



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 11:19 am BST

PDB ID : 5MDW / pdb_00005mdw
EMDB ID : EMD-3490
Title : Structure of ArfA(A18T) and RF2 bound to the 70S ribosome (pre-accommodated state)
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2016-11-13
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

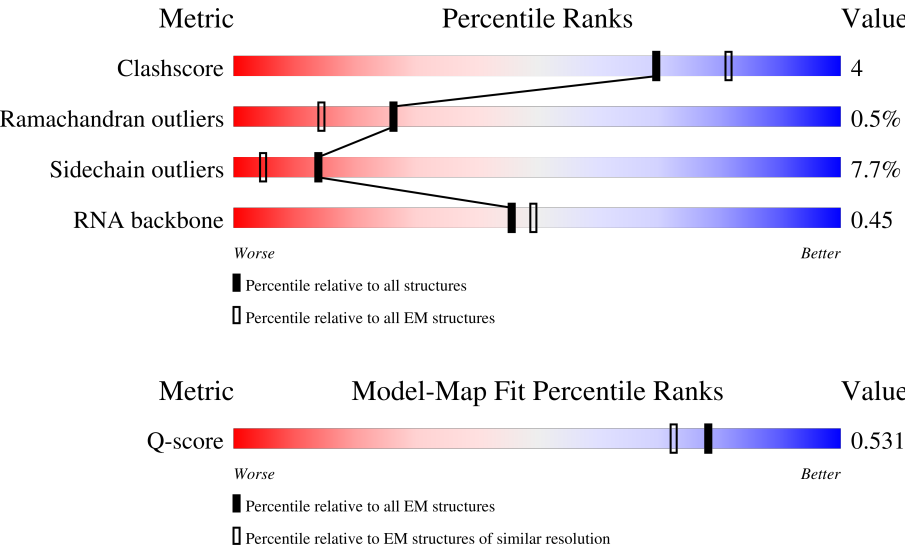
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.06 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.



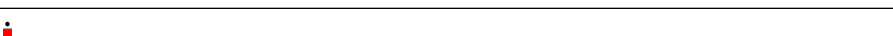
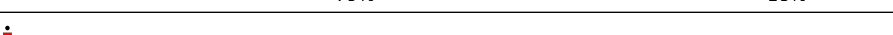
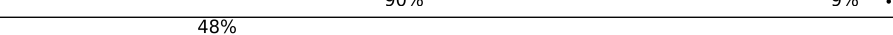
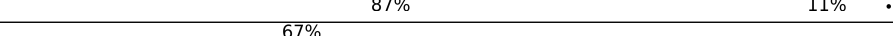
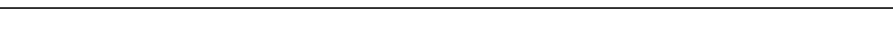
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13976 (2.56 - 3.56)

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	1	2904	70% 25% . .
2	2	1534	68% 27% . .
3	3	120	79% 19% .

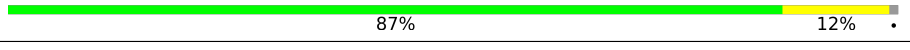
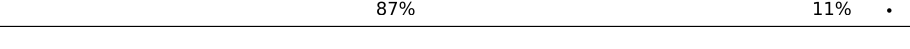
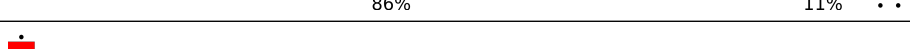
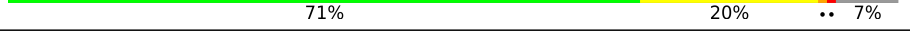
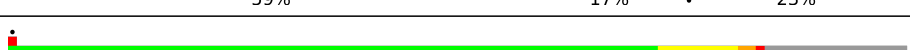
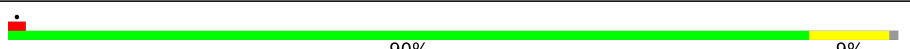
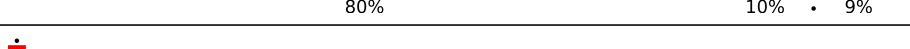
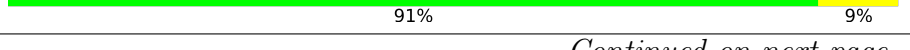
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Mol	Chain	Length	Quality of chain
4	4	18	
5	5	78	
6	6	61	
7	7	365	
8	B	273	
9	C	209	
10	D	201	
11	E	179	
12	F	177	
13	G	149	
14	H	165	
15	I	142	
16	J	142	
17	K	123	
18	L	144	
19	M	136	
20	N	127	
21	O	117	
22	P	115	
23	Q	118	
24	R	103	
25	S	110	
26	T	100	
27	U	104	
28	V	94	

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Mol	Chain	Length	Quality of chain
29	W	85	
30	X	78	
31	Y	63	
32	Z	59	
33	a	70	
34	b	57	
35	c	55	
36	d	46	
37	e	65	
38	f	38	
39	g	241	
40	h	233	
41	i	206	
42	j	167	
43	k	135	
44	l	179	
45	m	130	
46	n	130	
47	o	103	
48	p	129	
49	q	124	
50	r	118	
51	s	101	
52	t	89	
53	u	82	

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Mol	Chain	Length	Quality of chain
54	v	84	81%13%5%
55	w	75	73%13%12%
56	x	92	76%13%10%
57	y	87	87%10%..
58	z	71	11%83%14%..

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 149607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	887	A	U	conflict	GB 802133627

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	5	Total	C	N	O	P	0	0
			109	49	22	33	5		

- Molecule 5 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace	
5	5	76	Total	C	N	O	P	S	0	0
			1622	725	292	528	76	1		

- Molecule 6 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	32	Total	C	N	O	S	0	0
			261	164	53	43	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	0	HIS	-	expression tag	UNP P36675
6	18	THR	ALA	engineered mutation	UNP P36675

- Molecule 7 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	341	Total	C	N	O	S	0	0
			2706	1669	470	558	9		

- Molecule 8 is a protein called 50S ribosomal protein L2.

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

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

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 14 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

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

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 21 is a protein called 50S ribosomal protein L18.

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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	103	Total	C	N	O	S	0	0
			788	498	148	142			

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

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

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	52	Total	C	N	O	S	0	0
			426	275	78	73			

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L35.

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

- Molecule 38 is a protein called 50S ribosomal protein L36.

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

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

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

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 56 is a protein called 30S ribosomal protein S19.

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

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

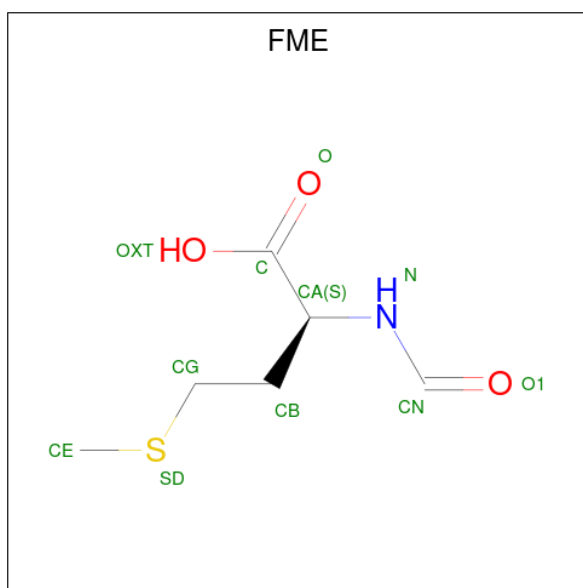
- Molecule 58 is a protein called 30S ribosomal protein S21.

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

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

Mol	Chain	Residues	Atoms		AltConf
59	1	295	Total	Mg	0
			295	295	
59	2	133	Total	Mg	0
			133	133	
59	3	6	Total	Mg	0
			6	6	
59	5	2	Total	Mg	0
			2	2	
59	b	1	Total	Mg	0
			1	1	
59	i	1	Total	Mg	0
			1	1	

- Molecule 60 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
60	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	a	1	Total	Zn	0
			1	1	
61	f	1	Total	Zn	0
			1	1	

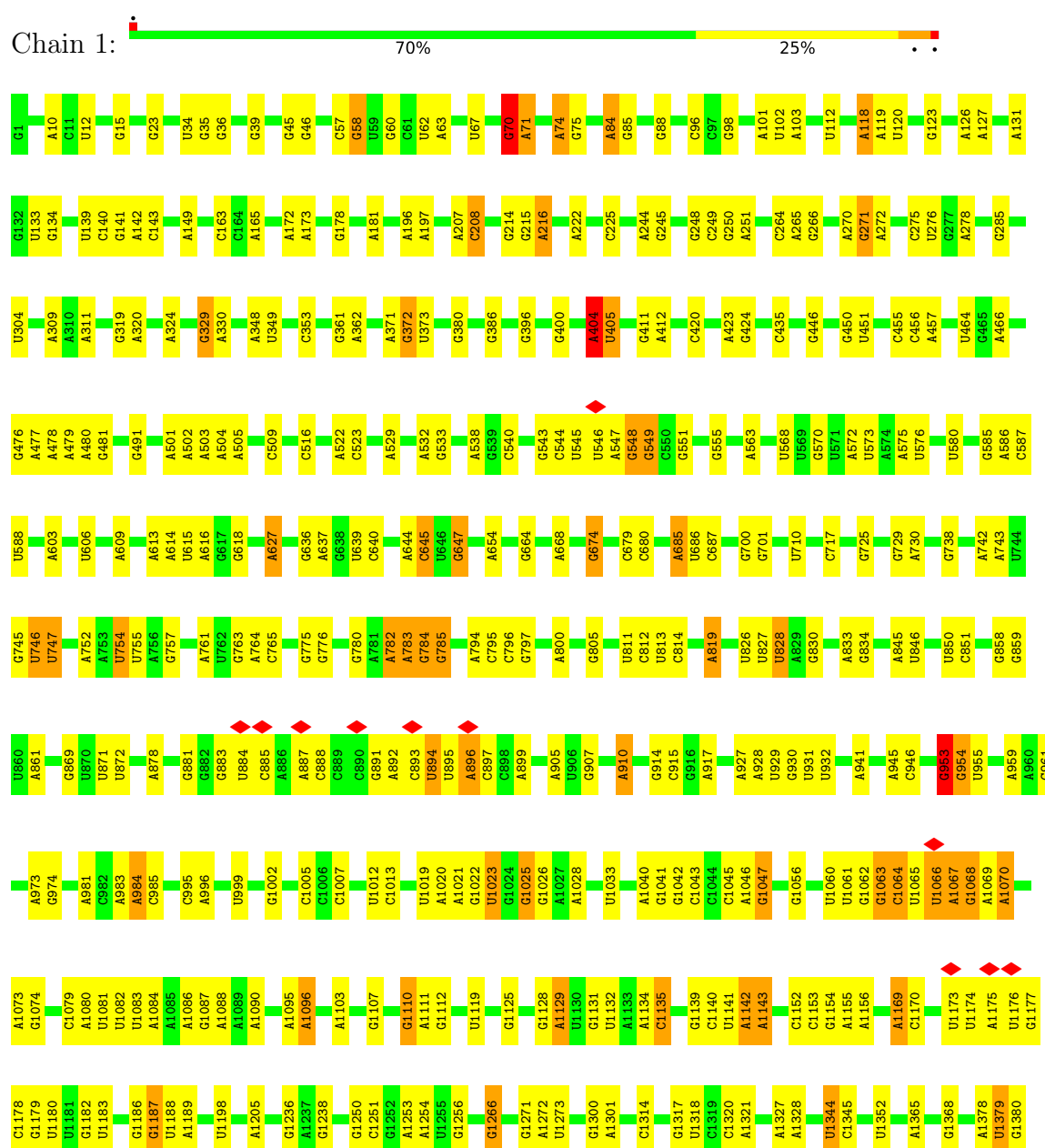
- Molecule 62 is water.

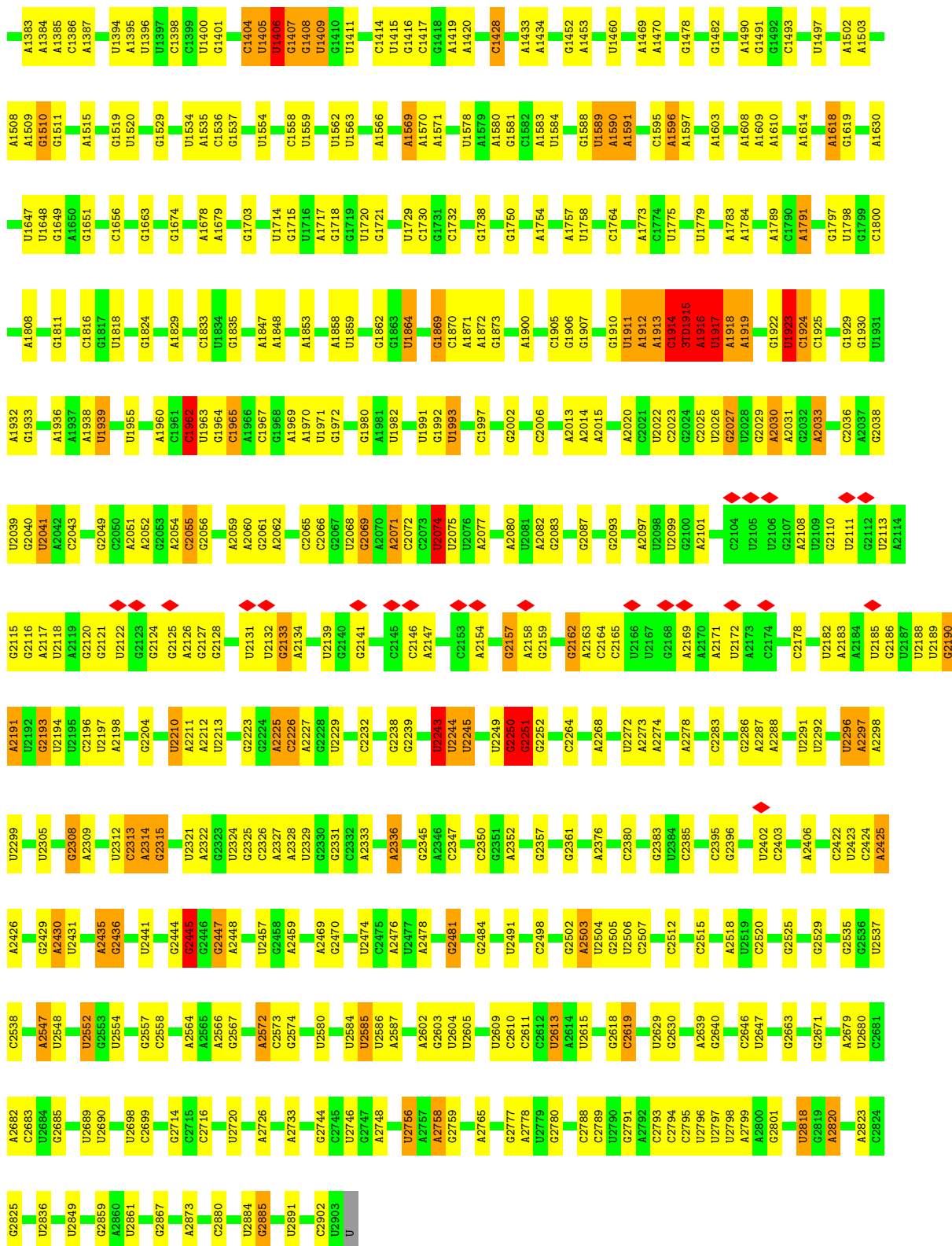
Mol	Chain	Residues	Atoms		AltConf
62	B	2	Total	O	0
			2	2	

3 Residue-property plots

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

• Molecule 1: 23S ribosomal RNA

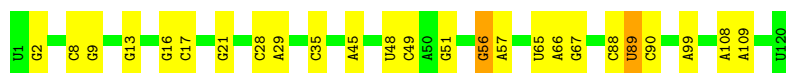




• Molecule 2: 16S ribosomal RNA



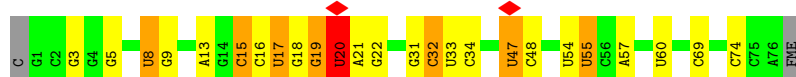




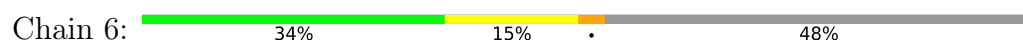
- Molecule 4: mRNA



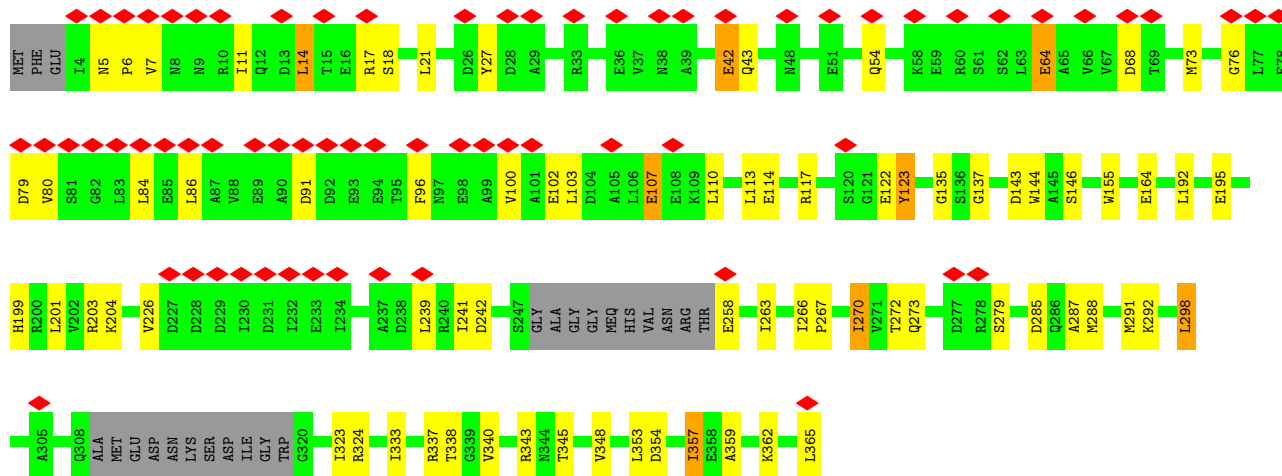
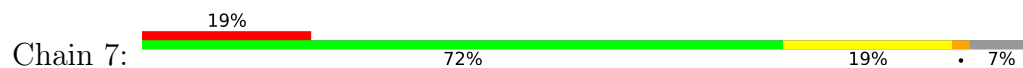
- Molecule 5: fMet-NH-tRNA(fMet)



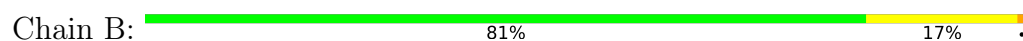
- Molecule 6: Alternative ribosome-rescue factor A

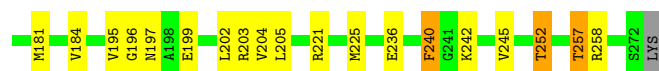


- Molecule 7: Peptide chain release factor 2

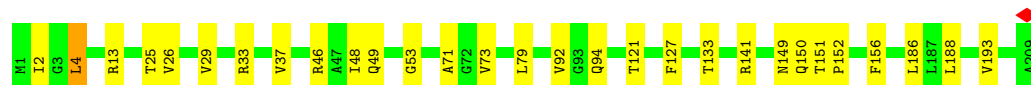
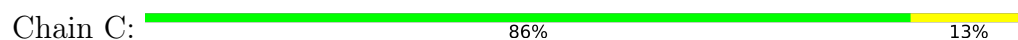


- Molecule 8: 50S ribosomal protein L2

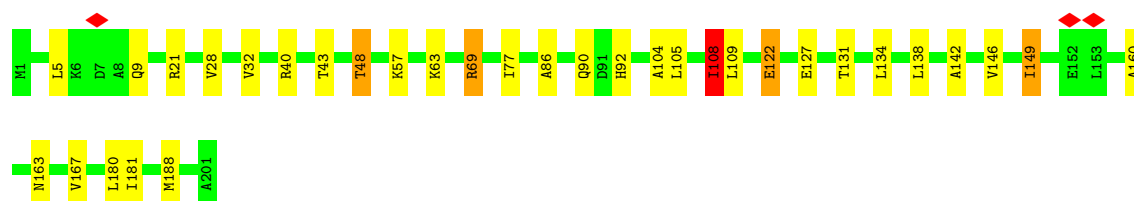
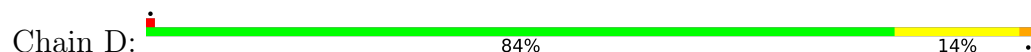




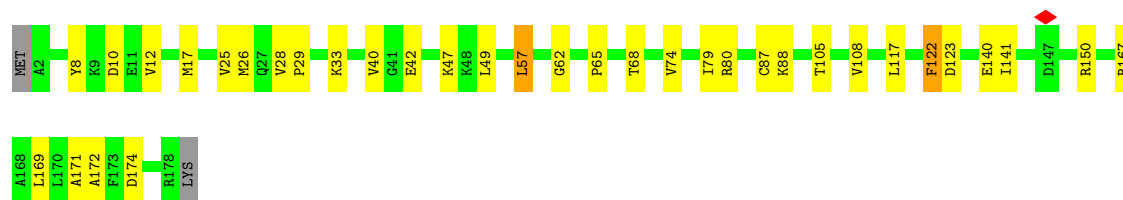
- Molecule 9: 50S ribosomal protein L3



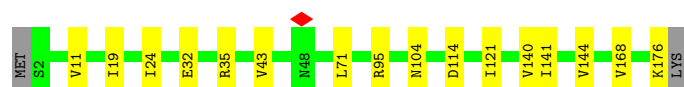
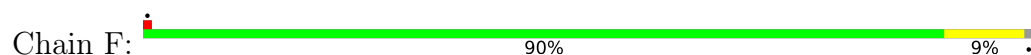
- Molecule 10: 50S ribosomal protein L4



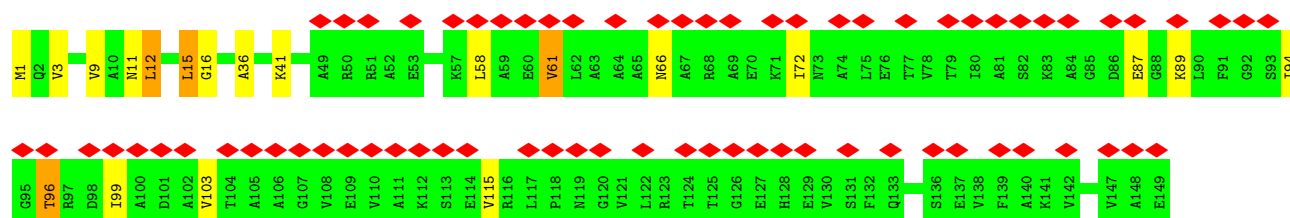
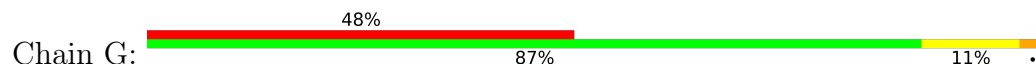
- Molecule 11: 50S ribosomal protein L5



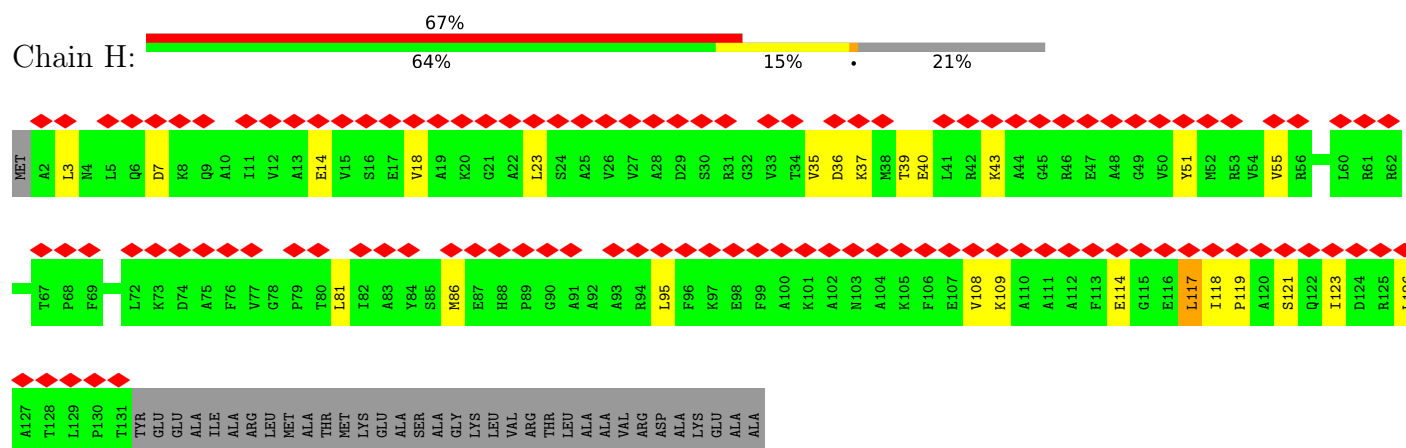
- Molecule 12: 50S ribosomal protein L6



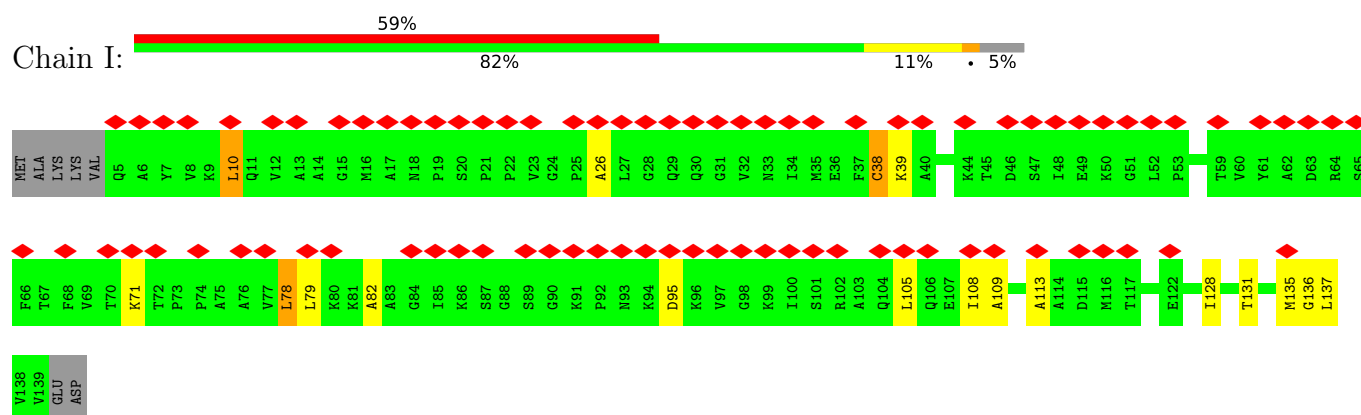
- Molecule 13: 50S ribosomal protein L9



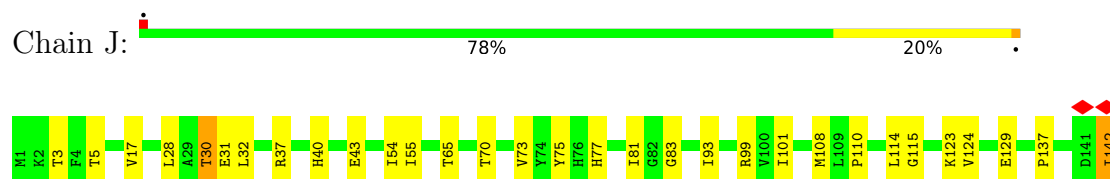
- Molecule 14: 50S ribosomal protein L10



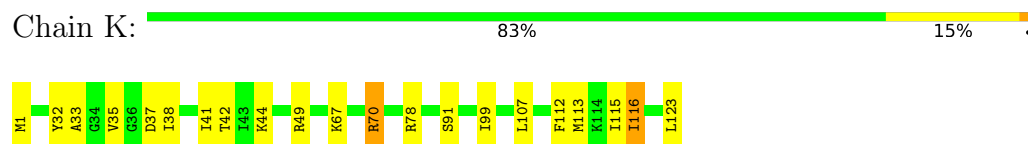
- Molecule 15: 50S ribosomal protein L11



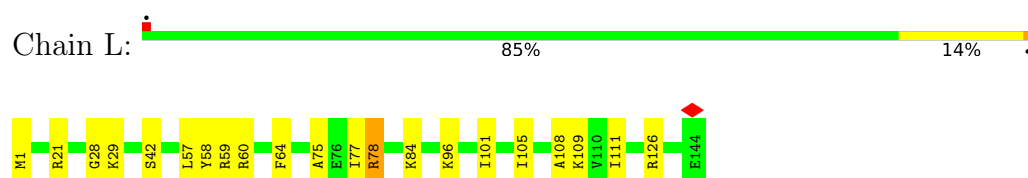
- Molecule 16: 50S ribosomal protein L13



- Molecule 17: 50S ribosomal protein L14



- Molecule 18: 50S ribosomal protein L15



- Molecule 19: 50S ribosomal protein L16

Chain M:  81% 18%



- Molecule 20: 50S ribosomal protein L17

Chain N:  78% 14% 6%



- Molecule 21: 50S ribosomal protein L18

Chain O:  81% 15%



- Molecule 22: 50S ribosomal protein L19

Chain P:  79% 19%



- Molecule 23: 50S ribosomal protein L20

Chain Q:  83% 15%



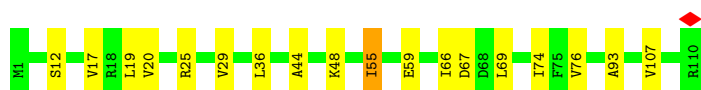
- Molecule 24: 50S ribosomal protein L21

Chain R:  83% 17%



- Molecule 25: 50S ribosomal protein L22

Chain S:  84% 15%



- Molecule 26: 50S ribosomal protein L23

Chain T:  83% 11% 6%



- Molecule 27: 50S ribosomal protein L24

Chain U:  83% 16% .



- Molecule 28: 50S ribosomal protein L25

Chain V:  89% 11%



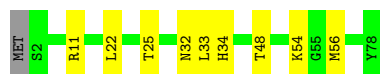
- Molecule 29: 50S ribosomal protein L27

Chain W:  79% 11% 11%



- Molecule 30: 50S ribosomal protein L28

Chain X:  87% 12% .



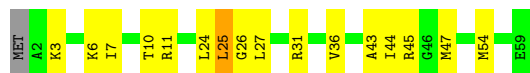
- Molecule 31: 50S ribosomal protein L29

Chain Y:  87% 11% .

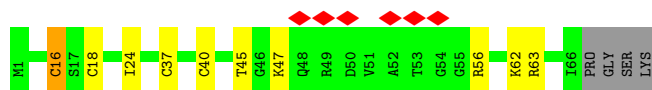
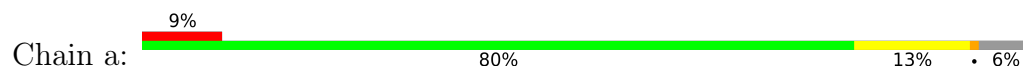


- Molecule 32: 50S ribosomal protein L30

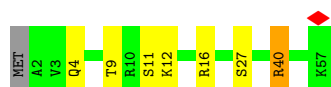
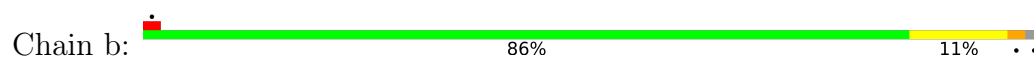
Chain Z:  71% 25% . .



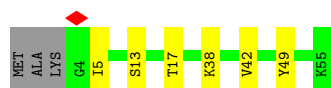
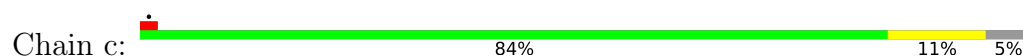
• Molecule 33: 50S ribosomal protein L31



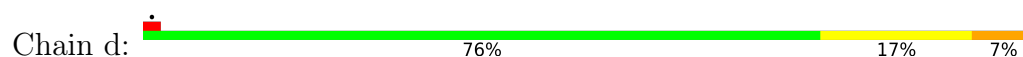
• Molecule 34: 50S ribosomal protein L32



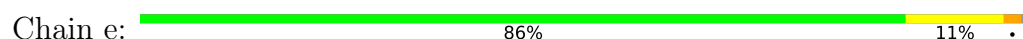
• Molecule 35: 50S ribosomal protein L33



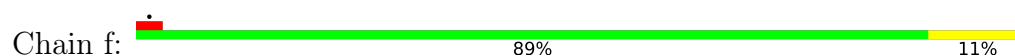
• Molecule 36: 50S ribosomal protein L34



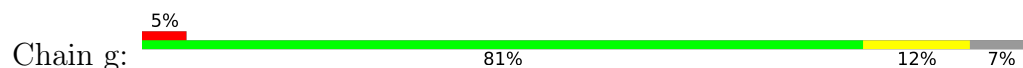
• Molecule 37: 50S ribosomal protein L35

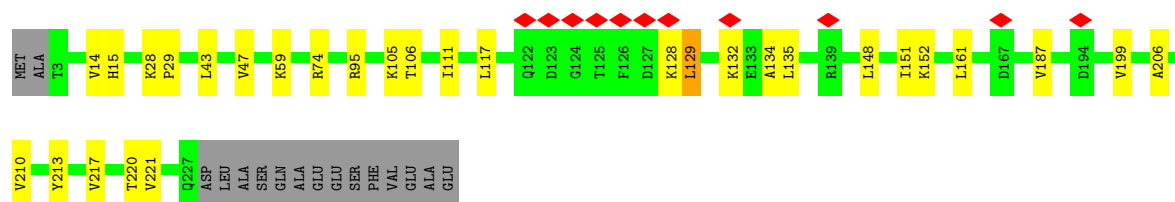


• Molecule 38: 50S ribosomal protein L36

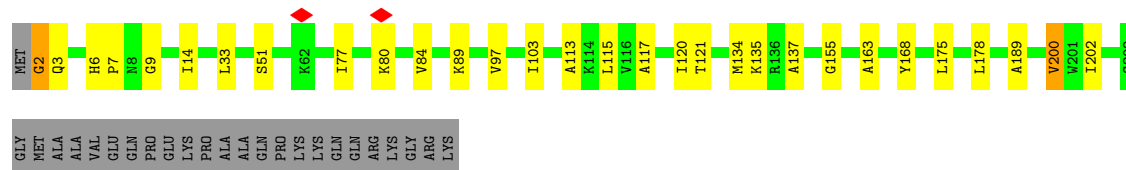
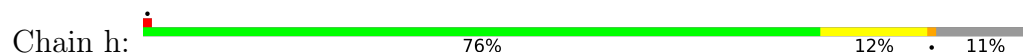


• Molecule 39: 30S ribosomal protein S2





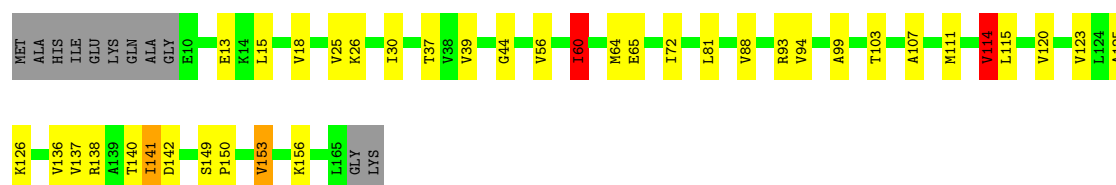
- Molecule 40: 30S ribosomal protein S3



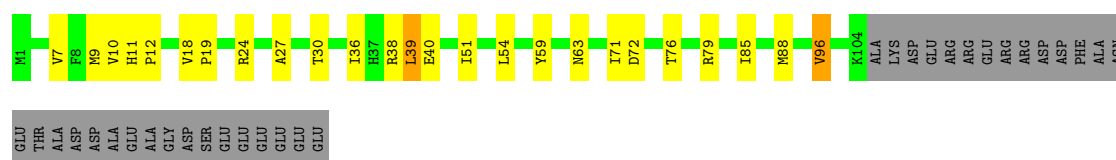
- Molecule 41: 30S ribosomal protein S4



- Molecule 42: 30S ribosomal protein S5

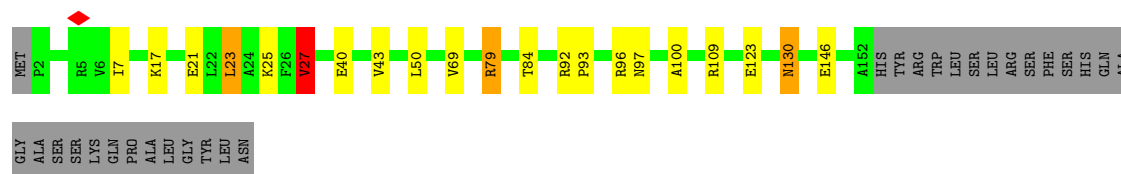


- Molecule 43: 30S ribosomal protein S6



- Molecule 44: 30S ribosomal protein S7

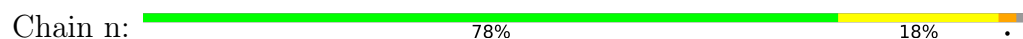




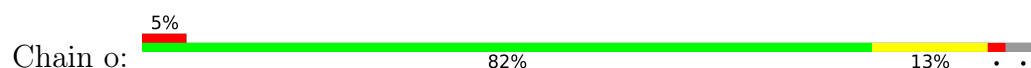
- Molecule 45: 30S ribosomal protein S8



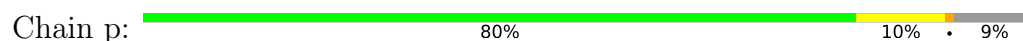
- Molecule 46: 30S ribosomal protein S9



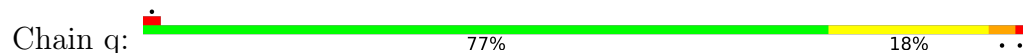
- Molecule 47: 30S ribosomal protein S10



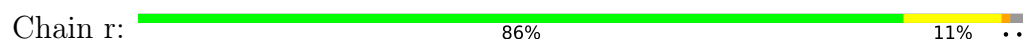
- Molecule 48: 30S ribosomal protein S11



- Molecule 49: 30S ribosomal protein S12

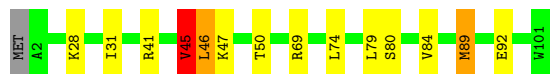


- Molecule 50: 30S ribosomal protein S13



- Molecule 51: 30S ribosomal protein S14

Chain s:  85% 11% ...



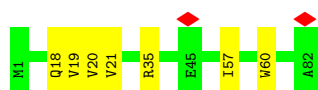
- Molecule 52: 30S ribosomal protein S15

Chain t:  82% 13% ..



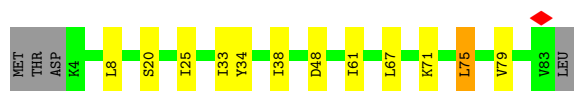
- Molecule 53: 30S ribosomal protein S16

Chain u:  91% 9%



- Molecule 54: 30S ribosomal protein S17

Chain v:  81% 13% • 5%



- Molecule 55: 30S ribosomal protein S18

Chain w:  73% 13% • 12%



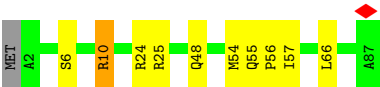
- Molecule 56: 30S ribosomal protein S19

Chain x:  76% 13% • 10%

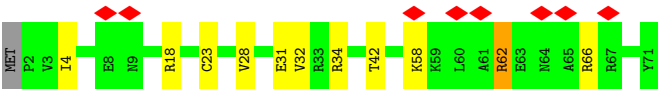
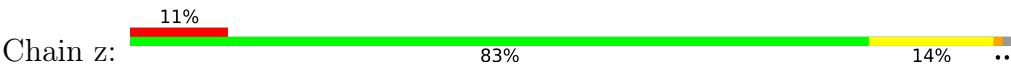


- Molecule 57: 30S ribosomal protein S20

Chain y:  87% 10% ..



• Molecule 58: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141950	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134615	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.807	Depositor
Minimum map value	-0.456	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, OMG, 0TD, G7M, PSU, ZN, UR3, MA6, 2MA, 4SU, H2U, FME, 5MC, MG, 1MG, 5MU, OMU, 6MZ, 2MG, OMC, 7MG, 3TD, 4OC

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	1	0.43	1/69285 (0.0%)	0.80	100/108083 (0.1%)
2	2	0.40	0/36590	0.80	61/57074 (0.1%)
3	3	0.39	0/2872	0.73	0/4478
4	4	0.47	0/122	0.70	0/188
5	5	0.40	0/1672	0.77	3/2603 (0.1%)
6	6	0.45	0/265	0.88	0/348
7	7	0.60	0/2741	1.11	4/3692 (0.1%)
8	B	0.72	0/2121	0.96	3/2852 (0.1%)
9	C	0.68	0/1586	0.89	0/2134
10	D	0.63	0/1571	1.03	1/2113 (0.0%)
11	E	0.62	0/1434	1.08	1/1926 (0.1%)
12	F	0.55	0/1333	0.88	0/1805
13	G	0.62	0/1122	0.98	1/1515 (0.1%)
14	H	0.72	0/993	1.05	1/1340 (0.1%)
15	I	0.66	0/998	1.04	0/1348
16	J	0.74	0/1152	1.06	0/1551
17	K	0.66	0/955	0.94	1/1279 (0.1%)
18	L	0.60	0/1062	0.99	3/1413 (0.2%)
19	M	0.71	0/1093	0.98	0/1460
20	N	0.69	0/964	1.11	0/1289
21	O	0.64	0/902	1.11	3/1209 (0.2%)
22	P	0.67	0/929	0.90	0/1242
23	Q	0.88	0/960	1.28	1/1278 (0.1%)
24	R	0.55	0/829	0.81	0/1107
25	S	0.72	0/864	1.09	0/1156
26	T	0.67	0/752	0.97	0/1005
27	U	0.47	0/796	0.76	0/1062
28	V	0.61	0/766	0.93	0/1025
29	W	0.64	0/589	0.80	1/779 (0.1%)
30	X	0.80	0/635	1.07	1/848 (0.1%)
31	Y	0.68	0/502	1.21	0/667

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.66	0/452	1.05	0/605
33	a	0.55	0/531	0.97	1/709 (0.1%)
34	b	0.60	0/450	0.92	0/599
35	c	0.50	0/433	0.81	0/576
36	d	0.76	0/380	1.27	0/498
37	e	0.63	0/513	1.10	1/676 (0.1%)
38	f	0.59	0/303	0.88	0/397
39	g	0.61	0/1791	1.05	1/2413 (0.0%)
40	h	0.59	0/1663	1.01	2/2241 (0.1%)
41	i	0.64	0/1665	1.09	0/2227
42	j	0.67	0/1165	1.06	4/1568 (0.3%)
43	k	0.64	0/867	0.97	0/1171
44	l	0.67	0/1195	1.20	3/1602 (0.2%)
45	m	0.58	0/989	0.95	0/1326
46	n	0.57	0/1034	1.00	0/1375
47	o	0.53	0/800	0.94	1/1082 (0.1%)
48	p	0.60	0/893	0.97	0/1205
49	q	0.61	0/960	0.89	1/1286 (0.1%)
50	r	0.64	0/909	1.13	0/1215
51	s	0.69	0/817	1.14	1/1088 (0.1%)
52	t	0.72	0/722	1.24	0/964
53	u	0.60	0/659	0.97	0/884
54	v	0.45	0/657	0.75	0/881
55	w	0.64	0/553	1.08	1/743 (0.1%)
56	x	0.53	0/680	0.84	0/915
57	y	0.77	0/675	1.33	0/895
58	z	0.73	0/597	1.22	0/792
All	All	0.50	1/160808 (0.0%)	0.87	201/239802 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2069	G7M	O3'-P	5.01	1.61	1.56

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1914	C	C4'-C3'-O3'	14.64	134.97	113.00
2	2	1276	G	C1'-C2'-O2'	-13.04	88.84	108.40
40	h	2	GLY	N-CA-C	-12.24	77.80	113.30
1	1	2313	C	C1'-C2'-O2'	-12.04	90.34	108.40
2	2	528	C	C1'-C2'-O2'	-10.65	92.42	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	928	G	N9-C1'-C2'	-9.82	97.26	112.00
2	2	198	G	C4'-C3'-O3'	9.52	127.28	113.00
1	1	2425	A	C2'-C3'-O3'	9.23	123.34	109.50
1	1	2296	U	C4'-C3'-O3'	9.17	123.15	109.40
2	2	1384	C	N1-C1'-C2'	-9.03	98.46	112.00
1	1	2250	G	C4'-C3'-O3'	-9.01	95.88	109.40
2	2	428	G	C4'-C3'-O3'	8.91	122.77	109.40
2	2	198	G	C1'-C2'-O2'	-8.68	95.38	108.40
2	2	480	U	C4'-C3'-O3'	8.48	125.72	113.00
2	2	1276	G	C4'-C3'-O3'	8.43	125.65	113.00
1	1	1595	C	C1'-C2'-O2'	-8.43	95.75	108.40
2	2	927	G	C1'-C2'-O2'	-8.41	95.78	108.40
2	2	1530	G	C4'-C3'-O3'	-8.33	100.51	113.00
1	1	2252	G	N9-C1'-C2'	-8.29	99.57	112.00
1	1	404	A	C2'-C3'-O3'	8.19	121.79	109.50
2	2	199	A	N9-C1'-C2'	-8.18	99.73	112.00
51	s	45	VAL	N-CA-CB	8.07	119.99	110.55
1	1	2193	G	C2'-C3'-O3'	8.02	125.73	113.70
1	1	2071	A	C4'-C3'-O3'	-8.00	101.00	113.00
2	2	1277	C	N1-C1'-C2'	-7.96	100.06	112.00
37	e	13	ARG	N-CA-C	7.89	122.67	112.89
1	1	2244	U	C1'-C2'-O2'	-7.82	96.67	108.40
1	1	2313	C	C4'-C3'-O3'	7.79	124.68	113.00
1	1	1404	C	C1'-C2'-O2'	-7.74	96.80	108.40
2	2	1499	A	N9-C1'-C2'	-7.69	100.47	112.00
44	l	27	VAL	N-CA-CB	7.67	119.53	110.55
1	1	1916	A	C3'-C2'-O2'	7.65	122.18	110.70
2	2	927	G	C4'-C3'-O3'	7.64	124.46	113.00
2	2	928	G	C4'-C3'-O3'	7.59	124.39	113.00
1	1	783	A	C4'-C3'-O3'	7.54	124.31	113.00
42	j	60	ILE	N-CA-CB	7.53	119.36	110.55
1	1	1916	A	C2'-C3'-O3'	-7.50	102.44	113.70
1	1	1923	U	C4'-C3'-O3'	7.50	120.65	109.40
1	1	1406	U	C1'-C2'-O2'	-7.42	97.27	108.40
1	1	754	U	N1-C1'-C2'	7.38	123.06	112.00
11	E	108	VAL	O-C-N	7.35	125.29	120.07
2	2	528	C	C4'-C3'-O3'	7.32	123.98	113.00
1	1	2252	G	C4'-C3'-O3'	7.28	123.92	113.00
1	1	2315	G	N9-C1'-C2'	-7.28	101.09	112.00
2	2	730	G	C2'-C3'-O3'	-7.14	102.98	113.70
7	7	357	ILE	CB-CA-C	-7.13	102.84	111.97
39	g	47	VAL	O-C-N	7.11	124.97	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1916	A	C4'-C3'-O3'	7.08	123.63	113.00
10	D	108	ILE	N-CA-CB	7.07	118.82	110.55
1	1	2162	G	C4'-C3'-O3'	7.05	119.98	109.40
2	2	927	G	N9-C1'-C2'	-6.98	101.53	112.00
2	2	1206	G	C4'-C3'-O3'	6.97	123.45	113.00
2	2	526	C	C4'-C3'-O3'	6.93	123.40	113.00
1	1	1757	A	C4'-C3'-O3'	-6.93	102.61	113.00
5	5	47	U	C2'-C3'-O3'	6.92	119.88	109.50
8	B	245	VAL	CB-CA-C	-6.90	105.25	111.74
1	1	896	A	C4'-C3'-O3'	6.89	119.73	109.40
1	1	2820	A	C4'-C3'-O3'	-6.82	102.76	113.00
1	1	2068	U	C4'-C3'-O3'	-6.80	102.80	113.00
2	2	148	G	N9-C1'-C2'	-6.76	101.86	112.00
1	1	1379	U	C2'-C3'-O3'	6.72	123.78	113.70
2	2	1390	U	C1'-C2'-O2'	-6.71	98.33	108.40
1	1	70	G	C4'-C3'-O3'	6.68	119.42	109.40
1	1	1914	C	C2'-C3'-O3'	-6.67	103.70	113.70
2	2	1390	U	C4'-C3'-O3'	6.63	122.94	113.00
1	1	1407	G	N9-C1'-C2'	-6.62	102.07	112.00
1	1	2315	G	C4'-C3'-O3'	6.61	122.92	113.00
2	2	776	G	C4'-C3'-O3'	-6.58	103.13	113.00
2	2	1206	G	N9-C1'-C2'	-6.53	102.20	112.00
2	2	147	G	C4'-C3'-O3'	6.51	122.76	113.00
5	5	17	U	C2'-C3'-O3'	6.47	119.21	109.50
1	1	894	U	C2'-C3'-O3'	6.46	119.20	109.50
1	1	2055	C	C2'-C3'-O3'	-6.45	104.02	113.70
1	1	2243	U	C4'-C3'-O3'	6.45	122.67	113.00
13	G	61	VAL	N-CA-CB	6.42	118.06	110.55
8	B	130	LEU	N-CA-C	6.42	113.99	108.22
1	1	1140	C	C4'-C3'-O3'	-6.36	103.46	113.00
1	1	1154	G	C2'-C3'-O3'	-6.32	104.22	113.70
1	1	2314	A	C4'-C3'-O3'	6.29	122.43	113.00
2	2	1383	C	C4'-C3'-O3'	6.26	122.40	113.00
2	2	1383	C	N1-C1'-C2'	-6.26	102.61	112.00
2	2	1499	A	C4'-C3'-O3'	6.24	122.35	113.00
2	2	1391	U	N1-C1'-C2'	-6.19	102.72	112.00
1	1	2425	A	C4'-C3'-O3'	6.18	118.67	109.40
1	1	1916	A	N9-C1'-C2'	-6.17	102.75	112.00
2	2	573	A	C4'-C3'-O3'	-6.11	103.83	113.00
1	1	2308	G	C2'-C3'-O3'	-6.09	104.56	113.70
1	1	2756	U	C4'-C3'-O3'	6.08	118.52	109.40
2	2	1299	A	C2'-C3'-O3'	6.05	118.58	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	776	G	C2'-C3'-O3'	6.05	122.77	113.70
2	2	864	A	N9-C1'-C2'	6.03	121.04	112.00
2	2	480	U	N1-C1'-C2'	-6.02	102.97	112.00
1	1	271	G	C4'-C3'-O3'	6.01	118.42	109.40
1	1	2225	A	C4'-C3'-O3'	6.00	118.40	109.40
2	2	198	G	N9-C1'-C2'	-5.99	103.02	112.00
2	2	1493	A	C3'-C2'-O2'	5.98	119.66	110.70
7	7	357	ILE	N-CA-CB	5.97	117.53	110.55
2	2	1395	C	C3'-C2'-O2'	5.96	119.63	110.70
1	1	126	A	C4'-C3'-O3'	-5.91	104.13	113.00
1	1	2020	A	C4'-C3'-O3'	-5.91	104.14	113.00
18	L	60	ARG	CB-CA-C	-5.91	100.81	110.85
1	1	2314	A	N9-C1'-C2'	-5.89	103.17	112.00
2	2	1384	C	C4'-C3'-O3'	5.89	121.83	113.00
2	2	1208	C	C4'-C3'-O3'	5.85	121.77	113.00
1	1	685	A	C4'-C3'-O3'	5.84	118.16	109.40
1	1	1002	G	C3'-C2'-O2'	5.82	119.42	110.70
1	1	1023	U	C1'-C2'-O2'	5.79	117.09	108.40
1	1	1969	A	C4'-C3'-O3'	-5.79	104.31	113.00
1	1	2074	U	N1-C1'-C2'	5.78	120.67	112.00
1	1	101	A	C3'-C2'-O2'	5.78	119.36	110.70
18	L	64	PHE	N-CA-C	5.77	118.05	108.99
1	1	479	A	C4'-C3'-O3'	5.76	118.05	109.40
1	1	1131	G	C4'-C3'-O3'	5.74	118.01	109.40
29	W	12	ASN	N-CA-C	5.72	122.63	114.16
1	1	2210	U	C4'-C3'-O3'	5.71	117.97	109.40
2	2	69	G	C4'-C3'-O3'	-5.71	104.44	113.00
2	2	978	A	C4'-C3'-O3'	-5.68	104.48	113.00
1	1	953	G	C2'-C3'-O3'	5.67	122.21	113.70
1	1	2313	C	N1-C1'-C2'	-5.67	103.49	112.00
2	2	199	A	C4'-C3'-O3'	5.67	121.50	113.00
2	2	1335	U	C4'-C3'-O3'	-5.67	104.50	113.00
1	1	2232	C	C1'-C2'-O2'	5.66	116.89	108.40
1	1	576	U	C4'-C3'-O3'	-5.65	104.52	113.00
55	w	14	THR	N-CA-C	-5.62	105.20	112.68
1	1	2244	U	C4'-C3'-O3'	5.61	121.42	113.00
1	1	2223	G	C3'-C2'-O2'	5.57	119.06	110.70
44	1	92	ARG	CA-C-N	5.57	124.77	118.97
44	1	92	ARG	C-N-CA	5.57	124.77	118.97
2	2	1225	A	C2'-C3'-O3'	5.52	117.78	109.50
1	1	380	G	C3'-C2'-O2'	5.52	118.97	110.70
2	2	928	G	C2'-C3'-O3'	-5.51	105.43	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	198	G	C2'-C3'-O3'	-5.50	105.45	113.70
1	1	127	A	C4'-C3'-O3'	-5.49	104.77	113.00
2	2	24	U	C3'-C2'-O2'	5.49	118.93	110.70
2	2	1276	G	N9-C1'-C2'	-5.48	103.77	112.00
1	1	850	U	C4'-C3'-O3'	-5.48	104.78	113.00
1	1	2619	C	C3'-C2'-O2'	5.47	118.91	110.70
1	1	763	G	C4'-C3'-O3'	-5.46	104.81	113.00
1	1	959	A	C4'-C3'-O3'	-5.46	104.81	113.00
1	1	2074	U	C2'-C3'-O3'	5.46	121.88	113.70
1	1	794	A	C4'-C3'-O3'	-5.45	104.83	113.00
2	2	1322	C	C2'-C3'-O3'	-5.42	101.37	109.50
1	1	2315	G	C2'-C3'-O3'	-5.40	105.61	113.70
17	K	116	ILE	N-CA-CB	5.39	117.87	110.54
7	7	64	GLU	CA-C-N	5.39	127.77	120.44
7	7	64	GLU	C-N-CA	5.39	127.77	120.44
2	2	574	A	C4'-C3'-O3'	-5.34	104.99	113.00
2	2	720	C	C4'-C3'-O3'	-5.33	105.00	113.00
1	1	123	G	C3'-C2'-O2'	5.32	118.68	110.70
1	1	1152	C	C3'-C2'-O2'	5.32	118.68	110.70
1	1	2272	U	C2'-C3'-O3'	-5.32	105.72	113.70
2	2	1145	A	C4'-C3'-O3'	-5.32	105.02	113.00
1	1	2054	A	C4'-C3'-O3'	-5.31	105.03	113.00
30	X	22	LEU	N-CA-C	5.31	119.34	112.86
2	2	1363	A	C4'-C3'-O3'	-5.31	101.44	109.40
18	L	29	LYS	N-CA-C	5.31	116.75	111.07
1	1	1791	A	C3'-C2'-O2'	5.30	118.65	110.70
40	h	3	GLN	N-CA-CB	5.29	119.55	110.34
2	2	529	G	C4'-C3'-O3'	5.29	120.93	113.00
1	1	516	C	C3'-C2'-O2'	5.28	118.62	110.70
8	B	158	ALA	N-CA-C	5.28	122.04	110.80
21	O	11	ALA	N-CA-C	5.26	118.96	112.54
33	a	62	LYS	N-CA-C	5.25	117.41	111.11
42	j	153	VAL	N-CA-CB	5.25	117.67	110.54
1	1	1155	A	C3'-C2'-O2'	5.24	118.56	110.70
1	1	2422	C	C4'-C3'-O3'	-5.24	105.14	113.00
1	1	1864	U	C4'-C3'-O3'	-5.23	105.16	113.00
1	1	2447	G	C2'-C3'-O3'	-5.22	101.67	109.50
1	1	1187	G	C4'-C3'-O3'	-5.22	105.17	113.00
1	1	2245	U	N1-C1'-C2'	-5.18	104.23	112.00
2	2	147	G	N9-C1'-C2'	-5.18	104.23	112.00
5	5	15	C	C2'-C3'-O3'	5.18	117.27	109.50
1	1	1663	G	C4'-C3'-O3'	-5.17	105.25	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	147	G	C1'-C2'-O2'	-5.16	100.67	108.40
14	H	81	LEU	N-CA-C	5.14	118.69	111.90
49	q	87	VAL	N-CA-C	-5.14	102.87	109.30
1	1	1025	G	C4'-C3'-O3'	5.14	117.11	109.40
42	j	120	VAL	N-CA-CB	5.13	116.12	110.53
1	1	826	U	C1'-C2'-O2'	5.12	116.08	108.40
1	1	208	C	C4'-C3'-O3'	-5.10	105.34	113.00
1	1	2481	G	C4'-C3'-O3'	-5.09	105.36	113.00
23	Q	6	ARG	N-CA-C	5.09	118.98	112.26
2	2	1277	C	C4'-C3'-O3'	5.09	120.63	113.00
1	1	1314	C	C4'-C3'-O3'	-5.08	105.37	113.00
1	1	725	G	C4'-C3'-O3'	-5.08	105.39	113.00
42	j	114	VAL	N-CA-CB	5.08	117.44	110.54
1	1	674	G	C1'-C2'-O2'	5.07	116.00	108.40
1	1	478	A	C4'-C3'-O3'	-5.06	105.41	113.00
1	1	2818	U	C3'-C2'-O2'	5.06	118.29	110.70
47	o	25	ILE	N-CA-CB	5.06	117.42	110.54
1	1	1135	C	C4'-C3'-O3'	-5.05	105.42	113.00
21	O	74	VAL	CA-C-N	5.05	125.54	119.94
21	O	74	VAL	C-N-CA	5.05	125.54	119.94
1	1	761	A	C4'-C3'-O3'	-5.05	105.43	113.00
2	2	481	G	C2'-C3'-O3'	-5.04	101.94	109.50
1	1	112	U	C3'-C2'-O2'	5.03	118.24	110.70
2	2	1395	C	C4'-C3'-O3'	-5.03	105.46	113.00
1	1	606	U	C3'-C2'-O2'	5.01	118.22	110.70
1	1	1398	C	C4'-C3'-O3'	-5.01	105.49	113.00
1	1	828	U	C4'-C3'-O3'	-5.00	105.49	113.00
1	1	423	A	C2'-C3'-O3'	-5.00	106.20	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31366	266	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	32929	0	16587	224	0
3	3	2569	0	1301	6	0
4	4	109	0	55	0	0
5	5	1622	0	829	3	0
6	6	261	0	276	18	0
7	7	2706	0	2616	43	0
8	B	2082	0	2154	26	0
9	C	1565	0	1616	16	0
10	D	1552	0	1619	18	0
11	E	1410	0	1444	17	0
12	F	1313	0	1358	5	0
13	G	1111	0	1148	6	0
14	H	980	0	1013	10	0
15	I	984	0	1035	10	0
16	J	1129	0	1162	13	0
17	K	946	0	1023	9	0
18	L	1053	0	1129	12	0
19	M	1074	0	1157	11	0
20	N	951	0	994	8	0
21	O	892	0	923	11	0
22	P	917	0	962	8	0
23	Q	947	0	1019	11	0
24	R	816	0	839	4	0
25	S	857	0	922	9	0
26	T	746	0	811	7	0
27	U	788	0	843	12	0
28	V	753	0	780	3	0
29	W	582	0	599	2	0
30	X	625	0	652	1	0
31	Y	501	0	531	5	0
32	Z	448	0	488	7	0
33	a	522	0	520	7	0
34	b	444	0	458	3	0
35	c	426	0	464	2	0
36	d	377	0	418	6	0
37	e	504	0	572	3	0
38	f	302	0	340	0	0
39	g	1760	0	1787	12	0
40	h	1636	0	1710	13	0
41	i	1643	0	1707	8	0
42	j	1152	0	1196	21	0
43	k	848	0	846	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	l	1181	0	1238	6	0
45	m	979	0	1031	5	0
46	n	1022	0	1070	13	0
47	o	790	0	831	6	0
48	p	877	0	887	7	0
49	q	957	0	1017	17	0
50	r	900	0	965	7	0
51	s	805	0	844	12	0
52	t	714	0	734	5	0
53	u	649	0	666	2	0
54	v	648	0	691	7	0
55	w	544	0	560	5	0
56	x	663	0	688	8	0
57	y	669	0	719	5	0
58	z	589	0	629	5	0
59	1	295	0	0	0	0
59	2	133	0	0	0	0
59	3	6	0	0	0	0
59	5	2	0	0	0	0
59	b	1	0	0	0	0
59	i	1	0	0	0	0
60	5	10	0	10	0	0
61	a	1	0	0	0	0
61	f	1	0	0	0	0
62	B	2	0	0	0	0
All	All	149607	0	101849	888	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 (888) 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)
1:1:1021:A:N1	1:1:1141:U:O4	1.60	1.34
2:2:827:U:O4	2:2:872:A:N1	1.59	1.34
2:2:37:U:O4	2:2:397:A:N1	1.62	1.33
2:2:1358:U:O4	2:2:1363:A:N1	1.59	1.31
1:1:1914:C:H5''	6:6:21:HIS:CE1	1.70	1.25
2:2:563:A:N1	2:2:884:U:O4	1.71	1.23
1:1:2074:U:N3	1:1:2435:A:N1	1.87	1.20
2:2:195:A:O2'	2:2:196:A:H5'	1.46	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:158:ALA:O	8:B:196:GLY:O	1.63	1.14
1:1:2297:A:N1	1:1:2321:U:C4	2.26	1.04
2:2:13:U:N3	2:2:915:A:C6	2.25	1.04
1:1:1596:A:O2'	1:1:1597:A:C8	2.13	1.01
1:1:1019:U:H3	1:1:1142:A:H61	1.07	0.99
33:a:18:CYS:HB3	33:a:40:CYS:HB3	1.46	0.96
1:1:1914:C:H5''	6:6:21:HIS:HE1	1.03	0.96
1:1:67:U:N3	1:1:74:A:C6	2.34	0.96
1:1:1019:U:H3	1:1:1142:A:N6	1.63	0.95
2:2:13:U:N3	2:2:915:A:N6	2.14	0.95
2:2:13:U:C4	2:2:915:A:N6	2.34	0.94
2:2:37:U:N3	2:2:397:A:N6	2.16	0.93
1:1:1596:A:HO2'	1:1:1597:A:H8	1.08	0.92
1:1:2297:A:N1	1:1:2321:U:O4	2.03	0.92
42:j:111:MET:HE2	42:j:125:ALA:HB1	1.51	0.92
1:1:1918:A:O2'	1:1:1919:A:N7	2.01	0.92
2:2:481:G:O2'	2:2:483:C:N4	2.03	0.91
1:1:1916:A:O2'	1:1:1917:PSU:O4'	1.89	0.90
2:2:13:U:O4	2:2:20:U:O4	1.90	0.89
7:7:73:MET:HE2	7:7:110:LEU:HD12	1.54	0.89
1:1:67:U:N3	1:1:74:A:N6	2.21	0.88
6:6:17:GLU:N	6:6:17:GLU:OE1	2.08	0.87
33:a:18:CYS:HB3	33:a:40:CYS:CB	2.04	0.87
1:1:2298:A:C4	1:1:2321:U:C5	2.62	0.87
1:1:783:A:H2'	1:1:783:A:N3	1.88	0.86
2:2:527:7MG:H3'	2:2:527:7MG:H81	1.55	0.86
1:1:1915:3TD:H2'	1:1:1916:A:C8	2.11	0.85
1:1:1916:A:H2'	1:1:1917:PSU:C6	2.11	0.85
2:2:13:U:C4	2:2:20:U:O4	2.29	0.85
1:1:1021:A:H61	1:1:1141:U:H3	1.24	0.85
1:1:1021:A:N6	1:1:1141:U:H3	1.75	0.84
6:6:22:ASP:OD1	6:6:23:PRO:HD2	1.75	0.84
1:1:1913:A:OP2	1:1:1913:A:H3'	1.77	0.84
1:1:1405:U:O2'	1:1:1406:U:C6	2.30	0.84
2:2:517:G:O2'	2:2:530:G:H4'	1.77	0.83
2:2:13:U:O4	2:2:21:G:C2	2.32	0.83
1:1:1914:C:H2'	1:1:1915:3TD:O4	1.77	0.83
1:1:2298:A:C4	1:1:2321:U:H5	1.93	0.83
1:1:585:G:N7	23:Q:6:ARG:NH1	2.27	0.82
27:U:36:VAL:HG11	27:U:39:ILE:HD12	1.61	0.82
1:1:1916:A:H2'	1:1:1917:PSU:H6	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2013:A:N6	1:1:2613:U:H3	1.78	0.82
2:2:37:U:H3	2:2:397:A:N6	1.77	0.82
1:1:1405:U:H2'	1:1:1406:U:C5	2.15	0.81
2:2:37:U:C4	2:2:397:A:N1	2.48	0.81
2:2:915:A:N6	2:2:916:U:C4	2.48	0.81
1:1:1405:U:H2'	1:1:1406:U:C6	2.15	0.81
1:1:572:A:OP2	24:R:80:ARG:NH2	2.13	0.81
2:2:827:U:H3	2:2:872:A:N6	1.80	0.80
33:a:18:CYS:CB	33:a:40:CYS:HB3	2.11	0.80
1:1:1915:3TD:O4	1:1:1915:3TD:OP2	1.98	0.80
1:1:2756:U:N3	1:1:2758:A:N6	2.30	0.79
1:1:2756:U:N3	1:1:2758:A:C6	2.50	0.79
2:2:1208:C:O2'	2:2:1209:C:O4'	2.01	0.78
1:1:1405:U:C2'	1:1:1406:U:C6	2.67	0.78
51:s:46:LEU:HD12	56:x:13:LEU:HD13	1.66	0.78
1:1:1914:C:C5'	6:6:21:HIS:HE1	1.92	0.77
7:7:64:GLU:O	7:7:68:ASP:N	2.17	0.77
1:1:742:A:H2'	1:1:743:A:C8	2.21	0.76
1:1:1021:A:N1	1:1:1141:U:C4	2.53	0.76
2:2:1358:U:C4	2:2:1363:A:N1	2.52	0.76
2:2:146:G:C2'	2:2:147:G:H5'	2.16	0.75
7:7:11:ILE:HA	7:7:103:LEU:HD21	1.68	0.75
42:j:137:VAL:O	42:j:140:THR:OG1	2.04	0.75
46:n:84:THR:HG21	46:n:103:PHE:HB3	1.67	0.75
2:2:1358:U:H3	2:2:1363:A:N6	1.85	0.74
1:1:67:U:C4	1:1:74:A:N6	2.55	0.74
2:2:927:G:C2'	2:2:928:G:H5'	2.18	0.73
21:O:31:THR:O	21:O:102:ARG:NH1	2.21	0.73
2:2:515:G:O2'	2:2:516:PSU:O4'	2.05	0.73
1:1:1779:U:H5	1:1:1784:A:N7	1.86	0.73
49:q:86:ARG:O	49:q:86:ARG:HG3	1.87	0.73
2:2:827:U:C4	2:2:872:A:N1	2.53	0.73
2:2:527:7MG:H3'	2:2:527:7MG:C8	2.23	0.73
28:V:75:GLN:HB2	28:V:92:VAL:HG23	1.70	0.72
1:1:2756:U:C4	1:1:2758:A:N6	2.58	0.72
2:2:197:A:O2'	2:2:220:G:N2	2.22	0.72
1:1:2312:U:H2'	1:1:2313:C:H5'	1.71	0.72
14:H:36:ASP:O	14:H:39:THR:OG1	2.05	0.72
55:w:11:CYS:SG	55:w:14:THR:HG23	2.28	0.72
1:1:2298:A:N3	1:1:2321:U:C5	2.59	0.71
33:a:16:CYS:HB3	33:a:37:CYS:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:158:ALA:O	8:B:195:VAL:HG13	1.90	0.71
1:1:2312:U:C2'	1:1:2313:C:H5'	2.21	0.71
7:7:298:LEU:C	7:7:298:LEU:HD23	2.15	0.71
2:2:927:G:H4'	2:2:927:G:OP2	1.91	0.71
7:7:14:LEU:HD11	7:7:107:GLU:HB2	1.71	0.71
1:1:1962:5MC:O2'	1:1:1964:G:OP2	2.08	0.70
2:2:1358:U:N3	2:2:1363:A:N6	2.40	0.69
2:2:827:U:O4	2:2:872:A:C2	2.45	0.69
2:2:827:U:N3	2:2:872:A:N6	2.40	0.69
1:1:1021:A:H3'	1:1:1021:A:N3	2.08	0.69
1:1:2013:A:N6	1:1:2613:U:N3	2.39	0.68
2:2:528:C:H41	49:q:46:ASN:CG	2.02	0.68
2:2:563:A:N1	2:2:884:U:C4	2.60	0.68
9:C:33:ARG:NH1	9:C:53:GLY:O	2.27	0.68
7:7:64:GLU:O	7:7:68:ASP:HB2	1.93	0.68
36:d:31:LEU:HD22	36:d:42:LEU:HD13	1.75	0.68
15:I:109:ALA:HB2	15:I:128:ILE:HD12	1.76	0.67
54:v:25:ILE:HD11	54:v:61:ILE:HD11	1.77	0.67
7:7:270:ILE:HG23	7:7:291:MET:HE1	1.76	0.67
1:1:1818:U:OP2	8:B:156:ARG:NH1	2.27	0.67
9:C:4:LEU:HD23	9:C:29:VAL:HG11	1.77	0.67
19:M:82:MET:HA	19:M:82:MET:HE2	1.76	0.67
54:v:8:LEU:HD23	54:v:25:ILE:HD13	1.76	0.66
2:2:974:A:OP1	51:s:69:ARG:NH1	2.29	0.66
2:2:1358:U:O4	2:2:1363:A:C2	2.46	0.65
33:a:16:CYS:CB	33:a:37:CYS:HB3	2.26	0.65
8:B:6:CYS:SG	8:B:13:ARG:NH1	2.69	0.65
19:M:66:ARG:NH1	19:M:104:GLU:OE1	2.29	0.65
1:1:2297:A:C2	1:1:2321:U:C4	2.84	0.65
1:1:2196:C:O3'	1:1:2197:U:P	2.55	0.64
2:2:146:G:H2'	2:2:147:G:H5'	1.79	0.64
16:J:17:VAL:HG23	16:J:137:PRO:HB2	1.79	0.64
40:h:77:ILE:HA	40:h:84:VAL:HG23	1.79	0.64
1:1:1021:A:C2	1:1:1141:U:O4	2.46	0.64
1:1:2435:A:O2'	1:1:2436:G:O5'	2.14	0.64
1:1:2315:G:OP1	11:E:33:LYS:NZ	2.31	0.64
15:I:82:ALA:HB2	15:I:108:ILE:HD11	1.79	0.64
2:2:37:U:O4	2:2:397:A:C2	2.48	0.63
1:1:1266:G:OP1	34:b:16:ARG:NE	2.31	0.63
7:7:21:LEU:HD21	7:7:113:LEU:HD12	1.80	0.63
27:U:34:VAL:HG13	27:U:67:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1824:G:O2'	8:B:252:THR:HG21	1.99	0.63
1:1:2298:A:C5	1:1:2321:U:O4	2.51	0.63
1:1:754:U:H2'	1:1:755:U:C6	2.34	0.63
2:2:439:U:O2	2:2:440:C:C5	2.51	0.63
1:1:2683:C:OP1	22:P:51:ARG:NH2	2.31	0.62
2:2:517:G:O2'	2:2:530:G:C5'	2.47	0.62
2:2:658:C:H1'	52:t:22:THR:HG21	1.81	0.62
1:1:1914:C:C5'	6:6:21:HIS:CE1	2.65	0.62
33:a:37:CYS:N	33:a:40:CYS:SG	2.71	0.62
2:2:528:C:N4	49:q:46:ASN:OD1	2.29	0.62
1:1:927:A:H2'	1:1:928:A:C8	2.34	0.62
1:1:1067:A:C6	7:7:54:GLN:HG3	2.35	0.62
2:2:35:G:N3	49:q:115:SER:OG	2.32	0.62
6:6:20:LEU:HD11	7:7:135:GLY:HA2	1.82	0.61
8:B:135:ILE:HD13	8:B:141:VAL:HG11	1.82	0.61
1:1:568:U:H1'	1:1:2030:6MZ:H9C1	1.81	0.61
1:1:1405:U:O2'	1:1:1406:U:O4'	2.17	0.61
1:1:1596:A:O2'	1:1:1597:A:O4'	2.18	0.61
26:T:61:LEU:HD12	26:T:61:LEU:C	2.25	0.61
36:d:31:LEU:HD22	36:d:42:LEU:CD1	2.30	0.61
9:C:37:VAL:HG22	9:C:48:ILE:HG22	1.82	0.61
2:2:517:G:O2'	2:2:530:G:C4'	2.45	0.61
2:2:517:G:O2'	2:2:530:G:H5''	2.00	0.61
2:2:527:7MG:H81	2:2:527:7MG:C3'	2.30	0.61
2:2:736:C:OP1	55:w:61:ARG:NH2	2.34	0.61
14:H:23:LEU:HD12	14:H:118:ILE:HG12	1.82	0.61
2:2:13:U:O2	2:2:915:A:N7	2.33	0.60
44:l:69:VAL:HG23	44:l:100:ALA:HB1	1.83	0.60
11:E:42:GLU:HG3	11:E:49:LEU:HD23	1.84	0.60
15:I:105:LEU:HD22	15:I:128:ILE:HG22	1.82	0.60
21:O:18:LEU:HD23	21:O:25:ARG:HD2	1.82	0.60
46:n:21:ILE:HD13	46:n:63:LEU:HB3	1.83	0.60
52:t:21:ASP:O	52:t:22:THR:HG22	2.02	0.59
3:3:48:U:H2'	3:3:49:C:C6	2.37	0.59
18:L:58:TYR:O	37:e:13:ARG:HD3	2.01	0.59
2:2:16:A:OP2	6:6:41:ARG:NH1	2.35	0.59
25:S:36:LEU:HD13	25:S:48:LYS:HA	1.84	0.59
43:k:63:ASN:HD22	43:k:96:VAL:HG23	1.67	0.59
2:2:527:7MG:C8	2:2:527:7MG:C3'	2.86	0.59
2:2:1061:G:OP2	40:h:2:GLY:O	2.20	0.59
2:2:563:A:N6	2:2:884:U:N3	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1218:C:H2'	2:2:1219:A:C8	2.36	0.59
7:7:338:THR:HG21	7:7:359:ALA:HB1	1.84	0.59
12:F:24:ILE:HD11	12:F:43:VAL:HG11	1.83	0.59
2:2:13:U:C4	2:2:21:G:C2	2.90	0.59
31:Y:49:ASP:O	31:Y:53:VAL:HG23	2.03	0.59
2:2:13:U:C5	2:2:20:U:O4	2.54	0.58
7:7:11:ILE:HD12	7:7:84:LEU:HD22	1.83	0.58
10:D:146:VAL:HG12	10:D:167:VAL:HG22	1.85	0.58
1:1:570:G:H2'	1:1:2030:6MZ:N7	2.18	0.58
44:l:23:LEU:O	44:l:27:VAL:HG13	2.03	0.58
2:2:13:U:C2	2:2:915:A:N6	2.70	0.58
2:2:515:G:O2'	2:2:516:PSU:O5'	2.21	0.58
2:2:563:A:N6	2:2:884:U:H3	2.02	0.58
20:N:67:PHE:O	20:N:71:ARG:N	2.36	0.58
24:R:5:PHE:HB3	24:R:59:ILE:HD12	1.86	0.58
2:2:966:2MG:HM22	5:5:34:C:H5''	1.84	0.58
26:T:50:LEU:HD23	31:Y:26:PHE:CZ	2.38	0.58
27:U:14:LEU:HD11	27:U:71:ALA:HB2	1.84	0.57
57:y:25:ARG:HA	57:y:66:LEU:HD21	1.86	0.57
1:1:2297:A:C2	1:1:2321:U:C5	2.92	0.57
1:1:1614:A:C2	25:S:93:ALA:HB2	2.39	0.57
2:2:146:G:O2'	2:2:147:G:H5'	2.05	0.57
42:j:94:VAL:HG13	42:j:111:MET:HE1	1.86	0.57
2:2:1499:A:O2'	2:2:1500:A:H5'	2.04	0.57
53:u:21:VAL:HG21	53:u:60:TRP:CD1	2.40	0.57
1:1:627:A:OP1	18:L:78:ARG:NH2	2.38	0.56
2:2:966:2MG:H5''	2:2:967:5MC:OP2	2.05	0.56
25:S:20:VAL:HG11	25:S:44:ALA:HA	1.87	0.56
1:1:1590:A:H2'	1:1:1591:A:C8	2.40	0.56
10:D:181:ILE:HG12	18:L:1:MET:HE3	1.85	0.56
21:O:35:ILE:HG21	21:O:71:ALA:HA	1.86	0.56
39:g:148:LEU:HD22	39:g:151:ILE:HD11	1.86	0.56
1:1:1020:A:C2	1:1:1141:U:C2	2.93	0.56
2:2:107:G:N7	57:y:10:ARG:NH2	2.51	0.56
2:2:927:G:H2'	2:2:928:G:H5'	1.87	0.56
1:1:929:U:H1'	32:Z:26:GLY:O	2.05	0.56
15:I:78:LEU:HD22	15:I:108:ILE:HG23	1.86	0.56
22:P:14:LYS:NZ	22:P:76:THR:O	2.39	0.56
51:s:47:LYS:O	51:s:50:THR:OG1	2.17	0.56
47:o:57:VAL:O	47:o:57:VAL:HG13	2.04	0.56
51:s:46:LEU:CD1	56:x:13:LEU:HD13	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:56:VAL:O	42:j:60:ILE:HG23	2.06	0.56
7:7:96:PHE:O	7:7:100:VAL:HG23	2.05	0.56
1:1:1433:A:H2'	1:1:1434:A:O4'	2.05	0.56
39:g:129:LEU:HD13	39:g:134:ALA:HB2	1.88	0.56
1:1:404:A:O2'	1:1:405:U:OP2	2.25	0.56
1:1:1082:U:N3	1:1:1086:A:N6	2.54	0.56
1:1:2646:C:O5'	1:1:2646:C:H6	1.89	0.56
2:2:1169:A:H2'	2:2:1170:A:C8	2.40	0.55
51:s:46:LEU:O	51:s:50:THR:HG23	2.06	0.55
1:1:1250:G:OP2	18:L:21:ARG:NH2	2.39	0.55
2:2:13:U:O4	2:2:21:G:N3	2.39	0.55
2:2:928:G:O2'	2:2:929:G:C5'	2.54	0.55
2:2:1275:A:H2'	2:2:1276:G:H5'	1.87	0.55
40:h:9:GLY:HA3	51:s:89:MET:HE3	1.88	0.55
1:1:1070:A:N7	1:1:1096:A:O2'	2.40	0.55
2:2:769:G:H4'	2:2:1513:A:H4'	1.87	0.55
16:J:17:VAL:HG22	16:J:55:ILE:HB	1.88	0.55
36:d:18:PHE:HA	36:d:43:THR:HG21	1.87	0.55
1:1:2328:A:H2'	1:1:2329:U:C6	2.41	0.55
2:2:515:G:H2'	2:2:516:PSU:C6	2.41	0.55
1:1:2245:U:O2'	1:1:2436:G:OP2	2.24	0.55
2:2:404:G:N7	41:i:2:ALA:HB3	2.21	0.55
42:j:13:GLU:HB3	42:j:39:VAL:HG12	1.88	0.55
1:1:2249:U:H3'	1:1:2250:G:H5'	1.89	0.55
12:F:35:ARG:HD3	12:F:71:LEU:HD13	1.88	0.55
41:i:37:ALA:HB1	41:i:38:PRO:HD2	1.89	0.55
10:D:108:ILE:HD11	10:D:180:LEU:HD13	1.87	0.55
2:2:1208:C:H2'	2:2:1209:C:C6	2.42	0.55
2:2:673:A:H2'	2:2:674:G:C8	2.42	0.54
2:2:915:A:C6	2:2:916:U:C4	2.94	0.54
2:2:1518:MA6:N6	2:2:1519:MA6:H93	2.22	0.54
7:7:14:LEU:HD13	7:7:103:LEU:CD1	2.38	0.54
47:o:8:ILE:HG23	47:o:100:ILE:HD13	1.89	0.54
51:s:41:ARG:O	51:s:45:VAL:HG13	2.06	0.54
1:1:2006:C:O2'	1:1:2823:A:N3	2.40	0.54
1:1:2082:A:H2'	1:1:2083:G:O4'	2.07	0.54
48:p:67:ALA:HB2	48:p:96:THR:HG23	1.89	0.54
2:2:13:U:C4	2:2:915:A:C6	2.88	0.54
13:G:9:VAL:HG11	13:G:12:LEU:HD21	1.88	0.54
48:p:89:PRO:HG3	58:z:32:VAL:HG11	1.89	0.54
2:2:195:A:O2'	2:2:196:A:C5'	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:32:4OC:HM43	5:5:33:U:C4	2.43	0.54
15:I:82:ALA:CB	15:I:108:ILE:HD11	2.36	0.54
1:1:1327:A:H2'	1:1:1328:A:O4'	2.08	0.54
2:2:13:U:C2	2:2:915:A:C6	2.96	0.54
2:2:1206:G:H2'	2:2:1207:2MG:C8	2.42	0.54
11:E:25:VAL:O	11:E:28:VAL:HG12	2.08	0.54
13:G:58:LEU:O	13:G:61:VAL:HG22	2.08	0.54
28:V:14:LYS:O	28:V:18:ARG:HG2	2.08	0.54
1:1:1570:A:H2'	1:1:1571:A:C8	2.43	0.54
7:7:155:TRP:CZ3	7:7:192:LEU:HD21	2.43	0.54
49:q:4:VAL:HG23	54:v:34:TYR:HB3	1.89	0.54
2:2:1130:A:O2'	46:n:5:GLN:NE2	2.41	0.54
2:2:1175:G:N3	2:2:1176:A:C8	2.76	0.54
7:7:11:ILE:CD1	7:7:84:LEU:HD22	2.38	0.54
8:B:78:VAL:HG21	8:B:110:LEU:HD21	1.89	0.54
1:1:1717:A:H2'	1:1:1718:G:O4'	2.07	0.54
2:2:915:A:H3'	2:2:915:A:C8	2.43	0.54
27:U:94:ARG:HB3	27:U:103:ILE:HD12	1.88	0.54
25:S:59:GLU:CG	25:S:66:ILE:HD11	2.38	0.54
35:c:17:THR:HG21	35:c:42:VAL:HG21	1.90	0.54
10:D:104:ALA:O	10:D:108:ILE:HG23	2.08	0.53
22:P:33:VAL:HG22	22:P:38:LYS:HG2	1.91	0.53
2:2:195:A:C2'	2:2:196:A:H5'	2.35	0.53
8:B:155:ALA:HB2	8:B:162:VAL:HG23	1.90	0.53
18:L:77:ILE:HD11	18:L:108:ALA:HB1	1.89	0.53
2:2:62:U:OP1	2:2:385:C:O2'	2.25	0.53
1:1:1385:A:O2'	1:1:1396:U:O2	2.26	0.53
1:1:1596:A:O2'	1:1:1597:A:H8	1.72	0.53
2:2:1275:A:C2'	2:2:1276:G:H5'	2.38	0.53
32:Z:7:ILE:HD13	32:Z:27:LEU:HD22	1.91	0.53
1:1:1797:G:O2'	8:B:257:THR:OG1	2.24	0.53
1:1:2298:A:C2	1:1:2321:U:C5	2.96	0.53
2:2:481:G:HO2'	2:2:483:C:H41	1.53	0.53
42:j:156:LYS:HG2	45:m:71:VAL:HG13	1.90	0.53
8:B:165:VAL:HG21	8:B:181:MET:HE1	1.91	0.53
1:1:811:U:H2'	18:L:21:ARG:HA	1.90	0.53
1:1:1153:C:OP1	23:Q:92:ARG:NH1	2.42	0.53
2:2:397:A:H3'	2:2:397:A:N3	2.23	0.53
2:2:1389:C:C2'	2:2:1390:U:H5'	2.39	0.53
17:K:123:LEU:HD21	22:P:70:VAL:HG11	1.91	0.53
1:1:1588:G:C6	1:1:1589:U:O4	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1174:G:H2'	2:2:1175:G:H5'	1.89	0.53
2:2:1366:C:O2'	47:o:62:ARG:NH2	2.42	0.53
8:B:240:PHE:CD2	8:B:240:PHE:O	2.61	0.53
2:2:915:A:N6	2:2:916:U:O4	2.42	0.53
43:k:88:MET:HE1	55:w:61:ARG:HG2	1.91	0.53
1:1:1869:G:N2	1:1:1871:A:O2'	2.42	0.52
2:2:13:U:O4	2:2:20:U:C4	2.61	0.52
2:2:712:A:H2'	2:2:713:G:O4'	2.09	0.52
21:O:53:THR:HG23	21:O:74:VAL:CG2	2.39	0.52
2:2:37:U:O2	2:2:548:G:C2	2.62	0.52
27:U:36:VAL:CG1	27:U:39:ILE:HD12	2.38	0.52
42:j:13:GLU:CB	42:j:39:VAL:HG12	2.39	0.52
1:1:2029:G:N1	1:1:2033:A:OP2	2.33	0.52
8:B:160:THR:H	8:B:195:VAL:HG12	1.75	0.52
17:K:107:LEU:HD21	17:K:115:ILE:HG21	1.92	0.52
41:i:48:LEU:HD23	41:i:53:VAL:HG12	1.90	0.52
2:2:109:A:H2'	2:2:326:G:N2	2.24	0.52
1:1:2557:G:H2'	1:1:2558:C:C6	2.45	0.52
7:7:17:ARG:HD3	7:7:110:LEU:HD22	1.92	0.52
7:7:80:VAL:HG11	7:7:103:LEU:HD13	1.91	0.52
7:7:239:LEU:HD11	7:7:241:ILE:HD11	1.91	0.52
51:s:74:LEU:HD12	51:s:84:VAL:HG21	1.92	0.52
2:2:864:A:H2'	2:2:865:A:C8	2.45	0.51
27:U:94:ARG:CB	27:U:103:ILE:HD12	2.40	0.51
16:J:32:LEU:CD2	16:J:54:ILE:HG21	2.39	0.51
55:w:12:ARG:O	55:w:16:GLU:HG3	2.10	0.51
1:1:783:A:N3	1:1:783:A:C2'	2.70	0.51
1:1:372:G:O2'	1:1:400:G:O6	2.28	0.51
2:2:966:2MG:H2'	2:2:966:2MG:N3	2.26	0.51
12:F:121:ILE:HD12	12:F:141:ILE:CG2	2.40	0.51
43:k:51:ILE:HG13	43:k:85:ILE:HG21	1.91	0.51
1:1:1020:A:C6	1:1:1141:U:O2	2.63	0.51
1:1:2683:C:O2	17:K:70:ARG:NH2	2.41	0.51
2:2:1225:A:N3	2:2:1225:A:C2'	2.72	0.51
42:j:149:SER:O	42:j:153:VAL:HG13	2.11	0.51
2:2:439:U:O2	2:2:440:C:C6	2.64	0.51
2:2:516:PSU:O2'	2:2:519:C:N3	2.42	0.51
21:O:51:ALA:HB3	21:O:78:VAL:HB	1.92	0.51
32:Z:25:LEU:C	32:Z:25:LEU:HD13	2.36	0.51
42:j:150:PRO:O	42:j:153:VAL:HG22	2.10	0.51
41:i:100:ASN:OD1	41:i:111:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:518:C:C5	2:2:529:G:H2'	2.46	0.51
1:1:1596:A:C2'	1:1:1597:A:C8	2.94	0.50
2:2:789:U:O2'	2:2:791:G:N7	2.37	0.50
18:L:57:LEU:HD22	37:e:54:ASP:HB3	1.93	0.50
46:n:10:GLY:HA3	46:n:78:ALA:O	2.11	0.50
47:o:56:HIS:O	47:o:57:VAL:HG12	2.11	0.50
50:r:23:TYR:CD1	50:r:69:LEU:HD23	2.45	0.50
7:7:144:TRP:CE3	7:7:201:LEU:HD22	2.47	0.50
40:h:121:THR:HG23	40:h:189:ALA:HA	1.94	0.50
42:j:107:ALA:HB2	42:j:125:ALA:HB3	1.92	0.50
1:1:476:G:H4'	1:1:502:A:N1	2.27	0.50
1:1:2547:A:H2'	1:1:2548:U:C6	2.46	0.50
41:i:61:VAL:HG21	41:i:200:ILE:HD11	1.94	0.50
2:2:664:G:H22	2:2:741:G:H1	1.59	0.50
1:1:1797:G:HO2'	8:B:257:THR:HG1	1.57	0.50
2:2:496:A:N3	2:2:496:A:H2'	2.27	0.50
2:2:975:A:H8	2:2:1357:A:HO2'	1.58	0.50
8:B:158:ALA:C	8:B:195:VAL:HG13	2.37	0.50
1:1:1408:G:H2'	1:1:1409:U:C6	2.47	0.50
2:2:371:A:H2'	2:2:372:C:O4'	2.11	0.50
2:2:481:G:HO2'	2:2:483:C:N4	2.05	0.50
2:2:552:U:O2'	49:q:83:ARG:O	2.24	0.50
2:2:563:A:C2	2:2:884:U:O4	2.59	0.50
11:E:12:VAL:HG13	11:E:172:ALA:CB	2.42	0.49
25:S:59:GLU:HG3	25:S:66:ILE:HD11	1.94	0.49
57:y:55:GLN:N	57:y:56:PRO:HD2	2.27	0.49
1:1:2298:A:C6	1:1:2299:U:C2	3.00	0.49
2:2:528:C:N4	49:q:46:ASN:CG	2.68	0.49
15:I:38:CYS:SG	15:I:39:LYS:N	2.85	0.49
50:r:17:ILE:O	50:r:20:THR:OG1	2.19	0.49
1:1:1405:U:HO2'	1:1:1406:U:H6	1.56	0.49
2:2:321:A:N7	2:2:328:C:O2'	2.45	0.49
1:1:2585:U:O2	1:1:2585:U:O4'	2.30	0.49
2:2:14:U:OP2	6:6:41:ARG:NH2	2.46	0.49
2:2:346:G:OP1	22:P:39:ARG:NH2	2.43	0.49
7:7:353:LEU:HD12	7:7:357:ILE:HD11	1.94	0.49
2:2:526:C:P	49:q:88:LYS:HE3	2.53	0.49
2:2:604:G:H2'	2:2:605:U:O4'	2.12	0.49
10:D:90:GLN:HG3	10:D:92:HIS:CE1	2.48	0.49
39:g:217:VAL:O	39:g:221:VAL:HG23	2.13	0.49
48:p:31:ILE:HG12	48:p:46:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:39:G:H1'	10:D:43:THR:HG21	1.95	0.49
1:1:2297:A:C6	1:1:2321:U:O4	2.64	0.49
2:2:1064:G:O2'	2:2:1190:G:N2	2.45	0.49
1:1:2291:U:H2'	1:1:2292:U:C6	2.47	0.49
9:C:26:VAL:HG22	9:C:188:LEU:CD2	2.43	0.49
13:G:3:VAL:HG22	13:G:36:ALA:HB1	1.95	0.49
21:O:27:VAL:HG21	21:O:40:ILE:HD12	1.94	0.49
26:T:34:VAL:HG21	26:T:43:ILE:HD11	1.95	0.49
1:1:207:A:H2'	1:1:208:C:O4'	2.13	0.49
1:1:2059:A:N6	1:1:2503:2MA:O2'	2.46	0.49
2:2:555:U:H2'	2:2:556:C:C6	2.48	0.49
29:W:37:ILE:HG22	29:W:38:VAL:HG23	1.95	0.49
49:q:67:ILE:HD13	49:q:74:LEU:HD23	1.95	0.49
7:7:64:GLU:O	7:7:68:ASP:CB	2.60	0.48
16:J:30:THR:HG22	16:J:31:GLU:N	2.27	0.48
1:1:70:G:H4'	1:1:71:A:OP1	2.13	0.48
2:2:13:U:C2	2:2:915:A:C5	3.01	0.48
1:1:464:U:O3'	36:d:12:ARG:NH2	2.45	0.48
2:2:373:A:O2'	2:2:451:A:N7	2.46	0.48
2:2:767:A:H2'	2:2:768:A:O4'	2.14	0.48
27:U:13:VAL:CG2	27:U:39:ILE:HD13	2.42	0.48
1:1:1789:A:OP2	8:B:221:ARG:NH1	2.47	0.48
1:1:2298:A:C6	1:1:2321:U:O4	2.66	0.48
2:2:1527:U:OP2	58:z:42:THR:HG22	2.14	0.48
21:O:53:THR:HG23	21:O:74:VAL:HG21	1.94	0.48
50:r:16:VAL:HG23	50:r:17:ILE:HD12	1.96	0.48
54:v:75:LEU:C	54:v:75:LEU:HD12	2.38	0.48
1:1:1469:A:H2'	1:1:1470:A:C8	2.49	0.48
1:1:2243:U:H2'	1:1:2244:U:C6	2.49	0.48
1:1:2291:U:OP1	1:1:2380:C:O2'	2.28	0.48
2:2:1054:C:O2'	7:7:204:LYS:NZ	2.46	0.48
8:B:88:SER:O	8:B:197:ASN:ND2	2.40	0.48
36:d:12:ARG:CG	36:d:44:VAL:HG11	2.43	0.48
1:1:2065:C:H4'	1:1:2251:OMG:CM2	2.43	0.48
49:q:57:LEU:HD21	49:q:82:ILE:CD1	2.43	0.48
1:1:1914:C:O2'	1:1:1915:3TD:H5'A	2.14	0.48
11:E:57:LEU:HD12	11:E:87:CYS:SG	2.54	0.48
46:n:52:LEU:HD11	46:n:63:LEU:HD21	1.96	0.48
8:B:157:SER:O	8:B:195:VAL:HG11	2.14	0.48
37:e:26:HIS:CE1	37:e:48:ALA:HB2	2.48	0.48
43:k:18:VAL:N	43:k:19:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:108:G:H5''	2:2:108:G:N3	2.29	0.48
7:7:239:LEU:HD11	7:7:241:ILE:CD1	2.44	0.48
16:J:73:VAL:HG11	16:J:75:TYR:CZ	2.48	0.48
39:g:111:ILE:HD12	39:g:152:LYS:HA	1.96	0.48
1:1:214:G:N2	1:1:216:A:N3	2.62	0.47
2:2:55:A:N1	2:2:368:U:H5	2.12	0.47
2:2:1473:G:H2'	2:2:1474:U:O4'	2.14	0.47
56:x:15:LEU:HD13	56:x:33:THR:HG21	1.96	0.47
7:7:263:ILE:HD13	7:7:287:ALA:CB	2.44	0.47
12:F:121:ILE:HD12	12:F:141:ILE:HG22	1.96	0.47
25:S:29:VAL:HB	25:S:55:ILE:HD11	1.96	0.47
36:d:30:VAL:HG22	36:d:33:ARG:NH1	2.29	0.47
39:g:129:LEU:HD13	39:g:134:ALA:CB	2.44	0.47
1:1:2038:G:H2'	1:1:2039:U:O4'	2.14	0.47
8:B:146:MET:HE3	8:B:154:LEU:HD21	1.96	0.47
33:a:16:CYS:CB	33:a:37:CYS:CB	2.93	0.47
1:1:1720:U:H2'	1:1:1721:G:O4'	2.15	0.47
2:2:37:U:N3	2:2:397:A:C6	2.83	0.47
6:6:19:LEU:C	6:6:19:LEU:HD23	2.40	0.47
40:h:155:GLY:HA2	40:h:163:ALA:HB1	1.97	0.47
2:2:195:A:HO2'	2:2:196:A:H5'	1.69	0.47
8:B:43:ARG:NH2	8:B:49:ILE:HD11	2.29	0.47
9:C:25:THR:HG21	9:C:193:VAL:HG22	1.96	0.47
1:1:1853:A:N1	1:1:2087:G:H1'	2.29	0.47
40:h:113:ALA:HA	40:h:202:ILE:HD12	1.97	0.47
43:k:39:LEU:HD12	43:k:40:GLU:N	2.29	0.47
44:l:93:PRO:O	44:l:96:ARG:HG2	2.14	0.47
52:t:4:SER:O	52:t:8:THR:HG23	2.15	0.47
1:1:2014:A:H2'	1:1:2015:A:C8	2.50	0.47
2:2:5:U:O2	2:2:5:U:O4'	2.33	0.47
2:2:148:G:O2'	2:2:149:A:C5'	2.62	0.47
2:2:1318:A:OP1	56:x:3:ARG:NH1	2.47	0.47
10:D:48:THR:HG23	10:D:86:ALA:HB3	1.97	0.47
13:G:99:ILE:O	13:G:103:VAL:HG23	2.15	0.47
23:Q:41:LYS:HE2	23:Q:45:TYR:CZ	2.49	0.47
27:U:13:VAL:HG23	27:U:39:ILE:HD13	1.96	0.47
1:1:244:A:H2'	1:1:245:G:O4'	2.15	0.47
1:1:2572:A:N7	9:C:150:GLN:NE2	2.63	0.47
16:J:77:HIS:HA	16:J:83:GLY:O	2.15	0.47
24:R:26:ASP:O	24:R:27:ILE:HD13	2.14	0.47
54:v:48:ASP:HB3	54:v:75:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1208:C:H2'	2:2:1209:C:H6	1.80	0.47
2:2:1526:G:OP2	58:z:42:THR:HG23	2.14	0.47
1:1:1317:G:H2'	1:1:1318:U:O4'	2.15	0.47
6:6:20:LEU:O	6:6:20:LEU:HD13	2.15	0.47
7:7:201:LEU:HD21	7:7:203:ARG:HD3	1.96	0.47
27:U:72:ILE:HD12	27:U:83:VAL:HG21	1.96	0.47
1:1:548:G:H3'	1:1:549:G:O4'	2.14	0.46
1:1:819:A:C4	1:1:1189:A:C2	3.03	0.46
1:1:910:A:N3	1:1:2264:C:O2'	2.46	0.46
8:B:158:ALA:HB1	8:B:197:ASN:O	2.15	0.46
11:E:171:ALA:O	11:E:174:ASP:N	2.49	0.46
18:L:75:ALA:HB2	18:L:105:ILE:HD12	1.95	0.46
1:1:639:U:H2'	1:1:640:C:C6	2.50	0.46
1:1:700:G:H2'	1:1:701:G:O4'	2.15	0.46
1:1:2615:U:C2	34:b:4:GLN:HA	2.50	0.46
2:2:1317:C:OP2	51:s:28:LYS:CE	2.63	0.46
2:2:1402:4OC:O2	2:2:1500:A:N1	2.47	0.46
49:q:110:ARG:NH1	49:q:112:GLN:O	2.45	0.46
51:s:80:SER:O	51:s:84:VAL:HG23	2.16	0.46
1:1:1067:A:O2'	1:1:1068:G:O4'	2.33	0.46
1:1:2469:A:N6	1:1:2481:G:O2'	2.48	0.46
2:2:1225:A:N3	2:2:1225:A:H2'	2.30	0.46
1:1:84:A:N1	1:1:98:G:O2'	2.37	0.46
1:1:813:U:H2'	1:1:814:C:C6	2.50	0.46
1:1:2788:C:H2'	1:1:2789:C:C6	2.51	0.46
42:j:99:ALA:HB1	42:j:103:THR:HG21	1.97	0.46
42:j:111:MET:CE	42:j:125:ALA:HB1	2.33	0.46
42:j:114:VAL:HG21	42:j:141:ILE:HD12	1.98	0.46
1:1:1824:G:O2'	8:B:252:THR:CG2	2.64	0.46
1:1:2074:U:C2	1:1:2435:A:N1	2.76	0.46
43:k:10:VAL:HG11	43:k:18:VAL:HG22	1.98	0.46
49:q:87:VAL:HG23	49:q:93:VAL:CG1	2.45	0.46
1:1:1980:G:O2'	1:1:1982:U:OP2	2.34	0.46
1:1:2245:U:O2	1:1:2435:A:H2'	2.15	0.46
2:2:1356:G:H2'	2:2:1357:A:C8	2.51	0.46
2:2:1375:A:OP1	44:l:25:LYS:NZ	2.49	0.46
14:H:118:ILE:HB	14:H:119:PRO:HD3	1.98	0.46
11:E:8:TYR:HA	11:E:12:VAL:HB	1.97	0.46
20:N:38:LEU:N	20:N:39:PRO:CD	2.79	0.46
25:S:25:ARG:NH1	25:S:74:ILE:O	2.49	0.46
39:g:206:ALA:O	39:g:210:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:17:GLU:H	6:6:17:GLU:CD	1.96	0.46
45:m:18:GLN:OE1	45:m:18:GLN:HA	2.14	0.46
1:1:1141:U:H4'	1:1:1142:A:O4'	2.16	0.46
1:1:2315:G:OP1	11:E:33:LYS:CE	2.64	0.46
2:2:626:G:OP1	53:u:35:ARG:NH2	2.48	0.46
2:2:915:A:C8	2:2:915:A:C3'	2.99	0.46
7:7:144:TRP:CD2	7:7:201:LEU:HB2	2.51	0.46
9:C:49:GLN:OE1	9:C:79:LEU:HD13	2.16	0.46
1:1:1614:A:N1	25:S:93:ALA:HB2	2.31	0.46
10:D:131:THR:HG22	10:D:160:ALA:O	2.16	0.46
32:Z:24:LEU:HD11	32:Z:54:MET:HE2	1.98	0.46
49:q:79:VAL:HG12	49:q:102:LEU:HD23	1.98	0.46
1:1:1056:G:O2'	1:1:1103:A:N6	2.49	0.45
2:2:517:G:HO2'	2:2:530:G:H5''	1.79	0.45
7:7:14:LEU:HD13	7:7:103:LEU:HD11	1.97	0.45
21:O:27:VAL:CG2	21:O:40:ILE:HD12	2.46	0.45
42:j:136:VAL:O	42:j:140:THR:HG23	2.17	0.45
1:1:1344:U:H5'	1:1:1384:A:C6	2.51	0.45
1:1:2445:2MG:P	10:D:69:ARG:HH22	2.38	0.45
2:2:945:G:C2	2:2:946:A:C8	3.05	0.45
2:2:1017:U:O2'	2:2:1018:G:O4'	2.34	0.45
14:H:18:VAL:HA	14:H:86:MET:HE2	1.98	0.45
45:m:3:MET:HE3	45:m:3:MET:HA	1.97	0.45
52:t:64:ARG:NH1	52:t:68:ASP:OD1	2.50	0.45
1:1:320:A:H2'	10:D:131:THR:HG21	1.99	0.45
1:1:1394:U:H4'	1:1:1603:A:H4'	1.97	0.45
7:7:76:GLY:O	7:7:80:VAL:HG23	2.17	0.45
8:B:91:ILE:HD12	8:B:103:TYR:CD1	2.51	0.45
8:B:94:VAL:HG11	8:B:116:ILE:HD11	1.98	0.45
9:C:121:THR:HB	9:C:127:PHE:CD2	2.50	0.45
23:Q:58:ARG:HA	23:Q:61:TRP:CE3	2.52	0.45
32:Z:44:ILE:HD13	32:Z:47:MET:HE3	1.97	0.45
1:1:784:G:H5'	1:1:785:G:OP1	2.16	0.45
1:1:1919:A:N1	2:2:1495:U:O2'	2.41	0.45
2:2:1526:G:P	58:z:42:THR:HG23	2.56	0.45
7:7:298:LEU:HD23	7:7:298:LEU:O	2.15	0.45
23:Q:76:TYR:CZ	23:Q:80:ILE:HG13	2.51	0.45
1:1:67:U:C2	1:1:74:A:N6	2.84	0.45
1:1:1047:G:N2	1:1:1110:G:O2'	2.49	0.45
1:1:2313:C:H5''	11:E:68:THR:HG21	1.97	0.45
2:2:1350:A:OP2	46:n:120:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:22:ASP:CG	6:6:23:PRO:HD2	2.41	0.45
7:7:353:LEU:CD1	7:7:357:ILE:HD11	2.45	0.45
9:C:152:PRO:HG3	9:C:156:PHE:CZ	2.51	0.45
10:D:5:LEU:HD23	10:D:122:GLU:OE1	2.17	0.45
26:T:2:ILE:HD13	26:T:42:GLU:HA	1.99	0.45
50:r:16:VAL:O	50:r:20:THR:HG23	2.16	0.45
2:2:716:A:N3	48:p:119:ASN:O	2.49	0.45
6:6:16:ILE:N	6:6:17:GLU:OE1	2.49	0.45
6:6:23:PRO:O	6:6:24:LEU:C	2.60	0.45
10:D:138:LEU:HD13	10:D:167:VAL:HG21	1.98	0.45
56:x:49:ILE:HD12	56:x:71:LEU:HD21	1.98	0.45
1:1:1510:G:H2'	1:1:1511:G:O4'	2.16	0.45
1:1:1783:A:N1	1:1:2587:A:H2'	2.31	0.45
1:1:1922:G:C2'	1:1:1923:U:H5'	2.47	0.45
1:1:1939:5MU:OP1	1:1:2604:U:O2'	2.35	0.45
2:2:1435:G:H2'	2:2:1436:U:C6	2.51	0.45
2:2:1493:A:O2'	2:2:1494:G:P	2.74	0.45
2:2:1499:A:O2'	2:2:1500:A:C5'	2.65	0.45
11:E:42:GLU:CG	11:E:49:LEU:HD23	2.47	0.45
16:J:110:PRO:O	16:J:115:GLY:HA3	2.17	0.45
42:j:81:LEU:HD13	42:j:123:VAL:HG12	1.99	0.45
1:1:2552:OMU:O5'	1:1:2552:OMU:H6	2.17	0.45
16:J:114:LEU:HD12	16:J:114:LEU:HA	1.81	0.45
17:K:1:MET:HE3	17:K:32:TYR:CE2	2.52	0.45
39:g:187:VAL:HG21	39:g:199:VAL:HG23	1.98	0.45
58:z:58:LYS:O	58:z:62:ARG:CG	2.65	0.45
1:1:729:G:H2'	1:1:1775:U:H1'	1.99	0.45
1:1:851:C:O2'	32:Z:43:ALA:O	2.30	0.45
1:1:197:A:N6	1:1:2430:A:H2'	2.32	0.45
1:1:348:A:H2'	1:1:349:U:O4'	2.17	0.45
13:G:96:THR:HG22	13:G:115:VAL:HB	1.99	0.45
1:1:1797:G:C5	1:1:1798:U:C5	3.05	0.44
7:7:5:ASN:N	7:7:6:PRO:CD	2.80	0.44
7:7:199:HIS:CE1	7:7:323:ILE:HD11	2.52	0.44
18:L:96:LYS:HG3	18:L:101:ILE:HD11	1.99	0.44
57:y:25:ARG:CA	57:y:66:LEU:HD21	2.47	0.44
1:1:319:G:H2'	1:1:320:A:O4'	2.17	0.44
1:1:782:A:C6	8:B:225:MET:HE2	2.52	0.44
2:2:1382:C:O2'	2:2:1383:C:H5'	2.17	0.44
3:3:28:C:H2'	3:3:29:A:O4'	2.17	0.44
23:Q:92:ARG:HA	23:Q:95:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:28:VAL:O	10:D:32:VAL:HG23	2.18	0.44
39:g:15:HIS:HB3	39:g:43:LEU:HD11	2.00	0.44
41:i:119:SER:O	41:i:131:ASN:ND2	2.44	0.44
1:1:981:A:H2	1:1:2027:G:N3	2.15	0.44
1:1:1993:U:H4'	9:C:133:THR:HG22	1.99	0.44
2:2:244:U:O4	2:2:906:A:H1'	2.17	0.44
2:2:529:G:O2'	2:2:530:G:H5'	2.17	0.44
2:2:798:U:H2'	2:2:799:G:O4'	2.16	0.44
2:2:928:G:O2'	2:2:929:G:O5'	2.36	0.44
2:2:1323:G:H2'	2:2:1324:A:C8	2.53	0.44
1:1:2537:U:H2'	1:1:2538:C:C6	2.52	0.44
2:2:140:U:H2'	2:2:141:G:O4'	2.18	0.44
2:2:515:G:H2'	2:2:516:PSU:H6	1.82	0.44
2:2:1176:A:H2'	2:2:1177:G:O4'	2.17	0.44
25:S:17:VAL:HG12	25:S:76:VAL:HG21	1.99	0.44
40:h:117:ALA:HB2	40:h:200:VAL:CG1	2.47	0.44
46:n:55:VAL:HG23	46:n:55:VAL:O	2.18	0.44
54:v:38:ILE:HD12	54:v:38:ILE:N	2.33	0.44
1:1:1064:C:H2'	1:1:1065:U:C6	2.51	0.44
1:1:1141:U:O2	1:1:1142:A:N6	2.51	0.44
1:1:1519:G:H2'	1:1:1520:U:O4'	2.18	0.44
2:2:872:A:N3	2:2:872:A:H2'	2.33	0.44
2:2:1207:2MG:C2'	2:2:1208:C:H5'	2.48	0.44
3:3:65:U:C4	3:3:108:A:C4	3.06	0.44
7:7:18:SER:HA	7:7:110:LEU:HD11	2.00	0.44
11:E:57:LEU:HD13	11:E:65:PRO:HB3	1.99	0.44
1:1:1028:A:N6	1:1:1125:G:H2'	2.32	0.44
1:1:1063:G:H4'	15:I:135:MET:HE2	1.99	0.44
1:1:2065:C:H2'	1:1:2066:C:O4'	2.18	0.44
1:1:2298:A:C5	1:1:2321:U:C4	3.06	0.44
2:2:399:G:H2'	2:2:400:C:C6	2.52	0.44
2:2:515:G:O2'	2:2:516:PSU:C5'	2.66	0.44
2:2:915:A:C5	2:2:916:U:C5	3.05	0.44
2:2:967:5MC:H5''	2:2:968:A:P	2.58	0.44
2:2:1103:C:OP1	39:g:95:ARG:NH2	2.50	0.44
8:B:19:VAL:HG13	8:B:199:GLU:HG3	1.99	0.44
14:H:35:VAL:O	14:H:39:THR:HG23	2.18	0.44
19:M:24:THR:HG22	19:M:24:THR:O	2.17	0.44
23:Q:14:HIS:O	23:Q:18:LEU:HD23	2.17	0.44
24:R:25:LEU:HD12	24:R:94:THR:HG21	2.00	0.44
27:U:13:VAL:HG21	27:U:39:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:x:49:ILE:CD1	56:x:71:LEU:HD21	2.48	0.44
1:1:1386:C:H2'	1:1:1387:A:C8	2.53	0.44
2:2:986:U:H2'	2:2:987:G:O4'	2.18	0.44
2:2:1394:A:N1	2:2:1500:A:O2'	2.37	0.44
7:7:266:ILE:HB	7:7:267:PRO:HD3	2.00	0.44
16:J:28:LEU:HD12	16:J:142:ILE:HG21	1.99	0.44
31:Y:26:PHE:CE1	31:Y:30:MET:HE3	2.52	0.44
1:1:754:U:O2	1:1:755:U:C2	2.71	0.44
2:2:37:U:C4	2:2:397:A:N6	2.82	0.44
2:2:860:A:H2'	2:2:861:G:O4'	2.18	0.44
2:2:1382:C:C2'	2:2:1383:C:H5'	2.48	0.44
6:6:22:ASP:OD1	6:6:23:PRO:CD	2.57	0.44
9:C:71:ALA:HB3	9:C:73:VAL:HG12	1.99	0.44
1:1:57:C:H2'	1:1:58:G:O4'	2.18	0.43
1:1:973:A:O4'	1:1:1188:U:C6	2.71	0.43
1:1:1169:A:N3	1:1:1169:A:H5''	2.33	0.43
2:2:1370:G:C2	2:2:1371:G:C8	3.06	0.43
1:1:36:G:N3	1:1:450:G:O2'	2.52	0.43
1:1:1062:G:O2'	15:I:131:THR:HG23	2.19	0.43
19:M:53:MET:HG3	19:M:63:ILE:HD13	2.00	0.43
48:p:52:PHE:CE1	48:p:65:VAL:HG21	2.53	0.43
2:2:421:U:O2	2:2:421:U:O4'	2.37	0.43
2:2:564:C:OP1	49:q:12:ARG:HD2	2.17	0.43
2:2:580:C:H2'	2:2:581:G:O4'	2.18	0.43
2:2:1518:MA6:C9	2:2:1519:MA6:H93	2.48	0.43
7:7:298:LEU:C	7:7:298:LEU:CD2	2.85	0.43
42:j:81:LEU:HD13	42:j:123:VAL:CG1	2.48	0.43
44:l:79:ARG:HB3	44:l:84:THR:HG23	1.99	0.43
57:y:54:MET:O	57:y:57:ILE:HG22	2.18	0.43
1:1:1656:C:OP1	9:C:141:ARG:NH1	2.52	0.43
1:1:2698:U:H2'	1:1:2699:C:C6	2.53	0.43
2:2:1302:C:C6	50:r:17:ILE:HG12	2.54	0.43
50:r:16:VAL:HG13	50:r:34:LEU:CD1	2.48	0.43
1:1:2273:A:H2'	1:1:2274:A:C8	2.53	0.43
1:1:2314:A:H2'	1:1:2315:G:C8	2.53	0.43
17:K:42:THR:HG23	17:K:44:LYS:HE2	2.01	0.43
17:K:113:MET:O	17:K:116:ILE:HG13	2.17	0.43
1:1:2133:G:O2'	1:1:2157:G:N2	2.50	0.43
2:2:1175:G:O2'	2:2:1176:A:P	2.76	0.43
2:2:1460:C:H2'	2:2:1461:G:O4'	2.18	0.43
14:H:14:GLU:O	14:H:18:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:679:C:H2'	1:1:680:C:C6	2.53	0.43
1:1:1182:G:H2'	1:1:1183:U:O4'	2.18	0.43
1:1:1912:A:N1	2:2:1407:5MC:O2'	2.51	0.43
1:1:2885:G:N7	34:b:40:ARG:NH2	2.58	0.43
2:2:657:U:O2	52:t:22:THR:HG23	2.18	0.43
2:2:1109:C:C3'	2:2:1109:C:C5'	2.97	0.43
3:3:8:C:O3'	21:O:25:ARG:NH1	2.47	0.43
15:I:105:LEU:HD22	15:I:128:ILE:CG2	2.49	0.43
18:L:111:ILE:HD12	18:L:111:ILE:N	2.34	0.43
19:M:41:LEU:HD21	19:M:126:ILE:HD13	2.00	0.43
3:3:29:A:C2	3:3:56:G:C2	3.06	0.43
45:m:78:VAL:HG21	45:m:128:TYR:CE1	2.54	0.43
1:1:12:U:O2	1:1:12:U:H2'	2.18	0.43
12:F:140:VAL:O	12:F:144:VAL:HG23	2.19	0.43
40:h:120:ILE:HD11	40:h:137:ALA:CB	2.49	0.43
1:1:1021:A:N6	1:1:1141:U:N3	2.45	0.43
1:1:1141:U:O2	1:1:1142:A:C6	2.72	0.43
1:1:2395:C:H2'	1:1:2396:G:O4'	2.19	0.43
2:2:148:G:O2'	2:2:149:A:O4'	2.31	0.43
2:2:382:A:H2'	2:2:383:A:C8	2.54	0.43
11:E:12:VAL:HG13	11:E:172:ALA:HB1	2.00	0.43
18:L:109:LYS:HA	18:L:126:ARG:O	2.19	0.43
20:N:28:LEU:HD23	20:N:48:VAL:HG21	1.99	0.43
22:P:106:LYS:HA	22:P:109:ARG:HD3	2.00	0.43
46:n:21:ILE:HD12	46:n:61:LEU:HD13	2.00	0.43
49:q:74:LEU:HD21	49:q:104:CYS:SG	2.59	0.43
1:1:2445:2MG:OP1	10:D:69:ARG:NH2	2.42	0.42
2:2:1124:G:O2'	2:2:1145:A:N6	2.52	0.42
11:E:122:PHE:CZ	11:E:167:ARG:HA	2.53	0.42
21:O:28:VAL:HG11	21:O:103:VAL:HG13	2.01	0.42
21:O:75:GLY:O	21:O:78:VAL:HG12	2.19	0.42
39:g:28:LYS:N	39:g:29:PRO:CD	2.81	0.42
56:x:50:ALA:HB1	56:x:57:HIS:HB3	2.01	0.42
1:1:1139:G:O2'	1:1:1143:A:N1	2.47	0.42
2:2:692:U:O2'	2:2:694:A:N7	2.48	0.42
2:2:827:U:C2	2:2:874:G:N2	2.87	0.42
9:C:26:VAL:HG22	9:C:188:LEU:HD22	2.00	0.42
15:I:10:LEU:HD22	15:I:26:ALA:HB1	2.00	0.42
29:W:37:ILE:HG21	29:W:80:ILE:HG21	2.01	0.42
49:q:80:ILE:HD12	49:q:97:THR:HG22	2.00	0.42
1:1:118:A:N3	1:1:178:G:H1'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2074:U:C4	1:1:2435:A:N1	2.79	0.42
2:2:110:C:H2'	2:2:111:G:O4'	2.19	0.42
2:2:842:U:H3'	2:2:843:U:C5'	2.48	0.42
2:2:928:G:O2'	2:2:929:G:H5'	2.19	0.42
10:D:149:ILE:CD1	10:D:188:MET:HE3	2.49	0.42
19:M:105:MET:HE3	19:M:117:PHE:CE1	2.54	0.42
1:1:67:U:O2	1:1:74:A:N7	2.52	0.42
1:1:1428:C:C5	1:1:1569:A:H5'	2.54	0.42
1:1:2071:A:H2'	1:1:2072:C:C6	2.55	0.42
1:1:2226:C:H2'	1:1:2227:A:O4'	2.19	0.42
2:2:373:A:C2	2:2:374:A:C8	3.08	0.42
26:T:50:LEU:HD23	31:Y:26:PHE:CE1	2.53	0.42
1:1:587:C:OP2	18:L:21:ARG:NH1	2.52	0.42
1:1:953:G:C2'	1:1:954:G:O5'	2.68	0.42
2:2:37:U:C4	2:2:397:A:C6	3.07	0.42
47:o:22:THR:HA	47:o:25:ILE:HG22	2.02	0.42
1:1:74:A:N7	1:1:88:G:C5	2.87	0.42
1:1:796:C:H2'	1:1:797:G:C8	2.54	0.42
1:1:861:A:C2	1:1:917:A:C4	3.08	0.42
1:1:984:A:N3	1:1:984:A:H2'	2.34	0.42
1:1:1007:C:OP1	16:J:37:ARG:NH2	2.52	0.42
2:2:337:G:H2'	2:2:338:A:C8	2.54	0.42
2:2:1389:C:O2'	2:2:1390:U:H5'	2.19	0.42
26:T:8:LEU:HD13	31:Y:22:LEU:HB3	2.01	0.42
27:U:7:ARG:O	27:U:25:VAL:O	2.38	0.42
35:c:38:LYS:HB2	35:c:49:TYR:CD1	2.55	0.42
1:1:627:A:N1	1:1:636:G:O2'	2.49	0.42
2:2:199:A:H2'	2:2:200:G:H8	1.84	0.42
14:H:43:LYS:HE3	14:H:95:LEU:HD22	2.02	0.42
42:j:94:VAL:HG13	42:j:111:MET:CE	2.50	0.42
42:j:99:ALA:CB	42:j:103:THR:HG21	2.49	0.42
46:n:19:VAL:HG11	46:n:83:ILE:HA	2.00	0.42
1:1:2618:G:C6	1:1:2619:C:C4	3.08	0.42
2:2:216:U:H2'	2:2:217:C:C6	2.55	0.42
27:U:5:ILE:N	27:U:5:ILE:HD12	2.34	0.42
28:V:8:VAL:HG22	28:V:38:LEU:HD11	2.00	0.42
43:k:9:MET:HE2	43:k:51:ILE:HD13	2.02	0.42
1:1:1065:U:HO2'	1:1:1066:U:C5'	2.32	0.42
2:2:1428:A:H2'	2:2:1429:A:O4'	2.20	0.42
7:7:7:VAL:HG22	7:7:100:VAL:HG13	2.01	0.42
9:C:156:PHE:CE1	16:J:81:ILE:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:74:THR:HA	19:M:88:ASN:O	2.19	0.42
48:p:61:PHE:O	48:p:65:VAL:HG13	2.20	0.42
1:1:580:U:O3'	23:Q:31:VAL:HG13	2.20	0.42
1:1:780:G:O2'	1:1:783:A:N6	2.53	0.42
1:1:1678:A:H2'	1:1:1679:A:O4'	2.20	0.42
2:2:381:C:H2'	2:2:382:A:O4'	2.19	0.42
7:7:17:ARG:CD	7:7:110:LEU:HD22	2.50	0.42
13:G:15:LEU:HD22	13:G:16:GLY:N	2.34	0.42
50:r:4:ILE:CG1	50:r:9:ILE:HD12	2.50	0.42
1:1:523:C:H4'	1:1:540:C:O2	2.20	0.41
1:1:2190:G:H2'	1:1:2191:A:O4'	2.20	0.41
2:2:104:G:H4'	2:2:174:A:O4'	2.20	0.41
42:j:25:VAL:HG11	42:j:30:ILE:HD12	2.01	0.41
1:1:644:A:H2'	1:1:645:C:O4'	2.20	0.41
1:1:2639:A:H2'	1:1:2640:G:O4'	2.20	0.41
14:H:121:SER:OG	14:H:126:LEU:HD11	2.20	0.41
23:Q:47:TYR:CD1	23:Q:47:TYR:C	2.97	0.41
51:s:31:ILE:HD11	51:s:45:VAL:HA	2.02	0.41
1:1:674:G:O2'	10:D:69:ARG:HD3	2.20	0.41
1:1:1589:U:C2	1:1:1590:A:C8	3.08	0.41
2:2:918:A:H2'	2:2:919:A:O4'	2.20	0.41
2:2:1493:A:HO2'	2:2:1494:G:P	2.43	0.41
3:3:89:U:O2	3:3:89:U:O4'	2.35	0.41
7:7:123:TYR:CZ	7:7:226:VAL:HG12	2.55	0.41
19:M:53:MET:HE1	19:M:103:TYR:CG	2.55	0.41
19:M:109:PRO:HD2	19:M:112:LEU:HD23	2.02	0.41
1:1:250:G:C6	1:1:251:A:C6	3.08	0.41
1:1:930:G:H1'	32:Z:25:LEU:HD11	2.03	0.41
1:1:1129:A:O2'	1:1:2515:C:O2	2.37	0.41
1:1:1198:U:H5'	23:Q:9:ILE:HD11	2.01	0.41
1:1:2297:A:H2	1:1:2321:U:C5	2.37	0.41
1:1:2780:G:O6	16:J:99:ARG:NH1	2.53	0.41
2:2:3:A:N1	2:2:628:G:O2'	2.52	0.41
2:2:976:G:C8	2:2:1358:U:C2	3.08	0.41
2:2:1103:C:O2	39:g:106:THR:HG21	2.21	0.41
7:7:143:ASP:O	7:7:146:SER:OG	2.37	0.41
7:7:333:ILE:HD13	7:7:348:VAL:HG11	2.02	0.41
17:K:38:ILE:HD11	17:K:112:PHE:CZ	2.55	0.41
44:l:27:VAL:HG12	44:l:43:VAL:HG11	2.03	0.41
45:m:8:ALA:HA	45:m:77:ARG:HG3	2.01	0.41
1:1:2249:U:H3'	1:1:2250:G:C5'	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2286:G:H5'	1:1:2286:G:C8	2.56	0.41
2:2:1371:G:O3'	46:n:71:GLY:HA3	2.21	0.41
2:2:1391:U:O2'	2:2:1392:G:O5'	2.38	0.41
9:C:186:LEU:HD21	22:P:4:ILE:HG21	2.03	0.41
1:1:74:A:N7	1:1:88:G:N7	2.68	0.41
1:1:133:U:H2'	1:1:134:G:O4'	2.20	0.41
1:1:2040:G:H2'	1:1:2041:U:O4'	2.21	0.41
1:1:2314:A:OP1	11:E:88:LYS:NZ	2.42	0.41
1:1:2756:U:C4	1:1:2759:G:C6	3.08	0.41
2:2:502:A:H2'	2:2:503:C:O4'	2.20	0.41
2:2:662:U:O2'	2:2:836:G:OP1	2.36	0.41
7:7:14:LEU:O	7:7:17:ARG:HG3	2.20	0.41
11:E:29:PRO:HB2	11:E:169:LEU:HD22	2.02	0.41
41:i:105:MET:HE1	41:i:143:VAL:HG13	2.02	0.41
1:1:2331:G:O2'	1:1:2336:A:N1	2.48	0.41
2:2:152:A:N6	2:2:170:U:C2	2.88	0.41
2:2:384:G:H2'	2:2:385:C:C6	2.55	0.41
11:E:74:VAL:HG22	11:E:79:ILE:HD11	2.02	0.41
42:j:88:VAL:HG12	42:j:93:ARG:CB	2.51	0.41
1:1:309:A:N3	1:1:329:G:O2'	2.50	0.41
1:1:811:U:C2	1:1:1251:C:C5	3.08	0.41
1:1:1913:A:H1'	2:2:1492:A:N1	2.36	0.41
1:1:2679:A:H2'	1:1:2680:U:O4'	2.21	0.41
2:2:16:A:OP1	6:6:41:ARG:HG3	2.20	0.41
2:2:525:C:C2'	2:2:526:C:H5'	2.51	0.41
40:h:134:MET:HE2	40:h:168:TYR:CD2	2.56	0.41
46:n:55:VAL:HG21	46:n:94:LEU:HD13	2.01	0.41
54:v:20:SER:OG	54:v:71:LYS:NZ	2.39	0.41
1:1:172:A:H2'	1:1:173:A:C8	2.56	0.41
1:1:466:A:H2	1:1:795:C:O2	2.04	0.41
1:1:645:C:H2'	1:1:647:G:C8	2.56	0.41
1:1:2444:G:OP2	10:D:63:LYS:HD2	2.20	0.41
1:1:2564:A:C2	1:1:2647:U:H4'	2.56	0.41
1:1:2794:C:H2'	1:1:2795:C:C6	2.55	0.41
2:2:1007:U:N3	2:2:1022:A:N1	2.67	0.41
2:2:1277:C:O2'	2:2:1279:G:H8	2.04	0.41
2:2:1499:A:OP2	2:2:1499:A:H3'	2.21	0.41
5:5:19:G:H3'	5:5:20:H2U:H5''	2.03	0.41
14:H:23:LEU:HA	14:H:118:ILE:HG12	2.03	0.41
20:N:67:PHE:O	20:N:71:ARG:HG2	2.20	0.41
22:P:43:PHE:CZ	22:P:63:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:37:THR:HG21	42:j:64:MET:HE2	2.02	0.41
43:k:11:HIS:CD2	43:k:12:PRO:HD2	2.56	0.41
55:w:14:THR:HG21	55:w:48:ARG:HG3	2.03	0.41
1:1:1198:U:C5'	23:Q:9:ILE:HD11	2.51	0.41
1:1:1562:U:H2'	1:1:1563:U:O4'	2.21	0.41
2:2:684:U:H2'	2:2:685:G:O4'	2.20	0.41
20:N:2:ARG:O	20:N:2:ARG:NH1	2.54	0.41
20:N:90:ARG:CZ	20:N:116:VAL:HG11	2.51	0.41
39:g:14:VAL:HG13	39:g:213:TYR:OH	2.20	0.41
51:s:79:LEU:HB2	51:s:84:VAL:HG22	2.03	0.41
1:1:833:A:H2'	1:1:834:G:C8	2.56	0.40
2:2:1384:C:H2'	2:2:1385:G:C8	2.56	0.40
40:h:6:HIS:HA	40:h:7:PRO:HD3	1.99	0.40
43:k:9:MET:HG2	43:k:59:TYR:CE2	2.57	0.40
1:1:742:A:C2	1:1:743:A:C6	3.09	0.40
1:1:1400:U:H2'	1:1:1401:G:O4'	2.21	0.40
1:1:1964:G:H4'	1:1:1965:C:OP2	2.21	0.40
2:2:8:A:C5	41:i:206:LYS:HB3	2.55	0.40
2:2:215:C:H2'	2:2:216:U:O4'	2.21	0.40
2:2:915:A:O5'	2:2:915:A:H8	2.04	0.40
7:7:42:GLU:HG3	7:7:43:GLN:N	2.35	0.40
20:N:55:ALA:HA	20:N:80:PHE:CE1	2.56	0.40
43:k:72:ASP:O	43:k:76:THR:HG23	2.21	0.40
47:o:25:ILE:HG12	47:o:87:LEU:HD11	2.03	0.40
1:1:1932:A:H2'	1:1:1933:G:O4'	2.22	0.40
8:B:31:ALA:N	8:B:32:PRO:CD	2.84	0.40
10:D:134:LEU:HB2	10:D:160:ALA:HB1	2.03	0.40
19:M:14:LYS:O	19:M:71:LYS:NZ	2.48	0.40
20:N:14:SER:HA	20:N:17:ARG:NH1	2.36	0.40
26:T:61:LEU:C	26:T:61:LEU:CD1	2.93	0.40
56:x:40:ILE:O	56:x:67:VAL:O	2.38	0.40
1:1:1797:G:C6	1:1:1798:U:C4	3.09	0.40
1:1:1924:C:H2'	1:1:1925:C:O4'	2.21	0.40
1:1:2025:C:H2'	1:1:2026:U:C6	2.56	0.40
1:1:2074:U:H2'	1:1:2075:U:C6	2.57	0.40
1:1:2685:G:OP1	17:K:78:ARG:NH2	2.53	0.40
2:2:567:G:H2'	2:2:568:G:O4'	2.22	0.40
2:2:1424:U:H2'	2:2:1425:U:O4'	2.21	0.40
16:J:30:THR:CG2	16:J:31:GLU:N	2.85	0.40
19:M:41:LEU:HD21	19:M:126:ILE:CD1	2.51	0.40
30:X:32:ASN:OD1	30:X:34:HIS:NE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:121:THR:HG23	40:h:189:ALA:CA	2.51	0.40
46:n:9:THR:O	46:n:85:ARG:HD2	2.21	0.40
1:1:871:U:H2'	1:1:872:U:C6	2.56	0.40
1:1:1021:A:N3	1:1:1021:A:C3'	2.79	0.40
1:1:1754:A:N1	1:1:2716:C:O2'	2.38	0.40
1:1:1910:G:H2'	1:1:1911:PSU:C6	2.57	0.40
1:1:1910:G:H2'	1:1:1911:PSU:H6	1.86	0.40
2:2:530:G:C5	6:6:30:GLU:HG3	2.57	0.40
2:2:953:G:H2'	2:2:954:G:O4'	2.21	0.40
9:C:149:ASN:O	9:C:151:THR:N	2.54	0.40
11:E:17:MET:HE2	11:E:25:VAL:HA	2.03	0.40
14:H:18:VAL:HG22	14:H:86:MET:HE2	2.03	0.40
17:K:33:ALA:HB1	17:K:37:ASP:HB2	2.03	0.40
40:h:51:SER:HB3	40:h:115:LEU:HD22	2.04	0.40
40:h:84:VAL:HG22	40:h:103:ILE:HD11	2.04	0.40
43:k:27:ALA:O	43:k:30:THR:OG1	2.30	0.40
46:n:127:PHE:CG	46:n:128:SER:N	2.90	0.40
48:p:62:ALA:O	48:p:65:VAL:HG22	2.21	0.40
49:q:21:VAL:HB	49:q:24:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	30/61 (49%)	24 (80%)	6 (20%)	0	100	100
7	7	335/365 (92%)	322 (96%)	11 (3%)	2 (1%)	21	48
8	B	269/273 (98%)	249 (93%)	18 (7%)	2 (1%)	18	45
9	C	207/209 (99%)	196 (95%)	10 (5%)	1 (0%)	24	52
10	D	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	24	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	21	48
12	F	173/177 (98%)	165 (95%)	8 (5%)	0	100	100
13	G	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	18	45
14	H	128/165 (78%)	106 (83%)	19 (15%)	3 (2%)	5	19
15	I	133/142 (94%)	116 (87%)	15 (11%)	2 (2%)	8	28
16	J	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
17	K	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
18	L	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	18	45
19	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
20	N	117/127 (92%)	106 (91%)	11 (9%)	0	100	100
21	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
22	P	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
23	Q	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	39
24	R	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6	21
25	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
26	T	92/100 (92%)	87 (95%)	5 (5%)	0	100	100
27	U	101/104 (97%)	96 (95%)	5 (5%)	0	100	100
28	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	W	74/85 (87%)	68 (92%)	5 (7%)	1 (1%)	9	29
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
31	Y	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
32	Z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
33	a	64/70 (91%)	58 (91%)	6 (9%)	0	100	100
34	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
35	c	50/55 (91%)	47 (94%)	3 (6%)	0	100	100
36	d	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
37	e	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
38	f	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
39	g	223/241 (92%)	208 (93%)	14 (6%)	1 (0%)	30	57
40	h	206/233 (88%)	193 (94%)	12 (6%)	1 (0%)	24	52
41	i	203/206 (98%)	196 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	j	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	21	48
43	k	102/135 (76%)	98 (96%)	3 (3%)	1 (1%)	12	37
44	l	149/179 (83%)	142 (95%)	6 (4%)	1 (1%)	18	45
45	m	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	7	26
46	n	125/130 (96%)	113 (90%)	11 (9%)	1 (1%)	16	42
47	o	97/103 (94%)	90 (93%)	6 (6%)	1 (1%)	12	37
48	p	115/129 (89%)	103 (90%)	10 (9%)	2 (2%)	7	25
49	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
50	r	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
51	s	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
52	t	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	32
53	u	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
54	v	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
55	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
56	x	81/92 (88%)	77 (95%)	4 (5%)	0	100	100
57	y	84/87 (97%)	84 (100%)	0	0	100	100
58	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	6234/6646 (94%)	5854 (94%)	350 (6%)	30 (0%)	26	52

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	B	158	ALA
46	n	56	ASP
7	7	137	GLY
11	E	62	GLY
14	H	117	LEU
23	Q	3	ARG
42	j	44	GLY
43	k	96	VAL
47	o	57	VAL
7	7	91	ASP
15	I	113	ALA
40	h	80	LYS
44	l	130	ASN
52	t	21	ASP

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Mol	Chain	Res	Type
8	B	240	PHE
10	D	142	ALA
14	H	51	TYR
24	R	37	GLU
48	p	119	ASN
13	G	89	LYS
14	H	55	VAL
9	C	94	GLN
29	W	29	GLU
39	g	74	ARG
45	m	6	PRO
15	I	136	GLY
48	p	74	VAL
18	L	28	GLY
24	R	44	GLY
45	m	75	ILE

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	
6	6	27/52 (52%)	24 (89%)	3 (11%)	6	21
7	7	292/310 (94%)	261 (89%)	31 (11%)	6	23
8	B	216/218 (99%)	199 (92%)	17 (8%)	11	34
9	C	164/164 (100%)	159 (97%)	5 (3%)	36	62
10	D	165/165 (100%)	151 (92%)	14 (8%)	10	31
11	E	148/150 (99%)	135 (91%)	13 (9%)	9	30
12	F	136/138 (99%)	128 (94%)	8 (6%)	18	44
13	G	114/114 (100%)	104 (91%)	10 (9%)	9	30
14	H	99/123 (80%)	90 (91%)	9 (9%)	9	28
15	I	104/110 (94%)	97 (93%)	7 (7%)	15	39
16	J	116/116 (100%)	102 (88%)	14 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	K	104/104 (100%)	97 (93%)	7 (7%)	15	39
18	L	103/103 (100%)	99 (96%)	4 (4%)	28	56
19	M	109/109 (100%)	98 (90%)	11 (10%)	7	24
20	N	99/103 (96%)	90 (91%)	9 (9%)	9	28
21	O	86/87 (99%)	79 (92%)	7 (8%)	11	33
22	P	99/100 (99%)	87 (88%)	12 (12%)	5	17
23	Q	89/90 (99%)	85 (96%)	4 (4%)	24	52
24	R	84/84 (100%)	75 (89%)	9 (11%)	6	22
25	S	93/93 (100%)	87 (94%)	6 (6%)	15	40
26	T	81/84 (96%)	77 (95%)	4 (5%)	22	50
27	U	84/85 (99%)	81 (96%)	3 (4%)	31	58
28	V	78/78 (100%)	74 (95%)	4 (5%)	21	48
29	W	58/63 (92%)	54 (93%)	4 (7%)	14	38
30	X	67/68 (98%)	61 (91%)	6 (9%)	9	29
31	Y	54/55 (98%)	52 (96%)	2 (4%)	30	57
32	Z	48/49 (98%)	40 (83%)	8 (17%)	2	8
33	a	59/62 (95%)	53 (90%)	6 (10%)	7	24
34	b	47/48 (98%)	42 (89%)	5 (11%)	6	23
35	c	47/49 (96%)	45 (96%)	2 (4%)	26	53
36	d	38/38 (100%)	32 (84%)	6 (16%)	2	10
37	e	51/52 (98%)	47 (92%)	4 (8%)	11	34
38	f	34/34 (100%)	30 (88%)	4 (12%)	5	18
39	g	187/199 (94%)	178 (95%)	9 (5%)	23	50
40	h	171/190 (90%)	163 (95%)	8 (5%)	23	51
41	i	172/173 (99%)	164 (95%)	8 (5%)	23	51
42	j	119/126 (94%)	107 (90%)	12 (10%)	7	24
43	k	91/116 (78%)	83 (91%)	8 (9%)	9	30
44	l	124/147 (84%)	111 (90%)	13 (10%)	6	23
45	m	104/105 (99%)	101 (97%)	3 (3%)	37	62
46	n	105/107 (98%)	97 (92%)	8 (8%)	12	35
47	o	86/90 (96%)	77 (90%)	9 (10%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	p	90/99 (91%)	87 (97%)	3 (3%)	33 60
49	q	102/103 (99%)	93 (91%)	9 (9%)	9 30
50	r	94/96 (98%)	87 (93%)	7 (7%)	13 36
51	s	83/84 (99%)	79 (95%)	4 (5%)	23 50
52	t	76/77 (99%)	65 (86%)	11 (14%)	3 12
53	u	65/65 (100%)	61 (94%)	4 (6%)	16 42
54	v	74/78 (95%)	70 (95%)	4 (5%)	20 46
55	w	57/65 (88%)	52 (91%)	5 (9%)	9 30
56	x	72/79 (91%)	68 (94%)	4 (6%)	19 45
57	y	65/66 (98%)	61 (94%)	4 (6%)	16 42
58	z	60/61 (98%)	52 (87%)	8 (13%)	4 14
All	All	5190/5424 (96%)	4791 (92%)	399 (8%)	14 35

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	17	GLU
6	6	18	THR
6	6	20	LEU
7	7	14	LEU
7	7	27	TYR
7	7	42	GLU
7	7	79	ASP
7	7	86	LEU
7	7	102	GLU
7	7	107	GLU
7	7	114	GLU
7	7	117	ARG
7	7	122	GLU
7	7	123	TYR
7	7	164	GLU
7	7	195	GLU
7	7	242	ASP
7	7	258	GLU
7	7	270	ILE
7	7	272	THR
7	7	273	GLN
7	7	279	SER

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Mol	Chain	Res	Type
7	7	285	ASP
7	7	288	MET
7	7	292	LYS
7	7	298	LEU
7	7	324	ARG
7	7	337	ARG
7	7	340	VAL
7	7	343	ARG
7	7	345	THR
7	7	354	ASP
7	7	362	LYS
7	7	365	LEU
8	B	51	THR
8	B	105	LEU
8	B	115	GLN
8	B	125	LYS
8	B	156	ARG
8	B	172	VAL
8	B	174	LEU
8	B	184	VAL
8	B	202	LEU
8	B	203	ARG
8	B	204	VAL
8	B	205	LEU
8	B	236	GLU
8	B	242	LYS
8	B	252	THR
8	B	257	THR
8	B	258	ARG
9	C	2	ILE
9	C	4	LEU
9	C	13	ARG
9	C	46	ARG
9	C	92	VAL
10	D	9	GLN
10	D	21	ARG
10	D	40	ARG
10	D	48	THR
10	D	57	LYS
10	D	69	ARG
10	D	77	ILE
10	D	105	LEU

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Mol	Chain	Res	Type
10	D	108	ILE
10	D	109	LEU
10	D	122	GLU
10	D	127	GLU
10	D	149	ILE
10	D	163	ASN
11	E	10	ASP
11	E	26	MET
11	E	40	VAL
11	E	47	LYS
11	E	57	LEU
11	E	80	ARG
11	E	105	THR
11	E	117	LEU
11	E	122	PHE
11	E	123	ASP
11	E	140	GLU
11	E	141	ILE
11	E	150	ARG
12	F	11	VAL
12	F	19	ILE
12	F	32	GLU
12	F	95	ARG
12	F	104	ASN
12	F	114	ASP
12	F	168	VAL
12	F	176	LYS
13	G	1	MET
13	G	11	ASN
13	G	12	LEU
13	G	15	LEU
13	G	41	LYS
13	G	66	ASN
13	G	72	ILE
13	G	87	GLU
13	G	94	ILE
13	G	96	THR
14	H	3	LEU
14	H	7	ASP
14	H	37	LYS
14	H	40	GLU
14	H	108	VAL

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Mol	Chain	Res	Type
14	H	109	LYS
14	H	114	GLU
14	H	117	LEU
14	H	123	ILE
15	I	10	LEU
15	I	38	CYS
15	I	71	LYS
15	I	78	LEU
15	I	79	LEU
15	I	95	ASP
15	I	137	LEU
16	J	3	THR
16	J	5	THR
16	J	30	THR
16	J	40	HIS
16	J	43	GLU
16	J	65	THR
16	J	70	THR
16	J	93	ILE
16	J	101	ILE
16	J	108	MET
16	J	123	LYS
16	J	124	VAL
16	J	129	GLU
16	J	142	ILE
17	K	35	VAL
17	K	41	ILE
17	K	49	ARG
17	K	67	LYS
17	K	70	ARG
17	K	91	SER
17	K	99	ILE
18	L	42	SER
18	L	59	ARG
18	L	78	ARG
18	L	84	LYS
19	M	6	ARG
19	M	14	LYS
19	M	40	ARG
19	M	59	ARG
19	M	60	GLN
19	M	110	GLU

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Mol	Chain	Res	Type
19	M	115	GLU
19	M	119	LEU
19	M	126	ILE
19	M	127	LYS
19	M	134	THR
20	N	2	ARG
20	N	17	ARG
20	N	20	MET
20	N	46	ARG
20	N	51	LEU
20	N	59	SER
20	N	65	LEU
20	N	69	ARG
20	N	95	THR
21	O	4	LYS
21	O	8	ILE
21	O	20	GLU
21	O	31	THR
21	O	47	VAL
21	O	48	LEU
21	O	102	ARG
22	P	8	LEU
22	P	11	GLU
22	P	26	VAL
22	P	27	GLU
22	P	40	LEU
22	P	68	GLU
22	P	71	GLU
22	P	80	VAL
22	P	81	VAL
22	P	109	ARG
22	P	110	ILE
22	P	114	LEU
23	Q	51	ARG
23	Q	75	SER
23	Q	91	ASP
23	Q	117	LEU
24	R	10	LYS
24	R	33	VAL
24	R	39	LEU
24	R	40	MET
24	R	47	VAL

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Mol	Chain	Res	Type
24	R	48	LYS
24	R	68	ARG
24	R	72	VAL
24	R	86	GLN
25	S	12	SER
25	S	19	LEU
25	S	55	ILE
25	S	67	ASP
25	S	69	LEU
25	S	107	VAL
26	T	1	MET
26	T	25	GLU
26	T	74	ILE
26	T	78	SER
27	U	22	ARG
27	U	52	LEU
27	U	99	ASN
28	V	1	MET
28	V	40	ILE
28	V	59	GLU
28	V	60	VAL
29	W	10	THR
29	W	11	ARG
29	W	41	ARG
29	W	70	GLU
30	X	11	ARG
30	X	25	THR
30	X	33	LEU
30	X	48	THR
30	X	54	LYS
30	X	56	MET
31	Y	18	LEU
31	Y	57	LEU
32	Z	3	LYS
32	Z	6	LYS
32	Z	10	THR
32	Z	11	ARG
32	Z	25	LEU
32	Z	31	ARG
32	Z	36	VAL
32	Z	45	ARG
33	a	16	CYS

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Mol	Chain	Res	Type
33	a	24	ILE
33	a	45	THR
33	a	47	LYS
33	a	56	ARG
33	a	63	ARG
34	b	9	THR
34	b	11	SER
34	b	12	LYS
34	b	27	SER
34	b	40	ARG
35	c	5	ILE
35	c	13	SER
36	d	3	ARG
36	d	12	ARG
36	d	24	THR
36	d	42	LEU
36	d	43	THR
36	d	45	SER
37	e	6	THR
37	e	16	LYS
37	e	30	ARG
37	e	55	LEU
38	f	3	VAL
38	f	6	SER
38	f	17	VAL
38	f	26	ILE
39	g	59	LYS
39	g	105	LYS
39	g	117	LEU
39	g	128	LYS
39	g	129	LEU
39	g	132	LYS
39	g	135	LEU
39	g	161	LEU
39	g	220	THR
40	h	14	ILE
40	h	33	LEU
40	h	89	LYS
40	h	97	VAL
40	h	135	LYS
40	h	175	LEU
40	h	178	LEU

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Mol	Chain	Res	Type
40	h	200	VAL
41	i	5	LEU
41	i	95	GLU
41	i	104	ARG
41	i	116	GLN
41	i	131	ASN
41	i	143	VAL
41	i	197	GLU
41	i	206	LYS
42	j	15	LEU
42	j	18	VAL
42	j	26	LYS
42	j	60	ILE
42	j	65	GLU
42	j	72	ILE
42	j	114	VAL
42	j	115	LEU
42	j	126	LYS
42	j	138	ARG
42	j	141	ILE
42	j	142	ASP
43	k	7	VAL
43	k	24	ARG
43	k	36	ILE
43	k	38	ARG
43	k	39	LEU
43	k	54	LEU
43	k	71	ILE
43	k	79	ARG
44	l	7	ILE
44	l	17	LYS
44	l	21	GLU
44	l	23	LEU
44	l	27	VAL
44	l	40	GLU
44	l	50	LEU
44	l	79	ARG
44	l	97	ASN
44	l	109	ARG
44	l	123	GLU
44	l	130	ASN
44	l	146	GLU

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Mol	Chain	Res	Type
45	m	96	MET
45	m	117	ARG
45	m	121	LEU
46	n	27	LYS
46	n	60	LYS
46	n	61	LEU
46	n	63	LEU
46	n	87	LEU
46	n	98	LEU
46	n	116	VAL
46	n	118	LEU
47	o	5	ARG
47	o	17	LEU
47	o	18	ILE
47	o	24	GLU
47	o	25	ILE
47	o	27	GLU
47	o	37	ARG
47	o	57	VAL
47	o	102	LEU
48	p	15	GLN
48	p	32	VAL
48	p	107	ILE
49	q	5	ASN
49	q	21	VAL
49	q	24	LEU
49	q	35	THR
49	q	58	THR
49	q	62	GLU
49	q	74	LEU
49	q	87	VAL
49	q	102	LEU
50	r	16	VAL
50	r	25	VAL
50	r	29	ARG
50	r	59	GLU
50	r	76	SER
50	r	93	ARG
50	r	104	THR
51	s	45	VAL
51	s	46	LEU
51	s	89	MET

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Mol	Chain	Res	Type
51	s	92	GLU
52	t	10	LYS
52	t	22	THR
52	t	39	LEU
52	t	40	GLN
52	t	61	SER
52	t	64	ARG
52	t	66	LEU
52	t	67	LEU
52	t	70	LEU
52	t	73	LYS
52	t	85	LEU
53	u	18	GLN
53	u	19	VAL
53	u	20	VAL
53	u	57	ILE
54	v	33	ILE
54	v	67	LEU
54	v	75	LEU
54	v	79	VAL
55	w	18	VAL
55	w	54	GLN
55	w	55	LEU
55	w	71	THR
55	w	74	HIS
56	x	21	LYS
56	x	33	THR
56	x	58	VAL
56	x	79	THR
57	y	6	SER
57	y	10	ARG
57	y	24	ARG
57	y	48	GLN
58	z	4	ILE
58	z	18	ARG
58	z	23	CYS
58	z	28	VAL
58	z	31	GLU
58	z	34	ARG
58	z	62	ARG
58	z	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60)

such sidechains are listed below:

Mol	Chain	Res	Type
6	6	27	GLN
7	7	54	GLN
7	7	273	GLN
7	7	276	ASN
7	7	283	ASN
7	7	344	ASN
8	B	25	HIS
9	C	149	ASN
11	E	5	HIS
12	F	38	ASN
12	F	104	ASN
13	G	18	GLN
13	G	133	GLN
14	H	4	ASN
15	I	30	GLN
16	J	136	GLN
18	L	4	ASN
18	L	99	ASN
19	M	22	GLN
20	N	9	GLN
21	O	67	ASN
21	O	116	GLN
22	P	75	GLN
22	P	77	HIS
23	Q	44	GLN
23	Q	71	GLN
24	R	82	HIS
26	T	28	ASN
26	T	59	ASN
27	U	54	GLN
32	Z	9	GLN
33	a	20	ASN
33	a	33	ASN
33	a	41	HIS
34	b	5	GLN
37	e	28	ASN
38	f	13	ASN
38	f	35	GLN
39	g	15	HIS
39	g	58	ASN
39	g	94	HIS
40	h	6	HIS

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Mol	Chain	Res	Type
40	h	25	ASN
40	h	123	GLN
41	i	40	GLN
41	i	136	GLN
42	j	97	GLN
43	k	3	HIS
43	k	11	HIS
43	k	46	GLN
44	l	148	ASN
46	n	110	GLN
46	n	126	GLN
47	o	99	GLN
48	p	15	GLN
48	p	40	ASN
52	t	20	ASN
56	x	52	HIS
57	y	48	GLN
57	y	55	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2904 (99%)	565 (19%)	70 (2%)
2	2	1531/1534 (99%)	314 (20%)	34 (2%)
3	3	119/120 (99%)	18 (15%)	0
4	4	4/18 (22%)	1 (25%)	0
5	5	74/78 (94%)	21 (28%)	8 (10%)
All	All	4630/4654 (99%)	919 (19%)	112 (2%)

All (919) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	23	G
1	1	34	U
1	1	35	G
1	1	45	G
1	1	46	G
1	1	58	G
1	1	60	G

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Mol	Chain	Res	Type
1	1	62	U
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	84	A
1	1	85	G
1	1	96	C
1	1	102	U
1	1	103	A
1	1	118	A
1	1	119	A
1	1	120	U
1	1	131	A
1	1	139	U
1	1	140	C
1	1	141	G
1	1	142	A
1	1	143	C
1	1	149	A
1	1	163	C
1	1	165	A
1	1	181	A
1	1	196	A
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	270	A
1	1	271	G
1	1	272	A
1	1	275	C
1	1	276	U
1	1	278	A
1	1	285	G
1	1	304	U
1	1	311	A

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Mol	Chain	Res	Type
1	1	324	A
1	1	329	G
1	1	330	A
1	1	353	C
1	1	361	G
1	1	362	A
1	1	371	A
1	1	372	G
1	1	373	U
1	1	386	G
1	1	396	G
1	1	405	U
1	1	411	G
1	1	412	A
1	1	420	C
1	1	424	G
1	1	435	C
1	1	451	U
1	1	455	C
1	1	456	C
1	1	457	A
1	1	477	A
1	1	480	A
1	1	481	G
1	1	491	G
1	1	501	A
1	1	503	A
1	1	504	A
1	1	505	A
1	1	509	C
1	1	522	A
1	1	529	A
1	1	532	A
1	1	533	G
1	1	538	A
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G

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Mol	Chain	Res	Type
1	1	563	A
1	1	573	U
1	1	575	A
1	1	586	A
1	1	588	U
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	618	G
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	664	G
1	1	668	A
1	1	685	A
1	1	686	U
1	1	687	C
1	1	710	U
1	1	717	C
1	1	730	A
1	1	738	G
1	1	746	PSU
1	1	747	5MU
1	1	757	G
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U

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Mol	Chain	Res	Type
1	1	830	G
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	869	G
1	1	878	A
1	1	881	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	899	A
1	1	905	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C
1	1	931	U
1	1	932	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	954	G
1	1	961	C
1	1	974	G
1	1	983	A
1	1	984	A
1	1	985	C
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C

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Mol	Chain	Res	Type
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1040	A
1	1	1041	G
1	1	1042	G
1	1	1043	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1073	A
1	1	1074	G
1	1	1079	C
1	1	1080	A
1	1	1081	U
1	1	1083	U
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1095	A
1	1	1096	A
1	1	1107	G
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1128	G
1	1	1129	A
1	1	1132	U
1	1	1134	A

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Mol	Chain	Res	Type
1	1	1135	C
1	1	1142	A
1	1	1143	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1180	U
1	1	1186	G
1	1	1187	G
1	1	1236	G
1	1	1238	G
1	1	1253	A
1	1	1254	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1395	A
1	1	1404	C
1	1	1405	U
1	1	1406	U
1	1	1407	G
1	1	1408	G

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Mol	Chain	Res	Type
1	1	1409	U
1	1	1411	U
1	1	1414	C
1	1	1415	U
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1428	C
1	1	1452	G
1	1	1453	A
1	1	1460	U
1	1	1478	G
1	1	1482	G
1	1	1490	A
1	1	1491	G
1	1	1493	C
1	1	1497	U
1	1	1502	A
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1529	G
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1558	C
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1583	A
1	1	1584	U
1	1	1589	U
1	1	1590	A
1	1	1591	A

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Mol	Chain	Res	Type
1	1	1596	A
1	1	1608	A
1	1	1609	A
1	1	1610	A
1	1	1618	6MZ
1	1	1619	G
1	1	1630	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1703	G
1	1	1714	U
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1750	G
1	1	1758	U
1	1	1764	C
1	1	1773	A
1	1	1791	A
1	1	1800	C
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1859	U
1	1	1862	G
1	1	1864	U
1	1	1869	G
1	1	1870	C
1	1	1872	A
1	1	1873	G
1	1	1905	C
1	1	1906	G

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Mol	Chain	Res	Type
1	1	1907	G
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1915	3TD
1	1	1916	A
1	1	1917	PSU
1	1	1918	A
1	1	1919	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1938	A
1	1	1955	U
1	1	1960	A
1	1	1963	U
1	1	1965	C
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2027	G
1	1	2031	A
1	1	2033	A
1	1	2036	C
1	1	2041	U
1	1	2043	C
1	1	2049	G
1	1	2051	A
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A

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Mol	Chain	Res	Type
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2077	A
1	1	2080	A
1	1	2093	G
1	1	2097	A
1	1	2099	U
1	1	2101	A
1	1	2108	A
1	1	2110	G
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2120	G
1	1	2121	G
1	1	2122	U
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2141	G
1	1	2146	C
1	1	2147	A
1	1	2154	A
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A

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Mol	Chain	Res	Type
1	1	2171	A
1	1	2172	U
1	1	2178	C
1	1	2182	U
1	1	2183	A
1	1	2185	U
1	1	2186	G
1	1	2188	U
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2225	A
1	1	2226	C
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2251	OMG
1	1	2268	A
1	1	2278	A
1	1	2283	C
1	1	2287	A
1	1	2288	A
1	1	2297	A
1	1	2305	U
1	1	2308	G
1	1	2309	A
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2336	A
1	1	2345	G

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Mol	Chain	Res	Type
1	1	2347	C
1	1	2350	C
1	1	2352	A
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2436	G
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2459	A
1	1	2470	G
1	1	2474	U
1	1	2476	A
1	1	2478	A
1	1	2484	G
1	1	2491	U
1	1	2502	G
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2512	C
1	1	2518	A
1	1	2520	C
1	1	2525	G
1	1	2529	G
1	1	2535	G
1	1	2547	A

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Mol	Chain	Res	Type
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2584	U
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2603	G
1	1	2609	U
1	1	2610	C
1	1	2611	C
1	1	2613	U
1	1	2629	U
1	1	2630	G
1	1	2663	G
1	1	2671	G
1	1	2682	A
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2720	U
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2746	U
1	1	2748	A
1	1	2758	A
1	1	2765	A
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2799	A
1	1	2801	G
1	1	2818	U
1	1	2820	A

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Mol	Chain	Res	Type
1	1	2825	G
1	1	2836	U
1	1	2859	G
1	1	2861	U
1	1	2867	G
1	1	2880	C
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2902	C
2	2	4	U
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	41	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	58	C
2	2	69	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	74	A
2	2	76	G
2	2	82	G
2	2	83	C
2	2	84	U
2	2	87	C
2	2	90	C
2	2	94	G
2	2	95	C
2	2	96	U
2	2	108	G
2	2	116	A
2	2	120	A
2	2	121	U
2	2	122	G

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Mol	Chain	Res	Type
2	2	128	G
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	161	A
2	2	164	G
2	2	173	U
2	2	181	A
2	2	182	A
2	2	196	A
2	2	197	A
2	2	198	G
2	2	204	G
2	2	208	U
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	214	C
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	258	G
2	2	262	A
2	2	266	G
2	2	267	C
2	2	271	C
2	2	279	A
2	2	289	G
2	2	299	G
2	2	306	A
2	2	321	A
2	2	328	C
2	2	329	A
2	2	330	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G

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Mol	Chain	Res	Type
2	2	355	C
2	2	367	U
2	2	372	C
2	2	373	A
2	2	374	A
2	2	376	G
2	2	382	A
2	2	384	G
2	2	392	C
2	2	393	A
2	2	397	A
2	2	406	G
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	428	G
2	2	429	U
2	2	446	G
2	2	451	A
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	478	A
2	2	479	U
2	2	480	U
2	2	481	G
2	2	482	A
2	2	484	G
2	2	485	U
2	2	486	U
2	2	505	G
2	2	511	C
2	2	515	G
2	2	516	PSU

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Mol	Chain	Res	Type
2	2	517	G
2	2	518	C
2	2	519	C
2	2	528	C
2	2	529	G
2	2	531	U
2	2	532	A
2	2	533	A
2	2	542	G
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	579	A
2	2	596	A
2	2	607	A
2	2	628	G
2	2	633	G
2	2	642	A
2	2	650	G
2	2	653	U
2	2	665	A
2	2	666	G
2	2	700	G
2	2	722	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	733	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	763	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	799	G
2	2	810	C

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Mol	Chain	Res	Type
2	2	815	A
2	2	817	C
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	844	G
2	2	845	A
2	2	846	G
2	2	849	G
2	2	851	G
2	2	874	G
2	2	876	C
2	2	887	G
2	2	902	G
2	2	914	A
2	2	916	U
2	2	926	G
2	2	928	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	960	U
2	2	961	U
2	2	963	G
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	968	A
2	2	969	A
2	2	972	C
2	2	975	A
2	2	976	G
2	2	977	A
2	2	978	A
2	2	989	U
2	2	991	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	999	C
2	2	1004	A

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Mol	Chain	Res	Type
2	2	1008	U
2	2	1009	U
2	2	1017	U
2	2	1018	G
2	2	1021	A
2	2	1024	G
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1033	G
2	2	1037	C
2	2	1042	A
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1056	U
2	2	1065	U
2	2	1085	U
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1124	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1143	G
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1154	G
2	2	1158	C
2	2	1159	U
2	2	1171	A
2	2	1174	G
2	2	1175	G

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Mol	Chain	Res	Type
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1206	G
2	2	1208	C
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1225	A
2	2	1226	C
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1246	A
2	2	1257	A
2	2	1260	G
2	2	1275	A
2	2	1277	C
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1299	A
2	2	1300	G
2	2	1302	C
2	2	1305	G
2	2	1311	A
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1329	A
2	2	1338	G
2	2	1340	A
2	2	1346	A
2	2	1347	G
2	2	1353	G
2	2	1363	A

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Mol	Chain	Res	Type
2	2	1370	G
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1396	A
2	2	1397	C
2	2	1419	G
2	2	1429	A
2	2	1432	G
2	2	1433	A
2	2	1441	A
2	2	1446	A
2	2	1447	A
2	2	1448	C
2	2	1452	C
2	2	1453	G
2	2	1475	G
2	2	1487	G
2	2	1492	A
2	2	1493	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1531	A
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	16	G
3	3	17	C
3	3	21	G
3	3	35	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	57	A
3	3	66	A

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Mol	Chain	Res	Type
3	3	67	G
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
4	4	15	A
5	5	3	G
5	5	5	G
5	5	8	4SU
5	5	9	G
5	5	13	A
5	5	15	C
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	21	A
5	5	22	G
5	5	31	G
5	5	47	U
5	5	48	C
5	5	55	PSU
5	5	57	A
5	5	60	U
5	5	69	C
5	5	74	C

All (112) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	62	U
1	1	70	G
1	1	140	C
1	1	142	A
1	1	271	G
1	1	404	A
1	1	446	G
1	1	503	A
1	1	532	A
1	1	545	U

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Mol	Chain	Res	Type
1	1	548	G
1	1	555	G
1	1	685	A
1	1	752	A
1	1	764	A
1	1	784	G
1	1	883	G
1	1	892	A
1	1	894	U
1	1	896	A
1	1	984	A
1	1	1045	C
1	1	1063	G
1	1	1064	C
1	1	1069	A
1	1	1110	G
1	1	1128	G
1	1	1142	A
1	1	1173	U
1	1	1177	G
1	1	1205	A
1	1	1253	A
1	1	1320	C
1	1	1344	U
1	1	1379	U
1	1	1415	U
1	1	1490	A
1	1	1509	A
1	1	1583	A
1	1	1584	U
1	1	1608	A
1	1	1847	A
1	1	1900	A
1	1	1912	A
1	1	1913	A
1	1	1918	A
1	1	1962	5MC
1	1	2062	A
1	1	2074	U
1	1	2146	C
1	1	2162	G
1	1	2193	G

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Mol	Chain	Res	Type
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2250	G
1	1	2296	U
1	1	2308	G
1	1	2324	U
1	1	2326	C
1	1	2425	A
1	1	2447	G
1	1	2506	U
1	1	2572	A
1	1	2585	U
1	1	2610	C
1	1	2798	U
1	1	2849	U
1	1	2873	A
2	2	70	U
2	2	106	C
2	2	181	A
2	2	183	C
2	2	197	A
2	2	209	U
2	2	428	G
2	2	438	U
2	2	481	G
2	2	517	G
2	2	527	7MG
2	2	531	U
2	2	560	A
2	2	641	U
2	2	722	G
2	2	793	U
2	2	966	2MG
2	2	967	5MC
2	2	991	U
2	2	992	U
2	2	1145	A
2	2	1196	A
2	2	1211	U
2	2	1213	A

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Mol	Chain	Res	Type
2	2	1214	C
2	2	1225	A
2	2	1299	A
2	2	1363	A
2	2	1396	A
2	2	1407	5MC
2	2	1432	G
2	2	1447	A
2	2	1493	A
2	2	1516	2MG
5	5	8	4SU
5	5	16	C
5	5	17	U
5	5	18	G
5	5	20	H2U
5	5	21	A
5	5	47	U
5	5	60	U

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

40 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$
1	PSU	1	1917	1	18,21,22	0.91	1 (5%)	22,30,33	1.01	1 (4%)
1	3TD	1	1915	1	18,22,23	2.35	2 (11%)	22,32,35	2.63	6 (27%)
1	5MU	1	1939	59,1	19,22,23	0.84	1 (5%)	28,32,35	0.99	3 (10%)
1	OMC	1	2498	59,1	19,22,23	1.14	2 (10%)	26,31,34	1.63	4 (15%)
5	4OC	5	32	5	20,23,24	0.59	0	26,32,35	1.21	2 (7%)
1	1MG	1	745	1	22,26,27	1.01	2 (9%)	33,39,42	1.50	4 (12%)
2	UR3	2	1498	2	19,22,23	1.35	2 (10%)	26,32,35	1.24	5 (19%)
2	MA6	2	1518	2	23,26,27	0.55	0	34,38,41	1.04	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	5	55	5	18,21,22	1.86	1 (5%)	22,30,33	1.57	3 (13%)
1	5MC	1	1962	1	18,22,23	0.85	1 (5%)	26,32,35	1.52	4 (15%)
5	4SU	5	8	5	18,21,22	1.64	3 (16%)	26,30,33	2.75	9 (34%)
5	H2U	5	20	5	18,21,22	0.63	0	21,30,33	1.93	4 (19%)
2	PSU	2	516	59,2	18,21,22	1.57	1 (5%)	22,30,33	1.61	2 (9%)
2	2MG	2	966	2	23,26,27	0.63	0	32,38,41	1.56	2 (6%)
1	PSU	1	2580	1	18,21,22	1.83	1 (5%)	22,30,33	1.61	3 (13%)
1	PSU	1	2504	1	18,21,22	1.64	1 (5%)	22,30,33	1.65	3 (13%)
2	4OC	2	1402	2	20,23,24	1.18	2 (10%)	26,32,35	1.12	2 (7%)
1	6MZ	1	1618	1	22,25,26	0.73	0	30,36,39	1.38	3 (10%)
2	5MC	2	1407	2	18,22,23	0.90	1 (5%)	26,32,35	1.30	3 (11%)
1	PSU	1	746	59,1	18,21,22	2.14	1 (5%)	22,30,33	2.11	3 (13%)
1	PSU	1	2457	1	18,21,22	2.15	1 (5%)	22,30,33	1.54	4 (18%)
1	PSU	1	2605	1	18,21,22	1.98	1 (5%)	22,30,33	1.70	3 (13%)
1	2MA	1	2503	59,1	22,25,26	1.42	4 (18%)	33,37,40	2.58	13 (39%)
1	PSU	1	955	1	18,21,22	2.17	2 (11%)	22,30,33	1.57	3 (13%)
1	G7M	1	2069	1	23,26,27	0.96	1 (4%)	35,39,42	2.20	8 (22%)
1	2MG	1	1835	1	23,26,27	0.64	0	32,38,41	1.12	2 (6%)
2	MA6	2	1519	2	23,26,27	0.59	0	34,38,41	1.10	3 (8%)
1	2MG	1	2445	1	23,26,27	0.69	0	32,38,41	1.13	3 (9%)
5	5MU	5	54	5	19,22,23	0.64	0	28,32,35	1.00	3 (10%)
1	6MZ	1	2030	1	22,25,26	0.89	0	30,36,39	1.61	5 (16%)
1	5MU	1	747	1	19,22,23	0.75	1 (5%)	28,32,35	1.01	3 (10%)
2	7MG	2	527	59,2	22,26,27	1.47	4 (18%)	29,39,42	2.86	12 (41%)
1	PSU	1	1911	1	18,21,22	1.44	4 (22%)	22,30,33	2.08	4 (18%)
1	OMU	1	2552	1	19,22,23	0.48	0	26,31,34	0.82	1 (3%)
2	5MC	2	967	2	18,22,23	0.85	1 (5%)	26,32,35	1.45	3 (11%)
2	2MG	2	1207	2	23,26,27	0.99	1 (4%)	32,38,41	0.93	1 (3%)
5	8AN	5	76	60,59,1,5	22,24,25	0.38	0	26,35,38	0.34	0
49	0TD	q	89	49	7,9,10	6.74	5 (71%)	6,11,13	4.11	2 (33%)
1	OMG	1	2251	1,5	23,26,27	1.61	2 (8%)	33,38,41	1.64	5 (15%)
2	2MG	2	1516	2	23,26,27	0.70	0	32,38,41	1.12	2 (6%)

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
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	5/7/25/26	0/2/2/2
1	5MU	1	1939	59,1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	59,1	-	2/9/27/28	0/2/2/2
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/11/29/30	0/3/3/3
5	PSU	5	55	5	-	3/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
5	4SU	5	8	5	-	2/7/25/26	0/2/2/2
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
2	PSU	2	516	59,2	-	2/7/25/26	0/2/2/2
2	2MG	2	966	2	-	5/9/27/28	0/3/3/3
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	1/7/25/26	0/2/2/2
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
1	6MZ	1	1618	1	-	4/9/27/28	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	746	59,1	-	2/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	2MA	1	2503	59,1	-	2/7/25/26	0/3/3/3
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	2/7/25/26	0/3/3/3
1	2MG	1	1835	1	-	0/9/27/28	0/3/3/3
2	MA6	2	1519	2	-	6/11/29/30	0/3/3/3
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/9/27/28	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	7MG	2	527	59,2	-	0/7/37/38	0/3/3/3
1	PSU	1	1911	1	-	1/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
2	5MC	2	967	2	-	5/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
5	8AN	5	76	60,59,1,5	-	3/7/25/26	0/3/3/3
49	0TD	q	89	49	-	2/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1	2251	1,5	-	0/9/27/28	0/3/3/3
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	q	89	0TD	CB-SB	-16.93	1.65	1.82
1	1	1915	3TD	C1'-C5	-9.08	1.29	1.50
1	1	746	PSU	C2'-C1'	-8.86	1.42	1.53
1	1	955	PSU	C2'-C1'	-8.65	1.42	1.53
1	1	2457	PSU	C2'-C1'	-8.61	1.42	1.53
1	1	2605	PSU	C2'-C1'	-7.97	1.43	1.53
5	5	55	PSU	C2'-C1'	-7.67	1.43	1.53
1	1	2580	PSU	C2'-C1'	-7.43	1.44	1.53
1	1	2504	PSU	C2'-C1'	-6.55	1.45	1.53
2	2	516	PSU	C2'-C1'	-6.32	1.45	1.53
1	1	2251	OMG	C2'-C1'	-4.94	1.40	1.53
5	5	8	4SU	C4-S4	-4.73	1.59	1.68
1	1	2251	OMG	C3'-C2'	-4.42	1.43	1.52
1	1	2503	2MA	C2-N1	3.87	1.40	1.34
2	2	527	7MG	C4-N9	-3.52	1.33	1.37
1	1	2498	OMC	C3'-C2'	-3.48	1.45	1.52
49	q	89	0TD	CA-N	-3.17	1.37	1.47
1	1	2503	2MA	C6-N1	2.98	1.39	1.35
5	5	8	4SU	C5-C4	-2.97	1.38	1.42
1	1	1911	PSU	C4-N3	-2.95	1.33	1.38
1	1	2069	G7M	C2'-C1'	-2.90	1.44	1.53
2	2	527	7MG	C5-N7	-2.88	1.32	1.35
2	2	527	7MG	C6-N1	-2.87	1.33	1.38
1	1	1962	5MC	C2'-C1'	-2.76	1.44	1.53
1	1	1939	5MU	C2'-C1'	-2.76	1.44	1.53
49	q	89	0TD	OD2-CG	-2.70	1.21	1.30
49	q	89	0TD	CB-CG	-2.68	1.47	1.52
1	1	2498	OMC	C2'-C1'	-2.66	1.46	1.53
1	1	2503	2MA	C6-N6	-2.64	1.27	1.34
1	1	745	1MG	C5-C6	-2.63	1.38	1.45
2	2	527	7MG	C5-C4	2.61	1.46	1.38
2	2	1498	UR3	O4-C4	-2.57	1.18	1.23
49	q	89	0TD	CSB-SB	-2.53	1.74	1.79
1	1	1911	PSU	C6-C5	2.50	1.38	1.35
2	2	967	5MC	C2'-C1'	-2.48	1.45	1.53
1	1	1915	3TD	C4-N3	-2.43	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1407	5MC	C2'-C1'	-2.39	1.45	1.53
1	1	2503	2MA	C2'-C3'	-2.38	1.46	1.53
2	2	1402	4OC	C6-N1	-2.30	1.32	1.38
1	1	1917	PSU	C2'-C1'	-2.22	1.50	1.53
1	1	955	PSU	C3'-C2'	-2.22	1.47	1.53
1	1	1911	PSU	C2-N3	-2.16	1.33	1.37
1	1	745	1MG	C2'-C1'	-2.14	1.46	1.53
1	1	747	5MU	C2'-C1'	-2.14	1.46	1.53
1	1	1911	PSU	C2-N1	-2.13	1.33	1.36
2	2	1498	UR3	C6-N1	-2.13	1.32	1.38
5	5	8	4SU	C4-N3	-2.05	1.35	1.37
2	2	1207	2MG	C6-N1	2.02	1.42	1.38
2	2	1402	4OC	C2-N3	-2.01	1.32	1.36

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	7MG	N9-C4-N3	8.97	138.88	125.47
1	1	746	PSU	C3'-C2'-C1'	7.73	110.64	101.64
1	1	1915	3TD	O5'-C5'-C4'	7.70	135.17	108.99
49	q	89	0TD	CB-CA-N	-7.52	93.08	109.10
1	1	2503	2MA	C3'-C2'-C1'	-7.23	87.69	101.43
5	5	8	4SU	C5-C4-N3	7.17	121.34	114.69
2	2	966	2MG	O3'-C3'-C4'	6.98	131.23	111.05
5	5	8	4SU	C4-N3-C2	-6.94	120.60	127.34
1	1	2069	G7M	O2'-C2'-C3'	6.63	133.26	111.82
1	1	1911	PSU	N1-C2-N3	6.31	122.28	115.13
49	q	89	0TD	CSB-SB-CB	6.19	113.63	102.44
1	1	1915	3TD	N1-C2-N3	6.01	120.88	116.14
5	5	8	4SU	C5-C4-S4	-5.98	116.77	124.47
2	2	967	5MC	O3'-C3'-C4'	5.70	127.52	111.05
2	2	527	7MG	C5-C4-N3	-5.51	117.62	128.13
2	2	516	PSU	O2'-C2'-C3'	5.47	129.52	111.82
2	2	527	7MG	N9-C8-N7	-5.24	95.89	103.38
1	1	1962	5MC	O3'-C3'-C4'	5.21	126.12	111.05
1	1	2498	OMC	O2'-C2'-C1'	5.21	119.24	109.08
1	1	2251	OMG	C3'-C2'-C1'	5.20	112.66	102.89
1	1	2503	2MA	O2'-C2'-C1'	5.20	127.40	110.02
1	1	1618	6MZ	O3'-C3'-C4'	5.14	125.90	111.05
1	1	2498	OMC	O3'-C3'-C2'	5.11	125.69	111.17
5	5	55	PSU	O2'-C2'-C3'	5.11	128.34	111.82
1	1	2580	PSU	O2'-C2'-C3'	4.98	127.93	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2504	PSU	O2'-C2'-C3'	4.92	127.73	111.82
5	5	20	H2U	O2'-C2'-C3'	4.89	127.66	111.82
1	1	2069	G7M	C2'-C1'-N9	4.86	126.98	113.22
2	2	1407	5MC	O3'-C3'-C2'	4.80	127.34	111.82
1	1	2504	PSU	O2'-C2'-C1'	4.73	122.52	111.23
1	1	2030	6MZ	O3'-C3'-C4'	4.69	124.60	111.05
1	1	955	PSU	O2'-C2'-C3'	4.67	126.93	111.82
2	2	1516	2MG	O3'-C3'-C2'	4.64	126.85	111.82
1	1	2605	PSU	O2'-C2'-C3'	4.61	126.74	111.82
1	1	2605	PSU	O2'-C2'-C1'	4.59	122.19	111.23
5	5	20	H2U	O3'-C3'-C2'	4.54	126.50	111.82
1	1	2457	PSU	O2'-C2'-C3'	4.53	126.49	111.82
1	1	2069	G7M	O2'-C2'-C1'	4.41	124.78	110.02
1	1	2069	G7M	C4'-O4'-C1'	-4.39	99.79	109.47
1	1	1911	PSU	C4-N3-C2	-4.38	120.03	126.34
1	1	746	PSU	O2'-C2'-C3'	4.36	125.94	111.82
1	1	2503	2MA	C4'-O4'-C1'	-4.36	99.85	109.47
1	1	2503	2MA	O3'-C3'-C4'	4.36	123.66	111.05
1	1	2445	2MG	O3'-C3'-C2'	4.33	125.82	111.82
5	5	32	4OC	O3'-C3'-C2'	4.31	123.40	111.17
1	1	2251	OMG	O3'-C3'-C4'	4.27	123.39	111.05
1	1	1915	3TD	C5'-C4'-C3'	-4.25	99.26	115.18
1	1	2069	G7M	C3'-C2'-C1'	-4.23	93.39	101.43
1	1	2503	2MA	O3'-C3'-C2'	4.20	125.40	111.82
1	1	745	1MG	C3'-C2'-C1'	4.18	109.37	101.43
2	2	527	7MG	C2-N3-C4	4.10	119.61	112.30
1	1	745	1MG	O3'-C3'-C4'	4.09	122.89	111.05
1	1	1835	2MG	O3'-C3'-C4'	4.05	122.76	111.05
5	5	20	H2U	O3'-C3'-C4'	4.05	122.76	111.05
1	1	745	1MG	O3'-C3'-C2'	4.03	124.85	111.82
5	5	55	PSU	O2'-C2'-C1'	4.01	120.80	111.23
1	1	1915	3TD	C4-N3-C2	-3.99	120.28	124.61
1	1	1911	PSU	O2-C2-N1	-3.96	118.43	122.79
1	1	2030	6MZ	C3'-C2'-C1'	-3.93	93.95	101.43
1	1	955	PSU	O2'-C2'-C1'	3.85	120.40	111.23
1	1	2251	OMG	O3'-C3'-C2'	3.79	121.93	111.17
2	2	1518	MA6	C2-N1-C6	3.66	120.39	111.75
1	1	2503	2MA	O4'-C1'-N9	-3.64	100.89	108.06
1	1	2580	PSU	O2'-C2'-C1'	3.60	119.82	111.23
2	2	516	PSU	O2'-C2'-C1'	3.53	119.66	111.23
2	2	1519	MA6	C2-N1-C6	3.48	119.98	111.75
1	1	2457	PSU	O2'-C2'-C1'	3.45	119.46	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	7MG	O4'-C4'-C3'	-3.44	98.30	105.11
1	1	1835	2MG	O3'-C3'-C2'	3.41	122.86	111.82
1	1	2580	PSU	C3'-C2'-C1'	3.41	105.61	101.64
1	1	2030	6MZ	C4-N9-C8	3.38	109.40	105.73
5	5	20	H2U	O2'-C2'-C1'	3.38	121.34	110.02
1	1	1618	6MZ	C4-N9-C8	3.29	109.29	105.73
2	2	527	7MG	O3'-C3'-C2'	3.29	122.45	111.82
2	2	1519	MA6	C4-N9-C8	3.26	109.26	105.73
5	5	8	4SU	C1'-N1-C2	3.24	123.43	117.57
2	2	1518	MA6	C4-N9-C8	3.23	109.23	105.73
1	1	1917	PSU	C3'-C2'-C1'	3.19	105.35	101.64
1	1	2030	6MZ	O3'-C3'-C2'	3.16	122.06	111.82
5	5	8	4SU	N3-C2-N1	3.16	119.08	114.89
1	1	2503	2MA	O4'-C1'-C2'	3.16	113.52	106.64
2	2	966	2MG	C2'-C3'-C4'	-3.14	96.54	102.64
1	1	2503	2MA	C1'-N9-C8	-3.02	120.31	127.14
5	5	32	4OC	O3'-C3'-C4'	2.98	119.68	111.05
1	1	955	PSU	C2'-C3'-C4'	-2.98	96.85	102.64
2	2	1498	UR3	O4'-C1'-C2'	-2.97	100.17	106.64
1	1	746	PSU	O2'-C2'-C1'	2.94	118.25	111.23
2	2	1516	2MG	O3'-C3'-C4'	2.93	119.53	111.05
1	1	1962	5MC	O3'-C3'-C2'	2.92	121.27	111.82
1	1	2251	OMG	O2'-C2'-C1'	2.89	114.72	109.08
1	1	2069	G7M	O3'-C3'-C2'	2.87	121.12	111.82
1	1	2503	2MA	C4-N9-C8	2.87	108.84	105.73
1	1	2605	PSU	C2'-C3'-C4'	-2.80	97.21	102.64
1	1	2445	2MG	O3'-C3'-C4'	2.78	119.09	111.05
2	2	527	7MG	O3'-C3'-C4'	2.78	119.09	111.05
1	1	2457	PSU	C2'-C3'-C4'	-2.77	97.27	102.64
1	1	745	1MG	O2'-C2'-C3'	2.72	120.63	111.82
1	1	2503	2MA	O2'-C2'-C3'	2.72	120.62	111.82
2	2	527	7MG	C5-C6-N1	2.68	115.72	110.99
1	1	1962	5MC	C2'-C1'-N1	2.66	120.76	113.22
1	1	2069	G7M	C2'-C3'-C4'	-2.65	97.50	102.64
5	5	54	5MU	C2'-C1'-N1	2.58	120.54	113.22
2	2	1402	4OC	O4'-C4'-C3'	-2.58	100.00	105.11
1	1	747	5MU	C2'-C1'-N1	2.58	120.52	113.22
5	5	8	4SU	C4'-O4'-C1'	-2.54	103.86	109.47
1	1	2251	OMG	C5'-C4'-C3'	2.54	124.71	115.18
1	1	1618	6MZ	C2'-C1'-N9	2.54	119.74	113.30
1	1	2503	2MA	C5-C4-N3	-2.51	124.37	127.19
1	1	1939	5MU	C2'-C1'-N1	2.51	120.32	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1498	UR3	O2-C2-N3	-2.44	117.90	121.34
2	2	527	7MG	C3'-C2'-C1'	-2.44	96.80	101.43
1	1	2498	OMC	O3'-C3'-C4'	2.43	118.07	111.05
2	2	1402	4OC	O2-C2-N3	-2.41	118.42	122.33
5	5	55	PSU	C3'-C2'-C1'	2.40	104.43	101.64
1	1	2504	PSU	C2'-C3'-C4'	-2.40	97.98	102.64
2	2	527	7MG	O6-C6-C5	-2.37	121.73	127.54
1	1	1962	5MC	C3'-C2'-C1'	2.36	105.92	101.43
2	2	1519	MA6	C2'-C3'-C4'	-2.36	98.05	102.64
5	5	8	4SU	O4'-C1'-N1	2.35	113.74	108.36
1	1	2503	2MA	N3-C4-N9	2.35	130.25	126.99
1	1	2030	6MZ	C4'-O4'-C1'	-2.32	104.35	109.47
5	5	8	4SU	O4'-C1'-C2'	-2.27	101.70	106.64
1	1	1939	5MU	C4-N3-C2	-2.26	124.43	127.35
1	1	1939	5MU	N3-C2-N1	2.26	117.88	114.89
2	2	1207	2MG	O2'-C2'-C1'	-2.24	102.52	110.02
1	1	2457	PSU	C3'-C2'-C1'	2.24	104.24	101.64
2	2	527	7MG	C5-C4-N9	-2.23	103.45	106.35
1	1	2503	2MA	N9-C8-N7	-2.22	110.88	113.91
1	1	1915	3TD	O4'-C4'-C5'	-2.18	102.19	109.37
1	1	747	5MU	N3-C2-N1	2.17	117.77	114.89
2	2	1407	5MC	O3'-C3'-C4'	2.15	117.28	111.05
2	2	1498	UR3	C1'-N1-C2	2.15	120.62	116.99
1	1	1915	3TD	C3'-C2'-C1'	2.12	104.11	101.64
5	5	54	5MU	N3-C2-N1	2.11	117.70	114.89
1	1	2552	OMU	N3-C2-N1	2.11	117.69	114.89
1	1	2498	OMC	C3'-C2'-C1'	2.10	106.84	102.89
2	2	967	5MC	O3'-C3'-C2'	2.10	118.61	111.82
2	2	1498	UR3	C4-N3-C2	-2.08	122.61	124.56
2	2	527	7MG	O4'-C1'-N9	2.08	112.13	109.30
1	1	2069	G7M	O4'-C1'-N9	2.07	113.10	108.36
5	5	8	4SU	C6-C5-C4	-2.07	118.16	119.95
2	2	967	5MC	C2'-C1'-N1	2.04	119.00	113.22
2	2	1498	UR3	O3'-C3'-C4'	-2.03	105.18	111.05
5	5	54	5MU	C4-N3-C2	-2.03	124.73	127.35
2	2	1407	5MC	O4'-C1'-C2'	2.01	111.03	106.64
1	1	1911	PSU	C5-C6-N1	-2.01	119.10	122.11
1	1	2445	2MG	C3'-C2'-C1'	2.00	105.23	101.43
1	1	747	5MU	C4-N3-C2	-2.00	124.76	127.35

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	746	PSU	C2'-C1'-C5-C4
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	N3-C2-N2-CM2
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C9
2	2	1519	MA6	C5-C6-N6-C10
49	q	89	0TD	SB-CB-CG-OD2
5	5	20	H2U	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C6
5	5	55	PSU	C3'-C4'-C5'-O5'
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C2
5	5	76	8AN	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	516	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
5	5	20	H2U	C3'-C4'-C5'-O5'
5	5	55	PSU	O4'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
5	5	76	8AN	C4'-C5'-O5'-P
5	5	76	8AN	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C5-C6-N6-C9
5	5	8	4SU	O4'-C1'-N1-C2
49	q	89	0TD	CG-CB-SB-CSB
5	5	8	4SU	O4'-C1'-N1-C6
1	1	2069	G7M	C4'-C5'-O5'-P
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C4'-C5'-O5'
1	1	1911	PSU	O4'-C4'-C5'-O5'
2	2	967	5MC	C4'-C5'-O5'-P
1	1	2498	OMC	C3'-C4'-C5'-O5'

Continued on next page...

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Mol	Chain	Res	Type	Atoms
2	2	967	5MC	C2'-C1'-N1-C6
1	1	2503	2MA	O4'-C1'-N9-C8
2	2	966	2MG	C2'-C1'-N9-C4
2	2	966	2MG	C2'-C1'-N9-C8
1	1	746	PSU	O4'-C1'-C5-C6
1	1	1915	3TD	C4'-C5'-O5'-P
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C2
2	2	1519	MA6	C4'-C5'-O5'-P
5	5	55	PSU	C4'-C5'-O5'-P
1	1	2504	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

21 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1917	PSU	3	0
1	1	1915	3TD	4	0
1	1	1939	5MU	1	0
5	5	32	4OC	1	0
2	2	1518	MA6	2	0
1	1	1962	5MC	1	0
5	5	20	H2U	1	0
2	2	516	PSU	6	0
2	2	966	2MG	3	0
2	2	1402	4OC	1	0
2	2	1407	5MC	1	0
1	1	2503	2MA	1	0
2	2	1519	MA6	2	0
1	1	2445	2MG	2	0
1	1	2030	6MZ	2	0
2	2	527	7MG	4	0
1	1	1911	PSU	2	0
1	1	2552	OMU	1	0
2	2	967	5MC	2	0
2	2	1207	2MG	2	0
1	1	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 441 ligands modelled in this entry, 440 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	FME	5	101	5	8,9,10	0.54	0	7,9,11	1.22	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	FME	5	101	5	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	5	101	FME	O-C-CA	-3.16	116.50	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	5	101	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	2196:C	O3'	2197:U	P	2.55

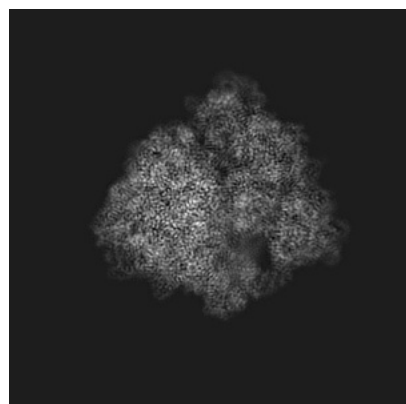
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3490. These allow visual inspection of the internal detail of the map and identification of artifacts.

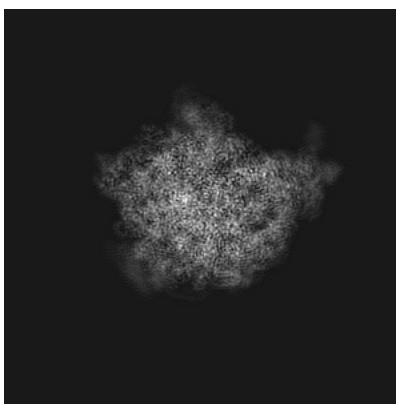
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

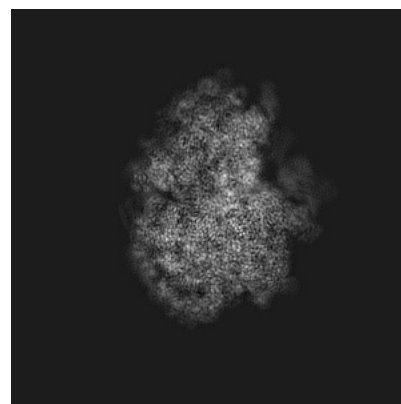
6.1.1 Primary map



X

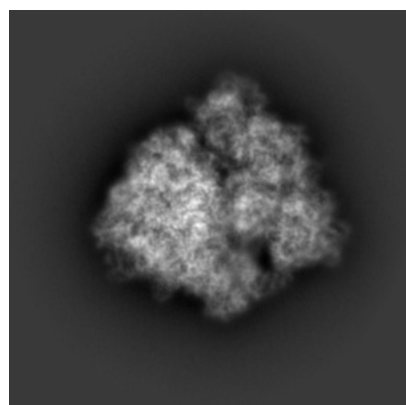


Y

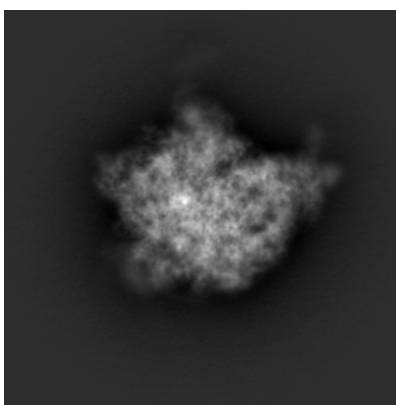


Z

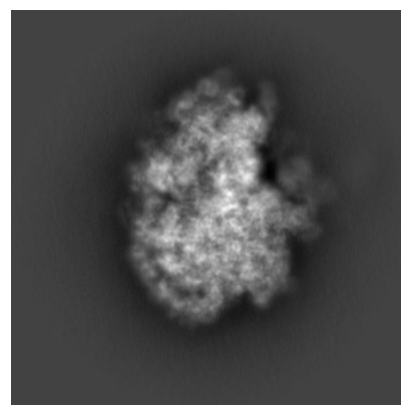
6.1.2 Raw map



X



Y

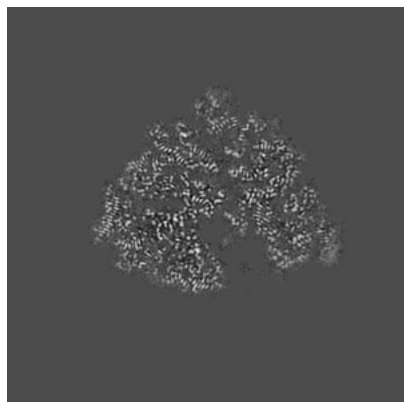


Z

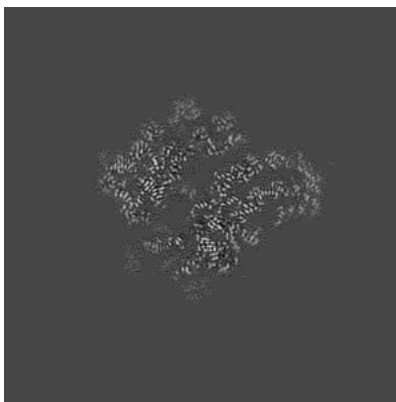
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

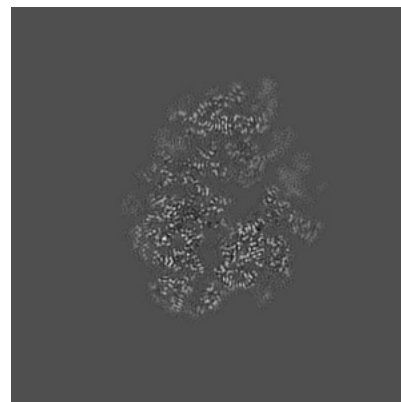
6.2.1 Primary map



X Index: 200

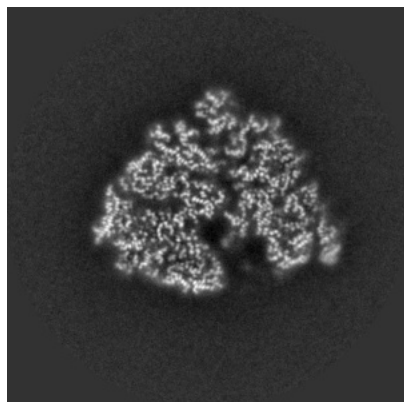


Y Index: 200

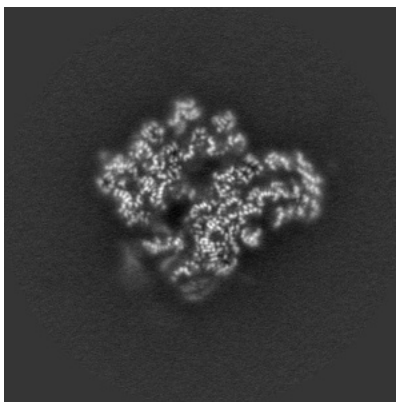


Z Index: 200

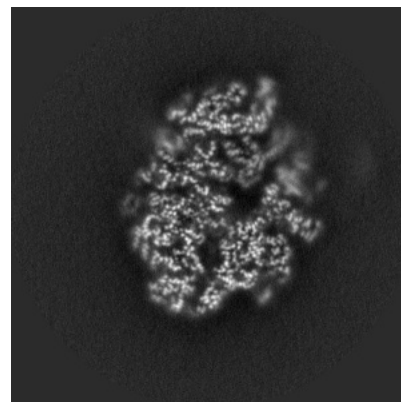
6.2.2 Raw map



X Index: 200



Y Index: 200

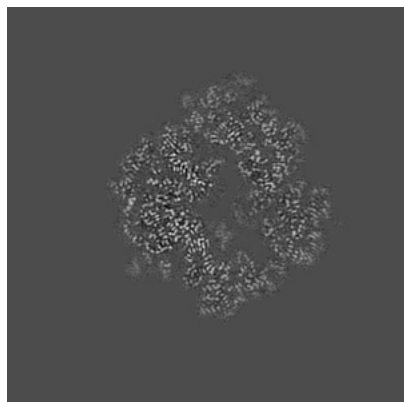


Z Index: 200

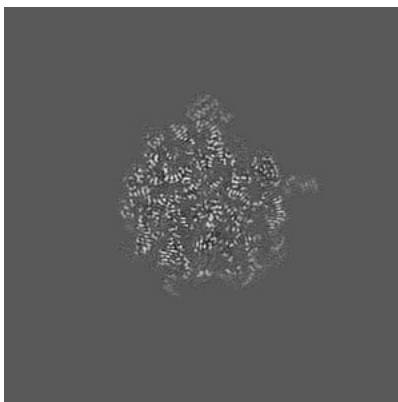
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

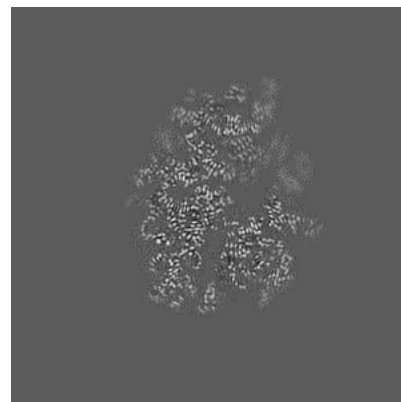
6.3.1 Primary map



X Index: 225

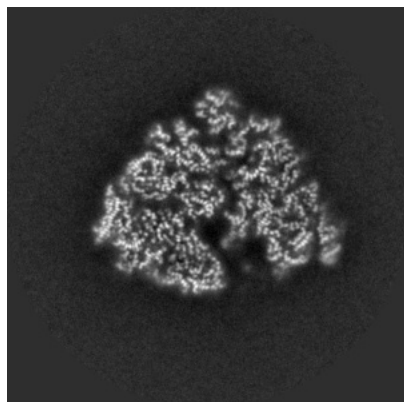


Y Index: 181

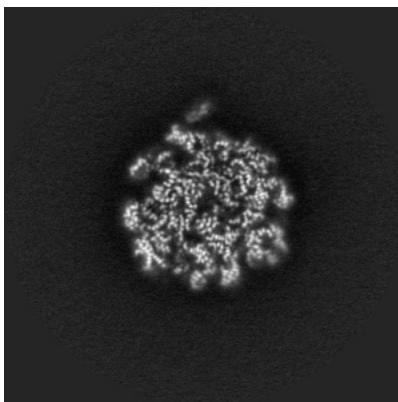


Z Index: 205

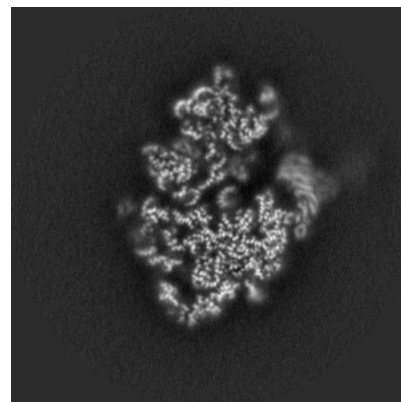
6.3.2 Raw map



X Index: 201



Y Index: 169

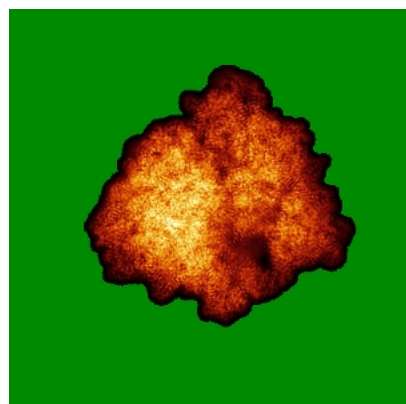


Z Index: 185

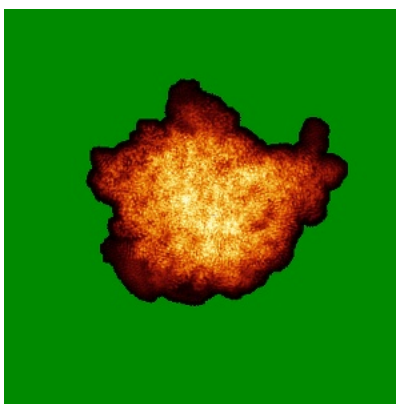
The images above show the largest variance slices of the map in three orthogonal directions.

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

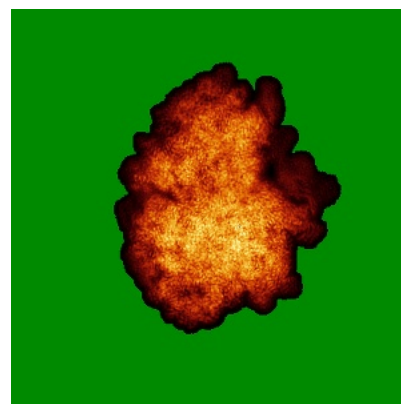
6.4.1 Primary map



X



Y

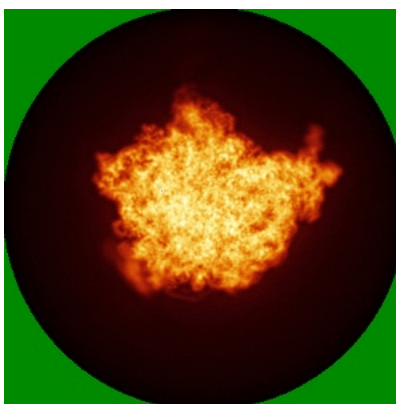


Z

6.4.2 Raw map



X



Y

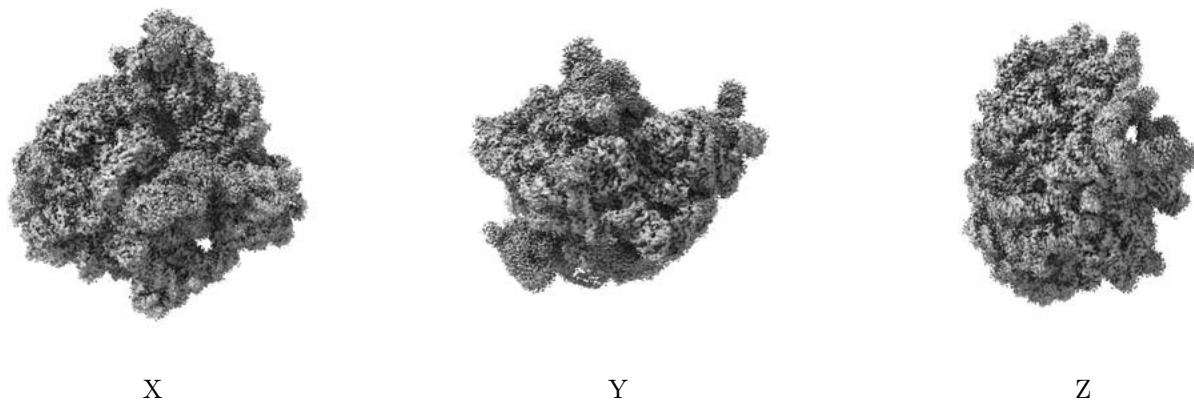


Z

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.

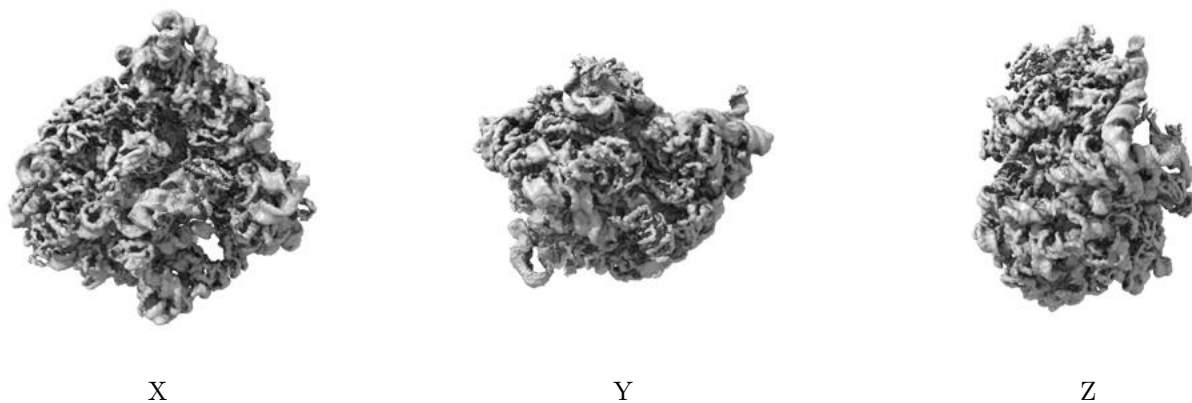
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

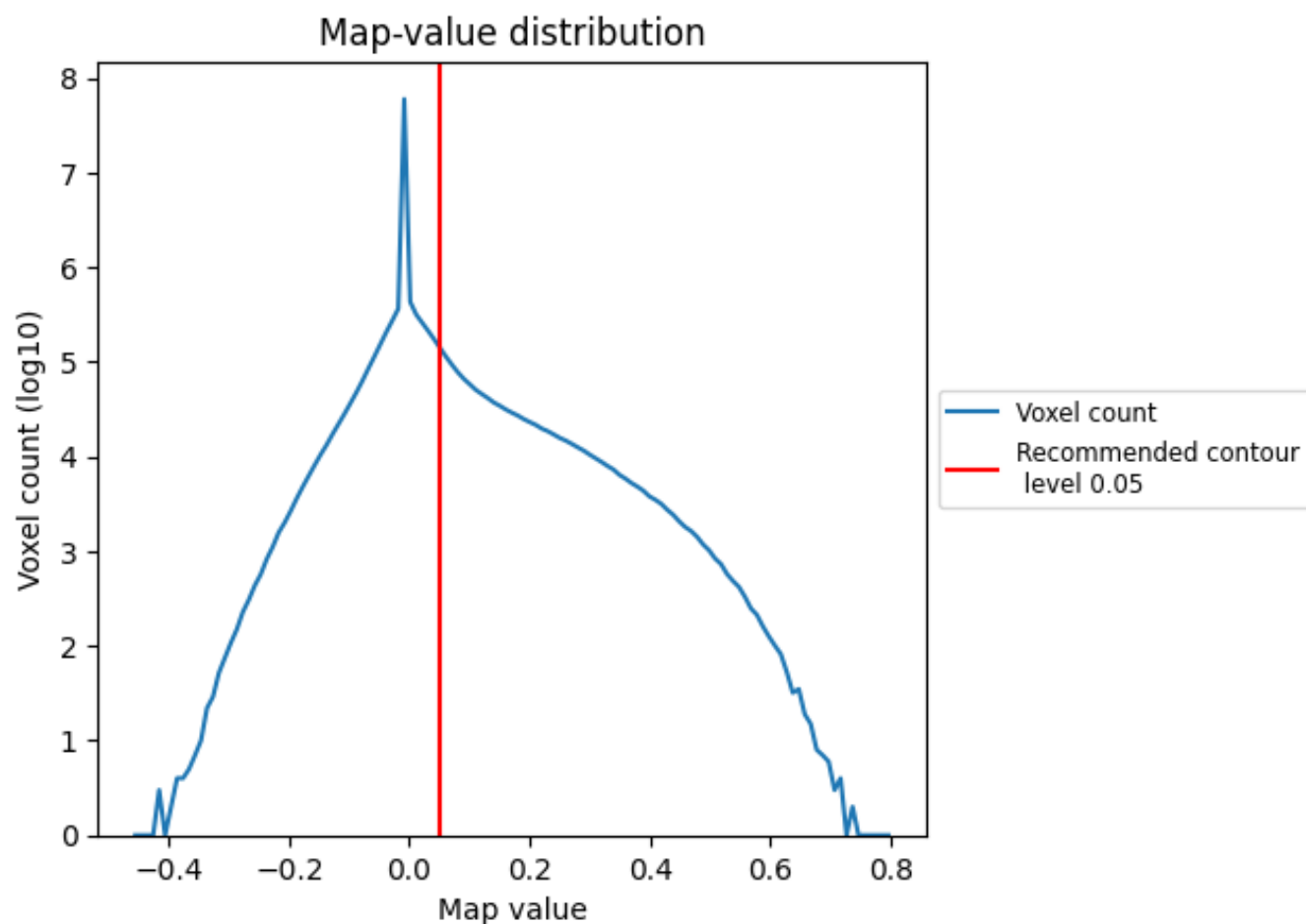
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

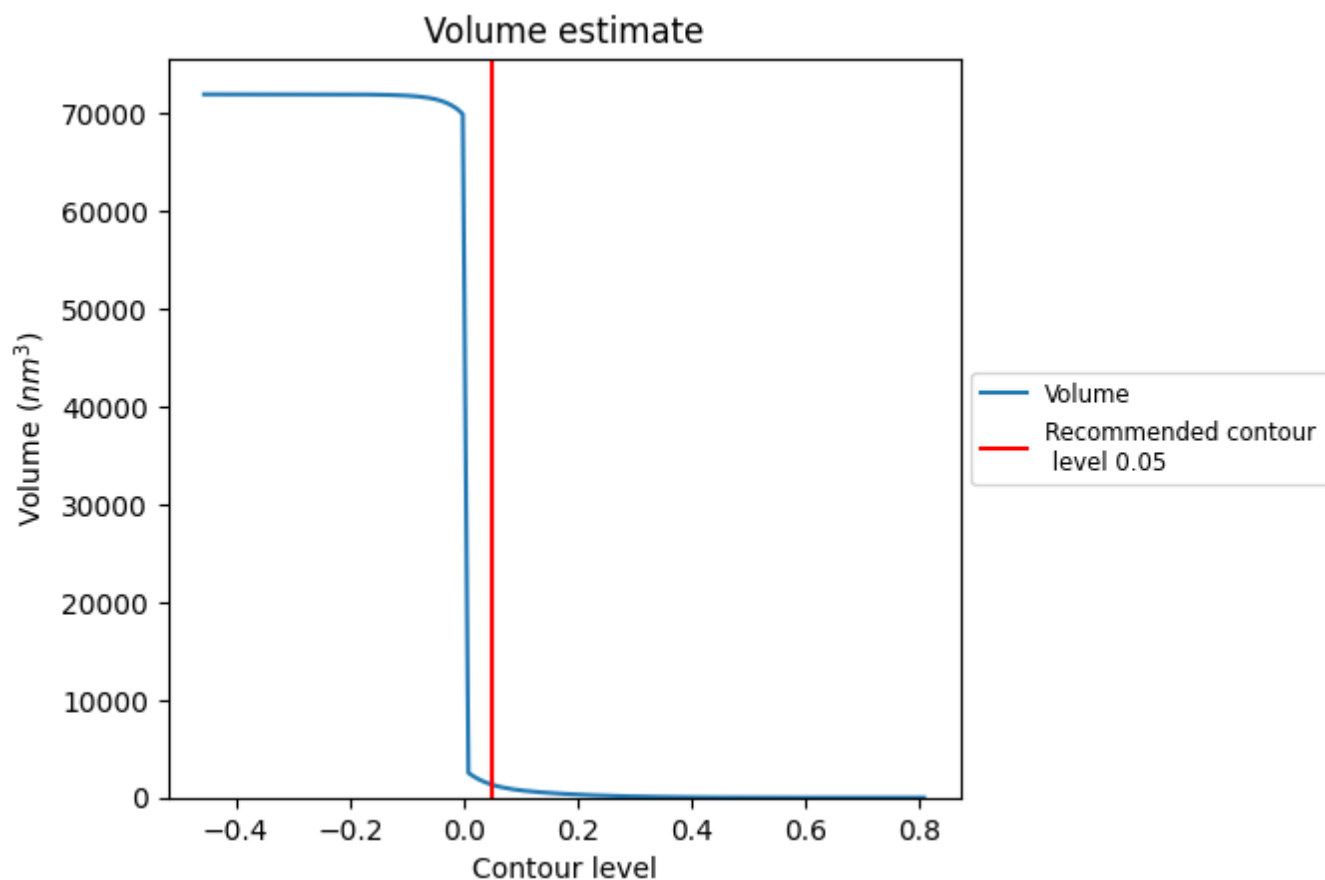
This section contains the results of statistical analysis of the map.

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.

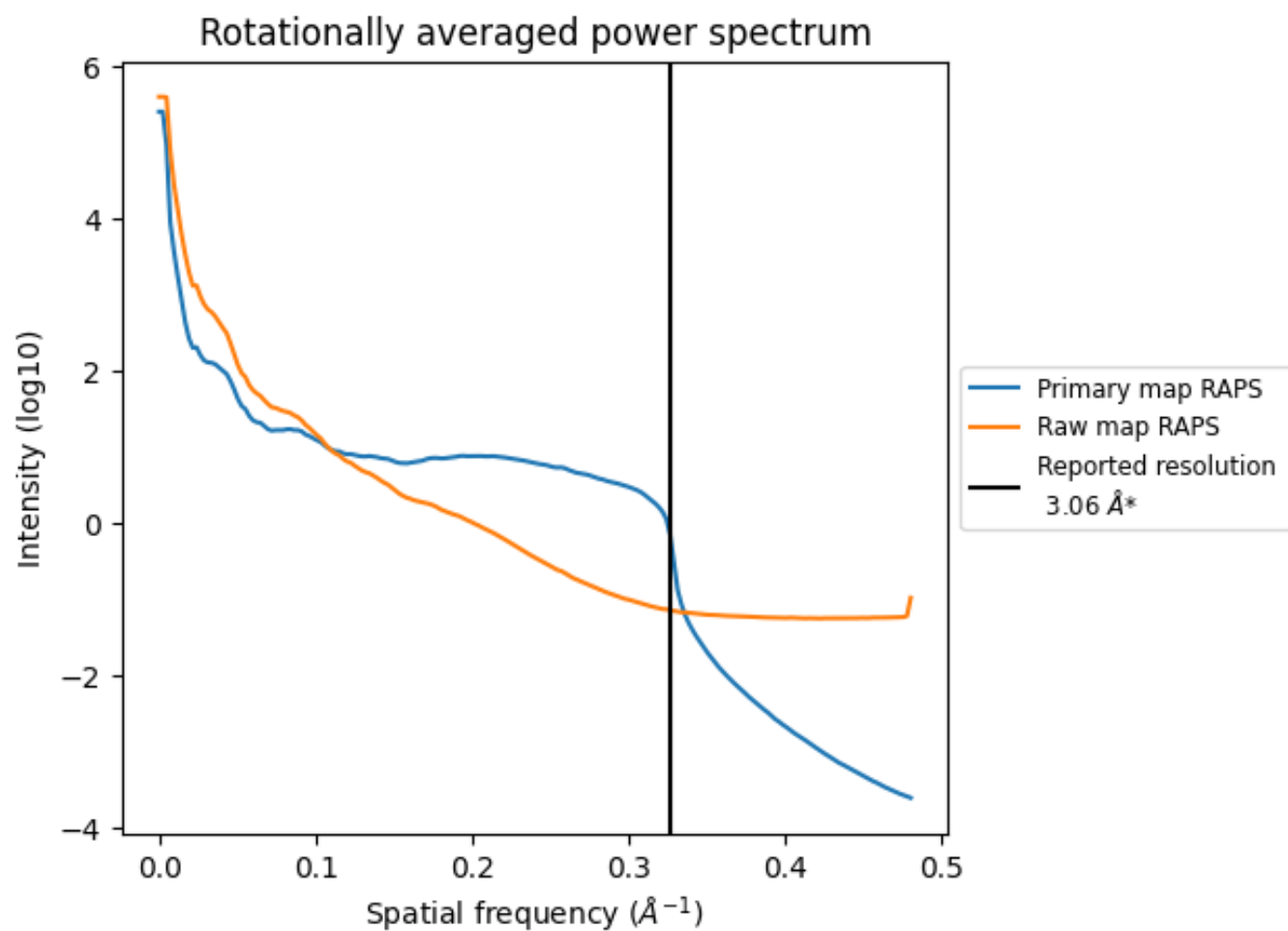
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1309 nm³; this corresponds to an approximate mass of 1182 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 ⓘ

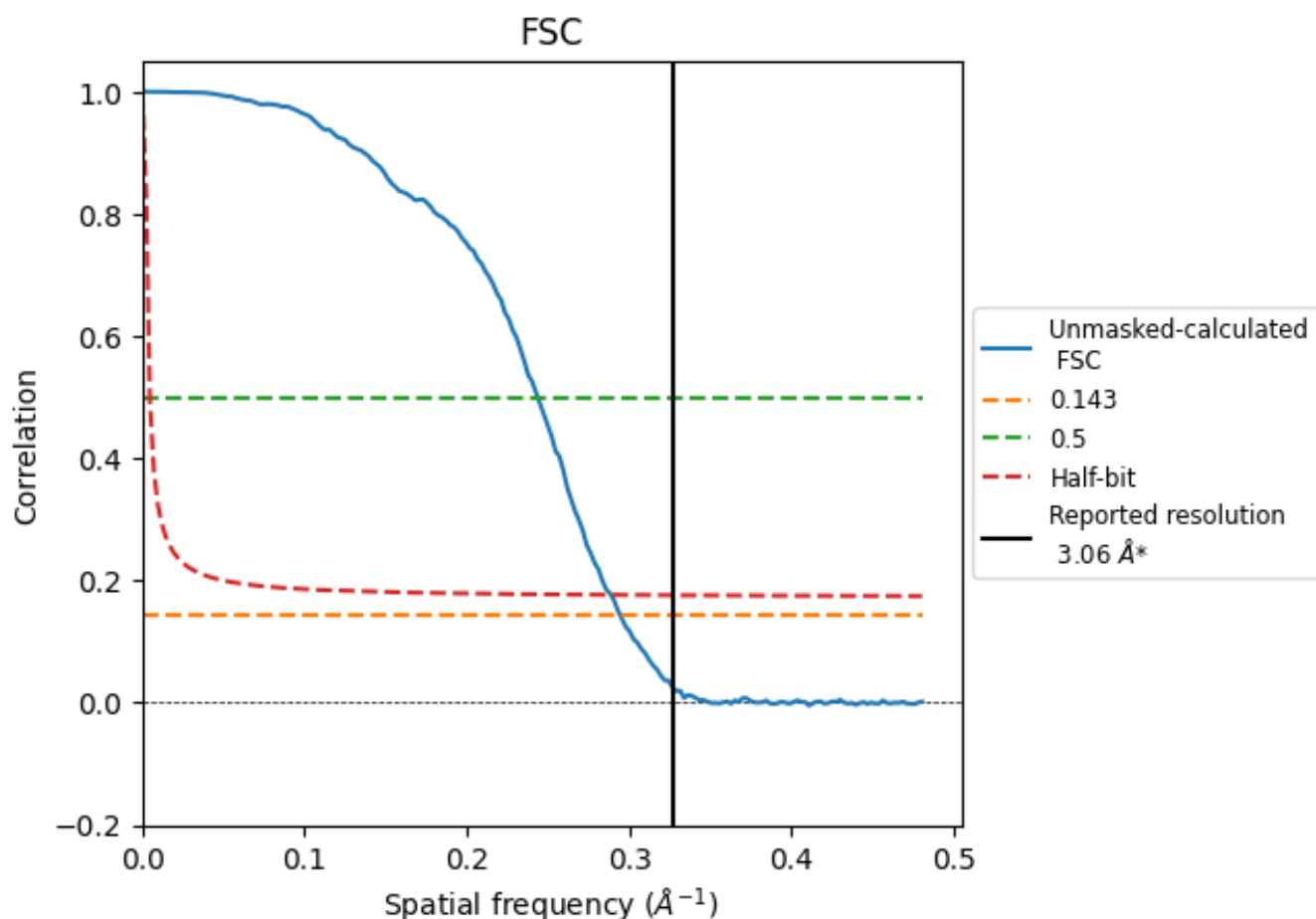


*Reported resolution corresponds to spatial frequency of $0.327 \text{ \AA}^{-1}$

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 0.327 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

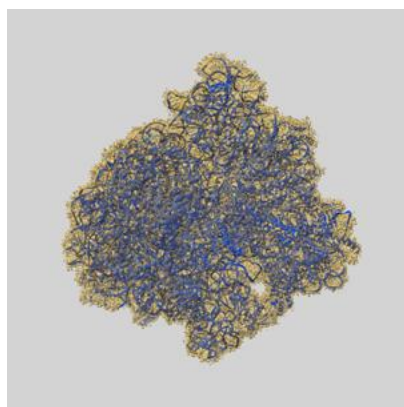
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	4.10	3.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.39 differs from the reported value 3.06 by more than 10 %

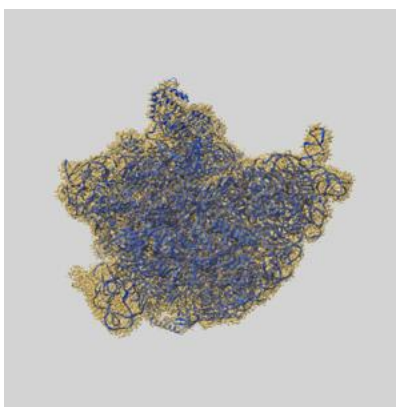
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3490 and PDB model 5MDW. Per-residue inclusion information can be found in section 3 on page 16.

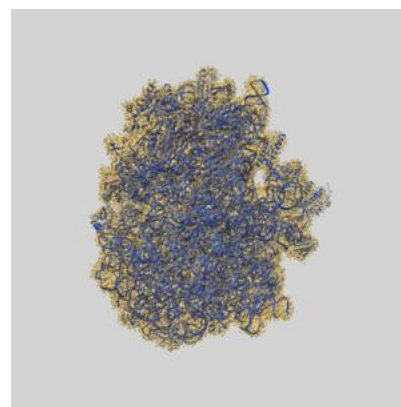
9.1 Map-model overlay [i](#)



X



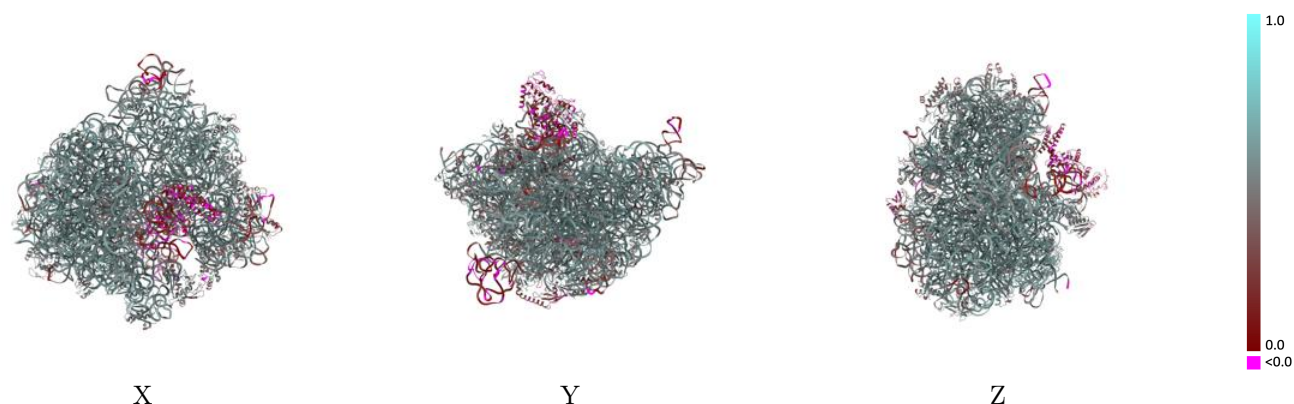
Y



Z

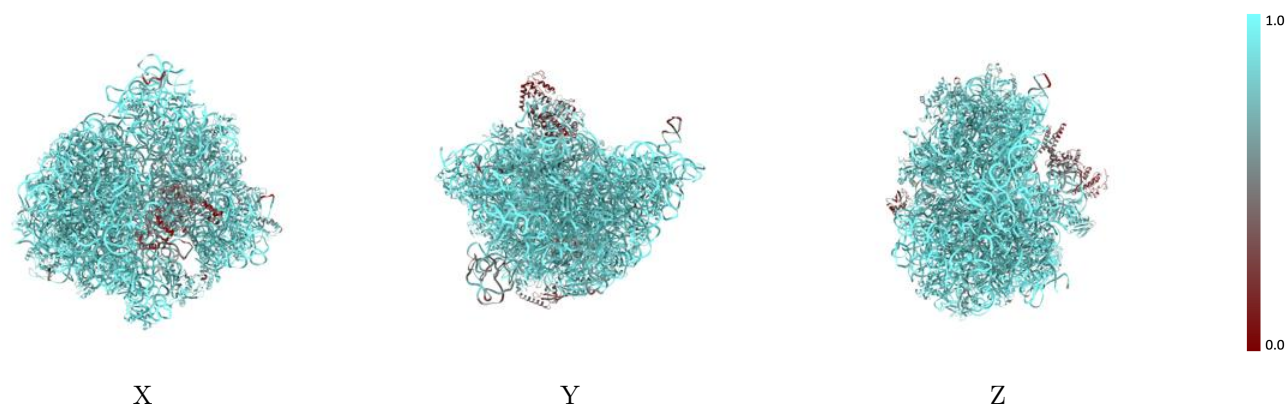
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



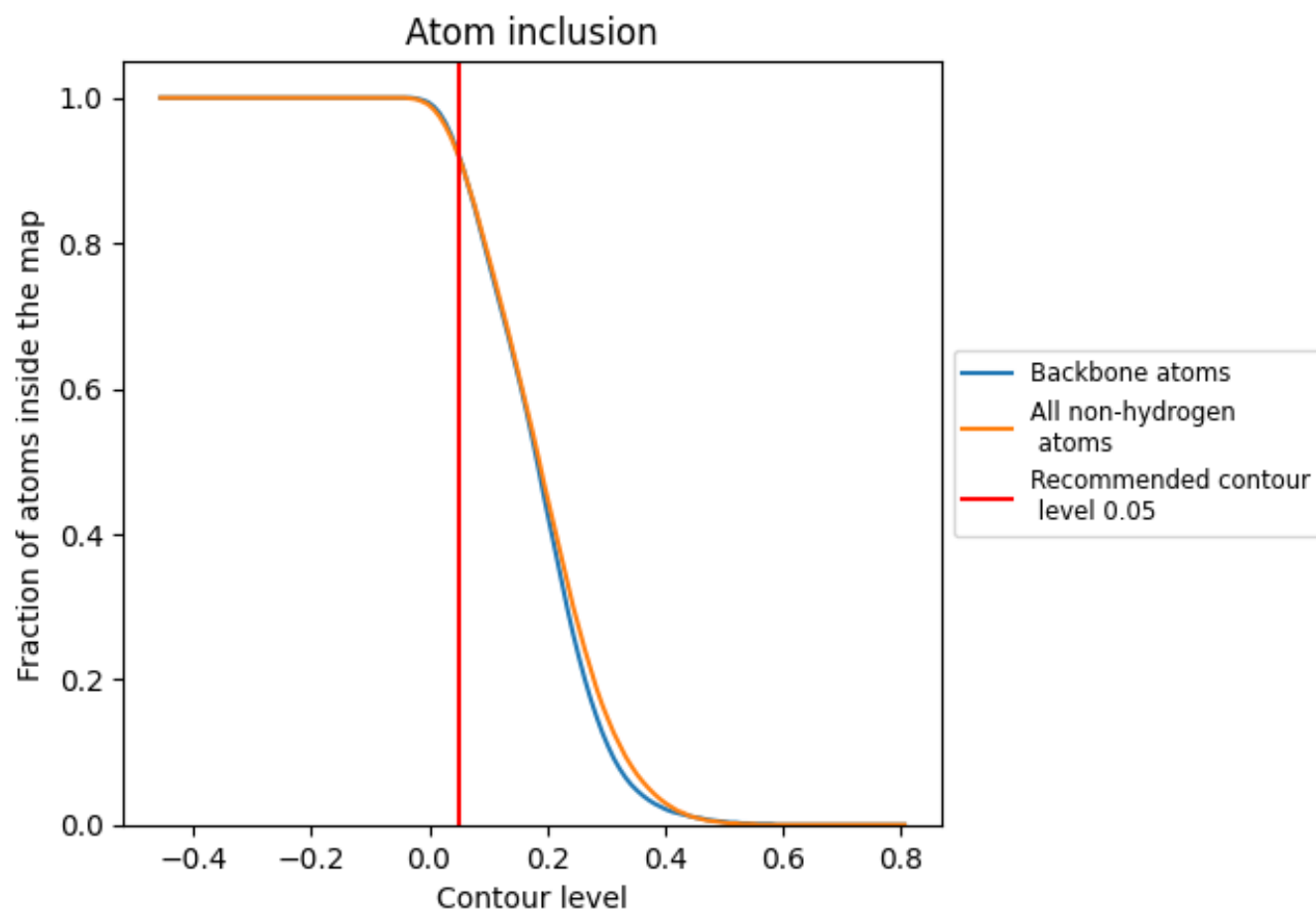
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9200	 0.5310
1	 0.9610	 0.5470
2	 0.9690	 0.5530
3	 0.9780	 0.5620
4	 0.9540	 0.5460
5	 0.9310	 0.5180
6	 0.8470	 0.5290
7	 0.6360	 0.3400
B	 0.9410	 0.5830
C	 0.9230	 0.5690
D	 0.8820	 0.5170
E	 0.8700	 0.4920
F	 0.8520	 0.4700
G	 0.4700	 0.2810
H	 0.1730	 0.0610
I	 0.3420	 0.0690
J	 0.9240	 0.5610
K	 0.9100	 0.5580
L	 0.9100	 0.5470
M	 0.9200	 0.5590
N	 0.9270	 0.5670
O	 0.9060	 0.5360
P	 0.9140	 0.5610
Q	 0.9260	 0.5720
R	 0.9310	 0.5570
S	 0.8990	 0.5530
T	 0.8780	 0.5240
U	 0.8890	 0.5150
V	 0.8860	 0.5270
W	 0.9280	 0.5780
X	 0.9270	 0.5720
Y	 0.8550	 0.4940
Z	 0.9150	 0.5520
a	 0.7890	 0.3910
b	 0.9040	 0.5640



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Chain	Atom inclusion	Q-score
c	 0.8590	 0.5320
d	 0.9100	 0.5820
e	 0.9350	 0.5860
f	 0.9250	 0.5600
g	 0.7430	 0.4440
h	 0.8830	 0.5130
i	 0.8770	 0.5150
j	 0.9110	 0.5540
k	 0.8560	 0.4870
l	 0.8370	 0.4720
m	 0.8850	 0.5400
n	 0.8660	 0.5010
o	 0.8180	 0.4560
p	 0.9040	 0.5410
q	 0.9090	 0.5620
r	 0.8720	 0.5070
s	 0.9000	 0.5350
t	 0.8990	 0.5320
u	 0.8950	 0.5340
v	 0.8670	 0.5130
w	 0.8950	 0.5280
x	 0.9040	 0.5140
y	 0.8850	 0.5150
z	 0.7570	 0.4250