



Full wwPDB EM Validation Report ⓘ

Aug 13, 2025 – 04:49 pm BST

PDB ID : 9I5X / pdb_00009i5x
EMDB ID : EMD-52641
Title : Porphyromonas gingivalis 70S ribosome (W83 Strain)
Authors : Hiregange, D.G.; Bashan, A.; Yonath, A.
Deposited on : 2025-01-28
Resolution : 3.00 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.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

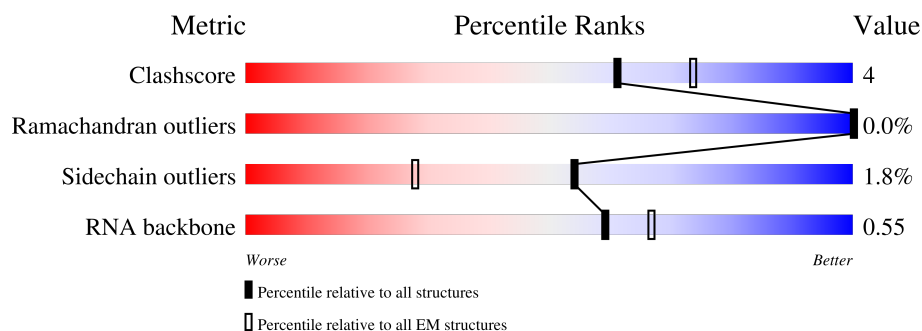
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.









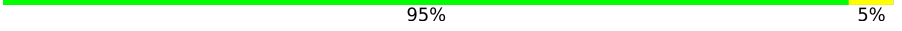




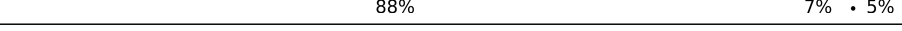




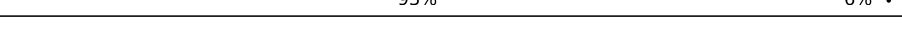


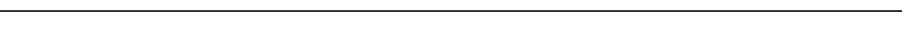

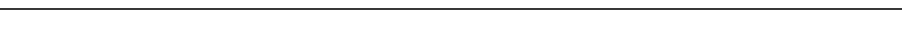
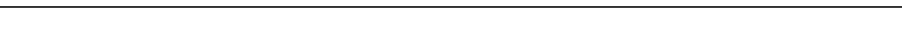


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	p	89	
2	0	79	
3	1	64	
4	2	58	
5	4	61	
6	5	62	
7	6	50	

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Mol	Chain	Length	Quality of chain
8	7	65	 88% 11% .
9	8	38	 82% 11% 8%
10	A	2889	 60% 19% . 19%
11	B	109	 61% 28% . 8%
12	D	274	 89% 11% .
13	E	205	 91% 7% .
14	F	209	 95% 5%
15	K	101	 64% 5% . 30%
16	L	128	 66% 8% 26%
17	M	151	 89% 11% .
18	N	121	 89% 11%
19	O	148	 88% 7% . 5%
20	P	144	 81% 15% ..
21	Q	160	 72% . 23%
22	R	114	 85% 8% . 6%
23	S	121	 87% 7% 6%
24	T	115	 93% 6% .
25	U	105	 89% 10% ..
26	V	134	 83% 12% . .
27	W	97	 73% 20% 7%
28	X	106	 92% 5% .
29	Z	85	 87% . 9%
30	a	1534	 52% 29% 5% 14%
31	b	117	 73% 11% 16%
32	c	192	 42% 9% 49%

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Mol	Chain	Length	Quality of chain
33	d	84	
34	e	84	
35	f	89	
36	g	89	
37	h	179	
38	i	126	
39	j	134	
40	k	246	
41	l	201	
42	m	158	
43	n	172	
44	Y	192	
45	o	131	
46	10	30	
47	J	128	
48	I	90	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 116574 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	p	71	Total	C	N	O	S	0	0
			510	325	95	88	2		

- Molecule 2 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	77	Total	C	N	O	S	0	0
			608	390	118	97	3		

- Molecule 3 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	63	Total	C	N	O	S	0	0
			450	281	87	79	3		

- Molecule 4 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	56	Total	C	N	O	S	0	0
			437	276	89	70	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	56	Total	C	N	O	S	0	0
			427	265	89	69	4		

- Molecule 6 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	47	Total	C	N	O	S	0	0
			342	213	62	66	1		

- Molecule 7 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	48	Total	C	N	O	S	0	0
			391	237	89	63	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	64	Total	C	N	O	S	0	0
			456	289	91	75	1		

- Molecule 9 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	35	Total	C	N	O	S	0	0
			262	164	53	43	2		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2344	Total	C	N	O	P	0	0
			50306	22463	9275	16224	2344		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	100	Total	C	N	O	P	0	0
			2142	955	391	696	100		

- Molecule 12 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	272	Total	C	N	O	S	0	0
			2058	1282	403	365	8		

- Molecule 13 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	204	Total	C	N	O	S	0	0
			1512	963	273	269	7		

- Molecule 14 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	209	Total	C	N	O	S	0	0
			1624	1029	295	298	2		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	71	Total	C	N	O	0	0
			511	330	91	90		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	95	Total	C	N	O	S	0	0
			550	331	113	105	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	150	Total	C	N	O	S	0	0
			1178	751	217	204	6		

- Molecule 18 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	121	Total	C	N	O	S	0	0
			904	565	173	162	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	141	Total	C	N	O	S	0	0
			991	620	189	180	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	141	Total	C	N	O	S	0	0
			1089	699	201	186	3		

- Molecule 21 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	123	Total	C	N	O	S	0	0
			989	630	184	169	6		

- Molecule 22 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	107	Total	C	N	O	S	0	0
			739	460	147	132			

- Molecule 23 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	114	Total	C	N	O	S	0	0
			945	602	178	164	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	114	Total	C	N	O	S	0	0
			919	581	189	146	3		

- Molecule 25 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	104	Total	C	N	O	S	0	0
			824	526	150	145	3		

- Molecule 26 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	128	Total	C	N	O	S	0	0
			1023	634	203	181	5		

- Molecule 27 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	90	Total	C	N	O	S	0	0
			683	434	122	124	3		

- Molecule 28 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	102	Total	C	N	O	S	0	0
			732	458	144	128	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	77	Total	C	N	O	S	0	0
			570	352	113	104	1		

- Molecule 30 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	1326	Total	C	N	O	P	0	0
			28463	12702	5226	9209	1326		

- Molecule 31 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	b	98	Total	C	N	O	0	0
			696	445	128	123		

- Molecule 32 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	97	Total	C	N	O	S	0	0
			712	446	135	130	1		

- Molecule 33 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	76	Total	C	N	O	S	0	0
			591	367	123	100	1		

- Molecule 34 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	81	Total	C	N	O	S	0	0
			639	403	124	109	3		

- Molecule 35 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	89	Total	C	N	O	S	0	0
			671	426	124	119	2		

- Molecule 36 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	88	Total	C	N	O	S	0	0
			659	415	132	107	5		

- Molecule 37 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	55	Total	C	N	O	S	0	0
			415	263	76	75	1		

- Molecule 38 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	82	Total	C	N	O	S	0	0
			616	392	114	109	1		

- Molecule 39 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	120	Total	C	N	O	S	0	0
			849	521	178	148	2		

- Molecule 40 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	106	Total	C	N	O	S	0	0
			691	433	123	131	4		

- Molecule 41 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	191	Total	C	N	O	S	0	0
			1383	889	250	243	1		

- Molecule 42 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	105	Total	C	N	O	S	0	0
			714	456	123	133	2		

- Molecule 43 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	160	Total	C	N	O	S	0	0
			1032	648	191	191	2		

- Molecule 44 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Y	128	Total	C	N	O	S	0	0
			851	549	152	149	1		

- Molecule 45 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	129	Total	C	N	O	S	0	0
			964	623	167	169	5		

- Molecule 46 is a protein called AURKAIP1/COX24 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	10	27	Total	C	N	O	S	0	0
			219	132	56	30	1		

- Molecule 47 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	J	124	Total	C	N	O		0	0
			827	528	162	137			

- Molecule 48 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	I	51	Total	C	N	O		0	0
			369	239	73	57			

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	4	1	Total 1	Mg 1	0
49	A	119	Total 119	Mg 119	0
49	F	1	Total 1	Mg 1	0
49	T	1	Total 1	Mg 1	0
49	V	2	Total 2	Mg 2	0
49	a	4	Total 4	Mg 4	0

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
50	4	1	Total 1	Zn 1	0

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
51	A	31	Total 31	K 31	0
51	B	1	Total 1	K 1	0
51	W	1	Total 1	K 1	0
51	X	1	Total 1	K 1	0
51	a	9	Total 9	K 9	0

- Molecule 52 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
52	A	12	Total 12	Na 12	0
52	B	2	Total 2	Na 2	0

- Molecule 53 is water.

Mol	Chain	Residues	Atoms	AltConf
53	4	2	Total O 2 2	0
53	A	741	Total O 741 741	0
53	B	6	Total O 6 6	0
53	D	4	Total O 4 4	0
53	E	10	Total O 10 10	0
53	F	4	Total O 4 4	0
53	M	2	Total O 2 2	0
53	O	13	Total O 13 13	0
53	Q	8	Total O 8 8	0
53	T	10	Total O 10 10	0
53	U	8	Total O 8 8	0
53	V	6	Total O 6 6	0
53	Z	1	Total O 1 1	0
53	a	40	Total O 40 40	0

3 Residue-property plots [i](#)

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

- Molecule 1: Small ribosomal subunit protein uS19

Chain p: 




- Molecule 2: Large ribosomal subunit protein bL28

Chain 0: 




- Molecule 3: Large ribosomal subunit protein uL29

Chain 1: 




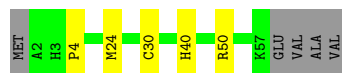
- Molecule 4: Large ribosomal subunit protein uL30

Chain 2: 



- Molecule 5: Large ribosomal subunit protein bL32

Chain 4: 



- Molecule 6: Large ribosomal subunit protein bL33

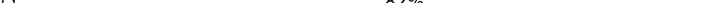
MET
ALA
LYS
LVS
VAL
LVS
GLY
ASN
ARG
VAL
GLN
VAL
IIE
L14
T17
K20
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P80
G26
T32
T33
K34
L43
K46
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Y48
N49
R53
R54
H55
T56
L57
I61
LVS

- Chain 6: 92% . .



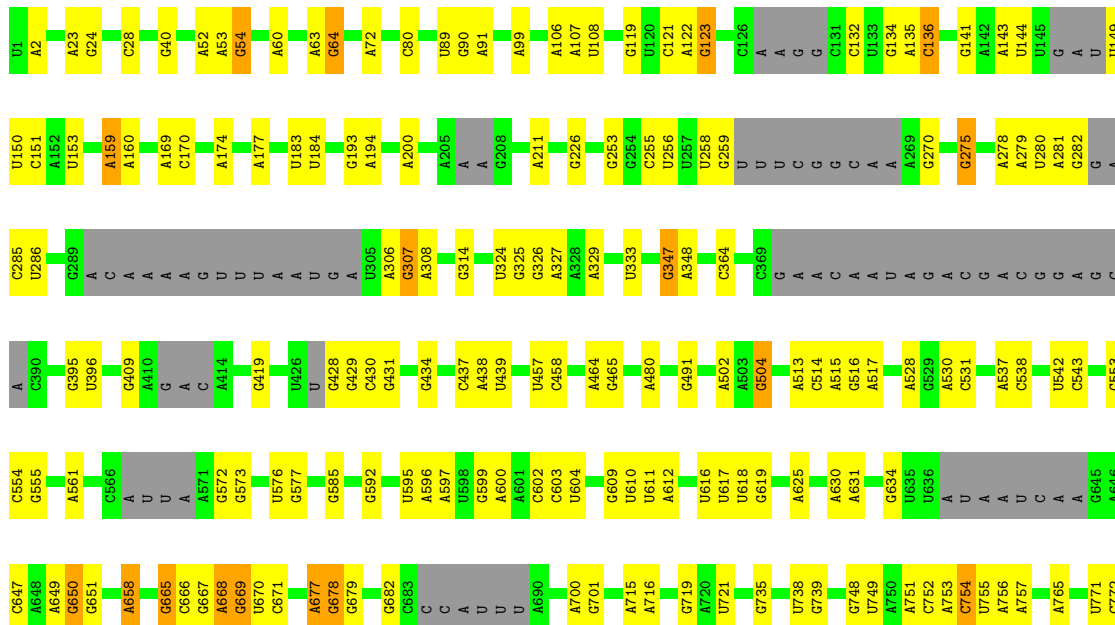
- Chain 7: 88% 11%



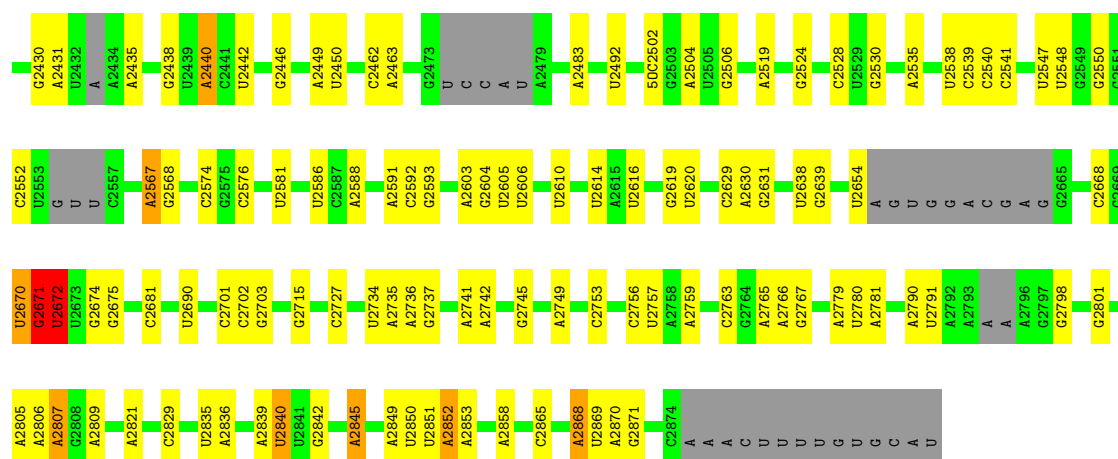
- Chain 8:  82% 11% 8%



- Chain A: 60% 19% 1% 19%

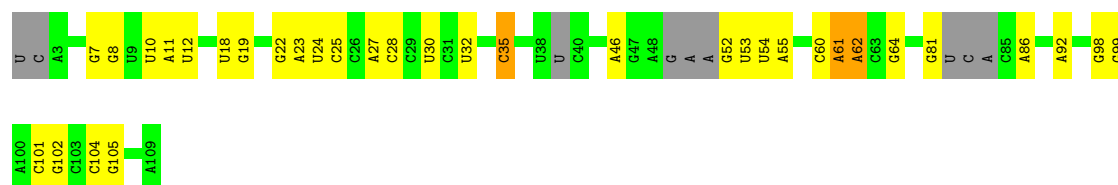






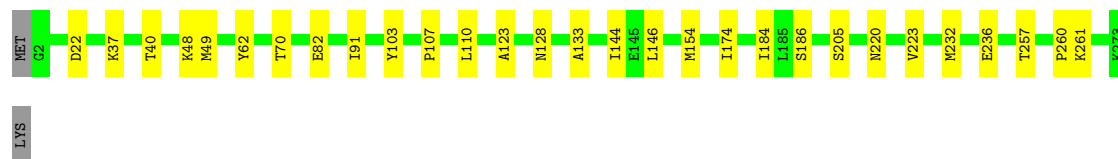
• Molecule 11: 5S rRNA

Chain B: 61% 28% 8%



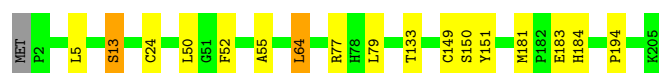
• Molecule 12: Large ribosomal subunit protein uL2

Chain D: 89% 11%



• Molecule 13: Large ribosomal subunit protein uL3

Chain E: 91% 7%



• Molecule 14: Large ribosomal subunit protein uL4

Chain F: 95% 5%



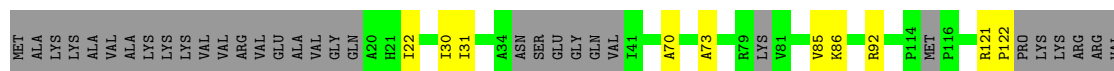
• Molecule 15: Small ribosomal subunit protein uS10

Chain K:  64% 5% 30%




- Molecule 16: Small ribosomal subunit protein uS11

Chain L:  66% 8% 26%




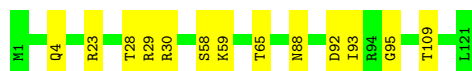
- Molecule 17: Large ribosomal subunit protein uL13

Chain M:  89% 11%




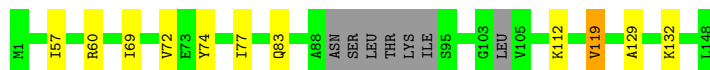
- Molecule 18: Large ribosomal subunit protein uL14

Chain N:  89% 11%




- Molecule 19: Large ribosomal subunit protein uL15

Chain O:  88% 7% 5%



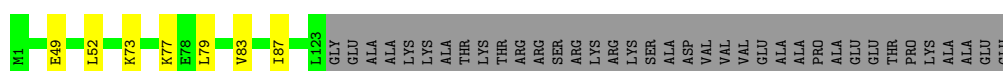
- Molecule 20: Large ribosomal subunit protein uL16

Chain P:  81% 15% 2%




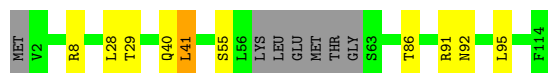
- Molecule 21: Large ribosomal subunit protein bL17

Chain Q:  72% 23%




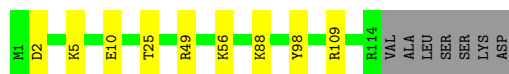
- Molecule 22: Large ribosomal subunit protein uL18

Chain R:  85% 8% 6%



- Molecule 23: Large ribosomal subunit protein bL19

Chain S:  87% 7% 6%




- Molecule 24: Large ribosomal subunit protein bL20

Chain T:  93% 6% .




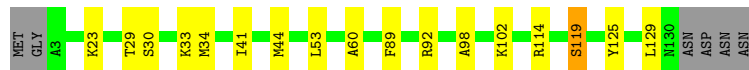
- Molecule 25: Large ribosomal subunit protein bL21

Chain U:  89% 10% ..



- Molecule 26: Large ribosomal subunit protein uL22

Chain V:  83% 12% . .



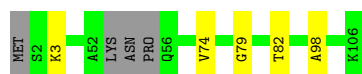
- Molecule 27: Large ribosomal subunit protein uL23

Chain W:  73% 20% 7%



- Molecule 28: Large ribosomal subunit protein uL24

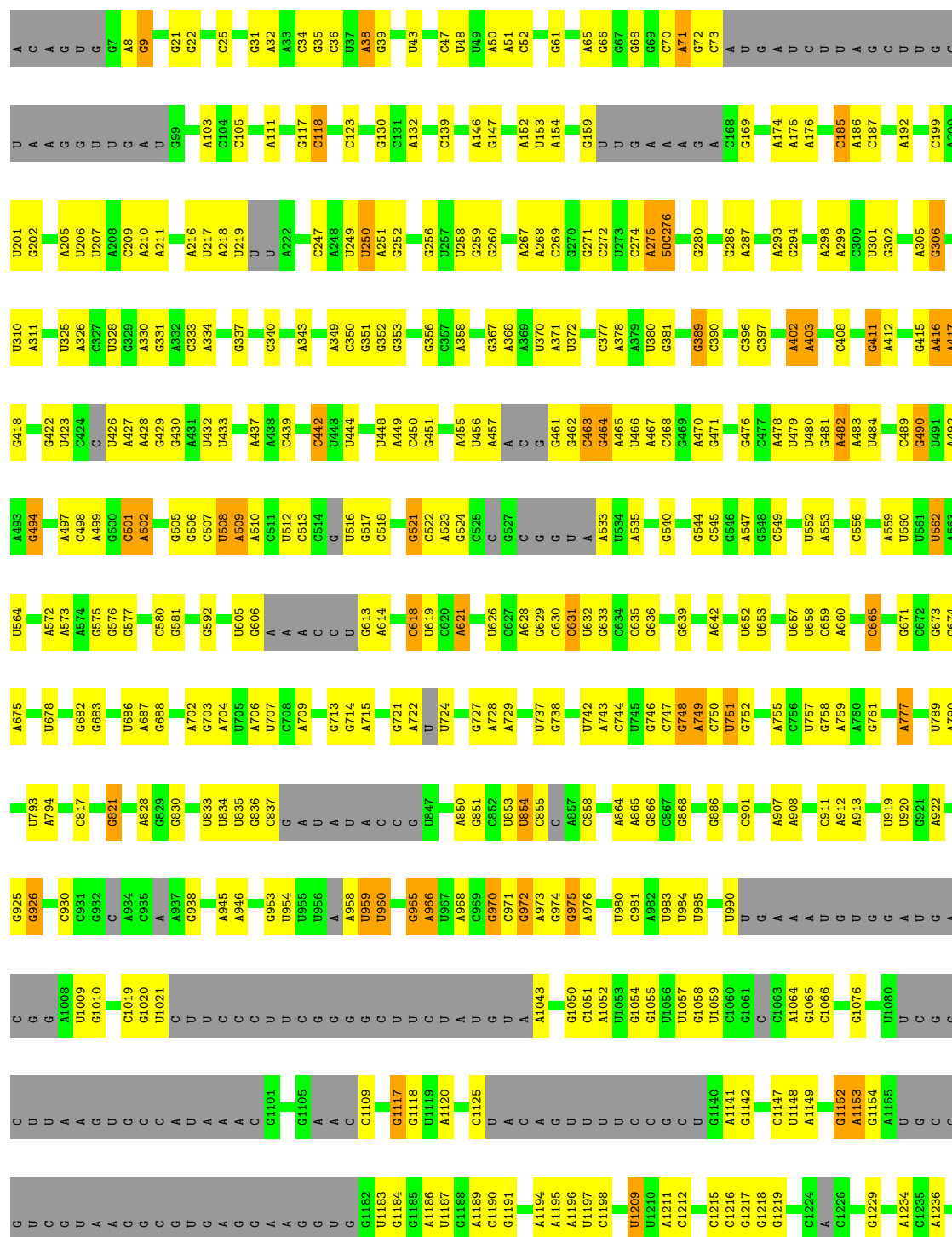
Chain X:  92% 5% .

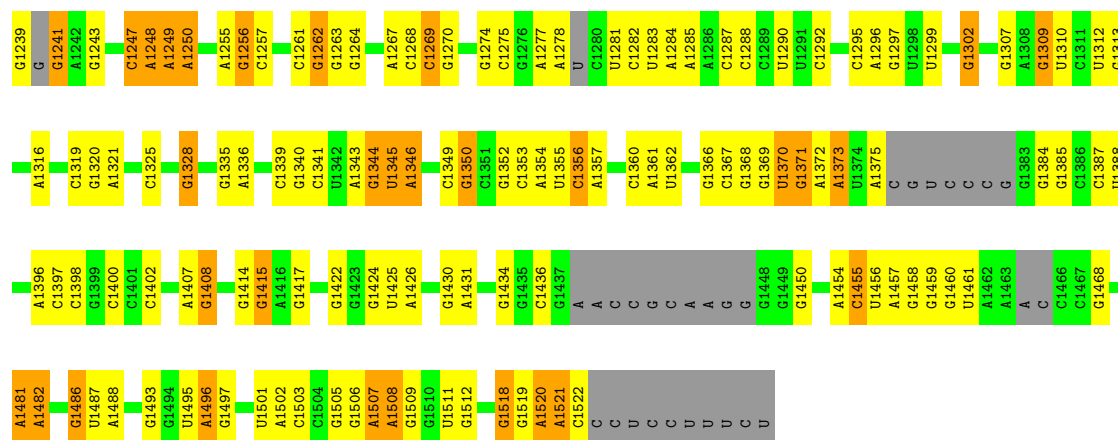


- Molecule 29: Large ribosomal subunit protein bL27

MET
ALA
HIS
LYS
LYS
GLY
VAL
G8
S9
E15
S18
E84
SER

Chain a: 52% 29% 5% 14%





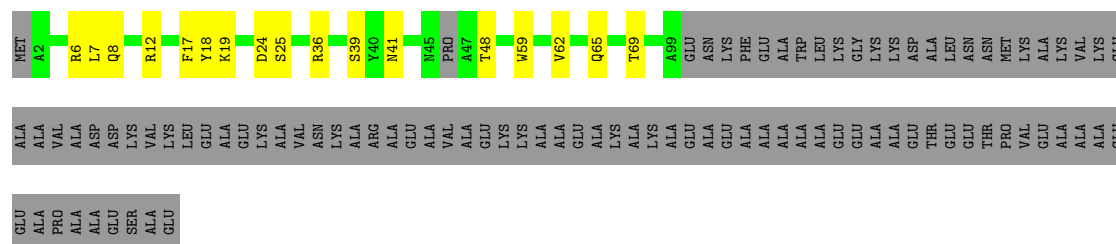
- Molecule 31: Small ribosomal subunit protein bS6

Chain b: 73% 11% 16%



- Molecule 32: Small ribosomal subunit protein bS16

Chain c: 42% 9% 49%



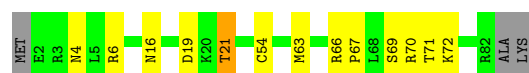
- Molecule 33: Small ribosomal subunit protein bS20

Chain d: 75% 14% 10%



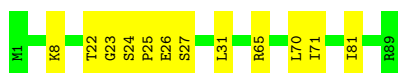
- Molecule 34: Small ribosomal subunit protein uS17

Chain e: 81% 14% 5%



- Molecule 35: Small ribosomal subunit protein uS15

Chain f: 87% 13%



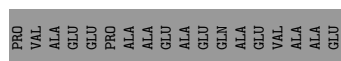
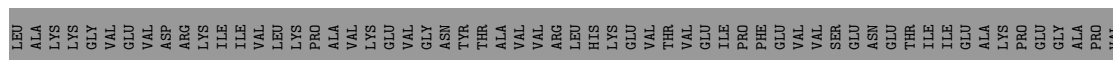
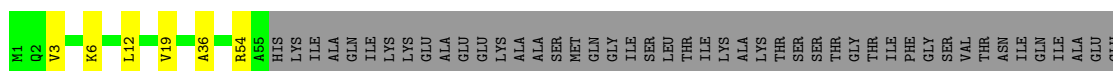
- Molecule 36: Small ribosomal subunit protein uS14

Chain g: 93% 6%



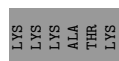
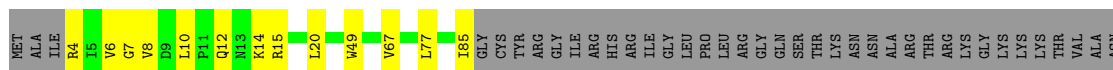
- Molecule 37: Large ribosomal subunit protein bL9

Chain h: 27% 69%



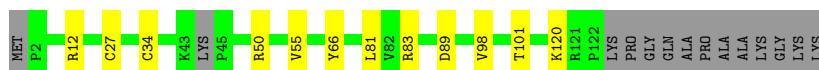
- Molecule 38: Small ribosomal subunit protein uS13

Chain i: 55% 10% 35%



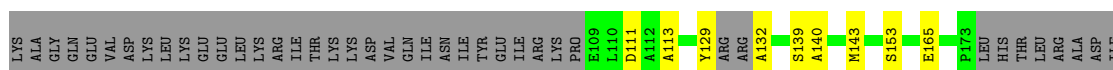
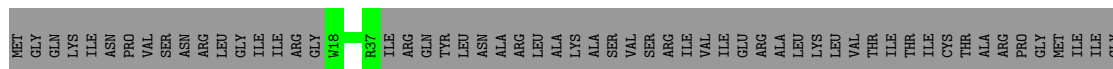
- Molecule 39: Small ribosomal subunit protein uS12

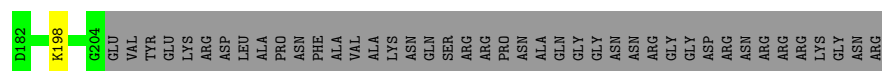
Chain j: 81% 9% 10%



- Molecule 40: Small ribosomal subunit protein uS3

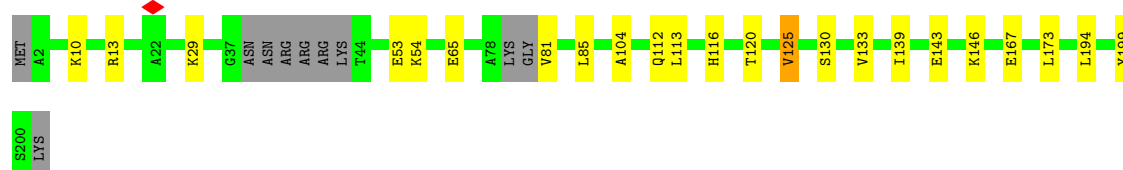
Chain k: 39% 57%





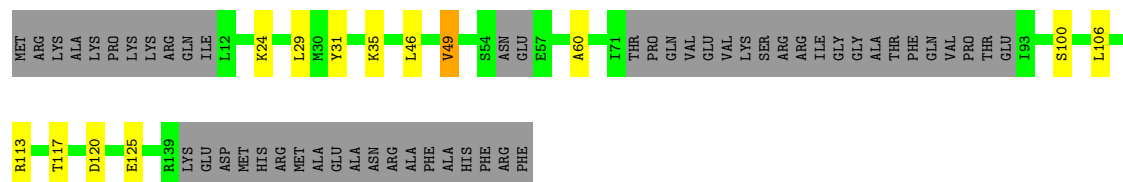
- Molecule 41: Small ribosomal subunit protein uS4

Chain l: 84% 11% 5%



- Molecule 42: Small ribosomal subunit protein uS7

Chain m: 58% 8% 34%



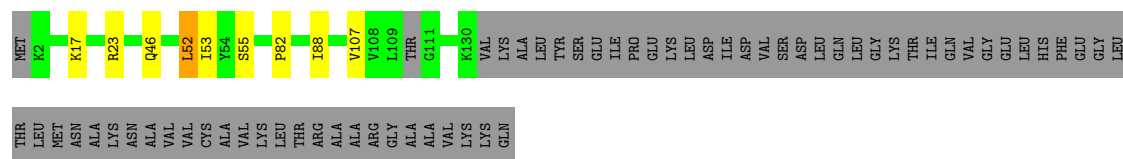
- Molecule 43: Small ribosomal subunit protein uS5

Chain n: 84% 8% 7%



- Molecule 44: Large ribosomal subunit protein bL25

Chain Y: 62% 33%



- Molecule 45: Small ribosomal subunit protein uS8

Chain o: 89% 9% 2%

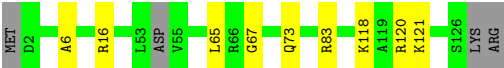
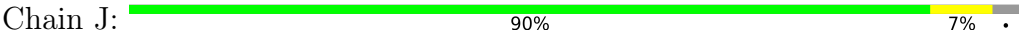


- Molecule 46: AURKAIP1/COX24 domain-containing protein

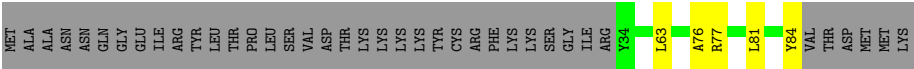
Chain 10: 73% 17% 10%



- Molecule 47: Small ribosomal subunit protein uS9



- Molecule 48: Small ribosomal subunit protein bS18



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	370.48, 370.48, 370.48	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MG, 2MA, 5MC, 5MU, 4OC, K, NA, UR3, ZN, MA6, OMG, 2MG, OMU, 7MG, 5OC, H2U

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	p	0.13	0/522	0.30	0/708
2	0	0.16	0/617	0.31	0/825
3	1	0.14	0/454	0.26	0/615
4	2	0.19	0/440	0.35	0/591
5	4	0.19	0/438	0.34	0/592
6	5	0.17	0/344	0.39	0/464
7	6	0.18	0/395	0.35	0/521
8	7	0.16	0/461	0.44	0/617
9	8	0.10	0/263	0.25	0/347
10	A	0.23	0/56035	0.35	5/87314 (0.0%)
11	B	0.15	0/2393	0.27	0/3723
12	D	0.19	0/2097	0.37	1/2814 (0.0%)
13	E	0.18	0/1541	0.39	0/2071
14	F	0.18	0/1647	0.34	0/2219
15	K	0.14	0/518	0.38	0/703
16	L	0.09	0/553	0.23	0/750
17	M	0.18	0/1203	0.31	0/1622
18	N	0.17	0/911	0.34	0/1225
19	O	0.16	0/1001	0.37	0/1341
20	P	0.17	0/1112	0.39	0/1495
21	Q	0.18	0/1006	0.36	0/1347
22	R	0.13	0/745	0.30	0/1000
23	S	0.15	0/960	0.26	0/1275
24	T	0.21	0/936	0.35	0/1252
25	U	0.20	0/834	0.44	0/1118
26	V	0.18	0/1036	0.33	0/1385
27	W	0.18	0/690	0.37	0/924
28	X	0.14	0/738	0.31	0/988
29	Z	0.16	0/577	0.29	0/772
30	a	0.15	0/31641	0.30	0/49284
31	b	0.10	0/708	0.30	0/967
32	c	0.14	0/723	0.32	0/977

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.16	0/597	0.37	0/799
34	e	0.11	0/650	0.28	0/872
35	f	0.15	0/680	0.34	0/914
36	g	0.11	0/670	0.27	0/897
37	h	0.20	0/417	0.54	0/559
38	i	0.13	0/622	0.32	0/839
39	j	0.10	0/860	0.30	0/1167
40	k	0.12	0/694	0.34	0/936
41	l	0.14	0/1412	0.38	0/1922
42	m	0.15	0/722	0.36	0/981
43	n	0.10	0/1043	0.28	0/1425
44	Y	0.15	0/863	0.38	0/1178
45	o	0.13	0/977	0.31	0/1317
46	10	0.10	0/222	0.23	0/289
47	J	0.12	0/838	0.30	0/1141
48	I	0.12	0/376	0.27	0/511
All	All	0.19	0/125182	0.33	6/187593 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2672	U	OP1-P-OP2	-13.12	80.23	119.60
10	A	2671	G	OP2-P-O3'	-12.05	71.84	108.00
10	A	2672	U	O5'-P-OP1	-10.34	76.98	108.00
10	A	2672	U	O5'-P-OP2	8.86	134.59	108.00
10	A	2671	G	OP1-P-O3'	8.36	133.08	108.00
12	D	260	PRO	CA-N-CD	-5.41	104.42	112.00

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	p	510	0	465	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	0	608	0	643	1	0
3	1	450	0	427	4	0
4	2	437	0	484	7	0
5	4	427	0	413	4	0
6	5	342	0	319	8	0
7	6	391	0	418	2	0
8	7	456	0	448	5	0
9	8	262	0	264	4	0
10	A	50306	0	25356	260	0
11	B	2142	0	1085	10	0
12	D	2058	0	2134	14	0
13	E	1512	0	1548	12	0
14	F	1624	0	1692	7	0
15	K	511	0	458	6	0
16	L	550	0	401	7	0
17	M	1178	0	1208	11	0
18	N	904	0	969	7	0
19	O	991	0	1005	5	0
20	P	1089	0	1108	15	0
21	Q	989	0	1035	4	0
22	R	739	0	692	5	0
23	S	945	0	998	6	0
24	T	919	0	964	5	0
25	U	824	0	869	5	0
26	V	1023	0	1065	9	0
27	W	683	0	709	12	0
28	X	732	0	756	3	0
29	Z	570	0	574	1	0
30	a	28463	0	14367	256	0
31	b	696	0	618	9	0
32	c	712	0	676	10	0
33	d	591	0	608	9	0
34	e	639	0	644	10	0
35	f	671	0	645	9	0
36	g	659	0	676	4	0
37	h	415	0	443	4	0
38	i	616	0	633	8	0
39	j	849	0	810	8	0
40	k	691	0	604	7	0
41	l	1383	0	1297	18	0
42	m	714	0	628	9	0
43	n	1032	0	952	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Y	851	0	777	6	0
45	o	964	0	983	8	0
46	10	219	0	228	4	0
47	J	827	0	751	9	0
48	I	369	0	347	3	0
49	4	1	0	0	0	0
49	A	119	0	0	0	0
49	F	1	0	0	0	0
49	T	1	0	0	0	0
49	V	2	0	0	0	0
49	a	4	0	0	0	0
50	4	1	0	0	0	0
51	A	31	0	0	0	0
51	B	1	0	0	0	0
51	W	1	0	0	0	0
51	X	1	0	0	0	0
51	a	9	0	0	0	0
52	A	12	0	0	0	0
52	B	2	0	0	0	0
53	4	2	0	0	0	0
53	A	741	0	0	13	0
53	B	6	0	0	1	0
53	D	4	0	0	0	0
53	E	10	0	0	0	0
53	F	4	0	0	0	0
53	M	2	0	0	1	0
53	O	13	0	0	0	0
53	Q	8	0	0	0	0
53	T	10	0	0	0	0
53	U	8	0	0	0	0
53	V	6	0	0	0	0
53	Z	1	0	0	0	0
53	a	40	0	0	3	0
All	All	116574	0	75194	748	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 (748) 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)
10:A:1949:5MU:C5	10:A:1949:5MU:C4	1.79	1.68
30:a:1426:A:H2	30:a:1459:G:H1	1.31	0.79
10:A:1436:G:H1	10:A:1632:U:H3	1.29	0.78
30:a:1117:G:H1	30:a:1148:U:H3	1.33	0.77
10:A:253:G:H22	10:A:275:G:H1	1.31	0.76
17:M:8:THR:HG21	24:T:61:TRP:HE1	1.49	0.76
30:a:1009:U:H3	30:a:1020:G:H1	1.33	0.76
33:d:57:ARG:O	33:d:61:LYS:HB2	1.90	0.72
10:A:1452:U:H3	10:A:1613:G:H1	1.41	0.69
10:A:2302:C:H42	10:A:2317:G:H1	1.39	0.69
30:a:1425:U:H3	30:a:1460:G:H22	1.39	0.68
10:A:677:A:H4'	10:A:678:G:H5'	1.74	0.68
30:a:1353:C:H2'	30:a:1354:A:H8	1.59	0.68
19:O:83:GLN:NE2	19:O:119:VAL:O	2.26	0.68
37:h:6:LYS:HB2	37:h:36:ALA:H	1.58	0.68
12:D:144:ILE:HB	12:D:154:MET:HB2	1.76	0.68
30:a:1109:C:H42	30:a:1186:A:H61	1.40	0.68
10:A:719:G:N7	53:A:3104:HOH:O	2.28	0.67
10:A:811:G:N2	10:A:812:G:O6	2.28	0.67
30:a:201:U:O2	34:e:66:ARG:NH1	2.28	0.67
10:A:123:G:H22	10:A:134:G:H22	1.43	0.66
40:k:140:ALA:HA	40:k:143:MET:HE3	1.77	0.66
30:a:513:C:HO2'	30:a:516:U:H3	1.43	0.65
10:A:2524:G:H1	10:A:2541:C:H5	1.43	0.65
13:E:55:ALA:HB2	13:E:77:ARG:HG2	1.79	0.65
44:Y:52:LEU:HD12	44:Y:53:ILE:HG12	1.79	0.65
10:A:1943:G:H5''	46:10:27:LYS:HA	1.78	0.64
10:A:1065:C:H5	10:A:1160:G:H1	1.46	0.64
30:a:1243:G:H1	30:a:1290:U:H3	1.45	0.64
34:e:6:ARG:HB2	34:e:63:MET:HE2	1.78	0.64
30:a:463:C:H42	30:a:470:A:H61	1.44	0.64
30:a:658:U:H3	30:a:747:C:H41	1.45	0.64
4:2:7:GLN:HB2	4:2:34:ILE:HG12	1.80	0.64
5:4:40:HIS:HD1	10:A:2801:G:HO2'	1.45	0.64
18:N:93:ILE:HG22	18:N:95:GLY:H	1.63	0.64
30:a:501:C:H2'	30:a:508:U:H3	1.63	0.64
34:e:69:SER:HB3	34:e:72:LYS:HB2	1.80	0.64
10:A:2348:C:H5	10:A:2371:G:H1	1.43	0.64
27:W:63:ASN:HB3	27:W:70:LEU:HD11	1.80	0.64
10:A:1169:A:O2'	10:A:1172:G:OP1	2.16	0.63
10:A:1827:U:O2'	12:D:154:MET:O	2.16	0.63
30:a:1426:A:N1	30:a:1459:G:O6	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1422:G:OP2	30:a:1422:G:N2	2.28	0.63
6:5:47:LYS:NZ	10:A:2348:C:OP1	2.30	0.63
17:M:2:ASP:OD1	17:M:7:LYS:NZ	2.31	0.63
30:a:462:G:H22	30:a:471:G:H1	1.47	0.63
10:A:1990:G:O2'	10:A:1992:U:OP2	2.16	0.63
30:a:1009:U:H3'	30:a:1010:G:H21	1.63	0.62
30:a:340:C:O2'	30:a:1431:A:N3	2.32	0.62
30:a:858:C:OP2	30:a:868:G:N1	2.31	0.62
30:a:1353:C:H2'	30:a:1354:A:C8	2.34	0.62
10:A:1234:G:H1	10:A:1269:U:H5	1.48	0.62
33:d:41:ARG:NH1	33:d:41:ARG:HB3	2.15	0.61
37:h:12:LEU:HD11	37:h:19:VAL:HG21	1.82	0.61
25:U:24:HIS:HA	25:U:96:THR:HG23	1.82	0.61
30:a:1249:A:OP1	47:J:73:GLN:NE2	2.33	0.61
10:A:1964:G:N2	53:A:3128:HOH:O	2.34	0.61
28:X:74:VAL:HG13	28:X:79:GLY:HA2	1.82	0.61
10:A:1596:G:H3'	10:A:1597:G:H21	1.66	0.60
30:a:1125:C:O3'	30:a:1142:G:N2	2.31	0.60
30:a:1355:U:OP2	30:a:1356:C:N4	2.34	0.60
30:a:1509:G:N7	46:10:15:HIS:NE2	2.48	0.60
20:P:58:MET:HE2	20:P:109:VAL:HG21	1.83	0.60
31:b:11:THR:HG23	31:b:55:LYS:HE3	1.83	0.60
30:a:1125:C:HO3'	30:a:1142:G:H22	1.50	0.60
10:A:2438:G:N7	53:A:3113:HOH:O	2.31	0.60
30:a:517:G:H1	30:a:533:A:H61	1.49	0.60
42:m:117:THR:HB	42:m:120:ASP:HB2	1.83	0.60
43:n:20:LEU:HD11	43:n:23:ILE:HG23	1.83	0.60
10:A:465:G:N7	53:A:3111:HOH:O	2.31	0.60
15:K:52:ARG:NH2	30:a:1187:U:OP1	2.35	0.60
41:l:167:GLU:N	41:l:167:GLU:OE1	2.35	0.60
10:A:123:G:H1	10:A:134:G:H1	1.49	0.60
23:S:49:ARG:NH1	23:S:98:TYR:OH	2.35	0.60
43:n:137:ASN:O	43:n:141:LEU:HB2	2.01	0.60
10:A:2550:G:N7	53:A:3118:HOH:O	2.32	0.59
30:a:678:U:H1'	30:a:777:A:H4'	1.84	0.59
10:A:2035:C:H2'	10:A:2036:G:C8	2.37	0.59
18:N:4:GLN:OE1	18:N:23:ARG:NH2	2.34	0.59
26:V:102:LYS:HG2	26:V:114:ARG:HD3	1.84	0.59
12:D:133:ALA:HB2	12:D:186:SER:HB3	1.83	0.59
6:5:20:LYS:HB3	6:5:57:LEU:HB3	1.85	0.58
30:a:830:G:H1	30:a:854:U:H3	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:36:ARG:NH2	1:p:75:SER:O	2.35	0.58
30:a:545:C:OP1	41:l:54:LYS:NZ	2.35	0.58
30:a:1346:A:H5'	47:J:121:LYS:HB2	1.85	0.58
31:b:5:GLU:OE1	31:b:93:GLN:NE2	2.31	0.58
33:d:58:LEU:HG	33:d:63:ILE:HB	1.85	0.58
3:1:49:MET:HG2	3:1:53:MET:HE3	1.84	0.58
30:a:412:A:H61	30:a:439:C:H42	1.50	0.58
30:a:1430:G:H21	30:a:1455:C:H5	1.51	0.58
40:k:165:GLU:N	40:k:165:GLU:OE1	2.37	0.58
20:P:54:VAL:HB	20:P:121:ALA:HB2	1.84	0.58
30:a:36:C:OP1	39:j:120:LYS:NZ	2.35	0.58
30:a:1292:C:O3'	38:i:15:ARG:NH1	2.37	0.58
10:A:848:U:H2'	10:A:849:C:C6	2.39	0.58
30:a:945:A:H2'	30:a:946:A:C8	2.39	0.58
41:l:133:VAL:HG11	41:l:139:ILE:HD11	1.85	0.58
42:m:46:LEU:HD22	42:m:60:ALA:HB1	1.85	0.58
10:A:1860:U:H2'	10:A:1861:A:C8	2.39	0.57
10:A:2201:G:H2'	10:A:2202:G:C5	2.39	0.57
20:P:35:LYS:NZ	44:Y:82:PRO:O	2.31	0.57
38:i:10:LEU:O	38:i:12:GLN:NE2	2.34	0.57
30:a:652:U:O4	30:a:752:G:O2'	2.23	0.57
10:A:258:U:H3	10:A:270:G:H22	1.52	0.57
30:a:367:G:N2	30:a:370:U:OP2	2.37	0.57
47:J:118:LYS:HB2	47:J:121:LYS:HB3	1.87	0.57
10:A:2292:U:H2'	10:A:2293:A:C8	2.40	0.56
18:N:88:ASN:HD21	18:N:92:ASP:HB3	1.70	0.56
26:V:98:ALA:HB3	26:V:119:SER:HB2	1.87	0.56
30:a:674:G:H2'	30:a:675:A:H8	1.70	0.56
41:l:143:GLU:N	41:l:143:GLU:OE2	2.37	0.56
47:J:65:LEU:HD22	47:J:73:GLN:HG2	1.88	0.56
10:A:1694:G:N7	53:A:3121:HOH:O	2.32	0.56
17:M:18:LYS:NZ	17:M:54:ASP:OD1	2.37	0.56
30:a:1313:G:N2	30:a:1316:A:OP2	2.33	0.56
20:P:138:ASP:HB3	44:Y:55:SER:HB2	1.88	0.56
30:a:562:U:H1'	39:j:12:ARG:HD2	1.87	0.56
30:a:835:U:H2'	30:a:836:G:H8	1.71	0.56
30:a:1312:U:O2'	30:a:1357:A:N3	2.32	0.56
6:5:47:LYS:O	6:5:54:ARG:NE	2.39	0.56
10:A:1756:C:H2'	10:A:1757:A:H8	1.71	0.56
34:e:16:ASN:ND2	34:e:54:CYS:O	2.39	0.56
10:A:2353:A:H2	10:A:2366:G:H21	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:107:PRO:HD2	12:D:110:LEU:HD22	1.87	0.56
10:A:1672:U:H2'	10:A:1673:A:C8	2.41	0.55
30:a:247:C:O2'	30:a:250:U:OP1	2.25	0.55
10:A:756:A:H2'	10:A:757:A:C8	2.42	0.55
10:A:834:G:N7	53:A:3124:HOH:O	2.33	0.55
10:A:1392:C:O2'	10:A:1818:A:N3	2.37	0.55
30:a:618:C:N4	30:a:621:A:OP2	2.39	0.55
30:a:463:C:O2'	30:a:464:G:O5'	2.25	0.55
30:a:606:G:H22	30:a:631:C:H2'	1.72	0.55
32:c:7:LEU:HB3	32:c:18:TYR:HB3	1.88	0.55
22:R:91:ARG:HH21	22:R:95:LEU:HA	1.72	0.55
30:a:958:A:O2'	30:a:959:U:O4'	2.25	0.55
10:A:753:A:H3'	10:A:754:C:H6	1.72	0.55
30:a:259:G:H4'	34:e:21:THR:HG21	1.88	0.55
30:a:130:G:OP1	34:e:4:ASN:ND2	2.40	0.54
30:a:835:U:H2'	30:a:836:G:C8	2.43	0.54
30:a:945:A:H2'	30:a:946:A:H8	1.72	0.54
30:a:683:G:O6	30:a:707:U:O2	2.25	0.54
30:a:1431:A:H62	30:a:1454:A:H2	1.55	0.54
30:a:975:G:OP2	30:a:1355:U:O2'	2.24	0.54
9:8:19:ARG:NE	10:A:2757:U:OP2	2.32	0.54
10:A:1369:U:OP1	27:W:12:LYS:NZ	2.41	0.54
10:A:169:A:H2'	10:A:170:C:C6	2.43	0.54
7:6:39:ARG:NH2	10:A:491:G:N7	2.47	0.54
8:7:39:LYS:NZ	10:A:2366:G:N7	2.54	0.54
10:A:2228:A:H5''	12:D:261:LYS:HE3	1.89	0.54
43:n:120:LEU:HD13	43:n:128:VAL:HG11	1.89	0.54
12:D:22:ASP:N	12:D:22:ASP:OD1	2.36	0.54
10:A:314:G:OP1	28:X:3:LYS:NZ	2.41	0.54
10:A:2675:G:H4'	18:N:30:ARG:HD2	1.90	0.54
30:a:513:C:O2'	30:a:516:U:N3	2.35	0.54
30:a:1426:A:C2	30:a:1459:G:N1	2.63	0.54
30:a:1249:A:OP1	47:J:67:GLY:N	2.41	0.53
41:l:65:GLU:OE2	41:l:199:TYR:OH	2.25	0.53
25:U:7:ILE:HG21	25:U:22:VAL:HG11	1.91	0.53
28:X:82:THR:HG21	28:X:98:ALA:HB1	1.90	0.53
30:a:1142:G:H21	47:J:16:ARG:NH1	2.06	0.53
30:a:217:U:H2'	30:a:218:A:C8	2.43	0.53
30:a:976:A:O2'	30:a:980:U:O4	2.27	0.53
10:A:1703:G:O2'	10:A:2001:U:O4	2.23	0.53
10:A:2329:A:H2'	10:A:2330:U:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:38:A:H61	30:a:402:A:H5''	1.72	0.53
10:A:64:G:H22	10:A:99:A:H2	1.57	0.53
30:a:153:U:H2'	30:a:154:A:H8	1.74	0.53
10:A:307:G:H2'	10:A:308:A:H8	1.73	0.53
10:A:883:U:H2'	10:A:884:U:C6	2.44	0.53
30:a:1249:A:H2'	30:a:1250:A:C8	2.44	0.53
10:A:1276:A:N7	53:A:3130:HOH:O	2.34	0.53
30:a:973:A:H4'	30:a:974:G:H3'	1.90	0.53
10:A:517:A:H4'	26:V:23:LYS:HB2	1.91	0.53
10:A:1415:A:H2'	10:A:1416:C:O4'	2.09	0.53
23:S:109:ARG:NH1	30:a:1450:G:OP1	2.40	0.53
30:a:983:U:H3	30:a:1219:G:H1	1.56	0.53
12:D:37:LYS:HD2	12:D:62:TYR:HB2	1.90	0.52
30:a:1295:C:O2	30:a:1296:A:N6	2.42	0.52
39:j:81:LEU:HD22	39:j:101:THR:HG21	1.90	0.52
30:a:742:U:H2'	30:a:743:A:H8	1.75	0.52
10:A:2440:A:O2'	10:A:2588:A:OP1	2.24	0.52
30:a:552:U:H2'	30:a:553:A:H8	1.74	0.52
30:a:1054:G:OP1	40:k:153:SER:OG	2.27	0.52
10:A:123:G:H1	10:A:134:G:H22	1.55	0.52
10:A:618:U:H2'	10:A:619:G:C8	2.44	0.52
10:A:2462:C:H2'	10:A:2463:A:C8	2.44	0.52
11:B:35:C:N3	11:B:46:A:O2'	2.40	0.52
34:e:71:THR:O	34:e:71:THR:OG1	2.26	0.52
8:7:59:LYS:O	8:7:64:LEU:N	2.37	0.52
10:A:1002:U:H2'	10:A:1003:C:C6	2.44	0.52
11:B:60:C:H2'	11:B:61:A:H8	1.74	0.52
10:A:307:G:H2'	10:A:308:A:C8	2.45	0.52
10:A:603:C:H2'	10:A:604:U:C6	2.44	0.52
10:A:2292:U:OP1	10:A:2381:U:O2'	2.28	0.52
11:B:99:G:N7	53:B:301:HOH:O	2.34	0.52
30:a:21:G:H2'	30:a:22:G:C8	2.44	0.52
30:a:671:G:O2'	31:b:76:GLU:OE1	2.26	0.52
10:A:1033:A:H2'	10:A:1034:A:C8	2.45	0.52
30:a:302:G:N2	30:a:305:A:OP2	2.37	0.52
30:a:448:U:H2'	30:a:449:A:H8	1.75	0.52
34:e:19:ASP:OD1	34:e:19:ASP:N	2.36	0.52
46:10:12:MET:HE2	46:10:16:LYS:HE2	1.91	0.52
4:2:48:ASN:OD1	4:2:51:ARG:NH2	2.43	0.52
26:V:92:ARG:HB2	26:V:125:TYR:HB2	1.92	0.52
30:a:478:A:O2'	30:a:480:U:O4	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1435:U:H2'	10:A:1436:G:H8	1.75	0.52
10:A:1949:5MU:OP1	10:A:2605:U:O2'	2.27	0.52
10:A:2074:C:H2'	10:A:2075:C:C6	2.44	0.52
20:P:64:VAL:HG22	20:P:106:VAL:HG12	1.92	0.52
30:a:1426:A:N1	30:a:1459:G:C6	2.78	0.52
32:c:17:PHE:HD1	32:c:41:ASN:HD22	1.57	0.52
33:d:28:ALA:O	33:d:32:VAL:HG23	2.10	0.52
10:A:327:A:N3	10:A:347:G:O2'	2.41	0.51
10:A:1429:C:H2'	10:A:1430:G:H8	1.75	0.51
20:P:32:PHE:HD2	20:P:133:VAL:HG12	1.76	0.51
30:a:498:C:H2'	30:a:499:A:H8	1.75	0.51
10:A:749:U:O2'	10:A:751:A:N7	2.42	0.51
10:A:898:G:N7	53:A:3131:HOH:O	2.34	0.51
10:A:1416:C:H2'	10:A:1417:C:C6	2.46	0.51
19:O:112:LYS:HG3	19:O:129:ALA:HB3	1.92	0.51
10:A:258:U:H2'	10:A:259:G:C8	2.46	0.51
30:a:371:A:N6	53:a:1706:HOH:O	2.36	0.51
30:a:402:A:H1'	30:a:403:A:H2'	1.90	0.51
3:1:25:TYR:HB2	3:1:46:GLN:HG2	1.93	0.51
14:F:159:GLU:OE2	14:F:198:ARG:NH1	2.40	0.51
30:a:1502:A:H2'	30:a:1503:C:C6	2.46	0.51
20:P:65:TRP:HB2	20:P:105:GLU:HG2	1.91	0.51
10:A:658:A:H61	10:A:668:A:H5''	1.76	0.51
24:T:83:LEU:HG	24:T:88:ILE:HD11	1.93	0.51
30:a:423:U:OP1	30:a:510:A:O2'	2.28	0.51
30:a:1518:G:N7	46:10:7:ARG:NH1	2.59	0.51
39:j:50:ARG:HB3	39:j:66:TYR:HE1	1.76	0.51
48:I:76:ALA:HB1	48:I:81:LEU:HB2	1.93	0.51
10:A:1811:A:H2'	10:A:1812:A:C8	2.47	0.50
10:A:2101:U:H3	10:A:2229:C:H42	1.60	0.50
12:D:123:ALA:O	12:D:128:ASN:ND2	2.35	0.50
30:a:1183:U:H2'	30:a:1184:G:C8	2.46	0.50
43:n:48:ASP:OD1	43:n:48:ASP:N	2.45	0.50
10:A:2295:C:OP1	22:R:91:ARG:NH2	2.38	0.50
10:A:890:G:H2'	10:A:891:A:C8	2.46	0.50
10:A:602:C:H2'	10:A:603:C:C6	2.45	0.50
10:A:1071:C:H5	10:A:1155:G:H1	1.59	0.50
17:M:135:HIS:CE1	17:M:137:HIS:HB2	2.46	0.50
10:A:2315:C:H2'	10:A:2316:G:C8	2.46	0.50
10:A:72:A:H2	10:A:91:A:H2	1.58	0.50
10:A:258:U:H3	10:A:270:G:H1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:14:VAL:HG21	25:U:100:VAL:HG21	1.92	0.50
12:D:48:LYS:NZ	12:D:49:MET:O	2.34	0.50
30:a:1320:G:H2'	30:a:1321:A:C8	2.47	0.50
30:a:1397:C:H4'	30:a:1398:C:H3'	1.92	0.50
10:A:715:A:H2'	10:A:716:A:C8	2.47	0.50
10:A:668:A:H8	10:A:682:G:H21	1.60	0.50
27:W:66:THR:OG1	27:W:67:LYS:N	2.44	0.50
1:p:74:PHE:HE1	38:i:85:ILE:HG23	1.76	0.49
30:a:498:C:H1'	30:a:549:C:H1'	1.94	0.49
10:A:1052:U:OP1	10:A:1070:U:O2'	2.23	0.49
30:a:1349:C:H2'	30:a:1350:G:C8	2.48	0.49
42:m:125:GLU:OE1	42:m:125:GLU:N	2.44	0.49
10:A:773:G:N7	53:A:3127:HOH:O	2.34	0.49
10:A:1435:U:H2'	10:A:1436:G:C8	2.47	0.49
30:a:217:U:H2'	30:a:218:A:H8	1.77	0.49
30:a:1384:G:H2'	30:a:1385:G:H8	1.77	0.49
39:j:50:ARG:NH1	39:j:89:ASP:OD2	2.44	0.49
10:A:610:U:H2'	10:A:611:U:C6	2.48	0.49
17:M:119:LEU:O	17:M:123:ILE:HG12	2.13	0.49
30:a:1057:U:H2'	30:a:1058:G:H8	1.77	0.49
11:B:61:A:H2'	11:B:62:A:C8	2.47	0.49
22:R:8:ARG:NH1	22:R:92:ASN:O	2.45	0.49
30:a:269:C:O2'	34:e:67:PRO:O	2.28	0.49
30:a:1256:G:H2'	30:a:1257:C:C6	2.48	0.49
39:j:83:ARG:HG2	39:j:98:VAL:HG22	1.95	0.49
9:8:31:PRO:HB2	10:A:2528:C:H5''	1.94	0.49
10:A:630:A:H2'	10:A:631:A:C8	2.48	0.49
10:A:1756:C:H2'	10:A:1757:A:C8	2.47	0.49
21:Q:49:GLU:HA	21:Q:52:LEU:HD12	1.95	0.49
30:a:268:A:OP1	33:d:71:ASN:ND2	2.46	0.49
30:a:301:U:O2	30:a:306:G:O6	2.30	0.49
30:a:613:G:H2'	30:a:614:A:C8	2.48	0.49
30:a:834:U:H4'	48:I:63:LEU:HD12	1.94	0.49
30:a:1520:A:H3'	30:a:1521:A:H8	1.78	0.49
30:a:174:A:H2'	30:a:175:A:C8	2.48	0.48
30:a:657:U:O2'	35:f:22:THR:O	2.23	0.48
30:a:451:G:H21	30:a:484:U:H5	1.60	0.48
30:a:1352:G:H2'	30:a:1353:C:C6	2.47	0.48
8:7:19:THR:HG23	10:A:682:G:H5'	1.96	0.48
10:A:2383:G:H3'	10:A:2384:A:H5'	1.94	0.48
15:K:62:GLU:OE1	15:K:62:GLU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:427:A:H2'	30:a:428:A:C8	2.47	0.48
30:a:728:A:H2'	30:a:729:A:C8	2.47	0.48
30:a:886:G:N7	53:a:1705:HOH:O	2.35	0.48
43:n:142:VAL:O	43:n:146:ILE:HG13	2.14	0.48
8:7:56:ASN:HA	8:7:59:LYS:HB2	1.95	0.48
10:A:939:A:H2'	10:A:940:G:H5''	1.96	0.48
10:A:1154:U:H2'	10:A:1155:G:C8	2.48	0.48
10:A:2547:U:OP1	18:N:29:ARG:NH1	2.39	0.48
30:a:259:G:H2'	30:a:260:G:H8	1.79	0.48
30:a:907:A:H2'	30:a:908:A:H8	1.79	0.48
30:a:976:A:H1'	30:a:981:C:H41	1.78	0.48
30:a:1458:G:H2'	30:a:1459:G:H8	1.78	0.48
31:b:43:TRP:HE1	31:b:62:LEU:HD22	1.78	0.48
30:a:581:G:OP1	35:f:65:ARG:NH2	2.34	0.48
30:a:1373:A:OP1	42:m:24:LYS:NZ	2.41	0.48
30:a:1407:A:H2'	30:a:1408:2MG:H8	1.78	0.48
32:c:19:LYS:HD3	32:c:36:ARG:HG3	1.95	0.48
45:o:112:MET:HE3	45:o:117:ALA:HA	1.96	0.48
10:A:278:A:N6	10:A:279:A:N1	2.61	0.48
10:A:2247:G:H2'	10:A:2248:A:C8	2.48	0.48
10:A:2671:G:H2'	10:A:2672:U:C6	2.49	0.48
11:B:60:C:H2'	11:B:61:A:C8	2.49	0.48
14:F:19:LEU:HA	14:F:204:ASN:HD21	1.78	0.48
24:T:83:LEU:HD12	24:T:113:VAL:HG11	1.96	0.48
10:A:700:A:H2'	10:A:701:G:C8	2.49	0.48
30:a:35:G:H2'	30:a:36:C:C6	2.49	0.48
30:a:1043:A:H61	30:a:1209:U:H3	1.61	0.48
8:7:48:SER:OG	8:7:49:THR:N	2.47	0.48
30:a:1183:U:H2'	30:a:1184:G:H8	1.79	0.48
30:a:1424:G:OP2	30:a:1424:G:N2	2.40	0.48
10:A:1834:U:H2'	10:A:1835:C:C6	2.49	0.48
14:F:156:VAL:HB	14:F:195:LEU:HD23	1.95	0.48
30:a:43:U:H5''	32:c:12:ARG:HD3	1.96	0.48
30:a:1344:G:N2	30:a:1371:G:H2'	2.29	0.48
30:a:1352:G:H2'	30:a:1353:C:H6	1.78	0.48
40:k:139:SER:O	40:k:143:MET:HG3	2.14	0.48
10:A:1429:C:H2'	10:A:1430:G:C8	2.48	0.47
36:g:52:CYS:HB3	36:g:56:GLY:H	1.79	0.47
41:l:120:THR:HA	41:l:125:VAL:HA	1.96	0.47
5:4:24:MET:HE1	26:V:44:MET:HE1	1.96	0.47
10:A:123:G:H22	10:A:134:G:N2	2.08	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1176:U:H4'	10:A:1177:A:O4'	2.14	0.47
30:a:381:G:H5''	32:c:6:ARG:HB2	1.95	0.47
30:a:1274:G:H2'	30:a:1275:C:O4'	2.14	0.47
31:b:11:THR:HG22	31:b:13:VAL:H	1.79	0.47
10:A:1210:A:H2'	10:A:1211:U:C6	2.50	0.47
10:A:1860:U:H2'	10:A:1861:A:H8	1.79	0.47
30:a:970:G:OP2	30:a:1229:G:N2	2.42	0.47
30:a:1505:G:N1	30:a:1508:MA6:OP2	2.47	0.47
10:A:1976:A:N3	10:A:2593:G:O2'	2.45	0.47
24:T:104:GLU:H	24:T:104:GLU:CD	2.23	0.47
30:a:1343:A:H61	30:a:1372:A:H3'	1.79	0.47
10:A:457:U:H1'	10:A:458:C:H5	1.79	0.47
10:A:1288:G:N7	53:A:3133:HOH:O	2.35	0.47
10:A:2292:U:H2'	10:A:2293:A:H8	1.79	0.47
16:L:22:ILE:HB	16:L:85:VAL:HG22	1.95	0.47
30:a:9:G:H1	30:a:25:C:H5	1.63	0.47
30:a:139:C:O2'	32:c:65:GLN:OE1	2.33	0.47
30:a:618:C:H5'	30:a:619:U:H5''	1.96	0.47
10:A:121:C:H42	10:A:136:C:N4	2.13	0.47
19:O:57:ILE:HA	19:O:60:ARG:HG2	1.96	0.47
20:P:118:LEU:HD12	20:P:131:PHE:HE1	1.79	0.47
32:c:24:ASP:OD1	32:c:25:SER:N	2.47	0.47
10:A:751:A:H2'	10:A:752:C:O4'	2.15	0.47
10:A:2315:C:H2'	10:A:2316:G:H8	1.79	0.47
10:A:2462:C:H2'	10:A:2463:A:H8	1.80	0.47
10:A:2702:C:O2'	21:Q:73:LYS:NZ	2.48	0.47
30:a:22:G:O2'	30:a:912:A:N1	2.43	0.47
10:A:253:G:N2	10:A:275:G:H1	2.08	0.47
20:P:68:ILE:HD11	20:P:103:ILE:HG23	1.97	0.47
10:A:611:U:H2'	10:A:612:A:H8	1.79	0.46
10:A:1438:U:H2'	10:A:1439:A:C8	2.50	0.46
10:A:2670:U:O2'	10:A:2671:G:OP1	2.28	0.46
30:a:575:G:O2'	30:a:821:7MG:OP2	2.31	0.46
13:E:183:GLU:HG2	13:E:184:HIS:CD2	2.50	0.46
10:A:1067:A:N6	10:A:1158:A:H61	2.14	0.46
12:D:82:GLU:HB3	12:D:91:ILE:HG13	1.98	0.46
30:a:1284:A:H2'	30:a:1285:A:C8	2.51	0.46
10:A:592:G:H2'	10:A:2040:A:N7	2.31	0.46
10:A:899:C:O2	10:A:943:A:N6	2.48	0.46
10:A:1901:G:O2'	10:A:2236:G:O2'	2.33	0.46
10:A:906:U:H2'	10:A:907:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:52:G:H2'	11:B:53:U:O4'	2.16	0.46
30:a:464:G:H3'	30:a:465:A:H8	1.80	0.46
30:a:613:G:H2'	30:a:614:A:H8	1.81	0.46
30:a:674:G:H2'	30:a:675:A:C8	2.48	0.46
30:a:1455:C:H2'	30:a:1456:U:O4'	2.16	0.46
10:A:2316:G:H2'	10:A:2317:G:C8	2.50	0.46
15:K:52:ARG:HB3	30:a:1057:U:H5''	1.98	0.46
16:L:22:ILE:HG12	16:L:31:ILE:HG12	1.97	0.46
26:V:30:SER:HB3	26:V:33:LYS:HD2	1.97	0.46
10:A:430:C:H2'	10:A:431:G:H8	1.81	0.46
18:N:58:SER:OG	18:N:59:LYS:N	2.47	0.46
21:Q:79:LEU:HA	21:Q:83:VAL:HB	1.97	0.46
30:a:984:U:H3	30:a:1218:G:H1	1.63	0.46
42:m:106:LEU:HD11	42:m:125:GLU:HB3	1.96	0.46
43:n:39:ALA:HA	43:n:56:GLY:O	2.16	0.46
44:Y:23:ARG:HD3	44:Y:88:ILE:HG22	1.97	0.46
10:A:537:A:H2'	10:A:538:C:C6	2.51	0.46
30:a:68:G:H22	30:a:103:A:H2	1.63	0.46
30:a:508:U:H5	30:a:540:G:H1	1.63	0.46
3:1:24:ALA:O	3:1:28:MET:HG3	2.16	0.46
9:8:28:LYS:NZ	10:A:2756:C:OP1	2.40	0.46
13:E:183:GLU:OE1	13:E:183:GLU:N	2.35	0.46
23:S:25:THR:HB	23:S:88:LYS:HG2	1.97	0.46
30:a:665:C:H41	30:a:724:U:H3	1.63	0.46
30:a:1239:G:H2'	30:a:1241:G:H8	1.81	0.46
10:A:909:G:H21	10:A:937:C:N4	2.14	0.45
10:A:1417:C:H2'	10:A:1418:G:O4'	2.16	0.45
30:a:1511:U:H2'	30:a:1512:G:H8	1.81	0.45
34:e:69:SER:OG	34:e:70:ARG:N	2.49	0.45
39:j:34:CYS:HA	39:j:55:VAL:HG12	1.97	0.45
10:A:54:G:H5'	27:W:64:ARG:HG3	1.99	0.45
10:A:771:U:H2'	10:A:772:C:C6	2.51	0.45
10:A:909:G:H2'	10:A:910:A:C5	2.51	0.45
10:A:1596:G:O5'	10:A:1597:G:N2	2.48	0.45
10:A:2328:A:H2'	10:A:2329:A:C8	2.52	0.45
10:A:2538:U:H2'	10:A:2539:C:C6	2.51	0.45
30:a:965:G:H2'	30:a:966:A:C8	2.52	0.45
44:Y:17:LYS:HE2	44:Y:17:LYS:HB3	1.77	0.45
30:a:743:A:H2'	30:a:744:C:C6	2.52	0.45
30:a:1339:C:H2'	30:a:1340:G:H8	1.80	0.45
10:A:324:U:H2'	10:A:325:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:958:G:H2'	10:A:959:A:C8	2.52	0.45
10:A:964:U:H5''	10:A:965:G:H21	1.80	0.45
10:A:1413:G:H21	10:A:1435:U:H1'	1.81	0.45
10:A:2242:A:H2'	10:A:2243:G:C8	2.51	0.45
10:A:2538:U:H2'	10:A:2539:C:H6	1.81	0.45
15:K:7:ILE:HB	15:K:73:ILE:HG13	1.97	0.45
27:W:68:SER:OG	27:W:69:GLY:N	2.48	0.45
30:a:185:C:H4'	30:a:186:A:H5'	1.99	0.45
30:a:521:G:H2'	30:a:522:C:C6	2.51	0.45
30:a:545:C:H5'	41:l:65:GLU:HB2	1.99	0.45
30:a:976:A:H4'	30:a:980:U:H5	1.81	0.45
30:a:1486:G:H1'	30:a:1507:MA6:H2	1.97	0.45
45:o:114:ASP:OD1	45:o:114:ASP:N	2.47	0.45
10:A:1042:A:N3	10:A:1188:C:O2'	2.43	0.45
10:A:1167:A:C6	17:M:82:HIS:HB2	2.52	0.45
10:A:1677:A:H2'	10:A:1678:G:O4'	2.17	0.45
44:Y:52:LEU:H	44:Y:52:LEU:HG	1.49	0.45
10:A:2629:C:H2'	10:A:2630:A:C2	2.52	0.45
27:W:13:MET:HA	27:W:13:MET:HE2	1.99	0.45
30:a:455:A:H4'	30:a:456:U:H5'	1.99	0.45
30:a:463:C:N4	30:a:470:A:H61	2.13	0.45
30:a:1247:C:H2'	30:a:1248:A:C8	2.52	0.45
40:k:129:TYR:HA	40:k:132:ALA:HB3	1.98	0.45
41:l:53:GLU:HG3	41:l:194:LEU:HD12	1.99	0.45
10:A:2619:G:C4	10:A:2620:H2U:H62	2.52	0.45
30:a:325:U:H2'	30:a:326:A:O4'	2.16	0.45
30:a:368:A:N6	39:j:27:CYS:SG	2.90	0.45
30:a:411:G:H21	41:l:112:GLN:NE2	2.14	0.45
30:a:1020:G:H2'	30:a:1021:U:C6	2.52	0.45
42:m:46:LEU:HD23	42:m:46:LEU:HA	1.86	0.45
10:A:326:G:N7	53:A:3136:HOH:O	2.36	0.45
10:A:2592:C:H2'	10:A:2593:G:H8	1.81	0.45
12:D:174:ILE:HD12	12:D:184:ILE:HG13	1.99	0.45
30:a:1313:G:OP2	36:g:28:LYS:NZ	2.49	0.45
41:l:146:LYS:HG2	41:l:173:LEU:HD23	1.99	0.45
10:A:735:G:O2'	10:A:1668:A:N3	2.48	0.45
10:A:965:G:H2'	10:A:966:A:C4	2.52	0.45
10:A:1607:A:H2'	10:A:1608:A:C8	2.52	0.45
10:A:611:U:H2'	10:A:612:A:C8	2.52	0.45
10:A:1860:U:O2	10:A:2234:U:O2'	2.30	0.45
10:A:2741:A:H2'	10:A:2742:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:56:VAL:HA	30:a:972:G:H5'	1.99	0.45
10:A:831:U:H2'	10:A:832:U:C6	2.52	0.44
16:L:30:ILE:HD11	30:a:706:A:H4'	1.98	0.44
20:P:25:ASN:OD1	20:P:25:ASN:N	2.42	0.44
27:W:30:PRO:HA	27:W:79:LYS:HB2	2.00	0.44
27:W:55:MET:HG3	27:W:80:LYS:HB2	1.99	0.44
30:a:748:G:H4'	30:a:749:A:O5'	2.15	0.44
30:a:834:U:H2'	30:a:835:U:C6	2.52	0.44
30:a:1148:U:H2'	30:a:1149:A:C8	2.52	0.44
36:g:70:ILE:H	36:g:70:ILE:HG13	1.62	0.44
10:A:502:A:N3	10:A:504:G:H5''	2.33	0.44
30:a:408:C:OP1	41:l:130:SER:OG	2.31	0.44
30:a:833:U:H2'	30:a:834:U:C6	2.52	0.44
10:A:255:C:H2'	10:A:256:U:H6	1.83	0.44
10:A:437:C:H2'	10:A:438:A:H8	1.80	0.44
10:A:1261:U:H2'	10:A:1262:C:C6	2.52	0.44
25:U:34:VAL:HG23	25:U:62:CYS:HB2	2.00	0.44
30:a:1302:G:H22	30:a:1328:G:H2'	1.83	0.44
30:a:1320:G:H2'	30:a:1321:A:H8	1.82	0.44
10:A:428:G:H2'	10:A:429:G:C8	2.52	0.44
10:A:602:C:H2'	10:A:603:C:H6	1.83	0.44
10:A:2347:A:H4'	10:A:2384:A:OP2	2.17	0.44
20:P:116:GLU:OE2	20:P:119:ARG:NH2	2.50	0.44
10:A:964:U:C6	10:A:965:G:H1'	2.53	0.44
10:A:2369:C:H2'	10:A:2370:A:H8	1.83	0.44
13:E:5:LEU:HD13	13:E:52:PHE:HB2	1.98	0.44
30:a:508:U:O2'	30:a:509:A:O5'	2.34	0.44
30:a:922:A:O2'	30:a:1397:C:OP2	2.33	0.44
10:A:437:C:H2'	10:A:438:A:C8	2.53	0.44
30:a:498:C:H2'	30:a:499:A:C8	2.52	0.44
30:a:1216:C:H2'	30:a:1217:G:C8	2.52	0.44
30:a:1424:G:H2'	30:a:1425:U:H6	1.83	0.44
30:a:1458:G:H2'	30:a:1459:G:C8	2.53	0.44
10:A:2851:U:H2'	10:A:2852:A:N7	2.33	0.44
14:F:135:LYS:HD2	14:F:135:LYS:HA	1.85	0.44
20:P:77:LYS:NZ	20:P:84:GLY:O	2.51	0.44
30:a:1370:U:HO2'	30:a:1371:G:H8	1.65	0.44
1:p:5:LEU:HD11	30:a:1309:G:H5'	2.00	0.44
10:A:1075:A:H2'	10:A:1076:A:C8	2.52	0.44
26:V:89:PHE:HB3	26:V:129:LEU:HD11	2.00	0.44
30:a:34:C:H2'	30:a:35:G:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:210:A:H2'	30:a:211:A:C8	2.53	0.44
30:a:258:U:H2'	30:a:259:G:H8	1.83	0.44
30:a:580:C:H2'	30:a:581:G:O4'	2.18	0.44
30:a:635:C:H2'	30:a:636:G:H8	1.83	0.44
30:a:742:U:H2'	30:a:743:A:C8	2.52	0.44
30:a:864:A:H2'	30:a:865:A:C8	2.53	0.44
30:a:1460:G:H2'	30:a:1461:U:C6	2.52	0.44
10:A:618:U:H2'	10:A:619:G:H8	1.81	0.44
10:A:989:G:N7	20:P:14:LYS:NZ	2.65	0.44
10:A:1387:U:H5	10:A:1401:A:N7	2.16	0.44
27:W:37:ILE:O	27:W:41:VAL:HG12	2.16	0.44
30:a:657:U:H1'	35:f:23:GLY:HA2	2.00	0.44
10:A:1310:G:H2'	10:A:1311:C:C6	2.53	0.43
10:A:1778:G:O2'	10:A:1968:C:OP1	2.35	0.43
10:A:1956:U:H2'	10:A:1957:C:C6	2.53	0.43
30:a:911:C:H2'	30:a:912:A:C8	2.53	0.43
4:2:7:GLN:HA	4:2:33:GLN:O	2.18	0.43
5:4:4:PRO:HA	10:A:2616:U:C2	2.53	0.43
10:A:169:A:H2'	10:A:170:C:H6	1.81	0.43
10:A:1260:U:H2'	10:A:1261:U:C6	2.53	0.43
10:A:2849:A:H2'	10:A:2850:U:C6	2.54	0.43
35:f:71:ILE:HD13	35:f:71:ILE:HA	1.79	0.43
40:k:111:ASP:O	40:k:113:ALA:N	2.52	0.43
10:A:1344:C:O2'	10:A:1422:A:N3	2.46	0.43
10:A:2272:G:OP1	29:Z:18:SER:HB3	2.18	0.43
13:E:50:LEU:O	13:E:79:LEU:HA	2.18	0.43
20:P:34:ILE:HD11	20:P:104:PHE:HB2	1.99	0.43
30:a:1302:G:N2	30:a:1328:G:H2'	2.33	0.43
30:a:1434:G:OP1	33:d:22:ARG:NH2	2.47	0.43
10:A:599:G:H2'	10:A:600:A:C8	2.53	0.43
10:A:1151:U:H2'	10:A:1152:U:O4'	2.18	0.43
30:a:448:U:H2'	30:a:449:A:C8	2.52	0.43
30:a:907:A:H2'	30:a:908:A:C8	2.54	0.43
30:a:926:G:H1	30:a:1388:U:H3	1.65	0.43
30:a:1371:G:H5''	42:m:35:LYS:HB2	2.00	0.43
31:b:89:LEU:HD12	31:b:89:LEU:HA	1.87	0.43
2:0:58:LEU:HD13	10:A:395:G:H5''	2.00	0.43
6:5:34:LYS:HD3	6:5:43:LEU:HD13	2.01	0.43
10:A:2591:A:H2'	10:A:2592:C:H6	1.83	0.43
10:A:2592:C:H2'	10:A:2593:G:C8	2.53	0.43
30:a:659:C:H2'	30:a:660:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:750:C:O2'	30:a:751:U:H5'	2.19	0.43
30:a:919:U:H2'	30:a:920:U:C6	2.53	0.43
37:h:3:VAL:HG11	37:h:36:ALA:HB1	1.99	0.43
10:A:616:U:H2'	10:A:617:U:C6	2.54	0.43
10:A:2576:C:H5'	13:E:149:CYS:HB2	2.01	0.43
10:A:2681:C:H5'	13:E:194:PRO:HA	2.01	0.43
10:A:1227:U:H2'	10:A:1228:U:C6	2.54	0.43
10:A:2334:A:H5'	10:A:2336:A:H1'	2.00	0.43
13:E:13:SER:O	23:S:56:LYS:NZ	2.42	0.43
30:a:428:A:H3'	30:a:429:G:H21	1.84	0.43
30:a:444:U:O2	30:a:494:G:O6	2.37	0.43
30:a:1055:G:OP1	40:k:198:LYS:NZ	2.49	0.43
31:b:22:ALA:HB2	31:b:84:ARG:HH12	1.83	0.43
30:a:642:A:N3	45:o:106:SER:OG	2.51	0.43
30:a:1142:G:H21	47:J:16:ARG:CZ	2.32	0.43
30:a:1196:A:H2'	30:a:1197:U:C6	2.53	0.43
30:a:1262:G:H1	30:a:1269:C:H5	1.66	0.43
41:l:173:LEU:HD12	41:l:173:LEU:HA	1.85	0.43
10:A:1063:A:H2'	10:A:1064:A:C8	2.53	0.43
30:a:461:G:H2'	30:a:462:G:C8	2.53	0.43
30:a:757:U:H2'	30:a:758:G:O4'	2.19	0.43
30:a:1501:U:H2'	30:a:1502:A:C8	2.54	0.43
10:A:143:A:H61	10:A:151:C:N4	2.17	0.43
10:A:2567:A:N1	18:N:28:THR:OG1	2.48	0.43
17:M:24:ASP:OD1	17:M:25:ALA:N	2.52	0.43
24:T:110:VAL:O	24:T:114:LYS:HB2	2.19	0.43
30:a:276:5OC:O5'	30:a:276:5OC:H6	2.19	0.43
30:a:642:A:C8	45:o:108:PRO:HA	2.54	0.43
31:b:43:TRP:NE1	31:b:62:LEU:HD22	2.34	0.43
3:l:9:LEU:HG	3:l:14:LEU:HD13	2.01	0.42
10:A:2835:U:H4'	10:A:2836:A:H5'	2.00	0.42
13:E:64:LEU:HD13	13:E:64:LEU:HA	1.91	0.42
13:E:181:MET:HE3	23:S:10:GLU:HG3	2.01	0.42
30:a:628:A:C6	30:a:629:G:H1'	2.54	0.42
35:f:24:SER:O	35:f:27:SER:OG	2.35	0.42
10:A:1382:A:H2'	10:A:1383:A:C8	2.54	0.42
16:L:92:ARG:HE	16:L:92:ARG:HB2	1.58	0.42
17:M:28:GLN:H	17:M:28:GLN:HG2	1.69	0.42
17:M:118:ARG:NH2	53:M:201:HOH:O	2.52	0.42
30:a:426:U:H1'	30:a:427:A:C4	2.52	0.42
30:a:626:U:OP1	32:c:36:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:o:105:VAL:HG12	45:o:107:THR:HG23	2.01	0.42
10:A:504:G:O2'	10:A:530:A:N1	2.47	0.42
10:A:669:G:H2'	10:A:670:U:C6	2.54	0.42
10:A:670:U:H2'	10:A:671:C:H6	1.84	0.42
25:U:65:LEU:HD11	25:U:99:LEU:HB2	2.01	0.42
30:a:380:U:OP1	32:c:69:THR:OG1	2.25	0.42
10:A:121:C:H2'	10:A:122:A:H8	1.84	0.42
10:A:149:U:H2'	10:A:150:U:C5	2.55	0.42
10:A:2591:A:H2'	10:A:2592:C:C6	2.54	0.42
16:L:70:ALA:HA	16:L:73:ALA:HB3	2.01	0.42
30:a:416:A:O2'	30:a:417:A:O5'	2.37	0.42
30:a:489:C:O2'	30:a:490:G:O5'	2.32	0.42
32:c:59:TRP:HA	32:c:62:VAL:HG22	2.02	0.42
45:o:28:SER:HB3	45:o:31:LYS:HE2	2.02	0.42
30:a:502:A:H61	30:a:523:A:N6	2.17	0.42
30:a:737:U:H2'	30:a:738:G:C8	2.55	0.42
30:a:938:G:O2'	30:a:1373:A:N3	2.47	0.42
30:a:1407:A:H2'	30:a:1408:2MG:C8	2.54	0.42
9:8:36:ARG:HH12	10:A:2540:C:H4'	1.85	0.42
10:A:464:A:H2'	10:A:465:G:C8	2.54	0.42
10:A:1152:U:H2'	10:A:1153:U:C6	2.55	0.42
12:D:232:MET:HE2	12:D:232:MET:HB3	1.96	0.42
30:a:727:G:N7	53:a:1707:HOH:O	2.37	0.42
30:a:959:U:H4'	30:a:960:U:O5'	2.19	0.42
30:a:1384:G:H2'	30:a:1385:G:C8	2.54	0.42
6:5:14:LEU:HD23	6:5:14:LEU:HA	1.84	0.42
10:A:255:C:H2'	10:A:256:U:C6	2.55	0.42
10:A:1942:A:H2'	10:A:1943:G:O4'	2.20	0.42
10:A:2077:G:N7	53:A:3139:HOH:O	2.37	0.42
10:A:2081:A:H2'	10:A:2082:C:C6	2.54	0.42
10:A:2387:A:H2'	10:A:2388:U:C6	2.55	0.42
11:B:61:A:H2'	11:B:62:A:H8	1.82	0.42
14:F:124:ILE:HG12	14:F:194:VAL:HG22	2.01	0.42
30:a:470:A:H2'	30:a:471:G:C8	2.54	0.42
30:a:581:G:N1	30:a:759:A:OP2	2.37	0.42
30:a:1043:A:N6	30:a:1209:U:H3	2.18	0.42
30:a:1057:U:H2'	30:a:1058:G:C8	2.53	0.42
30:a:1250:A:N3	30:a:1367:C:O2'	2.49	0.42
38:i:6:VAL:O	38:i:8:VAL:N	2.53	0.42
10:A:2638:U:H2'	10:A:2639:G:O4'	2.19	0.42
10:A:2845:A:H8	10:A:2845:A:OP2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:l:54:LYS:HE2	41:l:54:LYS:HB3	1.86	0.42
41:l:104:ALA:HB2	41:l:113:LEU:HD12	2.01	0.42
10:A:2299:A:H61	10:A:2319:C:H41	1.68	0.42
10:A:2424:U:H2'	10:A:2425:C:O4'	2.20	0.42
10:A:2805:A:H2'	10:A:2807:A:N7	2.35	0.42
30:a:218:A:H2'	30:a:219:U:C6	2.55	0.42
30:a:714:G:H2'	30:a:715:A:C8	2.55	0.42
30:a:1426:A:H2	30:a:1459:G:N1	2.08	0.42
38:i:14:LYS:HD3	38:i:14:LYS:HA	1.79	0.42
10:A:650:G:H5'	10:A:651:G:OP2	2.19	0.42
10:A:738:U:H2'	10:A:739:G:O4'	2.20	0.42
10:A:938:C:H2'	10:A:939:A:C8	2.55	0.42
10:A:1351:A:N1	10:A:1362:A:O2'	2.47	0.42
10:A:2440:A:N3	10:A:2440:A:H2'	2.35	0.42
16:L:121:ARG:HA	16:L:122:PRO:HD3	1.90	0.42
21:Q:83:VAL:O	21:Q:87:ILE:HG13	2.19	0.42
30:a:442:C:H1'	41:l:116:HIS:CE1	2.55	0.42
42:m:46:LEU:O	42:m:49:VAL:HG12	2.20	0.42
42:m:113:ARG:NE	42:m:125:GLU:OE2	2.52	0.42
47:J:6:ALA:HB1	47:J:83:ARG:HG3	2.02	0.42
10:A:159:A:H2'	10:A:160:A:C8	2.55	0.41
10:A:2701:C:H2'	10:A:2702:C:C6	2.55	0.41
11:B:7:G:H2'	11:B:8:G:C8	2.54	0.41
17:M:97:PHE:HB3	17:M:105:LEU:HB2	2.02	0.41
38:i:85:ILE:HD13	38:i:85:ILE:HA	1.83	0.41
1:p:64:GLU:OE2	1:p:64:GLU:N	2.46	0.41
6:5:49:ASN:HB2	6:5:53:ARG:O	2.20	0.41
10:A:253:G:H22	10:A:275:G:H22	1.69	0.41
10:A:1230:C:H2'	10:A:1231:A:C8	2.55	0.41
10:A:2654:U:H3	10:A:2668:C:H42	1.68	0.41
30:a:70:C:H4'	30:a:71:A:C8	2.55	0.41
30:a:258:U:H2'	30:a:259:G:C8	2.54	0.41
30:a:865:A:C5	30:a:866:G:H1'	2.55	0.41
37:h:54:ARG:HA	37:h:54:ARG:HD3	1.82	0.41
4:2:14:ARG:HA	10:A:1002:U:O3'	2.20	0.41
5:4:50:ARG:NH1	10:A:2868:A:OP2	2.53	0.41
10:A:515:A:H2'	10:A:516:G:O4'	2.20	0.41
10:A:576:U:H2'	10:A:577:G:O4'	2.20	0.41
10:A:1806:A:O2'	12:D:257:THR:OG1	2.38	0.41
30:a:105:C:OP2	33:d:9:LYS:HE3	2.20	0.41
30:a:117:G:H4'	30:a:118:C:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:4:ARG:HA	38:i:4:ARG:HD2	1.79	0.41
10:A:123:G:N2	10:A:134:G:H22	2.13	0.41
10:A:2346:G:N3	10:A:2382:A:H2'	2.35	0.41
19:O:74:TYR:HB3	19:O:112:LYS:HB2	2.01	0.41
26:V:34:MET:SD	26:V:60:ALA:HB1	2.61	0.41
30:a:451:G:H1	30:a:482:A:H1'	1.85	0.41
30:a:1345:U:H4'	47:J:120:ARG:HG3	2.01	0.41
30:a:1414:G:H2'	30:a:1415:G:C8	2.55	0.41
31:b:7:VAL:HG22	31:b:62:LEU:HB2	2.03	0.41
10:A:667:G:OP1	19:O:132:LYS:HG3	2.21	0.41
10:A:885:A:H2'	10:A:886:U:C6	2.55	0.41
10:A:1211:U:H2'	10:A:1212:A:O4'	2.21	0.41
30:a:299:A:O2'	30:a:311:A:N6	2.54	0.41
30:a:1481:A:C4	30:a:1482:A:H1'	2.55	0.41
33:d:40:ASP:HB3	33:d:43:GLU:HB3	2.03	0.41
35:f:26:GLU:HB3	35:f:81:ILE:HD13	2.01	0.41
35:f:70:LEU:HD23	35:f:70:LEU:HA	1.84	0.41
45:o:9:LEU:HD11	45:o:128:CYS:HB3	2.03	0.41
6:5:46:LYS:HA	6:5:56:THR:HA	2.01	0.41
7:6:7:PRO:HB2	10:A:1338:G:H4'	2.01	0.41
10:A:438:A:H2'	10:A:439:U:C6	2.55	0.41
10:A:876:H2U:H52	10:A:877:U:C5	2.55	0.41
10:A:1460:G:H2'	10:A:1461:A:C8	2.55	0.41
10:A:1464:A:H2'	10:A:1465:G:C8	2.55	0.41
10:A:2247:G:H2'	10:A:2248:A:H8	1.84	0.41
16:L:86:LYS:HB2	16:L:86:LYS:HE3	1.76	0.41
23:S:2:ASP:HB3	23:S:5:LYS:HB3	2.03	0.41
27:W:13:MET:HA	27:W:16:VAL:HG12	2.02	0.41
30:a:1019:C:H2'	30:a:1020:G:C8	2.55	0.41
30:a:1502:A:H2'	30:a:1503:C:H6	1.84	0.41
10:A:2287:A:H4'	10:A:2288:A:O4'	2.21	0.41
11:B:18:U:H2'	11:B:19:G:C8	2.56	0.41
22:R:40:GLN:HE21	22:R:40:GLN:HB2	1.62	0.41
4:2:16:PRO:HB2	4:2:18:ASP:OD1	2.20	0.41
10:A:2839:A:H2'	10:A:2840:U:C6	2.55	0.41
15:K:39:ILE:HD12	15:K:39:ILE:H	1.85	0.41
30:a:267:A:H2'	30:a:268:A:C8	2.56	0.41
4:2:46:MET:O	4:2:50:VAL:HG22	2.20	0.41
10:A:650:G:H5''	10:A:650:G:H8	1.85	0.41
10:A:1028:C:O2	17:M:8:THR:HG23	2.21	0.41
10:A:1228:U:H2'	10:A:1229:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2383:G:H4'	10:A:2384:A:OP2	2.21	0.41
10:A:2540:C:H2'	10:A:2541:C:O2	2.20	0.41
14:F:204:ASN:O	14:F:208:LYS:HB3	2.21	0.41
26:V:41:ILE:HG21	26:V:53:LEU:HD21	2.01	0.41
30:a:328:U:O3'	33:d:17:ARG:HD2	2.21	0.41
30:a:389:G:H2'	30:a:390:C:C6	2.56	0.41
30:a:605:U:H2'	30:a:606:G:C8	2.55	0.41
30:a:984:U:H2'	30:a:985:U:C6	2.56	0.41
30:a:274:C:H2'	30:a:275:A:C8	2.56	0.41
30:a:449:A:H2'	30:a:450:C:C6	2.56	0.41
35:f:8:LYS:HE2	35:f:31:LEU:HD11	2.03	0.41
10:A:135:A:H2'	10:A:136:C:H5''	2.03	0.40
10:A:141:G:H1	10:A:153:U:H3	1.69	0.40
10:A:665:G:H2'	10:A:666:C:C6	2.57	0.40
10:A:944:A:H2'	10:A:945:A:C8	2.56	0.40
10:A:2084:U:H2'	10:A:2085:U:C6	2.56	0.40
10:A:2252:OMG:H1'	10:A:2252:OMG:HM23	1.67	0.40
11:B:27:A:H2'	11:B:28:C:C6	2.55	0.40
27:W:38:LYS:O	27:W:42:GLU:HG3	2.21	0.40
38:i:20:LEU:HD21	38:i:49:TRP:HH2	1.86	0.40
43:n:159:ALA:HB1	43:n:165:SER:HA	2.02	0.40
22:R:28:LEU:HG	22:R:41:LEU:HD12	2.03	0.40
30:a:427:A:H2'	30:a:428:A:H8	1.86	0.40
30:a:1152:G:H2'	30:a:1153:A:H4'	2.03	0.40
30:a:1215:C:P	36:g:9:ARG:HH21	2.44	0.40
30:a:1496:A:H2'	30:a:1497:G:C8	2.57	0.40
10:A:542:U:H2'	10:A:543:C:C6	2.55	0.40
10:A:553:G:H1'	10:A:2045:G:H4'	2.03	0.40
10:A:1716:U:H2'	10:A:1717:G:O4'	2.21	0.40
27:W:38:LYS:HD3	27:W:49:VAL:HB	2.03	0.40
30:a:497:A:N6	30:a:545:C:H42	2.18	0.40
30:a:1370:U:O2'	30:a:1371:G:H8	2.03	0.40
10:A:819:G:H5'	10:A:820:G:OP1	2.21	0.40
10:A:2003:U:H4'	13:E:133:THR:OG1	2.21	0.40
12:D:82:GLU:OE2	12:D:103:TYR:OH	2.30	0.40
14:F:1:MET:HG3	14:F:19:LEU:HD13	2.01	0.40
20:P:118:LEU:HD12	20:P:131:PHE:CE1	2.56	0.40
30:a:432:U:H5''	41:l:10:LYS:HD2	2.04	0.40
30:a:953:G:H2'	30:a:954:U:C6	2.57	0.40
30:a:1335:G:H2'	30:a:1336:A:C8	2.57	0.40
35:f:25:PRO:C	35:f:27:SER:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:o:41:LYS:HD3	45:o:41:LYS:HA	1.77	0.40
48:I:77:ARG:HB3	48:I:84:TYR:CZ	2.57	0.40
4:2:31:LEU:HD23	4:2:31:LEU:HA	1.81	0.40
6:5:47:LYS:HE2	6:5:47:LYS:HB3	1.83	0.40
10:A:1711:C:O2	13:E:133:THR:HB	2.21	0.40
30:a:251:A:C2	30:a:287:A:C5	3.09	0.40
30:a:274:C:H2'	30:a:275:A:H8	1.87	0.40
41:l:13:ARG:HD2	41:l:29:LYS:O	2.22	0.40
41:l:81:VAL:O	41:l:85:LEU:HD23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	p	67/89 (75%)	65 (97%)	2 (3%)	0	100	100
2	0	75/79 (95%)	75 (100%)	0	0	100	100
3	1	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	2	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
5	4	54/61 (88%)	53 (98%)	1 (2%)	0	100	100
6	5	43/62 (69%)	33 (77%)	10 (23%)	0	100	100
7	6	46/50 (92%)	46 (100%)	0	0	100	100
8	7	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
9	8	31/38 (82%)	29 (94%)	2 (6%)	0	100	100
12	D	270/274 (98%)	264 (98%)	6 (2%)	0	100	100
13	E	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
14	F	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
15	K	65/101 (64%)	63 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	L	87/128 (68%)	77 (88%)	10 (12%)	0	100	100
17	M	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
18	N	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
19	O	135/148 (91%)	127 (94%)	8 (6%)	0	100	100
20	P	139/144 (96%)	133 (96%)	6 (4%)	0	100	100
21	Q	121/160 (76%)	118 (98%)	3 (2%)	0	100	100
22	R	103/114 (90%)	95 (92%)	8 (8%)	0	100	100
23	S	112/121 (93%)	108 (96%)	4 (4%)	0	100	100
24	T	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
25	U	102/105 (97%)	96 (94%)	6 (6%)	0	100	100
26	V	126/134 (94%)	124 (98%)	2 (2%)	0	100	100
27	W	88/97 (91%)	86 (98%)	2 (2%)	0	100	100
28	X	98/106 (92%)	91 (93%)	7 (7%)	0	100	100
29	Z	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
31	b	96/117 (82%)	95 (99%)	1 (1%)	0	100	100
32	c	93/192 (48%)	85 (91%)	8 (9%)	0	100	100
33	d	74/84 (88%)	73 (99%)	1 (1%)	0	100	100
34	e	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
35	f	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
36	g	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
37	h	53/179 (30%)	48 (91%)	5 (9%)	0	100	100
38	i	80/126 (64%)	75 (94%)	4 (5%)	1 (1%)	10	39
39	j	116/134 (87%)	110 (95%)	6 (5%)	0	100	100
40	k	98/246 (40%)	91 (93%)	7 (7%)	0	100	100
41	l	185/201 (92%)	172 (93%)	13 (7%)	0	100	100
42	m	99/158 (63%)	94 (95%)	5 (5%)	0	100	100
43	n	156/172 (91%)	151 (97%)	5 (3%)	0	100	100
44	Y	124/192 (65%)	110 (89%)	14 (11%)	0	100	100
45	o	125/131 (95%)	122 (98%)	3 (2%)	0	100	100
46	10	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
47	J	120/128 (94%)	116 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	I	49/90 (54%)	47 (96%)	2 (4%)	0	100	100
All	All	4547/5526 (82%)	4331 (95%)	215 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	i	7	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	46/75 (61%)	46 (100%)	0	100	100
2	0	62/66 (94%)	61 (98%)	1 (2%)	58	82
3	1	38/56 (68%)	38 (100%)	0	100	100
4	2	48/53 (91%)	48 (100%)	0	100	100
5	4	40/50 (80%)	39 (98%)	1 (2%)	42	73
6	5	33/58 (57%)	30 (91%)	3 (9%)	7	30
7	6	39/40 (98%)	39 (100%)	0	100	100
8	7	40/58 (69%)	40 (100%)	0	100	100
9	8	24/35 (69%)	24 (100%)	0	100	100
12	D	213/218 (98%)	206 (97%)	7 (3%)	33	67
13	E	157/163 (96%)	152 (97%)	5 (3%)	34	67
14	F	174/177 (98%)	174 (100%)	0	100	100
15	K	45/92 (49%)	44 (98%)	1 (2%)	47	76
16	L	28/102 (28%)	28 (100%)	0	100	100
17	M	124/128 (97%)	124 (100%)	0	100	100
18	N	97/100 (97%)	95 (98%)	2 (2%)	48	77
19	O	95/117 (81%)	91 (96%)	4 (4%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	P	107/118 (91%)	105 (98%)	2 (2%)	52	79
21	Q	102/129 (79%)	101 (99%)	1 (1%)	73	88
22	R	57/90 (63%)	53 (93%)	4 (7%)	12	41
23	S	101/107 (94%)	101 (100%)	0	100	100
24	T	89/93 (96%)	89 (100%)	0	100	100
25	U	91/92 (99%)	89 (98%)	2 (2%)	47	76
26	V	107/113 (95%)	105 (98%)	2 (2%)	52	79
27	W	70/85 (82%)	70 (100%)	0	100	100
28	X	72/89 (81%)	72 (100%)	0	100	100
29	Z	58/69 (84%)	56 (97%)	2 (3%)	32	66
31	b	55/101 (54%)	54 (98%)	1 (2%)	54	80
32	c	63/137 (46%)	60 (95%)	3 (5%)	21	55
33	d	55/69 (80%)	54 (98%)	1 (2%)	54	80
34	e	65/77 (84%)	64 (98%)	1 (2%)	60	83
35	f	61/79 (77%)	61 (100%)	0	100	100
36	g	60/69 (87%)	60 (100%)	0	100	100
37	h	43/146 (30%)	43 (100%)	0	100	100
38	i	60/102 (59%)	58 (97%)	2 (3%)	33	67
39	j	76/111 (68%)	76 (100%)	0	100	100
40	k	48/197 (24%)	48 (100%)	0	100	100
41	l	125/174 (72%)	124 (99%)	1 (1%)	79	90
42	m	56/132 (42%)	52 (93%)	4 (7%)	12	40
43	n	81/130 (62%)	78 (96%)	3 (4%)	29	63
44	Y	68/159 (43%)	65 (96%)	3 (4%)	24	58
45	o	95/112 (85%)	93 (98%)	2 (2%)	48	77
46	10	20/28 (71%)	20 (100%)	0	100	100
47	J	58/106 (55%)	58 (100%)	0	100	100
48	I	29/80 (36%)	29 (100%)	0	100	100
All	All	3275/4582 (72%)	3217 (98%)	58 (2%)	54	80

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	0	26	LYS
5	4	30	CYS
6	5	17	THR
6	5	32	THR
6	5	56	THR
12	D	40	THR
12	D	70	THR
12	D	146	LEU
12	D	205	SER
12	D	220	ASN
12	D	223	VAL
12	D	236	GLU
13	E	13	SER
13	E	24	CYS
13	E	64	LEU
13	E	150	SER
13	E	151	TYR
15	K	56	VAL
18	N	65	THR
18	N	109	THR
19	O	69	ILE
19	O	72	VAL
19	O	77	ILE
19	O	119	VAL
20	P	25	ASN
20	P	34	ILE
21	Q	77	LYS
22	R	29	THR
22	R	41	LEU
22	R	55	SER
22	R	86	THR
25	U	34	VAL
25	U	50	VAL
26	V	29	THR
26	V	119	SER
29	Z	9	SER
29	Z	15	GLU
31	b	63	VAL
32	c	8	GLN
32	c	39	SER
32	c	48	THR
33	d	61	LYS
34	e	21	THR

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Mol	Chain	Res	Type
38	i	67	VAL
38	i	77	LEU
41	l	125	VAL
42	m	29	LEU
42	m	31	TYR
42	m	49	VAL
42	m	100	SER
43	n	43	VAL
43	n	51	ILE
43	n	141	LEU
44	Y	46	GLN
44	Y	52	LEU
44	Y	107	VAL
45	o	41	LYS
45	o	104	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	p	12	ASN
2	0	17	ASN
3	1	46	GLN
3	1	59	GLN
12	D	143	ASN
14	F	67	GLN
14	F	173	ASN
15	K	63	GLN
16	L	117	HIS
17	M	52	HIS
17	M	89	GLN
20	P	135	HIS
21	Q	31	HIS
21	Q	71	GLN
23	S	83	ASN
24	T	101	ASN
25	U	8	GLN
26	V	47	ASN
27	W	53	ASN
32	c	8	GLN
32	c	43	ASN
32	c	45	ASN
32	c	52	ASN

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Mol	Chain	Res	Type
33	d	13	GLN
36	g	37	GLN
36	g	42	ASN
41	l	35	GLN
41	l	50	GLN
41	l	73	HIS
41	l	137	GLN
44	Y	41	ASN
46	10	3	ASN
48	I	71	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2306/2889 (79%)	292 (12%)	10 (0%)
11	B	96/109 (88%)	22 (22%)	1 (1%)
30	a	1297/1534 (84%)	270 (20%)	0
All	All	3699/4532 (81%)	584 (15%)	11 (0%)

All (584) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	2	A
10	A	23	A
10	A	24	G
10	A	28	C
10	A	40	G
10	A	52	A
10	A	53	A
10	A	54	G
10	A	60	A
10	A	63	A
10	A	64	G
10	A	80	C
10	A	89	U
10	A	90	G
10	A	106	A
10	A	107	A
10	A	108	U
10	A	119	G
10	A	123	G

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Mol	Chain	Res	Type
10	A	132	C
10	A	136	C
10	A	144	U
10	A	159	A
10	A	174	A
10	A	177	A
10	A	183	U
10	A	184	U
10	A	193	G
10	A	194	A
10	A	200	A
10	A	211	A
10	A	226	G
10	A	275	G
10	A	280	U
10	A	281	A
10	A	282	G
10	A	286	U
10	A	306	A
10	A	307	G
10	A	329	A
10	A	333	U
10	A	347	G
10	A	348	A
10	A	364	C
10	A	396	U
10	A	409	G
10	A	419	G
10	A	434	G
10	A	480	A
10	A	504	G
10	A	513	A
10	A	514	C
10	A	528	A
10	A	531	C
10	A	554	C
10	A	555	G
10	A	561	A
10	A	572	G
10	A	573	G
10	A	585	G
10	A	595	U

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Mol	Chain	Res	Type
10	A	596	A
10	A	597	A
10	A	609	G
10	A	625	A
10	A	634	G
10	A	647	C
10	A	649	A
10	A	650	G
10	A	658	A
10	A	665	G
10	A	668	A
10	A	669	G
10	A	677	A
10	A	678	G
10	A	679	G
10	A	721	U
10	A	754	C
10	A	755	U
10	A	765	A
10	A	782	U
10	A	783	G
10	A	799	A
10	A	810	G
10	A	817	A
10	A	819	G
10	A	820	G
10	A	827	A
10	A	840	G
10	A	847	C
10	A	862	U
10	A	880	A
10	A	882	G
10	A	893	G
10	A	900	G
10	A	901	A
10	A	908	G
10	A	910	A
10	A	940	G
10	A	944	A
10	A	946	C
10	A	965	G
10	A	966	A

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Mol	Chain	Res	Type
10	A	967	C
10	A	974	A
10	A	978	A
10	A	979	G
10	A	994	G
10	A	1007	G
10	A	1013	A
10	A	1029	G
10	A	1045	U
10	A	1046	A
10	A	1050	G
10	A	1054	A
10	A	1064	A
10	A	1066	G
10	A	1067	A
10	A	1068	A
10	A	1069	G
10	A	1074	G
10	A	1076	A
10	A	1155	G
10	A	1163	U
10	A	1164	A
10	A	1168	C
10	A	1170	C
10	A	1174	C
10	A	1177	A
10	A	1203	U
10	A	1235	A
10	A	1239	A
10	A	1252	G
10	A	1253	C
10	A	1267	G
10	A	1285	G
10	A	1300	G
10	A	1301	A
10	A	1305	A
10	A	1329	A
10	A	1330	A
10	A	1381	U
10	A	1394	A
10	A	1408	U
10	A	1412	A

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Mol	Chain	Res	Type
10	A	1413	G
10	A	1414	A
10	A	1418	G
10	A	1433	A
10	A	1458	C
10	A	1603	A
10	A	1606	A
10	A	1632	U
10	A	1643	U
10	A	1644	A
10	A	1645	A
10	A	1654	A
10	A	1668	A
10	A	1683	U
10	A	1684	C
10	A	1710	G
10	A	1765	G
10	A	1767	A
10	A	1773	G
10	A	1782	A
10	A	1791	C
10	A	1795	A
10	A	1809	C
10	A	1810	A
10	A	1811	A
10	A	1815	A
10	A	1826	G
10	A	1838	A
10	A	1901	G
10	A	1939	G
10	A	1940	G
10	A	1947	A
10	A	1951	C
10	A	1965	U
10	A	1973	U
10	A	1977	C
10	A	1980	A
10	A	1981	U
10	A	1982	G
10	A	1992	U
10	A	2001	U
10	A	2002	G

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Mol	Chain	Res	Type
10	A	2003	U
10	A	2041	A
10	A	2042	G
10	A	2043	A
10	A	2053	C
10	A	2065	C
10	A	2066	G
10	A	2070	A
10	A	2071	G
10	A	2072	A
10	A	2079	G
10	A	2103	G
10	A	2107	U
10	A	2202	G
10	A	2208	A
10	A	2222	G
10	A	2226	A
10	A	2239	G
10	A	2240	G
10	A	2280	G
10	A	2284	U
10	A	2288	A
10	A	2289	A
10	A	2316	G
10	A	2317	G
10	A	2318	U
10	A	2323	A
10	A	2324	G
10	A	2326	G
10	A	2334	A
10	A	2336	A
10	A	2341	U
10	A	2346	G
10	A	2348	C
10	A	2351	G
10	A	2383	G
10	A	2384	A
10	A	2386	C
10	A	2392	G
10	A	2423	C
10	A	2426	A
10	A	2430	G

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Mol	Chain	Res	Type
10	A	2431	A
10	A	2435	A
10	A	2440	A
10	A	2442	U
10	A	2449	A
10	A	2483	A
10	A	2492	U
10	A	2506	G
10	A	2519	A
10	A	2530	G
10	A	2535	A
10	A	2548	U
10	A	2552	C
10	A	2567	A
10	A	2568	G
10	A	2574	C
10	A	2586	U
10	A	2603	A
10	A	2604	G
10	A	2610	U
10	A	2614	U
10	A	2631	G
10	A	2671	G
10	A	2672	U
10	A	2674	G
10	A	2690	U
10	A	2703	G
10	A	2715	G
10	A	2727	C
10	A	2734	U
10	A	2735	A
10	A	2736	A
10	A	2737	G
10	A	2745	G
10	A	2749	A
10	A	2753	C
10	A	2759	A
10	A	2763	C
10	A	2765	A
10	A	2766	A
10	A	2767	G
10	A	2779	A

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Mol	Chain	Res	Type
10	A	2780	U
10	A	2781	A
10	A	2790	A
10	A	2791	U
10	A	2798	G
10	A	2806	A
10	A	2807	A
10	A	2809	A
10	A	2821	A
10	A	2829	C
10	A	2840	U
10	A	2842	G
10	A	2845	A
10	A	2852	A
10	A	2853	A
10	A	2858	A
10	A	2865	C
10	A	2868	A
10	A	2869	U
10	A	2870	A
10	A	2871	G
11	B	10	U
11	B	11	A
11	B	12	U
11	B	22	G
11	B	23	A
11	B	24	U
11	B	25	C
11	B	30	U
11	B	32	U
11	B	35	C
11	B	54	U
11	B	55	A
11	B	62	A
11	B	64	G
11	B	81	G
11	B	86	A
11	B	92	A
11	B	98	G
11	B	101	C
11	B	102	G
11	B	104	C

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Mol	Chain	Res	Type
11	B	105	G
30	a	8	A
30	a	9	G
30	a	31	G
30	a	32	A
30	a	38	A
30	a	39	G
30	a	47	C
30	a	48	U
30	a	50	A
30	a	51	A
30	a	52	C
30	a	61	G
30	a	65	A
30	a	66	G
30	a	71	A
30	a	72	G
30	a	73	C
30	a	111	A
30	a	118	C
30	a	123	C
30	a	132	A
30	a	146	A
30	a	147	G
30	a	152	A
30	a	159	G
30	a	169	G
30	a	176	A
30	a	185	C
30	a	187	C
30	a	192	A
30	a	199	C
30	a	202	G
30	a	205	A
30	a	206	U
30	a	207	U
30	a	209	C
30	a	216	A
30	a	249	U
30	a	250	U
30	a	252	G
30	a	256	G

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Mol	Chain	Res	Type
30	a	271	G
30	a	272	C
30	a	275	A
30	a	280	G
30	a	286	G
30	a	293	A
30	a	294	G
30	a	298	A
30	a	306	G
30	a	310	U
30	a	330	A
30	a	331	G
30	a	333	C
30	a	334	A
30	a	337	G
30	a	343	A
30	a	349	A
30	a	350	C
30	a	351	G
30	a	352	G
30	a	353	G
30	a	356	G
30	a	358	A
30	a	372	U
30	a	377	C
30	a	378	A
30	a	389	G
30	a	396	C
30	a	397	C
30	a	402	A
30	a	403	A
30	a	411	G
30	a	415	G
30	a	416	A
30	a	417	A
30	a	418	G
30	a	422	G
30	a	430	G
30	a	433	U
30	a	437	A
30	a	442	C
30	a	457	A

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Mol	Chain	Res	Type
30	a	463	C
30	a	464	G
30	a	466	U
30	a	467	A
30	a	468	C
30	a	476	G
30	a	479	U
30	a	481	G
30	a	482	A
30	a	483	A
30	a	490	G
30	a	492	A
30	a	494	G
30	a	501	C
30	a	502	A
30	a	505	G
30	a	506	G
30	a	507	C
30	a	508	U
30	a	509	A
30	a	512	U
30	a	518	C
30	a	521	G
30	a	524	G
30	a	535	A
30	a	544	G
30	a	547	A
30	a	556	C
30	a	559	A
30	a	560	U
30	a	562	U
30	a	564	U
30	a	572	A
30	a	573	A
30	a	576	G
30	a	577	G
30	a	592	G
30	a	618	C
30	a	621	A
30	a	630	C
30	a	631	C
30	a	632	U

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Mol	Chain	Res	Type
30	a	633	G
30	a	639	G
30	a	653	U
30	a	665	C
30	a	673	G
30	a	682	G
30	a	686	U
30	a	687	A
30	a	688	G
30	a	702	A
30	a	703	G
30	a	704	A
30	a	709	A
30	a	713	G
30	a	721	G
30	a	722	A
30	a	746	G
30	a	748	G
30	a	749	A
30	a	751	U
30	a	755	A
30	a	761	G
30	a	777	A
30	a	789	U
30	a	790	A
30	a	793	U
30	a	794	A
30	a	817	C
30	a	828	A
30	a	837	C
30	a	850	A
30	a	851	G
30	a	853	U
30	a	854	U
30	a	855	C
30	a	901	C
30	a	913	A
30	a	925	G
30	a	926	G
30	a	930	C
30	a	959	U
30	a	960	U

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Mol	Chain	Res	Type
30	a	965	G
30	a	966	A
30	a	968	A
30	a	970	G
30	a	971	C
30	a	972	G
30	a	975	G
30	a	990	U
30	a	1050	G
30	a	1051	C
30	a	1052	A
30	a	1059	U
30	a	1064	A
30	a	1065	G
30	a	1066	C
30	a	1076	G
30	a	1117	G
30	a	1118	G
30	a	1120	A
30	a	1141	A
30	a	1147	C
30	a	1152	G
30	a	1153	A
30	a	1154	G
30	a	1189	A
30	a	1190	C
30	a	1191	G
30	a	1194	A
30	a	1195	A
30	a	1198	C
30	a	1209	U
30	a	1211	A
30	a	1212	C
30	a	1234	A
30	a	1236	A
30	a	1241	G
30	a	1247	C
30	a	1248	A
30	a	1249	A
30	a	1250	A
30	a	1255	A
30	a	1256	G

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Mol	Chain	Res	Type
30	a	1261	C
30	a	1262	G
30	a	1263	G
30	a	1264	G
30	a	1267	A
30	a	1268	C
30	a	1269	C
30	a	1270	G
30	a	1277	A
30	a	1278	A
30	a	1281	U
30	a	1282	C
30	a	1283	U
30	a	1287	C
30	a	1288	C
30	a	1297	G
30	a	1299	U
30	a	1302	G
30	a	1307	G
30	a	1309	G
30	a	1310	U
30	a	1319	C
30	a	1325	C
30	a	1328	G
30	a	1341	C
30	a	1344	G
30	a	1345	U
30	a	1346	A
30	a	1350	G
30	a	1356	C
30	a	1360	C
30	a	1361	A
30	a	1362	U
30	a	1366	G
30	a	1368	G
30	a	1369	G
30	a	1370	U
30	a	1371	G
30	a	1373	A
30	a	1375	A
30	a	1387	C
30	a	1396	A

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Mol	Chain	Res	Type
30	a	1415	G
30	a	1417	G
30	a	1436	C
30	a	1455	C
30	a	1457	A
30	a	1468	G
30	a	1481	A
30	a	1482	A
30	a	1486	G
30	a	1488	A
30	a	1493	G
30	a	1495	U
30	a	1496	A
30	a	1506	G
30	a	1518	G
30	a	1519	G
30	a	1520	A
30	a	1521	A
30	a	1522	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	285	C
10	A	677	A
10	A	748	G
10	A	862	U
10	A	1255	A
10	A	1309	G
10	A	2221	C
10	A	2670	U
10	A	2671	G
10	A	2852	A
11	B	61	A

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

20 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
10	H2U	A	2620	10	18,21,22	0.43	0	21,30,33	0.37	0
30	5OC	a	276	30	18,21,22	4.40	13 (72%)	25,30,33	1.18	1 (4%)
10	5MU	A	1949	10	19,22,23	7.25	8 (42%)	28,32,35	3.41	10 (35%)
10	5MC	A	1972	10	18,22,23	3.67	7 (38%)	26,32,35	1.00	2 (7%)
30	7MG	a	821	30	22,26,27	3.70	10 (45%)	29,39,42	2.04	9 (31%)
10	OMG	A	2252	10	18,26,27	2.51	8 (44%)	19,38,41	1.49	4 (21%)
30	4OC	a	1400	30	20,23,24	3.14	8 (40%)	26,32,35	0.90	1 (3%)
10	H2U	A	781	10	18,21,22	0.31	0	21,30,33	0.50	0
10	5OC	A	2502	10,51	18,21,22	4.26	13 (72%)	25,30,33	1.17	3 (12%)
10	2MA	A	2504	10,51,49	19,25,26	3.59	6 (31%)	21,37,40	2.51	4 (19%)
30	2MG	a	1408	30	18,26,27	2.50	7 (38%)	16,38,41	1.36	3 (18%)
10	PSU	A	2606	10	18,21,22	1.01	1 (5%)	22,30,33	1.73	4 (18%)
30	MA6	a	1508	30	18,26,27	1.04	2 (11%)	19,38,41	4.07	2 (10%)
30	MA6	a	1507	30	18,26,27	1.02	2 (11%)	19,38,41	4.21	3 (15%)
10	PSU	A	2581	10	18,21,22	1.10	2 (11%)	22,30,33	1.88	5 (22%)
30	5MC	a	1402	30	18,22,23	3.72	7 (38%)	26,32,35	0.98	1 (3%)
10	H2U	A	876	10	18,21,22	0.40	0	21,30,33	0.39	0
10	OMU	A	2450	10	19,22,23	2.98	8 (42%)	26,31,34	1.74	5 (19%)
10	2MG	A	2446	10	18,26,27	2.42	7 (38%)	16,38,41	1.35	3 (18%)
30	UR3	a	1487	30	19,22,23	3.21	8 (42%)	26,32,35	1.30	2 (7%)

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
10	H2U	A	2620	10	-	0/7/38/39	0/2/2/2
30	5OC	a	276	30	-	1/7/21/22	0/2/2/2
10	5MU	A	1949	10	-	0/7/25/26	0/2/2/2
10	5MC	A	1972	10	-	0/7/25/26	0/2/2/2
30	7MG	a	821	30	-	0/7/37/38	0/3/3/3
10	OMG	A	2252	10	-	1/5/27/28	0/3/3/3
30	4OC	a	1400	30	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	H2U	A	781	10	-	0/7/38/39	0/2/2/2
10	5OC	A	2502	10,51	-	5/7/21/22	0/2/2/2
10	2MA	A	2504	10,51,49	-	1/3/25/26	0/3/3/3
30	2MG	a	1408	30	-	0/5/27/28	0/3/3/3
10	PSU	A	2606	10	-	0/7/25/26	0/2/2/2
30	MA6	a	1508	30	-	5/7/29/30	0/3/3/3
30	MA6	a	1507	30	-	3/7/29/30	0/3/3/3
10	PSU	A	2581	10	-	0/7/25/26	0/2/2/2
30	5MC	a	1402	30	-	0/7/25/26	0/2/2/2
10	H2U	A	876	10	-	0/7/38/39	0/2/2/2
10	OMU	A	2450	10	-	0/9/27/28	0/2/2/2
10	2MG	A	2446	10	-	2/5/27/28	0/3/3/3
30	UR3	a	1487	30	-	0/7/25/26	0/2/2/2

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1949	5MU	C4-C5	21.01	1.79	1.44
10	A	1949	5MU	C6-N1	15.49	1.64	1.38
10	A	1949	5MU	C6-C5	-11.72	1.15	1.34
10	A	1949	5MU	C4-N3	-11.71	1.17	1.38
30	a	1402	5MC	C6-C5	9.37	1.50	1.34
10	A	1972	5MC	C6-C5	9.36	1.50	1.34
10	A	2504	2MA	C4-N3	9.35	1.50	1.35
30	a	821	7MG	C8-N9	8.75	1.50	1.46
30	a	1487	UR3	C2-N1	8.73	1.51	1.38
30	a	276	5OC	C2'-C3'	-8.55	1.30	1.52
10	A	2502	5OC	C2'-C3'	-8.43	1.30	1.52
30	a	821	7MG	C5-N7	8.17	1.45	1.35
10	A	2504	2MA	C2-N3	7.81	1.47	1.34
30	a	1400	4OC	C4-N3	6.94	1.44	1.32
10	A	2450	OMU	C2-N1	6.88	1.49	1.38
30	a	1487	UR3	C6-C5	6.71	1.50	1.35
30	a	1402	5MC	C4-N3	6.66	1.45	1.34
10	A	1972	5MC	C4-N3	6.62	1.45	1.34
10	A	2450	OMU	C2-N3	6.54	1.49	1.38
30	a	1402	5MC	C2-N3	6.33	1.49	1.36
10	A	1972	5MC	C2-N3	6.21	1.49	1.36
30	a	276	5OC	C2-N3	6.15	1.48	1.36
30	a	276	5OC	C4-N3	5.96	1.44	1.34
30	a	1400	4OC	C4-N4	5.88	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	1487	UR3	C2-N3	5.88	1.50	1.39
10	A	2502	5OC	C2-N3	5.85	1.48	1.36
10	A	2502	5OC	O4'-C1'	-5.84	1.29	1.42
30	a	1400	4OC	C6-C5	5.79	1.48	1.35
10	A	2504	2MA	C6-N1	5.73	1.44	1.33
30	a	276	5OC	C5-C4	5.70	1.49	1.42
30	a	821	7MG	C2-N3	5.65	1.46	1.33
30	a	276	5OC	O4'-C1'	-5.64	1.29	1.42
10	A	2504	2MA	C2-N1	5.63	1.44	1.34
10	A	2450	OMU	C6-C5	5.62	1.48	1.35
30	a	1400	4OC	C2-N3	5.51	1.47	1.36
30	a	1408	2MG	C2-N2	5.48	1.45	1.33
30	a	821	7MG	C4-N3	5.46	1.47	1.34
10	A	2252	OMG	C2-N3	5.44	1.46	1.33
10	A	2502	5OC	C5-C4	5.44	1.49	1.42
10	A	2502	5OC	C4-N3	5.36	1.43	1.34
30	a	821	7MG	C4-N9	5.31	1.43	1.37
10	A	2446	2MG	C2-N2	5.23	1.45	1.33
30	a	1408	2MG	C4-N3	5.06	1.49	1.37
30	a	1402	5MC	C6-N1	5.04	1.46	1.38
30	a	276	5OC	O4'-C4'	5.01	1.56	1.45
10	A	2446	2MG	C4-N3	4.93	1.49	1.37
30	a	276	5OC	C4-N4	4.87	1.46	1.34
10	A	1972	5MC	C6-N1	4.87	1.46	1.38
10	A	2252	OMG	C4-N3	4.85	1.49	1.37
10	A	2502	5OC	C4-N4	4.70	1.46	1.34
30	a	1408	2MG	C2-N1	4.69	1.44	1.36
10	A	2502	5OC	O4'-C4'	4.68	1.55	1.45
30	a	821	7MG	C2-N2	4.63	1.45	1.34
30	a	1402	5MC	C4-N4	4.58	1.46	1.34
10	A	2252	OMG	C2-N2	4.53	1.45	1.34
30	a	276	5OC	C2-N1	4.47	1.49	1.40
10	A	2446	2MG	C2-N1	4.45	1.43	1.36
10	A	1972	5MC	C4-N4	4.44	1.45	1.34
30	a	1400	4OC	C2-N1	4.44	1.49	1.40
30	a	1402	5MC	C2-N1	4.39	1.49	1.40
30	a	276	5OC	C6-N1	4.29	1.45	1.38
10	A	1972	5MC	C2-N1	4.24	1.49	1.40
30	a	276	5OC	C2'-C1'	4.18	1.64	1.52
10	A	2502	5OC	C2-N1	4.15	1.49	1.40
10	A	2502	5OC	C6-N1	4.13	1.45	1.38
10	A	2502	5OC	C2'-C1'	4.11	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	1487	UR3	C6-N1	3.92	1.47	1.38
10	A	2450	OMU	C4-N3	3.86	1.45	1.38
10	A	1949	5MU	C2-N3	3.83	1.44	1.38
30	a	1400	4OC	C5-C4	3.68	1.48	1.40
10	A	2502	5OC	C5'-C4'	-3.65	1.40	1.51
30	a	821	7MG	C2-N1	3.63	1.46	1.37
10	A	1949	5MU	C2-N1	3.61	1.44	1.38
30	a	276	5OC	C5'-C4'	-3.59	1.40	1.51
30	a	821	7MG	C5-C6	3.55	1.52	1.43
30	a	1408	2MG	C6-N1	3.49	1.43	1.37
10	A	2504	2MA	CM2-C2	3.43	1.59	1.49
10	A	2252	OMG	C6-N1	3.35	1.42	1.37
10	A	2450	OMU	O4-C4	-3.29	1.18	1.24
30	a	1400	4OC	C6-N1	3.17	1.45	1.38
10	A	2581	PSU	C6-C5	3.17	1.39	1.35
10	A	2502	5OC	O3'-C3'	3.10	1.49	1.43
10	A	2606	PSU	C6-C5	3.09	1.38	1.35
30	a	821	7MG	C6-N1	3.08	1.44	1.38
30	a	1408	2MG	C5-C6	3.02	1.53	1.47
30	a	276	5OC	O3'-C3'	3.02	1.49	1.43
10	A	2446	2MG	C6-N1	3.00	1.42	1.37
10	A	2504	2MA	C6-C5	2.93	1.54	1.43
10	A	2252	OMG	C5-C6	2.87	1.53	1.47
10	A	2446	2MG	C5-C4	-2.81	1.35	1.43
10	A	2446	2MG	C5-C6	2.75	1.53	1.47
10	A	2450	OMU	C6-N1	2.73	1.44	1.38
10	A	1972	5MC	O2-C2	-2.73	1.18	1.23
30	a	1487	UR3	C5-C4	2.72	1.50	1.43
10	A	2450	OMU	O2-C2	-2.68	1.18	1.23
30	a	821	7MG	O6-C6	-2.65	1.18	1.23
30	a	1487	UR3	C4-N3	2.62	1.46	1.40
10	A	1949	5MU	O4-C4	-2.62	1.18	1.23
10	A	2252	OMG	C5-C4	-2.61	1.36	1.43
10	A	2446	2MG	O6-C6	-2.60	1.18	1.23
30	a	1507	MA6	C5-C4	-2.60	1.34	1.40
30	a	1402	5MC	O2-C2	-2.58	1.18	1.23
30	a	1408	2MG	C5-C4	-2.51	1.36	1.43
30	a	1508	MA6	C5-C4	-2.50	1.34	1.40
10	A	1949	5MU	O2-C2	-2.47	1.18	1.23
10	A	2252	OMG	O6-C6	-2.46	1.18	1.23
30	a	1508	MA6	C2-N3	2.43	1.36	1.32
10	A	2252	OMG	C2-N1	2.43	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	276	5OC	O5-C5	2.40	1.40	1.34
30	a	1507	MA6	C2-N3	2.32	1.35	1.32
30	a	1408	2MG	O6-C6	-2.31	1.18	1.23
10	A	2450	OMU	C5-C4	2.29	1.48	1.43
10	A	2581	PSU	O4'-C1'	-2.21	1.40	1.43
10	A	2502	5OC	O5-C5	2.09	1.39	1.34
30	a	1487	UR3	O4-C4	-2.08	1.19	1.23
30	a	1487	UR3	O2-C2	-2.07	1.18	1.22
30	a	1400	4OC	O2-C2	-2.07	1.19	1.23

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1507	MA6	N1-C6-N6	-17.14	99.02	117.06
30	a	1508	MA6	N1-C6-N6	-16.56	99.63	117.06
10	A	1949	5MU	C5-C4-N3	10.60	124.36	115.31
10	A	1949	5MU	C5-C6-N1	-8.70	114.39	123.34
10	A	2504	2MA	C2-N3-C4	7.76	121.83	115.52
10	A	1949	5MU	C4-N3-C2	-7.07	118.20	127.35
10	A	2504	2MA	C1'-N9-C4	-6.91	114.50	126.64
30	a	1507	MA6	N3-C2-N1	-5.71	119.75	128.68
30	a	1508	MA6	N3-C2-N1	-5.58	119.95	128.68
10	A	2450	OMU	C4-N3-C2	-5.42	119.42	126.58
30	a	821	7MG	C5-C6-N1	5.06	119.91	110.99
30	a	1487	UR3	C4-N3-C2	-4.78	120.06	124.56
10	A	2581	PSU	N1-C2-N3	4.74	120.50	115.13
10	A	1949	5MU	N3-C2-N1	4.60	121.00	114.89
10	A	2606	PSU	C4-N3-C2	-4.53	119.81	126.34
30	a	821	7MG	C2-N3-C4	4.48	120.29	112.30
10	A	2606	PSU	N1-C2-N3	4.46	120.18	115.13
10	A	2581	PSU	C4-N3-C2	-4.44	119.94	126.34
10	A	1949	5MU	C5M-C5-C6	-4.06	117.42	122.85
30	a	821	7MG	C5-C4-N3	-3.98	120.55	128.13
10	A	2450	OMU	N3-C2-N1	3.94	120.12	114.89
10	A	1949	5MU	O4-C4-C5	-3.89	120.39	124.90
30	a	276	5OC	O5-C5-C4	3.81	120.17	114.43
10	A	2252	OMG	C5-C6-N1	3.60	120.30	113.95
10	A	2446	2MG	C5-C6-N1	3.53	120.18	113.95
10	A	2502	5OC	O5-C5-C4	3.49	119.69	114.43
30	a	1408	2MG	C5-C6-N1	3.44	120.02	113.95
10	A	2450	OMU	C5-C4-N3	3.39	119.92	114.84
10	A	1972	5MC	C5-C6-N1	-3.30	119.94	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2252	OMG	C2-N1-C6	-3.29	119.04	125.10
10	A	1949	5MU	C6-C5-C4	3.26	120.75	118.03
10	A	2504	2MA	N3-C2-N1	-3.17	119.94	125.73
30	a	821	7MG	C5-C4-N9	3.13	110.41	106.35
30	a	1402	5MC	C5-C6-N1	-3.09	120.16	123.34
30	a	821	7MG	C4-C5-N7	3.06	109.78	105.53
10	A	2450	OMU	O4-C4-C5	-2.88	120.09	125.16
10	A	1949	5MU	C5M-C5-C4	2.78	121.83	118.77
30	a	821	7MG	C2-N1-C6	-2.73	120.12	125.10
30	a	821	7MG	O6-C6-C5	-2.66	121.01	127.54
10	A	2446	2MG	C8-N7-C5	2.66	108.05	102.99
30	a	821	7MG	N9-C8-N7	2.63	107.14	103.38
10	A	2581	PSU	O4'-C1'-C2'	2.61	108.83	105.14
10	A	2252	OMG	C8-N7-C5	2.61	107.96	102.99
10	A	2581	PSU	O2-C2-N1	-2.60	119.93	122.79
10	A	2581	PSU	C6-N1-C2	-2.55	120.08	122.68
10	A	1949	5MU	O4-C4-N3	-2.54	115.25	120.12
30	a	1408	2MG	C8-N7-C5	2.53	107.82	102.99
30	a	1400	4OC	C6-C5-C4	2.41	119.91	116.96
30	a	821	7MG	N9-C4-N3	2.39	129.04	125.47
10	A	2446	2MG	O6-C6-C5	-2.37	119.74	124.37
30	a	1408	2MG	O6-C6-C5	-2.28	119.92	124.37
30	a	1487	UR3	C6-N1-C2	-2.25	119.78	121.79
10	A	2606	PSU	O2-C2-N1	-2.20	120.36	122.79
10	A	2252	OMG	O6-C6-C5	-2.17	120.13	124.37
10	A	1972	5MC	CM5-C5-C6	-2.17	119.95	122.85
10	A	1949	5MU	O2-C2-N1	-2.15	119.93	122.79
10	A	2504	2MA	CM2-C2-N3	2.12	120.46	117.16
10	A	2450	OMU	O2-C2-N1	-2.11	119.98	122.79
10	A	2502	5OC	C3'-C2'-C1'	2.07	107.72	102.54
30	a	1507	MA6	C1'-N9-C4	-2.06	123.01	126.64
10	A	2502	5OC	C2'-C3'-C4'	2.06	107.04	102.76
10	A	2606	PSU	C6-N1-C2	-2.04	120.60	122.68

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2252	OMG	C1'-C2'-O2'-CM2
30	a	1507	MA6	C5-C6-N6-C9
30	a	1507	MA6	C5-C6-N6-C10
30	a	1508	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
30	a	1508	MA6	O4'-C4'-C5'-O5'
30	a	1507	MA6	N1-C6-N6-C10
30	a	1508	MA6	N1-C6-N6-C10
10	A	2502	5OC	C2'-C1'-N1-C6
10	A	2502	5OC	C2'-C1'-N1-C2
30	a	1508	MA6	C5-C6-N6-C9
10	A	2446	2MG	C3'-C4'-C5'-O5'
10	A	2502	5OC	O4'-C1'-N1-C6
10	A	2502	5OC	O4'-C1'-N1-C2
30	a	1508	MA6	C3'-C4'-C5'-O5'
30	a	276	5OC	C3'-C4'-C5'-O5'
10	A	2502	5OC	O4'-C4'-C5'-O5'
10	A	2504	2MA	O4'-C4'-C5'-O5'
10	A	2446	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2620	H2U	1	0
30	a	276	5OC	1	0
10	A	1949	5MU	2	0
30	a	821	7MG	1	0
10	A	2252	OMG	1	0
30	a	1408	2MG	2	0
30	a	1508	MA6	1	0
30	a	1507	MA6	1	0
10	A	876	H2U	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 186 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

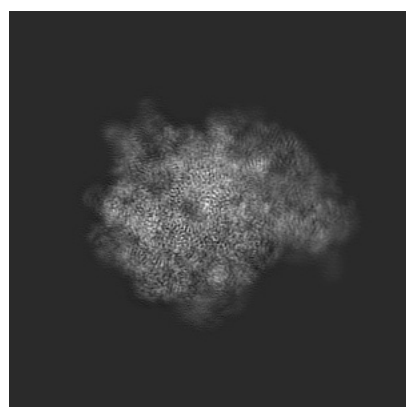
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52641. These allow visual inspection of the internal detail of the map and identification of artifacts.

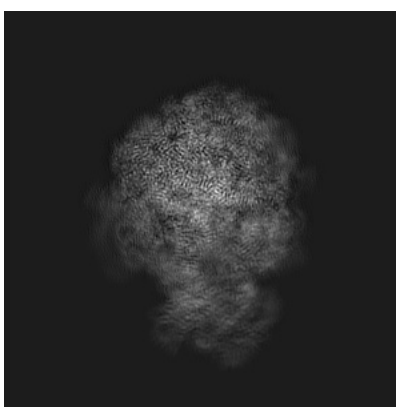
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

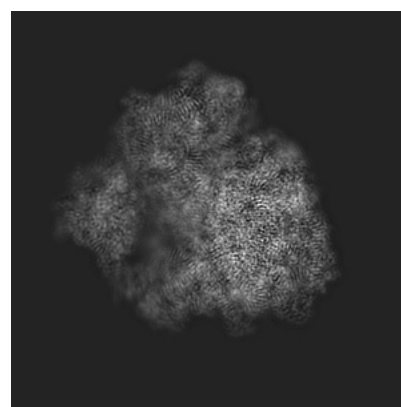
6.1.1 Primary map



X



Y

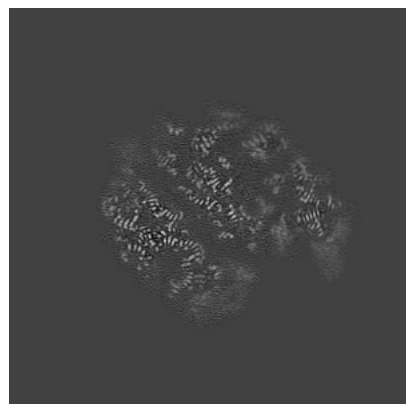


Z

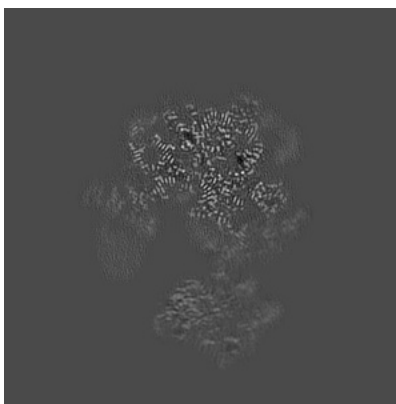
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

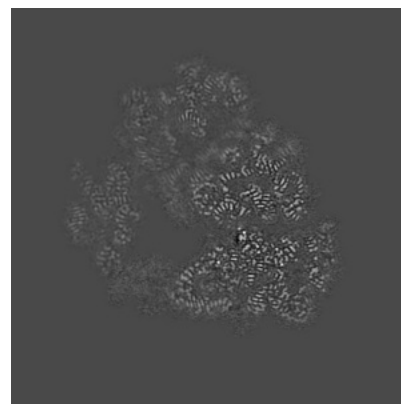
6.2.1 Primary map



X Index: 220



Y Index: 220

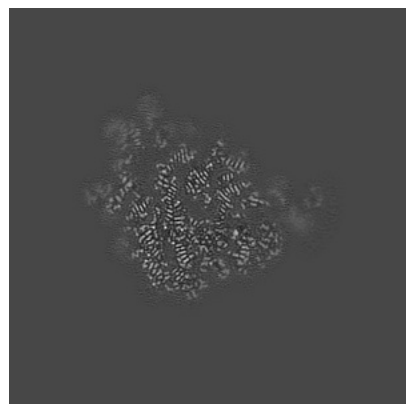


Z Index: 220

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

6.3 Largest variance slices [i](#)

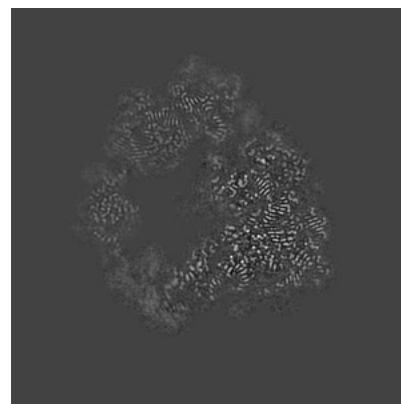
6.3.1 Primary map



X Index: 262



Y Index: 184

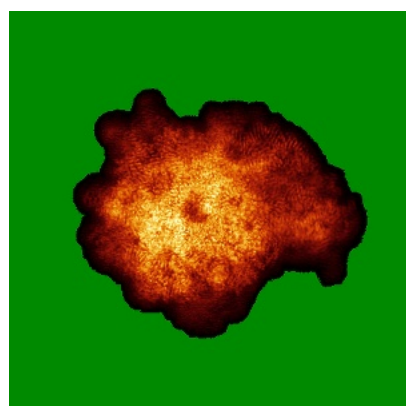


Z Index: 201

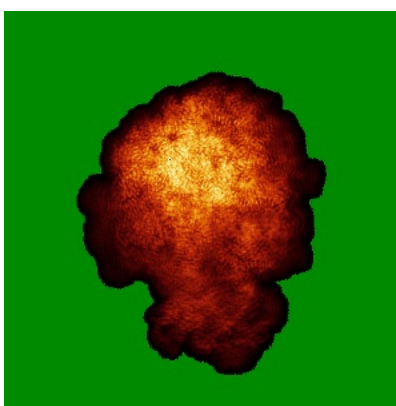
The images above show the largest variance slices of the map in three orthogonal directions.

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

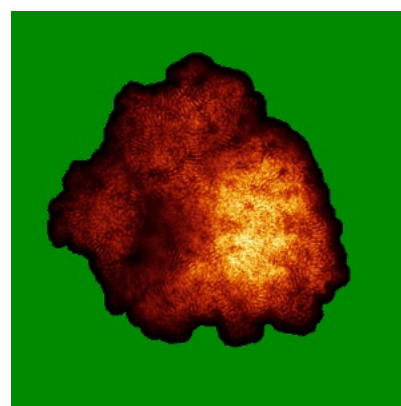
6.4.1 Primary map



X



Y

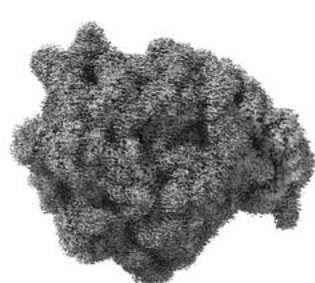


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

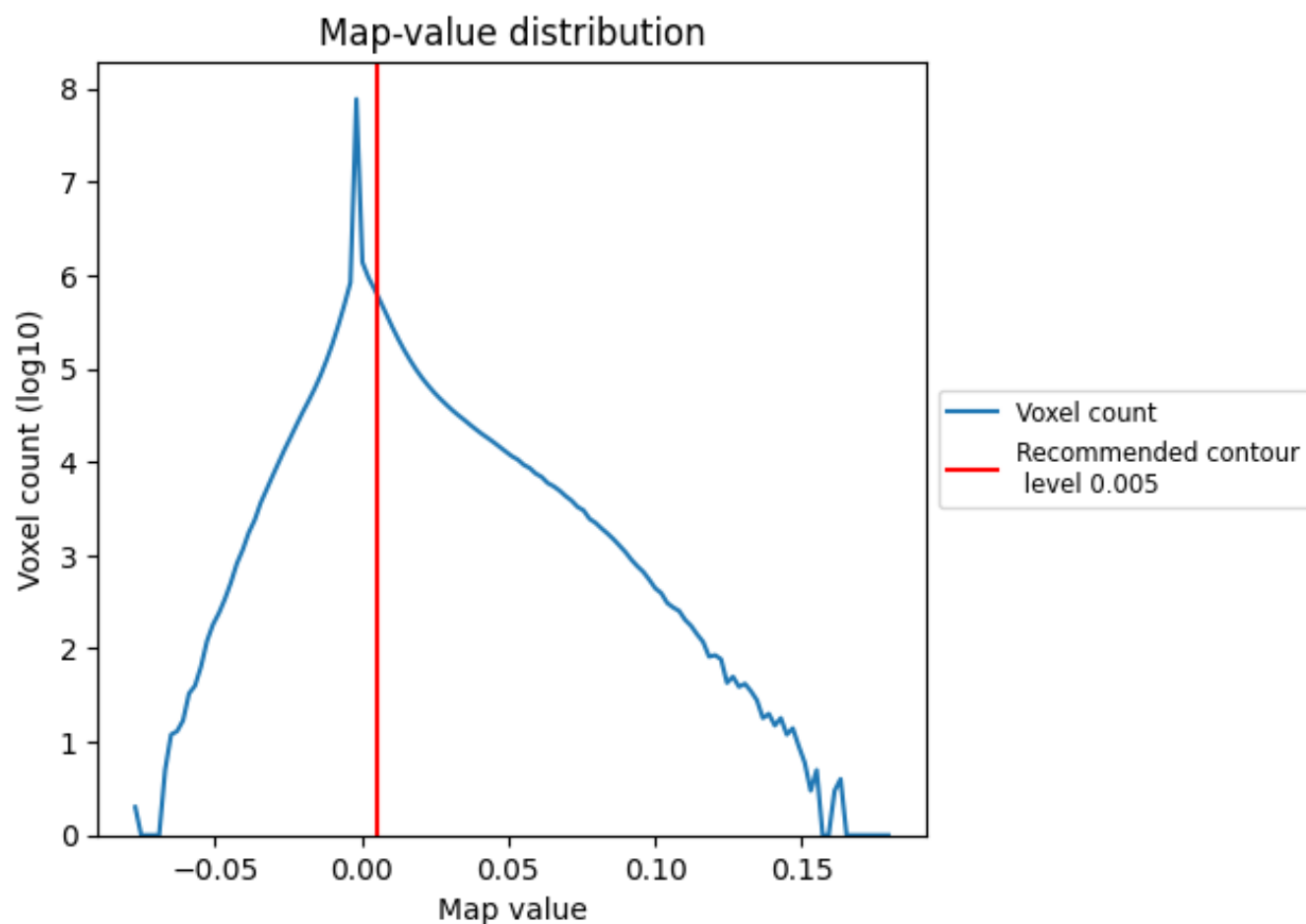
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

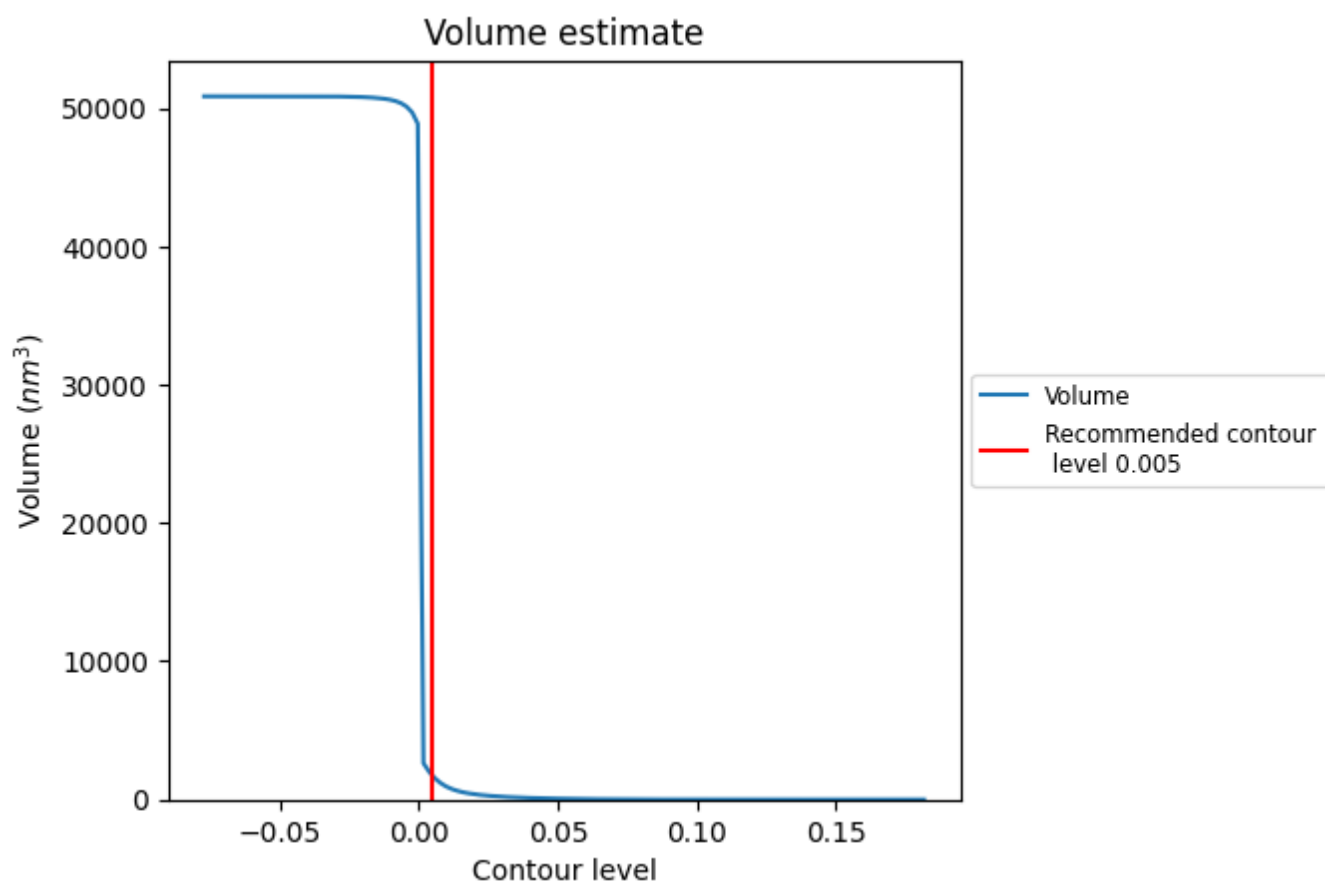
This section contains the results of statistical analysis of the map.

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.

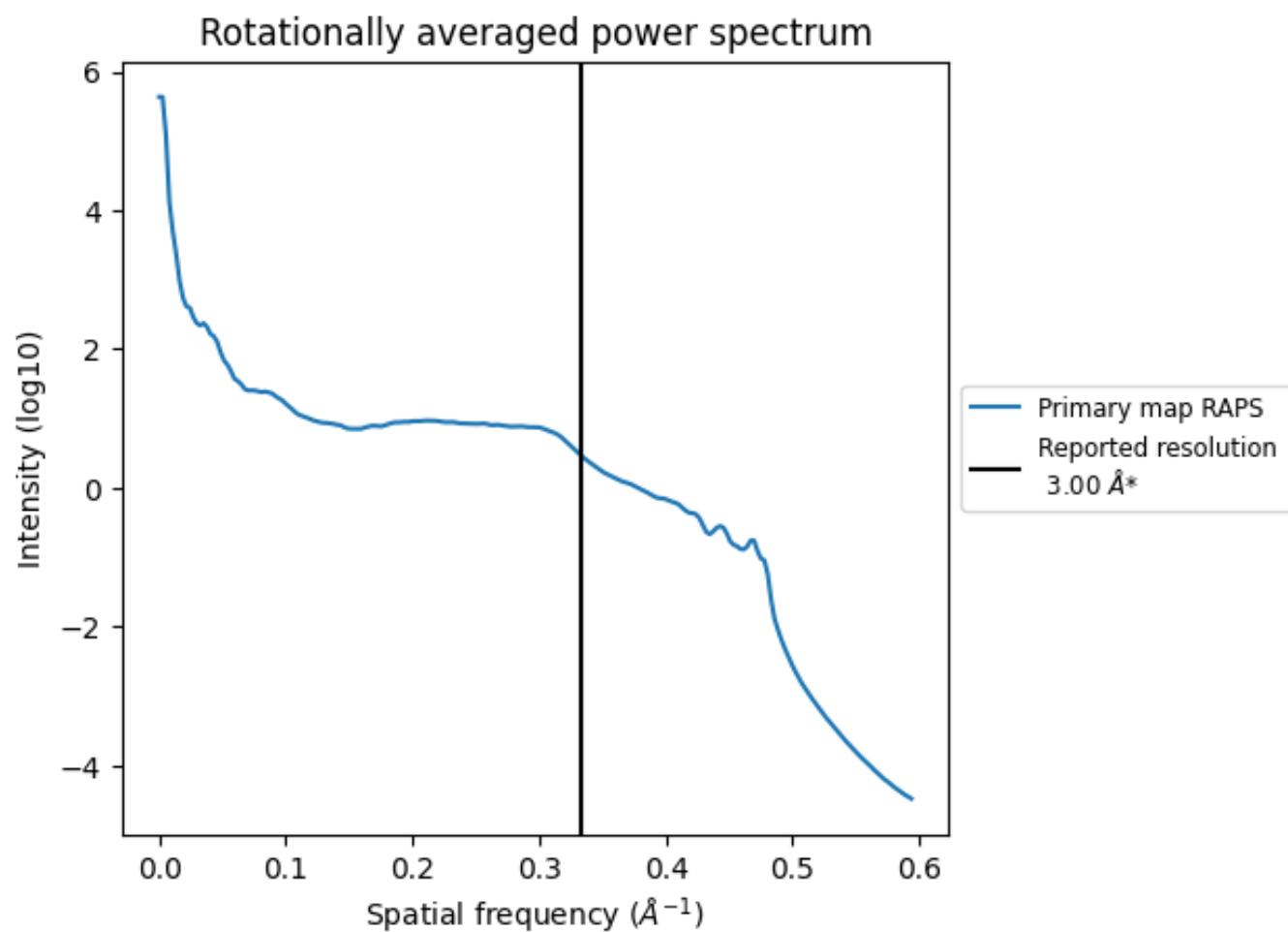
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1735 nm³; this corresponds to an approximate mass of 1567 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 0.333 Å⁻¹

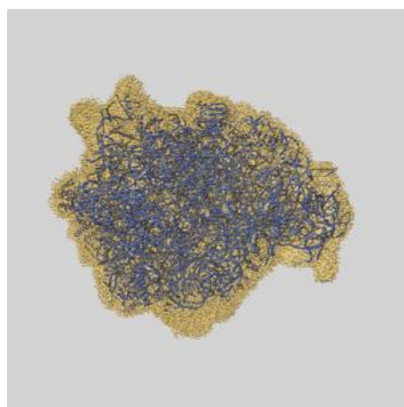
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

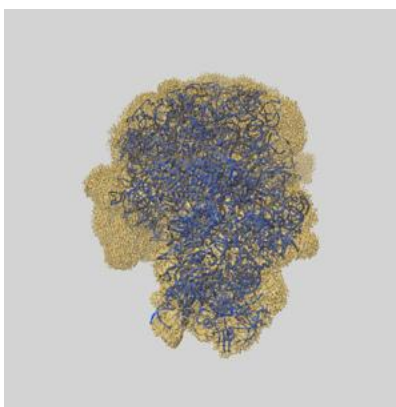
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52641 and PDB model 9I5X. Per-residue inclusion information can be found in section 3 on page 14.

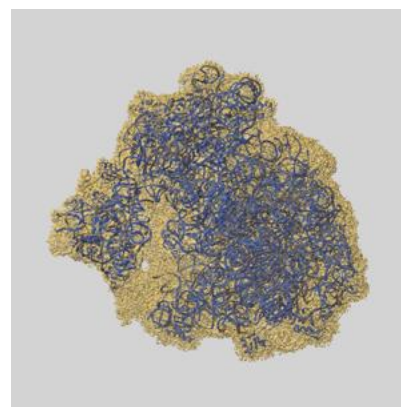
9.1 Map-model overlay [i](#)



X



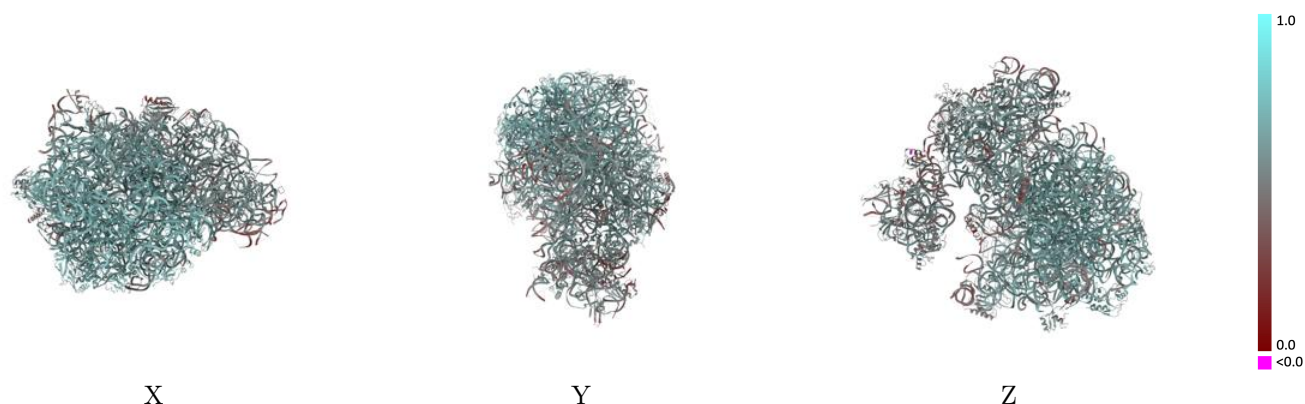
Y



Z

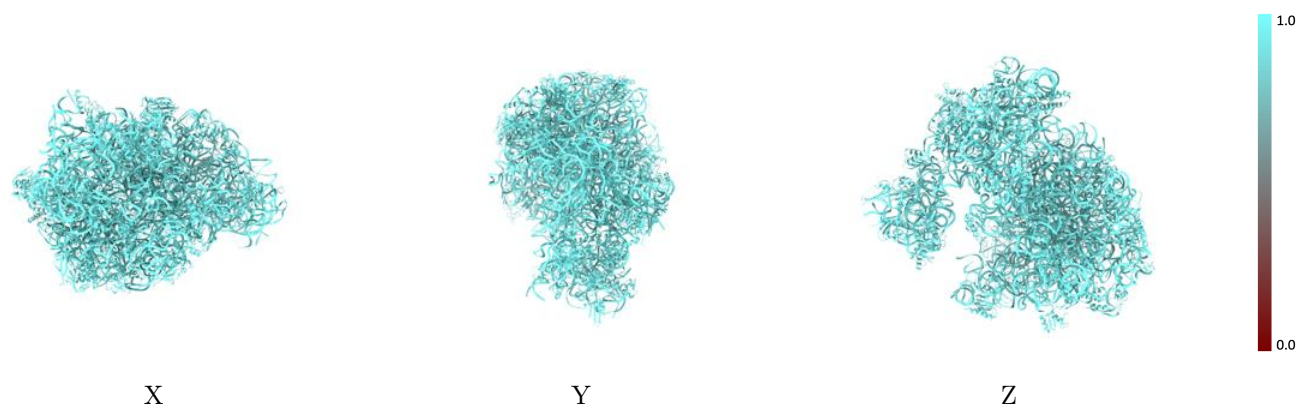
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



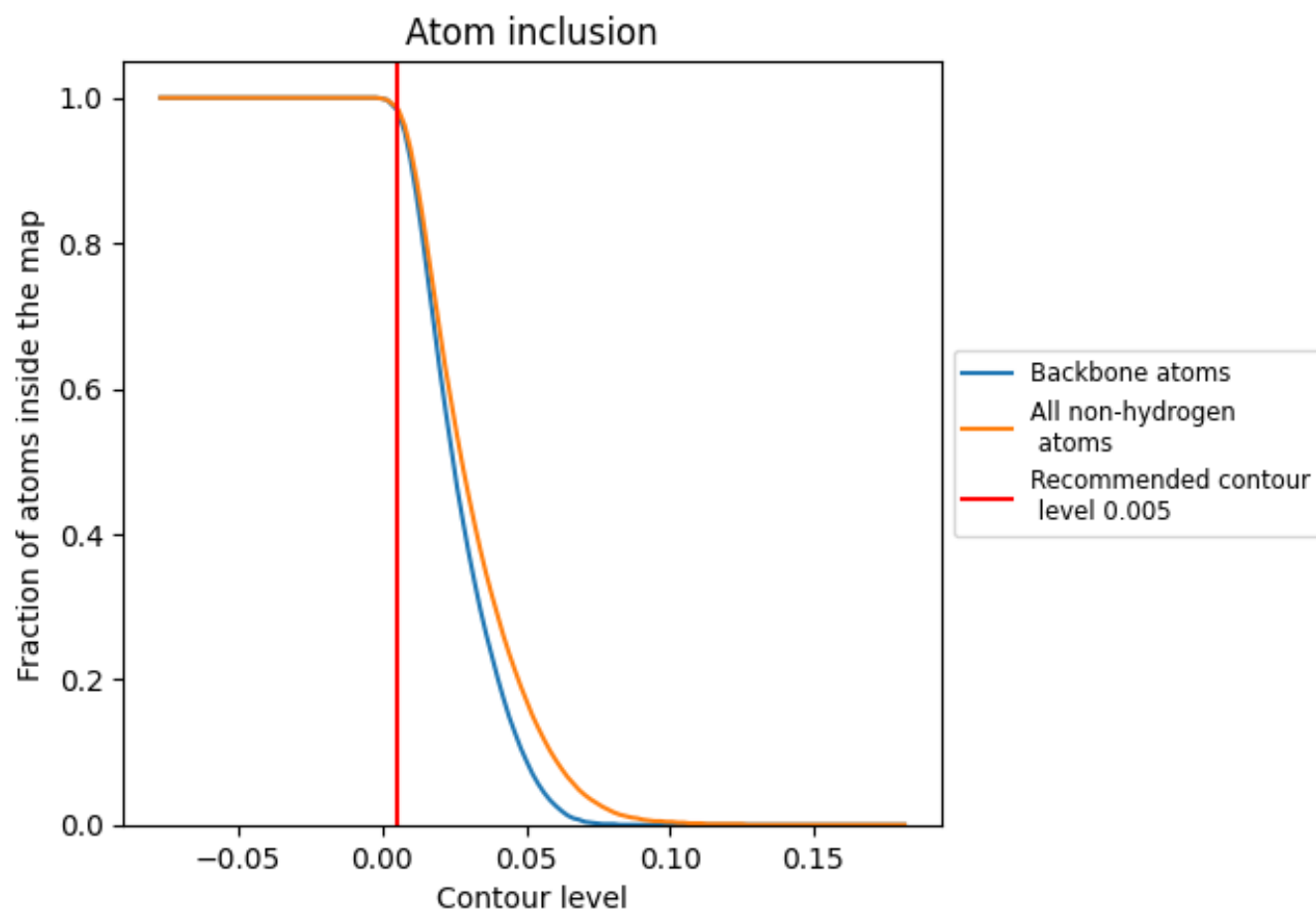
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 99% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9870	 0.5910
0	 0.9950	 0.6430
1	 0.9770	 0.5490
10	 0.9330	 0.5720
2	 0.9950	 0.6480
4	 0.9950	 0.6550
5	 0.9760	 0.5690
6	 0.9920	 0.6860
7	 0.9780	 0.6130
8	 0.9760	 0.5920
A	 0.9960	 0.6320
B	 0.9850	 0.4980
D	 0.9910	 0.6550
E	 0.9950	 0.6600
F	 0.9910	 0.6510
I	 0.9780	 0.5250
J	 0.9760	 0.5370
K	 0.9580	 0.5220
L	 0.9470	 0.4580
M	 0.9890	 0.6480
N	 0.9870	 0.6350
O	 0.9900	 0.6110
P	 0.9810	 0.6040
Q	 0.9960	 0.6640
R	 0.9750	 0.5130
S	 0.9900	 0.6260
T	 0.9970	 0.6810
U	 0.9890	 0.6440
V	 0.9950	 0.6680
W	 0.9840	 0.5970
X	 0.9900	 0.6140
Y	 0.9910	 0.5550
Z	 0.9960	 0.6660
a	 0.9820	 0.5240
b	 0.9570	 0.4690



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Chain	Atom inclusion	Q-score
c	 0.9740	 0.5530
d	 0.9720	 0.5450
e	 0.9840	 0.5630
f	 0.9660	 0.5330
g	 0.9690	 0.5530
h	 0.9490	 0.5170
i	 0.9770	 0.5210
j	 0.9530	 0.5570
k	 0.9430	 0.4990
l	 0.9680	 0.5060
m	 0.9530	 0.4960
n	 0.9650	 0.5290
o	 0.9840	 0.5680
p	 0.9860	 0.5570