



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:58 PM UTC

PDB ID : 8UU5 / pdb_00008uu5
EMDB ID : EMD-42557
Title : Cryo-EM structure of the *Listeria innocua* 70S ribosome (head-swiveled) in complex with pe/E-tRNA (structure I-B)
Authors : Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on : 2023-10-31
Resolution : 3.00 Å(reported)
Based on initial model : 7NHN

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

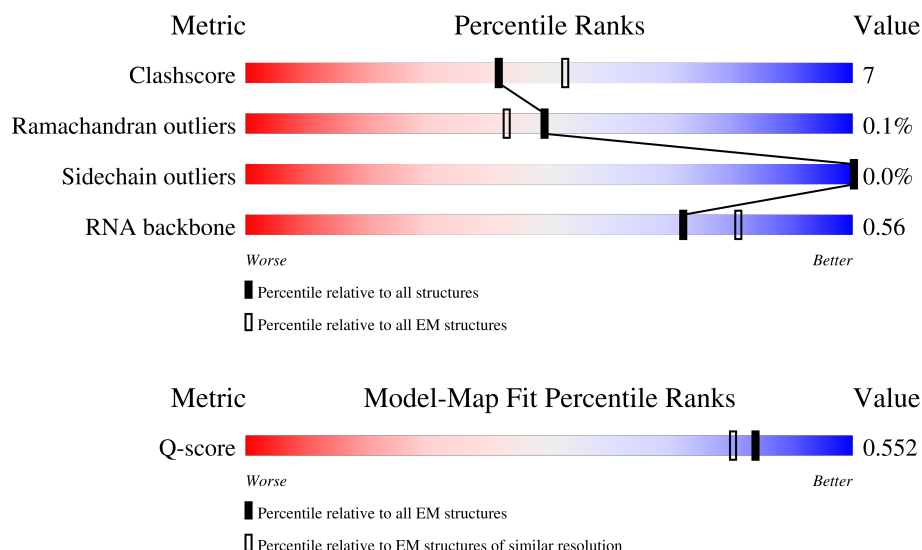
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	a	1550	
2	b	249	
3	c	218	

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Mol	Chain	Length	Quality of chain
4	d	200	
5	e	167	
6	f	97	
7	g	156	
8	h	132	
9	i	130	
10	j	102	
11	k	129	
12	l	137	
13	m	121	
14	n	61	
15	o	89	
16	p	90	
17	q	87	
18	r	79	
19	s	92	
20	t	84	
21	x	76	
22	w	21	
23	A	2932	
24	B	116	
25	C	277	
26	D	209	
27	E	207	
28	F	179	

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Mol	Chain	Length	Quality of chain
29	G	178	
30	L	145	
31	M	122	
32	N	146	
33	O	144	
34	P	135	
35	Q	119	
36	R	114	
37	S	119	
38	T	102	
39	U	118	
40	V	94	
41	W	103	
42	Y	96	
43	Z	62	
44	1	63	
45	2	59	
46	3	81	
47	4	57	
48	5	49	
49	6	44	
50	7	66	
51	8	37	

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 140861 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1523	Total	C	N	O	P	0	0
			32665	14571	5988	10583	1523		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	221	Total	C	N	O	S	0	0
			1765	1128	308	322	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	204	Total	C	N	O	S	0	0
			1547	967	296	282	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	199	Total	C	N	O	S	0	0
			1562	978	289	293	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	156	Total	C	N	O	S	0	0
			1146	719	210	215	2		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	93	Total	C	N	O	S	0	0
			771	488	132	149	2		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	149	Total	C	N	O	S	0	0
			1143	709	216	209	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	130	Total	C	N	O	S	0	0
			1002	641	178	181	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			998	629	195	173	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	97	Total	C	N	O	S	0	0
			738	463	139	135	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	115	Total	C	N	O	S	0	0
			845	520	163	159	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	134	Total	C	N	O	S	0	0
			1003	623	199	179	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			900	554	177	168	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			490	313	97	75	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	86	Total	C	N	O	S	0	0
			716	445	142	127	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	87	Total	C	N	O	S	0	0
			691	439	130	119	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			612	391	112	108	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	64	Total	C	N	O	S	0	0
			509	328	92	87	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	81	Total	C	N	O	S	0	0
			632	405	115	110	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	81	Total	C	N	O	S	0	0
			610	369	123	117	1		

- Molecule 21 is a RNA chain called pe/E Hybrid State Phenylalanine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	x	74	Total	C	N	O	P	S	0	0
			1591	713	285	517	74	2		

- Molecule 22 is a RNA chain called F-Stop mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	w	14	Total	C	N	O	P		0	0
			304	136	59	95	14			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
23	A	2902	Total	C	N	O	P		0	0
			62340	27821	11532	20085	2902			

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	B	114	Total	C	N	O	P		0	0
			2428	1082	428	804	114			

- Molecule 25 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	C	273	Total	C	N	O	S		0	0
			2108	1307	415	379	7			

- Molecule 26 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	D	206	Total	C	N	O	S		0	0
			1583	995	291	293	4			

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	E	204	Total	C	N	O			0	0
			1537	974	285	278				

- Molecule 28 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	F	174	Total	C	N	O	S	0	0
			1189	745	210	229	5		

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	G	172	Total	C	N	O	S	0	0
			1283	802	239	241	1		

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L	143	Total	C	N	O	S	0	0
			1124	713	205	203	3		

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	122	Total	C	N	O	S	0	0
			915	569	174	167	5		

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	N	145	Total	C	N	O	0	0
			1040	644	209	187		

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	O	134	Total	C	N	O	S	0	0
			1045	669	201	169	6		

- Molecule 34 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	P	123	Total	C	N	O	S	0	0
			967	607	188	171	1		

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Q	118	Total	C	N	O	0	0
			846	522	169	155		

- Molecule 36 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	R	113	Total	C	N	O	S	0
			893	564	177	151	1	0

- Molecule 37 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	S	118	Total	C	N	O	S	0
			953	605	188	156	4	0

- Molecule 38 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	T	101	Total	C	N	O	S	0
			774	502	134	137	1	0

- Molecule 39 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	U	112	Total	C	N	O	0	0
			858	541	159	158		

- Molecule 40 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	V	92	Total	C	N	O	S	0
			720	461	123	134	2	0

- Molecule 41 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	W	101	Total	C	N	O	S	0
			755	479	140	133	3	0

- Molecule 42 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y	76	Total	C	N	O	S	0	0
			572	350	110	111	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Z	60	Total	C	N	O	S	0	0
			451	277	95	77	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	61	Total	C	N	O	S	0	0
			504	310	97	96	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	56	Total	C	N	O	S	0	0
			421	265	81	74	1		

- Molecule 46 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	72	Total	C	N	O	S	0	0
			555	352	95	107	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	53	Total	C	N	O	S	0	0
			410	251	85	69	5		

- Molecule 48 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	47	Total	C	N	O	S	0	0
			377	231	73	70	3		

- Molecule 49 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	6	44	Total	C	N	O	S	0	0
			370	225	89	54	2		

- Molecule 50 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	7	64	Total	C	N	O	S	0	0
			520	322	114	79	5		

- Molecule 51 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	8	36	Total	C	N	O	S	0	0
			266	166	52	42	6		

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	a	219	Total	Mg	0
			219	219	
52	c	2	Total	Mg	0
			2	2	
52	g	2	Total	Mg	0
			2	2	
52	i	7	Total	Mg	0
			7	7	
52	j	1	Total	Mg	0
			1	1	
52	m	1	Total	Mg	0
			1	1	
52	s	1	Total	Mg	0
			1	1	
52	t	1	Total	Mg	0
			1	1	
52	w	1	Total	Mg	0
			1	1	
52	A	248	Total	Mg	0
			248	248	
52	B	3	Total	Mg	0
			3	3	
52	C	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
52	N	1	Total 1	Mg 1	0
52	S	1	Total 1	Mg 1	0
52	6	1	Total 1	Mg 1	0

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	n	1	Total 1	Zn 1	0
53	4	1	Total 1	Zn 1	0
53	5	1	Total 1	Zn 1	0
53	8	1	Total 1	Zn 1	0

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	a	122	Total 122	O 122	0
54	c	1	Total 1	O 1	0
54	d	1	Total 1	O 1	0
54	g	2	Total 2	O 2	0
54	i	2	Total 2	O 2	0
54	m	3	Total 3	O 3	0
54	n	2	Total 2	O 2	0
54	t	1	Total 1	O 1	0
54	A	175	Total 175	O 175	0
54	B	1	Total 1	O 1	0

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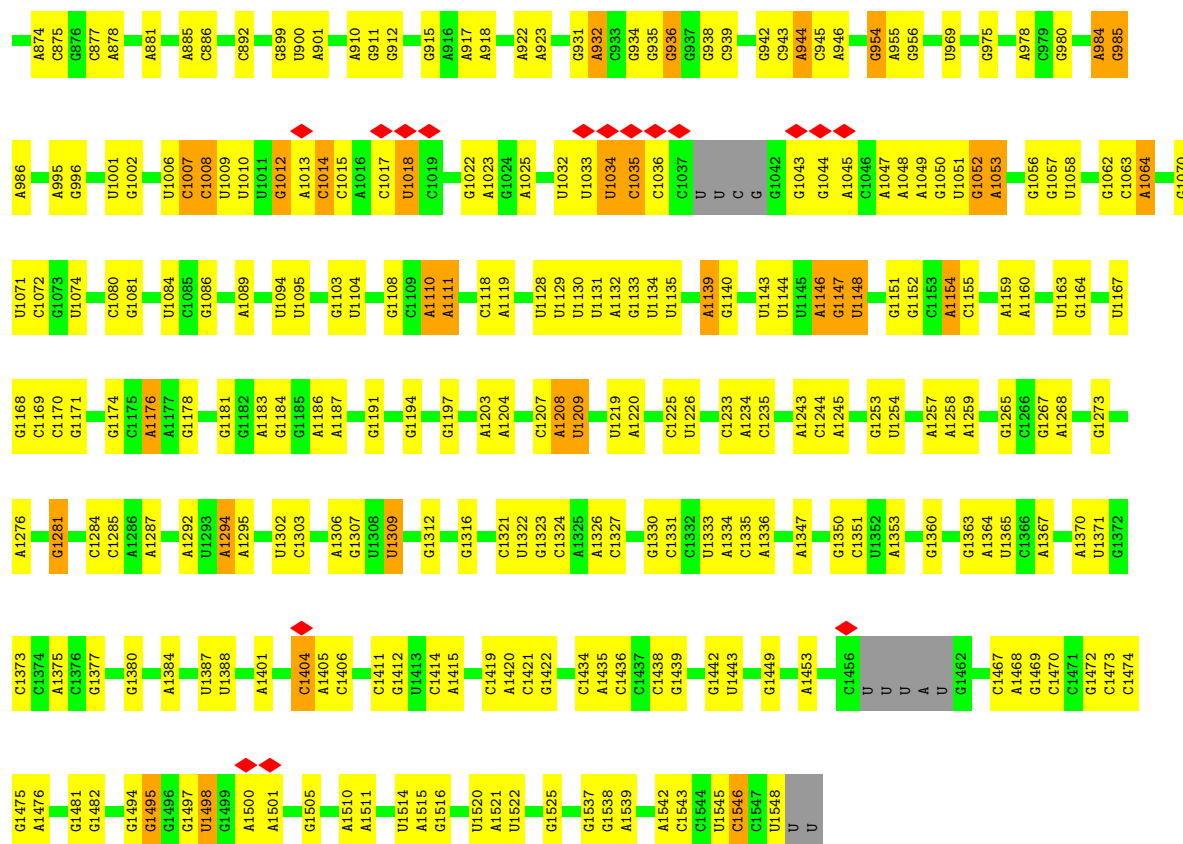
Mol	Chain	Residues	Atoms		AltConf
54	C	4	Total 4	O 4	0
54	D	1	Total 1	O 1	0
54	N	2	Total 2	O 2	0
54	O	1	Total 1	O 1	0
54	P	1	Total 1	O 1	0
54	S	1	Total 1	O 1	0
54	T	1	Total 1	O 1	0
54	U	2	Total 2	O 2	0

3 Residue-property plots

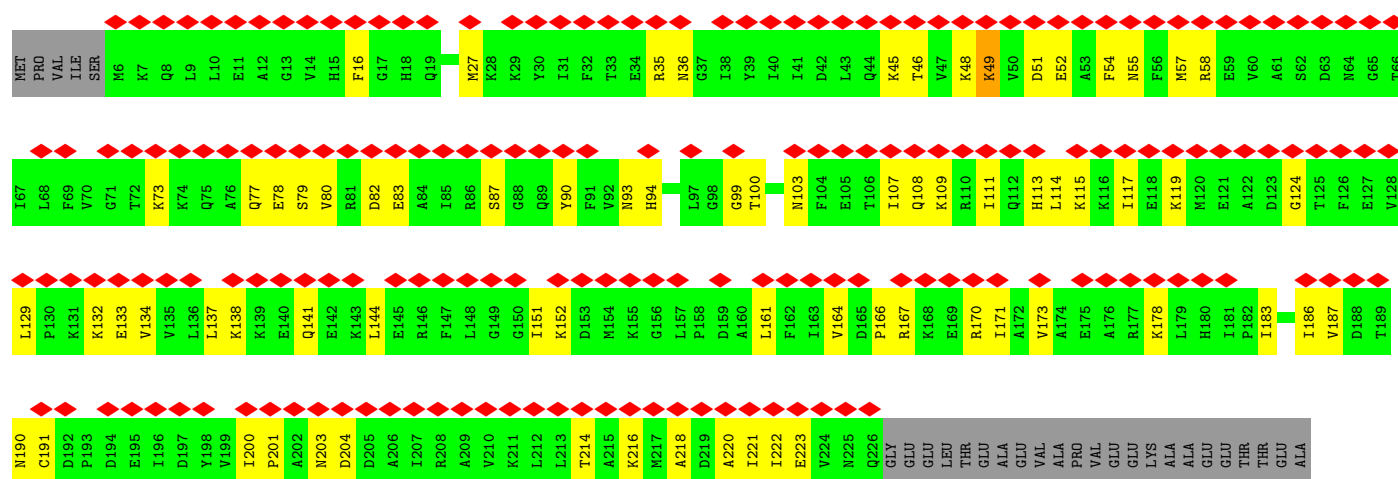
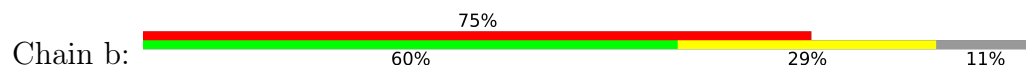
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S Ribosomal RNA



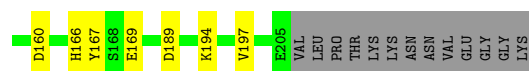


• Molecule 2: Small ribosomal subunit protein uS2

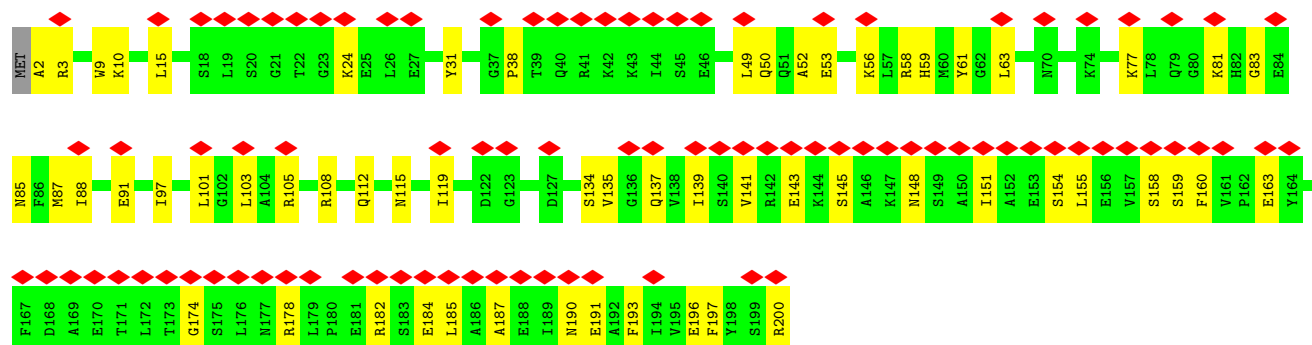


• Molecule 3: Small ribosomal subunit protein uS3

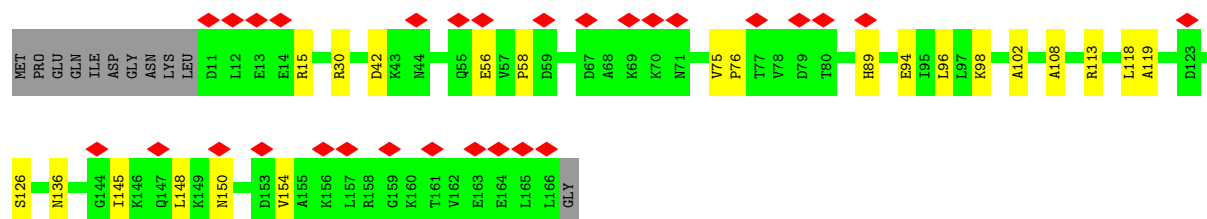
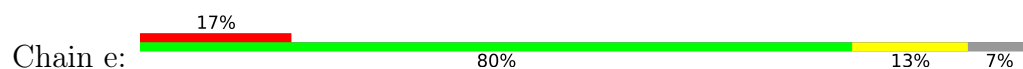




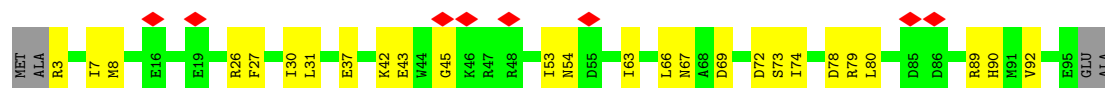
- Molecule 4: Small ribosomal subunit protein uS4



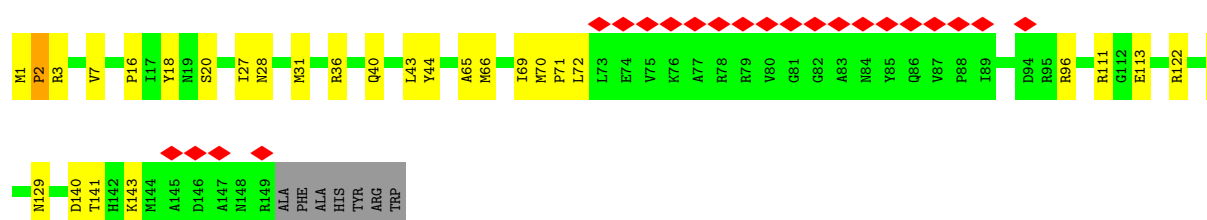
- Molecule 5: Small ribosomal subunit protein uS5



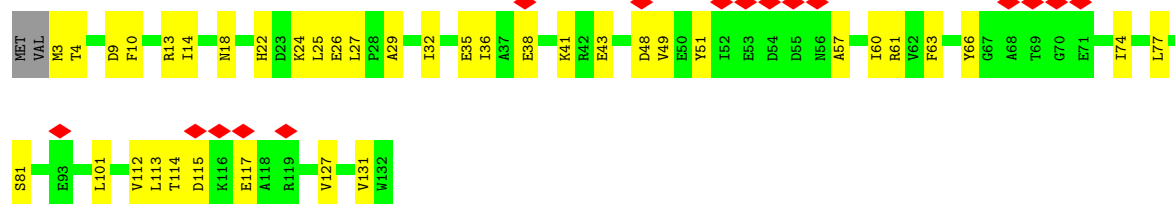
- Molecule 6: Small ribosomal subunit protein bS6



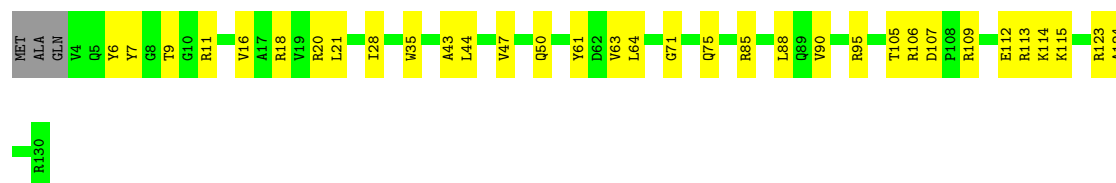
- Molecule 7: Small ribosomal subunit protein uS7



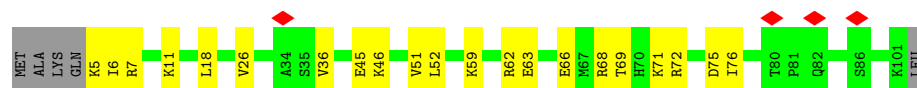
- Molecule 8: Small ribosomal subunit protein uS8



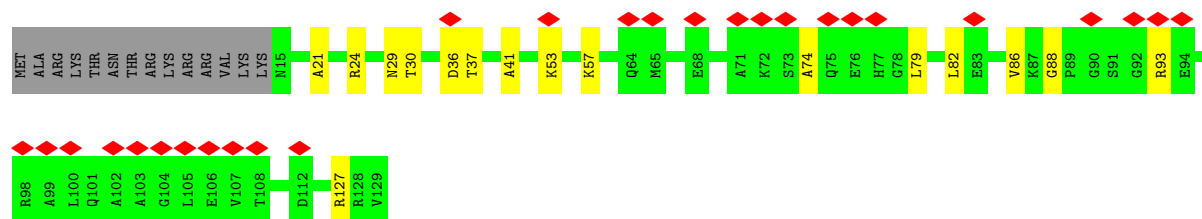
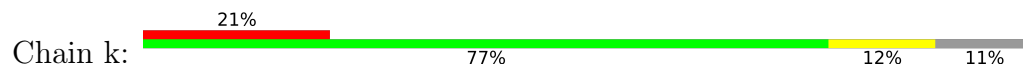
- Molecule 9: Small ribosomal subunit protein uS9



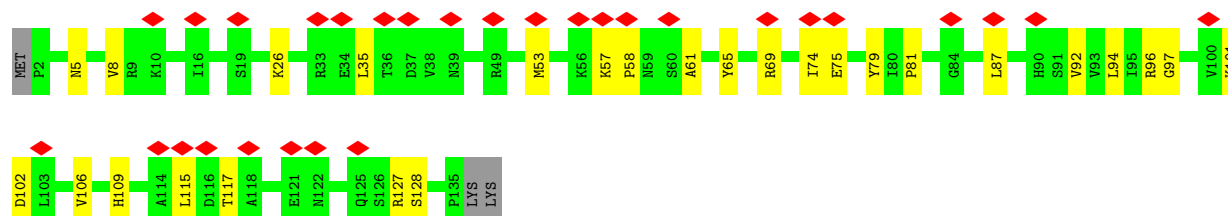
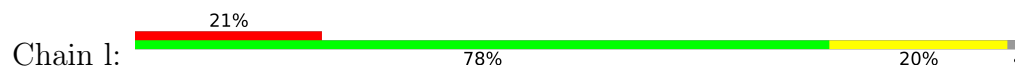
- Molecule 10: Small ribosomal subunit protein uS10



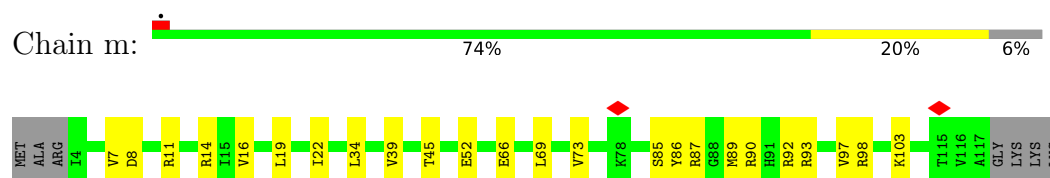
- Molecule 11: Small ribosomal subunit protein uS11



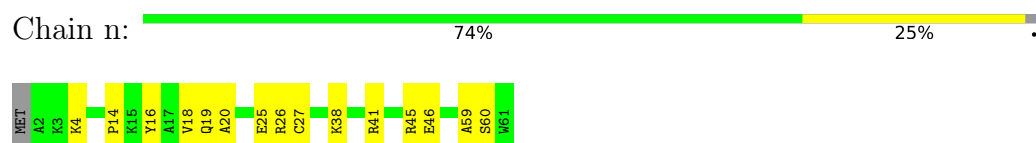
- Molecule 12: Small ribosomal subunit protein uS12



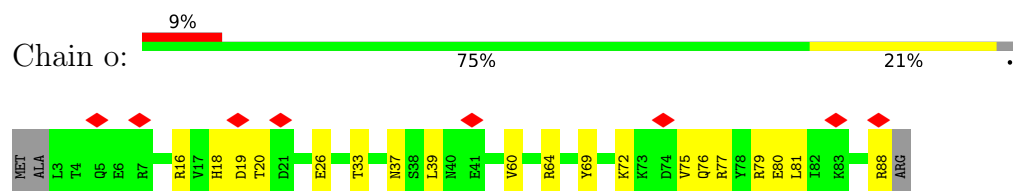
- Molecule 13: Small ribosomal subunit protein uS13



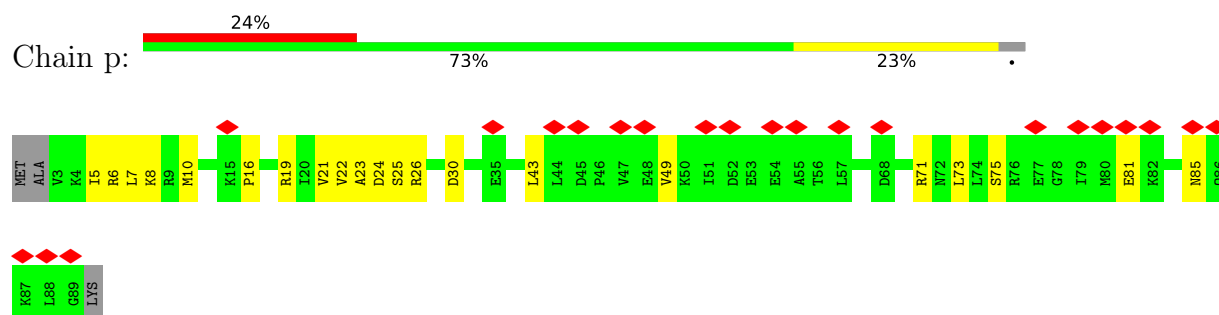
- Molecule 14: Small ribosomal subunit protein uS14



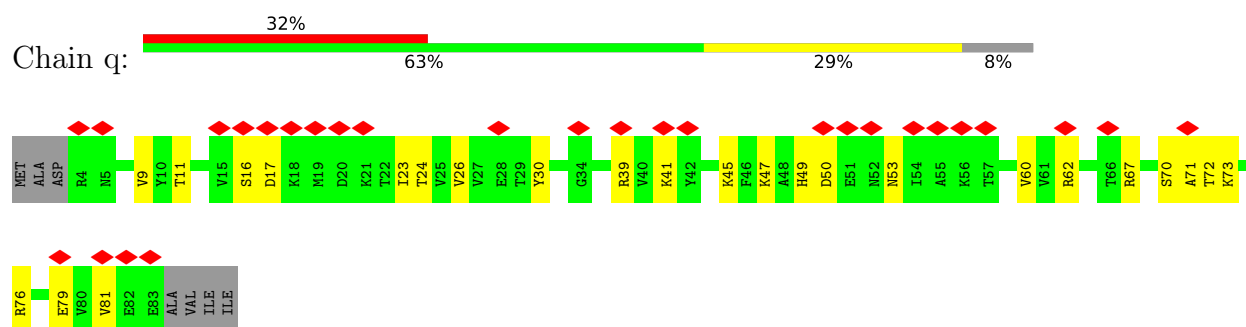
- Molecule 15: Small ribosomal subunit protein uS15



- Molecule 16: Small ribosomal subunit protein bS16

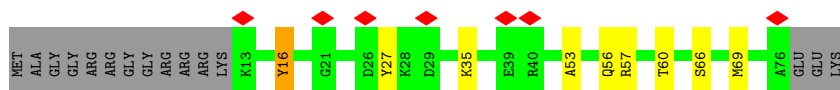


- Molecule 17: Small ribosomal subunit protein uS17

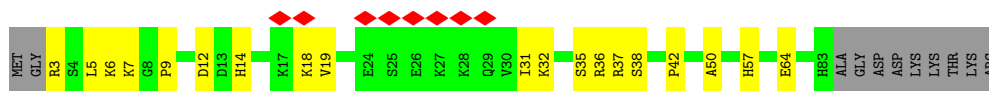


- Molecule 18: Small ribosomal subunit protein bS18

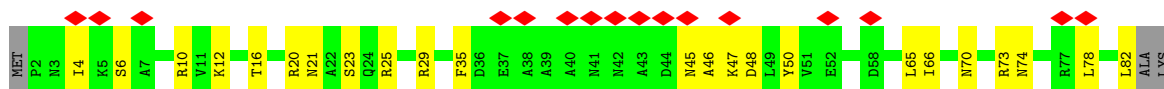




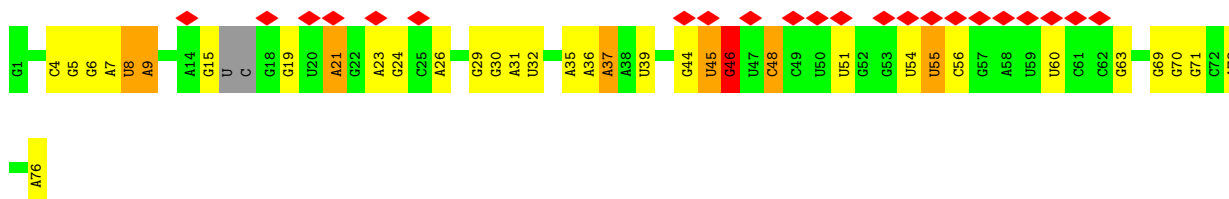
- Molecule 19: Small ribosomal subunit protein uS19



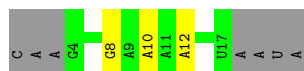
- Molecule 20: Small ribosomal subunit protein bS20



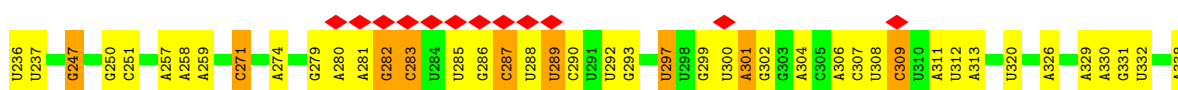
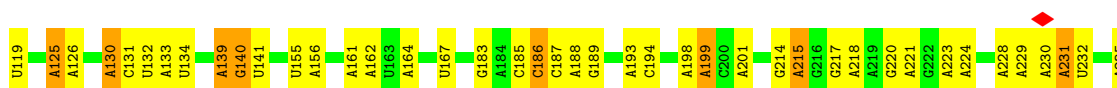
- Molecule 21: pe/E Hybrid State Phenylalanine tRNA



- Molecule 22: F-Stop mRNA



- Molecule 23: 23S Ribosomal RNA



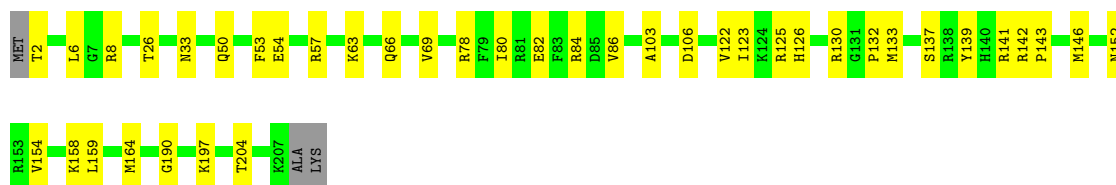


Chain C:  86% 13% .



- Molecule 26: Large ribosomal subunit protein uL3

Chain D:  79% 19% .



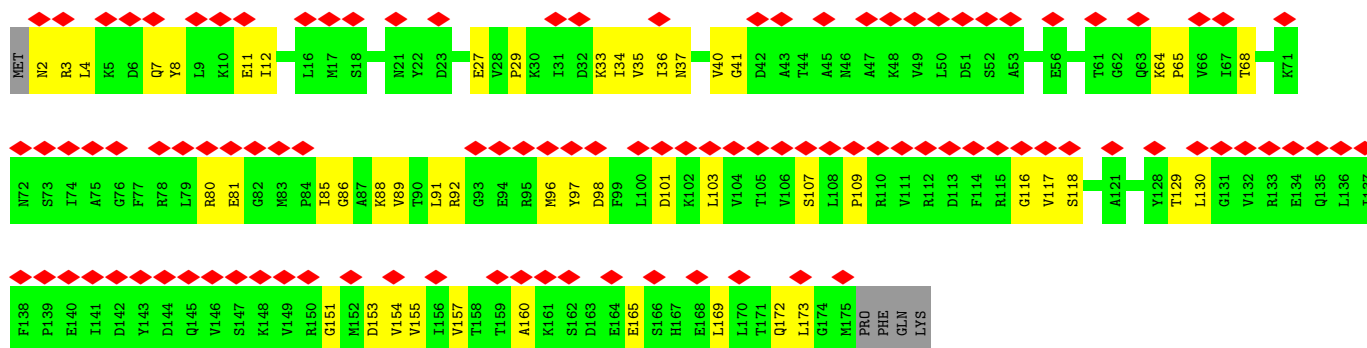
- Molecule 27: Large ribosomal subunit protein uL4

Chain E:  89% 10% .



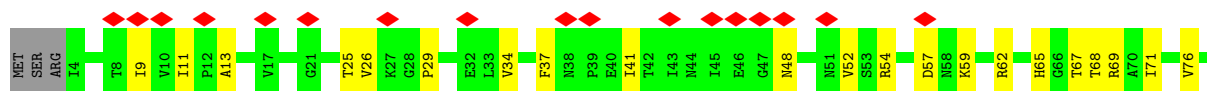
- Molecule 28: Large ribosomal subunit protein uL5

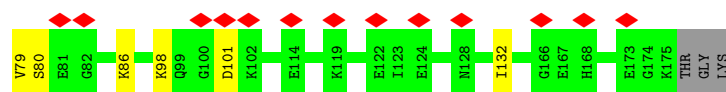
Chain F:  59% 70% 27% .



- Molecule 29: Large ribosomal subunit protein uL6

Chain G:  17% 81% 15% .





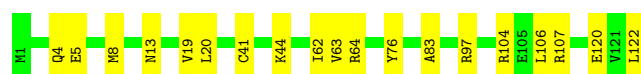
- Molecule 30: Large ribosomal subunit protein uL13

Chain L: 88% 11% .



- Molecule 31: Large ribosomal subunit protein uL14

Chain M: 84% 16%



- Molecule 32: Large ribosomal subunit protein uL15

Chain N: 92% 8% .



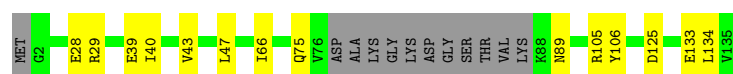
- Molecule 33: Large ribosomal subunit protein uL16

Chain O: 82% 11% 7%



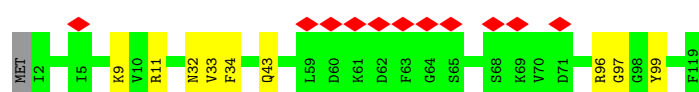
- Molecule 34: Large ribosomal subunit protein bL17

Chain P: 81% 10% 9%



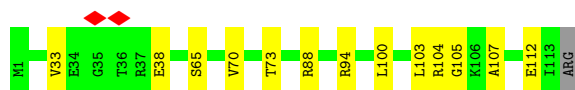
- Molecule 35: Large ribosomal subunit protein uL18

Chain Q: 9% 92% 8% .

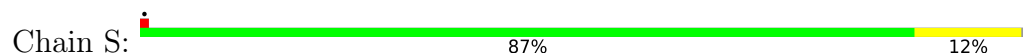


- Molecule 36: Large ribosomal subunit protein bL19

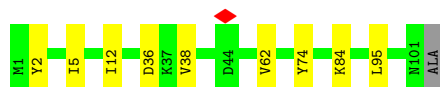
Chain R: 88% 11% .



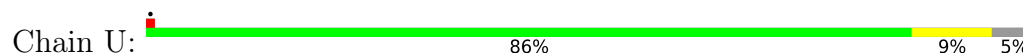
- Molecule 37: Large ribosomal subunit protein bL20



- Molecule 38: Large ribosomal subunit protein bL21



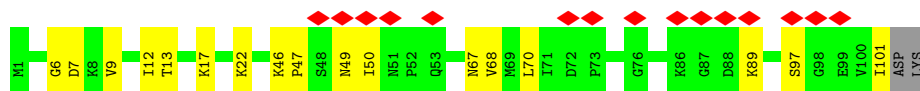
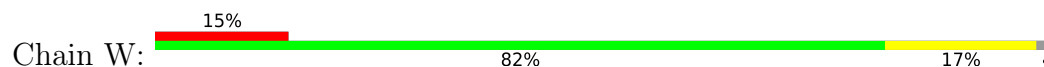
- Molecule 39: Large ribosomal subunit protein uL22



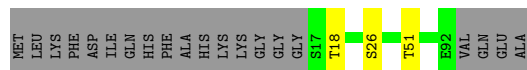
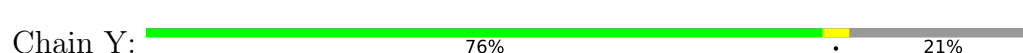
- Molecule 40: Large ribosomal subunit protein uL23



- Molecule 41: Large ribosomal subunit protein uL24



- Molecule 42: Large ribosomal subunit protein bL27



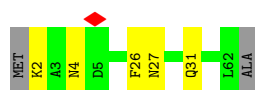
- Molecule 43: Large ribosomal subunit protein bL28

Chain Z:  71% 26% .



- Molecule 44: Large ribosomal subunit protein uL29

Chain 1:  89% 8% .



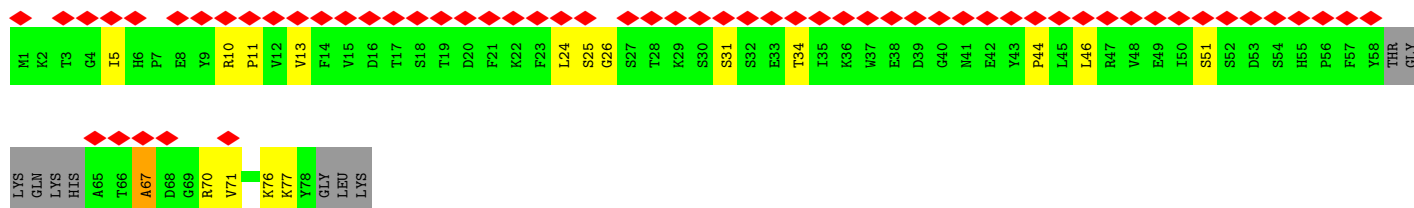
- Molecule 45: Large ribosomal subunit protein uL30

Chain 2:  86% 8% 5%



- Molecule 46: Large ribosomal subunit protein bL31B

Chain 3:  74% 68% 20% 11%



- Molecule 47: Large ribosomal subunit protein bL32

Chain 4:  82% 11% 7%



- Molecule 48: Large ribosomal subunit protein bL33

Chain 5:  82% 14% .



- Molecule 49: Large ribosomal subunit protein bL34

Chain 6:  91% 9%



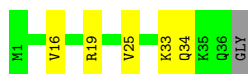
- Molecule 50: Large ribosomal subunit protein bL35

Chain 7: 82% 15% .



- Molecule 51: Large ribosomal subunit protein bL36

Chain 8: 84% 14% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196886	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	47.649	Depositor
Minimum map value	-27.659	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.089	Depositor
Recommended contour level	3.28	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 4SU, 5MU, MIA, MG, PSU, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.11	0/36571	0.27	0/57040
2	b	0.22	0/1794	0.52	1/2414 (0.0%)
3	c	0.11	0/1572	0.32	0/2129
4	d	0.10	0/1590	0.30	0/2142
5	e	0.10	0/1159	0.28	0/1565
6	f	0.14	0/783	0.38	0/1051
7	g	0.12	0/1156	0.31	0/1552
8	h	0.11	0/1015	0.31	0/1365
9	i	0.14	0/1017	0.39	0/1369
10	j	0.12	0/747	0.34	0/1006
11	k	0.10	0/859	0.30	0/1159
12	l	0.12	0/1019	0.32	0/1376
13	m	0.17	0/906	0.43	0/1213
14	n	0.15	0/500	0.42	0/664
15	o	0.15	0/726	0.38	0/973
16	p	0.10	0/704	0.33	0/945
17	q	0.08	0/621	0.26	0/836
18	r	0.13	0/516	0.39	0/692
19	s	0.13	0/648	0.48	1/876 (0.1%)
20	t	0.15	0/612	0.36	0/816
21	x	0.20	0/1605	0.27	0/2497
22	w	0.08	0/341	0.23	0/530
23	A	0.11	0/69843	0.29	0/108955
24	B	0.08	0/2711	0.20	0/4224
25	C	0.15	0/2144	0.36	0/2875
26	D	0.11	0/1605	0.29	0/2156
27	E	0.10	0/1557	0.33	0/2103
28	F	0.18	0/1202	0.39	0/1634
29	G	0.11	0/1304	0.30	0/1762
30	L	0.11	0/1147	0.26	0/1541
31	M	0.11	0/922	0.30	0/1235
32	N	0.08	0/1050	0.26	0/1401

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	O	0.09	0/1067	0.24	0/1429
34	P	0.10	0/978	0.31	0/1310
35	Q	0.09	0/854	0.25	0/1149
36	R	0.13	0/905	0.33	0/1215
37	S	0.10	0/966	0.30	0/1284
38	T	0.08	0/787	0.26	0/1057
39	U	0.09	0/868	0.28	0/1175
40	V	0.08	0/729	0.24	0/981
41	W	0.10	0/764	0.30	0/1021
42	Y	0.12	0/579	0.41	0/773
43	Z	0.11	0/456	0.42	0/607
44	1	0.09	0/505	0.27	0/673
45	2	0.10	0/424	0.30	0/571
46	3	0.10	0/566	0.31	0/763
47	4	0.09	0/418	0.34	0/559
48	5	0.09	0/381	0.26	0/514
49	6	0.08	0/373	0.27	0/486
50	7	0.09	0/527	0.29	0/685
51	8	0.09	0/269	0.24	0/359
All	All	0.12	0/152362	0.29	2/228707 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	g	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	s	19	VAL	N-CA-C	-7.94	106.17	113.71
2	b	49	LYS	CB-CG-CD	6.69	126.68	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	g	1	MET	Peptide

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Mol	Chain	Res	Type	Group
7	g	2	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32665	0	16443	370	0
2	b	1765	0	1807	54	0
3	c	1547	0	1501	25	0
4	d	1562	0	1543	47	0
5	e	1146	0	1202	16	0
6	f	771	0	753	18	0
7	g	1143	0	1164	22	0
8	h	1002	0	1057	26	0
9	i	998	0	1034	27	0
10	j	738	0	725	14	0
11	k	845	0	859	11	0
12	l	1003	0	1028	19	0
13	m	900	0	949	18	0
14	n	490	0	525	16	0
15	o	716	0	736	15	0
16	p	691	0	714	20	0
17	q	612	0	621	16	0
18	r	509	0	544	7	0
19	s	632	0	619	16	0
20	t	610	0	638	16	0
21	x	1591	0	818	17	0
22	w	304	0	152	1	0
23	A	62340	0	31344	613	0
24	B	2428	0	1229	21	0
25	C	2108	0	2183	24	0
26	D	1583	0	1646	24	0
27	E	1537	0	1612	16	0
28	F	1189	0	1067	34	0
29	G	1283	0	1259	16	0
30	L	1124	0	1154	11	0
31	M	915	0	972	12	0
32	N	1040	0	1053	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	O	1045	0	1100	9	0
34	P	967	0	1007	8	0
35	Q	846	0	822	6	0
36	R	893	0	951	9	0
37	S	953	0	1029	12	0
38	T	774	0	812	7	0
39	U	858	0	909	10	0
40	V	720	0	731	3	0
41	W	755	0	817	10	0
42	Y	572	0	562	4	0
43	Z	451	0	467	13	0
44	1	504	0	528	3	0
45	2	421	0	460	4	0
46	3	555	0	519	14	0
47	4	410	0	400	6	0
48	5	377	0	369	5	0
49	6	370	0	422	3	0
50	7	520	0	571	9	0
51	8	266	0	275	4	0
52	6	1	0	0	0	0
52	A	248	0	0	0	0
52	B	3	0	0	0	0
52	C	1	0	0	0	0
52	N	1	0	0	0	0
52	S	1	0	0	0	0
52	a	219	0	0	0	0
52	c	2	0	0	0	0
52	g	2	0	0	0	0
52	i	7	0	0	0	0
52	j	1	0	0	0	0
52	m	1	0	0	0	0
52	s	1	0	0	0	0
52	t	1	0	0	0	0
52	w	1	0	0	0	0
53	4	1	0	0	0	0
53	5	1	0	0	0	0
53	8	1	0	0	0	0
53	n	1	0	0	0	0
54	A	175	0	0	0	0
54	B	1	0	0	0	0
54	C	4	0	0	0	0
54	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	N	2	0	0	0	0
54	O	1	0	0	0	0
54	P	1	0	0	0	0
54	S	1	0	0	0	0
54	T	1	0	0	0	0
54	U	2	0	0	0	0
54	a	122	0	0	0	0
54	c	1	0	0	0	0
54	d	1	0	0	0	0
54	g	2	0	0	0	0
54	i	2	0	0	0	0
54	m	3	0	0	0	0
54	n	2	0	0	0	0
54	t	1	0	0	1	0
All	All	140861	0	91702	1538	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 7.

All (1538) 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)
6:f:8:MET:HG3	6:f:63:ILE:HG12	1.40	1.03
23:A:304:A:H62	23:A:410:G:N2	1.57	1.01
23:A:1763:U:H3	23:A:1778:A:N6	1.57	1.01
23:A:304:A:N6	23:A:410:G:H21	1.59	1.00
23:A:1580:A:H62	23:A:1594:G:N2	1.58	1.00
23:A:304:A:H62	23:A:410:G:H21	1.08	0.99
1:a:72:G:H1	1:a:95:A:N6	1.62	0.98
1:a:72:G:H1	1:a:95:A:H61	1.04	0.96
23:A:1580:A:N6	23:A:1594:G:H21	1.63	0.95
23:A:1580:A:H62	23:A:1594:G:H21	1.06	0.95
23:A:2173:G:H1	23:A:2184:U:H3	1.03	0.91
21:x:15:G:H22	21:x:48:C:H42	1.20	0.89
23:A:332:U:H3	23:A:393:G:H1	1.10	0.89
23:A:1087:U:H3	23:A:1160:G:H1	1.24	0.86
1:a:849:U:H3	1:a:854:G:H1	1.19	0.86
21:x:51:U:H3	21:x:63:G:H1	0.84	0.84
1:a:467:U:H3	1:a:482:G:H1	0.85	0.83
23:A:925:A:N7	23:A:946:G:N2	2.27	0.82
7:g:122:ARG:NH2	7:g:125:MET:SD	2.54	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:112:GLU:HG2	9:i:113:ARG:H	1.46	0.80
24:B:57:G:O2'	35:Q:9:LYS:NZ	2.17	0.78
14:n:14:PRO:HB2	14:n:19:GLN:HB2	1.67	0.76
23:A:2424:G:O2'	23:A:2462:G:N2	2.18	0.76
23:A:2361:A:H2'	23:A:2362:A:C8	2.21	0.75
23:A:1248:A:H2'	23:A:1249:A:C8	2.22	0.75
19:s:5:LEU:HD23	19:s:6:LYS:H	1.52	0.74
21:x:15:G:N2	21:x:48:C:H42	1.85	0.74
4:d:50:GLN:HE22	4:d:200:ARG:HH21	1.35	0.74
21:x:15:G:H22	21:x:48:C:N4	1.86	0.74
1:a:109:G:H1	1:a:338:C:H41	1.34	0.73
23:A:1093:G:N2	23:A:1156:G:O2'	2.21	0.73
2:b:87:SER:HA	2:b:222:ILE:HD11	1.71	0.72
23:A:2338:A:H8	28:F:151:GLY:HA3	1.53	0.72
19:s:5:LEU:HD22	19:s:7:LYS:HG3	1.71	0.72
23:A:101:G:O6	41:W:89:LYS:NZ	2.23	0.72
4:d:101:LEU:HD11	4:d:174:GLY:HA3	1.69	0.72
47:4:24:LEU:HD12	47:4:25:PRO:HD2	1.72	0.72
1:a:1194:G:H21	14:n:60:SER:HB3	1.52	0.72
23:A:2167:A:N6	23:A:2190:G:N3	2.38	0.72
46:3:11:PRO:HA	46:3:26:GLY:HA2	1.70	0.72
1:a:682:G:H2'	1:a:683:A:H8	1.54	0.72
14:n:26:ARG:NH2	14:n:46:GLU:OE2	2.22	0.72
23:A:1199:C:OP1	37:S:92:ARG:NH2	2.22	0.72
12:l:87:LEU:HD21	12:l:117:THR:HG22	1.71	0.71
3:c:140:THR:HG21	3:c:148:ILE:HD13	1.71	0.71
1:a:1302:U:O2'	13:m:14:ARG:NH2	2.24	0.71
1:a:305:G:N2	1:a:308:A:OP2	2.24	0.71
1:a:681:G:H2'	1:a:682:G:C8	2.26	0.71
23:A:2915:G:H1'	47:4:28:ASN:HD21	1.55	0.71
2:b:167:ARG:NH2	2:b:190:ASN:O	2.24	0.70
10:j:11:LYS:HG2	10:j:71:LYS:HG2	1.73	0.70
1:a:550:U:OP1	4:d:10:LYS:NZ	2.24	0.70
7:g:3:ARG:HH22	7:g:7:VAL:HB	1.56	0.70
3:c:118:ASN:O	3:c:122:GLN:NE2	2.25	0.70
23:A:286:G:H21	23:A:287:C:N4	1.89	0.70
1:a:21:G:H2'	1:a:22:G:C8	2.27	0.70
23:A:2361:A:H2'	23:A:2362:A:H8	1.54	0.70
24:B:5:G:H21	35:Q:43:GLN:HE22	1.37	0.70
23:A:897:G:H21	45:2:46:MET:HE3	1.57	0.69
1:a:1404:C:OP2	5:e:30:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1130:A:HO2'	23:A:1151:U:HO2'	1.41	0.69
23:A:1891:G:O2'	23:A:1917:A:N6	2.26	0.69
9:i:106:ARG:NH1	9:i:107:ASP:O	2.26	0.69
33:O:58:MET:HE1	33:O:106:ILE:HD12	1.74	0.69
39:U:16:ARG:O	39:U:16:ARG:NH1	2.20	0.69
1:a:419:A:H61	1:a:438:A:H62	1.42	0.68
1:a:984:A:H4'	1:a:985:G:H5''	1.74	0.68
4:d:50:GLN:HB3	4:d:197:PHE:HB2	1.74	0.68
23:A:1824:A:C2	23:A:1862:A:H4'	2.29	0.68
1:a:722:G:H2'	1:a:723:A:C8	2.28	0.68
3:c:14:VAL:HG12	3:c:15:ILE:HG23	1.75	0.68
23:A:84:A:N6	23:A:101:G:O2'	2.26	0.68
28:F:8:TYR:HA	28:F:12:ILE:HD12	1.76	0.68
1:a:1131:U:O4	1:a:1132:A:N6	2.27	0.68
23:A:1763:U:H3	23:A:1778:A:H62	0.74	0.68
23:A:220:G:H22	23:A:237:U:H4'	1.59	0.67
1:a:1363:G:H2'	1:a:1364:A:C8	2.29	0.67
43:Z:59:VAL:HG12	43:Z:60:GLU:H	1.59	0.67
23:A:632:U:H2'	23:A:633:A:H8	1.60	0.67
1:a:224:U:O2'	1:a:476:C:N4	2.26	0.67
3:c:53:ARG:NH1	3:c:55:GLU:OE1	2.28	0.67
30:L:2:ARG:HG2	30:L:3:THR:HG23	1.77	0.67
35:Q:11:ARG:NH1	35:Q:97:GLY:O	2.28	0.66
8:h:24:LYS:HD2	8:h:61:ARG:HD2	1.78	0.66
1:a:1494:G:H2'	1:a:1495:G:C8	2.29	0.66
23:A:1151:U:H2'	23:A:1152:G:H8	1.60	0.66
23:A:1685:U:H2'	23:A:1686:C:C6	2.31	0.66
24:B:29:C:H1'	24:B:51:A:H61	1.60	0.66
8:h:35:GLU:HB3	8:h:112:VAL:HG21	1.76	0.66
23:A:251:C:O2	50:7:12:LYS:NZ	2.29	0.66
23:A:625:G:H2'	23:A:626:G:H8	1.61	0.66
23:A:2279:G:H2'	23:A:2280:A:H8	1.60	0.66
23:A:1763:U:HO2'	23:A:1764:A:H8	1.43	0.65
26:D:6:LEU:H	26:D:33:ASN:HD21	1.43	0.65
34:P:29:ARG:NH1	34:P:133:GLU:OE1	2.29	0.65
1:a:955:A:H2'	1:a:956:G:C8	2.31	0.65
23:A:1763:U:O4	23:A:1778:A:N7	2.29	0.65
23:A:1397:A:H2'	23:A:1398:A:H8	1.61	0.65
23:A:2133:U:H3	23:A:2222:G:N2	1.95	0.65
16:p:6:ARG:N	16:p:21:VAL:O	2.28	0.65
23:A:1248:A:H2'	23:A:1249:A:H8	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:18:ASN:ND2	8:h:74:ILE:O	2.29	0.65
23:A:2148:G:O2'	23:A:2199:G:N2	2.25	0.65
46:3:13:VAL:HG22	46:3:24:LEU:HA	1.78	0.65
20:t:45:ASN:O	20:t:47:LYS:N	2.31	0.65
20:t:70:ASN:OD1	20:t:73:ARG:NH2	2.30	0.65
23:A:665:G:H4'	23:A:666:A:H5'	1.77	0.65
23:A:2279:G:H2'	23:A:2280:A:C8	2.32	0.65
35:Q:96:ARG:NH1	35:Q:99:TYR:O	2.30	0.65
1:a:605:G:O2'	17:q:39:ARG:NH2	2.29	0.64
2:b:100:THR:HA	2:b:107:ILE:HG13	1.80	0.64
1:a:1481:G:H2'	1:a:1482:G:C8	2.32	0.64
23:A:878:G:H2'	23:A:879:C:H6	1.62	0.64
23:A:2927:A:N1	23:A:2928:A:N6	2.43	0.64
37:S:102:ASP:OD2	38:T:2:TYR:OH	2.15	0.64
1:a:546:U:H2'	1:a:547:A:H8	1.60	0.64
1:a:1333:U:H2'	1:a:1334:A:H8	1.63	0.64
28:F:2:ASN:N	28:F:98:ASP:OD1	2.31	0.64
1:a:721:G:H2'	1:a:722:G:C8	2.32	0.64
15:o:88:ARG:NH2	23:A:760:U:OP2	2.29	0.64
1:a:698:G:OP1	11:k:24:ARG:NH2	2.30	0.64
9:i:112:GLU:OE1	9:i:115:LYS:NZ	2.30	0.64
20:t:45:ASN:HB2	20:t:48:ASP:HB3	1.80	0.64
28:F:92:ARG:HA	28:F:96:MET:HE2	1.78	0.64
1:a:187:U:H3	1:a:202:G:H1	1.45	0.64
1:a:199:C:H2'	1:a:200:A:H8	1.63	0.64
23:A:1530:G:H3'	23:A:1531:U:H5''	1.80	0.64
23:A:1172:A:H4'	23:A:1173:A:H5''	1.80	0.63
1:a:72:G:N2	1:a:95:A:N1	2.40	0.63
9:i:20:ARG:HH21	9:i:64:LEU:HD12	1.64	0.63
23:A:1397:A:H2'	23:A:1398:A:C8	2.34	0.63
1:a:133:G:O6	16:p:26:ARG:NH2	2.32	0.63
6:f:3:ARG:N	6:f:69:ASP:OD1	2.32	0.63
23:A:1253:C:O2'	23:A:1254:G:H8	1.81	0.63
1:a:1363:G:H2'	1:a:1364:A:H8	1.63	0.63
8:h:13:ARG:HD2	8:h:27:LEU:HD13	1.81	0.63
2:b:186:ILE:HA	2:b:200:ILE:O	1.99	0.63
23:A:292:U:H2'	23:A:293:G:H8	1.63	0.63
23:A:1046:A:H2'	23:A:1047:A:C8	2.33	0.63
23:A:2345:U:O2	28:F:37:ASN:ND2	2.32	0.63
18:r:27:TYR:O	18:r:66:SER:OG	2.16	0.63
1:a:69:A:N7	1:a:70:A:N6	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1130:A:O2'	23:A:1151:U:O2'	2.14	0.62
23:A:1549:G:O2'	25:C:99:GLY:O	2.15	0.62
1:a:409:C:O2'	1:a:629:A:N3	2.30	0.62
23:A:1136:U:N3	23:A:1137:G:O6	2.33	0.62
23:A:632:U:H2'	23:A:633:A:C8	2.33	0.62
23:A:2154:G:OP1	23:A:2203:G:N2	2.31	0.62
28:F:64:LYS:HD3	46:3:5:ILE:HG22	1.81	0.62
1:a:1434:C:H2'	1:a:1435:A:H8	1.64	0.62
1:a:1327:C:O2	19:s:36:ARG:NH2	2.33	0.62
23:A:2133:U:H3	23:A:2222:G:H22	1.48	0.62
28:F:103:LEU:HA	28:F:107:SER:HB3	1.81	0.62
1:a:995:A:H2'	1:a:996:G:C8	2.34	0.62
23:A:827:A:OP1	25:C:217:ARG:NH2	2.32	0.62
23:A:2149:G:H2'	23:A:2150:A:C5	2.35	0.62
28:F:29:PRO:HG2	28:F:169:LEU:HD12	1.82	0.62
31:M:20:LEU:HD13	31:M:44:LYS:HE3	1.81	0.62
23:A:1148:C:H2'	23:A:1149:A:H8	1.64	0.62
28:F:65:PRO:HA	28:F:89:VAL:HG22	1.82	0.62
2:b:35:ARG:HG3	2:b:36:ASN:H	1.65	0.61
6:f:53:ILE:HG22	6:f:54:ASN:H	1.64	0.61
41:W:13:THR:OG1	41:W:67:ASN:OD1	2.17	0.61
23:A:1309:G:OP1	47:4:16:ARG:NH2	2.26	0.61
28:F:160:ALA:HB1	28:F:165:GLU:HG2	1.81	0.61
1:a:467:U:O2	1:a:482:G:N2	2.25	0.61
23:A:2112:U:O2'	43:Z:23:ASN:ND2	2.32	0.61
23:A:2380:C:OP1	48:5:34:LYS:NZ	2.30	0.61
23:A:1429:A:O2'	23:A:1440:U:O2	2.18	0.61
23:A:2142:U:H2'	23:A:2143:G:C8	2.35	0.61
1:a:587:G:H5'	1:a:736:A:H1'	1.82	0.61
1:a:955:A:H2'	1:a:956:G:H8	1.64	0.61
1:a:1225:C:H2'	1:a:1226:U:C6	2.35	0.61
2:b:114:LEU:HD13	2:b:144:LEU:HD22	1.81	0.61
5:e:15:ARG:HD3	5:e:118:LEU:HD21	1.82	0.61
23:A:842:U:H2'	23:A:843:U:C6	2.36	0.61
26:D:125:ARG:HG3	26:D:164:MET:HG3	1.82	0.61
1:a:35:G:O2'	12:l:128:SER:O	2.15	0.61
16:p:8:LYS:HD2	16:p:30:ASP:HA	1.83	0.61
1:a:660:U:O4	1:a:760:G:O2'	2.16	0.61
23:A:139:A:H2'	23:A:140:G:C8	2.35	0.61
23:A:1131:A:O2'	23:A:1150:C:O2'	2.19	0.61
1:a:1095:U:H3	1:a:1108:G:H22	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1457:A:N1	23:A:1638:G:O6	2.33	0.61
1:a:416:A:O2'	4:d:105:ARG:NH1	2.34	0.60
23:A:1787:C:H5	36:R:94:ARG:HH21	1.49	0.60
21:x:26:A:H61	21:x:44:G:H1	1.48	0.60
1:a:560:U:H2'	1:a:561:G:H8	1.67	0.60
23:A:1088:G:O6	23:A:1159:U:O2	2.18	0.60
23:A:2167:A:H2'	23:A:2168:G:H8	1.67	0.60
1:a:595:G:H4'	8:h:4:THR:HA	1.83	0.60
11:k:88:GLY:O	11:k:93:ARG:NH2	2.34	0.60
17:q:62:ARG:NH1	17:q:79:GLU:OE2	2.30	0.60
23:A:1835:A:H2'	23:A:1836:A:C8	2.35	0.60
37:S:43:TYR:HB3	38:T:74:TYR:HB3	1.83	0.60
2:b:90:TYR:HB3	2:b:151:ILE:HG22	1.83	0.60
23:A:422:G:H2'	23:A:423:A:H8	1.67	0.60
23:A:280:A:H2'	23:A:281:A:C8	2.35	0.60
23:A:1072:A:OP2	23:A:1180:C:O2'	2.12	0.60
23:A:1112:U:N3	23:A:1115:A:OP2	2.27	0.60
23:A:1129:G:H1'	23:A:1132:A:H61	1.66	0.60
1:a:603:A:N6	1:a:649:A:O2'	2.35	0.60
19:s:50:ALA:HB1	19:s:57:HIS:HB3	1.83	0.60
23:A:2338:A:N6	28:F:153:ASP:OD2	2.35	0.60
23:A:199:A:N6	23:A:2463:A:O2'	2.35	0.60
23:A:2104:A:H2'	23:A:2105:G:C8	2.36	0.60
23:A:2187:G:N2	23:A:2188:A:N7	2.49	0.60
23:A:703:U:H2'	23:A:704:A:C8	2.37	0.60
3:c:33:HIS:HE1	14:n:38:LYS:HB2	1.67	0.59
23:A:625:G:H2'	23:A:626:G:C8	2.36	0.59
25:C:110:LEU:HD11	25:C:116:ILE:HD11	1.84	0.59
1:a:19:C:OP1	5:e:136:ASN:ND2	2.34	0.59
15:o:64:ARG:NH2	23:A:761:A:OP1	2.33	0.59
23:A:1022:G:HO2'	23:A:1201:A:HO2'	1.49	0.59
23:A:2149:G:H5''	23:A:2150:A:N7	2.16	0.59
1:a:1159:A:HO2'	1:a:1160:A:H8	1.48	0.59
3:c:33:HIS:CE1	14:n:38:LYS:HB2	2.37	0.59
31:M:64:ARG:HG2	31:M:83:ALA:HB3	1.84	0.59
1:a:8:A:N1	4:d:200:ARG:NH2	2.50	0.59
1:a:280:C:H2'	1:a:281:A:H8	1.66	0.59
1:a:911:G:H2'	1:a:912:G:H8	1.67	0.59
6:f:31:LEU:HD21	6:f:66:LEU:HD11	1.84	0.59
23:A:185:C:H2'	23:A:186:C:H5'	1.84	0.59
28:F:129:THR:HG22	28:F:155:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:553:C:OP2	4:d:58:ARG:NH2	2.35	0.59
4:d:52:ALA:O	4:d:56:LYS:HG2	2.03	0.59
23:A:2104:A:H2'	23:A:2105:G:H8	1.68	0.59
18:r:16:TYR:OH	18:r:35:LYS:NZ	2.34	0.59
39:U:15:VAL:HG11	39:U:51:ILE:HG21	1.85	0.59
1:a:38:G:H22	1:a:405:A:H5'	1.68	0.58
23:A:629:A:H5'	27:E:89:VAL:HG21	1.84	0.58
3:c:30:ASP:OD1	3:c:31:PHE:N	2.36	0.58
23:A:703:U:H2'	23:A:704:A:H8	1.68	0.58
46:3:34:THR:HA	46:3:44:PRO:HA	1.85	0.58
23:A:789:A:O2'	23:A:1708:U:OP1	2.20	0.58
23:A:899:C:H2'	23:A:900:A:H8	1.67	0.58
23:A:350:G:N1	23:A:353:A:OP2	2.32	0.58
23:A:1531:U:O2	23:A:1561:G:O6	2.21	0.58
2:b:83:GLU:OE2	2:b:214:THR:HB	2.02	0.58
23:A:945:C:H2'	23:A:946:G:H4'	1.84	0.58
23:A:2097:C:H2'	23:A:2098:C:C6	2.38	0.58
23:A:2107:U:H2'	23:A:2108:U:C6	2.39	0.58
23:A:2362:A:H2'	23:A:2363:G:C8	2.38	0.58
13:m:39:VAL:HG23	13:m:52:GLU:OE2	2.04	0.58
14:n:16:TYR:HB2	14:n:19:GLN:HG2	1.86	0.58
15:o:26:GLU:HA	15:o:81:LEU:HD11	1.85	0.58
1:a:695:A:H61	1:a:711:G:H1'	1.69	0.58
12:l:96:ARG:NH1	12:l:97:GLY:O	2.36	0.58
1:a:221:G:OP2	1:a:221:G:N2	2.32	0.58
1:a:1273:G:N2	1:a:1276:A:OP2	2.29	0.58
4:d:134:SER:H	4:d:137:GLN:HG3	1.68	0.58
15:o:18:HIS:CD2	15:o:20:THR:H	2.21	0.58
23:A:1598:G:OP2	23:A:1598:G:N2	2.26	0.58
23:A:1698:G:O2'	34:P:125:ASP:OD2	2.14	0.58
39:U:16:ARG:NH2	39:U:103:LYS:HD2	2.19	0.58
1:a:67:C:O2	1:a:68:G:N1	2.36	0.57
1:a:113:G:H4'	1:a:114:A:O5'	2.03	0.57
12:l:79:TYR:HB2	12:l:106:VAL:HG11	1.85	0.57
27:E:148:VAL:HG23	27:E:149:ASP:H	1.69	0.57
23:A:193:A:H2'	23:A:194:C:H6	1.69	0.57
23:A:329:A:H2'	23:A:330:A:C8	2.40	0.57
23:A:591:A:H4'	23:A:592:A:H5'	1.85	0.57
23:A:1114:G:N2	23:A:1141:A:O2'	2.37	0.57
32:N:92:THR:HG22	32:N:94:GLU:H	1.69	0.57
1:a:682:G:H2'	1:a:683:A:C8	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:88:LYS:O	3:c:92:GLU:HG3	2.03	0.57
9:i:28:ILE:HB	9:i:35:TRP:CD1	2.39	0.57
23:A:280:A:H2'	23:A:281:A:H8	1.69	0.57
23:A:1452:U:H2'	23:A:1453:G:H8	1.69	0.57
43:Z:7:ILE:HD13	43:Z:58:LYS:HD2	1.86	0.57
1:a:7:G:N7	5:e:98:LYS:NZ	2.52	0.57
1:a:900:U:H2'	1:a:901:A:H8	1.69	0.57
4:d:159:SER:OG	4:d:160:PHE:N	2.37	0.57
4:d:182:ARG:HH12	4:d:187:ALA:H	1.49	0.57
23:A:281:A:H2'	23:A:282:G:C8	2.39	0.57
23:A:2086:G:H4'	26:D:152:ASN:HD22	1.68	0.57
1:a:414:G:H21	4:d:112:GLN:HE22	1.52	0.57
2:b:117:ILE:HD12	2:b:141:GLN:HE21	1.69	0.57
23:A:2438:G:O2'	23:A:2439:C:OP2	2.20	0.57
1:a:73:G:O2'	1:a:74:A:OP1	2.21	0.57
2:b:166:PRO:HD3	2:b:187:VAL:HG12	1.87	0.57
9:i:28:ILE:HD12	9:i:63:VAL:HG22	1.87	0.57
23:A:880:U:C2	23:A:881:A:C8	2.93	0.57
23:A:2164:A:H5'	23:A:2165:A:H8	1.69	0.57
28:F:7:GLN:NE2	28:F:11:GLU:OE2	2.37	0.57
1:a:388:G:N2	1:a:391:A:OP2	2.29	0.57
1:a:415:U:H5''	4:d:108:ARG:HB3	1.87	0.57
10:j:5:LYS:N	10:j:76:ILE:O	2.38	0.57
20:t:25:ARG:HB3	20:t:29:ARG:NH1	2.20	0.57
4:d:119:ILE:HD12	4:d:139:ILE:HD11	1.86	0.57
23:A:1482:G:H2'	23:A:1483:A:C8	2.39	0.57
4:d:3:ARG:HH22	4:d:59:HIS:HA	1.68	0.56
23:A:341:A:N3	23:A:362:C:O2'	2.37	0.56
1:a:384:G:H5''	16:p:6:ARG:HG3	1.86	0.56
1:a:746:U:OP1	6:f:3:ARG:NH1	2.39	0.56
1:a:1147:G:H5''	1:a:1148:U:H5	1.70	0.56
23:A:879:C:H2'	23:A:880:U:C6	2.41	0.56
23:A:1569:U:H2'	23:A:1570:G:H8	1.70	0.56
30:L:142:GLU:O	30:L:144:ARG:NH1	2.37	0.56
1:a:622:C:OP2	4:d:77:LYS:NZ	2.36	0.56
1:a:931:G:O2'	1:a:932:A:OP1	2.23	0.56
6:f:27:PHE:HA	6:f:30:ILE:HG12	1.88	0.56
13:m:89:MET:HE2	13:m:93:ARG:HH12	1.69	0.56
23:A:637:U:H2'	23:A:638:U:C6	2.40	0.56
23:A:891:U:O2'	23:A:893:A:OP1	2.23	0.56
23:A:925:A:H62	23:A:946:G:H21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2167:A:H2'	23:A:2168:G:C8	2.41	0.56
23:A:2184:U:H2'	23:A:2185:A:C8	2.40	0.56
32:N:55:LEU:O	32:N:60:ARG:NH1	2.38	0.56
1:a:332:G:N1	1:a:335:A:OP2	2.38	0.56
23:A:363:A:N3	27:E:169:ASN:ND2	2.49	0.56
23:A:1297:G:H1	37:S:37:GLN:HE21	1.53	0.56
23:A:2412:G:H2'	23:A:2413:U:C6	2.40	0.56
1:a:352:A:H5'	1:a:353:C:H5	1.71	0.56
1:a:847:G:H2'	1:a:848:G:H8	1.69	0.56
23:A:4:U:H2'	23:A:5:A:H8	1.71	0.56
23:A:676:A:OP2	50:7:15:LYS:NZ	2.38	0.56
2:b:49:LYS:HE3	2:b:200:ILE:HA	1.88	0.56
23:A:684:U:H2'	23:A:685:C:C6	2.41	0.56
1:a:583:G:O2'	1:a:829:G:OP2	2.23	0.56
1:a:1439:G:O2'	1:a:1476:A:N6	2.39	0.56
27:E:126:LEU:HD23	27:E:128:GLY:H	1.71	0.56
1:a:424:G:H2'	1:a:425:G:H8	1.71	0.56
23:A:2052:U:OP2	47:4:6:ARG:NH2	2.39	0.56
28:F:4:LEU:O	28:F:8:TYR:N	2.37	0.56
37:S:97:ASP:OD2	37:S:101:ASN:ND2	2.39	0.56
2:b:133:GLU:HG3	2:b:137:LEU:HD12	1.88	0.56
23:A:878:G:H2'	23:A:879:C:C6	2.40	0.56
23:A:1480:C:H2'	23:A:1481:A:C8	2.41	0.56
31:M:104:ARG:HH12	31:M:107:ARG:HH21	1.53	0.56
1:a:525:G:N2	1:a:538:G:OP1	2.39	0.55
1:a:843:A:OP1	18:r:57:ARG:NH2	2.39	0.55
15:o:16:ARG:NH1	15:o:19:ASP:O	2.39	0.55
23:A:2362:A:H2'	23:A:2363:G:H8	1.71	0.55
39:U:87:LEU:HB2	39:U:103:LYS:HB2	1.87	0.55
1:a:1155:C:O2	9:i:18:ARG:NH1	2.39	0.55
16:p:16:PRO:HD2	16:p:43:LEU:HD21	1.87	0.55
23:A:292:U:H2'	23:A:293:G:C8	2.41	0.55
4:d:148:ASN:HB3	4:d:151:ILE:HG12	1.88	0.55
1:a:415:U:OP1	4:d:108:ARG:NH1	2.40	0.55
1:a:1442:G:H2'	1:a:1443:U:C6	2.41	0.55
23:A:1639:U:H2'	23:A:1640:A:H8	1.71	0.55
1:a:277:U:H2'	1:a:278:A:C8	2.42	0.55
8:h:41:LYS:HD3	8:h:49:VAL:HG12	1.88	0.55
1:a:36:C:O2'	12:l:127:ARG:NH2	2.40	0.55
1:a:1139:A:H2'	1:a:1140:G:C8	2.41	0.55
17:q:30:TYR:HE1	17:q:41:LYS:HG2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1336:U:H2'	23:A:1337:U:C6	2.42	0.55
1:a:1014:C:H1'	1:a:1047:A:H4'	1.88	0.55
7:g:140:ASP:OD1	7:g:141:THR:N	2.40	0.55
23:A:1151:U:H2'	23:A:1152:G:C8	2.41	0.55
23:A:1213:A:H2'	23:A:1214:A:C8	2.42	0.55
1:a:412:G:OP1	4:d:115:ASN:ND2	2.37	0.55
1:a:1071:U:H2'	1:a:1072:C:C6	2.41	0.55
12:l:92:VAL:HG12	12:l:115:LEU:HD13	1.88	0.55
23:A:1213:A:H2'	23:A:1214:A:H8	1.70	0.55
1:a:839:U:O2'	1:a:1548:U:OP1	2.22	0.55
21:x:9:A:H5''	21:x:46:G7M:H22	1.72	0.55
23:A:1187:U:H2'	30:L:66:THR:HG21	1.89	0.55
23:A:1321:A:H2'	23:A:1322:A:C8	2.42	0.55
23:A:859:U:H2'	23:A:860:C:C6	2.42	0.55
23:A:2166:G:N2	23:A:2190:G:O2'	2.39	0.54
32:N:58:PHE:O	50:7:13:ARG:NH1	2.40	0.54
1:a:470:G:H2'	1:a:471:A:C8	2.42	0.54
1:a:1419:C:H2'	1:a:1420:A:C8	2.42	0.54
7:g:16:PRO:HG2	9:i:43:ALA:HB1	1.87	0.54
10:j:51:VAL:HG13	14:n:41:ARG:HB2	1.89	0.54
23:A:579:U:O2'	37:S:49:ASP:OD2	2.24	0.54
23:A:1366:A:C2	23:A:1367:G:C8	2.95	0.54
23:A:2788:C:O2'	23:A:2789:U:O2	2.16	0.54
2:b:200:ILE:O	2:b:200:ILE:HG13	2.07	0.54
23:A:2058:C:H2'	23:A:2059:U:C6	2.43	0.54
23:A:2319:A:H4'	23:A:2320:A:O4'	2.08	0.54
23:A:2580:U:H2'	23:A:2581:G:H8	1.72	0.54
1:a:531:A:H61	12:l:102:ASP:HB2	1.73	0.54
23:A:1369:C:OP1	23:A:1696:G:O2'	2.25	0.54
23:A:1897:U:OP1	23:A:2443:G:O2'	2.26	0.54
23:A:2256:A:OP1	25:C:171:TYR:OH	2.23	0.54
13:m:7:VAL:HG22	13:m:8:ASP:H	1.72	0.54
23:A:27:G:H1'	23:A:558:A:N6	2.23	0.54
1:a:302:C:OP1	1:a:618:G:O2'	2.20	0.54
12:l:57:LYS:HE2	12:l:58:PRO:HA	1.89	0.54
17:q:60:VAL:HG23	17:q:81:VAL:HB	1.89	0.54
23:A:13:A:O2'	23:A:15:G:N7	2.38	0.54
26:D:8:ARG:NH1	26:D:197:LYS:O	2.40	0.54
1:a:277:U:H2'	1:a:278:A:H8	1.73	0.54
2:b:16:PHE:O	2:b:203:ASN:ND2	2.34	0.54
23:A:903:G:H2'	23:A:904:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:L:92:GLU:OE2	30:L:96:ASN:ND2	2.40	0.54
31:M:8:MET:HE1	31:M:62:ILE:HG12	1.89	0.54
2:b:82:ASP:OD1	2:b:83:GLU:N	2.40	0.54
2:b:166:PRO:CD	2:b:187:VAL:HG12	2.38	0.54
3:c:16:ARG:HG2	3:c:17:ASP:H	1.72	0.54
34:P:28:GLU:OE2	34:P:105:ARG:NH2	2.39	0.54
2:b:115:LYS:HB3	2:b:119:LYS:NZ	2.22	0.54
8:h:13:ARG:HB3	8:h:25:LEU:HD11	1.90	0.54
17:q:26:VAL:HG22	17:q:45:LYS:HG2	1.89	0.54
19:s:5:LEU:HD23	19:s:6:LYS:N	2.22	0.54
23:A:1833:C:H5'	25:C:146:MET:HE1	1.90	0.54
23:A:2863:G:H2'	23:A:2908:A:H61	1.72	0.54
1:a:415:U:H2'	1:a:416:A:C8	2.42	0.54
1:a:546:U:H2'	1:a:547:A:C8	2.41	0.54
1:a:736:A:H2'	1:a:737:A:C8	2.43	0.54
13:m:11:ARG:HA	13:m:45:THR:HB	1.90	0.54
23:A:799:G:H2'	23:A:800:U:H6	1.73	0.54
23:A:1055:A:N3	23:A:1199:C:O2'	2.39	0.54
28:F:130:LEU:N	28:F:154:VAL:O	2.41	0.54
1:a:21:G:H2'	1:a:22:G:H8	1.72	0.53
1:a:467:U:O4	1:a:482:G:O6	2.25	0.53
1:a:1129:U:H2'	1:a:1130:U:C6	2.41	0.53
8:h:10:PHE:O	8:h:14:ILE:HD12	2.08	0.53
8:h:51:TYR:HD1	8:h:60:ILE:HG22	1.73	0.53
23:A:66:C:H2'	23:A:67:A:H8	1.72	0.53
23:A:1239:G:OP1	32:N:14:LYS:NZ	2.30	0.53
23:A:2324:U:H2'	23:A:2325:U:C6	2.42	0.53
23:A:2369:A:H61	42:Y:51:THR:HG21	1.73	0.53
1:a:280:C:H2'	1:a:281:A:C8	2.43	0.53
1:a:1543:C:H42	22:w:8:G:H1	1.56	0.53
2:b:73:LYS:NZ	2:b:204:ASP:OD1	2.41	0.53
23:A:1716:G:O2'	23:A:2024:U:O4	2.20	0.53
28:F:41:GLY:HA2	28:F:85:ILE:HD12	1.90	0.53
2:b:54:PHE:HB2	2:b:216:LYS:HZ3	1.73	0.53
1:a:41:G:H2'	1:a:42:G:H8	1.74	0.53
1:a:749:G:H5''	15:o:39:LEU:HD11	1.89	0.53
1:a:954:G:C2	1:a:955:A:C8	2.96	0.53
1:a:1064:A:O2'	3:c:160:ASP:O	2.22	0.53
23:A:288:U:O2'	23:A:289:U:O5'	2.27	0.53
23:A:1111:U:H3	23:A:1115:A:H8	1.55	0.53
21:x:5:G:H2'	21:x:6:G:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:720:G:H1'	27:E:74:ARG:HD3	1.90	0.53
23:A:1452:U:H2'	23:A:1453:G:C8	2.42	0.53
23:A:1851:U:O2'	25:C:154:LEU:O	2.27	0.53
48:5:29:ARG:NH2	48:5:47:GLU:O	2.36	0.53
1:a:723:A:H2'	1:a:724:A:C8	2.43	0.53
12:l:94:LEU:HB2	12:l:115:LEU:HD12	1.89	0.53
23:A:1212:G:H2'	23:A:1213:A:H8	1.73	0.53
1:a:1434:C:H2'	1:a:1435:A:C8	2.43	0.53
7:g:111:ARG:NH2	7:g:113:GLU:OE2	2.34	0.53
28:F:3:ARG:NH1	28:F:101:ASP:OD1	2.41	0.53
1:a:146:G:H2'	1:a:147:G:C8	2.43	0.53
1:a:262:G:O6	1:a:281:A:N6	2.41	0.53
1:a:384:G:H4'	16:p:6:ARG:HD3	1.91	0.53
26:D:54:GLU:O	26:D:78:ARG:N	2.39	0.53
17:q:70:SER:OG	17:q:71:ALA:N	2.42	0.53
23:A:2064:A:N3	23:A:2488:G:O2'	2.34	0.53
1:a:8:A:N6	4:d:196:GLU:O	2.42	0.53
4:d:182:ARG:HA	4:d:185:LEU:HD12	1.91	0.53
9:i:28:ILE:HB	9:i:35:TRP:CG	2.45	0.53
10:j:52:LEU:HD23	10:j:62:ARG:HD3	1.90	0.53
23:A:2471:U:O3'	23:A:2472:A:H3'	2.09	0.53
1:a:1330:G:H2'	1:a:1331:C:C6	2.44	0.52
1:a:1323:G:N1	1:a:1326:A:OP2	2.38	0.52
2:b:161:LEU:HB2	2:b:183:ILE:HG22	1.91	0.52
20:t:25:ARG:HB3	20:t:29:ARG:HH12	1.73	0.52
1:a:849:U:O2	1:a:854:G:N2	2.36	0.52
1:a:1497:G:H2'	1:a:1498:U:C6	2.45	0.52
6:f:53:ILE:HD12	6:f:89:ARG:HH21	1.73	0.52
10:j:63:GLU:OE2	14:n:45:ARG:NH1	2.36	0.52
25:C:82:GLU:OE2	25:C:103:TYR:OH	2.22	0.52
1:a:413:U:OP2	4:d:2:ALA:N	2.42	0.52
23:A:404:A:N6	23:A:405:G:O6	2.43	0.52
23:A:525:A:N3	23:A:527:G:H5''	2.24	0.52
23:A:597:U:H2'	23:A:598:G:O4'	2.10	0.52
23:A:2463:A:H2'	23:A:2463:A:N3	2.24	0.52
1:a:819:C:O2'	1:a:910:A:N1	2.42	0.52
23:A:1212:G:H2'	23:A:1213:A:C8	2.45	0.52
8:h:38:GLU:OE2	8:h:51:TYR:OH	2.26	0.52
8:h:113:LEU:HD13	8:h:117:GLU:HB3	1.92	0.52
23:A:329:A:H2'	23:A:330:A:H8	1.73	0.52
38:T:5:ILE:HG22	38:T:38:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:917:A:H2'	1:a:918:A:H8	1.74	0.52
4:d:97:ILE:O	4:d:101:LEU:HB2	2.09	0.52
5:e:56:GLU:HG3	5:e:58:PRO:HD2	1.92	0.52
23:A:899:C:H2'	23:A:900:A:C8	2.44	0.52
1:a:588:C:H2'	1:a:589:G:O4'	2.09	0.52
23:A:1311:G:H5''	39:U:20:ARG:HH22	1.75	0.52
23:A:1404:G:N7	23:A:1405:G:C8	2.78	0.52
23:A:1763:U:N3	23:A:1778:A:N6	2.33	0.52
23:A:1823:C:H2'	23:A:1824:A:N7	2.25	0.52
23:A:2347:A:H2'	23:A:2348:U:C6	2.44	0.52
6:f:89:ARG:HG2	18:r:69:MET:SD	2.49	0.52
23:A:487:U:O2'	27:E:46:GLN:NE2	2.43	0.52
24:B:22:G:O6	24:B:54:U:O2'	2.26	0.52
24:B:28:C:H2'	24:B:29:C:H5'	1.92	0.52
31:M:122:LEU:HD13	36:R:70:VAL:HG11	1.91	0.52
1:a:121:C:OP1	1:a:319:C:O2'	2.25	0.51
1:a:508:G:H2'	1:a:509:C:C6	2.45	0.51
1:a:942:G:N7	7:g:2:PRO:HG3	2.24	0.51
32:N:47:ARG:HB2	32:N:50:PHE:HB2	1.92	0.51
1:a:370:G:N2	1:a:370:G:OP2	2.42	0.51
2:b:111:ILE:HD12	2:b:152:LYS:HA	1.92	0.51
19:s:64:GLU:HA	46:3:70:ARG:HH22	1.74	0.51
21:x:51:U:O4	21:x:63:G:O6	2.28	0.51
23:A:1320:G:OP2	23:A:1694:G:O2'	2.21	0.51
23:A:2217:U:H2'	23:A:2218:G:H8	1.75	0.51
24:B:18:G:H2'	24:B:19:A:H8	1.74	0.51
1:a:343:C:H2'	1:a:344:A:H8	1.75	0.51
1:a:469:A:H2'	1:a:470:G:H8	1.75	0.51
1:a:1133:G:N2	1:a:1134:U:O4	2.38	0.51
1:a:1515:A:H2'	1:a:1516:G:C8	2.45	0.51
10:j:26:VAL:HG13	10:j:36:VAL:HG11	1.92	0.51
23:A:577:A:H4'	23:A:578:G:C8	2.45	0.51
23:A:1095:C:C2	23:A:1096:A:C8	2.99	0.51
23:A:2360:A:H2'	23:A:2361:A:C8	2.45	0.51
1:a:1186:A:OP2	9:i:95:ARG:NH2	2.42	0.51
1:a:1294:A:H2'	1:a:1295:A:C8	2.45	0.51
15:o:26:GLU:HG3	15:o:81:LEU:HD11	1.92	0.51
23:A:631:U:H2'	23:A:632:U:C6	2.45	0.51
26:D:146:MET:HA	26:D:158:LYS:HE3	1.92	0.51
23:A:1187:U:H4'	23:A:1188:A:O4'	2.10	0.51
47:4:28:ASN:N	47:4:37:ARG:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:8:25:VAL:HG22	51:8:34:GLN:HB2	1.92	0.51
1:a:672:G:H22	1:a:749:G:H1	1.58	0.51
10:j:66:GLU:HB3	14:n:59:ALA:HB2	1.93	0.51
12:l:81:PRO:HG3	12:l:109:HIS:HD2	1.73	0.51
23:A:40:U:H2'	23:A:41:A:H8	1.75	0.51
23:A:2389:U:H2'	23:A:2390:G:O4'	2.11	0.51
1:a:642:C:H2'	1:a:643:A:H8	1.74	0.51
1:a:944:A:N6	7:g:2:PRO:HG2	2.25	0.51
1:a:1050:G:H2'	1:a:1051:U:C6	2.46	0.51
1:a:1080:C:H2'	1:a:1081:G:H8	1.75	0.51
2:b:58:ARG:NE	2:b:58:ARG:HA	2.26	0.51
23:A:139:A:H2	23:A:1453:G:H1'	1.75	0.51
23:A:193:A:H2'	23:A:194:C:C6	2.46	0.51
23:A:1430:C:H2'	23:A:1431:A:C8	2.46	0.51
23:A:1961:A:H2'	23:A:1962:G:O4'	2.11	0.51
23:A:2337:G:N2	28:F:153:ASP:OD2	2.44	0.51
1:a:701:G:N2	21:x:37:MIA:S10	2.84	0.51
23:A:1247:U:H2'	23:A:1248:A:H8	1.75	0.51
23:A:1464:A:N6	23:A:1634:A:N7	2.58	0.51
23:A:2109:U:OP2	23:A:2271:G:N2	2.42	0.51
21:x:9:A:N3	21:x:45:U:O2'	2.40	0.51
1:a:307:G:H2'	1:a:308:A:C8	2.46	0.51
5:e:96:LEU:O	5:e:126:SER:HA	2.11	0.51
23:A:1109:G:H1	23:A:1121:C:H42	1.59	0.51
23:A:1622:A:H2'	23:A:1623:A:C8	2.46	0.51
23:A:1639:U:H2'	23:A:1640:A:C8	2.46	0.51
23:A:2135:U:H2'	23:A:2136:A:C8	2.46	0.51
23:A:2202:G:H2'	23:A:2203:G:C8	2.46	0.51
23:A:2328:C:HO2'	23:A:2329:U:H6	1.59	0.51
26:D:103:ALA:N	26:D:106:ASP:OD2	2.44	0.51
34:P:75:GLN:HA	34:P:89:ASN:HA	1.93	0.51
2:b:134:VAL:HA	2:b:138:LYS:HD2	1.93	0.50
23:A:1245:U:H1'	37:S:4:VAL:HG22	1.92	0.50
23:A:1253:C:O2'	23:A:1254:G:O5'	2.25	0.50
23:A:1569:U:H2'	23:A:1570:G:C8	2.46	0.50
23:A:1823:C:H2'	23:A:1824:A:C8	2.46	0.50
23:A:2506:U:OP1	23:A:2508:C:N4	2.41	0.50
23:A:140:G:H2'	23:A:141:U:C6	2.46	0.50
41:W:46:LYS:HD3	41:W:47:PRO:HD2	1.94	0.50
1:a:199:C:H2'	1:a:200:A:C8	2.45	0.50
1:a:1014:C:H2'	1:a:1015:C:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:7:ILE:HG12	6:f:92:VAL:HG22	1.93	0.50
23:A:133:A:H2'	23:A:134:U:C6	2.46	0.50
23:A:1115:A:N7	23:A:1119:A:N6	2.59	0.50
23:A:1726:A:H2'	23:A:1727:A:H8	1.76	0.50
23:A:2873:G:H2'	23:A:2874:A:H8	1.74	0.50
30:L:50:ASP:OD1	30:L:122:LYS:NZ	2.45	0.50
1:a:728:C:O2'	18:r:60:THR:HG21	2.11	0.50
1:a:1380:G:H5''	7:g:36:ARG:HG3	1.93	0.50
2:b:220:ALA:O	2:b:223:GLU:HG3	2.12	0.50
23:A:214:G:H2'	23:A:215:A:O4'	2.12	0.50
23:A:489:A:H5''	23:A:490:C:OP1	2.12	0.50
1:a:1043:G:H2'	1:a:1044:G:C8	2.46	0.50
5:e:154:VAL:HG21	8:h:101:LEU:HD12	1.93	0.50
9:i:21:LEU:HD21	9:i:61:TYR:CG	2.47	0.50
18:r:53:ALA:O	18:r:57:ARG:HG2	2.11	0.50
23:A:809:G:O2'	23:A:810:A:OP1	2.24	0.50
23:A:1623:A:H2'	23:A:1624:A:C8	2.47	0.50
23:A:2624:C:H2'	23:A:2625:G:H8	1.77	0.50
27:E:126:LEU:HD11	27:E:142:PHE:HZ	1.77	0.50
28:F:80:ARG:NH1	28:F:81:GLU:O	2.44	0.50
1:a:917:A:H2'	1:a:918:A:C8	2.47	0.50
6:f:79:ARG:NH2	25:C:123:ASP:OD2	2.45	0.50
23:A:923:C:H2'	23:A:924:U:H4'	1.93	0.50
23:A:2339:U:H5''	23:A:2340:G:H2'	1.94	0.50
2:b:77:GLN:HE22	2:b:94:HIS:CD2	2.29	0.50
16:p:10:MET:HE1	16:p:19:ARG:HH11	1.77	0.50
23:A:651:A:H2'	23:A:652:A:C8	2.47	0.50
23:A:1010:C:O2'	23:A:2306:A:N3	2.42	0.50
34:P:106:TYR:OH	34:P:134:LEU:O	2.29	0.50
1:a:504:G:H21	1:a:505:A:H3'	1.77	0.50
23:A:301:A:H2'	23:A:302:G:C8	2.47	0.50
23:A:338:A:H2'	23:A:339:U:C6	2.47	0.50
23:A:2130:G:H2'	23:A:2131:U:C6	2.46	0.50
23:A:2170:C:H2'	23:A:2171:G:H8	1.76	0.50
27:E:170:LEU:HD23	27:E:173:ILE:HG13	1.93	0.50
1:a:1411:C:H2'	1:a:1412:G:C8	2.46	0.50
1:a:1438:C:H2'	1:a:1439:G:O4'	2.12	0.50
2:b:77:GLN:HG3	2:b:93:ASN:HB2	1.94	0.50
2:b:164:VAL:O	2:b:186:ILE:HG13	2.12	0.50
8:h:114:THR:OG1	8:h:117:GLU:OE1	2.30	0.50
10:j:59:LYS:HE2	10:j:62:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1549:G:N2	25:C:98:ASP:O	2.43	0.50
1:a:1209:U:O2'	14:n:27:CYS:SG	2.63	0.49
1:a:1322:U:O2'	1:a:1367:A:N3	2.33	0.49
3:c:141:MET:HE2	3:c:169:GLU:HG2	1.94	0.49
11:k:29:ASN:OD1	11:k:30:THR:N	2.44	0.49
13:m:89:MET:HG2	13:m:92:ARG:HH21	1.77	0.49
23:A:2098:C:H2'	23:A:2099:C:H6	1.77	0.49
1:a:46:G:O2'	1:a:373:U:O2	2.30	0.49
1:a:1303:C:H4'	1:a:1309:U:O4	2.11	0.49
2:b:49:LYS:HZ2	2:b:201:PRO:HG2	1.77	0.49
3:c:52:SER:HB2	3:c:114:LEU:HD21	1.92	0.49
23:A:75:G:N3	23:A:75:G:H2'	2.27	0.49
23:A:140:G:H2'	23:A:141:U:H6	1.76	0.49
23:A:1480:C:H2'	23:A:1481:A:H8	1.75	0.49
23:A:2269:U:H2'	23:A:2270:G:O4'	2.12	0.49
1:a:1139:A:H4'	9:i:20:ARG:NH1	2.27	0.49
13:m:89:MET:HB3	13:m:93:ARG:NH1	2.26	0.49
23:A:945:C:H42	23:A:946:G:N2	2.10	0.49
23:A:2617:U:H2'	23:A:2618:U:H2'	1.95	0.49
43:Z:49:VAL:HG11	43:Z:54:LEU:HD13	1.94	0.49
1:a:35:G:H2'	1:a:36:C:C6	2.48	0.49
1:a:995:A:H2'	1:a:996:G:H8	1.74	0.49
1:a:1035:C:H2'	1:a:1036:C:C6	2.47	0.49
13:m:16:VAL:HG22	13:m:34:LEU:HD12	1.95	0.49
23:A:2586:G:N2	23:A:2616:G:H1'	2.27	0.49
25:C:247:MET:HE2	25:C:251:GLY:HA2	1.92	0.49
29:G:9:ILE:HA	29:G:69:ARG:HH21	1.78	0.49
33:O:67:LYS:NZ	33:O:105:GLU:OE2	2.41	0.49
1:a:985:G:OP2	1:a:1365:U:O2'	2.31	0.49
1:a:1022:G:N2	1:a:1025:A:OP2	2.29	0.49
2:b:83:GLU:HG3	2:b:218:ALA:HB2	1.95	0.49
3:c:189:ASP:OD2	3:c:194:LYS:NZ	2.45	0.49
23:A:349:U:H2'	23:A:350:G:O4'	2.12	0.49
23:A:755:U:H2'	23:A:756:A:H8	1.78	0.49
23:A:800:U:H2'	23:A:801:G:H8	1.77	0.49
23:A:860:C:O2'	23:A:1269:G:N2	2.45	0.49
23:A:1093:G:H21	23:A:1157:A:H62	1.60	0.49
23:A:1243:G:C2	23:A:1244:U:C5	3.00	0.49
23:A:1640:A:H2'	23:A:1641:G:C8	2.47	0.49
23:A:2378:G:N3	23:A:2414:C:H2'	2.28	0.49
23:A:2860:G:OP1	26:D:57:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:537:G:H22	12:l:61:ALA:HB2	1.76	0.49
1:a:1084:U:H5'	2:b:178:LYS:HE3	1.95	0.49
1:a:1129:U:H2'	1:a:1130:U:H6	1.78	0.49
8:h:81:SER:OG	8:h:127:VAL:O	2.29	0.49
23:A:1384:U:OP2	40:V:58:TYR:OH	2.29	0.49
23:A:1527:A:N6	23:A:1565:G:O2'	2.44	0.49
29:G:54:ARG:NE	29:G:57:ASP:OD1	2.46	0.49
23:A:2043:G:H5''	39:U:47:SER:HB3	1.95	0.49
24:B:88:C:H5'	33:O:18:ARG:HB3	1.95	0.49
34:P:40:ILE:HA	34:P:43:VAL:HG22	1.94	0.49
23:A:911:G:H2'	23:A:912:C:C6	2.48	0.49
23:A:27:G:HO2'	23:A:28:A:P	2.34	0.49
23:A:125:A:H5'	49:6:19:ARG:HG3	1.95	0.49
23:A:2147:A:C2	23:A:2201:G:H1'	2.48	0.49
30:L:99:GLU:O	30:L:103:GLU:HG3	2.13	0.49
2:b:99:GLY:O	2:b:103:ASN:HB2	2.13	0.49
23:A:221:A:N3	23:A:236:U:O2'	2.43	0.49
23:A:889:G:H2'	23:A:890:G:C8	2.48	0.49
23:A:1294:U:OP1	23:A:1294:U:H3'	2.13	0.49
23:A:1365:A:C4	23:A:1366:A:C8	3.00	0.49
23:A:1699:A:HO2'	23:A:1700:G:C5'	2.26	0.49
23:A:2624:C:H2'	23:A:2625:G:C8	2.48	0.49
31:M:76:TYR:HB2	36:R:73:THR:HB	1.95	0.49
9:i:107:ASP:OD2	9:i:109:ARG:HG2	2.13	0.48
23:A:509:G:N2	23:A:512:A:OP2	2.40	0.48
23:A:756:A:H2'	23:A:757:A:C8	2.47	0.48
23:A:1483:A:H2'	23:A:1484:A:C8	2.48	0.48
23:A:2565:G:N2	23:A:2696:G:O2'	2.46	0.48
25:C:30:GLU:HG2	25:C:33:LEU:HD13	1.95	0.48
29:G:37:PHE:HE1	29:G:71:ILE:HD11	1.78	0.48
1:a:670:A:H2'	1:a:671:A:C8	2.48	0.48
1:a:765:U:H2'	1:a:766:G:O4'	2.13	0.48
2:b:187:VAL:HB	2:b:191:CYS:HB2	1.94	0.48
23:A:228:A:H2'	23:A:229:A:C8	2.48	0.48
23:A:1297:G:H1	37:S:37:GLN:NE2	2.11	0.48
23:A:2590:G:H2'	23:A:2591:C:C6	2.48	0.48
24:B:37:A:H2'	24:B:38:U:C6	2.49	0.48
38:T:36:ASP:OD1	38:T:36:ASP:N	2.44	0.48
12:l:5:ASN:HA	12:l:8:VAL:HG22	1.95	0.48
23:A:1620:G:H4'	25:C:59:LYS:HG3	1.95	0.48
23:A:2347:A:H2'	23:A:2348:U:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1335:C:C2	1:a:1336:A:C8	3.02	0.48
2:b:57:MET:SD	2:b:221:ILE:HB	2.53	0.48
23:A:155:U:H2'	23:A:156:A:H8	1.77	0.48
23:A:680:C:O2'	23:A:684:U:OP1	2.30	0.48
23:A:735:A:H2'	23:A:736:C:C6	2.48	0.48
23:A:2276:U:H2'	23:A:2277:U:C6	2.48	0.48
50:7:16:ARG:HD2	50:7:65:MET:HE1	1.95	0.48
1:a:532:G:H2'	1:a:533:C:C6	2.48	0.48
1:a:1521:A:H2'	1:a:1522:U:C6	2.48	0.48
16:p:10:MET:HE2	16:p:19:ARG:HD2	1.94	0.48
23:A:2580:U:H2'	23:A:2581:G:C8	2.48	0.48
28:F:40:VAL:HG22	28:F:86:GLY:H	1.78	0.48
1:a:1110:A:H4'	1:a:1111:A:O5'	2.13	0.48
4:d:31:TYR:CZ	4:d:38:PRO:HB3	2.49	0.48
11:k:86:VAL:HG13	11:k:93:ARG:NH1	2.29	0.48
21:x:21:A:N6	21:x:46:G7M:O2'	2.47	0.48
23:A:684:U:H2'	23:A:685:C:H6	1.78	0.48
27:E:17:ILE:HG21	27:E:125:VAL:HG11	1.95	0.48
1:a:1128:U:OP1	9:i:85:ARG:NH2	2.46	0.48
1:a:1414:C:H2'	1:a:1415:A:H8	1.78	0.48
2:b:46:THR:HA	2:b:49:LYS:HD3	1.95	0.48
23:A:636:A:H5''	50:7:64:LYS:HE2	1.96	0.48
23:A:755:U:H2'	23:A:756:A:C8	2.49	0.48
23:A:2546:G:H2'	23:A:2547:U:C6	2.48	0.48
34:P:47:LEU:HD21	34:P:66:ILE:HD11	1.94	0.48
1:a:41:G:H2'	1:a:42:G:C8	2.49	0.48
1:a:704:A:H2'	1:a:705:U:H6	1.79	0.48
2:b:79:SER:O	2:b:82:ASP:N	2.47	0.48
23:A:2097:C:H2'	23:A:2098:C:H6	1.74	0.48
23:A:2219:U:H2'	23:A:2220:A:C8	2.48	0.48
24:B:30:C:N4	24:B:31:G:O6	2.46	0.48
1:a:1316:G:OP2	13:m:98:ARG:NH1	2.47	0.48
4:d:15:LEU:HD21	4:d:56:LYS:HA	1.96	0.48
8:h:24:LYS:NZ	8:h:26:GLU:OE2	2.33	0.48
23:A:799:G:H2'	23:A:800:U:C6	2.49	0.48
23:A:1823:C:O2'	25:C:208:ALA:HB2	2.13	0.48
1:a:397:A:H3'	1:a:398:C:H6	1.79	0.48
1:a:523:G:H2'	1:a:524:U:H6	1.79	0.48
23:A:287:C:H2'	23:A:288:U:C6	2.48	0.48
23:A:629:A:N1	23:A:855:G:O2'	2.46	0.48
23:A:2494:C:H2'	23:A:2495:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:R:100:LEU:HD23	36:R:103:LEU:HD23	1.96	0.48
4:d:103:LEU:HD23	4:d:155:LEU:HD11	1.96	0.47
23:A:183:G:O6	27:E:58:ARG:NH2	2.47	0.47
23:A:1469:A:H2'	23:A:1471:G:N7	2.29	0.47
23:A:1712:U:O2'	23:A:2719:G:H4'	2.14	0.47
23:A:1829:U:H2'	23:A:1830:C:H6	1.79	0.47
30:L:2:ARG:HH21	38:T:12:ILE:HD11	1.78	0.47
1:a:445:U:H2'	1:a:446:G:C8	2.49	0.47
1:a:1373:C:O2'	10:j:62:ARG:NH2	2.46	0.47
23:A:130:A:H2'	23:A:131:C:C6	2.49	0.47
23:A:749:U:H2'	23:A:750:G:O4'	2.15	0.47
23:A:2873:G:H2'	23:A:2874:A:C8	2.49	0.47
27:E:148:VAL:HG12	27:E:191:LYS:HD2	1.94	0.47
1:a:494:U:H2'	1:a:495:A:C8	2.49	0.47
18:r:56:GLN:O	18:r:60:THR:HG23	2.14	0.47
23:A:2148:G:HO2'	23:A:2199:G:H22	1.55	0.47
29:G:98:LYS:HZ2	29:G:101:ASP:C	2.22	0.47
1:a:392:G:H2'	1:a:393:U:C6	2.50	0.47
1:a:653:G:C2	1:a:654:G:C8	3.03	0.47
1:a:1155:C:O2'	9:i:7:TYR:OH	2.27	0.47
5:e:89:HIS:ND1	5:e:94:GLU:OE2	2.47	0.47
23:A:1449:C:H2'	23:A:1450:A:H8	1.79	0.47
23:A:1595:G:HO2'	23:A:1596:A:H8	1.57	0.47
23:A:2152:A:H2	23:A:2204:A:H5'	1.79	0.47
23:A:2682:U:H2'	23:A:2683:C:H6	1.78	0.47
1:a:196:U:O2	17:q:67:ARG:NH1	2.47	0.47
1:a:398:C:H2'	1:a:399:G:C8	2.49	0.47
10:j:46:LYS:HB3	10:j:68:ARG:HG2	1.96	0.47
12:l:53:MET:HG2	12:l:65:TYR:CE1	2.49	0.47
23:A:155:U:H2'	23:A:156:A:C8	2.49	0.47
23:A:1117:G:N3	23:A:1135:G:O2'	2.42	0.47
23:A:1249:A:N3	32:N:4:HIS:HB3	2.29	0.47
23:A:2238:C:H2'	23:A:2239:A:H8	1.79	0.47
23:A:2676:G:H2'	23:A:2677:A:H8	1.79	0.47
2:b:129:LEU:HD12	2:b:132:LYS:HE2	1.97	0.47
8:h:22:HIS:O	8:h:66:TYR:OH	2.27	0.47
15:o:75:VAL:O	15:o:79:ARG:HG3	2.14	0.47
23:A:395:U:H2'	23:A:396:U:C6	2.49	0.47
23:A:579:U:H2'	23:A:580:U:C6	2.50	0.47
23:A:622:A:H2'	23:A:623:C:C6	2.50	0.47
23:A:1311:G:OP1	47:4:16:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1457:A:H2	23:A:1638:G:H1	1.62	0.47
33:O:44:ASN:HB3	33:O:70:PRO:HG3	1.97	0.47
1:a:45:U:H2'	1:a:46:G:H8	1.79	0.47
1:a:225:A:H2'	1:a:226:U:C6	2.50	0.47
1:a:1033:U:H5''	1:a:1034:U:H5'	1.95	0.47
1:a:1044:G:H2'	1:a:1045:A:C8	2.50	0.47
2:b:46:THR:HA	2:b:49:LYS:CD	2.45	0.47
4:d:163:GLU:OE2	4:d:178:ARG:NH2	2.48	0.47
7:g:27:ILE:HG13	7:g:43:LEU:HD22	1.96	0.47
7:g:71:PRO:O	7:g:96:ARG:NH1	2.48	0.47
20:t:20:ARG:O	20:t:23:SER:OG	2.29	0.47
23:A:4:U:H2'	23:A:5:A:C8	2.49	0.47
23:A:133:A:H2'	23:A:134:U:H6	1.79	0.47
23:A:258:A:H2'	23:A:259:A:C8	2.49	0.47
23:A:1409:A:OP1	43:Z:30:LYS:NZ	2.40	0.47
23:A:1430:C:H2'	23:A:1431:A:H8	1.79	0.47
23:A:1922:A:H2'	23:A:1923:A:C8	2.49	0.47
23:A:2114:C:OP1	43:Z:17:LYS:NZ	2.45	0.47
23:A:2114:C:H2'	23:A:2115:A:H8	1.80	0.47
23:A:2886:G:N2	23:A:2889:A:OP2	2.39	0.47
25:C:37:LEU:HG	25:C:62:TYR:HB2	1.95	0.47
26:D:132:PRO:O	26:D:137:SER:OG	2.29	0.47
1:a:1257:A:H2'	1:a:1258:A:C8	2.49	0.47
23:A:1055:A:OP2	30:L:40:LYS:NZ	2.48	0.47
23:A:1886:A:H2'	23:A:1887:A:C8	2.49	0.47
28:F:27:GLU:N	28:F:27:GLU:OE1	2.48	0.47
28:F:36:ILE:O	28:F:88:LYS:HA	2.14	0.47
23:A:348:C:H2'	23:A:349:U:C6	2.50	0.47
23:A:1763:U:C2	23:A:1778:A:N6	2.79	0.47
28:F:130:LEU:HB3	28:F:154:VAL:HB	1.97	0.47
41:W:70:LEU:HD22	41:W:101:ILE:HD13	1.97	0.47
1:a:722:G:H2'	1:a:723:A:H8	1.77	0.47
7:g:125:MET:O	7:g:129:ASN:ND2	2.48	0.47
8:h:115:ASP:N	8:h:115:ASP:OD1	2.46	0.47
23:A:59:G:O2'	23:A:74:U:OP2	2.27	0.47
23:A:1137:G:H1	23:A:1147:U:H1'	1.80	0.47
23:A:1352:A:H2'	23:A:1353:G:O4'	2.16	0.47
23:A:1364:G:OP2	23:A:1364:G:N2	2.35	0.47
23:A:2324:U:H2'	23:A:2325:U:H6	1.80	0.47
29:G:41:ILE:HD12	29:G:52:VAL:HG23	1.97	0.47
1:a:523:G:H2'	1:a:524:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:609:G:H2'	1:a:610:A:H8	1.80	0.46
1:a:621:C:H2'	1:a:622:C:C6	2.51	0.46
1:a:1151:G:H2'	1:a:1152:G:H8	1.79	0.46
1:a:1334:A:H2'	1:a:1335:C:H6	1.80	0.46
9:i:71:GLY:O	9:i:75:GLN:HG2	2.15	0.46
23:A:688:A:O2'	23:A:689:A:OP1	2.31	0.46
23:A:1760:U:H5''	23:A:1761:A:H2'	1.97	0.46
23:A:1812:U:OP2	23:A:1817:A:N6	2.43	0.46
23:A:1987:G:O2'	23:A:1989:U:O4	2.30	0.46
1:a:71:C:H2'	1:a:72:G:C8	2.51	0.46
2:b:58:ARG:HH12	2:b:220:ALA:HB1	1.80	0.46
3:c:90:LEU:HD12	3:c:100:ILE:HD11	1.96	0.46
5:e:76:PRO:HB3	5:e:150:ASN:HD21	1.80	0.46
23:A:69:C:H4'	23:A:75:G:N7	2.30	0.46
23:A:999:A:C2	23:A:1000:G:C8	3.02	0.46
23:A:1129:G:N2	23:A:1131:A:H3'	2.30	0.46
23:A:1829:U:H2'	23:A:1830:C:C6	2.51	0.46
23:A:2125:G:H4'	23:A:2126:G:H5''	1.97	0.46
23:A:2668:U:O2'	26:D:82:GLU:OE2	2.24	0.46
33:O:54:MET:SD	33:O:106:ILE:HD11	2.56	0.46
50:7:8:ARG:HA	50:7:8:ARG:HD2	1.78	0.46
1:a:521:A:H2'	1:a:522:C:C6	2.51	0.46
4:d:9:TRP:HE1	4:d:24:LYS:NZ	2.13	0.46
5:e:75:VAL:HG12	5:e:145:ILE:HG21	1.96	0.46
9:i:123:ARG:NH1	9:i:124:ALA:O	2.45	0.46
23:A:514:G:N7	49:6:39:ARG:NH2	2.63	0.46
23:A:1227:U:H2'	23:A:1228:U:C6	2.51	0.46
23:A:2216:C:H2'	23:A:2217:U:C6	2.49	0.46
23:A:2225:C:H2'	23:A:2226:A:H8	1.80	0.46
26:D:2:THR:HA	26:D:204:THR:HG21	1.98	0.46
26:D:123:ILE:HD11	26:D:141:ARG:CZ	2.46	0.46
1:a:560:U:H2'	1:a:561:G:C8	2.50	0.46
1:a:695:A:N6	1:a:711:G:H1'	2.30	0.46
1:a:934:G:O2'	1:a:936:G:OP1	2.24	0.46
1:a:1321:C:H2'	1:a:1322:U:C6	2.51	0.46
17:q:49:HIS:H	17:q:76:ARG:HA	1.79	0.46
20:t:35:PHE:HE2	20:t:78:LEU:HB2	1.80	0.46
23:A:639:U:H2'	23:A:640:G:H8	1.79	0.46
23:A:1459:U:H2'	23:A:1460:G:C8	2.51	0.46
23:A:1727:A:C4	23:A:1728:A:C8	3.03	0.46
23:A:2141:U:H3	23:A:2214:G:H1	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2586:G:C2	23:A:2616:G:H1'	2.50	0.46
23:A:2778:C:H2'	23:A:2779:U:C6	2.50	0.46
44:1:2:LYS:O	44:1:4:ASN:N	2.48	0.46
1:a:563:C:H2'	1:a:564:C:C6	2.50	0.46
1:a:945:C:C2	1:a:946:A:C8	3.03	0.46
3:c:33:HIS:NE2	14:n:25:GLU:HB2	2.31	0.46
7:g:72:LEU:HG	7:g:96:ARG:HH12	1.81	0.46
14:n:14:PRO:HG3	14:n:20:ALA:HB2	1.98	0.46
23:A:985:G:OP1	50:7:59:ARG:NH1	2.47	0.46
23:A:1117:G:H2'	23:A:1118:C:C6	2.50	0.46
23:A:1130:A:H2'	23:A:1131:A:C4	2.51	0.46
23:A:1140:U:H1'	23:A:1143:U:H5	1.79	0.46
23:A:2107:U:H2'	23:A:2108:U:H6	1.80	0.46
25:C:67:PHE:HE1	25:C:105:ILE:HD11	1.80	0.46
29:G:59:LYS:HE2	29:G:62:ARG:HD2	1.97	0.46
31:M:63:VAL:HG12	31:M:106:LEU:HD11	1.98	0.46
1:a:847:G:H2'	1:a:848:G:C8	2.50	0.46
1:a:942:G:OP2	7:g:2:PRO:HB2	2.14	0.46
1:a:1017:C:H2'	1:a:1018:U:H6	1.81	0.46
2:b:108:GLN:HE22	2:b:109:LYS:HE3	1.81	0.46
23:A:1129:G:N2	23:A:1132:A:OP2	2.40	0.46
23:A:1623:A:H2'	23:A:1624:A:H8	1.81	0.46
24:B:19:A:H2'	24:B:20:A:H8	1.81	0.46
28:F:34:ILE:HD11	28:F:91:LEU:HD11	1.98	0.46
1:a:1135:U:OP1	10:j:7:ARG:NH2	2.41	0.46
1:a:1334:A:H2'	1:a:1335:C:C6	2.51	0.46
1:a:1387:U:O4	7:g:3:ARG:HB2	2.16	0.46
4:d:184:GLU:O	4:d:184:GLU:HG2	2.15	0.46
20:t:21:ASN:HD22	20:t:65:LEU:HB3	1.81	0.46
23:A:139:A:C2	23:A:1453:G:H1'	2.51	0.46
23:A:422:G:H2'	23:A:423:A:C8	2.48	0.46
23:A:910:A:H2'	23:A:911:G:H8	1.81	0.46
23:A:2173:G:N2	23:A:2184:U:O2	2.29	0.46
28:F:33:LYS:HA	28:F:96:MET:HE1	1.97	0.46
48:5:7:LEU:HD11	48:5:32:LEU:HD12	1.98	0.46
8:h:29:ALA:HB2	8:h:60:ILE:HG23	1.98	0.46
23:A:115:C:O2'	23:A:125:A:N3	2.45	0.46
23:A:879:C:C2	23:A:880:U:C5	3.04	0.46
23:A:942:U:H3'	23:A:945:C:H5	1.81	0.46
24:B:41:C:O2	28:F:92:ARG:NH1	2.44	0.46
28:F:97:TYR:O	28:F:101:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:415:U:H2'	1:a:416:A:H8	1.80	0.46
1:a:1375:A:OP2	9:i:114:LYS:HG3	2.16	0.46
10:j:45:GLU:HG2	10:j:69:THR:HB	1.98	0.46
23:A:5:A:H2'	23:A:6:A:C8	2.51	0.46
23:A:1360:U:H2'	23:A:1361:G:H8	1.81	0.46
23:A:1479:A:H2'	23:A:1480:C:C6	2.51	0.46
23:A:2547:U:H2'	23:A:2548:C:H6	1.80	0.46
29:G:26:VAL:HG12	29:G:79:VAL:HG11	1.97	0.46
2:b:115:LYS:HB3	2:b:119:LYS:HZ3	1.79	0.46
19:s:64:GLU:O	46:3:70:ARG:NH1	2.49	0.46
23:A:74:U:H5''	23:A:75:G:O4'	2.16	0.46
23:A:993:A:H2'	23:A:994:C:C6	2.51	0.46
23:A:2299:A:H4'	23:A:2300:A:N3	2.31	0.46
24:B:34:C:N3	24:B:47:C:O2'	2.49	0.46
27:E:148:VAL:HG23	27:E:149:ASP:N	2.31	0.46
46:3:67:ALA:H	46:3:71:VAL:HG21	1.81	0.46
1:a:1152:G:N2	1:a:1154:A:H62	2.14	0.45
16:p:5:ILE:HA	16:p:22:VAL:HA	1.97	0.45
23:A:1806:A:N7	23:A:1862:A:H1'	2.31	0.45
28:F:116:GLY:O	28:F:118:SER:N	2.49	0.45
36:R:105:GLY:C	36:R:107:ALA:H	2.24	0.45
41:W:9:VAL:HG13	41:W:68:VAL:HG13	1.97	0.45
45:2:7:THR:OG1	45:2:34:VAL:HG22	2.16	0.45
1:a:201:C:H2'	1:a:202:G:H8	1.82	0.45
1:a:343:C:H2'	1:a:344:A:C8	2.51	0.45
2:b:49:LYS:NZ	2:b:201:PRO:HG2	2.30	0.45
16:p:6:ARG:NH2	16:p:25:SER:HA	2.31	0.45
23:A:66:C:H2'	23:A:67:A:C8	2.50	0.45
23:A:1129:G:H1'	23:A:1132:A:N6	2.30	0.45
23:A:1242:C:C2	23:A:1243:G:C8	3.04	0.45
23:A:1906:G:H2'	23:A:1907:C:C6	2.51	0.45
23:A:2319:A:H2'	48:5:26:ASN:HD21	1.82	0.45
26:D:50:GLN:HE21	26:D:80:ILE:HG21	1.80	0.45
31:M:19:VAL:CG1	31:M:41:CYS:HB2	2.46	0.45
46:3:76:LYS:HD3	46:3:77:LYS:HZ2	1.82	0.45
1:a:1419:C:H2'	1:a:1420:A:H8	1.80	0.45
1:a:1442:G:H2'	1:a:1443:U:H6	1.80	0.45
16:p:5:ILE:O	16:p:5:ILE:HG13	2.16	0.45
23:A:2184:U:H2'	23:A:2185:A:H8	1.79	0.45
23:A:2789:U:O2'	23:A:2790:A:OP2	2.29	0.45
1:a:238:G:H5'	16:p:24:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:69:ARG:NH1	12:l:75:GLU:HG2	2.31	0.45
23:A:924:U:H1'	23:A:946:G:C6	2.52	0.45
23:A:1287:U:H2'	23:A:1288:U:C6	2.51	0.45
23:A:2182:C:H2'	23:A:2183:A:H8	1.82	0.45
41:W:49:ASN:OD1	41:W:50:ILE:N	2.49	0.45
43:Z:12:SER:HB2	43:Z:30:LYS:HD3	1.97	0.45
46:3:31:SER:HB2	46:3:46:LEU:HD13	1.99	0.45
50:7:55:PHE:O	50:7:59:ARG:HG3	2.16	0.45
1:a:17:U:H2'	1:a:18:C:C6	2.52	0.45
1:a:22:G:O2'	1:a:922:A:N1	2.47	0.45
1:a:850:U:O2'	1:a:853:C:N4	2.50	0.45
1:a:1208:A:H1'	1:a:1209:U:OP2	2.17	0.45
1:a:1268:A:N6	1:a:1281:G:H1'	2.30	0.45
2:b:79:SER:O	2:b:80:VAL:C	2.57	0.45
9:i:28:ILE:HG23	9:i:63:VAL:CG2	2.46	0.45
13:m:19:LEU:HD11	13:m:34:LEU:HD21	1.99	0.45
23:A:879:C:H2'	23:A:880:U:H6	1.80	0.45
23:A:910:A:H2'	23:A:911:G:C8	2.51	0.45
35:Q:32:ASN:OD1	35:Q:33:VAL:N	2.50	0.45
43:Z:8:THR:O	43:Z:10:ARG:N	2.46	0.45
1:a:499:A:H2'	1:a:500:A:H8	1.80	0.45
1:a:1497:G:H2'	1:a:1498:U:H6	1.82	0.45
2:b:27:MET:HE1	2:b:187:VAL:HG21	1.98	0.45
17:q:49:HIS:HB2	17:q:73:LYS:HE2	1.98	0.45
21:x:30:G:C2	21:x:31:A:C8	3.05	0.45
23:A:65:A:H2'	23:A:66:C:H6	1.82	0.45
23:A:339:U:H2'	23:A:340:G:O4'	2.17	0.45
23:A:994:C:H1'	23:A:1030:G:C8	2.51	0.45
23:A:1642:U:H2'	23:A:1643:A:C8	2.52	0.45
23:A:2176:C:H2'	23:A:2177:G:O4'	2.16	0.45
30:L:137:LYS:HE3	30:L:137:LYS:HB2	1.80	0.45
46:3:25:SER:OG	46:3:26:GLY:N	2.50	0.45
1:a:193:G:N1	1:a:196:U:OP2	2.40	0.45
1:a:563:C:H2'	1:a:564:C:H6	1.79	0.45
1:a:874:A:H2'	1:a:875:C:C6	2.52	0.45
15:o:33:THR:O	15:o:37:ASN:ND2	2.50	0.45
23:A:487:U:H2'	23:A:488:G:C8	2.51	0.45
23:A:713:U:H2'	23:A:714:A:O4'	2.17	0.45
23:A:1456:A:H2'	23:A:1457:A:C8	2.51	0.45
23:A:1528:G:O2'	23:A:1529:U:OP1	2.34	0.45
23:A:2141:U:H2'	23:A:2142:U:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2773:A:H2'	23:A:2774:A:C8	2.52	0.45
23:A:2776:C:OP1	51:8:33:LYS:NZ	2.50	0.45
23:A:2834:A:O2'	23:A:2835:A:H8	2.00	0.45
1:a:550:U:P	4:d:10:LYS:HZ3	2.39	0.45
1:a:1387:U:H5	7:g:3:ARG:HB3	1.82	0.45
23:A:332:U:O2	23:A:393:G:N2	2.41	0.45
23:A:1015:G:H2'	23:A:1016:U:C6	2.52	0.45
23:A:2876:U:H2'	23:A:2877:G:O4'	2.17	0.45
24:B:110:G:H2'	24:B:111:C:C6	2.51	0.45
28:F:33:LYS:O	28:F:157:VAL:HG22	2.16	0.45
43:Z:59:VAL:HG12	43:Z:60:GLU:N	2.28	0.45
16:p:5:ILE:HG22	16:p:22:VAL:HB	1.99	0.45
23:A:525:A:H1'	23:A:526:A:H5''	1.99	0.45
23:A:578:G:H2'	23:A:579:U:C6	2.52	0.45
23:A:1824:A:C2	23:A:1862:A:C4'	3.00	0.45
23:A:1922:A:H2'	23:A:1923:A:H8	1.81	0.45
23:A:2488:G:H2'	23:A:2489:C:C6	2.52	0.45
29:G:76:VAL:HA	29:G:79:VAL:HG12	1.99	0.45
1:a:328:G:H2'	1:a:329:A:C8	2.52	0.45
1:a:550:U:H2'	1:a:551:G:H8	1.81	0.45
13:m:87:ARG:HG2	13:m:97:VAL:HG13	1.98	0.45
16:p:10:MET:CE	16:p:19:ARG:HD2	2.46	0.45
23:A:746:G:O2'	23:A:1681:A:N3	2.47	0.45
23:A:1129:G:H21	23:A:1131:A:H3'	1.82	0.45
23:A:1548:C:C2	23:A:1549:G:C8	3.05	0.45
23:A:2167:A:N6	23:A:2190:G:H1'	2.31	0.45
23:A:2488:G:H2'	23:A:2489:C:H6	1.82	0.45
24:B:21:G:H2'	24:B:22:G:C8	2.51	0.45
25:C:108:LYS:HB2	25:C:196:GLY:HA2	1.99	0.45
1:a:414:G:H21	4:d:112:GLN:NE2	2.15	0.44
1:a:430:C:H4'	1:a:431:G:C2	2.52	0.44
1:a:560:U:C2	1:a:561:G:C8	3.04	0.44
4:d:85:ASN:HA	4:d:88:ILE:HG12	1.99	0.44
16:p:49:VAL:HG21	16:p:73:LEU:HD22	1.98	0.44
23:A:52:A:H2'	23:A:53:A:C8	2.51	0.44
23:A:800:U:H2'	23:A:801:G:C8	2.52	0.44
23:A:810:A:H5'	25:C:209:GLY:HA3	1.98	0.44
23:A:1046:A:H2'	23:A:1047:A:H8	1.78	0.44
23:A:1244:U:H2'	23:A:1245:U:C6	2.52	0.44
23:A:1580:A:H2'	23:A:1581:G:O4'	2.16	0.44
23:A:2225:C:H2'	23:A:2226:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2547:U:H2'	23:A:2548:C:C6	2.52	0.44
29:G:86:LYS:NZ	29:G:132:ILE:HD11	2.32	0.44
36:R:88:ARG:NH2	36:R:112:GLU:HB2	2.32	0.44
38:T:62:VAL:HA	38:T:95:LEU:HD23	1.99	0.44
13:m:7:VAL:HG22	13:m:8:ASP:N	2.32	0.44
19:s:18:LYS:HD2	19:s:18:LYS:HA	1.85	0.44
23:A:1525:U:H2'	23:A:1526:G:C8	2.53	0.44
1:a:1047:A:H2'	1:a:1048:A:C8	2.52	0.44
1:a:1421:C:H2'	1:a:1422:G:H8	1.83	0.44
1:a:1520:U:H2'	1:a:1521:A:C8	2.52	0.44
7:g:66:MET:HE3	7:g:70:MET:HE3	1.99	0.44
8:h:77:LEU:HG	8:h:131:VAL:HG23	1.99	0.44
23:A:247:G:O2'	23:A:430:A:N1	2.44	0.44
23:A:1640:A:H2'	23:A:1641:G:H8	1.82	0.44
23:A:2867:G:C4	23:A:2868:G:C8	3.05	0.44
24:B:11:A:O2'	24:B:13:G:OP2	2.35	0.44
26:D:66:GLN:HA	26:D:69:VAL:HG22	1.99	0.44
27:E:154:ILE:HB	27:E:175:VAL:HG22	1.99	0.44
1:a:381:A:H2'	1:a:382:A:H8	1.82	0.44
1:a:547:A:H2'	1:a:548:G:H8	1.82	0.44
1:a:899:G:O2'	1:a:915:G:O6	2.32	0.44
1:a:1258:A:H2'	1:a:1259:A:C8	2.52	0.44
6:f:78:ASP:OD1	6:f:90:HIS:NE2	2.43	0.44
11:k:74:ALA:HB1	11:k:79:LEU:HD21	2.00	0.44
15:o:18:HIS:HD2	15:o:20:THR:H	1.64	0.44
23:A:1074:A:N3	23:A:2519:G:O2'	2.46	0.44
23:A:1551:U:H2'	23:A:1552:U:C6	2.52	0.44
24:B:42:G:C2	24:B:46:A:C2	3.05	0.44
28:F:12:ILE:HG12	28:F:172:GLN:HG2	2.00	0.44
28:F:109:PRO:HG2	46:3:51:SER:HA	1.99	0.44
1:a:212:G:H2'	1:a:213:A:C8	2.52	0.44
1:a:547:A:H2'	1:a:548:G:C8	2.53	0.44
1:a:853:C:H2'	1:a:854:G:O4'	2.18	0.44
1:a:1233:C:C5	13:m:103:LYS:HA	2.52	0.44
16:p:6:ARG:HG2	16:p:7:LEU:H	1.82	0.44
23:A:1551:U:H2'	23:A:1552:U:H6	1.82	0.44
23:A:1727:A:H2'	23:A:1728:A:H8	1.83	0.44
23:A:1835:A:H2'	23:A:1836:A:H8	1.78	0.44
30:L:126:TYR:OH	30:L:133:HIS:NE2	2.49	0.44
41:W:6:GLY:O	41:W:22:LYS:NZ	2.49	0.44
1:a:522:C:H2'	1:a:523:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:792:A:H2'	1:a:793:G:H8	1.82	0.44
1:a:885:A:H2'	1:a:886:C:C6	2.52	0.44
3:c:8:ILE:O	3:c:12:ILE:HG12	2.17	0.44
8:h:9:ASP:O	8:h:13:ARG:HG3	2.16	0.44
23:A:650:U:C5	23:A:665:G:C5	3.05	0.44
1:a:216:G:H2'	1:a:217:U:C6	2.52	0.44
1:a:561:G:H2'	1:a:562:U:H6	1.83	0.44
1:a:792:A:H2'	1:a:793:G:C8	2.53	0.44
1:a:1333:U:H2'	1:a:1334:A:C8	2.46	0.44
1:a:1384:A:C5	7:g:7:VAL:HG11	2.53	0.44
2:b:170:ARG:HA	2:b:173:VAL:HG12	1.98	0.44
23:A:66:C:C2	23:A:67:A:C8	3.05	0.44
23:A:679:G:H2'	23:A:680:C:C6	2.53	0.44
23:A:1322:A:H2'	23:A:1323:G:H8	1.83	0.44
23:A:1405:G:H2'	23:A:1406:C:C6	2.53	0.44
6:f:43:GLU:OE2	6:f:45:GLY:HA2	2.18	0.44
13:m:22:ILE:HG23	13:m:66:GLU:OE2	2.17	0.44
13:m:89:MET:HB3	13:m:93:ARG:HH12	1.83	0.44
23:A:897:G:H2'	23:A:898:U:C6	2.53	0.44
23:A:1354:G:N2	23:A:1357:U:C4	2.85	0.44
23:A:1464:A:N7	23:A:1634:A:N6	2.66	0.44
43:Z:25:SER:OG	43:Z:26:LYS:N	2.49	0.44
1:a:45:U:H2'	1:a:46:G:C8	2.53	0.44
1:a:1170:C:H2'	1:a:1171:G:H8	1.83	0.44
2:b:49:LYS:NZ	2:b:201:PRO:O	2.43	0.44
2:b:78:GLU:N	2:b:78:GLU:OE2	2.50	0.44
2:b:114:LEU:CD1	2:b:144:LEU:HD22	2.47	0.44
11:k:53:LYS:O	11:k:57:LYS:HG3	2.18	0.44
13:m:90:ARG:HA	13:m:90:ARG:HD2	1.89	0.44
21:x:26:A:N6	21:x:44:G:H1	2.14	0.44
23:A:311:A:H2	23:A:312:U:H3	1.64	0.44
23:A:1602:C:OP1	23:A:1768:U:O2'	2.33	0.44
23:A:2349:U:H2'	23:A:2350:C:C6	2.53	0.44
23:A:2587:U:H2'	23:A:2588:U:C6	2.53	0.44
25:C:21:PHE:HB3	25:C:24:ILE:HD12	1.99	0.44
44:1:27:ASN:O	44:1:31:GLN:HG3	2.17	0.44
1:a:218:U:H2'	1:a:219:U:H2'	1.99	0.43
1:a:468:A:C6	1:a:482:G:C6	3.06	0.43
1:a:499:A:H2'	1:a:500:A:C8	2.53	0.43
1:a:1406:C:O2	1:a:1510:A:N6	2.51	0.43
15:o:60:VAL:HG11	23:A:761:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:81:GLU:CD	16:p:85:ASN:HD21	2.26	0.43
19:s:35:SER:OG	19:s:38:SER:OG	2.27	0.43
23:A:279:G:H2'	23:A:280:A:C8	2.53	0.43
23:A:566:U:H2'	23:A:567:G:C8	2.53	0.43
23:A:775:G:C8	25:C:207:LYS:HD2	2.53	0.43
23:A:2084:A:OP2	23:A:2084:A:H8	2.00	0.43
33:O:11:ARG:HG2	33:O:87:LYS:HD3	1.99	0.43
36:R:104:ARG:HD3	36:R:104:ARG:HA	1.88	0.43
41:W:9:VAL:CG1	41:W:68:VAL:HG13	2.48	0.43
51:8:16:VAL:HG22	51:8:25:VAL:HG12	1.99	0.43
1:a:1023:A:C2	1:a:1226:U:H1'	2.53	0.43
9:i:11:ARG:HG3	9:i:16:VAL:HG23	1.98	0.43
12:l:26:LYS:HD2	12:l:35:LEU:HD23	2.00	0.43
23:A:271:C:H5''	23:A:297:U:O4	2.18	0.43
23:A:2899:C:H2'	23:A:2900:G:O4'	2.18	0.43
1:a:494:U:H2'	1:a:495:A:H8	1.82	0.43
1:a:877:C:H2'	1:a:878:A:O4'	2.18	0.43
7:g:40:GLN:HG2	7:g:44:TYR:CE2	2.53	0.43
23:A:756:A:H2'	23:A:757:A:H8	1.83	0.43
23:A:861:U:OP2	38:T:84:LYS:NZ	2.47	0.43
23:A:1311:G:OP2	39:U:20:ARG:NH2	2.51	0.43
23:A:1749:A:H3'	23:A:1750:A:H8	1.83	0.43
23:A:1903:U:O2'	23:A:1904:C:O2	2.31	0.43
1:a:57:G:H2'	1:a:58:C:C6	2.54	0.43
1:a:868:C:H2'	1:a:869:A:H8	1.83	0.43
5:e:42:ASP:N	5:e:42:ASP:OD1	2.49	0.43
20:t:4:ILE:HG22	20:t:6:SER:H	1.83	0.43
23:A:88:G:O2'	23:A:89:U:OP1	2.36	0.43
23:A:685:C:H2'	23:A:686:U:C6	2.54	0.43
23:A:859:U:H2'	23:A:860:C:H6	1.82	0.43
23:A:1253:C:HO2'	23:A:1254:G:P	2.40	0.43
23:A:2324:U:OP1	23:A:2413:U:O2'	2.37	0.43
23:A:2710:A:H2'	23:A:2711:C:C6	2.53	0.43
23:A:2832:G:H2'	23:A:2833:A:H8	1.83	0.43
24:B:18:G:H2'	24:B:19:A:C8	2.53	0.43
1:a:56:U:H2'	1:a:57:G:C8	2.53	0.43
1:a:1057:G:H5'	1:a:1058:U:OP1	2.19	0.43
1:a:1110:A:OP1	2:b:170:ARG:NH2	2.51	0.43
16:p:6:ARG:NH1	16:p:23:ALA:HB3	2.32	0.43
19:s:32:LYS:HA	19:s:50:ALA:HB3	2.00	0.43
23:A:30:G:H2'	23:A:31:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:363:A:H4'	23:A:365:A:N7	2.34	0.43
23:A:1225:G:H2'	23:A:1226:G:H8	1.83	0.43
23:A:1462:U:H1'	23:A:1464:A:C4	2.53	0.43
24:B:19:A:H2'	24:B:20:A:C8	2.54	0.43
29:G:41:ILE:HD11	29:G:68:THR:HG21	1.99	0.43
1:a:885:A:H2'	1:a:886:C:H6	1.83	0.43
1:a:1014:C:O2'	1:a:1048:A:H5'	2.19	0.43
1:a:1014:C:OP2	1:a:1033:U:H2'	2.18	0.43
1:a:1168:G:C2	1:a:1169:C:C6	3.07	0.43
4:d:145:SER:HB3	4:d:148:ASN:HB2	1.99	0.43
6:f:26:ARG:HH22	6:f:80:LEU:HD12	1.83	0.43
7:g:143:LYS:HB3	7:g:143:LYS:HE3	1.74	0.43
20:t:21:ASN:ND2	20:t:65:LEU:HB3	2.33	0.43
20:t:35:PHE:CE1	20:t:50:TYR:HB2	2.54	0.43
20:t:66:ILE:HD11	20:t:70:ASN:HD22	1.83	0.43
23:A:1136:U:C2	23:A:1148:C:H1'	2.54	0.43
23:A:2047:A:H2'	23:A:2048:A:C8	2.54	0.43
23:A:2160:G:N2	23:A:2195:A:H1'	2.34	0.43
23:A:2790:A:N1	29:G:67:THR:OG1	2.35	0.43
27:E:174:THR:HB	27:E:189:HIS:HE1	1.83	0.43
1:a:1174:G:N2	1:a:1176:A:H3'	2.33	0.43
4:d:87:MET:HE2	4:d:185:LEU:HD13	2.00	0.43
23:A:463:C:H2'	23:A:464:U:C6	2.53	0.43
23:A:651:A:H2'	23:A:652:A:H8	1.83	0.43
29:G:29:PRO:HD2	29:G:80:SER:HA	2.01	0.43
1:a:212:G:H2'	1:a:213:A:H8	1.84	0.43
1:a:266:G:H2'	1:a:267:G:H8	1.84	0.43
1:a:1183:A:H2'	1:a:1184:G:C8	2.54	0.43
3:c:152:VAL:HG12	3:c:156:LEU:HD21	2.01	0.43
17:q:50:ASP:OD1	17:q:53:ASN:N	2.49	0.43
23:A:688:A:HO2'	23:A:689:A:P	2.41	0.43
23:A:831:U:H4'	23:A:1812:U:H4'	1.99	0.43
23:A:1244:U:C2	23:A:1245:U:C5	3.07	0.43
23:A:1827:U:H2'	23:A:1828:C:H6	1.83	0.43
33:O:43:THR:HG22	33:O:94:VAL:HG12	2.01	0.43
1:a:1110:A:H8	2:b:171:ILE:HD12	1.83	0.43
1:a:1130:U:H2'	1:a:1131:U:C6	2.53	0.43
1:a:1144:U:O2'	1:a:1146:A:N7	2.45	0.43
3:c:152:VAL:HG22	3:c:197:VAL:HG22	2.01	0.43
8:h:32:ILE:O	8:h:36:ILE:HG12	2.18	0.43
10:j:18:LEU:HD21	10:j:72:ARG:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:5:A:H2'	23:A:6:A:H8	1.84	0.43
23:A:132:U:H2'	23:A:133:A:H8	1.83	0.43
23:A:788:C:H2'	23:A:789:A:C8	2.54	0.43
23:A:1389:C:C2	23:A:1390:G:N7	2.86	0.43
23:A:2070:A:H2'	23:A:2071:G:C8	2.53	0.43
25:C:4:LYS:N	25:C:18:SER:O	2.51	0.43
1:a:224:U:H2'	1:a:225:A:H8	1.84	0.43
1:a:413:U:OP1	1:a:414:G:O2'	2.37	0.43
1:a:469:A:H2'	1:a:470:G:C8	2.53	0.43
1:a:934:G:C2	1:a:936:G:C8	3.07	0.43
1:a:1474:C:H2'	1:a:1475:G:O4'	2.18	0.43
2:b:119:LYS:O	2:b:124:GLY:N	2.40	0.43
5:e:75:VAL:HG21	5:e:119:ALA:HB1	2.01	0.43
9:i:43:ALA:O	9:i:47:VAL:HG13	2.18	0.43
15:o:76:GLN:O	15:o:80:GLU:HG2	2.19	0.43
17:q:11:THR:HG23	17:q:62:ARG:HG2	2.01	0.43
19:s:9:PRO:HB3	46:3:77:LYS:HE2	2.01	0.43
23:A:981:C:H2'	23:A:982:U:H6	1.84	0.43
23:A:1763:U:O2'	23:A:1764:A:H5'	2.19	0.43
29:G:86:LYS:HZ2	29:G:132:ILE:HD11	1.84	0.43
42:Y:51:THR:HG23	42:Y:51:THR:O	2.19	0.43
1:a:57:G:H2'	1:a:58:C:H6	1.84	0.42
1:a:141:G:O2'	1:a:210:A:N1	2.42	0.42
1:a:217:U:H2'	1:a:218:U:O4'	2.19	0.42
1:a:534:C:OP2	12:l:101:LYS:NZ	2.49	0.42
1:a:1062:G:H4'	1:a:1063:C:H3'	2.01	0.42
1:a:1243:A:H2'	1:a:1244:C:C6	2.54	0.42
13:m:85:SER:OG	13:m:86:TYR:N	2.52	0.42
17:q:16:SER:OG	17:q:24:THR:OG1	2.32	0.42
17:q:30:TYR:CE1	17:q:41:LYS:HG2	2.53	0.42
23:A:29:U:H2'	23:A:30:G:C8	2.54	0.42
23:A:40:U:H2'	23:A:41:A:C8	2.52	0.42
23:A:613:G:H2'	23:A:2063:A:N7	2.34	0.42
23:A:2149:G:H2'	23:A:2150:A:C6	2.54	0.42
23:A:2520:G:H2'	23:A:2521:A:H8	1.83	0.42
26:D:130:ARG:HH11	26:D:133:MET:HE3	1.84	0.42
1:a:424:G:H2'	1:a:425:G:C8	2.53	0.42
1:a:723:A:H2'	1:a:724:A:H8	1.82	0.42
4:d:190:ASN:HB3	4:d:193:PHE:HD2	1.84	0.42
9:i:47:VAL:HA	9:i:50:GLN:HG3	2.01	0.42
23:A:623:C:H2'	23:A:624:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:686:U:H2'	23:A:687:G:O4'	2.20	0.42
23:A:869:A:H2'	23:A:870:G:C8	2.53	0.42
23:A:1874:U:C2	23:A:1875:G:C8	3.07	0.42
23:A:2545:C:H2'	23:A:2546:G:O4'	2.19	0.42
24:B:5:G:H4'	35:Q:34:PHE:CD2	2.54	0.42
31:M:120:GLU:OE1	36:R:65:SER:OG	2.30	0.42
1:a:787:C:H2'	1:a:788:A:O4'	2.19	0.42
1:a:1086:G:N2	1:a:1089:A:OP2	2.46	0.42
20:t:74:ASN:O	20:t:78:LEU:HG	2.19	0.42
23:A:873:U:O2'	23:A:2101:U:C2	2.71	0.42
23:A:1449:C:H2'	23:A:1450:A:C8	2.54	0.42
31:M:13:ASN:HD22	31:M:97:ARG:HG2	1.84	0.42
1:a:571:A:H2'	1:a:575:G:C8	2.53	0.42
1:a:1007:C:H5''	1:a:1008:C:OP2	2.18	0.42
4:d:61:TYR:OH	4:d:91:GLU:OE1	2.28	0.42
8:h:3:MET:HG3	8:h:4:THR:HG23	2.00	0.42
21:x:23:A:H2'	21:x:24:G:C8	2.53	0.42
23:A:636:A:H2'	23:A:637:U:C6	2.54	0.42
23:A:924:U:O2	23:A:945:C:N4	2.53	0.42
23:A:1653:C:O2'	23:A:1659:A:N1	2.44	0.42
23:A:2348:U:H2'	23:A:2349:U:H6	1.84	0.42
1:a:28:G:O2'	1:a:304:U:OP1	2.37	0.42
1:a:72:G:N1	1:a:95:A:N6	2.31	0.42
1:a:366:U:C2	1:a:367:A:C8	3.07	0.42
1:a:581:A:N3	1:a:892:C:O2'	2.49	0.42
4:d:81:LYS:NZ	5:e:102:ALA:HB1	2.35	0.42
5:e:76:PRO:HD2	5:e:148:LEU:HD12	2.01	0.42
20:t:12:LYS:O	20:t:16:THR:HG23	2.19	0.42
23:A:869:A:H2'	23:A:870:G:H8	1.84	0.42
23:A:1089:C:H2'	23:A:1090:U:C6	2.55	0.42
23:A:2170:C:H2'	23:A:2171:G:C8	2.53	0.42
23:A:2369:A:H61	42:Y:51:THR:CG2	2.32	0.42
25:C:144:ILE:HB	25:C:154:LEU:HB2	2.02	0.42
29:G:65:HIS:CD2	29:G:65:HIS:C	2.98	0.42
30:L:54:PHE:CD2	30:L:122:LYS:HG3	2.54	0.42
1:a:619:C:C4	1:a:620:C:C5	3.08	0.42
1:a:1009:U:H2'	1:a:1010:U:H6	1.84	0.42
1:a:1542:A:N3	1:a:1542:A:H2'	2.34	0.42
16:p:6:ARG:HG2	16:p:7:LEU:N	2.34	0.42
23:A:778:C:H2'	23:A:779:G:O4'	2.20	0.42
23:A:1161:A:H2'	23:A:1162:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1442:C:C2	23:A:1443:C:C5	3.08	0.42
23:A:1550:C:H2'	23:A:1551:U:H6	1.85	0.42
39:U:26:ILE:HG13	39:U:81:VAL:HG23	2.02	0.42
49:6:8:SER:HB3	49:6:11:LYS:HB2	2.01	0.42
1:a:390:A:H2'	1:a:391:A:H8	1.83	0.42
1:a:509:C:H2'	1:a:510:C:C6	2.55	0.42
1:a:521:A:H2'	1:a:522:C:H6	1.85	0.42
1:a:642:C:H2'	1:a:643:A:C8	2.53	0.42
1:a:720:A:H2'	1:a:721:G:C8	2.54	0.42
1:a:1469:G:H2'	1:a:1470:C:H6	1.84	0.42
6:f:30:ILE:HD12	6:f:80:LEU:HG	2.02	0.42
23:A:775:G:H5'	23:A:776:U:H5''	2.01	0.42
23:A:788:C:H2'	23:A:789:A:H8	1.84	0.42
23:A:1087:U:O2	23:A:1160:G:N2	2.42	0.42
23:A:1894:U:C2	23:A:1895:G:C8	3.07	0.42
23:A:2162:C:H2'	23:A:2163:G:C8	2.54	0.42
23:A:2349:U:H2'	23:A:2350:C:H6	1.85	0.42
23:A:2719:G:H2'	23:A:2720:U:C6	2.54	0.42
23:A:2735:G:C2	23:A:2736:C:C6	3.08	0.42
1:a:181:A:H4'	1:a:182:U:OP1	2.20	0.42
1:a:421:G:H4'	1:a:422:A:H5''	2.01	0.42
1:a:938:G:H2'	1:a:939:C:C6	2.55	0.42
4:d:197:PHE:O	4:d:200:ARG:HG2	2.19	0.42
8:h:48:ASP:HB3	8:h:63:PHE:CD2	2.54	0.42
9:i:7:TYR:OH	9:i:9:THR:OG1	2.35	0.42
23:A:390:A:H2'	23:A:391:U:C6	2.54	0.42
23:A:972:G:O3'	23:A:973:U:H2'	2.19	0.42
23:A:2304:G:OP1	42:Y:26:SER:HB3	2.19	0.42
26:D:122:VAL:HG21	26:D:143:PRO:HA	2.01	0.42
1:a:686:U:H2'	1:a:687:C:H6	1.85	0.42
1:a:1520:U:H2'	1:a:1521:A:H8	1.83	0.42
2:b:48:LYS:O	2:b:51:ASP:HB2	2.20	0.42
6:f:74:ILE:HD12	6:f:74:ILE:H	1.85	0.42
8:h:10:PHE:CD1	8:h:27:LEU:HD11	2.54	0.42
10:j:6:ILE:O	10:j:75:ASP:HA	2.20	0.42
11:k:21:ALA:HB2	11:k:82:LEU:HD21	2.01	0.42
23:A:330:A:H2'	23:A:331:G:C8	2.55	0.42
23:A:735:A:H2'	23:A:736:C:H6	1.85	0.42
23:A:929:G:H2'	23:A:930:C:C6	2.55	0.42
23:A:1488:U:H2'	23:A:1489:A:H8	1.85	0.42
24:B:63:C:O2'	24:B:106:C:N4	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:26:THR:OG1	26:D:190:GLY:O	2.38	0.42
26:D:126:HIS:CD2	26:D:159:LEU:HB3	2.55	0.42
46:3:10:ARG:HG2	46:3:11:PRO:HD2	2.01	0.42
1:a:35:G:H2'	1:a:36:C:H6	1.85	0.42
1:a:586:C:O2'	1:a:736:A:N3	2.48	0.42
4:d:3:ARG:NH1	4:d:63:LEU:O	2.52	0.42
4:d:154:SER:O	4:d:158:SER:HB3	2.20	0.42
23:A:271:C:O2	23:A:271:C:H2'	2.20	0.42
23:A:395:U:H2'	23:A:396:U:H6	1.85	0.42
23:A:1553:C:H2'	23:A:1554:U:C6	2.54	0.42
1:a:181:A:O2'	1:a:182:U:O5'	2.31	0.41
1:a:428:U:H4'	1:a:429:U:H5	1.85	0.41
1:a:561:G:C4	1:a:562:U:C5	3.08	0.41
1:a:833:G:H2'	1:a:834:C:C6	2.55	0.41
1:a:931:G:H2'	1:a:932:A:C8	2.54	0.41
2:b:113:HIS:O	2:b:117:ILE:HG12	2.20	0.41
4:d:49:LEU:O	4:d:53:GLU:HG2	2.20	0.41
6:f:72:ASP:OD1	6:f:73:SER:N	2.53	0.41
9:i:88:LEU:HD11	9:i:95:ARG:HD3	2.01	0.41
23:A:139:A:H4'	23:A:140:G:OP1	2.20	0.41
23:A:301:A:H2'	23:A:302:G:H8	1.85	0.41
23:A:1388:U:O2	23:A:1429:A:H5''	2.19	0.41
23:A:1401:C:H2'	23:A:1402:G:O4'	2.20	0.41
23:A:1685:U:H2'	23:A:1686:C:H6	1.82	0.41
23:A:2044:U:H2'	23:A:2045:G:O4'	2.20	0.41
23:A:2067:U:O2'	23:A:2068:G:H5'	2.20	0.41
23:A:2292:G:C8	23:A:2460:C:C4	3.08	0.41
23:A:2348:U:H2'	23:A:2349:U:C6	2.55	0.41
23:A:2731:U:H2'	23:A:2732:U:C6	2.55	0.41
26:D:146:MET:O	26:D:154:VAL:HG23	2.20	0.41
28:F:68:THR:OG1	28:F:85:ILE:O	2.38	0.41
33:O:42:ILE:HD12	33:O:97:VAL:HG21	2.01	0.41
39:U:64:GLU:HG2	39:U:71:ILE:HD11	2.02	0.41
1:a:104:C:H2'	1:a:105:G:O4'	2.19	0.41
1:a:528:A:OP2	12:l:61:ALA:HB1	2.20	0.41
1:a:1056:G:H5''	14:n:4:LYS:HD3	2.02	0.41
1:a:1070:G:OP2	3:c:3:GLN:NE2	2.47	0.41
1:a:1187:A:OP1	9:i:105:THR:OG1	2.31	0.41
1:a:1472:G:H2'	1:a:1473:C:H6	1.85	0.41
4:d:15:LEU:HD12	4:d:15:LEU:HA	1.87	0.41
23:A:448:A:H2'	23:A:449:U:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:906:G:O2'	23:A:963:G:O6	2.27	0.41
23:A:909:G:H2'	23:A:910:A:O4'	2.20	0.41
23:A:1336:U:H2'	23:A:1337:U:H6	1.84	0.41
23:A:2266:A:H2'	23:A:2267:G:C8	2.55	0.41
23:A:2809:A:H4'	23:A:2810:G:O5'	2.20	0.41
25:C:43:ARG:NH1	25:C:49:LEU:HD13	2.35	0.41
31:M:4:GLN:HG2	31:M:5:GLU:HG2	2.02	0.41
41:W:7:ASP:OD1	41:W:7:ASP:N	2.52	0.41
43:Z:61:ARG:O	43:Z:61:ARG:NH1	2.44	0.41
1:a:329:A:H2'	1:a:330:C:H6	1.84	0.41
1:a:444:C:H2'	1:a:445:U:C6	2.55	0.41
1:a:562:U:C2	1:a:563:C:C5	3.08	0.41
1:a:1411:C:H2'	1:a:1412:G:H8	1.85	0.41
1:a:1467:C:H2'	1:a:1468:A:H8	1.84	0.41
2:b:49:LYS:HA	2:b:52:GLU:OE1	2.19	0.41
11:k:36:ASP:OD1	11:k:37:THR:N	2.47	0.41
14:n:14:PRO:CB	14:n:19:GLN:HB2	2.46	0.41
21:x:70:G:H4'	23:A:1926:C:O2'	2.21	0.41
23:A:188:A:H2'	23:A:189:G:H8	1.85	0.41
23:A:330:A:H2'	23:A:331:G:H8	1.85	0.41
23:A:860:C:H2'	23:A:861:U:H6	1.84	0.41
23:A:2261:G:H22	43:Z:34:GLN:HE22	1.66	0.41
1:a:562:U:H2'	1:a:563:C:H6	1.84	0.41
3:c:151:GLN:HB3	3:c:166:HIS:HB3	2.01	0.41
6:f:37:GLU:HG3	6:f:67:ASN:HB3	2.02	0.41
7:g:65:ALA:O	7:g:69:ILE:HG12	2.19	0.41
19:s:12:ASP:OD2	19:s:14:HIS:NE2	2.52	0.41
23:A:229:A:O4'	23:A:231:A:N6	2.53	0.41
23:A:396:U:H2'	23:A:397:U:C6	2.56	0.41
23:A:731:A:N1	23:A:833:C:H1'	2.35	0.41
23:A:897:G:H2'	23:A:898:U:H6	1.84	0.41
23:A:1405:G:H2'	23:A:1406:C:H6	1.85	0.41
23:A:2139:G:H2'	23:A:2140:C:H6	1.86	0.41
23:A:2398:G:N7	50:7:39:LYS:NZ	2.56	0.41
23:A:2807:C:H2'	23:A:2808:A:O4'	2.20	0.41
23:A:2829:U:H2'	23:A:2830:C:C6	2.56	0.41
29:G:25:THR:HA	29:G:34:VAL:HG12	2.03	0.41
39:U:16:ARG:HH21	39:U:103:LYS:HD2	1.85	0.41
43:Z:59:VAL:CG1	43:Z:60:GLU:H	2.29	0.41
1:a:755:U:H2'	1:a:756:A:C8	2.55	0.41
1:a:1326:A:OP1	19:s:3:ARG:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1435:A:H2'	1:a:1436:C:H6	1.86	0.41
3:c:135:GLN:HG2	3:c:139:ARG:NH1	2.36	0.41
4:d:83:GLY:HA3	4:d:191:GLU:OE1	2.21	0.41
11:k:29:ASN:ND2	11:k:57:LYS:HD2	2.36	0.41
17:q:17:ASP:HA	17:q:23:ILE:HG22	2.03	0.41
23:A:1129:G:H21	23:A:1131:A:H8	1.67	0.41
23:A:1178:U:H3'	23:A:1179:A:H5''	2.02	0.41
23:A:2141:U:H2'	23:A:2142:U:C6	2.55	0.41
23:A:2472:A:H4'	23:A:2473:C:O5'	2.20	0.41
23:A:2682:U:H2'	23:A:2683:C:C6	2.55	0.41
23:A:2925:U:H2'	23:A:2926:U:C6	2.56	0.41
26:D:84:ARG:O	26:D:86:VAL:HG23	2.20	0.41
1:a:621:C:H2'	1:a:622:C:H6	1.85	0.41
1:a:675:G:H2'	1:a:676:A:H8	1.86	0.41
1:a:1324:C:O2	19:s:37:ARG:NH2	2.46	0.41
1:a:1545:U:H2'	1:a:1546:C:C6	2.55	0.41
6:f:42:LYS:HG3	6:f:43:GLU:H	1.86	0.41
12:l:26:LYS:NZ	12:l:74:ILE:HD11	2.35	0.41
14:n:16:TYR:H	14:n:19:GLN:HG3	1.86	0.41
15:o:69:TYR:HA	15:o:72:LYS:HG2	2.02	0.41
23:A:75:G:C2	23:A:76:C:C5	3.09	0.41
23:A:498:G:OP1	27:E:57:VAL:HG13	2.21	0.41
23:A:1108:G:C4	23:A:1109:G:C8	3.09	0.41
23:A:1372:G:H2'	23:A:1374:C:C5	2.56	0.41
23:A:2166:G:H1'	23:A:2191:A:N6	2.34	0.41
23:A:2789:U:H5''	51:8:19:ARG:HG2	2.02	0.41
23:A:2842:U:H2'	23:A:2843:C:H6	1.85	0.41
26:D:2:THR:HG23	26:D:204:THR:HG22	2.02	0.41
1:a:248:U:O2'	1:a:249:G:H8	2.03	0.41
1:a:271:A:H2'	1:a:272:U:C6	2.56	0.41
1:a:341:C:C2	1:a:342:C:C5	3.09	0.41
1:a:390:A:H2'	1:a:391:A:C8	2.56	0.41
1:a:955:A:C2	1:a:956:G:C5	3.09	0.41
1:a:1008:C:N4	1:a:1050:G:O6	2.53	0.41
1:a:1350:G:H2'	1:a:1351:C:C6	2.56	0.41
4:d:50:GLN:HE22	4:d:200:ARG:NH2	2.12	0.41
19:s:42:PRO:HB3	46:3:70:ARG:HG3	2.02	0.41
23:A:77:U:H2'	23:A:78:U:C6	2.56	0.41
23:A:282:G:H3'	23:A:283:C:H4'	2.02	0.41
23:A:1300:U:O5'	23:A:1301:G:H5''	2.20	0.41
23:A:1319:A:H4'	23:A:1320:G:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1337:U:H2'	23:A:1338:C:H6	1.85	0.41
23:A:1700:G:C4	23:A:1701:A:C8	3.09	0.41
23:A:2232:A:N1	23:A:2259:C:N4	2.67	0.41
23:A:2789:U:H5	23:A:2791:A:N7	2.18	0.41
1:a:230:U:H2'	1:a:231:U:C6	2.56	0.41
1:a:1009:U:H2'	1:a:1010:U:C6	2.56	0.41
1:a:1012:G:C6	1:a:1047:A:C6	3.08	0.41
1:a:1052:G:O2'	1:a:1053:A:O4'	2.39	0.41
11:k:127:ARG:HG2	11:k:127:ARG:HH11	1.85	0.41
19:s:31:ILE:O	19:s:50:ALA:N	2.33	0.41
23:A:491:C:H2'	23:A:492:G:O4'	2.21	0.41
23:A:622:A:H2'	23:A:623:C:H6	1.86	0.41
23:A:1453:G:H2'	23:A:1454:C:H6	1.86	0.41
23:A:1706:U:H2'	23:A:1707:C:H6	1.86	0.41
23:A:2189:G:H2'	23:A:2190:G:C8	2.56	0.41
37:S:24:TYR:O	37:S:29:HIS:ND1	2.43	0.41
1:a:177:A:H2'	1:a:178:A:H8	1.85	0.41
1:a:221:G:H21	1:a:221:G:P	2.42	0.41
1:a:336:C:H4'	1:a:337:A:H5'	2.03	0.41
1:a:419:A:N6	1:a:438:A:H62	2.13	0.41
1:a:644:U:H2'	1:a:645:U:O4'	2.20	0.41
1:a:736:A:H2'	1:a:737:A:H8	1.85	0.41
1:a:775:A:H2'	1:a:776:A:H8	1.86	0.41
3:c:62:ARG:NH2	3:c:99:HIS:HB2	2.36	0.41
12:l:69:ARG:CZ	12:l:75:GLU:HG2	2.51	0.41
17:q:47:LYS:HD2	17:q:72:THR:O	2.21	0.41
20:t:47:LYS:HE2	20:t:82:LEU:HD13	2.02	0.41
21:x:15:G:O6	21:x:48:C:O2	2.39	0.41
23:A:687:G:N2	23:A:690:U:OP2	2.48	0.41
23:A:1433:G:H2'	23:A:1434:U:O4'	2.21	0.41
23:A:1947:C:H5'	23:A:1948:U:OP2	2.21	0.41
23:A:2155:U:H2'	23:A:2156:A:H8	1.86	0.41
23:A:2169:A:H2'	23:A:2170:C:H6	1.85	0.41
23:A:2195:A:H5''	23:A:2205:U:H2'	2.03	0.41
23:A:2336:G:H2'	23:A:2337:G:O4'	2.20	0.41
28:F:35:VAL:HG22	28:F:155:VAL:HB	2.02	0.41
37:S:5:LYS:HB2	37:S:5:LYS:HE3	1.95	0.41
1:a:230:U:H2'	1:a:231:U:H6	1.85	0.41
7:g:28:ASN:HA	7:g:31:MET:HE3	2.02	0.41
9:i:6:TYR:CG	9:i:90:VAL:HG22	2.56	0.41
16:p:71:ARG:NH1	16:p:75:SER:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:x:70:G:H2'	21:x:71:G:C8	2.56	0.41
23:A:638:U:H2'	23:A:639:U:C6	2.56	0.41
23:A:941:U:O2'	23:A:943:A:H2'	2.21	0.41
23:A:1864:G:H2'	23:A:1865:C:C6	2.56	0.41
23:A:2057:C:H2'	23:A:2058:C:H6	1.86	0.41
23:A:2187:G:H22	23:A:2188:A:H62	1.69	0.41
23:A:2908:A:O2'	23:A:2909:C:OP2	2.32	0.41
26:D:8:ARG:HG3	26:D:53:PHE:HE2	1.86	0.41
41:W:12:ILE:O	41:W:17:LYS:HG3	2.21	0.41
1:a:107:A:H5'	1:a:108:C:H5	1.86	0.40
1:a:640:G:O2'	1:a:641:U:H5''	2.21	0.40
1:a:1118:C:C2	1:a:1119:A:C8	3.09	0.40
1:a:1253:G:H2'	1:a:1254:U:O4'	2.21	0.40
4:d:141:VAL:HG13	4:d:143:GLU:H	1.85	0.40
5:e:108:ALA:HB3	5:e:113:ARG:HG3	2.04	0.40
15:o:26:GLU:OE1	15:o:26:GLU:N	2.54	0.40
23:A:29:U:H2'	23:A:30:G:H8	1.86	0.40
23:A:130:A:H2'	23:A:131:C:H6	1.87	0.40
23:A:1487:A:H2'	23:A:1488:U:C6	2.56	0.40
23:A:1804:C:H2'	23:A:1805:G:C8	2.55	0.40
23:A:1827:U:H2'	23:A:1828:C:C6	2.55	0.40
23:A:2191:A:H4'	23:A:2192:G:H5'	2.02	0.40
23:A:2325:U:H2'	23:A:2326:C:H6	1.85	0.40
24:B:4:G:H5'	24:B:25:A:H8	1.85	0.40
25:C:69:ARG:HH22	25:C:116:ILE:CG2	2.34	0.40
27:E:126:LEU:HD23	27:E:128:GLY:N	2.35	0.40
31:M:104:ARG:NH1	31:M:107:ARG:HH21	2.18	0.40
37:S:118:ALA:O	37:S:119:LYS:HB2	2.21	0.40
4:d:134:SER:OG	4:d:135:VAL:N	2.55	0.40
15:o:26:GLU:OE2	15:o:77:ARG:NH2	2.54	0.40
20:t:10:ARG:NH2	54:t:201:HOH:O	2.53	0.40
23:A:1497:G:O2'	23:A:1596:A:N3	2.50	0.40
23:A:1512:U:H2'	23:A:1513:G:H8	1.87	0.40
23:A:2126:G:O2'	23:A:2127:A:H5'	2.22	0.40
23:A:2318:C:OP2	48:5:2:ARG:NH2	2.33	0.40
40:V:1:MET:HB3	40:V:5:ASP:HB2	2.03	0.40
45:2:15:ARG:HD3	45:2:15:ARG:HA	1.86	0.40
45:2:26:LEU:HG	45:2:46:MET:SD	2.62	0.40
1:a:1323:G:H4'	14:n:18:VAL:HG11	2.04	0.40
3:c:137:ILE:HG23	3:c:148:ILE:HG21	2.03	0.40
4:d:185:LEU:HD23	4:d:185:LEU:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:18:TYR:O	7:g:20:SER:N	2.54	0.40
8:h:43:GLU:OE2	8:h:114:THR:HG21	2.21	0.40
23:A:1366:A:N3	23:A:1367:G:C8	2.90	0.40
23:A:2217:U:C2	23:A:2218:G:C8	3.10	0.40
23:A:2820:C:H4'	26:D:63:LYS:HG3	2.03	0.40
23:A:2879:A:H2'	23:A:2880:A:C8	2.56	0.40
28:F:12:ILE:HD13	28:F:173:LEU:HD22	2.02	0.40
37:S:95:LEU:HD23	37:S:95:LEU:HA	1.97	0.40
40:V:4:ARG:HG2	44:1:26:PHE:HB2	2.02	0.40
1:a:331:U:H2'	1:a:332:G:O4'	2.21	0.40
1:a:373:U:H5'	1:a:374:C:OP1	2.21	0.40
1:a:468:A:H2'	1:a:469:A:H8	1.85	0.40
1:a:508:G:H2'	1:a:509:C:H6	1.85	0.40
1:a:661:G:O6	8:h:57:ALA:HB2	2.21	0.40
1:a:1163:U:H2'	1:a:1164:G:O4'	2.20	0.40
1:a:1515:A:H2'	1:a:1516:G:H8	1.86	0.40
5:e:150:ASN:O	5:e:154:VAL:HG22	2.22	0.40
9:i:44:LEU:O	9:i:47:VAL:HG22	2.21	0.40
13:m:69:LEU:O	13:m:73:VAL:HG12	2.21	0.40
17:q:9:VAL:HG11	17:q:62:ARG:NH2	2.37	0.40
23:A:1808:U:O4	23:A:1822:A:H2	2.04	0.40
23:A:2485:C:H2'	23:A:2486:A:C8	2.56	0.40
23:A:2507:C:H5''	23:A:2508:C:H5	1.86	0.40
23:A:2723:A:N6	34:P:39:GLU:OE2	2.48	0.40
25:C:44:ASN:N	25:C:48:LYS:O	2.52	0.40
26:D:139:TYR:CZ	26:D:142:ARG:HB2	2.57	0.40
29:G:11:ILE:N	29:G:48:ASN:O	2.55	0.40
1:a:407:G:H2'	1:a:408:C:C6	2.56	0.40
1:a:692:U:O2'	11:k:41:ALA:O	2.33	0.40
1:a:1370:A:N3	1:a:1370:A:H2'	2.37	0.40
2:b:55:ASN:O	2:b:58:ARG:HB2	2.22	0.40
3:c:115:VAL:O	3:c:119:ILE:HG13	2.21	0.40
3:c:130:ARG:HG2	3:c:167:TYR:OH	2.21	0.40
23:A:308:U:H3'	23:A:309:C:H5''	2.03	0.40
23:A:806:G:H2'	23:A:807:A:O4'	2.22	0.40
23:A:1308:U:H2'	23:A:1309:G:C8	2.57	0.40
23:A:1404:G:C8	23:A:1405:G:C8	3.10	0.40
23:A:2103:G:H2'	23:A:2104:A:C8	2.57	0.40
23:A:2576:G:H2'	23:A:2577:G:C8	2.57	0.40
23:A:2901:G:O2'	23:A:2902:A:H5'	2.21	0.40
32:N:93:PRO:HD3	32:N:124:LYS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:O:112:ASP:OD1	33:O:113:VAL:N	2.54	0.40
36:R:33:VAL:HG23	36:R:38:GLU:OE2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	219/249 (88%)	192 (88%)	27 (12%)	0	100	100
3	c	202/218 (93%)	185 (92%)	17 (8%)	0	100	100
4	d	197/200 (98%)	184 (93%)	13 (7%)	0	100	100
5	e	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
6	f	91/97 (94%)	84 (92%)	7 (8%)	0	100	100
7	g	147/156 (94%)	144 (98%)	3 (2%)	0	100	100
8	h	128/132 (97%)	123 (96%)	5 (4%)	0	100	100
9	i	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	j	95/102 (93%)	91 (96%)	4 (4%)	0	100	100
11	k	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
12	l	132/137 (96%)	129 (98%)	3 (2%)	0	100	100
13	m	112/121 (93%)	105 (94%)	7 (6%)	0	100	100
14	n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	o	84/89 (94%)	84 (100%)	0	0	100	100
16	p	85/90 (94%)	82 (96%)	3 (4%)	0	100	100
17	q	78/87 (90%)	73 (94%)	5 (6%)	0	100	100
18	r	62/79 (78%)	60 (97%)	1 (2%)	1 (2%)	7	34
19	s	79/92 (86%)	76 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	t	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	9	38
25	C	271/277 (98%)	260 (96%)	11 (4%)	0	100	100
26	D	204/209 (98%)	195 (96%)	9 (4%)	0	100	100
27	E	202/207 (98%)	194 (96%)	8 (4%)	0	100	100
28	F	172/179 (96%)	154 (90%)	17 (10%)	1 (1%)	21	56
29	G	170/178 (96%)	150 (88%)	19 (11%)	1 (1%)	21	56
30	L	141/145 (97%)	141 (100%)	0	0	100	100
31	M	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
32	N	143/146 (98%)	136 (95%)	7 (5%)	0	100	100
33	O	132/144 (92%)	132 (100%)	0	0	100	100
34	P	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
35	Q	116/119 (98%)	112 (97%)	4 (3%)	0	100	100
36	R	111/114 (97%)	104 (94%)	7 (6%)	0	100	100
37	S	116/119 (98%)	113 (97%)	3 (3%)	0	100	100
38	T	99/102 (97%)	96 (97%)	3 (3%)	0	100	100
39	U	110/118 (93%)	108 (98%)	2 (2%)	0	100	100
40	V	90/94 (96%)	88 (98%)	2 (2%)	0	100	100
41	W	99/103 (96%)	95 (96%)	3 (3%)	1 (1%)	12	45
42	Y	74/96 (77%)	68 (92%)	5 (7%)	1 (1%)	9	36
43	Z	58/62 (94%)	49 (84%)	9 (16%)	0	100	100
44	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
45	2	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
46	3	68/81 (84%)	63 (93%)	4 (6%)	1 (2%)	8	35
47	4	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
48	5	45/49 (92%)	45 (100%)	0	0	100	100
49	6	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
50	7	62/66 (94%)	55 (89%)	7 (11%)	0	100	100
51	8	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	5202/5545 (94%)	4941 (95%)	254 (5%)	7 (0%)	49	80

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	r	16	TYR
20	t	46	ALA
42	Y	18	THR
41	W	97	SER
29	G	13	ALA
46	3	67	ALA
28	F	117	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	188/214 (88%)	187 (100%)	1 (0%)	81	89
3	c	145/177 (82%)	145 (100%)	0	100	100
4	d	162/170 (95%)	162 (100%)	0	100	100
5	e	122/131 (93%)	122 (100%)	0	100	100
6	f	81/85 (95%)	81 (100%)	0	100	100
7	g	116/130 (89%)	116 (100%)	0	100	100
8	h	104/110 (94%)	104 (100%)	0	100	100
9	i	100/102 (98%)	100 (100%)	0	100	100
10	j	73/93 (78%)	73 (100%)	0	100	100
11	k	87/100 (87%)	87 (100%)	0	100	100
12	l	105/118 (89%)	105 (100%)	0	100	100
13	m	96/102 (94%)	96 (100%)	0	100	100
14	n	51/52 (98%)	51 (100%)	0	100	100
15	o	78/81 (96%)	78 (100%)	0	100	100
16	p	74/80 (92%)	74 (100%)	0	100	100
17	q	63/78 (81%)	63 (100%)	0	100	100
18	r	55/67 (82%)	55 (100%)	0	100	100
19	s	64/78 (82%)	64 (100%)	0	100	100
20	t	62/66 (94%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	C	221/225 (98%)	221 (100%)	0	100	100
26	D	169/171 (99%)	169 (100%)	0	100	100
27	E	162/174 (93%)	162 (100%)	0	100	100
28	F	101/155 (65%)	101 (100%)	0	100	100
29	G	127/147 (86%)	127 (100%)	0	100	100
30	L	119/121 (98%)	119 (100%)	0	100	100
31	M	98/101 (97%)	98 (100%)	0	100	100
32	N	97/115 (84%)	97 (100%)	0	100	100
33	O	102/113 (90%)	102 (100%)	0	100	100
34	P	97/111 (87%)	97 (100%)	0	100	100
35	Q	77/97 (79%)	77 (100%)	0	100	100
36	R	94/99 (95%)	94 (100%)	0	100	100
37	S	96/97 (99%)	96 (100%)	0	100	100
38	T	78/82 (95%)	78 (100%)	0	100	100
39	U	92/97 (95%)	92 (100%)	0	100	100
40	V	74/84 (88%)	74 (100%)	0	100	100
41	W	82/88 (93%)	82 (100%)	0	100	100
42	Y	58/76 (76%)	58 (100%)	0	100	100
43	Z	45/53 (85%)	45 (100%)	0	100	100
44	1	54/55 (98%)	54 (100%)	0	100	100
45	2	47/52 (90%)	47 (100%)	0	100	100
46	3	57/73 (78%)	57 (100%)	0	100	100
47	4	43/50 (86%)	43 (100%)	0	100	100
48	5	41/48 (85%)	41 (100%)	0	100	100
49	6	39/39 (100%)	39 (100%)	0	100	100
50	7	54/56 (96%)	54 (100%)	0	100	100
51	8	29/35 (83%)	29 (100%)	0	100	100
All	All	4179/4648 (90%)	4178 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	45	LYS

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

Mol	Chain	Res	Type
2	b	77	GLN
2	b	94	HIS
3	c	122	GLN
3	c	151	GLN
4	d	36	HIS
4	d	50	GLN
4	d	70	ASN
4	d	85	ASN
4	d	118	HIS
4	d	137	GLN
4	d	190	ASN
5	e	150	ASN
6	f	62	HIS
6	f	67	ASN
6	f	75	ASN
7	g	129	ASN
8	h	16	ASN
8	h	122	GLN
9	i	60	ASN
9	i	68	HIS
10	j	56	HIS
12	l	6	GLN
12	l	59	ASN
12	l	109	HIS
13	m	76	ASN
15	o	18	HIS
15	o	37	ASN
15	o	42	HIS
15	o	46	HIS
15	o	65	ASN
16	p	62	ASN
16	p	85	ASN
18	r	20	ASN
18	r	56	GLN
20	t	21	ASN
20	t	42	ASN
25	C	15	HIS
25	C	70	ASN
26	D	33	ASN
26	D	126	HIS
26	D	140	HIS

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Mol	Chain	Res	Type
26	D	152	ASN
26	D	201	GLN
27	E	9	GLN
27	E	46	GLN
29	G	106	ASN
31	M	13	ASN
31	M	82	ASN
34	P	27	HIS
34	P	61	GLN
34	P	110	GLN
35	Q	15	HIS
35	Q	43	GLN
37	S	37	GLN
37	S	72	GLN
38	T	81	ASN
38	T	101	ASN
39	U	73	ASN
40	V	37	GLN
42	Y	20	ASN
43	Z	23	ASN
43	Z	34	GLN
44	1	36	GLN
45	2	40	ASN
46	3	6	HIS
47	4	32	ASN
47	4	48	GLN
48	5	16	ASN
48	5	26	ASN
50	7	35	ASN
50	7	40	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1519/1550 (98%)	242 (15%)	0
21	x	72/76 (94%)	18 (25%)	0
22	w	13/21 (61%)	2 (15%)	0
23	A	2898/2932 (98%)	453 (15%)	28 (0%)
24	B	113/116 (97%)	14 (12%)	0
All	All	4615/4695 (98%)	729 (15%)	28 (0%)

All (729) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	17	U
1	a	31	G
1	a	32	A
1	a	39	G
1	a	44	G
1	a	47	C
1	a	48	C
1	a	51	A
1	a	60	A
1	a	63	C
1	a	67	C
1	a	68	G
1	a	69	A
1	a	70	A
1	a	71	C
1	a	74	A
1	a	91	C
1	a	92	C
1	a	93	A
1	a	95	A
1	a	96	G
1	a	97	U
1	a	98	U
1	a	99	A
1	a	100	G
1	a	101	U
1	a	102	G
1	a	112	U
1	a	114	A
1	a	119	C
1	a	128	A
1	a	129	A
1	a	130	C
1	a	143	U
1	a	148	A
1	a	149	U
1	a	150	A
1	a	154	C
1	a	156	G
1	a	158	G
1	a	159	A
1	a	162	C

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Mol	Chain	Res	Type
1	a	164	G
1	a	172	U
1	a	173	A
1	a	182	U
1	a	188	G
1	a	195	A
1	a	197	G
1	a	209	A
1	a	211	A
1	a	212	G
1	a	214	U
1	a	215	G
1	a	219	U
1	a	220	C
1	a	249	G
1	a	255	G
1	a	259	G
1	a	274	G
1	a	275	C
1	a	288	C
1	a	297	G
1	a	336	C
1	a	340	G
1	a	352	A
1	a	354	G
1	a	355	G
1	a	359	G
1	a	360	C
1	a	362	G
1	a	371	A
1	a	372	A
1	a	373	U
1	a	375	U
1	a	380	C
1	a	381	A
1	a	382	A
1	a	405	A
1	a	414	G
1	a	419	A
1	a	420	A
1	a	421	G
1	a	422	A

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Mol	Chain	Res	Type
1	a	423	A
1	a	424	G
1	a	425	G
1	a	427	U
1	a	429	U
1	a	430	C
1	a	431	G
1	a	432	G
1	a	437	U
1	a	447	U
1	a	454	A
1	a	456	A
1	a	461	C
1	a	467	U
1	a	470	G
1	a	471	A
1	a	473	U
1	a	475	A
1	a	476	C
1	a	492	G
1	a	493	G
1	a	503	A
1	a	505	A
1	a	518	A
1	a	519	C
1	a	520	U
1	a	526	C
1	a	529	G
1	a	535	G
1	a	539	U
1	a	540	A
1	a	555	A
1	a	572	U
1	a	576	G
1	a	581	A
1	a	584	C
1	a	585	G
1	a	596	G
1	a	624	G
1	a	626	C
1	a	643	A
1	a	661	G

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Mol	Chain	Res	Type
1	a	673	A
1	a	695	A
1	a	702	A
1	a	703	A
1	a	711	G
1	a	712	A
1	a	731	U
1	a	739	G
1	a	741	G
1	a	757	A
1	a	763	G
1	a	769	G
1	a	786	G
1	a	789	A
1	a	801	U
1	a	802	A
1	a	823	A
1	a	825	C
1	a	829	G
1	a	848	G
1	a	855	C
1	a	881	A
1	a	923	A
1	a	932	A
1	a	935	G
1	a	936	G
1	a	943	C
1	a	944	A
1	a	954	G
1	a	969	U
1	a	975	G
1	a	978	A
1	a	980	G
1	a	984	A
1	a	985	G
1	a	986	A
1	a	1001	U
1	a	1002	G
1	a	1006	U
1	a	1007	C
1	a	1008	C
1	a	1012	G

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Mol	Chain	Res	Type
1	a	1013	A
1	a	1014	C
1	a	1018	U
1	a	1032	U
1	a	1034	U
1	a	1035	C
1	a	1049	A
1	a	1052	G
1	a	1053	A
1	a	1064	A
1	a	1074	U
1	a	1094	U
1	a	1103	G
1	a	1104	U
1	a	1110	A
1	a	1111	A
1	a	1139	A
1	a	1143	U
1	a	1146	A
1	a	1147	G
1	a	1148	U
1	a	1154	A
1	a	1167	U
1	a	1176	A
1	a	1178	G
1	a	1181	G
1	a	1191	G
1	a	1197	G
1	a	1203	A
1	a	1204	A
1	a	1207	C
1	a	1208	A
1	a	1209	U
1	a	1219	U
1	a	1220	A
1	a	1234	A
1	a	1235	C
1	a	1245	A
1	a	1265	G
1	a	1267	G
1	a	1281	G
1	a	1284	C

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Mol	Chain	Res	Type
1	a	1285	C
1	a	1287	A
1	a	1292	A
1	a	1294	A
1	a	1306	A
1	a	1307	G
1	a	1309	U
1	a	1312	G
1	a	1347	A
1	a	1353	A
1	a	1360	G
1	a	1371	U
1	a	1377	G
1	a	1388	U
1	a	1401	A
1	a	1404	C
1	a	1405	A
1	a	1449	G
1	a	1453	A
1	a	1495	G
1	a	1498	U
1	a	1500	A
1	a	1501	A
1	a	1505	G
1	a	1511	A
1	a	1514	U
1	a	1525	G
1	a	1537	G
1	a	1538	G
1	a	1539	A
1	a	1546	C
21	x	4	C
21	x	7	A
21	x	8	4SU
21	x	9	A
21	x	19	G
21	x	21	A
21	x	29	G
21	x	35	A
21	x	36	A
21	x	45	U
21	x	46	G7M

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Mol	Chain	Res	Type
21	x	48	C
21	x	55	PSU
21	x	56	C
21	x	60	U
21	x	69	G
21	x	73	A
21	x	76	A
22	w	10	A
22	w	12	A
23	A	13	A
23	A	14	A
23	A	28	A
23	A	34	U
23	A	46	C
23	A	60	G
23	A	71	A
23	A	75	G
23	A	89	U
23	A	90	A
23	A	92	G
23	A	93	U
23	A	100	U
23	A	101	G
23	A	117	A
23	A	118	A
23	A	119	U
23	A	125	A
23	A	126	A
23	A	130	A
23	A	140	G
23	A	161	A
23	A	162	A
23	A	164	A
23	A	167	U
23	A	186	C
23	A	187	C
23	A	198	A
23	A	199	A
23	A	201	A
23	A	215	A
23	A	217	G
23	A	218	A

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Mol	Chain	Res	Type
23	A	223	A
23	A	224	A
23	A	230	A
23	A	231	A
23	A	232	U
23	A	235	A
23	A	247	G
23	A	250	G
23	A	257	A
23	A	271	C
23	A	274	A
23	A	282	G
23	A	283	C
23	A	285	U
23	A	287	C
23	A	289	U
23	A	290	C
23	A	297	U
23	A	299	G
23	A	300	U
23	A	301	A
23	A	306	A
23	A	307	C
23	A	309	C
23	A	313	A
23	A	320	U
23	A	326	A
23	A	345	G
23	A	354	A
23	A	372	A
23	A	373	A
23	A	375	A
23	A	388	A
23	A	404	A
23	A	406	A
23	A	410	G
23	A	411	A
23	A	417	A
23	A	418	G
23	A	429	C
23	A	432	G
23	A	433	U

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Mol	Chain	Res	Type
23	A	457	G
23	A	470	G
23	A	489	A
23	A	490	C
23	A	501	C
23	A	503	A
23	A	513	G
23	A	526	A
23	A	527	G
23	A	550	A
23	A	553	U
23	A	554	C
23	A	555	C
23	A	567	G
23	A	576	U
23	A	577	A
23	A	578	G
23	A	591	A
23	A	592	A
23	A	594	G
23	A	606	G
23	A	616	G
23	A	618	A
23	A	646	A
23	A	659	A
23	A	666	A
23	A	667	G
23	A	672	A
23	A	679	G
23	A	682	A
23	A	689	A
23	A	690	U
23	A	699	U
23	A	700	A
23	A	718	C
23	A	732	U
23	A	776	U
23	A	786	C
23	A	792	U
23	A	793	U
23	A	794	G
23	A	810	A

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Mol	Chain	Res	Type
23	A	811	G
23	A	821	G
23	A	823	G
23	A	825	A
23	A	828	A
23	A	830	U
23	A	836	U
23	A	838	G
23	A	851	G
23	A	858	C
23	A	865	A
23	A	873	U
23	A	876	G
23	A	891	U
23	A	892	A
23	A	893	A
23	A	913	A
23	A	925	A
23	A	926	G
23	A	927	G
23	A	928	G
23	A	940	G
23	A	941	U
23	A	942	U
23	A	943	A
23	A	944	C
23	A	946	G
23	A	947	A
23	A	949	U
23	A	957	A
23	A	959	C
23	A	964	A
23	A	973	U
23	A	979	U
23	A	980	A
23	A	987	A
23	A	992	G
23	A	1007	G
23	A	1020	A
23	A	1025	A
23	A	1029	A
23	A	1036	A

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Mol	Chain	Res	Type
23	A	1042	A
23	A	1055	A
23	A	1058	U
23	A	1059	A
23	A	1072	A
23	A	1073	A
23	A	1079	U
23	A	1085	G
23	A	1092	A
23	A	1093	G
23	A	1097	A
23	A	1106	U
23	A	1107	U
23	A	1116	A
23	A	1117	G
23	A	1122	C
23	A	1129	G
23	A	1130	A
23	A	1131	A
23	A	1134	A
23	A	1135	G
23	A	1137	G
23	A	1157	A
23	A	1158	G
23	A	1160	G
23	A	1162	C
23	A	1173	A
23	A	1176	U
23	A	1178	U
23	A	1179	A
23	A	1181	C
23	A	1182	G
23	A	1188	A
23	A	1203	A
23	A	1230	G
23	A	1249	A
23	A	1250	G
23	A	1252	G
23	A	1254	G
23	A	1283	G
23	A	1298	A
23	A	1300	U

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Mol	Chain	Res	Type
23	A	1301	G
23	A	1311	G
23	A	1316	G
23	A	1317	A
23	A	1320	G
23	A	1344	A
23	A	1345	A
23	A	1365	A
23	A	1369	C
23	A	1373	U
23	A	1394	C
23	A	1396	U
23	A	1404	G
23	A	1409	A
23	A	1423	U
23	A	1429	A
23	A	1435	A
23	A	1439	A
23	A	1440	U
23	A	1455	U
23	A	1462	U
23	A	1463	U
23	A	1464	A
23	A	1465	A
23	A	1469	A
23	A	1470	U
23	A	1478	C
23	A	1502	A
23	A	1509	A
23	A	1519	A
23	A	1528	G
23	A	1529	U
23	A	1531	U
23	A	1532	G
23	A	1533	A
23	A	1534	G
23	A	1539	A
23	A	1542	C
23	A	1543	A
23	A	1546	U
23	A	1553	C
23	A	1556	G

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Mol	Chain	Res	Type
23	A	1557	C
23	A	1559	A
23	A	1562	C
23	A	1563	A
23	A	1564	U
23	A	1570	G
23	A	1573	A
23	A	1574	U
23	A	1575	G
23	A	1581	G
23	A	1611	C
23	A	1618	A
23	A	1621	A
23	A	1630	U
23	A	1638	G
23	A	1642	U
23	A	1656	C
23	A	1657	A
23	A	1659	A
23	A	1683	A
23	A	1695	A
23	A	1696	G
23	A	1697	C
23	A	1700	G
23	A	1701	A
23	A	1712	U
23	A	1723	G
23	A	1724	C
23	A	1749	A
23	A	1761	A
23	A	1762	U
23	A	1763	U
23	A	1764	A
23	A	1771	A
23	A	1773	G
23	A	1781	G
23	A	1782	A
23	A	1783	G
23	A	1787	C
23	A	1789	G
23	A	1795	A
23	A	1796	G

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Mol	Chain	Res	Type
23	A	1797	G
23	A	1806	A
23	A	1809	G
23	A	1815	C
23	A	1818	A
23	A	1819	A
23	A	1833	C
23	A	1834	A
23	A	1849	C
23	A	1862	A
23	A	1880	A
23	A	1881	A
23	A	1887	A
23	A	1889	A
23	A	1891	G
23	A	1903	U
23	A	1904	C
23	A	1905	G
23	A	1915	C
23	A	1939	G
23	A	1946	A
23	A	1947	C
23	A	1949	A
23	A	1962	G
23	A	1963	G
23	A	1969	A
23	A	1971	A
23	A	1973	U
23	A	1988	U
23	A	2000	C
23	A	2003	A
23	A	2004	A
23	A	2005	G
23	A	2024	U
23	A	2026	U
23	A	2029	C
23	A	2030	A
23	A	2056	A
23	A	2064	A
23	A	2065	G
23	A	2066	A
23	A	2069	C

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Mol	Chain	Res	Type
23	A	2072	G
23	A	2076	C
23	A	2088	C
23	A	2089	G
23	A	2093	A
23	A	2094	G
23	A	2095	A
23	A	2102	G
23	A	2126	G
23	A	2127	A
23	A	2149	G
23	A	2150	A
23	A	2165	A
23	A	2191	A
23	A	2192	G
23	A	2204	A
23	A	2205	U
23	A	2206	A
23	A	2223	A
23	A	2236	G
23	A	2237	C
23	A	2245	A
23	A	2256	A
23	A	2258	A
23	A	2259	C
23	A	2271	G
23	A	2272	G
23	A	2312	G
23	A	2316	C
23	A	2320	A
23	A	2321	A
23	A	2329	U
23	A	2337	G
23	A	2338	A
23	A	2341	G
23	A	2342	A
23	A	2344	A
23	A	2352	C
23	A	2353	A
23	A	2354	G
23	A	2355	A
23	A	2358	G

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Mol	Chain	Res	Type
23	A	2360	A
23	A	2367	C
23	A	2368	A
23	A	2380	C
23	A	2383	C
23	A	2394	A
23	A	2412	G
23	A	2416	G
23	A	2418	C
23	A	2435	U
23	A	2439	C
23	A	2455	C
23	A	2458	A
23	A	2462	G
23	A	2463	A
23	A	2473	C
23	A	2474	C
23	A	2481	A
23	A	2492	A
23	A	2498	C
23	A	2501	A
23	A	2506	U
23	A	2507	C
23	A	2509	A
23	A	2531	C
23	A	2535	G
23	A	2536	A
23	A	2538	G
23	A	2551	A
23	A	2553	C
23	A	2562	G
23	A	2567	C
23	A	2568	G
23	A	2587	U
23	A	2599	A
23	A	2600	G
23	A	2611	G
23	A	2615	G
23	A	2635	A
23	A	2636	G
23	A	2643	C
23	A	2646	U

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Mol	Chain	Res	Type
23	A	2648	U
23	A	2663	G
23	A	2679	C
23	A	2694	G
23	A	2715	G
23	A	2722	U
23	A	2724	C
23	A	2747	G
23	A	2759	U
23	A	2766	C
23	A	2768	G
23	A	2781	A
23	A	2783	A
23	A	2789	U
23	A	2790	A
23	A	2797	A
23	A	2798	A
23	A	2799	G
23	A	2810	G
23	A	2811	A
23	A	2812	U
23	A	2813	G
23	A	2822	C
23	A	2824	U
23	A	2827	C
23	A	2828	U
23	A	2831	G
23	A	2832	G
23	A	2835	A
23	A	2837	U
23	A	2849	A
23	A	2862	A
23	A	2864	A
23	A	2872	G
23	A	2877	G
23	A	2890	U
23	A	2896	G
23	A	2901	G
23	A	2902	A
23	A	2909	C
23	A	2922	G
23	A	2929	C

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Mol	Chain	Res	Type
24	B	10	U
24	B	11	A
24	B	23	U
24	B	33	U
24	B	39	C
24	B	40	C
24	B	49	G
24	B	54	U
24	B	55	A
24	B	59	U
24	B	87	U
24	B	88	C
24	B	107	G
24	B	114	G

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	27	G
23	A	88	G
23	A	92	G
23	A	139	A
23	A	410	G
23	A	525	A
23	A	553	U
23	A	688	A
23	A	756	A
23	A	809	G
23	A	847	G
23	A	854	G
23	A	946	G
23	A	1017	C
23	A	1248	A
23	A	1249	A
23	A	1497	G
23	A	1528	G
23	A	1532	G
23	A	1533	A
23	A	1569	U
23	A	1817	A
23	A	1886	A
23	A	1888	G

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Mol	Chain	Res	Type
23	A	2438	G
23	A	2472	A
23	A	2809	A
23	A	2908	A

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

7 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$
21	PSU	x	32	21	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
21	PSU	x	55	21	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
21	G7M	x	46	21	23,26,27	2.39	5 (21%)	34,39,42	2.98	10 (29%)
21	PSU	x	39	21	18,21,22	1.23	1 (5%)	21,30,33	2.55	4 (19%)
21	4SU	x	8	21	18,21,22	1.85	5 (27%)	25,30,33	2.22	5 (20%)
21	5MU	x	54	21	19,22,23	1.41	5 (26%)	27,32,35	2.05	7 (25%)
21	MIA	x	37	21	28,31,32	2.33	6 (21%)	38,44,47	2.75	14 (36%)

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
21	PSU	x	32	21	-	0/7/25/26	0/2/2/2
21	PSU	x	55	21	-	3/7/25/26	0/2/2/2
21	G7M	x	46	21	-	2/7/25/26	0/3/3/3
21	PSU	x	39	21	-	0/7/25/26	0/2/2/2
21	4SU	x	8	21	-	1/7/25/26	0/2/2/2
21	5MU	x	54	21	-	0/7/25/26	0/2/2/2
21	MIA	x	37	21	-	1/15/33/34	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	46	G7M	C8-N7	7.80	1.46	1.33
21	x	37	MIA	C2-S10	-6.93	1.70	1.75
21	x	37	MIA	C13-C14	6.88	1.53	1.32
21	x	8	4SU	C4-S4	-4.95	1.59	1.68
21	x	37	MIA	C5-C4	4.65	1.47	1.39
21	x	46	G7M	C5-N7	-4.63	1.33	1.39
21	x	46	G7M	C8-N9	4.19	1.47	1.35
21	x	46	G7M	C5-C4	3.80	1.47	1.38
21	x	55	PSU	C6-C5	3.42	1.39	1.35
21	x	8	4SU	C4-N3	-3.30	1.34	1.37
21	x	32	PSU	C6-C5	3.18	1.38	1.35
21	x	39	PSU	C6-C5	2.98	1.38	1.35
21	x	37	MIA	C5-C6	2.79	1.48	1.41
21	x	54	5MU	C6-C5	2.76	1.39	1.34
21	x	32	PSU	C4-N3	-2.73	1.33	1.38
21	x	8	4SU	C5-C4	-2.69	1.39	1.42
21	x	55	PSU	C4-N3	-2.58	1.34	1.38
21	x	54	5MU	C4-N3	-2.55	1.34	1.38
21	x	54	5MU	C2-N1	2.52	1.42	1.38
21	x	8	4SU	C2-N1	2.37	1.42	1.38
21	x	46	G7M	C6-N1	-2.36	1.34	1.38
21	x	54	5MU	C4-C5	2.30	1.48	1.44
21	x	37	MIA	C8-N7	2.29	1.36	1.31
21	x	37	MIA	C5-N7	-2.28	1.34	1.39
21	x	54	5MU	C6-N1	-2.20	1.34	1.38
21	x	8	4SU	C2-N3	-2.12	1.34	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	37	MIA	C12-C13-C14	-8.55	111.66	127.01
21	x	37	MIA	C5-C4-N3	-7.99	118.76	127.18
21	x	46	G7M	CN7-N7-C8	-7.88	112.85	124.79
21	x	39	PSU	N1-C2-N3	7.44	123.02	115.17
21	x	46	G7M	N9-C8-N7	-6.80	95.97	112.48
21	x	46	G7M	C8-N7-C5	6.53	115.95	107.78
21	x	8	4SU	C4-N3-C2	-6.48	121.10	127.31
21	x	32	PSU	N1-C2-N3	6.43	121.95	115.17
21	x	55	PSU	N1-C2-N3	6.41	121.93	115.17
21	x	37	MIA	N3-C4-N9	6.32	135.01	126.99
21	x	46	G7M	N9-C4-N3	6.24	138.44	125.95
21	x	39	PSU	C4-N3-C2	-5.88	118.27	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	8	4SU	C5-C4-N3	5.71	120.06	114.75
21	x	46	G7M	C5-C4-N3	-5.41	117.94	128.15
21	x	39	PSU	O2-C2-N1	-5.18	117.45	122.79
21	x	54	5MU	C4-N3-C2	-4.77	121.08	127.34
21	x	54	5MU	N3-C2-N1	4.74	121.06	114.89
21	x	46	G7M	C2-N3-C4	4.43	119.92	112.30
21	x	46	G7M	C8-N9-C4	4.28	117.68	107.09
21	x	54	5MU	C5-C4-N3	4.22	118.99	115.32
21	x	55	PSU	C4-N3-C2	-4.03	120.82	126.37
21	x	54	5MU	O4-C4-C5	-3.99	120.36	124.92
21	x	8	4SU	N3-C2-N1	3.96	120.05	114.89
21	x	32	PSU	C4-N3-C2	-3.90	121.00	126.37
21	x	37	MIA	C15-C14-C13	-3.87	111.06	122.66
21	x	8	4SU	C5-C4-S4	-3.82	119.94	124.31
21	x	37	MIA	C16-C14-C13	-3.75	111.40	122.66
21	x	55	PSU	O2-C2-N1	-3.69	118.98	122.79
21	x	46	G7M	C1'-N9-C8	-3.55	114.74	126.74
21	x	46	G7M	CN7-N7-C5	3.53	131.20	126.80
21	x	37	MIA	C4-C5-N7	-3.45	106.64	110.58
21	x	32	PSU	O2-C2-N1	-3.37	119.31	122.79
21	x	37	MIA	C2-N3-C4	3.37	121.11	112.29
21	x	37	MIA	C6-C5-N7	3.09	135.80	132.43
21	x	54	5MU	C5-C6-N1	-3.09	119.96	123.31
21	x	8	4SU	C1'-N1-C2	2.73	122.49	117.59
21	x	37	MIA	C11-S10-C2	-2.65	100.26	102.25
21	x	37	MIA	C4-N9-C8	2.63	108.50	105.74
21	x	37	MIA	C5-N7-C8	2.56	107.47	103.45
21	x	39	PSU	C5-C6-N1	-2.56	118.59	122.14
21	x	46	G7M	O6-C6-C5	-2.46	122.51	128.01
21	x	54	5MU	C1'-N1-C2	2.34	121.80	117.59
21	x	37	MIA	C2-N1-C6	2.31	121.92	117.54
21	x	37	MIA	N3-C2-N1	-2.31	122.79	127.00
21	x	37	MIA	N6-C6-N1	2.21	121.30	118.33
21	x	54	5MU	C1'-N1-C6	-2.11	117.67	121.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	x	37	MIA	C12-C13-C14-C16
21	x	55	PSU	C3'-C4'-C5'-O5'
21	x	55	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
21	x	46	G7M	O4'-C1'-N9-C4
21	x	46	G7M	O4'-C1'-N9-C8
21	x	55	PSU	C4'-C5'-O5'-P
21	x	8	4SU	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	x	46	G7M	2	0
21	x	37	MIA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 494 ligands modelled in this entry, 494 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

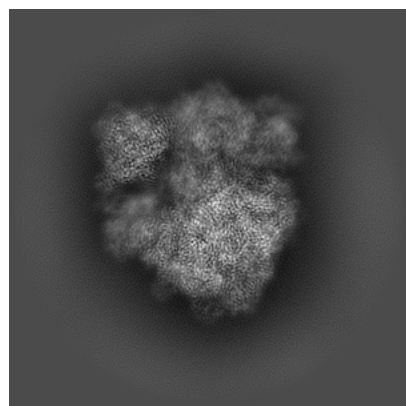
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42557. These allow visual inspection of the internal detail of the map and identification of artifacts.

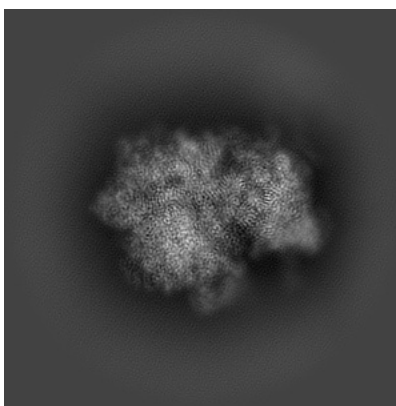
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

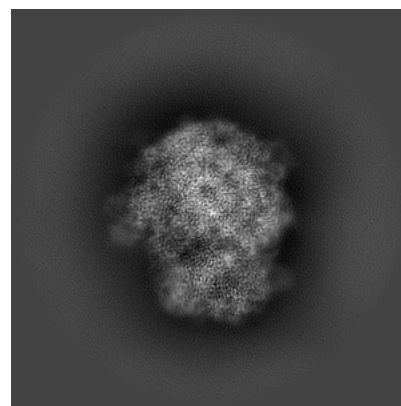
6.1.1 Primary map



X

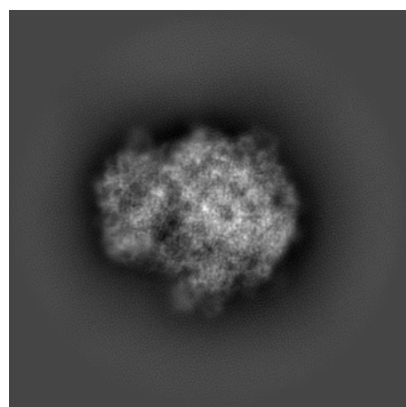


Y

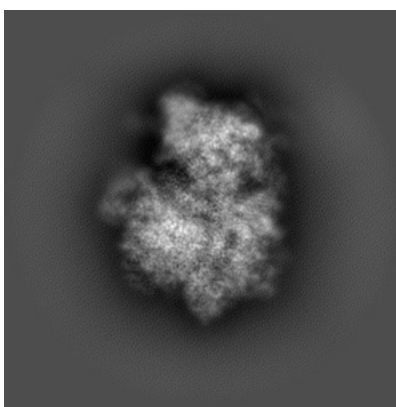


Z

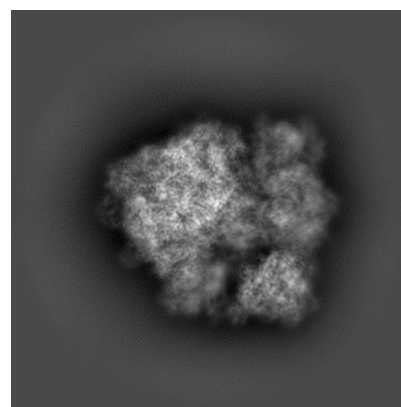
6.1.2 Raw map



X



Y

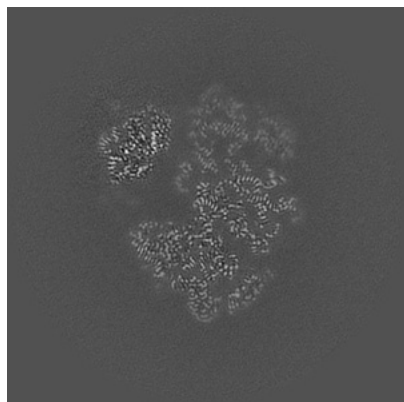


Z

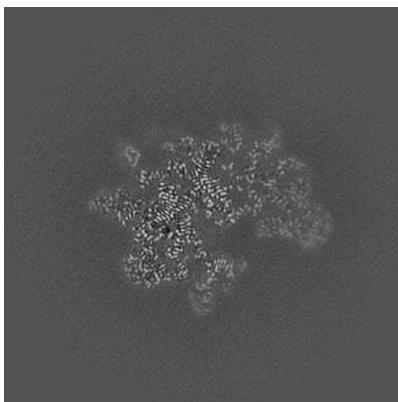
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

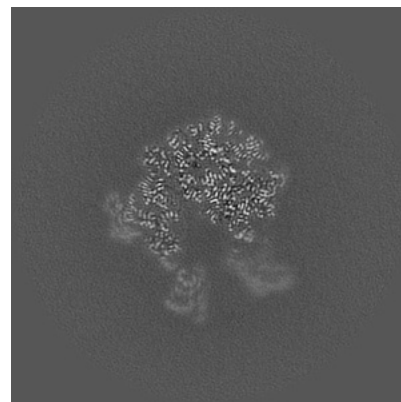
6.2.1 Primary map



X Index: 256

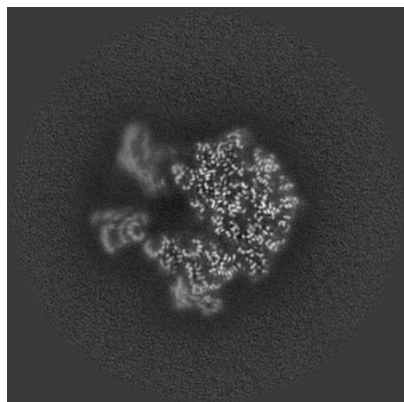


Y Index: 256

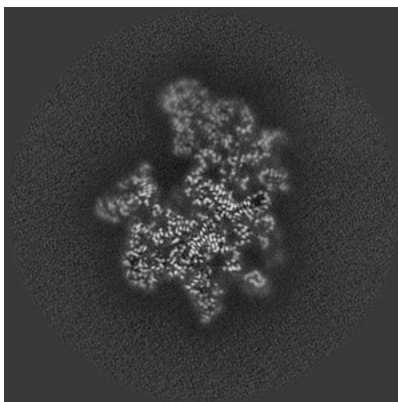


Z Index: 256

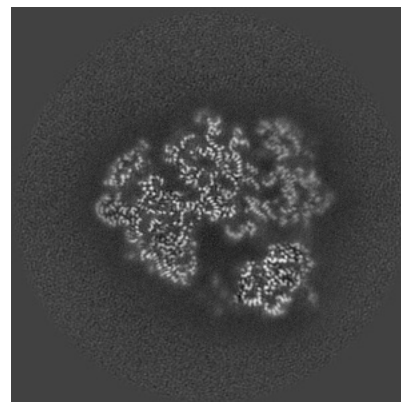
6.2.2 Raw map



X Index: 256



Y Index: 256

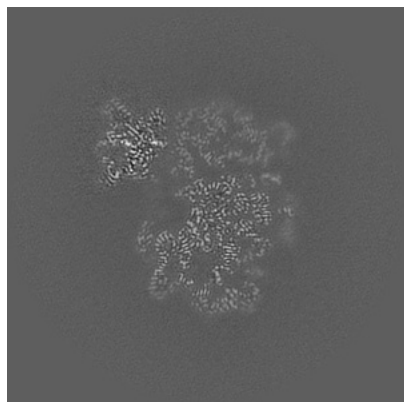


Z Index: 256

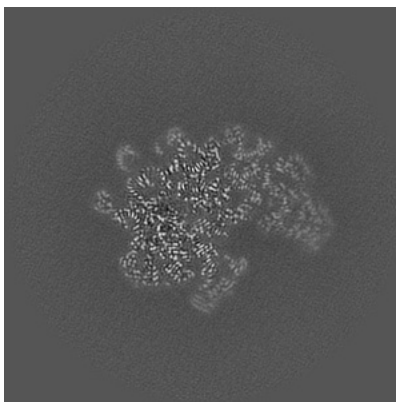
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

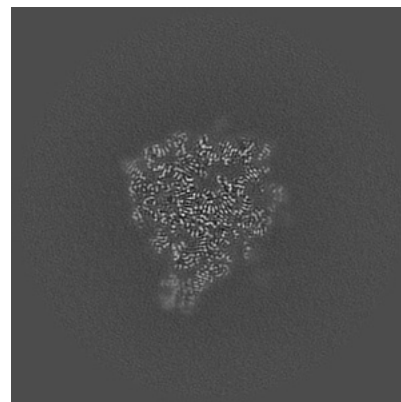
6.3.1 Primary map



X Index: 269

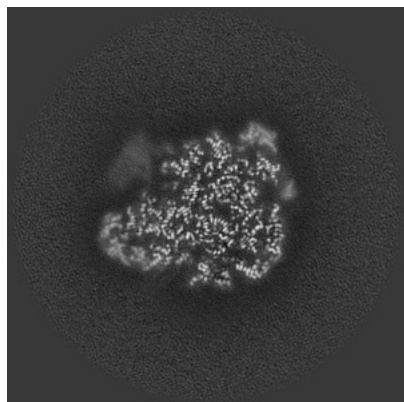


Y Index: 265

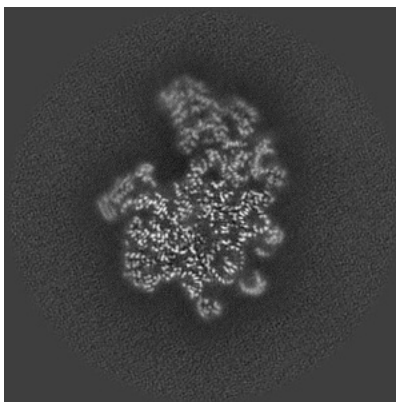


Z Index: 209

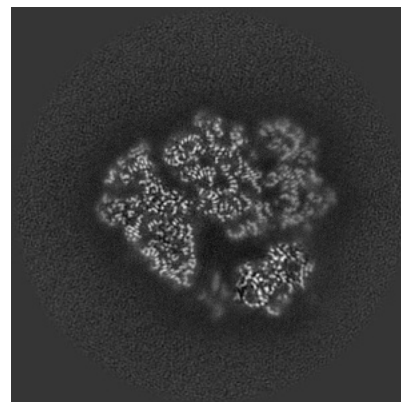
6.3.2 Raw map



X Index: 228



Y Index: 265

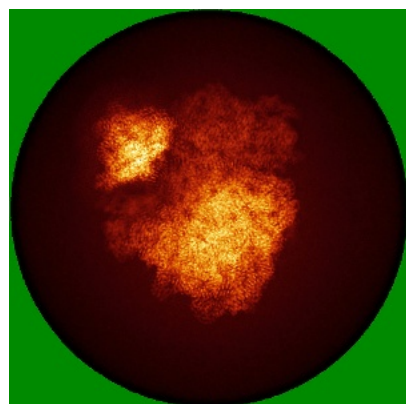


Z Index: 252

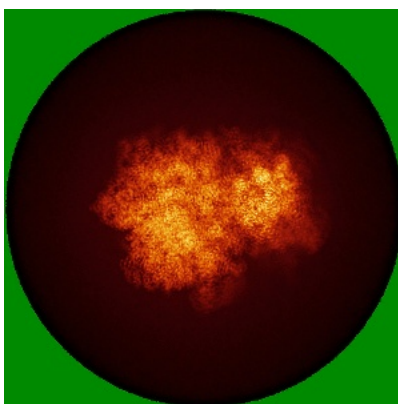
The images above show the largest variance slices of the map in three orthogonal directions.

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

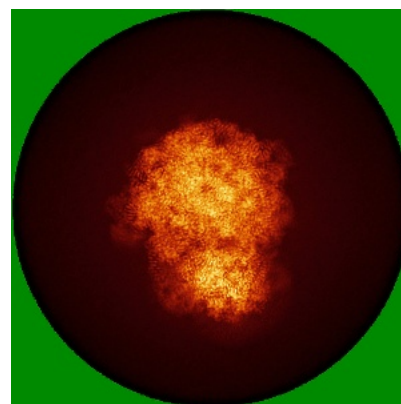
6.4.1 Primary map



X

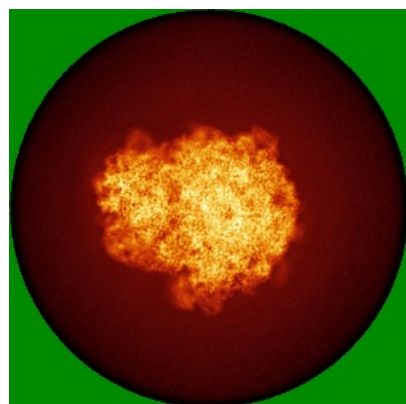


Y

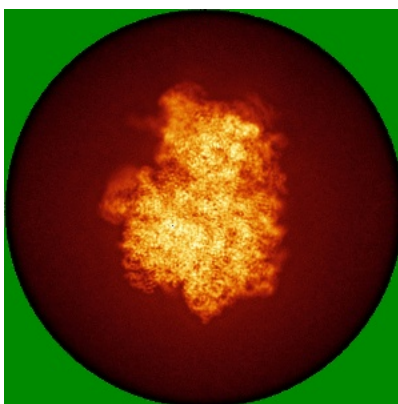


Z

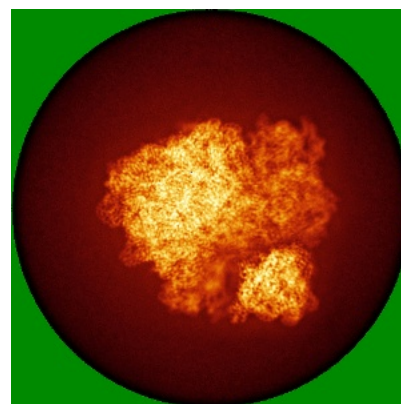
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

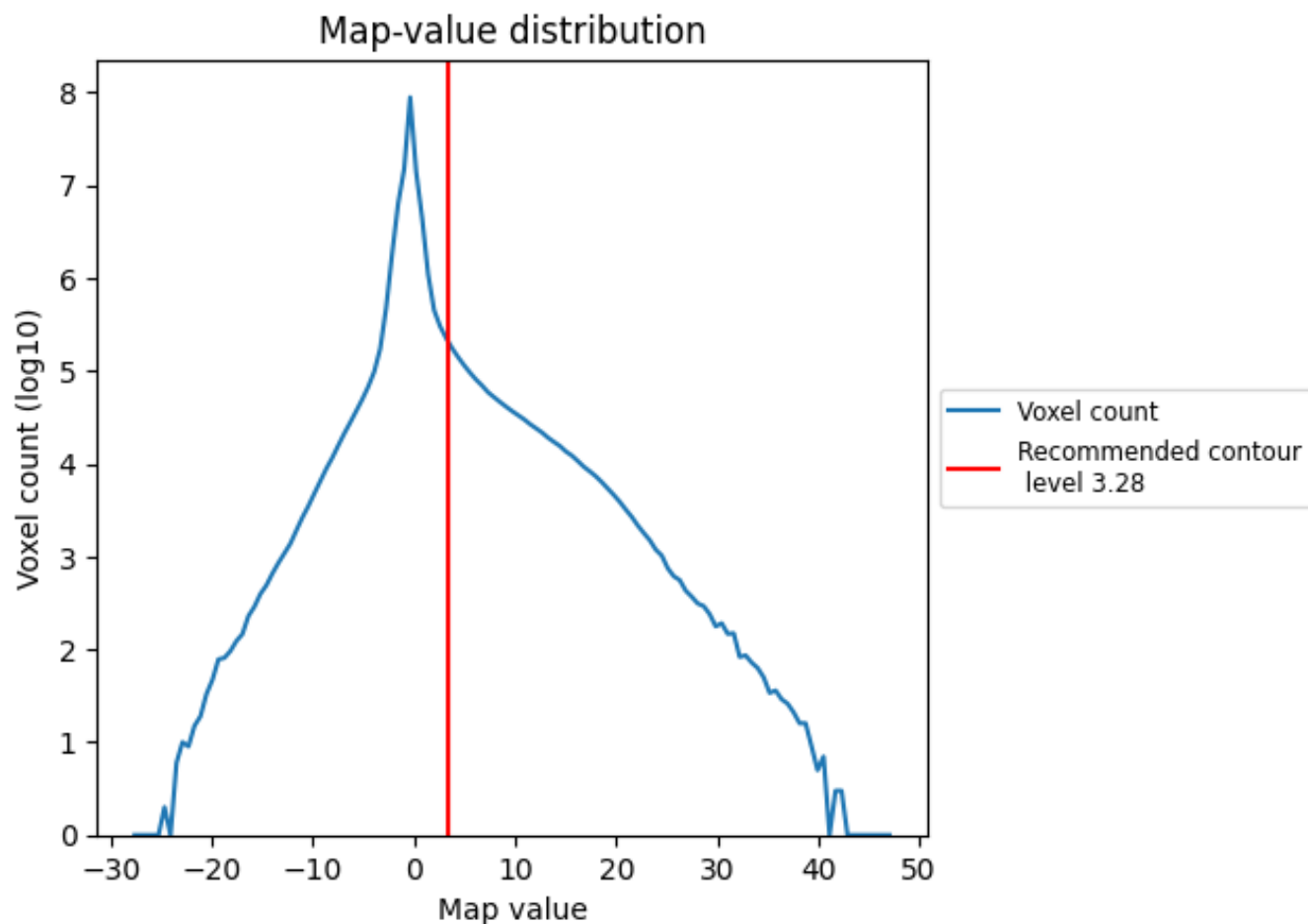
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

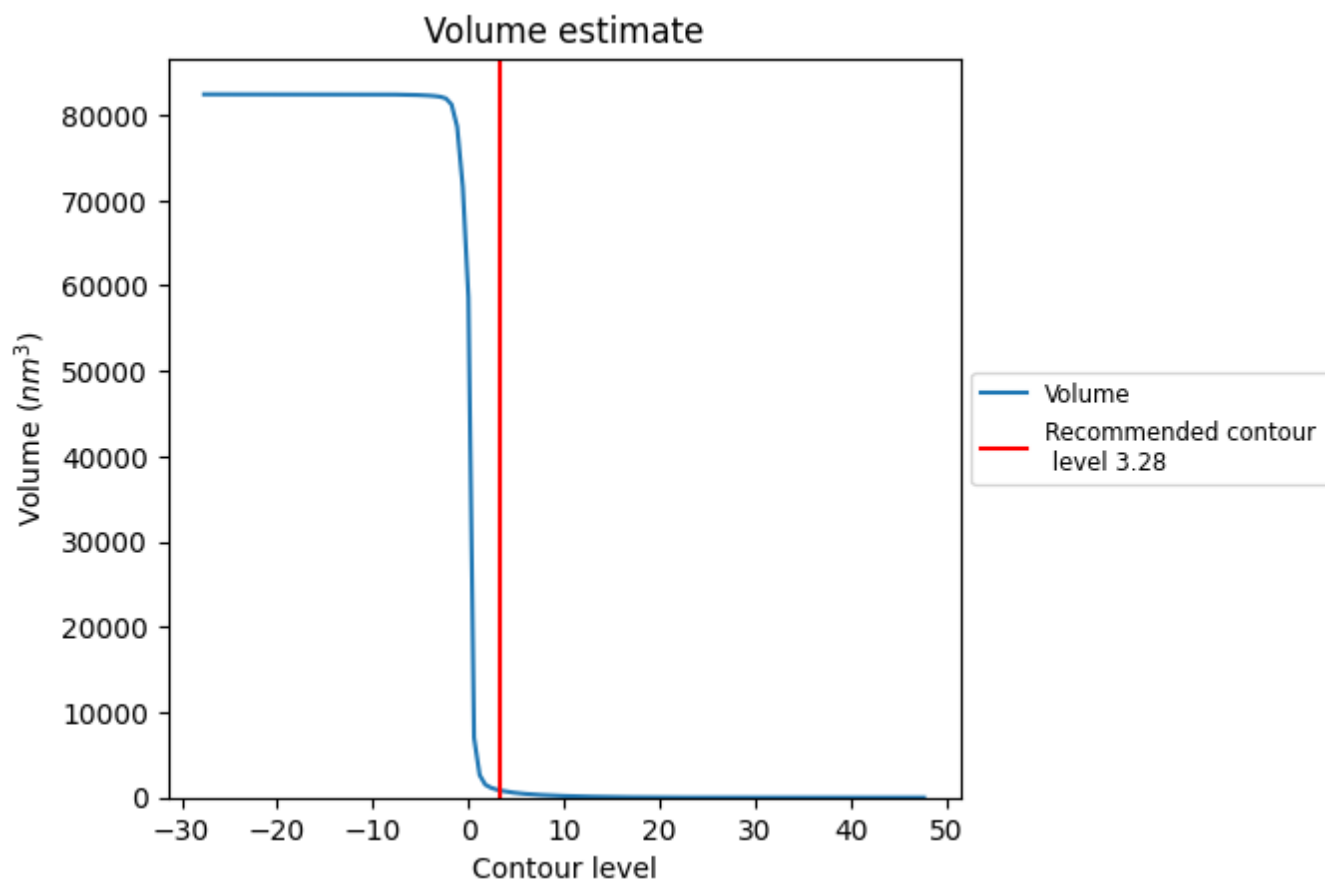
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

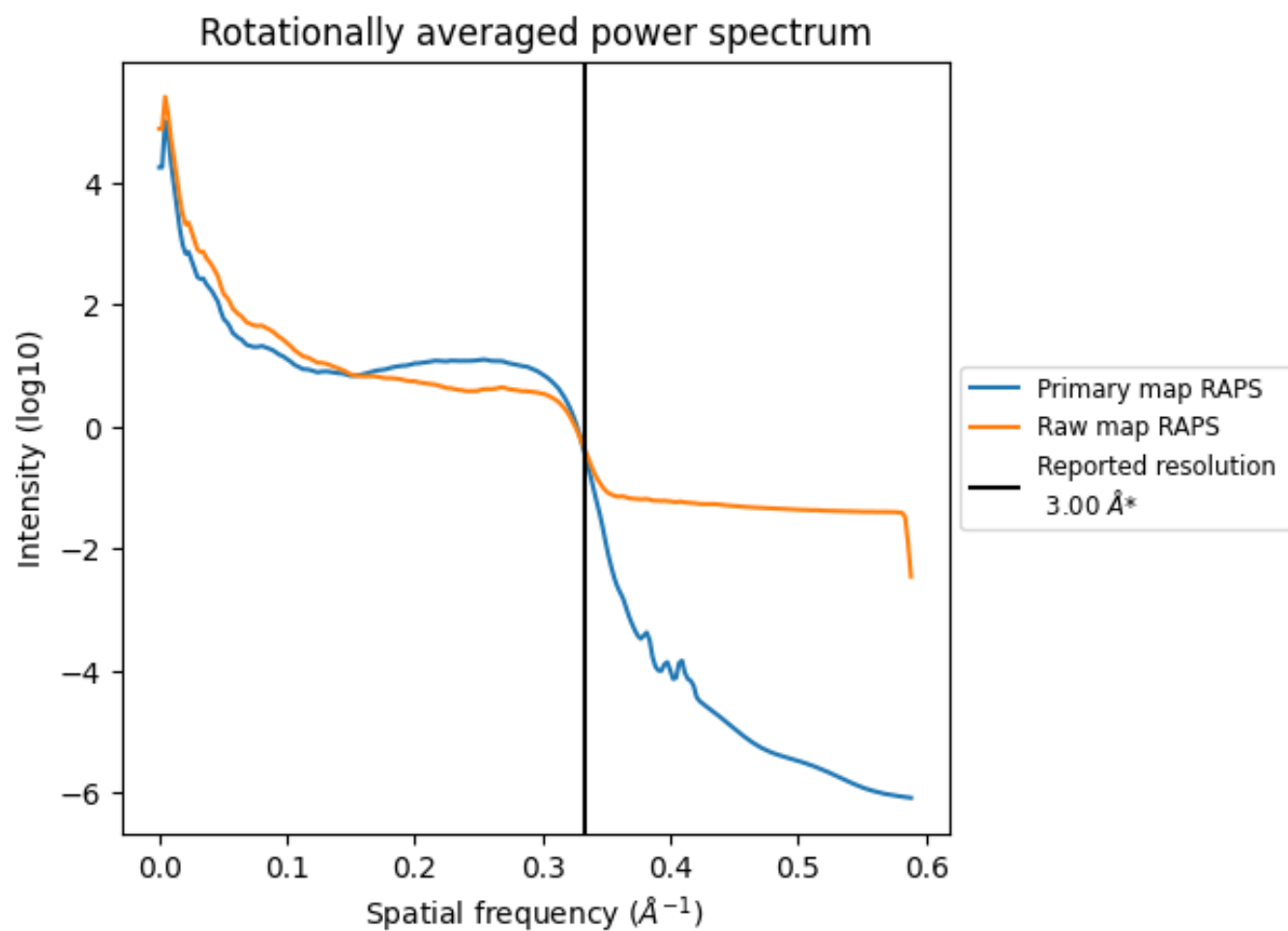
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 853 nm^3 ; this corresponds to an approximate mass of 770 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 ⓘ

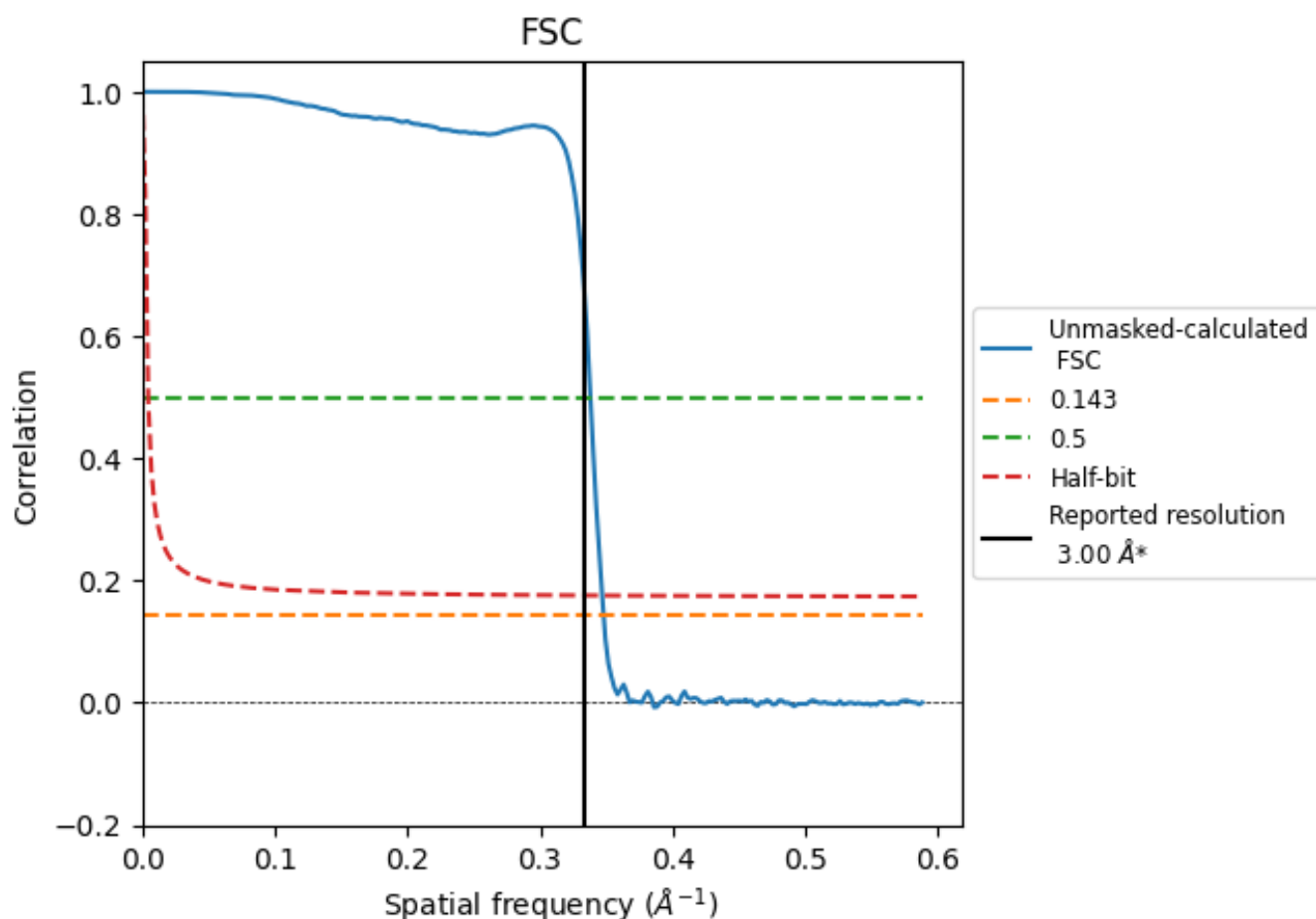


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

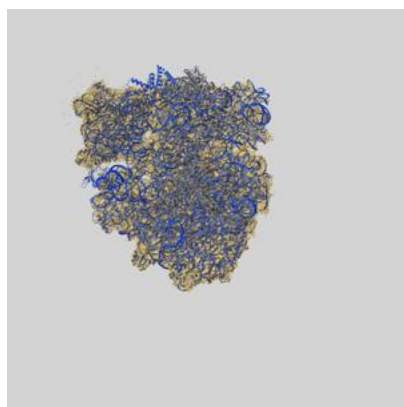
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.87	2.96	2.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

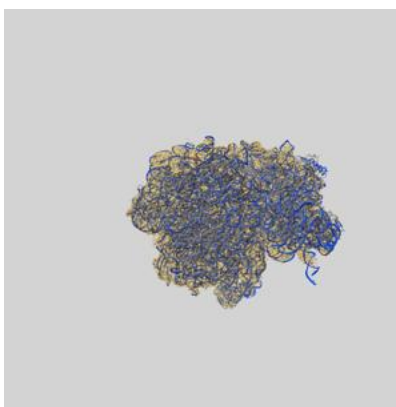
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42557 and PDB model 8UU5. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

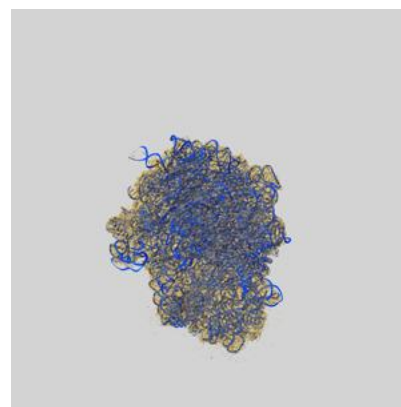
9.1 Map-model overlay [i](#)



X



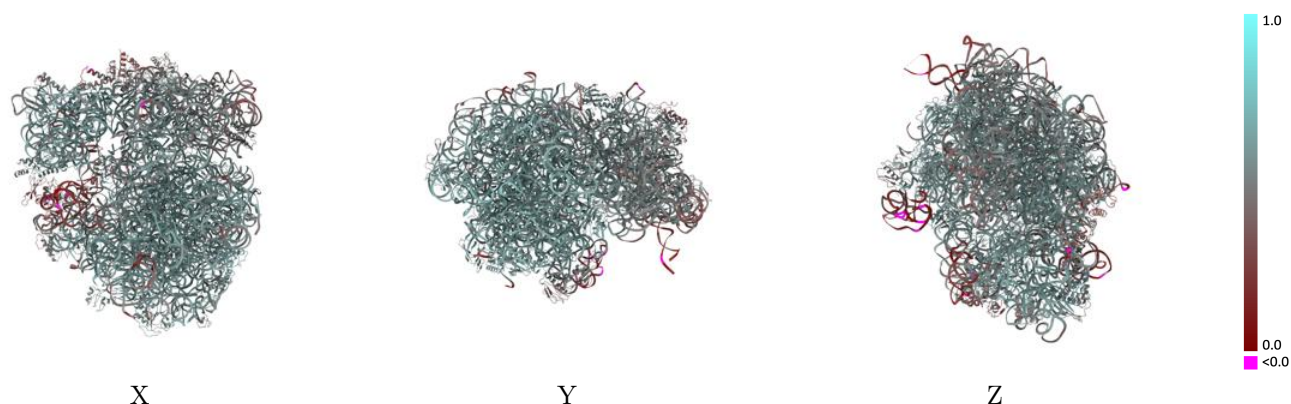
Y



Z

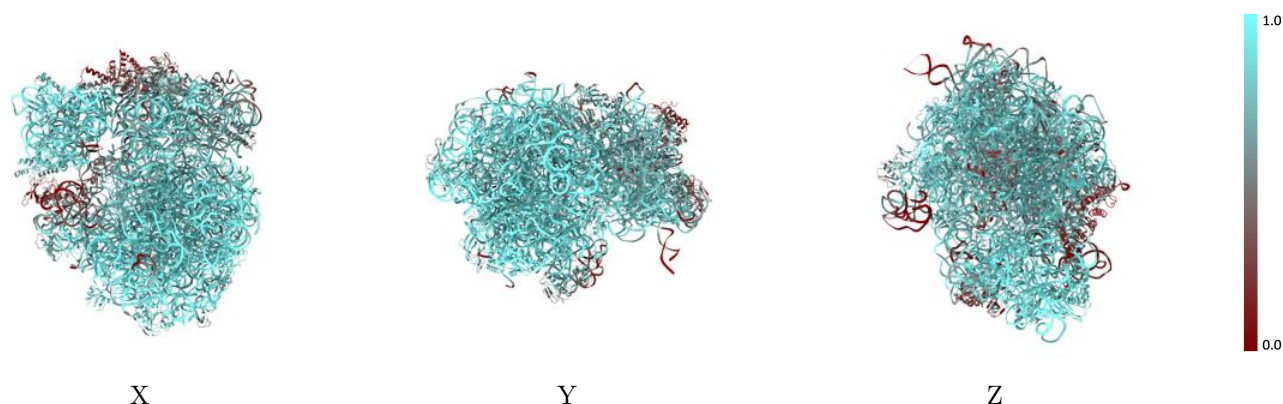
The images above show the 3D surface view of the map at the recommended contour level 3.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



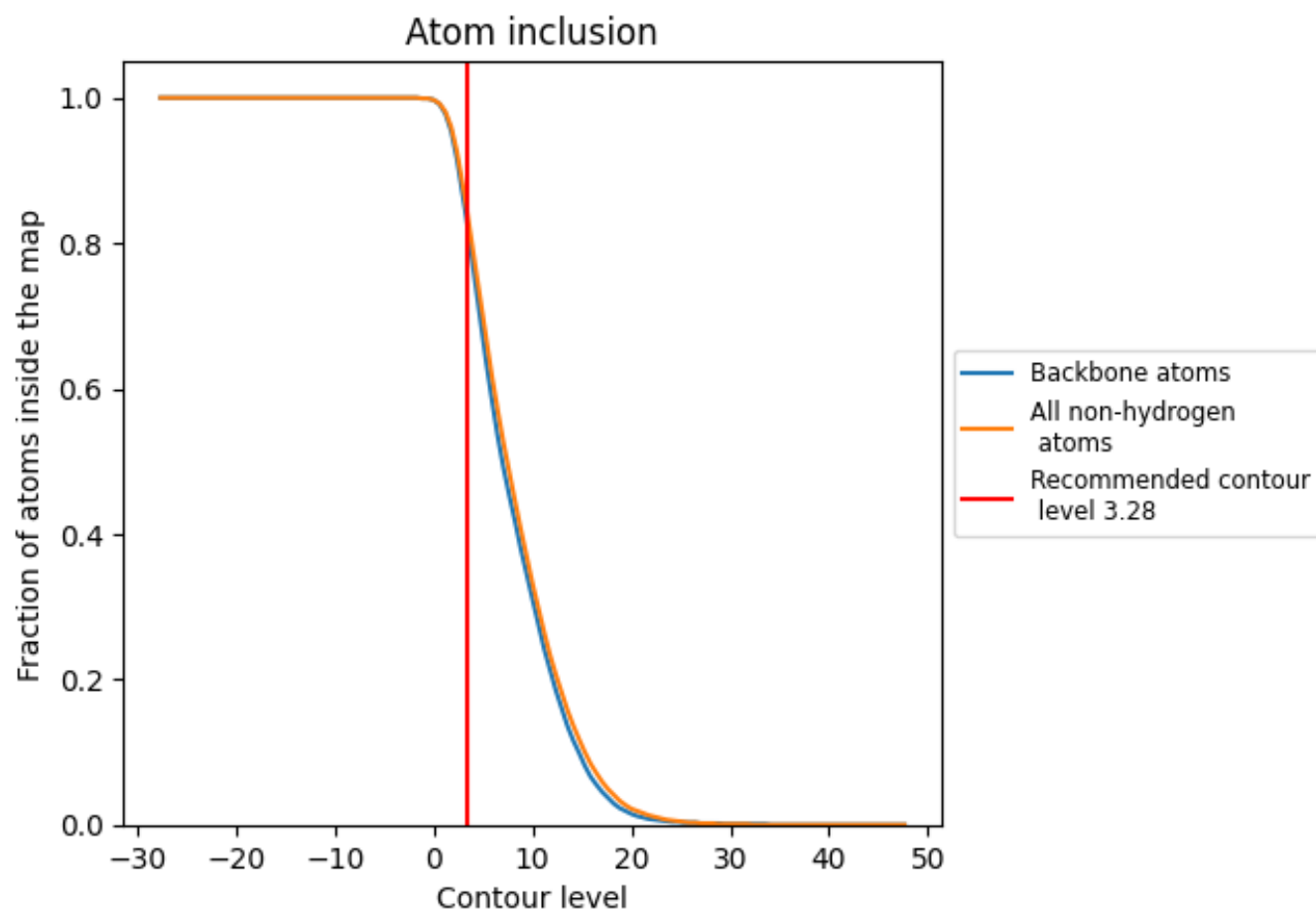
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 85% 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 (3.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8520	 0.5520
1	 0.8320	 0.5580
2	 0.9180	 0.6050
3	 0.2040	 0.3190
4	 0.9520	 0.6120
5	 0.8960	 0.5820
6	 0.9660	 0.6290
7	 0.9540	 0.6170
8	 0.9430	 0.6080
A	 0.9140	 0.5690
B	 0.8790	 0.5050
C	 0.9320	 0.6110
D	 0.9230	 0.6070
E	 0.8890	 0.5920
F	 0.3700	 0.4020
G	 0.6550	 0.4780
L	 0.9390	 0.6130
M	 0.9040	 0.6030
N	 0.8850	 0.5890
O	 0.9110	 0.5940
P	 0.9180	 0.6010
Q	 0.7360	 0.5110
R	 0.9120	 0.6020
S	 0.9390	 0.6110
T	 0.9110	 0.6070
U	 0.9240	 0.6060
V	 0.9080	 0.6020
W	 0.7460	 0.5400
Y	 0.9220	 0.6060
Z	 0.9130	 0.5870
a	 0.8610	 0.5340
b	 0.2210	 0.4040
c	 0.9030	 0.5760
d	 0.4380	 0.4600
e	 0.6020	 0.5280



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Chain	Atom inclusion	Q-score
f	 0.6990	 0.5330
g	 0.7930	 0.5240
h	 0.6400	 0.5250
i	 0.9250	 0.5700
j	 0.8650	 0.5480
k	 0.5810	 0.4960
l	 0.6010	 0.5150
m	 0.8410	 0.5460
n	 0.9510	 0.5990
o	 0.7170	 0.5190
p	 0.5510	 0.4960
q	 0.5020	 0.4830
r	 0.6920	 0.5430
s	 0.8080	 0.5590
t	 0.5710	 0.4800
w	 0.6980	 0.5240
x	 0.6070	 0.4390