



## Full wwPDB EM Validation Report ⓘ

May 26, 2026 – 02:54 pm BST

PDB ID : 9RBF / pdb\_00009rbf  
EMDB ID : EMD-53892  
Title : Structure of a stalled E. coli 70S RNC-NuoK-86 in complex with the membrane protein insertase SecYEG-YidC  
Authors : Rosales-Hernandez, C.; Busch, M.; Kamel, M.; Beckmann, R.; Kedrov, A.  
Deposited on : 2025-05-22  
Resolution : 2.44 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

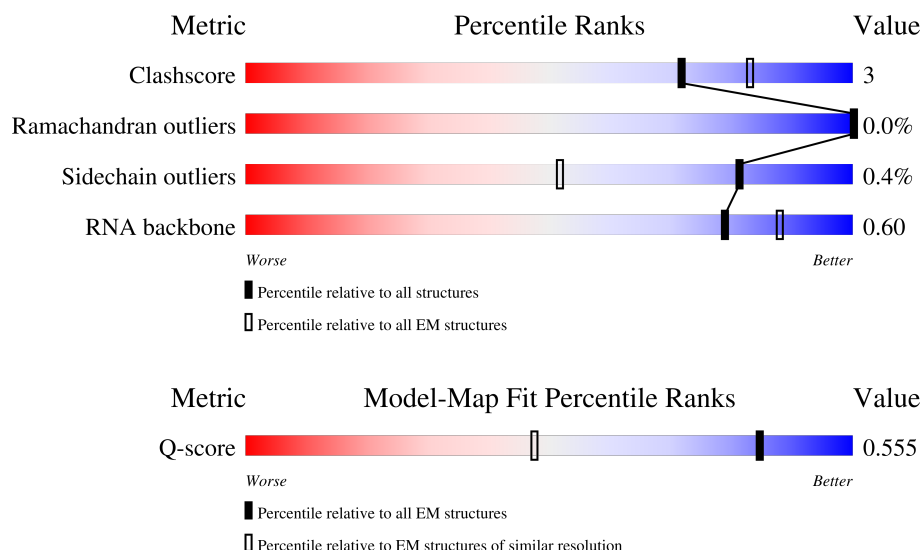
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 2.44 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.



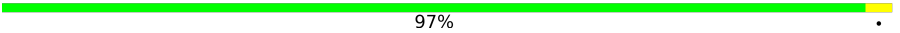


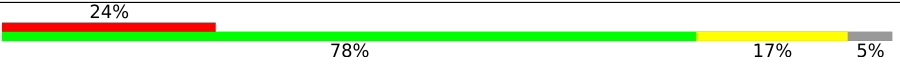



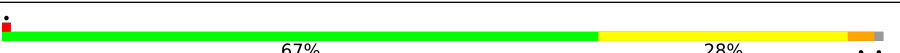
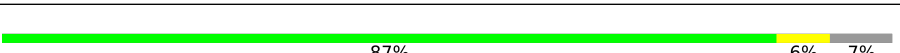
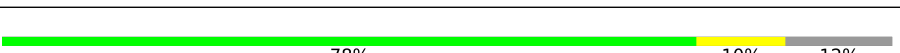
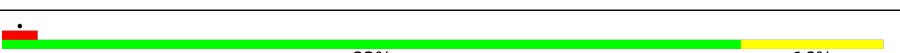
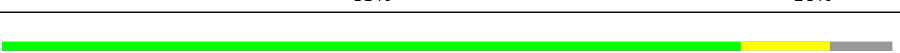

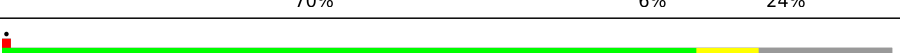
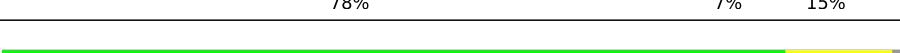

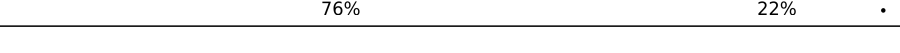
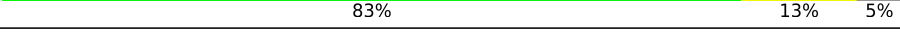




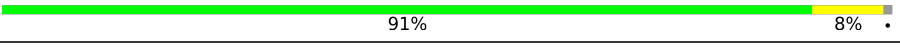
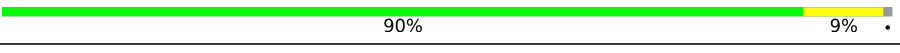
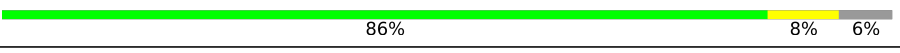
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5856 ( 1.94 - 2.94 )

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

Mol	Chain	Length	Quality of chain
1	0	55	 82% 11% 7%
2	1	46	 96%
3	2	65	 89% 9%







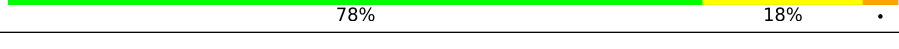
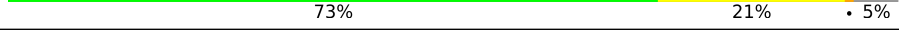
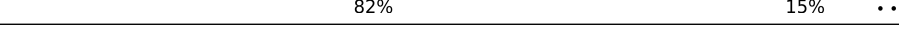
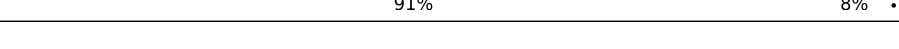
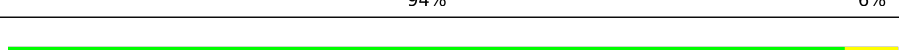
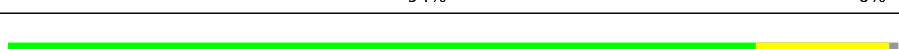
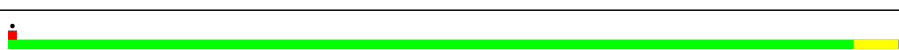

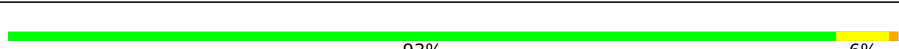
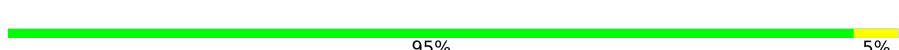
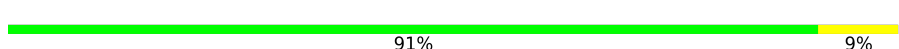


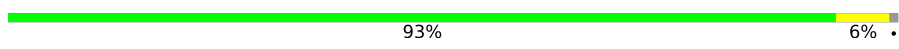
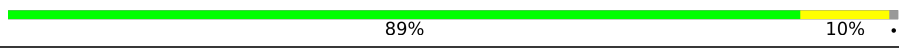
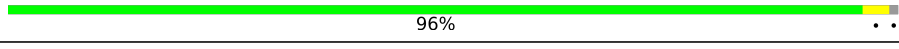
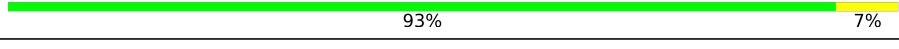
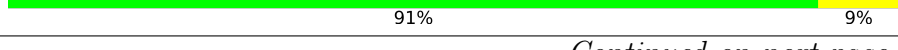

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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	5	2	
7	6	443	
8	7	127	
9	8	110	
10	9	548	
11	A	1542	
12	B	241	
13	C	233	
14	D	206	
15	E	167	
16	F	135	
17	G	179	
18	H	130	
19	I	130	
20	J	103	
21	K	129	
22	L	124	
23	M	118	
24	N	101	
25	O	89	
26	P	82	
27	Q	84	
28	R	75	



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Mol	Chain	Length	Quality of chain
29	S	92	
30	T	87	
31	U	71	
32	V	119	
33	X	9	
34	Y	77	
35	Z	77	
36	a	2904	
37	b	120	
38	c	273	
39	d	209	
40	e	201	
41	f	179	
42	g	177	
43	h	149	
44	i	142	
45	j	123	
46	k	144	
47	l	136	
48	m	127	
49	n	117	
50	o	115	
51	p	118	
52	q	103	
53	r	110	

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Mol	Chain	Length	Quality of chain
54	s	100	 89% 7%
55	t	104	 95%
56	u	94	 81% 19%
57	v	85	 86% 6% 8%
58	w	78	 91% 8%
59	x	63	 87% 11%
60	y	59	 90% 8%
61	z	57	 91% 7%

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 150736 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	51	Total	C	N	O	0	0
			417	269	76	72		

- 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 Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	421	Total	C	N	O	S	0	0
			3260	2158	535	550	17		

- Molecule 8 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	114	Total	C	N	O	S	0	0
			873	579	149	142	3		

- Molecule 9 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	56	Total	C	N	O	S	0	0
			431	287	68	72	4		

- Molecule 10 is a protein called Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	467	Total	C	N	O	S	0	0
			3716	2419	606	670	21		

- Molecule 11 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 12 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 16 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS9.

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

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

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

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



Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 23 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 25 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 26 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 27 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 28 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 29 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 30 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 31 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 32 is a protein called NuoK-86 nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	V	89	Total	C	N	O	0	0
			542	344	99	99		

- Molecule 33 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	X	9	Total	C	N	O	P	0	0
			189	84	31	65	9		

- Molecule 34 is a RNA chain called A-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Y	77	Total	C	N	O	P	0	0
			1646	734	297	539	76		

- Molecule 35 is a RNA chain called P-site tRNA-Pro.

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

- Molecule 36 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	2753	Total	C	N	O	P	0	0
			59127	26381	10897	19096	2753		

- Molecule 37 is a RNA chain called 5S rRNA.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 40 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 45 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 46 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 47 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	l	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 48 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 50 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 51 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 54 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 55 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 56 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 57 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 58 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 59 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 60 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 61 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

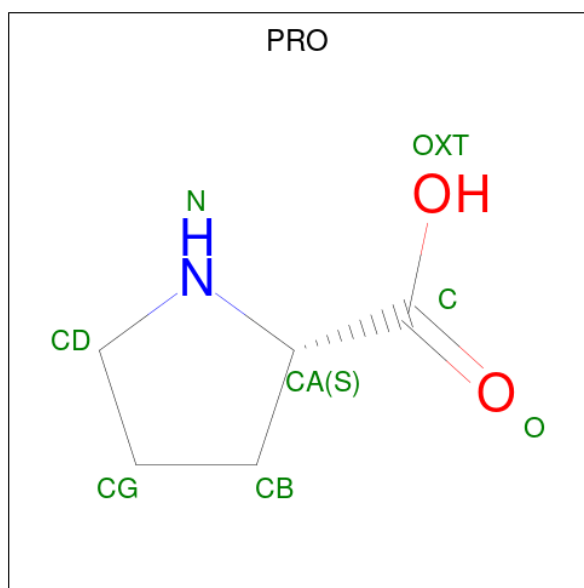
- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	3	1	Total	Zn	0
			1	1	
62	4	1	Total	Zn	0
			1	1	

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

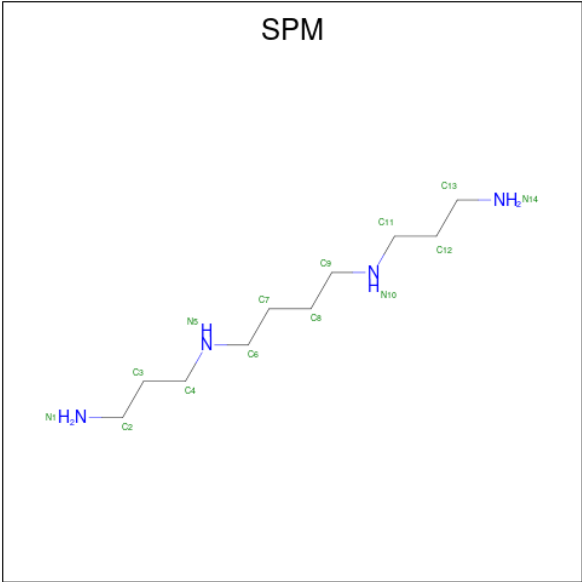
Mol	Chain	Residues	Atoms		AltConf
63	A	91	Total	Mg	0
			91	91	
63	N	1	Total	Mg	0
			1	1	
63	Q	1	Total	Mg	0
			1	1	
63	a	208	Total	Mg	0
			208	208	
63	b	5	Total	Mg	0
			5	5	
63	c	1	Total	Mg	0
			1	1	
63	d	1	Total	Mg	0
			1	1	
63	z	1	Total	Mg	0
			1	1	

- Molecule 64 is PROLINE (CCD ID: PRO) (formula:  $C_5H_9NO_2$ ).



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

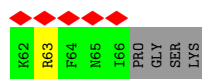
- Molecule 65 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			AltConf
65	a	1	Total	C	N	0
			14	10	4	







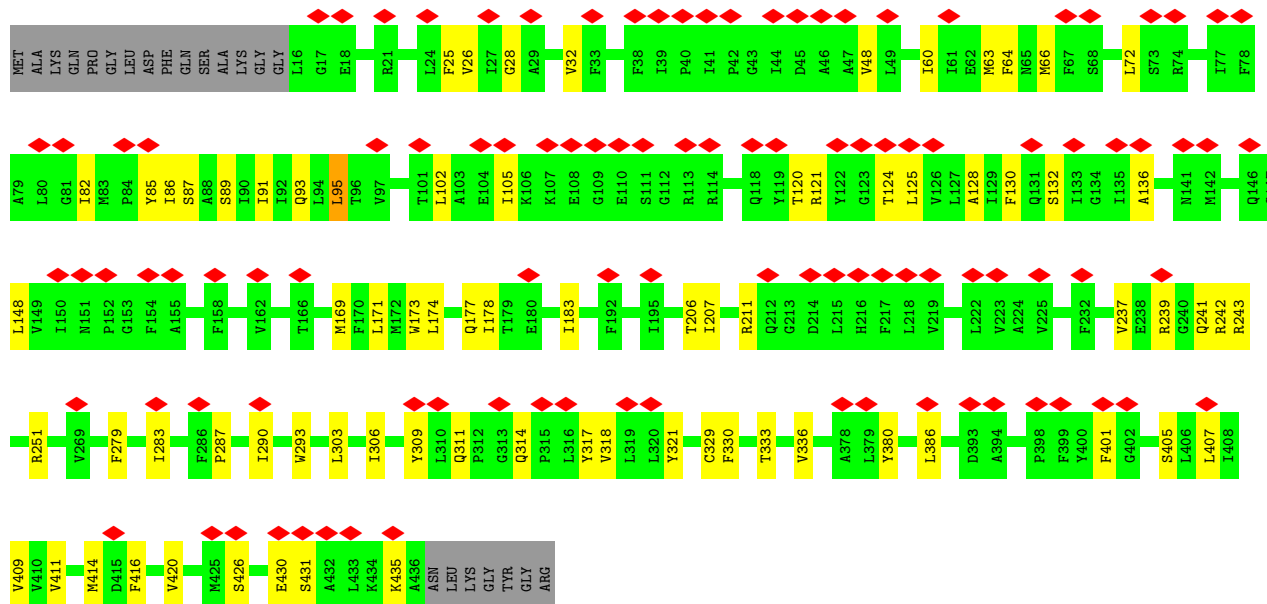
• Molecule 6: E-site tRNA

Chain 5: 50% 50%



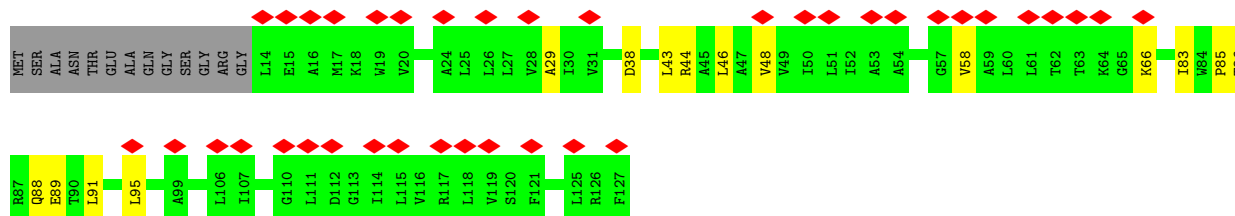
• Molecule 7: Protein translocase subunit SecY

Chain 6: 24% 78% 17% 5%



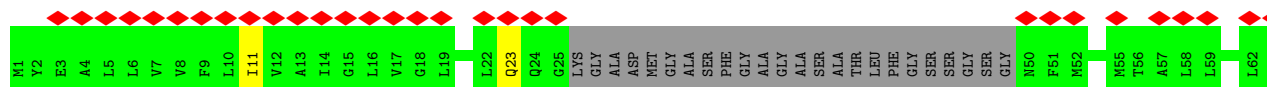
• Molecule 8: Protein translocase subunit SecE

Chain 7: 30% 78% 12% 10%

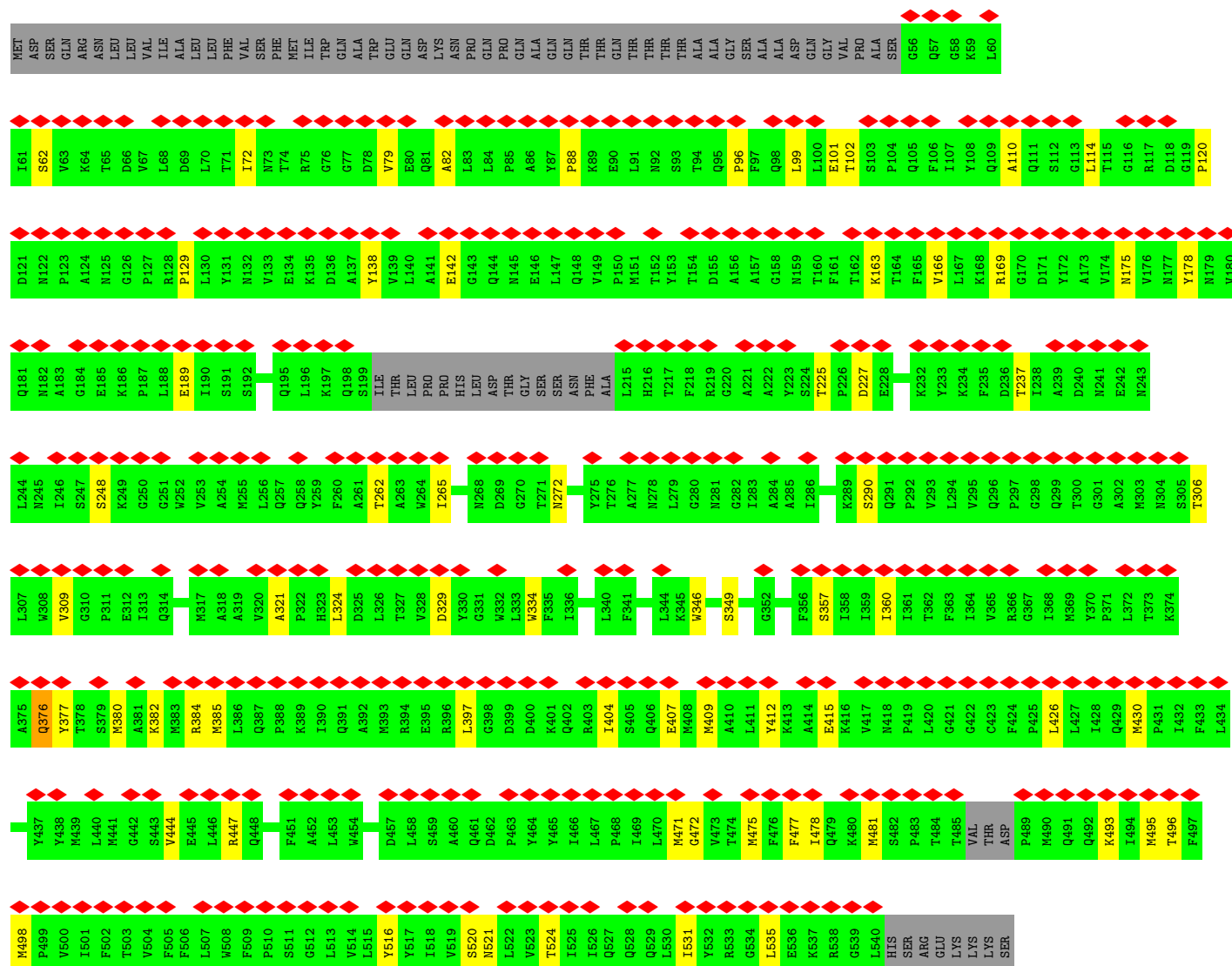


• Molecule 9: Protein-export membrane protein SecG

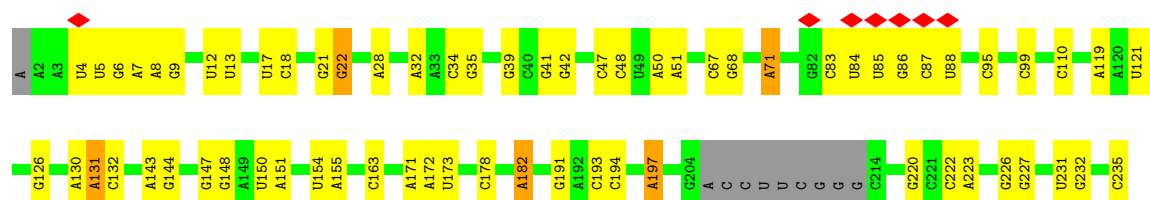
Chain 8: 37% 47% 49%

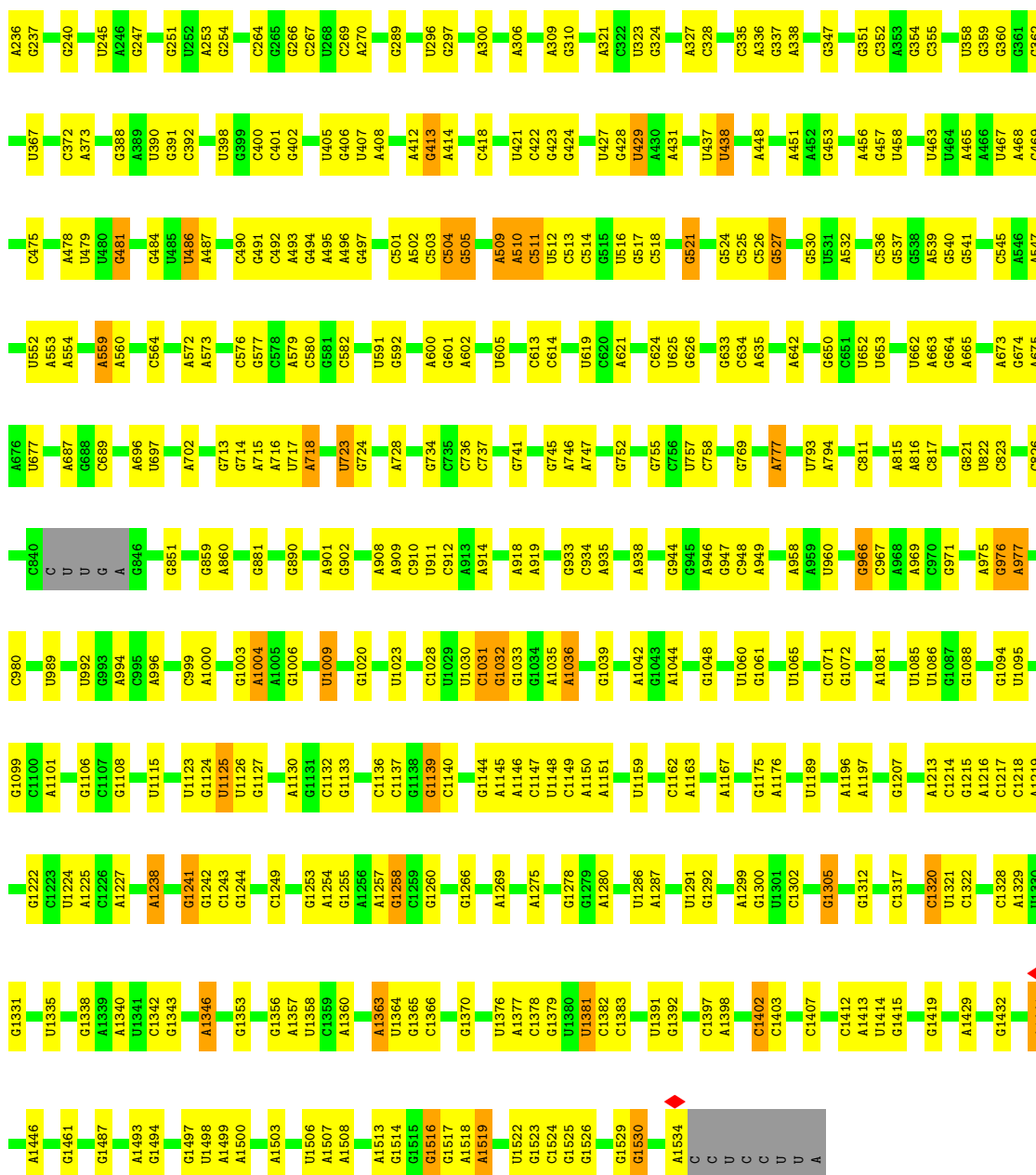


- Molecule 10: Membrane protein insertase YidC



- Molecule 11: 16S rRNA





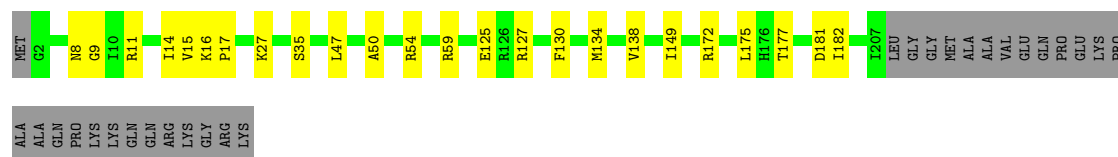
- Molecule 12: Small ribosomal subunit protein uS2

Chain B: 87% 6% 7%

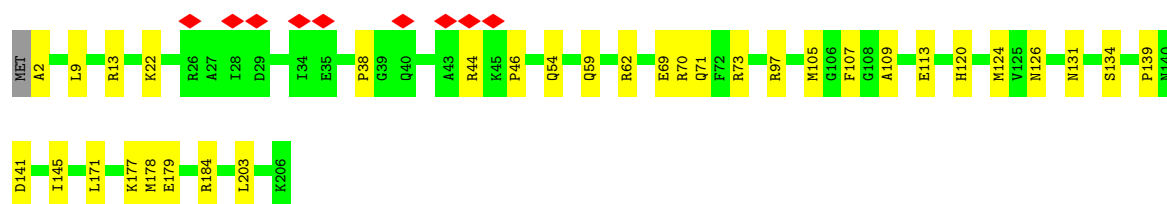
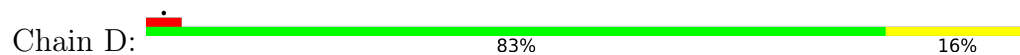


- Molecule 13: Small ribosomal subunit protein uS3

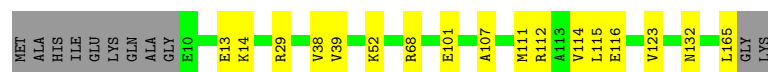
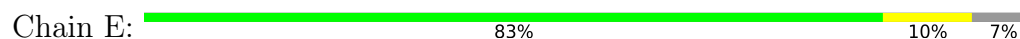
Chain C: 78% 10% 12%



- Molecule 14: Small ribosomal subunit protein uS4



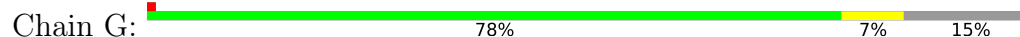
- Molecule 15: Small ribosomal subunit protein uS5



- Molecule 16: Small ribosomal subunit protein bS6, fully modified isoform



- Molecule 17: Small ribosomal subunit protein uS7

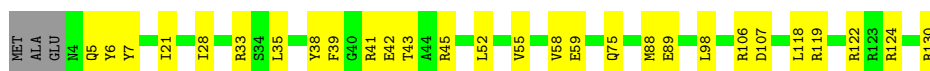


- Molecule 18: Small ribosomal subunit protein uS8



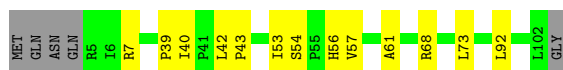
- Molecule 19: Small ribosomal subunit protein uS9





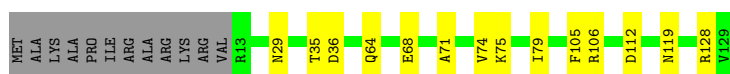
- Molecule 20: Small ribosomal subunit protein uS10

Chain J: 83% 13% 5%



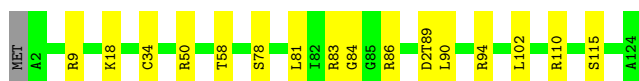
- Molecule 21: Small ribosomal subunit protein uS11

Chain K: 80% 11% 9%



- Molecule 22: Small ribosomal subunit protein uS12

Chain L: 86% 13% .



- Molecule 23: Small ribosomal subunit protein uS13

Chain M: 82% 15% .



- Molecule 24: Small ribosomal subunit protein uS14

Chain N: 82% 16% ..



- Molecule 25: Small ribosomal subunit protein uS15

Chain O: 91% 8% .



- Molecule 26: Small ribosomal subunit protein bS16

Chain P: 90% 9% .



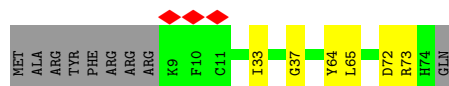
- Molecule 27: Small ribosomal subunit protein uS17

Chain Q: 86% 8% 6%



- Molecule 28: Small ribosomal subunit protein bS18

Chain R: 80% 8% 12%



- Molecule 29: Small ribosomal subunit protein uS19

Chain S: 74% 17% 9%



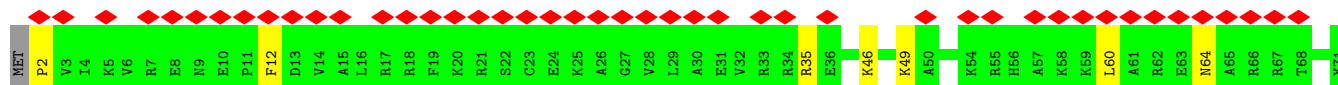
- Molecule 30: Small ribosomal subunit protein bS20

Chain T: 80% 18% 2%



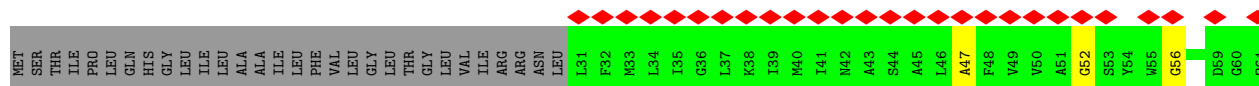
- Molecule 31: Small ribosomal subunit protein bS21

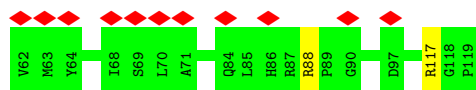
Chain U: 63% 89% 10%



- Molecule 32: NuoK-86 nascent peptide

Chain V: 32% 71% 25%





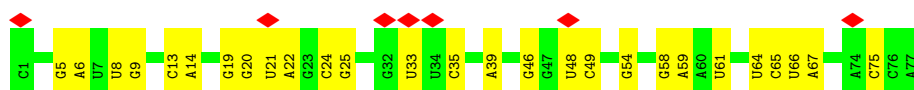
• Molecule 33: mRNA

Chain X: 89% 11%



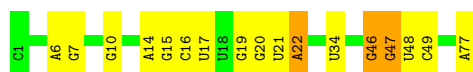
• Molecule 34: A-site tRNA-Pro

Chain Y: 9% 65% 35%



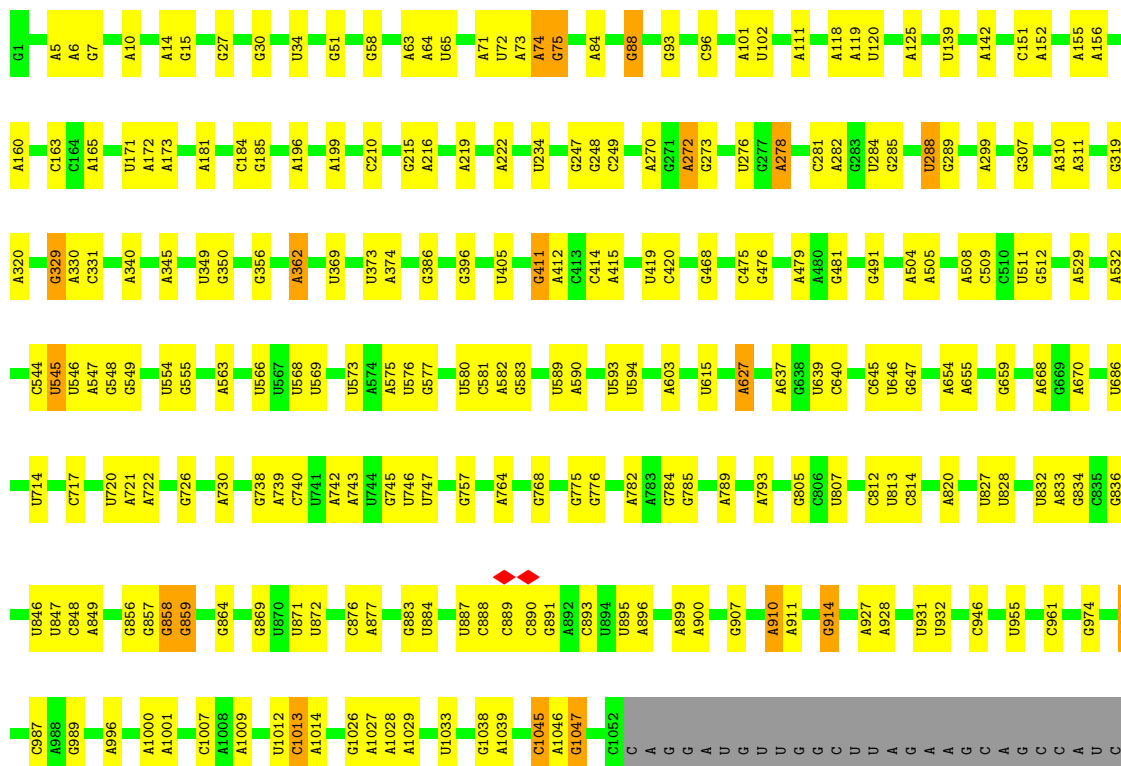
• Molecule 35: P-site tRNA-Pro

Chain Z: 78% 18%



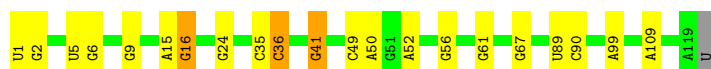
• Molecule 36: 23S rRNA

Chain a: 73% 21% 5%









- Molecule 38: Large ribosomal subunit protein uL2

Chain c: 91% 8%



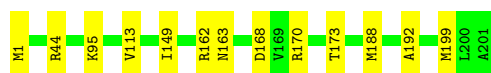
- Molecule 39: Large ribosomal subunit protein uL3

Chain d: 94% 6%



- Molecule 40: Large ribosomal subunit protein uL4

Chain e: 94% 6%



- Molecule 41: Large ribosomal subunit protein uL5

Chain f: 84% 15%



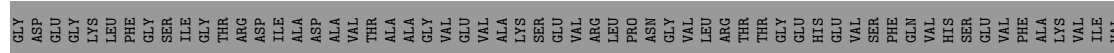
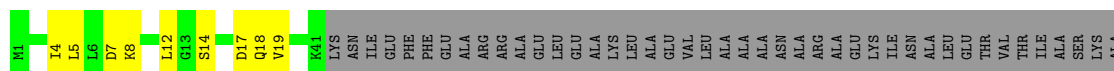
- Molecule 42: Large ribosomal subunit protein uL6

Chain g: 95% 5%



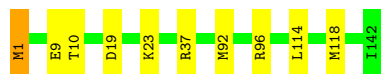
- Molecule 43: Large ribosomal subunit protein bL9

Chain h: 21% 6% 72%



- Molecule 44: Large ribosomal subunit protein uL13

Chain i:  93% 6%



- Molecule 45: Large ribosomal subunit protein uL14

Chain j:  95% 5%




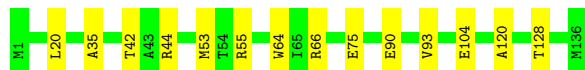
- Molecule 46: Large ribosomal subunit protein uL15

Chain k:  91% 9%




- Molecule 47: 50S ribosomal protein L16

Chain l:  90% 10%



- Molecule 48: Large ribosomal subunit protein bL17

Chain m:  88% 5% 7%




- Molecule 49: Large ribosomal subunit protein uL18

Chain n:  93% 6%



- Molecule 50: Large ribosomal subunit protein bL19

Chain o:  89% 10%



- Molecule 51: Large ribosomal subunit protein bL20

Chain p:  96%




- Molecule 52: Large ribosomal subunit protein bL21

Chain q:  93% 7%




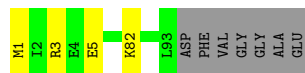
- Molecule 53: Large ribosomal subunit protein uL22

Chain r:  91% 9%



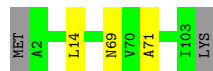
- Molecule 54: Large ribosomal subunit protein uL23

Chain s:  89% 7%




- Molecule 55: Large ribosomal subunit protein uL24

Chain t:  95%




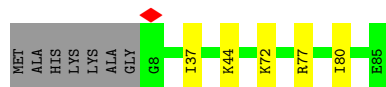
- Molecule 56: Large ribosomal subunit protein bL25

Chain u:  81% 19%




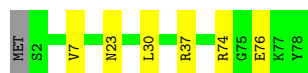
- Molecule 57: Large ribosomal subunit protein bL27

Chain v:  86% 6% 8%




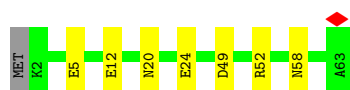
- Molecule 58: Large ribosomal subunit protein bL28

Chain w:  91% 8%




- Molecule 59: Large ribosomal subunit protein uL29

Chain x:  87% 11%



- Molecule 60: Large ribosomal subunit protein uL30

Chain y:  90% 8%



- Molecule 61: Large ribosomal subunit protein bL32

Chain z:  91% 7%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113368	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.073	Depositor
Minimum map value	-0.651	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	494.36, 494.36, 494.36	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, MEQ, MG, 2MA, ZN, G7M, 1MG, H2U, 6MZ, MA6, PSU, 5MC, OMG, 4OC, UR3, 2MG, SPM, OMU, D2T

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.17	0/424	0.38	0/565
2	1	0.21	0/380	0.31	0/498
3	2	0.22	0/513	0.37	0/676
4	3	0.21	0/303	0.37	0/397
5	4	0.16	0/488	0.38	0/649
6	5	0.11	0/46	0.12	0/69
7	6	0.23	0/3335	0.59	0/4526
8	7	0.21	0/886	0.57	0/1209
9	8	0.20	0/434	0.46	0/584
10	9	0.21	0/3813	0.50	0/5179
11	A	0.16	0/36236	0.29	0/56520
12	B	0.18	0/1784	0.43	0/2403
13	C	0.17	0/1651	0.38	0/2225
14	D	0.16	0/1665	0.38	0/2227
15	E	0.20	0/1165	0.44	0/1568
16	F	0.22	0/858	0.53	0/1160
17	G	0.19	0/1219	0.47	0/1635
18	H	0.17	0/989	0.39	0/1326
19	I	0.18	0/1034	0.50	0/1375
20	J	0.22	0/796	0.54	0/1077
21	K	0.19	0/893	0.48	0/1205
22	L	0.17	0/960	0.42	0/1286
23	M	0.17	0/900	0.49	0/1204
24	N	0.17	0/817	0.43	1/1088 (0.1%)
25	O	0.15	0/722	0.34	0/964
26	P	0.19	0/653	0.43	0/877
27	Q	0.20	0/650	0.53	0/871
28	R	0.18	0/553	0.45	0/742
29	S	0.15	0/685	0.40	0/922
30	T	0.24	0/676	0.48	0/895
31	U	0.16	0/597	0.40	0/792

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	V	0.19	0/559	0.48	0/777
33	X	0.15	0/209	0.26	0/323
34	Y	0.13	0/1840	0.30	0/2869
35	Z	0.13	0/1837	0.25	0/2864
36	a	0.24	0/65718	0.31	0/102519
37	b	0.19	0/2850	0.27	0/4444
38	c	0.23	0/2121	0.38	0/2852
39	d	0.23	0/1576	0.37	0/2119
40	e	0.21	0/1571	0.35	0/2113
41	f	0.21	0/1434	0.51	0/1926
42	g	0.21	0/1343	0.50	0/1816
43	h	0.22	0/306	0.62	0/413
44	i	0.21	0/1152	0.35	0/1551
45	j	0.23	0/955	0.37	0/1279
46	k	0.21	0/1062	0.37	0/1413
47	l	0.24	0/1093	0.37	0/1460
48	m	0.22	0/958	0.40	0/1281
49	n	0.18	0/902	0.40	0/1209
50	o	0.21	0/929	0.32	0/1242
51	p	0.23	0/960	0.36	0/1278
52	q	0.23	0/829	0.46	0/1107
53	r	0.22	0/864	0.37	0/1156
54	s	0.21	0/744	0.37	0/994
55	t	0.20	0/787	0.38	0/1051
56	u	0.19	0/766	0.39	0/1025
57	v	0.20	0/599	0.36	0/792
58	w	0.21	0/635	0.35	0/848
59	x	0.19	0/502	0.38	0/667
60	y	0.22	0/453	0.47	0/605
61	z	0.21	0/450	0.37	0/599
All	All	0.21	0/162129	0.35	1/241306 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	89	MET	CB-CG-SD	5.52	129.27	112.70

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	4	0
2	1	377	0	418	2	0
3	2	504	0	572	6	0
4	3	302	0	340	1	0
5	4	480	0	478	8	0
6	5	42	0	23	0	0
7	6	3260	0	3416	47	0
8	7	873	0	966	9	0
9	8	431	0	475	2	0
10	9	3716	0	3720	41	0
11	A	32612	0	16428	216	0
12	B	1753	0	1780	8	0
13	C	1624	0	1696	14	0
14	D	1643	0	1707	23	0
15	E	1152	0	1196	12	0
16	F	839	0	833	5	0
17	G	1203	0	1254	9	0
18	H	979	0	1031	10	0
19	I	1022	0	1070	18	0
20	J	786	0	828	9	0
21	K	877	0	887	12	0
22	L	957	0	1017	10	0
23	M	891	0	952	12	0
24	N	805	0	844	15	0
25	O	714	0	734	5	0
26	P	643	0	661	5	0
27	Q	641	0	682	5	0
28	R	544	0	565	4	0
29	S	668	0	693	13	0
30	T	670	0	719	11	0
31	U	589	0	629	6	0
32	V	542	0	379	3	0
33	X	189	0	98	0	0
34	Y	1646	0	832	8	0
35	Z	1644	0	832	6	0
36	a	59127	0	29762	256	0
37	b	2549	0	1291	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	c	2082	0	2154	13	0
39	d	1566	0	1618	9	0
40	e	1552	0	1619	9	0
41	f	1410	0	1444	15	0
42	g	1323	0	1371	4	0
43	h	303	0	327	5	0
44	i	1129	0	1162	8	0
45	j	946	0	1023	5	0
46	k	1053	0	1129	10	0
47	l	1074	0	1157	10	0
48	m	945	0	989	3	0
49	n	892	0	923	5	0
50	o	917	0	962	9	0
51	p	947	0	1019	3	0
52	q	816	0	839	6	0
53	r	857	0	922	5	0
54	s	738	0	807	3	0
55	t	779	0	831	2	0
56	u	753	0	780	10	0
57	v	592	0	607	4	0
58	w	625	0	652	5	0
59	x	501	0	531	5	0
60	y	449	0	488	3	0
61	z	444	0	458	3	0
62	3	1	0	0	0	0
62	4	1	0	0	0	0
63	A	91	0	0	0	0
63	N	1	0	0	0	0
63	Q	1	0	0	0	0
63	a	208	0	0	0	0
63	b	5	0	0	0	0
63	c	1	0	0	0	0
63	d	1	0	0	0	0
63	z	1	0	0	0	0
64	Y	7	0	7	0	0
65	a	14	0	26	1	0
All	All	150736	0	104104	838	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (838) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1441:A:N6	11:A:1461:G:H21	1.54	1.03
11:A:1441:A:H62	11:A:1461:G:N2	1.59	1.01
11:A:1009:U:H3	11:A:1020:G:H1	1.29	0.79
11:A:1441:A:H62	11:A:1461:G:H21	0.83	0.76
34:Y:33:U:H3	34:Y:39:A:H61	1.38	0.71
11:A:1127:G:H1	11:A:1145:A:H61	1.40	0.69
11:A:664:G:H22	11:A:741:G:H1	1.41	0.68
7:6:306:ILE:HA	7:6:309:TYR:HB3	1.76	0.67
36:a:2343:U:HO2'	36:a:2373:G:HO2'	1.41	0.67
19:I:58:VAL:HG13	19:I:59:GLU:HG3	1.78	0.65
43:h:14:SER:HB2	43:h:17:ASP:HB2	1.79	0.65
11:A:1088:G:H21	11:A:1167:A:H61	1.45	0.64
11:A:1031:C:O2'	11:A:1032:G:N2	2.31	0.64
11:A:1086:U:H3	11:A:1099:G:H22	1.46	0.63
21:K:119:ASN:OD1	31:U:35:ARG:NH2	2.32	0.63
36:a:2469:A:H4'	47:l:55:ARG:HD3	1.80	0.63
36:a:1724:G:O6	36:a:1737:G:N2	2.31	0.63
11:A:958:A:N6	29:S:77:THR:O	2.32	0.63
11:A:71:A:H61	11:A:99:C:H1'	1.65	0.62
35:Z:22:A:N6	35:Z:47:G:O2'	2.33	0.62
19:I:28:ILE:HG21	19:I:35:LEU:HD22	1.81	0.62
36:a:568:U:H1'	36:a:2030:6MZ:H9C1	1.81	0.62
7:6:329:CYS:SG	7:6:330:PHE:N	2.73	0.62
11:A:823:C:HO2'	18:H:2:SER:N	1.98	0.61
11:A:407:U:O2'	14:D:113:GLU:OE1	2.16	0.61
10:9:426:LEU:HD21	32:V:47:ALA:HB1	1.81	0.61
36:a:848:C:H2'	36:a:849:A:H8	1.65	0.61
10:9:380:MET:HE1	10:9:481:MET:HE2	1.81	0.61
11:A:1150:A:H4'	20:J:43:PRO:HG3	1.82	0.61
11:A:1081:A:OP2	15:E:52:LYS:NZ	2.32	0.61
36:a:768:G:N7	65:a:6209:SPM:N14	2.48	0.61
35:Z:10:G:O6	35:Z:46:G:N2	2.27	0.61
36:a:1434:A:H2'	36:a:1435:G:H8	1.64	0.60
11:A:335:C:H2'	11:A:336:A:H8	1.65	0.60
11:A:910:C:OP2	22:L:18:LYS:NZ	2.33	0.60
19:I:130:ARG:NH2	35:Z:34:U:OP2	2.34	0.60
36:a:2848:G:O2'	36:a:2867:G:N2	2.31	0.59
3:2:31:HIS:NE2	36:a:2421:G:N7	2.50	0.59
51:p:97:ASP:OD2	52:q:13:ARG:NH1	2.36	0.59
7:6:121:ARG:NH1	9:8:23:GLN:O	2.36	0.59
11:A:1149:C:H2'	11:A:1150:A:H8	1.67	0.59
47:l:66:ARG:NH1	47:l:104:GLU:OE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:39:LYS:NZ	36:a:2365:G:N7	2.49	0.58
11:A:362:G:H5''	22:L:58:THR:HG21	1.85	0.58
11:A:826:C:O2	18:H:16:ASN:ND2	2.36	0.58
16:F:38:ARG:NH1	16:F:99:ALA:O	2.36	0.58
11:A:1071:C:H2'	11:A:1072:G:H8	1.69	0.58
47:l:64:TRP:HB2	47:l:104:GLU:HB2	1.84	0.58
13:C:16:LYS:NZ	13:C:181:ASP:OD1	2.36	0.58
11:A:674:G:H2'	11:A:675:A:H8	1.67	0.57
53:r:37:THR:OG1	53:r:48:LYS:NZ	2.36	0.57
36:a:1590:A:H2'	36:a:1591:A:H8	1.69	0.57
47:l:53:MET:HG3	47:l:120:ALA:HB2	1.85	0.57
24:N:92:GLU:N	24:N:92:GLU:OE1	2.37	0.57
39:d:46:ARG:NH1	39:d:85:ALA:O	2.36	0.57
11:A:1144:G:H21	11:A:1146:A:H62	1.51	0.57
19:I:39:PHE:O	19:I:45:ARG:NH1	2.37	0.57
11:A:1397:C:OP2	15:E:29:ARG:NH2	2.37	0.57
17:G:111:ARG:NH2	17:G:123:GLU:OE1	2.37	0.57
50:o:88:ARG:NH2	50:o:110:ILE:O	2.36	0.57
19:I:52:LEU:HG	19:I:58:VAL:HG23	1.87	0.57
46:k:108:ALA:HB3	46:k:125:LEU:HD22	1.86	0.57
11:A:405:U:O4	14:D:2:ALA:N	2.37	0.57
11:A:501:C:H2'	11:A:502:A:H8	1.70	0.57
5:4:42:PRO:HB3	5:4:47:LYS:HB3	1.85	0.57
7:6:251:ARG:NH2	36:a:1335:C:O3'	2.38	0.57
11:A:401:C:O2'	11:A:621:A:N3	2.36	0.57
22:L:83:ARG:NH1	22:L:84:GLY:O	2.38	0.57
36:a:2469:A:N6	36:a:2481:G:O2'	2.36	0.57
36:a:284:U:H3	36:a:356:G:H1	1.51	0.56
11:A:1106:G:H5''	13:C:172:ARG:HG2	1.87	0.56
15:E:14:LYS:NZ	15:E:116:GLU:OE2	2.37	0.56
30:T:17:ALA:O	30:T:21:ASN:ND2	2.39	0.56
36:a:1007:C:OP1	44:i:37:ARG:NH1	2.37	0.56
11:A:677:U:H3	11:A:713:G:H22	1.52	0.56
15:E:115:LEU:HD13	15:E:123:VAL:HG11	1.88	0.56
41:f:58:ALA:HB2	41:f:65:PRO:HD3	1.87	0.56
7:6:333:THR:HA	7:6:336:VAL:HG12	1.88	0.56
11:A:517:G:N2	11:A:530:G:OP1	2.38	0.56
5:4:42:PRO:O	5:4:45:THR:C	2.49	0.56
11:A:1088:G:N2	11:A:1167:A:H61	2.03	0.56
36:a:1434:A:H2'	36:a:1435:G:C8	2.40	0.56
11:A:451:A:H61	11:A:481:G:H5'	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:43:LEU:HA	12:B:46:THR:HG22	1.87	0.56
15:E:38:VAL:HG11	15:E:114:VAL:HG22	1.88	0.56
11:A:110:C:O2'	26:P:25:ARG:O	2.23	0.55
11:A:178:C:OP2	30:T:60:ARG:NH1	2.39	0.55
12:B:104:TRP:HA	12:B:107:VAL:HG22	1.88	0.55
23:M:87:ARG:NH2	29:S:73:GLU:OE1	2.39	0.55
36:a:1432:G:H2'	36:a:1433:A:C8	2.40	0.55
36:a:1796:U:H2'	36:a:1797:G:H8	1.70	0.55
60:y:6:LYS:HD3	60:y:37:GLU:HG3	1.86	0.55
44:i:19:ASP:O	44:i:23:LYS:NZ	2.37	0.55
10:9:79:VAL:HB	10:9:110:ALA:HB3	1.88	0.55
10:9:321:ALA:HB3	10:9:324:LEU:HD13	1.88	0.55
10:9:376:GLN:HG2	10:9:377:TYR:HD1	1.71	0.55
11:A:264:C:O2'	27:Q:66:PRO:O	2.24	0.55
11:A:559:A:H4'	11:A:560:A:H3'	1.88	0.55
14:D:59:GLN:OE1	14:D:62:ARG:NH1	2.39	0.55
11:A:552:U:H2'	11:A:553:A:H8	1.72	0.55
11:A:933:G:O6	17:G:3:ARG:NH2	2.38	0.55
3:2:54:ASP:HB3	46:k:57:LEU:HD22	1.89	0.55
7:6:130:PHE:HZ	7:6:290:ILE:HG23	1.72	0.55
11:A:713:G:H2'	11:A:714:G:C8	2.42	0.55
50:o:9:GLU:OE2	50:o:56:HIS:NE2	2.40	0.55
56:u:35:GLU:N	56:u:35:GLU:OE1	2.39	0.55
14:D:97:ARG:HH21	14:D:134:SER:HB3	1.72	0.55
36:a:1045:C:O2	36:a:1111:A:N6	2.39	0.55
51:p:49:ASP:HA	51:p:52:GLN:HB2	1.89	0.55
19:I:106:ARG:NH1	19:I:107:ASP:O	2.41	0.54
7:6:85:TYR:HA	7:6:124:THR:HG22	1.89	0.54
54:s:3:ARG:NH1	54:s:5:GLU:OE2	2.40	0.54
47:l:20:LEU:HD13	56:u:81:PRO:HG2	1.89	0.54
7:6:125:LEU:HA	7:6:169:MET:HE1	1.89	0.54
11:A:946:A:H2'	11:A:947:G:C8	2.42	0.54
11:A:1060:U:H2'	11:A:1061:G:H8	1.71	0.54
43:h:5:LEU:HD23	43:h:17:ASP:HB3	1.90	0.54
11:A:1530:G:N7	31:U:46:LYS:NZ	2.56	0.54
27:Q:47:HIS:HB3	27:Q:74:THR:HG22	1.89	0.54
56:u:1:MET:SD	56:u:53:LYS:NZ	2.81	0.54
7:6:293:TRP:HE1	7:6:303:LEU:HD21	1.73	0.54
56:u:51:GLN:OE1	56:u:57:TYR:OH	2.26	0.54
5:4:28:VAL:HG22	41:f:140:GLU:HA	1.89	0.54
17:G:15:ASP:OD1	17:G:19:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:H:77:ARG:NH1	18:H:79:SER:O	2.41	0.54
26:P:69:ASP:OD1	26:P:70:ARG:N	2.40	0.54
7:6:242:ARG:NH2	7:6:243:ARG:O	2.41	0.54
11:A:980:C:O2'	24:N:13:ARG:NH1	2.40	0.54
11:A:1127:G:H1	11:A:1145:A:N6	2.05	0.54
45:j:121:GLU:OE1	50:o:65:SER:OG	2.26	0.54
11:A:402:G:OP2	14:D:71:GLN:NE2	2.37	0.54
13:C:35:SER:OG	13:C:59:ARG:NH2	2.41	0.54
36:a:1386:C:H2'	36:a:1387:A:C8	2.43	0.54
11:A:227:G:O2'	26:P:63:GLN:OE1	2.26	0.53
11:A:717:U:H4'	21:K:119:ASN:HD22	1.73	0.53
38:c:29:PRO:HG2	38:c:34:LEU:HD11	1.91	0.53
5:4:42:PRO:O	5:4:45:THR:O	2.27	0.53
36:a:864:G:O2'	36:a:914:G:O6	2.26	0.53
21:K:64:GLN:NE2	21:K:68:GLU:OE2	2.40	0.53
36:a:1278:C:H2'	36:a:1279:G:H8	1.73	0.53
36:a:1590:A:H2'	36:a:1591:A:C8	2.43	0.53
11:A:1218:C:H2'	11:A:1219:A:H8	1.73	0.53
11:A:1278:G:N7	13:C:27:LYS:NZ	2.57	0.53
37:b:1:U:H2'	37:b:2:G:H8	1.74	0.53
12:B:58:ASN:ND2	12:B:220:THR:O	2.41	0.53
25:O:88:ARG:NH2	36:a:714:U:OP2	2.39	0.53
11:A:673:A:H2'	11:A:674:G:C8	2.43	0.53
11:A:323:U:OP1	30:T:25:ARG:NH2	2.38	0.52
11:A:335:C:H2'	11:A:336:A:C8	2.42	0.52
30:T:55:GLN:HG3	30:T:76:LYS:HD3	1.91	0.52
36:a:93:G:N2	36:a:93:G:OP2	2.42	0.52
38:c:107:PRO:HD2	38:c:110:LEU:HD22	1.90	0.52
38:c:144:VAL:HB	38:c:154:LEU:HB2	1.90	0.52
11:A:1124:G:N2	11:A:1125:U:O4	2.37	0.52
17:G:68:ASN:O	17:G:138:ARG:NH2	2.43	0.52
8:7:86:THR:HG23	8:7:89:GLU:H	1.73	0.52
36:a:270:A:N1	36:a:369:U:O2'	2.32	0.52
36:a:807:U:OP2	46:k:41:ARG:NH2	2.42	0.52
11:A:811:C:O2'	11:A:901:A:N1	2.42	0.52
7:6:26:VAL:HG21	7:6:183:ILE:HG13	1.90	0.52
11:A:1360:A:OP2	24:N:75:ARG:NH2	2.42	0.52
24:N:52:PRO:O	24:N:55:SER:OG	2.28	0.52
36:a:627:A:OP1	46:k:78:ARG:NH1	2.43	0.52
36:a:1248:G:OP1	40:e:44:ARG:NH1	2.42	0.52
11:A:946:A:OP1	23:M:113:ARG:NH1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:107:ALA:O	15:E:112:ARG:NH1	2.43	0.52
36:a:577:G:O2'	36:a:1254:A:OP1	2.28	0.52
36:a:832:U:H2'	36:a:833:A:H8	1.74	0.52
11:A:1218:C:H2'	11:A:1219:A:C8	2.45	0.52
11:A:1381:U:H2'	17:G:79:ARG:HE	1.74	0.52
30:T:39:ILE:HG23	30:T:86:LEU:HD12	1.91	0.52
36:a:411:G:OP2	36:a:2406:A:O2'	2.26	0.52
41:f:162:SER:OG	41:f:165:GLU:OE1	2.28	0.52
11:A:1088:G:H21	11:A:1167:A:N6	2.07	0.52
20:J:53:ILE:HD11	20:J:61:ALA:HB1	1.92	0.52
58:w:74:ARG:NH1	58:w:76:GLU:OE2	2.43	0.52
10:9:225:THR:HG23	10:9:248:SER:HB2	1.92	0.52
10:9:272:ASN:HA	10:9:290:SER:HA	1.91	0.52
11:A:1222:G:OP2	11:A:1322:C:N4	2.40	0.52
11:A:1377:A:OP1	17:G:92:ARG:NH2	2.43	0.52
7:6:237:VAL:HG21	7:6:380:TYR:CZ	2.45	0.51
10:9:88:PRO:HA	10:9:96:PRO:HA	1.90	0.51
10:9:397:LEU:HB3	10:9:404:ILE:HG23	1.92	0.51
11:A:714:G:H2'	11:A:715:A:C8	2.45	0.51
13:C:130:PHE:O	13:C:134:MET:HG2	2.10	0.51
20:J:40:ILE:HB	20:J:73:LEU:HD23	1.92	0.51
23:M:17:ILE:O	23:M:20:THR:OG1	2.28	0.51
11:A:41:G:H2'	11:A:42:G:H8	1.74	0.51
11:A:946:A:H2'	11:A:947:G:H8	1.75	0.51
11:A:1522:U:H2'	11:A:1523:G:H8	1.74	0.51
35:Z:15:G:H22	35:Z:49:C:H42	1.58	0.51
36:a:476:G:N1	36:a:479:A:OP2	2.40	0.51
36:a:2200:C:OP2	58:w:37:ARG:NH1	2.42	0.51
51:p:89:GLU:O	52:q:11:GLN:NE2	2.40	0.51
36:a:1819:A:H5''	38:c:160:THR:HG21	1.91	0.51
36:a:2303:G:O2'	41:f:121:SER:O	2.28	0.51
46:k:143:GLU:OE1	46:k:143:GLU:N	2.44	0.51
49:n:69:ASP:OD1	49:n:69:ASP:N	2.37	0.51
5:4:63:ARG:NH1	11:A:1312:G:OP2	2.44	0.51
10:9:521:ASN:HA	10:9:524:THR:HB	1.93	0.51
36:a:887:U:O2'	36:a:889:C:OP2	2.29	0.51
37:b:15:A:H3'	37:b:16:G:H8	1.75	0.51
11:A:501:C:H2'	11:A:502:A:C8	2.46	0.51
13:C:125:GLU:O	13:C:127:ARG:NH1	2.42	0.51
13:C:138:VAL:HG23	13:C:149:ILE:HG23	1.91	0.51
36:a:1800:C:OP2	38:c:182:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:f:2:ALA:N	41:f:98:GLU:OE2	2.43	0.51
56:u:76:ASP:H	56:u:90:ASP:HB2	1.75	0.51
10:9:265:ILE:HB	10:9:306:THR:HB	1.91	0.51
15:E:13:GLU:OE2	15:E:68:ARG:NH1	2.39	0.51
15:E:101:GLU:N	15:E:101:GLU:OE1	2.43	0.51
18:H:91:GLU:N	18:H:91:GLU:OE1	2.44	0.51
23:M:87:ARG:HH22	29:S:69:HIS:CE1	2.28	0.51
36:a:2831:G:OP2	39:d:59:ARG:NH1	2.41	0.51
11:A:723:U:O2	31:U:49:LYS:NZ	2.44	0.51
11:A:1366:C:OP1	19:I:119:ARG:NH1	2.44	0.51
11:A:309:A:H2'	11:A:310:G:H8	1.74	0.51
11:A:1305:G:N2	11:A:1331:G:O2'	2.43	0.51
36:a:340:A:O2'	40:e:162:ARG:NH2	2.44	0.51
36:a:568:U:O4	52:q:81:LYS:NZ	2.44	0.51
36:a:2515:C:H2'	36:a:2516:A:H8	1.75	0.51
44:i:9:GLU:OE1	44:i:9:GLU:N	2.44	0.51
11:A:126:G:OP1	11:A:605:U:O2'	2.24	0.50
11:A:437:U:O2'	14:D:120:HIS:ND1	2.40	0.50
12:B:11:LYS:O	12:B:208:ARG:NH1	2.43	0.50
29:S:44:MET:HG3	29:S:62:VAL:HG11	1.92	0.50
36:a:545:U:O2'	36:a:548:G:N2	2.45	0.50
36:a:2372:U:H2'	36:a:2373:G:H8	1.77	0.50
48:m:24:MET:HE1	48:m:40:LYS:HB3	1.93	0.50
10:9:382:LYS:NZ	10:9:415:GLU:O	2.40	0.50
2:l:29:GLN:NE2	36:a:210:C:OP1	2.45	0.50
7:6:239:ARG:HG3	8:7:85:PRO:HG3	1.92	0.50
10:9:516:TYR:O	10:9:520:SER:OG	2.19	0.50
36:a:581:C:H2'	36:a:582:A:C8	2.46	0.50
36:a:793:A:OP2	36:a:2071:A:O2'	2.27	0.50
59:x:49:ASP:OD1	59:x:52:ARG:NH1	2.44	0.50
11:A:50:A:O2'	11:A:360:G:N2	2.44	0.50
7:6:86:ILE:HD11	7:6:279:PHE:HA	1.94	0.50
11:A:1321:U:O2'	29:S:78:ARG:NH1	2.44	0.50
34:Y:59:A:O2'	34:Y:61:U:OP2	2.29	0.50
36:a:151:C:H2'	36:a:152:A:H8	1.76	0.50
1:0:29:THR:HG22	1:0:30:LYS:HD3	1.93	0.50
7:6:318:VAL:HG12	7:6:386:LEU:HD12	1.92	0.50
10:9:82:ALA:HB3	10:9:99:LEU:HD12	1.94	0.50
24:N:66:GLN:HG3	24:N:79:LEU:HD22	1.94	0.50
7:6:407:LEU:O	7:6:411:VAL:HG22	2.12	0.50
14:D:105:MET:HG3	14:D:171:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:6:TYR:HB2	19:I:21:ILE:HG23	1.93	0.50
36:a:1796:U:H2'	36:a:1797:G:C8	2.46	0.50
52:q:46:GLU:OE1	52:q:46:GLU:N	2.44	0.50
36:a:2229:U:H2'	36:a:2230:G:H8	1.77	0.50
36:a:2484:G:OP1	47:l:44:ARG:NH1	2.39	0.50
53:r:20:VAL:HG11	53:r:44:ALA:HA	1.94	0.50
7:6:26:VAL:HG22	7:6:178:ILE:HD11	1.94	0.49
8:7:43:LEU:HD13	8:7:46:LEU:HD12	1.93	0.49
11:A:938:A:N3	11:A:1376:U:O2'	2.39	0.49
11:A:1255:G:O2'	11:A:1258:G:N3	2.38	0.49
11:A:1507:A:H2'	11:A:1508:A:C8	2.47	0.49
22:L:86:ARG:HG2	22:L:94:ARG:HA	1.93	0.49
36:a:75:G:H22	36:a:111:A:H2	1.59	0.49
36:a:475:C:O2	36:a:479:A:N6	2.40	0.49
11:A:1253:G:H2'	11:A:1254:A:H8	1.77	0.49
14:D:126:ASN:ND2	14:D:141:ASP:OD1	2.44	0.49
17:G:87:VAL:HG21	17:G:154:TYR:HB2	1.93	0.49
36:a:2898:U:H2'	36:a:2899:A:H8	1.78	0.49
11:A:34:C:H2'	11:A:35:G:H8	1.77	0.49
36:a:1476:U:H2'	36:a:1477:A:H8	1.77	0.49
36:a:2313:C:O4'	41:f:37:ASN:ND2	2.32	0.49
36:a:2571:U:O2'	39:d:151:THR:O	2.29	0.49
7:6:89:SER:O	7:6:93:GLN:NE2	2.46	0.49
7:6:207:ILE:HD11	10:9:334:TRP:H	1.78	0.49
11:A:634:C:H2'	11:A:635:A:H8	1.78	0.49
11:A:1414:U:H2'	11:A:1415:G:H8	1.77	0.49
13:C:17:PRO:HG2	13:C:54:ARG:HH22	1.78	0.49
36:a:2314:A:OP1	41:f:88:LYS:NZ	2.44	0.49
45:j:43:ILE:HD12	45:j:56:ASP:HB2	1.94	0.49
12:B:15:HIS:HB3	12:B:43:LEU:HD11	1.94	0.49
14:D:145:ILE:HD13	14:D:178:MET:HB3	1.95	0.49
36:a:1028:A:N3	36:a:2486:C:O2'	2.40	0.49
36:a:1433:A:H2'	36:a:1434:A:C8	2.47	0.49
11:A:150:U:H2'	11:A:151:A:H8	1.78	0.49
11:A:231:U:H2'	11:A:232:G:H8	1.77	0.49
23:M:58:ASP:OD1	23:M:58:ASP:N	2.45	0.49
7:6:173:TRP:HD1	7:6:174:LEU:HD23	1.76	0.49
11:A:1004:A:O2'	11:A:1036:A:N6	2.46	0.49
11:A:1241:G:H2'	11:A:1242:G:H8	1.77	0.49
36:a:742:A:H2'	36:a:743:A:C8	2.48	0.49
36:a:832:U:H2'	36:a:833:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:2564:A:OP1	36:a:2648:G:O2'	2.26	0.49
11:A:413:G:N2	11:A:429:U:OP2	2.44	0.49
11:A:490:C:H2'	11:A:491:G:H8	1.78	0.49
11:A:1356:G:H2'	11:A:1357:A:C8	2.47	0.49
48:m:28:LEU:HD23	48:m:48:VAL:HG21	1.94	0.49
11:A:147:G:H2'	11:A:148:G:C8	2.48	0.49
11:A:521:G:HO2'	11:A:536:C:HO2'	1.60	0.49
11:A:1402:4OC:H2'	11:A:1403:C:O4'	2.12	0.49
29:S:36:ARG:NH2	29:S:75:ALA:O	2.45	0.49
36:a:5:A:H2'	36:a:6:A:C8	2.48	0.49
36:a:1319:C:O2'	36:a:1321:A:N6	2.46	0.49
8:7:88:GLN:HA	8:7:91:LEU:HD12	1.94	0.49
10:9:409:MET:HA	10:9:412:TYR:HB2	1.95	0.49
36:a:856:G:H2'	36:a:857:G:C8	2.47	0.49
56:u:40:ILE:HD12	56:u:42:LEU:HD21	1.94	0.49
11:A:222:C:H2'	11:A:223:A:H8	1.78	0.48
11:A:1139:G:H4'	11:A:1140:C:H5'	1.95	0.48
12:B:46:THR:HB	12:B:201:PRO:HG2	1.93	0.48
18:H:29:SER:HB2	18:H:59:LEU:HB2	1.95	0.48
43:h:12:LEU:HD22	43:h:19:VAL:HG21	1.94	0.48
46:k:132:ARG:O	46:k:136:GLU:HG2	2.13	0.48
1:0:37:LYS:HE3	1:0:37:LYS:HB2	1.69	0.48
37:b:49:C:H2'	37:b:50:A:H8	1.76	0.48
41:f:136:ILE:HA	41:f:141:ILE:HD11	1.95	0.48
11:A:624:C:H4'	26:P:10:GLY:HA2	1.96	0.48
36:a:74:A:O2'	36:a:88:G:OP2	2.30	0.48
36:a:1028:A:H2'	36:a:1029:A:C8	2.48	0.48
36:a:1406:U:H2'	36:a:1407:G:H8	1.78	0.48
60:y:9:GLN:NE2	60:y:11:ARG:O	2.40	0.48
7:6:317:TYR:O	7:6:321:TYR:HB2	2.13	0.48
11:A:1513:A:H2'	11:A:1514:G:C8	2.48	0.48
36:a:2640:G:OP1	44:i:96:ARG:NH1	2.45	0.48
49:n:99:TYR:OH	49:n:111:ARG:NH2	2.46	0.48
7:6:64:PHE:HD1	7:6:72:LEU:HD23	1.77	0.48
59:x:20:ASN:O	59:x:24:GLU:HG3	2.13	0.48
7:6:431:SER:O	7:6:435:LYS:NZ	2.40	0.48
11:A:545:C:H5'	14:D:69:GLU:HB2	1.95	0.48
11:A:662:U:H2'	11:A:663:A:C8	2.49	0.48
36:a:219:A:N3	36:a:234:U:O2'	2.40	0.48
36:a:987:C:O2'	36:a:1000:A:N3	2.39	0.48
14:D:13:ARG:HG3	14:D:38:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:118:LEU:HD22	19:I:124:ARG:HG2	1.95	0.48
36:a:581:C:H2'	36:a:582:A:H8	1.79	0.48
42:g:2:SER:OG	42:g:3:ARG:N	2.47	0.48
5:4:48:GLN:NE2	41:f:114:PHE:O	2.46	0.48
35:Z:15:G:O6	35:Z:49:C:O2	2.31	0.48
36:a:1047:G:O2'	36:a:1110:G:N1	2.38	0.48
36:a:1429:G:H2'	36:a:1430:G:H8	1.79	0.48
11:A:816:A:OP1	11:A:1526:G:O2'	2.28	0.48
13:C:11:ARG:NH2	13:C:177:THR:O	2.42	0.48
15:E:13:GLU:HG2	15:E:39:VAL:HG12	1.96	0.48
11:A:1147:C:O2'	19:I:7:TYR:OH	2.24	0.48
18:H:102:ALA:HB3	18:H:113:ASP:HB3	1.96	0.48
36:a:307:G:N1	36:a:310:A:OP2	2.39	0.48
36:a:1385:A:O2'	36:a:1396:U:O2	2.32	0.48
36:a:1386:C:H2'	36:a:1387:A:H8	1.78	0.48
36:a:1419:A:O2'	36:a:1421:G:N7	2.44	0.48
19:I:52:LEU:HA	19:I:55:VAL:HG22	1.96	0.47
28:R:72:ASP:OD1	28:R:73:ARG:N	2.47	0.47
36:a:668:A:H2'	36:a:670:A:H62	1.78	0.47
36:a:1296:G:OP1	36:a:2709:G:O2'	2.30	0.47
56:u:55:GLU:OE1	56:u:55:GLU:N	2.38	0.47
11:A:537:G:OP1	22:L:110:ARG:NH2	2.47	0.47
11:A:1071:C:H2'	11:A:1072:G:C8	2.49	0.47
36:a:2339:C:O2'	37:b:41:G:N2	2.47	0.47
10:9:531:ILE:O	10:9:535:LEU:N	2.42	0.47
11:A:652:U:O4	11:A:752:G:O2'	2.25	0.47
11:A:689:C:OP1	21:K:29:ASN:ND2	2.44	0.47
11:A:715:A:H2'	11:A:716:A:C8	2.49	0.47
11:A:999:C:H2'	11:A:1000:A:H8	1.78	0.47
11:A:1243:C:H2'	11:A:1244:G:H8	1.79	0.47
36:a:721:A:H2'	36:a:722:A:C8	2.50	0.47
36:a:1406:U:H2'	36:a:1407:G:C8	2.49	0.47
36:a:1469:A:H2'	36:a:1470:A:C8	2.49	0.47
36:a:2547:A:H2'	36:a:2548:U:C6	2.49	0.47
43:h:4:ILE:HG22	43:h:18:GLN:HG2	1.97	0.47
13:C:47:LEU:HB3	13:C:50:ALA:HB3	1.95	0.47
21:K:71:ALA:O	21:K:75:LYS:HG3	2.14	0.47
36:a:2246:G:H2'	36:a:2247:A:C8	2.49	0.47
36:a:2305:U:H5''	41:f:131:GLY:HA3	1.96	0.47
59:x:5:GLU:OE1	59:x:5:GLU:N	2.42	0.47
7:6:128:ALA:O	7:6:132:SER:OG	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:155:A:H2'	36:a:156:A:C8	2.50	0.47
36:a:877:A:O2'	36:a:900:A:N6	2.48	0.47
36:a:2233:U:H2'	36:a:2234:G:C8	2.50	0.47
36:a:2676:C:OP1	45:j:31:ARG:NH2	2.48	0.47
43:h:7:ASP:OD1	43:h:8:LYS:N	2.48	0.47
11:A:154:U:O4	11:A:155:A:N6	2.48	0.47
23:M:24:GLY:O	23:M:29:ARG:NH1	2.47	0.47
36:a:72:U:O4	59:x:58:ASN:ND2	2.47	0.47
36:a:2245:U:H5''	36:a:2246:G:H5'	1.97	0.47
7:6:287:PRO:HA	7:6:290:ILE:HD12	1.97	0.47
8:7:29:ALA:HB2	8:7:48:VAL:HG11	1.96	0.47
11:A:1516:2MG:N2	11:A:1519:MA6:OP2	2.45	0.47
18:H:11:LEU:HD22	18:H:75:ILE:HD11	1.96	0.47
30:T:35:VAL:O	30:T:39:ILE:HG13	2.15	0.47
36:a:1417:C:HO2'	36:a:1587:G:HO2'	1.48	0.47
36:a:2328:A:H2'	36:a:2329:U:C6	2.50	0.47
36:a:2698:U:H2'	36:a:2699:C:C6	2.50	0.47
42:g:73:ASN:O	42:g:77:ILE:HG13	2.15	0.47
44:i:9:GLU:HG2	44:i:10:THR:HG23	1.97	0.47
52:q:16:GLU:OE2	52:q:101:ILE:N	2.45	0.47
11:A:253:A:O2'	27:Q:17:MET:SD	2.73	0.47
36:a:1791:A:N6	36:a:1828:G:O2'	2.43	0.47
36:a:2618:G:H21	39:d:155:VAL:HG21	1.80	0.47
56:u:73:LYS:HG3	56:u:94:ALA:HB2	1.97	0.47
21:K:64:GLN:O	21:K:68:GLU:HG3	2.15	0.47
36:a:833:A:H2'	36:a:834:G:C8	2.50	0.47
36:a:2540:C:O2'	36:a:2740:A:N3	2.46	0.47
36:a:2788:C:O2'	36:a:2809:A:N3	2.42	0.47
7:6:120:THR:O	7:6:124:THR:HG23	2.15	0.47
14:D:70:ARG:HD2	14:D:73:ARG:HH21	1.80	0.47
36:a:743:A:O2'	36:a:1659:G:OP1	2.28	0.47
11:A:745:G:H2'	11:A:746:A:H8	1.80	0.46
13:C:14:ILE:HG22	13:C:15:VAL:HG13	1.97	0.46
36:a:329:G:OP2	55:t:69:ASN:ND2	2.47	0.46
36:a:1266:G:O2'	36:a:2012:G:O6	2.30	0.46
36:a:2012:G:N7	53:r:16:LYS:NZ	2.59	0.46
36:a:2241:A:H2'	36:a:2242:G:C8	2.50	0.46
37:b:1:U:H2'	37:b:2:G:C8	2.50	0.46
56:u:55:GLU:HB2	56:u:59:GLU:HG3	1.98	0.46
10:9:189:GLU:N	10:9:189:GLU:OE1	2.48	0.46
14:D:107:PHE:CG	14:D:145:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:16:PRO:HB3	19:I:42:GLU:HG3	1.96	0.46
21:K:106:ARG:HG2	31:U:12:PHE:HZ	1.80	0.46
36:a:807:U:O2'	36:a:2060:A:N1	2.46	0.46
36:a:1047:G:N2	36:a:1110:G:O2'	2.44	0.46
36:a:1340:U:OP2	54:s:82:LYS:NZ	2.45	0.46
36:a:2039:U:H2'	36:a:2040:G:C8	2.50	0.46
11:A:486:U:H2'	11:A:487:A:H8	1.80	0.46
12:B:19:GLN:OE1	12:B:19:GLN:N	2.45	0.46
20:J:54:SER:OG	20:J:56:HIS:O	2.32	0.46
36:a:576:U:H2'	36:a:577:G:C8	2.51	0.46
36:a:2079:U:O2'	58:w:23:ASN:OD1	2.30	0.46
8:7:91:LEU:O	8:7:95:LEU:HD22	2.15	0.46
14:D:9:LEU:HG	14:D:22:LYS:HE3	1.98	0.46
27:Q:15:ASP:HA	27:Q:21:ILE:HG22	1.97	0.46
34:Y:19:G:O2'	34:Y:58:G:N2	2.31	0.46
36:a:1734:G:H2'	36:a:1735:A:H8	1.81	0.46
36:a:2291:U:H2'	36:a:2292:U:C6	2.49	0.46
11:A:503:C:O2'	11:A:509:A:N6	2.49	0.46
11:A:674:G:H2'	11:A:675:A:C8	2.49	0.46
25:O:71:LYS:HB2	25:O:71:LYS:HE3	1.66	0.46
26:P:50:THR:HG23	26:P:74:LEU:HD13	1.97	0.46
34:Y:66:U:H2'	34:Y:67:A:H8	1.80	0.46
38:c:142:HIS:ND1	38:c:193:GLY:O	2.38	0.46
11:A:21:G:H2'	11:A:22:G:C8	2.49	0.46
36:a:1278:C:H2'	36:a:1279:G:C8	2.51	0.46
36:a:1667:G:O2'	36:a:1991:U:O4	2.28	0.46
36:a:2246:G:H2'	36:a:2247:A:H8	1.80	0.46
5:4:41:HIS:O	5:4:45:THR:OG1	2.31	0.46
7:6:28:GLY:O	7:6:32:VAL:HG23	2.16	0.46
11:A:1253:G:H2'	11:A:1254:A:C8	2.51	0.46
14:D:109:ALA:HB3	14:D:113:GLU:HG3	1.98	0.46
23:M:3:ARG:NH2	41:f:110:ARG:O	2.48	0.46
36:a:2070:A:H2'	36:a:2071:A:C8	2.51	0.46
36:a:2258:C:O2'	36:a:2427:C:OP2	2.29	0.46
47:l:75:GLU:HB2	47:l:90:GLU:HG3	1.97	0.46
10:9:101:GLU:OE1	10:9:102:THR:N	2.49	0.46
11:A:324:G:N1	11:A:327:A:OP2	2.46	0.46
11:A:769:G:H4'	11:A:1513:A:H4'	1.98	0.46
18:H:52:GLU:OE1	18:H:52:GLU:N	2.49	0.46
36:a:1799:G:O2'	38:c:180:GLU:OE2	2.32	0.46
41:f:4:LEU:N	41:f:101:GLU:OE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:z:46:ASP:OD1	61:z:46:ASP:N	2.39	0.46
7:6:95:LEU:HD11	7:6:102:LEU:HD12	1.97	0.46
20:J:42:LEU:HD21	20:J:73:LEU:HD22	1.98	0.46
36:a:1306:C:H41	36:a:1606:C:H2'	1.81	0.46
36:a:1802:A:H2'	36:a:1803:A:C8	2.50	0.46
38:c:133:ARG:NH1	38:c:187:ASP:OD1	2.40	0.46
49:n:76:LYS:NZ	49:n:80:GLU:OE2	2.45	0.46
10:9:72:ILE:HG22	10:9:79:VAL:HG13	1.97	0.46
36:a:414:C:H2'	36:a:415:A:C8	2.51	0.46
36:a:910:A:H2'	36:a:911:A:C8	2.51	0.46
36:a:2591:C:H2'	36:a:2592:G:C8	2.50	0.46
36:a:2788:C:H2'	36:a:2789:C:C6	2.51	0.46
11:A:634:C:H2'	11:A:635:A:C8	2.52	0.45
36:a:1115:G:O2'	36:a:1116:G:O5'	2.34	0.45
36:a:2273:A:H2'	36:a:2274:A:C8	2.51	0.45
40:e:173:THR:HA	40:e:199:MET:HE1	1.97	0.45
59:x:12:GLU:OE1	59:x:12:GLU:N	2.45	0.45
10:9:357:SER:HA	10:9:360:ILE:HG22	1.97	0.45
11:A:197:A:N1	11:A:220:G:O2'	2.47	0.45
11:A:1291:U:H2'	11:A:1292:G:H8	1.82	0.45
23:M:89:LEU:HD13	23:M:92:ARG:HD2	1.98	0.45
36:a:1114:C:H2'	36:a:1115:G:C8	2.51	0.45
2:1:39:ARG:NH2	36:a:468:G:N7	2.57	0.45
11:A:235:C:H2'	11:A:236:A:C8	2.52	0.45
11:A:1048:G:H5''	24:N:3:LYS:HD2	1.98	0.45
14:D:44:ARG:HG3	14:D:46:PRO:HD3	1.97	0.45
22:L:50:ARG:HG3	22:L:90:LEU:HD21	1.99	0.45
36:a:1447:C:H2'	36:a:1448:G:H8	1.82	0.45
36:a:2087:G:H2'	36:a:2088:A:H8	1.81	0.45
36:a:2230:G:H5''	58:w:30:LEU:HD12	1.98	0.45
36:a:2514:U:H2'	36:a:2515:C:C6	2.51	0.45
39:d:39:ASP:N	39:d:39:ASP:OD1	2.49	0.45
61:z:38:HIS:ND1	61:z:39:LEU:O	2.49	0.45
11:A:171:A:H2'	11:A:172:A:C8	2.52	0.45
11:A:1391:U:H2'	11:A:1392:G:C8	2.52	0.45
36:a:349:U:H2'	36:a:350:G:H8	1.81	0.45
36:a:589:U:H2'	36:a:590:A:C8	2.52	0.45
36:a:2333:A:OP2	57:v:77:ARG:NH2	2.47	0.45
10:9:114:LEU:HB2	10:9:120:PRO:HD2	1.97	0.45
10:9:493:LYS:HA	10:9:496:THR:HG22	1.98	0.45
11:A:1500:A:H5''	11:A:1508:A:H5''	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:175:LEU:HD23	13:C:182:ILE:HD13	1.97	0.45
36:a:272:A:H2'	36:a:273:G:C8	2.52	0.45
36:a:639:U:H2'	36:a:640:C:C6	2.52	0.45
36:a:1794:A:H2'	36:a:1795:C:C6	2.52	0.45
36:a:1853:A:H2'	36:a:1854:A:C8	2.52	0.45
56:u:77:VAL:HG23	56:u:89:ILE:HG12	1.98	0.45
7:6:63:MET:SD	7:6:63:MET:N	2.89	0.45
10:9:163:LYS:HD3	10:9:178:TYR:HB3	1.98	0.45
47:l:42:THR:HG22	47:l:93:VAL:HG12	1.97	0.45
11:A:17:U:H2'	11:A:18:C:C6	2.52	0.45
11:A:1126:U:OP1	20:J:7:ARG:NH1	2.38	0.45
36:a:1469:A:H2'	36:a:1470:A:H8	1.82	0.45
7:6:132:SER:O	7:6:136:ALA:HB2	2.16	0.45
11:A:41:G:H2'	11:A:42:G:C8	2.51	0.45
16:F:72:ASP:O	16:F:76:THR:HG23	2.17	0.45
32:V:117:ARG:O	36:a:2061:G:N2	2.46	0.45
36:a:2243:U:H2'	36:a:2244:U:C6	2.52	0.45
53:r:17:VAL:HG11	53:r:103:ILE:HG12	1.98	0.45
54:s:5:GLU:OE1	54:s:5:GLU:N	2.42	0.45
1:0:23:THR:OG1	1:0:24:THR:N	2.50	0.45
11:A:1320:C:N3	29:S:36:ARG:NH1	2.65	0.45
23:M:90:ARG:HD3	23:M:95:LEU:HB2	1.98	0.45
34:Y:24:C:H2'	34:Y:25:G:C8	2.52	0.45
36:a:2291:U:OP1	36:a:2380:C:O2'	2.35	0.45
36:a:2591:C:H2'	36:a:2592:G:H8	1.82	0.45
46:k:82:LEU:HD22	46:k:90:VAL:HG21	1.98	0.45
9:8:65:ILE:O	9:8:69:VAL:HG23	2.17	0.45
36:a:320:A:N3	40:e:163:ASN:ND2	2.51	0.45
47:l:35:ALA:HA	47:l:128:THR:HG22	1.99	0.45
7:6:63:MET:HA	7:6:66:MET:HG2	1.99	0.44
36:a:1799:G:OP1	38:c:258:ARG:NH1	2.38	0.44
7:6:102:LEU:HD23	7:6:105:ILE:HD12	1.99	0.44
7:6:311:GLN:O	7:6:314:GLN:NE2	2.50	0.44
10:9:346:TRP:O	10:9:349:SER:OG	2.33	0.44
11:A:757:U:OP1	11:A:822:U:O2'	2.33	0.44
42:g:17:VAL:HG11	42:g:50:LEU:HD21	1.99	0.44
48:m:86:ARG:NE	48:m:117:ASP:OD2	2.42	0.44
11:A:1123:U:O2'	20:J:39:PRO:O	2.27	0.44
11:A:1342:C:H2'	11:A:1343:G:C8	2.52	0.44
36:a:593:U:H2'	36:a:594:U:C6	2.52	0.44
36:a:1864:U:OP1	36:a:2410:G:O2'	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1149:C:H2'	11:A:1150:A:C8	2.50	0.44
22:L:34:CYS:HB2	22:L:78:SER:H	1.82	0.44
24:N:82:ILE:O	24:N:86:GLU:HG3	2.17	0.44
36:a:2047:C:H2'	36:a:2048:G:H8	1.82	0.44
10:9:384:ARG:HG3	10:9:385:MET:HG3	2.00	0.44
11:A:1162:C:H2'	11:A:1163:A:H8	1.82	0.44
36:a:1353:A:H2'	36:a:1354:A:C8	2.53	0.44
37:b:5:U:OP1	37:b:61:G:O2'	2.25	0.44
10:9:477:PHE:O	10:9:481:MET:HG2	2.18	0.44
11:A:539:A:H2'	11:A:540:G:C8	2.53	0.44
11:A:1305:G:H22	11:A:1331:G:HO2'	1.66	0.44
36:a:1438:U:H2'	36:a:1439:A:H8	1.83	0.44
36:a:2845:U:H5''	50:o:52:ASN:O	2.17	0.44
11:A:947:G:O3'	23:M:108:THR:OG1	2.36	0.44
25:O:74:ASP:OD1	25:O:74:ASP:N	2.49	0.44
34:Y:54:G:O3'	47:l:55:ARG:NH2	2.48	0.44
36:a:58:G:O2'	36:a:73:A:N1	2.50	0.44
36:a:582:A:H2'	36:a:583:G:C8	2.53	0.44
36:a:1009:A:N3	36:a:1153:C:O2'	2.47	0.44
36:a:1754:A:C8	50:o:94:LYS:HE2	2.53	0.44
36:a:2405:G:O2'	36:a:2411:A:N6	2.50	0.44
37:b:49:C:H2'	37:b:50:A:C8	2.52	0.44
7:6:60:ILE:HA	7:6:63:MET:HG2	2.00	0.44
36:a:1744:A:H3'	36:a:1745:A:H8	1.83	0.44
11:A:677:U:O2	11:A:777:A:O2'	2.28	0.44
11:A:1147:C:H2'	11:A:1148:U:C6	2.53	0.44
36:a:580:U:H2'	36:a:581:C:C6	2.53	0.44
36:a:1734:G:H2'	36:a:1735:A:C8	2.53	0.44
36:a:2014:A:H2'	36:a:2015:A:C8	2.53	0.44
11:A:976:G:OP2	11:A:1358:U:O2'	2.35	0.43
57:v:44:LYS:HB2	57:v:44:LYS:HE2	1.79	0.43
11:A:490:C:H2'	11:A:491:G:C8	2.54	0.43
58:w:7:VAL:O	58:w:74:ARG:NH2	2.51	0.43
11:A:505:G:OP1	11:A:510:A:N6	2.51	0.43
23:M:15:ALA:HB3	23:M:34:LEU:HD21	2.00	0.43
36:a:278:A:N6	36:a:362:A:N7	2.67	0.43
36:a:589:U:H2'	36:a:590:A:H8	1.83	0.43
36:a:1013:C:H2'	36:a:1014:A:H8	1.84	0.43
36:a:1808:A:H3'	36:a:1809:A:C8	2.54	0.43
4:3:1:MET:HE2	4:3:1:MET:HB2	1.93	0.43
36:a:151:C:H2'	36:a:152:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:288:U:H2'	36:a:289:G:H8	1.82	0.43
36:a:1563:U:H2'	36:a:1564:C:C6	2.53	0.43
40:e:1:MET:HE1	40:e:113:VAL:HG11	2.00	0.43
11:A:1144:G:N2	11:A:1146:A:H62	2.15	0.43
11:A:1382:C:H2'	11:A:1383:C:H6	1.84	0.43
36:a:1571:A:H2'	36:a:1572:A:C8	2.53	0.43
36:a:1604:C:H2'	36:a:1605:C:H6	1.83	0.43
36:a:1654:A:O2'	39:d:118:PHE:O	2.28	0.43
36:a:2087:G:H2'	36:a:2088:A:C8	2.54	0.43
10:9:471:MET:HE3	10:9:471:MET:HB3	1.91	0.43
11:A:337:G:H2'	11:A:338:A:H8	1.83	0.43
11:A:552:U:H2'	11:A:553:A:C8	2.53	0.43
11:A:1249:C:O3'	19:I:75:GLN:NE2	2.51	0.43
36:a:5:A:H2'	36:a:6:A:H8	1.82	0.43
36:a:1000:A:H2'	36:a:1001:A:C8	2.54	0.43
36:a:2836:U:H2'	36:a:2837:A:C8	2.54	0.43
11:A:358:U:H2'	11:A:359:G:H8	1.82	0.43
11:A:390:U:H2'	11:A:391:G:C8	2.54	0.43
11:A:1189:U:OP1	24:N:98:LYS:NZ	2.52	0.43
11:A:1291:U:H2'	11:A:1292:G:C8	2.54	0.43
11:A:1412:C:H2'	11:A:1413:A:C8	2.53	0.43
12:B:97:LEU:H	12:B:100:MET:HE3	1.84	0.43
30:T:31:PHE:O	30:T:35:VAL:HG23	2.17	0.43
36:a:171:U:H2'	36:a:172:A:H8	1.82	0.43
36:a:414:C:H2'	36:a:415:A:H8	1.84	0.43
36:a:582:A:H2'	36:a:583:G:H8	1.84	0.43
36:a:659:G:O2'	40:e:95:LYS:O	2.35	0.43
7:6:121:ARG:O	7:6:124:THR:OG1	2.28	0.43
11:A:400:C:OP1	14:D:70:ARG:NH2	2.51	0.43
24:N:54:ASP:OD1	24:N:59:ARG:NH2	2.40	0.43
36:a:848:C:H2'	36:a:849:A:C8	2.49	0.43
3:2:25:LYS:HB3	46:k:62:PRO:HG2	2.01	0.43
8:7:38:ASP:O	8:7:44:ARG:NH2	2.50	0.43
11:A:582:C:OP2	11:A:758:C:N4	2.46	0.43
36:a:349:U:H2'	36:a:350:G:C8	2.54	0.43
36:a:813:U:H2'	36:a:814:C:C6	2.53	0.43
36:a:2567:G:H2'	36:a:2568:U:C6	2.54	0.43
36:a:2898:U:H2'	36:a:2899:A:C8	2.53	0.43
40:e:149:ILE:HG22	40:e:192:ALA:HB1	2.00	0.43
44:i:1:MET:HE1	52:q:12:HIS:HB3	1.99	0.43
1:0:6:ARG:NE	36:a:2285:C:OP2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:211:ARG:NH1	10:9:329:ASP:OD1	2.52	0.43
15:E:165:LEU:HD12	15:E:165:LEU:HA	1.91	0.43
19:I:88:MET:HE3	19:I:98:LEU:HD12	2.01	0.43
22:L:81:LEU:HB2	22:L:102:LEU:HD12	2.00	0.43
24:N:49:GLN:OE1	29:S:13:LEU:N	2.46	0.43
29:S:28:LYS:NZ	29:S:46:GLY:O	2.52	0.43
36:a:1197:G:H2'	36:a:1198:U:H6	1.84	0.43
37:b:5:U:H2'	37:b:6:G:H8	1.84	0.43
7:6:82:ILE:HD13	7:6:171:LEU:HD13	2.01	0.42
10:9:472:GLY:HA2	10:9:475:MET:HE2	2.01	0.42
11:A:438:U:H1'	14:D:120:HIS:CE1	2.54	0.42
11:A:524:G:H2'	11:A:525:C:C6	2.54	0.42
11:A:1115:U:OP1	20:J:68:ARG:NH1	2.45	0.42
11:A:1130:A:O2'	19:I:5:GLN:OE1	2.29	0.42
11:A:1266:G:N2	11:A:1269:A:OP2	2.38	0.42
11:A:1522:U:OP1	21:K:128:ARG:NH2	2.51	0.42
36:a:720:U:H2'	36:a:721:A:C8	2.54	0.42
36:a:1394:U:H4'	36:a:1603:A:H4'	2.00	0.42
36:a:2229:U:H2'	36:a:2230:G:C8	2.53	0.42
36:a:2251:OMG:HM23	36:a:2251:OMG:H1'	1.59	0.42
41:f:119:ALA:HB1	41:f:167:ARG:HE	1.84	0.42
36:a:247:G:OP2	36:a:249:C:N4	2.49	0.42
36:a:272:A:H2'	36:a:273:G:H8	1.83	0.42
36:a:820:A:H4'	36:a:836:G:H22	1.83	0.42
36:a:1224:U:H2'	36:a:1225:G:C8	2.54	0.42
36:a:1570:A:H2'	36:a:1571:A:C8	2.53	0.42
36:a:2329:U:H2'	36:a:2330:G:C8	2.54	0.42
36:a:2372:U:H2'	36:a:2373:G:C8	2.53	0.42
41:f:106:ILE:HG21	41:f:139:PRO:HG3	2.01	0.42
7:6:87:SER:O	7:6:91:ILE:HG12	2.18	0.42
13:C:8:ASN:ND2	24:N:90:ARG:O	2.52	0.42
21:K:112:ASP:HB3	31:U:2:PRO:HB2	2.01	0.42
30:T:76:LYS:O	30:T:80:THR:OG1	2.28	0.42
36:a:373:U:H2'	36:a:374:A:H8	1.84	0.42
36:a:989:G:OP2	60:y:12:SER:OG	2.38	0.42
36:a:1607:C:N4	36:a:1622:G:OP2	2.40	0.42
36:a:1997:C:OP2	39:d:129:THR:OG1	2.28	0.42
41:f:57:LEU:O	41:f:61:SER:OG	2.23	0.42
50:o:87:LYS:HA	50:o:87:LYS:HD2	1.94	0.42
7:6:241:GLN:HB2	8:7:83:ILE:HD11	2.01	0.42
14:D:54:GLN:HB3	14:D:203:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:90:MET:HE3	16:F:90:MET:HB2	1.86	0.42
30:T:27:MET:HB3	30:T:27:MET:HE3	1.80	0.42
36:a:155:A:H2'	36:a:156:A:H8	1.85	0.42
36:a:1447:C:H2'	36:a:1448:G:C8	2.54	0.42
5:4:13:THR:O	5:4:13:THR:OG1	2.33	0.42
28:R:65:LEU:HD23	28:R:65:LEU:HA	1.89	0.42
29:S:51:VAL:HG21	29:S:71:LEU:HB3	2.01	0.42
32:V:52:GLY:O	32:V:56:GLY:N	2.47	0.42
36:a:569:U:O2'	36:a:983:A:N1	2.44	0.42
36:a:739:A:H1'	36:a:740:C:H5	1.84	0.42
36:a:1038:G:H2'	36:a:1039:A:C8	2.54	0.42
10:9:62:SER:O	10:9:138:TYR:N	2.47	0.42
10:9:407:GLU:OE1	10:9:407:GLU:N	2.51	0.42
11:A:512:U:H2'	11:A:513:C:C6	2.54	0.42
11:A:948:C:H2'	11:A:949:A:H8	1.85	0.42
11:A:1524:C:H2'	11:A:1525:G:C8	2.55	0.42
29:S:41:PHE:H	29:S:44:MET:HE3	1.85	0.42
35:Z:6:A:H2'	35:Z:7:G:C8	2.55	0.42
36:a:566:U:H5''	46:k:29:LYS:HE3	2.01	0.42
36:a:2377:A:O2'	49:n:117:PHE:O	2.32	0.42
36:a:2443:C:H2'	36:a:2444:G:H8	1.84	0.42
38:c:145:GLU:HB2	38:c:188:CYS:HB3	2.01	0.42
15:E:111:MET:HB3	15:E:111:MET:HE2	1.80	0.42
31:U:60:LEU:O	31:U:64:ASN:ND2	2.44	0.42
44:i:114:LEU:HG	44:i:118:MET:HE3	2.01	0.42
55:t:14:LEU:HD11	55:t:71:ALA:HB2	2.00	0.42
10:9:166:VAL:N	10:9:175:ASN:O	2.50	0.42
10:9:262:THR:HG22	10:9:309:VAL:HG13	2.01	0.42
11:A:977:A:N6	11:A:1224:U:O5'	2.53	0.42
11:A:1175:G:H2'	11:A:1176:A:H8	1.85	0.42
36:a:1689:A:H2'	36:a:1690:A:C8	2.54	0.42
36:a:2615:U:C2	61:z:4:GLN:HA	2.54	0.42
36:a:2646:C:OP2	36:a:2732:G:O2'	2.37	0.42
10:9:120:PRO:HB2	10:9:129:PRO:HG3	2.01	0.42
11:A:28:A:O2'	11:A:296:U:OP1	2.26	0.42
18:H:111:MET:HB3	18:H:111:MET:HE2	1.75	0.42
25:O:17:ARG:HH21	25:O:77:ARG:HH11	1.67	0.42
36:a:172:A:H2'	36:a:173:A:C8	2.55	0.42
36:a:2394:C:H5''	46:k:63:LYS:HE2	2.02	0.42
10:9:227:ASP:OD1	10:9:227:ASP:N	2.53	0.42
17:G:129:GLU:N	17:G:129:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Y:5:G:H2'	34:Y:6:A:H8	1.85	0.42
36:a:299:A:N3	36:a:319:G:O2'	2.44	0.42
36:a:1754:A:O3'	50:o:103:ARG:NH2	2.52	0.42
36:a:1889:A:H2'	36:a:1890:A:C8	2.55	0.42
45:j:114:LYS:HE3	45:j:114:LYS:HB2	1.70	0.42
11:A:493:A:H2'	11:A:494:G:C4	2.55	0.41
11:A:1346:A:OP1	19:I:122:ARG:NH1	2.43	0.41
37:b:36:C:N4	37:b:49:C:O2	2.52	0.41
44:i:92:MET:HE3	44:i:92:MET:HB3	1.81	0.41
11:A:182:A:N1	11:A:223:A:O2'	2.53	0.41
11:A:254:G:N2	27:Q:18:GLU:OE2	2.51	0.41
11:A:579:A:O2'	25:O:54:ARG:NH1	2.46	0.41
11:A:579:A:H5'	11:A:728:A:H1'	2.02	0.41
11:A:736:C:H2'	11:A:737:C:H6	1.85	0.41
11:A:1363:A:O2'	11:A:1365:G:N7	2.44	0.41
18:H:25:VAL:HG13	18:H:63:LEU:HD21	2.01	0.41
36:a:742:A:H2'	36:a:743:A:H8	1.84	0.41
36:a:927:A:H2'	36:a:928:A:C8	2.55	0.41
36:a:1443:U:H2'	36:a:1444:G:H8	1.86	0.41
36:a:2086:U:H2'	36:a:2087:G:C8	2.55	0.41
11:A:944:G:N1	11:A:1338:G:OP2	2.48	0.41
36:a:1683:U:H2'	36:a:1684:G:C8	2.55	0.41
36:a:1716:U:H2'	36:a:1717:A:H8	1.85	0.41
7:6:206:THR:HG21	7:6:401:PHE:HE2	1.85	0.41
11:A:67:C:H2'	11:A:68:G:C8	2.55	0.41
11:A:390:U:H2'	11:A:391:G:H8	1.85	0.41
11:A:1006:G:H1	11:A:1023:U:H3	1.67	0.41
16:F:88:MET:HE2	28:R:64:TYR:HD2	1.85	0.41
21:K:35:THR:OG1	21:K:36:ASP:N	2.52	0.41
7:6:279:PHE:O	7:6:283:ILE:HB	2.21	0.41
11:A:579:A:H2'	11:A:580:C:C6	2.56	0.41
11:A:619:U:H3	14:D:131:ASN:HB3	1.86	0.41
11:A:696:A:H2'	11:A:697:U:H6	1.86	0.41
11:A:1216:A:OP1	24:N:3:LYS:NZ	2.42	0.41
19:I:41:ARG:NH2	19:I:43:THR:OG1	2.54	0.41
23:M:78:LYS:HA	23:M:81:MET:HG3	2.03	0.41
29:S:49:ILE:HD12	29:S:49:ILE:HA	1.84	0.41
30:T:28:MET:HG3	30:T:58:VAL:HG12	2.02	0.41
36:a:184:C:H2'	36:a:185:G:H8	1.84	0.41
36:a:284:U:O2	36:a:356:G:N2	2.44	0.41
36:a:1668:A:O2'	36:a:1674:G:N7	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:o:22:PRO:HD3	50:o:50:ILE:HD12	2.03	0.41
7:6:130:PHE:HE2	7:6:290:ILE:HG12	1.85	0.41
10:9:495:MET:HA	10:9:498:MET:HE3	2.02	0.41
11:A:193:C:H2'	11:A:194:C:C6	2.55	0.41
11:A:235:C:H2'	11:A:236:A:H8	1.83	0.41
11:A:600:A:H2'	11:A:601:G:H8	1.86	0.41
14:D:139:PRO:HB3	14:D:184:ARG:HA	2.02	0.41
36:a:64:A:H2'	36:a:65:U:C6	2.56	0.41
36:a:876:C:H2'	36:a:877:A:O4'	2.20	0.41
36:a:1231:U:H2'	36:a:1232:G:H8	1.85	0.41
36:a:1571:A:H2'	36:a:1572:A:H8	1.86	0.41
36:a:1682:G:H2'	36:a:1683:U:C6	2.56	0.41
38:c:5:LYS:HD2	38:c:17:VAL:HG22	2.02	0.41
11:A:12:U:H4'	11:A:526:C:H4'	2.03	0.41
11:A:35:G:N3	22:L:115:SER:OG	2.48	0.41
11:A:908:A:H2'	11:A:909:A:H8	1.84	0.41
19:I:33:ARG:HE	19:I:38:TYR:HD1	1.69	0.41
36:a:160:A:N3	36:a:2208:C:O2'	2.44	0.41
36:a:511:U:H4'	36:a:1235:G:H4'	2.03	0.41
36:a:871:U:H2'	36:a:872:U:C6	2.56	0.41
36:a:1292:G:H2'	36:a:1293:C:C6	2.56	0.41
36:a:1564:C:H2'	36:a:1565:C:C6	2.56	0.41
38:c:72:ASP:OD2	38:c:189:ARG:NH2	2.54	0.41
40:e:149:ILE:HB	40:e:188:MET:HG2	2.03	0.41
11:A:402:G:P	14:D:71:GLN:HE22	2.43	0.41
11:A:427:U:O2'	11:A:541:G:OP1	2.35	0.41
28:R:33:ILE:HD12	28:R:37:GLY:HA2	2.03	0.41
36:a:554:U:H2'	36:a:555:G:O4'	2.21	0.41
53:r:84:ARG:HB2	53:r:96:ILE:HB	2.03	0.41
3:2:45:ARG:NH2	36:a:2349:G:OP1	2.53	0.41
3:2:52:LYS:HB3	3:2:52:LYS:HE3	1.80	0.41
7:6:405:SER:O	7:6:409:VAL:HG13	2.21	0.41
7:6:416:PHE:O	7:6:420:VAL:HG13	2.20	0.41
7:6:426:SER:O	7:6:430:GLU:N	2.53	0.41
11:A:236:A:H2'	11:A:237:G:C8	2.55	0.41
11:A:337:G:H2'	11:A:338:A:C8	2.55	0.41
11:A:407:U:H2'	11:A:408:A:C8	2.55	0.41
11:A:512:U:H2'	11:A:513:C:H6	1.85	0.41
11:A:718:A:H5'	21:K:119:ASN:HD21	1.86	0.41
11:A:859:G:H2'	11:A:860:A:C8	2.56	0.41
11:A:881:G:OP2	22:L:9:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1217:C:OP1	24:N:9:ARG:NE	2.44	0.41
24:N:49:GLN:NE2	29:S:11:ILE:O	2.47	0.41
34:Y:64:U:H2'	34:Y:65:C:C6	2.56	0.41
36:a:6:A:H2'	36:a:7:G:C8	2.56	0.41
36:a:27:G:N2	36:a:512:G:H1'	2.36	0.41
36:a:2081:U:H2'	36:a:2082:A:H8	1.86	0.41
36:a:2443:C:H2'	36:a:2444:G:C8	2.56	0.41
36:a:2705:A:O2'	36:a:2852:G:OP1	2.31	0.41
39:d:181:ASP:OD2	39:d:184:ARG:NE	2.54	0.41
45:j:106:GLU:OE1	45:j:106:GLU:N	2.53	0.41
11:A:297:G:N2	11:A:300:A:OP2	2.36	0.41
11:A:625:U:H2'	11:A:626:G:H8	1.86	0.41
16:F:6:ILE:HG13	16:F:89:VAL:HG23	2.03	0.41
36:a:1412:U:H2'	36:a:1413:A:C8	2.56	0.41
38:c:165:VAL:HG21	38:c:181:MET:HE1	2.02	0.41
57:v:72:LYS:HB2	57:v:72:LYS:HE2	1.91	0.41
10:9:444:VAL:HG12	10:9:447:ARG:HA	2.02	0.40
11:A:269:C:H2'	11:A:270:A:C8	2.55	0.40
11:A:504:C:O2	11:A:511:C:N4	2.53	0.40
11:A:553:A:H2'	11:A:554:A:C8	2.56	0.40
11:A:918:A:H2'	11:A:919:A:C8	2.56	0.40
30:T:29:ARG:O	30:T:33:LYS:HG3	2.21	0.40
36:a:1880:U:H2'	36:a:1881:C:C6	2.57	0.40
11:A:613:C:H2'	11:A:614:C:C6	2.56	0.40
11:A:911:U:H2'	11:A:912:C:C6	2.56	0.40
11:A:1238:A:OP1	11:A:1335:U:O2'	2.32	0.40
36:a:30:G:O2'	36:a:1214:A:N3	2.50	0.40
36:a:1794:A:H2'	36:a:1795:C:H6	1.86	0.40
36:a:2314:A:H2'	36:a:2315:G:C8	2.56	0.40
50:o:5:ILE:O	50:o:9:GLU:HG3	2.20	0.40
7:6:48:VAL:HG23	7:6:148:LEU:HD23	2.03	0.40
8:7:58:VAL:HG12	8:7:66:LYS:HE3	2.02	0.40
10:9:142:GLU:O	10:9:169:ARG:NH2	2.54	0.40
11:A:591:U:H2'	11:A:592:G:H8	1.86	0.40
14:D:177:LYS:NZ	14:D:179:GLU:OE1	2.38	0.40
21:K:79:ILE:HB	21:K:105:PHE:HE1	1.86	0.40
36:a:2857:G:N2	36:a:2860:A:OP2	2.39	0.40
37:b:52:A:N7	49:n:64:TYR:OH	2.48	0.40
39:d:152:PRO:HG3	39:d:156:PHE:CZ	2.56	0.40
40:e:168:ASP:OD2	40:e:170:ARG:NE	2.53	0.40
57:v:37:ILE:HG21	57:v:80:ILE:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:25:PHE:HZ	7:6:177:GLN:HG3	1.85	0.40
10:9:475:MET:HA	10:9:478:ILE:HG22	2.04	0.40
11:A:18:C:OP1	15:E:132:ASN:ND2	2.51	0.40
11:A:131:A:H2'	11:A:132:C:C6	2.57	0.40
13:C:9:GLY:HA3	24:N:89:MET:HE3	2.04	0.40
20:J:92:LEU:HD23	20:J:92:LEU:HA	1.85	0.40
36:a:419:U:H2'	36:a:420:C:C6	2.56	0.40
36:a:858:G:H3'	36:a:859:G:C8	2.55	0.40
10:9:426:LEU:O	10:9:430:MET:HG2	2.21	0.40
11:A:486:U:H2'	11:A:487:A:C8	2.57	0.40
11:A:513:C:H2'	11:A:514:C:H6	1.87	0.40
11:A:601:G:H2'	11:A:602:A:H8	1.87	0.40
11:A:601:G:H2'	11:A:602:A:C8	2.57	0.40
11:A:1328:C:H2'	11:A:1329:A:H8	1.86	0.40
36:a:171:U:H2'	36:a:172:A:C8	2.56	0.40
36:a:1715:G:O2'	36:a:1743:G:O6	2.32	0.40
42:g:107:LEU:O	42:g:152:ARG:NH2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
7	6	419/443 (95%)	404 (96%)	15 (4%)	0	100	100
8	7	112/127 (88%)	107 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	8	52/110 (47%)	49 (94%)	3 (6%)	0	100	100
10	9	461/548 (84%)	436 (95%)	25 (5%)	0	100	100
12	B	222/241 (92%)	215 (97%)	7 (3%)	0	100	100
13	C	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
14	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
15	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
16	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
17	G	151/179 (84%)	146 (97%)	5 (3%)	0	100	100
18	H	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
19	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
20	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	13
21	K	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
22	L	120/124 (97%)	110 (92%)	10 (8%)	0	100	100
23	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
24	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
25	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
26	P	79/82 (96%)	77 (98%)	2 (2%)	0	100	100
27	Q	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
28	R	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
29	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
30	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
31	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
32	V	87/119 (73%)	82 (94%)	4 (5%)	1 (1%)	11	12
38	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
39	d	206/209 (99%)	203 (98%)	3 (2%)	0	100	100
40	e	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
41	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
42	g	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
43	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
44	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
45	j	121/123 (98%)	120 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
47	l	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
48	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
49	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
50	o	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
51	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
52	q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
53	r	108/110 (98%)	108 (100%)	0	0	100	100
54	s	91/100 (91%)	91 (100%)	0	0	100	100
55	t	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
56	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
57	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
58	w	75/78 (96%)	75 (100%)	0	0	100	100
59	x	60/63 (95%)	60 (100%)	0	0	100	100
60	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
61	z	54/57 (95%)	54 (100%)	0	0	100	100
All	All	6616/7260 (91%)	6420 (97%)	194 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	V	88	ARG
20	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	46/49 (94%)	46 (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	344/359 (96%)	342 (99%)	2 (1%)	78	85
8	7	91/99 (92%)	91 (100%)	0	100	100
9	8	48/84 (57%)	47 (98%)	1 (2%)	47	60
10	9	400/469 (85%)	398 (100%)	2 (0%)	81	87
12	B	186/199 (94%)	184 (99%)	2 (1%)	65	75
13	C	170/190 (90%)	170 (100%)	0	100	100
14	D	172/173 (99%)	171 (99%)	1 (1%)	78	85
15	E	119/126 (94%)	119 (100%)	0	100	100
16	F	90/116 (78%)	90 (100%)	0	100	100
17	G	126/147 (86%)	126 (100%)	0	100	100
18	H	104/105 (99%)	104 (100%)	0	100	100
19	I	105/107 (98%)	104 (99%)	1 (1%)	68	77
20	J	86/90 (96%)	86 (100%)	0	100	100
21	K	90/99 (91%)	89 (99%)	1 (1%)	65	75
22	L	102/103 (99%)	102 (100%)	0	100	100
23	M	93/96 (97%)	92 (99%)	1 (1%)	65	75
24	N	83/84 (99%)	83 (100%)	0	100	100
25	O	76/77 (99%)	75 (99%)	1 (1%)	61	72
26	P	65/65 (100%)	65 (100%)	0	100	100
27	Q	73/78 (94%)	73 (100%)	0	100	100
28	R	57/65 (88%)	57 (100%)	0	100	100
29	S	72/79 (91%)	72 (100%)	0	100	100
30	T	65/66 (98%)	65 (100%)	0	100	100
31	U	60/61 (98%)	60 (100%)	0	100	100
32	V	25/93 (27%)	25 (100%)	0	100	100
38	c	216/218 (99%)	215 (100%)	1 (0%)	81	87
39	d	163/163 (100%)	162 (99%)	1 (1%)	78	85
40	e	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	f	148/150 (99%)	145 (98%)	3 (2%)	48	62
42	g	137/138 (99%)	137 (100%)	0	100	100
43	h	32/114 (28%)	32 (100%)	0	100	100
44	i	116/116 (100%)	115 (99%)	1 (1%)	70	80
45	j	104/104 (100%)	104 (100%)	0	100	100
46	k	103/103 (100%)	103 (100%)	0	100	100
47	l	109/109 (100%)	109 (100%)	0	100	100
48	m	98/103 (95%)	98 (100%)	0	100	100
49	n	86/87 (99%)	86 (100%)	0	100	100
50	o	99/100 (99%)	99 (100%)	0	100	100
51	p	89/90 (99%)	89 (100%)	0	100	100
52	q	84/84 (100%)	84 (100%)	0	100	100
53	r	93/93 (100%)	92 (99%)	1 (1%)	65	75
54	s	80/84 (95%)	79 (99%)	1 (1%)	61	72
55	t	83/85 (98%)	83 (100%)	0	100	100
56	u	78/78 (100%)	76 (97%)	2 (3%)	40	53
57	v	59/63 (94%)	59 (100%)	0	100	100
58	w	67/68 (98%)	67 (100%)	0	100	100
59	x	54/55 (98%)	54 (100%)	0	100	100
60	y	48/49 (98%)	48 (100%)	0	100	100
61	z	47/48 (98%)	47 (100%)	0	100	100
All	All	5484/5932 (92%)	5462 (100%)	22 (0%)	81	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	6	95	LEU
7	6	414	MET
9	8	11	ILE
10	9	237	THR
10	9	376	GLN
12	B	10	LEU
12	B	94	HIS
14	D	124	MET
19	I	89	GLU

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Mol	Chain	Res	Type
21	K	74	VAL
23	M	42	ASP
25	O	24	SER
38	c	97	LYS
39	d	1	MET
41	f	49	LEU
41	f	50	LEU
41	f	85	ILE
44	i	1	MET
53	r	4	ILE
54	s	1	MET
56	u	61	LEU
56	u	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	26	ASN
5	4	20	ASN
7	6	252	GLN
7	6	264	HIS
9	8	72	ASN
10	9	57	GLN
10	9	323	HIS
10	9	448	GLN
10	9	527	GLN
12	B	109	GLN
12	B	177	ASN
13	C	100	GLN
13	C	102	ASN
13	C	123	GLN
14	D	74	ASN
15	E	122	ASN
15	E	146	ASN
16	F	55	HIS
17	G	28	ASN
17	G	122	ASN
21	K	24	HIS
24	N	43	ASN
25	O	35	GLN
26	P	40	ASN
30	T	48	GLN

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Mol	Chain	Res	Type
30	T	52	ASN
38	c	25	HIS
40	e	9	GLN
40	e	136	GLN
45	j	93	GLN
47	l	13	HIS
48	m	31	HIS
50	o	66	ASN
51	p	44	GLN
53	r	9	HIS
54	s	48	GLN
58	w	36	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1516/1542 (98%)	214 (14%)	2 (0%)
33	X	8/9 (88%)	1 (12%)	0
34	Y	76/77 (98%)	10 (13%)	2 (2%)
35	Z	76/77 (98%)	11 (14%)	0
36	a	2749/2904 (94%)	309 (11%)	0
37	b	118/120 (98%)	12 (10%)	0
6	5	1/2 (50%)	1 (100%)	0
All	All	4544/4731 (96%)	558 (12%)	4 (0%)

All (558) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
11	A	4	U
11	A	5	U
11	A	6	G
11	A	7	A
11	A	8	A
11	A	9	G
11	A	13	U
11	A	22	G
11	A	32	A
11	A	39	G
11	A	47	C
11	A	48	C

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Mol	Chain	Res	Type
11	A	51	A
11	A	71	A
11	A	83	C
11	A	84	U
11	A	85	U
11	A	86	G
11	A	87	C
11	A	88	U
11	A	95	C
11	A	119	A
11	A	121	U
11	A	122	G
11	A	130	A
11	A	131	A
11	A	143	A
11	A	144	G
11	A	163	C
11	A	173	U
11	A	182	A
11	A	191	G
11	A	197	A
11	A	226	G
11	A	240	G
11	A	245	U
11	A	247	G
11	A	251	G
11	A	266	G
11	A	267	C
11	A	289	G
11	A	306	A
11	A	321	A
11	A	328	C
11	A	347	G
11	A	351	G
11	A	352	C
11	A	354	G
11	A	355	C
11	A	367	U
11	A	372	C
11	A	373	A
11	A	388	G
11	A	392	C

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Mol	Chain	Res	Type
11	A	398	U
11	A	406	G
11	A	412	A
11	A	413	G
11	A	414	A
11	A	418	C
11	A	421	U
11	A	422	C
11	A	423	G
11	A	424	G
11	A	429	U
11	A	431	A
11	A	438	U
11	A	448	A
11	A	453	G
11	A	456	A
11	A	457	G
11	A	458	U
11	A	463	U
11	A	465	A
11	A	467	U
11	A	468	A
11	A	469	C
11	A	475	C
11	A	478	A
11	A	479	U
11	A	481	G
11	A	484	G
11	A	486	U
11	A	492	C
11	A	495	A
11	A	496	A
11	A	497	G
11	A	504	C
11	A	505	G
11	A	509	A
11	A	510	A
11	A	511	C
11	A	518	C
11	A	521	G
11	A	527	G7M
11	A	532	A

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Mol	Chain	Res	Type
11	A	547	A
11	A	559	A
11	A	564	C
11	A	572	A
11	A	573	A
11	A	576	C
11	A	577	G
11	A	633	G
11	A	642	A
11	A	650	G
11	A	653	U
11	A	665	A
11	A	687	A
11	A	702	A
11	A	718	A
11	A	723	U
11	A	724	G
11	A	734	G
11	A	747	A
11	A	755	G
11	A	777	A
11	A	793	U
11	A	794	A
11	A	815	A
11	A	817	C
11	A	821	G
11	A	851	G
11	A	890	G
11	A	902	G
11	A	914	A
11	A	934	C
11	A	935	A
11	A	960	U
11	A	966	2MG
11	A	969	A
11	A	971	G
11	A	975	A
11	A	976	G
11	A	977	A
11	A	989	U
11	A	992	U
11	A	994	A

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Mol	Chain	Res	Type
11	A	996	A
11	A	1003	G
11	A	1004	A
11	A	1009	U
11	A	1028	C
11	A	1030	U
11	A	1031	C
11	A	1032	G
11	A	1033	G
11	A	1035	A
11	A	1036	A
11	A	1039	G
11	A	1042	A
11	A	1044	A
11	A	1065	U
11	A	1085	U
11	A	1094	G
11	A	1095	U
11	A	1101	A
11	A	1108	G
11	A	1125	U
11	A	1132	C
11	A	1133	G
11	A	1136	C
11	A	1137	C
11	A	1139	G
11	A	1151	A
11	A	1159	U
11	A	1196	A
11	A	1197	A
11	A	1213	A
11	A	1214	C
11	A	1215	G
11	A	1225	A
11	A	1227	A
11	A	1238	A
11	A	1241	G
11	A	1257	A
11	A	1258	G
11	A	1260	G
11	A	1275	A
11	A	1280	A

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Mol	Chain	Res	Type
11	A	1286	U
11	A	1287	A
11	A	1299	A
11	A	1300	G
11	A	1302	C
11	A	1305	G
11	A	1317	C
11	A	1320	C
11	A	1340	A
11	A	1346	A
11	A	1353	G
11	A	1363	A
11	A	1364	U
11	A	1370	G
11	A	1378	C
11	A	1379	G
11	A	1381	U
11	A	1398	A
11	A	1419	G
11	A	1429	A
11	A	1432	G
11	A	1441	A
11	A	1446	A
11	A	1487	G
11	A	1493	A
11	A	1494	G
11	A	1497	G
11	A	1499	A
11	A	1503	A
11	A	1506	U
11	A	1517	G
11	A	1529	G
11	A	1530	G
11	A	1534	A
33	X	7	C
34	Y	8	U
34	Y	9	G
34	Y	14	A
34	Y	20	G
34	Y	21	U
34	Y	22	A
34	Y	35	C

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Mol	Chain	Res	Type
34	Y	46	G
34	Y	49	C
34	Y	75	C
35	Z	14	A
35	Z	16	C
35	Z	17	U
35	Z	19	G
35	Z	20	G
35	Z	21	U
35	Z	22	A
35	Z	46	G
35	Z	47	G
35	Z	48	U
35	Z	77	A
36	a	10	A
36	a	14	A
36	a	15	G
36	a	34	U
36	a	51	G
36	a	63	A
36	a	71	A
36	a	74	A
36	a	75	G
36	a	84	A
36	a	88	G
36	a	96	C
36	a	101	A
36	a	102	U
36	a	118	A
36	a	119	A
36	a	120	U
36	a	125	A
36	a	139	U
36	a	142	A
36	a	163	C
36	a	165	A
36	a	181	A
36	a	196	A
36	a	199	A
36	a	215	G
36	a	216	A
36	a	222	A

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Mol	Chain	Res	Type
36	a	248	G
36	a	272	A
36	a	276	U
36	a	278	A
36	a	281	C
36	a	282	A
36	a	285	G
36	a	288	U
36	a	311	A
36	a	329	G
36	a	330	A
36	a	331	C
36	a	345	A
36	a	362	A
36	a	386	G
36	a	396	G
36	a	405	U
36	a	411	G
36	a	412	A
36	a	481	G
36	a	491	G
36	a	504	A
36	a	505	A
36	a	508	A
36	a	509	C
36	a	529	A
36	a	532	A
36	a	544	C
36	a	545	U
36	a	546	U
36	a	547	A
36	a	549	G
36	a	563	A
36	a	573	U
36	a	575	A
36	a	603	A
36	a	615	U
36	a	627	A
36	a	637	A
36	a	645	C
36	a	646	U
36	a	647	G

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Mol	Chain	Res	Type
36	a	654	A
36	a	655	A
36	a	686	U
36	a	717	C
36	a	726	G
36	a	730	A
36	a	738	G
36	a	747	U
36	a	757	G
36	a	764	A
36	a	775	G
36	a	776	G
36	a	782	A
36	a	784	G
36	a	785	G
36	a	789	A
36	a	805	G
36	a	812	C
36	a	827	U
36	a	828	U
36	a	846	U
36	a	847	U
36	a	858	G
36	a	859	G
36	a	869	G
36	a	883	G
36	a	884	U
36	a	888	C
36	a	890	C
36	a	891	G
36	a	893	C
36	a	895	U
36	a	896	A
36	a	899	A
36	a	907	G
36	a	910	A
36	a	914	G
36	a	931	U
36	a	932	U
36	a	946	C
36	a	961	C
36	a	974	G

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Mol	Chain	Res	Type
36	a	983	A
36	a	996	A
36	a	1012	U
36	a	1013	C
36	a	1026	G
36	a	1027	A
36	a	1033	U
36	a	1045	C
36	a	1046	A
36	a	1047	G
36	a	1108	U
36	a	1110	G
36	a	1111	A
36	a	1112	G
36	a	1116	G
36	a	1122	G
36	a	1130	U
36	a	1132	U
36	a	1133	A
36	a	1135	C
36	a	1142	A
36	a	1206	G
36	a	1212	G
36	a	1236	G
36	a	1250	G
36	a	1253	A
36	a	1256	G
36	a	1271	G
36	a	1272	A
36	a	1273	U
36	a	1300	G
36	a	1301	A
36	a	1321	A
36	a	1322	A
36	a	1329	U
36	a	1352	U
36	a	1365	A
36	a	1378	A
36	a	1379	U
36	a	1383	A
36	a	1416	G
36	a	1428	C

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Mol	Chain	Res	Type
36	a	1437	C
36	a	1452	G
36	a	1453	A
36	a	1482	G
36	a	1493	C
36	a	1508	A
36	a	1509	A
36	a	1510	G
36	a	1515	A
36	a	1529	G
36	a	1535	A
36	a	1536	C
36	a	1537	G
36	a	1566	A
36	a	1569	A
36	a	1578	U
36	a	1583	A
36	a	1585	C
36	a	1607	C
36	a	1608	A
36	a	1647	U
36	a	1648	U
36	a	1649	G
36	a	1674	G
36	a	1715	G
36	a	1729	U
36	a	1730	C
36	a	1731	G
36	a	1732	C
36	a	1738	G
36	a	1764	C
36	a	1773	A
36	a	1782	U
36	a	1800	C
36	a	1801	A
36	a	1808	A
36	a	1816	C
36	a	1829	A
36	a	1847	A
36	a	1848	A
36	a	1858	A
36	a	1869	G

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Mol	Chain	Res	Type
36	a	1870	C
36	a	1871	A
36	a	1872	A
36	a	1906	G
36	a	1913	A
36	a	1914	C
36	a	1929	G
36	a	1930	G
36	a	1937	A
36	a	1939	U
36	a	1955	U
36	a	1964	G
36	a	1966	A
36	a	1967	C
36	a	1970	A
36	a	1971	U
36	a	1972	G
36	a	1991	U
36	a	1993	U
36	a	2020	A
36	a	2023	C
36	a	2030	6MZ
36	a	2031	A
36	a	2033	A
36	a	2043	C
36	a	2055	C
36	a	2056	G
36	a	2060	A
36	a	2061	G
36	a	2062	A
36	a	2069	G7M
36	a	2093	G
36	a	2198	A
36	a	2204	G
36	a	2211	A
36	a	2225	A
36	a	2238	G
36	a	2239	G
36	a	2279	G
36	a	2283	C
36	a	2287	A
36	a	2288	A

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Mol	Chain	Res	Type
36	a	2305	U
36	a	2308	G
36	a	2309	A
36	a	2312	U
36	a	2322	A
36	a	2325	G
36	a	2333	A
36	a	2334	U
36	a	2345	G
36	a	2347	C
36	a	2350	C
36	a	2357	G
36	a	2361	G
36	a	2383	G
36	a	2385	C
36	a	2402	U
36	a	2403	C
36	a	2406	A
36	a	2425	A
36	a	2429	G
36	a	2435	A
36	a	2441	U
36	a	2448	A
36	a	2476	A
36	a	2478	A
36	a	2491	U
36	a	2498	OMC
36	a	2502	G
36	a	2505	G
36	a	2518	A
36	a	2520	C
36	a	2525	G
36	a	2529	G
36	a	2535	G
36	a	2547	A
36	a	2566	A
36	a	2567	G
36	a	2572	A
36	a	2602	A
36	a	2609	U
36	a	2613	U
36	a	2615	U

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Mol	Chain	Res	Type
36	a	2629	U
36	a	2630	G
36	a	2646	C
36	a	2663	G
36	a	2689	U
36	a	2690	U
36	a	2714	G
36	a	2716	C
36	a	2718	G
36	a	2726	A
36	a	2732	G
36	a	2733	A
36	a	2744	G
36	a	2748	A
36	a	2757	A
36	a	2765	A
36	a	2778	A
36	a	2798	U
36	a	2818	U
36	a	2820	A
36	a	2821	A
36	a	2835	A
36	a	2836	U
36	a	2861	U
36	a	2873	A
36	a	2880	C
36	a	2883	A
36	a	2884	U
36	a	2891	U
37	b	9	G
37	b	16	G
37	b	24	G
37	b	35	C
37	b	36	C
37	b	41	G
37	b	56	G
37	b	67	G
37	b	89	U
37	b	90	C
37	b	99	A
37	b	109	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	428	G
11	A	1035	A
34	Y	13	C
34	Y	48	U

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

34 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	$\# Z  > 2$
36	G7M	a	2069	36	23,26,27	2.42	5 (21%)	35,39,42	1.64	6 (17%)
11	5MC	A	967	11	18,22,23	2.16	7 (38%)	26,32,35	1.21	1 (3%)
11	2MG	A	1207	11	23,26,27	2.65	6 (26%)	32,38,41	2.06	10 (31%)
11	MA6	A	1519	11	23,26,27	1.16	3 (13%)	34,38,41	2.25	10 (29%)
36	H2U	a	2449	36	18,21,22	4.21	5 (27%)	21,30,33	4.65	6 (28%)
36	6MZ	a	1618	36	22,25,26	2.31	3 (13%)	30,36,39	2.41	11 (36%)
11	2MG	A	1516	11	23,26,27	2.65	6 (26%)	32,38,41	2.08	11 (34%)
11	2MG	A	966	11	23,26,27	2.66	5 (21%)	32,38,41	2.19	10 (31%)
36	2MG	a	1835	36	23,26,27	2.64	5 (21%)	32,38,41	2.22	11 (34%)
36	PSU	a	2457	36	18,21,22	2.15	8 (44%)	22,30,33	1.78	5 (22%)
11	PSU	A	516	11	18,21,22	2.01	8 (44%)	22,30,33	1.75	4 (18%)
36	PSU	a	2605	36	18,21,22	2.11	8 (44%)	22,30,33	1.76	4 (18%)
11	4OC	A	1402	11	20,23,24	2.53	5 (25%)	26,32,35	1.05	2 (7%)
36	6MZ	a	2030	36	22,25,26	2.28	3 (13%)	30,36,39	2.59	11 (36%)
11	MA6	A	1518	11	23,26,27	1.18	3 (13%)	34,38,41	2.25	9 (26%)
36	OMC	a	2498	36,63	19,22,23	1.85	5 (26%)	26,31,34	0.97	1 (3%)
39	MEQ	d	150	39	8,9,10	0.88	0	5,10,12	0.49	0
36	PSU	a	1917	36	18,21,22	2.08	8 (44%)	22,30,33	1.61	3 (13%)
36	2MG	a	2445	36	23,26,27	2.67	6 (26%)	32,38,41	2.05	11 (34%)
11	5MC	A	1407	11	18,22,23	2.17	8 (44%)	26,32,35	1.17	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	PSU	a	746	36,63	18,21,22	2.08	9 (50%)	22,30,33	1.66	4 (18%)
36	PSU	a	1911	36	18,21,22	2.05	8 (44%)	22,30,33	1.77	4 (18%)
36	5MC	a	1962	36	18,22,23	2.17	7 (38%)	26,32,35	1.24	2 (7%)
36	PSU	a	2504	36	18,21,22	2.14	8 (44%)	22,30,33	1.70	3 (13%)
36	OMG	a	2251	35,36	23,26,27	2.70	5 (21%)	33,38,41	1.96	10 (30%)
36	1MG	a	745	36	22,26,27	2.44	6 (27%)	33,39,42	1.91	10 (30%)
36	OMU	a	2552	36	19,22,23	2.59	7 (36%)	26,31,34	1.87	5 (19%)
36	PSU	a	2604	36	18,21,22	2.09	8 (44%)	22,30,33	1.74	4 (18%)
36	PSU	a	2580	36	18,21,22	2.16	9 (50%)	22,30,33	1.76	4 (18%)
11	UR3	A	1498	11	19,22,23	2.38	6 (31%)	26,32,35	1.14	1 (3%)
36	2MA	a	2503	36,63	22,25,26	1.37	2 (9%)	33,37,40	2.10	7 (21%)
36	PSU	a	955	36	18,21,22	2.13	8 (44%)	22,30,33	1.77	4 (18%)
11	G7M	A	527	11	23,26,27	2.39	5 (21%)	35,39,42	1.65	7 (20%)
22	D2T	L	89	22	7,9,10	1.36	1 (14%)	6,11,13	1.43	1 (16%)

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
36	G7M	a	2069	36	-	1/7/25/26	0/3/3/3
11	5MC	A	967	11	-	0/7/25/26	0/2/2/2
11	2MG	A	1207	11	-	2/9/27/28	0/3/3/3
11	MA6	A	1519	11	-	5/11/29/30	0/3/3/3
36	H2U	a	2449	36	-	0/7/38/39	0/2/2/2
36	6MZ	a	1618	36	-	0/9/27/28	0/3/3/3
11	2MG	A	1516	11	-	0/9/27/28	0/3/3/3
11	2MG	A	966	11	-	2/9/27/28	0/3/3/3
36	2MG	a	1835	36	-	2/9/27/28	0/3/3/3
36	PSU	a	2457	36	-	0/7/25/26	0/2/2/2
11	PSU	A	516	11	-	0/7/25/26	0/2/2/2
36	PSU	a	2605	36	-	0/7/25/26	0/2/2/2
11	4OC	A	1402	11	-	2/9/29/30	0/2/2/2
36	6MZ	a	2030	36	-	2/9/27/28	0/3/3/3
11	MA6	A	1518	11	-	2/11/29/30	0/3/3/3
36	OMC	a	2498	36,63	-	0/9/27/28	0/2/2/2
39	MEQ	d	150	39	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PSU	a	1917	36	-	0/7/25/26	0/2/2/2
36	2MG	a	2445	36	-	2/9/27/28	0/3/3/3
11	5MC	A	1407	11	-	0/7/25/26	0/2/2/2
36	PSU	a	746	36,63	-	1/7/25/26	0/2/2/2
36	PSU	a	1911	36	-	0/7/25/26	0/2/2/2
36	5MC	a	1962	36	-	0/7/25/26	0/2/2/2
36	PSU	a	2504	36	-	2/7/25/26	0/2/2/2
36	OMG	a	2251	35,36	-	1/9/27/28	0/3/3/3
36	1MG	a	745	36	-	0/7/25/26	0/3/3/3
36	OMU	a	2552	36	-	0/9/27/28	0/2/2/2
36	PSU	a	2604	36	-	0/7/25/26	0/2/2/2
36	PSU	a	2580	36	-	0/7/25/26	0/2/2/2
11	UR3	A	1498	11	-	0/7/25/26	0/2/2/2
36	2MA	a	2503	36,63	-	2/7/25/26	0/3/3/3
36	PSU	a	955	36	-	0/7/25/26	0/2/2/2
11	G7M	A	527	11	-	3/7/25/26	0/3/3/3
22	D2T	L	89	22	-	1/7/12/14	-

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	966	2MG	O6-C6	9.91	1.42	1.23
11	A	1207	2MG	O6-C6	9.89	1.42	1.23
11	A	1516	2MG	O6-C6	9.86	1.42	1.23
36	a	2449	H2U	O4-C4	9.85	1.43	1.23
36	a	1835	2MG	O6-C6	9.76	1.42	1.23
36	a	2445	2MG	O6-C6	9.73	1.42	1.23
36	a	1618	6MZ	C6-N6	9.69	1.44	1.34
36	a	2251	OMG	O6-C6	9.67	1.42	1.23
36	a	2030	6MZ	C6-N6	9.32	1.44	1.34
11	A	1402	4OC	O2-C2	8.91	1.40	1.23
11	A	527	G7M	O6-C6	8.74	1.40	1.23
36	a	2449	H2U	O2-C2	8.70	1.39	1.23
36	a	2069	G7M	O6-C6	8.66	1.40	1.23
36	a	2449	H2U	C2-N1	8.32	1.47	1.35
36	a	2552	OMU	O4-C4	8.08	1.40	1.24
11	A	1498	UR3	O4-C4	7.85	1.40	1.23
36	a	745	1MG	O6-C6	7.41	1.38	1.23
36	a	2449	H2U	C2-N3	7.06	1.50	1.38
36	a	2251	OMG	C2-N2	7.05	1.50	1.34
36	a	745	1MG	C2-N2	6.79	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	966	2MG	C2-N2	5.25	1.45	1.33
11	A	1207	2MG	C2-N2	5.23	1.45	1.33
11	A	967	5MC	C4-N4	5.16	1.47	1.34
11	A	1516	2MG	C2-N2	5.16	1.44	1.33
11	A	1407	5MC	C4-N4	5.13	1.47	1.34
36	a	1962	5MC	C4-N4	5.09	1.47	1.34
36	a	2445	2MG	C2-N2	5.04	1.44	1.33
36	a	1835	2MG	C2-N2	5.04	1.44	1.33
36	a	2449	H2U	C4-N3	4.89	1.45	1.37
36	a	2498	OMC	C4-N4	4.78	1.45	1.33
11	A	527	G7M	C2-N2	4.77	1.45	1.34
36	a	2069	G7M	C2-N2	4.64	1.45	1.34
11	A	1402	4OC	C4-N4	4.47	1.45	1.35
36	a	2503	2MA	C6-N6	4.31	1.44	1.34
36	a	1962	5MC	O2-C2	-4.25	1.15	1.23
11	A	1407	5MC	O2-C2	-4.20	1.15	1.23
11	A	967	5MC	O2-C2	-4.13	1.16	1.23
11	A	1498	UR3	C4-N3	-4.05	1.31	1.40
36	a	2552	OMU	C2-N1	-4.02	1.32	1.38
36	a	2580	PSU	C2-N1	-3.85	1.31	1.36
36	a	2457	PSU	C4-N3	-3.84	1.31	1.38
36	a	2504	PSU	C2-N1	-3.83	1.31	1.36
36	a	2580	PSU	C4-N3	-3.78	1.31	1.38
36	a	955	PSU	C4-N3	-3.76	1.31	1.38
36	a	955	PSU	C2-N1	-3.74	1.31	1.36
36	a	2457	PSU	C2-N1	-3.72	1.31	1.36
36	a	2605	PSU	C4-N3	-3.69	1.32	1.38
36	a	1917	PSU	C2-N1	-3.68	1.31	1.36
36	a	2604	PSU	C2-N1	-3.66	1.31	1.36
36	a	2504	PSU	C4-N3	-3.66	1.32	1.38
36	a	2604	PSU	C4-N3	-3.66	1.32	1.38
36	a	746	PSU	C4-N3	-3.66	1.32	1.38
36	a	2605	PSU	C2-N1	-3.63	1.31	1.36
11	A	1402	4OC	C2-N1	-3.61	1.32	1.40
36	a	2498	OMC	C2-N1	-3.60	1.32	1.40
36	a	2552	OMU	C4-N3	-3.59	1.32	1.38
36	a	2069	G7M	C5-N7	-3.57	1.35	1.39
36	a	1917	PSU	C4-N3	-3.56	1.32	1.38
36	a	2457	PSU	C2-N3	-3.54	1.31	1.37
36	a	1911	PSU	C4-N3	-3.54	1.32	1.38
36	a	746	PSU	C2-N1	-3.51	1.32	1.36
36	a	2069	G7M	C6-N1	-3.50	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	1911	PSU	C2-N1	-3.48	1.32	1.36
36	a	2605	PSU	C2-N3	-3.48	1.31	1.37
36	a	955	PSU	C2-N3	-3.44	1.31	1.37
36	a	2580	PSU	C2-N3	-3.42	1.31	1.37
36	a	2604	PSU	C2-N3	-3.42	1.31	1.37
11	A	516	PSU	C2-N1	-3.42	1.32	1.36
36	a	2504	PSU	C2-N3	-3.41	1.31	1.37
11	A	1207	2MG	CM2-N2	3.40	1.51	1.45
11	A	966	2MG	CM2-N2	3.40	1.51	1.45
36	a	2552	OMU	C2-N3	-3.39	1.31	1.38
36	a	1917	PSU	C2-N3	-3.38	1.31	1.37
11	A	516	PSU	C4-N3	-3.37	1.32	1.38
36	a	746	PSU	C2-N3	-3.35	1.31	1.37
11	A	1516	2MG	CM2-N2	3.35	1.51	1.45
11	A	527	G7M	C5-N7	-3.34	1.35	1.39
36	a	1962	5MC	C6-N1	-3.31	1.32	1.38
11	A	527	G7M	C6-N1	-3.29	1.32	1.38
36	a	2030	6MZ	C8-N9	-3.29	1.31	1.37
36	a	1911	PSU	C2-N3	-3.27	1.31	1.37
36	a	1835	2MG	CM2-N2	3.22	1.51	1.45
36	a	2445	2MG	C2-N1	-3.22	1.31	1.36
36	a	1911	PSU	C6-C5	3.20	1.39	1.35
11	A	1518	MA6	C6-N6	3.17	1.46	1.36
36	a	1618	6MZ	C8-N9	-3.14	1.31	1.37
11	A	516	PSU	C6-C5	3.13	1.39	1.35
11	A	516	PSU	C2-N3	-3.12	1.32	1.37
11	A	967	5MC	C6-N1	-3.12	1.32	1.38
36	a	2445	2MG	CM2-N2	3.12	1.51	1.45
11	A	1407	5MC	C6-N1	-3.11	1.32	1.38
11	A	1519	MA6	C6-N6	3.08	1.46	1.36
36	a	1917	PSU	C6-C5	3.08	1.38	1.35
36	a	2605	PSU	C6-C5	3.06	1.38	1.35
11	A	1498	UR3	C2-N1	-3.04	1.34	1.38
36	a	1962	5MC	C2-N1	-3.04	1.33	1.40
36	a	2604	PSU	C6-C5	3.03	1.38	1.35
36	a	2504	PSU	C6-C5	3.03	1.38	1.35
11	A	1518	MA6	C8-N9	-3.02	1.32	1.37
36	a	1835	2MG	C2-N1	-3.02	1.31	1.36
11	A	967	5MC	C2-N1	-2.98	1.33	1.40
36	a	955	PSU	C6-C5	2.97	1.38	1.35
11	A	1407	5MC	C2-N1	-2.95	1.33	1.40
36	a	746	PSU	C6-C5	2.95	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1519	MA6	C8-N9	-2.95	1.32	1.37
36	a	2503	2MA	C8-N9	-2.91	1.32	1.37
36	a	2457	PSU	C6-C5	2.89	1.38	1.35
36	a	2580	PSU	C6-C5	2.83	1.38	1.35
11	A	966	2MG	C2-N1	-2.83	1.32	1.36
36	a	2445	2MG	C6-N1	-2.80	1.33	1.38
36	a	2498	OMC	O2-C2	-2.79	1.18	1.23
11	A	967	5MC	CM5-C5	2.77	1.57	1.50
36	a	1962	5MC	CM5-C5	2.71	1.57	1.50
11	A	1407	5MC	CM5-C5	2.70	1.57	1.50
36	a	2457	PSU	O4-C4	-2.70	1.18	1.23
11	A	1516	2MG	C2-N1	-2.69	1.32	1.36
36	a	745	1MG	C5-N7	-2.68	1.33	1.39
11	A	1207	2MG	C2-N1	-2.68	1.32	1.36
36	a	745	1MG	C6-N1	-2.67	1.34	1.40
36	a	2580	PSU	O4-C4	-2.67	1.18	1.23
36	a	746	PSU	O4-C4	-2.67	1.18	1.23
36	a	955	PSU	O4-C4	-2.66	1.18	1.23
36	a	2605	PSU	O4-C4	-2.66	1.18	1.23
36	a	1917	PSU	C1'-C5	2.63	1.56	1.50
36	a	2504	PSU	C6-N1	-2.62	1.31	1.36
36	a	2504	PSU	O4-C4	-2.59	1.18	1.23
36	a	2604	PSU	O4-C4	-2.59	1.18	1.23
36	a	2457	PSU	C6-N1	-2.59	1.31	1.36
36	a	955	PSU	C6-N1	-2.58	1.31	1.36
36	a	2580	PSU	C6-N1	-2.57	1.32	1.36
36	a	2504	PSU	C1'-C5	2.54	1.56	1.50
36	a	1835	2MG	C6-N1	-2.53	1.34	1.38
36	a	1917	PSU	O4-C4	-2.51	1.18	1.23
36	a	2604	PSU	C6-N1	-2.51	1.32	1.36
36	a	1911	PSU	O4-C4	-2.51	1.18	1.23
36	a	2552	OMU	O2-C2	-2.48	1.18	1.23
11	A	516	PSU	O4-C4	-2.47	1.18	1.23
11	A	516	PSU	C1'-C5	2.47	1.55	1.50
11	A	1498	UR3	C6-C5	2.47	1.40	1.35
36	a	2605	PSU	C6-N1	-2.46	1.32	1.36
36	a	2030	6MZ	C5-N7	-2.46	1.34	1.39
11	A	516	PSU	C6-N1	-2.45	1.32	1.36
36	a	955	PSU	O2-C2	-2.44	1.18	1.23
11	A	966	2MG	C6-N1	-2.44	1.34	1.38
11	A	1516	2MG	C6-N1	-2.44	1.34	1.38
36	a	1618	6MZ	C5-N7	-2.42	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	1917	PSU	C6-N1	-2.42	1.32	1.36
36	a	2251	OMG	C6-N1	-2.41	1.34	1.38
36	a	1911	PSU	C6-N1	-2.40	1.32	1.36
36	a	955	PSU	C1'-C5	2.38	1.55	1.50
11	A	1207	2MG	C6-N1	-2.38	1.34	1.38
36	a	2504	PSU	O2-C2	-2.37	1.18	1.23
36	a	1911	PSU	C1'-C5	2.37	1.55	1.50
11	A	1519	MA6	C5-N7	-2.37	1.34	1.39
36	a	2580	PSU	O2-C2	-2.36	1.18	1.23
36	a	746	PSU	C6-N1	-2.36	1.32	1.36
36	a	2498	OMC	C6-N1	-2.35	1.32	1.38
36	a	2457	PSU	C1'-C5	2.34	1.55	1.50
36	a	2604	PSU	C1'-C5	2.34	1.55	1.50
36	a	2457	PSU	O2-C2	-2.34	1.18	1.23
36	a	2605	PSU	C1'-C5	2.33	1.55	1.50
36	a	2605	PSU	O2-C2	-2.31	1.18	1.23
11	A	1498	UR3	C6-N1	-2.30	1.32	1.38
36	a	2604	PSU	O2-C2	-2.30	1.18	1.23
36	a	2552	OMU	C5-C4	-2.29	1.38	1.43
36	a	2580	PSU	O4'-C1'	-2.28	1.40	1.43
36	a	2069	G7M	C2-N1	-2.27	1.32	1.37
36	a	2251	OMG	C5-N7	-2.27	1.34	1.39
11	A	1402	4OC	C6-N1	-2.26	1.32	1.38
36	a	2552	OMU	C6-N1	-2.25	1.32	1.38
36	a	745	1MG	C4-N9	-2.24	1.32	1.38
36	a	1911	PSU	O2-C2	-2.23	1.18	1.23
36	a	746	PSU	C1'-C5	2.22	1.55	1.50
36	a	2580	PSU	C1'-C5	2.22	1.55	1.50
36	a	2445	2MG	C4-N9	-2.22	1.32	1.38
11	A	1516	2MG	C4-N9	-2.21	1.32	1.38
36	a	2498	OMC	C2-N3	-2.21	1.31	1.36
11	A	1402	4OC	C2-N3	-2.21	1.31	1.36
36	a	746	PSU	O2-C2	-2.20	1.18	1.23
11	A	1518	MA6	C5-N7	-2.19	1.34	1.39
11	A	1498	UR3	C2-N3	-2.17	1.34	1.39
11	A	516	PSU	O2-C2	-2.17	1.18	1.23
36	a	1917	PSU	O2-C2	-2.16	1.18	1.23
11	A	967	5MC	C6-C5	2.16	1.38	1.34
11	A	1407	5MC	C6-C5	2.15	1.38	1.34
36	a	745	1MG	C5-C6	-2.14	1.40	1.45
36	a	2251	OMG	C8-N9	-2.14	1.32	1.37
11	A	1407	5MC	C4-N3	-2.14	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	527	G7M	C2-N1	-2.08	1.32	1.37
36	a	1962	5MC	C4-N3	-2.07	1.30	1.34
11	A	1207	2MG	C4-N9	-2.07	1.32	1.38
36	a	746	PSU	O4'-C1'	-2.06	1.41	1.43
36	a	1962	5MC	C2-N3	-2.05	1.32	1.36
11	A	967	5MC	C4-N3	-2.03	1.30	1.34
11	A	1407	5MC	C2-N3	-2.02	1.32	1.36
22	L	89	D2T	CB1-SB	-2.01	1.75	1.79

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	2449	H2U	C4-N3-C2	-13.69	114.44	125.79
36	a	2449	H2U	O2-C2-N1	-10.63	109.77	123.11
36	a	2449	H2U	O4-C4-N3	-7.52	108.36	120.28
36	a	2503	2MA	C5-C4-N3	-6.91	119.42	127.19
36	a	1835	2MG	C2-N3-C4	6.86	120.54	112.04
11	A	966	2MG	C2-N3-C4	6.67	120.31	112.04
36	a	2030	6MZ	C9-N6-C6	-6.61	117.18	122.87
11	A	1207	2MG	C2-N3-C4	6.36	119.92	112.04
36	a	2449	H2U	O4-C4-C5	-6.32	108.66	122.17
36	a	2445	2MG	C2-N3-C4	6.32	119.88	112.04
11	A	1516	2MG	C2-N3-C4	6.32	119.87	112.04
36	a	2552	OMU	N3-C2-N1	5.99	122.84	114.89
36	a	2251	OMG	C5-C4-N3	-5.94	118.83	128.46
36	a	2449	H2U	O2-C2-N3	-5.83	110.64	121.50
11	A	1519	MA6	C5-C4-N3	-5.81	119.17	126.75
36	a	745	1MG	C5-C4-N3	-5.76	119.11	128.46
11	A	966	2MG	C5-C4-N3	-5.59	119.39	128.46
36	a	1835	2MG	C5-C4-N3	-5.54	119.47	128.46
36	a	1618	6MZ	C5-C4-N3	-5.52	119.55	126.75
36	a	1618	6MZ	N1-C2-N3	-5.50	120.00	128.60
36	a	2457	PSU	N1-C2-N3	5.47	121.33	115.13
36	a	2030	6MZ	N1-C2-N3	-5.47	120.05	128.60
36	a	955	PSU	N1-C2-N3	5.45	121.31	115.13
36	a	1911	PSU	N1-C2-N3	5.42	121.27	115.13
11	A	1518	MA6	C5-C4-N3	-5.41	119.69	126.75
11	A	516	PSU	N1-C2-N3	5.38	121.22	115.13
36	a	2580	PSU	N1-C2-N3	5.34	121.18	115.13
36	a	2604	PSU	N1-C2-N3	5.32	121.15	115.13
36	a	2605	PSU	N1-C2-N3	5.31	121.15	115.13
36	a	2504	PSU	N1-C2-N3	5.23	121.06	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	746	PSU	N1-C2-N3	5.13	120.94	115.13
11	A	1207	2MG	C5-C4-N3	-5.05	120.26	128.46
36	a	1917	PSU	N1-C2-N3	5.03	120.83	115.13
36	a	2445	2MG	C5-C4-N3	-5.01	120.34	128.46
36	a	2030	6MZ	C5-C4-N3	-5.00	120.23	126.75
11	A	1516	2MG	C5-C4-N3	-4.94	120.44	128.46
36	a	2251	OMG	C2-N3-C4	4.94	121.09	112.30
36	a	2503	2MA	N3-C4-N9	4.83	133.69	126.99
11	A	967	5MC	C5-C6-N1	-4.73	118.47	123.34
11	A	527	G7M	C2-N3-C4	4.64	120.56	112.30
36	a	1962	5MC	C5-C6-N1	-4.62	118.59	123.34
36	a	2552	OMU	C4-N3-C2	-4.55	120.57	126.58
36	a	2069	G7M	C2-N3-C4	4.49	120.30	112.30
11	A	1518	MA6	N1-C2-N3	-4.46	121.62	128.60
11	A	1407	5MC	C5-C6-N1	-4.44	118.77	123.34
11	A	1518	MA6	C5-N7-C8	4.34	109.68	103.51
11	A	1519	MA6	C5-N7-C8	4.28	109.59	103.51
11	A	966	2MG	N9-C4-N3	4.22	134.41	125.94
36	a	745	1MG	N9-C4-N3	4.21	134.40	125.94
11	A	1519	MA6	N1-C2-N3	-4.20	122.03	128.60
36	a	1618	6MZ	N3-C4-N9	4.19	133.99	127.08
11	A	527	G7M	C5-C4-N3	-4.18	120.13	128.15
11	A	1518	MA6	C2-N1-C6	4.15	121.56	111.75
36	a	1618	6MZ	C2-N3-C4	4.15	121.55	111.75
11	A	1518	MA6	N9-C8-N7	-4.10	108.30	113.91
11	A	1518	MA6	C4-C5-N7	-4.09	105.64	110.62
11	A	1519	MA6	N3-C4-N9	4.08	133.81	127.08
36	a	1618	6MZ	C9-N6-C6	-4.05	119.39	122.87
36	a	2449	H2U	N3-C2-N1	-4.03	112.39	116.65
36	a	2030	6MZ	N9-C8-N7	-4.03	108.40	113.91
36	a	1835	2MG	N9-C4-N3	4.02	134.00	125.94
36	a	2030	6MZ	C2-N3-C4	3.97	121.12	111.75
36	a	2251	OMG	N9-C4-N3	3.96	133.90	125.94
36	a	2069	G7M	C5-C4-N3	-3.94	120.60	128.15
11	A	1519	MA6	C2-N1-C6	3.90	120.95	111.75
11	A	1519	MA6	C4-C5-N7	-3.88	105.89	110.62
36	a	745	1MG	C2-N3-C4	3.88	120.69	111.98
11	A	1519	MA6	N9-C8-N7	-3.88	108.61	113.91
11	A	1519	MA6	C2-N3-C4	3.86	120.88	111.75
36	a	2030	6MZ	C5-N7-C8	3.85	108.98	103.51
11	A	1518	MA6	C2-N3-C4	3.84	120.82	111.75
36	a	2503	2MA	N9-C8-N7	-3.84	108.67	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	2069	G7M	C6-C5-N7	3.82	136.86	132.25
36	a	2503	2MA	C5-N7-C8	3.77	108.86	103.51
36	a	2445	2MG	N9-C4-N3	3.74	133.46	125.94
36	a	1618	6MZ	N9-C8-N7	-3.68	108.88	113.91
11	A	1518	MA6	N3-C4-N9	3.67	133.12	127.08
36	a	1835	2MG	C2-N1-C6	-3.65	120.28	124.48
11	A	527	G7M	C6-C5-N7	3.64	136.65	132.25
36	a	1618	6MZ	C5-N7-C8	3.63	108.67	103.51
36	a	2605	PSU	C4-N3-C2	-3.62	121.13	126.34
11	A	1207	2MG	N9-C4-N3	3.60	133.16	125.94
11	A	1498	UR3	C4-N3-C2	-3.60	121.18	124.56
36	a	2030	6MZ	N3-C4-N9	3.60	133.01	127.08
11	A	966	2MG	C2-N1-C6	-3.56	120.39	124.48
11	A	527	G7M	C5-C6-N1	3.53	119.17	111.79
36	a	2069	G7M	C5-C6-N1	3.51	119.13	111.79
36	a	1911	PSU	C4-N3-C2	-3.50	121.29	126.34
36	a	955	PSU	C4-N3-C2	-3.49	121.31	126.34
36	a	746	PSU	C4-N3-C2	-3.47	121.33	126.34
36	a	2604	PSU	C4-N3-C2	-3.43	121.39	126.34
36	a	2457	PSU	C4-N3-C2	-3.41	121.42	126.34
36	a	2030	6MZ	C6-C5-N7	3.40	136.07	132.39
11	A	516	PSU	C4-N3-C2	-3.35	121.50	126.34
11	A	1516	2MG	C2-N1-C6	-3.35	120.63	124.48
11	A	1516	2MG	N9-C4-N3	3.30	132.57	125.94
36	a	2503	2MA	C4-C5-N7	-3.29	106.61	110.62
36	a	2504	PSU	C4-N3-C2	-3.28	121.61	126.34
11	A	527	G7M	N9-C4-N3	3.24	132.44	125.94
36	a	955	PSU	O2-C2-N1	-3.24	119.23	122.79
11	A	516	PSU	O2-C2-N1	-3.23	119.24	122.79
36	a	2030	6MZ	C4-C5-N7	-3.20	106.72	110.62
11	A	1518	MA6	C4-N9-C8	3.20	109.19	105.73
11	A	1207	2MG	C2-N1-C6	-3.18	120.82	124.48
36	a	2504	PSU	O2-C2-N1	-3.18	119.29	122.79
36	a	2457	PSU	O2-C2-N1	-3.16	119.31	122.79
36	a	745	1MG	C5-C6-N1	3.15	120.99	114.91
36	a	2030	6MZ	C4-N9-C8	3.14	109.13	105.73
36	a	2604	PSU	O2-C2-N1	-3.14	119.33	122.79
36	a	2580	PSU	O2-C2-N1	-3.13	119.35	122.79
36	a	2580	PSU	C4-N3-C2	-3.12	121.84	126.34
36	a	1911	PSU	O2-C2-N1	-3.10	119.38	122.79
36	a	2069	G7M	N9-C4-N3	3.05	132.07	125.94
11	A	1516	2MG	C6-C5-N7	3.05	135.93	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	2503	2MA	C4-N9-C8	2.99	108.97	105.73
36	a	1917	PSU	O2-C2-N1	-2.94	119.56	122.79
36	a	2605	PSU	O2-C2-N1	-2.93	119.57	122.79
36	a	1917	PSU	C4-N3-C2	-2.92	122.13	126.34
36	a	2552	OMU	O2-C2-N1	-2.92	118.91	122.79
11	A	1519	MA6	C4-N9-C8	2.91	108.89	105.73
36	a	1618	6MZ	C4-N9-C8	2.90	108.87	105.73
36	a	1618	6MZ	C4-C5-N7	-2.87	107.12	110.62
11	A	1207	2MG	C6-C5-N7	2.86	135.57	130.25
36	a	2445	2MG	C6-C5-N7	2.80	135.46	130.25
36	a	2251	OMG	C4-C5-N7	-2.79	106.31	110.72
36	a	1835	2MG	C6-C5-N7	2.75	135.36	130.25
11	A	1402	4OC	C5-C4-N3	-2.74	118.18	122.59
36	a	746	PSU	O2-C2-N1	-2.73	119.78	122.79
36	a	1835	2MG	C5-C6-N1	2.71	120.08	113.19
36	a	2251	OMG	C8-N7-C5	2.70	109.13	104.24
36	a	2445	2MG	C2-N1-C6	-2.69	121.39	124.48
11	A	966	2MG	C5-C6-N1	2.68	120.00	113.19
36	a	2552	OMU	C5-C4-N3	2.67	118.83	114.84
36	a	2251	OMG	C6-C5-N7	2.65	135.17	130.25
36	a	2069	G7M	O6-C6-C5	-2.60	122.19	128.06
36	a	745	1MG	C6-C5-N7	2.60	135.23	129.35
11	A	1516	2MG	C5-C6-N1	2.60	119.78	113.19
36	a	2498	OMC	O2-C2-N3	-2.59	118.11	122.33
11	A	527	G7M	O6-C6-C5	-2.57	122.25	128.06
11	A	1207	2MG	C5-C6-N1	2.56	119.69	113.19
36	a	1618	6MZ	C6-C5-N7	2.54	135.13	132.39
36	a	745	1MG	C2-N1-C6	-2.53	118.89	120.95
36	a	2552	OMU	O4-C4-C5	-2.53	120.72	125.16
36	a	2251	OMG	C2-N1-C6	-2.52	120.51	125.10
11	A	966	2MG	O6-C6-C5	-2.50	119.97	126.60
36	a	2445	2MG	C5-C6-N1	2.50	119.53	113.19
11	A	966	2MG	C6-C5-N7	2.50	134.89	130.25
36	a	1835	2MG	C8-N7-C5	2.46	108.69	104.24
11	A	1516	2MG	C4-C5-N7	-2.45	106.85	110.72
11	A	1516	2MG	O6-C6-C5	-2.44	120.12	126.60
36	a	1835	2MG	O6-C6-C5	-2.44	120.14	126.60
36	a	2445	2MG	N9-C8-N7	-2.39	108.88	113.39
11	A	966	2MG	C8-N7-C5	2.39	108.57	104.24
36	a	2445	2MG	C8-N7-C5	2.38	108.55	104.24
36	a	2580	PSU	O4'-C1'-C2'	2.38	108.50	105.14
36	a	2251	OMG	C5-C6-N1	2.37	119.20	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1207	2MG	O6-C6-C5	-2.35	120.36	126.60
11	A	1207	2MG	C8-N7-C5	2.35	108.50	104.24
11	A	1516	2MG	C8-N7-C5	2.35	108.49	104.24
36	a	2445	2MG	O6-C6-C5	-2.32	120.44	126.60
36	a	746	PSU	C5-C6-N1	-2.32	118.64	122.11
36	a	1835	2MG	C4-C5-N7	-2.31	107.06	110.72
36	a	2251	OMG	N9-C8-N7	-2.31	109.05	113.39
11	A	1207	2MG	C4-C5-N7	-2.30	107.08	110.72
36	a	1835	2MG	CM2-N2-C2	-2.30	118.79	123.86
11	A	1207	2MG	N9-C8-N7	-2.28	109.11	113.39
36	a	745	1MG	C6-C5-C4	-2.26	117.47	119.97
36	a	1835	2MG	N9-C8-N7	-2.26	109.14	113.39
11	A	1516	2MG	N9-C8-N7	-2.25	109.15	113.39
36	a	2605	PSU	C5-C6-N1	-2.23	118.76	122.11
36	a	1911	PSU	C5-C6-N1	-2.22	118.78	122.11
36	a	2251	OMG	O6-C6-C5	-2.21	120.73	126.60
36	a	2457	PSU	C5-C6-N1	-2.21	118.80	122.11
36	a	745	1MG	C8-N7-C5	2.20	108.22	104.24
11	A	966	2MG	N9-C8-N7	-2.19	109.26	113.39
36	a	745	1MG	N9-C8-N7	-2.19	109.27	113.39
22	L	89	D2T	O-C-CA	-2.18	119.05	124.78
36	a	2445	2MG	C4-C5-N7	-2.17	107.28	110.72
36	a	745	1MG	C4-C5-N7	-2.16	107.31	110.72
11	A	966	2MG	C4-C5-N7	-2.15	107.31	110.72
36	a	2604	PSU	C5-C6-N1	-2.15	118.89	122.11
36	a	2030	6MZ	C2-N1-C6	2.14	122.44	115.25
36	a	2503	2MA	N3-C2-N1	-2.12	121.82	125.72
36	a	1618	6MZ	C2-N1-C6	2.11	122.33	115.25
11	A	1407	5MC	O2-C2-N3	-2.10	118.91	122.33
36	a	955	PSU	C5-C6-N1	-2.08	118.99	122.11
36	a	2445	2MG	CM2-N2-C2	-2.08	119.27	123.86
11	A	516	PSU	O4'-C1'-C2'	2.07	108.07	105.14
11	A	527	G7M	C2-N1-C6	-2.06	121.35	125.10
11	A	1519	MA6	C4-C5-C6	2.05	118.18	115.88
36	a	1962	5MC	O2-C2-N3	-2.05	119.00	122.33
11	A	1516	2MG	CM2-N2-C2	-2.03	119.39	123.86
36	a	2457	PSU	O4'-C1'-C2'	2.00	107.97	105.14
11	A	1402	4OC	C4-N3-C2	2.00	122.84	120.12

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	527	G7M	C3'-C4'-C5'-O5'
11	A	1207	2MG	N1-C2-N2-CM2
11	A	1207	2MG	N3-C2-N2-CM2
11	A	1519	MA6	C5-C6-N6-C9
11	A	1519	MA6	C5-C6-N6-C10
22	L	89	D2T	O-C-CA-CB
39	d	150	MEQ	N-CA-CB-CG
39	d	150	MEQ	O-C-CA-CB
36	a	2251	OMG	C1'-C2'-O2'-CM2
36	a	2030	6MZ	O4'-C4'-C5'-O5'
36	a	2030	6MZ	C3'-C4'-C5'-O5'
36	a	2504	PSU	O4'-C4'-C5'-O5'
11	A	1402	4OC	O4'-C4'-C5'-O5'
36	a	2504	PSU	C3'-C4'-C5'-O5'
11	A	1519	MA6	N1-C6-N6-C10
39	d	150	MEQ	OE1-CD-CG-CB
39	d	150	MEQ	NE2-CD-CG-CB
11	A	527	G7M	O4'-C4'-C5'-O5'
11	A	966	2MG	C3'-C4'-C5'-O5'
11	A	1402	4OC	C3'-C4'-C5'-O5'
39	d	150	MEQ	C-CA-CB-CG
11	A	1518	MA6	C5-C6-N6-C10
36	a	2445	2MG	C3'-C4'-C5'-O5'
11	A	1519	MA6	O4'-C4'-C5'-O5'
11	A	966	2MG	O4'-C4'-C5'-O5'
11	A	1518	MA6	C5-C6-N6-C9
11	A	527	G7M	C4'-C5'-O5'-P
39	d	150	MEQ	CA-CB-CG-CD
11	A	1519	MA6	C3'-C4'-C5'-O5'
36	a	1835	2MG	C3'-C4'-C5'-O5'
36	a	2503	2MA	O4'-C4'-C5'-O5'
36	a	1835	2MG	O4'-C4'-C5'-O5'
36	a	2069	G7M	O4'-C4'-C5'-O5'
36	a	2445	2MG	O4'-C4'-C5'-O5'
36	a	746	PSU	O4'-C1'-C5-C6
36	a	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1519	MA6	1	0
11	A	1516	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1402	4OC	1	0
36	a	2030	6MZ	1	0
36	a	2251	OMG	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 311 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
65	SPM	a	6209	-	13,13,13	0.35	0	12,12,12	0.82	0
64	PRO	Y	101	34	5,7,8	0.57	0	7,8,10	1.27	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
65	SPM	a	6209	-	-	7/11/11/11	-
64	PRO	Y	101	34	-	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(°)
64	Y	101	PRO	O-C-CA	-2.27	118.84	124.78

There are no chirality outliers.



All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
65	a	6209	SPM	C7-C8-C9-N10
65	a	6209	SPM	C2-C3-C4-N5
65	a	6209	SPM	C7-C6-N5-C4
65	a	6209	SPM	C11-C12-C13-N14
65	a	6209	SPM	C6-C7-C8-C9
65	a	6209	SPM	C8-C9-N10-C11
65	a	6209	SPM	N10-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	a	6209	SPM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

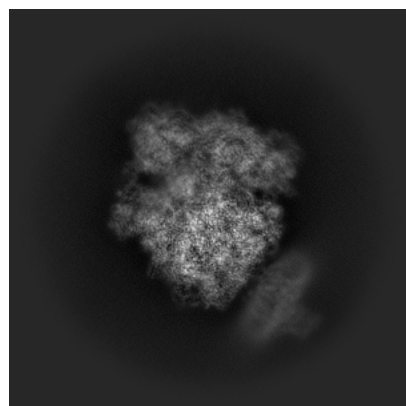
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53892. These allow visual inspection of the internal detail of the map and identification of artifacts.

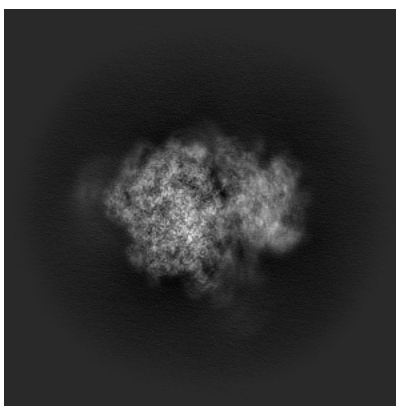
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

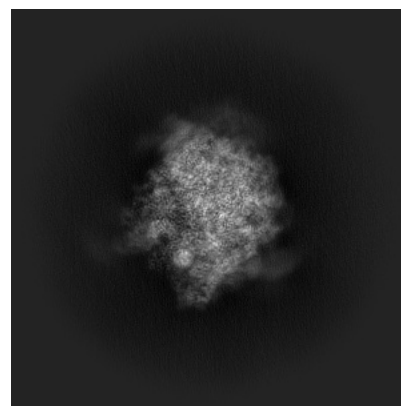
#### 6.1.1 Primary map



X

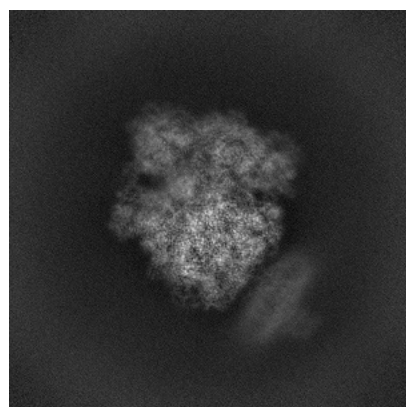


Y

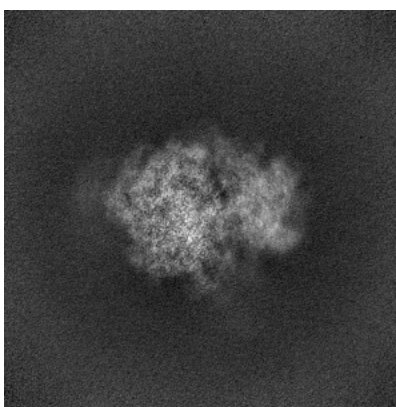


Z

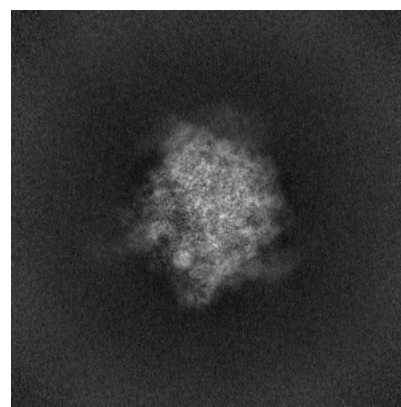
#### 6.1.2 Raw map



X



Y

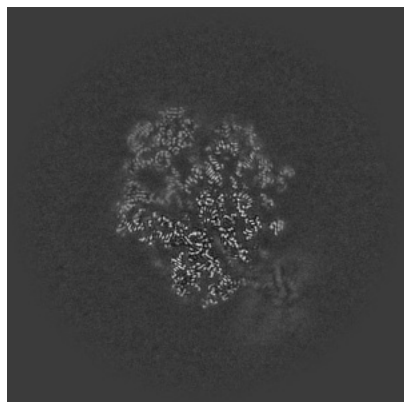


Z

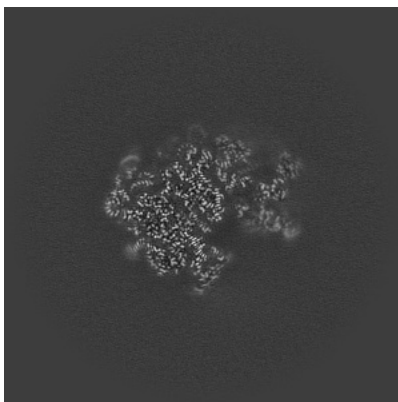
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

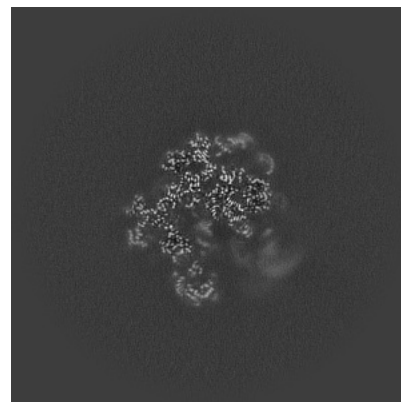
### 6.2.1 Primary map



X Index: 340

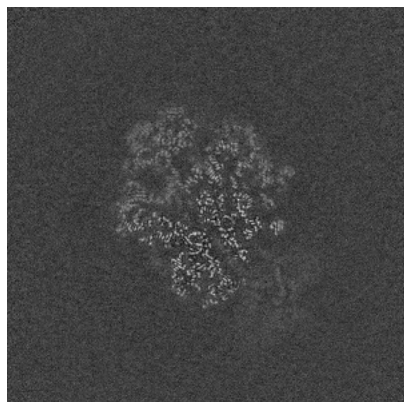


Y Index: 340

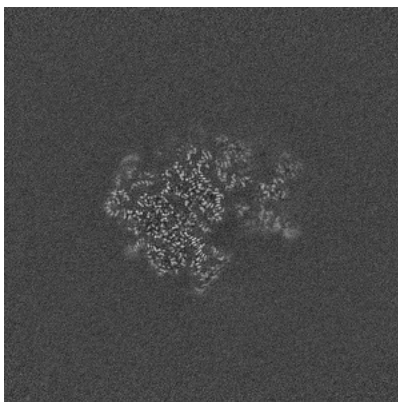


Z Index: 340

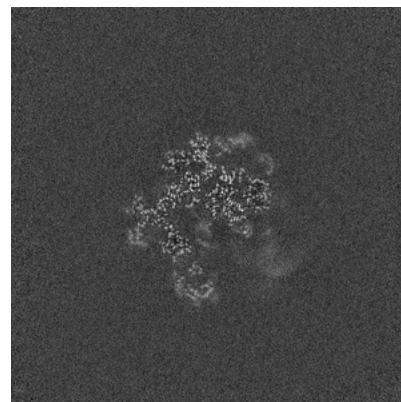
### 6.2.2 Raw map



X Index: 340



Y Index: 340

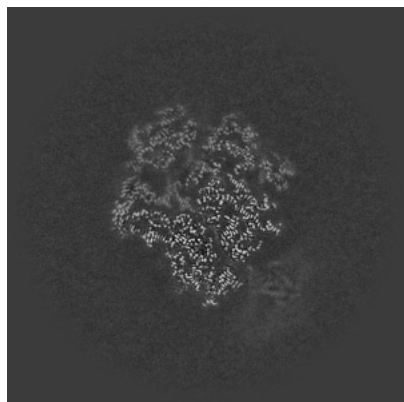


Z Index: 340

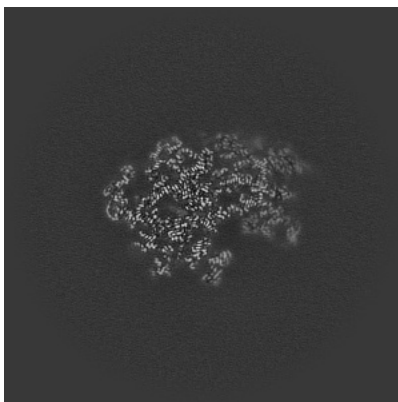
The images above show central slices of the map in three orthogonal directions.

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

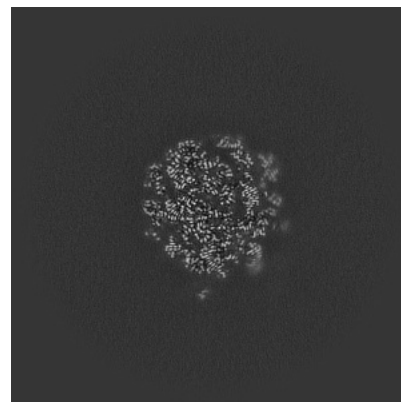
### 6.3.1 Primary map



X Index: 334

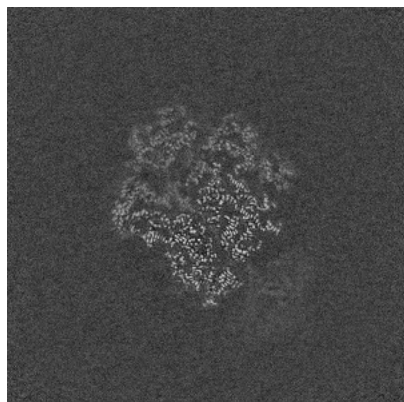


Y Index: 354

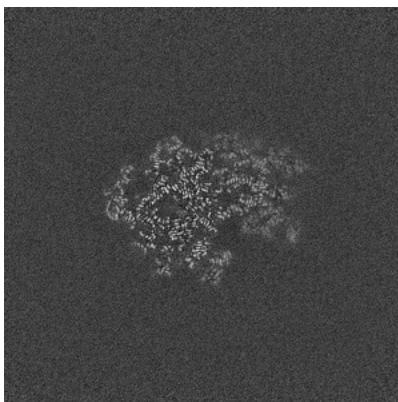


Z Index: 288

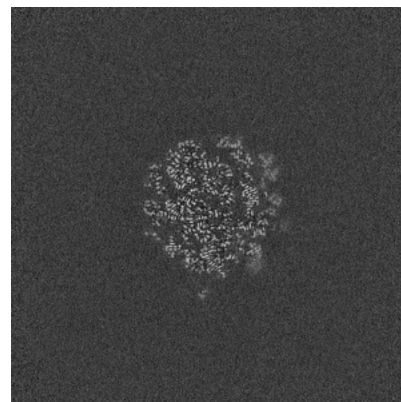
### 6.3.2 Raw map



X Index: 334



Y Index: 353



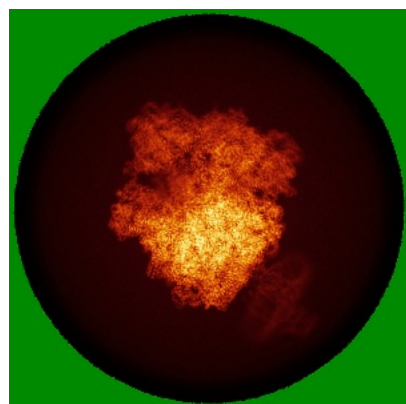
Z Index: 288

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

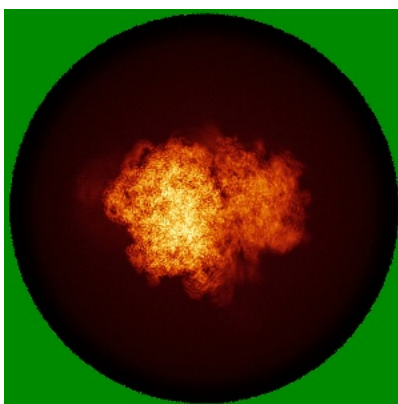


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

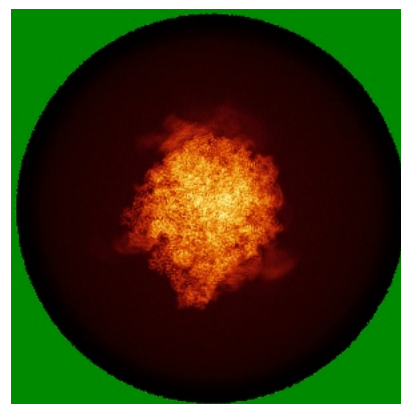
### 6.4.1 Primary map



X

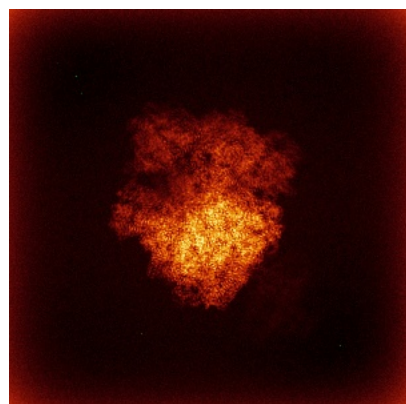


Y

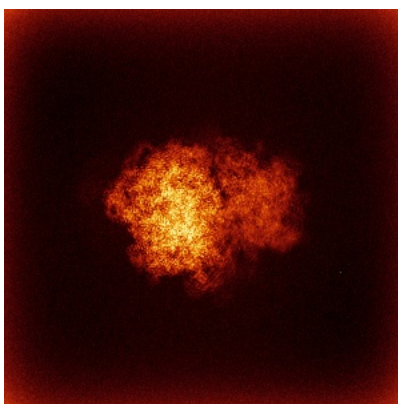


Z

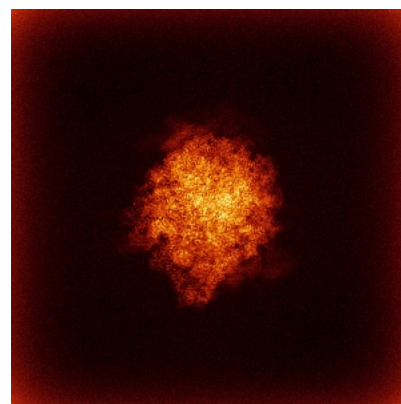
### 6.4.2 Raw map



X



Y



Z

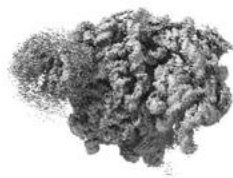
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



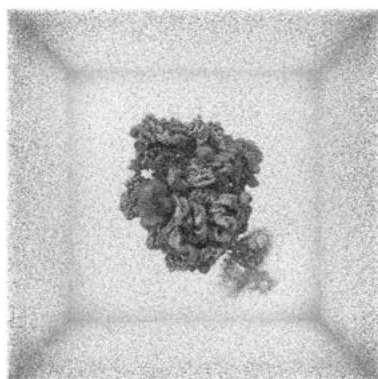
Y



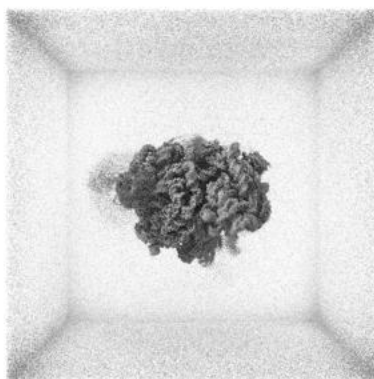
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

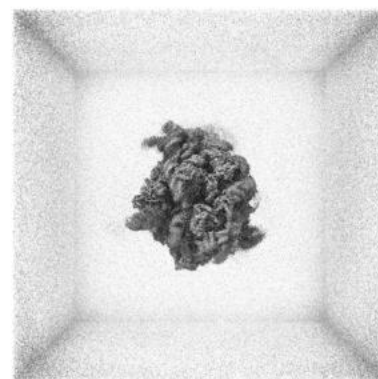
### 6.5.2 Raw map



X



Y



Z

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

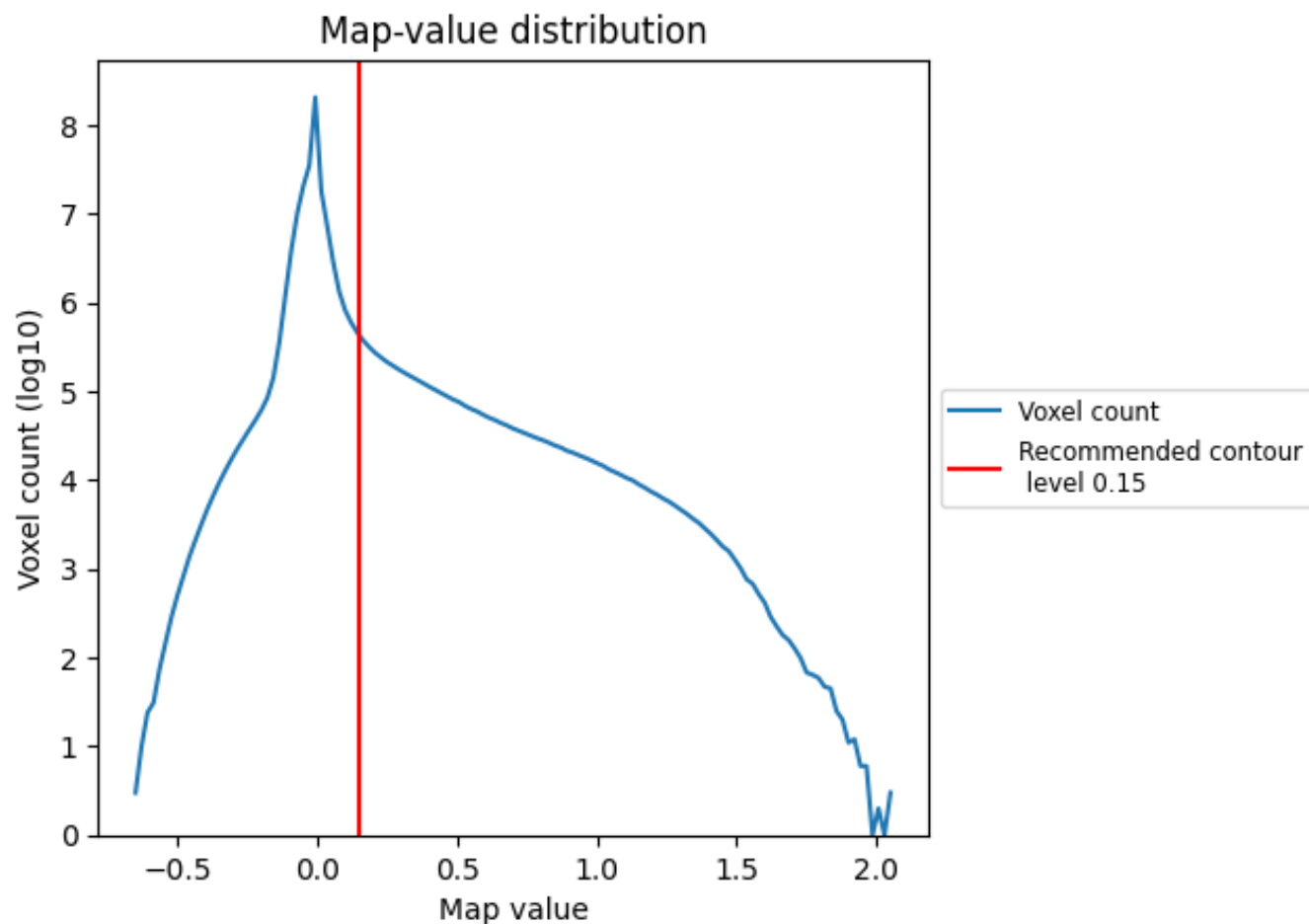
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

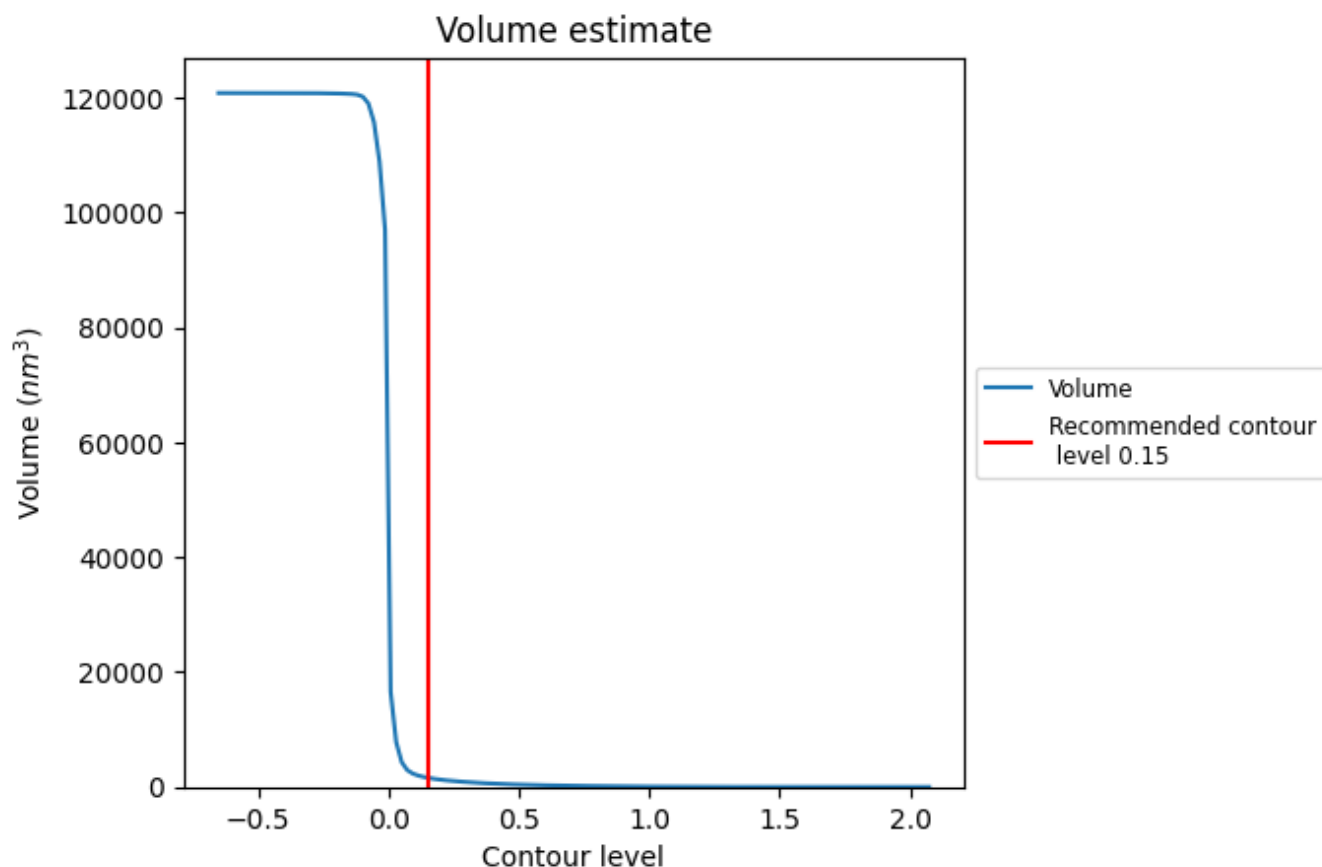
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

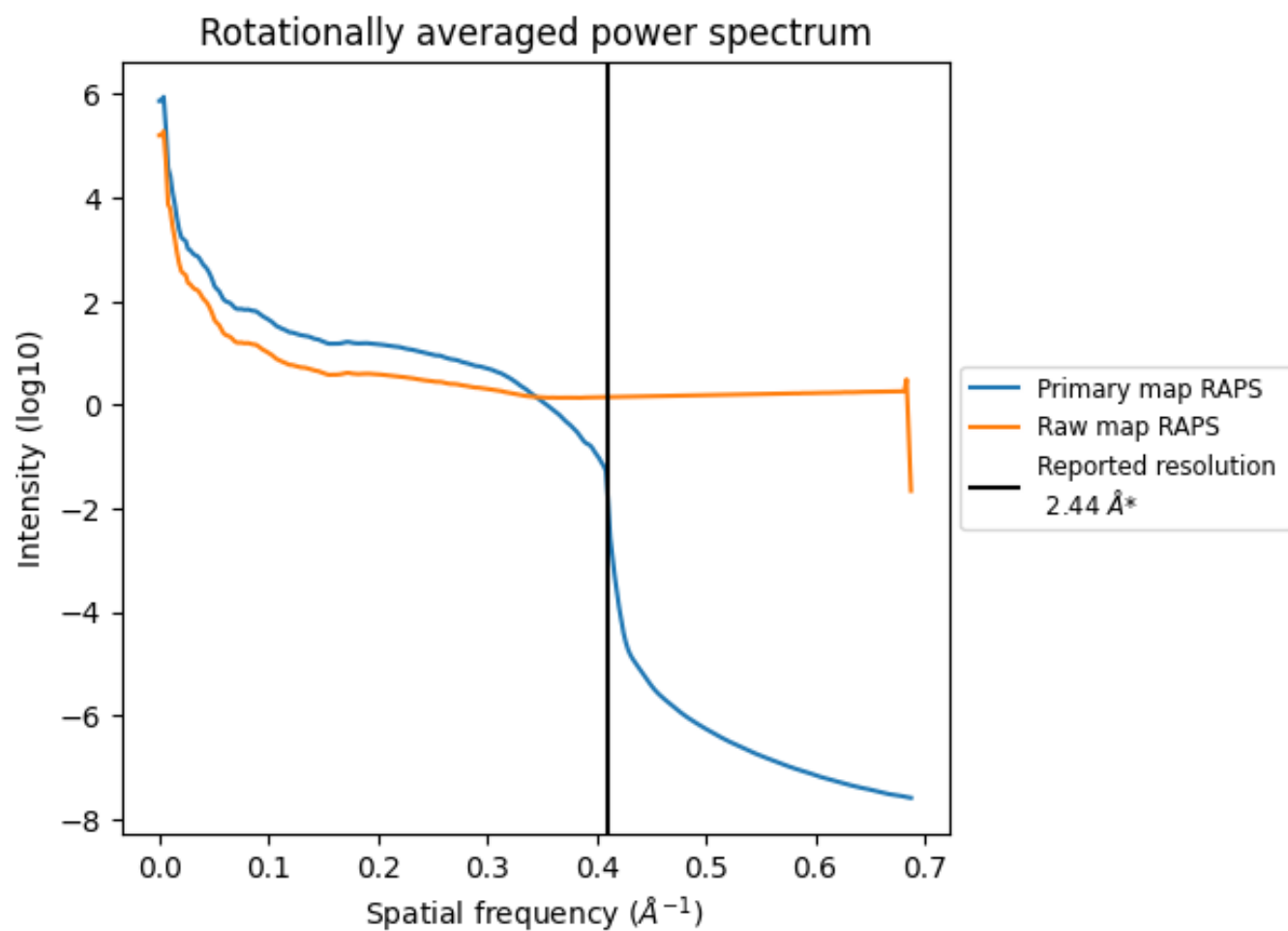


The volume at the recommended contour level is 1607  $\text{nm}^3$ ; this corresponds to an approximate mass of 1452 kDa.

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 ⓘ

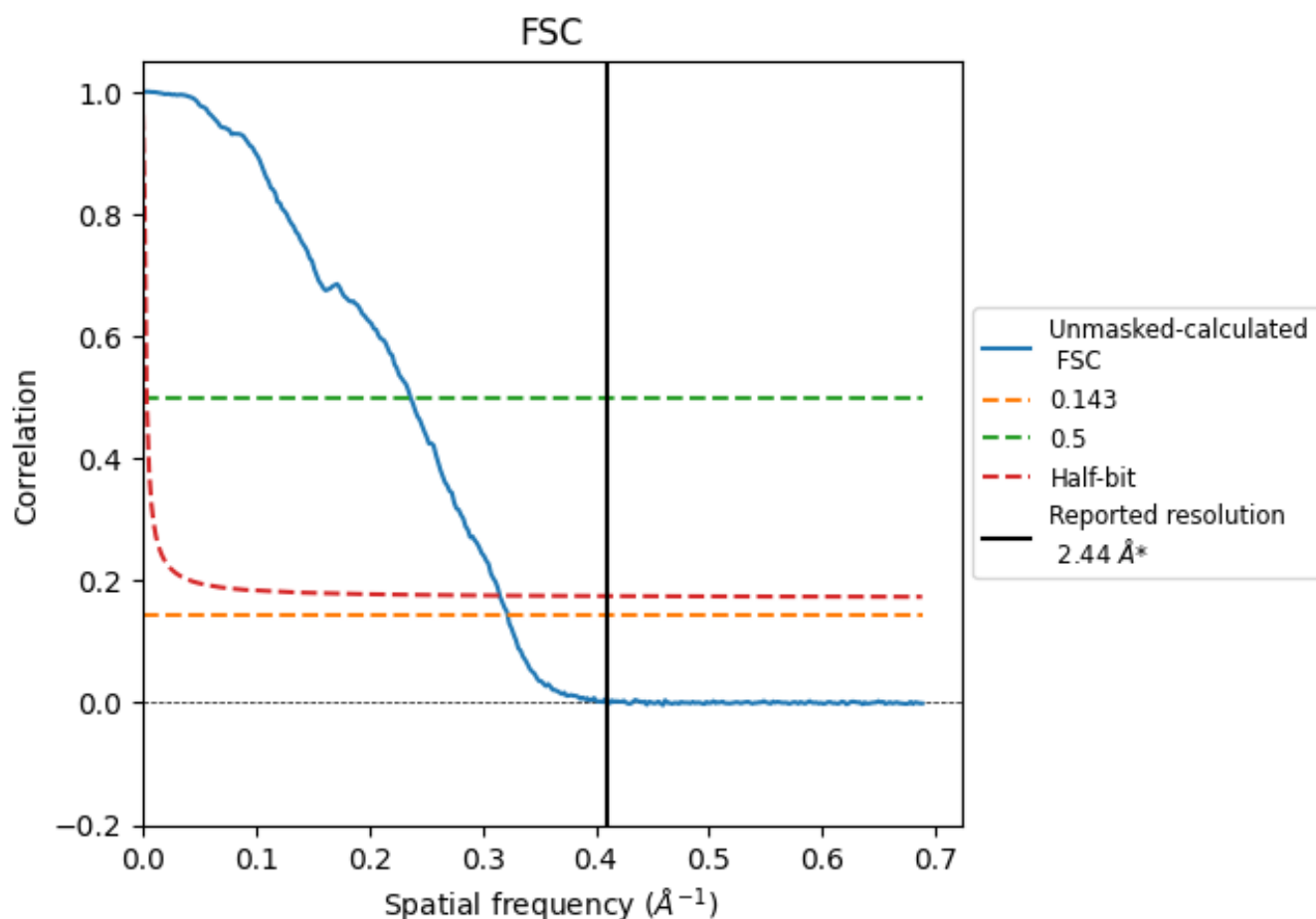


\*Reported resolution corresponds to spatial frequency of 0.410 Å<sup>-1</sup>

## 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 0.410 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

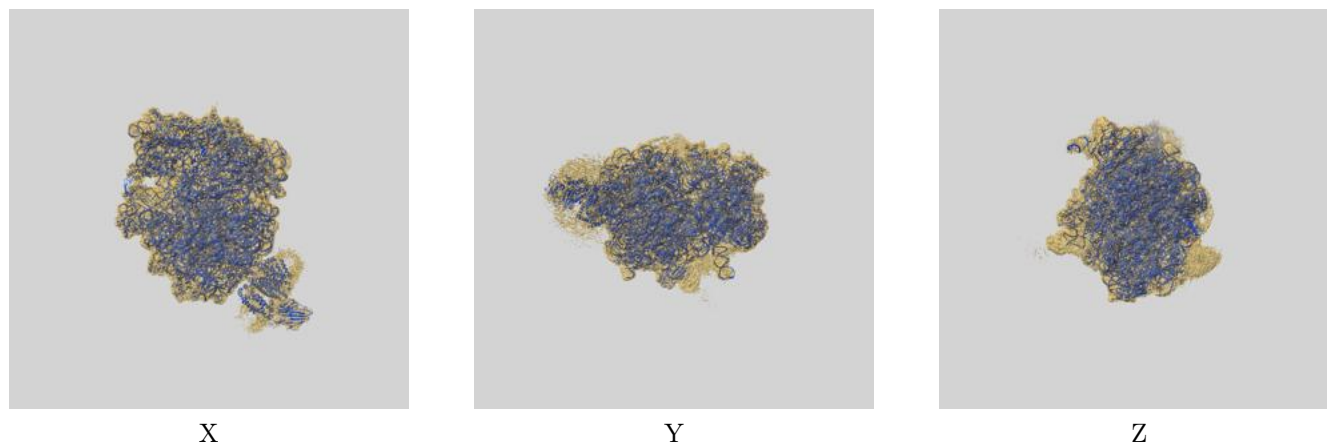
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.10	4.23	3.17

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.10 differs from the reported value 2.44 by more than 10 %

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

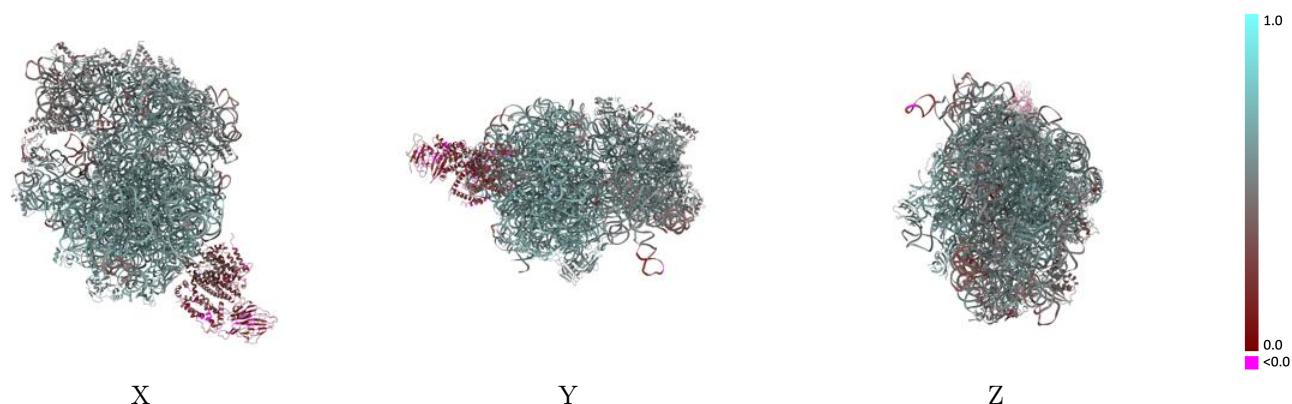
This section contains information regarding the fit between EMDB map EMD-53892 and PDB model 9RBF. Per-residue inclusion information can be found in section 3 on page 17.

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



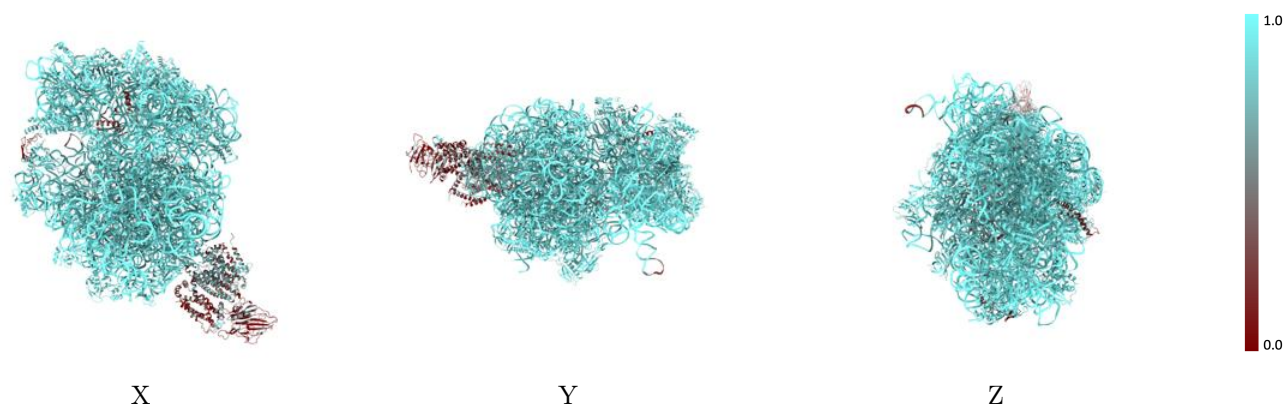
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



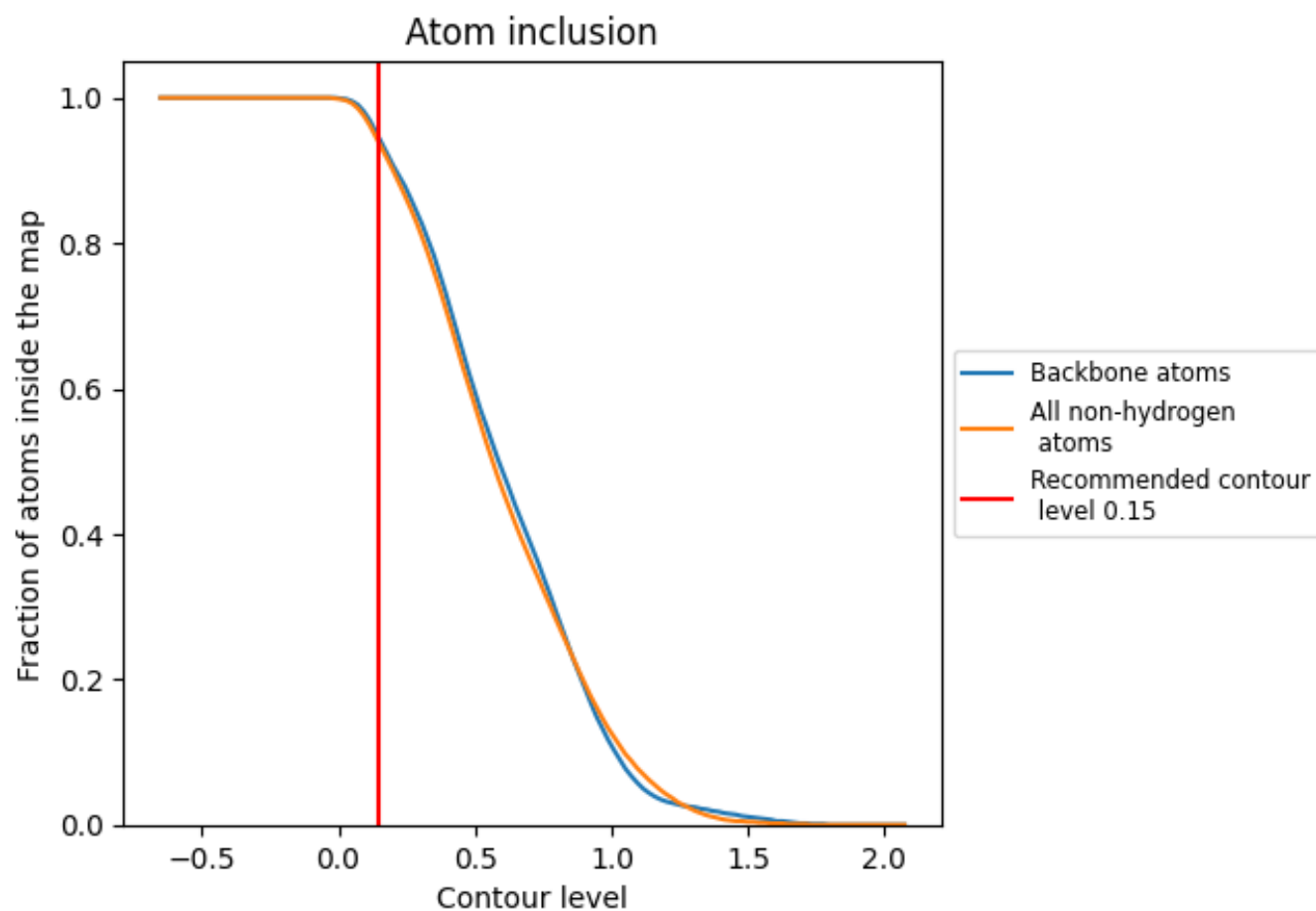
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9370	 0.5550
0	 0.9120	 0.6000
1	 0.9780	 0.6350
2	 0.9780	 0.6360
3	 0.9830	 0.6280
4	 0.0640	 0.2500
5	 0.8570	 0.5940
6	 0.5600	 0.2810
7	 0.5080	 0.2350
8	 0.2800	 0.1990
9	 0.2210	 0.1610
A	 0.9870	 0.5320
B	 0.9070	 0.4980
C	 0.9310	 0.5320
D	 0.8620	 0.4940
E	 0.9590	 0.5730
F	 0.9390	 0.5270
G	 0.8880	 0.4460
H	 0.9560	 0.5750
I	 0.9410	 0.4650
J	 0.9360	 0.4800
K	 0.9250	 0.5160
L	 0.8930	 0.5210
M	 0.9060	 0.4700
N	 0.9510	 0.4990
O	 0.9570	 0.5360
P	 0.9360	 0.5290
Q	 0.9380	 0.5240
R	 0.8740	 0.5010
S	 0.9030	 0.4760
T	 0.9300	 0.5210
U	 0.3090	 0.4000
V	 0.6160	 0.3750
X	 0.8730	 0.5140
Y	 0.7360	 0.5090



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Chain	Atom inclusion	Q-score
Z	 0.9640	 0.4950
a	 0.9950	 0.6140
b	 0.9980	 0.5780
c	 0.9890	 0.6390
d	 0.9740	 0.6320
e	 0.9740	 0.6070
f	 0.9200	 0.4980
g	 0.9520	 0.5510
h	 0.9570	 0.5490
i	 0.9790	 0.6260
j	 0.9810	 0.6300
k	 0.9840	 0.6240
l	 0.9780	 0.6240
m	 0.9950	 0.6450
n	 0.9720	 0.5720
o	 0.9720	 0.6290
p	 0.9910	 0.6380
q	 0.9670	 0.6170
r	 0.9710	 0.6300
s	 0.9600	 0.6160
t	 0.9530	 0.5900
u	 0.9610	 0.5980
v	 0.9670	 0.6270
w	 0.9680	 0.6130
x	 0.9320	 0.5610
y	 0.9700	 0.6160
z	 0.9770	 0.6270