



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 11:02 am BST

PDB ID : 8AYE / pdb_00008aye
EMDB ID : EMD-15712
Title : E. coli 70S ribosome bound to thermorubin and fMet-tRNA
Authors : Sanyal, S.; Parajuli, N.P.; Emmerich, A.G.
Deposited on : 2022-09-02
Resolution : 1.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

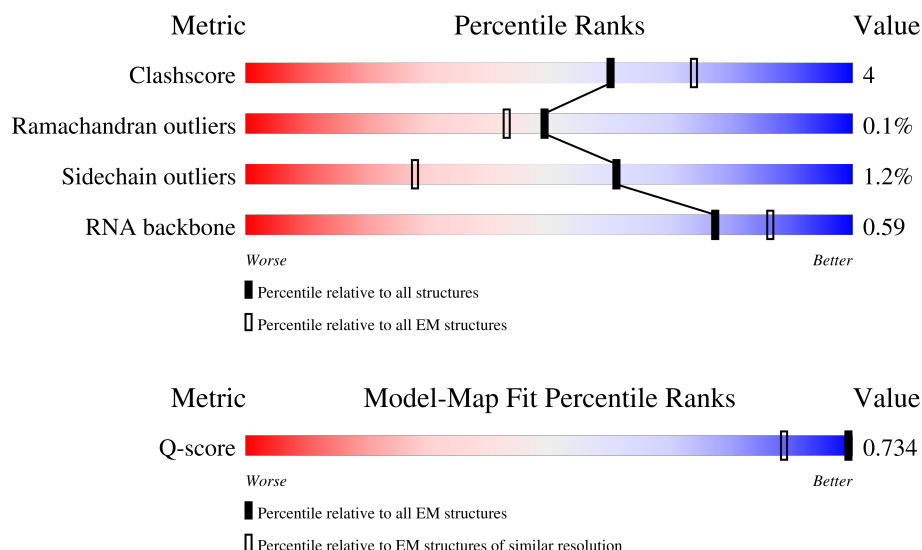
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

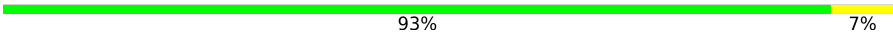
The reported resolution of this entry is 1.96 Å.

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.



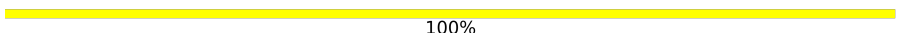
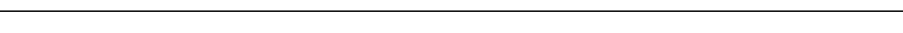
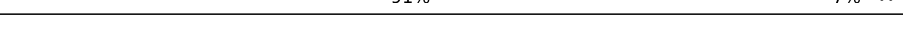
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1340 (1.46 - 2.46)

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

Mol	Chain	Length	Quality of chain
1	0	55	 82% 11% 7%
2	1	46	 93% 7%
3	2	65	 94% 5% .

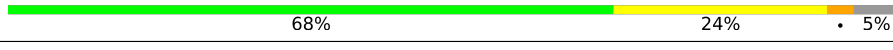
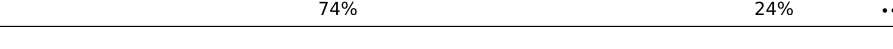
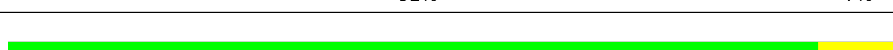
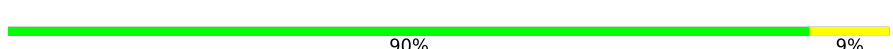
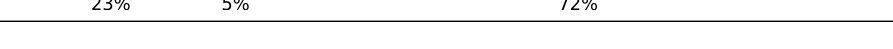
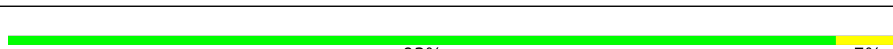
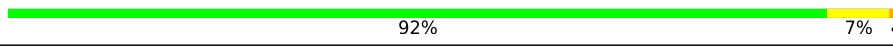
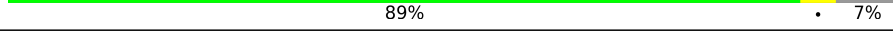
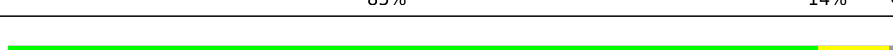
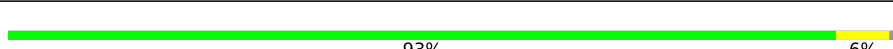
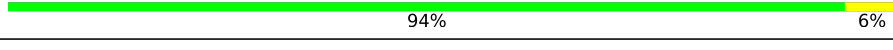
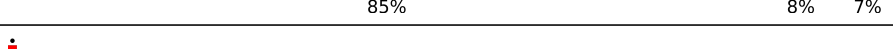
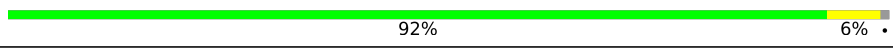
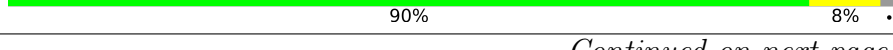
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Mol	Chain	Length	Quality of chain
4	3	38	 82% 16%
5	4	70	 67% 19% 14%
6	5	2	 100%
7	A	1542	 67% 28%
8	B	241	 76% 17% 7%
9	C	233	 72% 16% 12%
10	D	206	 73% 25%
11	E	167	 84% 10% 7%
12	F	135	 56% 21% 24%
13	G	179	 71% 14% 15%
14	H	130	 92% 8%
15	I	130	 82% 16%
16	J	103	 6% 69% 24% 5%
17	K	129	 73% 16% 9%
18	L	124	 91% 7% 2%
19	M	118	 78% 19% 3%
20	N	101	 86% 13% 1%
21	O	89	 87% 12% 1%
22	P	82	 89% 10% 1%
23	Q	84	 82% 10% 6%
24	R	75	 75% 11% 12%
25	S	92	 83% 9% 9%
26	T	87	 91% 8% 1%
27	U	71	 85% 14% 1%
28	X	6	 100%

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Mol	Chain	Length	Quality of chain
29	Z	76	
30	a	2903	
31	b	120	
32	c	273	
33	d	209	
34	e	201	
35	f	179	
36	g	177	
37	h	149	
38	i	142	
39	j	123	
40	k	144	
41	l	136	
42	m	127	
43	n	117	
44	o	115	
45	p	118	
46	q	103	
47	r	110	
48	s	100	
49	t	104	
50	u	94	
51	v	85	
52	w	78	
53	x	63	

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Mol	Chain	Length	Quality of chain
54	y	59	86% 10%
55	z	57	79% 19%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 140205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

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

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

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

- Molecule 7 is a RNA chain called 16S rRNA.

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

- Molecule 8 is a protein called 30S ribosomal protein S2.

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

- Molecule 9 is a protein called 30S ribosomal protein S3.

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

- Molecule 10 is a protein called 30S ribosomal protein S4.

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

- Molecule 11 is a protein called 30S ribosomal protein S5.

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

- Molecule 12 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

- Molecule 13 is a protein called 30S ribosomal protein S7.

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

- Molecule 14 is a protein called 30S ribosomal protein S8.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

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

- Molecule 16 is a protein called 30S ribosomal protein S10.

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

- Molecule 17 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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	ASP	ASN	conflict	UNP P0A7R9

- Molecule 18 is a protein called 30S ribosomal protein S12.

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

- Molecule 19 is a protein called 30S ribosomal protein S13.

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

- Molecule 20 is a protein called 30S ribosomal protein S14.

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

- Molecule 21 is a protein called 30S ribosomal protein S15.

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

- Molecule 22 is a protein called 30S ribosomal protein S16.

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

- Molecule 23 is a protein called 30S ribosomal protein S17.

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

- Molecule 24 is a protein called 30S ribosomal protein S18.

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

- Molecule 25 is a protein called 30S ribosomal protein S19.

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

- Molecule 26 is a protein called 30S ribosomal protein S20.

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

- Molecule 27 is a protein called 30S ribosomal protein S21.

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

- Molecule 28 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 29 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2753	Total	C	N	O	P	0	0
			59129	26383	10897	19096	2753		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	2163	G	A	conflict	GB 937521852

- Molecule 31 is a RNA chain called 5S rRNA.

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

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

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

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L9.

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

- Molecule 38 is a protein called 50S ribosomal protein L13.

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

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

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

- Molecule 48 is a protein called 50S ribosomal protein L23.

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

- Molecule 49 is a protein called 50S ribosomal protein L24.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

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

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

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

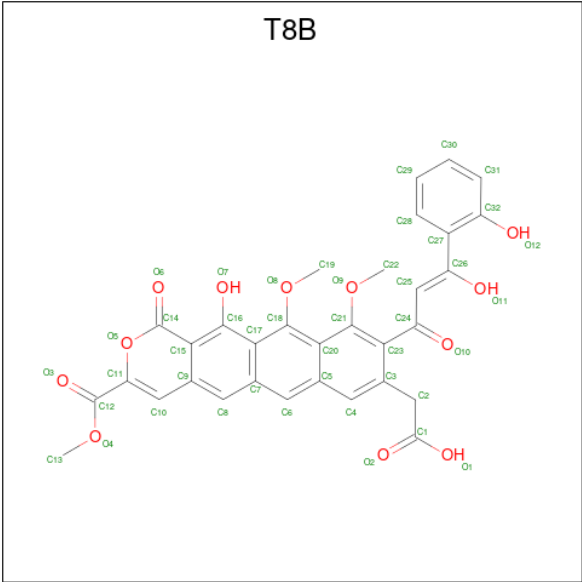
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	89	Total	Mg	0
			89	89	
57	E	1	Total	Mg	0
			1	1	
57	N	1	Total	Mg	0
			1	1	
57	Q	1	Total	Mg	0
			1	1	
57	a	207	Total	Mg	0
			207	207	
57	b	5	Total	Mg	0
			5	5	
57	d	1	Total	Mg	0
			1	1	
57	k	1	Total	Mg	0
			1	1	
57	p	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is Thermorubin (CCD ID: T8B) (formula: C₃₂H₂₄O₁₂) (labeled as "Ligand of Interest" by depositor).

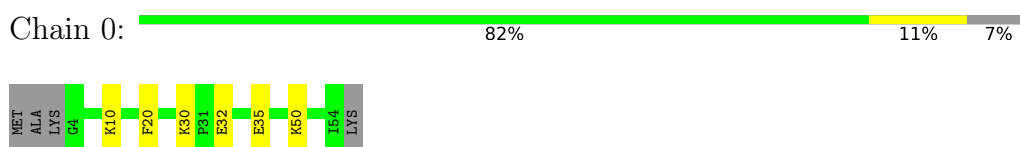


Mol	Chain	Residues	Atoms			AltConf
58	A	1	Total	C	O	0
			44	32	12	

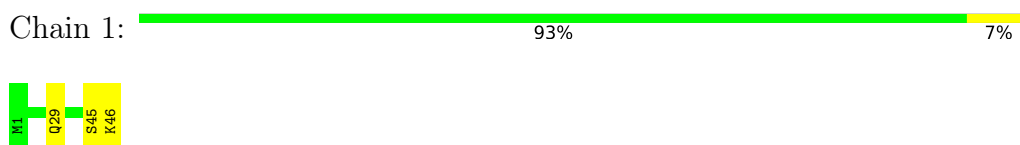
3 Residue-property plots [i](#)

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

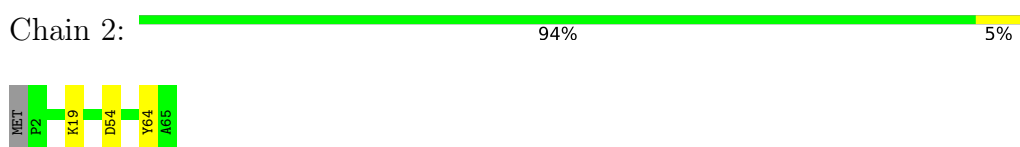
- Molecule 1: 50S ribosomal protein L33



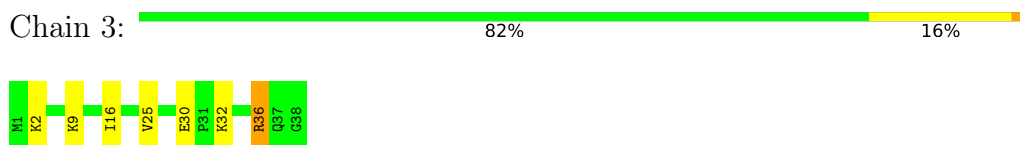
- Molecule 2: 50S ribosomal protein L34



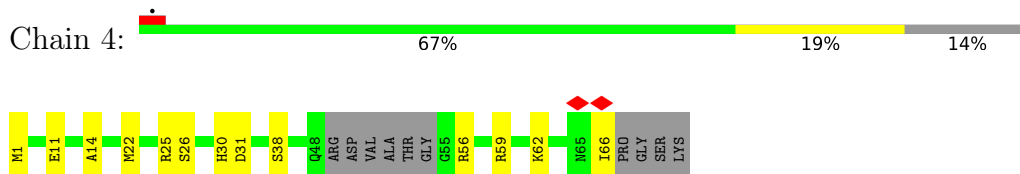
- Molecule 3: 50S ribosomal protein L35



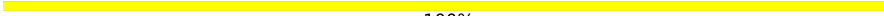
- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 50S ribosomal protein L31



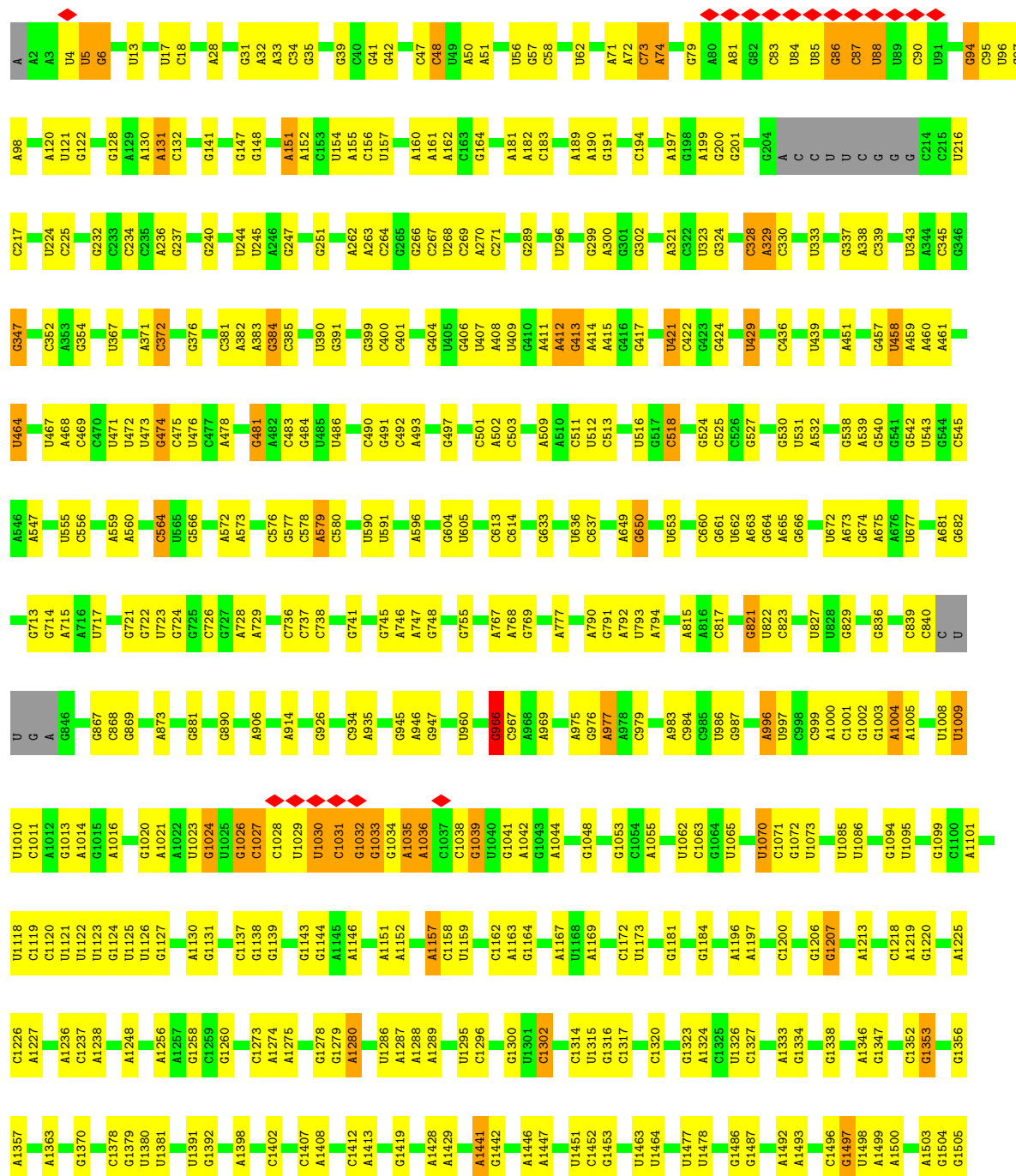
- Molecule 6: E-site tRNA

Chain 5:  100%

C75
A76

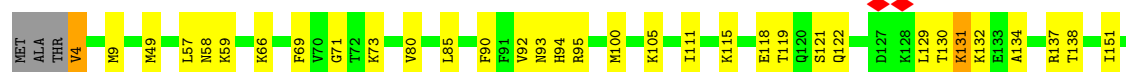
- Molecule 7: 16S rRNA

Chain A:  67% 28% . .

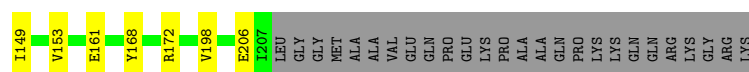




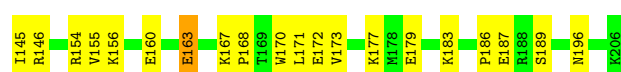
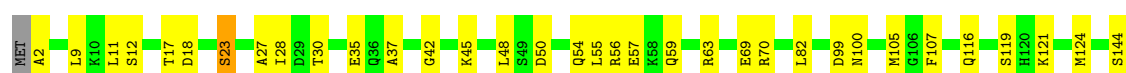
• Molecule 8: 30S ribosomal protein S2



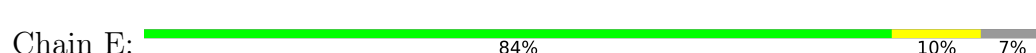
• Molecule 9: 30S ribosomal protein S3



• Molecule 10: 30S ribosomal protein S4



• Molecule 11: 30S ribosomal protein S5



• Molecule 12: 30S ribosomal protein S6, fully modified isoform



GLU
THR
ALA
ASP
ASP
GLU
GLU
GLU
GLU

- Molecule 13: 30S ribosomal protein S7

Chain G:  71% 14% 15%

MET PHE SER HIS GLN ALA GLY ALA SER SER LYS GLN PRO ALA LEU TYR LEU ASN
F2 R3 R4 R5 V6 L22 F26 K36 E40 E48 Q52 E60 A61 F62 E63 L66 R70 P71 R96 N97 M101 D113 L120 S125 E129 V135 R138 E139 D140 V141 H142 K149 Y154 ARG TRP LEU SER LEU ARG SER

- Molecule 14: 30S ribosomal protein S8

Chain H:  92% 8%

MET S2 Q18 M27 K50 L63 K64 Y65 Q67 V71 M96 A130

- Molecule 15: 30S ribosomal protein S9

Chain I:  82% 16%

MET ALA GLU N4 Q5 Y6 K13 R41 V47 L52 E53 L54 V55 D56 M57 V58 L63 R80 E89 Y90 D91 L94 L98 E112 V116 A121 R130

- Molecule 16: 30S ribosomal protein S10

Chain J:  6% 69% 24% 5%

MET GLN ASN GLN R5 I6 R7 L10 H15 VAL I13 T22 T25 T28 A34 Q35 V36 R37 I40 T44 L52 V57 R62 E66 H70 L71 D75 I76 V77 E78 P79 T80 E81 K82 D85 R89 L90 D91 S101 L102 GLY

- Molecule 17: 30S ribosomal protein S11

Chain K:  73% 16% 9%

MET ALA LYS ALA PRO TLE ARG ALA ARG LYS ARG VAL R13 V16 S17 D18 T35 A41 L42 S50 G51 F52 R53 F61 R69 Y77 G78 I79 E83 V84 R85 V86 K87 M109 V113 T114 P115 I116 P117 H118 D119 V129

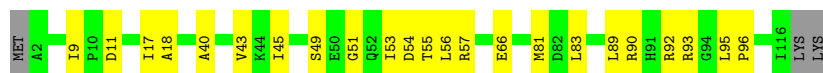
- Molecule 18: 30S ribosomal protein S12

Chain L:  91% 7% 2%

MET R2 R9 K10 K15 R54 E62 R110 K111 R114 V119 K120 R121 A124

- Molecule 19: 30S ribosomal protein S13

Chain M:  78% 19%



- Molecule 20: 30S ribosomal protein S14

Chain N:  86% 13%



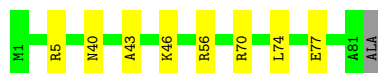
- Molecule 21: 30S ribosomal protein S15

Chain O:  87% 12%



- Molecule 22: 30S ribosomal protein S16

Chain P:  89% 10%



- Molecule 23: 30S ribosomal protein S17

Chain Q:  82% 10% 6%



- Molecule 24: 30S ribosomal protein S18

Chain R:  75% 11% 12%



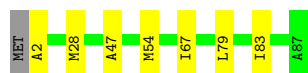
- Molecule 25: 30S ribosomal protein S19

Chain S:  83% 9% 9%



- Molecule 26: 30S ribosomal protein S20

Chain T:  91% 8%



- Molecule 27: 30S ribosomal protein S21

Chain U:  85% 14%



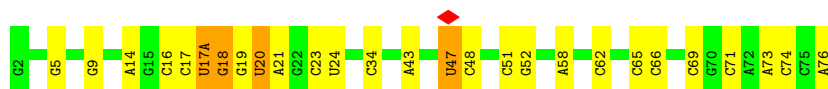
- Molecule 28: mRNA

Chain X:  100%

There are no outlier residues recorded for this chain.

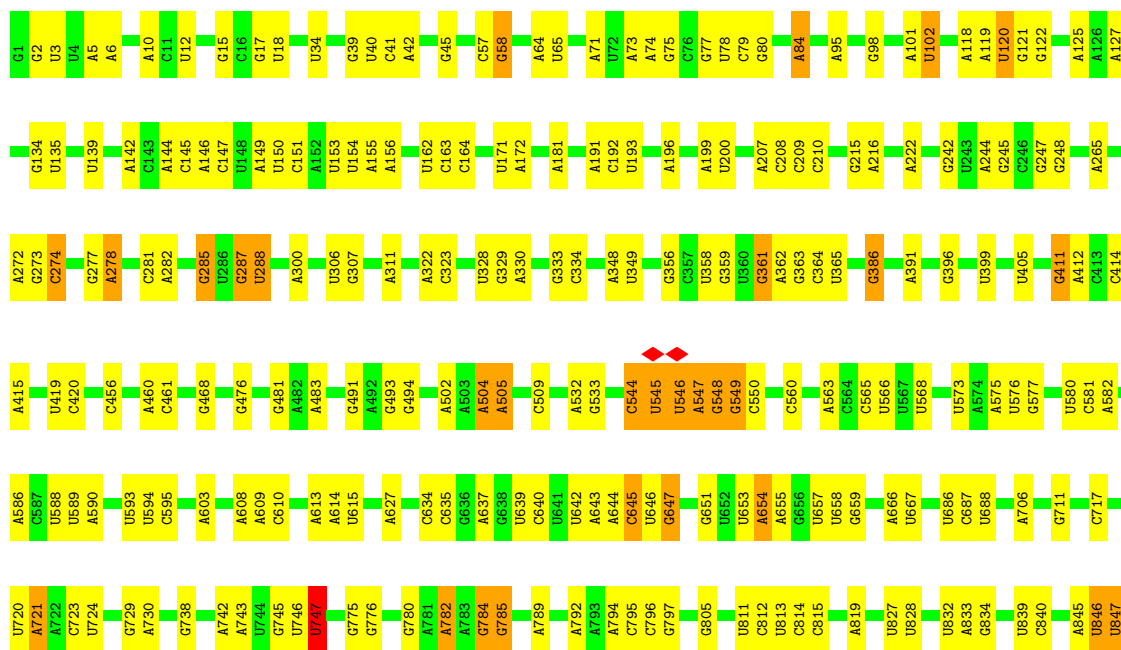
- Molecule 29: P-site tRNA-fMet

Chain Z:  64% 30% 5%

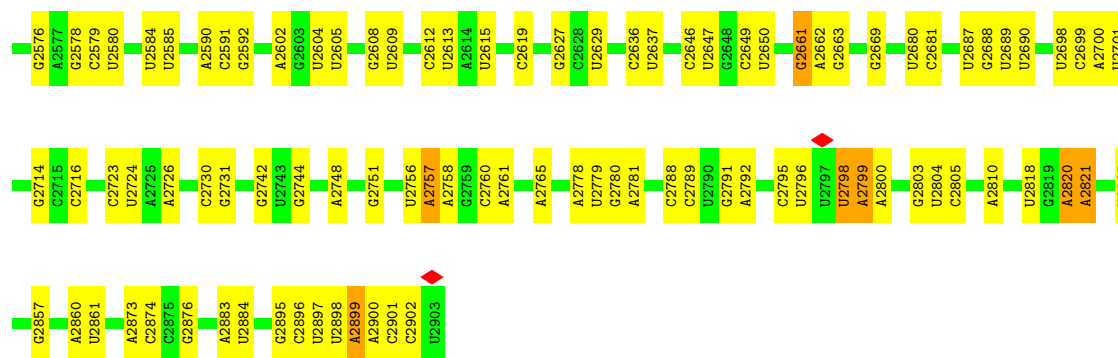


- Molecule 30: 23S rRNA

Chain a:  68% 24% 5%

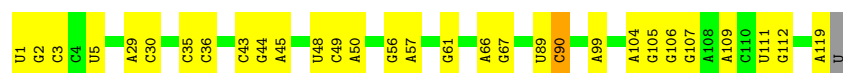


C2462	A2335	G2223	C	A2071	U1939	U1796	G1649	U1487	G1361	G1149	G	C848
C2463	A2336	G2224	A	C2072	U1946	G1797	C1656	C1493	G1362	C1150	A	A849
G2464	G2345	A2225	G	C2073	C1947	C1800	U1657	A1494	A1365	G1168	A	U850
A2469	G2346	G2228	U	U2074	A1801	C1800	A1668	A1495	A1366	A1169	C	C851
G2470	C2347	U2229	C	U2075	U1955	A1805	A1668	A1496	C1370	C1170	A	U852
U2473	G2361	U2233	C	U2086	G1962	A1808	G1674	U1497	G1371	G1171	G	C853
A2476	A2369	G2234	A	G2087	C1962	A1808	G1674	U1506	A1383	C1172	C	G856
U2477	G2373	G2234	A	U2092	C1965	A1808	G1681	C1507	A1378	U	C	G857
A2478	G2374	G2238	G	A2097	A1966	C1816	G1682	A1508	A1379	A	U	G858
G2481	C2380	U2239	G	U2098	C1967	U1820	U1683	A1509	G1380	U	C	G859
G2488	A2381	U2243	G	U	A1970	U1714	U1714	G1510	A1383	G1177	A	U860
U2491	G2382	U2244	C	G	U1971	G1715	G1715	U1513	U1405	C1178	A	A861
C2496	G2383	G2250	C	A	G1972	A1717	A1717	C1507	U1406	G1179	U	G862
A2497	U2384	G2251	G	G	U1991	G1835	G1718	A1508	A1387	U1180	U	A863
C2498	G2385	A2288	G	C	U1992	C1838	G1719	U1534	A1383	U1181	A	C965
C2499	U2393	A2273	C	U	U1993	G1842	U1720	A1535	U1405	G1182	A	U871
G2502	G2395	A2274	U	U	C1999	C1843	G1722	C1536	U1406	U1183	G	G872
A2503	G2396	G2277	A	G	A2014	A1847	C1726	G1542	G1410	U1184	A	C873
U2504	U2402	C2283	A	U	A2015	A1848	C1727	U1544	U1411	A1189	A	G874
G2505	C2403	G2283	U	G	U2016	A1853	G1728	A1545	G1416	U1198	U	G875
U2506	U2406	G2286	C	U	U2017	A1858	U1729	G1546	A1419	U1199	A	C876
C2512	G2415	A2287	C	G	G2018	A1858	G1731	C1547	A1427	C1200	U	A877
A2513	C2416	G2291	C	A	A2019	C1868	G1732	A1548	G1428	U1223	A	G878
U2514	G2422	U2292	C	G	A2020	C1874	G1733	A1549	G1429	U1224	C	G879
U2518	U2423	G2293	U	U	G2023	A1871	G1734	U1563	G1430	G1225	C	G880
C2520	C2424	G2294	U	G	G2024	A1872	G1738	C1565	A1434	A1226	U	G881
G2529	G2429	A2298	A	G	A2026	C1874	A1744	C1566	G1435	G1227	C	G882
U2537	U2430	G2304	U	C	G2027	G1875	A1745	A1569	U1442	A1253	C	G883
C2538	A2432	U2305	U	G	A2031	U1898	A1746	A1569	U1443	G1256	U	U884
A2547	G2435	G2308	U	U	A2032	C1902	U1747	U1578	G1444	A1264	A	C885
U2548	U2441	U2312	G	U	A2033	C1902	C1748	U1583	A1452	U1269	G	A886
U2552	C2442	A2322	A	G	G2038	G1906	A1762	U1584	A1453	C1270	U	U887
G2553	G2443	G2325	U	C	U2039	G1907	G1763	C1585	G1459	G1271	C	C888
U2554	G2444	C2326	U	U	G2043	U1911	A1773	A1590	A1469	A1272	C	C889
G2557	A2448	A2327	A	A	C2043	C1914	U1778	A1591	A1470	U1273	U	C890
C2558	U2449	G2328	G	G	G2055	U1915	U1782	C1595	A1475	G1300	G	G891
A2566	G2455	U2329	U	U	G2056	A1916	A1783	U1594	G1476	A1301	A	A909
G2567	C2456	G2330	G	G	A2059	U1917	A1784	C1595	U1477	G1338	U	A910
U2570	U2457	G2331	A	A	G2060	G1929	A1785	C1607	G1478	U1352	U	G911
C2573	G2461	U2332	C	C	G2061	U1932	A1791	A1618	G1482	A1353	G	G912
		U2334	G	G	A2062	G1933	A1791	G1622	G1483	G1355	U	U913
			C	C	G2063	G1933	A1791	G1622	U1484	G1356	U	G914
			C	C	G2065	G1933	A1791	G1622	G1357	A1141	U	G930
			C	C	G2069	A1937	A1794	U1647	U1485	A1142	A	U931
			C	C	A2070	A1938	C1795	U1648	U1486			U932
			C	C								U933
			C	C								U934



• Molecule 31: 5S rRNA

Chain b: 74% 24% ..



• Molecule 32: 50S ribosomal protein L2

Chain c: 92% 7% .



• Molecule 33: 50S ribosomal protein L3

Chain d: 91% 9%



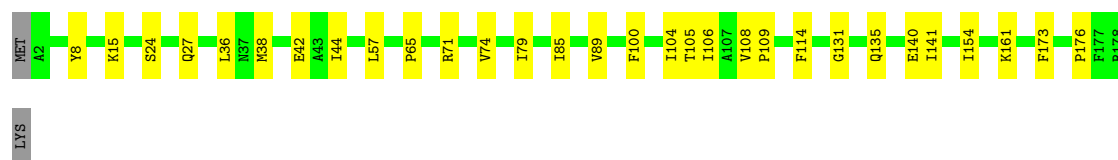
• Molecule 34: 50S ribosomal protein L4

Chain e: 90% 9%

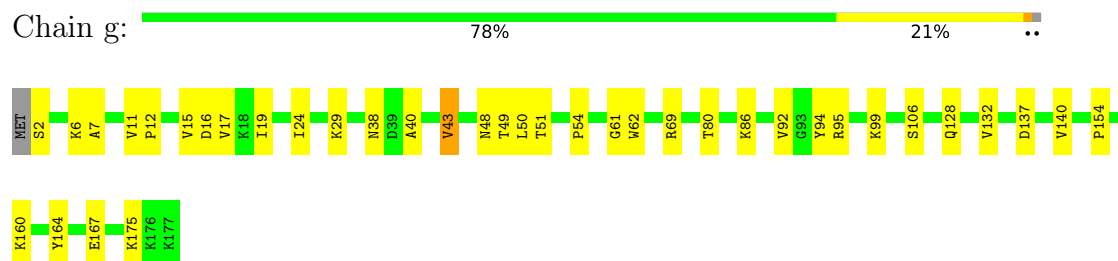


• Molecule 35: 50S ribosomal protein L5

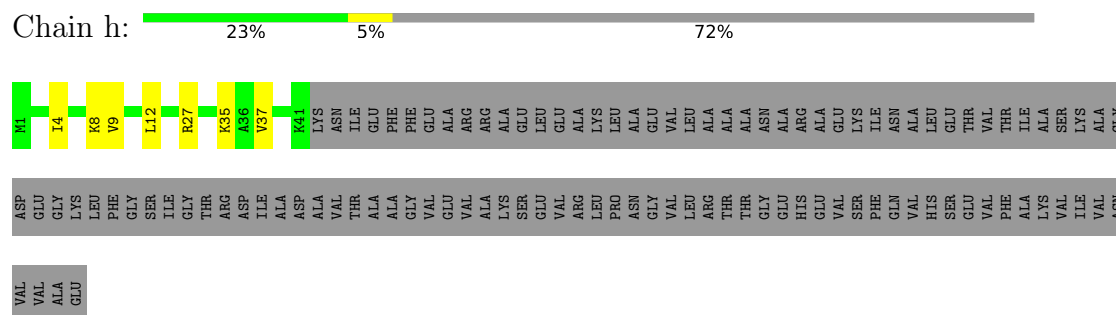
Chain f: 82% 17% .



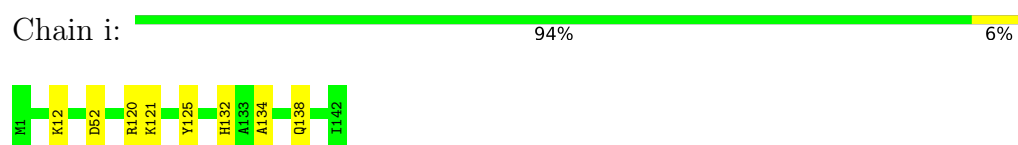
• Molecule 36: 50S ribosomal protein L6



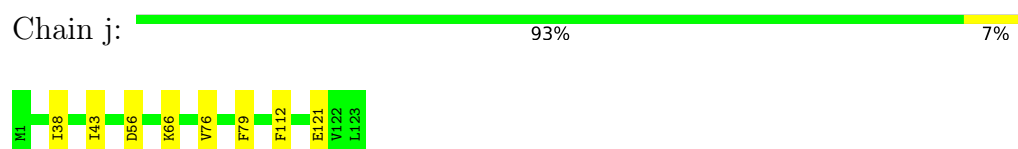
- Molecule 37: 50S ribosomal protein L9



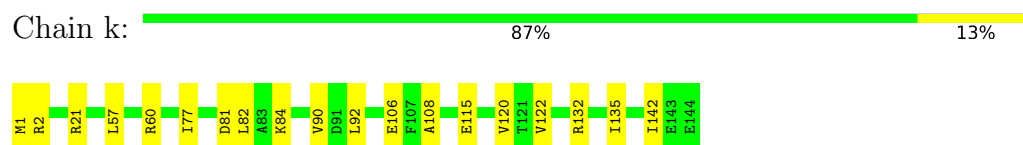
- Molecule 38: 50S ribosomal protein L13



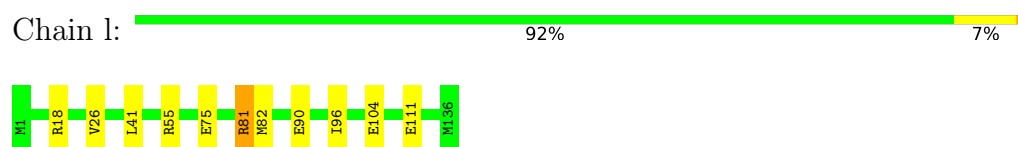
- Molecule 39: 50S ribosomal protein L14



- Molecule 40: 50S ribosomal protein L15



- Molecule 41: 50S ribosomal protein L16



- Molecule 42: 50S ribosomal protein L17

Chain m:  89% 7%



- Molecule 43: 50S ribosomal protein L18

Chain n:  85% 14%



- Molecule 44: 50S ribosomal protein L19

Chain o:  91% 8%



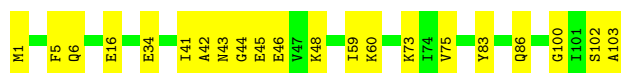
- Molecule 45: 50S ribosomal protein L20

Chain p:  93% 6%



- Molecule 46: 50S ribosomal protein L21

Chain q:  80% 20%



- Molecule 47: 50S ribosomal protein L22

Chain r:  94% 6%

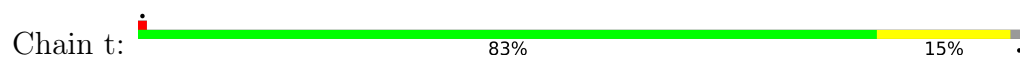


- Molecule 48: 50S ribosomal protein L23

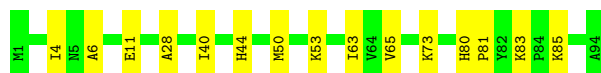
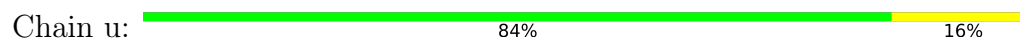
Chain s:  85% 8% 7%



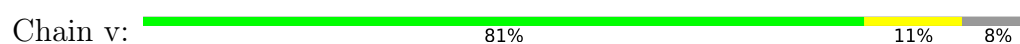
- Molecule 49: 50S ribosomal protein L24



- Molecule 50: 50S ribosomal protein L25



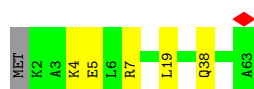
- Molecule 51: 50S ribosomal protein L27



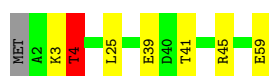
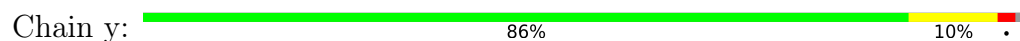
- Molecule 52: 50S ribosomal protein L28



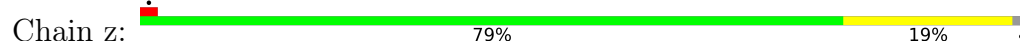
- Molecule 53: 50S ribosomal protein L29



- Molecule 54: 50S ribosomal protein L30



- Molecule 55: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1088035	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.745	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.598	Depositor
Minimum map value	-1.927	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	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, 1MG, MEQ, OMC, 6MZ, OMG, 5MU, MG, 5MC, OMU, MA6, 4OC, G7M, T8B, PSU, 2MA, ZN, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.33	0/424	0.46	0/565
2	1	0.34	0/380	0.51	0/498
3	2	0.34	0/513	0.44	0/676
4	3	0.33	0/303	0.39	0/397
5	4	0.22	0/488	0.44	0/649
6	5	0.26	0/46	0.24	0/69
7	A	0.38	0/36236	0.43	0/56520
8	B	0.28	0/1784	0.49	0/2403
9	C	0.28	0/1651	0.45	0/2225
10	D	0.26	0/1665	0.45	0/2227
11	E	0.32	0/1165	0.50	0/1568
12	F	0.35	1/858 (0.1%)	0.62	3/1160 (0.3%)
13	G	0.26	0/1219	0.46	0/1635
14	H	0.31	0/989	0.48	0/1326
15	I	0.30	0/1034	0.44	0/1375
16	J	0.31	0/796	0.49	0/1077
17	K	0.28	0/893	0.55	2/1205 (0.2%)
18	L	0.30	0/969	0.48	0/1300
19	M	0.27	0/900	0.44	1/1204 (0.1%)
20	N	0.28	0/817	0.39	0/1088
21	O	0.26	0/722	0.41	0/964
22	P	0.29	0/653	0.50	0/877
23	Q	0.31	0/650	0.47	0/871
24	R	0.29	0/553	0.51	0/742
25	S	0.24	0/685	0.44	0/922
26	T	0.28	0/676	0.43	0/895
27	U	0.27	0/597	0.47	0/792
28	X	0.35	0/147	0.41	0/227
29	Z	0.31	0/1813	0.43	0/2825
30	a	0.46	1/65696 (0.0%)	0.48	0/102485
31	b	0.36	0/2850	0.37	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.36	0/2121	0.49	0/2852
33	d	0.33	0/1576	0.47	0/2119
34	e	0.30	0/1571	0.46	0/2113
35	f	0.27	0/1434	0.44	0/1926
36	g	0.27	0/1343	0.46	0/1816
37	h	0.26	0/306	0.57	0/413
38	i	0.32	0/1152	0.46	0/1551
39	j	0.37	0/955	0.53	0/1279
40	k	0.31	0/1062	0.45	0/1413
41	l	0.33	0/1092	0.51	1/1457 (0.1%)
42	m	0.36	0/958	0.52	0/1281
43	n	0.28	0/902	0.46	0/1209
44	o	0.33	0/929	0.47	0/1242
45	p	0.33	0/960	0.47	0/1278
46	q	0.31	0/829	0.45	0/1107
47	r	0.34	0/864	0.46	0/1156
48	s	0.29	0/744	0.46	0/994
49	t	0.29	0/787	0.48	0/1051
50	u	0.30	0/766	0.43	0/1025
51	v	0.33	0/593	0.46	0/785
52	w	0.31	0/635	0.42	0/848
53	x	0.25	0/502	0.36	0/667
54	y	0.33	0/453	0.51	0/605
55	z	0.33	0/450	0.43	0/599
All	All	0.40	2/151156 (0.0%)	0.46	7/225997 (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
52	w	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2449	U	C5-C6	7.93	1.50	1.34
12	F	101	PRO	CG-CD	-6.43	1.28	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	101	PRO	N-CD-CG	-10.47	87.50	103.20
17	K	118	HIS	CA-C-N	6.98	134.87	121.54
17	K	118	HIS	C-N-CA	6.98	134.87	121.54
41	l	81	ARG	N-CA-C	-6.49	102.14	110.19
12	F	101	PRO	CA-N-CD	-6.01	103.59	112.00
12	F	101	PRO	CA-CB-CG	-5.85	93.39	104.50
19	M	66	GLU	CB-CA-C	-5.57	110.13	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	w	16	ASN	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	0	417	0	451	6	0
2	1	377	0	418	3	0
3	2	504	0	572	3	0
4	3	302	0	340	5	0
5	4	480	0	478	9	0
6	5	42	0	23	1	0
7	A	32612	0	16432	257	0
8	B	1753	0	1780	28	0
9	C	1624	0	1696	23	0
10	D	1643	0	1707	32	0
11	E	1152	0	1196	9	0
12	F	839	0	833	16	0
13	G	1203	0	1254	19	0
14	H	979	0	1031	6	0
15	I	1022	0	1070	16	0
16	J	786	0	828	17	0
17	K	877	0	885	13	0
18	L	955	0	1016	6	0
19	M	891	0	952	15	0
20	N	805	0	844	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	O	714	0	734	6	0
22	P	643	0	661	5	0
23	Q	641	0	682	10	0
24	R	544	0	565	10	0
25	S	668	0	693	4	0
26	T	670	0	719	6	0
27	U	589	0	629	7	0
28	X	131	0	66	0	0
29	Z	1623	0	825	7	0
30	a	59129	0	29761	369	0
31	b	2549	0	1291	16	0
32	c	2082	0	2154	12	0
33	d	1566	0	1618	11	0
34	e	1552	0	1619	15	0
35	f	1410	0	1444	20	0
36	g	1323	0	1371	23	0
37	h	303	0	327	4	0
38	i	1129	0	1162	5	0
39	j	946	0	1023	5	0
40	k	1053	0	1129	12	0
41	l	1074	0	1156	10	0
42	m	945	0	989	3	0
43	n	892	0	923	9	0
44	o	917	0	962	7	0
45	p	947	0	1019	5	0
46	q	816	0	839	11	0
47	r	857	0	922	5	0
48	s	738	0	807	4	0
49	t	779	0	831	9	0
50	u	753	0	780	9	0
51	v	586	0	596	8	0
52	w	625	0	652	3	0
53	x	501	0	531	6	0
54	y	449	0	488	4	0
55	z	444	0	458	7	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	89	0	0	0	0
57	E	1	0	0	0	0
57	N	1	0	0	0	0
57	Q	1	0	0	0	0
57	a	207	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	b	5	0	0	0	0
57	d	1	0	0	0	0
57	k	1	0	0	0	0
57	p	1	0	0	0	0
57	z	1	0	0	0	0
58	A	44	0	20	1	0
All	All	140205	0	94252	1036	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1036) 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)
30:a:747:5MU:C5	30:a:747:5MU:C4	1.78	1.62
30:a:1939:5MU:C4	30:a:1939:5MU:C5	1.78	1.62
12:F:37:HIS:HB3	12:F:97:THR:HG22	1.53	0.91
7:A:1028:C:N4	7:A:1033:G:O6	2.06	0.89
30:a:2796:U:H3	30:a:2799:A:H61	1.16	0.88
7:A:1009:U:H3	7:A:1020:G:H1	1.24	0.83
30:a:881:G:H1	30:a:895:U:H3	1.27	0.83
7:A:677:U:H3	7:A:713:G:H22	1.26	0.82
8:B:92:VAL:HG21	8:B:100:MET:HE1	1.60	0.82
9:C:50:ALA:HA	9:C:75:ILE:HD11	1.62	0.82
49:t:50:PRO:HA	49:t:54:GLN:HG3	1.62	0.82
7:A:458:U:H3	7:A:474:G:H1	1.27	0.81
30:a:568:U:H1'	30:a:2030:6MZ:H9C1	1.63	0.80
8:B:100:MET:HE3	8:B:151:ILE:HD13	1.64	0.80
51:v:10:THR:HG22	51:v:12:ASN:H	1.45	0.79
15:I:55:VAL:HG23	15:I:57:MET:HG3	1.65	0.78
36:g:95:ARG:HB2	36:g:128:GLN:HG2	1.66	0.77
17:K:85:MET:HE3	17:K:113:VAL:HG11	1.65	0.76
12:F:5:GLU:OE2	24:R:24:LYS:NZ	2.19	0.75
8:B:121:SER:OG	8:B:122:GLN:NE2	2.20	0.75
16:J:66:GLU:HB2	20:N:99:ALA:HB2	1.67	0.75
23:Q:25:ILE:HB	23:Q:42:THR:HG23	1.67	0.75
30:a:549:G:H2'	30:a:550:C:C6	2.23	0.74
7:A:79:G:H1	7:A:90:C:H42	1.34	0.73
16:J:10:LEU:HD13	16:J:22:THR:HG22	1.70	0.72
7:A:1048:G:H5''	20:N:3:LYS:HG2	1.72	0.72
30:a:1478:G:H1	30:a:1513:U:H3	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1086:U:H3	7:A:1099:G:H22	1.39	0.71
7:A:664:G:H22	7:A:741:G:H1	1.36	0.71
9:C:135:LYS:O	9:C:139:GLN:HG2	1.92	0.70
7:A:131:A:H2'	7:A:132:C:C6	2.28	0.69
24:R:9:LYS:HG2	24:R:10:PHE:H	1.57	0.69
48:s:25:GLU:HG3	48:s:26:LYS:HG2	1.73	0.69
54:y:45:ARG:HH22	54:y:59:GLU:HG2	1.58	0.69
8:B:129:LEU:HD21	8:B:137:ARG:HD3	1.75	0.68
7:A:946:A:H2'	7:A:947:G:C8	2.28	0.68
35:f:36:LEU:HD22	35:f:154:ILE:HG12	1.75	0.68
30:a:2328:A:H2'	30:a:2329:U:C6	2.29	0.67
7:A:1391:U:H2'	7:A:1392:G:C8	2.29	0.67
30:a:881:G:N2	30:a:895:U:O2	2.27	0.67
25:S:15:LEU:HD12	25:S:35:SER:HB3	1.77	0.67
30:a:2547:A:H2'	30:a:2548:U:C6	2.30	0.67
10:D:124:MET:HE3	10:D:146:ARG:HG2	1.76	0.66
13:G:113:ASP:OD1	13:G:113:ASP:N	2.27	0.66
30:a:1469:A:H2'	30:a:1470:A:C8	2.30	0.65
39:j:121:GLU:OE2	44:o:65:SER:OG	2.13	0.65
7:A:17:U:H2'	7:A:18:C:C6	2.31	0.65
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.78	0.65
7:A:460:A:H2'	7:A:461:A:H8	1.62	0.65
36:g:11:VAL:O	36:g:48:ASN:ND2	2.26	0.65
30:a:363:G:H2'	30:a:364:C:C6	2.31	0.64
7:A:673:A:H2'	7:A:674:G:C8	2.33	0.64
30:a:2291:U:H2'	30:a:2292:U:C6	2.32	0.64
41:l:75:GLU:HB2	41:l:90:GLU:HG3	1.78	0.64
30:a:887:U:O2'	30:a:889:C:OP2	2.16	0.64
10:D:11:LEU:HD13	10:D:63:ARG:HG2	1.81	0.63
7:A:337:G:H2'	7:A:338:A:C8	2.34	0.63
5:4:11:GLU:HA	5:4:25:ARG:HA	1.80	0.63
41:l:81:ARG:C	41:l:82:MET:N	2.56	0.63
30:a:544:C:H4'	30:a:545:U:C5	2.34	0.63
30:a:2277:G:OP2	51:v:10:THR:HG21	1.99	0.62
13:G:22:LEU:HD12	13:G:62:PHE:HE1	1.64	0.62
29:Z:16:C:OP1	29:Z:17:C:N4	2.32	0.62
10:D:163:GLU:HA	10:D:167:LYS:NZ	2.13	0.62
30:a:813:U:H2'	30:a:814:C:C6	2.35	0.62
18:L:110:ARG:HB3	18:L:119:VAL:HG21	1.82	0.62
50:u:6:ALA:HB3	50:u:65:VAL:HG12	1.81	0.62
7:A:1027:C:H2'	7:A:1028:C:C6	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:823:C:HO2'	14:H:2:SER:N	1.98	0.62
32:c:29:PRO:HG2	32:c:34:LEU:HD11	1.82	0.62
7:A:460:A:H2'	7:A:461:A:C8	2.35	0.61
27:U:55:ARG:O	27:U:59:LYS:HG2	2.00	0.61
30:a:1733:G:H2'	30:a:1734:G:H8	1.65	0.61
7:A:1323:G:H2'	7:A:1324:A:C8	2.35	0.61
15:I:47:VAL:HG13	15:I:80:ARG:HD3	1.83	0.61
7:A:96:U:H2'	7:A:97:G:C8	2.35	0.61
23:Q:17:MET:HB3	23:Q:20:SER:HB2	1.82	0.61
54:y:39:GLU:HG3	54:y:41:THR:HG23	1.83	0.61
7:A:5:U:H4'	7:A:6:G:O5'	2.00	0.61
7:A:1071:C:H2'	7:A:1072:G:H8	1.66	0.61
30:a:639:U:H2'	30:a:640:C:C6	2.36	0.61
30:a:876:C:H2'	30:a:877:A:O4'	2.01	0.61
8:B:73:LYS:NZ	8:B:204:ASP:O	2.34	0.61
7:A:613:C:H2'	7:A:614:C:C6	2.36	0.61
41:l:26:VAL:HA	41:l:104:GLU:OE1	2.00	0.61
7:A:216:U:H2'	7:A:217:C:C6	2.35	0.60
24:R:14:THR:OG1	24:R:48:ARG:HD3	2.00	0.60
30:a:2298:A:OP1	35:f:71:ARG:NH1	2.33	0.60
50:u:4:ILE:HG12	50:u:50:MET:HE1	1.83	0.60
7:A:769:G:H4'	7:A:1513:A:H4'	1.83	0.60
12:F:38:ARG:HB3	12:F:63:ASN:HB2	1.82	0.60
34:e:1:MET:HE1	34:e:20:GLY:HA3	1.82	0.60
40:k:77:ILE:HD11	40:k:108:ALA:HB1	1.83	0.60
7:A:1130:A:H2'	7:A:1131:G:H8	1.67	0.60
12:F:88:MET:HE3	12:F:90:MET:SD	2.42	0.60
15:I:57:MET:HE1	15:I:90:TYR:CE1	2.37	0.60
32:c:182:ARG:HG2	32:c:183:LYS:N	2.17	0.60
30:a:546:U:H6	30:a:548:G:H21	1.50	0.60
31:b:66:A:H61	31:b:107:G:H2'	1.67	0.60
7:A:1218:C:H2'	7:A:1219:A:C8	2.37	0.60
7:A:1356:G:H2'	7:A:1357:A:C8	2.36	0.59
36:g:86:LYS:HG2	36:g:132:VAL:HG22	1.84	0.59
12:F:18:VAL:O	12:F:22:ILE:HG13	2.02	0.59
9:C:129:MET:HG3	9:C:132:ARG:NH1	2.18	0.59
7:A:451:A:H61	7:A:481:G:H5'	1.66	0.59
7:A:518:C:O2'	7:A:530:G:N2	2.35	0.59
12:F:41:ASP:OD1	12:F:58:HIS:NE2	2.25	0.59
30:a:594:U:H2'	30:a:595:C:C6	2.37	0.59
7:A:181:A:O2'	7:A:194:C:N4	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1410:G:H2'	30:a:1411:U:C6	2.37	0.59
7:A:1013:G:N2	7:A:1016:A:OP2	2.30	0.59
11:E:160:SER:OG	11:E:163:GLU:HG3	2.03	0.59
17:K:42:LEU:HD12	17:K:79:ILE:HD11	1.83	0.59
17:K:83:GLU:HG2	17:K:109:ASN:HB3	1.85	0.59
34:e:1:MET:HE3	34:e:16:GLU:HG3	1.85	0.59
7:A:1014:A:C2	7:A:1219:A:H1'	2.37	0.59
30:a:851:C:H2'	30:a:852:U:C6	2.38	0.59
30:a:2557:G:H2'	30:a:2558:C:C6	2.38	0.58
44:o:3:ASN:HA	44:o:6:LYS:HG2	1.84	0.58
30:a:1746:A:H2'	30:a:1747:U:C6	2.38	0.58
30:a:2895:G:H2'	30:a:2896:C:C6	2.37	0.58
33:d:149:ASN:OD1	33:d:150:MEQ:N	2.36	0.58
43:n:87:ILE:O	43:n:88:LYS:HG2	2.02	0.58
17:K:13:ARG:HD2	17:K:77:TYR:OH	2.04	0.58
40:k:132:ARG:HG3	40:k:142:ILE:HD13	1.85	0.58
46:q:41:ILE:HD12	46:q:103:ALA:HA	1.84	0.58
9:C:9:GLY:HA3	20:N:89:MET:HE3	1.84	0.58
7:A:545:C:H5'	10:D:69:GLU:HB2	1.85	0.58
7:A:1001:C:H2'	7:A:1002:G:H8	1.68	0.58
15:I:91:ASP:HB3	15:I:94:LEU:HG	1.84	0.58
7:A:216:U:H4'	7:A:464:U:H4'	1.86	0.58
7:A:1071:C:H2'	7:A:1072:G:C8	2.38	0.58
30:a:706:A:OP1	32:c:7:LYS:NZ	2.29	0.58
49:t:81:ASP:OD2	49:t:96:PHE:HB3	2.04	0.58
40:k:77:ILE:CD1	40:k:108:ALA:HB1	2.34	0.58
7:A:1020:G:H2'	7:A:1021:A:H8	1.68	0.58
12:F:1:MET:HE3	12:F:65:GLU:HG2	1.84	0.58
30:a:1199:U:H2'	30:a:1200:C:H6	1.69	0.58
7:A:409:U:OP1	10:D:23:SER:OG	2.22	0.57
14:H:64:LYS:HG3	14:H:71:VAL:HG21	1.85	0.57
30:a:273:G:H2'	30:a:274:C:C6	2.39	0.57
35:f:44:ILE:HD13	35:f:79:ILE:HG22	1.84	0.57
30:a:144:A:H2'	30:a:145:C:C6	2.39	0.57
48:s:69:ARG:NH1	48:s:72:GLN:OE1	2.37	0.57
15:I:112:GLU:HG2	15:I:121:ALA:HB1	1.85	0.57
30:a:278:A:N1	30:a:361:G:O2'	2.36	0.57
30:a:1906:G:H2'	30:a:1907:G:H5''	1.85	0.57
11:E:45:ARG:HB3	11:E:71:MET:HE2	1.87	0.57
30:a:2193:G:H2'	30:a:2194:U:C6	2.40	0.57
10:D:107:PHE:CG	10:D:145:ILE:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:414:C:H2'	30:a:415:A:C8	2.38	0.57
7:A:1041:G:H2'	7:A:1042:A:O4'	2.04	0.57
9:C:14:ILE:HG22	9:C:15:VAL:HG13	1.85	0.57
30:a:1405:U:H2'	30:a:1406:U:C6	2.40	0.57
30:a:2331:G:O2'	30:a:2336:A:N1	2.37	0.57
30:a:2591:C:H2'	30:a:2592:G:C8	2.39	0.57
26:T:28:MET:HE1	26:T:67:ILE:HG21	1.86	0.57
30:a:1722:A:N6	30:a:1738:G:O2'	2.38	0.57
11:E:14:LYS:HE3	11:E:116:GLU:OE1	2.04	0.57
30:a:64:A:H2'	30:a:65:U:C6	2.39	0.57
7:A:1225:A:H2'	7:A:1226:C:C5	2.40	0.57
30:a:1197:G:H2'	30:a:1198:U:H6	1.70	0.57
5:4:38:SER:HB2	35:f:105:THR:HA	1.87	0.56
7:A:87:C:H2'	7:A:88:U:C6	2.40	0.56
7:A:269:C:H2'	7:A:270:A:C8	2.40	0.56
7:A:299:G:H2'	7:A:300:A:C8	2.41	0.56
31:b:1:U:H2'	31:b:2:G:H8	1.71	0.56
7:A:539:A:H2'	7:A:540:G:C8	2.39	0.56
7:A:1009:U:H2'	7:A:1010:U:C6	2.40	0.56
7:A:1302:C:C5	19:M:17:ILE:HG13	2.41	0.56
30:a:871:U:H2'	30:a:872:U:C6	2.41	0.56
10:D:154:ARG:HG3	10:D:155:VAL:N	2.21	0.56
8:B:131:LYS:HD3	8:B:131:LYS:C	2.30	0.56
30:a:930:G:H1'	54:y:25:LEU:HD11	1.87	0.56
7:A:1273:C:H2'	7:A:1274:A:O4'	2.05	0.56
15:I:52:LEU:HD11	15:I:63:LEU:HD21	1.87	0.56
19:M:49:SER:O	19:M:53:ILE:HG12	2.05	0.56
8:B:49:MET:HE2	8:B:199:VAL:O	2.06	0.56
10:D:50:ASP:OD1	10:D:54:GLN:NE2	2.38	0.56
46:q:34:GLU:OE2	46:q:60:LYS:HE3	2.06	0.56
45:p:49:ASP:HA	45:p:52:GLN:HB2	1.88	0.56
12:F:67:PRO:HB2	12:F:69:GLU:OE1	2.05	0.56
30:a:2649:C:H2'	30:a:2650:U:H6	1.70	0.56
7:A:31:G:O2'	7:A:48:C:N4	2.39	0.56
30:a:2243:U:H2'	30:a:2244:U:C6	2.41	0.56
7:A:475:C:H2'	7:A:476:U:C6	2.41	0.55
7:A:666:G:H5'	7:A:726:C:H1'	1.87	0.55
7:A:728:A:H2'	7:A:729:A:C8	2.42	0.55
7:A:384:G:H2'	7:A:385:C:C6	2.41	0.55
7:A:1004:A:H2'	7:A:1005:A:O4'	2.07	0.55
7:A:1162:C:H2'	7:A:1163:A:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:580:U:H2'	30:a:581:C:C6	2.41	0.55
52:w:3:ARG:O	52:w:12:PRO:HD3	2.06	0.55
7:A:717:U:H4'	17:K:119:ASP:OD2	2.05	0.55
19:M:9:ILE:HG23	19:M:18:ALA:HB1	1.86	0.55
30:a:720:U:H2'	30:a:721:A:C8	2.41	0.55
36:g:164:TYR:HB2	36:g:167:GLU:HB2	1.89	0.55
38:i:125:TYR:HH	38:i:132:HIS:HE2	1.49	0.55
20:N:16:LEU:HD12	20:N:54:ASP:HB2	1.88	0.55
7:A:1408:A:C2	58:A:1689:T8B:H5	2.42	0.55
20:N:64:CYS:HB2	20:N:80:SER:HB3	1.88	0.55
8:B:115:LYS:O	8:B:119:THR:HG23	2.05	0.55
10:D:163:GLU:HA	10:D:167:LYS:HZ3	1.71	0.55
47:r:4:ILE:HG12	47:r:106:VAL:HG22	1.88	0.55
13:G:5:ARG:O	13:G:5:ARG:HG3	2.05	0.55
30:a:1475:G:O2'	30:a:1514:G:O6	2.24	0.55
36:g:2:SER:O	36:g:6:LYS:HG2	2.07	0.55
13:G:63:GLU:OE2	13:G:70:ARG:NH2	2.37	0.55
30:a:1199:U:H2'	30:a:1200:C:C6	2.41	0.55
30:a:856:G:H2'	30:a:857:G:C8	2.42	0.55
30:a:2900:A:H2'	30:a:2901:C:C6	2.42	0.55
30:a:1796:U:H2'	30:a:1797:G:H8	1.72	0.55
34:e:1:MET:HE1	34:e:20:GLY:CA	2.37	0.55
7:A:636:U:H2'	7:A:637:C:C6	2.42	0.54
7:A:1121:U:H2'	7:A:1122:U:C6	2.42	0.54
30:a:634:C:H2'	30:a:635:C:C6	2.42	0.54
30:a:1720:U:H2'	30:a:1721:G:O4'	2.07	0.54
30:a:2064:C:H2'	30:a:2065:C:C6	2.43	0.54
7:A:1032:G:H2'	7:A:1033:G:H4'	1.89	0.54
30:a:77:G:O3'	53:x:7:ARG:NH2	2.40	0.54
23:Q:17:MET:HE3	23:Q:20:SER:CB	2.38	0.54
30:a:2327:A:H2'	30:a:2328:A:C8	2.43	0.54
30:a:277:G:H4'	30:a:278:A:O5'	2.08	0.54
30:a:2780:G:OP2	38:i:120:ARG:HD3	2.08	0.54
30:a:2798:U:H4'	30:a:2799:A:H5'	1.88	0.54
7:A:713:G:H2'	7:A:714:G:C8	2.42	0.54
23:Q:26:GLU:OE1	23:Q:39:LYS:HD2	2.07	0.54
30:a:1485:U:H2'	30:a:1486:U:H6	1.72	0.54
39:j:43:ILE:HD12	39:j:56:ASP:HB2	1.89	0.54
30:a:1141:U:H4'	30:a:1142:A:O4'	2.08	0.54
30:a:2649:C:H2'	30:a:2650:U:C6	2.43	0.54
30:a:2900:A:H2'	30:a:2901:C:H6	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2074:U:H2'	30:a:2075:U:C6	2.43	0.54
4:3:2:LYS:NZ	30:a:2478:A:OP2	2.37	0.54
30:a:593:U:H2'	30:a:594:U:C6	2.42	0.54
30:a:1187:G:H5''	46:q:83:TYR:CE1	2.43	0.54
7:A:471:U:H2'	7:A:472:U:C6	2.42	0.54
7:A:492:C:H2'	7:A:493:A:C8	2.43	0.54
7:A:86:G:O2'	7:A:87:C:O5'	2.26	0.53
30:a:1607:C:N4	30:a:1622:G:OP2	2.25	0.53
30:a:2020:A:H5'	55:z:9:THR:CG2	2.38	0.53
7:A:1062:U:H2'	7:A:1063:C:C6	2.43	0.53
7:A:1446:A:OP1	7:A:1446:A:H8	1.90	0.53
8:B:163:VAL:HG11	8:B:173:ILE:HD11	1.91	0.53
9:C:86:LYS:O	9:C:90:VAL:HG23	2.07	0.53
12:F:25:TYR:O	12:F:29:ILE:HG12	2.07	0.53
30:a:191:A:H2'	30:a:192:C:C6	2.43	0.53
30:a:1168:G:H2'	30:a:1169:A:H8	1.73	0.53
7:A:404:G:N7	10:D:2:ALA:HB3	2.24	0.53
7:A:1144:G:N2	7:A:1146:A:H62	2.06	0.53
30:a:547:A:H1'	30:a:548:G:C5	2.44	0.53
30:a:2552:OMU:HM23	30:a:2554:U:C6	2.43	0.53
51:v:37:ILE:HG21	51:v:80:ILE:HG21	1.89	0.53
7:A:147:G:H2'	7:A:148:G:C8	2.43	0.53
30:a:1269:A:H2'	30:a:1270:C:C6	2.44	0.53
30:a:851:C:H2'	30:a:852:U:H6	1.73	0.53
9:C:130:PHE:O	9:C:134:MET:HG3	2.08	0.53
30:a:5:A:H2'	30:a:6:A:C8	2.44	0.53
30:a:858:G:OP1	51:v:78:LYS:HE2	2.09	0.53
10:D:48:LEU:HD21	10:D:56:ARG:HG3	1.91	0.53
12:F:20:GLY:O	12:F:24:ARG:HG3	2.09	0.53
30:a:1486:U:H2'	30:a:1487:U:H6	1.74	0.53
7:A:1001:C:H2'	7:A:1002:G:C8	2.44	0.53
10:D:18:ASP:OD1	10:D:28:ILE:HD12	2.09	0.53
13:G:48:GLU:O	13:G:52:GLN:HG2	2.08	0.53
30:a:1434:A:H2'	30:a:1435:G:C8	2.44	0.53
16:J:34:ALA:HB2	16:J:79:PRO:HA	1.91	0.52
30:a:414:C:H2'	30:a:415:A:H8	1.74	0.52
30:a:849:A:H2'	30:a:850:U:C6	2.44	0.52
30:a:2537:U:H2'	30:a:2538:C:C6	2.44	0.52
7:A:1053:G:N7	7:A:1200:C:H5''	2.24	0.52
7:A:1152:A:OP1	16:J:70:HIS:ND1	2.40	0.52
30:a:2071:A:H2'	30:a:2072:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:73:C:O2'	7:A:74:A:H8	1.93	0.52
30:a:1778:U:H2'	30:a:1784:A:N6	2.25	0.52
9:C:5:VAL:HG21	9:C:10:ILE:HD13	1.92	0.52
30:a:2491:U:H5''	30:a:2570:G:H5''	1.89	0.52
30:a:742:A:H2'	30:a:743:A:C8	2.45	0.52
7:A:996:A:H2'	7:A:997:U:C6	2.45	0.52
7:A:1412:C:H2'	7:A:1413:A:C8	2.44	0.52
8:B:130:THR:O	8:B:132:LYS:N	2.42	0.52
43:n:99:TYR:CE2	43:n:104:GLN:HG3	2.44	0.52
7:A:490:C:H2'	7:A:491:G:H8	1.74	0.52
7:A:564:C:C6	23:Q:33:ILE:HD11	2.45	0.52
8:B:111:ILE:O	8:B:115:LYS:HG2	2.10	0.52
30:a:813:U:H2'	30:a:814:C:H6	1.75	0.52
30:a:2014:A:H2'	30:a:2015:A:C8	2.45	0.52
7:A:1236:A:H2'	7:A:1237:C:C6	2.45	0.52
10:D:35:GLU:CD	10:D:35:GLU:H	2.18	0.52
30:a:1168:G:H2'	30:a:1169:A:C8	2.44	0.52
30:a:1548:A:H2'	30:a:1549:A:C8	2.44	0.52
30:a:1733:G:H2'	30:a:1734:G:C8	2.45	0.52
3:2:54:ASP:HB3	40:k:57:LEU:HD22	1.91	0.52
7:A:1532:U:H2'	7:A:1533:C:O4'	2.10	0.52
55:z:52:ARG:CZ	55:z:54:VAL:HG12	2.40	0.52
16:J:52:LEU:HD12	16:J:62:ARG:HD3	1.92	0.51
30:a:2250:G:C5	41:l:82:MET:HB2	2.44	0.51
30:a:2430:A:N3	30:a:2430:A:H2'	2.24	0.51
30:a:2627:G:O2'	30:a:2781:A:N1	2.43	0.51
5:4:14:ALA:HB3	5:4:22:MET:HG3	1.91	0.51
7:A:1124:G:H4'	16:J:40:ILE:HD11	1.91	0.51
30:a:155:A:H2'	30:a:156:A:C8	2.44	0.51
30:a:811:U:H2'	40:k:21:ARG:HA	1.92	0.51
7:A:382:A:H2'	7:A:383:A:C8	2.45	0.51
30:a:1796:U:H2'	30:a:1797:G:C8	2.46	0.51
12:F:20:GLY:O	12:F:23:GLU:HG2	2.10	0.51
30:a:84:A:N1	30:a:98:G:O2'	2.36	0.51
30:a:1443:U:H2'	30:a:1444:G:C8	2.45	0.51
7:A:1032:G:H22	7:A:1033:G:H21	1.59	0.51
36:g:12:PRO:HD2	36:g:15:VAL:HG11	1.92	0.51
7:A:1070:U:H2'	7:A:1071:C:C6	2.46	0.51
30:a:1682:G:H2'	30:a:1683:U:C6	2.45	0.51
7:A:459:A:H2'	7:A:460:A:C8	2.45	0.51
13:G:138:ARG:HD3	13:G:142:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:17:MET:HE3	23:Q:20:SER:HB2	1.92	0.51
29:Z:19:G:H4'	29:Z:20:U:OP2	2.11	0.51
30:a:857:G:H2'	30:a:858:G:O4'	2.10	0.51
2:1:45:SER:C	2:1:46:LYS:HD2	2.36	0.51
30:a:784:G:H5'	30:a:785:G:OP1	2.10	0.51
30:a:2373:G:H2'	30:a:2374:C:C6	2.46	0.51
7:A:736:C:H2'	7:A:737:C:C6	2.44	0.51
13:G:22:LEU:HD12	13:G:62:PHE:CE1	2.45	0.51
21:O:45:GLU:HG2	21:O:46:HIS:CD2	2.46	0.51
30:a:287:G:H2'	30:a:288:U:C6	2.46	0.51
30:a:2304:G:H22	30:a:2312:U:H3	1.59	0.51
30:a:2646:C:H2'	30:a:2647:U:O4'	2.10	0.51
27:U:17:ARG:O	27:U:21:ARG:HG2	2.11	0.51
30:a:58:G:O2'	30:a:73:A:N1	2.39	0.51
34:e:7:ASP:OD2	34:e:7:ASP:N	2.35	0.51
48:s:39:THR:OG1	48:s:42:GLU:HG3	2.11	0.51
7:A:156:C:H2'	7:A:157:U:O4'	2.11	0.50
7:A:262:A:H2'	7:A:263:A:C8	2.47	0.50
36:g:40:ALA:HB1	36:g:61:GLY:HA2	1.93	0.50
8:B:66:LYS:HB3	8:B:90:PHE:HE2	1.76	0.50
9:C:153:VAL:HG22	9:C:198:VAL:HG22	1.94	0.50
10:D:187:GLU:OE1	10:D:187:GLU:HA	2.12	0.50
7:A:41:G:H2'	7:A:42:G:H8	1.76	0.50
7:A:501:C:H2'	7:A:502:A:C8	2.47	0.50
19:M:89:LEU:O	19:M:93:ARG:HG3	2.11	0.50
30:a:102:U:C5	53:x:4:LYS:HE3	2.46	0.50
30:a:2455:G:H2'	30:a:2456:C:C6	2.46	0.50
32:c:107:PRO:HD2	32:c:110:LEU:HD22	1.92	0.50
5:4:30:HIS:ND1	5:4:31:ASP:O	2.37	0.50
7:A:160:A:H2'	7:A:161:A:O4'	2.11	0.50
30:a:2469:A:H4'	41:l:55:ARG:HD3	1.94	0.50
10:D:172:GLU:HB2	10:D:183:LYS:HD3	1.94	0.50
11:E:81:LEU:HD11	11:E:96:MET:HB3	1.93	0.50
15:I:53:GLU:OE1	15:I:58:VAL:HG21	2.11	0.50
30:a:399:U:H5	52:w:54:LYS:HE3	1.76	0.50
30:a:2469:A:H4'	41:l:55:ARG:CD	2.42	0.50
35:f:38:MET:HE3	35:f:57:LEU:HD13	1.94	0.50
7:A:161:A:H2'	7:A:162:A:C8	2.47	0.50
16:J:35:GLN:NE2	16:J:77:VAL:HB	2.27	0.50
49:t:29:LEU:HD21	49:t:35:ILE:HD12	1.93	0.50
7:A:538:G:H5''	18:L:111:LYS:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:555:U:H2'	7:A:556:C:C6	2.47	0.50
30:a:306:U:H2'	30:a:307:G:O4'	2.12	0.50
30:a:2233:U:H2'	30:a:2234:G:C8	2.46	0.50
36:g:94:TYR:HA	36:g:106:SER:O	2.12	0.50
44:o:5:ILE:O	44:o:9:GLU:HG3	2.12	0.50
7:A:381:C:H2'	7:A:382:A:O4'	2.12	0.50
7:A:1352:C:H2'	7:A:1353:G:C8	2.46	0.50
9:C:134:MET:HE2	9:C:168:TYR:CD2	2.47	0.50
31:b:66:A:N6	31:b:107:G:H2'	2.27	0.50
7:A:636:U:H2'	7:A:637:C:H6	1.77	0.50
7:A:1020:G:H2'	7:A:1021:A:C8	2.46	0.50
7:A:1256:A:O2'	7:A:1278:G:O6	2.23	0.50
30:a:476:G:H4'	30:a:502:A:N1	2.27	0.50
30:a:1378:A:O2'	30:a:1380:G:N7	2.45	0.50
30:a:2529:G:H4'	36:g:175:LYS:HD2	1.94	0.50
33:d:149:ASN:CG	33:d:150:MEQ:H	2.20	0.50
7:A:512:U:H2'	7:A:513:C:C6	2.46	0.49
25:S:30:PRO:HA	25:S:48:THR:O	2.12	0.49
30:a:2496:C:OP1	41:l:82:MET:N	2.44	0.49
7:A:96:U:H2'	7:A:97:G:H8	1.76	0.49
18:L:114:ARG:NH2	18:L:121:ARG:HG3	2.27	0.49
30:a:1028:A:N6	30:a:1125:G:H2'	2.27	0.49
7:A:41:G:H2'	7:A:42:G:C8	2.48	0.49
7:A:234:C:H4'	23:Q:66:PRO:HG3	1.95	0.49
7:A:663:A:H5'	7:A:836:G:OP1	2.12	0.49
8:B:92:VAL:CG2	8:B:100:MET:HE1	2.37	0.49
30:a:150:U:H2'	30:a:151:C:C6	2.47	0.49
30:a:1485:U:H2'	30:a:1486:U:C6	2.47	0.49
30:a:1902:C:H4'	32:c:242:LYS:O	2.12	0.49
7:A:269:C:H2'	7:A:270:A:H8	1.78	0.49
7:A:1162:C:H2'	7:A:1163:A:C8	2.46	0.49
17:K:16:VAL:HG12	17:K:18:ASP:H	1.77	0.49
30:a:1149:G:H2'	30:a:1150:C:C6	2.47	0.49
36:g:95:ARG:HG2	36:g:106:SER:HB2	1.95	0.49
13:G:26:PHE:HZ	13:G:120:LEU:HD11	1.76	0.49
30:a:581:C:H2'	30:a:582:A:C8	2.47	0.49
35:f:114:PHE:HZ	35:f:176:PRO:HB2	1.77	0.49
7:A:977:A:O2'	7:A:979:C:OP2	2.26	0.49
7:A:1119:C:H2'	7:A:1120:C:H6	1.78	0.49
24:R:9:LYS:HG2	24:R:10:PHE:N	2.24	0.49
30:a:1484:U:H2'	30:a:1485:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2097:A:H2'	30:a:2098:U:C6	2.48	0.49
7:A:56:U:H2'	7:A:57:G:C8	2.48	0.49
30:a:1486:U:H2'	30:a:1487:U:C6	2.48	0.49
13:G:71:PRO:O	13:G:96:ARG:HG2	2.13	0.49
30:a:1443:U:H2'	30:a:1444:G:H8	1.78	0.49
30:a:1794:A:H2'	30:a:1795:C:C6	2.48	0.49
41:l:41:LEU:HG	41:l:96:ILE:HG13	1.94	0.49
7:A:1009:U:H2'	7:A:1010:U:H6	1.78	0.49
30:a:121:G:H4'	30:a:149:A:H5'	1.95	0.49
30:a:1495:A:H2'	30:a:1496:A:C8	2.48	0.49
35:f:42:GLU:OE1	35:f:42:GLU:N	2.32	0.49
7:A:376:G:H5''	22:P:5:ARG:HB2	1.95	0.48
10:D:144:SER:HB3	10:D:179:GLU:HB2	1.95	0.48
43:n:35:ILE:HG21	43:n:71:ALA:HA	1.94	0.48
7:A:579:A:H2'	7:A:580:C:C6	2.48	0.48
19:M:90:ARG:HD3	19:M:96:PRO:O	2.12	0.48
30:a:1932:A:H2'	30:a:1933:G:O4'	2.13	0.48
55:z:43:ILE:HG22	55:z:49:TYR:HB2	1.94	0.48
7:A:502:A:H2'	7:A:503:C:O4'	2.14	0.48
30:a:1442:U:H2'	30:a:1443:U:C6	2.48	0.48
54:y:3:LYS:O	54:y:4:THR:HG22	2.13	0.48
7:A:28:A:O2'	7:A:296:U:OP1	2.27	0.48
14:H:18:GLN:HG2	14:H:63:LEU:HD13	1.96	0.48
30:a:864:G:O2'	30:a:914:G:O6	2.27	0.48
30:a:2505:G:N2	30:a:2506:U:O4	2.26	0.48
30:a:2756:U:H1'	30:a:2757:A:H5''	1.96	0.48
7:A:429:U:H3'	10:D:9:LEU:HD12	1.95	0.48
17:K:35:THR:HG22	17:K:41:ALA:HA	1.95	0.48
27:U:58:LYS:HE3	27:U:59:LYS:CE	2.44	0.48
50:u:44:HIS:CE1	50:u:85:LYS:HE3	2.49	0.48
7:A:867:G:O2'	7:A:873:A:N1	2.43	0.48
7:A:1314:C:OP2	25:S:4:SER:OG	2.20	0.48
18:L:15:LYS:H	18:L:15:LYS:HG2	1.40	0.48
7:A:79:G:H1	7:A:90:C:N4	2.08	0.48
7:A:1513:A:H2'	7:A:1514:G:C8	2.49	0.48
10:D:45:LYS:HD2	10:D:45:LYS:HA	1.53	0.48
29:Z:23:C:H2'	29:Z:24:U:C6	2.48	0.48
30:a:589:U:H2'	30:a:590:A:C8	2.49	0.48
30:a:645:C:O2'	30:a:646:U:H5''	2.13	0.48
30:a:2092:U:OP2	37:h:27:ARG:NH1	2.45	0.48
7:A:1326:U:H2'	7:A:1327:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:134:ALA:O	8:B:138:THR:OG1	2.29	0.48
30:a:588:U:H2'	30:a:589:U:C6	2.48	0.48
30:a:880:G:C4	30:a:881:G:C8	3.02	0.48
30:a:2584:U:H2'	30:a:2585:U:H2'	1.96	0.48
30:a:2758:A:O2'	36:g:38:ASN:ND2	2.42	0.48
7:A:439:U:H4'	10:D:121:LYS:HG3	1.96	0.48
9:C:22:TRP:HB3	9:C:59:ARG:HB2	1.94	0.48
30:a:2273:A:H2'	30:a:2274:A:C8	2.48	0.48
5:4:1:MET:HG3	31:b:43:C:H5''	1.96	0.48
10:D:105:MET:HG2	10:D:173:VAL:HG22	1.95	0.48
30:a:642:U:O2'	30:a:644:A:N7	2.35	0.48
30:a:882:G:C2	30:a:895:U:H1'	2.49	0.48
30:a:909:A:H2'	30:a:912:C:C5	2.49	0.48
30:a:1183:U:H2'	30:a:1184:U:C6	2.49	0.48
49:t:86:ARG:HG3	49:t:95:PHE:CE2	2.49	0.48
7:A:1288:A:H2'	7:A:1289:A:O4'	2.14	0.47
16:J:36:VAL:HG12	16:J:76:ILE:HD13	1.96	0.47
20:N:24:ARG:NH1	20:N:55:SER:OG	2.47	0.47
30:a:933:A:H5'	30:a:934:U:OP2	2.14	0.47
30:a:2328:A:H2'	30:a:2329:U:H6	1.78	0.47
30:a:2876:G:OP1	44:o:2:SER:OG	2.25	0.47
45:p:58:ARG:HA	45:p:61:TRP:CE3	2.49	0.47
13:G:4:ARG:HG3	13:G:4:ARG:HH11	1.79	0.47
30:a:1386:C:H2'	30:a:1387:A:C8	2.48	0.47
30:a:1484:U:H2'	30:a:1485:U:H6	1.79	0.47
35:f:8:TYR:HB2	35:f:173:PHE:HZ	1.79	0.47
41:l:111:GLU:CD	41:l:111:GLU:H	2.22	0.47
42:m:66:ALA:O	42:m:69:ARG:O	2.32	0.47
46:q:75:VAL:HG22	46:q:86:GLN:OE1	2.14	0.47
30:a:364:C:H2'	30:a:365:U:C6	2.49	0.47
30:a:687:C:H2'	30:a:688:U:O4'	2.14	0.47
30:a:984:A:N3	30:a:984:A:H2'	2.29	0.47
30:a:1003:G:O2'	30:a:1010:A:N1	2.44	0.47
7:A:1314:C:H2'	7:A:1315:U:C6	2.48	0.47
9:C:6:HIS:CG	20:N:89:MET:HB3	2.50	0.47
11:E:38:VAL:HG11	11:E:114:VAL:HG22	1.96	0.47
30:a:608:A:H2'	30:a:609:A:C8	2.50	0.47
30:a:2469:A:N6	30:a:2481:G:O2'	2.48	0.47
34:e:127:GLU:O	34:e:156:ASN:ND2	2.48	0.47
7:A:1000:A:H2'	7:A:1001:C:C6	2.49	0.47
7:A:1004:A:N6	7:A:1026:G:H1'	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:58:ASN:HB2	8:B:220:THR:HG22	1.95	0.47
9:C:50:ALA:O	9:C:70:THR:OG1	2.31	0.47
30:a:2030:6MZ:C2	30:a:2499:C:H5''	2.44	0.47
12:F:97:THR:O	12:F:97:THR:OG1	2.32	0.47
23:Q:39:LYS:C	23:Q:40:ARG:HD2	2.39	0.47
30:a:494:G:H4'	47:r:6:LYS:HB2	1.95	0.47
30:a:2799:A:O2'	30:a:2800:A:H5''	2.14	0.47
2:1:46:LYS:HE2	30:a:127:A:N7	2.29	0.47
7:A:263:A:H2'	7:A:264:C:C6	2.49	0.47
7:A:1163:A:H2'	7:A:1164:G:C8	2.49	0.47
13:G:22:LEU:HD11	13:G:66:LEU:HD11	1.96	0.47
15:I:89:GLU:HA	15:I:89:GLU:OE2	2.13	0.47
16:J:7:ARG:HB3	16:J:101:SER:HB3	1.97	0.47
22:P:74:LEU:HA	22:P:77:GLU:HG2	1.97	0.47
30:a:947:A:H2'	30:a:948:C:C6	2.50	0.47
30:a:1838:C:N4	30:a:1898:U:H2'	2.30	0.47
30:a:2529:G:H4'	36:g:175:LYS:CD	2.45	0.47
50:u:83:LYS:HB3	50:u:85:LYS:HG3	1.97	0.47
24:R:9:LYS:CG	24:R:10:PHE:N	2.78	0.47
30:a:39:G:H2'	30:a:40:U:C6	2.50	0.47
30:a:419:U:H2'	30:a:420:C:C6	2.49	0.47
30:a:1542:U:H2'	30:a:1543:G:O4'	2.15	0.47
30:a:2299:U:H2'	30:a:2300:C:C6	2.49	0.47
35:f:44:ILE:CD1	35:f:79:ILE:HG22	2.45	0.47
36:g:17:VAL:HG11	36:g:50:LEU:HD11	1.96	0.47
12:F:102:MET:HE1	24:R:24:LYS:O	2.15	0.47
17:K:87:LYS:HB2	17:K:113:VAL:HG23	1.97	0.47
30:a:493:G:H2'	30:a:494:G:O4'	2.15	0.47
33:d:1:MET:HG2	33:d:88:GLU:OE2	2.15	0.47
7:A:999:C:H2'	7:A:1000:A:H8	1.79	0.47
30:a:2:G:H2'	30:a:3:U:C6	2.50	0.47
30:a:645:C:H2'	30:a:647:G:C8	2.49	0.47
30:a:1545:A:H2'	30:a:1546:G:O4'	2.15	0.47
30:a:2443:C:OP1	34:e:63:LYS:HD3	2.15	0.47
1:0:10:LYS:HE2	1:0:20:PHE:CD1	2.50	0.46
7:A:524:G:H2'	7:A:525:C:C6	2.50	0.46
8:B:71:GLY:O	8:B:93:ASN:HA	2.15	0.46
9:C:108:LYS:HB3	9:C:144:LEU:HD12	1.96	0.46
21:O:45:GLU:HG2	21:O:46:HIS:NE2	2.30	0.46
22:P:56:ARG:HD2	22:P:56:ARG:HA	1.71	0.46
30:a:729:G:C6	32:c:207:LYS:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1790:C:H2'	30:a:1791:A:C5	2.50	0.46
21:O:26:GLU:HG3	21:O:81:LEU:HD22	1.95	0.46
30:a:328:U:O3'	49:t:66:GLN:HG3	2.13	0.46
31:b:106:G:H2'	31:b:107:G:O4'	2.14	0.46
16:J:37:ARG:HB2	16:J:75:ASP:HB2	1.97	0.46
30:a:969:G:H2'	30:a:970:U:C6	2.50	0.46
30:a:1370:C:H2'	30:a:1371:G:O4'	2.14	0.46
30:a:1590:A:H2'	30:a:1591:A:C8	2.51	0.46
36:g:12:PRO:O	36:g:15:VAL:HG12	2.16	0.46
51:v:38:VAL:HG12	51:v:59:LEU:HB2	1.97	0.46
7:A:1014:A:N3	7:A:1219:A:H1'	2.30	0.46
7:A:1130:A:H2'	7:A:1131:G:C8	2.49	0.46
16:J:10:LEU:O	16:J:71:LEU:HA	2.15	0.46
24:R:9:LYS:CG	24:R:10:PHE:H	2.27	0.46
35:f:74:VAL:HB	35:f:79:ILE:HG12	1.98	0.46
30:a:1853:A:N1	30:a:2087:G:H1'	2.31	0.46
34:e:147:LEU:HD11	34:e:170:ARG:HG3	1.97	0.46
30:a:208:C:H2'	30:a:209:C:C6	2.50	0.46
30:a:1197:G:H2'	30:a:1198:U:C6	2.51	0.46
31:b:49:C:H2'	31:b:50:A:C8	2.51	0.46
36:g:29:LYS:HE2	36:g:80:THR:O	2.15	0.46
7:A:714:G:H2'	7:A:715:A:C8	2.51	0.46
30:a:1594:U:H2'	30:a:1595:C:C6	2.51	0.46
30:a:2329:U:H2'	30:a:2330:G:C8	2.51	0.46
7:A:120:A:H4'	7:A:121:U:OP1	2.16	0.46
7:A:1477:U:H2'	7:A:1478:U:C6	2.50	0.46
10:D:27:ALA:HB3	10:D:30:THR:HG23	1.98	0.46
23:Q:39:LYS:O	23:Q:40:ARG:HD2	2.16	0.46
27:U:58:LYS:HG3	27:U:59:LYS:N	2.31	0.46
30:a:1506:U:H2'	30:a:1507:C:C6	2.51	0.46
35:f:106:ILE:C	35:f:109:PRO:HD2	2.41	0.46
3:2:64:TYR:CE2	30:a:242:G:H5''	2.50	0.46
7:A:1302:C:C4	19:M:17:ILE:HG13	2.51	0.46
7:A:1499:A:O2'	7:A:1500:A:H5'	2.16	0.46
8:B:66:LYS:HB3	8:B:90:PHE:CE2	2.51	0.46
30:a:814:C:H2'	30:a:815:C:H6	1.81	0.46
30:a:832:U:H2'	30:a:833:A:C8	2.50	0.46
30:a:2038:G:H2'	30:a:2039:U:O4'	2.15	0.46
39:j:38:ILE:HD11	39:j:112:PHE:CZ	2.51	0.46
46:q:43:ASN:O	46:q:43:ASN:ND2	2.41	0.46
7:A:244:U:O4	7:A:906:A:H1'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:471:U:H2'	7:A:472:U:H6	1.80	0.45
7:A:604:G:H2'	7:A:605:U:O4'	2.16	0.45
7:A:1121:U:H2'	7:A:1122:U:H6	1.79	0.45
7:A:1127:G:H5'	7:A:1280:A:O2'	2.16	0.45
7:A:1486:G:H2'	7:A:1487:G:O4'	2.15	0.45
30:a:1027:A:C2	30:a:2488:G:H5'	2.51	0.45
30:a:2086:U:H2'	30:a:2087:G:C8	2.51	0.45
30:a:2615:U:C2	55:z:4:GLN:HA	2.50	0.45
30:a:2636:C:H2'	30:a:2637:U:C6	2.51	0.45
7:A:662:U:H2'	7:A:663:A:C8	2.51	0.45
9:C:110:GLU:CD	9:C:110:GLU:H	2.24	0.45
15:I:6:TYR:CE1	15:I:90:TYR:HD2	2.34	0.45
19:M:40:ALA:HB3	19:M:43:VAL:HG23	1.99	0.45
30:a:40:U:H2'	30:a:41:C:C6	2.51	0.45
30:a:549:G:H2'	30:a:550:C:H6	1.77	0.45
30:a:1429:G:H2'	30:a:1430:G:C8	2.52	0.45
30:a:1746:A:H2'	30:a:1747:U:H6	1.80	0.45
34:e:191:ASP:O	34:e:195:GLN:HG3	2.16	0.45
40:k:82:LEU:HD22	40:k:90:VAL:HG21	1.99	0.45
7:A:390:U:H2'	7:A:391:G:C8	2.51	0.45
7:A:945:G:C2	7:A:946:A:C8	3.04	0.45
7:A:1504:G:H4'	7:A:1505:G:C4	2.50	0.45
8:B:4:VAL:HG11	8:B:9:MET:HE3	1.97	0.45
16:J:28:THR:HG21	16:J:90:LEU:HD22	1.97	0.45
29:Z:17:C:H2'	29:Z:17(A):U:C5	2.52	0.45
30:a:207:A:H2'	30:a:208:C:O4'	2.16	0.45
30:a:2619:C:H5'	33:d:155:VAL:O	2.16	0.45
31:b:1:U:H2'	31:b:2:G:C8	2.50	0.45
1:O:35:GLU:OE1	1:O:50:LYS:HE3	2.17	0.45
9:C:49:LYS:O	9:C:72:ARG:NH2	2.48	0.45
14:H:27:MET:HE2	14:H:27:MET:HB3	1.82	0.45
16:J:85:ASP:O	16:J:89:ARG:HG2	2.17	0.45
19:M:54:ASP:OD1	19:M:57:ARG:NH1	2.49	0.45
30:a:244:A:H2'	30:a:245:G:O4'	2.16	0.45
30:a:594:U:H2'	30:a:595:C:H6	1.80	0.45
30:a:1805:A:N3	32:c:50:THR:HB	2.32	0.45
30:a:2895:G:H2'	30:a:2896:C:H6	1.82	0.45
7:A:412:A:O2'	7:A:413:G:H4'	2.17	0.45
7:A:675:A:O2'	17:K:116:ILE:O	2.33	0.45
7:A:790:A:H2'	7:A:791:G:C8	2.52	0.45
15:I:6:TYR:CE2	15:I:90:TYR:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:11:ASP:HA	19:M:45:ILE:HB	1.98	0.45
22:P:40:ASN:HB3	22:P:43:ALA:HB2	1.97	0.45
30:a:460:A:H2'	30:a:461:C:O4'	2.15	0.45
30:a:909:A:H2'	30:a:912:C:H5	1.81	0.45
7:A:224:U:H2'	7:A:225:C:C6	2.52	0.45
7:A:401:C:OP2	10:D:70:ARG:NH1	2.46	0.45
7:A:999:C:H2'	7:A:1000:A:C8	2.52	0.45
7:A:1391:U:H2'	7:A:1392:G:H8	1.81	0.45
30:a:898:C:H2'	30:a:899:A:O4'	2.17	0.45
30:a:1509:A:O2'	30:a:1510:G:H8	2.00	0.45
7:A:737:C:H2'	7:A:738:C:H6	1.81	0.45
7:A:1023:U:H2'	7:A:1024:G:H8	1.82	0.45
9:C:58:GLU:OE1	9:C:65:ARG:NH1	2.49	0.45
30:a:576:U:H2'	30:a:577:G:C8	2.52	0.45
30:a:580:U:H2'	30:a:581:C:H6	1.81	0.45
30:a:711:G:H1	30:a:720:U:H3	1.62	0.45
33:d:179:ARG:HB3	33:d:188:LEU:HD22	1.99	0.45
43:n:80:GLU:O	43:n:84:GLU:HG2	2.17	0.45
46:q:46:GLU:OE1	46:q:48:LYS:NZ	2.42	0.45
30:a:17:G:H2'	30:a:18:U:C6	2.52	0.45
30:a:1842:G:H2'	30:a:1843:C:C6	2.51	0.45
30:a:2025:C:H2'	30:a:2026:U:C6	2.51	0.45
30:a:2415:G:H2'	30:a:2416:C:C6	2.51	0.45
10:D:99:ASP:OD1	10:D:100:ASN:N	2.49	0.45
30:a:2193:G:H2'	30:a:2194:U:H6	1.82	0.45
30:a:2393:U:H5'	40:k:60:ARG:O	2.16	0.45
30:a:2788:C:H2'	30:a:2789:C:C6	2.52	0.45
36:g:24:ILE:HD11	36:g:43:VAL:HG11	1.99	0.45
36:g:137:ASP:HB3	36:g:140:VAL:HB	1.99	0.45
7:A:1446:A:O2'	7:A:1447:A:H5'	2.17	0.45
12:F:69:GLU:CD	12:F:69:GLU:H	2.25	0.45
13:G:70:ARG:NH1	13:G:97:ASN:OD1	2.42	0.45
30:a:2395:C:H2'	30:a:2396:G:O4'	2.17	0.45
8:B:90:PHE:CD2	8:B:154:MET:HG3	2.52	0.44
11:E:151:GLU:OE1	11:E:151:GLU:N	2.43	0.44
19:M:83:LEU:HA	19:M:83:LEU:HD23	1.85	0.44
26:T:79:LEU:HD23	26:T:79:LEU:HA	1.87	0.44
30:a:659:G:H4'	34:e:95:LYS:HG2	2.00	0.44
30:a:723:C:H2'	30:a:724:U:O4'	2.17	0.44
30:a:1494:A:H2'	30:a:1495:A:C8	2.52	0.44
30:a:1668:A:O2'	30:a:1674:G:N7	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1872:A:C5	30:a:1873:G:H1'	2.52	0.44
30:a:2512:C:H2'	30:a:2513:A:O4'	2.16	0.44
31:b:29:A:H2'	31:b:30:C:C6	2.52	0.44
47:r:59:GLU:OE1	47:r:66:ILE:HD11	2.17	0.44
7:A:328:C:H4'	7:A:329:A:H5''	1.99	0.44
7:A:881:G:OP2	18:L:9:ARG:NH2	2.51	0.44
30:a:2723:C:H2'	30:a:2724:U:O4'	2.16	0.44
33:d:184:ARG:NH1	44:o:7:GLN:OE1	2.50	0.44
7:A:983:A:H5'	7:A:984:C:OP2	2.17	0.44
16:J:10:LEU:HD21	16:J:25:ILE:HD12	2.00	0.44
30:a:819:A:C4	30:a:1189:A:C2	3.05	0.44
30:a:1874:C:H2'	30:a:1875:G:O4'	2.18	0.44
30:a:2820:A:O2'	30:a:2821:A:OP1	2.31	0.44
35:f:15:LYS:HE3	35:f:15:LYS:HB2	1.69	0.44
7:A:590:U:H2'	7:A:591:U:C6	2.52	0.44
7:A:1000:A:H2'	7:A:1001:C:H6	1.82	0.44
30:a:2779:U:H5'	30:a:2781:A:O4'	2.18	0.44
37:h:8:LYS:HA	37:h:8:LYS:HD2	1.87	0.44
53:x:4:LYS:NZ	53:x:5:GLU:OE1	2.50	0.44
7:A:154:U:H2'	7:A:155:A:C8	2.52	0.44
7:A:649:A:H2'	7:A:650:G:O4'	2.17	0.44
30:a:833:A:H2'	30:a:834:G:C8	2.53	0.44
30:a:1656:C:H2'	30:a:1657:U:H6	1.82	0.44
30:a:2299:U:H2'	30:a:2300:C:H6	1.82	0.44
30:a:2514:U:H2'	30:a:2515:C:C6	2.53	0.44
42:m:69:ARG:O	42:m:71:ARG:N	2.49	0.44
49:t:14:LEU:HD11	49:t:71:ALA:HB2	2.00	0.44
1:0:32:GLU:OE1	1:0:32:GLU:N	2.42	0.44
4:3:9:LYS:HE2	4:3:9:LYS:HB2	1.71	0.44
10:D:82:LEU:HD23	10:D:82:LEU:HA	1.88	0.44
13:G:36:LYS:HG2	15:I:41:ARG:NH2	2.32	0.44
13:G:70:ARG:HD3	13:G:97:ASN:OD1	2.18	0.44
30:a:886:A:H2'	30:a:887:U:O4'	2.17	0.44
30:a:1177:G:H2'	30:a:1178:C:C6	2.53	0.44
43:n:56:LYS:O	43:n:60:GLU:HG2	2.17	0.44
7:A:333:U:OP1	26:T:2:ALA:N	2.51	0.44
7:A:1356:G:H2'	7:A:1357:A:H8	1.83	0.44
8:B:66:LYS:NZ	8:B:154:MET:O	2.33	0.44
21:O:48:LYS:HD2	21:O:48:LYS:HA	1.73	0.44
30:a:78:U:H2'	30:a:79:C:C6	2.52	0.44
30:a:468:G:H5''	34:e:55:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:794:A:H2'	30:a:795:C:C6	2.53	0.44
30:a:2576:G:O2'	30:a:2579:C:OP2	2.25	0.44
33:d:55:LYS:HG2	33:d:60:VAL:HG22	1.98	0.44
7:A:539:A:H2'	7:A:540:G:H8	1.83	0.44
8:B:59:LYS:N	8:B:59:LYS:HD3	2.32	0.44
8:B:85:LEU:HD23	8:B:85:LEU:HA	1.85	0.44
26:T:54:MET:HE2	26:T:79:LEU:CD1	2.48	0.44
29:Z:17:C:OP2	29:Z:18:G:H5''	2.18	0.44
30:a:1357:C:H2'	30:a:1358:G:O4'	2.17	0.44
30:a:1410:G:H2'	30:a:1411:U:H6	1.79	0.44
30:a:2730:C:O2'	30:a:2731:G:H5'	2.18	0.44
36:g:48:ASN:ND2	36:g:48:ASN:O	2.51	0.44
37:h:4:ILE:O	37:h:37:VAL:HG12	2.18	0.44
40:k:81:ASP:HA	40:k:84:LYS:HD2	1.99	0.44
7:A:1463:U:H2'	7:A:1464:U:C6	2.53	0.44
7:A:1530:G:H2'	7:A:1531:A:C8	2.53	0.44
30:a:967:U:H2'	30:a:968:C:C6	2.53	0.44
30:a:1429:G:H2'	30:a:1430:G:H8	1.82	0.44
4:3:30:GLU:CD	4:3:32:LYS:HB2	2.43	0.43
7:A:57:G:H2'	7:A:58:C:C6	2.53	0.43
7:A:737:C:H2'	7:A:738:C:C6	2.53	0.43
10:D:156:LYS:O	10:D:160:GLU:HG3	2.18	0.43
12:F:45:ARG:O	12:F:56:LYS:HG2	2.18	0.43
17:K:114:THR:HG21	27:U:32:VAL:HG21	2.00	0.43
30:a:1179:G:H2'	30:a:1180:U:H6	1.83	0.43
30:a:2228:G:H2'	30:a:2229:U:C6	2.53	0.43
7:A:472:U:H2'	7:A:473:U:C6	2.53	0.43
7:A:613:C:H2'	7:A:614:C:H6	1.83	0.43
7:A:1413:A:H2	7:A:1487:G:H22	1.66	0.43
13:G:36:LYS:HG2	15:I:41:ARG:HH22	1.84	0.43
30:a:171:U:H2'	30:a:172:A:H8	1.83	0.43
30:a:2312:U:H5'	35:f:85:ILE:HD11	2.00	0.43
7:A:33:A:H2'	7:A:34:C:C6	2.53	0.43
7:A:1008:U:H3'	7:A:1009:U:H5''	1.99	0.43
7:A:1524:C:H2'	7:A:1525:G:C8	2.53	0.43
18:L:54:ARG:CZ	18:L:62:GLU:HG2	2.48	0.43
21:O:35:GLN:HA	21:O:35:GLN:OE1	2.18	0.43
30:a:644:A:H2'	30:a:645:C:O4'	2.18	0.43
30:a:2898:U:O2	38:i:134:ALA:HB1	2.18	0.43
35:f:65:PRO:HA	35:f:89:VAL:HG12	1.99	0.43
7:A:459:A:H2'	7:A:460:A:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:660:C:H2'	7:A:661:G:O4'	2.19	0.43
7:A:1206:G:H2'	7:A:1207:2MG:O4'	2.19	0.43
7:A:1347:G:N7	15:I:13:LYS:HE2	2.34	0.43
15:I:116:VAL:HG11	16:J:62:ARG:HG3	2.01	0.43
31:b:104:A:H2'	31:b:105:G:O4'	2.18	0.43
55:z:29:SER:O	55:z:37:LYS:HA	2.18	0.43
7:A:86:G:H1'	7:A:87:C:O4'	2.18	0.43
13:G:140:ASP:N	13:G:140:ASP:OD2	2.51	0.43
30:a:162:U:O4	30:a:2218:G:H4'	2.18	0.43
30:a:322:A:OP2	34:e:163:ASN:HB2	2.17	0.43
30:a:720:U:H2'	30:a:721:A:H8	1.82	0.43
30:a:1047:G:O2'	30:a:1110:G:N2	2.49	0.43
7:A:1035:A:C4	7:A:1036:A:C2	3.06	0.43
17:K:52:PHE:O	17:K:53:ARG:HD2	2.18	0.43
30:a:1179:G:H2'	30:a:1180:U:C6	2.53	0.43
30:a:2698:U:H2'	30:a:2699:C:C6	2.53	0.43
36:g:7:ALA:O	36:g:69:ARG:NE	2.51	0.43
50:u:73:LYS:HB3	50:u:73:LYS:HE2	1.57	0.43
53:x:19:LEU:HD23	53:x:19:LEU:HA	1.90	0.43
7:A:399:G:H2'	7:A:400:C:C6	2.53	0.43
7:A:1032:G:N2	7:A:1033:G:N3	2.67	0.43
30:a:285:G:C6	30:a:356:G:C6	3.06	0.43
30:a:874:G:H2'	30:a:875:G:H8	1.84	0.43
30:a:1747:U:H2'	30:a:1748:C:C6	2.53	0.43
40:k:82:LEU:HD13	40:k:120:VAL:HG21	2.00	0.43
7:A:458:U:H2'	7:A:459:A:C8	2.54	0.43
7:A:1124:G:N2	7:A:1125:U:O4	2.34	0.43
15:I:54:LEU:HD23	15:I:98:LEU:HD23	2.00	0.43
30:a:247:G:H4'	30:a:386:G:C5	2.54	0.43
30:a:1871:A:H8	30:a:1871:A:OP2	2.01	0.43
30:a:2059:A:H2'	30:a:2503:2MA:HM23	2.00	0.43
30:a:2857:G:N2	30:a:2860:A:OP2	2.43	0.43
43:n:60:GLU:OE2	43:n:61:GLN:NE2	2.52	0.43
7:A:97:G:H2'	7:A:98:A:O4'	2.19	0.43
7:A:509:A:N3	7:A:543:U:O2'	2.45	0.43
19:M:56:LEU:HD23	19:M:56:LEU:HA	1.84	0.43
30:a:323:C:C4	30:a:333:G:C8	3.07	0.43
30:a:780:G:H2'	30:a:782:A:N7	2.33	0.43
30:a:1563:U:H2'	30:a:1564:C:C6	2.53	0.43
30:a:1717:A:H2'	30:a:1718:G:O4'	2.18	0.43
40:k:122:VAL:HG21	40:k:135:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:30:LYS:HD3	1:0:32:GLU:OE2	2.19	0.43
7:A:270:A:H2'	7:A:271:C:C6	2.54	0.43
7:A:1020:G:C4	7:A:1021:A:C8	3.06	0.43
7:A:1220:G:P	20:N:53:ARG:HH12	2.42	0.43
26:T:54:MET:HE2	26:T:79:LEU:HD12	2.00	0.43
30:a:273:G:H2'	30:a:274:C:H6	1.84	0.43
30:a:504:A:O2'	30:a:505:A:OP1	2.31	0.43
30:a:1820:U:C2	32:c:201:MET:HG2	2.53	0.43
30:a:2291:U:OP1	30:a:2380:C:O2'	2.29	0.43
34:e:7:ASP:CG	34:e:122:GLU:H	2.26	0.43
23:Q:17:MET:HE3	23:Q:20:SER:HB3	2.01	0.42
30:a:639:U:H2'	30:a:640:C:H6	1.84	0.42
30:a:657:U:H2'	30:a:658:U:C6	2.54	0.42
30:a:1794:A:H2'	30:a:1795:C:H6	1.84	0.42
30:a:2016:U:H2'	30:a:2017:U:C6	2.54	0.42
30:a:2251:OMG:HM23	30:a:2251:OMG:H1'	1.90	0.42
30:a:2803:G:H2'	30:a:2804:U:H6	1.84	0.42
1:0:32:GLU:H	1:0:32:GLU:CD	2.16	0.42
7:A:371:A:H2'	7:A:372:C:O4'	2.19	0.42
7:A:421:U:H1'	9:C:127:ARG:NH2	2.34	0.42
16:J:15:HIS:HA	16:J:18:ILE:HG22	2.01	0.42
30:a:391:A:H1'	30:a:411:G:O4'	2.19	0.42
30:a:396:G:H1'	52:w:29:PHE:HB3	2.01	0.42
30:a:846:U:H5'	30:a:847:U:OP1	2.19	0.42
30:a:852:U:H2'	30:a:853:C:C6	2.54	0.42
30:a:2520:C:C6	30:a:2567:G:H1'	2.55	0.42
30:a:2803:G:H2'	30:a:2804:U:C6	2.54	0.42
50:u:28:ALA:HB3	50:u:40:ILE:HG13	2.01	0.42
7:A:1225:A:H2'	7:A:1226:C:C6	2.55	0.42
13:G:125:SER:O	13:G:129:GLU:HG2	2.19	0.42
14:H:66:PHE:CD2	14:H:67:GLN:HG2	2.55	0.42
27:U:40:LYS:HE2	27:U:42:THR:HG22	2.01	0.42
30:a:609:A:H2'	30:a:610:C:O4'	2.19	0.42
30:a:2345:G:N3	30:a:2381:A:H2'	2.34	0.42
30:a:2804:U:H2'	30:a:2805:C:C6	2.54	0.42
31:b:29:A:H2'	31:b:30:C:O4'	2.19	0.42
50:u:80:HIS:CG	50:u:81:PRO:HD2	2.54	0.42
6:5:75:C:O4'	30:a:2432:A:H1'	2.20	0.42
7:A:1041:G:N1	7:A:1042:A:N7	2.68	0.42
7:A:1151:A:HO2'	7:A:1152:A:H8	1.64	0.42
9:C:77:ILE:HA	9:C:84:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:54:PRO:HD3	36:g:62:TRP:CZ3	2.54	0.42
49:t:26:LYS:CD	49:t:37:GLU:HG3	2.49	0.42
7:A:94:G:H5''	7:A:95:C:H5	1.84	0.42
7:A:821:G:H2'	7:A:822:U:C6	2.54	0.42
7:A:986:U:H2'	7:A:987:G:C8	2.54	0.42
8:B:57:LEU:HD13	8:B:217:VAL:HG13	2.01	0.42
10:D:57:GLU:OE2	10:D:196:ASN:N	2.36	0.42
13:G:149:LYS:HD2	17:K:61:PHE:CE1	2.54	0.42
30:a:864:G:O2'	30:a:865:C:H5'	2.19	0.42
30:a:1405:U:H2'	30:a:1406:U:H6	1.82	0.42
30:a:2897:U:H2'	30:a:2898:U:C6	2.55	0.42
34:e:46:GLN:O	34:e:88:ARG:NH2	2.47	0.42
35:f:100:PHE:CZ	35:f:104:ILE:HD11	2.54	0.42
1:0:10:LYS:HE3	1:0:10:LYS:HB3	1.74	0.42
2:1:29:GLN:NE2	30:a:210:C:OP1	2.48	0.42
4:3:36:ARG:HD3	30:a:2742:G:OP1	2.19	0.42
5:4:26:SER:OG	35:f:140:GLU:OE1	2.21	0.42
7:A:161:A:N1	7:A:347:G:O2'	2.45	0.42
7:A:343:U:H2'	7:A:345:C:C5	2.54	0.42
7:A:1151:A:H5''	16:J:44:THR:HG22	2.00	0.42
7:A:1326:U:H2'	7:A:1327:C:H6	1.85	0.42
7:A:1333:A:H2'	7:A:1334:G:O4'	2.20	0.42
14:H:50:LYS:HB3	14:H:50:LYS:HE3	1.93	0.42
15:I:56:ASP:C	15:I:57:MET:HG2	2.44	0.42
30:a:364:C:H2'	30:a:365:U:H6	1.84	0.42
30:a:2464:G:H8	30:a:2464:G:H5''	1.85	0.42
35:f:135:GLN:HG2	35:f:141:ILE:HG21	2.01	0.42
43:n:2:ASP:OD2	43:n:3:LYS:N	2.48	0.42
7:A:236:A:H2'	7:A:237:G:C8	2.54	0.42
7:A:672:U:H2'	7:A:673:A:C8	2.53	0.42
7:A:721:G:H4'	7:A:722:G:O4'	2.19	0.42
11:E:19:ASN:HB3	11:E:34:THR:OG1	2.20	0.42
30:a:134:G:H2'	30:a:135:U:C6	2.55	0.42
30:a:1681:G:N3	30:a:1762:A:H2'	2.35	0.42
30:a:2760:C:O2'	30:a:2761:A:H5'	2.19	0.42
7:A:578:C:H2'	7:A:579:A:O4'	2.20	0.42
7:A:1157:A:C2	7:A:1181:G:C4	3.07	0.42
30:a:1946:U:H2'	30:a:1947:C:C6	2.55	0.42
30:a:2680:U:O2'	30:a:2681:C:H5'	2.19	0.42
30:a:2700:A:H2'	30:a:2701:U:C6	2.54	0.42
30:a:2898:U:H2'	30:a:2899:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:111:U:H2'	31:b:112:G:H8	1.84	0.42
33:d:38:LYS:O	33:d:46:ARG:HA	2.20	0.42
38:i:138:GLN:OE1	38:i:138:GLN:HA	2.20	0.42
49:t:40:ASN:HB3	49:t:63:ALA:O	2.20	0.42
7:A:268:U:H2'	7:A:269:C:C6	2.55	0.42
7:A:407:U:H2'	7:A:408:A:C8	2.55	0.42
7:A:1003:G:C2	7:A:1038:C:C2	3.08	0.42
7:A:1041:G:C6	7:A:1042:A:N7	2.88	0.42
7:A:1163:A:H2'	7:A:1164:G:H8	1.84	0.42
7:A:1226:C:P	19:M:90:ARG:HH22	2.43	0.42
8:B:118:GLU:O	8:B:122:GLN:HG2	2.19	0.42
11:E:165:LEU:HD23	11:E:165:LEU:HA	1.75	0.42
19:M:51:GLY:O	19:M:55:THR:HG23	2.19	0.42
30:a:1361:G:H2'	30:a:1362:C:C6	2.55	0.42
30:a:1726:C:H2'	30:a:1727:C:C6	2.55	0.42
7:A:1315:U:H2'	7:A:1316:G:O4'	2.18	0.42
30:a:1168:G:H1	30:a:1181:U:H3	1.68	0.42
30:a:1264:A:H5'	55:z:8:PRO:HG2	2.02	0.42
30:a:2026:U:H2'	30:a:2027:G:O4'	2.20	0.42
30:a:2293:G:H2'	30:a:2294:G:O4'	2.19	0.42
30:a:2845:U:H5''	44:o:52:ASN:O	2.20	0.42
42:m:55:ALA:HA	42:m:80:PHE:CE2	2.54	0.42
7:A:530:G:H8	7:A:530:G:H2'	1.71	0.41
12:F:6:ILE:HG12	12:F:89:VAL:HG22	2.01	0.41
27:U:20:LYS:HB3	27:U:20:LYS:HE2	1.60	0.41
30:a:12:U:O2	30:a:12:U:H2'	2.20	0.41
30:a:146:A:H2'	30:a:147:C:C6	2.55	0.41
30:a:1050:A:C2	30:a:2751:G:C4	3.08	0.41
30:a:1182:G:H2'	30:a:1183:U:O4'	2.20	0.41
30:a:1338:G:O2'	30:a:1393:A:N1	2.52	0.41
30:a:2308:G:H2'	30:a:2308:G:N3	2.34	0.41
30:a:2804:U:H2'	30:a:2805:C:H6	1.85	0.41
39:j:38:ILE:HD11	39:j:112:PHE:HZ	1.84	0.41
7:A:986:U:H2'	7:A:987:G:O4'	2.19	0.41
7:A:1496:C:H2'	7:A:1497:G:O4'	2.21	0.41
11:E:44:GLY:O	11:E:74:VAL:N	2.48	0.41
20:N:19:LYS:HG2	20:N:20:TYR:CD1	2.56	0.41
24:R:24:LYS:HB2	24:R:24:LYS:HE2	1.84	0.41
30:a:348:A:H2'	30:a:349:U:O4'	2.20	0.41
30:a:747:5MU:C5M	30:a:2612:C:H4'	2.50	0.41
31:b:90:C:H5'	41:l:18:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:108:VAL:HG11	35:f:176:PRO:HG2	2.02	0.41
40:k:92:LEU:HD11	40:k:106:GLU:O	2.20	0.41
46:q:1:MET:HA	46:q:42:ALA:O	2.20	0.41
47:r:23:LEU:HD22	55:z:24:ALA:HB2	2.01	0.41
7:A:767:A:H2'	7:A:768:A:O4'	2.20	0.41
7:A:839:C:H2'	7:A:840:C:C6	2.54	0.41
7:A:1010:U:H2'	7:A:1011:C:H6	1.84	0.41
8:B:73:LYS:HE3	8:B:165:ASP:OD2	2.21	0.41
10:D:55:LEU:O	10:D:59:GLN:HG2	2.21	0.41
17:K:50:SER:OG	17:K:69:ARG:NH1	2.48	0.41
30:a:102:U:H5	53:x:4:LYS:HE3	1.85	0.41
30:a:560:C:O2	45:p:48:ARG:NH2	2.50	0.41
30:a:747:5MU:C4	30:a:747:5MU:C5M	2.84	0.41
30:a:839:U:H2'	30:a:840:C:C6	2.55	0.41
31:b:2:G:H2'	31:b:3:C:C6	2.55	0.41
35:f:161:LYS:HA	35:f:161:LYS:HD3	1.82	0.41
39:j:66:LYS:HA	39:j:79:PHE:O	2.20	0.41
5:4:62:LYS:HB2	5:4:62:LYS:HZ3	1.86	0.41
7:A:232:G:H1'	7:A:262:A:N1	2.35	0.41
7:A:1295:U:H2'	7:A:1296:C:C6	2.55	0.41
7:A:1441:A:C8	7:A:1442:G:C8	3.08	0.41
26:T:47:ALA:HB1	26:T:83:ILE:HG12	2.02	0.41
29:Z:47:U:H5'	29:Z:48:C:H5'	2.00	0.41
30:a:95:A:H4'	53:x:38:GLN:O	2.20	0.41
30:a:483:A:C8	49:t:45:HIS:HD2	2.39	0.41
30:a:654:A:H3'	30:a:654:A:N3	2.35	0.41
30:a:945:A:C4	30:a:2448:A:C2	3.08	0.41
30:a:2687:U:H2'	30:a:2688:G:O4'	2.21	0.41
32:c:160:THR:HB	32:c:177:ARG:HG3	2.03	0.41
33:d:152:PRO:HG3	33:d:156:PHE:CZ	2.56	0.41
36:g:19:ILE:HD13	36:g:43:VAL:HG22	2.02	0.41
36:g:99:LYS:HB3	36:g:99:LYS:HE2	1.76	0.41
46:q:5:PHE:HB3	46:q:59:ILE:HD12	2.02	0.41
46:q:44:GLY:O	46:q:45:GLU:HB2	2.20	0.41
7:A:151:A:H5''	7:A:152:A:OP2	2.20	0.41
30:a:861:A:H2'	30:a:862:G:O4'	2.21	0.41
30:a:1001:A:H2'	30:a:1002:G:O4'	2.21	0.41
30:a:1722:A:N6	30:a:1738:G:H1'	2.36	0.41
30:a:2590:A:H2'	30:a:2591:C:C6	2.56	0.41
3:2:19:LYS:HG3	30:a:651:G:H5'	2.02	0.41
7:A:1030:U:H5'	7:A:1031:C:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1118:U:H2'	7:A:1119:C:H6	1.85	0.41
7:A:1172:C:H2'	7:A:1173:U:C6	2.55	0.41
10:D:12:SER:HB3	10:D:17:THR:O	2.21	0.41
31:b:5:U:OP1	31:b:61:G:O2'	2.32	0.41
7:A:189:A:H2'	7:A:190:A:C8	2.56	0.41
7:A:1508:A:H2'	7:A:1509:C:O4'	2.21	0.41
7:A:1510:C:H2'	7:A:1511:G:C8	2.56	0.41
30:a:1730:C:H1'	30:a:1731:G:C2	2.56	0.41
32:c:5:LYS:HD2	32:c:17:VAL:HG22	2.02	0.41
37:h:9:VAL:HG11	37:h:12:LEU:HD12	2.01	0.41
50:u:63:ILE:HG22	50:u:65:VAL:HG13	2.03	0.41
7:A:1428:A:H2'	7:A:1429:A:O4'	2.21	0.41
10:D:168:PRO:HB2	10:D:171:LEU:HD12	2.03	0.41
19:M:95:LEU:HD23	19:M:95:LEU:HA	1.82	0.41
30:a:565:C:H2'	30:a:566:U:O4'	2.20	0.41
30:a:2205:A:H2'	30:a:2206:C:C6	2.55	0.41
30:a:2473:U:O2	30:a:2473:U:H2'	2.21	0.41
31:b:48:U:H2'	31:b:49:C:C6	2.56	0.41
46:q:16:GLU:OE1	46:q:100:GLY:HA2	2.21	0.41
7:A:34:C:H2'	7:A:35:G:H8	1.86	0.41
7:A:62:U:OP1	7:A:385:C:O2'	2.37	0.41
7:A:130:A:H1'	7:A:263:A:O2'	2.21	0.41
7:A:473:U:H2'	7:A:474:G:C8	2.54	0.41
7:A:560:A:H5'	7:A:566:G:N2	2.36	0.41
7:A:736:C:H2'	7:A:737:C:H6	1.84	0.41
7:A:1009:U:C2	7:A:1010:U:C5	3.09	0.41
7:A:1073:U:O2'	8:B:105:LYS:HE2	2.21	0.41
7:A:1157:A:H4'	7:A:1158:C:O5'	2.20	0.41
8:B:94:HIS:O	8:B:95:ARG:C	2.64	0.41
9:C:18:TRP:CH2	20:N:97:LYS:HD2	2.56	0.41
13:G:26:PHE:HB2	13:G:101:MET:SD	2.60	0.41
25:S:50:ALA:HB1	25:S:57:HIS:HB3	2.03	0.41
30:a:57:C:H2'	30:a:58:G:O4'	2.21	0.41
30:a:155:A:H2'	30:a:156:A:H8	1.86	0.41
30:a:884:U:C2	30:a:885:C:C5	3.09	0.41
30:a:1224:U:H2'	30:a:1225:G:C8	2.55	0.41
30:a:1999:C:H5''	30:a:2723:C:O2'	2.21	0.41
30:a:2286:G:N3	30:a:2286:G:H2'	2.36	0.41
30:a:2305:U:H5''	35:f:131:GLY:HA3	2.03	0.41
30:a:2810:A:H5''	33:d:62:LYS:HD2	2.01	0.41
32:c:182:ARG:HG2	32:c:183:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:15:SER:HB3	34:e:197:GLU:OE2	2.20	0.41
34:e:129:PRO:HB3	34:e:156:ASN:HA	2.03	0.41
38:i:52:ASP:O	38:i:121:LYS:HE2	2.20	0.41
40:k:1:MET:C	40:k:2:ARG:HD2	2.45	0.41
46:q:73:LYS:HE2	46:q:86:GLN:OE1	2.21	0.41
50:u:53:LYS:HE2	50:u:53:LYS:HB2	1.96	0.41
51:v:44:LYS:HB2	51:v:44:LYS:HE2	1.75	0.41
5:4:59:ARG:O	5:4:62:LYS:HG2	2.20	0.41
7:A:323:U:H2'	7:A:324:G:O4'	2.21	0.41
7:A:408:A:H2'	7:A:409:U:C6	2.56	0.41
7:A:681:A:H2'	7:A:682:G:O4'	2.21	0.41
7:A:1055:A:O2'	9:C:161:GLU:O	2.31	0.41
7:A:1143:G:H2'	7:A:1144:G:C8	2.56	0.41
7:A:1143:G:H2'	7:A:1144:G:H8	1.86	0.41
21:O:69:TYR:CZ	21:O:73:LYS:HD3	2.56	0.41
24:R:69:PRO:HB2	24:R:71:THR:O	2.20	0.41
30:a:547:A:H1'	30:a:548:G:C6	2.56	0.41
30:a:1786:A:H1'	30:a:1938:A:N6	2.36	0.41
31:b:29:A:OP2	43:n:32:PRO:HD2	2.21	0.41
47:r:6:LYS:HA	47:r:103:ILE:O	2.21	0.41
51:v:41:ARG:HD3	51:v:41:ARG:HA	1.85	0.41
7:A:1038:C:H5'	7:A:1039:G:OP2	2.21	0.40
24:R:23:TYR:HA	24:R:29:LEU:HD11	2.02	0.40
30:a:120:U:H5''	30:a:122:G:OP2	2.21	0.40
30:a:796:C:H2'	30:a:797:G:C8	2.56	0.40
30:a:1223:G:C6	30:a:1227:G:C6	3.09	0.40
30:a:2019:A:H4'	45:p:34:VAL:HG21	2.02	0.40
7:A:481:G:O2'	7:A:483:C:N4	2.55	0.40
7:A:745:G:H2'	7:A:746:A:C8	2.56	0.40
9:C:148:GLY:HA3	9:C:172:ARG:O	2.21	0.40
10:D:37:ALA:O	10:D:42:GLY:HA3	2.21	0.40
19:M:81:MET:HG2	19:M:92:ARG:HG3	2.02	0.40
30:a:1199:U:H1'	45:p:4:VAL:HG22	2.04	0.40
30:a:2443:C:H2'	30:a:2444:G:C8	2.56	0.40
30:a:2461:A:H2'	30:a:2462:C:C6	2.56	0.40
44:o:114:LEU:HD23	44:o:114:LEU:HA	1.89	0.40
48:s:54:GLU:HB2	48:s:91:GLN:HG3	2.03	0.40
5:4:56:ARG:CZ	5:4:59:ARG:HE	2.35	0.40
8:B:69:PHE:HB3	8:B:80:VAL:HG22	2.03	0.40
30:a:643:A:N1	30:a:2369:A:O2'	2.45	0.40
30:a:1583:A:O2'	30:a:1585:C:N4	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2661:G:H2'	30:a:2662:A:C8	2.57	0.40
33:d:35:THR:HG22	33:d:73:VAL:HG21	2.03	0.40
36:g:154:PRO:HA	36:g:160:LYS:O	2.21	0.40
7:A:302:G:O2'	7:A:556:C:H5''	2.22	0.40
7:A:747:A:OP2	7:A:747:A:H8	2.04	0.40
7:A:1120:C:H2'	7:A:1121:U:H6	1.86	0.40
7:A:1286:U:N3	7:A:1288:A:OP1	2.55	0.40
9:C:73:PRO:O	9:C:77:ILE:HG13	2.21	0.40
30:a:153:U:H2'	30:a:154:U:C6	2.57	0.40
30:a:192:C:H2'	30:a:193:U:H5'	2.03	0.40
30:a:300:A:H2'	30:a:334:C:H1'	2.04	0.40
30:a:1013:C:H2'	30:a:1014:A:C8	2.56	0.40
30:a:1354:A:H2'	30:a:1355:G:O4'	2.21	0.40
30:a:2590:A:H2'	30:a:2591:C:H6	1.86	0.40
51:v:59:LEU:HD12	51:v:80:ILE:HD12	2.04	0.40
7:A:451:A:H5'	22:P:70:ARG:NH2	2.36	0.40
7:A:868:C:H2'	7:A:869:G:O4'	2.21	0.40
7:A:966:2MG:C2	29:Z:34:C:H5'	2.57	0.40
10:D:107:PHE:HB3	10:D:145:ILE:HD11	2.04	0.40
10:D:170:TRP:CD2	10:D:186:PRO:HB3	2.56	0.40
30:a:613:A:H8	30:a:613:A:OP1	2.04	0.40
30:a:666:A:H2'	30:a:667:U:C6	2.56	0.40
30:a:1783:A:H5'	30:a:2608:G:H4'	2.03	0.40
30:a:2294:G:OP1	43:n:10:ARG:HD2	2.22	0.40
32:c:76:ALA:HB2	32:c:96:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
8	B	222/241 (92%)	216 (97%)	5 (2%)	1 (0%)	24	16
9	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
10	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
11	E	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
12	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
13	G	151/179 (84%)	143 (95%)	8 (5%)	0	100	100
14	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
15	I	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
16	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	5
17	K	115/129 (89%)	109 (95%)	5 (4%)	1 (1%)	14	6
18	L	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
22	P	79/82 (96%)	71 (90%)	7 (9%)	1 (1%)	9	3
23	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
24	R	64/75 (85%)	61 (95%)	2 (3%)	1 (2%)	7	2
25	S	82/92 (89%)	82 (100%)	0	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
32	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
33	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
34	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
35	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
36	g	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
37	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
38	i	140/142 (99%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
40	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
41	l	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
42	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
43	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
44	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
45	p	115/118 (98%)	115 (100%)	0	0	100	100
46	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
47	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
48	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
49	t	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
50	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
51	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	60/63 (95%)	60 (100%)	0	0	100	100
54	y	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	6	1
55	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5484/5913 (93%)	5333 (97%)	145 (3%)	6 (0%)	49	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	R	10	PHE
16	J	57	VAL
17	K	119	ASP
22	P	46	LYS
54	y	4	THR
8	B	131	LYS

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	29
5	4	55/62 (89%)	54 (98%)	1 (2%)	51	47
8	B	186/199 (94%)	184 (99%)	2 (1%)	65	64
9	C	170/190 (90%)	167 (98%)	3 (2%)	51	47
10	D	172/173 (99%)	166 (96%)	6 (4%)	32	22
11	E	119/126 (94%)	119 (100%)	0	100	100
12	F	90/116 (78%)	88 (98%)	2 (2%)	45	40
13	G	126/147 (86%)	122 (97%)	4 (3%)	34	25
14	H	104/105 (99%)	103 (99%)	1 (1%)	68	67
15	I	105/107 (98%)	105 (100%)	0	100	100
16	J	86/90 (96%)	84 (98%)	2 (2%)	44	38
17	K	90/99 (91%)	88 (98%)	2 (2%)	45	40
18	L	103/104 (99%)	101 (98%)	2 (2%)	50	45
19	M	93/96 (97%)	93 (100%)	0	100	100
20	N	83/84 (99%)	83 (100%)	0	100	100
21	O	76/77 (99%)	73 (96%)	3 (4%)	28	18
22	P	65/65 (100%)	65 (100%)	0	100	100
23	Q	73/78 (94%)	70 (96%)	3 (4%)	27	17
24	R	57/65 (88%)	55 (96%)	2 (4%)	32	22
25	S	72/79 (91%)	71 (99%)	1 (1%)	59	56
26	T	65/66 (98%)	65 (100%)	0	100	100
27	U	60/61 (98%)	59 (98%)	1 (2%)	53	49
32	c	216/218 (99%)	214 (99%)	2 (1%)	70	70
33	d	163/163 (100%)	162 (99%)	1 (1%)	78	79
34	e	165/165 (100%)	164 (99%)	1 (1%)	78	79
35	f	148/150 (99%)	146 (99%)	2 (1%)	59	56
36	g	137/138 (99%)	132 (96%)	5 (4%)	31	21
37	h	32/114 (28%)	31 (97%)	1 (3%)	35	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	i	116/116 (100%)	115 (99%)	1 (1%)	70	70
39	j	104/104 (100%)	103 (99%)	1 (1%)	68	67
40	k	103/103 (100%)	102 (99%)	1 (1%)	68	67
41	l	109/109 (100%)	109 (100%)	0	100	100
42	m	98/103 (95%)	98 (100%)	0	100	100
43	n	86/87 (99%)	85 (99%)	1 (1%)	63	61
44	o	99/100 (99%)	99 (100%)	0	100	100
45	p	89/90 (99%)	89 (100%)	0	100	100
46	q	84/84 (100%)	82 (98%)	2 (2%)	43	36
47	r	93/93 (100%)	93 (100%)	0	100	100
48	s	80/84 (95%)	80 (100%)	0	100	100
49	t	83/85 (98%)	83 (100%)	0	100	100
50	u	78/78 (100%)	77 (99%)	1 (1%)	61	58
51	v	58/63 (92%)	58 (100%)	0	100	100
52	w	67/68 (98%)	67 (100%)	0	100	100
53	x	54/55 (98%)	54 (100%)	0	100	100
54	y	48/49 (98%)	47 (98%)	1 (2%)	47	41
55	z	47/48 (98%)	46 (98%)	1 (2%)	47	41
All	All	4576/4829 (95%)	4519 (99%)	57 (1%)	61	61

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	3	36	ARG
5	4	66	ILE
8	B	4	VAL
8	B	211	THR
9	C	86	LYS
9	C	149	ILE
9	C	206	GLU
10	D	23	SER
10	D	116	GLN
10	D	119	SER
10	D	163	GLU
10	D	177	LYS
10	D	189	SER

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Mol	Chain	Res	Type
12	F	64	VAL
12	F	100	SER
13	G	40	GLU
13	G	60	GLU
13	G	113	ASP
13	G	135	VAL
14	H	96	MET
16	J	25	ILE
16	J	44	THR
17	K	116	ILE
17	K	129	VAL
18	L	10	LYS
18	L	15	LYS
21	O	75	VAL
21	O	79	THR
21	O	80	GLN
23	Q	13	VAL
23	Q	17	MET
23	Q	42	THR
24	R	14	THR
24	R	66	SER
25	S	71	LEU
27	U	4	ILE
32	c	162	VAL
32	c	272	SER
33	d	95	SER
34	e	127	GLU
35	f	24	SER
35	f	27	GLN
36	g	16	ASP
36	g	43	VAL
36	g	49	THR
36	g	51	THR
36	g	92	VAL
37	h	35	LYS
38	i	12	LYS
39	j	76	VAL
40	k	115	GLU
43	n	83	LEU
46	q	6	GLN
46	q	102	SER
50	u	11	GLU

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Mol	Chain	Res	Type
54	y	4	THR
55	z	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	45	GLN
8	B	58	ASN
8	B	120	GLN
8	B	122	GLN
9	C	123	GLN
10	D	59	GLN
10	D	164	GLN
11	E	73	ASN
13	G	68	ASN
13	G	148	ASN
14	H	4	GLN
15	I	110	GLN
16	J	15	HIS
16	J	58	ASN
21	O	40	GLN
21	O	50	HIS
22	P	59	HIS
22	P	63	GLN
24	R	52	GLN
25	S	56	GLN
26	T	3	ASN
26	T	61	GLN
32	c	25	HIS
32	c	86	ASN
32	c	117	GLN
32	c	134	ASN
33	d	42	ASN
34	e	156	ASN
35	f	5	HIS
35	f	21	ASN
36	g	30	ASN
36	g	104	ASN
37	h	2	GLN
38	i	58	ASN
38	i	80	HIS
39	j	3	GLN

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Mol	Chain	Res	Type
41	l	13	HIS
41	l	60	GLN
42	m	18	GLN
44	o	66	ASN
47	r	9	HIS
52	w	36	HIS
53	x	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	X	5/6 (83%)	0	0
29	Z	75/76 (98%)	20 (26%)	0
30	a	2749/2903 (94%)	311 (11%)	0
31	b	118/120 (98%)	12 (10%)	0
6	5	1/2 (50%)	1 (100%)	0
7	A	1516/1542 (98%)	186 (12%)	6 (0%)
All	All	4464/4649 (96%)	530 (11%)	6 (0%)

All (530) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
7	A	4	U
7	A	5	U
7	A	6	G
7	A	13	U
7	A	32	A
7	A	39	G
7	A	47	C
7	A	48	C
7	A	50	A
7	A	51	A
7	A	71	A
7	A	72	A
7	A	73	C
7	A	74	A
7	A	81	A
7	A	83	C
7	A	84	U
7	A	85	U

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Mol	Chain	Res	Type
7	A	86	G
7	A	87	C
7	A	88	U
7	A	94	G
7	A	122	G
7	A	128	G
7	A	131	A
7	A	141	G
7	A	151	A
7	A	164	G
7	A	182	A
7	A	183	C
7	A	191	G
7	A	197	A
7	A	200	G
7	A	201	G
7	A	240	G
7	A	245	U
7	A	247	G
7	A	251	G
7	A	266	G
7	A	267	C
7	A	289	G
7	A	321	A
7	A	328	C
7	A	329	A
7	A	330	C
7	A	339	C
7	A	347	G
7	A	352	C
7	A	354	G
7	A	367	U
7	A	372	C
7	A	384	G
7	A	406	G
7	A	411	A
7	A	412	A
7	A	413	G
7	A	414	A
7	A	415	A
7	A	417	G
7	A	421	U

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Mol	Chain	Res	Type
7	A	422	C
7	A	424	G
7	A	429	U
7	A	436	C
7	A	457	G
7	A	458	U
7	A	464	U
7	A	467	U
7	A	468	A
7	A	469	C
7	A	474	G
7	A	478	A
7	A	481	G
7	A	484	G
7	A	486	U
7	A	497	G
7	A	511	C
7	A	518	C
7	A	531	U
7	A	532	A
7	A	542	G
7	A	547	A
7	A	559	A
7	A	564	C
7	A	572	A
7	A	573	A
7	A	576	C
7	A	577	G
7	A	579	A
7	A	596	A
7	A	633	G
7	A	650	G
7	A	653	U
7	A	665	A
7	A	723	U
7	A	724	G
7	A	748	G
7	A	755	G
7	A	777	A
7	A	792	A
7	A	793	U
7	A	794	A

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Mol	Chain	Res	Type
7	A	815	A
7	A	817	C
7	A	821	G
7	A	829	G
7	A	890	G
7	A	914	A
7	A	926	G
7	A	934	C
7	A	935	A
7	A	960	U
7	A	966	2MG
7	A	969	A
7	A	975	A
7	A	976	G
7	A	977	A
7	A	996	A
7	A	1004	A
7	A	1009	U
7	A	1024	G
7	A	1027	C
7	A	1029	U
7	A	1030	U
7	A	1031	C
7	A	1032	G
7	A	1033	G
7	A	1034	G
7	A	1036	A
7	A	1039	G
7	A	1044	A
7	A	1065	U
7	A	1070	U
7	A	1085	U
7	A	1094	G
7	A	1095	U
7	A	1101	A
7	A	1123	U
7	A	1126	U
7	A	1137	C
7	A	1138	G
7	A	1139	G
7	A	1157	A
7	A	1159	U

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Mol	Chain	Res	Type
7	A	1167	A
7	A	1169	A
7	A	1184	G
7	A	1196	A
7	A	1197	A
7	A	1213	A
7	A	1227	A
7	A	1238	A
7	A	1248	A
7	A	1258	G
7	A	1260	G
7	A	1275	A
7	A	1279	G
7	A	1280	A
7	A	1287	A
7	A	1300	G
7	A	1302	C
7	A	1317	C
7	A	1320	C
7	A	1338	G
7	A	1346	A
7	A	1353	G
7	A	1363	A
7	A	1370	G
7	A	1378	C
7	A	1379	G
7	A	1380	U
7	A	1381	U
7	A	1398	A
7	A	1419	G
7	A	1441	A
7	A	1451	U
7	A	1452	C
7	A	1453	G
7	A	1492	A
7	A	1493	A
7	A	1497	G
7	A	1503	A
7	A	1506	U
7	A	1517	G
7	A	1529	G
7	A	1530	G

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Mol	Chain	Res	Type
29	Z	5	G
29	Z	9	G
29	Z	14	A
29	Z	17(A)	U
29	Z	18	G
29	Z	20	U
29	Z	21	A
29	Z	43	A
29	Z	47	U
29	Z	51	C
29	Z	52	G
29	Z	58	A
29	Z	62	C
29	Z	65	C
29	Z	66	C
29	Z	69	C
29	Z	71	C
29	Z	73	A
29	Z	74	C
29	Z	76	A
30	a	10	A
30	a	15	G
30	a	34	U
30	a	42	A
30	a	45	G
30	a	58	G
30	a	71	A
30	a	74	A
30	a	75	G
30	a	80	G
30	a	84	A
30	a	101	A
30	a	102	U
30	a	118	A
30	a	119	A
30	a	120	U
30	a	125	A
30	a	139	U
30	a	142	A
30	a	163	C
30	a	164	C
30	a	181	A

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Mol	Chain	Res	Type
30	a	196	A
30	a	199	A
30	a	200	U
30	a	215	G
30	a	216	A
30	a	222	A
30	a	248	G
30	a	265	A
30	a	272	A
30	a	274	C
30	a	278	A
30	a	281	C
30	a	282	A
30	a	285	G
30	a	287	G
30	a	288	U
30	a	311	A
30	a	329	G
30	a	330	A
30	a	358	U
30	a	359	G
30	a	361	G
30	a	362	A
30	a	386	G
30	a	405	U
30	a	411	G
30	a	412	A
30	a	456	C
30	a	481	G
30	a	491	G
30	a	504	A
30	a	505	A
30	a	509	C
30	a	532	A
30	a	533	G
30	a	544	C
30	a	545	U
30	a	546	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	563	A

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Mol	Chain	Res	Type
30	a	573	U
30	a	575	A
30	a	586	A
30	a	603	A
30	a	614	A
30	a	615	U
30	a	627	A
30	a	637	A
30	a	645	C
30	a	647	G
30	a	653	U
30	a	654	A
30	a	655	A
30	a	686	U
30	a	717	C
30	a	721	A
30	a	730	A
30	a	738	G
30	a	747	5MU
30	a	775	G
30	a	776	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	789	A
30	a	792	A
30	a	805	G
30	a	812	C
30	a	827	U
30	a	828	U
30	a	845	A
30	a	846	U
30	a	847	U
30	a	859	G
30	a	877	A
30	a	879	G
30	a	881	G
30	a	882	G
30	a	883	G
30	a	884	U
30	a	885	C
30	a	888	C

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Mol	Chain	Res	Type
30	a	890	C
30	a	891	G
30	a	895	U
30	a	896	A
30	a	897	C
30	a	898	C
30	a	903	C
30	a	910	A
30	a	914	G
30	a	931	U
30	a	946	C
30	a	961	C
30	a	974	G
30	a	983	A
30	a	996	A
30	a	1012	U
30	a	1013	C
30	a	1022	G
30	a	1033	U
30	a	1046	A
30	a	1047	G
30	a	1108	U
30	a	1110	G
30	a	1111	A
30	a	1112	G
30	a	1115	G
30	a	1116	G
30	a	1122	G
30	a	1132	U
30	a	1135	C
30	a	1142	A
30	a	1169	A
30	a	1170	C
30	a	1171	G
30	a	1172	C
30	a	1253	A
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1273	U
30	a	1300	G
30	a	1301	A

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Mol	Chain	Res	Type
30	a	1352	U
30	a	1365	A
30	a	1379	U
30	a	1383	A
30	a	1416	G
30	a	1419	A
30	a	1427	A
30	a	1428	C
30	a	1434	A
30	a	1452	G
30	a	1453	A
30	a	1459	G
30	a	1476	U
30	a	1482	G
30	a	1493	C
30	a	1497	U
30	a	1508	A
30	a	1509	A
30	a	1510	G
30	a	1515	A
30	a	1534	U
30	a	1535	A
30	a	1536	C
30	a	1537	G
30	a	1566	A
30	a	1569	A
30	a	1578	U
30	a	1583	A
30	a	1585	C
30	a	1608	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1714	U
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1731	G
30	a	1738	G
30	a	1744	A
30	a	1764	C

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Mol	Chain	Res	Type
30	a	1773	A
30	a	1782	U
30	a	1800	C
30	a	1801	A
30	a	1808	A
30	a	1816	C
30	a	1829	A
30	a	1847	A
30	a	1848	A
30	a	1858	A
30	a	1868	C
30	a	1871	A
30	a	1872	A
30	a	1873	G
30	a	1874	C
30	a	1906	G
30	a	1907	G
30	a	1914	C
30	a	1915	U
30	a	1929	G
30	a	1930	G
30	a	1937	A
30	a	1938	A
30	a	1955	U
30	a	1965	C
30	a	1967	C
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1992	G
30	a	1993	U
30	a	2023	C
30	a	2030	6MZ
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A

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Mol	Chain	Res	Type
30	a	2069	G7M
30	a	2198	A
30	a	2203	U
30	a	2204	G
30	a	2211	A
30	a	2223	G
30	a	2225	A
30	a	2238	G
30	a	2239	G
30	a	2268	A
30	a	2283	C
30	a	2287	A
30	a	2305	U
30	a	2308	G
30	a	2322	A
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2347	C
30	a	2361	G
30	a	2383	G
30	a	2385	C
30	a	2396	G
30	a	2402	U
30	a	2403	C
30	a	2406	A
30	a	2422	C
30	a	2424	C
30	a	2425	A
30	a	2429	G
30	a	2430	A
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2470	G
30	a	2476	A
30	a	2491	U
30	a	2502	G
30	a	2505	G
30	a	2518	A
30	a	2529	G
30	a	2547	A

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Mol	Chain	Res	Type
30	a	2554	U
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2578	G
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2661	G
30	a	2663	G
30	a	2669	G
30	a	2689	U
30	a	2690	U
30	a	2714	G
30	a	2716	C
30	a	2726	A
30	a	2744	G
30	a	2748	A
30	a	2757	A
30	a	2765	A
30	a	2778	A
30	a	2791	G
30	a	2792	A
30	a	2795	C
30	a	2798	U
30	a	2799	A
30	a	2818	U
30	a	2820	A
30	a	2821	A
30	a	2861	U
30	a	2873	A
30	a	2874	C
30	a	2883	A
30	a	2884	U
30	a	2899	A
30	a	2902	C
31	b	35	C
31	b	36	C
31	b	44	G
31	b	45	A
31	b	56	G

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Mol	Chain	Res	Type
31	b	57	A
31	b	67	G
31	b	89	U
31	b	90	C
31	b	99	A
31	b	109	A
31	b	119	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	5	U
7	A	199	A
7	A	827	U
7	A	1026	G
7	A	1035	A
7	A	1492	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	PSU	a	2605	30	18,21,22	1.14	1 (5%)	22,30,33	1.74	4 (18%)
7	2MG	A	1207	7	23,26,27	3.00	7 (30%)	32,38,41	2.49	11 (34%)
7	5MC	A	967	7	18,22,23	3.61	7 (38%)	26,32,35	1.05	2 (7%)
7	2MG	A	1516	7	23,26,27	2.88	7 (30%)	32,38,41	2.41	11 (34%)
30	PSU	a	2604	30	18,21,22	1.10	1 (5%)	22,30,33	1.80	4 (18%)
30	PSU	a	1911	30	18,21,22	1.14	1 (5%)	22,30,33	1.88	4 (18%)
30	PSU	a	2457	30	18,21,22	1.15	1 (5%)	22,30,33	1.90	4 (18%)
7	G7M	A	527	7	23,26,27	2.55	9 (39%)	35,39,42	1.94	10 (28%)
30	1MG	a	745	30	22,26,27	2.70	6 (27%)	33,39,42	2.19	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMG	a	2251	29,30	23,26,27	2.31	9 (39%)	33,38,41	1.96	13 (39%)
33	MEQ	d	150	33	8,9,10	0.83	0	5,10,12	0.98	0
30	G7M	a	2069	30	23,26,27	2.55	9 (39%)	35,39,42	1.67	8 (22%)
7	UR3	A	1498	57,7	19,22,23	2.76	8 (42%)	26,32,35	1.47	1 (3%)
30	2MA	a	2503	57,30	22,25,26	3.45	9 (40%)	33,37,40	2.71	10 (30%)
30	PSU	a	2580	30	18,21,22	1.14	2 (11%)	22,30,33	1.80	5 (22%)
30	OMC	a	2498	57,30	19,22,23	2.89	8 (42%)	26,31,34	0.96	1 (3%)
30	5MU	a	1939	30	19,22,23	7.11	8 (42%)	28,32,35	3.45	8 (28%)
7	5MC	A	1407	7	18,22,23	3.48	7 (38%)	26,32,35	1.18	3 (11%)
30	OMU	a	2552	30	19,22,23	2.94	8 (42%)	26,31,34	1.72	4 (15%)
7	2MG	A	966	7	23,26,27	2.89	7 (30%)	32,38,41	2.43	12 (37%)
7	4OC	A	1402	7	20,23,24	2.92	8 (40%)	26,32,35	1.19	2 (7%)
30	5MU	a	747	30	19,22,23	7.18	8 (42%)	28,32,35	3.41	8 (28%)
30	2MG	a	1835	30	23,26,27	2.81	7 (30%)	32,38,41	2.50	13 (40%)
7	MA6	A	1518	7	23,26,27	1.63	5 (21%)	34,38,41	3.31	13 (38%)
30	6MZ	a	1618	30	22,25,26	2.94	5 (22%)	30,36,39	2.51	11 (36%)
30	6MZ	a	2030	30	22,25,26	2.78	5 (22%)	30,36,39	2.66	11 (36%)
7	PSU	A	516	7	18,21,22	1.20	1 (5%)	22,30,33	1.79	5 (22%)
30	2MG	a	2445	30	23,26,27	3.03	8 (34%)	32,38,41	2.57	11 (34%)
30	PSU	a	2504	30	18,21,22	1.14	1 (5%)	22,30,33	1.89	2 (9%)
30	5MC	a	1962	30	18,22,23	3.47	7 (38%)	26,32,35	1.05	1 (3%)
30	PSU	a	746	57,30	18,21,22	1.23	1 (5%)	22,30,33	1.67	4 (18%)
30	PSU	a	955	30	18,21,22	1.20	1 (5%)	22,30,33	2.04	3 (13%)
7	MA6	A	1519	7	23,26,27	1.63	6 (26%)	34,38,41	3.53	13 (38%)
30	PSU	a	1917	30	18,21,22	1.06	1 (5%)	22,30,33	1.70	3 (13%)

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
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
7	2MG	A	1207	7	-	0/9/27/28	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
7	2MG	A	1516	7	-	0/9/27/28	0/3/3/3
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	a	1911	30	-	1/7/25/26	0/2/2/2
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
7	G7M	A	527	7	-	0/7/25/26	0/3/3/3
30	1MG	a	745	30	-	0/7/25/26	0/3/3/3
30	OMG	a	2251	29,30	-	1/9/27/28	0/3/3/3
33	MEQ	d	150	33	-	2/8/9/11	-
30	G7M	a	2069	30	-	2/7/25/26	0/3/3/3
7	UR3	A	1498	57,7	-	0/7/25/26	0/2/2/2
30	2MA	a	2503	57,30	-	2/7/25/26	0/3/3/3
30	PSU	a	2580	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	57,30	-	0/9/27/28	0/2/2/2
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
30	OMU	a	2552	30	-	1/9/27/28	0/2/2/2
7	2MG	A	966	7	-	0/9/27/28	0/3/3/3
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2
30	2MG	a	1835	30	-	0/9/27/28	0/3/3/3
7	MA6	A	1518	7	-	0/11/29/30	0/3/3/3
30	6MZ	a	1618	30	-	0/9/27/28	0/3/3/3
30	6MZ	a	2030	30	-	2/9/27/28	0/3/3/3
7	PSU	A	516	7	-	0/7/25/26	0/2/2/2
30	2MG	a	2445	30	-	0/9/27/28	0/3/3/3
30	PSU	a	2504	30	-	0/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	0/7/25/26	0/2/2/2
30	PSU	a	746	57,30	-	3/7/25/26	0/2/2/2
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
7	MA6	A	1519	7	-	2/11/29/30	0/3/3/3
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	747	5MU	C4-C5	20.47	1.78	1.44
30	a	1939	5MU	C4-C5	20.34	1.78	1.44
30	a	747	5MU	C6-N1	15.03	1.63	1.38
30	a	1939	5MU	C6-N1	14.78	1.63	1.38
30	a	1618	6MZ	C6-N6	12.37	1.47	1.34
30	a	747	5MU	C6-C5	-12.22	1.14	1.34
30	a	1939	5MU	C6-C5	-12.14	1.14	1.34
30	a	1939	5MU	C4-N3	-11.74	1.17	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	747	5MU	C4-N3	-11.63	1.17	1.38
30	a	2503	2MA	C4-N3	11.06	1.48	1.34
30	a	2030	6MZ	C6-N6	11.00	1.46	1.34
30	a	1962	5MC	C6-C5	9.63	1.50	1.34
7	A	1407	5MC	C6-C5	9.54	1.50	1.34
7	A	967	5MC	C6-C5	9.52	1.50	1.34
7	A	1207	2MG	C2-N3	8.25	1.47	1.31
30	a	2445	2MG	C2-N3	7.81	1.46	1.31
7	A	966	2MG	C2-N3	7.72	1.46	1.31
7	A	1516	2MG	C2-N3	7.54	1.46	1.31
30	a	1835	2MG	C2-N3	7.53	1.46	1.31
7	A	1498	UR3	C2-N1	6.94	1.48	1.38
7	A	966	2MG	C4-N3	6.68	1.50	1.34
7	A	1207	2MG	C4-N3	6.65	1.50	1.34
30	a	745	1MG	C2-N3	6.63	1.46	1.34
7	A	1207	2MG	C2-N2	6.43	1.47	1.33
30	a	2445	2MG	C2-N2	6.41	1.47	1.33
30	a	2552	OMU	C2-N1	6.40	1.48	1.38
30	a	745	1MG	C4-N3	6.36	1.49	1.34
7	A	967	5MC	C4-N3	6.31	1.44	1.34
7	A	1516	2MG	C4-N3	6.26	1.49	1.34
7	A	966	2MG	C2-N2	6.26	1.47	1.33
30	a	2503	2MA	C2-N3	6.24	1.45	1.34
7	A	1498	UR3	C6-C5	6.18	1.49	1.35
30	a	2445	2MG	C4-N3	6.18	1.48	1.34
7	A	967	5MC	C2-N3	6.10	1.48	1.36
7	A	1516	2MG	C2-N2	6.09	1.46	1.33
30	a	1835	2MG	C2-N2	6.08	1.46	1.33
7	A	1402	4OC	C4-N3	6.04	1.43	1.32
30	a	2069	G7M	C5-N7	-6.04	1.32	1.39
7	A	1402	4OC	C6-C5	6.00	1.49	1.35
30	a	1835	2MG	C4-N3	5.97	1.48	1.34
30	a	2552	OMU	C2-N3	5.95	1.48	1.38
7	A	527	G7M	C4-N3	5.87	1.48	1.34
7	A	1407	5MC	C4-N3	5.67	1.43	1.34
30	a	2498	OMC	C6-C5	5.66	1.48	1.35
30	a	2069	G7M	C4-N3	5.65	1.47	1.34
30	a	2552	OMU	C6-C5	5.65	1.48	1.35
30	a	2445	2MG	C2-N1	5.62	1.45	1.36
7	A	1407	5MC	C2-N3	5.56	1.47	1.36
30	a	1962	5MC	C2-N3	5.45	1.47	1.36
30	a	2251	OMG	C4-N3	5.41	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	745	1MG	C2-N2	5.34	1.43	1.34
30	a	1962	5MC	C4-N3	5.25	1.43	1.34
30	a	2498	OMC	C2-N3	5.23	1.47	1.36
30	a	2503	2MA	C6-N1	5.21	1.42	1.35
7	A	527	G7M	C5-N7	-5.12	1.33	1.39
7	A	527	G7M	C2-N3	5.06	1.45	1.33
30	a	2498	OMC	C4-N4	5.03	1.45	1.33
7	A	1207	2MG	C2-N1	4.95	1.44	1.36
7	A	1402	4OC	C2-N3	4.90	1.46	1.36
7	A	1516	2MG	C2-N1	4.83	1.44	1.36
7	A	967	5MC	C4-N4	4.70	1.46	1.34
7	A	966	2MG	C2-N1	4.65	1.44	1.36
30	a	1835	2MG	C2-N1	4.64	1.44	1.36
30	a	2069	G7M	C2-N3	4.64	1.44	1.33
7	A	1407	5MC	C4-N4	4.56	1.45	1.34
30	a	2251	OMG	C2-N3	4.52	1.44	1.33
7	A	1498	UR3	C2-N3	4.49	1.47	1.39
30	a	2503	2MA	C6-N6	-4.43	1.23	1.34
7	A	1402	4OC	C4-N4	4.40	1.44	1.35
30	a	2498	OMC	C4-N3	4.39	1.43	1.34
7	A	527	G7M	C2-N2	4.36	1.44	1.34
30	a	2552	OMU	O4-C4	-4.30	1.16	1.24
30	a	745	1MG	C5-N7	-4.21	1.30	1.39
30	a	1962	5MC	C4-N4	4.19	1.45	1.34
30	a	1962	5MC	C6-N1	4.15	1.45	1.38
30	a	747	5MU	C2-N3	4.15	1.45	1.38
30	a	2498	OMC	O2-C2	-4.15	1.16	1.23
30	a	2251	OMG	C2-N2	4.13	1.44	1.34
7	A	967	5MC	C6-N1	4.05	1.45	1.38
30	a	2498	OMC	C2-N1	4.03	1.48	1.40
7	A	1402	4OC	O2-C2	-4.01	1.16	1.23
30	a	1962	5MC	C2-N1	3.98	1.48	1.40
7	A	1407	5MC	C6-N1	3.87	1.44	1.38
7	A	967	5MC	C2-N1	3.87	1.48	1.40
30	a	2503	2MA	C2-N1	3.83	1.40	1.34
30	a	1939	5MU	C2-N3	3.81	1.44	1.38
30	a	746	PSU	C6-C5	3.79	1.39	1.35
30	a	745	1MG	C5-C6	3.75	1.55	1.45
30	a	2069	G7M	C2-N2	3.75	1.43	1.34
7	A	1402	4OC	C5-C4	3.72	1.48	1.40
7	A	1519	MA6	C6-N6	3.72	1.47	1.36
30	a	1962	5MC	O2-C2	-3.69	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1518	MA6	C6-N6	3.65	1.47	1.36
30	a	2503	2MA	C5-C6	3.65	1.51	1.41
7	A	516	PSU	C6-C5	3.65	1.39	1.35
7	A	1407	5MC	C2-N1	3.65	1.47	1.40
7	A	1402	4OC	C2-N1	3.64	1.47	1.40
30	a	2504	PSU	C6-C5	3.61	1.39	1.35
7	A	527	G7M	C5-C6	3.58	1.53	1.43
30	a	2251	OMG	O6-C6	-3.53	1.16	1.23
7	A	1407	5MC	O2-C2	-3.51	1.17	1.23
7	A	1498	UR3	O4-C4	-3.47	1.16	1.23
30	a	2503	2MA	C5-N7	-3.44	1.32	1.39
30	a	2069	G7M	C5-C6	3.44	1.52	1.43
30	a	2605	PSU	C6-C5	3.43	1.39	1.35
30	a	2251	OMG	C4-N9	-3.36	1.29	1.38
7	A	1518	MA6	C5-C4	-3.34	1.32	1.39
30	a	1939	5MU	O2-C2	-3.33	1.17	1.23
30	a	2498	OMC	C6-N1	3.31	1.46	1.38
30	a	747	5MU	O2-C2	-3.31	1.17	1.23
30	a	955	PSU	C6-C5	3.31	1.39	1.35
30	a	2604	PSU	C6-C5	3.29	1.39	1.35
30	a	2030	6MZ	C5-N7	-3.25	1.32	1.39
30	a	2457	PSU	C6-C5	3.24	1.39	1.35
7	A	967	5MC	O2-C2	-3.21	1.17	1.23
7	A	527	G7M	O6-C6	-3.21	1.17	1.23
30	a	1917	PSU	C6-C5	3.19	1.39	1.35
30	a	2069	G7M	O6-C6	-3.16	1.17	1.23
30	a	747	5MU	C2-N1	3.14	1.43	1.38
30	a	2552	OMU	C4-N3	3.12	1.44	1.38
30	a	2552	OMU	O2-C2	-3.11	1.17	1.23
30	a	747	5MU	O4-C4	-3.08	1.17	1.23
30	a	1911	PSU	C6-C5	3.08	1.38	1.35
30	a	1618	6MZ	C5-N7	-3.08	1.33	1.39
30	a	2445	2MG	C5-N7	-3.07	1.33	1.39
30	a	2030	6MZ	C5-C4	-3.06	1.33	1.39
30	a	2251	OMG	C5-N7	-3.03	1.33	1.39
30	a	2030	6MZ	C4-N9	-3.00	1.31	1.37
30	a	1939	5MU	O4-C4	-3.00	1.17	1.23
30	a	1835	2MG	C5-C6	2.98	1.55	1.44
7	A	1519	MA6	C5-C4	-2.96	1.33	1.39
7	A	1518	MA6	C9-N6	2.93	1.52	1.45
7	A	1498	UR3	O2-C2	-2.92	1.17	1.22
30	a	2069	G7M	C4-N9	-2.92	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2552	OMU	C6-N1	2.92	1.45	1.38
30	a	2580	PSU	C6-C5	2.86	1.38	1.35
7	A	1519	MA6	C5-N7	-2.85	1.33	1.39
7	A	1516	2MG	C5-N7	-2.85	1.33	1.39
7	A	1516	2MG	C5-C6	2.82	1.54	1.44
30	a	2498	OMC	C5-C4	2.80	1.49	1.42
7	A	1519	MA6	C9-N6	2.78	1.52	1.45
7	A	1207	2MG	C5-C6	2.75	1.54	1.44
7	A	1402	4OC	C6-N1	2.75	1.44	1.38
30	a	2445	2MG	C6-N1	2.72	1.43	1.38
7	A	1498	UR3	C6-N1	2.70	1.44	1.38
7	A	1207	2MG	C5-N7	-2.65	1.33	1.39
30	a	2445	2MG	C5-C6	2.64	1.54	1.44
30	a	1618	6MZ	C5-C4	-2.63	1.34	1.39
30	a	2030	6MZ	C8-N9	-2.63	1.32	1.37
7	A	1518	MA6	C5-N7	-2.63	1.34	1.39
7	A	966	2MG	C5-N7	-2.60	1.34	1.39
7	A	966	2MG	C5-C6	2.59	1.54	1.44
30	a	1835	2MG	C5-N7	-2.57	1.34	1.39
30	a	1939	5MU	C2-N1	2.55	1.42	1.38
30	a	1835	2MG	O6-C6	-2.49	1.18	1.23
30	a	2445	2MG	O6-C6	-2.44	1.19	1.23
7	A	1518	MA6	C8-N9	-2.43	1.33	1.37
30	a	2580	PSU	O4'-C1'	-2.40	1.40	1.43
30	a	2251	OMG	C5-C6	2.40	1.53	1.44
7	A	527	G7M	C2-N1	2.39	1.43	1.37
30	a	745	1MG	O6-C6	-2.37	1.18	1.23
7	A	1516	2MG	O6-C6	-2.37	1.19	1.23
30	a	2552	OMU	C5-C4	2.35	1.48	1.43
7	A	527	G7M	C4-N9	-2.30	1.32	1.38
30	a	2251	OMG	C2-N1	2.29	1.43	1.37
7	A	1519	MA6	C8-N9	-2.29	1.33	1.37
30	a	2251	OMG	C6-N1	2.29	1.43	1.38
30	a	2069	G7M	C2-N1	2.28	1.43	1.37
30	a	1618	6MZ	C8-N9	-2.26	1.33	1.37
7	A	1207	2MG	O6-C6	-2.25	1.19	1.23
7	A	1519	MA6	C10-N6	2.17	1.50	1.45
30	a	2503	2MA	C8-N9	-2.17	1.33	1.37
7	A	527	G7M	C6-N1	2.14	1.42	1.38
7	A	1498	UR3	C4-N3	2.12	1.45	1.40
7	A	966	2MG	O6-C6	-2.12	1.19	1.23
30	a	2503	2MA	C5-C4	-2.10	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1498	UR3	C5-C4	2.04	1.49	1.43
30	a	1618	6MZ	C9-N6	2.03	1.48	1.45
30	a	2069	G7M	C6-N1	2.00	1.42	1.38

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1519	MA6	N1-C6-N6	-13.75	102.05	117.08
7	A	1518	MA6	N1-C6-N6	-11.92	104.05	117.08
30	a	1939	5MU	C5-C4-N3	10.68	124.43	115.31
30	a	747	5MU	C5-C4-N3	9.36	123.30	115.31
30	a	1939	5MU	C5-C6-N1	-9.07	114.01	123.34
30	a	747	5MU	C5-C6-N1	-8.98	114.10	123.34
30	a	2503	2MA	C5-C4-N3	-8.75	117.35	127.19
30	a	1835	2MG	C2-N3-C4	7.47	121.30	112.04
30	a	747	5MU	C4-N3-C2	-7.16	118.08	127.35
30	a	2445	2MG	C2-N3-C4	7.09	120.83	112.04
30	a	1939	5MU	C4-N3-C2	-7.07	118.20	127.35
7	A	1519	MA6	C5-C6-N6	6.87	137.27	125.30
7	A	1207	2MG	C2-N3-C4	6.84	120.52	112.04
30	a	2030	6MZ	C9-N6-C6	-6.76	117.05	122.87
7	A	966	2MG	C2-N3-C4	6.72	120.38	112.04
30	a	2030	6MZ	N1-C2-N3	-6.57	118.32	128.60
30	a	1618	6MZ	N1-C2-N3	-6.40	118.60	128.60
30	a	2503	2MA	N3-C4-N9	6.37	135.83	126.99
30	a	1835	2MG	C5-C4-N3	-6.21	118.38	128.46
30	a	1939	5MU	O4-C4-C5	-6.20	117.71	124.90
7	A	1519	MA6	C5-C4-N3	-6.08	118.82	126.75
7	A	1207	2MG	C5-C4-N3	-6.03	118.67	128.46
7	A	1516	2MG	C2-N3-C4	6.03	119.52	112.04
30	a	745	1MG	C5-C4-N3	-6.02	118.70	128.46
7	A	966	2MG	C5-C4-N3	-6.01	118.72	128.46
7	A	1498	UR3	C4-N3-C2	-5.91	119.00	124.56
30	a	2445	2MG	C5-C4-N3	-5.82	119.02	128.46
7	A	1518	MA6	C5-C6-N6	5.65	135.13	125.30
30	a	2030	6MZ	N9-C8-N7	-5.56	106.30	113.91
7	A	1518	MA6	C5-C4-N3	-5.55	119.51	126.75
30	a	955	PSU	N1-C2-N3	5.48	121.33	115.13
7	A	1518	MA6	N1-C2-N3	-5.47	120.04	128.60
30	a	955	PSU	C4-N3-C2	-5.47	118.46	126.34
30	a	2552	OMU	C4-N3-C2	-5.43	119.42	126.58
7	A	1519	MA6	N1-C2-N3	-5.31	120.29	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2445	2MG	C2-N1-C6	-5.29	118.39	124.48
30	a	747	5MU	O4-C4-C5	-5.25	118.82	124.90
30	a	2503	2MA	C4-N9-C1'	-5.15	114.32	126.59
30	a	1835	2MG	C2-N1-C6	-5.09	118.62	124.48
30	a	747	5MU	N3-C2-N1	5.06	121.60	114.89
30	a	2504	PSU	N1-C2-N3	5.05	120.85	115.13
30	a	2504	PSU	C4-N3-C2	-5.04	119.07	126.34
7	A	1516	2MG	C5-C4-N3	-5.01	120.33	128.46
7	A	1516	2MG	C1'-N9-C4	-5.00	111.65	126.50
30	a	745	1MG	C1'-N9-C4	-4.99	111.67	126.50
30	a	1911	PSU	C4-N3-C2	-4.93	119.23	126.34
30	a	2503	2MA	C1'-N9-C8	4.92	138.25	127.14
30	a	1618	6MZ	C9-N6-C6	-4.91	118.64	122.87
30	a	2457	PSU	N1-C2-N3	4.90	120.69	115.13
30	a	2604	PSU	N1-C2-N3	4.89	120.67	115.13
30	a	1618	6MZ	C5-C4-N3	-4.88	120.38	126.75
30	a	747	5MU	C6-C5-C4	4.87	122.10	118.03
7	A	966	2MG	C2-N1-C6	-4.85	118.89	124.48
30	a	2457	PSU	C4-N3-C2	-4.84	119.37	126.34
7	A	1518	MA6	N3-C4-N9	4.82	135.03	127.08
30	a	1911	PSU	N1-C2-N3	4.81	120.58	115.13
7	A	1207	2MG	C2-N1-C6	-4.81	118.95	124.48
7	A	1518	MA6	N9-C8-N7	-4.79	107.37	113.91
30	a	2605	PSU	N1-C2-N3	4.73	120.49	115.13
30	a	2580	PSU	C4-N3-C2	-4.63	119.67	126.34
7	A	516	PSU	C4-N3-C2	-4.63	119.67	126.34
30	a	745	1MG	C1'-N9-C8	4.62	139.86	126.70
7	A	527	G7M	C2-N3-C4	4.62	120.53	112.30
30	a	1618	6MZ	N9-C8-N7	-4.57	107.66	113.91
30	a	746	PSU	C4-N3-C2	-4.56	119.76	126.34
30	a	1917	PSU	C4-N3-C2	-4.50	119.86	126.34
7	A	1516	2MG	C1'-N9-C8	4.45	139.38	126.70
30	a	2552	OMU	C5-C4-N3	4.45	121.50	114.84
30	a	746	PSU	N1-C2-N3	4.40	120.12	115.13
30	a	2604	PSU	C4-N3-C2	-4.40	120.00	126.34
7	A	1519	MA6	N9-C8-N7	-4.39	107.91	113.91
7	A	516	PSU	N1-C2-N3	4.35	120.06	115.13
7	A	966	2MG	N9-C4-N3	4.34	134.66	125.94
30	a	1917	PSU	N1-C2-N3	4.32	120.03	115.13
7	A	1516	2MG	C2-N1-C6	-4.31	119.52	124.48
7	A	1207	2MG	N9-C4-N3	4.29	134.55	125.94
30	a	745	1MG	N9-C4-N3	4.27	134.50	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1519	MA6	N3-C4-N9	4.26	134.10	127.08
30	a	2605	PSU	C4-N3-C2	-4.24	120.22	126.34
7	A	527	G7M	C5-C6-N1	4.23	120.61	111.79
30	a	2251	OMG	C2-N3-C4	4.20	119.79	112.30
30	a	2069	G7M	C2-N3-C4	4.18	119.75	112.30
30	a	2580	PSU	N1-C2-N3	4.18	119.87	115.13
30	a	2251	OMG	N9-C8-N7	-4.17	105.53	113.39
7	A	527	G7M	C5-C4-N3	-4.03	120.43	128.15
7	A	1519	MA6	C2-N3-C4	4.01	121.23	111.75
30	a	2445	2MG	C1'-N9-C4	-3.99	114.66	126.50
7	A	967	5MC	C5-C6-N1	-3.97	119.25	123.34
30	a	2445	2MG	N9-C4-N3	3.97	133.90	125.94
30	a	1618	6MZ	C2-N3-C4	3.96	121.11	111.75
7	A	527	G7M	O6-C6-C5	-3.93	119.20	128.06
30	a	1939	5MU	N3-C2-N1	3.92	120.10	114.89
7	A	1519	MA6	C4-C5-C6	3.92	120.26	115.88
7	A	1518	MA6	C4-N9-C8	3.89	109.94	105.73
7	A	1207	2MG	C1'-N9-C4	-3.88	114.96	126.50
7	A	1518	MA6	C4-C5-C6	3.83	120.16	115.88
30	a	1835	2MG	N9-C4-N3	3.82	133.62	125.94
30	a	2030	6MZ	C4-N9-C8	3.81	109.86	105.73
30	a	2030	6MZ	C5-C4-N3	-3.81	121.78	126.75
30	a	745	1MG	C2-N3-C4	3.80	120.52	111.98
7	A	1407	5MC	C5-C6-N1	-3.77	119.46	123.34
30	a	1618	6MZ	C5-N7-C8	3.70	108.77	103.51
30	a	2069	G7M	C5-C6-N1	3.68	119.47	111.79
30	a	2030	6MZ	C2-N3-C4	3.67	120.42	111.75
7	A	1518	MA6	C4-N9-C1'	-3.64	117.92	126.59
7	A	1518	MA6	C2-N3-C4	3.60	120.25	111.75
30	a	1962	5MC	C5-C6-N1	-3.59	119.65	123.34
7	A	1402	4OC	C6-C5-C4	3.53	121.28	116.96
30	a	2030	6MZ	C5-N7-C8	3.52	108.50	103.51
30	a	2069	G7M	C5-C4-N3	-3.50	121.44	128.15
30	a	2445	2MG	C1'-N9-C8	3.49	136.63	126.70
30	a	2503	2MA	N9-C8-N7	-3.47	109.17	113.91
7	A	527	G7M	CN7-N7-C5	3.43	131.03	126.77
30	a	2552	OMU	N3-C2-N1	3.42	119.42	114.89
7	A	1207	2MG	C1'-N9-C8	3.39	136.35	126.70
7	A	966	2MG	C1'-N9-C4	-3.36	116.52	126.50
30	a	2445	2MG	O6-C6-C5	-3.35	117.71	126.60
7	A	1516	2MG	N9-C8-N7	-3.35	107.08	113.39
7	A	527	G7M	C2-N1-C6	-3.31	119.06	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2445	2MG	N9-C8-N7	-3.28	107.22	113.39
30	a	2457	PSU	O2-C2-N1	-3.22	119.25	122.79
30	a	1939	5MU	C6-C5-C4	3.19	120.70	118.03
30	a	2503	2MA	C6-C5-C4	3.18	121.46	117.18
7	A	1518	MA6	C2-N1-C6	3.16	119.21	111.75
30	a	2251	OMG	C5-C4-N3	-3.08	123.46	128.46
30	a	2503	2MA	C5-N7-C8	3.08	107.89	103.51
30	a	747	5MU	O2-C2-N1	-3.08	118.69	122.79
7	A	1519	MA6	C5-N7-C8	3.07	107.87	103.51
7	A	1207	2MG	N9-C8-N7	-3.06	107.63	113.39
30	a	2251	OMG	C1'-N9-C8	-3.05	118.02	126.70
30	a	2251	OMG	C6-C5-N7	3.03	135.89	130.25
30	a	745	1MG	N9-C8-N7	-3.03	107.69	113.39
30	a	2503	2MA	N3-C2-N1	-3.00	120.20	125.72
30	a	1835	2MG	CM2-N2-C2	-3.00	117.23	123.86
7	A	1516	2MG	N9-C4-N3	2.99	131.94	125.94
7	A	1519	MA6	C4-N9-C1'	-2.96	119.53	126.59
7	A	1519	MA6	C2-N1-C6	2.96	118.74	111.75
30	a	745	1MG	C2-N1-C6	-2.96	118.54	120.95
30	a	747	5MU	C5M-C5-C6	-2.95	118.91	122.85
30	a	2069	G7M	CN7-N7-C5	2.92	130.40	126.77
30	a	1939	5MU	O2-C2-N1	-2.92	118.91	122.79
7	A	1207	2MG	C5-C6-N1	2.92	120.60	113.19
30	a	1835	2MG	C1'-N9-C4	-2.91	117.84	126.50
7	A	966	2MG	C5-C6-N1	2.91	120.57	113.19
7	A	1518	MA6	C5-N7-C8	2.89	107.61	103.51
7	A	966	2MG	C1'-N9-C8	2.86	134.84	126.70
30	a	2069	G7M	O6-C6-C5	-2.85	121.63	128.06
30	a	1835	2MG	C5-C6-N1	2.84	120.39	113.19
30	a	2251	OMG	C5-C6-N1	2.82	120.35	113.19
7	A	527	G7M	CN7-N7-C8	-2.77	120.56	124.84
30	a	1835	2MG	C1'-N9-C8	2.77	134.59	126.70
7	A	966	2MG	N9-C8-N7	-2.77	108.18	113.39
30	a	1618	6MZ	C4-C5-N7	-2.75	107.27	110.62
30	a	2445	2MG	C8-N7-C5	2.74	109.20	104.24
30	a	2445	2MG	C5-C6-N1	2.72	120.09	113.19
30	a	745	1MG	C5-C6-N1	2.67	120.07	114.91
7	A	527	G7M	N9-C4-N3	2.66	131.28	125.94
30	a	2030	6MZ	C6-C5-N7	2.65	135.26	132.39
7	A	1207	2MG	O6-C6-C5	-2.64	119.60	126.60
30	a	2604	PSU	O2-C2-N1	-2.63	119.89	122.79
30	a	2030	6MZ	C5-C6-N1	2.63	121.00	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2580	PSU	C6-C5-C4	2.62	120.03	118.20
7	A	1519	MA6	C4-N9-C8	2.62	108.56	105.73
7	A	966	2MG	O6-C6-C5	-2.61	119.66	126.60
7	A	1516	2MG	C5-C6-N1	2.61	119.82	113.19
30	a	2605	PSU	C6-N1-C2	-2.60	120.02	122.68
30	a	1835	2MG	N9-C8-N7	-2.59	108.51	113.39
30	a	2069	G7M	C2-N1-C6	-2.58	120.39	125.10
30	a	2251	OMG	N2-C2-N1	2.58	122.21	116.71
30	a	2251	OMG	C2-N1-C6	-2.53	120.49	125.10
30	a	1618	6MZ	N3-C4-N9	2.52	131.23	127.08
30	a	2251	OMG	C8-N7-C5	2.51	108.79	104.24
7	A	1407	5MC	C5-C4-N3	-2.51	118.97	121.67
30	a	2457	PSU	C6-C5-C4	2.50	119.94	118.20
7	A	1516	2MG	C8-N7-C5	2.43	108.64	104.24
30	a	2580	PSU	O4'-C1'-C2'	2.41	108.54	105.14
30	a	2030	6MZ	C4-C5-N7	-2.39	107.70	110.62
7	A	966	2MG	CM2-N2-C2	-2.38	118.60	123.86
7	A	1207	2MG	N1-C2-N3	-2.38	120.27	123.95
30	a	1917	PSU	O2-C2-N1	-2.38	120.17	122.79
30	a	2580	PSU	O2-C2-N1	-2.38	120.18	122.79
30	a	1911	PSU	O2-C2-N1	-2.36	120.19	122.79
30	a	745	1MG	C8-N7-C5	2.33	108.47	104.24
30	a	2552	OMU	O4-C4-C5	-2.32	121.08	125.16
30	a	2251	OMG	N1-C2-N3	-2.30	119.03	123.32
30	a	1939	5MU	C5M-C5-C6	-2.30	119.78	122.85
30	a	1835	2MG	C8-N7-C5	2.29	108.39	104.24
7	A	1407	5MC	CM5-C5-C6	-2.29	119.79	122.85
7	A	1516	2MG	O6-C6-C5	-2.28	120.56	126.60
30	a	2604	PSU	C6-N1-C2	-2.27	120.37	122.68
30	a	746	PSU	O2-C2-N3	-2.26	117.56	121.82
7	A	516	PSU	O2-C2-N1	-2.26	120.31	122.79
30	a	2498	OMC	C2'-C1'-N1	-2.25	109.86	114.22
30	a	2069	G7M	CN7-N7-C8	-2.24	121.38	124.84
30	a	2445	2MG	N1-C2-N3	-2.24	120.49	123.95
30	a	1618	6MZ	C5-C4-N9	2.24	108.39	105.78
7	A	1518	MA6	C1'-N9-C8	2.22	132.14	127.14
30	a	2503	2MA	CM2-C2-N3	2.21	120.60	117.15
30	a	2251	OMG	C4-C5-N7	-2.21	107.23	110.72
30	a	2605	PSU	O2-C2-N3	-2.20	117.67	121.82
7	A	516	PSU	O4'-C1'-C2'	2.19	108.24	105.14
30	a	1911	PSU	C6-N1-C2	-2.19	120.44	122.68
30	a	2503	2MA	N6-C6-N1	2.17	120.10	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	516	PSU	C6-N1-C2	-2.14	120.50	122.68
7	A	967	5MC	CM5-C5-C6	-2.14	120.00	122.85
7	A	1207	2MG	C8-N7-C5	2.13	108.09	104.24
30	a	2030	6MZ	N3-C4-N9	2.13	130.59	127.08
30	a	955	PSU	O2-C2-N3	-2.12	117.81	121.82
30	a	2251	OMG	C8-N9-C4	2.12	110.08	106.05
7	A	966	2MG	N1-C2-N3	-2.10	120.70	123.95
7	A	1402	4OC	C5-C6-N1	-2.09	118.31	121.81
30	a	2069	G7M	N9-C4-N3	2.09	130.13	125.94
30	a	1835	2MG	N1-C2-N3	-2.08	120.74	123.95
7	A	1516	2MG	N1-C2-N3	-2.08	120.74	123.95
7	A	527	G7M	N9-C8-N7	-2.06	107.13	112.21
30	a	1618	6MZ	C5-C6-N1	2.05	120.39	118.20
7	A	1519	MA6	C1'-N9-C8	2.05	131.76	127.14
30	a	1835	2MG	O6-C6-C5	-2.04	121.19	126.60
30	a	2251	OMG	O6-C6-C5	-2.03	121.21	126.60
7	A	966	2MG	C8-N7-C5	2.02	107.90	104.24
30	a	746	PSU	C5-C4-N3	2.02	121.15	116.58
30	a	1618	6MZ	C4-N9-C8	2.01	107.90	105.73
7	A	527	G7M	N2-C2-N1	2.00	120.98	116.71
30	a	1835	2MG	C4-C5-N7	-2.00	107.55	110.72

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	a	746	PSU	C2'-C1'-C5-C4
30	a	746	PSU	O4'-C1'-C5-C6
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2030	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	NE2-CD-CG-CB
33	d	150	MEQ	OE1-CD-CG-CB
7	A	1519	MA6	O4'-C4'-C5'-O5'
7	A	1519	MA6	C3'-C4'-C5'-O5'
30	a	2552	OMU	C3'-C2'-O2'-CM2
30	a	2069	G7M	C4'-C5'-O5'-P
30	a	747	5MU	C3'-C4'-C5'-O5'
30	a	1911	PSU	C3'-C4'-C5'-O5'
30	a	746	PSU	O4'-C1'-C5-C4
30	a	2503	2MA	C4'-C5'-O5'-P
30	a	2251	OMG	C1'-C2'-O2'-CM2
30	a	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
30	a	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1207	2MG	1	0
30	a	2251	OMG	1	0
33	d	150	MEQ	2	0
30	a	2503	2MA	1	0
30	a	1939	5MU	1	0
30	a	2552	OMU	1	0
7	A	966	2MG	1	0
30	a	747	5MU	3	0
30	a	2030	6MZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 311 ligands modelled in this entry, 310 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	T8B	A	1689	57	48,48,48	0.80	2 (4%)	63,71,71	1.07	2 (3%)

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
58	T8B	A	1689	57	-	2/26/26/26	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	A	1689	T8B	C10-C11	3.91	1.38	1.34
58	A	1689	T8B	O1-C1	-2.19	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	A	1689	T8B	C21-C23-C24	-5.27	118.89	125.03
58	A	1689	T8B	O7-C16-C15	-2.61	116.08	121.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

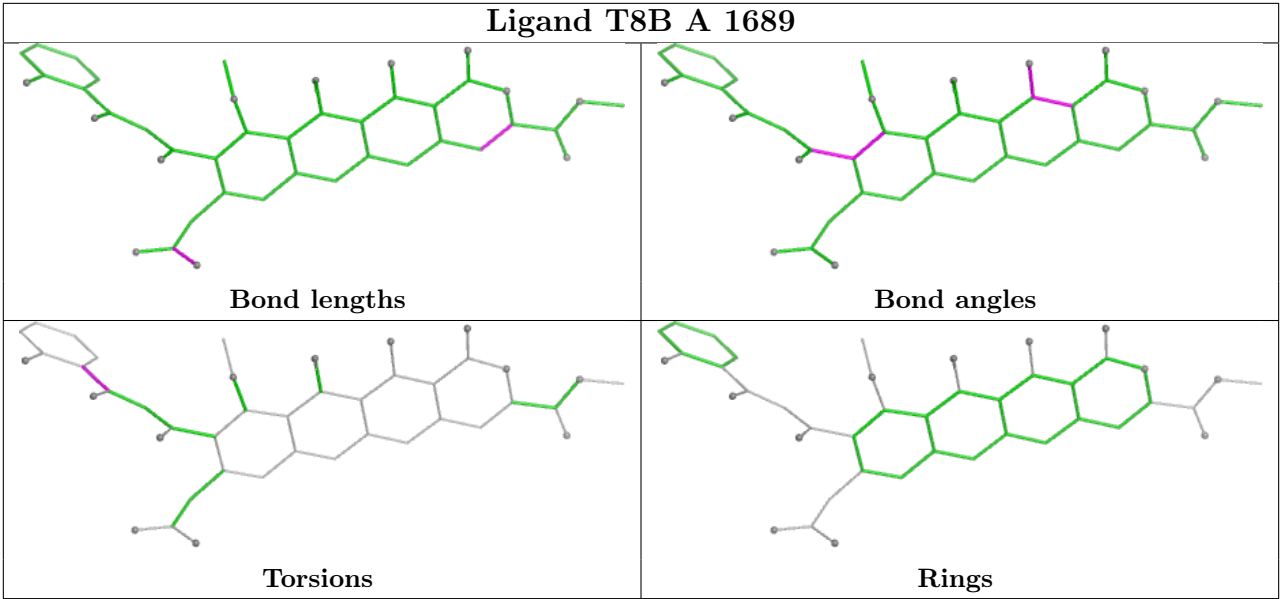
Mol	Chain	Res	Type	Atoms
58	A	1689	T8B	O11-C26-C27-C32
58	A	1689	T8B	C25-C26-C27-C28

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	A	1689	T8B	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	81:ARG	C	82:MET	N	2.56

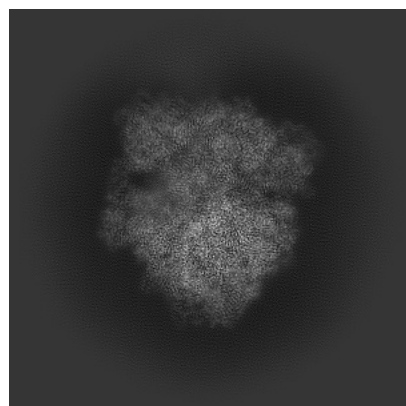
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15712. These allow visual inspection of the internal detail of the map and identification of artifacts.

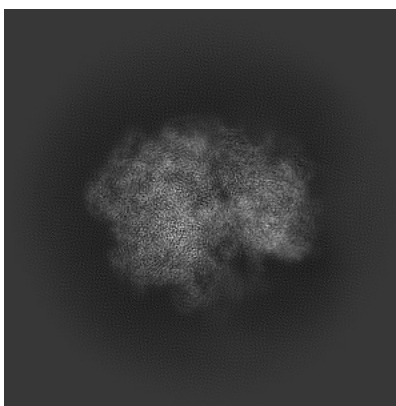
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

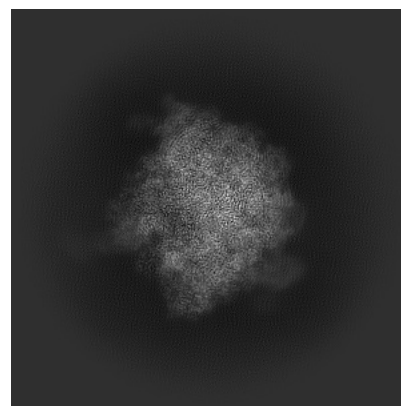
6.1.1 Primary map



X

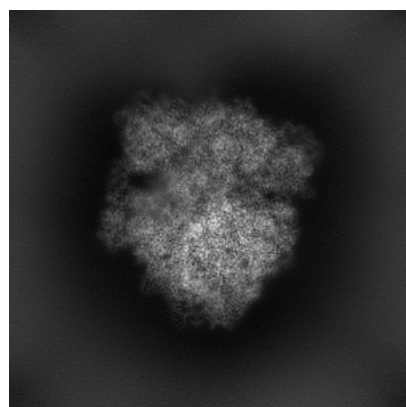


Y

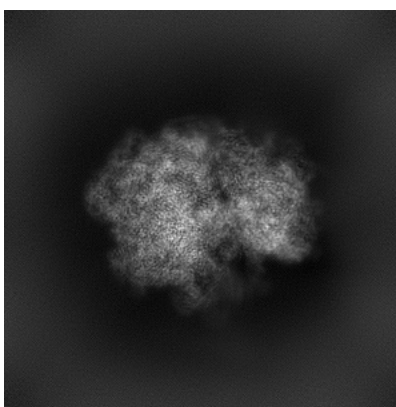


Z

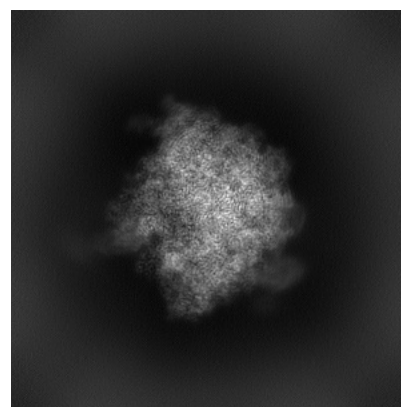
6.1.2 Raw map



X



Y

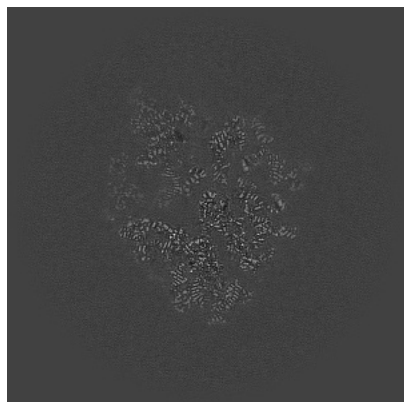


Z

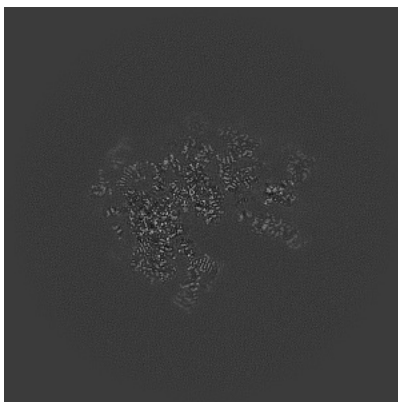
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

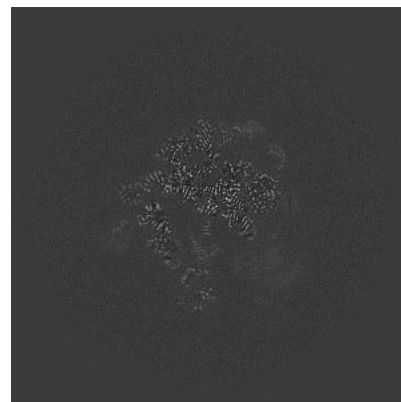
6.2.1 Primary map



X Index: 256

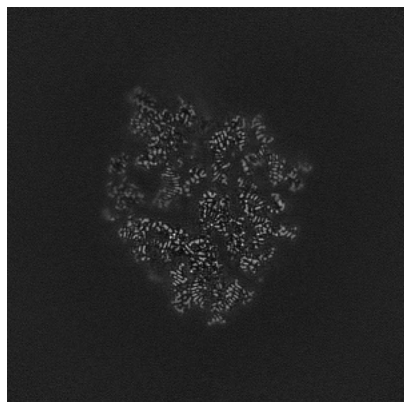


Y Index: 256

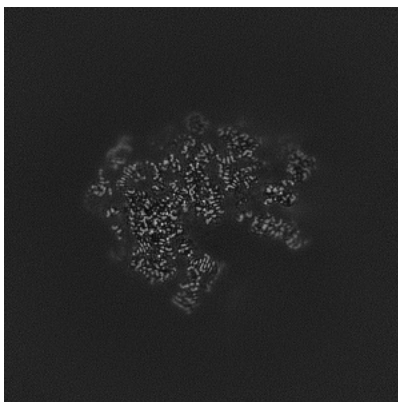


Z Index: 256

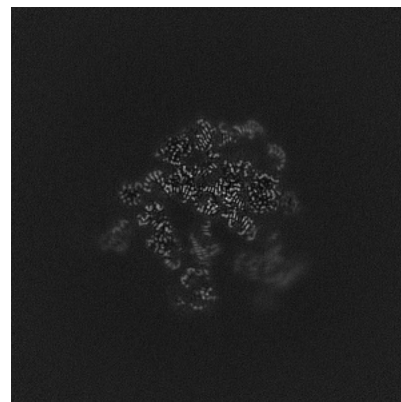
6.2.2 Raw map



X Index: 256



Y Index: 256

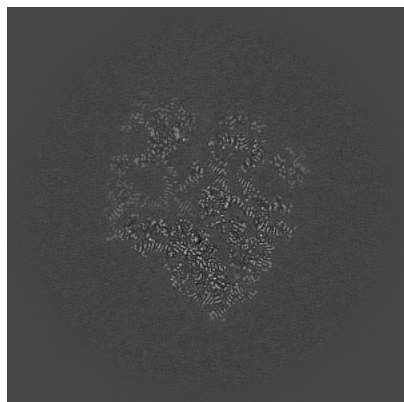


Z Index: 256

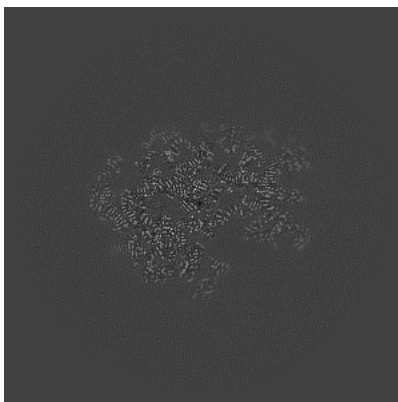
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

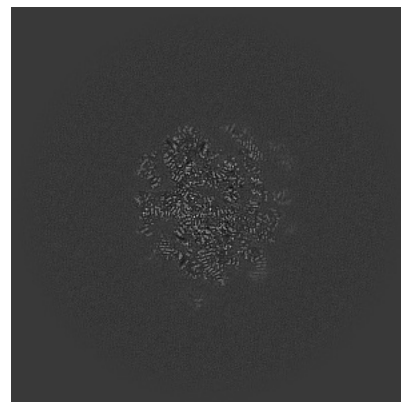
6.3.1 Primary map



X Index: 250

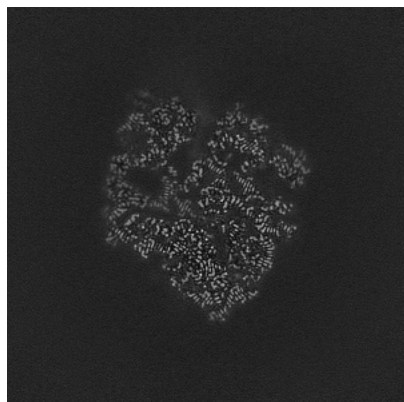


Y Index: 270

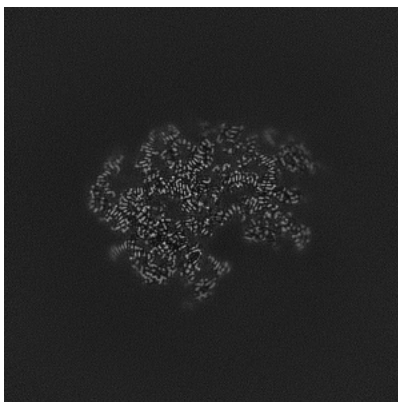


Z Index: 205

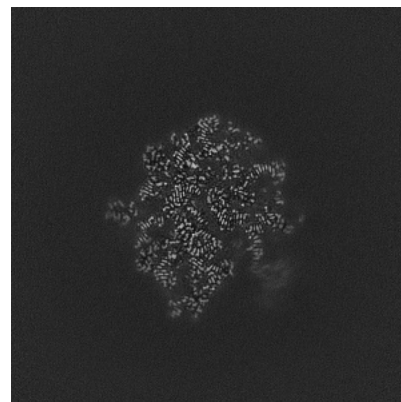
6.3.2 Raw map



X Index: 249



Y Index: 268

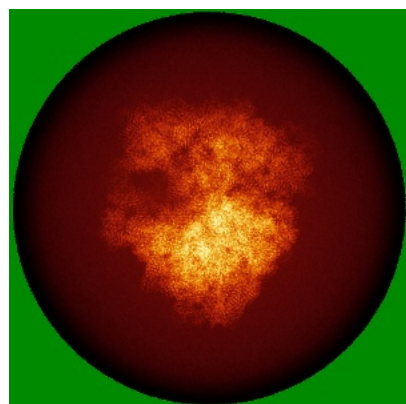


Z Index: 228

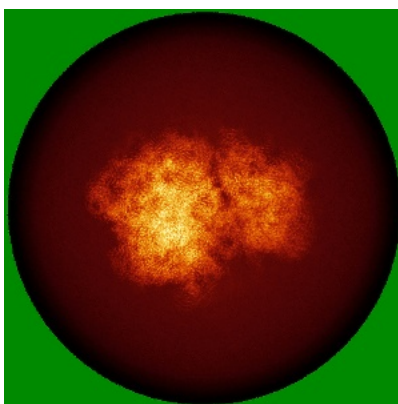
The images above show the largest variance slices of the map in three orthogonal directions.

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

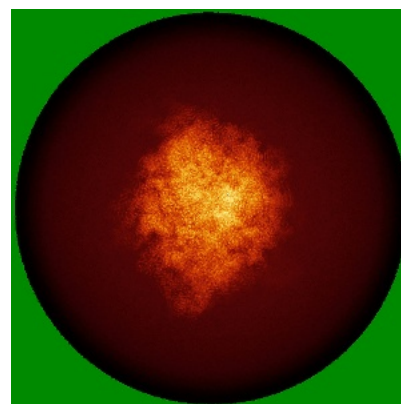
6.4.1 Primary map



X

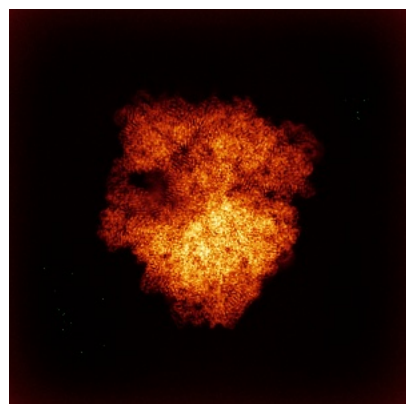


Y

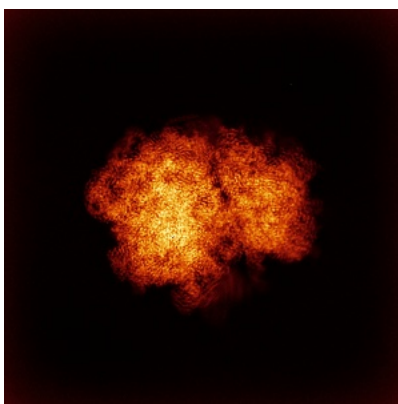


Z

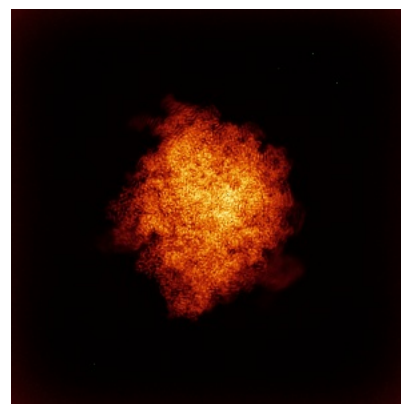
6.4.2 Raw map



X



Y

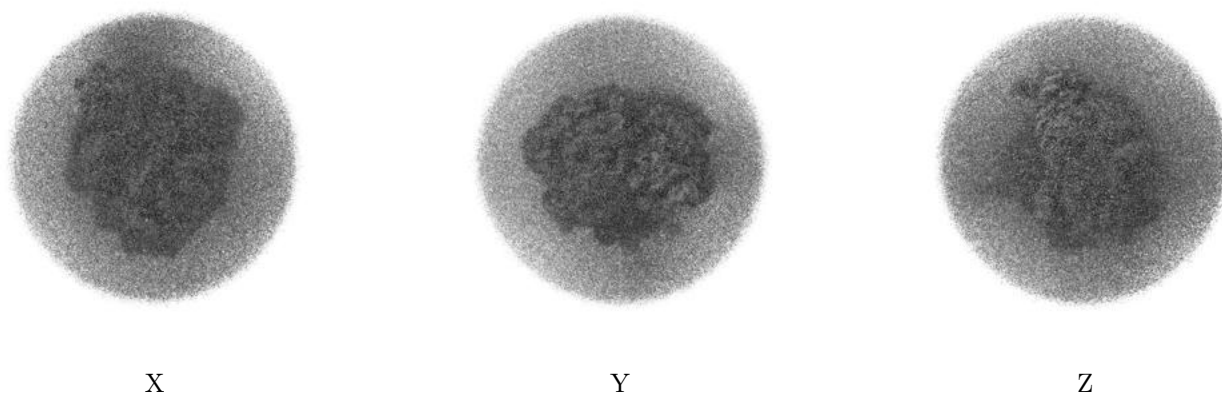


Z

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

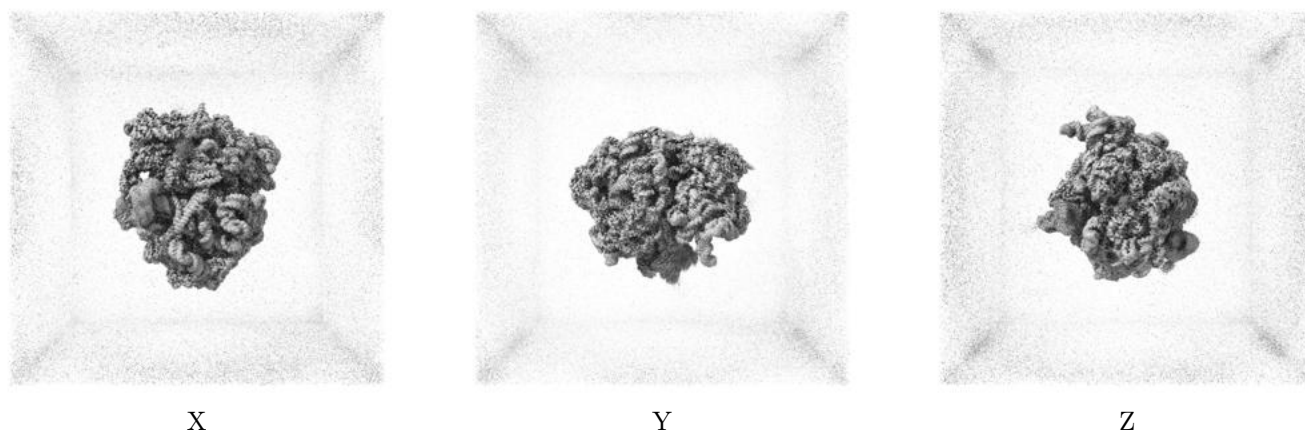
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

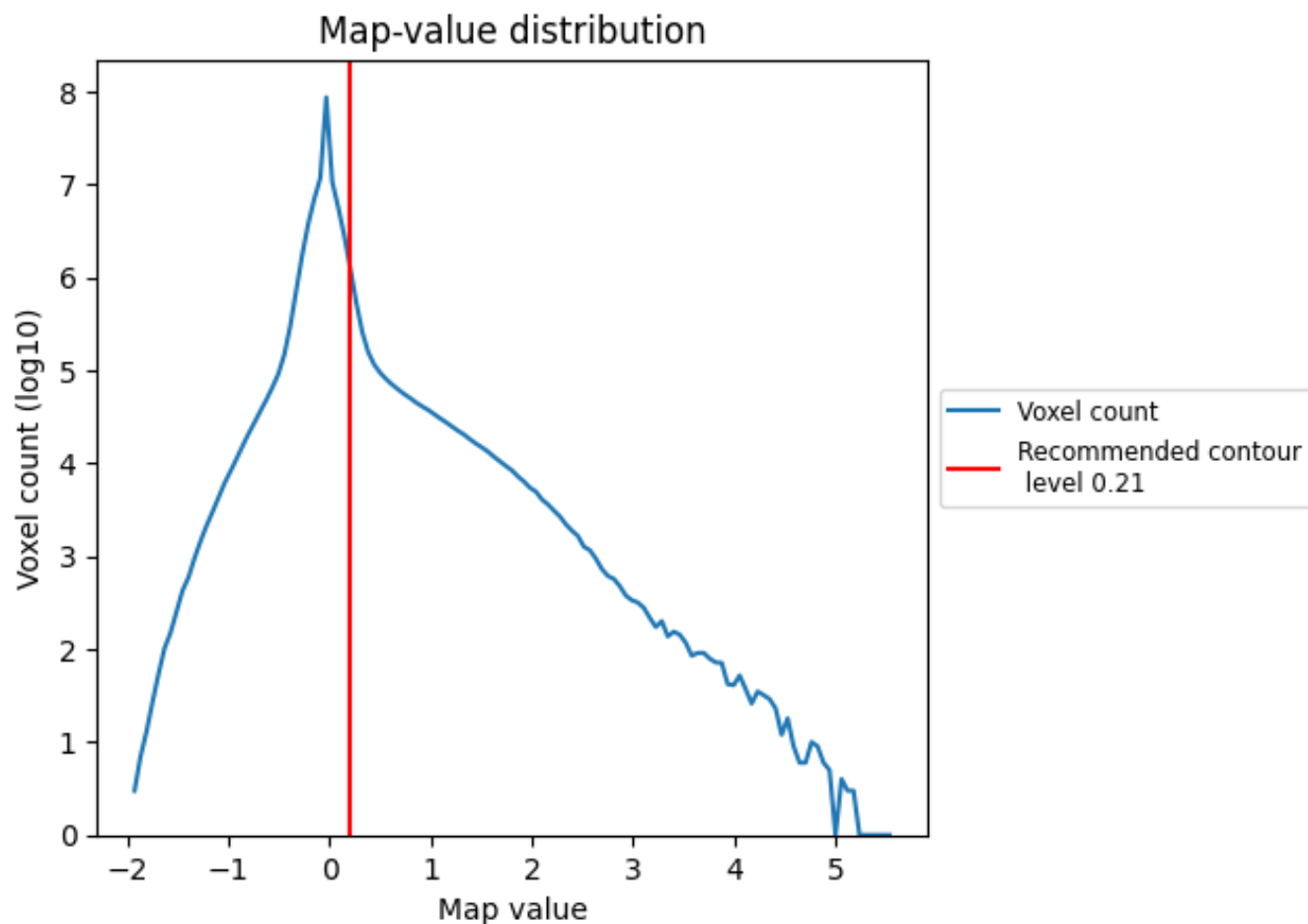
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

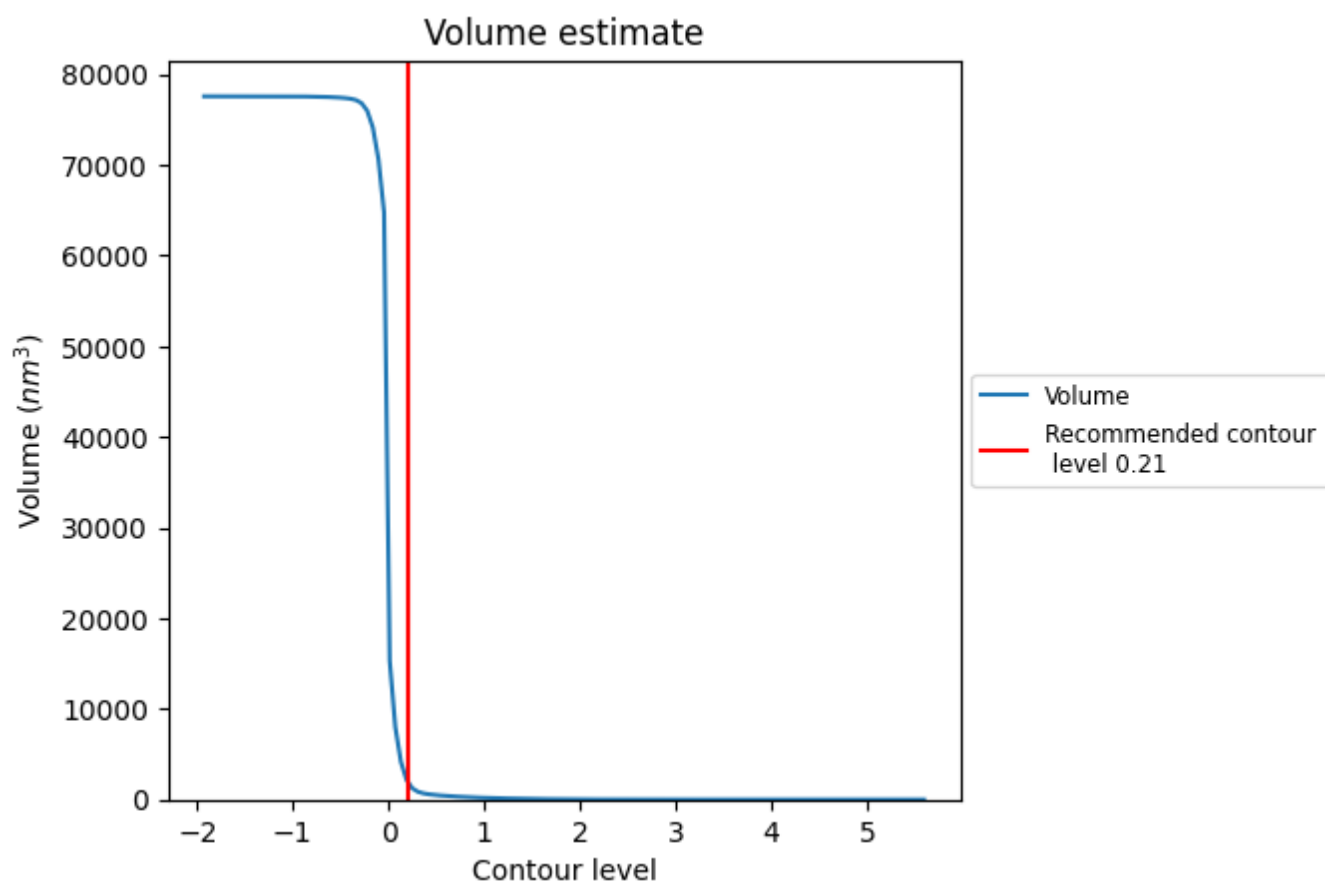
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

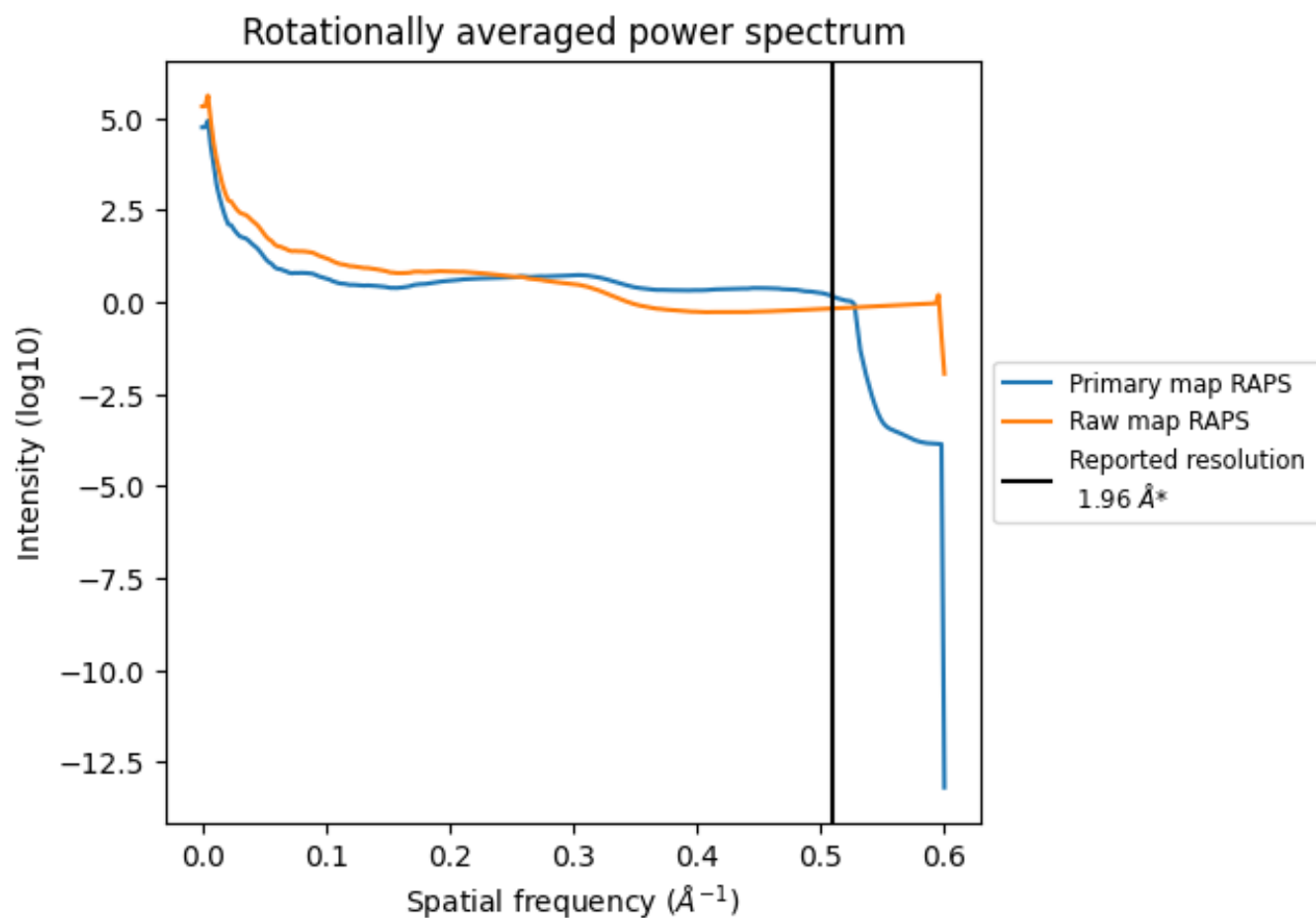
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1845 nm³; this corresponds to an approximate mass of 1666 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 ⓘ

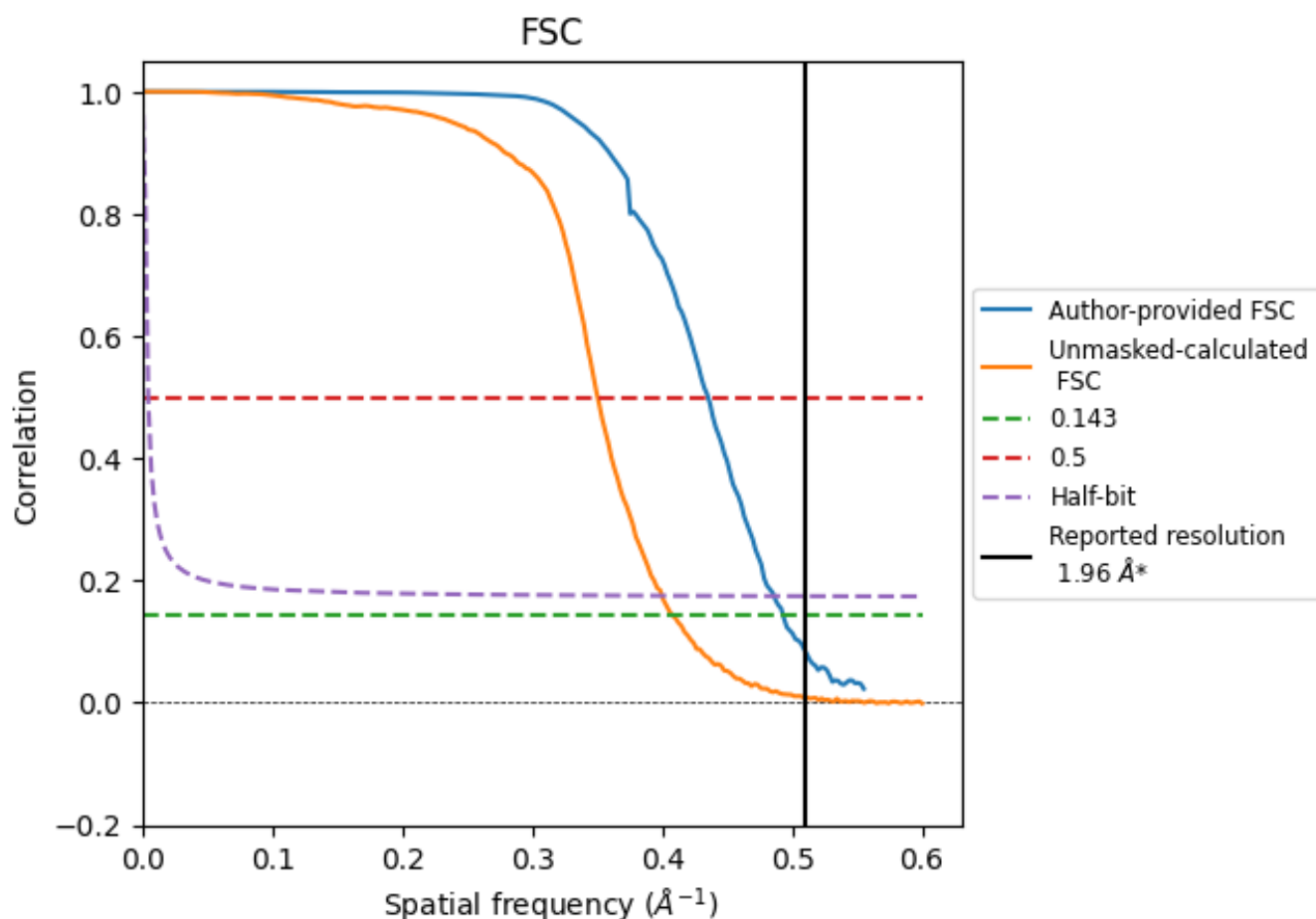


*Reported resolution corresponds to spatial frequency of 0.510 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.510 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

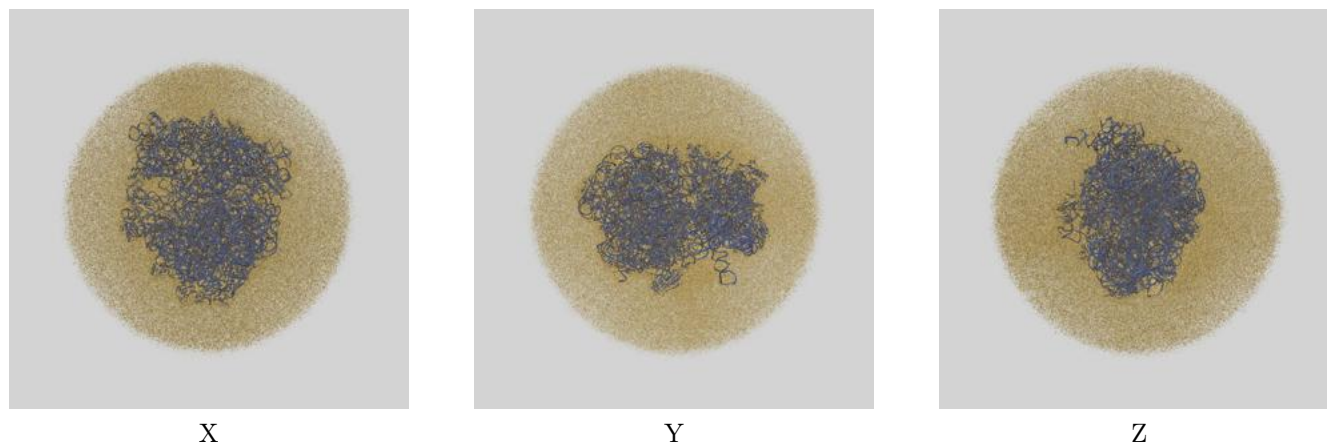
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.96	-	-
Author-provided FSC curve	2.03	2.30	2.06
Unmasked-calculated*	2.45	2.85	2.50

*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 2.45 differs from the reported value 1.96 by more than 10 %

9 Map-model fit [i](#)

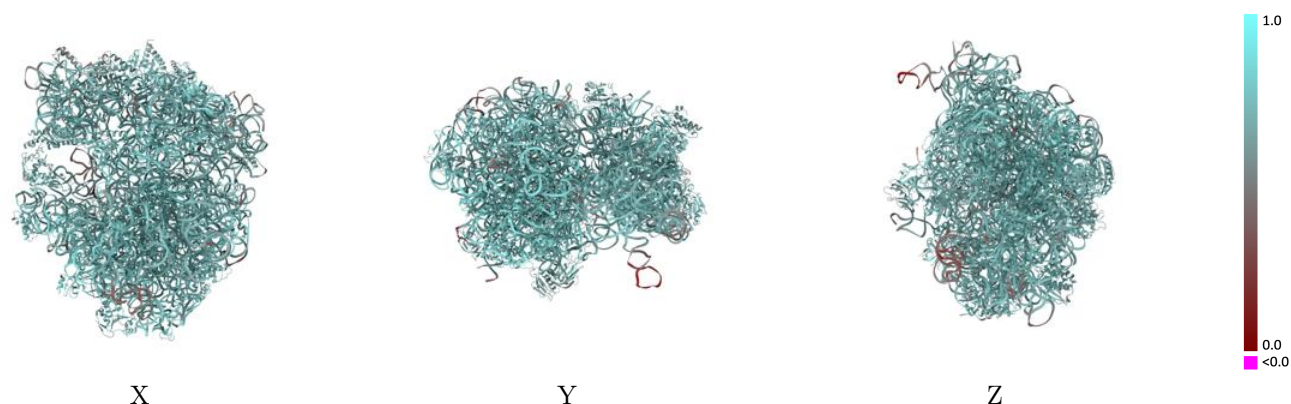
This section contains information regarding the fit between EMDB map EMD-15712 and PDB model 8AYE. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



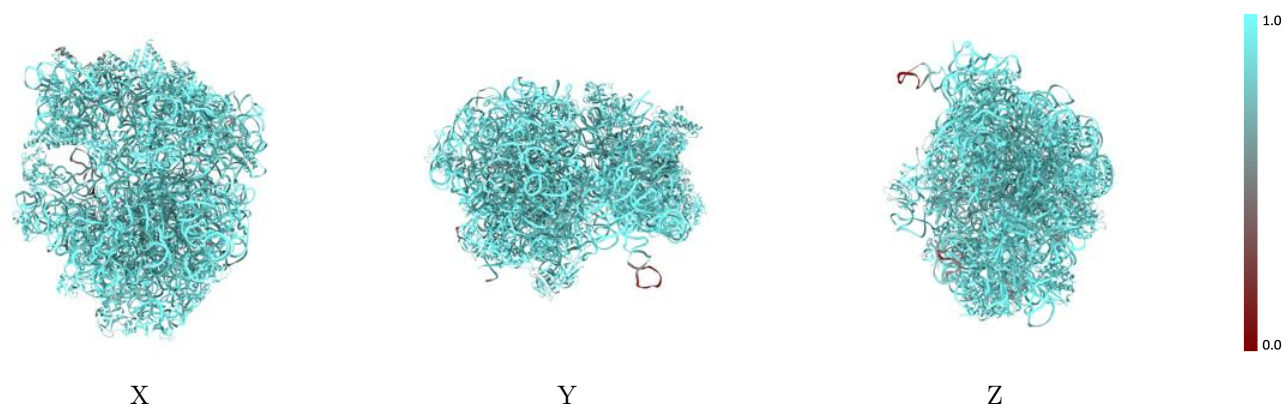
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



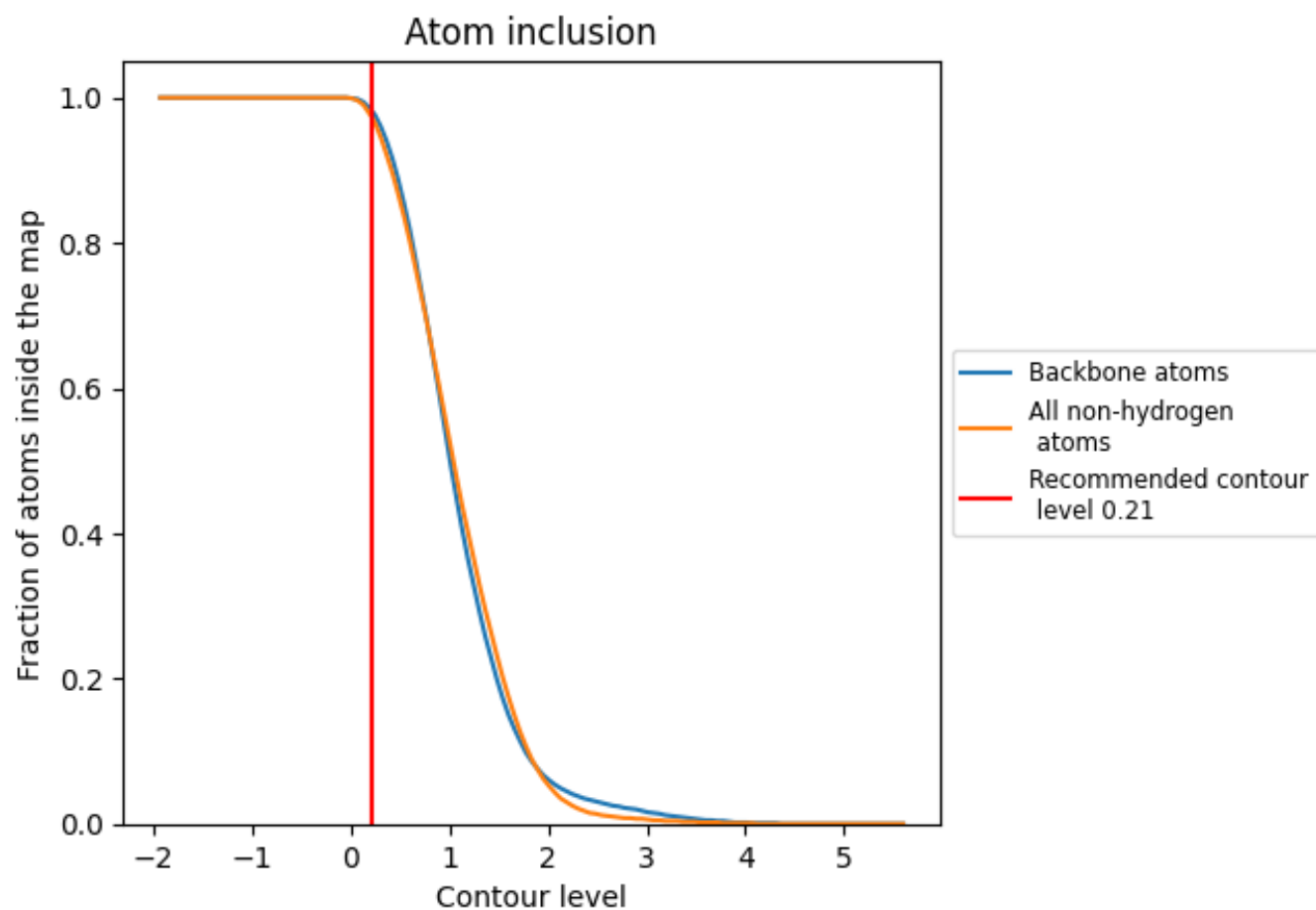
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.7340
0	 0.9830	 0.7670
1	 0.9920	 0.8020
2	 1.0000	 0.8050
3	 0.9930	 0.7800
4	 0.8390	 0.6080
5	 0.7860	 0.6560
A	 0.9710	 0.7100
B	 0.9240	 0.6760
C	 0.9610	 0.7160
D	 0.9570	 0.7160
E	 0.9800	 0.7650
F	 0.9490	 0.6870
G	 0.9420	 0.6930
H	 0.9770	 0.7630
I	 0.9500	 0.6980
J	 0.8400	 0.6310
K	 0.9660	 0.7280
L	 0.9760	 0.7520
M	 0.9640	 0.7110
N	 0.9690	 0.7190
O	 0.9770	 0.7490
P	 0.9570	 0.7210
Q	 0.9550	 0.7000
R	 0.9500	 0.7160
S	 0.9290	 0.6770
T	 0.9740	 0.7370
U	 0.8710	 0.6500
X	 0.9620	 0.7100
Z	 0.9360	 0.6540
a	 0.9850	 0.7480
b	 0.9840	 0.7100
c	 0.9950	 0.7970
d	 0.9850	 0.7890
e	 0.9630	 0.7510



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Chain	Atom inclusion	Q-score
f	 0.9590	 0.6970
g	 0.9290	 0.6630
h	 0.9400	 0.6800
i	 0.9890	 0.7860
j	 0.9920	 0.7910
k	 0.9820	 0.7750
l	 0.9910	 0.7800
m	 1.0000	 0.8040
n	 0.9690	 0.7320
o	 0.9820	 0.7780
p	 0.9980	 0.8040
q	 0.9770	 0.7670
r	 0.9840	 0.7870
s	 0.9630	 0.7490
t	 0.9640	 0.7200
u	 0.9630	 0.7330
v	 0.9830	 0.7820
w	 0.9920	 0.7810
x	 0.9410	 0.7130
y	 0.9790	 0.7810
z	 0.9770	 0.7820