



Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 02:32 AM EDT

PDB ID : 9Q3R / pdb_00009q3r
EMDB ID : EMD-72205
Title : Cryo-EM structure of the Escherichia coli 70S ribosome bound to mRNA, P-site fMet-tRNA^{fMet}, glycyl-tRNA^{Gly} in A/T conformation, EF-Tu-GDPCP, and bottromycin at 1.99Å resolution
Authors : Travin, D.Y.; Basu, R.S.; Paranjpe, M.; Klepacki, D.; Zhurakovskaya, A.I.; Vazquez-Laslop, N.; Mankin, A.S.; Polikanov, Y.S.; Gagnon, M.G.
Deposited on : 2025-08-19
Resolution : 1.99 Å(reported)
Based on initial model : 8G7P

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

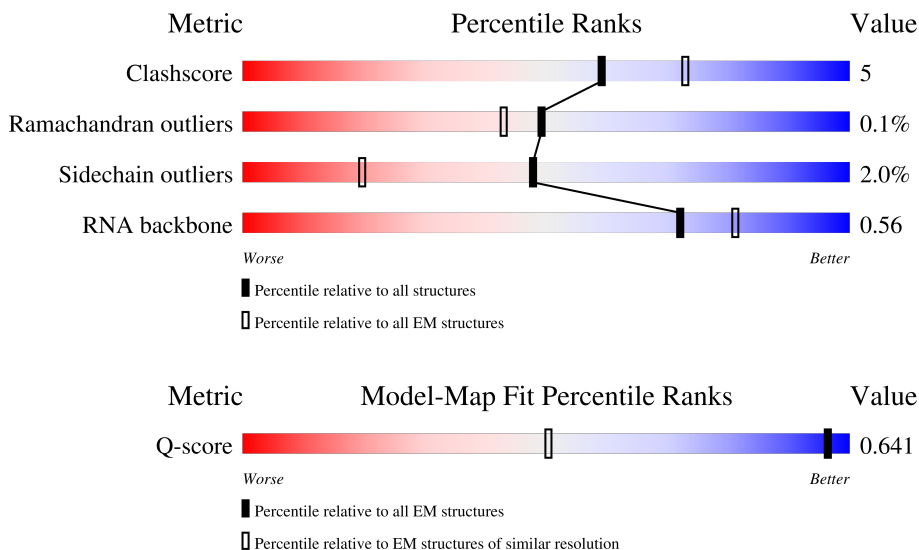
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

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 1.99 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	1416 (1.50 - 2.49)

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

Mol	Chain	Length	Quality of chain
1	a	1542	

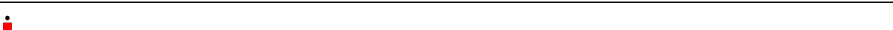
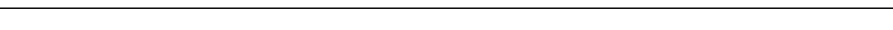
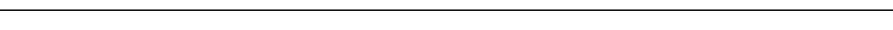
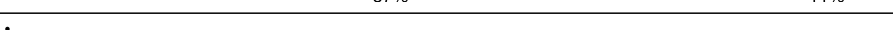
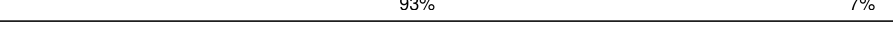
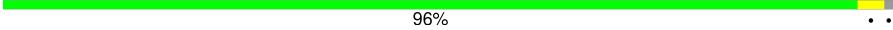
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Mol	Chain	Length	Quality of chain
2	b	241	
3	c	233	
4	d	206	
5	e	167	
6	f	131	
7	g	156	
8	h	130	
9	i	130	
10	j	103	
11	k	129	
12	l	124	
13	m	118	
14	n	101	
15	o	89	
16	p	82	
17	q	84	
18	r	75	
19	s	92	
20	t	87	
21	u	71	
22	v	24	
23	w	74	
24	x	77	
25	z	394	
26	A	2904	

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Mol	Chain	Length	Quality of chain
27	B	120	
28	C	273	
29	D	209	
30	E	201	
31	F	179	
32	G	177	
33	H	149	
34	J	142	
35	L	142	
36	M	123	
37	N	144	
38	O	136	
39	P	127	
40	Q	117	
41	R	115	
42	S	118	
43	T	103	
44	U	110	
45	V	100	
46	W	104	
47	X	94	
48	Y	85	
49	Z	78	
50	1	63	
51	2	59	

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Mol	Chain	Length	Quality of chain
52	3	70	
53	4	57	
54	5	55	
55	6	46	
56	7	65	
57	8	38	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 151455 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 RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1529	Total	C	N	O	P	0	0
			32825	14647	6024	10625	1529		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1754	1110	315	321	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	conflict	UNP A7ZSI6

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			446	283	85	78		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 22 is a RNA chain called 24MG mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	11	Total	C	N	O	P	0	0
			242	108	49	74	11		

- Molecule 23 is a RNA chain called A/T-site glycine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	w	73	Total	C	N	O	P	S	0	0
			1556	695	275	512	73	1		

- Molecule 24 is a RNA chain called P-site initiator tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	x	76	Total	C	N	O	P	S	0	0
			1635	731	295	531	76	2		

- Molecule 25 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	371	Total	C	N	O	S	0	0
			2876	1823	492	548	13		

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 33 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	J	141	Total	C	N	O	0	0
			693	411	141	141		

- Molecule 35 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	N	144	Total	C	N	O	S	0
			1052	653	207	190	2	0

- Molecule 38 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 39 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called Ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	60	Total	C	N	O	S	0	0
			476	296	89	85	6		

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	5	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	46	Total	C	N	O	S	0	0
			373	225	89	57	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	a	189	Total	Mg	0
			189	189	
58	d	1	Total	Mg	0
			1	1	
58	j	1	Total	Mg	0
			1	1	
58	k	1	Total	Mg	0
			1	1	
58	v	2	Total	Mg	0
			2	2	
58	x	1	Total	Mg	0
			1	1	
58	A	751	Total	Mg	0
			751	751	
58	B	3	Total	Mg	0
			3	3	
58	C	17	Total	Mg	0
			17	17	
58	D	6	Total	Mg	0
			6	6	
58	E	4	Total	Mg	0
			4	4	
58	M	1	Total	Mg	0
			1	1	

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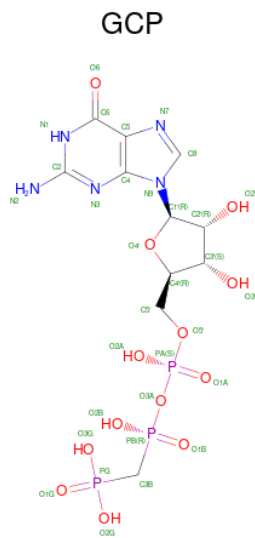
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Mol	Chain	Residues	Atoms		AltConf
58	N	4	Total 4	Mg 4	0
58	O	1	Total 1	Mg 1	0
58	R	1	Total 1	Mg 1	0
58	S	6	Total 6	Mg 6	0
58	T	4	Total 4	Mg 4	0
58	U	1	Total 1	Mg 1	0
58	V	1	Total 1	Mg 1	0
58	Z	1	Total 1	Mg 1	0
58	4	7	Total 7	Mg 7	0
58	6	3	Total 3	Mg 3	0
58	7	1	Total 1	Mg 1	0

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

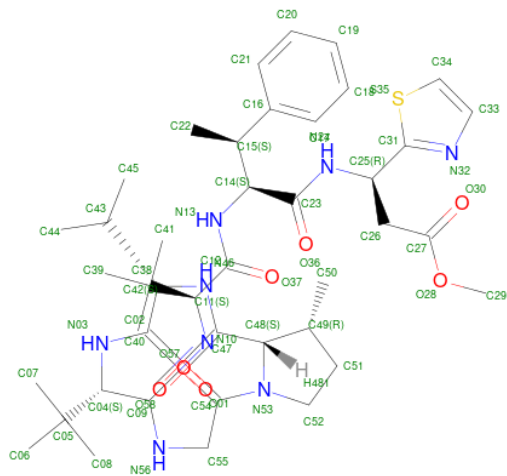
Mol	Chain	Residues	Atoms		AltConf
59	a	30	Total 30	K 30	0
59	f	1	Total 1	K 1	0
59	A	88	Total 88	K 88	0
59	B	1	Total 1	K 1	0
59	C	1	Total 1	K 1	0
59	D	1	Total 1	K 1	0
59	E	1	Total 1	K 1	0

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
60	z	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 61 is Bottromycin A2 (CCD ID: MQH) (formula: $C_{42}H_{62}N_8O_7S$).



Mol	Chain	Residues	Atoms					AltConf
61	z	1	Total	C	N	O	S	0
			58	42	8	7	1	

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

Mol	Chain	Residues	Atoms		AltConf
62	3	1	Total 1	Zn 1	0
62	8	1	Total 1	Zn 1	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		AltConf
63	a	327	Total 327	O 327	0
63	c	1	Total 1	O 1	0
63	k	4	Total 4	O 4	0
63	l	4	Total 4	O 4	0
63	v	6	Total 6	O 6	0
63	w	1	Total 1	O 1	0
63	x	1	Total 1	O 1	0
63	A	1490	Total 1490	O 1490	0
63	B	11	Total 11	O 11	0
63	C	34	Total 34	O 34	0
63	D	15	Total 15	O 15	0
63	E	18	Total 18	O 18	0
63	H	1	Total 1	O 1	0
63	M	2	Total 2	O 2	0
63	N	12	Total 12	O 12	0
63	O	6	Total 6	O 6	0
63	P	2	Total 2	O 2	0
63	R	2	Total 2	O 2	0

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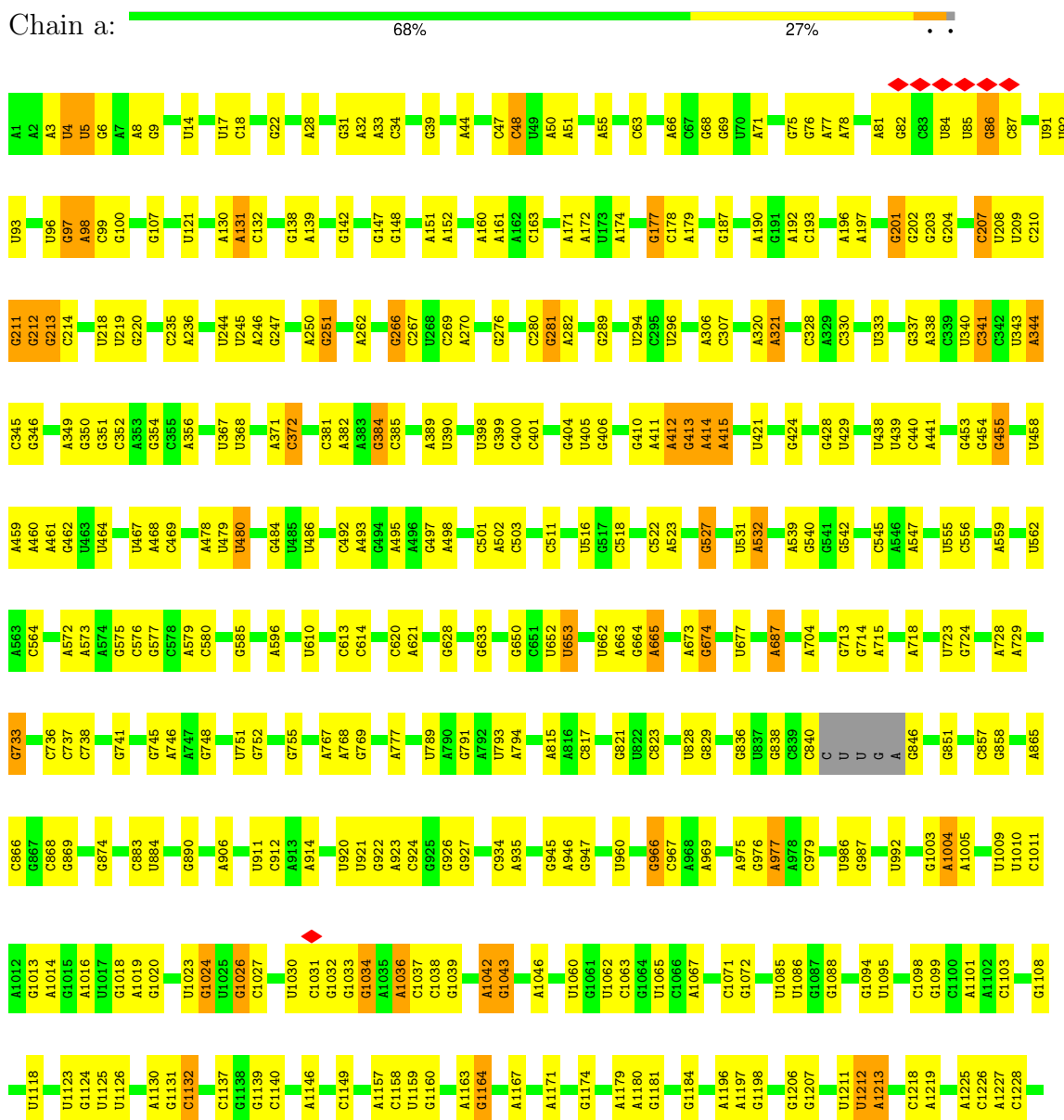
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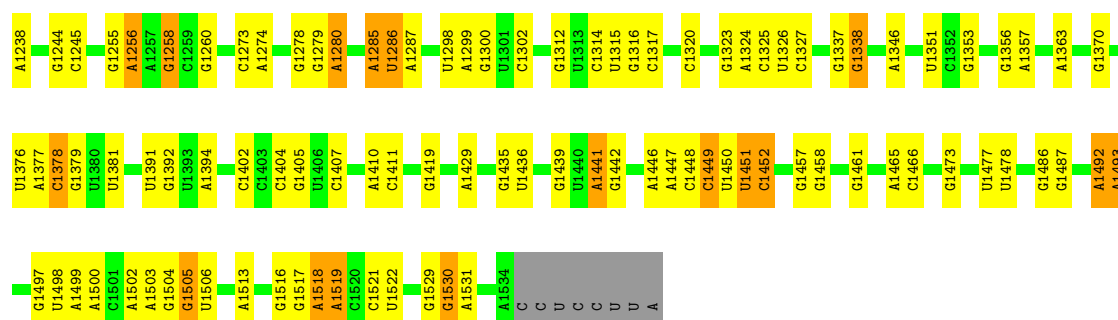
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63	T	3	Total 3	O 3	0
63	U	3	Total 3	O 3	0
63	V	1	Total 1	O 1	0
63	X	1	Total 1	O 1	0
63	Z	1	Total 1	O 1	0
63	4	14	Total 14	O 14	0
63	6	3	Total 3	O 3	0
63	7	4	Total 4	O 4	0
63	8	1	Total 1	O 1	0

3 Residue-property plots

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

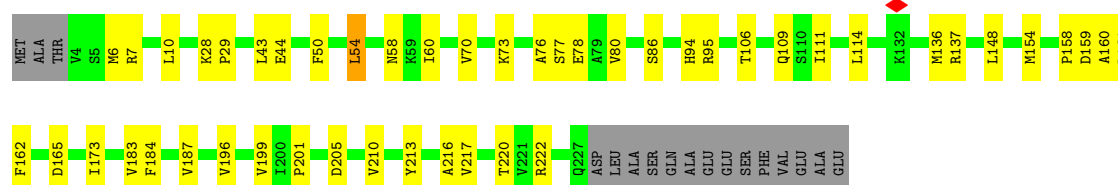
• Molecule 1: 16S Ribosomal RNA





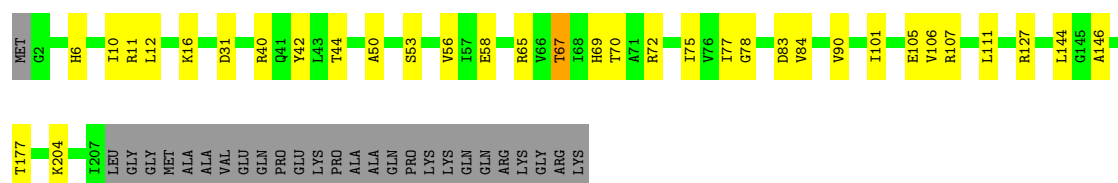
• Molecule 2: 30S ribosomal protein S2

Chain b: 73% 20% 7%



• Molecule 3: Small ribosomal subunit protein uS3

Chain c: 74% 14% 12%



• Molecule 4: Small ribosomal subunit protein uS4

Chain d: 84% 16%

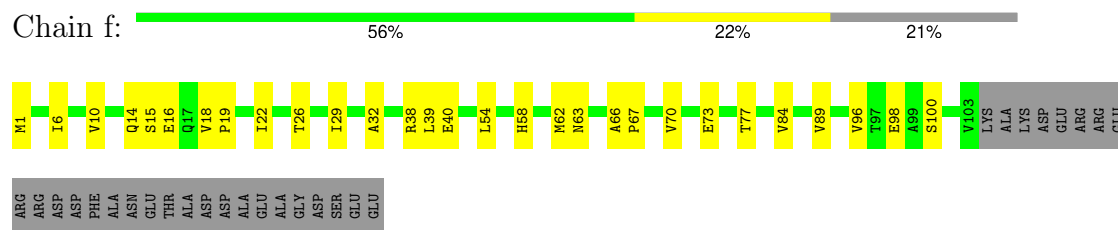


• Molecule 5: Small ribosomal subunit protein uS5

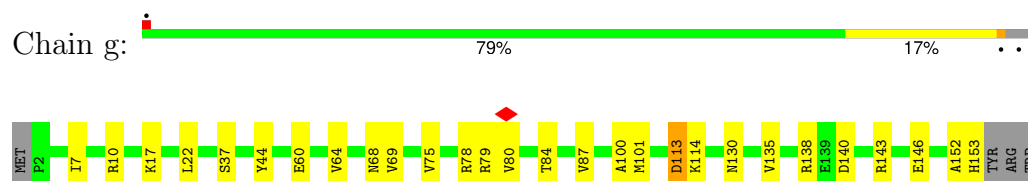
Chain e: 81% 13% 7%



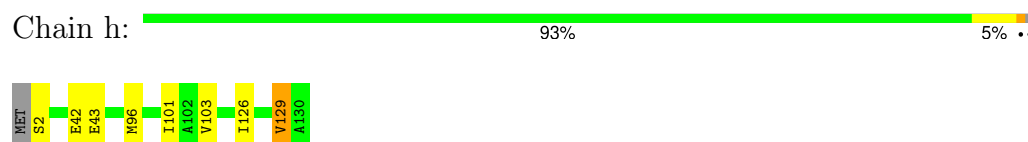
• Molecule 6: 30S ribosomal protein S6



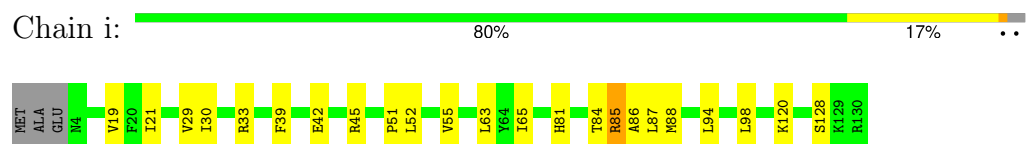
- Molecule 7: 30S ribosomal protein S7



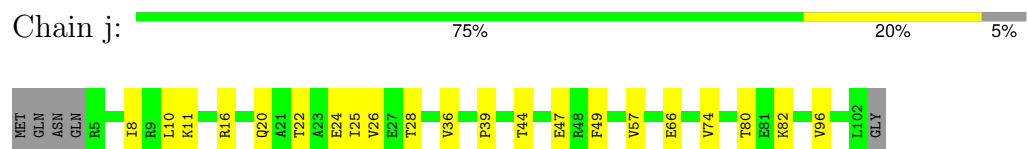
- Molecule 8: Small ribosomal subunit protein uS8



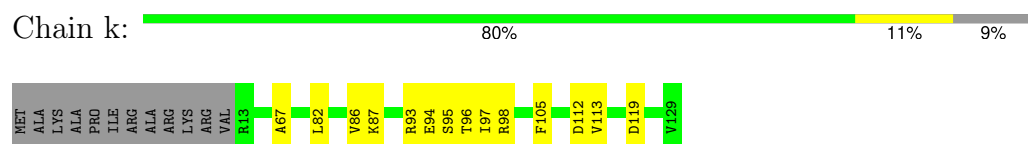
- Molecule 9: Small ribosomal subunit protein uS9



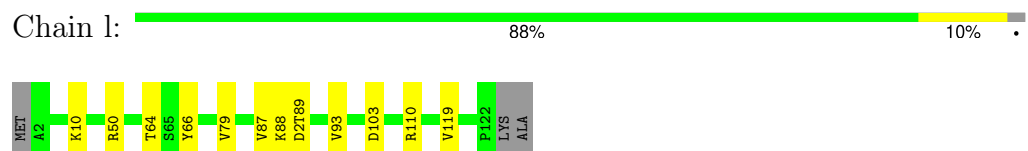
- Molecule 10: Small ribosomal subunit protein uS10



- Molecule 11: Small ribosomal subunit protein uS11

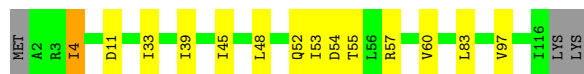


- Molecule 12: Small ribosomal subunit protein uS12



- Molecule 13: Small ribosomal subunit protein uS13

Chain m:  86% 11% ..



- Molecule 14: Small ribosomal subunit protein uS14

Chain n:  85% 14% .



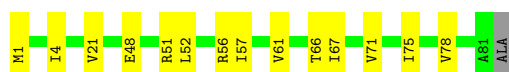
- Molecule 15: Small ribosomal subunit protein uS15

Chain o:  84% 15% .



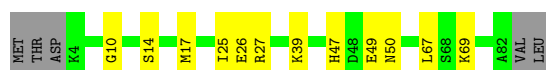
- Molecule 16: Small ribosomal subunit protein bS16

Chain p:  82% 17% .



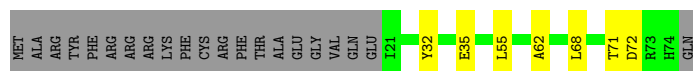
- Molecule 17: Small ribosomal subunit protein uS17

Chain q:  80% 14% 6%



- Molecule 18: Small ribosomal subunit protein bS18

Chain r:  63% 9% 28%



- Molecule 19: Small ribosomal subunit protein uS19

Chain s:  71% 17% 10%



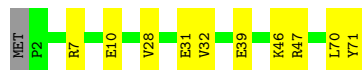
- Molecule 20: Small ribosomal subunit protein bS20

Chain t:  86% 13%



- Molecule 21: Small ribosomal subunit protein bS21

Chain u:  85% 14%



- Molecule 22: 24MG mRNA

Chain v:  38% 54%



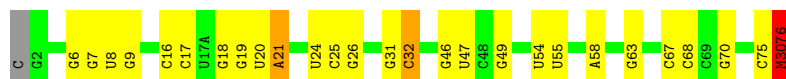
- Molecule 23: A/T-site glycine tRNA

Chain w:  50% 35% 14%



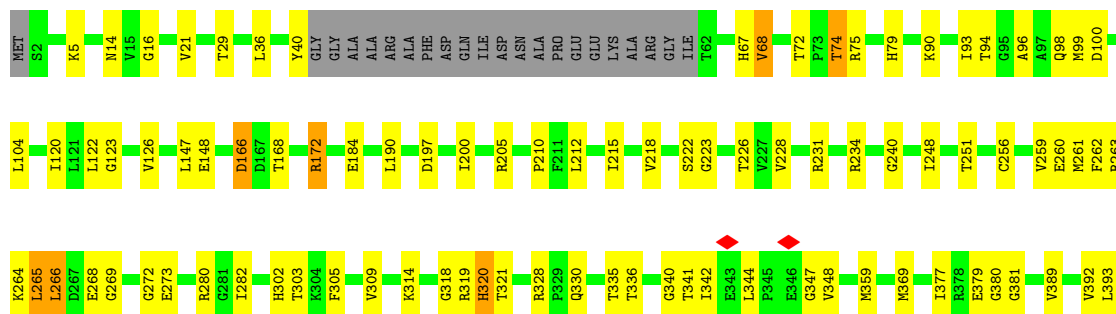
- Molecule 24: P-site initiator tRNA fMet

Chain x:  64% 31%



- Molecule 25: Elongation factor Tu 2

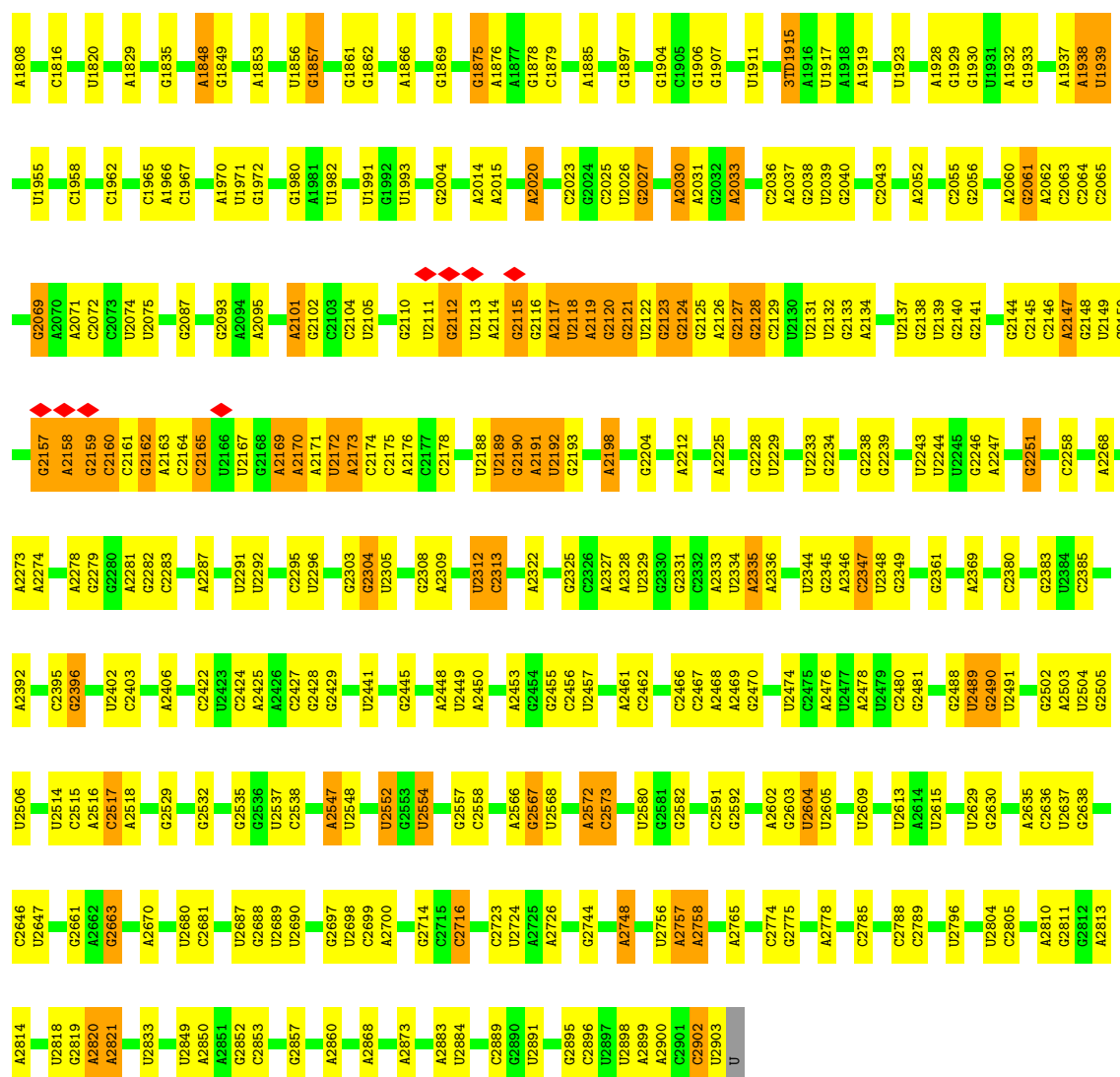
Chain z:  71% 21% 6%



- Molecule 26: 23S Ribosomal RNA

Chain A:  69% 26% 5%

G1	G2	G3	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	G14	G15	G16	G17	G18	G19	G20	G21	G22	G23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33	G34	G35	G36	G37	G38	G39	G40	G41	G42	G43	G44	G45	G46	G47	G48	G49	G50	G51	G52	G53	G54	G55	G56	G57	G58	G59	G60	G61	G62	G63	G64	G65	G66	G67	G68	G69	G70	G71	G72	G73	G74	G75	G76	G77	G78	G79	G80	G81	G82	G83	G84	G85	G86	G87	G88	G89	G90	G91	G92	G93	G94	G95	G96	G97	G98	G99	G100	G101	G102	G103	G104	G105	G106	G107	G108	G109	G110	G111	G112	G113	G114	G115	G116	G117	G118	G119	G120	G121	G122	G123	G124	G125	G126	G127	G128	G129	G130	G131	G132	G133	G134	G135	G136	G137	G138	G139	G140	G141	G142	G143	G144	G145	G146	G147	G148	G149	G150	G151	G152	G153	G154	G155	G156	G157	G158	G159	G160	G161	G162	G163	G164	G165	G166	G167	G168	G169	G170	G171	G172	G173	G174	G175	G176	G177	G178	G179	G180	G181	G182	G183	G184	G185	G186	G187	G188	G189	G190	G191	G192	G193	G194	G195	G196	G197	G198	G199	G200	G201	G202	G203	G204	G205	G206	G207	G208	G209	G210	G211	G212	G213	G214	G215	G216	G217	G218	G219	G220	G221	G222	G223	G224	G225	G226	G227	G228	G229	G230	G231	G232	G233	G234	G235	G236	G237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G147
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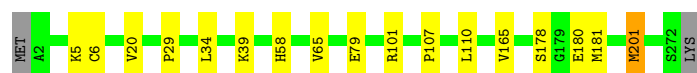
• Molecule 27: 5S Ribosomal RNA

Chain B: 74% 19% 7%



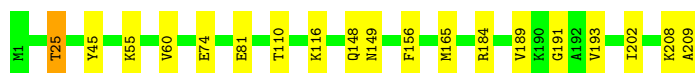
• Molecule 28: 50S ribosomal protein L2

Chain C: 93% 6%



• Molecule 29: 50S ribosomal protein L3

Chain D: 91% 9%



- Molecule 30: Large ribosomal subunit protein uL4

Chain E: 89% 10% .



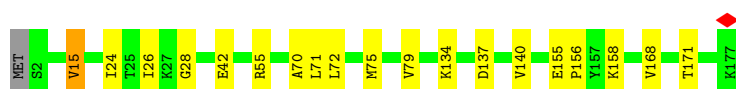
- Molecule 31: Large ribosomal subunit protein uL5

Chain F: 83% 15% ..



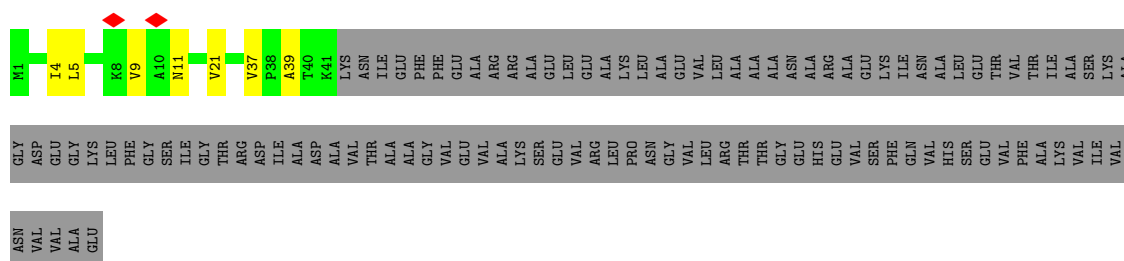
- Molecule 32: Large ribosomal subunit protein uL6

Chain G: 89% 10% ..



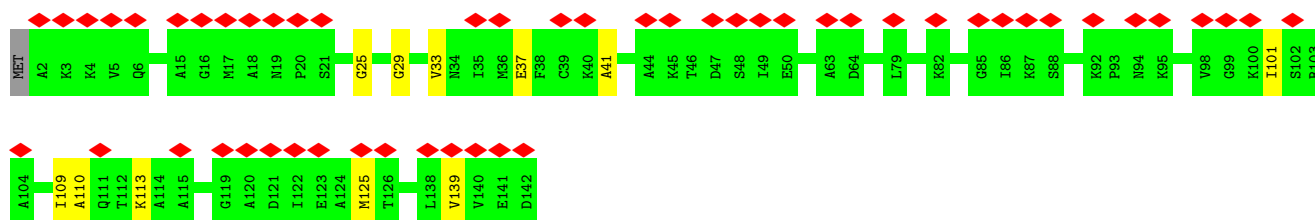
- Molecule 33: Large ribosomal subunit protein bL9

Chain H: 23% 5% 72%



- Molecule 34: 50S ribosomal protein L11

Chain J: 37% 92% 8% .



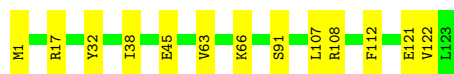
- Molecule 35: Large ribosomal subunit protein uL13

Chain L:  92% 8%

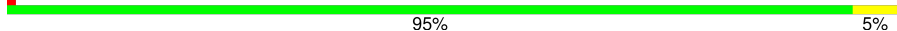


- Molecule 36: Large ribosomal subunit protein uL14

Chain M:  89% 11%



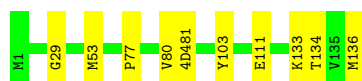
- Molecule 37: 50S ribosomal protein L15

Chain N:  95% 5%



- Molecule 38: Large ribosomal subunit protein uL16

Chain O:  93% 7%



- Molecule 39: Large ribosomal subunit protein bL17

Chain P:  84% 9% 7%



- Molecule 40: Large ribosomal subunit protein uL18

Chain Q:  87% 11% ..



- Molecule 41: Large ribosomal subunit protein bL19

Chain R:  92% 7%



- Molecule 42: 50S ribosomal protein L20

Chain S:  91% 8%



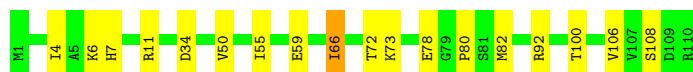
- Molecule 43: Ribosomal protein L21

Chain T:  93% 7%



- Molecule 44: 50S ribosomal protein L22

Chain U:  84% 15%



- Molecule 45: 50S ribosomal protein L23

Chain V:  86% 7% 7%



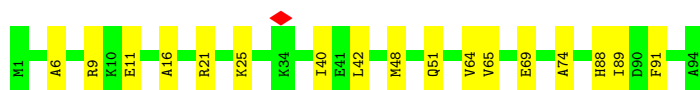
- Molecule 46: 50S ribosomal protein L24

Chain W:  75% 22%



- Molecule 47: Large ribosomal subunit protein bL25

Chain X:  82% 18%

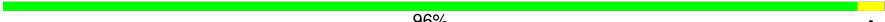


- Molecule 48: 50S ribosomal protein L27

Chain Y:  79% 11% 11%



- Molecule 49: 50S ribosomal protein L28

Chain Z:  96% ..



- Molecule 50: Large ribosomal subunit protein uL29

Chain 1:  76% 21% .



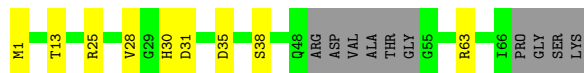
- Molecule 51: 50S ribosomal protein L30

Chain 2:  92% 7% .



- Molecule 52: 50S ribosomal protein L31

Chain 3:  73% 13% 14%



- Molecule 53: 50S ribosomal protein L32

Chain 4:  84% 12% .



- Molecule 54: 50S ribosomal protein L33

Chain 5:  87% 5% 7%



- Molecule 55: 50S ribosomal protein L34

Chain 6:  91% 9%



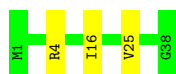
- Molecule 56: 50S ribosomal protein L35

Chain 7:  91% 8% •



• Molecule 57: 50S ribosomal protein L36

Chain 8:  92% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	443440	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 ($e^-/\text{\AA}^2$)	39.238	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.575	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	425.9328, 425.9328, 425.9328	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8319, 0.8319, 0.8319	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, IAS, 4SU, 4D4, 2MA, UR3, OMC, OMG, MQH, 3TD, L3X, 4OC, MS6, 5MU, OMU, H2U, G7M, PSU, D2T, GCP, MEQ, 6MZ, K, M3O, MA6, ZN, 5MC, 1MG, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.30	1/36475 (0.0%)	0.36	0/56895
2	b	0.19	0/1785	0.40	0/2404
3	c	0.22	0/1651	0.39	0/2225
4	d	0.20	0/1665	0.34	0/2227
5	e	0.25	0/1165	0.38	0/1568
6	f	0.24	0/858	0.45	0/1160
7	g	0.20	0/1206	0.35	0/1617
8	h	0.24	0/989	0.37	0/1326
9	i	0.21	0/1034	0.39	0/1375
10	j	0.23	0/796	0.42	0/1077
11	k	0.22	0/884	0.36	0/1191
12	l	0.24	0/945	0.36	0/1268
13	m	0.20	0/900	0.39	0/1204
14	n	0.21	0/817	0.33	0/1088
15	o	0.20	0/722	0.35	0/964
16	p	0.23	0/653	0.40	0/877
17	q	0.24	0/650	0.38	0/871
18	r	0.22	0/453	0.34	0/609
19	s	0.21	0/680	0.35	0/915
20	t	0.22	0/676	0.42	0/895
21	u	0.19	0/597	0.33	0/792
22	v	0.34	0/272	0.35	0/423
23	w	0.25	0/1639	0.34	0/2548
24	x	0.29	0/1700	0.35	0/2650
25	z	0.20	0/2929	0.40	0/3964
26	A	0.36	0/69147	0.41	1/107869 (0.0%)
27	B	0.27	0/2876	0.35	0/4483
28	C	0.26	0/2121	0.37	0/2852
29	D	0.26	0/1576	0.36	0/2119
30	E	0.24	0/1571	0.34	0/2113
31	F	0.19	0/1434	0.33	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	G	0.19	0/1343	0.34	0/1816
33	H	0.20	0/306	0.37	0/413
34	J	0.16	0/692	0.43	0/960
35	L	0.24	0/1152	0.35	0/1551
36	M	0.25	0/955	0.38	0/1279
37	N	0.25	0/1061	0.36	0/1412
38	O	0.25	0/1073	0.35	0/1433
39	P	0.26	0/958	0.40	0/1281
40	Q	0.21	0/902	0.36	0/1209
41	R	0.25	0/929	0.34	0/1242
42	S	0.24	0/960	0.34	0/1278
43	T	0.24	0/829	0.34	0/1107
44	U	0.27	0/864	0.35	0/1156
45	V	0.23	0/744	0.34	0/994
46	W	0.23	0/787	0.40	0/1051
47	X	0.26	0/766	0.38	0/1025
48	Y	0.26	0/587	0.38	0/776
49	Z	0.23	0/635	0.33	0/848
50	1	0.20	0/496	0.36	0/660
51	2	0.22	0/453	0.31	0/605
52	3	0.21	0/484	0.36	0/645
53	4	0.26	0/440	0.39	0/588
54	5	0.20	0/424	0.34	0/565
55	6	0.25	0/376	0.39	0/494
56	7	0.26	0/513	0.35	0/676
57	8	0.26	0/303	0.38	0/397
All	All	0.31	1/159898 (0.0%)	0.39	1/238956 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
25	z	0	1
56	7	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	527	G7M	O3'-P	5.16	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
26	A	512	G	O4'-C1'-N9	5.51	116.46	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	7	30	ARG	Peptide
25	z	264	LYS	Peptide

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	a	32825	0	16531	222	0
2	b	1754	0	1782	32	0
3	c	1624	0	1696	21	0
4	d	1643	0	1707	20	0
5	e	1152	0	1196	10	0
6	f	839	0	833	18	0
7	g	1191	0	1245	16	0
8	h	979	0	1031	4	0
9	i	1022	0	1070	23	0
10	j	786	0	828	10	0
11	k	877	0	883	6	0
12	l	942	0	999	6	0
13	m	891	0	952	10	0
14	n	805	0	844	13	0
15	o	714	0	734	10	0
16	p	643	0	661	9	0
17	q	641	0	682	7	0
18	r	446	0	472	6	0
19	s	663	0	688	11	0
20	t	670	0	719	9	0
21	u	589	0	628	7	0
22	v	242	0	120	2	0
23	w	1556	0	779	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	x	1635	0	838	11	0
25	z	2876	0	2898	62	0
26	A	62252	0	31312	435	0
27	B	2572	0	1301	22	0
28	C	2082	0	2154	12	0
29	D	1566	0	1618	15	0
30	E	1552	0	1619	12	0
31	F	1410	0	1444	21	0
32	G	1323	0	1371	9	0
33	H	303	0	327	6	0
34	J	693	0	344	5	0
35	L	1129	0	1162	10	0
36	M	946	0	1023	8	0
37	N	1052	0	1127	5	0
38	O	1075	0	1145	6	0
39	P	945	0	989	6	0
40	Q	892	0	923	8	0
41	R	917	0	962	5	0
42	S	947	0	1019	7	0
43	T	816	0	839	3	0
44	U	857	0	922	15	0
45	V	738	0	807	5	0
46	W	779	0	831	16	0
47	X	753	0	780	11	0
48	Y	580	0	594	6	0
49	Z	625	0	652	1	0
50	1	495	0	526	12	0
51	2	449	0	488	2	0
52	3	476	0	467	8	0
53	4	434	0	445	5	0
54	5	417	0	451	1	0
55	6	373	0	407	2	0
56	7	504	0	572	3	0
57	8	302	0	340	3	0
58	4	7	0	0	0	0
58	6	3	0	0	0	0
58	7	1	0	0	0	0
58	A	751	0	0	0	0
58	B	3	0	0	0	0
58	C	17	0	0	0	0
58	D	6	0	0	0	0
58	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	M	1	0	0	0	0
58	N	4	0	0	0	0
58	O	1	0	0	0	0
58	R	1	0	0	0	0
58	S	6	0	0	0	0
58	T	4	0	0	0	0
58	U	1	0	0	0	0
58	V	1	0	0	0	0
58	Z	1	0	0	0	0
58	a	189	0	0	0	0
58	d	1	0	0	0	0
58	j	1	0	0	0	0
58	k	1	0	0	0	0
58	v	2	0	0	0	0
58	x	1	0	0	0	0
59	A	88	0	0	0	0
59	B	1	0	0	0	0
59	C	1	0	0	0	0
59	D	1	0	0	0	0
59	E	1	0	0	0	0
59	a	30	0	0	0	0
59	f	1	0	0	0	0
60	z	32	0	14	0	0
61	z	58	0	0	5	0
62	3	1	0	0	0	0
62	8	1	0	0	0	0
63	4	14	0	0	0	0
63	6	3	0	0	0	0
63	7	4	0	0	0	0
63	8	1	0	0	0	0
63	A	1490	0	0	12	0
63	B	11	0	0	0	0
63	C	34	0	0	0	0
63	D	15	0	0	0	0
63	E	18	0	0	0	0
63	H	1	0	0	0	0
63	M	2	0	0	0	0
63	N	12	0	0	0	0
63	O	6	0	0	0	0
63	P	2	0	0	0	0
63	R	2	0	0	0	0
63	S	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	T	3	0	0	0	0
63	U	3	0	0	0	0
63	V	1	0	0	0	0
63	X	1	0	0	0	0
63	Z	1	0	0	0	0
63	a	327	0	0	4	0
63	c	1	0	0	0	0
63	k	4	0	0	0	0
63	l	4	0	0	0	0
63	v	6	0	0	0	0
63	w	1	0	0	0	0
63	x	1	0	0	0	0
All	All	151455	0	99791	1146	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 5.

All (1146) 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)
26:A:1915:3TD:C1'	26:A:1915:3TD:O4'	1.65	1.26
45:V:4:GLU:OE1	45:V:49:LYS:NZ	1.84	1.10
27:B:8:C:O2'	27:B:9:G:O5'	1.73	1.06
26:A:1084:A:O2'	26:A:1085:A:O5'	1.77	1.00
26:A:1044:C:O2'	26:A:1111:A:N6	1.98	0.96
1:a:1211:U:O2'	1:a:1212:U:OP2	1.86	0.93
29:D:184:ARG:NH1	41:R:7:GLN:OE1	2.05	0.88
1:a:1314:C:OP2	19:s:4:SER:OG	1.96	0.84
11:k:67:ALA:HB2	11:k:96:THR:HG23	1.58	0.84
31:F:26:MET:HE2	31:F:26:MET:HA	1.61	0.83
25:z:342:ILE:HD12	25:z:359:MET:HE1	1.60	0.82
3:c:105:GLU:OE1	3:c:107:ARG:NH1	2.12	0.82
44:U:59:GLU:CD	44:U:66:ILE:HD11	2.04	0.81
1:a:1518:MA6:H103	1:a:1519:MA6:N6	1.95	0.81
26:A:2169:A:O2'	26:A:2170:A:N3	2.12	0.81
1:a:413:G:O2'	1:a:414:A:OP2	1.98	0.81
14:n:89:MET:HE2	14:n:89:MET:HA	1.63	0.81
1:a:1013:G:N2	1:a:1016:A:OP2	2.13	0.80
26:A:2159:G:O2'	26:A:2160:C:O4'	1.99	0.80
7:g:60:GLU:O	7:g:64:VAL:HG23	1.82	0.80
26:A:1857:G:O2'	26:A:1885:A:N6	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:12:U:O2'	26:A:13:A:O5'	2.01	0.79
25:z:75:ARG:NH2	25:z:200:ILE:O	2.16	0.78
50:1:51:ALA:O	50:1:55:THR:HG23	1.83	0.78
1:a:97:G:O2'	1:a:98:A:OP2	2.01	0.78
26:A:1064:C:O2'	26:A:1065:U:O5'	2.01	0.78
27:B:50:A:O2'	27:B:51:G:O4'	2.01	0.78
26:A:1046:A:O2'	26:A:1047:G:OP2	2.01	0.78
6:f:15:SER:OG	6:f:58:HIS:ND1	2.17	0.78
34:J:109:ILE:O	34:J:113:LYS:N	2.16	0.77
32:G:137:ASP:OD2	32:G:140:VAL:HG23	1.85	0.77
23:w:17:G:HO2'	23:w:57:G:H1	1.33	0.76
27:B:8:C:HO2'	27:B:9:G:P	2.08	0.76
26:A:652:U:OP1	26:A:654:A:N6	2.18	0.76
26:A:1417:C:O2'	26:A:1587:G:O2'	2.04	0.75
5:e:72:ILE:HD13	5:e:145:GLU:HG3	1.69	0.75
30:E:106:LYS:NZ	30:E:201:ALA:OXT	2.18	0.75
6:f:22:ILE:O	6:f:26:THR:HG23	1.86	0.75
35:L:125:TYR:OH	35:L:132:HIS:NE2	2.19	0.75
26:A:546:U:OP2	26:A:548:G:N2	2.19	0.75
1:a:201:G:O2'	1:a:469:C:O2'	2.01	0.75
9:i:55:VAL:CG1	9:i:94:LEU:HD21	2.17	0.74
9:i:21:ILE:HG22	9:i:63:LEU:HD22	1.66	0.74
1:a:1448:C:O2'	1:a:1449:C:O5'	2.04	0.74
26:A:2027:G:H1	26:A:2036:C:H5	1.34	0.74
47:X:11:GLU:HG3	47:X:16:ALA:HB1	1.71	0.73
30:E:149:ILE:HD13	30:E:175:ILE:HD11	1.69	0.73
26:A:1361:G:N7	63:A:3903:HOH:O	2.20	0.73
23:w:17:G:HO2'	23:w:57:G:N2	1.87	0.73
1:a:673:A:O2'	1:a:674:G:OP1	2.07	0.72
1:a:1124:G:N2	1:a:1125:U:O4	2.18	0.72
26:A:2697:G:N7	63:A:3905:HOH:O	2.21	0.72
1:a:652:U:O2'	1:a:653:U:OP2	2.08	0.72
2:b:77:SER:OG	2:b:78:GLU:OE1	2.07	0.72
16:p:48:GLU:OE2	16:p:51:ARG:NE	2.23	0.72
26:A:1416:G:O2'	26:A:1417:C:OP2	2.06	0.72
1:a:677:U:H3	1:a:713:G:H22	1.37	0.71
47:X:40:ILE:HD12	47:X:42:LEU:HD21	1.72	0.71
1:a:673:A:H2'	1:a:674:G:C8	2.24	0.71
26:A:1721:G:O2'	26:A:1739:A:N6	2.23	0.71
6:f:73:GLU:O	6:f:77:THR:HG23	1.91	0.71
16:p:1:MET:HE2	16:p:66:THR:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:54:ASP:OD1	13:m:57:ARG:NH2	2.24	0.71
50:1:9:LYS:O	50:1:60:LYS:NZ	2.24	0.71
26:A:624:C:O2'	26:A:625:G:O5'	2.09	0.70
26:A:2489:U:O2'	26:A:2490:G:OP1	2.09	0.70
57:8:16:ILE:CD1	57:8:25:VAL:HG22	2.22	0.70
26:A:2189:U:O2'	26:A:2190:G:O5'	2.09	0.70
26:A:2117:A:O2'	26:A:2119:A:OP1	2.07	0.70
2:b:111:ILE:HD13	2:b:148:LEU:HD13	1.74	0.70
26:A:1729:U:O2'	26:A:1730:C:OP2	2.08	0.70
1:a:664:G:H22	1:a:741:G:H1	1.40	0.69
26:A:145:C:O2'	26:A:146:A:OP2	2.11	0.69
26:A:2189:U:HO2'	26:A:2190:G:C5'	2.05	0.69
1:a:28:A:O2'	1:a:296:U:OP1	2.08	0.69
26:A:1897:G:N7	63:A:3910:HOH:O	2.25	0.69
1:a:1312:G:OP2	52:3:63:ARG:NH1	2.26	0.69
9:i:84:THR:HG22	9:i:88:MET:HE2	1.75	0.69
26:A:1084:A:HO2'	26:A:1085:A:P	2.16	0.68
44:U:59:GLU:CG	44:U:66:ILE:HD11	2.24	0.68
9:i:55:VAL:HG11	9:i:94:LEU:HD21	1.76	0.68
10:j:26:VAL:HG23	10:j:36:VAL:HG11	1.75	0.68
44:U:4:ILE:HG12	44:U:106:VAL:HG22	1.74	0.68
11:k:93:ARG:NH2	11:k:112:ASP:OD1	2.24	0.67
26:A:534:U:O2'	42:S:49:ASP:OD2	2.05	0.67
1:a:343:U:O2'	1:a:346:G:O6	2.11	0.67
26:A:2116:G:N2	26:A:2163:A:OP2	2.28	0.67
26:A:1085:A:O2'	26:A:1086:A:O4'	2.07	0.67
26:A:627:A:H61	26:A:637:A:H5''	1.61	0.66
26:A:1064:C:HO2'	26:A:1065:U:P	2.16	0.66
30:E:176:ASP:OD1	30:E:179:SER:OG	2.12	0.66
2:b:213:TYR:O	2:b:217:VAL:HG23	1.95	0.66
3:c:75:ILE:HD12	3:c:75:ILE:H	1.60	0.66
9:i:85:ARG:HA	9:i:88:MET:HE3	1.77	0.66
26:A:2134:A:H1'	26:A:2159:G:H21	1.61	0.66
13:m:4:ILE:HD11	13:m:60:VAL:HG21	1.77	0.66
26:A:2453:A:H4'	26:A:2573:C:OP2	1.96	0.65
7:g:69:VAL:HG23	7:g:100:ALA:HB1	1.78	0.65
24:x:7:G:O2'	24:x:49:G:OP2	2.09	0.65
23:w:14:A:N1	23:w:21:A:O2'	2.30	0.65
1:a:1473:G:N7	63:a:3308:HOH:O	2.30	0.64
18:r:32:TYR:CG	18:r:55:LEU:HD21	2.31	0.64
2:b:6:MET:HE3	2:b:43:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:154:MET:HE3	2:b:158:PRO:HD3	1.79	0.64
1:a:1086:U:H3	1:a:1099:G:H22	1.45	0.64
26:A:2004:G:N7	63:A:3919:HOH:O	2.30	0.64
28:C:79:GLU:OE2	28:C:101:ARG:NE	2.29	0.64
19:s:10:PHE:O	19:s:39:THR:HG22	1.98	0.64
30:E:149:ILE:HD13	30:E:175:ILE:CD1	2.28	0.63
19:s:12:ASP:OD2	19:s:35:SER:OG	2.13	0.62
26:A:1082:U:H2'	26:A:1083:U:O4'	1.98	0.62
1:a:160:A:H2'	1:a:161:A:O4'	2.00	0.62
3:c:111:LEU:O	3:c:204:LYS:NZ	2.31	0.61
1:a:1530:G:O6	21:u:46:LYS:NZ	2.32	0.61
10:j:10:LEU:HD21	10:j:25:ILE:HD12	1.82	0.61
33:H:9:VAL:O	33:H:9:VAL:HG23	2.01	0.61
29:D:25:THR:HG22	29:D:191:GLY:O	2.00	0.61
36:M:121:GLU:OE2	41:R:65:SER:OG	2.17	0.61
8:h:42:GLU:OE1	8:h:43:GLU:OE1	2.18	0.61
1:a:187:G:N2	1:a:190:A:OP2	2.29	0.61
1:a:1042:A:H2'	1:a:1043:G:C8	2.36	0.61
34:J:101:ILE:N	34:J:139:VAL:O	2.33	0.61
3:c:58:GLU:OE1	3:c:65:ARG:NH1	2.33	0.61
23:w:17:G:HO2'	23:w:57:G:H22	1.47	0.61
26:A:1110:G:O2'	26:A:1111:A:O5'	2.18	0.61
26:A:2128:G:H21	26:A:2173:A:H4'	1.66	0.60
35:L:125:TYR:HH	35:L:132:HIS:CD2	2.19	0.60
46:W:98:SER:OG	46:W:98:SER:O	2.20	0.60
1:a:769:G:H4'	1:a:1513:A:H4'	1.84	0.60
19:s:50:ALA:HB1	19:s:57:HIS:HB3	1.84	0.60
26:A:568:U:H1'	26:A:2030:6MZ:H9C1	1.83	0.60
26:A:2159:G:O2'	26:A:2160:C:O5'	2.18	0.60
35:L:3:THR:HG21	42:S:61:TRP:HE1	1.66	0.60
30:E:171:ASP:OD2	30:E:173:THR:HG22	2.01	0.60
1:a:1255:G:O2'	1:a:1258:G:N3	2.34	0.60
25:z:93:ILE:HG12	25:z:122:LEU:HD22	1.84	0.59
28:C:107:PRO:HD2	28:C:110:LEU:HD22	1.82	0.59
31:F:102:ARG:NH1	52:3:25:ARG:O	2.34	0.59
26:A:278:A:N1	26:A:361:G:O2'	2.18	0.59
25:z:104:LEU:HD22	25:z:120:ILE:HD11	1.84	0.59
26:A:2757:A:O2'	26:A:2758:A:O5'	2.20	0.59
26:A:483:A:O2'	46:W:57:GLY:N	2.33	0.59
1:a:1088:G:H5'	21:u:70:LEU:HD22	1.85	0.59
26:A:144:A:O2'	26:A:145:C:OP2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:7:ARG:HA	2:b:10:LEU:HD12	1.85	0.58
1:a:411:A:C4	1:a:413:G:H1'	2.37	0.58
35:L:91:GLU:O	35:L:95:ARG:HD3	2.03	0.58
5:e:36:LEU:HD22	5:e:134:ILE:HD13	1.84	0.58
9:i:84:THR:HG22	9:i:88:MET:CE	2.33	0.58
27:B:75:G:HO2'	47:X:88:HIS:HE2	1.50	0.58
1:a:1376:U:O4	7:g:10:ARG:NH2	2.35	0.57
25:z:379:GLU:O	25:z:381:GLY:N	2.37	0.57
26:A:2065:C:H4'	26:A:2251:OMG:HM22	1.86	0.57
1:a:1391:U:H2'	1:a:1392:G:C8	2.40	0.57
9:i:55:VAL:HG13	9:i:94:LEU:HD21	1.86	0.57
26:A:1939:5MU:OP1	26:A:2604:PSU:O2'	2.21	0.57
26:A:2052:A:H4'	29:D:148:GLN:O	2.04	0.57
1:a:131:A:O2'	1:a:262:A:N3	2.30	0.57
18:r:62:ALA:CB	18:r:68:LEU:HD12	2.33	0.57
26:A:2123:G:O2'	26:A:2124:G:N7	2.36	0.57
4:d:27:ALA:O	4:d:30:THR:OG1	2.21	0.57
18:r:62:ALA:HB3	18:r:68:LEU:HD12	1.86	0.57
26:A:2291:U:H2'	26:A:2292:U:C6	2.39	0.57
25:z:147:LEU:HD13	25:z:172:ARG:HD2	1.87	0.57
26:A:1534:U:O2'	26:A:1537:G:O6	2.07	0.57
41:R:100:LEU:HD11	41:R:110:ILE:HD11	1.85	0.57
24:x:16:C:OP1	24:x:17:C:N4	2.38	0.57
26:A:1067:A:H2'	26:A:1068:G:O4'	2.05	0.57
26:A:2547:A:H2'	26:A:2548:U:C6	2.40	0.57
51:2:45:ARG:NH1	51:2:59:GLU:OE2	2.37	0.56
1:a:1225:A:H2'	1:a:1226:C:C5	2.40	0.56
23:w:65:U:H4'	25:z:330:GLN:NE2	2.20	0.56
25:z:342:ILE:HG23	25:z:359:MET:HE1	1.86	0.56
26:A:784:G:H5'	26:A:785:G:OP1	2.05	0.56
25:z:74:THR:OG1	25:z:197:ASP:OD2	2.22	0.56
30:E:1:MET:N	30:E:14:VAL:O	2.39	0.56
1:a:1279:G:OP2	10:j:11:LYS:NZ	2.30	0.56
9:i:55:VAL:HG21	9:i:87:LEU:HD13	1.87	0.56
25:z:14:ASN:O	25:z:100:ASP:N	2.38	0.56
26:A:1061:U:H3'	26:A:1062:G:C5'	2.36	0.56
1:a:31:G:O2'	1:a:48:C:N4	2.39	0.56
1:a:823:C:HO2'	8:h:2:SER:N	2.03	0.56
26:A:2811:G:H1	26:A:2889:C:H5	1.53	0.56
26:A:2857:G:N2	26:A:2860:A:OP2	2.31	0.56
23:w:17:G:O2'	23:w:57:G:N2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:639:U:H2'	26:A:640:C:C6	2.40	0.56
1:a:333:U:OP1	20:t:2:ALA:N	2.39	0.56
26:A:271:G:O2'	26:A:272:A:OP2	2.19	0.56
55:6:45:SER:O	55:6:46:LYS:CB	2.54	0.56
26:A:2163:A:H2'	26:A:2164:C:O4'	2.06	0.55
13:m:39:ILE:HD11	13:m:52:GLN:HB3	1.88	0.55
26:A:642:U:O2'	26:A:644:A:N7	2.33	0.55
14:n:37:SER:OG	14:n:39:GLU:OE1	2.24	0.55
44:U:72:THR:HG21	44:U:108:SER:OG	2.07	0.55
1:a:371:A:H2'	1:a:372:C:O4'	2.07	0.55
26:A:191:A:H2'	26:A:192:C:C6	2.42	0.55
3:c:77:ILE:HA	3:c:84:VAL:HG13	1.89	0.55
13:m:83:LEU:HD11	19:s:65:GLU:HB3	1.89	0.55
26:A:282:A:N6	26:A:359:G:O6	2.40	0.55
26:A:2192:U:H2'	26:A:2193:G:O4'	2.07	0.55
3:c:31:ASP:OD2	14:n:65:ARG:NH2	2.40	0.55
7:g:130:ASN:HA	7:g:135:VAL:HG21	1.88	0.55
25:z:218:VAL:HG22	25:z:228:VAL:HG12	1.89	0.55
34:J:37:GLU:O	34:J:41:ALA:N	2.40	0.55
10:j:66:GLU:HB2	14:n:99:ALA:HB2	1.89	0.54
26:A:428:A:C2'	26:A:429:A:H5'	2.36	0.54
1:a:545:C:OP1	4:d:58:LYS:NZ	2.41	0.54
2:b:86:SER:O	2:b:222:ARG:NH1	2.40	0.54
26:A:1028:A:N6	26:A:1125:G:H2'	2.22	0.54
3:c:11:ARG:NH2	3:c:177:THR:O	2.40	0.54
26:A:849:A:H2'	26:A:850:U:C6	2.42	0.54
26:A:1790:C:H2'	26:A:1791:A:C5	2.42	0.54
1:a:414:A:O2'	1:a:415:A:OP1	2.25	0.54
26:A:58:G:O2'	26:A:73:A:N1	2.41	0.54
1:a:946:A:H2'	1:a:947:G:C8	2.43	0.54
26:A:279:A:C6	26:A:362:A:H4'	2.42	0.54
26:A:930:G:H1'	51:2:25:LEU:HD11	1.90	0.54
26:A:2303:G:O2'	26:A:2304:G:OP2	2.26	0.54
27:B:9:G:O2'	27:B:10:G:P	2.66	0.54
1:a:17:U:H2'	1:a:18:C:C6	2.43	0.53
1:a:977:A:O2'	1:a:979:C:OP2	2.23	0.53
26:A:76:C:H1'	50:1:55:THR:HG21	1.90	0.53
24:x:21:A:H61	24:x:46:G:H2'	1.73	0.53
26:A:276:U:O2	26:A:277:G:N2	2.41	0.53
26:A:428:A:O2'	26:A:429:A:H5'	2.08	0.53
26:A:2128:G:H21	26:A:2173:A:C4'	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:404:G:O2'	1:a:498:A:N1	2.41	0.53
26:A:362:A:H3'	26:A:363:G:H8	1.73	0.53
1:a:579:A:H2'	1:a:580:C:C6	2.43	0.53
1:a:1492:A:O2'	1:a:1493:A:OP2	2.18	0.53
26:A:147:C:O2'	26:A:148:U:OP2	2.24	0.53
26:A:1583:A:O2'	26:A:1585:C:N4	2.42	0.53
4:d:58:LYS:HA	4:d:200:ILE:CD1	2.39	0.53
25:z:226:THR:OG1	25:z:282:ILE:O	2.24	0.53
1:a:492:C:H2'	1:a:493:A:C8	2.44	0.52
26:A:75:G:H22	26:A:111:A:H2	1.56	0.52
26:A:1419:A:O2'	26:A:1421:G:N7	2.39	0.52
26:A:2902:C:H3'	26:A:2903:U:H5''	1.91	0.52
57:8:16:ILE:HD13	57:8:25:VAL:HG22	1.91	0.52
11:k:82:LEU:HD12	11:k:105:PHE:CG	2.44	0.52
26:A:1542:U:H2'	26:A:1543:G:O4'	2.09	0.52
26:A:2243:U:H2'	26:A:2244:U:C6	2.44	0.52
6:f:10:VAL:HG12	6:f:84:VAL:HA	1.90	0.52
26:A:2328:A:H2'	26:A:2329:U:C6	2.45	0.52
24:x:31:G:C8	24:x:32:5MC:HM53	2.44	0.52
26:A:1065:U:H2'	26:A:1066:U:O4'	2.08	0.52
36:M:108:ARG:HH12	36:M:122:VAL:HG11	1.74	0.52
39:P:86:ARG:NH2	39:P:117:ASP:OD1	2.41	0.52
26:A:72:U:N3	50:1:55:THR:HG22	2.24	0.52
26:A:644:A:H2'	26:A:645:C:O4'	2.10	0.52
26:A:1508:A:H2'	26:A:1509:A:O4'	2.10	0.52
26:A:1666:G:OP1	36:M:66:LYS:NZ	2.30	0.52
30:E:108:ILE:HG23	37:N:1:MET:HE1	1.91	0.52
1:a:276:G:OP1	17:q:14:SER:OG	2.18	0.52
28:C:39:LYS:NZ	28:C:58:HIS:O	2.41	0.52
42:S:111:GLU:OE1	42:S:111:GLU:HA	2.09	0.52
46:W:18:ASP:OD1	46:W:21:LYS:NZ	2.33	0.52
1:a:1062:U:H2'	1:a:1063:C:C6	2.45	0.52
4:d:198:HIS:ND1	4:d:202:GLU:OE2	2.43	0.52
5:e:76:LEU:HD23	5:e:76:LEU:H	1.74	0.52
26:A:1046:A:HO2'	26:A:1047:G:P	2.29	0.52
26:A:1:G:H2'	26:A:2:G:C8	2.45	0.52
3:c:127:ARG:HH11	3:c:127:ARG:HG2	1.75	0.52
1:a:107:G:O6	20:t:10:ARG:HD2	2.10	0.51
25:z:260:GLU:HG2	25:z:265:LEU:HA	1.93	0.51
25:z:320:HIS:HD2	25:z:321:THR:HG23	1.75	0.51
39:P:8:ARG:NH1	39:P:43:GLU:OE2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1820:U:C6	28:C:201:MET:HE3	2.45	0.51
38:O:111:GLU:CD	38:O:111:GLU:H	2.19	0.51
40:Q:52:SER:OG	40:Q:54:VAL:HG22	2.09	0.51
10:j:25:ILE:O	10:j:28:THR:HG22	2.11	0.51
1:a:662:U:O2'	1:a:836:G:OP1	2.29	0.51
26:A:1141:U:H4'	26:A:1142:A:O4'	2.11	0.51
29:D:156:PHE:CE1	35:L:81:ILE:HD13	2.46	0.51
1:a:613:C:H2'	1:a:614:C:C6	2.46	0.51
22:v:24:A:N3	22:v:24:A:O2'	2.31	0.51
26:A:1932:A:H2'	26:A:1933:G:O4'	2.10	0.51
30:E:46:GLN:O	30:E:88:ARG:NH2	2.43	0.51
1:a:532:A:N6	1:a:1206:G:O2'	2.41	0.51
6:f:39:LEU:HD13	6:f:39:LEU:C	2.36	0.51
15:o:35:GLN:NE2	15:o:35:GLN:HA	2.26	0.51
25:z:98:GLN:O	25:z:231:ARG:NH1	2.44	0.51
4:d:105:MET:HE1	4:d:143:VAL:HB	1.93	0.51
18:r:71:THR:HG22	18:r:72:ASP:N	2.25	0.51
1:a:714:G:H2'	1:a:715:A:C8	2.46	0.51
26:A:2124:G:O6	26:A:2125:G:N2	2.44	0.51
26:A:554:U:H2'	26:A:555:G:O4'	2.11	0.51
26:A:588:U:H2'	26:A:589:U:C6	2.46	0.51
32:G:42:GLU:OE1	32:G:55:ARG:NE	2.44	0.51
40:Q:35:ILE:HG23	40:Q:74:VAL:HG21	1.92	0.51
48:Y:11:ARG:O	48:Y:14:ARG:NH2	2.37	0.51
14:n:88:ALA:HB2	14:n:96:LEU:HD23	1.92	0.51
26:A:856:G:H2'	26:A:857:G:C8	2.45	0.51
27:B:9:G:O2'	27:B:10:G:OP1	2.28	0.51
25:z:248:ILE:HD12	25:z:248:ILE:H	1.75	0.50
26:A:594:U:H2'	26:A:595:C:C6	2.45	0.50
26:A:2532:G:N2	26:A:2663:G:O2'	2.43	0.50
1:a:97:G:O2'	1:a:98:A:P	2.69	0.50
26:A:624:C:O2'	26:A:625:G:P	2.69	0.50
26:A:1327:A:H2'	26:A:1328:A:O4'	2.12	0.50
42:S:58:ARG:HA	42:S:61:TRP:CE3	2.46	0.50
1:a:4:U:H2'	1:a:5:U:H5''	1.93	0.50
2:b:196:VAL:HG23	2:b:199:VAL:HG22	1.94	0.50
26:A:2115:G:O2'	26:A:2117:A:N6	2.45	0.50
37:N:82:LEU:HD22	37:N:90:VAL:HG21	1.94	0.50
46:W:96:PHE:O	46:W:100:SER:N	2.45	0.50
1:a:337:G:H2'	1:a:338:A:C8	2.47	0.50
1:a:1530:G:H2'	1:a:1531:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:W:18:ASP:OD2	46:W:39:ILE:O	2.30	0.50
1:a:405:U:O4	4:d:2:ALA:N	2.45	0.50
2:b:109:GLN:OE1	2:b:109:GLN:HA	2.10	0.50
13:m:48:LEU:HD23	13:m:53:ILE:HG12	1.93	0.50
16:p:51:ARG:O	16:p:52:LEU:HD23	2.12	0.50
26:A:84:A:N1	26:A:98:G:O2'	2.40	0.50
26:A:226:A:N1	26:A:418:C:O2'	2.44	0.50
26:A:243:U:OP1	56:7:6:THR:HG21	2.10	0.50
26:A:1073:A:C6	26:A:1074:G:H1'	2.47	0.50
26:A:1083:U:H2'	26:A:1084:A:H3'	1.93	0.50
26:A:1418:G:O2'	26:A:1579:A:N6	2.45	0.50
1:a:789:U:O2'	1:a:791:G:N7	2.44	0.50
13:m:11:ASP:OD1	13:m:45:ILE:HD11	2.12	0.50
23:w:50:A:O2'	23:w:51:G:P	2.69	0.50
23:w:74:C:O2	61:z:402:MQH:C51	2.60	0.50
26:A:2335:A:OP1	40:Q:13:ARG:NE	2.41	0.50
31:F:44:ILE:HA	31:F:83:TYR:CE1	2.47	0.50
25:z:265:LEU:O	25:z:266:LEU:O	2.30	0.50
26:A:2188:U:H2'	26:A:2189:U:C1'	2.42	0.50
26:A:2304:G:O5'	31:F:121:SER:OG	2.30	0.50
26:A:2788:C:H2'	26:A:2789:C:C6	2.47	0.50
39:P:32:GLU:HG2	39:P:115:LEU:HD12	1.92	0.50
39:P:56:LYS:NZ	39:P:90:ARG:O	2.43	0.50
1:a:142:G:O2'	1:a:196:A:N1	2.38	0.50
1:a:986:U:H2'	1:a:987:G:O4'	2.12	0.50
3:c:50:ALA:O	3:c:70:THR:OG1	2.30	0.50
6:f:96:VAL:O	6:f:98:GLU:N	2.40	0.50
1:a:1486:G:H2'	1:a:1487:G:O4'	2.12	0.49
12:l:79:VAL:O	12:l:103:ASP:HB2	2.12	0.49
5:e:142:ASP:O	5:e:146:ASN:ND2	2.45	0.49
28:C:29:PRO:HG2	28:C:34:LEU:HD11	1.95	0.49
4:d:57:GLU:OE2	4:d:60:LYS:NZ	2.46	0.49
11:k:87:LYS:HB3	11:k:113:VAL:HG23	1.94	0.49
21:u:7:ARG:N	21:u:10:GLU:OE2	2.45	0.49
26:A:2025:C:H2'	26:A:2026:U:C6	2.47	0.49
1:a:555:U:H2'	1:a:556:C:C6	2.47	0.49
4:d:188:ARG:NH2	4:d:195:ILE:O	2.46	0.49
25:z:5:LYS:HE3	25:z:265:LEU:HD11	1.95	0.49
26:A:593:U:H2'	26:A:594:U:C6	2.47	0.49
26:A:1338:G:O2'	26:A:1393:A:N1	2.36	0.49
26:A:2191:A:HO2'	26:A:2192:U:P	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:134:GLU:OE2	31:F:134:GLU:N	2.45	0.49
1:a:1457:G:H5'	20:t:30:THR:HG21	1.94	0.49
6:f:16:GLU:OE1	6:f:16:GLU:N	2.39	0.49
26:A:277:G:H5'	26:A:278:A:OP1	2.12	0.49
26:A:995:C:O2	35:L:3:THR:HG22	2.12	0.49
26:A:1778:U:H2'	26:A:1784:A:N6	2.28	0.49
27:B:3:C:HO2'	27:B:4:C:P	2.36	0.49
38:O:53:MET:HE1	38:O:103:TYR:CG	2.47	0.49
1:a:138:G:O2'	1:a:139:A:H5'	2.13	0.49
1:a:1356:G:H2'	1:a:1357:A:C8	2.48	0.49
2:b:6:MET:HE1	2:b:44:GLU:HG3	1.94	0.49
26:A:2480:C:H2'	26:A:2481:G:H5'	1.94	0.49
31:F:147:ASP:OD2	31:F:147:ASP:N	2.44	0.49
1:a:1060:U:OP1	14:n:85:ARG:NH2	2.41	0.49
26:A:340:A:H2'	26:A:341:C:O4'	2.13	0.49
26:A:460:A:H2'	26:A:461:C:O4'	2.13	0.49
26:A:801:G:OP1	63:A:3901:HOH:O	2.20	0.49
29:D:25:THR:HG21	29:D:193:VAL:HG13	1.94	0.49
1:a:1004:A:O2'	1:a:1036:A:N6	2.45	0.49
1:a:1018:G:H2'	1:a:1019:A:O4'	2.13	0.49
1:a:1435:G:H2'	1:a:1436:U:C6	2.48	0.49
25:z:328:ARG:HD3	25:z:341:THR:HG23	1.95	0.49
1:a:414:A:HO2'	1:a:415:A:P	2.35	0.49
1:a:1256:A:O2'	1:a:1278:G:O6	2.13	0.49
10:j:47:GLU:HG2	10:j:49:PHE:CZ	2.47	0.49
26:A:635:C:OP2	37:N:126:ARG:NH1	2.45	0.49
26:A:813:U:H2'	26:A:814:C:C6	2.48	0.49
26:A:1009:A:N3	26:A:1153:C:O2'	2.44	0.49
56:7:17:THR:HG21	56:7:49:MET:HE1	1.94	0.49
1:a:8:A:N6	4:d:202:GLU:O	2.45	0.49
1:a:857:C:H2'	1:a:858:G:O4'	2.13	0.49
1:a:1004:A:H2'	1:a:1005:A:O4'	2.13	0.49
6:f:18:VAL:N	6:f:19:PRO:CD	2.76	0.49
14:n:79:LEU:HB2	14:n:84:VAL:HG23	1.95	0.49
26:A:811:U:OP1	63:A:3902:HOH:O	2.20	0.49
1:a:244:U:O4	1:a:906:A:H1'	2.13	0.48
1:a:413:G:O2'	1:a:428:G:N2	2.45	0.48
1:a:413:G:C2'	1:a:414:A:OP2	2.61	0.48
28:C:20:VAL:HG23	28:C:20:VAL:O	2.13	0.48
1:a:713:G:H2'	1:a:714:G:C8	2.48	0.48
1:a:1071:C:H2'	1:a:1072:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1071:C:H2'	1:a:1072:G:H8	1.78	0.48
1:a:1448:C:HO2'	1:a:1449:C:P	2.34	0.48
2:b:160:ALA:HB1	2:b:184:PHE:HE2	1.77	0.48
15:o:88:ARG:NH2	26:A:716:A:OP2	2.43	0.48
26:A:2064:C:H2'	26:A:2065:C:C6	2.48	0.48
1:a:147:G:H2'	1:a:148:G:C8	2.48	0.48
1:a:1394:A:N1	1:a:1500:A:O2'	2.41	0.48
23:w:64:U:H4'	25:z:380:GLY:HA2	1.95	0.48
25:z:348:VAL:O	25:z:348:VAL:HG22	2.13	0.48
26:A:2327:A:H2'	26:A:2328:A:C8	2.48	0.48
1:a:1179:A:H2'	1:a:1180:A:O4'	2.13	0.48
2:b:76:ALA:O	2:b:80:VAL:HG23	2.13	0.48
7:g:152:ALA:O	7:g:153:HIS:HB2	2.13	0.48
1:a:346:G:OP1	41:R:39:ARG:NH1	2.46	0.48
1:a:662:U:H2'	1:a:663:A:C8	2.49	0.48
9:i:30:ILE:N	9:i:33:ARG:O	2.40	0.48
13:m:45:ILE:C	13:m:45:ILE:HD12	2.38	0.48
26:A:624:C:O2'	26:A:625:G:H8	1.97	0.48
26:A:2095:A:OP1	33:H:11:ASN:ND2	2.41	0.48
32:G:155:GLU:OE2	32:G:158:LYS:N	2.41	0.48
44:U:66:ILE:N	44:U:66:ILE:HD13	2.29	0.48
53:4:43:ILE:HG22	53:4:49:TYR:HB2	1.95	0.48
1:a:269:C:H2'	1:a:270:A:C8	2.49	0.48
1:a:1042:A:O2'	1:a:1043:G:O5'	2.31	0.48
26:A:1820:U:N1	28:C:201:MET:HE3	2.27	0.48
26:A:2603:G:N7	63:A:3936:HOH:O	2.35	0.48
26:A:2820:A:C8	39:P:4:ARG:HD2	2.48	0.48
29:D:25:THR:HG23	29:D:189:VAL:CG2	2.44	0.48
46:W:49:VAL:O	46:W:52:LEU:O	2.31	0.48
48:Y:31:VAL:HB	48:Y:35:SER:OG	2.13	0.48
6:f:32:ALA:CB	6:f:70:VAL:HG11	2.44	0.48
25:z:335:THR:O	25:z:335:THR:HG22	2.13	0.48
41:R:6:LYS:O	41:R:10:GLN:HG2	2.14	0.48
1:a:945:G:C2	1:a:946:A:C8	3.01	0.48
9:i:51:PRO:O	9:i:55:VAL:HG23	2.13	0.48
15:o:40:GLN:HA	15:o:40:GLN:NE2	2.27	0.48
26:A:871:U:H2'	26:A:872:U:C6	2.49	0.48
26:A:1211:C:H3'	26:A:1212:G:H5'	1.96	0.48
26:A:1386:C:H2'	26:A:1387:A:C8	2.49	0.48
26:A:1848:A:H2'	26:A:1849:G:O4'	2.13	0.48
26:A:2636:C:HO2'	29:D:45:TYR:HH	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:52:LEU:HD21	9:i:63:LEU:HD11	1.96	0.48
19:s:22:ALA:HB2	19:s:31:LEU:HD11	1.95	0.48
26:A:2159:G:H2'	26:A:2160:C:C6	2.49	0.48
26:A:2273:A:H2'	26:A:2274:A:C8	2.49	0.48
1:a:414:A:O2'	1:a:415:A:P	2.72	0.47
2:b:78:GLU:OE1	2:b:78:GLU:N	2.45	0.47
12:l:110:ARG:HB3	12:l:119:VAL:HG21	1.95	0.47
13:m:11:ASP:HA	13:m:45:ILE:HD11	1.96	0.47
26:A:742:A:H2'	26:A:743:A:C8	2.49	0.47
33:H:5:LEU:HD13	33:H:9:VAL:HG22	1.96	0.47
33:H:9:VAL:O	33:H:9:VAL:CG2	2.62	0.47
38:O:136:MET:HE1	47:X:74:ALA:O	2.14	0.47
26:A:1069:A:H5'	26:A:1070:A:OP1	2.13	0.47
26:A:2191:A:O2'	26:A:2192:U:O5'	2.32	0.47
52:3:30:HIS:ND1	52:3:31:ASP:O	2.45	0.47
1:a:3:A:N1	1:a:628:G:O2'	2.47	0.47
12:l:66:TYR:HB2	12:l:87:VAL:HG21	1.95	0.47
26:A:1297:C:O2'	26:A:1302:A:N1	2.45	0.47
26:A:2191:A:C2'	26:A:2192:U:O5'	2.61	0.47
1:a:502:A:H2'	1:a:503:C:O4'	2.14	0.47
1:a:522:C:H41	12:l:50:ARG:NH2	2.12	0.47
1:a:585:G:OP1	17:q:39:LYS:HE2	2.15	0.47
4:d:35:GLU:HA	4:d:35:GLU:OE1	2.15	0.47
26:A:876:C:H2'	26:A:877:A:O4'	2.15	0.47
26:A:1434:A:H2'	26:A:1435:G:C8	2.49	0.47
6:f:29:ILE:N	6:f:29:ILE:HD13	2.29	0.47
26:A:2159:G:H2'	26:A:2160:C:C5	2.49	0.47
45:V:4:GLU:OE2	50:1:23:ARG:NH1	2.46	0.47
46:W:46:GLN:OE1	46:W:46:GLN:HA	2.14	0.47
52:3:13:THR:N	52:3:31:ASP:OD1	2.36	0.47
26:A:277:G:C5'	26:A:278:A:OP1	2.62	0.47
26:A:914:G:H5'	26:A:915:C:OP2	2.14	0.47
26:A:1370:C:H2'	26:A:1371:G:O4'	2.14	0.47
27:B:3:C:O2'	27:B:4:C:P	2.73	0.47
44:U:59:GLU:HG3	44:U:66:ILE:HD11	1.96	0.47
1:a:208:U:O2'	1:a:211:G:N1	2.48	0.47
1:a:539:A:H2'	1:a:540:G:C8	2.50	0.47
9:i:55:VAL:HG13	9:i:94:LEU:HD11	1.97	0.47
26:A:791:C:OP2	63:A:3904:HOH:O	2.20	0.47
26:A:1019:U:O2'	26:A:1021:A:N7	2.45	0.47
26:A:1045:C:H5'	26:A:1046:A:H5'	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1478:G:H1	26:A:1513:U:H3	1.63	0.47
26:A:1539:U:C2	26:A:1540:G:C8	3.03	0.47
42:S:76:TYR:CZ	42:S:80:ILE:HG13	2.49	0.47
9:i:39:PHE:O	9:i:45:ARG:NE	2.48	0.47
13:m:33:ILE:HD13	13:m:60:VAL:HG22	1.97	0.47
25:z:314:LYS:NZ	25:z:318:GLY:O	2.48	0.47
26:A:279:A:N1	26:A:362:A:H4'	2.29	0.47
26:A:2635:A:O2'	29:D:81:GLU:OE2	2.20	0.47
3:c:12:LEU:O	3:c:16:LYS:O	2.33	0.47
5:e:44:GLY:O	5:e:74:VAL:N	2.46	0.47
26:A:76:C:O2'	50:1:55:THR:HG21	2.14	0.47
26:A:493:G:H2'	26:A:494:G:O4'	2.15	0.47
26:A:1128:G:C8	26:A:2490:G:OP1	2.68	0.47
26:A:2052:A:O2'	29:D:148:GLN:O	2.31	0.47
31:F:135:GLN:HG2	31:F:141:ILE:CD1	2.45	0.47
1:a:1211:U:HO2'	1:a:1212:U:P	2.26	0.47
6:f:54:LEU:HD12	6:f:54:LEU:O	2.14	0.47
25:z:305:PHE:HB2	25:z:389:VAL:HG13	1.95	0.47
26:A:2123:G:H4'	26:A:2124:G:OP1	2.15	0.47
26:A:2303:G:O2'	26:A:2304:G:P	2.73	0.47
27:B:106:G:H2'	27:B:107:G:O4'	2.14	0.47
31:F:58:ALA:O	31:F:62:GLY:N	2.48	0.47
54:5:11:LEU:HB3	54:5:49:TYR:HB3	1.96	0.47
2:b:187:VAL:HG21	2:b:199:VAL:HG13	1.96	0.46
7:g:113:ASP:OD1	7:g:113:ASP:N	2.47	0.46
15:o:80:GLN:O	15:o:83:GLU:HG3	2.15	0.46
16:p:57:ILE:O	16:p:61:VAL:HG23	2.15	0.46
26:A:1820:U:C2	28:C:201:MET:HE3	2.50	0.46
26:A:2191:A:H2'	26:A:2192:U:C6	2.50	0.46
26:A:2552:OMU:HM23	26:A:2554:U:C6	2.50	0.46
35:L:10:THR:HG22	35:L:10:THR:O	2.15	0.46
46:W:35:ILE:HD13	46:W:64:ALA:HA	1.96	0.46
25:z:342:ILE:HD12	25:z:359:MET:CE	2.41	0.46
31:F:140:GLU:N	31:F:140:GLU:OE1	2.48	0.46
46:W:49:VAL:HB	46:W:52:LEU:O	2.14	0.46
1:a:207:C:H2'	1:a:208:U:H5'	1.96	0.46
1:a:320:A:H2'	1:a:321:A:O4'	2.15	0.46
1:a:922:G:H2'	1:a:923:A:C8	2.51	0.46
1:a:1032:G:H3'	1:a:1032:G:N3	2.29	0.46
11:k:86:VAL:HG21	11:k:97:ILE:HD11	1.97	0.46
11:k:94:GLU:CD	11:k:98:ARG:HE	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2279:G:O6	48:Y:14:ARG:HG3	2.16	0.46
26:A:2514:U:H2'	26:A:2515:C:C6	2.50	0.46
50:1:12:GLU:H	50:1:12:GLU:CD	2.23	0.46
52:3:35:ASP:OD1	52:3:35:ASP:N	2.49	0.46
1:a:33:A:H2'	1:a:34:C:C6	2.51	0.46
1:a:131:A:H2'	1:a:132:C:C6	2.50	0.46
1:a:266:G:H3'	17:q:69:LYS:HB2	1.96	0.46
1:a:344:A:H4'	1:a:345:C:OP2	2.14	0.46
4:d:99:ASP:OD1	4:d:99:ASP:N	2.49	0.46
25:z:240:GLY:N	25:z:256:CYS:O	2.45	0.46
26:A:223:A:N1	26:A:407:G:O2'	2.45	0.46
26:A:1469:A:H2'	26:A:1470:A:C8	2.51	0.46
26:A:1570:A:H2'	26:A:1571:A:C8	2.51	0.46
26:A:2258:C:O2'	26:A:2427:C:OP2	2.25	0.46
1:a:673:A:HO2'	1:a:674:G:P	2.34	0.46
1:a:920:U:H2'	1:a:921:U:C6	2.50	0.46
26:A:1526:C:H2'	26:A:1527:G:O4'	2.16	0.46
26:A:1563:U:H2'	26:A:1564:C:C6	2.50	0.46
26:A:2140:G:N2	26:A:2141:G:O6	2.48	0.46
26:A:2489:U:O2'	26:A:2490:G:H5'	2.15	0.46
29:D:25:THR:HG23	29:D:189:VAL:HG22	1.98	0.46
35:L:110:PRO:O	35:L:115:GLY:HA3	2.15	0.46
25:z:262:PHE:HD1	61:z:402:MQH:C22	2.27	0.46
26:A:391:A:H1'	26:A:411:G:O4'	2.16	0.46
26:A:1405:U:H2'	26:A:1406:U:C6	2.50	0.46
26:A:1437:C:H2'	26:A:1438:U:C6	2.50	0.46
26:A:1799:G:O2'	28:C:180:GLU:OE2	2.30	0.46
29:D:208:LYS:O	29:D:209:ALA:O	2.33	0.46
1:a:523:A:C2	12:l:88:LYS:HB3	2.50	0.46
14:n:89:MET:HE2	14:n:89:MET:CA	2.40	0.46
26:A:1361:G:H2'	26:A:1362:C:C6	2.51	0.46
26:A:2036:C:O2	26:A:2036:C:O4'	2.32	0.46
26:A:1433:A:H2'	26:A:1434:A:O4'	2.16	0.46
29:D:110:THR:CG2	29:D:202:ILE:HB	2.46	0.46
31:F:133:ARG:HG2	31:F:133:ARG:HH11	1.80	0.46
1:a:151:A:H2'	1:a:152:A:O4'	2.16	0.46
9:i:21:ILE:HG22	9:i:63:LEU:CD2	2.41	0.46
15:o:35:GLN:HA	15:o:35:GLN:HE21	1.80	0.46
23:w:75:C:OP1	61:z:402:MQH:N56	2.49	0.46
26:A:1607:C:H4'	26:A:1608:A:O5'	2.16	0.46
26:A:1746:A:H2'	26:A:1747:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2557:G:H2'	26:A:2558:C:C6	2.51	0.46
44:U:55:ILE:HG23	44:U:66:ILE:HD12	1.97	0.46
1:a:1441:A:H62	1:a:1461:G:H21	1.64	0.46
3:c:6:HIS:CG	14:n:89:MET:HB3	2.51	0.46
5:e:81:LEU:HD22	5:e:147:MET:HE1	1.98	0.46
26:A:717:C:O2	26:A:717:C:O4'	2.34	0.46
33:H:4:ILE:HG23	33:H:39:ALA:HB2	1.98	0.46
34:J:25:GLY:O	34:J:29:GLY:N	2.48	0.46
50:1:11:VAL:O	50:1:15:ASN:ND2	2.48	0.46
2:b:173:ILE:HD12	2:b:183:VAL:HG11	1.97	0.45
20:t:27:MET:HE3	20:t:27:MET:HB3	1.89	0.45
22:v:23:A:H4'	22:v:24:A:H5'	1.98	0.45
26:A:2189:U:O2'	26:A:2190:G:P	2.74	0.45
27:B:50:A:O2'	27:B:51:G:C5'	2.64	0.45
32:G:156:PRO:O	32:G:171:THR:HA	2.15	0.45
40:Q:76:LYS:O	40:Q:80:GLU:HG3	2.15	0.45
1:a:96:U:O2'	1:a:97:G:H2'	2.16	0.45
24:x:76:M3O:CG	26:A:2061:G:H22	2.28	0.45
26:A:548:G:H2'	26:A:549:G:C4	2.51	0.45
26:A:1085:A:H2'	26:A:1086:A:C4	2.52	0.45
26:A:1668:A:O2'	26:A:1674:G:N7	2.45	0.45
26:A:2331:G:O2'	26:A:2336:A:N1	2.35	0.45
26:A:2516:A:H2'	26:A:2517:C:H5''	1.97	0.45
44:U:80:PRO:O	44:U:100:THR:OG1	2.30	0.45
1:a:410:G:OP1	4:d:26:ARG:HD3	2.16	0.45
26:A:2071:A:H2'	26:A:2072:C:C6	2.52	0.45
26:A:2698:U:H2'	26:A:2699:C:C6	2.51	0.45
1:a:413:G:O2'	1:a:414:A:P	2.74	0.45
1:a:1010:U:H2'	1:a:1011:C:C6	2.52	0.45
1:a:1458:G:H5''	20:t:26:SER:HB2	1.98	0.45
2:b:54:LEU:HD23	2:b:220:THR:HB	1.99	0.45
7:g:22:LEU:O	7:g:101:MET:HE1	2.17	0.45
15:o:8:THR:O	15:o:12:VAL:HG23	2.15	0.45
26:A:12:U:O2'	26:A:13:A:C8	2.68	0.45
26:A:283:G:H2'	26:A:284:U:C6	2.52	0.45
26:A:306:U:H2'	26:A:307:G:O4'	2.17	0.45
26:A:2191:A:O2'	26:A:2192:U:P	2.73	0.45
31:F:26:MET:HA	31:F:26:MET:CE	2.40	0.45
13:m:52:GLN:HA	13:m:55:THR:OG1	2.17	0.45
25:z:215:ILE:O	25:z:335:THR:HG21	2.16	0.45
26:A:72:U:C2	50:1:55:THR:HG22	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:643:A:N1	26:A:2369:A:O2'	2.46	0.45
26:A:947:A:H2'	26:A:948:C:C6	2.51	0.45
26:A:1106:G:C2	26:A:1107:G:C8	3.04	0.45
26:A:2291:U:OP1	26:A:2380:C:O2'	2.29	0.45
27:B:110:C:H2'	27:B:111:U:O4'	2.17	0.45
42:S:102:ASP:OD2	42:S:105:ALA:HB2	2.16	0.45
46:W:99:ASN:C	46:W:99:ASN:OD1	2.59	0.45
47:X:11:GLU:HG3	47:X:16:ALA:CB	2.44	0.45
1:a:330:C:O2	1:a:330:C:O4'	2.32	0.45
3:c:56:VAL:HB	3:c:67:THR:HG23	1.98	0.45
6:f:38:ARG:NH2	6:f:63:ASN:OD1	2.48	0.45
15:o:3:LEU:HD13	15:o:35:GLN:HE21	1.82	0.45
26:A:849:A:H2'	26:A:850:U:H6	1.80	0.45
46:W:97:LYS:O	46:W:98:SER:CB	2.65	0.45
1:a:479:U:H2'	1:a:480:U:H5''	1.98	0.45
1:a:1337:G:H5''	1:a:1338:G:OP1	2.17	0.45
3:c:53:SER:N	3:c:69:HIS:O	2.46	0.45
29:D:55:LYS:HE3	29:D:60:VAL:HG22	1.99	0.45
1:a:96:U:H1'	1:a:97:G:P	2.56	0.45
1:a:1131:G:H2'	1:a:1132:C:H5''	1.99	0.45
7:g:17:LYS:HG2	7:g:44:TYR:CZ	2.51	0.45
25:z:96:ALA:HA	25:z:99:MET:SD	2.57	0.45
25:z:261:MET:HE1	25:z:273:GLU:HB3	1.98	0.45
25:z:263:ARG:HH11	25:z:263:ARG:HG3	1.82	0.45
25:z:344:LEU:HD23	25:z:359:MET:HE2	1.99	0.45
26:A:839:U:H2'	26:A:840:C:C6	2.52	0.45
26:A:2014:A:H2'	26:A:2015:A:C8	2.52	0.45
47:X:89:ILE:HG21	47:X:91:PHE:CZ	2.52	0.45
1:a:294:U:OP1	1:a:610:U:O2'	2.18	0.45
1:a:1149:C:O2'	1:a:1280:A:N1	2.46	0.45
2:b:216:ALA:O	2:b:220:THR:HG22	2.17	0.45
18:r:35:GLU:H	18:r:35:GLU:CD	2.23	0.45
19:s:45:ILE:CD1	19:s:64:ASP:HA	2.47	0.45
25:z:29:THR:HG23	25:z:79:HIS:CD2	2.52	0.45
26:A:580:U:H2'	26:A:581:C:C6	2.51	0.45
32:G:15:VAL:HG12	32:G:28:GLY:HA3	1.99	0.45
1:a:1298:U:OP2	7:g:114:LYS:NZ	2.45	0.45
4:d:12:SER:OG	4:d:17:THR:O	2.32	0.45
7:g:69:VAL:CG2	7:g:100:ALA:HB1	2.47	0.45
9:i:19:VAL:HG12	9:i:65:ILE:HG12	1.98	0.45
26:A:1019:U:OP1	26:A:1035:U:O2'	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1035:U:C2'	26:A:1036:G:H5''	2.47	0.45
26:A:1866:A:N6	26:A:1875:G:O2'	2.42	0.45
26:A:2344:U:H4'	26:A:2345:G:OP1	2.17	0.45
26:A:2850:A:N7	26:A:2868:A:O2'	2.40	0.45
4:d:188:ARG:NH2	4:d:197:GLU:OE1	2.49	0.44
5:e:151:GLU:CD	5:e:151:GLU:H	2.25	0.44
16:p:4:ILE:HD12	16:p:67:ILE:HD13	1.99	0.44
25:z:16:GLY:C	25:z:99:MET:HE2	2.42	0.44
25:z:68:VAL:HG22	25:z:79:HIS:HB3	1.99	0.44
26:A:445:C:O2'	26:A:446:G:H5'	2.17	0.44
26:A:586:A:N1	26:A:809:G:O2'	2.36	0.44
26:A:2144:G:C2	26:A:2148:G:C6	3.06	0.44
26:A:2757:A:HO2'	26:A:2758:A:P	2.39	0.44
1:a:55:A:C5	25:z:223:GLY:HA3	2.52	0.44
24:x:24:U:O2'	26:A:1923:U:OP1	2.28	0.44
26:A:26:G:H1'	26:A:514:A:N6	2.32	0.44
26:A:819:A:C4	26:A:1189:A:C2	3.05	0.44
26:A:861:A:H2'	26:A:862:G:O4'	2.17	0.44
1:a:728:A:H2'	1:a:729:A:C8	2.52	0.44
1:a:1465:A:H2'	1:a:1466:C:C6	2.53	0.44
7:g:79:ARG:HG3	7:g:84:THR:HA	2.00	0.44
16:p:56:ARG:HD2	16:p:56:ARG:HA	1.84	0.44
26:A:494:G:H4'	44:U:6:LYS:HB2	1.99	0.44
26:A:811:U:H2'	37:N:21:ARG:HA	1.98	0.44
26:A:881:G:C2	26:A:882:G:N7	2.85	0.44
27:B:76:G:OP1	47:X:9:ARG:NH1	2.48	0.44
1:a:1067:A:N1	1:a:1108:G:O2'	2.42	0.44
19:s:19:VAL:HG21	19:s:44:MET:HG2	1.98	0.44
23:w:4:G:O2'	23:w:5:G:H5'	2.18	0.44
25:z:166:ASP:OD2	25:z:166:ASP:N	2.51	0.44
25:z:305:PHE:CD1	25:z:369:MET:HE1	2.53	0.44
26:A:12:U:O2'	26:A:13:A:P	2.75	0.44
26:A:75:G:N3	26:A:75:G:H2'	2.33	0.44
26:A:1796:U:H2'	26:A:1797:G:C8	2.53	0.44
36:M:17:ARG:HB2	36:M:45:GLU:HG3	1.99	0.44
1:a:235:C:H2'	1:a:236:A:C8	2.53	0.44
1:a:454:G:H2'	1:a:455:G:H5''	2.00	0.44
9:i:21:ILE:O	9:i:21:ILE:HG13	2.18	0.44
24:x:67:C:O2'	24:x:68:C:H5'	2.18	0.44
25:z:100:ASP:OD2	25:z:205:ARG:NH2	2.45	0.44
26:A:888:C:H2'	26:A:889:C:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1416:G:C4	26:A:1417:C:C5	3.06	0.44
26:A:2172:U:H4'	26:A:2174:C:OP2	2.17	0.44
26:A:2461:A:H2'	26:A:2462:C:C6	2.53	0.44
26:A:2804:U:H2'	26:A:2805:C:C6	2.53	0.44
36:M:38:ILE:HD11	36:M:112:PHE:CZ	2.53	0.44
1:a:687:A:C2	1:a:704:A:C5	3.05	0.44
1:a:1218:C:H2'	1:a:1219:A:C8	2.53	0.44
25:z:21:VAL:HG21	26:A:2661:G:H5'	2.00	0.44
25:z:320:HIS:CD2	25:z:321:THR:HG23	2.52	0.44
26:A:142:A:O2'	26:A:143:C:P	2.75	0.44
26:A:1048:A:C2	26:A:1049:C:C6	3.06	0.44
26:A:2134:A:N6	26:A:2157:G:O2'	2.51	0.44
26:A:2895:G:H2'	26:A:2896:C:C6	2.52	0.44
28:C:5:LYS:HD2	28:C:6:CYS:N	2.32	0.44
40:Q:88:LYS:O	40:Q:88:LYS:NZ	2.44	0.44
46:W:62:GLU:OE1	46:W:62:GLU:N	2.50	0.44
1:a:1157:A:H4'	1:a:1158:C:O5'	2.18	0.44
3:c:42:TYR:CZ	3:c:90:VAL:HG21	2.52	0.44
21:u:39:GLU:OE2	21:u:47:ARG:NH1	2.51	0.44
26:A:419:U:H2'	26:A:420:C:C6	2.52	0.44
26:A:894:U:H2'	26:A:895:U:H4'	2.00	0.44
26:A:1786:A:H1'	26:A:1938:A:N6	2.33	0.44
26:A:2615:U:C2	53:4:4:GLN:HA	2.52	0.44
50:1:10:SER:O	50:1:14:LEU:HG	2.18	0.44
1:a:368:U:OP2	25:z:280:ARG:HD3	2.18	0.44
1:a:575:G:O2'	1:a:821:G:OP2	2.32	0.44
1:a:1158:C:H3'	1:a:1158:C:O2	2.18	0.44
1:a:1285:A:H4'	1:a:1286:U:OP1	2.17	0.44
17:q:49:GLU:O	17:q:50:ASN:CG	2.61	0.44
26:A:283:G:C2'	26:A:284:U:O5'	2.66	0.44
26:A:541:A:H2'	26:A:542:C:O4'	2.18	0.44
26:A:851:C:H2'	26:A:852:U:C6	2.52	0.44
1:a:868:C:H2'	1:a:869:G:O4'	2.18	0.44
1:a:1211:U:H1'	1:a:1213:A:C2	2.53	0.44
1:a:1324:A:H2'	1:a:1325:C:O4'	2.18	0.44
2:b:76:ALA:HB1	2:b:210:VAL:HG11	2.00	0.44
5:e:22:SER:HB3	5:e:31:PHE:CD1	2.53	0.44
26:A:526:A:H2'	63:A:4303:HOH:O	2.18	0.44
26:A:634:C:H2'	26:A:635:C:C6	2.52	0.44
26:A:2228:G:H2'	26:A:2229:U:C6	2.53	0.44
26:A:2466:C:OP1	57:8:4:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2567:G:H2'	26:A:2568:U:C6	2.53	0.44
27:B:114:C:O2'	27:B:115:A:P	2.76	0.44
28:C:165:VAL:HG21	28:C:181:MET:HE1	1.99	0.44
38:O:134:THR:OG1	38:O:136:MET:O	2.32	0.44
43:T:37:GLU:O	43:T:37:GLU:CG	2.65	0.44
1:a:1273:C:H2'	1:a:1274:A:O4'	2.18	0.43
3:c:53:SER:HB3	3:c:106:VAL:HG21	1.99	0.43
4:d:78:GLU:OE2	4:d:81:ARG:NH2	2.51	0.43
9:i:29:VAL:O	9:i:29:VAL:HG13	2.17	0.43
25:z:342:ILE:HG23	25:z:359:MET:CE	2.47	0.43
26:A:207:A:H2'	26:A:208:C:O4'	2.18	0.43
26:A:242:G:H5''	56:7:64:TYR:CE2	2.53	0.43
26:A:857:G:H2'	26:A:858:G:O4'	2.18	0.43
26:A:1637:A:H5'	26:A:1760:C:O2'	2.18	0.43
26:A:1720:U:H2'	26:A:1721:G:O4'	2.18	0.43
27:B:66:A:H4'	27:B:67:G:OP1	2.18	0.43
31:F:105:THR:HA	52:3:38:SER:HB3	1.99	0.43
32:G:26:ILE:HG22	32:G:79:VAL:HG11	1.99	0.43
46:W:7:ARG:O	46:W:8:ASP:HB2	2.18	0.43
1:a:399:G:H2'	1:a:400:C:C6	2.53	0.43
1:a:412:A:O2'	1:a:413:G:H4'	2.19	0.43
9:i:21:ILE:CG2	9:i:63:LEU:HD22	2.44	0.43
23:w:21:A:H61	23:w:46:A:H2'	1.83	0.43
26:A:172:A:H2'	26:A:173:A:C8	2.53	0.43
26:A:366:C:H2'	26:A:367:G:O4'	2.18	0.43
26:A:909:A:H2'	26:A:912:C:H5	1.83	0.43
26:A:984:A:N3	26:A:984:A:H2'	2.33	0.43
26:A:2480:C:C2'	26:A:2481:G:H5'	2.48	0.43
26:A:2537:U:H2'	26:A:2538:C:C6	2.53	0.43
45:V:24:MET:HE3	45:V:24:MET:HA	2.00	0.43
2:b:60:ILE:HD11	2:b:159:ASP:HB3	1.99	0.43
15:o:21:ASP:OD1	15:o:24:SER:HB3	2.18	0.43
26:A:1703:G:H2'	26:A:1704:C:C6	2.53	0.43
26:A:1980:G:O2'	26:A:1982:U:OP2	2.36	0.43
26:A:2165:C:OP2	26:A:2165:C:H2'	2.18	0.43
29:D:110:THR:HG23	29:D:202:ILE:HB	2.00	0.43
1:a:171:A:H2'	1:a:172:A:C8	2.53	0.43
1:a:212:G:H2'	1:a:213:G:O4'	2.18	0.43
1:a:911:U:H2'	1:a:912:C:C6	2.53	0.43
1:a:1004:A:C2	1:a:1026:G:C2	3.07	0.43
26:A:479:A:N3	26:A:481:G:H5''	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:756:A:H2'	26:A:757:G:O4'	2.18	0.43
26:A:1966:A:N3	26:A:2592:G:O2'	2.51	0.43
26:A:2038:G:H2'	26:A:2039:U:O4'	2.19	0.43
26:A:2687:U:H2'	26:A:2688:G:O4'	2.18	0.43
1:a:212:G:C4	1:a:213:G:C8	3.06	0.43
1:a:438:U:O2'	1:a:439:U:C5	2.71	0.43
1:a:1504:G:H4'	1:a:1505:G:C4	2.54	0.43
3:c:40:ARG:O	3:c:44:THR:HG23	2.18	0.43
9:i:81:HIS:CE1	9:i:85:ARG:HE	2.36	0.43
14:n:31:ILE:HD13	14:n:31:ILE:N	2.31	0.43
25:z:16:GLY:CA	25:z:99:MET:HE2	2.49	0.43
25:z:268:GLU:O	25:z:269:GLY:C	2.61	0.43
1:a:340:U:H5'	1:a:341:C:OP2	2.18	0.43
1:a:381:C:H2'	1:a:382:A:O4'	2.18	0.43
1:a:1123:U:O2'	1:a:1124:G:H5'	2.18	0.43
6:f:1:MET:HE1	6:f:67:PRO:HD3	2.01	0.43
24:x:76:M3O:SD	26:A:2061:G:N2	2.88	0.43
26:A:1750:G:O2'	26:A:2860:A:N1	2.43	0.43
26:A:2118:U:P	26:A:2147:A:HO2'	2.42	0.43
26:A:2312:U:C5'	31:F:85:ILE:HD11	2.49	0.43
31:F:140:GLU:HA	52:3:28:VAL:HG13	2.00	0.43
42:S:80:ILE:O	42:S:84:LYS:HG2	2.19	0.43
50:1:17:GLU:OE2	50:1:21:LEU:HD11	2.19	0.43
1:a:1448:C:O2'	1:a:1449:C:C5'	2.66	0.43
9:i:84:THR:HG23	9:i:98:LEU:HD13	2.00	0.43
19:s:30:PRO:HA	19:s:48:THR:HG23	2.00	0.43
26:A:155:A:H2'	26:A:156:A:C8	2.52	0.43
26:A:1198:U:H2'	26:A:1199:U:C6	2.53	0.43
26:A:1682:G:H2'	26:A:1683:U:C6	2.54	0.43
26:A:1904:G:O2'	26:A:1928:A:N1	2.50	0.43
26:A:2190:G:C4	26:A:2191:A:C8	3.06	0.43
36:M:1:MET:HE3	36:M:32:TYR:CZ	2.54	0.43
1:a:86:G:H4'	1:a:87:C:C6	2.54	0.43
1:a:1103:C:O2	2:b:106:THR:HG21	2.18	0.43
1:a:1439:G:OP1	20:t:33:LYS:NZ	2.51	0.43
6:f:6:ILE:HG12	6:f:89:VAL:HG22	2.00	0.43
26:A:441:U:O2'	30:E:41:GLN:OE1	2.22	0.43
26:A:1061:U:H3'	26:A:1062:G:H5'	2.01	0.43
45:V:2:ILE:HD13	45:V:42:GLU:HA	2.00	0.43
1:a:280:C:H3'	1:a:281:G:H5'	2.01	0.43
17:q:26:GLU:OE2	17:q:39:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2:G:H2'	26:A:3:U:C6	2.54	0.43
26:A:833:A:H2'	26:A:834:G:C8	2.54	0.43
26:A:1001:A:H2'	26:A:1002:G:O4'	2.17	0.43
26:A:1269:A:H2'	26:A:1270:C:C6	2.54	0.43
26:A:1432:G:O2'	26:A:1433:A:H5'	2.18	0.43
27:B:104:A:H2'	27:B:105:G:O4'	2.18	0.43
32:G:24:ILE:HD13	32:G:72:LEU:HD11	1.99	0.43
1:a:1163:A:H2'	1:a:1164:G:O4'	2.19	0.43
23:w:56:C:H1'	26:A:1067:A:C4	2.54	0.43
26:A:927:A:H2'	26:A:928:A:C8	2.54	0.43
26:A:969:G:H2'	26:A:970:U:C6	2.54	0.43
26:A:2063:C:O2	26:A:2450:A:N1	2.51	0.43
26:A:2572:A:C4'	26:A:2573:C:OP2	2.65	0.43
1:a:736:C:H2'	1:a:737:C:C6	2.54	0.42
1:a:1157:A:C2	1:a:1181:G:C4	3.06	0.42
1:a:1351:U:O4	9:i:120:LYS:NZ	2.53	0.42
4:d:160:GLU:O	4:d:163:GLU:HG2	2.18	0.42
9:i:21:ILE:HG12	9:i:86:ALA:HB1	2.01	0.42
10:j:16:ARG:O	10:j:20:GLN:HG3	2.18	0.42
23:w:4:G:C2'	23:w:5:G:H5'	2.49	0.42
24:x:20:U:O5'	24:x:20:U:H6	2.02	0.42
26:A:430:A:H5''	26:A:431:U:OP2	2.19	0.42
26:A:548:G:H2'	26:A:549:G:N9	2.35	0.42
26:A:2149:U:H2'	26:A:2150:C:C6	2.53	0.42
26:A:2748:A:OP1	32:G:70:ALA:HB2	2.19	0.42
1:a:86:G:H4'	1:a:87:C:H6	1.83	0.42
1:a:192:A:H2'	1:a:193:C:O4'	2.18	0.42
1:a:1521:C:H2'	1:a:1522:U:C6	2.54	0.42
2:b:50:PHE:O	2:b:54:LEU:HD12	2.19	0.42
8:h:101:ILE:HG13	8:h:129:VAL:HG13	2.01	0.42
23:w:61:C:H2'	23:w:62:C:C6	2.54	0.42
25:z:319:ARG:NH2	25:z:321:THR:O	2.52	0.42
26:A:572:A:C2	26:A:2033:A:C2	3.07	0.42
26:A:1418:G:HO2'	26:A:1579:A:H62	1.66	0.42
26:A:1436:G:O2'	26:A:1515:A:N1	2.50	0.42
26:A:1485:U:H2'	26:A:1486:U:C6	2.54	0.42
26:A:1664:A:H2	36:M:1:MET:HE1	1.83	0.42
26:A:2104:C:H2'	26:A:2105:U:C6	2.55	0.42
26:A:2112:G:C2	26:A:2113:U:C6	3.07	0.42
26:A:2281:A:O2'	26:A:2282:G:H5'	2.19	0.42
26:A:2455:G:H2'	26:A:2456:C:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2646:C:H2'	26:A:2647:U:O4'	2.19	0.42
27:B:42:C:O2'	31:F:63:GLN:HG2	2.19	0.42
1:a:177:G:C8	1:a:178:C:C6	3.07	0.42
1:a:349:A:O2'	1:a:350:G:H5'	2.18	0.42
20:t:42:GLY:HA2	20:t:86:LEU:HD11	2.01	0.42
26:A:68:G:H2'	26:A:69:C:O4'	2.20	0.42
26:A:858:G:OP1	48:Y:78:LYS:NZ	2.44	0.42
26:A:1081:U:O2'	26:A:1082:U:P	2.77	0.42
26:A:1527:G:N1	26:A:1544:A:OP2	2.36	0.42
26:A:2037:A:H2'	26:A:2038:G:C8	2.54	0.42
26:A:2112:G:N3	26:A:2112:G:H2'	2.33	0.42
26:A:2898:U:O2	35:L:134:ALA:HB1	2.18	0.42
1:a:76:G:H2'	1:a:77:A:C8	2.54	0.42
1:a:401:C:O2'	1:a:621:A:N3	2.45	0.42
4:d:8:LYS:HG3	4:d:21:LEU:HD13	2.01	0.42
6:f:66:ALA:HB1	6:f:70:VAL:CG2	2.50	0.42
26:A:265:A:N1	26:A:427:U:O2'	2.52	0.42
26:A:274:C:H2'	26:A:275:C:C6	2.54	0.42
26:A:289:G:H8	26:A:289:G:OP2	2.02	0.42
26:A:881:G:H21	26:A:896:A:H62	1.67	0.42
26:A:1577:C:H2'	26:A:1578:U:C1'	2.49	0.42
26:A:2591:C:H2'	26:A:2592:G:C8	2.54	0.42
30:E:141:MET:HE2	30:E:143:LEU:HD12	2.00	0.42
47:X:6:ALA:HB2	47:X:42:LEU:CD2	2.50	0.42
48:Y:37:ILE:HG21	48:Y:80:ILE:HG21	2.00	0.42
1:a:767:A:H2'	1:a:768:A:O4'	2.19	0.42
1:a:1023:U:H2'	1:a:1024:G:O4'	2.18	0.42
1:a:1033:G:H2'	1:a:1034:G:C8	2.55	0.42
1:a:1315:U:H2'	1:a:1316:G:O4'	2.20	0.42
3:c:42:TYR:CE2	3:c:90:VAL:HG21	2.54	0.42
23:w:75:C:N3	25:z:222:SER:OG	2.53	0.42
26:A:1047:G:H2'	26:A:1110:G:N2	2.34	0.42
26:A:1558:C:O4'	26:A:1560:G:C8	2.73	0.42
26:A:1784:A:OP1	63:A:3907:HOH:O	2.21	0.42
26:A:1856:U:H2'	26:A:1857:G:O4'	2.20	0.42
26:A:2139:U:H2'	26:A:2140:G:O4'	2.20	0.42
26:A:2158:A:O2'	26:A:2159:G:C2	2.73	0.42
26:A:2233:U:H2'	26:A:2234:G:C8	2.55	0.42
31:F:95:ARG:CZ	52:3:1:MET:HE2	2.49	0.42
34:J:110:ALA:HB1	34:J:125:MET:CB	2.50	0.42
47:X:48:MET:HE3	47:X:51:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:306:A:C5	1:a:307:C:C5	3.07	0.42
1:a:924:C:O2'	1:a:1502:A:N1	2.48	0.42
1:a:1211:U:O2'	1:a:1212:U:P	2.77	0.42
1:a:1298:U:H4'	1:a:1299:A:O4'	2.20	0.42
16:p:4:ILE:HD12	16:p:67:ILE:CD1	2.50	0.42
26:A:272:A:H2'	26:A:273:G:C8	2.54	0.42
26:A:720:U:H2'	26:A:721:A:C8	2.54	0.42
26:A:744:U:OP1	63:A:3906:HOH:O	2.21	0.42
26:A:1187:G:H5''	43:T:83:TYR:CE1	2.54	0.42
26:A:1545:A:H2'	26:A:1546:G:O4'	2.19	0.42
26:A:1548:A:H2'	26:A:1549:A:C8	2.54	0.42
26:A:1794:A:H2'	26:A:1795:C:C6	2.55	0.42
26:A:1853:A:N1	26:A:2087:G:H1'	2.34	0.42
26:A:2395:C:H2'	26:A:2396:G:O4'	2.19	0.42
30:E:170:ARG:NH1	30:E:176:ASP:OD1	2.52	0.42
44:U:7:HIS:HB2	44:U:50:VAL:HG22	2.01	0.42
26:A:549:G:H2'	26:A:550:C:O4'	2.19	0.42
26:A:898:C:H2'	26:A:899:A:O4'	2.20	0.42
26:A:2114:A:O2'	26:A:2115:G:OP1	2.32	0.42
26:A:2813:A:H2'	26:A:2814:A:O4'	2.20	0.42
31:F:132:VAL:HG22	31:F:152:LEU:HD23	2.02	0.42
40:Q:106:LEU:HD23	40:Q:106:LEU:C	2.44	0.42
46:W:74:ASN:O	46:W:75:ALA:HB3	2.19	0.42
47:X:64:VAL:HG22	47:X:69:GLU:HG2	2.02	0.42
1:a:620:C:C6	4:d:132:ILE:HD13	2.54	0.42
2:b:76:ALA:O	2:b:77:SER:C	2.61	0.42
3:c:78:GLY:HA3	3:c:83:ASP:HB2	2.01	0.42
15:o:24:SER:OG	15:o:27:VAL:HG23	2.19	0.42
23:w:9:A:O2'	23:w:10:G:N7	2.51	0.42
25:z:259:VAL:O	25:z:265:LEU:O	2.38	0.42
26:A:612:G:O2'	26:A:614:A:N7	2.48	0.42
26:A:747:5MU:O2'	44:U:92:ARG:NH2	2.52	0.42
26:A:2348:U:O2'	26:A:2349:G:H5'	2.19	0.42
1:a:246:A:C2	1:a:282:A:C5	3.08	0.42
1:a:665:A:H1'	1:a:733:G:O4'	2.19	0.42
1:a:927:G:N7	63:a:3317:HOH:O	2.37	0.42
2:b:94:HIS:O	2:b:95:ARG:C	2.62	0.42
20:t:10:ARG:HA	20:t:13:GLN:HB2	2.00	0.42
26:A:297:G:H2'	26:A:298:G:O4'	2.20	0.42
26:A:609:A:H2'	26:A:610:C:O4'	2.19	0.42
26:A:668:A:H2'	26:A:670:A:H62	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1070:A:N6	26:A:1096:A:O2'	2.45	0.42
26:A:1105:U:O2	26:A:1106:G:C8	2.73	0.42
38:O:77:PRO:O	38:O:80:VAL:HG22	2.19	0.42
1:a:652:U:O2'	1:a:653:U:P	2.78	0.42
1:a:737:C:H2'	1:a:738:C:H6	1.85	0.42
1:a:745:G:H2'	1:a:746:A:C8	2.55	0.42
6:f:32:ALA:HB2	6:f:70:VAL:HG11	2.02	0.42
7:g:78:ARG:HB2	7:g:87:VAL:HG21	2.02	0.42
25:z:36:LEU:HD22	25:z:40:TYR:OH	2.20	0.42
25:z:210:PRO:O	25:z:234:ARG:NE	2.51	0.42
26:A:1064:C:HO2'	26:A:1065:U:C5'	2.22	0.42
26:A:1079:C:C2	26:A:1088:A:C2	3.08	0.42
26:A:2101:A:H2'	26:A:2102:G:H8	1.84	0.42
26:A:2159:G:HO2'	26:A:2160:C:C1'	2.28	0.42
27:B:66:A:H5''	27:B:67:G:OP1	2.20	0.42
35:L:131:ASN:OD1	35:L:131:ASN:N	2.53	0.42
45:V:13:ALA:HB1	50:1:33:ALA:HB1	2.02	0.42
55:6:25:LYS:O	55:6:29:GLN:HG3	2.19	0.42
1:a:98:A:O2'	1:a:99:C:H5'	2.20	0.41
1:a:501:C:H2'	1:a:502:A:C8	2.55	0.41
1:a:1404:C:H2'	1:a:1405:G:C8	2.54	0.41
2:b:70:VAL:CG2	2:b:161:LEU:HD11	2.50	0.41
7:g:69:VAL:HG23	7:g:100:ALA:CB	2.46	0.41
17:q:10:GLY:HA3	17:q:25:ILE:HD13	2.02	0.41
23:w:11:U:H2'	23:w:12:U:C6	2.55	0.41
23:w:65:U:H2'	23:w:66:C:C6	2.55	0.41
25:z:90:LYS:O	25:z:94:THR:HG23	2.20	0.41
25:z:347:GLY:O	25:z:348:VAL:C	2.63	0.41
26:A:1442:U:H2'	26:A:1443:U:C6	2.55	0.41
26:A:1541:C:O2'	26:A:1542:U:H5'	2.20	0.41
26:A:1680:U:H2'	26:A:1681:G:O4'	2.19	0.41
26:A:2039:U:H2'	26:A:2040:G:C8	2.55	0.41
26:A:2246:G:H2'	26:A:2247:A:C8	2.55	0.41
26:A:2819:G:H2'	26:A:2821:A:N7	2.35	0.41
33:H:4:ILE:HG12	33:H:37:VAL:HG23	2.02	0.41
44:U:11:ARG:HD3	44:U:82:MET:HE2	2.02	0.41
49:Z:3:ARG:O	49:Z:12:PRO:HD3	2.20	0.41
1:a:177:G:C5	1:a:178:C:C5	3.08	0.41
1:a:440:C:C2	1:a:441:A:C8	3.08	0.41
1:a:718:A:O2'	21:u:31:GLU:OE2	2.38	0.41
1:a:1198:G:N7	63:a:3320:HOH:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1244:G:H2'	1:a:1245:C:C6	2.55	0.41
2:b:196:VAL:CG2	2:b:199:VAL:HG22	2.49	0.41
16:p:52:LEU:CD1	16:p:75:ILE:HG12	2.51	0.41
24:x:75:C:H2'	24:x:76:M3O:C1'	2.50	0.41
26:A:64:A:H2'	26:A:65:U:C6	2.54	0.41
26:A:144:A:O2'	26:A:145:C:C6	2.73	0.41
26:A:900:A:H2'	26:A:901:C:O4'	2.20	0.41
26:A:1534:U:O3'	26:A:1535:A:H2'	2.20	0.41
39:P:31:HIS:O	39:P:32:GLU:HB2	2.19	0.41
40:Q:83:LEU:HD21	40:Q:114:GLY:HA3	2.03	0.41
1:a:1042:A:H2'	1:a:1043:G:H8	1.83	0.41
1:a:1451:U:H5'	1:a:1452:C:H5	1.85	0.41
6:f:40:GLU:OE1	6:f:100:SER:OG	2.36	0.41
14:n:49:GLN:OE1	19:s:12:ASP:HA	2.21	0.41
21:u:28:VAL:O	21:u:32:VAL:HG23	2.20	0.41
26:A:1532:A:H2'	26:A:1533:C:O4'	2.20	0.41
26:A:2074:U:H2'	26:A:2075:U:C6	2.55	0.41
26:A:2127:G:N2	26:A:2162:G:C8	2.88	0.41
26:A:2810:A:H2'	26:A:2811:G:O4'	2.20	0.41
38:O:29:GLY:O	38:O:133:LYS:HE2	2.20	0.41
1:a:389:A:H3'	1:a:390:U:H6	1.85	0.41
1:a:840:C:O2'	1:a:846:G:N1	2.33	0.41
23:w:64:U:C4'	25:z:380:GLY:HA2	2.50	0.41
26:A:544:C:O3'	26:A:545:U:H2'	2.20	0.41
26:A:1528:A:H2'	26:A:1529:G:O4'	2.21	0.41
26:A:1728:C:N3	26:A:1730:C:O2	2.54	0.41
26:A:2295:C:O2'	26:A:2296:U:H5'	2.21	0.41
27:B:114:C:O2'	27:B:115:A:H8	2.04	0.41
32:G:71:LEU:O	32:G:75:MET:HG2	2.20	0.41
46:W:48:PRO:HB3	46:W:54:GLN:O	2.21	0.41
1:a:178:C:C2	1:a:179:A:C8	3.09	0.41
14:n:26:GLU:OE1	14:n:27:LEU:HD23	2.20	0.41
16:p:71:VAL:O	16:p:75:ILE:HG13	2.21	0.41
26:A:282:A:C6	26:A:359:G:O6	2.74	0.41
26:A:1769:U:O2'	26:A:1958:C:OP1	2.38	0.41
26:A:2346:A:H3'	26:A:2347:C:H5''	2.02	0.41
26:A:2723:C:H2'	26:A:2724:U:O4'	2.19	0.41
36:M:63:VAL:HG12	36:M:107:LEU:HD11	2.02	0.41
46:W:54:GLN:N	46:W:55:PRO:HD2	2.35	0.41
1:a:458:U:H2'	1:a:459:A:C8	2.55	0.41
1:a:865:A:H2'	1:a:866:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:58:ASN:HB2	2:b:220:THR:OG1	2.21	0.41
2:b:114:LEU:HD22	2:b:148:LEU:HD12	2.03	0.41
5:e:115:LEU:HD13	5:e:123:VAL:HG11	2.03	0.41
26:A:57:C:H2'	26:A:58:G:O4'	2.20	0.41
26:A:142:A:O2'	26:A:143:C:O5'	2.30	0.41
26:A:936:A:H2'	26:A:937:C:C6	2.56	0.41
26:A:1754:A:N1	26:A:2716:C:O2'	2.42	0.41
26:A:2158:A:OP2	26:A:2158:A:C8	2.73	0.41
26:A:2774:C:H2'	26:A:2775:G:O4'	2.20	0.41
27:B:113:C:O2'	27:B:114:C:H5'	2.20	0.41
31:F:30:ARG:N	31:F:159:THR:OG1	2.43	0.41
44:U:73:LYS:HB2	44:U:106:VAL:HB	2.03	0.41
1:a:14:U:OP2	63:a:3301:HOH:O	2.22	0.41
1:a:1158:C:C5	1:a:1160:G:H1'	2.56	0.41
24:x:25:C:C2	24:x:26:G:C8	3.09	0.41
26:A:150:U:H2'	26:A:151:C:C6	2.55	0.41
26:A:365:U:H2'	26:A:366:C:O4'	2.21	0.41
26:A:909:A:H2'	26:A:912:C:C5	2.55	0.41
26:A:1076:C:H2'	26:A:1077:A:O4'	2.19	0.41
26:A:1083:U:C2'	26:A:1084:A:H3'	2.50	0.41
26:A:1394:U:H4'	26:A:1603:A:H4'	2.02	0.41
26:A:1672:A:C2	26:A:2582:G:H5'	2.56	0.41
26:A:2488:G:O2'	26:A:2489:U:H5'	2.20	0.41
26:A:2491:U:H5	63:A:4585:HOH:O	2.03	0.41
1:a:1042:A:O2'	1:a:1043:G:C5'	2.69	0.41
2:b:28:LYS:N	2:b:29:PRO:HD2	2.36	0.41
20:t:39:ILE:HD13	20:t:82:GLN:HB3	2.02	0.41
25:z:328:ARG:HA	25:z:340:GLY:O	2.21	0.41
26:A:144:A:O2'	26:A:145:C:H5'	2.21	0.41
26:A:657:U:H2'	26:A:658:U:C6	2.56	0.41
26:A:2121:G:C6	26:A:2122:U:C4	3.08	0.41
29:D:116:LYS:HB2	29:D:165:MET:HB3	2.03	0.41
30:E:127:GLU:OE2	30:E:127:GLU:N	2.44	0.41
31:F:8:TYR:HA	31:F:12:VAL:HB	2.03	0.41
40:Q:35:ILE:HG21	40:Q:71:ALA:HA	2.03	0.41
1:a:736:C:H2'	1:a:737:C:H6	1.85	0.41
1:a:751:U:H2'	1:a:752:G:O4'	2.21	0.41
1:a:1410:A:H2'	1:a:1411:C:C6	2.55	0.41
1:a:1441:A:C8	1:a:1442:G:C8	3.09	0.41
2:b:162:PHE:HA	2:b:184:PHE:O	2.20	0.41
10:j:22:THR:HG21	10:j:39:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:64:THR:CG2	12:l:93:VAL:HG22	2.51	0.41
17:q:47:HIS:HB2	17:q:67:LEU:HD12	2.03	0.41
23:w:51:G:H2'	23:w:52:G:O4'	2.21	0.41
26:A:24:G:O2'	44:U:78:GLU:O	2.36	0.41
26:A:225:C:H2'	26:A:226:A:O4'	2.20	0.41
26:A:545:U:HO2'	26:A:546:U:P	2.44	0.41
26:A:832:U:H2'	26:A:833:A:C8	2.55	0.41
26:A:1028:A:H2'	26:A:1029:A:C8	2.56	0.41
26:A:2118:U:OP1	26:A:2147:A:O2'	2.39	0.41
26:A:2467:C:H2'	26:A:2468:A:O4'	2.21	0.41
26:A:2680:U:O2'	26:A:2681:C:H5'	2.21	0.41
26:A:2757:A:O2'	26:A:2758:A:P	2.79	0.41
43:T:38:VAL:HG22	43:T:59:ILE:HD12	2.03	0.41
44:U:34:ASP:OD1	53:4:37:LYS:NZ	2.52	0.41
1:a:460:A:H2'	1:a:461:A:C8	2.56	0.41
1:a:1014:A:C2	1:a:1219:A:H1'	2.56	0.41
3:c:10:ILE:HG23	3:c:11:ARG:HG3	2.02	0.41
14:n:49:GLN:HE22	19:s:13:LEU:H	1.67	0.41
25:z:261:MET:CE	25:z:273:GLU:HB3	2.50	0.41
26:A:2312:U:H5'	31:F:85:ILE:HD11	2.03	0.41
26:A:2646:C:H6	26:A:2646:C:O5'	2.03	0.41
27:B:42:C:C6	31:F:66:LEU:HB2	2.56	0.41
1:a:1118:U:H1'	1:a:1179:A:C5	2.55	0.40
1:a:1326:U:H2'	1:a:1327:C:H6	1.87	0.40
7:g:140:ASP:HA	7:g:143:ARG:HG2	2.02	0.40
23:w:50:A:O2'	23:w:51:G:OP1	2.39	0.40
25:z:302:HIS:ND1	25:z:392:VAL:HG11	2.35	0.40
26:A:208:C:H2'	26:A:209:C:C6	2.56	0.40
26:A:476:G:H4'	26:A:502:A:N1	2.36	0.40
26:A:555:G:O2'	26:A:556:A:C8	2.74	0.40
26:A:608:A:H2'	26:A:609:A:C8	2.56	0.40
26:A:1035:U:O2'	26:A:1036:G:H5''	2.22	0.40
26:A:1080:A:H2'	26:A:1081:U:H5'	2.03	0.40
26:A:1727:C:H2'	26:A:1728:C:O4'	2.22	0.40
26:A:1799:G:N7	28:C:178:SER:OG	2.50	0.40
26:A:2020:A:H5'	53:4:9:THR:CG2	2.50	0.40
1:a:384:G:H2'	1:a:385:C:C6	2.56	0.40
1:a:542:G:H5'	4:d:39:GLY:HA3	2.02	0.40
2:b:73:LYS:HE2	2:b:165:ASP:OD2	2.21	0.40
10:j:24:GLU:OE2	10:j:24:GLU:C	2.65	0.40
23:w:17:G:H21	23:w:57:G:H2'	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1317:G:H2'	26:A:1318:U:O4'	2.21	0.40
26:A:1394:U:H2'	26:A:1395:A:O4'	2.21	0.40
26:A:2849:U:H4'	26:A:2868:A:C2	2.55	0.40
26:A:2852:G:H2'	26:A:2853:C:O4'	2.21	0.40
27:B:51:G:O2'	27:B:52:A:H5'	2.21	0.40
1:a:840:C:O2	1:a:846:G:O6	2.40	0.40
1:a:883:C:O2'	1:a:884:U:H5'	2.21	0.40
1:a:1130:A:C8	1:a:1146:A:N1	2.90	0.40
1:a:1377:A:O3'	1:a:1378:C:H6	2.04	0.40
1:a:1378:C:OP1	7:g:7:ILE:HD11	2.22	0.40
1:a:1477:U:H2'	1:a:1478:U:C6	2.56	0.40
4:d:87:GLY:HA3	4:d:197:GLU:HG3	2.02	0.40
10:j:80:THR:OG1	10:j:82:LYS:HG2	2.22	0.40
18:r:32:TYR:CB	18:r:55:LEU:HD21	2.50	0.40
23:w:65:U:C2	23:w:66:C:C5	3.09	0.40
25:z:205:ARG:HD3	25:z:272:GLY:HA3	2.04	0.40
25:z:328:ARG:HH11	25:z:328:ARG:HG3	1.86	0.40
26:A:581:C:H2'	26:A:582:A:C8	2.56	0.40
26:A:1021:A:H3'	26:A:1021:A:N3	2.36	0.40
26:A:1062:G:N7	26:A:1076:C:N3	2.69	0.40
26:A:1083:U:C2	26:A:1085:A:OP2	2.74	0.40
26:A:1103:A:N3	26:A:1103:A:H2'	2.36	0.40
26:A:1275:A:N1	26:A:1295:C:O2'	2.51	0.40
26:A:1330:C:O2'	26:A:1331:G:H5'	2.21	0.40
26:A:1497:U:C2	26:A:1578:U:OP1	2.74	0.40
26:A:2093:G:O2'	26:A:2198:A:N1	2.48	0.40
26:A:2120:G:H2'	26:A:2121:G:C8	2.57	0.40
26:A:2637:U:C2'	26:A:2638:G:H5'	2.52	0.40
47:X:21:ARG:HA	47:X:25:LYS:O	2.21	0.40
1:a:250:A:H4'	1:a:251:G:O5'	2.21	0.40
1:a:1211:U:C2'	1:a:1212:U:OP2	2.66	0.40
1:a:1314:C:H2'	1:a:1315:U:C6	2.56	0.40
1:a:1323:G:H2'	1:a:1324:A:C8	2.56	0.40
6:f:96:VAL:O	6:f:96:VAL:HG22	2.21	0.40
7:g:68:ASN:O	7:g:138:ARG:NH2	2.54	0.40
25:z:72:THR:OG1	25:z:197:ASP:OD2	2.39	0.40
26:A:139:U:H4'	26:A:140:C:OP2	2.21	0.40
26:A:543:G:C6	26:A:551:G:C6	3.09	0.40
26:A:2312:U:O2'	26:A:2313:C:P	2.79	0.40
27:B:3:C:O2'	27:B:4:C:OP1	2.31	0.40
1:a:1098:C:O2'	21:u:71:TYR:O	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:136:MET:HG3	2:b:137:ARG:N	2.37	0.40
2:b:187:VAL:O	2:b:201:PRO:HA	2.22	0.40
3:c:72:ARG:HB3	3:c:75:ILE:HD13	2.03	0.40
3:c:111:LEU:HD22	3:c:146:ALA:HB2	2.03	0.40
5:e:132:ASN:O	5:e:136:VAL:HG23	2.22	0.40
8:h:103:VAL:HG12	8:h:126:ILE:HD12	2.03	0.40
9:i:42:GLU:HA	9:i:45:ARG:HD2	2.04	0.40
15:o:7:ALA:O	15:o:11:ILE:HG13	2.21	0.40
25:z:67:HIS:HB2	61:z:402:MQH:C21	2.52	0.40
25:z:123:GLY:HA2	25:z:126:VAL:HG22	2.03	0.40
25:z:262:PHE:CD1	61:z:402:MQH:C22	3.04	0.40
26:A:479:A:H4'	26:A:480:A:OP1	2.22	0.40
26:A:910:A:H2'	26:A:911:A:C8	2.55	0.40
26:A:1114:C:H2'	26:A:1115:G:C8	2.56	0.40
26:A:1739:A:H2'	26:A:1740:G:O4'	2.22	0.40
26:A:2392:A:O2'	37:N:60:ARG:O	2.36	0.40
48:Y:83:GLU:O	48:Y:84:ALA:C	2.64	0.40
53:4:52:ARG:CZ	53:4:54:VAL:HG12	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
3	c	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	d	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	e	154/167 (92%)	154 (100%)	0	0	100	100
6	f	101/131 (77%)	97 (96%)	4 (4%)	0	100	100
7	g	150/156 (96%)	142 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	h	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	i	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
10	j	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	8
11	k	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
12	l	118/124 (95%)	113 (96%)	5 (4%)	0	100	100
13	m	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
14	n	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	p	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	r	52/75 (69%)	52 (100%)	0	0	100	100
19	s	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
20	t	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	u	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
25	z	367/394 (93%)	342 (93%)	24 (6%)	1 (0%)	36	35
28	C	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
29	D	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	21
30	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
31	F	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
32	G	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
33	H	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
34	J	139/142 (98%)	117 (84%)	21 (15%)	1 (1%)	18	14
35	L	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
36	M	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
37	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
38	O	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
39	P	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
40	Q	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
41	R	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
42	S	115/118 (98%)	115 (100%)	0	0	100	100
43	T	101/103 (98%)	98 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	U	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
45	V	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
46	W	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
47	X	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
48	Y	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
49	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
50	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
51	2	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
52	3	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
53	4	53/57 (93%)	52 (98%)	1 (2%)	0	100	100
54	5	49/55 (89%)	49 (100%)	0	0	100	100
55	6	44/46 (96%)	44 (100%)	0	0	100	100
56	7	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
57	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5967/6422 (93%)	5758 (96%)	205 (3%)	4 (0%)	49	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	z	266	LEU
34	J	33	VAL
10	j	57	VAL
29	D	149	ASN

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	
2	b	186/199 (94%)	184 (99%)	2 (1%)	65	73
3	c	170/190 (90%)	167 (98%)	3 (2%)	51	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	172/173 (99%)	168 (98%)	4 (2%)	44	49
5	e	119/126 (94%)	116 (98%)	3 (2%)	42	45
6	f	90/112 (80%)	88 (98%)	2 (2%)	45	50
7	g	125/129 (97%)	120 (96%)	5 (4%)	28	27
8	h	104/105 (99%)	102 (98%)	2 (2%)	50	56
9	i	105/107 (98%)	103 (98%)	2 (2%)	50	56
10	j	86/90 (96%)	82 (95%)	4 (5%)	23	22
11	k	89/98 (91%)	88 (99%)	1 (1%)	65	73
12	l	101/103 (98%)	100 (99%)	1 (1%)	68	75
13	m	93/96 (97%)	91 (98%)	2 (2%)	45	50
14	n	83/84 (99%)	83 (100%)	0	100	100
15	o	76/77 (99%)	76 (100%)	0	100	100
16	p	65/65 (100%)	63 (97%)	2 (3%)	35	37
17	q	73/78 (94%)	71 (97%)	2 (3%)	39	42
18	r	47/65 (72%)	47 (100%)	0	100	100
19	s	72/79 (91%)	69 (96%)	3 (4%)	26	25
20	t	65/66 (98%)	65 (100%)	0	100	100
21	u	60/61 (98%)	60 (100%)	0	100	100
25	z	312/327 (95%)	295 (95%)	17 (5%)	20	17
28	C	216/218 (99%)	214 (99%)	2 (1%)	70	78
29	D	163/163 (100%)	161 (99%)	2 (1%)	63	70
30	E	165/165 (100%)	158 (96%)	7 (4%)	26	25
31	F	148/150 (99%)	141 (95%)	7 (5%)	23	22
32	G	137/138 (99%)	134 (98%)	3 (2%)	45	50
33	H	32/114 (28%)	31 (97%)	1 (3%)	35	37
35	L	116/116 (100%)	114 (98%)	2 (2%)	53	60
36	M	104/104 (100%)	103 (99%)	1 (1%)	68	75
37	N	103/103 (100%)	102 (99%)	1 (1%)	68	75
38	O	107/107 (100%)	107 (100%)	0	100	100
39	P	98/103 (95%)	97 (99%)	1 (1%)	68	75
40	Q	86/87 (99%)	83 (96%)	3 (4%)	32	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	R	99/100 (99%)	98 (99%)	1 (1%)	68	75
42	S	89/90 (99%)	88 (99%)	1 (1%)	65	73
43	T	84/84 (100%)	81 (96%)	3 (4%)	31	31
44	U	93/93 (100%)	92 (99%)	1 (1%)	65	73
45	V	80/84 (95%)	79 (99%)	1 (1%)	61	68
46	W	83/85 (98%)	80 (96%)	3 (4%)	31	31
47	X	78/78 (100%)	77 (99%)	1 (1%)	61	68
48	Y	57/63 (90%)	57 (100%)	0	100	100
49	Z	67/68 (98%)	67 (100%)	0	100	100
50	1	54/55 (98%)	54 (100%)	0	100	100
51	2	48/49 (98%)	47 (98%)	1 (2%)	47	52
52	3	54/62 (87%)	54 (100%)	0	100	100
53	4	46/48 (96%)	46 (100%)	0	100	100
54	5	46/49 (94%)	45 (98%)	1 (2%)	45	50
55	6	37/38 (97%)	37 (100%)	0	100	100
56	7	51/52 (98%)	51 (100%)	0	100	100
57	8	34/34 (100%)	34 (100%)	0	100	100
All	All	4868/5130 (95%)	4770 (98%)	98 (2%)	48	54

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	54	LEU
2	b	205	ASP
3	c	67	THR
3	c	101	ILE
3	c	144	LEU
4	d	144	SER
4	d	181	THR
4	d	189	SER
4	d	192	SER
5	e	32	SER
5	e	116	GLU
5	e	160	SER
6	f	14	GLN
6	f	62	MET

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Mol	Chain	Res	Type
7	g	37	SER
7	g	75	VAL
7	g	80	VAL
7	g	113	ASP
7	g	146	GLU
8	h	96	MET
8	h	129	VAL
9	i	85	ARG
9	i	128	SER
10	j	8	ILE
10	j	44	THR
10	j	74	VAL
10	j	96	VAL
11	k	95	SER
12	l	10	LYS
13	m	4	ILE
13	m	97	VAL
16	p	21	VAL
16	p	78	VAL
17	q	17	MET
17	q	27	ARG
19	s	27	ASP
19	s	35	SER
19	s	48	THR
25	z	68	VAL
25	z	74	THR
25	z	148	GLU
25	z	166	ASP
25	z	168	THR
25	z	172	ARG
25	z	184	GLU
25	z	190	LEU
25	z	212	LEU
25	z	251	THR
25	z	265	LEU
25	z	303	THR
25	z	309	VAL
25	z	320	HIS
25	z	336	THR
25	z	377	ILE
25	z	393	LEU
28	C	65	VAL

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Mol	Chain	Res	Type
28	C	201	MET
29	D	25	THR
29	D	74	GLU
30	E	1	MET
30	E	15	SER
30	E	69	ARG
30	E	105	LEU
30	E	107	SER
30	E	165	HIS
30	E	179	SER
31	F	36	LEU
31	F	132	VAL
31	F	136	ILE
31	F	141	ILE
31	F	149	VAL
31	F	153	ASP
31	F	164	GLU
32	G	15	VAL
32	G	134	LYS
32	G	168	VAL
33	H	21	VAL
35	L	3	THR
35	L	70	THR
36	M	91	SER
37	N	141	LYS
39	P	6	SER
40	Q	15	ARG
40	Q	35	ILE
40	Q	116	GLN
41	R	88	ARG
42	S	31	VAL
43	T	20	VAL
43	T	40	MET
43	T	45	GLU
44	U	66	ILE
45	V	88	LYS
46	W	39	ILE
46	W	59	VAL
46	W	83	VAL
47	X	65	VAL
51	2	55	VAL
54	5	54	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	94	HIS
2	b	120	GLN
2	b	168	HIS
2	b	177	ASN
3	c	8	ASN
3	c	102	ASN
3	c	123	GLN
4	d	136	GLN
4	d	140	ASN
5	e	89	HIS
5	e	97	GLN
5	e	146	ASN
5	e	148	ASN
6	f	11	HIS
6	f	46	GLN
7	g	86	GLN
7	g	97	ASN
7	g	122	ASN
7	g	148	ASN
9	i	5	GLN
9	i	110	GLN
10	j	35	GLN
11	k	40	ASN
11	k	109	ASN
11	k	118	HIS
13	m	14	HIS
13	m	52	GLN
14	n	66	GLN
15	o	35	GLN
15	o	40	GLN
16	p	59	HIS
18	r	74	HIS
19	s	56	GLN
20	t	13	GLN
20	t	48	GLN
20	t	61	GLN
20	t	82	GLN
25	z	64	ASN
25	z	67	HIS
25	z	91	ASN
30	E	94	GLN

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Mol	Chain	Res	Type
31	F	27	GLN
31	F	63	GLN
31	F	81	GLN
32	G	22	GLN
32	G	88	GLN
32	G	104	ASN
32	G	139	GLN
35	L	80	HIS
35	L	136	GLN
36	M	29	HIS
38	O	60	GLN
38	O	97	GLN
39	P	31	HIS
40	Q	98	GLN
40	Q	100	HIS
40	Q	104	GLN
42	S	81	ASN
44	U	31	GLN
47	X	12	GLN
47	X	87	GLN
48	Y	12	ASN
48	Y	50	ASN
48	Y	57	HIS
49	Z	36	HIS
50	1	20	ASN
50	1	27	ASN
50	1	31	GLN
50	1	45	GLN
52	3	20	ASN
57	8	13	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1527/1542 (99%)	215 (14%)	0
22	v	10/24 (41%)	1 (10%)	0
23	w	70/74 (94%)	20 (28%)	0
24	x	75/77 (97%)	10 (13%)	0
26	A	2897/2904 (99%)	420 (14%)	18 (0%)
27	B	119/120 (99%)	15 (12%)	3 (2%)
All	All	4698/4741 (99%)	681 (14%)	21 (0%)

All (681) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	44	A
1	a	47	C
1	a	48	C
1	a	50	A
1	a	51	A
1	a	63	C
1	a	66	A
1	a	68	G
1	a	69	G
1	a	71	A
1	a	75	G
1	a	78	A
1	a	81	A
1	a	82	G
1	a	84	U
1	a	85	U
1	a	86	G
1	a	91	U
1	a	92	U
1	a	93	U
1	a	97	G
1	a	98	A
1	a	100	G
1	a	121	U
1	a	130	A
1	a	131	A
1	a	163	C
1	a	174	A
1	a	177	G
1	a	197	A
1	a	201	G
1	a	202	G
1	a	203	G
1	a	204	G
1	a	207	C

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Mol	Chain	Res	Type
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	213	G
1	a	214	C
1	a	218	U
1	a	219	U
1	a	220	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	289	G
1	a	321	A
1	a	328	C
1	a	341	C
1	a	344	A
1	a	351	G
1	a	352	C
1	a	354	G
1	a	356	A
1	a	367	U
1	a	372	C
1	a	384	G
1	a	398	U
1	a	406	G
1	a	412	A
1	a	413	G
1	a	414	A
1	a	415	A
1	a	421	U
1	a	424	G
1	a	429	U
1	a	453	G
1	a	455	G
1	a	462	G
1	a	464	U
1	a	467	U
1	a	468	A

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Mol	Chain	Res	Type
1	a	478	A
1	a	480	U
1	a	484	G
1	a	486	U
1	a	495	A
1	a	497	G
1	a	511	C
1	a	518	C
1	a	527	G7M
1	a	531	U
1	a	532	A
1	a	547	A
1	a	559	A
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	596	A
1	a	633	G
1	a	650	G
1	a	653	U
1	a	665	A
1	a	674	G
1	a	687	A
1	a	723	U
1	a	724	G
1	a	733	G
1	a	748	G
1	a	755	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	828	U
1	a	829	G
1	a	838	G
1	a	851	G
1	a	874	G
1	a	890	G

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Mol	Chain	Res	Type
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	966	2MG
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	1003	G
1	a	1004	A
1	a	1009	U
1	a	1020	G
1	a	1024	G
1	a	1026	G
1	a	1027	C
1	a	1030	U
1	a	1031	C
1	a	1034	G
1	a	1036	A
1	a	1037	C
1	a	1038	C
1	a	1039	G
1	a	1042	A
1	a	1043	G
1	a	1046	A
1	a	1065	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1126	U
1	a	1132	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1159	U
1	a	1164	G
1	a	1167	A
1	a	1171	A

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Mol	Chain	Res	Type
1	a	1174	G
1	a	1184	G
1	a	1196	A
1	a	1197	A
1	a	1212	U
1	a	1213	A
1	a	1227	A
1	a	1228	C
1	a	1238	A
1	a	1256	A
1	a	1258	G
1	a	1260	G
1	a	1280	A
1	a	1285	A
1	a	1286	U
1	a	1287	A
1	a	1300	G
1	a	1302	C
1	a	1317	C
1	a	1320	C
1	a	1338	G
1	a	1346	A
1	a	1353	G
1	a	1363	A
1	a	1370	G
1	a	1378	C
1	a	1379	G
1	a	1381	U
1	a	1419	G
1	a	1429	A
1	a	1441	A
1	a	1446	A
1	a	1447	A
1	a	1449	C
1	a	1450	U
1	a	1451	U
1	a	1452	C
1	a	1492	A
1	a	1493	A
1	a	1497	G
1	a	1499	A
1	a	1503	A

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Mol	Chain	Res	Type
1	a	1505	G
1	a	1506	U
1	a	1517	G
1	a	1529	G
1	a	1530	G
22	v	24	A
23	w	5	G
23	w	8	4SU
23	w	9	A
23	w	11	U
23	w	15	A
23	w	17	G
23	w	18	G
23	w	24	A
23	w	33	U
23	w	45	U
23	w	47	C
23	w	51	G
23	w	52	G
23	w	55	PSU
23	w	56	C
23	w	59	U
23	w	67	G
23	w	68	C
23	w	71	G
23	w	75	C
24	x	6	G
24	x	9	G
24	x	18	G
24	x	19	G
24	x	21	A
24	x	47	U
24	x	58	A
24	x	63	G
24	x	70	G
24	x	76	M3O
26	A	2	G
26	A	5	A
26	A	9	G
26	A	13	A
26	A	34	U
26	A	58	G

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Mol	Chain	Res	Type
26	A	60	G
26	A	71	A
26	A	74	A
26	A	75	G
26	A	100	U
26	A	101	A
26	A	103	A
26	A	118	A
26	A	119	A
26	A	120	U
26	A	133	U
26	A	135	U
26	A	137	U
26	A	141	G
26	A	142	A
26	A	143	C
26	A	145	C
26	A	146	A
26	A	147	C
26	A	148	U
26	A	163	C
26	A	165	A
26	A	181	A
26	A	196	A
26	A	215	G
26	A	216	A
26	A	222	A
26	A	228	C
26	A	233	A
26	A	248	G
26	A	267	C
26	A	271	G
26	A	272	A
26	A	276	U
26	A	277	G
26	A	278	A
26	A	281	C
26	A	282	A
26	A	284	U
26	A	287	G
26	A	289	G
26	A	291	G

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Mol	Chain	Res	Type
26	A	295	G
26	A	311	A
26	A	329	G
26	A	330	A
26	A	352	A
26	A	353	C
26	A	354	A
26	A	356	G
26	A	362	A
26	A	386	G
26	A	404	A
26	A	405	U
26	A	411	G
26	A	412	A
26	A	424	G
26	A	429	A
26	A	430	A
26	A	448	U
26	A	451	U
26	A	456	C
26	A	481	G
26	A	491	G
26	A	505	A
26	A	509	C
26	A	530	G
26	A	531	C
26	A	532	A
26	A	533	G
26	A	544	C
26	A	545	U
26	A	546	U
26	A	547	A
26	A	549	G
26	A	563	A
26	A	573	U
26	A	575	A
26	A	602	A
26	A	603	A
26	A	615	U
26	A	625	G
26	A	627	A
26	A	637	A

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Mol	Chain	Res	Type
26	A	642	U
26	A	645	C
26	A	646	U
26	A	647	G
26	A	654	A
26	A	655	A
26	A	686	U
26	A	706	A
26	A	707	G
26	A	711	G
26	A	715	A
26	A	717	C
26	A	730	A
26	A	747	5MU
26	A	775	G
26	A	776	G
26	A	782	A
26	A	784	G
26	A	785	G
26	A	789	A
26	A	805	G
26	A	812	C
26	A	827	U
26	A	828	U
26	A	845	A
26	A	846	U
26	A	847	U
26	A	859	G
26	A	877	A
26	A	885	C
26	A	891	G
26	A	892	A
26	A	895	U
26	A	896	A
26	A	900	A
26	A	907	G
26	A	910	A
26	A	912	C
26	A	914	G
26	A	915	C
26	A	931	U
26	A	932	U

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Mol	Chain	Res	Type
26	A	934	U
26	A	946	C
26	A	961	C
26	A	974	G
26	A	983	A
26	A	996	A
26	A	1012	U
26	A	1013	C
26	A	1026	G
26	A	1033	U
26	A	1035	U
26	A	1036	G
26	A	1038	G
26	A	1039	A
26	A	1046	A
26	A	1047	G
26	A	1059	G
26	A	1061	U
26	A	1062	G
26	A	1064	C
26	A	1065	U
26	A	1069	A
26	A	1070	A
26	A	1071	G
26	A	1073	A
26	A	1075	C
26	A	1076	C
26	A	1078	U
26	A	1079	C
26	A	1080	A
26	A	1082	U
26	A	1084	A
26	A	1085	A
26	A	1087	G
26	A	1088	A
26	A	1091	G
26	A	1095	A
26	A	1097	U
26	A	1104	C
26	A	1111	A
26	A	1113	U
26	A	1118	C

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Mol	Chain	Res	Type
26	A	1132	U
26	A	1133	A
26	A	1134	A
26	A	1135	C
26	A	1142	A
26	A	1150	C
26	A	1151	A
26	A	1152	C
26	A	1168	G
26	A	1182	G
26	A	1212	G
26	A	1227	G
26	A	1253	A
26	A	1256	G
26	A	1271	G
26	A	1272	A
26	A	1300	G
26	A	1301	A
26	A	1352	U
26	A	1365	A
26	A	1379	U
26	A	1383	A
26	A	1409	U
26	A	1411	U
26	A	1414	C
26	A	1415	U
26	A	1416	G
26	A	1417	C
26	A	1419	A
26	A	1420	A
26	A	1428	C
26	A	1434	A
26	A	1451	C
26	A	1453	A
26	A	1460	U
26	A	1465	G
26	A	1482	G
26	A	1483	G
26	A	1486	U
26	A	1493	C
26	A	1505	A
26	A	1508	A

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Mol	Chain	Res	Type
26	A	1509	A
26	A	1510	G
26	A	1515	A
26	A	1524	G
26	A	1535	A
26	A	1536	C
26	A	1537	G
26	A	1538	G
26	A	1566	A
26	A	1569	A
26	A	1578	U
26	A	1580	A
26	A	1581	G
26	A	1584	U
26	A	1585	C
26	A	1608	A
26	A	1618	6MZ
26	A	1619	G
26	A	1647	U
26	A	1648	U
26	A	1649	G
26	A	1674	G
26	A	1715	G
26	A	1729	U
26	A	1730	C
26	A	1731	G
26	A	1732	C
26	A	1733	G
26	A	1738	G
26	A	1764	C
26	A	1773	A
26	A	1776	G
26	A	1782	U
26	A	1784	A
26	A	1800	C
26	A	1801	A
26	A	1808	A
26	A	1816	C
26	A	1829	A
26	A	1848	A
26	A	1857	G
26	A	1861	G

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Mol	Chain	Res	Type
26	A	1862	G
26	A	1869	G
26	A	1875	G
26	A	1876	A
26	A	1878	G
26	A	1879	C
26	A	1906	G
26	A	1907	G
26	A	1919	A
26	A	1929	G
26	A	1930	G
26	A	1937	A
26	A	1938	A
26	A	1955	U
26	A	1965	C
26	A	1967	C
26	A	1970	A
26	A	1971	U
26	A	1972	G
26	A	1991	U
26	A	1993	U
26	A	2020	A
26	A	2023	C
26	A	2027	G
26	A	2031	A
26	A	2033	A
26	A	2043	C
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G
26	A	2062	A
26	A	2069	G7M
26	A	2101	A
26	A	2110	G
26	A	2111	U
26	A	2112	G
26	A	2115	G
26	A	2117	A
26	A	2118	U
26	A	2119	A
26	A	2120	G

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Mol	Chain	Res	Type
26	A	2121	G
26	A	2124	G
26	A	2126	A
26	A	2127	G
26	A	2128	G
26	A	2129	C
26	A	2131	U
26	A	2132	U
26	A	2133	G
26	A	2137	U
26	A	2138	G
26	A	2145	C
26	A	2146	C
26	A	2147	A
26	A	2157	G
26	A	2158	A
26	A	2159	G
26	A	2160	C
26	A	2161	C
26	A	2162	G
26	A	2165	C
26	A	2167	U
26	A	2169	A
26	A	2170	A
26	A	2171	A
26	A	2172	U
26	A	2173	A
26	A	2175	C
26	A	2176	A
26	A	2178	C
26	A	2189	U
26	A	2190	G
26	A	2192	U
26	A	2198	A
26	A	2204	G
26	A	2212	A
26	A	2225	A
26	A	2238	G
26	A	2239	G
26	A	2268	A
26	A	2278	A
26	A	2283	C

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Mol	Chain	Res	Type
26	A	2287	A
26	A	2304	G
26	A	2305	U
26	A	2308	G
26	A	2309	A
26	A	2312	U
26	A	2313	C
26	A	2322	A
26	A	2325	G
26	A	2333	A
26	A	2334	U
26	A	2335	A
26	A	2347	C
26	A	2361	G
26	A	2383	G
26	A	2385	C
26	A	2396	G
26	A	2402	U
26	A	2403	C
26	A	2406	A
26	A	2422	C
26	A	2424	C
26	A	2425	A
26	A	2428	G
26	A	2429	G
26	A	2441	U
26	A	2448	A
26	A	2469	A
26	A	2470	G
26	A	2474	U
26	A	2476	A
26	A	2478	A
26	A	2490	G
26	A	2502	G
26	A	2505	G
26	A	2506	U
26	A	2517	C
26	A	2518	A
26	A	2529	G
26	A	2535	G
26	A	2547	A
26	A	2554	U

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Mol	Chain	Res	Type
26	A	2566	A
26	A	2567	G
26	A	2572	A
26	A	2573	C
26	A	2602	A
26	A	2609	U
26	A	2613	U
26	A	2629	U
26	A	2630	G
26	A	2663	G
26	A	2670	A
26	A	2689	U
26	A	2690	U
26	A	2700	A
26	A	2714	G
26	A	2716	C
26	A	2726	A
26	A	2744	G
26	A	2748	A
26	A	2757	A
26	A	2758	A
26	A	2765	A
26	A	2778	A
26	A	2785	C
26	A	2796	U
26	A	2818	U
26	A	2820	A
26	A	2821	A
26	A	2833	U
26	A	2873	A
26	A	2883	A
26	A	2884	U
26	A	2891	U
26	A	2899	A
26	A	2900	A
26	A	2902	C
27	B	4	C
27	B	9	G
27	B	10	G
27	B	16	G
27	B	25	U
27	B	35	C

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Mol	Chain	Res	Type
27	B	51	G
27	B	56	G
27	B	65	U
27	B	67	G
27	B	89	U
27	B	108	A
27	B	109	A
27	B	115	A
27	B	120	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	142	A
26	A	277	G
26	A	764	A
26	A	784	G
26	A	899	A
26	A	984	A
26	A	1026	G
26	A	1046	A
26	A	1084	A
26	A	1110	G
26	A	1440	U
26	A	1729	U
26	A	2123	G
26	A	2189	U
26	A	2191	A
26	A	2489	U
26	A	2572	A
26	A	2756	U
27	B	3	C
27	B	9	G
27	B	66	A

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

49 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
26	5MC	A	1962	59,26	19,22,23	1.52	3 (15%)	26,32,35	1.17	4 (15%)
24	5MC	x	32	24	19,22,23	1.39	3 (15%)	26,32,35	1.25	2 (7%)
26	5MU	A	1939	59,26	19,22,23	1.49	6 (31%)	27,32,35	2.14	6 (22%)
26	G7M	A	2069	59,26	23,26,27	1.63	4 (17%)	34,39,42	1.44	3 (8%)
1	5MC	a	1407	58,1	19,22,23	1.52	3 (15%)	26,32,35	1.37	5 (19%)
1	5MC	a	967	1	19,22,23	1.63	3 (15%)	26,32,35	1.14	4 (15%)
1	2MG	a	966	1	23,26,27	1.27	3 (13%)	33,38,41	2.24	7 (21%)
24	5MU	x	54	24	19,22,23	1.40	5 (26%)	27,32,35	2.00	7 (25%)
26	PSU	A	2504	59,58,26	18,21,22	1.48	3 (16%)	21,30,33	1.99	4 (19%)
24	M3O	x	76	58,24	31,34,35	1.36	4 (12%)	41,47,50	2.40	14 (34%)
1	4OC	a	1402	58,1	20,23,24	0.78	0	25,32,35	1.11	2 (8%)
23	L3X	w	76	23	24,28,29	1.34	3 (12%)	27,40,43	2.17	9 (33%)
26	5MU	A	747	26	19,22,23	1.43	5 (26%)	27,32,35	1.82	7 (25%)
1	MA6	a	1519	1	23,26,27	1.53	4 (17%)	33,38,41	2.37	14 (42%)
26	6MZ	A	1618	58,26	22,25,26	1.50	4 (18%)	29,36,39	2.25	10 (34%)
29	MEQ	D	150	29	8,9,10	0.94	0	5,10,12	1.02	0
26	PSU	A	2604	58,26	18,21,22	1.60	4 (22%)	21,30,33	1.78	3 (14%)
12	D2T	l	89	12	8,9,10	1.52	1 (12%)	6,11,13	1.64	2 (33%)
26	OMU	A	2552	58,26	19,22,23	1.26	3 (15%)	25,31,34	1.88	6 (24%)
1	2MG	a	1207	1	23,26,27	1.28	4 (17%)	33,38,41	2.03	7 (21%)
26	PSU	A	2580	58,59,26	18,21,22	1.62	5 (27%)	21,30,33	1.89	5 (23%)
1	MA6	a	1518	1	23,26,27	1.55	6 (26%)	33,38,41	2.27	13 (39%)
11	IAS	k	119	11,21	6,7,8	1.02	0	3,8,10	1.50	1 (33%)
26	PSU	A	2457	26	18,21,22	1.61	4 (22%)	21,30,33	2.05	4 (19%)
26	1MG	A	745	58,26	23,26,27	1.17	4 (17%)	33,39,42	2.18	9 (27%)
38	MS6	O	82	38	5,7,8	0.62	0	2,7,9	0.85	0
24	PSU	x	55	24	18,21,22	1.38	3 (16%)	21,30,33	2.06	3 (14%)
26	PSU	A	1911	26	18,21,22	1.44	4 (22%)	21,30,33	2.08	5 (23%)
1	PSU	a	516	58,1	18,21,22	1.59	4 (22%)	21,30,33	1.87	5 (23%)
26	PSU	A	2605	26	18,21,22	1.62	4 (22%)	21,30,33	1.88	5 (23%)
26	OMC	A	2498	58,26	19,22,23	0.73	0	25,31,34	0.96	0
1	UR3	a	1498	1	19,22,23	0.89	0	26,32,35	1.83	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	H2U	A	2449	58,26	18,21,22	0.64	0	19,30,33	0.82	1 (5%)
23	4SU	w	8	23	18,21,22	1.92	4 (22%)	25,30,33	2.21	5 (20%)
1	2MG	a	1516	1	23,26,27	1.28	4 (17%)	33,38,41	2.34	9 (27%)
26	2MA	A	2503	59,58,26	22,25,26	1.43	4 (18%)	32,37,40	2.36	9 (28%)
24	4SU	x	8	24	18,21,22	1.88	4 (22%)	25,30,33	1.95	5 (20%)
23	PSU	w	55	23	18,21,22	1.36	2 (11%)	21,30,33	2.18	4 (19%)
26	PSU	A	746	58,26	18,21,22	1.57	5 (27%)	21,30,33	1.95	5 (23%)
26	6MZ	A	2030	58,26	22,25,26	1.40	5 (22%)	29,36,39	2.33	12 (41%)
26	OMG	A	2251	59,58,24,26	23,26,27	1.27	4 (17%)	32,38,41	1.89	5 (15%)
26	2MG	A	2445	58,26	23,26,27	1.30	4 (17%)	33,38,41	2.09	6 (18%)
26	PSU	A	1917	26	18,21,22	1.58	4 (22%)	21,30,33	1.86	5 (23%)
38	4D4	O	81	38	9,11,12	2.14	2 (22%)	7,13,15	1.53	2 (28%)
26	PSU	A	955	58,26	18,21,22	1.55	4 (22%)	21,30,33	2.04	4 (19%)
26	2MG	A	1835	26	23,26,27	1.30	4 (17%)	33,38,41	2.02	6 (18%)
26	3TD	A	1915	26	19,22,23	6.75	12 (63%)	23,32,35	2.01	4 (17%)
1	G7M	a	527	1	23,26,27	1.56	4 (17%)	34,39,42	1.72	4 (11%)
23	5MU	w	54	23	19,22,23	1.36	6 (31%)	27,32,35	2.11	7 (25%)

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
26	5MC	A	1962	59,26	-	0/7/25/26	0/2/2/2
24	5MC	x	32	24	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	59,26	-	0/7/25/26	0/2/2/2
26	G7M	A	2069	59,26	-	2/7/25/26	0/3/3/3
1	5MC	a	1407	58,1	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
24	5MU	x	54	24	-	0/7/25/26	0/2/2/2
26	PSU	A	2504	59,58,26	-	1/7/25/26	0/2/2/2
24	M3O	x	76	58,24	-	6/22/40/41	0/3/3/3
1	4OC	a	1402	58,1	-	0/9/29/30	0/2/2/2
23	L3X	w	76	23	-	2/13/31/32	0/3/3/3
26	5MU	A	747	26	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	4/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	6MZ	A	1618	58,26	-	2/9/27/28	0/3/3/3
29	MEQ	D	150	29	-	3/8/9/11	-
26	PSU	A	2604	58,26	-	0/7/25/26	0/2/2/2
12	D2T	l	89	12	-	4/7/12/14	-
26	OMU	A	2552	58,26	-	0/9/27/28	0/2/2/2
1	2MG	a	1207	1	-	0/9/27/28	0/3/3/3
26	PSU	A	2580	58,59,26	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/11/29/30	0/3/3/3
11	IAS	k	119	11,21	-	0/7/7/8	-
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
26	1MG	A	745	58,26	-	0/7/25/26	0/3/3/3
38	MS6	O	82	38	-	1/4/6/8	-
24	PSU	x	55	24	-	0/7/25/26	0/2/2/2
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
1	PSU	a	516	58,1	-	0/7/25/26	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	58,26	-	0/9/27/28	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
26	H2U	A	2449	58,26	-	0/7/38/39	0/2/2/2
23	4SU	w	8	23	-	2/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
26	2MA	A	2503	59,58,26	-	2/7/25/26	0/3/3/3
24	4SU	x	8	24	-	1/7/25/26	0/2/2/2
23	PSU	w	55	23	-	1/7/25/26	0/2/2/2
26	PSU	A	746	58,26	-	1/7/25/26	0/2/2/2
26	6MZ	A	2030	58,26	-	2/9/27/28	0/3/3/3
26	OMG	A	2251	59,58,24,26	-	0/9/27/28	0/3/3/3
26	2MG	A	2445	58,26	-	0/9/27/28	0/3/3/3
26	PSU	A	1917	26	-	0/7/25/26	0/2/2/2
38	4D4	O	81	38	-	0/11/12/14	-
26	PSU	A	955	58,26	-	0/7/25/26	0/2/2/2
26	2MG	A	1835	26	-	0/9/27/28	0/3/3/3
26	3TD	A	1915	26	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
23	5MU	w	54	23	-	2/7/25/26	0/2/2/2

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1915	3TD	O4'-C1'	15.72	1.65	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1915	3TD	C2'-C1'	-15.31	1.33	1.53
26	A	1915	3TD	C6-C5	12.52	1.49	1.35
26	A	1915	3TD	C2-N1	9.35	1.48	1.37
26	A	1915	3TD	O4'-C4'	-6.31	1.31	1.45
1	a	967	5MC	C5-C4	5.88	1.48	1.44
26	A	1915	3TD	C6-N1	5.81	1.45	1.36
1	a	1407	5MC	C5-C4	5.60	1.48	1.44
26	A	1962	5MC	C5-C4	5.54	1.48	1.44
38	O	81	4D4	CZ-NE	5.35	1.43	1.33
1	a	527	G7M	C5-N7	-5.27	1.33	1.39
26	A	2069	G7M	C5-N7	-5.11	1.33	1.39
23	w	8	4SU	C4-S4	-5.10	1.59	1.68
24	x	8	4SU	C4-S4	-4.96	1.59	1.68
26	A	1915	3TD	C2-N3	4.66	1.48	1.38
24	x	32	5MC	C5-C4	4.62	1.47	1.44
26	A	1618	6MZ	C5-C4	4.34	1.46	1.39
1	a	1518	MA6	C5-C4	4.30	1.46	1.39
23	w	8	4SU	C4-N3	-4.06	1.33	1.37
1	a	1519	MA6	C5-C4	4.01	1.46	1.39
24	x	76	M3O	C5-N7	-4.00	1.31	1.39
23	w	76	L3X	C5-N7	-3.96	1.31	1.39
26	A	2503	2MA	C5-C4	3.93	1.46	1.39
24	x	8	4SU	C4-N3	-3.75	1.33	1.37
26	A	2604	PSU	C4-N3	-3.71	1.31	1.38
24	x	76	M3O	O3'-C	3.68	1.42	1.34
1	a	516	PSU	C6-C5	3.68	1.39	1.35
26	A	2504	PSU	C6-C5	3.62	1.39	1.35
26	A	2030	6MZ	C5-C4	3.59	1.45	1.39
26	A	1915	3TD	O3'-C3'	-3.58	1.34	1.43
26	A	1917	PSU	C4-N3	-3.56	1.32	1.38
26	A	746	PSU	C6-C5	3.56	1.39	1.35
26	A	2605	PSU	C4-N3	-3.54	1.32	1.38
26	A	955	PSU	C4-N3	-3.44	1.32	1.38
26	A	2457	PSU	C6-C5	3.41	1.39	1.35
26	A	2605	PSU	C6-C5	3.41	1.39	1.35
23	w	55	PSU	C6-C5	3.40	1.39	1.35
26	A	1911	PSU	C4-N3	-3.38	1.32	1.38
26	A	2552	OMU	C4-N3	-3.31	1.32	1.38
26	A	2580	PSU	C4-N3	-3.29	1.32	1.38
26	A	746	PSU	C4-N3	-3.26	1.32	1.38
24	x	8	4SU	C5-C4	-3.26	1.38	1.42
26	A	2457	PSU	C4-N3	-3.23	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2504	PSU	C4-N3	-3.21	1.32	1.38
23	w	76	L3X	C5-C4	-3.20	1.33	1.39
26	A	2604	PSU	C6-C5	3.15	1.38	1.35
26	A	1835	2MG	C6-N1	-3.13	1.33	1.38
26	A	747	5MU	C2-N3	-3.13	1.32	1.38
26	A	2605	PSU	C2-N3	-3.13	1.32	1.37
26	A	2030	6MZ	C5-N7	-3.12	1.33	1.39
26	A	2604	PSU	C2-N3	-3.10	1.32	1.37
26	A	955	PSU	C6-C5	3.10	1.38	1.35
26	A	1939	5MU	C4-N3	-3.09	1.33	1.38
24	x	76	M3O	C5-C4	-3.09	1.33	1.39
1	a	516	PSU	C4-N3	-3.08	1.33	1.38
26	A	2069	G7M	C6-N1	-3.07	1.33	1.38
26	A	2580	PSU	C6-C5	3.07	1.38	1.35
26	A	1917	PSU	C6-C5	3.03	1.38	1.35
24	x	55	PSU	C6-C5	3.01	1.38	1.35
1	a	1516	2MG	C6-N1	-3.00	1.33	1.38
1	a	516	PSU	C2-N3	-2.99	1.32	1.37
26	A	747	5MU	C4-N3	-2.97	1.33	1.38
26	A	1915	3TD	O2-C2	-2.96	1.17	1.23
26	A	2580	PSU	C2-N3	-2.94	1.32	1.37
1	a	966	2MG	C5-C4	2.93	1.46	1.38
1	a	1207	2MG	C6-N1	-2.91	1.33	1.38
26	A	2251	OMG	C6-N1	-2.90	1.33	1.38
24	x	32	5MC	C6-C5	2.89	1.39	1.34
26	A	2251	OMG	C5-C4	2.87	1.46	1.38
1	a	1519	MA6	C5-C6	2.87	1.48	1.41
23	w	55	PSU	C4-N3	-2.87	1.33	1.38
26	A	1618	6MZ	C5-N7	-2.87	1.33	1.39
1	a	966	2MG	C6-N1	-2.87	1.33	1.38
26	A	2069	G7M	C4-N9	-2.85	1.30	1.38
26	A	1911	PSU	C6-C5	2.83	1.38	1.35
26	A	1835	2MG	C5-C4	2.82	1.46	1.38
24	x	55	PSU	C4-N3	-2.82	1.33	1.38
26	A	1939	5MU	C6-C5	2.81	1.39	1.34
1	a	1519	MA6	C4-N9	-2.81	1.31	1.37
26	A	2445	2MG	C6-N1	-2.81	1.33	1.38
38	O	81	4D4	CZ-NH1	2.79	1.44	1.34
26	A	1917	PSU	C2-N3	-2.79	1.32	1.37
26	A	745	1MG	C5-C4	2.77	1.46	1.38
26	A	2069	G7M	C5-C4	2.77	1.45	1.38
1	a	967	5MC	C6-C5	2.76	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2030	6MZ	C4-N9	-2.76	1.31	1.37
26	A	745	1MG	C2-N1	2.74	1.42	1.37
1	a	1518	MA6	C5-C6	2.73	1.48	1.41
1	a	1207	2MG	C5-C4	2.72	1.46	1.38
1	a	527	G7M	C5-C4	2.72	1.45	1.38
24	x	54	5MU	C2-N3	-2.70	1.33	1.38
24	x	54	5MU	C6-C5	2.68	1.39	1.34
26	A	2445	2MG	C5-C4	2.67	1.46	1.38
24	x	54	5MU	C4-N3	-2.67	1.33	1.38
26	A	2445	2MG	C5-N7	-2.67	1.33	1.39
23	w	8	4SU	C2-N3	-2.67	1.33	1.38
26	A	955	PSU	C2-N3	-2.66	1.33	1.37
1	a	1518	MA6	C5-N7	-2.65	1.34	1.39
26	A	2503	2MA	C5-N7	-2.64	1.34	1.39
23	w	76	L3X	C5-C6	-2.63	1.33	1.41
24	x	8	4SU	C2-N3	-2.62	1.33	1.38
12	l	89	D2T	CB-CA	-2.62	1.53	1.54
1	a	1516	2MG	C5-C4	2.62	1.45	1.38
26	A	2457	PSU	C2-N3	-2.60	1.33	1.37
23	w	8	4SU	C5-C4	-2.59	1.39	1.42
26	A	1939	5MU	C6-N1	-2.59	1.33	1.38
26	A	2457	PSU	C2-N1	-2.58	1.33	1.36
24	x	76	M3O	C5-C6	-2.58	1.33	1.41
26	A	1939	5MU	C2-N3	-2.57	1.33	1.38
23	w	54	5MU	C4-N3	-2.57	1.34	1.38
1	a	1518	MA6	C4-N9	-2.55	1.32	1.37
1	a	1519	MA6	C5-N7	-2.55	1.34	1.39
26	A	2251	OMG	C5-N7	-2.55	1.34	1.39
26	A	747	5MU	C6-C5	2.54	1.38	1.34
1	a	1516	2MG	C5-N7	-2.54	1.34	1.39
1	a	1207	2MG	C5-N7	-2.53	1.34	1.39
26	A	2580	PSU	C2-N1	-2.51	1.33	1.36
26	A	2251	OMG	C4-N9	-2.50	1.31	1.38
26	A	1835	2MG	C5-N7	-2.50	1.34	1.39
26	A	746	PSU	C2-N3	-2.50	1.33	1.37
26	A	1939	5MU	C4-C5	2.47	1.48	1.44
26	A	1618	6MZ	C5-C6	2.45	1.47	1.41
26	A	2445	2MG	C4-N9	-2.44	1.31	1.38
26	A	1915	3TD	O4-C4	-2.44	1.18	1.23
24	x	54	5MU	C6-N1	-2.43	1.33	1.38
26	A	1915	3TD	C4-N3	2.41	1.45	1.40
26	A	2552	OMU	C2-N3	-2.40	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	967	5MC	C6-N1	-2.40	1.33	1.38
26	A	1618	6MZ	C4-N9	-2.39	1.32	1.37
1	a	527	G7M	C6-N1	-2.39	1.34	1.38
26	A	2503	2MA	C5-C6	2.39	1.47	1.41
1	a	966	2MG	C5-N7	-2.38	1.34	1.39
26	A	745	1MG	C5-N7	-2.38	1.34	1.39
26	A	1911	PSU	C2-N3	-2.38	1.33	1.37
26	A	955	PSU	C2-N1	-2.37	1.33	1.36
26	A	2503	2MA	C4-N9	-2.36	1.32	1.37
1	a	1407	5MC	C6-C5	2.35	1.38	1.34
26	A	745	1MG	C4-N9	-2.35	1.32	1.38
23	w	54	5MU	C6-C5	2.33	1.38	1.34
1	a	527	G7M	C4-N9	-2.32	1.32	1.38
1	a	1207	2MG	C4-N9	-2.31	1.32	1.38
26	A	2580	PSU	O4'-C1'	-2.31	1.40	1.43
26	A	1962	5MC	C6-C5	2.30	1.38	1.34
26	A	747	5MU	C4-C5	2.29	1.48	1.44
1	a	1516	2MG	C4-N9	-2.27	1.32	1.38
23	w	54	5MU	C2-N3	-2.26	1.34	1.38
23	w	54	5MU	C2-N1	2.26	1.42	1.38
26	A	1915	3TD	C3'-C4'	2.25	1.58	1.53
26	A	1917	PSU	C2-N1	-2.24	1.33	1.36
26	A	2504	PSU	C2-N3	-2.20	1.33	1.37
1	a	1407	5MC	C6-N1	-2.20	1.34	1.38
26	A	746	PSU	O4'-C1'	-2.19	1.40	1.43
26	A	1962	5MC	C6-N1	-2.19	1.34	1.38
26	A	1835	2MG	C4-N9	-2.19	1.32	1.38
26	A	2030	6MZ	C5-C6	2.18	1.47	1.41
24	x	55	PSU	C2-N3	-2.18	1.33	1.37
26	A	747	5MU	C6-N1	-2.18	1.34	1.38
23	w	54	5MU	C6-N1	-2.18	1.34	1.38
1	a	1518	MA6	C8-N9	-2.15	1.33	1.37
26	A	2552	OMU	C5-C4	-2.15	1.39	1.43
23	w	54	5MU	C4-C5	2.11	1.48	1.44
1	a	1518	MA6	C6-N6	2.10	1.42	1.36
26	A	746	PSU	C2-N1	-2.10	1.33	1.36
24	x	54	5MU	C4-C5	2.09	1.48	1.44
24	x	32	5MC	C6-N1	-2.06	1.34	1.38
26	A	2604	PSU	C2-N1	-2.05	1.34	1.36
26	A	1911	PSU	O4'-C1'	-2.04	1.41	1.43
26	A	2605	PSU	C2-N1	-2.04	1.34	1.36
26	A	1939	5MU	C2-N1	2.00	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	516	PSU	C2-N1	-2.00	1.34	1.36
26	A	2030	6MZ	C8-N9	-2.00	1.34	1.37

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2503	2MA	C5-C4-N3	-7.83	118.93	127.18
24	x	76	M3O	C3'-O3'-C	-7.46	105.37	117.76
1	a	1498	UR3	C4-N3-C2	-7.42	118.61	124.58
1	a	1516	2MG	C2-N3-C4	7.41	121.27	112.00
1	a	966	2MG	C2-N3-C4	7.15	120.94	112.00
26	A	2445	2MG	C2-N3-C4	6.97	120.72	112.00
26	A	1835	2MG	C2-N3-C4	6.78	120.49	112.00
23	w	55	PSU	N1-C2-N3	6.75	122.28	115.17
23	w	8	4SU	C4-N3-C2	-6.71	120.88	127.31
1	a	1207	2MG	C2-N3-C4	6.65	120.32	112.00
26	A	2503	2MA	N3-C4-N9	6.57	135.33	126.99
26	A	1911	PSU	N1-C2-N3	6.54	122.06	115.17
26	A	955	PSU	N1-C2-N3	6.52	122.05	115.17
26	A	2457	PSU	N1-C2-N3	6.50	122.03	115.17
24	x	55	PSU	N1-C2-N3	6.41	121.93	115.17
26	A	1917	PSU	N1-C2-N3	6.35	121.86	115.17
1	a	966	2MG	C5-C4-N3	-6.34	118.30	128.39
26	A	745	1MG	N2-C2-N1	6.29	123.85	118.79
26	A	1915	3TD	N1-C2-N3	6.25	120.67	116.13
26	A	2605	PSU	N1-C2-N3	6.22	121.73	115.17
1	a	516	PSU	N1-C2-N3	6.12	121.62	115.17
26	A	746	PSU	N1-C2-N3	6.06	121.56	115.17
26	A	2504	PSU	N1-C2-N3	6.06	121.56	115.17
26	A	2604	PSU	N1-C2-N3	5.90	121.39	115.17
23	w	8	4SU	C5-C4-N3	5.87	120.21	114.75
26	A	2580	PSU	N1-C2-N3	5.84	121.33	115.17
23	w	76	L3X	N1-C2-N3	-5.75	119.88	128.58
1	a	1516	2MG	C5-C4-N3	-5.72	119.28	128.39
24	x	76	M3O	N1-C2-N3	-5.72	119.92	128.58
24	x	8	4SU	C4-N3-C2	-5.62	121.93	127.31
26	A	2251	OMG	C5-C4-N3	-5.49	119.65	128.39
26	A	1618	6MZ	C5-C4-N3	-5.49	119.16	126.72
26	A	1939	5MU	N3-C2-N1	5.46	122.00	114.89
26	A	1939	5MU	C4-N3-C2	-5.42	120.24	127.34
26	A	2445	2MG	C5-C4-N3	-5.30	119.96	128.39
1	a	1207	2MG	C5-C4-N3	-5.27	120.00	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1835	2MG	C5-C4-N3	-5.23	120.07	128.39
1	a	1519	MA6	C5-C4-N3	-5.11	119.68	126.72
26	A	745	1MG	C5-C4-N3	-5.07	120.32	128.39
24	x	76	M3O	C5-C4-N3	-5.05	119.77	126.72
23	w	54	5MU	N3-C2-N1	5.02	121.42	114.89
26	A	2251	OMG	C2-N3-C4	4.99	120.90	112.30
24	x	54	5MU	N3-C2-N1	4.99	121.38	114.89
1	a	527	G7M	C5-C4-N3	-4.98	118.74	128.15
1	a	1518	MA6	C2-N1-C6	4.97	123.97	111.83
23	w	76	L3X	C5-C4-N3	-4.97	119.88	126.72
23	w	54	5MU	C4-N3-C2	-4.89	120.92	127.34
24	x	76	M3O	O3'-C-CA	4.88	122.56	111.41
26	A	2552	OMU	N3-C2-N1	4.87	121.22	114.89
26	A	2030	6MZ	C5-C4-N3	-4.86	120.03	126.72
1	a	1518	MA6	C5-C4-N3	-4.76	120.17	126.72
1	a	527	G7M	N9-C4-N3	4.72	135.39	125.95
24	x	8	4SU	C5-C4-N3	4.68	119.10	114.75
1	a	527	G7M	C2-N3-C4	4.64	120.30	112.30
26	A	2552	OMU	C4-N3-C2	-4.63	120.86	126.61
24	x	54	5MU	C4-N3-C2	-4.61	121.29	127.34
26	A	1939	5MU	C5-C4-N3	4.61	119.33	115.32
26	A	1915	3TD	C4-N3-C2	-4.61	119.73	124.61
26	A	1618	6MZ	N3-C4-N9	4.61	135.00	127.17
1	a	1519	MA6	C2-N1-C6	4.57	122.99	111.83
1	a	1519	MA6	C4-C5-N7	-4.56	105.36	110.58
26	A	745	1MG	C2-N3-C4	4.55	122.22	111.98
26	A	747	5MU	N3-C2-N1	4.50	120.75	114.89
1	a	966	2MG	N9-C4-N3	4.45	134.84	125.95
23	w	55	PSU	C4-N3-C2	-4.41	120.30	126.37
1	a	1518	MA6	C4-C5-N7	-4.35	105.61	110.58
23	w	8	4SU	N3-C2-N1	4.31	120.51	114.89
26	A	2030	6MZ	C6-C5-N7	4.31	137.13	132.43
26	A	1911	PSU	C4-N3-C2	-4.29	120.47	126.37
24	x	55	PSU	C4-N3-C2	-4.25	120.52	126.37
23	w	54	5MU	C5-C4-N3	4.20	118.98	115.32
26	A	2030	6MZ	N1-C2-N3	-4.15	122.30	128.58
24	x	8	4SU	N3-C2-N1	4.12	120.25	114.89
26	A	2030	6MZ	N3-C4-N9	4.12	134.17	127.17
26	A	2069	G7M	C5-C4-N3	-4.09	120.41	128.15
26	A	2445	2MG	N9-C4-N3	4.07	134.10	125.95
26	A	1939	5MU	C5-C6-N1	-4.03	118.94	123.31
24	x	54	5MU	O4-C4-C5	-4.02	120.31	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1207	2MG	N9-C4-N3	4.01	133.98	125.95
1	a	1516	2MG	N9-C4-N3	4.00	133.96	125.95
26	A	747	5MU	C4-N3-C2	-3.98	122.12	127.34
23	w	54	5MU	O4-C4-C5	-3.97	120.37	124.92
26	A	1835	2MG	C6-C5-N7	3.97	137.51	130.29
26	A	2069	G7M	C2-N3-C4	3.95	119.10	112.30
26	A	2251	OMG	C6-C5-N7	3.90	137.39	130.29
26	A	2069	G7M	N9-C4-N3	3.89	133.73	125.95
26	A	2504	PSU	C4-N3-C2	-3.86	121.06	126.37
26	A	955	PSU	C4-N3-C2	-3.85	121.06	126.37
1	a	1516	2MG	C6-C5-N7	3.85	137.29	130.29
24	x	54	5MU	C5-C4-N3	3.85	118.67	115.32
26	A	2457	PSU	O2-C2-N1	-3.79	118.88	122.79
26	A	2251	OMG	N9-C4-N3	3.78	133.51	125.95
26	A	2030	6MZ	C2-N3-C4	3.77	121.03	111.83
1	a	1519	MA6	C10-N6-C6	-3.76	110.95	120.52
1	a	1518	MA6	N1-C2-N3	-3.75	122.90	128.58
26	A	1835	2MG	N9-C4-N3	3.74	133.44	125.95
1	a	1519	MA6	C2-N3-C4	3.72	120.92	111.83
1	a	1518	MA6	N3-C4-N9	3.69	133.45	127.17
26	A	2030	6MZ	C4-N9-C8	3.69	109.62	105.74
1	a	1519	MA6	N1-C2-N3	-3.68	123.00	128.58
26	A	2457	PSU	C4-N3-C2	-3.67	121.31	126.37
1	a	1498	UR3	C5-C4-N3	3.67	119.88	115.04
26	A	2445	2MG	C6-C5-N7	3.67	136.97	130.29
26	A	747	5MU	C5-C4-N3	3.63	118.48	115.32
24	x	32	5MC	C5-C6-N1	-3.63	119.37	123.31
26	A	2503	2MA	C4-N9-C8	3.63	109.55	105.74
1	a	1519	MA6	N3-C4-N9	3.61	133.30	127.17
26	A	1618	6MZ	C4-C5-N7	-3.60	106.47	110.58
26	A	1618	6MZ	C4-N9-C8	3.59	109.51	105.74
26	A	745	1MG	N9-C4-N3	3.56	133.08	125.95
24	x	32	5MC	C5-C4-N3	-3.56	118.11	121.75
1	a	1518	MA6	C4-N9-C8	3.54	109.46	105.74
26	A	746	PSU	C6-C5-C4	-3.52	115.80	118.17
23	w	55	PSU	O2-C2-N1	-3.52	119.16	122.79
26	A	955	PSU	O2-C2-N1	-3.51	119.17	122.79
24	x	76	M3O	O3'-C-O	-3.50	117.62	123.95
1	a	1207	2MG	C6-C5-N7	3.49	136.65	130.29
26	A	746	PSU	C4-N3-C2	-3.49	121.56	126.37
26	A	2552	OMU	C5-C4-N3	3.49	119.68	114.80
23	w	76	L3X	N9-C8-N7	-3.48	108.99	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	x	76	M3O	N9-C8-N7	-3.45	109.04	113.94
26	A	747	5MU	O4-C4-C5	-3.45	120.97	124.92
24	x	55	PSU	O2-C2-N1	-3.45	119.23	122.79
26	A	1618	6MZ	C2-N3-C4	3.44	120.24	111.83
26	A	2504	PSU	O2-C2-N1	-3.43	119.25	122.79
26	A	747	5MU	C5-C6-N1	-3.43	119.59	123.31
1	a	966	2MG	C6-C5-N7	3.42	136.52	130.29
26	A	2030	6MZ	C4-C5-N7	-3.41	106.69	110.58
24	x	76	M3O	C2-N3-C4	3.40	120.14	111.83
1	a	1518	MA6	C2-N3-C4	3.39	120.12	111.83
26	A	2552	OMU	O2-C2-N1	-3.38	118.40	122.80
23	w	76	L3X	C2-N3-C4	3.36	120.03	111.83
26	A	1618	6MZ	C6-C5-N7	3.36	136.09	132.43
1	a	1519	MA6	C5-N7-C8	3.34	108.70	103.45
1	a	1519	MA6	C4-N9-C8	3.34	109.24	105.74
1	a	1518	MA6	C5-N7-C8	3.31	108.65	103.45
26	A	2503	2MA	C4-C5-N7	-3.30	106.81	110.58
1	a	1407	5MC	O3'-C3'-C4'	3.24	120.38	111.08
24	x	8	4SU	C5-C4-S4	-3.24	120.61	124.31
26	A	1618	6MZ	N1-C2-N3	-3.21	123.73	128.58
1	a	516	PSU	C4-N3-C2	-3.20	121.96	126.37
24	x	54	5MU	C5-C6-N1	-3.18	119.86	123.31
26	A	2580	PSU	C4-N3-C2	-3.17	122.00	126.37
1	a	1516	2MG	N1-C2-N2	3.16	119.78	116.56
26	A	745	1MG	C6-C5-N7	3.10	136.26	129.36
26	A	2030	6MZ	C9-N6-C6	-3.07	120.00	122.85
24	x	76	M3O	C5-N7-C8	3.06	108.26	103.45
26	A	2503	2MA	N6-C6-N1	3.05	121.15	117.03
23	w	76	L3X	C5-N7-C8	3.05	108.25	103.45
26	A	1939	5MU	O4-C4-C5	-3.05	121.43	124.92
26	A	2605	PSU	C4-N3-C2	-3.05	122.17	126.37
1	a	1519	MA6	N9-C8-N7	-3.02	109.66	113.94
1	a	967	5MC	C5-C4-N3	-3.01	118.67	121.75
26	A	2030	6MZ	C5-N7-C8	3.01	108.17	103.45
26	A	1618	6MZ	C5-N7-C8	3.00	108.16	103.45
26	A	2030	6MZ	N9-C8-N7	-2.97	109.72	113.94
26	A	745	1MG	C4-C5-N7	-2.94	106.02	110.67
26	A	1962	5MC	C5-C4-N3	-2.93	118.75	121.75
23	w	54	5MU	C5M-C5-C4	2.93	121.91	118.78
1	a	966	2MG	C4-C5-N7	-2.92	106.05	110.67
1	a	1407	5MC	O3'-C3'-C2'	2.89	121.10	111.82
23	w	8	4SU	C5-C4-S4	-2.89	121.00	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1407	5MC	C5-C6-N1	-2.88	120.19	123.31
1	a	1518	MA6	N9-C8-N7	-2.85	109.89	113.94
1	a	967	5MC	C5-C6-N1	-2.85	120.22	123.31
1	a	1402	4OC	C6-C5-C4	2.85	120.43	117.00
26	A	1835	2MG	C4-C5-N7	-2.81	106.22	110.67
26	A	2503	2MA	C5-N7-C8	2.79	107.84	103.45
23	w	54	5MU	C5-C6-N1	-2.79	120.28	123.31
26	A	1911	PSU	O2-C2-N1	-2.78	119.92	122.79
1	a	527	G7M	O6-C6-C5	-2.77	121.83	128.01
26	A	1618	6MZ	N9-C8-N7	-2.76	110.02	113.94
26	A	1915	3TD	C3'-C2'-C1'	2.73	104.92	101.69
26	A	2503	2MA	N9-C8-N7	-2.73	110.06	113.94
26	A	745	1MG	N2-C2-N3	-2.72	113.54	119.75
26	A	1962	5MC	C5-C6-N1	-2.72	120.36	123.31
38	O	81	4D4	O-C-CA	-2.72	117.78	124.77
26	A	1917	PSU	C4-N3-C2	-2.71	122.64	126.37
26	A	2580	PSU	O2-C2-N1	-2.70	120.00	122.79
26	A	2604	PSU	C4-N3-C2	-2.70	122.65	126.37
1	a	1519	MA6	C6-C5-N7	2.69	137.73	133.43
1	a	1516	2MG	C4-C5-N7	-2.69	106.40	110.67
23	w	76	L3X	C5-C4-N9	2.69	108.75	105.81
24	x	8	4SU	O2-C2-N1	-2.65	119.35	122.80
24	x	76	M3O	C5-C4-N9	2.64	108.69	105.81
26	A	2251	OMG	C4-C5-N7	-2.62	106.51	110.67
1	a	1518	MA6	N1-C6-N6	2.59	120.01	116.86
26	A	2503	2MA	C2-N1-C6	2.59	122.08	118.10
24	x	76	M3O	N3-C4-N9	2.57	131.54	127.17
26	A	1915	3TD	C6-C5-C4	2.56	119.91	118.19
26	A	747	5MU	O2-C2-N1	-2.56	119.46	122.80
1	a	1518	MA6	C6-C5-N7	2.56	137.52	133.43
24	x	54	5MU	O2-C2-N1	-2.55	119.48	122.80
26	A	1939	5MU	O2-C2-N1	-2.54	119.49	122.80
1	a	1407	5MC	C5-C4-N3	-2.52	119.17	121.75
1	a	1402	4OC	O2-C2-N3	-2.52	118.36	122.33
26	A	2604	PSU	O2-C2-N3	-2.51	117.40	121.86
23	w	8	4SU	O2-C2-N1	-2.51	119.53	122.80
11	k	119	IAS	OD1-CG-CB	-2.51	118.08	125.38
26	A	2580	PSU	C6-C5-C4	-2.49	116.49	118.17
26	A	1917	PSU	O2-C2-N3	-2.47	117.47	121.86
23	w	76	L3X	N3-C4-N9	2.47	131.37	127.17
26	A	2445	2MG	C4-C5-N7	-2.46	106.76	110.67
24	x	76	M3O	CA-N-CN	-2.45	119.05	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	746	PSU	O2-C2-N1	-2.43	120.28	122.79
26	A	1962	5MC	CM5-C5-C6	-2.41	119.59	122.85
26	A	2445	2MG	N1-C2-N2	2.40	119.02	116.56
26	A	2580	PSU	O4'-C1'-C2'	2.39	108.46	105.15
26	A	2552	OMU	O4-C4-C5	-2.39	121.05	125.16
1	a	966	2MG	C2-N1-C6	-2.39	121.67	124.55
38	O	81	4D4	NE-CZ-NH2	2.37	124.73	120.67
26	A	745	1MG	C2-N1-C6	-2.36	119.02	120.99
26	A	2605	PSU	O2-C2-N3	-2.35	117.69	121.86
12	l	89	D2T	O-C-CA	-2.34	118.75	124.77
1	a	1207	2MG	C4-C5-N7	-2.34	106.96	110.67
26	A	2504	PSU	C6-C5-C4	-2.34	116.60	118.17
1	a	516	PSU	O2-C2-N3	-2.33	117.72	121.86
26	A	1962	5MC	O2-C2-N3	-2.33	118.66	122.33
1	a	1407	5MC	O2-C2-N3	-2.32	118.68	122.33
23	w	54	5MU	C5M-C5-C6	-2.32	119.72	122.85
12	l	89	D2T	OD2-CG-CB	2.30	118.12	113.15
26	A	2030	6MZ	C2-N1-C6	2.29	122.83	115.24
26	A	1911	PSU	C5-C6-N1	-2.28	118.98	122.14
1	a	1516	2MG	C5'-C4'-C3'	2.27	123.37	115.21
26	A	2503	2MA	C6-C5-N7	2.24	136.41	132.09
24	x	76	M3O	O4'-C1'-N9	-2.22	103.83	108.09
23	w	55	PSU	C5-C6-N1	-2.21	119.08	122.14
1	a	1516	2MG	O4'-C4'-C5'	2.21	116.40	109.33
24	x	54	5MU	C5M-C5-C4	2.20	121.13	118.78
1	a	967	5MC	CM5-C5-C6	-2.20	119.88	122.85
1	a	1207	2MG	O6-C6-C5	-2.19	120.76	126.53
23	w	76	L3X	C6-C5-C4	2.18	120.16	117.18
24	x	76	M3O	C6-C5-C4	2.18	120.16	117.18
24	x	76	M3O	C4-C5-N7	-2.18	108.09	110.58
23	w	76	L3X	C4-C5-N7	-2.17	108.11	110.58
26	A	1911	PSU	O2-C2-N3	-2.16	118.02	121.86
1	a	1518	MA6	C9-N6-C6	-2.16	115.03	120.52
1	a	966	2MG	C8-N7-C5	2.15	108.10	104.26
26	A	2605	PSU	O2-C2-N1	-2.15	120.57	122.79
26	A	1618	6MZ	C2-N1-C6	2.14	122.33	115.24
1	a	1519	MA6	C9-N6-C6	-2.13	115.09	120.52
26	A	745	1MG	C8-N7-C5	2.13	108.05	104.26
26	A	747	5MU	C5M-C5-C4	2.11	121.04	118.78
26	A	1835	2MG	C8-N7-C5	2.10	108.00	104.26
26	A	2605	PSU	C5-C6-N1	-2.10	119.23	122.14
1	a	1518	MA6	C10-N6-C6	-2.10	115.19	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2457	PSU	C5-C6-N1	-2.09	119.24	122.14
26	A	746	PSU	O2-C2-N3	-2.08	118.16	121.86
26	A	2449	H2U	O2-C2-N3	-2.08	117.65	121.49
26	A	955	PSU	C5-C6-N1	-2.07	119.26	122.14
1	a	516	PSU	O4'-C1'-C2'	2.07	108.02	105.15
1	a	1516	2MG	C5-C6-N1	2.07	118.52	113.25
26	A	2030	6MZ	C4-N9-C1'	-2.07	121.80	126.63
1	a	516	PSU	O2-C2-N1	-2.06	120.66	122.79
1	a	1498	UR3	C3U-N3-C2	2.06	120.92	117.33
26	A	2552	OMU	C6-N1-C2	-2.05	118.50	121.00
26	A	1917	PSU	O2-C2-N1	-2.05	120.67	122.79
1	a	967	5MC	O2-C2-N3	-2.05	119.10	122.33
1	a	1519	MA6	C10-N6-C9	-2.04	109.62	116.18
26	A	1917	PSU	C6-N1-C2	-2.04	120.80	122.69
1	a	1519	MA6	C4-N9-C1'	-2.02	121.91	126.63
1	a	1207	2MG	N1-C2-N2	2.02	118.62	116.56

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C10
1	a	1519	MA6	C5-C6-N6-C10
12	l	89	D2T	CG-CB-SB-CB1
12	l	89	D2T	CA-CB-CG-OD2
29	D	150	MEQ	C-CA-CB-CG
23	w	76	L3X	O4'-C4'-C5'-O5'
24	x	76	M3O	C-CA-CB-CG
24	x	76	M3O	OCN-CN-N-CA
26	A	1618	6MZ	O4'-C4'-C5'-O5'
1	a	527	G7M	C3'-C4'-C5'-O5'
1	a	1519	MA6	O4'-C4'-C5'-O5'
23	w	8	4SU	C3'-C4'-C5'-O5'
23	w	54	5MU	C3'-C4'-C5'-O5'
23	w	54	5MU	O4'-C4'-C5'-O5'
26	A	1618	6MZ	C3'-C4'-C5'-O5'
24	x	76	M3O	C4'-C5'-O5'-P
23	w	8	4SU	O4'-C4'-C5'-O5'
1	a	1518	MA6	N1-C6-N6-C10
1	a	1519	MA6	N1-C6-N6-C10
29	D	150	MEQ	OE1-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
29	D	150	MEQ	NE2-CD-CG-CB
23	w	76	L3X	C3'-C4'-C5'-O5'
24	x	76	M3O	N-CA-CB-CG
1	a	1519	MA6	C3'-C4'-C5'-O5'
26	A	2030	6MZ	O4'-C4'-C5'-O5'
26	A	2030	6MZ	C3'-C4'-C5'-O5'
23	w	55	PSU	O4'-C4'-C5'-O5'
12	l	89	D2T	CA-CB-CG-OD1
38	O	82	MS6	CB-CG-SD-CE
26	A	2503	2MA	C4'-C5'-O5'-P
26	A	2504	PSU	O4'-C4'-C5'-O5'
12	l	89	D2T	SB-CB-CG-OD2
26	A	746	PSU	O4'-C1'-C5-C6
26	A	2503	2MA	O4'-C4'-C5'-O5'
24	x	76	M3O	O-C-CA-CB
24	x	76	M3O	O3'-C-CA-CB
24	x	8	4SU	O4'-C4'-C5'-O5'
26	A	2069	G7M	C4'-C5'-O5'-P
26	A	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	x	32	5MC	1	0
26	A	1939	5MU	1	0
24	x	76	M3O	3	0
26	A	747	5MU	1	0
1	a	1519	MA6	1	0
26	A	2604	PSU	1	0
26	A	2552	OMU	1	0
1	a	1518	MA6	1	0
26	A	2030	6MZ	1	0
26	A	2251	OMG	1	0
26	A	1915	3TD	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1134 ligands modelled in this entry, 1132 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
61	MQH	z	402	-	56,61,61	2.63	15 (26%)	77,89,89	2.37	17 (22%)
60	GCP	z	401	-	32,34,34	1.36	6 (18%)	49,54,54	1.72	8 (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
61	MQH	z	402	-	-	13/81/96/96	0/3/4/4
60	GCP	z	401	-	-	1/19/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	402	MQH	C23-N24	8.24	1.51	1.34
61	z	402	MQH	C12-N13	7.94	1.51	1.34
61	z	402	MQH	C02-N03	7.46	1.50	1.34
61	z	402	MQH	C47-N46	7.21	1.49	1.34
61	z	402	MQH	C54-N53	5.89	1.52	1.35
61	z	402	MQH	C09-N10	3.84	1.36	1.28
61	z	402	MQH	O28-C27	3.28	1.43	1.33
61	z	402	MQH	C33-C34	3.07	1.41	1.34
60	z	401	GCP	C5-C4	2.86	1.46	1.38
60	z	401	GCP	PG-O2G	2.73	1.61	1.55
61	z	402	MQH	O58-C47	-2.71	1.18	1.23
60	z	401	GCP	C6-N1	-2.69	1.33	1.38
61	z	402	MQH	C41-C38	2.59	1.59	1.53
61	z	402	MQH	O01-C02	-2.52	1.18	1.23
61	z	402	MQH	C16-C15	2.52	1.55	1.52
60	z	401	GCP	PG-O3G	2.39	1.60	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	402	MQH	O36-C23	-2.34	1.18	1.23
61	z	402	MQH	C55-N56	2.27	1.51	1.45
60	z	401	GCP	C5-N7	-2.13	1.34	1.39
60	z	401	GCP	C4-N9	-2.08	1.32	1.38
61	z	402	MQH	O37-C12	-2.04	1.19	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	z	402	MQH	C34-S35-C31	11.89	97.17	89.70
61	z	402	MQH	S35-C31-N32	-7.44	106.95	114.22
60	z	401	GCP	C5-C4-N3	-5.65	119.40	128.39
60	z	401	GCP	C2-N3-C4	4.85	120.65	112.30
61	z	402	MQH	C12-C11-N10	-4.73	102.67	111.22
61	z	402	MQH	C05-C04-C09	-4.37	107.83	113.04
61	z	402	MQH	O28-C27-C26	4.31	120.79	111.47
60	z	401	GCP	N9-C4-N3	4.21	134.38	125.95
61	z	402	MQH	C11-C12-N13	4.16	121.03	115.69
61	z	402	MQH	C33-C34-S35	-3.79	105.44	110.27
60	z	401	GCP	C6-C5-N7	3.51	136.67	130.29
61	z	402	MQH	C33-N32-C31	3.50	116.51	109.86
61	z	402	MQH	C25-C31-S35	3.35	126.25	121.79
60	z	401	GCP	PB-O3A-PA	-2.91	122.87	132.37
61	z	402	MQH	C48-N53-C54	2.85	120.89	118.50
60	z	401	GCP	C4-C5-N7	-2.57	106.59	110.67
61	z	402	MQH	C09-C04-N03	2.55	112.49	108.14
61	z	402	MQH	C50-C49-C51	-2.54	105.57	113.64
61	z	402	MQH	C04-C09-N56	2.50	123.49	115.99
61	z	402	MQH	C47-C48-N53	-2.27	106.76	112.01
61	z	402	MQH	O30-C27-C26	-2.21	119.52	124.65
61	z	402	MQH	O37-C12-N13	-2.12	119.17	122.96
61	z	402	MQH	C54-C55-N56	-2.10	105.72	110.90
60	z	401	GCP	O6-C6-C5	-2.05	121.11	126.53
60	z	401	GCP	C2'-C3'-C4'	2.02	106.51	102.61

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	z	402	MQH	C38-C11-N10-C09
61	z	402	MQH	C31-C25-N24-C23
61	z	402	MQH	O30-C27-O28-C29

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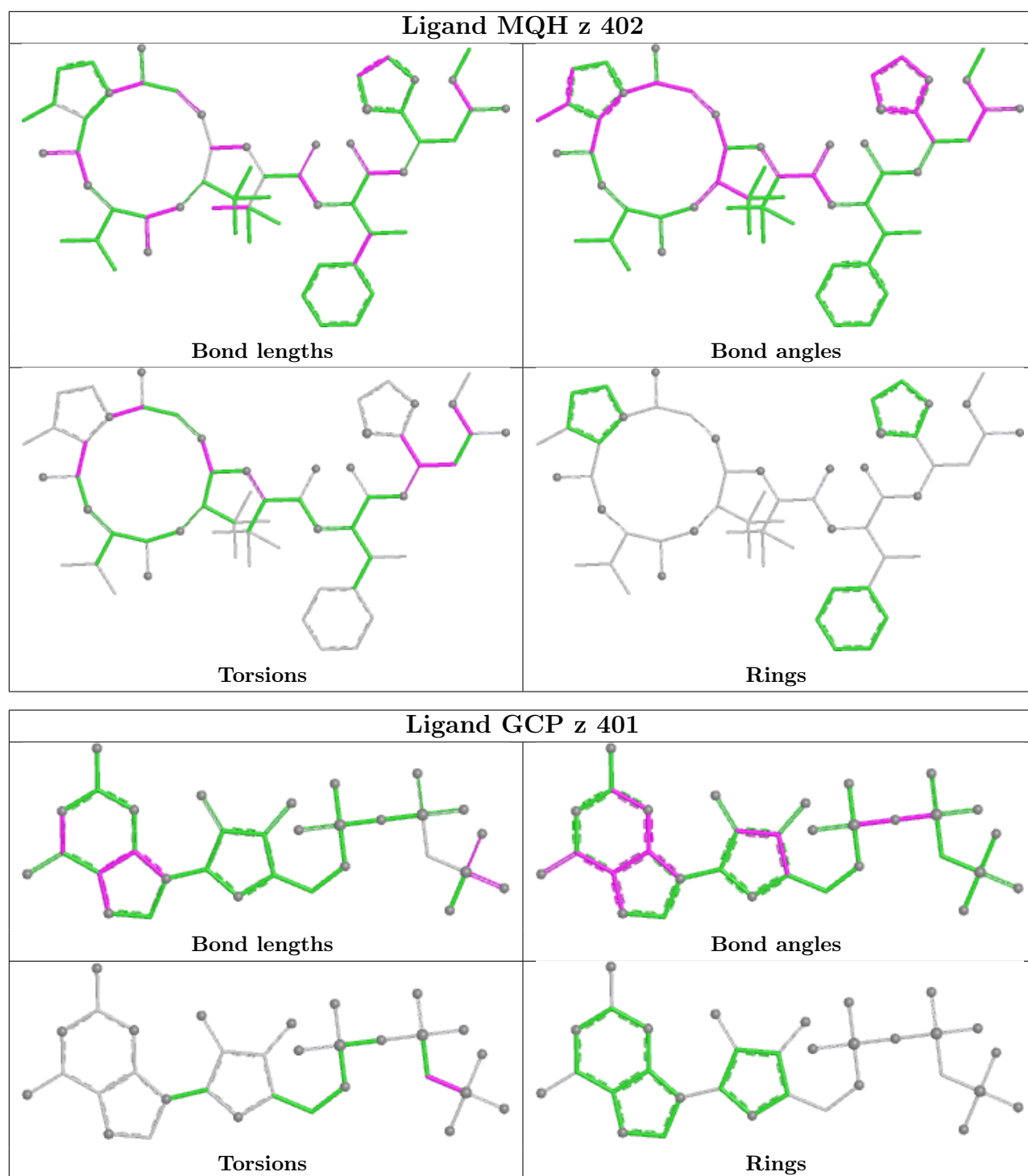
Mol	Chain	Res	Type	Atoms
61	z	402	MQH	C26-C27-O28-C29
61	z	402	MQH	C04-C09-N56-C55
61	z	402	MQH	N24-C25-C26-C27
61	z	402	MQH	N10-C09-N56-C55
61	z	402	MQH	C55-C54-N53-C48
61	z	402	MQH	N46-C47-C48-N53
61	z	402	MQH	O58-C47-C48-N53
61	z	402	MQH	N24-C25-C31-N32
61	z	402	MQH	N24-C25-C31-S35
61	z	402	MQH	C55-C54-N53-C52
60	z	401	GCP	PB-C3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	z	402	MQH	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

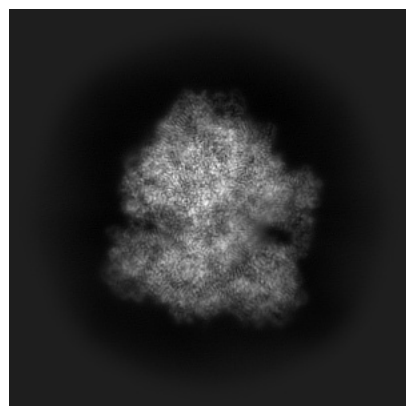
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72205. These allow visual inspection of the internal detail of the map and identification of artifacts.

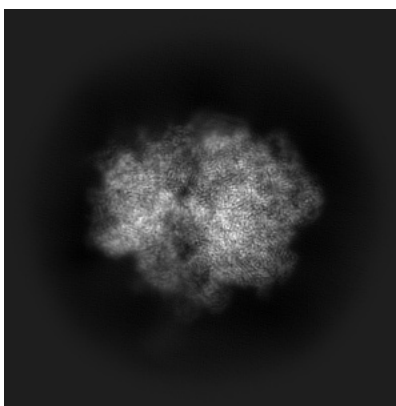
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

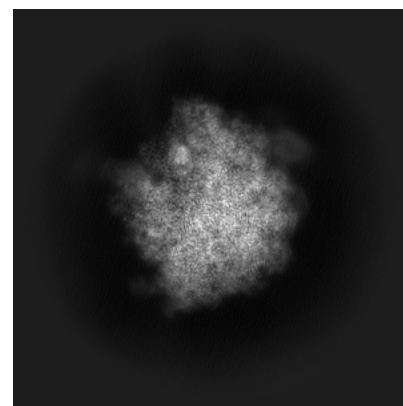
6.1.1 Primary map



X

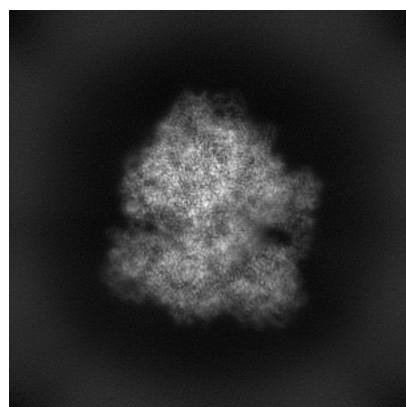


Y

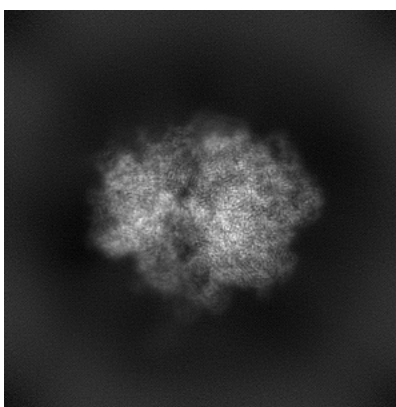


Z

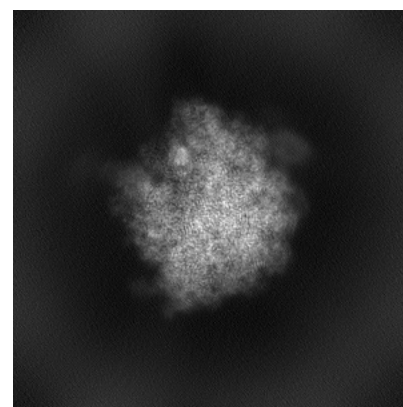
6.1.2 Raw map



X



Y

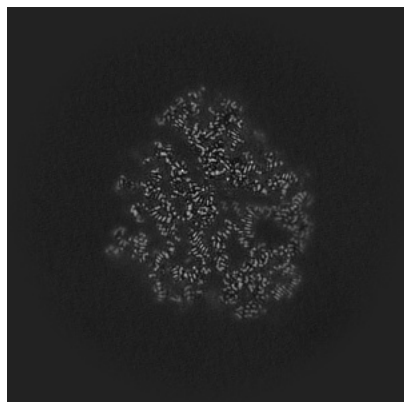


Z

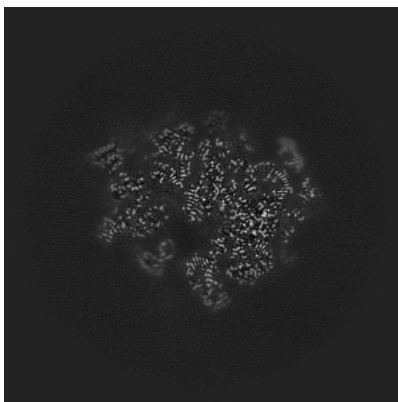
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

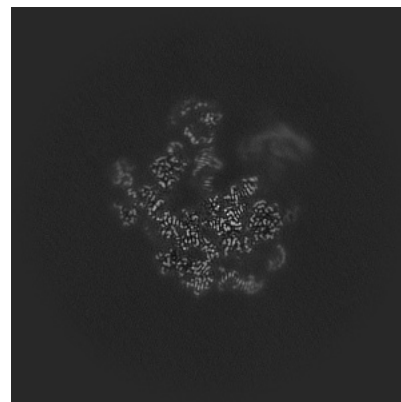
6.2.1 Primary map



X Index: 256

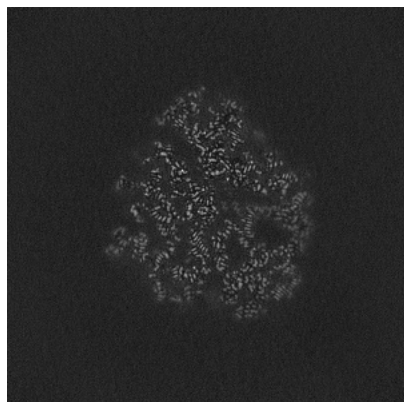


Y Index: 256

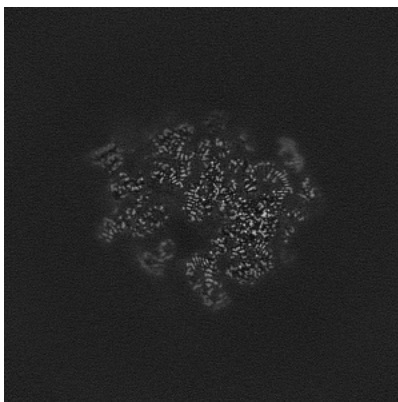


Z Index: 256

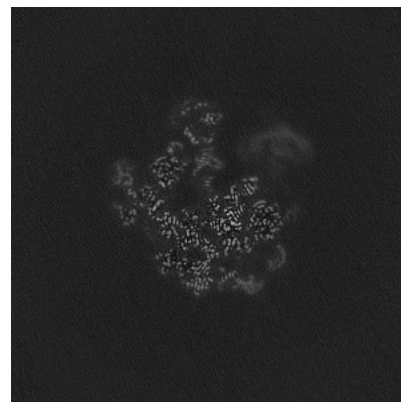
6.2.2 Raw map



X Index: 256



Y Index: 256

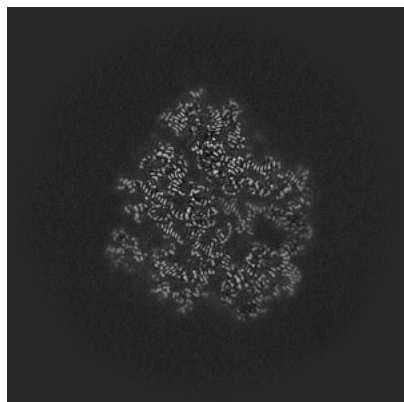


Z Index: 256

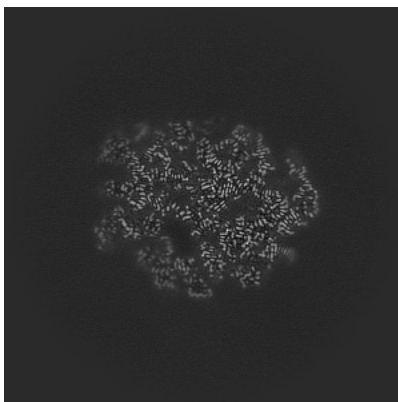
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

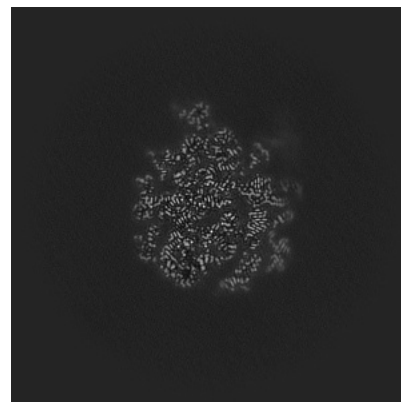
6.3.1 Primary map



X Index: 252

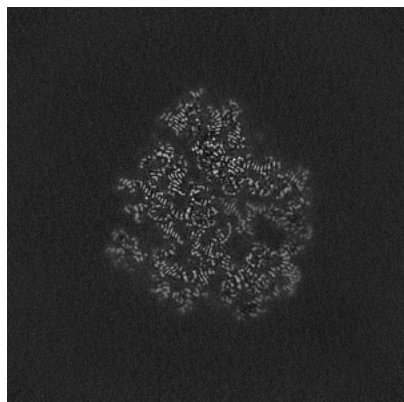


Y Index: 242

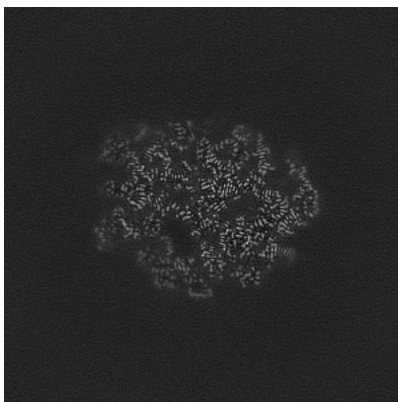


Z Index: 302

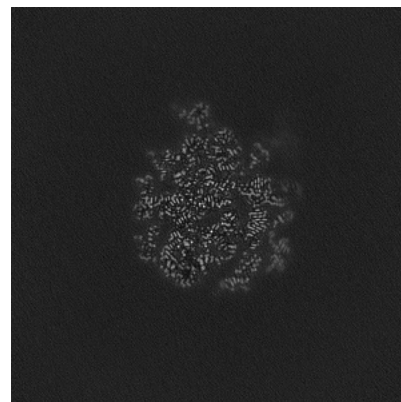
6.3.2 Raw map



X Index: 252



Y Index: 242

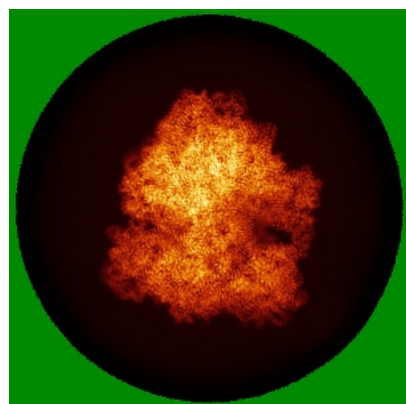


Z Index: 302

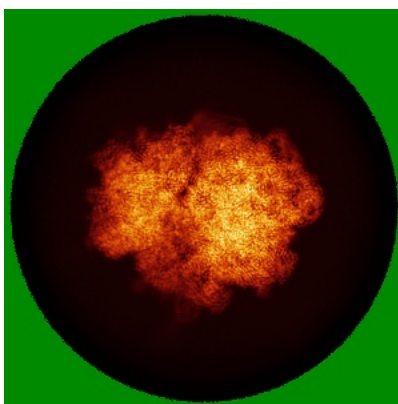
The images above show the largest variance slices of the map in three orthogonal directions.

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

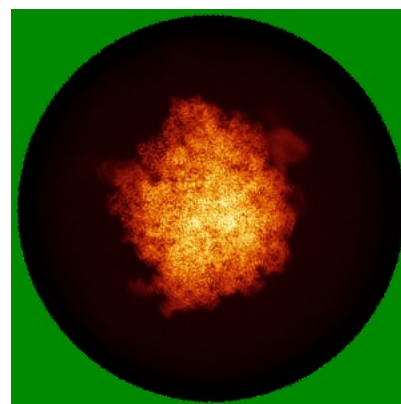
6.4.1 Primary map



X

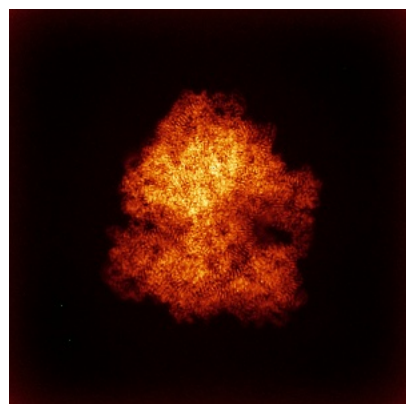


Y

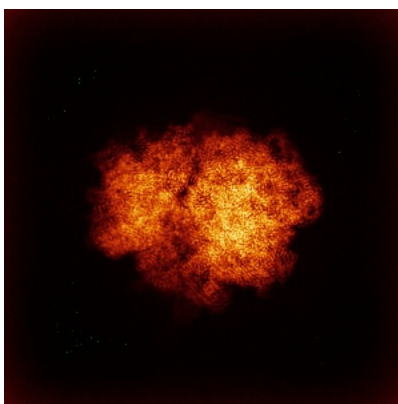


Z

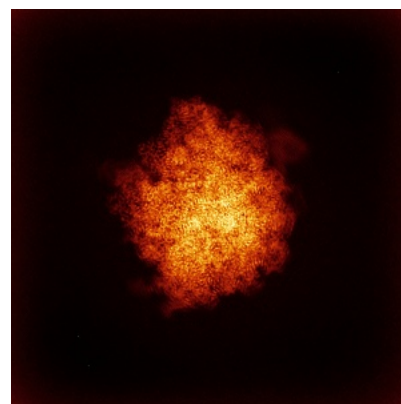
6.4.2 Raw map



X



Y

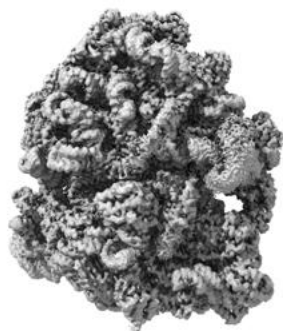


Z

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](#)

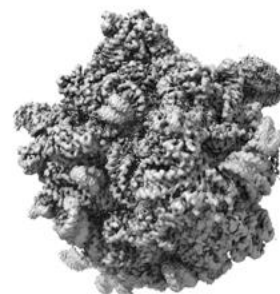
6.5.1 Primary map



X



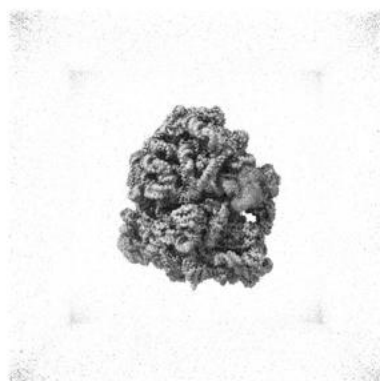
Y



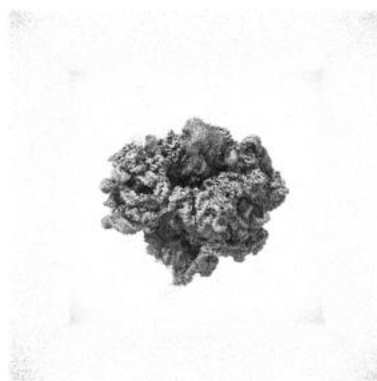
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

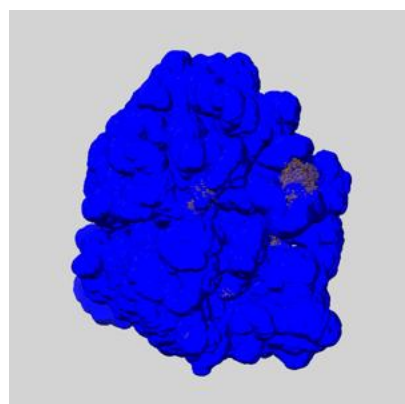
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

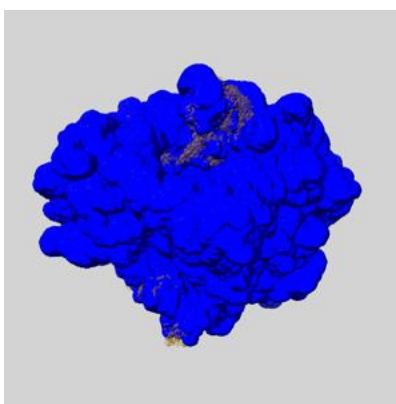
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

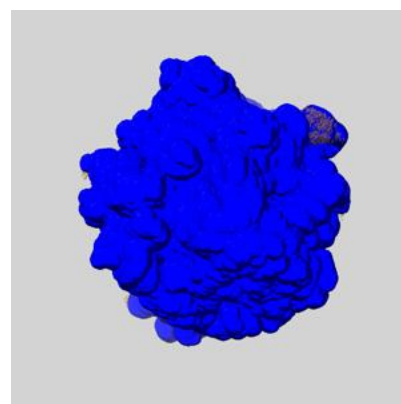
6.6.1 emd_72205_msk_1.map [i](#)



X



Y

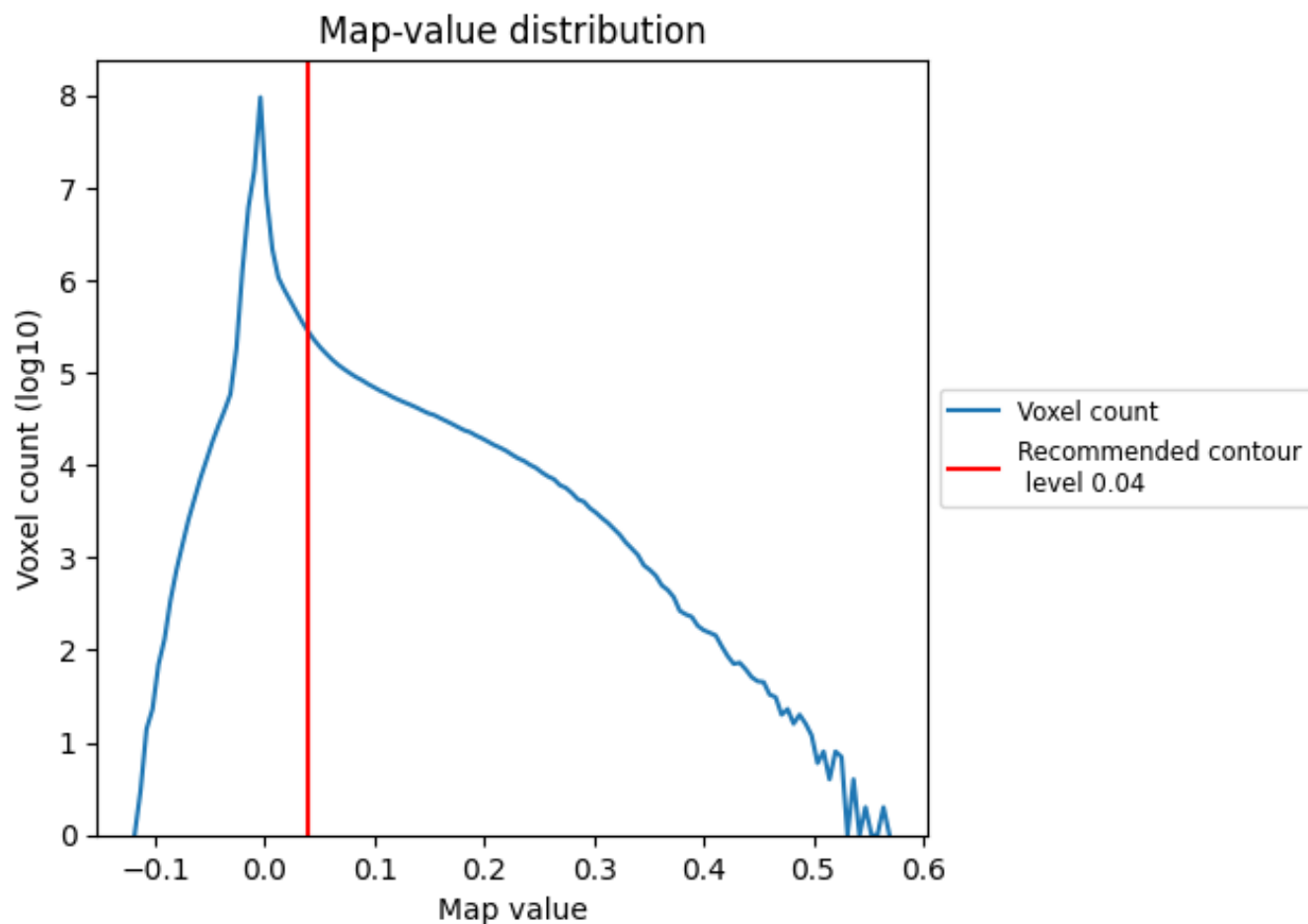


Z

7 Map analysis [i](#)

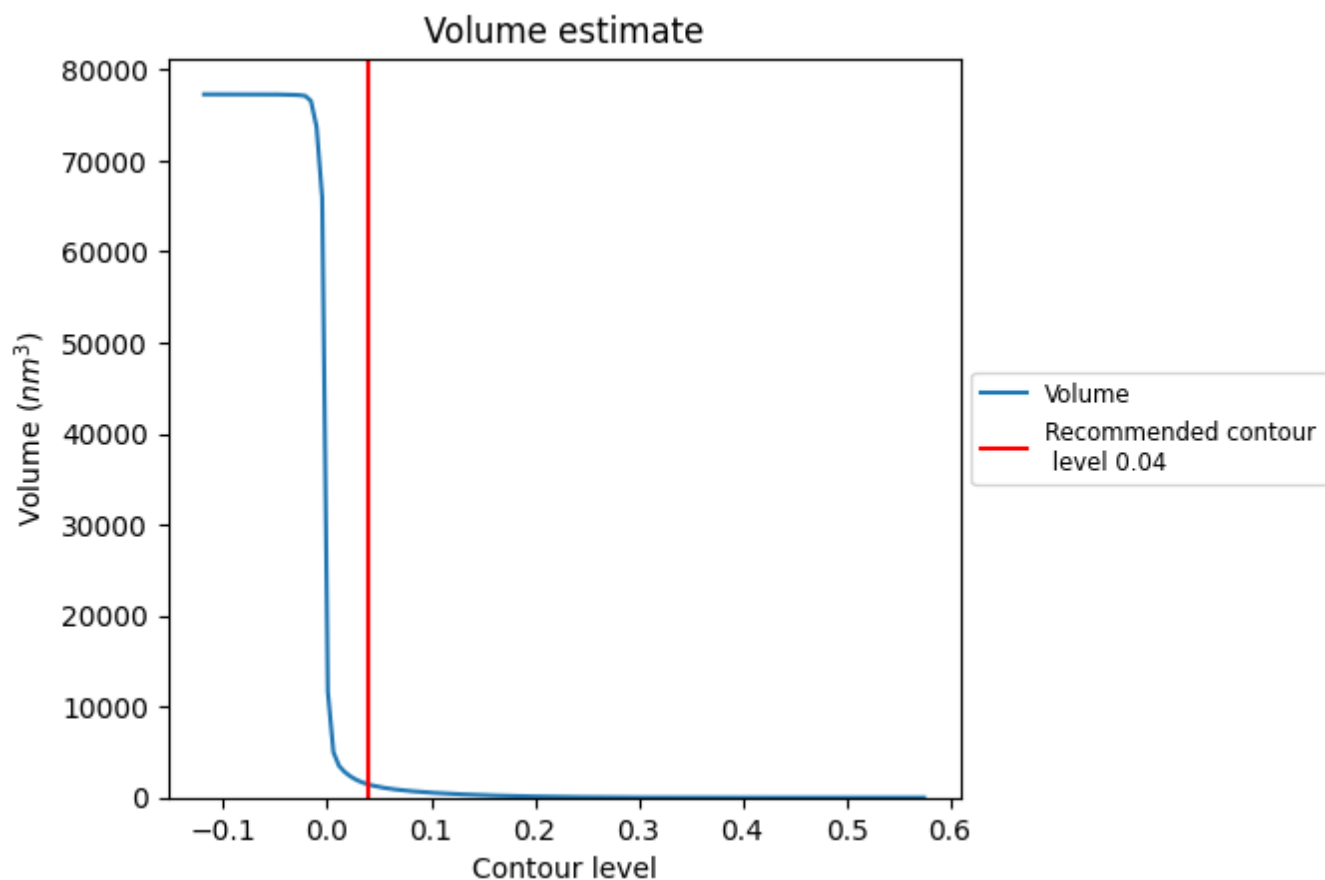
This section contains the results of statistical analysis of the map.

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.

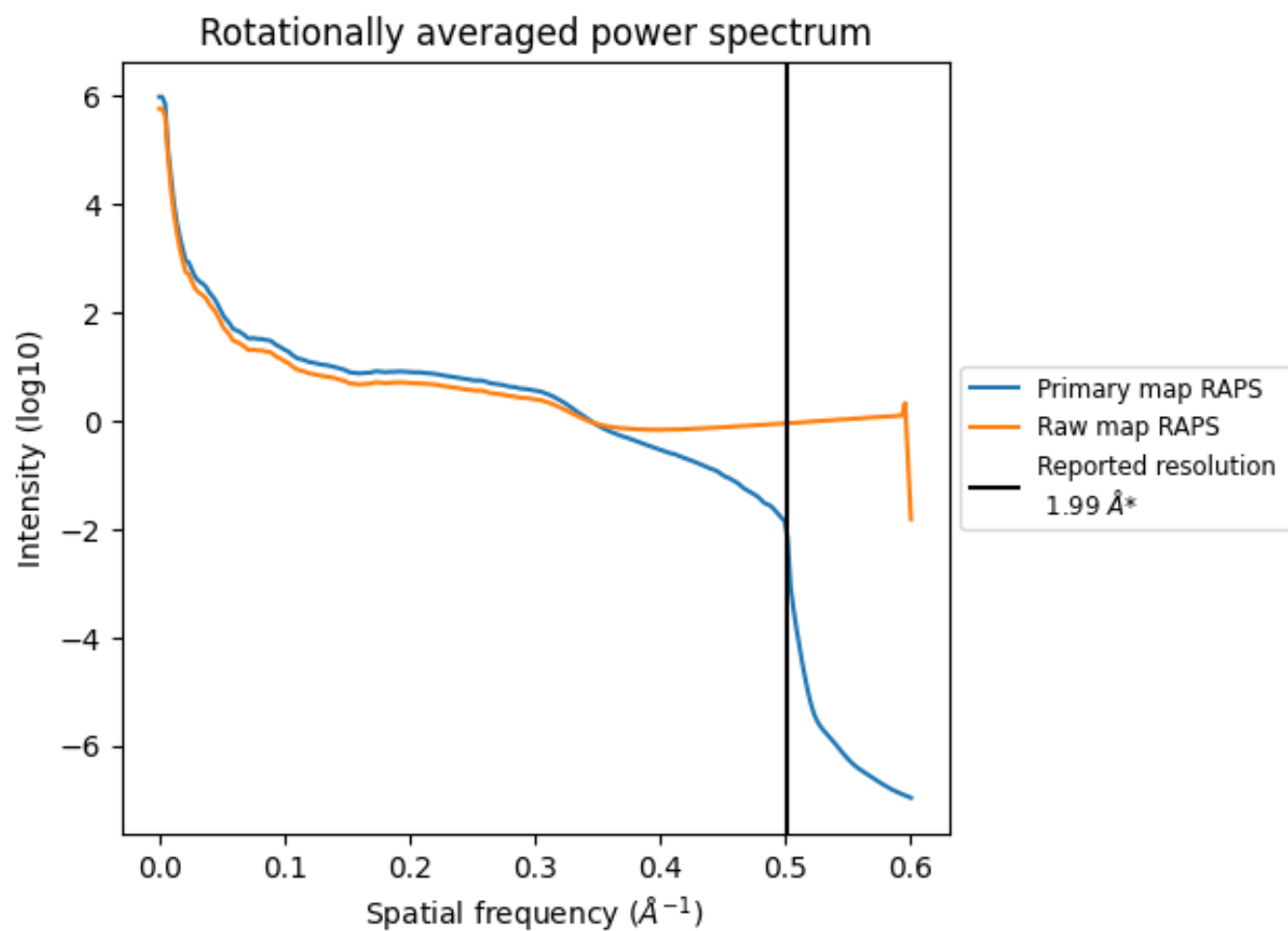
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1436 nm³; this corresponds to an approximate mass of 1297 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 ⓘ

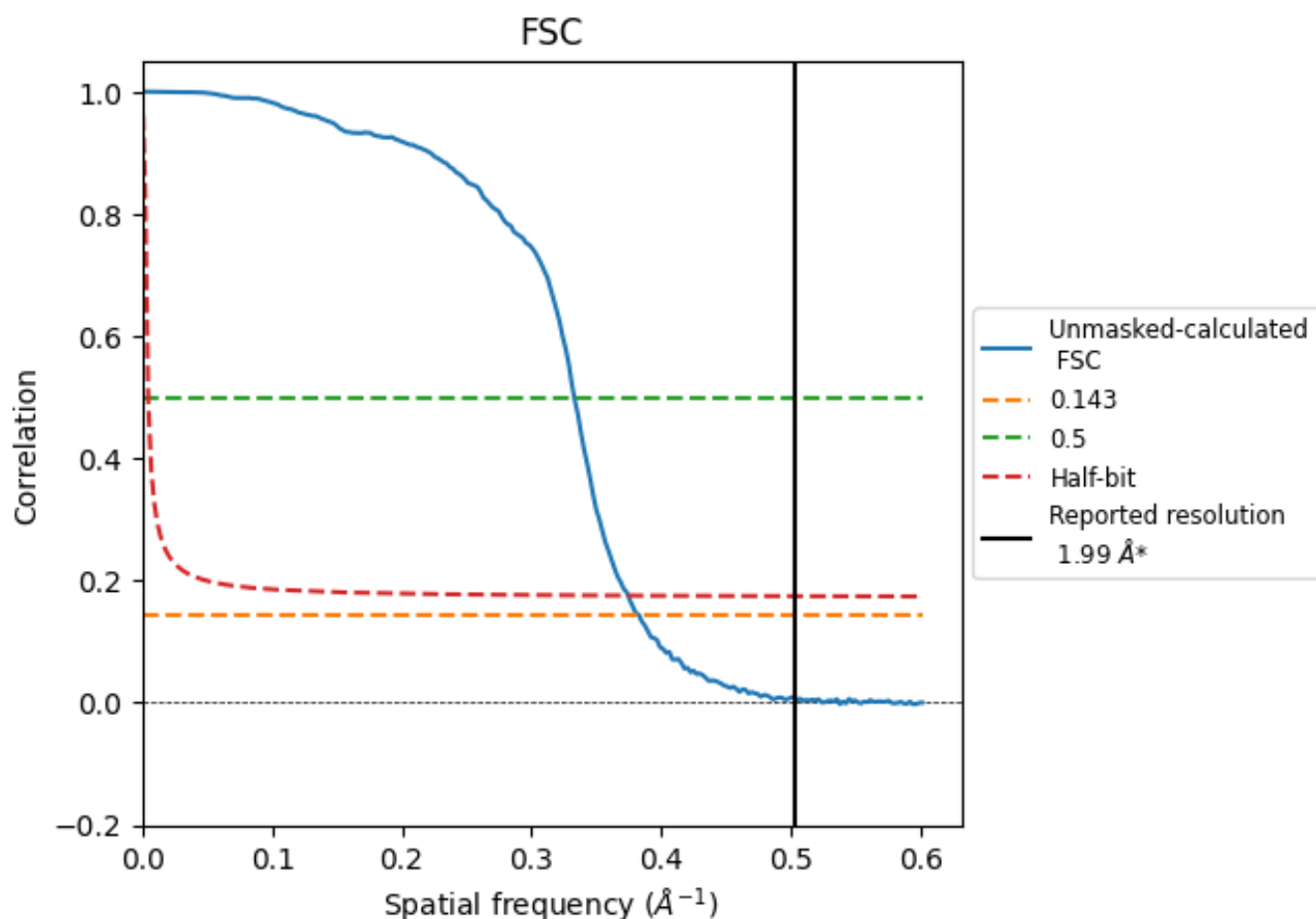


*Reported resolution corresponds to spatial frequency of 0.503 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.503 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

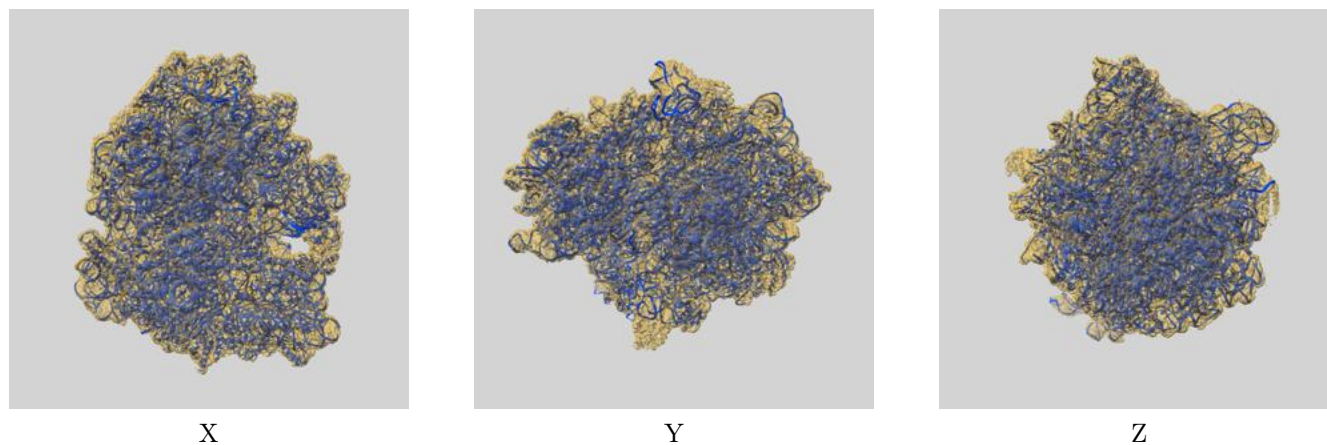
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.99	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.61	3.00	2.67

*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 2.61 differs from the reported value 1.99 by more than 10 %

9 Map-model fit [i](#)

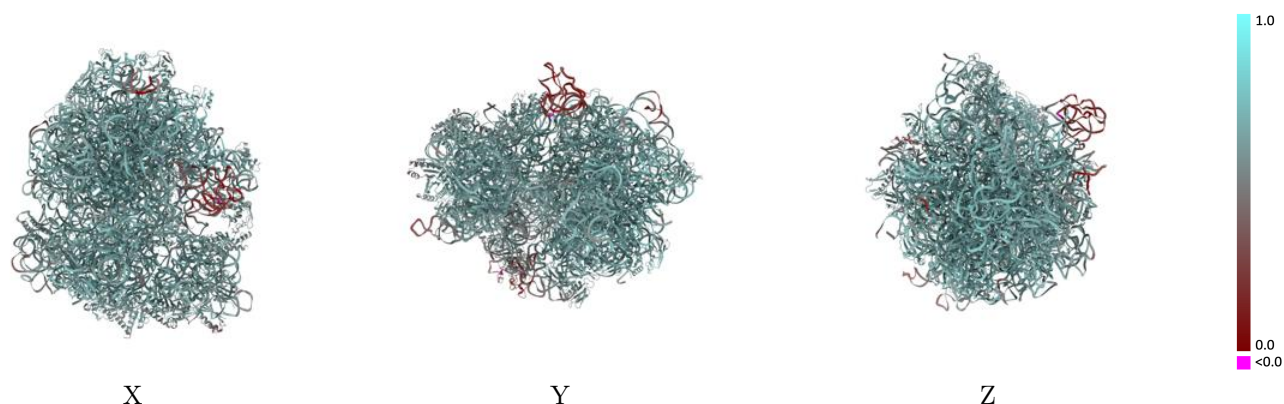
This section contains information regarding the fit between EMDB map EMD-72205 and PDB model 9Q3R. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



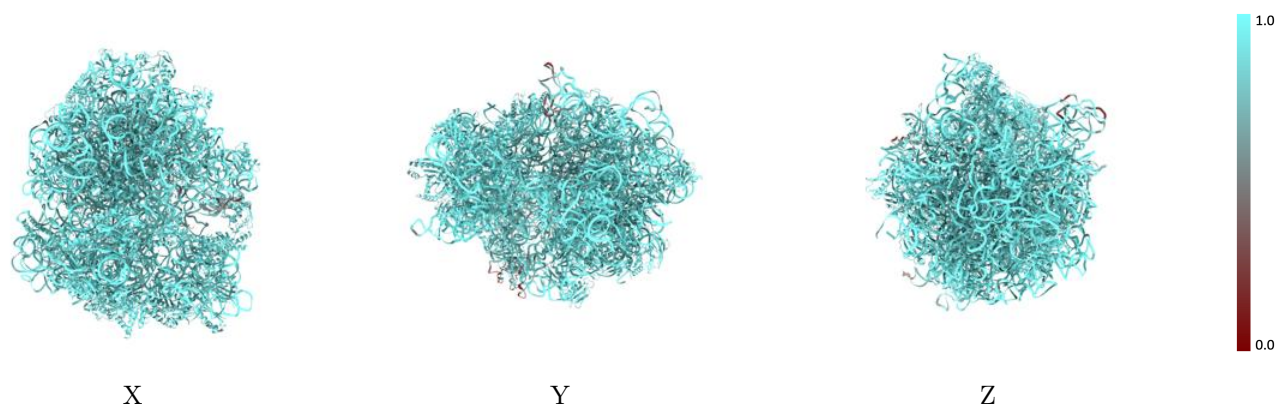
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



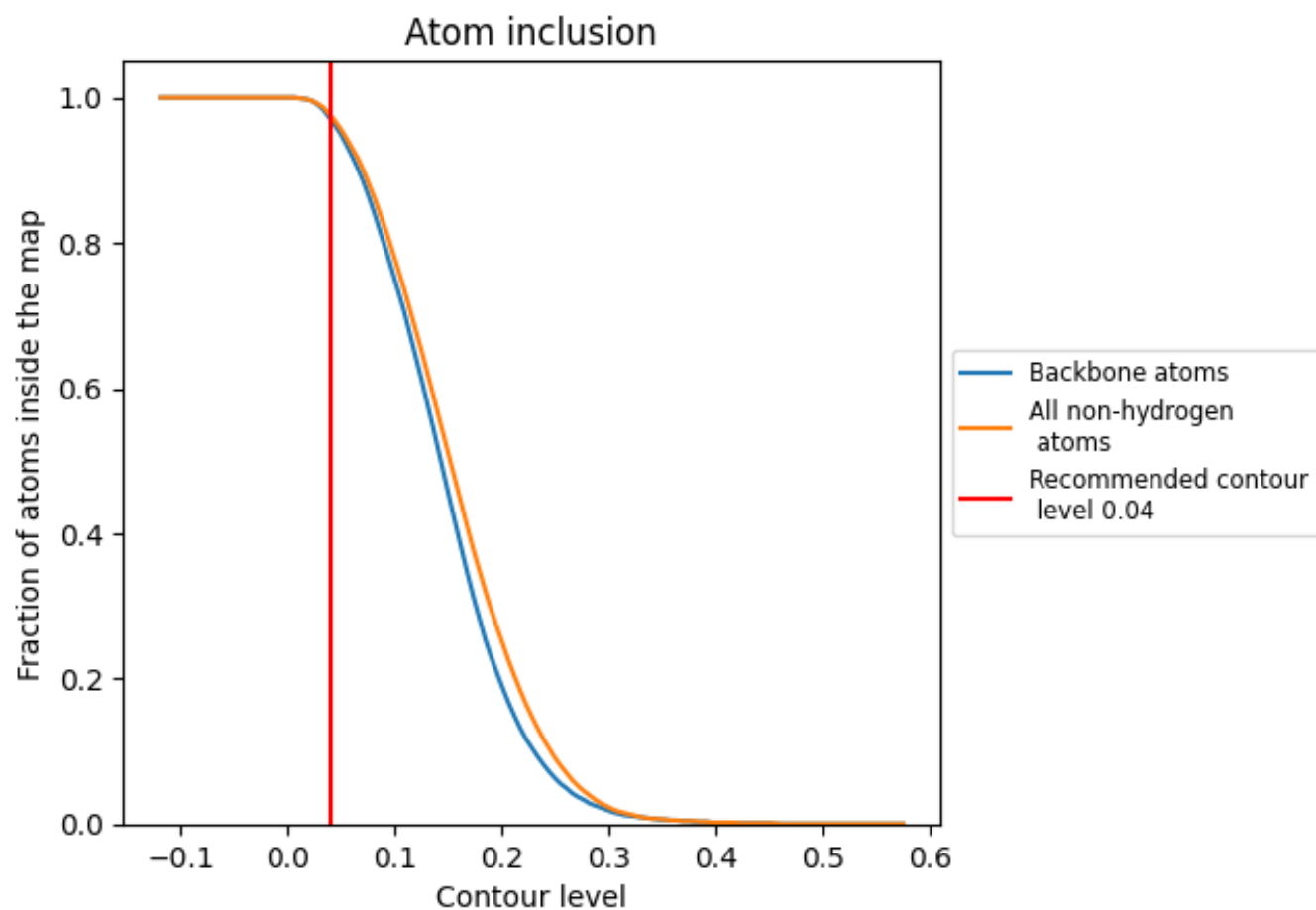
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9760	 0.6410
1	 0.9500	 0.6170
2	 0.9570	 0.6700
3	 0.9190	 0.5670
4	 0.9950	 0.6890
5	 0.9410	 0.6600
6	 0.9970	 0.7160
7	 0.9920	 0.6980
8	 0.9860	 0.6740
A	 0.9860	 0.6500
B	 0.9940	 0.6250
C	 0.9900	 0.7010
D	 0.9730	 0.6810
E	 0.9590	 0.6580
F	 0.9500	 0.5990
G	 0.9370	 0.5920
H	 0.8430	 0.5710
J	 0.5930	 0.3080
L	 0.9800	 0.6800
M	 0.9750	 0.6820
N	 0.9750	 0.6750
O	 0.9730	 0.6740
P	 0.9960	 0.6950
Q	 0.9650	 0.6190
R	 0.9560	 0.6660
S	 0.9920	 0.7010
T	 0.9560	 0.6660
U	 0.9700	 0.6830
V	 0.9540	 0.6530
W	 0.9670	 0.6210
X	 0.9380	 0.6310
Y	 0.9770	 0.6780
Z	 0.9750	 0.6760
a	 0.9910	 0.6400
b	 0.9070	 0.5740



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Chain	Atom inclusion	Q-score
c	 0.9510	 0.6340
d	 0.9570	 0.6260
e	 0.9660	 0.6530
f	 0.9410	 0.5930
g	 0.9220	 0.5800
h	 0.9580	 0.6540
i	 0.9460	 0.6100
j	 0.9090	 0.5740
k	 0.9660	 0.6300
l	 0.9780	 0.6850
m	 0.9530	 0.6170
n	 0.9690	 0.6360
o	 0.9640	 0.6370
p	 0.9740	 0.6330
q	 0.9620	 0.6360
r	 0.9720	 0.6300
s	 0.9580	 0.6090
t	 0.9620	 0.6250
u	 0.8870	 0.5790
v	 1.0000	 0.6700
w	 0.9880	 0.5860
x	 0.9880	 0.6230
z	 0.9270	 0.5800