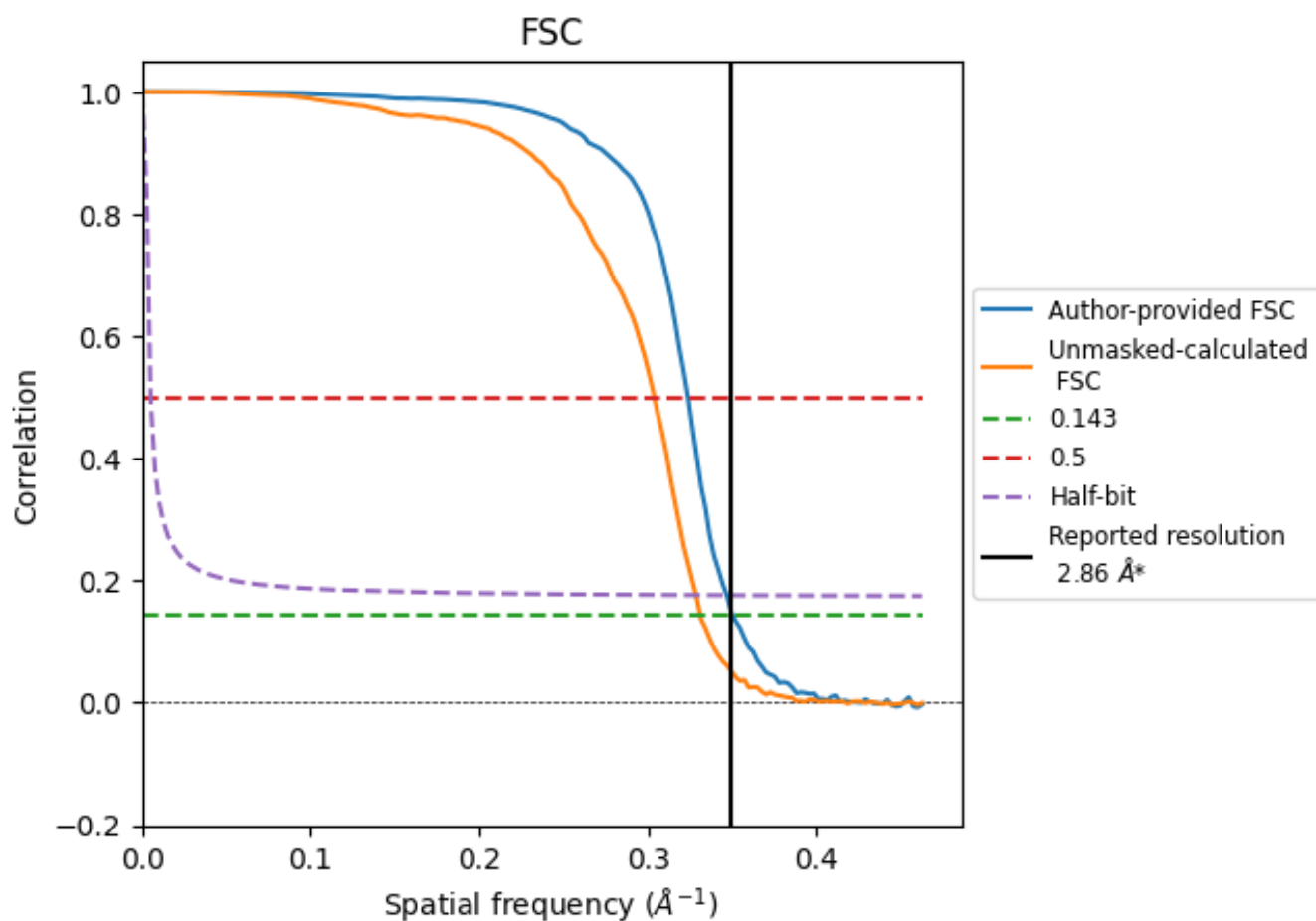


*Reported resolution corresponds to spatial frequency of 0.350 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.350 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

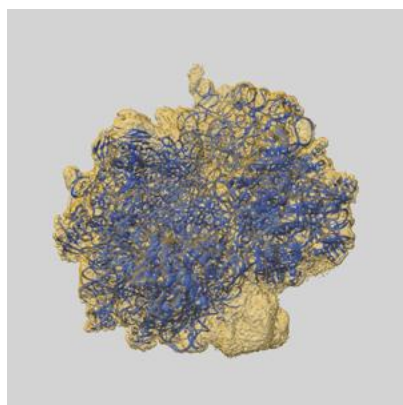
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.85	3.09	2.88
Unmasked-calculated*	3.02	3.29	3.04

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

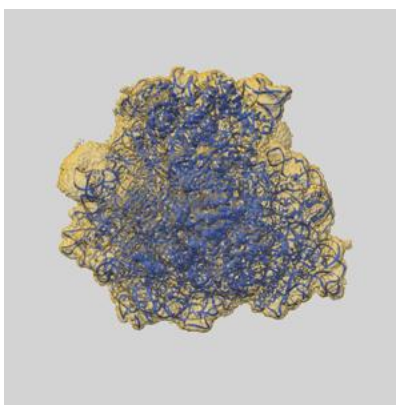
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53553 and PDB model 9R3A. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

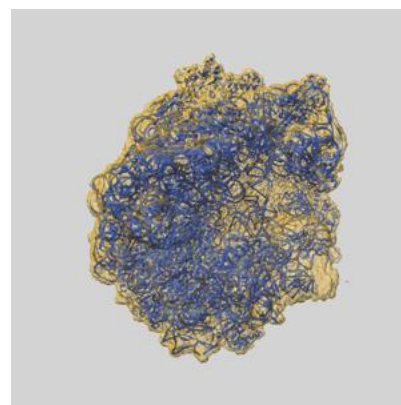
9.1 Map-model overlay [i](#)



X



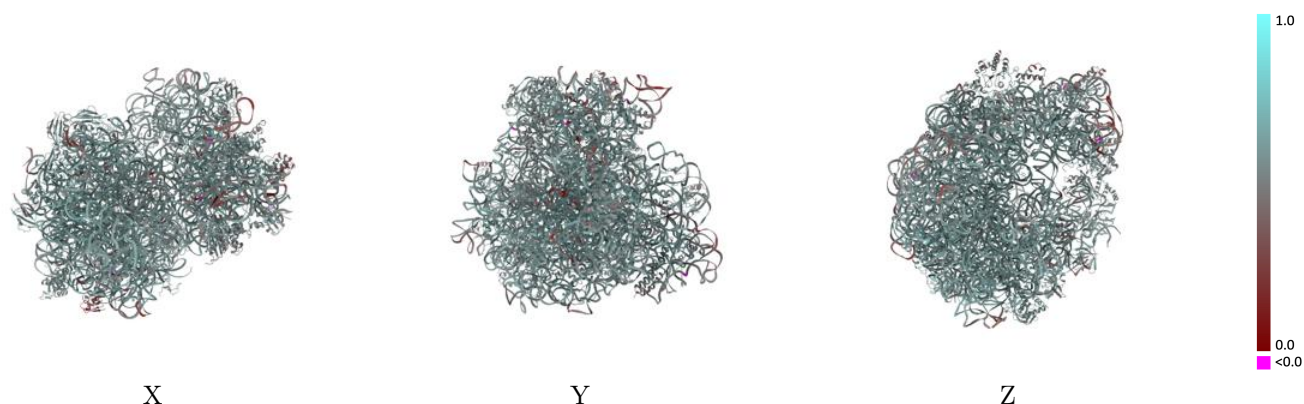
Y



Z

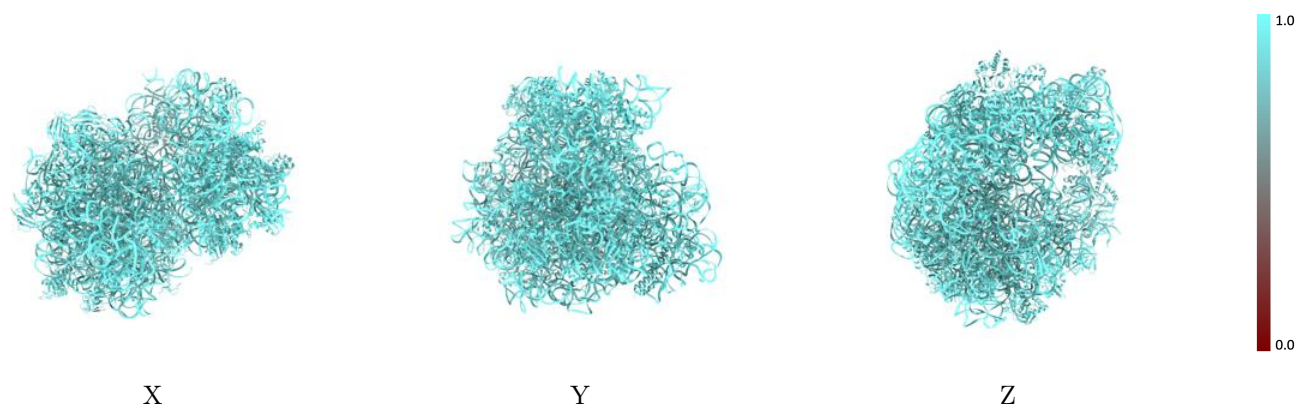
The images above show the 3D surface view of the map at the recommended contour level 0.00692 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



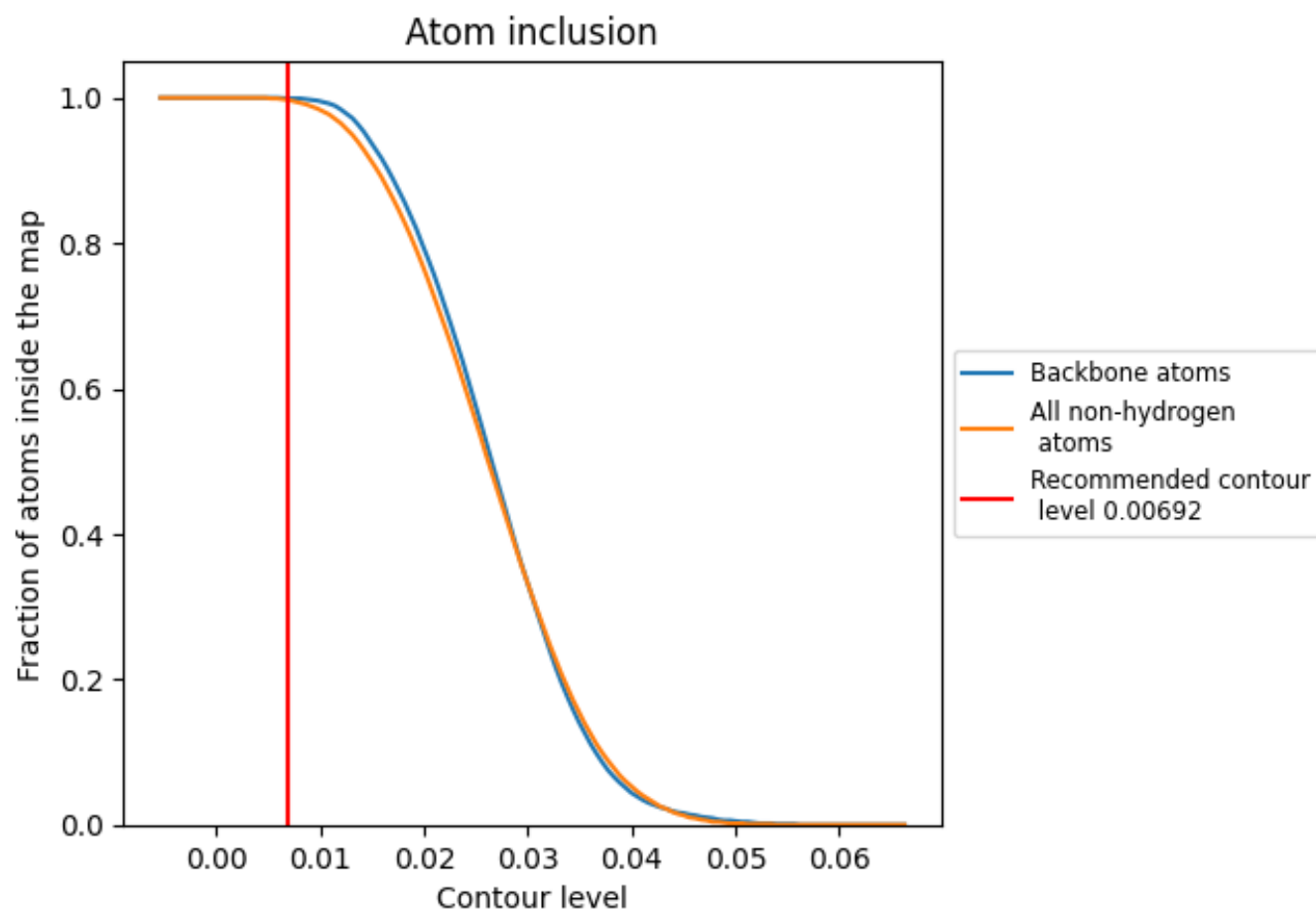
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00692).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00692) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9970	 0.5740
0	 1.0000	 0.5800
1	 1.0000	 0.6170
2	 1.0000	 0.6160
3	 1.0000	 0.5990
4	 0.9770	 0.5040
5	 1.0000	 0.6030
6	 1.0000	 0.4860
A	 0.9990	 0.5620
C	 0.9870	 0.5500
D	 0.9840	 0.5400
E	 1.0000	 0.5780
F	 0.9930	 0.5510
G	 0.9970	 0.5160
H	 0.9950	 0.5710
I	 0.9860	 0.5480
J	 0.9570	 0.5180
K	 0.9990	 0.4980
L	 1.0000	 0.5780
M	 0.9970	 0.5440
N	 0.9950	 0.5530
O	 1.0000	 0.5600
P	 0.9820	 0.5440
Q	 1.0000	 0.5510
R	 1.0000	 0.5580
S	 0.9940	 0.5630
T	 0.9970	 0.5280
U	 1.0000	 0.4940
V	 0.9810	 0.5080
Y	 1.0000	 0.5680
Z	 1.0000	 0.5610
a	 1.0000	 0.5930
b	 1.0000	 0.5790
c	 1.0000	 0.6120
d	 0.9950	 0.5990



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Chain	Atom inclusion	Q-score
e	 0.9680	 0.5660
f	 0.9920	 0.5450
g	 0.9800	 0.5420
h	 0.9970	 0.5520
i	 0.9990	 0.5960
j	 1.0000	 0.5940
k	 0.9590	 0.3750
l	 1.0000	 0.5280
m	 1.0000	 0.6040
n	 0.9720	 0.5620
o	 1.0000	 0.5960
p	 1.0000	 0.5980
q	 0.9720	 0.5870
r	 0.9990	 0.5940
s	 0.9970	 0.5660
t	 0.9840	 0.5530
u	 0.9780	 0.5680
v	 1.0000	 0.6040
w	 1.0000	 0.5950
x	 0.9750	 0.5260
y	 1.0000	 0.5880
z	 1.0000	 0.6010