Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 11:38 AM EDT

PDB ID	:	11EL / pdb_000011el
EMDB ID	:	EMD-75650
Title	:	Chimeric Escherichia coli 70S ribosome containing an evolved 16S rRNA from Vibrio cholerae (VC-ST)
Authors	:	Raskar, T.
Deposited on	:	2026-02-19
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

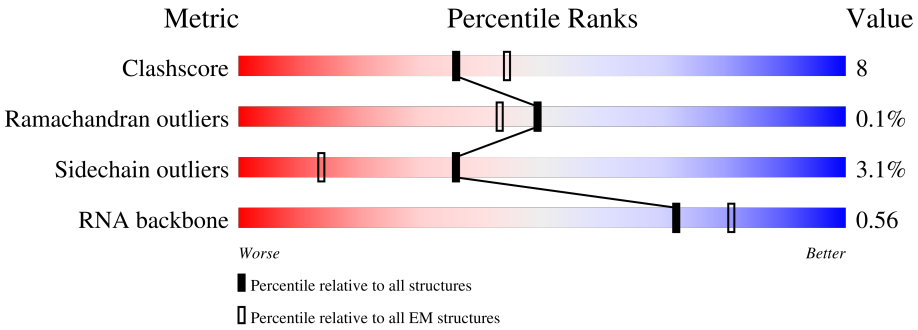
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

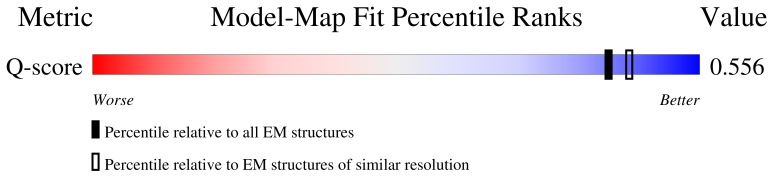
1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	11% 76% 16% 7%
2	1	46	87% 13%
3	2	65	77% 22%

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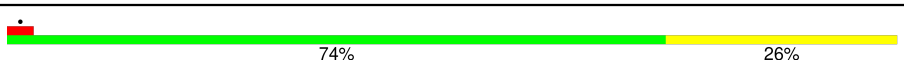
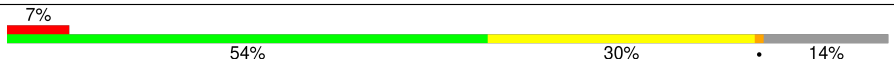
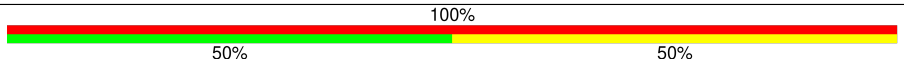
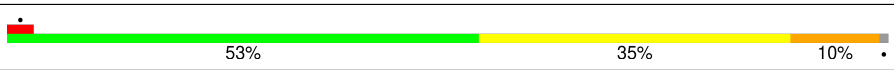
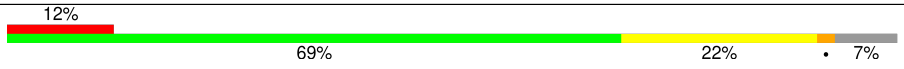
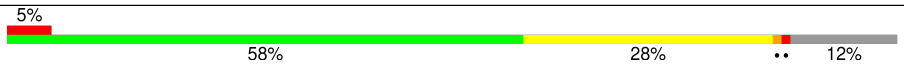
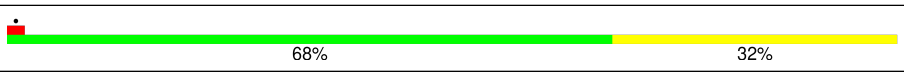
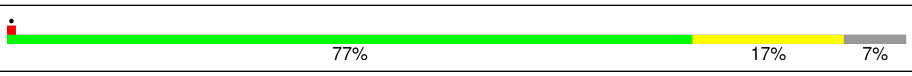
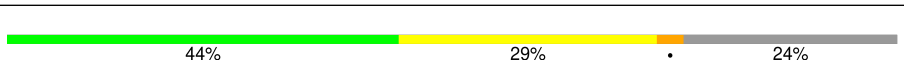
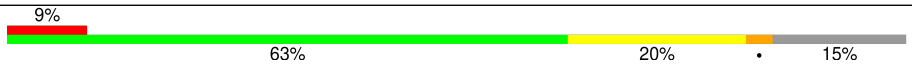
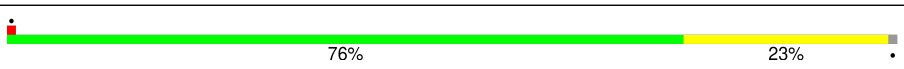
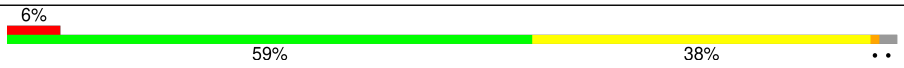
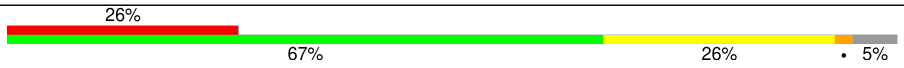
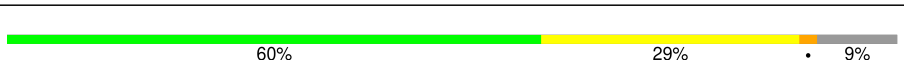
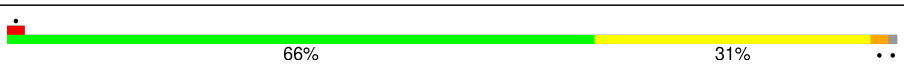
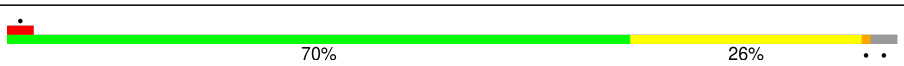
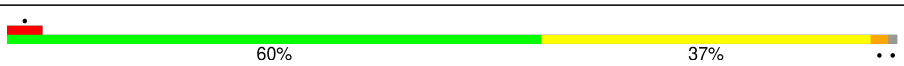
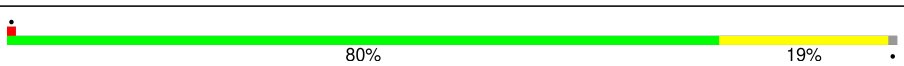
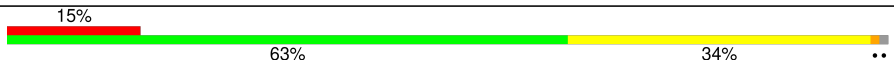
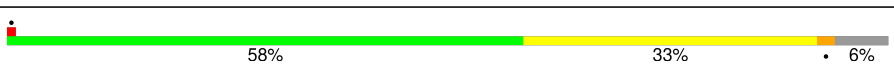
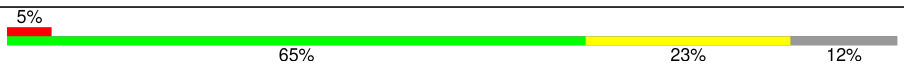
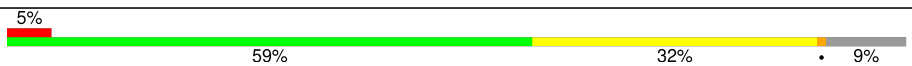
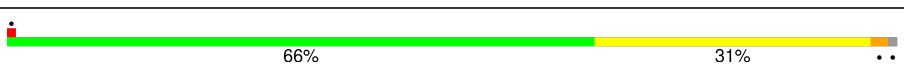
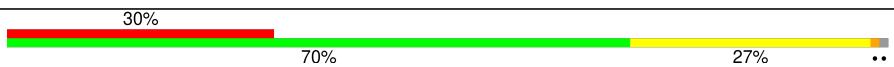
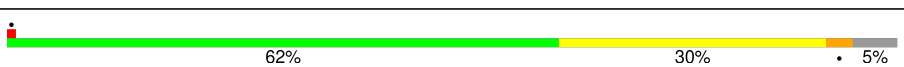
Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	5	2	
7	A	1543	
8	B	241	
9	C	233	
10	D	206	
11	E	167	
12	F	135	
13	G	179	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	U	71	
28	a	2904	

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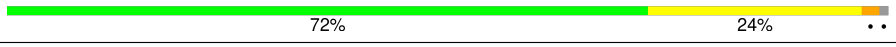
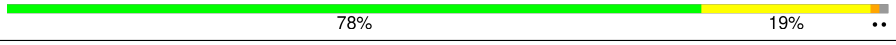
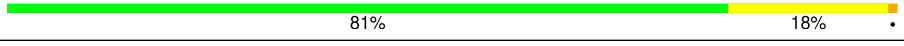
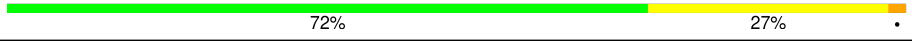
Mol	Chain	Length	Quality of chain
29	b	120	
30	c	273	
31	d	209	
32	e	201	
33	f	179	
34	g	177	
35	h	149	
36	i	142	
37	j	123	
38	k	144	
39	l	136	
40	m	127	
41	n	117	
42	o	115	
43	p	118	
44	q	103	
45	r	110	
46	s	100	
47	t	104	
48	u	94	
49	v	85	
50	w	78	
51	x	63	
52	y	59	
53	z	57	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 138616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

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

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

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

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1520	Total	C	N	O	P	0	0
			32643	14567	5995	10561	1520		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	847	G	U	conflict	GB 3166933093

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 12 is a protein called Small ribosomal subunit protein bS6.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS10.

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

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

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 22 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 27 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 35 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

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

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

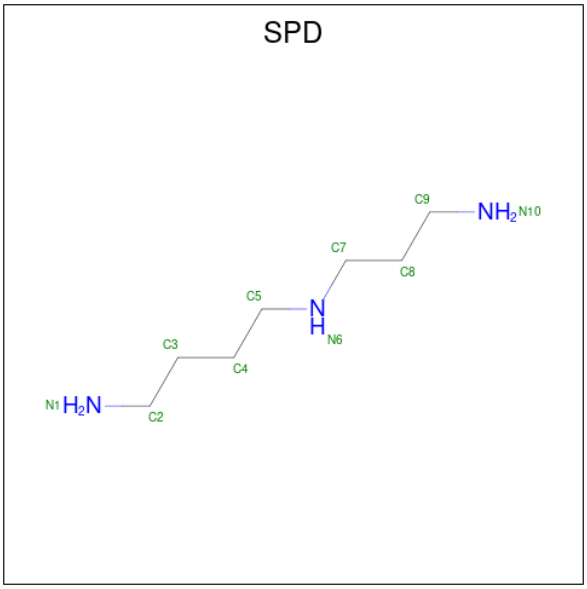
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
55	A	90	Total Mg 90 90	0
55	D	1	Total Mg 1 1	0
55	N	1	Total Mg 1 1	0
55	a	207	Total Mg 207 207	0
55	b	5	Total Mg 5 5	0
55	c	1	Total Mg 1 1	0
55	m	1	Total Mg 1 1	0
55	p	1	Total Mg 1 1	0
55	z	1	Total Mg 1 1	0

- Molecule 56 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
56	A	1	Total C N 10 7 3	0
56	A	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0

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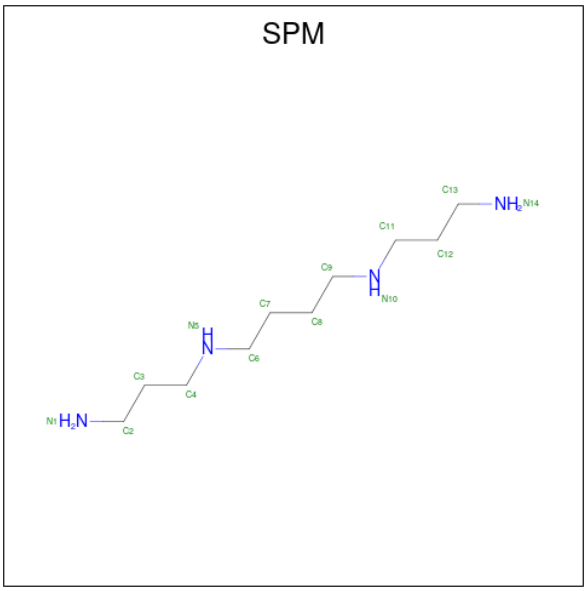
Mol	Chain	Residues	Atoms	AltConf
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0

- Molecule 57 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



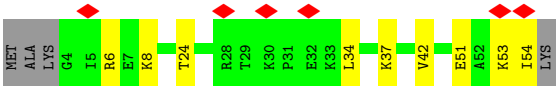
Mol	Chain	Residues	Atoms			AltConf
57	a	1	Total	C	N	0
			14	10	4	

3 Residue-property plots (i)

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

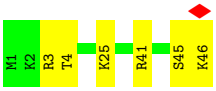
• Molecule 1: 50S ribosomal protein L33

Chain 0:



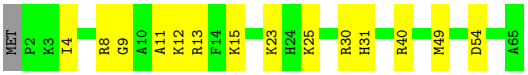
• Molecule 2: Large ribosomal subunit protein bL34

Chain 1:



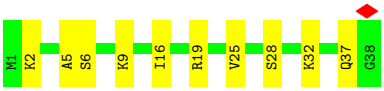
• Molecule 3: 50S ribosomal protein L35

Chain 2:



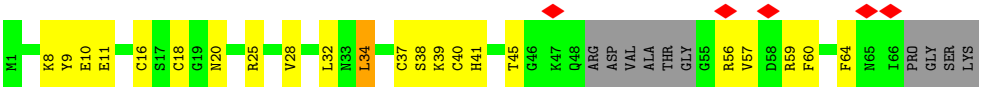
• Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:



• Molecule 5: 50S ribosomal protein L31

Chain 4:

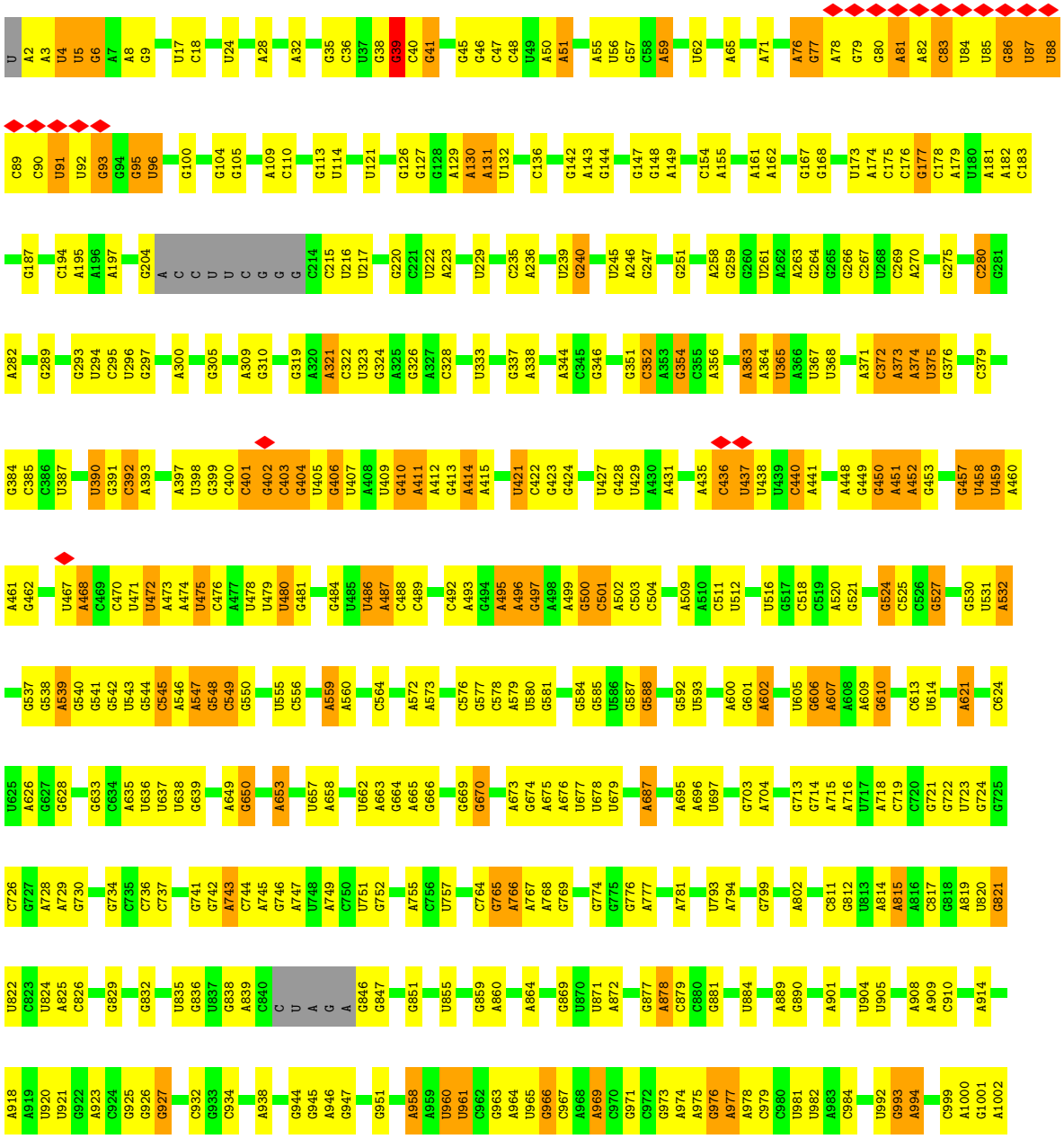


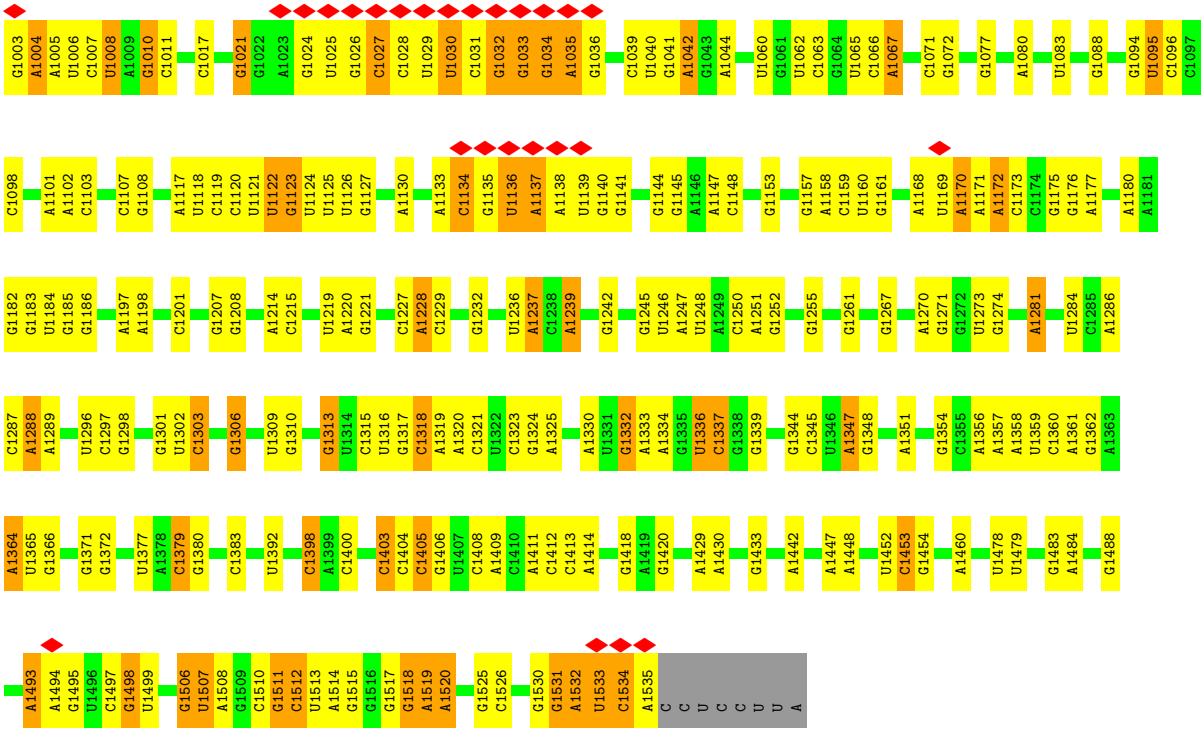
• Molecule 6: E-site tRNA

Chain 5:

• Molecule 7: 16S ribosomal RNA

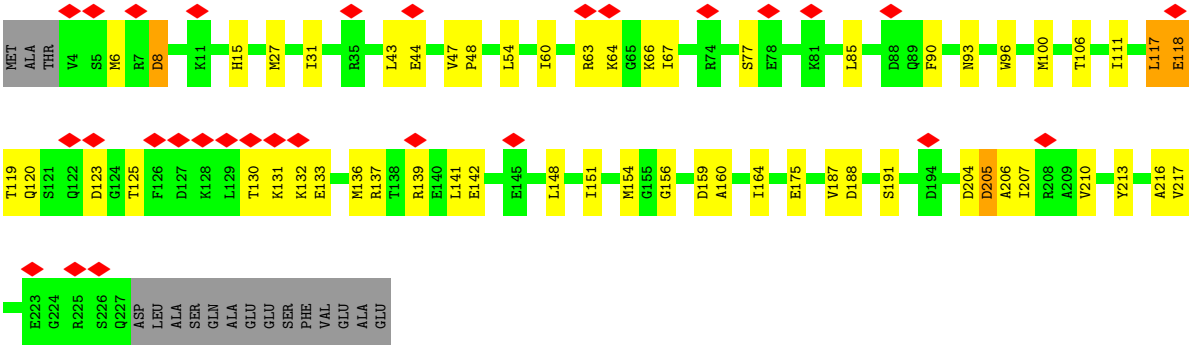
Chain A:





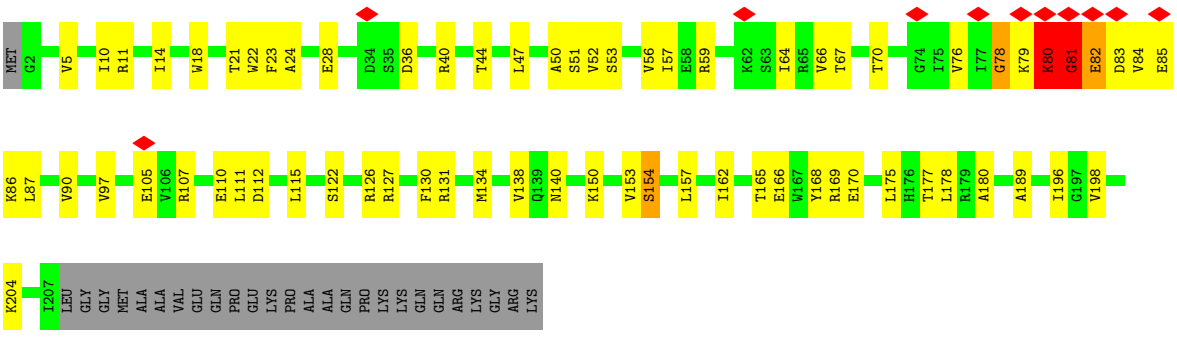
• Molecule 8: Small ribosomal subunit protein uS2

Chain B:



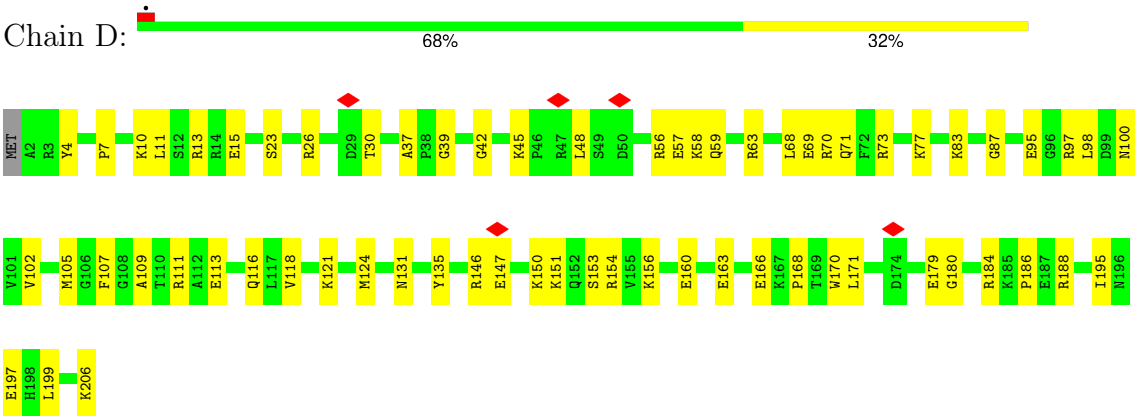
• Molecule 9: Small ribosomal subunit protein uS3

Chain C:



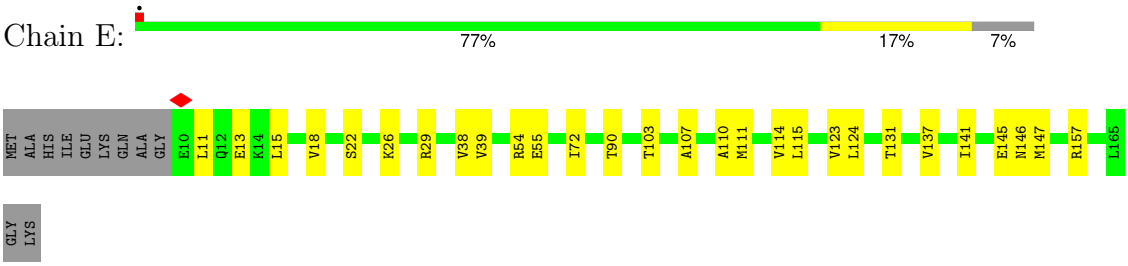
• Molecule 10: Small ribosomal subunit protein uS4

Chain D:



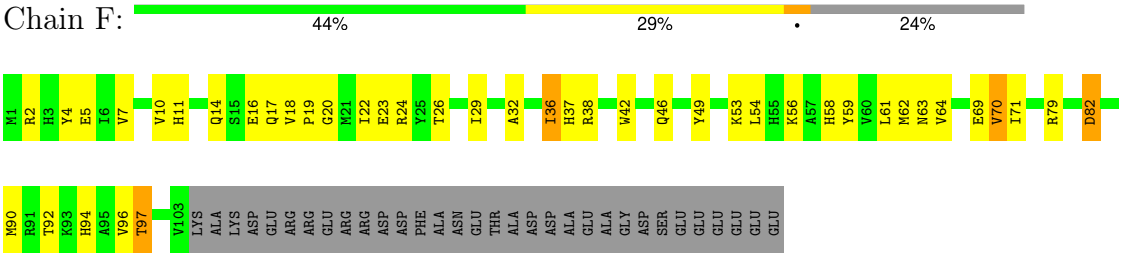
• Molecule 11: Small ribosomal subunit protein uS5

Chain E:



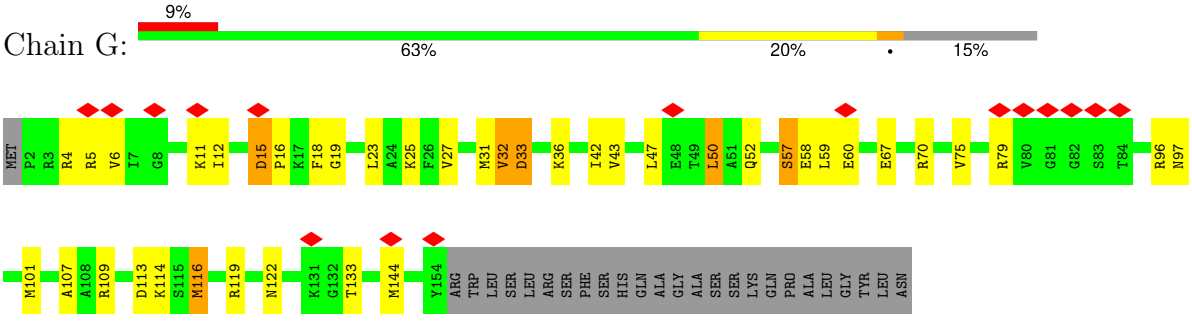
• Molecule 12: Small ribosomal subunit protein bS6

Chain F:



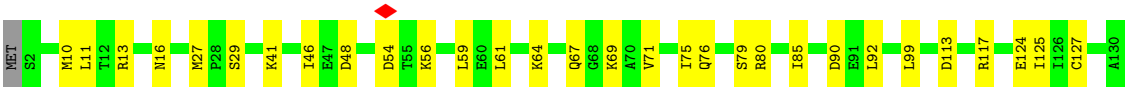
• Molecule 13: Small ribosomal subunit protein uS7

Chain G:



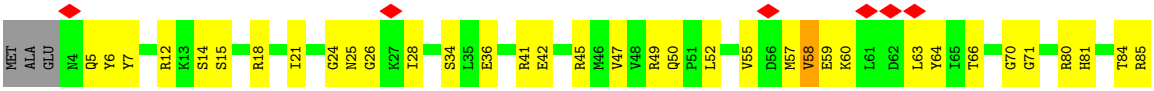
• Molecule 14: Small ribosomal subunit protein uS8

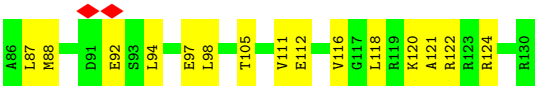
Chain H:



• Molecule 15: Small ribosomal subunit protein uS9

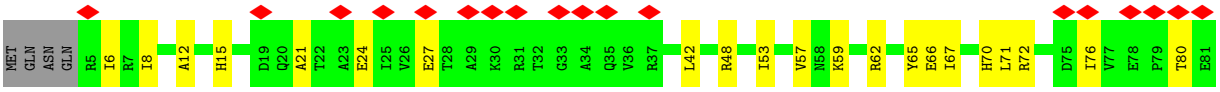
Chain I:

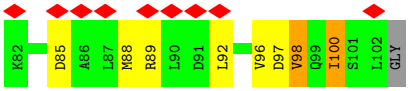




• Molecule 16: Small ribosomal subunit protein uS10

Chain J:



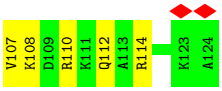


• Molecule 17: 30S ribosomal protein S11

Chain K:

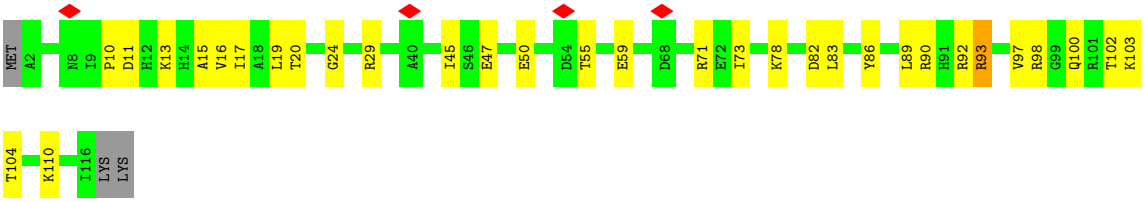
• Molecule 18: Small ribosomal subunit protein uS12

Chain L:



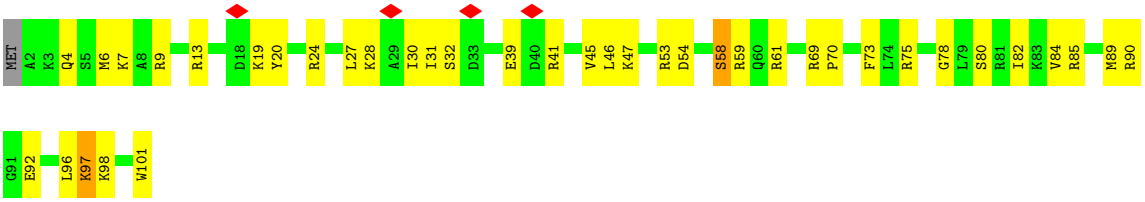
• Molecule 19: Small ribosomal subunit protein uS13

Chain M:



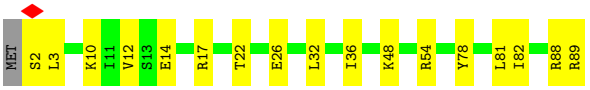
• Molecule 20: Small ribosomal subunit protein uS14

Chain N:



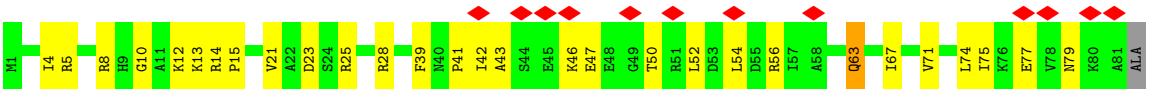
• Molecule 21: Small ribosomal subunit protein uS15

Chain O:



• Molecule 22: Small ribosomal subunit protein bS16

Chain P:



• Molecule 23: Small ribosomal subunit protein uS17

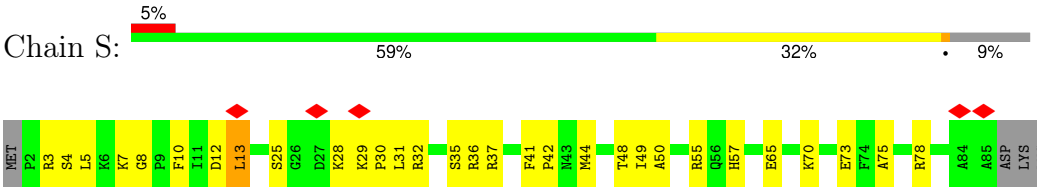
Chain Q:

• Molecule 24: Small ribosomal subunit protein bS18

Chain R:

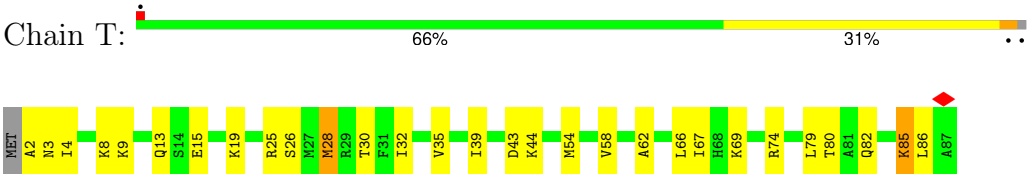
• Molecule 25: Small ribosomal subunit protein uS19

Chain S:



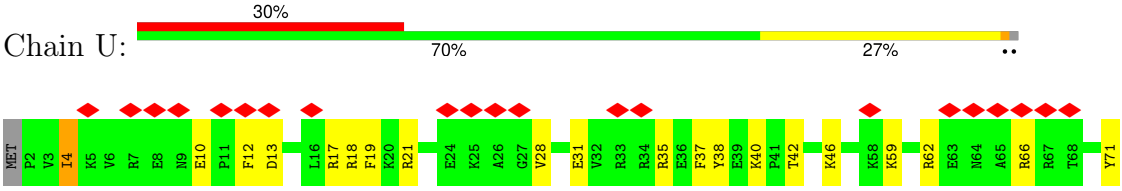
• Molecule 26: Small ribosomal subunit protein bS20

Chain T:



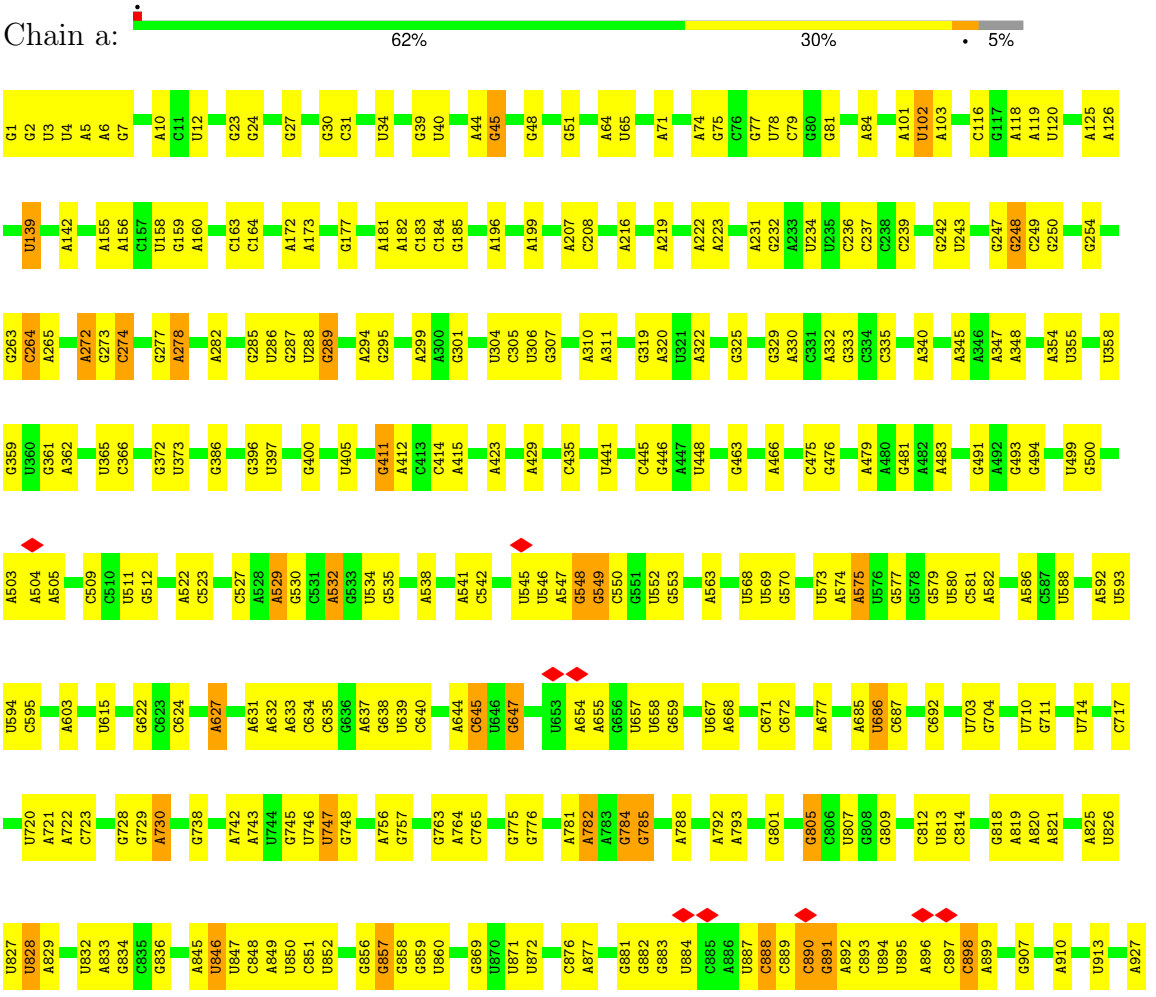
• Molecule 27: Small ribosomal subunit protein bS21

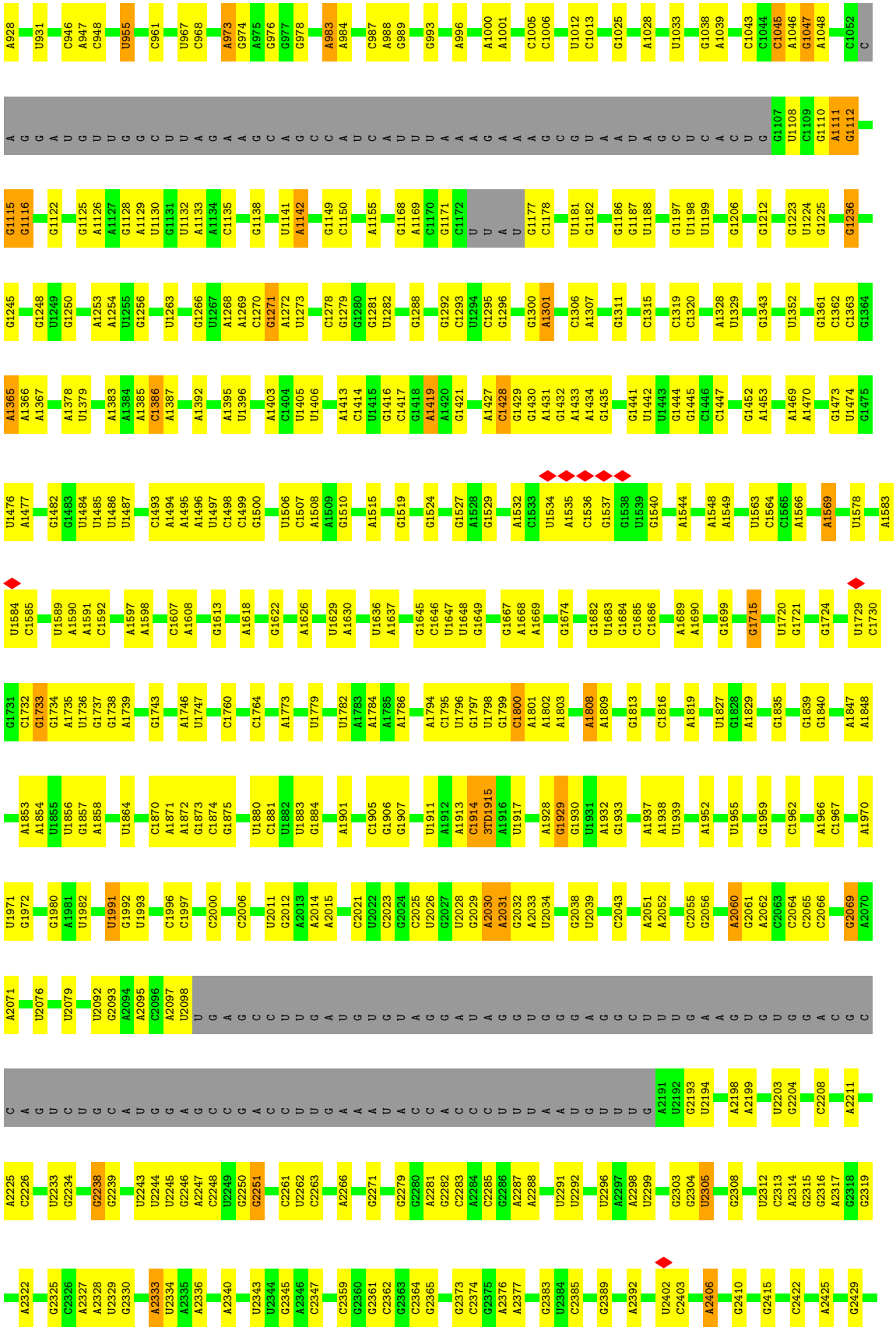
Chain U:

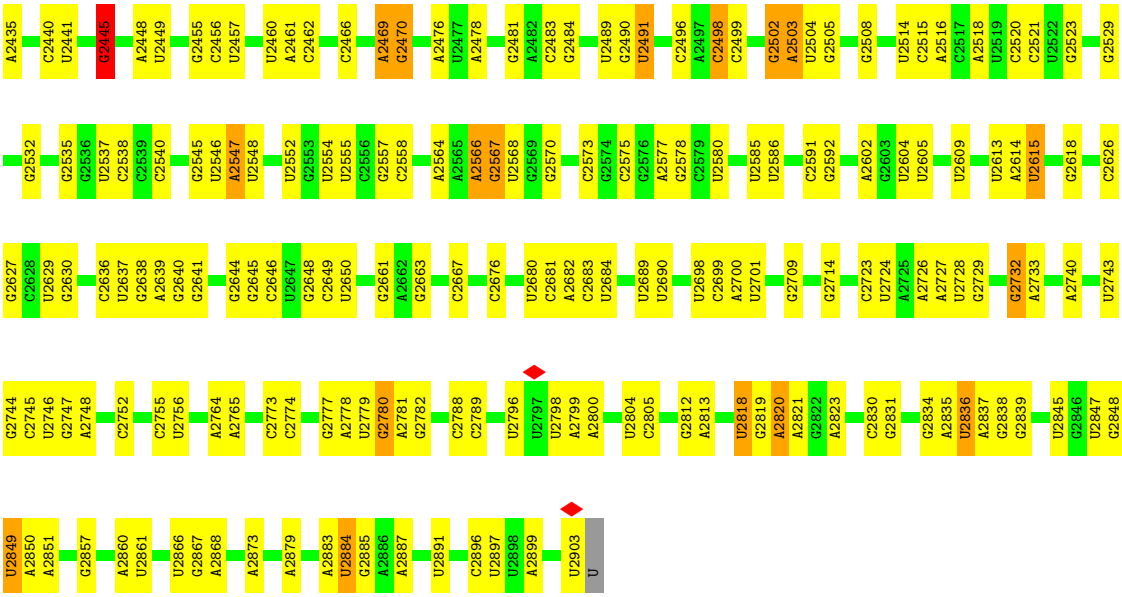


• Molecule 28: 23S ribosomal RNA

Chain a:

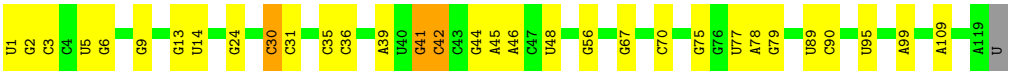






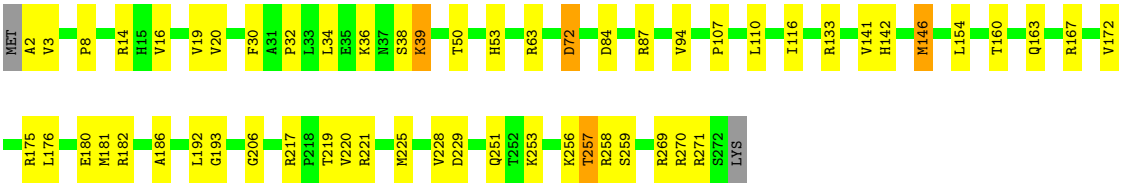
• Molecule 29: 5S ribosomal RNA

Chain b:



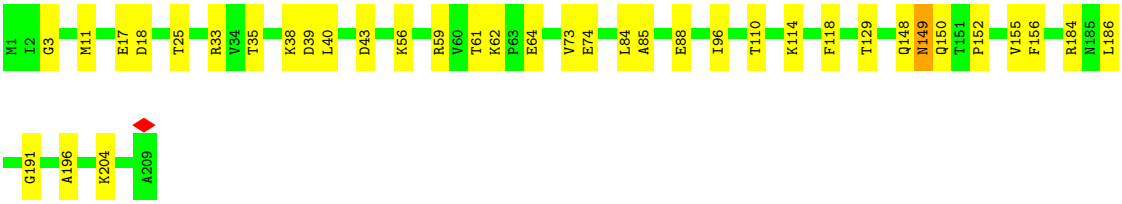
• Molecule 30: 50S ribosomal protein L2

Chain c:



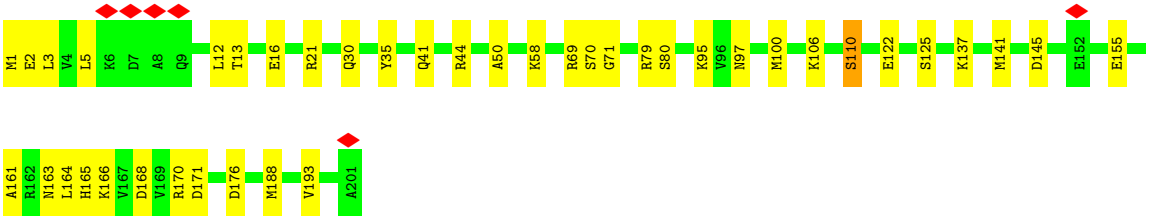
• Molecule 31: 50S ribosomal protein L3

Chain d:

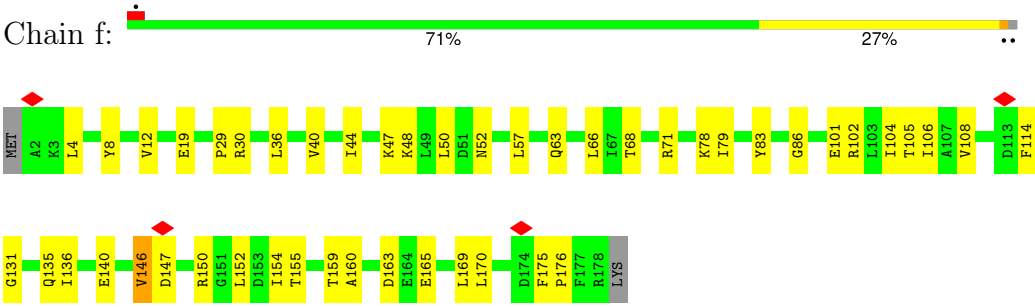


• Molecule 32: Large ribosomal subunit protein uL4

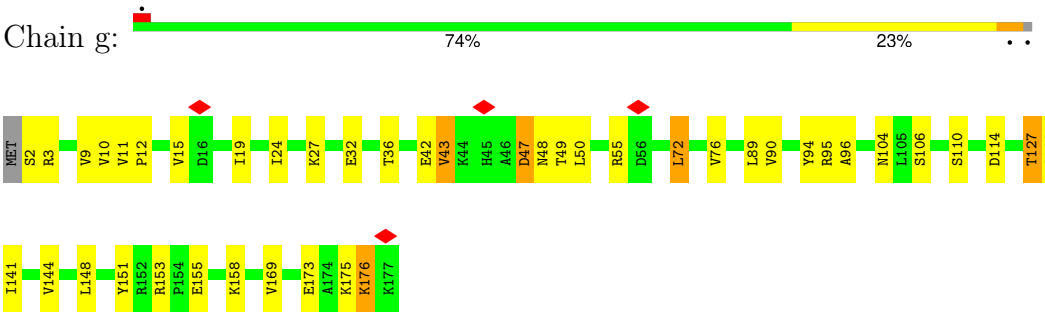
Chain e:



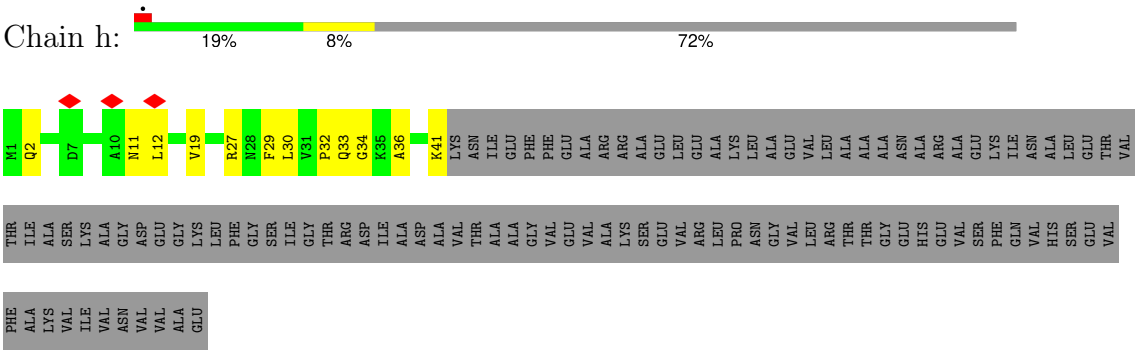
• Molecule 33: Large ribosomal subunit protein uL5



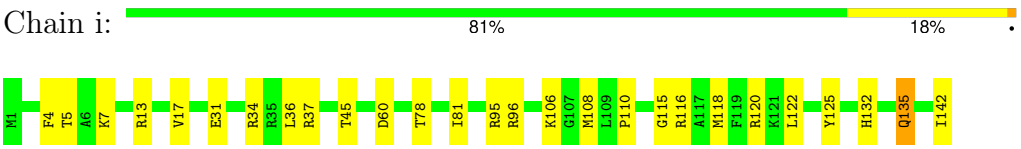
• Molecule 34: Large ribosomal subunit protein uL6



• Molecule 35: Large ribosomal subunit protein bL9

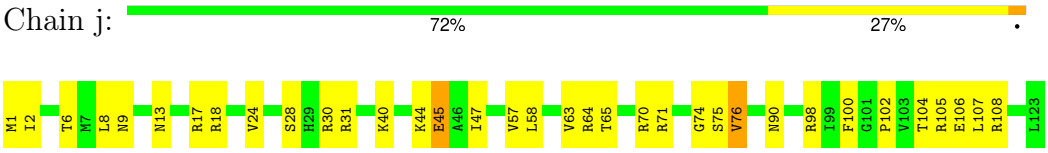


• Molecule 36: Large ribosomal subunit protein uL13



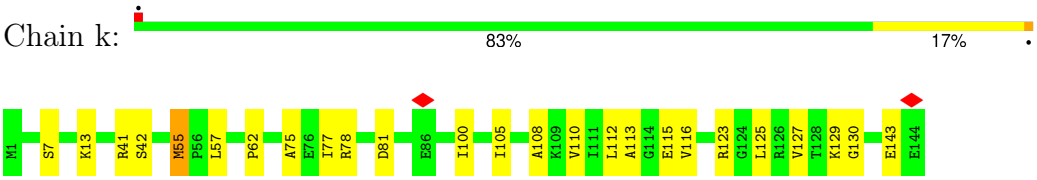
• Molecule 37: Large ribosomal subunit protein uL14

Chain j:



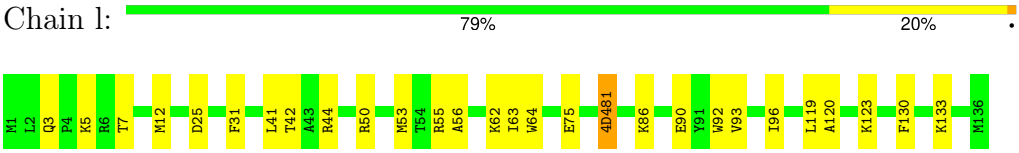
• Molecule 38: Large ribosomal subunit protein uL15

Chain k:



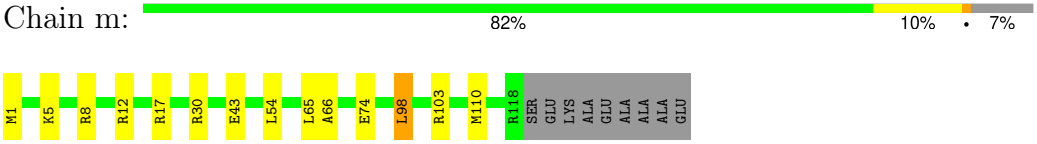
• Molecule 39: Large ribosomal subunit protein uL16

Chain l:



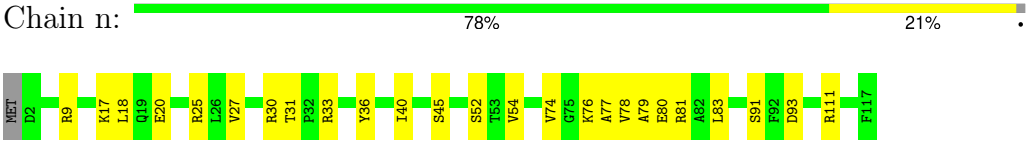
• Molecule 40: Large ribosomal subunit protein bL17

Chain m:



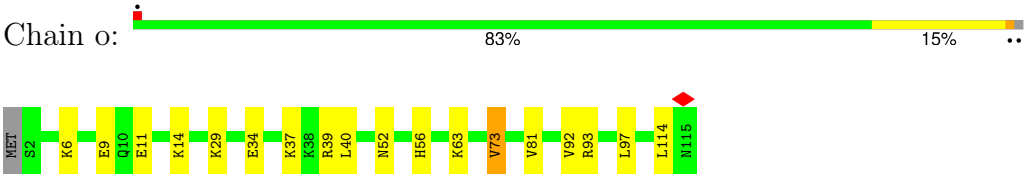
• Molecule 41: Large ribosomal subunit protein uL18

Chain n:



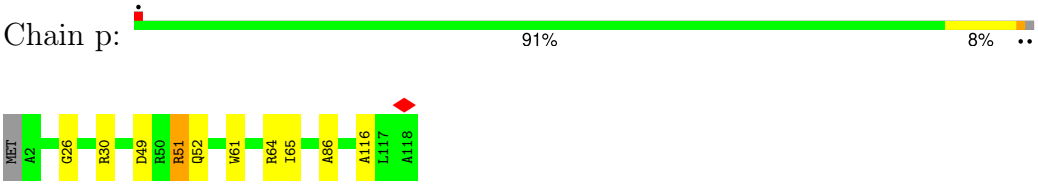
• Molecule 42: Large ribosomal subunit protein bL19

Chain o:



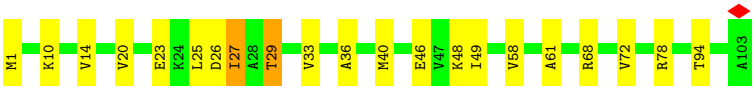
• Molecule 43: 50S ribosomal protein L20

Chain p:



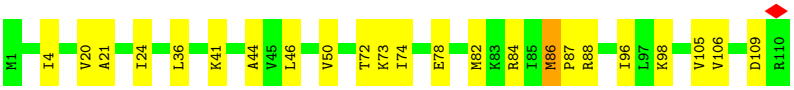
• Molecule 44: Large ribosomal subunit protein bL21

Chain q:



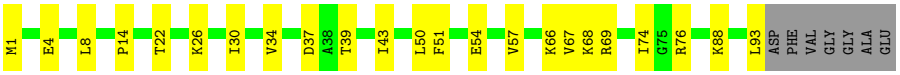
• Molecule 45: Large ribosomal subunit protein uL22

Chain r:



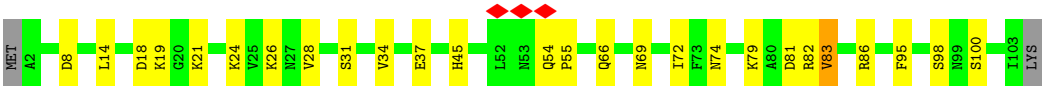
• Molecule 46: 50S ribosomal protein L23

Chain s:



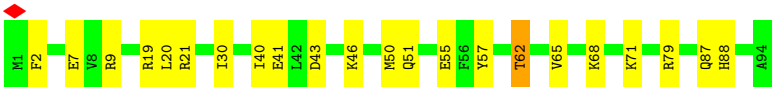
• Molecule 47: 50S ribosomal protein L24

Chain t:



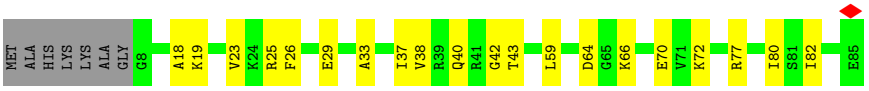
• Molecule 48: Large ribosomal subunit protein bL25

Chain u:



• Molecule 49: 50S ribosomal protein L27

Chain v:



• Molecule 50: 50S ribosomal protein L28

Chain w:

• Molecule 51: Large ribosomal subunit protein uL29

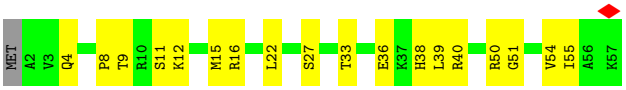
Chain x:

• Molecule 52: 50S ribosomal protein L30

Chain y:

• Molecule 53: 50S ribosomal protein L32

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	577128	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	27.798	Depositor
Minimum map value	-18.382	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.17	0/424	0.30	0/565
2	1	0.36	0/380	0.30	0/498
3	2	0.32	0/513	0.32	0/676
4	3	0.32	0/303	0.31	0/397
5	4	0.19	0/488	0.39	0/649
6	5	0.10	0/46	0.09	0/69
7	A	0.31	2/36275 (0.0%)	0.34	2/56582 (0.0%)
8	B	0.19	0/1784	0.36	0/2403
9	C	0.26	0/1651	0.41	0/2225
10	D	0.22	0/1665	0.37	0/2227
11	E	0.29	0/1165	0.34	0/1568
12	F	0.24	0/858	0.41	0/1160
13	G	0.18	0/1219	0.33	0/1635
14	H	0.27	0/989	0.29	0/1326
15	I	0.21	0/1034	0.41	0/1375
16	J	0.20	0/796	0.40	0/1077
17	K	0.25	0/893	0.39	0/1205
18	L	0.28	0/960	0.35	0/1286
19	M	0.19	0/900	0.34	0/1204
20	N	0.23	0/817	0.39	0/1088
21	O	0.27	0/722	0.32	0/964
22	P	0.28	0/653	0.47	0/877
23	Q	0.26	0/650	0.49	0/871
24	R	0.25	0/553	0.33	0/742
25	S	0.20	0/685	0.33	0/922
26	T	0.26	0/676	0.35	0/895
27	U	0.17	0/597	0.27	0/792
28	a	0.36	0/65651	0.31	0/102413
29	b	0.27	0/2850	0.25	0/4444
30	c	0.36	0/2121	0.33	0/2852
31	d	0.34	0/1576	0.31	0/2119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.27	0/1571	0.30	0/2113
33	f	0.20	0/1434	0.35	0/1926
34	g	0.21	0/1343	0.42	0/1816
35	h	0.22	0/306	0.48	0/413
36	i	0.30	0/1152	0.28	0/1551
37	j	0.34	0/955	0.30	0/1279
38	k	0.31	0/1062	0.32	0/1413
39	l	0.31	0/1073	0.30	0/1433
40	m	0.33	0/958	0.33	0/1281
41	n	0.22	0/902	0.35	0/1209
42	o	0.32	0/929	0.31	0/1242
43	p	0.35	0/960	0.28	0/1278
44	q	0.29	0/829	0.29	0/1107
45	r	0.30	0/864	0.28	0/1156
46	s	0.27	0/744	0.37	0/994
47	t	0.23	0/787	0.39	0/1051
48	u	0.26	0/766	0.29	0/1025
49	v	0.33	0/593	0.33	0/785
50	w	0.32	0/635	0.26	0/848
51	x	0.22	0/502	0.33	0/667
52	y	0.31	0/453	0.34	0/605
53	z	0.32	0/450	0.35	0/599
All	All	0.32	2/149162 (0.0%)	0.33	2/222897 (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
9	C	0	5
23	Q	0	1
34	g	0	1
39	l	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	39	G	C2-N2	-11.28	1.11	1.34
7	A	39	G	C6-N1	8.22	1.55	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	39	G	N1-C2-N2	-28.51	30.68	116.20
7	A	39	G	N3-C2-N2	-10.54	88.27	119.90

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	C	78	GLY	Peptide
9	C	80	LYS	Mainchain,Peptide
9	C	81	GLY	Peptide
9	C	82	GLU	Peptide
23	Q	16	LYS	Peptide
34	g	47	ASP	Peptide
39	l	81	4D4	Mainchain

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	0	417	0	451	4	0
2	1	377	0	418	6	0
3	2	504	0	572	14	0
4	3	302	0	340	7	0
5	4	480	0	478	19	0
6	5	42	0	23	0	0
7	A	32643	0	16433	452	0
8	B	1753	0	1780	39	0
9	C	1624	0	1696	51	0
10	D	1643	0	1707	49	0
11	E	1152	0	1196	20	0
12	F	839	0	833	33	0
13	G	1203	0	1254	29	0
14	H	979	0	1031	20	0
15	I	1022	0	1070	46	0
16	J	786	0	828	20	0
17	K	877	0	887	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	957	0	1017	29	0
19	M	891	0	952	25	0
20	N	805	0	844	36	0
21	O	714	0	734	13	0
22	P	643	0	661	27	0
23	Q	641	0	682	22	0
24	R	544	0	565	15	0
25	S	668	0	693	25	0
26	T	670	0	719	21	0
27	U	589	0	629	18	0
28	a	59130	0	29769	514	0
29	b	2549	0	1291	19	0
30	c	2082	0	2154	40	0
31	d	1566	0	1618	25	0
32	e	1552	0	1619	27	0
33	f	1410	0	1444	37	0
34	g	1323	0	1371	26	0
35	h	303	0	327	10	0
36	i	1129	0	1162	22	0
37	j	946	0	1023	23	0
38	k	1053	0	1129	17	0
39	l	1075	0	1145	18	0
40	m	945	0	989	8	0
41	n	892	0	923	15	0
42	o	917	0	962	15	0
43	p	947	0	1019	8	0
44	q	816	0	839	11	0
45	r	857	0	922	16	0
46	s	738	0	807	17	0
47	t	779	0	831	16	0
48	u	753	0	780	18	0
49	v	586	0	596	14	0
50	w	625	0	652	7	0
51	x	501	0	531	11	0
52	y	449	0	488	5	0
53	z	444	0	458	13	0
54	3	1	0	0	0	0
54	4	1	0	0	0	0
55	A	90	0	0	0	0
55	D	1	0	0	0	0
55	N	1	0	0	0	0
55	a	207	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	b	5	0	0	0	0
55	c	1	0	0	0	0
55	m	1	0	0	0	0
55	p	1	0	0	0	0
55	z	1	0	0	0	0
56	A	20	0	36	2	0
56	a	140	0	266	15	0
57	a	14	0	26	1	0
All	All	138616	0	93670	1767	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 8.

All (1767) 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)
9:C:80:LYS:O	9:C:82:GLU:N	1.70	1.24
7:A:76:A:N6	7:A:93:G:H1	1.49	1.09
28:a:627:A:OP1	38:k:78:ARG:NH2	2.02	0.91
24:R:42:SER:HB2	24:R:52:GLN:HG3	1.55	0.89
5:4:16:CYS:SG	5:4:37:CYS:HB3	2.16	0.86
7:A:401:C:N4	7:A:402:G:N7	2.25	0.84
7:A:451:A:N6	7:A:480:U:O2'	2.14	0.80
28:a:2469:A:H4'	39:l:55:ARG:HD2	1.64	0.80
7:A:403:C:H42	7:A:547:A:H5"	1.47	0.79
11:E:15:LEU:HD11	11:E:18:VAL:HG23	1.64	0.79
20:N:27:LEU:HD11	20:N:47:LYS:HG3	1.64	0.79
7:A:765:G:N1	7:A:812:G:N3	2.31	0.78
23:Q:47:HIS:HB3	23:Q:74:THR:HG22	1.65	0.78
28:a:2683:C:O2	37:j:70:ARG:NH2	2.16	0.78
7:A:501:C:OP2	18:L:114:ARG:NH2	2.14	0.78
7:A:718:A:H5'	17:K:119:ASN:HB2	1.64	0.78
7:A:1002:A:H2'	7:A:1003:G:C8	2.19	0.77
28:a:475:C:O2	28:a:479:A:N6	2.17	0.77
7:A:993:G:O2'	7:A:994:A:N7	2.18	0.76
9:C:80:LYS:C	9:C:82:GLU:N	2.42	0.76
7:A:427:U:OP1	10:D:13:ARG:NH2	2.19	0.76
8:B:117:LEU:HB3	8:B:141:LEU:HD23	1.68	0.76
7:A:1008:U:H3	7:A:1021:G:H1	1.33	0.76
46:s:54:GLU:HG2	46:s:88:LYS:HE2	1.68	0.76
34:g:104:ASN:ND2	34:g:114:ASP:OD1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:36:LYS:HB3	15:I:41:ARG:HH22	1.51	0.75
24:R:22:ASP:OD1	24:R:24:LYS:NZ	2.19	0.75
11:E:72:ILE:HD12	11:E:145:GLU:HB3	1.69	0.74
17:K:116:ILE:HD11	27:U:28:VAL:HG13	1.67	0.74
12:F:37:HIS:HB3	12:F:97:THR:HG22	1.69	0.74
28:a:976:G:HO2'	28:a:1155:A:HO2'	1.32	0.74
7:A:451:A:O2'	56:A:1691:SPD:N1	2.21	0.74
7:A:835:U:OP1	24:R:53:ARG:NH2	2.21	0.74
32:e:188:MET:HG2	32:e:193:VAL:HG23	1.70	0.74
45:r:74:ILE:HD12	45:r:105:VAL:HG22	1.70	0.74
28:a:2261:C:OP1	49:v:19:LYS:NZ	2.21	0.73
7:A:673:A:H2'	7:A:674:G:C8	2.23	0.73
30:c:107:PRO:HD2	30:c:110:LEU:HD22	1.71	0.72
28:a:820:A:H4'	28:a:836:G:H22	1.54	0.72
40:m:103:ARG:HD3	40:m:110:MET:HE2	1.70	0.72
41:n:25:ARG:NH1	41:n:93:ASP:OD2	2.23	0.72
7:A:537:G:OP1	18:L:110:ARG:NH2	2.23	0.71
42:o:37:LYS:HD3	42:o:37:LYS:H	1.54	0.71
52:y:8:THR:HG1	52:y:35:THR:HG1	1.34	0.71
7:A:401:C:O2'	7:A:621:A:N3	2.21	0.71
7:A:261:U:OP2	26:T:74:ARG:NH2	2.22	0.71
30:c:167:ARG:HG2	30:c:172:VAL:HG12	1.73	0.71
7:A:457:G:H1	7:A:475:U:H3	1.36	0.71
7:A:974:A:OP1	20:N:69:ARG:NH2	2.23	0.71
34:g:42:GLU:OE1	34:g:55:ARG:NH2	2.24	0.71
17:K:13:ARG:HB3	17:K:14:LYS:HE2	1.73	0.71
7:A:391:G:O2'	7:A:392:C:O4'	2.09	0.70
28:a:2566:A:N1	37:j:28:SER:OG	2.24	0.70
8:B:119:THR:O	8:B:123:ASP:HB2	1.91	0.70
56:a:6217:SPD:H52	45:r:87:PRO:HD2	1.74	0.70
34:g:2:SER:OG	34:g:3:ARG:N	2.19	0.70
28:a:2076:U:OP2	28:a:2238:G:N2	2.23	0.70
7:A:1219:U:H2'	7:A:1220:A:C8	2.27	0.70
7:A:826:C:O2	14:H:16:ASN:ND2	2.25	0.69
7:A:765:G:H1	7:A:812:G:H1'	1.57	0.69
33:f:40:VAL:HG21	33:f:50:LEU:HD13	1.74	0.69
16:J:65:TYR:HB3	20:N:96:LEU:HD11	1.75	0.69
28:a:1043:C:O2	28:a:1112:G:N2	2.19	0.69
38:k:108:ALA:HB3	38:k:125:LEU:HD22	1.75	0.69
7:A:77:G:H1	7:A:92:U:H3	1.40	0.69
8:B:205:ASP:OD1	8:B:205:ASP:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:207:ILE:H	8:B:207:ILE:HD12	1.56	0.69
28:a:807:U:OP2	38:k:41:ARG:NH2	2.26	0.69
28:a:2445:2MG:OP1	32:e:69:ARG:NH1	2.25	0.69
48:u:55:GLU:N	48:u:55:GLU:OE2	2.24	0.69
51:x:13:GLU:OE2	51:x:13:GLU:N	2.19	0.69
7:A:264:G:O2'	23:Q:66:PRO:O	2.09	0.69
7:A:824:U:H2'	7:A:825:A:H8	1.58	0.69
9:C:82:GLU:O	9:C:86:LYS:HG2	1.93	0.69
29:b:77:U:OP1	48:u:21:ARG:NH2	2.26	0.69
7:A:391:G:O2'	7:A:392:C:O5'	2.08	0.69
17:K:88:GLY:H	17:K:114:THR:HB	1.58	0.69
18:L:110:ARG:NH1	18:L:112:GLN:O	2.26	0.69
7:A:1025:U:H5"	7:A:1026:G:H5'	1.74	0.68
41:n:31:THR:HG22	41:n:33:ARG:H	1.58	0.68
7:A:76:A:H61	7:A:93:G:H1	0.75	0.68
13:G:67:GLU:OE1	13:G:70:ARG:NH1	2.24	0.68
7:A:269:C:H2'	7:A:270:A:H8	1.58	0.68
7:A:1348:G:O6	15:I:12:ARG:NH2	2.23	0.68
16:J:48:ARG:NH1	16:J:66:GLU:OE2	2.26	0.68
5:4:9:TYR:OH	33:f:102:ARG:NH1	2.26	0.68
45:r:4:ILE:HG12	45:r:106:VAL:HG22	1.75	0.68
7:A:392:C:OP2	22:P:8:ARG:NH2	2.27	0.68
7:A:1153:G:OP1	16:J:70:HIS:ND1	2.26	0.68
7:A:440:C:O2	7:A:497:G:N2	2.14	0.68
9:C:36:ASP:OD1	9:C:59:ARG:NH1	2.27	0.68
13:G:113:ASP:OD1	13:G:122:ASN:ND2	2.27	0.68
7:A:838:G:H2'	7:A:839:A:C8	2.29	0.68
50:w:72:ARG:NH1	50:w:78:TYR:OH	2.27	0.67
21:O:88:ARG:NH2	28:a:714:U:OP2	2.28	0.67
28:a:1043:C:N3	28:a:1112:G:N1	2.38	0.67
28:a:639:U:H2'	28:a:640:C:C6	2.30	0.67
47:t:74:ASN:ND2	47:t:81:ASP:OD2	2.27	0.67
28:a:2483:C:N3	39:l:123:LYS:NZ	2.42	0.67
49:v:38:VAL:HG12	49:v:59:LEU:HB2	1.75	0.67
7:A:960:U:H4'	7:A:961:U:OP2	1.94	0.67
7:A:664:G:OP1	24:R:57:ARG:NH2	2.28	0.67
12:F:16:GLU:OE2	12:F:16:GLU:N	2.20	0.67
48:u:62:THR:HB	48:u:71:LYS:HE3	1.75	0.67
14:H:29:SER:HB2	14:H:59:LEU:HB2	1.77	0.66
28:a:1115:G:O2'	28:a:1116:G:O5'	2.13	0.66
29:b:1:U:H2'	29:b:2:G:H8	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:846:G:H2'	7:A:847:G:C8	2.30	0.66
9:C:40:ARG:O	9:C:44:THR:HG23	1.95	0.66
7:A:1357:A:H2'	7:A:1358:A:C8	2.31	0.66
30:c:146:MET:HE2	30:c:154:LEU:HD21	1.76	0.66
7:A:1315:C:OP2	25:S:4:SER:OG	2.11	0.66
22:P:4:ILE:HG12	22:P:21:VAL:HG22	1.75	0.66
28:a:538:A:H4'	36:i:7:LYS:HG2	1.77	0.66
30:c:142:HIS:ND1	30:c:193:GLY:O	2.25	0.66
48:u:46:LYS:O	48:u:50:MET:HG3	1.95	0.66
30:c:256:LYS:HE2	30:c:270:ARG:NH1	2.12	0.66
23:Q:9:GLN:HE21	23:Q:58:VAL:HG12	1.61	0.65
3:2:30:ARG:HH21	38:k:62:PRO:HB2	1.59	0.65
19:M:78:LYS:NZ	19:M:82:ASP:OD1	2.29	0.65
31:d:33:ARG:NH2	31:d:74:GLU:O	2.28	0.65
52:y:6:LYS:NZ	52:y:37:GLU:OE1	2.30	0.65
7:A:1148:C:O2	15:I:18:ARG:NH1	2.30	0.65
28:a:1245:G:OP1	38:k:13:LYS:NZ	2.28	0.65
7:A:1318:C:O2	25:S:37:ARG:NH2	2.30	0.65
28:a:1779:U:OP2	28:a:1784:A:N6	2.27	0.65
28:a:1901:A:OP2	30:c:253:LYS:NZ	2.26	0.65
7:A:1219:U:H2'	7:A:1220:A:H8	1.61	0.65
7:A:545:C:OP1	10:D:58:LYS:NZ	2.29	0.65
22:P:8:ARG:HB3	22:P:28:ARG:NH1	2.11	0.65
7:A:40:C:H5	7:A:402:G:H21	1.46	0.64
28:a:860:U:OP2	56:a:6218:SPD:N1	2.29	0.64
1:0:6:ARG:NH1	28:a:2285:C:OP2	2.31	0.64
18:L:57:LEU:HD21	18:L:82:ILE:HD11	1.79	0.64
7:A:1357:A:H2'	7:A:1358:A:H8	1.61	0.64
10:D:98:LEU:HB2	10:D:135:TYR:HB3	1.78	0.64
16:J:85:ASP:HA	16:J:88:MET:SD	2.37	0.64
12:F:46:GLN:OE1	12:F:56:LYS:NZ	2.31	0.64
28:a:639:U:H2'	28:a:640:C:H6	1.62	0.64
10:D:166:GLU:OE2	10:D:166:GLU:N	2.25	0.64
26:T:28:MET:O	26:T:32:ILE:HD12	1.97	0.64
28:a:219:A:N3	28:a:234:U:O2'	2.27	0.64
7:A:532:A:N6	7:A:1207:G:O2'	2.30	0.64
7:A:127:G:H4'	23:Q:6:ARG:HH12	1.63	0.64
17:K:83:GLU:HG2	17:K:109:ASN:HB2	1.80	0.64
28:a:1447:C:O2'	28:a:1544:A:N3	2.30	0.64
12:F:26:THR:HG23	12:F:36:ILE:HD12	1.80	0.63
28:a:2728:U:HO2'	28:a:2729:G:H8	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1452:U:H3'	7:A:1453:C:H6	1.63	0.63
28:a:2305:U:H5"	33:f:131:GLY:HA3	1.79	0.63
28:a:2328:A:H2'	28:a:2329:U:C6	2.33	0.63
15:I:6:TYR:HB2	15:I:21:ILE:HD11	1.81	0.63
7:A:28:A:O2'	7:A:296:U:OP1	2.15	0.63
7:A:714:G:H2'	7:A:715:A:C8	2.33	0.63
28:a:1296:G:OP1	28:a:2709:G:O2'	2.16	0.63
7:A:1306:G:N2	7:A:1332:G:O2'	2.24	0.63
10:D:26:ARG:NH2	10:D:30:THR:O	2.31	0.63
39:l:53:MET:HG3	39:l:120:ALA:HB2	1.81	0.63
3:2:23:LYS:NZ	28:a:631:A:OP2	2.31	0.63
8:B:8:ASP:OD1	8:B:8:ASP:N	2.31	0.63
28:a:987:C:O2'	28:a:1000:A:N3	2.30	0.63
38:k:115:GLU:OE1	38:k:116:VAL:N	2.32	0.63
13:G:4:ARG:HA	13:G:4:ARG:NH1	2.14	0.63
19:M:100:GLN:N	19:M:100:GLN:OE1	2.30	0.63
28:a:2523:G:HO2'	28:a:2764:A:HO2'	1.44	0.63
15:I:55:VAL:HG23	15:I:57:MET:HB2	1.80	0.62
28:a:2304:G:H22	28:a:2312:U:H3	1.46	0.62
41:n:17:LYS:NZ	41:n:20:GLU:OE2	2.31	0.62
28:a:2575:C:OP1	31:d:149:ASN:ND2	2.32	0.62
28:a:2681:C:OP2	31:d:114:LYS:NZ	2.23	0.62
7:A:1030:U:H3'	7:A:1032:G:H8	1.64	0.62
7:A:76:A:N1	7:A:93:G:N2	2.41	0.62
7:A:815:A:N7	7:A:1510:C:O2'	2.31	0.62
9:C:168:TYR:OH	11:E:55:GLU:OE2	2.13	0.62
10:D:57:GLU:HG3	10:D:199:LEU:HD12	1.82	0.62
15:I:36:GLU:HA	15:I:45:ARG:HH21	1.64	0.62
15:I:47:VAL:HG13	15:I:80:ARG:HD3	1.81	0.62
28:a:2502:G:H5"	28:a:2503:2MA:H5"	1.82	0.62
48:u:9:ARG:HG2	48:u:41:GLU:HG3	1.80	0.62
7:A:664:G:H22	7:A:741:G:H1	1.47	0.62
7:A:1227:C:H2'	19:M:102:THR:HG22	1.82	0.62
10:D:100:ASN:OD1	10:D:111:ARG:NH1	2.32	0.62
19:M:47:GLU:N	19:M:47:GLU:OE2	2.32	0.62
13:G:42:ILE:HD13	13:G:116:MET:HG2	1.80	0.62
18:L:73:ASN:OD1	18:L:105:SER:OG	2.16	0.62
28:a:1952:A:OP1	37:j:44:LYS:NZ	2.31	0.62
7:A:472:U:H2'	7:A:473:A:H8	1.65	0.62
20:N:61:ARG:NH1	20:N:70:PRO:O	2.32	0.62
31:d:17:GLU:OE1	31:d:17:GLU:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:12:PRO:HD2	34:g:15:VAL:HG21	1.80	0.62
10:D:11:LEU:HD13	10:D:63:ARG:HG2	1.81	0.62
3:2:54:ASP:HB3	38:k:57:LEU:HD22	1.82	0.61
28:a:2796:U:H3	28:a:2799:A:H61	1.46	0.61
7:A:1336:U:H5'	7:A:1337:C:H5'	1.81	0.61
13:G:18:PHE:HB3	13:G:59:LEU:HD11	1.81	0.61
7:A:398:U:H2'	7:A:399:G:H8	1.65	0.61
51:x:4:LYS:H	51:x:4:LYS:HD2	1.64	0.61
7:A:6:G:H2'	11:E:124:LEU:HD21	1.81	0.61
50:w:6:GLN:NE2	50:w:76:GLU:OE2	2.32	0.61
7:A:427:U:O2'	7:A:541:G:OP1	2.18	0.61
17:K:69:ARG:NH1	17:K:69:ARG:HB2	2.16	0.61
14:H:46:ILE:HD12	14:H:61:LEU:HD22	1.82	0.61
28:a:299:A:N3	28:a:319:G:O2'	2.30	0.61
28:a:2848:G:O2'	28:a:2867:G:N2	2.30	0.61
7:A:1302:U:O2'	7:A:1303:C:OP1	2.19	0.61
30:c:53:HIS:CE1	30:c:219:THR:HG23	2.36	0.61
25:S:36:ARG:NH2	25:S:75:ALA:O	2.34	0.61
28:a:1223:G:OP1	44:q:68:ARG:NH1	2.33	0.61
28:a:2333:A:OP2	49:v:77:ARG:NH2	2.34	0.61
37:j:2:ILE:HG12	37:j:8:LEU:HD21	1.82	0.61
38:k:78:ARG:HB3	38:k:113:ALA:HB3	1.83	0.61
28:a:2484:G:OP1	39:l:44:ARG:NH1	2.34	0.61
14:H:54:ASP:OD1	14:H:54:ASP:N	2.32	0.60
28:a:2849:U:OP1	42:o:93:ARG:NH2	2.20	0.60
7:A:486:U:H2'	7:A:487:A:H8	1.66	0.60
20:N:89:MET:HA	20:N:89:MET:HE2	1.83	0.60
28:a:1248:G:OP1	32:e:44:ARG:NH1	2.33	0.60
37:j:17:ARG:NH2	37:j:45:GLU:OE1	2.35	0.60
3:2:8:ARG:NH1	28:a:243:U:OP2	2.34	0.60
9:C:78:GLY:HA2	9:C:81:GLY:H	1.67	0.60
30:c:270:ARG:HG2	30:c:271:ARG:H	1.65	0.60
3:2:54:ASP:OD2	28:a:2359:C:O2'	2.17	0.60
28:a:1721:G:O2'	28:a:1739:A:N6	2.33	0.60
9:C:131:ARG:NH1	9:C:166:GLU:OE1	2.34	0.60
28:a:871:U:H2'	28:a:872:U:C6	2.37	0.60
7:A:83:C:H5"	7:A:86:G:H22	1.66	0.60
7:A:409:U:OP1	10:D:23:SER:OG	2.19	0.60
7:A:460:A:H2'	7:A:461:A:H8	1.66	0.60
12:F:29:ILE:HD13	12:F:64:VAL:HG11	1.84	0.60
12:F:82:ASP:OD1	12:F:82:ASP:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1385:A:O2'	28:a:1396:U:O2	2.20	0.60
7:A:765:G:C2	7:A:812:G:N3	2.69	0.60
28:a:2298:A:OP1	33:f:71:ARG:NH1	2.34	0.60
42:o:29:LYS:HB3	42:o:40:LEU:HD12	1.84	0.60
8:B:133:GLU:O	8:B:137:ARG:HG2	2.01	0.59
8:B:111:ILE:HD13	8:B:148:LEU:HD13	1.83	0.59
20:N:28:LYS:HA	20:N:31:ILE:HG22	1.83	0.59
28:a:574:A:N6	28:a:2034:U:OP1	2.35	0.59
22:P:67:ILE:HG23	22:P:71:VAL:HB	1.84	0.59
3:2:12:LYS:NZ	28:a:247:G:O6	2.29	0.59
7:A:1004:A:H5'	7:A:1024:G:H22	1.67	0.59
25:S:37:ARG:O	25:S:70:LYS:NZ	2.31	0.59
28:a:2095:A:H4'	35:h:11:ASN:HD21	1.67	0.59
7:A:337:G:H2'	7:A:338:A:C8	2.38	0.59
7:A:1351:A:OP2	15:I:120:LYS:NZ	2.30	0.59
8:B:187:VAL:HG13	8:B:191:SER:HB2	1.83	0.59
14:H:41:LYS:HD2	14:H:48:ASP:HA	1.85	0.59
28:a:463:G:N2	28:a:466:A:OP2	2.32	0.59
48:u:20:LEU:HD11	48:u:41:GLU:HG2	1.83	0.59
3:2:25:LYS:HG2	38:k:62:PRO:HG2	1.83	0.59
28:a:1434:A:H2'	28:a:1435:G:H8	1.67	0.59
15:I:60:LYS:HE2	15:I:60:LYS:N	2.18	0.59
44:q:14:VAL:HG12	44:q:20:VAL:HG21	1.85	0.59
20:N:4:GLN:H	20:N:4:GLN:CD	2.11	0.59
28:a:549:G:H2'	28:a:550:C:H6	1.68	0.59
28:a:1797:G:O2'	30:c:257:THR:OG1	2.20	0.59
28:a:2340:A:H5'	29:b:41:G:H21	1.67	0.59
31:d:184:ARG:NH2	42:o:11:GLU:OE2	2.36	0.59
28:a:2682:A:C8	31:d:11:MET:HE2	2.38	0.59
28:a:2831:G:OP2	31:d:59:ARG:NH1	2.35	0.59
49:v:25:ARG:HH11	49:v:25:ARG:HG2	1.68	0.59
7:A:376:G:H5"	22:P:5:ARG:HB2	1.84	0.58
25:S:10:PHE:HE2	25:S:37:ARG:HE	1.51	0.58
7:A:500:G:O2'	7:A:501:C:OP1	2.19	0.58
8:B:136:MET:SD	8:B:139:ARG:NH2	2.75	0.58
25:S:12:ASP:OD2	25:S:35:SER:OG	2.21	0.58
7:A:450:G:H4'	22:P:41:PRO:HB2	1.84	0.58
7:A:743:A:H2'	7:A:743:A:N3	2.18	0.58
9:C:80:LYS:HB3	9:C:82:GLU:HB2	1.84	0.58
9:C:130:PHE:O	9:C:134:MET:HG3	2.03	0.58
37:j:9:ASN:OD1	37:j:18:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:q:40:MET:HE2	44:q:49:ILE:HG12	1.84	0.58
7:A:674:G:H2'	7:A:675:A:H8	1.69	0.58
28:a:2491:U:H5'	28:a:2570:G:H5"	1.85	0.58
3:2:15:LYS:HB2	3:2:23:LYS:HE3	1.85	0.58
9:C:81:GLY:C	9:C:84:VAL:HB	2.28	0.58
28:a:891:G:O6	28:a:892:A:N6	2.37	0.58
30:c:2:ALA:N	30:c:20:VAL:O	2.36	0.58
9:C:177:THR:HG22	9:C:180:ALA:H	1.68	0.58
1:0:34:LEU:H	1:0:51:GLU:HG2	1.67	0.58
12:F:69:GLU:H	12:F:69:GLU:CD	2.11	0.58
10:D:95:GLU:HA	10:D:100:ASN:ND2	2.18	0.58
26:T:35:VAL:HG11	26:T:79:LEU:HD13	1.86	0.58
7:A:384:G:H2'	7:A:385:C:C6	2.39	0.58
7:A:695:A:H2'	7:A:696:A:C8	2.39	0.58
20:N:13:ARG:NH1	20:N:54:ASP:OD1	2.35	0.58
7:A:110:C:O2'	22:P:25:ARG:O	2.21	0.57
7:A:923:A:O2'	7:A:1400:C:OP2	2.20	0.57
34:g:95:ARG:HG2	34:g:106:SER:HB2	1.86	0.57
47:t:54:GLN:HG2	47:t:55:PRO:HD3	1.84	0.57
7:A:460:A:H2'	7:A:461:A:C8	2.37	0.57
7:A:492:C:H2'	7:A:493:A:C8	2.39	0.57
28:a:2092:U:OP2	35:h:27:ARG:NH1	2.35	0.57
28:a:569:U:O2'	28:a:983:A:N1	2.35	0.57
28:a:1794:A:H2'	28:a:1795:C:C6	2.39	0.57
28:a:2343:U:HO2'	28:a:2373:G:HO2'	1.48	0.57
7:A:1506:G:O2'	7:A:1507:U:OP2	2.15	0.57
17:K:23:ILE:HG12	17:K:96:THR:HG21	1.86	0.57
28:a:184:C:H2'	28:a:185:G:H8	1.68	0.57
28:a:272:A:H2'	28:a:273:G:H8	1.69	0.57
28:a:2376:A:N3	41:n:111:ARG:NH2	2.53	0.57
28:a:2618:G:H21	31:d:155:VAL:HG21	1.69	0.57
7:A:1493:A:H2'	7:A:1494:A:H8	1.68	0.57
15:I:28:ILE:HG12	15:I:63:LEU:HD23	1.85	0.57
18:L:76:GLU:OE2	18:L:76:GLU:N	2.35	0.57
28:a:1802:A:H2'	28:a:1803:A:C8	2.40	0.57
7:A:537:G:H5"	18:L:110:ARG:HH21	1.70	0.57
14:H:79:SER:OG	14:H:124:GLU:OE2	2.20	0.57
27:U:13:ASP:HB3	27:U:17:ARG:HH22	1.69	0.57
28:a:1799:G:OP1	30:c:258:ARG:NH1	2.31	0.57
44:q:10:LYS:NZ	44:q:23:GLU:OE2	2.37	0.57
7:A:104:G:OP2	26:T:13:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:154:MET:HE3	8:B:156:GLY:O	2.05	0.57
9:C:10:ILE:HD12	20:N:98:LYS:HD3	1.86	0.57
14:H:11:LEU:HD22	14:H:75:ILE:HD11	1.86	0.57
28:a:2246:G:H2'	28:a:2247:A:C8	2.40	0.57
28:a:2850:A:OP2	56:a:6208:SPD:N10	2.38	0.57
7:A:2:A:H2	7:A:613:C:H1'	1.70	0.57
7:A:1071:C:H2'	7:A:1072:G:H8	1.69	0.57
16:J:12:ALA:HB2	16:J:96:VAL:HG22	1.86	0.57
25:S:41:PHE:H	25:S:44:MET:HE3	1.70	0.57
28:a:529:A:OP2	36:i:116:ARG:NH2	2.30	0.57
7:A:976:G:OP2	7:A:1359:U:O2'	2.22	0.57
10:D:70:ARG:NE	10:D:73:ARG:HH21	2.02	0.57
28:a:748:G:OP2	56:a:6217:SPD:N10	2.38	0.57
18:L:44:LYS:HG3	18:L:45:PRO:HA	1.85	0.57
5:4:11:GLU:HA	5:4:25:ARG:HA	1.85	0.56
28:a:1469:A:H2'	28:a:1470:A:C8	2.40	0.56
38:k:75:ALA:HB2	38:k:105:ILE:HD12	1.87	0.56
7:A:1418:G:O2'	7:A:1484:A:N6	2.38	0.56
28:a:1715:G:O2'	28:a:1743:G:O6	2.19	0.56
7:A:764:C:C2'	7:A:765:G:H5'	2.35	0.56
7:A:824:U:H2'	7:A:825:A:C8	2.40	0.56
7:A:1130:A:H5"	15:I:64:TYR:HE2	1.70	0.56
10:D:109:ALA:N	10:D:113:GLU:OE1	2.25	0.56
12:F:96:VAL:O	12:F:96:VAL:HG12	2.05	0.56
15:I:112:GLU:HG2	15:I:121:ALA:HB1	1.87	0.56
28:a:411:G:OP2	28:a:2406:A:O2'	2.21	0.56
28:a:2547:A:H2'	28:a:2548:U:C6	2.41	0.56
28:a:2667:C:N3	34:g:110:SER:OG	2.37	0.56
42:o:9:GLU:OE2	42:o:56:HIS:NE2	2.38	0.56
47:t:8:ASP:OD1	47:t:24:LYS:NZ	2.36	0.56
4:3:5:ALA:O	4:3:37:GLN:NE2	2.37	0.56
21:O:32:LEU:O	21:O:36:ILE:HG12	2.05	0.56
24:R:66:SER:O	24:R:66:SER:OG	2.23	0.56
7:A:4:U:O2'	7:A:5:U:OP1	2.20	0.56
13:G:12:ILE:HD12	13:G:12:ILE:O	2.05	0.56
28:a:893:C:H2'	28:a:894:U:C6	2.41	0.56
7:A:127:G:O2'	23:Q:6:ARG:NH1	2.39	0.56
28:a:1292:G:H2'	28:a:1293:C:C6	2.40	0.56
7:A:1060:U:OP1	20:N:85:ARG:NH2	2.38	0.56
28:a:955:PSU:OP1	39:l:86:LYS:NZ	2.29	0.56
28:a:1292:G:H2'	28:a:1293:C:H6	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2866:U:O4	56:a:6208:SPD:N10	2.38	0.56
7:A:744:C:H2'	7:A:745:A:C8	2.41	0.56
9:C:22:TRP:NE1	9:C:36:ASP:OD2	2.37	0.56
7:A:176:C:O2'	7:A:177:G:H5"	2.05	0.56
28:a:856:G:H2'	28:a:857:G:C8	2.39	0.56
30:c:269:ARG:HG2	30:c:269:ARG:HH11	1.71	0.56
32:e:58:LYS:HG3	32:e:71:GLY:HA2	1.88	0.56
12:F:20:GLY:O	12:F:24:ARG:HG3	2.06	0.56
34:g:137:ASP:O	34:g:141:ILE:HG22	2.06	0.56
12:F:18:VAL:HG11	12:F:58:HIS:CE1	2.40	0.55
16:J:8:ILE:HG13	16:J:100:ILE:HG13	1.88	0.55
28:a:102:U:O4	51:x:2:LYS:N	2.39	0.55
28:a:532:A:N7	28:a:2021:C:O2'	2.39	0.55
7:A:275:G:OP2	23:Q:16:LYS:NZ	2.38	0.55
7:A:1227:C:N4	19:M:103:LYS:HG3	2.21	0.55
7:A:1324:G:H2'	7:A:1325:A:C8	2.41	0.55
8:B:206:ALA:O	8:B:210:VAL:HG23	2.07	0.55
28:a:1363:C:O2'	28:a:1809:A:N3	2.36	0.55
28:a:1992:G:N2	28:a:1996:C:O2'	2.39	0.55
9:C:24:ALA:HB1	9:C:28:GLU:HG2	1.87	0.55
17:K:126:LYS:NZ	27:U:37:PHE:HB2	2.21	0.55
7:A:39:G:N1	7:A:403:C:C5	2.74	0.55
7:A:1121:U:O2'	7:A:1122:U:H5'	2.06	0.55
9:C:56:VAL:HB	9:C:67:THR:HB	1.88	0.55
28:a:577:G:O2'	28:a:1254:A:OP1	2.24	0.55
7:A:1007:C:OP1	20:N:19:LYS:NZ	2.38	0.55
12:F:38:ARG:NH1	12:F:63:ASN:OD1	2.39	0.55
17:K:28:ASN:O	17:K:57:LYS:NZ	2.33	0.55
7:A:1364:A:O2'	7:A:1366:G:N7	2.33	0.55
18:L:46:ASN:ND2	18:L:89:D2T:SB	2.80	0.55
7:A:713:G:H2'	7:A:714:G:C8	2.42	0.55
7:A:1000:A:H2'	7:A:1001:G:H8	1.72	0.55
9:C:11:ARG:NH2	9:C:175:LEU:O	2.39	0.55
10:D:156:LYS:O	10:D:160:GLU:HG3	2.06	0.55
28:a:729:G:H5'	28:a:730:A:H5"	1.89	0.55
28:a:2296:U:OP2	41:n:9:ARG:NH2	2.39	0.55
44:q:36:ALA:HA	44:q:58:VAL:HG23	1.88	0.55
2:1:4:THR:HG22	28:a:687:C:H1'	1.88	0.55
27:U:4:ILE:HD13	27:U:19:PHE:HB2	1.87	0.55
28:a:742:A:H2'	28:a:743:A:C8	2.41	0.55
46:s:14:PRO:HD3	51:x:30:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:587:G:O2'	7:A:588:G:OP2	2.22	0.55
7:A:1497:C:O2	7:A:1518:G:N2	2.34	0.55
10:D:87:GLY:HA3	10:D:197:GLU:HG3	1.89	0.55
25:S:31:LEU:HB2	25:S:49:ILE:HD13	1.89	0.55
7:A:269:C:H2'	7:A:270:A:C8	2.39	0.55
7:A:653:A:O5'	14:H:56:LYS:NZ	2.40	0.55
7:A:765:G:H2'	7:A:765:G:N3	2.22	0.55
7:A:910:C:OP2	18:L:18:LYS:NZ	2.40	0.55
7:A:1347:A:OP1	15:I:122:ARG:NH1	2.37	0.55
16:J:92:LEU:HG	16:J:98:VAL:HG11	1.88	0.55
20:N:32:SER:O	20:N:41:ARG:NH2	2.39	0.55
22:P:54:LEU:HD22	22:P:75:ILE:HG12	1.88	0.55
28:a:1720:U:H2'	28:a:1721:G:O4'	2.07	0.55
28:a:1980:G:O2'	28:a:1982:U:OP2	2.21	0.55
42:o:92:VAL:HG21	42:o:97:LEU:HD11	1.88	0.55
7:A:40:C:H5	7:A:402:G:N2	2.04	0.54
8:B:66:LYS:HG2	8:B:90:PHE:HE2	1.72	0.54
28:a:320:A:N3	32:e:163:ASN:ND2	2.49	0.54
28:a:1733:G:H2'	28:a:1734:G:H8	1.72	0.54
7:A:946:A:H2'	7:A:947:G:C8	2.42	0.54
8:B:213:TYR:O	8:B:217:VAL:HG22	2.07	0.54
12:F:22:ILE:O	12:F:26:THR:OG1	2.24	0.54
18:L:68:GLY:O	18:L:99:ARG:NH1	2.40	0.54
28:a:500:G:N1	28:a:503:A:OP2	2.39	0.54
34:g:127:THR:OG1	34:g:128:GLN:N	2.39	0.54
7:A:297:G:N2	7:A:300:A:OP2	2.41	0.54
7:A:1004:A:H2'	7:A:1005:A:O4'	2.08	0.54
10:D:188:ARG:NH2	10:D:195:ILE:O	2.40	0.54
25:S:50:ALA:HB1	25:S:57:HIS:HB3	1.90	0.54
28:a:782:A:N7	30:c:220:VAL:HG21	2.22	0.54
28:a:2291:U:H2'	28:a:2292:U:C6	2.42	0.54
7:A:1323:C:OP1	25:S:78:ARG:NH2	2.39	0.54
14:H:41:LYS:NZ	14:H:48:ASP:OD1	2.37	0.54
19:M:15:ALA:O	19:M:19:LEU:HD12	2.08	0.54
46:s:66:LYS:HD3	46:s:68:LYS:HE2	1.87	0.54
47:t:28:VAL:HG22	47:t:34:VAL:HG12	1.90	0.54
7:A:839:A:H2	7:A:847:G:H22	1.55	0.54
28:a:1315:C:O2'	28:a:1392:A:N3	2.41	0.54
28:a:1607:C:N4	28:a:1622:G:OP2	2.36	0.54
28:a:2031:A:N3	28:a:2455:G:O2'	2.36	0.54
32:e:97:ASN:HB2	32:e:100:MET:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:r:20:VAL:HG11	45:r:44:ALA:HA	1.90	0.54
7:A:1526:C:OP2	27:U:40:LYS:NZ	2.39	0.54
9:C:153:VAL:HG22	9:C:198:VAL:HG22	1.89	0.54
7:A:1003:G:N2	7:A:1005:A:H5'	2.22	0.54
18:L:5:ASN:OD1	23:Q:36:LYS:HE3	2.08	0.54
40:m:8:ARG:HD2	40:m:43:GLU:HG2	1.90	0.54
7:A:87:U:H2'	7:A:88:U:C6	2.42	0.54
7:A:472:U:H2'	7:A:473:A:C8	2.43	0.54
7:A:769:G:H4'	7:A:1514:A:H4'	1.89	0.54
7:A:1288:A:H2'	7:A:1289:A:C8	2.43	0.54
7:A:1379:C:OP1	13:G:5:ARG:NH1	2.41	0.54
8:B:67:ILE:HD12	8:B:160:ALA:HB3	1.89	0.54
24:R:73:ARG:HB3	24:R:73:ARG:CZ	2.37	0.54
28:a:2557:G:H2'	28:a:2558:C:C6	2.42	0.54
53:z:11:SER:O	53:z:15:MET:HG3	2.07	0.54
7:A:1119:C:OP1	15:I:85:ARG:NH2	2.41	0.54
10:D:70:ARG:HG2	10:D:70:ARG:HH11	1.71	0.54
33:f:47:LYS:HD2	33:f:47:LYS:O	2.08	0.54
48:u:21:ARG:NH1	48:u:87:GLN:O	2.40	0.54
7:A:741:G:C4	7:A:742:G:H8	2.26	0.53
7:A:1267:G:N2	7:A:1270:A:OP2	2.30	0.53
20:N:80:SER:O	20:N:84:VAL:HG12	2.07	0.53
33:f:8:TYR:HA	33:f:12:VAL:HB	1.90	0.53
7:A:405:U:H5'	7:A:406:G:O4'	2.08	0.53
7:A:1118:U:H2'	7:A:1119:C:H6	1.74	0.53
22:P:43:ALA:HB1	22:P:47:GLU:OE2	2.08	0.53
36:i:125:TYR:OH	36:i:132:HIS:NE2	2.28	0.53
42:o:92:VAL:HG11	42:o:97:LEU:HD21	1.90	0.53
43:p:26:GLY:O	43:p:30:ARG:NH1	2.39	0.53
7:A:452:A:OP2	56:A:1691:SPD:N1	2.41	0.53
7:A:1117:A:N6	7:A:1157:G:H22	2.06	0.53
8:B:77:SER:OG	8:B:93:ASN:O	2.24	0.53
28:a:2788:C:H2'	28:a:2789:C:C6	2.43	0.53
31:d:35:THR:HG22	31:d:73:VAL:HG21	1.89	0.53
19:M:11:ASP:HA	19:M:45:ILE:HB	1.91	0.53
27:U:31:GLU:OE2	27:U:35:ARG:NH2	2.41	0.53
33:f:68:THR:N	33:f:86:GLY:O	2.41	0.53
2:1:45:SER:OG	28:a:126:A:OP1	2.25	0.53
5:4:57:VAL:HG13	25:S:42:PRO:HB3	1.90	0.53
7:A:390:U:H4'	22:P:28:ARG:HH21	1.73	0.53
7:A:402:G:H4'	7:A:403:C:O5'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:736:C:H2'	7:A:737:C:H6	1.74	0.53
7:A:1413:C:H2'	7:A:1414:A:C8	2.44	0.53
15:I:18:ARG:HE	15:I:66:THR:HG23	1.74	0.53
19:M:71:ARG:NH2	33:f:115:ARG:HD2	2.23	0.53
22:P:74:LEU:HA	22:P:77:GLU:HG2	1.89	0.53
28:a:155:A:H2'	28:a:156:A:H8	1.72	0.53
34:g:155:GLU:OE1	34:g:158:LYS:N	2.42	0.53
47:t:66:GLN:HB2	47:t:69:ASN:ND2	2.24	0.53
7:A:275:G:P	23:Q:16:LYS:HZ3	2.32	0.53
7:A:1533:U:H4'	7:A:1534:C:H5'	1.90	0.53
15:I:28:ILE:HG12	15:I:63:LEU:HB2	1.91	0.53
38:k:129:LYS:HB3	38:k:129:LYS:NZ	2.24	0.53
49:v:33:ALA:N	49:v:64:ASP:OD1	2.41	0.53
5:4:10:GLU:HA	5:4:10:GLU:OE2	2.08	0.53
23:Q:53:CYS:SG	23:Q:75:LEU:HD11	2.49	0.53
28:a:64:A:H2'	28:a:65:U:C6	2.42	0.53
28:a:155:A:H2'	28:a:156:A:C8	2.43	0.53
28:a:1914:C:O2'	28:a:1915:3TD:O4'	2.27	0.53
28:a:2469:A:N6	28:a:2481:G:O2'	2.35	0.53
28:a:2836:U:H2'	28:a:2837:A:C8	2.44	0.53
33:f:136:ILE:HD11	33:f:146:VAL:HG21	1.90	0.53
28:a:720:U:H2'	28:a:721:A:C8	2.44	0.53
28:a:876:C:H2'	28:a:877:A:O4'	2.09	0.53
30:c:133:ARG:HB3	30:c:186:ALA:HB1	1.89	0.53
7:A:1239:A:OP1	7:A:1336:U:O2'	2.20	0.53
28:a:1433:A:H2'	28:a:1434:A:C8	2.44	0.53
30:c:141:VAL:HG12	30:c:192:LEU:HD13	1.90	0.53
37:j:76:VAL:HG13	42:o:73:VAL:HG13	1.91	0.53
46:s:69:ARG:NH1	46:s:69:ARG:HB3	2.24	0.53
7:A:78:A:H2'	7:A:79:G:C8	2.44	0.52
7:A:674:G:H2'	7:A:675:A:C8	2.44	0.52
7:A:764:C:H2'	7:A:765:G:H5'	1.91	0.52
28:a:1386:C:H2'	28:a:1387:A:C8	2.45	0.52
28:a:1794:A:H2'	28:a:1795:C:H6	1.74	0.52
29:b:1:U:H2'	29:b:2:G:C8	2.42	0.52
32:e:168:ASP:OD2	32:e:170:ARG:NH2	2.41	0.52
36:i:31:GLU:HG2	36:i:142:ILE:HG12	1.91	0.52
46:s:39:THR:O	46:s:43:ILE:HG13	2.09	0.52
7:A:346:G:OP1	42:o:39:ARG:NH1	2.40	0.52
30:c:154:LEU:HD13	30:c:176:LEU:HD21	1.90	0.52
31:d:38:LYS:HG2	31:d:43:ASP:OD1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1118:U:H2'	7:A:1119:C:C6	2.44	0.52
8:B:131:LYS:O	8:B:131:LYS:NZ	2.34	0.52
28:a:2857:G:N2	28:a:2860:A:OP2	2.33	0.52
46:s:4:GLU:O	46:s:8:LEU:HD22	2.09	0.52
1:0:8:LYS:HA	1:0:24:THR:HA	1.89	0.52
7:A:216:U:H2'	7:A:217:U:C6	2.44	0.52
7:A:730:G:N3	7:A:765:G:H4'	2.24	0.52
7:A:1356:A:H2'	7:A:1357:A:C8	2.45	0.52
29:b:48:U:P	41:n:30:ARG:HH12	2.32	0.52
33:f:104:ILE:HD11	33:f:175:PHE:CE1	2.45	0.52
43:p:61:TRP:O	43:p:65:ILE:HD12	2.08	0.52
7:A:973:G:OP1	16:J:59:LYS:NZ	2.35	0.52
8:B:60:ILE:HD12	8:B:63:ARG:HD3	1.91	0.52
22:P:52:LEU:HD11	22:P:74:LEU:HB3	1.90	0.52
22:P:75:ILE:O	22:P:79:ASN:HB2	2.10	0.52
28:a:335:C:OP2	47:t:82:ARG:NH1	2.42	0.52
37:j:18:ARG:HB3	37:j:45:GLU:HG3	1.92	0.52
7:A:41:G:O6	7:A:402:G:C6	2.62	0.52
7:A:549:C:O2'	7:A:550:G:H8	1.93	0.52
25:S:3:ARG:HH21	25:S:7:LYS:HD3	1.75	0.52
36:i:95:ARG:HE	36:i:96:ARG:NH2	2.06	0.52
7:A:1040:U:H2'	7:A:1041:G:C8	2.45	0.52
28:a:2461:A:H2'	28:a:2462:C:C6	2.45	0.52
28:a:2836:U:H2'	28:a:2837:A:H8	1.74	0.52
47:t:98:SER:O	47:t:98:SER:OG	2.26	0.52
7:A:131:A:H2'	7:A:132:U:C6	2.44	0.52
7:A:399:G:H2'	7:A:400:C:C6	2.45	0.52
7:A:977:A:OP1	20:N:61:ARG:NH2	2.43	0.52
24:R:21:ILE:HG13	24:R:54:GLN:HB3	1.91	0.52
28:a:568:U:H1'	28:a:2030:6MZ:H9C1	1.92	0.52
28:a:1386:C:H2'	28:a:1387:A:H8	1.75	0.52
28:a:2250:G:O2'	28:a:2496:C:OP1	2.26	0.52
35:h:2:GLN:OE1	35:h:2:GLN:HA	2.10	0.52
7:A:1318:C:OP1	20:N:24:ARG:NH2	2.43	0.52
17:K:35:THR:HG22	17:K:41:ALA:HA	1.92	0.52
28:a:1266:G:O2'	28:a:2012:G:O6	2.22	0.52
28:a:2025:C:H2'	28:a:2026:U:C6	2.45	0.52
7:A:811:C:O2'	7:A:901:A:N1	2.43	0.51
8:B:139:ARG:HA	8:B:142:GLU:OE2	2.10	0.51
19:M:15:ALA:HA	19:M:45:ILE:HD11	1.91	0.51
19:M:90:ARG:HB2	19:M:97:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1798:U:OP2	30:c:271:ARG:NH2	2.41	0.51
31:d:114:LYS:HD3	31:d:196:ALA:HB2	1.92	0.51
40:m:30:ARG:NH1	40:m:74:GLU:OE2	2.43	0.51
17:K:97:ILE:HG22	27:U:12:PHE:HZ	1.75	0.51
28:a:1278:C:H2'	28:a:1279:G:H8	1.75	0.51
28:a:1419:A:O2'	28:a:1421:G:N7	2.40	0.51
28:a:2887:A:N3	53:z:27:SER:OG	2.41	0.51
30:c:256:LYS:HE2	30:c:270:ARG:HH12	1.76	0.51
7:A:500:G:H2'	7:A:501:C:C6	2.46	0.51
7:A:1077:G:N2	7:A:1080:A:OP2	2.38	0.51
7:A:1318:C:H42	20:N:53:ARG:HH11	1.57	0.51
9:C:153:VAL:HG12	9:C:157:LEU:HD11	1.93	0.51
31:d:25:THR:OG1	31:d:191:GLY:O	2.25	0.51
32:e:161:ALA:HA	32:e:164:LEU:HD12	1.91	0.51
41:n:76:LYS:O	41:n:80:GLU:HG2	2.10	0.51
42:o:6:LYS:NZ	42:o:6:LYS:HB3	2.26	0.51
5:4:38:SER:HB2	33:f:105:THR:HA	1.92	0.51
7:A:601:G:H2'	7:A:602:A:H8	1.75	0.51
28:a:2327:A:H2'	28:a:2328:A:C8	2.45	0.51
39:l:42:THR:HG22	39:l:93:VAL:HG12	1.92	0.51
39:l:75:GLU:HB2	39:l:90:GLU:HG3	1.92	0.51
43:p:86:ALA:HB2	43:p:116:ALA:HB2	1.92	0.51
7:A:881:G:P	18:L:9:ARG:HH22	2.32	0.51
7:A:946:A:O2'	7:A:1334:A:N3	2.36	0.51
15:I:52:LEU:HD11	15:I:63:LEU:HD21	1.91	0.51
18:L:79:VAL:O	18:L:103:ASP:HB2	2.10	0.51
26:T:62:ALA:HB1	26:T:69:LYS:HA	1.92	0.51
28:a:1281:G:H2'	28:a:1282:U:C6	2.46	0.51
28:a:1808:A:H3'	28:a:1809:A:C8	2.45	0.51
39:l:41:LEU:HD13	39:l:96:ILE:HG13	1.93	0.51
18:L:50:ARG:HD2	18:L:90:LEU:HD11	1.93	0.51
28:a:1819:A:H5"	30:c:160:THR:HG21	1.92	0.51
46:s:22:THR:O	46:s:26:LYS:HB2	2.10	0.51
7:A:501:C:H2'	7:A:502:A:H8	1.76	0.51
7:A:1083:U:O2'	7:A:1102:A:OP2	2.29	0.51
7:A:1148:C:H4'	15:I:7:TYR:CE2	2.46	0.51
9:C:47:LEU:HB3	9:C:50:ALA:HB3	1.92	0.51
23:Q:25:ILE:HB	23:Q:42:THR:HG23	1.93	0.51
28:a:552:U:H2'	28:a:553:G:H8	1.76	0.51
28:a:1266:G:OP2	53:z:16:ARG:NH1	2.43	0.51
37:j:108:ARG:NH2	42:o:34:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:40:C:C4	7:A:403:C:C6	2.99	0.51
7:A:80:G:H2'	7:A:81:A:C8	2.46	0.51
7:A:1533:U:H4'	7:A:1534:C:OP1	2.10	0.51
27:U:10:GLU:OE2	27:U:18:ARG:NH2	2.43	0.51
7:A:559:A:H4'	7:A:560:A:H3'	1.93	0.51
7:A:744:C:H2'	7:A:745:A:H8	1.76	0.51
7:A:932:C:OP1	13:G:4:ARG:NH1	2.44	0.51
7:A:1098:C:O2'	27:U:71:TYR:O	2.27	0.51
10:D:15:GLU:OE1	10:D:63:ARG:NH1	2.44	0.51
19:M:86:TYR:CE2	19:M:90:ARG:HD2	2.46	0.51
28:a:549:G:H2'	28:a:550:C:C6	2.45	0.51
28:a:1636:U:H2'	28:a:1637:A:C8	2.45	0.51
33:f:160:ALA:HB1	33:f:165:GLU:HB2	1.93	0.51
34:g:11:VAL:HB	34:g:48:ASN:HB2	1.93	0.51
7:A:609:A:O2'	7:A:610:G:O5'	2.27	0.50
12:F:97:THR:O	12:F:97:THR:OG1	2.29	0.50
28:a:805:G:N2	28:a:829:A:OP1	2.45	0.50
28:a:1047:G:O2'	28:a:1110:G:N2	2.38	0.50
28:a:1434:A:H2'	28:a:1435:G:C8	2.45	0.50
28:a:2646:C:OP2	28:a:2732:G:O2'	2.29	0.50
34:g:24:ILE:HG21	34:g:72:LEU:HD21	1.92	0.50
42:o:14:LYS:NZ	42:o:81:VAL:O	2.40	0.50
47:t:86:ARG:NH2	47:t:100:SER:O	2.43	0.50
48:u:79:ARG:HG2	48:u:79:ARG:HH11	1.76	0.50
53:z:12:LYS:HD3	53:z:15:MET:HE2	1.93	0.50
7:A:398:U:H2'	7:A:399:G:C8	2.45	0.50
17:K:81:ASN:HB3	17:K:106:ARG:NH2	2.26	0.50
7:A:45:G:H2'	7:A:46:G:H8	1.75	0.50
7:A:293:G:C8	7:A:294:U:H5	2.30	0.50
7:A:501:C:H2'	7:A:502:A:C8	2.46	0.50
28:a:1:G:H2'	28:a:2:G:C8	2.46	0.50
28:a:527:C:O2'	28:a:2779:U:O2'	2.27	0.50
28:a:1856:U:H2'	28:a:1857:G:O4'	2.10	0.50
28:a:2246:G:H2'	28:a:2247:A:H8	1.75	0.50
51:x:9:LYS:HB3	51:x:13:GLU:HG2	1.92	0.50
10:D:48:LEU:HD21	10:D:56:ARG:HG3	1.92	0.50
16:J:67:ILE:HG13	20:N:96:LEU:HD13	1.92	0.50
28:a:414:C:H2'	28:a:415:A:H8	1.76	0.50
28:a:851:C:H2'	28:a:852:U:C6	2.47	0.50
28:a:1796:U:H2'	28:a:1797:G:C8	2.46	0.50
28:a:2006:C:O2'	28:a:2823:A:N3	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2804:U:H2'	28:a:2805:C:H6	1.77	0.50
38:k:112:LEU:HD12	38:k:130:GLY:HA3	1.92	0.50
7:A:126:G:OP1	7:A:605:U:O2'	2.26	0.50
7:A:1136:U:H4'	7:A:1137:A:C6	2.46	0.50
10:D:37:ALA:HB3	10:D:42:GLY:HA2	1.94	0.50
18:L:50:ARG:HB3	18:L:66:TYR:HE1	1.77	0.50
28:a:1548:A:H2'	28:a:1549:A:C8	2.46	0.50
5:4:8:LYS:HA	5:4:8:LYS:HE3	1.94	0.50
7:A:486:U:H2'	7:A:487:A:C8	2.46	0.50
7:A:1315:C:H2'	7:A:1316:U:C6	2.47	0.50
13:G:116:MET:HG3	13:G:116:MET:O	2.11	0.50
28:a:411:G:N7	56:a:6212:SPD:N10	2.59	0.50
28:a:1494:A:H2'	28:a:1495:A:C8	2.47	0.50
32:e:79:ARG:O	32:e:80:SER:OG	2.28	0.50
33:f:29:PRO:HB2	33:f:169:LEU:HD22	1.94	0.50
7:A:1356:A:H2'	7:A:1357:A:H8	1.76	0.50
13:G:58:GLU:OE1	13:G:58:GLU:N	2.41	0.50
15:I:94:LEU:O	15:I:98:LEU:HD12	2.12	0.50
21:O:78:TYR:O	21:O:82:ILE:HG23	2.10	0.50
28:a:184:C:H2'	28:a:185:G:C8	2.45	0.50
28:a:333:G:O3'	56:a:6214:SPD:N1	2.45	0.50
28:a:593:U:H2'	28:a:594:U:C6	2.46	0.50
28:a:820:A:H4'	28:a:836:G:N2	2.26	0.50
28:a:1129:A:N6	28:a:2491:U:OP1	2.42	0.50
28:a:1645:G:H5"	28:a:1646:C:H5'	1.93	0.50
28:a:1724:G:O6	28:a:1737:G:N2	2.44	0.50
28:a:2000:C:OP1	40:m:5:LYS:NZ	2.36	0.50
28:a:2796:U:H3	28:a:2799:A:N6	2.09	0.50
33:f:135:GLN:OE1	33:f:150:ARG:N	2.33	0.50
7:A:41:G:O6	7:A:402:G:C5	2.65	0.50
7:A:337:G:H2'	7:A:338:A:H8	1.76	0.50
7:A:1315:C:H2'	7:A:1316:U:H6	1.77	0.50
15:I:116:VAL:CG1	16:J:62:ARG:HD2	2.42	0.50
28:a:1432:G:H2'	28:a:1433:A:C8	2.47	0.50
51:x:12:GLU:HG2	51:x:13:GLU:N	2.26	0.50
7:A:56:U:H2'	7:A:57:G:H8	1.77	0.50
7:A:113:G:H1'	7:A:354:G:H5'	1.94	0.50
7:A:946:A:H2'	7:A:947:G:H8	1.77	0.50
10:D:71:GLN:OE1	10:D:97:ARG:NH1	2.40	0.50
15:I:36:GLU:OE2	15:I:49:ARG:NH2	2.45	0.50
17:K:21:ALA:HB2	17:K:82:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:645:C:H2'	28:a:647:G:C8	2.47	0.50
28:a:2038:G:H2'	28:a:2039:U:O4'	2.12	0.50
28:a:2639:A:H2'	28:a:2640:G:O4'	2.12	0.50
7:A:776:G:N2	7:A:802:A:OP2	2.43	0.49
7:A:1005:A:H2'	7:A:1006:U:O4'	2.12	0.49
28:a:2079:U:O2'	50:w:23:ASN:OD1	2.29	0.49
36:i:110:PRO:O	36:i:115:GLY:HA3	2.12	0.49
5:4:56:ARG:CZ	5:4:59:ARG:HH21	2.24	0.49
7:A:945:G:C2	7:A:946:A:C8	3.00	0.49
11:E:38:VAL:HG11	11:E:114:VAL:HG22	1.93	0.49
7:A:1030:U:H3'	7:A:1032:G:C8	2.47	0.49
12:F:42:TRP:HE3	12:F:59:TYR:HB3	1.77	0.49
13:G:25:LYS:HB3	13:G:101:MET:HE1	1.94	0.49
15:I:57:MET:HA	15:I:60:LYS:HE3	1.94	0.49
28:a:742:A:H2'	28:a:743:A:H8	1.77	0.49
31:d:152:PRO:HG3	31:d:156:PHE:CZ	2.48	0.49
46:s:8:LEU:O	51:x:29:ARG:NH2	2.44	0.49
7:A:56:U:H2'	7:A:57:G:C8	2.46	0.49
7:A:1531:G:O6	27:U:46:LYS:NZ	2.45	0.49
15:I:28:ILE:HA	15:I:63:LEU:HB2	1.92	0.49
17:K:106:ARG:HD2	17:K:108:THR:HG22	1.94	0.49
17:K:113:VAL:HG22	24:R:73:ARG:NE	2.26	0.49
23:Q:62:ARG:HG2	23:Q:62:ARG:HH11	1.76	0.49
28:a:1125:G:OP2	28:a:1126:A:O2'	2.26	0.49
30:c:34:LEU:HD11	30:c:63:ARG:HD3	1.94	0.49
39:l:50:ARG:HA	39:l:53:MET:HE2	1.93	0.49
7:A:663:A:H61	7:A:743:A:N6	2.11	0.49
7:A:938:A:N3	7:A:1377:U:O2'	2.32	0.49
7:A:1134:C:H2'	7:A:1135:G:C8	2.46	0.49
13:G:23:LEU:HD21	13:G:47:LEU:HD11	1.94	0.49
21:O:12:VAL:HG21	21:O:22:THR:HG22	1.93	0.49
28:a:365:U:H2'	28:a:366:C:C6	2.47	0.49
28:a:1484:U:H2'	28:a:1485:U:H6	1.78	0.49
32:e:35:TYR:OH	32:e:176:ASP:OD1	2.26	0.49
7:A:154:C:H2'	7:A:155:A:H8	1.78	0.49
7:A:579:A:O2'	21:O:54:ARG:NH1	2.45	0.49
10:D:95:GLU:HA	10:D:100:ASN:HD22	1.77	0.49
13:G:70:ARG:HB3	13:G:96:ARG:HD2	1.95	0.49
28:a:306:U:H2'	28:a:307:G:O4'	2.13	0.49
28:a:2392:A:H2	38:k:55:MET:SD	2.35	0.49
40:m:98:LEU:HD22	53:z:54:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:5:U:H5'	7:A:6:G:C4	2.47	0.49
7:A:39:G:N1	7:A:404:G:C2	2.80	0.49
7:A:524:G:H2'	7:A:525:C:C6	2.47	0.49
7:A:736:C:H2'	7:A:737:C:C6	2.48	0.49
13:G:97:ASN:O	13:G:101:MET:HG3	2.13	0.49
28:a:27:G:N2	28:a:512:G:H1'	2.28	0.49
28:a:624:C:O2'	28:a:657:U:OP1	2.29	0.49
28:a:659:G:O2'	32:e:95:LYS:O	2.30	0.49
28:a:2831:G:N2	28:a:2884:U:OP2	2.45	0.49
7:A:609:A:O2'	7:A:610:G:O4'	2.30	0.49
7:A:1062:U:H2'	7:A:1063:C:C6	2.48	0.49
10:D:102:VAL:HG13	10:D:107:PHE:HB2	1.95	0.49
15:I:52:LEU:HB3	15:I:58:VAL:HB	1.94	0.49
21:O:10:LYS:O	21:O:14:GLU:HG3	2.12	0.49
28:a:2314:A:H1'	33:f:155:THR:HG21	1.94	0.49
28:a:2830:C:H5"	31:d:56:LYS:HE3	1.95	0.49
41:n:36:TYR:HA	41:n:52:SER:HB2	1.94	0.49
49:v:37:ILE:HD11	49:v:82:ILE:HD11	1.95	0.49
28:a:1361:G:H2'	28:a:1362:C:C6	2.48	0.49
28:a:1405:U:H2'	28:a:1406:U:C6	2.47	0.49
28:a:1682:G:H2'	28:a:1683:U:C6	2.47	0.49
28:a:2469:A:H2'	28:a:2470:G:O4'	2.11	0.49
28:a:2540:C:O2'	28:a:2740:A:N3	2.41	0.49
37:j:24:VAL:HG12	37:j:30:ARG:HD3	1.94	0.49
7:A:2:A:O2'	10:D:83:LYS:NZ	2.45	0.49
7:A:1027:C:H42	7:A:1035:A:N6	2.11	0.49
28:a:639:U:C2	28:a:640:C:C5	3.01	0.49
28:a:1484:U:H2'	28:a:1485:U:C6	2.47	0.49
36:i:13:ARG:HG3	36:i:13:ARG:HH11	1.77	0.49
47:t:26:LYS:HG3	47:t:37:GLU:HG2	1.95	0.49
7:A:1071:C:H2'	7:A:1072:G:C8	2.47	0.48
7:A:1411:A:H2'	7:A:1412:C:C6	2.48	0.48
9:C:18:TRP:HZ2	20:N:97:LYS:HG2	1.78	0.48
20:N:39:GLU:HA	20:N:39:GLU:OE2	2.12	0.48
28:a:1746:A:H2'	28:a:1747:U:C6	2.48	0.48
36:i:36:LEU:HD11	36:i:122:LEU:HB2	1.94	0.48
36:i:37:ARG:HA	36:i:118:MET:SD	2.53	0.48
7:A:45:G:H2'	7:A:46:G:C8	2.48	0.48
7:A:1125:U:O2'	7:A:1126:U:O5'	2.28	0.48
15:I:5:GLN:OE1	15:I:5:GLN:N	2.45	0.48
28:a:833:A:H2'	28:a:834:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1288:G:OP2	28:a:1288:G:N2	2.37	0.48
41:n:52:SER:OG	41:n:54:VAL:HG22	2.12	0.48
13:G:16:PRO:HB3	15:I:42:GLU:OE2	2.13	0.48
32:e:3:LEU:HB2	32:e:12:LEU:HB3	1.96	0.48
23:Q:8:LEU:HD13	23:Q:25:ILE:HG21	1.95	0.48
28:a:414:C:H2'	28:a:415:A:C8	2.48	0.48
32:e:125:SER:O	32:e:137:LYS:NZ	2.43	0.48
37:j:71:ARG:HB2	37:j:75:SER:HB2	1.95	0.48
45:r:86:MET:HB3	45:r:96:ILE:HD13	1.96	0.48
3:2:9:GLY:O	3:2:13:ARG:NH1	2.41	0.48
8:B:54:LEU:HD11	8:B:216:ALA:HB1	1.95	0.48
14:H:10:MET:HE2	14:H:61:LEU:HD11	1.96	0.48
27:U:62:ARG:O	27:U:66:ARG:HG2	2.13	0.48
28:a:3:U:H2'	28:a:4:U:C6	2.49	0.48
28:a:570:G:H2'	28:a:2030:6MZ:N7	2.28	0.48
28:a:1295:C:C2	28:a:1296:G:C8	3.01	0.48
28:a:2680:U:O2'	28:a:2681:C:H5'	2.14	0.48
34:g:173:GLU:OE1	34:g:173:GLU:N	2.46	0.48
7:A:17:U:H2'	7:A:18:C:C6	2.47	0.48
12:F:32:ALA:HB2	12:F:70:VAL:HG21	1.95	0.48
14:H:79:SER:HB3	14:H:125:ILE:O	2.13	0.48
32:e:145:ASP:HA	32:e:166:LYS:HB3	1.95	0.48
39:l:62:LYS:HD3	39:l:64:TRP:CZ2	2.49	0.48
48:u:43:ASP:OD1	48:u:46:LYS:HG3	2.13	0.48
53:z:54:VAL:HG12	53:z:55:ILE:HG23	1.95	0.48
7:A:246:A:C2	7:A:282:A:C5	3.01	0.48
19:M:92:ARG:HD3	28:a:888:C:C5	2.49	0.48
28:a:671:C:H2'	28:a:672:C:C6	2.48	0.48
28:a:1263:U:O2'	53:z:8:PRO:HD2	2.13	0.48
30:c:84:ASP:OD2	30:c:87:ARG:NE	2.30	0.48
36:i:115:GLY:HA2	36:i:118:MET:HG3	1.96	0.48
45:r:82:MET:HB2	45:r:98:LYS:HB2	1.94	0.48
5:4:60:PHE:CE2	25:S:42:PRO:HD3	2.49	0.48
7:A:90:C:H2'	7:A:91:U:C5	2.49	0.48
7:A:592:G:H2'	7:A:593:U:H6	1.78	0.48
7:A:1220:A:H2'	7:A:1221:G:C8	2.49	0.48
13:G:32:VAL:HG12	13:G:33:ASP:HB2	1.95	0.48
17:K:126:LYS:HZ3	27:U:37:PHE:HB2	1.78	0.48
28:a:1629:U:O4	28:a:1630:A:N6	2.46	0.48
28:a:1796:U:H2'	28:a:1797:G:H8	1.77	0.48
28:a:1813:G:H1'	30:c:50:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2243:U:H2'	28:a:2244:U:C6	2.49	0.48
28:a:2245:U:H5"	28:a:2246:G:H5'	1.95	0.48
28:a:2637:U:C2	28:a:2782:G:N2	2.82	0.48
36:i:60:ASP:OD1	36:i:60:ASP:N	2.40	0.48
7:A:384:G:H2'	7:A:385:C:H6	1.78	0.48
7:A:606:G:H4'	7:A:607:A:OP2	2.13	0.48
7:A:901:A:O2'	7:A:1514:A:OP1	2.27	0.48
8:B:188:ASP:HB2	8:B:204:ASP:OD2	2.14	0.48
17:K:64:GLN:O	17:K:68:GLU:HG3	2.14	0.48
28:a:24:G:O2'	45:r:78:GLU:O	2.30	0.48
28:a:160:A:N3	28:a:2208:C:O2'	2.41	0.48
28:a:1799:G:O2'	30:c:180:GLU:OE2	2.22	0.48
5:4:60:PHE:O	5:4:64:PHE:HB2	2.14	0.48
7:A:2:A:N3	7:A:2:A:H2'	2.28	0.48
9:C:28:GLU:N	9:C:28:GLU:OE1	2.42	0.48
25:S:28:LYS:HZ3	25:S:29:LYS:HB2	1.78	0.48
28:a:441:U:O2'	32:e:41:GLN:NE2	2.47	0.48
28:a:2780:G:OP2	36:i:120:ARG:HD3	2.14	0.48
31:d:156:PHE:CE1	36:i:81:ILE:HD13	2.49	0.48
46:s:51:PHE:HZ	51:x:30:MET:HE2	1.79	0.48
51:x:2:LYS:HE3	51:x:6:LEU:HD21	1.95	0.48
51:x:10:SER:H	51:x:13:GLU:CD	2.22	0.48
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.95	0.47
7:A:696:A:H2'	7:A:697:U:H6	1.79	0.47
7:A:859:G:H2'	7:A:860:A:C8	2.49	0.47
7:A:1245:G:H2'	7:A:1246:U:C6	2.49	0.47
14:H:113:ASP:OD2	14:H:117:ARG:NH2	2.46	0.47
20:N:4:GLN:HA	20:N:7:LYS:HG3	1.96	0.47
28:a:2591:C:H2'	28:a:2592:G:H8	1.78	0.47
28:a:2885:G:N7	53:z:40:ARG:NH2	2.60	0.47
29:b:9:G:O2'	41:n:45:SER:OG	2.32	0.47
33:f:29:PRO:HB3	33:f:160:ALA:HB2	1.96	0.47
34:g:175:LYS:HD3	34:g:176:LYS:HE2	1.96	0.47
5:4:41:HIS:O	5:4:45:THR:HG22	2.15	0.47
7:A:662:U:H2'	7:A:663:A:C8	2.48	0.47
7:A:673:A:H2'	7:A:674:G:H8	1.76	0.47
7:A:718:A:C2	24:R:38:LYS:HG2	2.50	0.47
7:A:878:A:OP1	14:H:80:ARG:HB2	2.14	0.47
7:A:963:G:C2	7:A:964:A:C8	3.01	0.47
12:F:90:MET:HE3	12:F:90:MET:HB3	1.68	0.47
15:I:97:GLU:HA	15:I:97:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:24:GLU:O	16:J:27:GLU:HG3	2.13	0.47
18:L:83:ARG:HG3	18:L:98:VAL:HG22	1.95	0.47
18:L:99:ARG:NE	18:L:104:CYS:SG	2.87	0.47
21:O:17:ARG:HD2	21:O:17:ARG:C	2.39	0.47
28:a:263:G:O2'	28:a:429:A:N3	2.39	0.47
28:a:301:G:OP2	47:t:82:ARG:NH2	2.41	0.47
28:a:659:G:N2	32:e:30:GLN:OE1	2.45	0.47
28:a:2097:A:H2'	28:a:2098:U:C6	2.49	0.47
29:b:5:U:H2'	29:b:6:G:H8	1.78	0.47
47:t:86:ARG:HG3	47:t:95:PHE:CD1	2.48	0.47
4:3:6:SER:O	4:3:6:SER:OG	2.30	0.47
8:B:100:MET:HE2	8:B:151:ILE:HD11	1.97	0.47
9:C:23:PHE:CD2	16:J:97:ASP:HB2	2.50	0.47
9:C:70:THR:HG21	9:C:76:VAL:HG11	1.96	0.47
13:G:47:LEU:HD13	13:G:58:GLU:HB3	1.95	0.47
28:a:263:G:H2'	28:a:264:C:O4'	2.14	0.47
28:a:493:G:H2'	28:a:494:G:O4'	2.14	0.47
28:a:2820:A:N3	28:a:2820:A:H2'	2.30	0.47
32:e:141:MET:HE3	32:e:141:MET:HB2	1.71	0.47
42:o:63:LYS:HB2	42:o:63:LYS:HE3	1.67	0.47
45:r:82:MET:HE3	45:r:84:ARG:NH2	2.29	0.47
3:2:11:ALA:O	3:2:15:LYS:NZ	2.45	0.47
3:2:40:ARG:NE	28:a:2362:C:OP1	2.45	0.47
15:I:60:LYS:HE2	15:I:60:LYS:H	1.78	0.47
19:M:10:PRO:HB2	19:M:13:LYS:HG3	1.95	0.47
28:a:2313:C:H2'	28:a:2314:A:H8	1.79	0.47
32:e:155:GLU:N	32:e:155:GLU:OE2	2.48	0.47
47:t:72:ILE:HG21	47:t:83:VAL:HG23	1.96	0.47
7:A:393:A:OP2	22:P:12:LYS:HD2	2.15	0.47
7:A:1398:C:OP2	11:E:29:ARG:NH2	2.47	0.47
25:S:32:ARG:HA	25:S:50:ALA:HB3	1.96	0.47
28:a:813:U:H2'	28:a:814:C:H6	1.78	0.47
28:a:2281:A:O2'	28:a:2282:G:H5'	2.14	0.47
43:p:49:ASP:HA	43:p:52:GLN:HB2	1.96	0.47
7:A:1000:A:H2'	7:A:1001:G:C8	2.48	0.47
8:B:130:THR:C	8:B:132:LYS:H	2.22	0.47
12:F:16:GLU:H	12:F:16:GLU:CD	2.18	0.47
13:G:11:LYS:HE3	13:G:12:ILE:O	2.15	0.47
13:G:27:VAL:HG22	13:G:43:VAL:HG21	1.95	0.47
16:J:6:ILE:HB	16:J:76:ILE:HB	1.96	0.47
28:a:2591:C:H2'	28:a:2592:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:27:LYS:HG2	34:g:32:GLU:OE2	2.15	0.47
7:A:95:G:HO2'	7:A:96:U:H6	1.61	0.47
7:A:678:U:H2'	7:A:679:U:C6	2.50	0.47
7:A:757:U:O2'	7:A:879:C:O2	2.32	0.47
7:A:881:G:OP1	18:L:9:ARG:NH2	2.45	0.47
7:A:1176:G:H2'	7:A:1177:A:H8	1.79	0.47
7:A:1511:G:C4	7:A:1512:C:C5	3.03	0.47
9:C:53:SER:HB3	9:C:115:LEU:HD21	1.96	0.47
9:C:78:GLY:O	9:C:80:LYS:O	2.32	0.47
12:F:79:ARG:HH11	12:F:79:ARG:HG3	1.80	0.47
23:Q:58:VAL:HB	23:Q:80:GLU:HB3	1.97	0.47
26:T:2:ALA:HB3	26:T:8:LYS:HG2	1.96	0.47
28:a:231:A:H2'	28:a:232:G:O4'	2.15	0.47
28:a:242:G:O2'	28:a:254:G:O6	2.30	0.47
28:a:247:G:OP2	28:a:249:C:N4	2.47	0.47
28:a:807:U:O2'	28:a:2060:A:N1	2.47	0.47
28:a:1476:U:H2'	28:a:1477:A:H8	1.79	0.47
28:a:1800:C:OP2	30:c:182:ARG:NH1	2.47	0.47
28:a:2577:A:H2'	28:a:2614:A:N6	2.30	0.47
30:c:163:GLN:OE1	30:c:175:ARG:NH1	2.47	0.47
33:f:44:ILE:HG21	33:f:79:ILE:HG22	1.97	0.47
36:i:4:PHE:O	43:p:64:ARG:NH1	2.46	0.47
48:u:79:ARG:HG2	48:u:79:ARG:NH1	2.28	0.47
7:A:864:A:H4'	11:E:90:THR:HG23	1.97	0.47
7:A:1170:A:H2'	7:A:1171:A:C8	2.49	0.47
28:a:581:C:H2'	28:a:582:A:C8	2.49	0.47
28:a:2804:U:H2'	28:a:2805:C:C6	2.49	0.47
29:b:44:G:N2	29:b:48:U:C2	2.83	0.47
45:r:109:ASP:OD1	45:r:109:ASP:N	2.47	0.47
46:s:76:ARG:HG2	46:s:76:ARG:HH11	1.80	0.47
2:1:25:LYS:HE2	28:a:1367:A:O2'	2.15	0.47
7:A:1003:G:H21	7:A:1005:A:H5'	1.78	0.47
7:A:1250:C:O2'	15:I:70:GLY:O	2.21	0.47
11:E:107:ALA:HB1	11:E:111:MET:HB2	1.97	0.47
18:L:55:VAL:HG21	18:L:80:ILE:HD11	1.97	0.47
19:M:93:ARG:NH2	28:a:888:C:OP2	2.48	0.47
28:a:5:A:H2'	28:a:6:A:H8	1.79	0.47
28:a:1186:G:H2'	28:a:1187:G:O4'	2.15	0.47
28:a:1441:G:H2'	28:a:1442:U:C6	2.50	0.47
28:a:1563:U:H2'	28:a:1564:C:C6	2.49	0.47
28:a:1590:A:H2'	28:a:1591:A:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2328:A:H2'	28:a:2329:U:H6	1.76	0.47
28:a:2698:U:H2'	28:a:2699:C:C6	2.49	0.47
33:f:130:MET:HG2	33:f:154:ILE:HB	1.97	0.47
7:A:392:C:C2	7:A:393:A:C8	3.03	0.47
7:A:470:C:H2'	7:A:471:U:C6	2.50	0.47
7:A:877:G:O2'	7:A:878:A:OP2	2.21	0.47
7:A:1236:U:H2'	7:A:1237:A:O4'	2.14	0.47
20:N:53:ARG:NH1	25:S:37:ARG:HH12	2.13	0.47
28:a:5:A:H2'	28:a:6:A:C8	2.50	0.47
28:a:1532:A:N6	28:a:1540:G:O6	2.48	0.47
46:s:8:LEU:HD13	46:s:50:LEU:HD21	1.95	0.47
7:A:86:G:H4'	7:A:87:U:O5'	2.13	0.46
7:A:364:A:O2'	7:A:365:U:O2	2.33	0.46
7:A:1122:U:HO2'	7:A:1123:G:H8	1.62	0.46
9:C:81:GLY:O	9:C:84:VAL:HB	2.15	0.46
28:a:78:U:H2'	28:a:79:C:C6	2.50	0.46
28:a:813:U:H2'	28:a:814:C:C6	2.50	0.46
28:a:927:A:H2'	28:a:928:A:C8	2.49	0.46
28:a:1428:C:C5	28:a:1569:A:H5"	2.50	0.46
28:a:1527:G:N1	28:a:1544:A:OP2	2.36	0.46
28:a:1667:G:O2'	28:a:1991:U:O4	2.28	0.46
28:a:2537:U:H2'	28:a:2538:C:H6	1.80	0.46
44:q:29:THR:O	44:q:29:THR:OG1	2.27	0.46
53:z:33:THR:HG22	53:z:51:GLY:HA2	1.96	0.46
7:A:258:A:H2'	7:A:259:G:H8	1.80	0.46
7:A:944:G:N1	7:A:1339:G:OP2	2.38	0.46
15:I:47:VAL:HA	15:I:50:GLN:HG3	1.97	0.46
15:I:84:THR:HG23	15:I:98:LEU:HD22	1.98	0.46
20:N:47:LYS:O	20:N:47:LYS:HD3	2.15	0.46
22:P:8:ARG:HB3	22:P:28:ARG:HH11	1.77	0.46
33:f:30:ARG:H	33:f:159:THR:HB	1.81	0.46
39:l:3:GLN:HE21	39:l:92:TRP:NE1	2.13	0.46
7:A:371:A:H2'	7:A:372:C:O4'	2.16	0.46
7:A:544:G:H2'	7:A:545:C:O4'	2.14	0.46
7:A:859:G:OP2	7:A:869:G:N1	2.38	0.46
21:O:89:ARG:NH2	28:a:714:U:OP2	2.49	0.46
26:T:39:ILE:HD13	26:T:82:GLN:HB3	1.97	0.46
34:g:19:ILE:HD13	34:g:43:VAL:HB	1.98	0.46
39:l:5:LYS:H	39:l:5:LYS:HG2	1.55	0.46
8:B:120:GLN:HB3	8:B:125:THR:HG21	1.96	0.46
9:C:122:SER:O	9:C:126:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:79:SER:HB2	14:H:85:ILE:H	1.80	0.46
28:a:1177:G:H2'	28:a:1178:C:C6	2.50	0.46
29:b:42:C:C5	33:f:66:LEU:HD12	2.50	0.46
37:j:105:ARG:HG3	37:j:108:ARG:HG3	1.96	0.46
7:A:374:A:H2'	7:A:375:U:H6	1.81	0.46
7:A:401:C:OP1	10:D:70:ARG:HD2	2.15	0.46
7:A:741:G:C2	7:A:742:G:H8	2.34	0.46
7:A:855:U:OP2	7:A:871:U:N3	2.44	0.46
11:E:115:LEU:HD13	11:E:123:VAL:HG11	1.97	0.46
23:Q:46:VAL:HG21	23:Q:61:ILE:HG21	1.97	0.46
28:a:1168:G:H2'	28:a:1169:A:H8	1.81	0.46
34:g:72:LEU:O	34:g:76:VAL:HG13	2.16	0.46
37:j:70:ARG:NH1	37:j:74:GLY:O	2.49	0.46
7:A:1273:U:H2'	7:A:1274:G:O4'	2.16	0.46
20:N:90:ARG:NH1	20:N:92:GLU:OE1	2.48	0.46
28:a:534:U:O2'	43:p:49:ASP:OD2	2.26	0.46
28:a:1548:A:H2'	28:a:1549:A:H8	1.80	0.46
28:a:2823:A:OP1	31:d:118:PHE:HB2	2.16	0.46
39:l:12:MET:HE2	39:l:12:MET:HB3	1.80	0.46
3:2:31:HIS:NE2	28:a:2392:A:OP2	2.45	0.46
7:A:715:A:H2'	7:A:716:A:C8	2.50	0.46
12:F:4:TYR:CD2	12:F:71:ILE:HG13	2.51	0.46
28:a:784:G:H5'	28:a:785:G:OP1	2.16	0.46
28:a:1429:G:H2'	28:a:1430:G:H8	1.81	0.46
28:a:1997:C:OP2	31:d:129:THR:OG1	2.22	0.46
33:f:30:ARG:NH2	33:f:159:THR:HG21	2.30	0.46
7:A:130:A:H5'	23:Q:65:ARG:HD2	1.98	0.46
7:A:473:A:H2'	7:A:474:A:H8	1.81	0.46
7:A:495:A:H4'	7:A:496:A:OP1	2.15	0.46
7:A:978:A:C4	7:A:1320:A:C2	3.04	0.46
8:B:130:THR:O	8:B:132:LYS:N	2.49	0.46
16:J:85:ASP:O	16:J:89:ARG:HG2	2.16	0.46
21:O:89:ARG:HB3	21:O:89:ARG:CZ	2.46	0.46
26:T:43:ASP:OD1	26:T:44:LYS:N	2.48	0.46
28:a:667:U:H2'	28:a:668:A:O4'	2.16	0.46
28:a:692:C:H5"	30:c:39:LYS:HB2	1.97	0.46
28:a:857:G:H2'	28:a:858:G:O4'	2.15	0.46
28:a:2329:U:H2'	28:a:2330:G:C8	2.51	0.46
28:a:2649:C:H2'	28:a:2650:U:C6	2.51	0.46
37:j:40:LYS:HE3	37:j:57:VAL:HG12	1.97	0.46
28:a:2199:A:N1	28:a:2226:C:N4	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:v:70:GLU:OE1	49:v:72:LYS:HE2	2.16	0.46
7:A:263:A:H2'	7:A:264:G:C8	2.51	0.46
7:A:964:A:C2	7:A:969:A:H1'	2.51	0.46
8:B:96:TRP:CZ2	8:B:100:MET:HB3	2.51	0.46
28:a:1197:G:H2'	28:a:1198:U:H6	1.81	0.46
28:a:1630:A:N6	28:a:1637:A:H61	2.14	0.46
28:a:1637:A:H5'	28:a:1760:C:O2'	2.15	0.46
28:a:2747:G:O6	28:a:2755:C:H5"	2.15	0.46
7:A:195:A:H1'	7:A:222:U:O2'	2.16	0.45
7:A:421:U:O2	9:C:127:ARG:NH2	2.48	0.45
7:A:555:U:H2'	7:A:556:C:C6	2.52	0.45
8:B:96:TRP:NE1	8:B:175:GLU:OE2	2.36	0.45
13:G:15:ASP:OD1	13:G:19:GLY:N	2.49	0.45
14:H:64:LYS:HG3	14:H:71:VAL:HG11	1.98	0.45
22:P:15:PRO:HG2	22:P:41:PRO:HG2	1.96	0.45
27:U:13:ASP:HB3	27:U:17:ARG:NH2	2.31	0.45
28:a:988:A:OP2	52:y:12:SER:OG	2.34	0.45
46:s:30:ILE:HD13	46:s:93:LEU:HD13	1.97	0.45
1:0:53:LYS:HB3	1:0:53:LYS:HE3	1.69	0.45
28:a:307:G:N1	28:a:310:A:OP2	2.36	0.45
28:a:397:U:H5"	50:w:32:ASN:HB2	1.99	0.45
28:a:1198:U:H2'	28:a:1199:U:C6	2.50	0.45
28:a:1413:A:H2'	28:a:1414:C:C6	2.51	0.45
28:a:2845:U:H5"	42:o:52:ASN:O	2.16	0.45
28:a:2849:U:H4'	28:a:2868:A:C2	2.52	0.45
31:d:84:LEU:HD22	31:d:88:GLU:HB2	1.98	0.45
7:A:601:G:H2'	7:A:602:A:C8	2.51	0.45
7:A:1120:C:H2'	7:A:1121:U:H6	1.81	0.45
9:C:79:LYS:HD2	9:C:79:LYS:HA	1.61	0.45
9:C:162:ILE:HD12	9:C:162:ILE:N	2.32	0.45
10:D:116:GLN:OE1	10:D:154:ARG:NH1	2.40	0.45
19:M:17:ILE:O	19:M:20:THR:OG1	2.28	0.45
19:M:71:ARG:HH21	33:f:115:ARG:HD2	1.82	0.45
28:a:1168:G:H2'	28:a:1169:A:C8	2.52	0.45
28:a:2030:6MZ:C2	28:a:2499:C:H5"	2.46	0.45
29:b:95:U:OP2	48:u:19:ARG:NH2	2.49	0.45
32:e:1:MET:HG2	32:e:16:GLU:CD	2.42	0.45
41:n:27:VAL:HG21	41:n:40:ILE:HD12	1.98	0.45
49:v:29:GLU:O	49:v:66:LYS:HA	2.17	0.45
4:3:9:LYS:HE3	4:3:9:LYS:HB3	1.57	0.45
7:A:321:A:H2'	7:A:322:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:61:LEU:HD23	12:F:62:MET:N	2.31	0.45
23:Q:48:ASP:OD2	23:Q:51:ASN:HA	2.17	0.45
28:a:511:U:O4	28:a:512:G:N1	2.49	0.45
28:a:1496:A:H2'	28:a:1498:C:C5	2.51	0.45
28:a:2837:A:H2'	28:a:2838:G:H8	1.80	0.45
32:e:2:GLU:OE2	32:e:13:THR:OG1	2.27	0.45
34:g:48:ASN:O	34:g:49:THR:HG23	2.16	0.45
5:4:18:CYS:SG	5:4:40:CYS:HB3	2.56	0.45
5:4:20:ASN:ND2	5:4:39:LYS:HG3	2.32	0.45
7:A:410:G:H4'	7:A:411:A:OP1	2.15	0.45
7:A:1227:C:H2'	19:M:102:THR:CG2	2.46	0.45
13:G:114:LYS:HB2	13:G:114:LYS:HE2	1.72	0.45
28:a:288:U:H2'	28:a:289:G:C8	2.52	0.45
28:a:1366:A:H2'	28:a:1367:A:O4'	2.17	0.45
28:a:2233:U:H2'	28:a:2234:G:C8	2.51	0.45
28:a:2455:G:H2'	28:a:2456:C:C6	2.52	0.45
29:b:2:G:H2'	29:b:3:C:C6	2.51	0.45
30:c:72:ASP:OD1	30:c:72:ASP:N	2.34	0.45
5:4:32:LEU:HD23	5:4:32:LEU:HA	1.80	0.45
7:A:624:C:H4'	22:P:10:GLY:HA2	1.98	0.45
7:A:718:A:H2	24:R:38:LYS:HG2	1.81	0.45
7:A:1002:A:H2'	7:A:1003:G:H8	1.73	0.45
15:I:25:ASN:OD1	15:I:26:GLY:N	2.50	0.45
17:K:94:GLU:CD	17:K:94:GLU:H	2.25	0.45
17:K:107:ILE:HD12	27:U:12:PHE:CE1	2.51	0.45
26:T:44:LYS:HG2	26:T:86:LEU:HD22	1.99	0.45
28:a:358:U:H2'	28:a:359:G:H8	1.81	0.45
28:a:581:C:H2'	28:a:582:A:H8	1.80	0.45
28:a:1473:G:H2'	28:a:1474:U:H6	1.82	0.45
28:a:2064:C:H2'	28:a:2065:C:C6	2.51	0.45
28:a:2615:U:C2	53:z:4:GLN:HA	2.52	0.45
37:j:2:ILE:HG13	37:j:6:THR:HG21	1.98	0.45
46:s:34:VAL:HG11	46:s:43:ILE:HD13	1.97	0.45
51:x:14:LEU:HD23	51:x:14:LEU:HA	1.82	0.45
7:A:321:A:H2'	7:A:322:C:H6	1.82	0.45
7:A:333:U:OP1	26:T:2:ALA:N	2.50	0.45
7:A:1228:A:OP2	19:M:110:LYS:NZ	2.46	0.45
8:B:164:ILE:HD13	8:B:210:VAL:HG13	1.99	0.45
10:D:77:LYS:HB2	10:D:77:LYS:HE3	1.73	0.45
12:F:42:TRP:CZ2	12:F:61:LEU:HD12	2.52	0.45
20:N:19:LYS:HG2	20:N:20:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:2:SER:HB3	21:O:3:LEU:H	1.59	0.45
28:a:30:G:H2'	28:a:31:C:C6	2.52	0.45
28:a:729:G:O2'	28:a:763:G:H4'	2.17	0.45
28:a:2251:OMG:HM23	28:a:2251:OMG:H1'	1.69	0.45
31:d:85:ALA:HB3	31:d:88:GLU:HG3	1.99	0.45
48:u:2:PHE:HB3	48:u:50:MET:HE3	1.98	0.45
49:v:23:VAL:HA	49:v:38:VAL:HG23	1.99	0.45
7:A:657:U:C2	7:A:658:A:C8	3.05	0.45
7:A:719:C:H1'	24:R:38:LYS:HB3	1.98	0.45
7:A:999:C:H2'	7:A:1000:A:H8	1.82	0.45
7:A:1172:A:H2'	7:A:1173:C:C6	2.51	0.45
21:O:48:LYS:HD3	21:O:48:LYS:HA	1.56	0.45
26:T:15:GLU:OE2	26:T:19:LYS:NZ	2.49	0.45
26:T:85:LYS:O	26:T:85:LYS:HG2	2.17	0.45
28:a:64:A:H2'	28:a:65:U:H6	1.79	0.45
28:a:720:U:H2'	28:a:721:A:H8	1.82	0.45
28:a:2649:C:H2'	28:a:2650:U:H6	1.82	0.45
40:m:65:LEU:HD23	40:m:65:LEU:HA	1.84	0.45
50:w:3:ARG:O	50:w:12:PRO:HD3	2.17	0.45
7:A:323:U:H2'	7:A:324:G:O4'	2.17	0.45
7:A:436:C:H2'	7:A:437:U:C6	2.52	0.45
7:A:676:A:H2'	7:A:677:U:H6	1.82	0.45
7:A:1148:C:O2'	15:I:7:TYR:OH	2.28	0.45
11:E:72:ILE:HD13	11:E:141:ILE:HG23	1.99	0.45
11:E:111:MET:HE2	11:E:111:MET:HB3	1.75	0.45
15:I:81:HIS:CE1	15:I:85:ARG:HH11	2.35	0.45
22:P:39:PHE:HD1	22:P:50:THR:HG23	1.82	0.45
28:a:2799:A:O2'	28:a:2800:A:H5"	2.17	0.45
33:f:170:LEU:O	33:f:175:PHE:HB2	2.17	0.45
45:r:73:LYS:HB2	45:r:106:VAL:HB	1.98	0.45
48:u:51:GLN:OE1	48:u:57:TYR:OH	2.34	0.45
49:v:26:PHE:O	49:v:29:GLU:HG2	2.17	0.45
7:A:154:C:H2'	7:A:155:A:C8	2.52	0.45
7:A:542:G:H5'	10:D:39:GLY:HA2	1.99	0.45
7:A:768:A:H5'	7:A:1525:G:H1'	1.99	0.45
7:A:1172:A:H2'	7:A:1173:C:H6	1.82	0.45
7:A:1532:A:N6	7:A:1534:C:O2	2.50	0.45
9:C:78:GLY:C	9:C:80:LYS:N	2.72	0.45
20:N:9:ARG:O	20:N:13:ARG:HG3	2.16	0.45
22:P:56:ARG:HD2	22:P:56:ARG:HA	1.72	0.45
28:a:638:G:H2'	28:a:639:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:851:C:H2'	28:a:852:U:H6	1.80	0.45
28:a:1486:U:H2'	28:a:1487:U:H6	1.82	0.45
31:d:61:THR:OG1	31:d:64:GLU:HG3	2.16	0.45
34:g:9:VAL:HG22	34:g:50:LEU:HB2	1.99	0.45
35:h:32:PRO:HA	50:w:39:TRP:CD1	2.52	0.45
44:q:25:LEU:HD12	44:q:94:THR:HG21	1.97	0.45
44:q:27:ILE:HD13	44:q:33:VAL:HG23	1.98	0.45
44:q:46:GLU:OE2	44:q:48:LYS:NZ	2.50	0.45
7:A:352:C:H4'	7:A:354:G:OP1	2.17	0.44
7:A:745:A:H2'	7:A:746:G:C8	2.52	0.44
11:E:54:ARG:HG2	11:E:54:ARG:HH11	1.82	0.44
11:E:103:THR:HG21	11:E:124:LEU:HD11	1.99	0.44
12:F:5:GLU:HG3	12:F:63:ASN:ND2	2.32	0.44
25:S:65:GLU:HA	25:S:65:GLU:OE2	2.16	0.44
28:a:569:U:H5"	28:a:821:A:N1	2.32	0.44
28:a:849:A:H2'	28:a:850:U:C6	2.53	0.44
40:m:12:ARG:O	40:m:17:ARG:NH1	2.50	0.44
5:4:64:PHE:HE2	25:S:8:GLY:C	2.25	0.44
7:A:129:A:H1'	7:A:130:A:C8	2.52	0.44
7:A:222:U:H2'	7:A:223:A:H8	1.83	0.44
7:A:293:G:N1	7:A:305:G:C6	2.85	0.44
7:A:964:A:H2	7:A:969:A:N3	2.16	0.44
10:D:150:LYS:O	10:D:150:LYS:HD2	2.16	0.44
12:F:69:GLU:OE2	12:F:69:GLU:N	2.29	0.44
28:a:27:G:H22	28:a:512:G:H1'	1.81	0.44
28:a:483:A:C8	47:t:45:HIS:HD2	2.35	0.44
28:a:499:U:H2'	28:a:500:G:O4'	2.17	0.44
28:a:541:A:N6	28:a:553:G:O6	2.51	0.44
28:a:781:A:P	30:c:217:ARG:HH22	2.39	0.44
28:a:828:U:H2'	28:a:829:A:C8	2.52	0.44
28:a:1000:A:H2'	28:a:1001:A:C8	2.52	0.44
28:a:1306:C:H2'	28:a:1307:A:H8	1.83	0.44
28:a:2521:C:O2'	28:a:2564:A:N3	2.42	0.44
33:f:44:ILE:HA	33:f:83:TYR:CE1	2.52	0.44
36:i:5:THR:HG23	36:i:45:THR:HG21	2.00	0.44
45:r:21:ALA:HB1	45:r:74:ILE:HG12	1.98	0.44
7:A:373:A:C2'	7:A:374:A:H5'	2.48	0.44
7:A:821:G:H2'	7:A:822:U:C6	2.52	0.44
7:A:958:A:C2	25:S:55:ARG:HB3	2.52	0.44
7:A:1033:G:C8	7:A:1034:G:H1'	2.53	0.44
10:D:48:LEU:HA	10:D:48:LEU:HD12	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:63:GLN:O	22:P:63:GLN:HG3	2.17	0.44
28:a:1469:A:H2'	28:a:1470:A:H8	1.81	0.44
28:a:1591:A:H2'	28:a:1592:C:C6	2.52	0.44
28:a:2052:A:O2'	31:d:148:GLN:O	2.28	0.44
29:b:2:G:H2'	29:b:3:C:H6	1.82	0.44
29:b:42:C:O2'	33:f:63:GLN:HG2	2.18	0.44
37:j:106:GLU:N	37:j:106:GLU:OE2	2.51	0.44
4:3:6:SER:HB3	28:a:2466:C:H5"	1.99	0.44
11:E:110:ALA:HB1	11:E:137:VAL:HG23	1.98	0.44
28:a:2847:U:H2'	28:a:2848:G:O4'	2.17	0.44
34:g:19:ILE:HG12	34:g:24:ILE:HD12	1.98	0.44
48:u:68:LYS:HE2	48:u:68:LYS:HB3	1.44	0.44
3:2:49:MET:HE3	3:2:49:MET:HB3	1.74	0.44
7:A:62:U:O2'	7:A:379:C:O2	2.36	0.44
7:A:229:U:O2'	22:P:23:ASP:OD2	2.35	0.44
7:A:435:A:H3'	7:A:436:C:H5"	1.99	0.44
9:C:53:SER:HB3	9:C:115:LEU:CD2	2.47	0.44
28:a:2193:G:H2'	28:a:2194:U:C6	2.52	0.44
28:a:2838:G:C4	28:a:2839:G:C8	3.05	0.44
38:k:77:ILE:CD1	38:k:108:ALA:HB1	2.48	0.44
7:A:1107:C:C4	7:A:1108:G:C8	3.05	0.44
7:A:1255:G:H1	7:A:1284:U:H3	1.66	0.44
7:A:1344:G:H2'	7:A:1345:C:C6	2.52	0.44
7:A:1361:A:C8	20:N:58:SER:HB2	2.53	0.44
12:F:49:TYR:HB3	24:R:74:HIS:CD2	2.51	0.44
28:a:1798:U:H5"	30:c:258:ARG:HB2	2.00	0.44
35:h:30:LEU:HB3	35:h:36:ALA:HB3	1.99	0.44
37:j:1:MET:N	37:j:65:THR:HG21	2.33	0.44
2:1:25:LYS:HE3	2:1:25:LYS:HB3	1.55	0.44
7:A:538:G:H2'	7:A:539:A:H8	1.82	0.44
7:A:1095:U:H2'	7:A:1096:C:C6	2.53	0.44
8:B:85:LEU:HD23	8:B:85:LEU:HA	1.86	0.44
9:C:138:VAL:CG1	9:C:170:GLU:HG3	2.47	0.44
14:H:92:LEU:HD12	14:H:117:ARG:HG3	1.98	0.44
20:N:6:MET:HE3	20:N:6:MET:HB3	1.87	0.44
26:T:9:LYS:O	26:T:13:GLN:HG3	2.18	0.44
28:a:644:A:H2'	28:a:645:C:O4'	2.17	0.44
28:a:756:A:H2'	28:a:757:G:O4'	2.18	0.44
28:a:1431:A:H4'	56:a:6215:SPD:H21	1.99	0.44
28:a:2011:U:H2'	28:a:2012:G:O4'	2.17	0.44
28:a:2032:G:C8	31:d:150:MEQ:HE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2065:C:H2'	28:a:2066:C:H6	1.82	0.44
28:a:2460:U:C2	28:a:2461:A:C8	3.05	0.44
33:f:36:LEU:HD22	33:f:154:ILE:HG13	2.00	0.44
35:h:29:PHE:O	35:h:33:GLN:HG3	2.18	0.44
7:A:8:A:N6	10:D:206:LYS:HB2	2.33	0.44
7:A:24:U:O2'	7:A:524:G:O2'	2.33	0.44
7:A:392:C:H5"	22:P:12:LYS:HG3	1.99	0.44
7:A:403:C:H42	7:A:547:A:C5'	2.21	0.44
7:A:520:A:O2'	18:L:70:GLU:OE1	2.32	0.44
7:A:1296:U:H2'	7:A:1297:C:C6	2.52	0.44
7:A:1310:G:N7	19:M:98:ARG:NH2	2.66	0.44
7:A:1383:C:H4'	13:G:79:ARG:HH21	1.83	0.44
7:A:1429:A:H2'	7:A:1430:A:O4'	2.18	0.44
8:B:6:MET:HE3	8:B:6:MET:C	2.43	0.44
9:C:86:LYS:O	9:C:90:VAL:HG23	2.18	0.44
16:J:21:ALA:O	16:J:24:GLU:HG3	2.18	0.44
18:L:108:LYS:HB2	18:L:108:LYS:HE3	1.57	0.44
19:M:86:TYR:CZ	19:M:90:ARG:HD2	2.53	0.44
20:N:28:LYS:O	20:N:31:ILE:HG22	2.18	0.44
26:T:25:ARG:HB2	26:T:66:LEU:HD11	1.99	0.44
28:a:347:A:H2'	28:a:348:A:C8	2.52	0.44
28:a:967:U:H2'	28:a:968:C:C6	2.53	0.44
30:c:3:VAL:HG22	30:c:19:VAL:HG22	2.00	0.44
7:A:502:A:H2'	7:A:503:C:C6	2.53	0.44
7:A:580:U:H2'	7:A:581:G:O4'	2.18	0.44
8:B:207:ILE:H	8:B:207:ILE:CD1	2.28	0.44
17:K:37:ARG:NE	17:K:83:GLU:OE2	2.51	0.44
23:Q:15:ASP:HA	23:Q:21:ILE:HG22	2.00	0.44
28:a:4:U:H2'	28:a:5:A:H8	1.83	0.44
28:a:2014:A:H2'	28:a:2015:A:C8	2.52	0.44
28:a:2271:G:OP1	49:v:18:ALA:HB1	2.17	0.44
29:b:78:A:H2'	29:b:79:G:O4'	2.18	0.44
31:d:43:ASP:OD2	31:d:43:ASP:N	2.50	0.44
33:f:78:LYS:HE2	33:f:78:LYS:HB2	1.79	0.44
47:t:18:ASP:HB3	47:t:21:LYS:HD2	1.99	0.44
7:A:147:G:H2'	7:A:148:G:C8	2.53	0.43
7:A:178:C:C2	7:A:179:A:C8	3.06	0.43
7:A:666:G:H5'	7:A:726:C:H1'	2.00	0.43
7:A:687:A:C2	7:A:704:A:C5	3.05	0.43
7:A:1145:G:N2	7:A:1147:A:H62	2.16	0.43
27:U:17:ARG:O	27:U:21:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:322:A:H5'	28:a:340:A:H1'	2.00	0.43
28:a:476:G:N1	28:a:479:A:OP2	2.46	0.43
28:a:1365:A:OP1	50:w:28:ARG:NH2	2.51	0.43
28:a:1735:A:H2'	28:a:1736:U:C6	2.53	0.43
28:a:2537:U:H2'	28:a:2538:C:C6	2.53	0.43
28:a:2627:G:O2'	28:a:2781:A:N1	2.44	0.43
2:1:41:ARG:HH11	2:1:46:LYS:HZ1	1.66	0.43
5:4:34:LEU:HD11	33:f:106:ILE:HG23	2.00	0.43
7:A:978:A:C6	7:A:1319:A:C6	3.06	0.43
7:A:1313:G:H5'	25:S:5:LEU:HD11	2.00	0.43
7:A:1514:A:H2'	7:A:1515:G:C8	2.54	0.43
14:H:76:GLN:O	14:H:127:CYS:HB2	2.18	0.43
23:Q:25:ILE:O	23:Q:41:THR:HA	2.18	0.43
28:a:277:G:H4'	28:a:278:A:O5'	2.18	0.43
28:a:721:A:H2'	28:a:722:A:H8	1.83	0.43
28:a:748:G:P	45:r:88:ARG:HH21	2.41	0.43
28:a:2051:A:H5'	28:a:2578:G:O4'	2.18	0.43
30:c:94:VAL:HG11	30:c:116:ILE:HD11	1.99	0.43
32:e:106:LYS:O	32:e:110:SER:OG	2.32	0.43
5:4:28:VAL:N	33:f:140:GLU:OE1	2.51	0.43
7:A:392:C:P	22:P:8:ARG:HH22	2.40	0.43
7:A:649:A:H2'	7:A:650:G:O4'	2.18	0.43
7:A:1130:A:C8	7:A:1147:A:N1	2.87	0.43
8:B:27:MET:HE2	8:B:188:ASP:O	2.18	0.43
10:D:45:LYS:HD2	10:D:45:LYS:HA	1.88	0.43
17:K:23:ILE:HD12	17:K:84:VAL:HG13	2.01	0.43
23:Q:62:ARG:HG2	23:Q:62:ARG:NH1	2.33	0.43
26:T:54:MET:HE3	26:T:58:VAL:HG21	1.98	0.43
28:a:44:A:H2'	28:a:45:G:O4'	2.18	0.43
30:c:270:ARG:HG2	30:c:271:ARG:N	2.33	0.43
34:g:148:LEU:HA	34:g:151:TYR:HD2	1.82	0.43
39:l:31:PHE:HB3	39:l:130:PHE:CZ	2.53	0.43
7:A:1103:C:O2	8:B:106:THR:HG21	2.17	0.43
28:a:116:C:O2'	28:a:126:A:N3	2.42	0.43
28:a:586:A:N1	28:a:809:G:O2'	2.41	0.43
28:a:1853:A:H2'	28:a:1854:A:C8	2.53	0.43
28:a:2851:A:N7	56:a:6208:SPD:H92	2.34	0.43
30:c:30:PHE:CE2	30:c:32:PRO:HG2	2.52	0.43
31:d:62:LYS:HE2	31:d:62:LYS:HB3	1.63	0.43
7:A:1447:A:O2'	7:A:1448:A:H5'	2.18	0.43
9:C:81:GLY:O	9:C:85:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:248:G:H5'	28:a:250:G:N7	2.33	0.43
28:a:671:C:H2'	28:a:672:C:H6	1.82	0.43
28:a:801:G:C8	32:e:50:ALA:HB2	2.53	0.43
28:a:1028:A:N6	28:a:1125:G:H2'	2.33	0.43
28:a:1045:C:O2	28:a:1111:A:N6	2.51	0.43
28:a:1141:U:H4'	28:a:1142:A:O4'	2.18	0.43
28:a:2316:G:H2'	28:a:2317:A:H8	1.84	0.43
28:a:2812:G:H2'	28:a:2813:A:C8	2.53	0.43
35:h:34:GLY:O	35:h:36:ALA:N	2.51	0.43
36:i:31:GLU:OE2	36:i:34:ARG:NH1	2.51	0.43
44:q:33:VAL:HG12	44:q:61:ALA:HB3	2.01	0.43
45:r:46:LEU:O	45:r:50:VAL:HG23	2.18	0.43
46:s:8:LEU:CD1	46:s:50:LEU:HD21	2.49	0.43
4:3:19:ARG:NE	28:a:2756:U:OP2	2.42	0.43
7:A:1118:U:H1'	7:A:1180:A:C8	2.54	0.43
11:E:131:THR:HG22	11:E:131:THR:O	2.19	0.43
13:G:107:ALA:HB1	13:G:133:THR:HB	2.00	0.43
28:a:848:C:H2'	28:a:849:A:H8	1.84	0.43
29:b:75:G:O2'	48:u:88:HIS:NE2	2.44	0.43
41:n:18:LEU:HD21	41:n:91:SER:HB2	2.01	0.43
46:s:76:ARG:HG2	46:s:76:ARG:NH1	2.33	0.43
7:A:637:U:H2'	7:A:638:U:C6	2.54	0.43
7:A:1144:G:H2'	7:A:1145:G:H8	1.84	0.43
7:A:1452:U:H3'	7:A:1453:C:C6	2.49	0.43
7:A:1497:C:H2'	7:A:1498:G:O4'	2.18	0.43
8:B:27:MET:O	8:B:31:ILE:HG13	2.19	0.43
9:C:154:SER:HB3	9:C:165:THR:HG23	2.00	0.43
10:D:147:GLU:OE2	10:D:147:GLU:HA	2.18	0.43
12:F:17:GLN:H	12:F:17:GLN:HG2	1.62	0.43
28:a:657:U:H2'	28:a:658:U:C6	2.53	0.43
28:a:782:A:H2	30:c:229:ASP:OD2	2.02	0.43
28:a:1311:G:OP2	28:a:1311:G:N2	2.41	0.43
28:a:1827:U:OP2	30:c:221:ARG:HD2	2.17	0.43
28:a:2247:A:H2'	28:a:2248:C:H6	1.84	0.43
28:a:2461:A:H2'	28:a:2462:C:H6	1.84	0.43
29:b:30:C:H2'	29:b:31:C:H5'	2.00	0.43
38:k:123:ARG:NH1	38:k:143:GLU:OE2	2.48	0.43
49:v:37:ILE:HG21	49:v:80:ILE:HG21	2.00	0.43
7:A:216:U:H2'	7:A:217:U:H6	1.84	0.43
7:A:407:U:O2'	10:D:113:GLU:HB2	2.18	0.43
7:A:1158:A:H4'	7:A:1159:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:57:ILE:HD13	9:C:66:VAL:HG22	2.01	0.43
18:L:87:VAL:HG11	18:L:90:LEU:HD12	2.01	0.43
20:N:27:LEU:HD23	20:N:27:LEU:HA	1.82	0.43
28:a:1486:U:H2'	28:a:1487:U:C6	2.54	0.43
34:g:140:VAL:O	34:g:144:VAL:HG23	2.19	0.43
38:k:81:ASP:HB3	38:k:100:ILE:HD12	2.01	0.43
42:o:114:LEU:HD23	42:o:114:LEU:HA	1.80	0.43
48:u:30:ILE:HD11	48:u:40:ILE:HD13	2.00	0.43
2:1:3:ARG:HD3	2:1:3:ARG:HA	1.69	0.43
7:A:280:C:N3	23:Q:41:THR:HG22	2.34	0.43
7:A:428:G:H5"	10:D:10:LYS:HE3	2.00	0.43
7:A:678:U:H2'	7:A:679:U:H6	1.84	0.43
7:A:728:A:H2'	7:A:729:A:C8	2.53	0.43
7:A:1133:A:H2'	7:A:1134:C:O4'	2.19	0.43
9:C:112:ASP:HB3	9:C:115:LEU:HD23	2.00	0.43
28:a:373:U:O2'	28:a:423:A:H1'	2.18	0.43
28:a:580:U:H2'	28:a:581:C:C6	2.53	0.43
28:a:1684:G:H2'	28:a:1685:C:H6	1.84	0.43
53:z:38:HIS:ND1	53:z:39:LEU:O	2.52	0.43
7:A:51:A:N7	7:A:114:U:O2'	2.48	0.43
7:A:109:A:C6	7:A:326:G:C6	3.07	0.43
9:C:150:LYS:HB2	9:C:169:ARG:HG3	2.01	0.43
10:D:151:LYS:C	10:D:153:SER:H	2.27	0.43
11:E:11:LEU:HD12	11:E:39:VAL:HG12	2.01	0.43
28:a:1597:A:H5"	28:a:1598:A:H5'	2.01	0.43
28:a:1864:U:OP1	28:a:2410:G:O2'	2.30	0.43
28:a:2314:A:H2'	28:a:2315:G:H8	1.84	0.43
37:j:64:ARG:NH1	37:j:102:PRO:O	2.45	0.43
45:r:72:THR:HG22	45:r:73:LYS:HG3	2.01	0.43
7:A:59:A:H5'	7:A:387:U:H5"	2.00	0.42
7:A:239:U:H5"	7:A:240:G:OP2	2.19	0.42
8:B:64:LYS:HB2	8:B:64:LYS:HE3	1.58	0.42
14:H:67:GLN:C	14:H:69:LYS:H	2.27	0.42
15:I:42:GLU:OE2	15:I:42:GLU:C	2.61	0.42
18:L:69:GLY:HA3	18:L:107:VAL:HG11	2.00	0.42
25:S:70:LYS:O	25:S:73:GLU:HG3	2.18	0.42
26:T:79:LEU:HD23	26:T:79:LEU:HA	1.84	0.42
28:a:272:A:H2'	28:a:273:G:C8	2.51	0.42
28:a:631:A:N3	28:a:2415:G:O2'	2.44	0.42
28:a:1473:G:C6	28:a:1519:G:C6	3.07	0.42
28:a:1684:G:H2'	28:a:1685:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2564:A:OP1	28:a:2648:G:O2'	2.29	0.42
28:a:2636:C:H2'	28:a:2637:U:C6	2.54	0.42
28:a:2684:U:H4'	37:j:76:VAL:HG11	2.01	0.42
30:c:8:PRO:HB3	30:c:14:ARG:HG3	2.01	0.42
35:h:41:LYS:HD3	35:h:41:LYS:HA	1.76	0.42
44:q:78:ARG:HE	44:q:78:ARG:HB2	1.50	0.42
49:v:25:ARG:HB3	49:v:29:GLU:HG3	2.01	0.42
7:A:293:G:C6	7:A:305:G:N1	2.86	0.42
7:A:545:C:OP2	10:D:59:GLN:NE2	2.51	0.42
7:A:999:C:N3	7:A:1042:A:N6	2.67	0.42
7:A:1010:G:H2'	7:A:1011:C:C6	2.54	0.42
7:A:1478:U:H2'	7:A:1479:U:C6	2.54	0.42
9:C:64:ILE:HG22	9:C:97:VAL:HG23	2.01	0.42
22:P:46:LYS:HD2	22:P:46:LYS:HA	1.67	0.42
28:a:182:A:H2'	28:a:183:C:H6	1.85	0.42
28:a:239:C:O2'	28:a:622:G:O2'	2.32	0.42
28:a:1668:A:H4'	28:a:1669:A:O5'	2.19	0.42
28:a:1880:U:H2'	28:a:1881:C:H6	1.84	0.42
28:a:2489:U:H2'	28:a:2490:G:O4'	2.19	0.42
57:a:6221:SPM:H31	57:a:6221:SPM:H62	1.77	0.42
30:c:175:ARG:HE	30:c:181:MET:HE2	1.84	0.42
30:c:228:VAL:HG13	30:c:229:ASP:OD1	2.18	0.42
32:e:21:ARG:HH11	32:e:21:ARG:HB2	1.85	0.42
4:3:2:LYS:HE2	4:3:32:LYS:O	2.18	0.42
5:4:37:CYS:SG	5:4:39:LYS:N	2.85	0.42
7:A:412:A:H62	7:A:431:A:H61	1.66	0.42
7:A:766:A:H5'	7:A:767:A:OP2	2.19	0.42
7:A:1121:U:C2'	7:A:1122:U:H5'	2.49	0.42
8:B:43:LEU:H	8:B:43:LEU:HD22	1.85	0.42
11:E:146:ASN:OD1	11:E:146:ASN:C	2.62	0.42
13:G:116:MET:HA	13:G:119:ARG:HB2	2.00	0.42
16:J:15:HIS:HB3	16:J:70:HIS:CE1	2.54	0.42
22:P:14:ARG:NE	22:P:42:ILE:HD11	2.34	0.42
28:a:81:G:HO2'	28:a:295:G:HO2'	1.61	0.42
28:a:522:A:H2'	28:a:523:C:C6	2.55	0.42
28:a:890:C:C4	28:a:891:G:H1'	2.54	0.42
31:d:3:GLY:HA3	31:d:204:LYS:HG2	2.01	0.42
41:n:74:VAL:O	41:n:78:VAL:HG12	2.19	0.42
49:v:40:GLN:HG3	49:v:42:GLY:O	2.19	0.42
3:2:4:ILE:HD11	28:a:592:A:C2	2.55	0.42
7:A:391:G:O2'	7:A:392:C:H6	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:500:G:HO2'	7:A:501:C:P	2.40	0.42
7:A:1067:A:H8	7:A:1067:A:OP2	2.02	0.42
7:A:1088:G:H21	7:A:1168:A:H61	1.67	0.42
7:A:1316:U:O2'	7:A:1361:A:N3	2.51	0.42
13:G:109:ARG:HG2	13:G:116:MET:HE1	2.02	0.42
17:K:84:VAL:HG11	17:K:97:ILE:HG12	2.00	0.42
17:K:85:MET:HG3	17:K:111:THR:HG23	2.00	0.42
17:K:113:VAL:HG22	24:R:73:ARG:HE	1.83	0.42
26:T:25:ARG:HA	26:T:66:LEU:HD21	2.01	0.42
28:a:2641:G:H5"	36:i:78:THR:HB	2.00	0.42
30:c:259:SER:O	30:c:259:SER:OG	2.30	0.42
39:l:56:ALA:HB2	39:l:119:LEU:HD12	2.01	0.42
48:u:71:LYS:N	48:u:71:LYS:HD2	2.35	0.42
7:A:161:A:H2'	7:A:162:A:C8	2.55	0.42
7:A:392:C:H5'	22:P:13:LYS:HG2	2.00	0.42
7:A:1287:C:H2'	7:A:1288:A:H4'	2.02	0.42
8:B:47:VAL:HG23	8:B:48:PRO:HD3	2.00	0.42
9:C:79:LYS:CB	9:C:83:ASP:HB2	2.50	0.42
9:C:178:LEU:HD13	9:C:178:LEU:HA	1.90	0.42
17:K:86:VAL:HG11	17:K:93:ARG:HB3	2.01	0.42
20:N:46:LEU:HD13	25:S:13:LEU:HD22	2.02	0.42
23:Q:17:MET:HB2	23:Q:20:SER:HB2	2.00	0.42
28:a:632:A:H2'	28:a:633:A:C8	2.55	0.42
28:a:846:U:O2	28:a:846:U:H2'	2.18	0.42
28:a:898:C:H2'	28:a:899:A:O4'	2.18	0.42
28:a:1236:G:OP2	56:a:6211:SPD:N1	2.53	0.42
28:a:1387:A:H5'	28:a:1469:A:H1'	2.01	0.42
28:a:1689:A:H2'	28:a:1690:A:C8	2.54	0.42
28:a:2314:A:H2'	28:a:2315:G:C8	2.54	0.42
28:a:2364:C:H2'	28:a:2365:G:O4'	2.20	0.42
34:g:95:ARG:HE	34:g:128:GLN:NE2	2.16	0.42
47:t:79:LYS:HE2	47:t:79:LYS:HB3	1.82	0.42
7:A:235:C:H2'	7:A:236:A:H8	1.85	0.42
7:A:951:G:C6	7:A:1232:G:C6	3.07	0.42
21:O:3:LEU:HD23	21:O:3:LEU:HA	1.80	0.42
28:a:2:G:H2'	28:a:3:U:C6	2.54	0.42
28:a:30:G:H2'	28:a:31:C:H6	1.85	0.42
28:a:48:G:N1	28:a:177:G:OP2	2.48	0.42
28:a:273:G:C6	28:a:274:C:N4	2.87	0.42
28:a:913:U:O4	56:a:6218:SPD:H21	2.20	0.42
28:a:1006:C:O2'	36:i:108:MET:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1532:A:C6	28:a:1540:G:C6	3.07	0.42
28:a:1591:A:H2'	28:a:1592:C:H6	1.85	0.42
33:f:108:VAL:HG11	33:f:176:PRO:HG2	2.01	0.42
7:A:1027:C:H2'	7:A:1028:C:C6	2.54	0.42
7:A:1220:A:H2'	7:A:1221:G:H8	1.84	0.42
7:A:1372:G:OP1	15:I:14:SER:OG	2.35	0.42
7:A:1403:4OC:HM22	7:A:1404:C:H5'	2.02	0.42
9:C:105:GLU:OE2	9:C:107:ARG:NE	2.53	0.42
16:J:42:LEU:HD12	16:J:71:LEU:HG	2.00	0.42
28:a:818:G:N1	28:a:1188:U:OP2	2.30	0.42
28:a:832:U:H2'	28:a:833:A:C8	2.55	0.42
28:a:892:A:H2'	28:a:893:C:C6	2.55	0.42
28:a:1224:U:H2'	28:a:1225:G:C8	2.54	0.42
28:a:1473:G:H2'	28:a:1474:U:C6	2.54	0.42
28:a:1883:U:H2'	28:a:1884:G:O4'	2.19	0.42
28:a:2554:U:H2'	28:a:2555:U:C6	2.54	0.42
28:a:2627:G:N2	28:a:2777:G:OP2	2.50	0.42
28:a:2637:U:H2'	28:a:2638:G:O4'	2.20	0.42
32:e:58:LYS:NZ	32:e:70:SER:O	2.50	0.42
7:A:637:U:OP1	23:Q:4:LYS:HD2	2.19	0.42
7:A:669:G:O2'	7:A:670:G:H8	2.03	0.42
7:A:999:C:H2'	7:A:1000:A:C8	2.55	0.42
10:D:58:LYS:NZ	10:D:69:GLU:OE1	2.41	0.42
15:I:81:HIS:CE1	15:I:85:ARG:HD2	2.55	0.42
22:P:52:LEU:HD21	22:P:74:LEU:HD13	2.02	0.42
28:a:372:G:O2'	28:a:400:G:O6	2.32	0.42
28:a:1880:U:H2'	28:a:1881:C:C6	2.55	0.42
28:a:2298:A:H2'	28:a:2299:U:O4'	2.19	0.42
33:f:19:GLU:C	33:f:19:GLU:OE2	2.63	0.42
33:f:52:ASN:ND2	33:f:147:ASP:OD2	2.52	0.42
35:h:12:LEU:HD13	35:h:19:VAL:HG21	2.02	0.42
37:j:98:ARG:HH21	37:j:100:PHE:HE1	1.68	0.42
45:r:24:ILE:HD13	45:r:36:LEU:HD11	2.01	0.42
7:A:600:A:C6	7:A:639:G:C6	3.08	0.42
7:A:820:U:H4'	7:A:821:G:OP2	2.20	0.42
7:A:1418:G:C6	7:A:1483:G:C6	3.08	0.42
12:F:11:HIS:NE2	12:F:54:LEU:HD21	2.34	0.42
15:I:21:ILE:HG22	15:I:63:LEU:HD13	2.02	0.42
28:a:448:U:P	56:a:6216:SPD:H101	2.42	0.42
33:f:163:ASP:OD1	33:f:163:ASP:N	2.52	0.42
5:4:37:CYS:SG	5:4:38:SER:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1127:G:H5'	7:A:1281:A:O2'	2.20	0.42
7:A:1159:C:C4	7:A:1161:G:C8	3.07	0.42
7:A:1317:G:N2	7:A:1319:A:H3'	2.34	0.42
9:C:110:GLU:HG2	9:C:140:ASN:HB3	2.02	0.42
10:D:4:TYR:CE2	10:D:11:LEU:HD11	2.55	0.42
17:K:52:PHE:O	17:K:53:ARG:HD2	2.20	0.42
25:S:25:SER:O	25:S:25:SER:OG	2.22	0.42
28:a:77:G:H2'	28:a:78:U:C6	2.55	0.42
28:a:322:A:OP2	32:e:163:ASN:HB2	2.19	0.42
28:a:2028:U:H2'	28:a:2029:G:O4'	2.20	0.42
28:a:2193:G:H2'	28:a:2194:U:H6	1.84	0.42
28:a:2515:C:H2'	28:a:2516:A:H8	1.84	0.42
28:a:2646:C:O5'	28:a:2646:C:H6	2.03	0.42
32:e:5:LEU:HD22	32:e:122:GLU:HG2	2.02	0.42
39:l:53:MET:HE3	39:l:63:ILE:HD12	2.01	0.42
15:I:58:VAL:HG13	15:I:59:GLU:OE2	2.19	0.41
17:K:117:PRO:HD2	27:U:35:ARG:HD2	2.02	0.41
24:R:34:THR:HG22	24:R:40:VAL:HG22	2.01	0.41
24:R:73:ARG:HB3	24:R:73:ARG:NH1	2.35	0.41
28:a:332:A:OP2	56:a:6214:SPD:N10	2.52	0.41
28:a:2316:G:N3	28:a:2317:A:C8	2.88	0.41
28:a:2818:U:H2'	28:a:2819:G:H8	1.85	0.41
28:a:2903:U:O5'	28:a:2903:U:H6	2.03	0.41
29:b:14:U:OP2	29:b:70:C:O2'	2.34	0.41
36:i:106:LYS:HB2	36:i:106:LYS:HE3	1.63	0.41
7:A:176:C:C2'	7:A:177:G:H21	2.33	0.41
7:A:999:C:N4	7:A:1042:A:H61	2.17	0.41
7:A:1060:U:H4'	16:J:53:ILE:HG13	2.01	0.41
7:A:1405:C:H2'	7:A:1406:G:C8	2.55	0.41
8:B:207:ILE:HD12	8:B:207:ILE:N	2.30	0.41
13:G:144:MET:HE2	13:G:144:MET:HB2	1.78	0.41
15:I:15:SER:OG	15:I:70:GLY:HA3	2.20	0.41
17:K:69:ARG:HB2	17:K:69:ARG:HH11	1.83	0.41
20:N:31:ILE:HD11	20:N:45:VAL:HG23	2.01	0.41
28:a:6:A:H2'	28:a:7:G:C8	2.55	0.41
28:a:445:C:H2'	28:a:446:G:O4'	2.19	0.41
28:a:887:U:O2'	28:a:889:C:OP2	2.27	0.41
28:a:1319:C:O2'	28:a:1320:C:H5'	2.20	0.41
28:a:1444:G:C4	28:a:1445:G:C8	3.07	0.41
7:A:546:A:P	10:D:69:GLU:HB3	2.60	0.41
7:A:548:G:O2'	7:A:549:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1118:U:H1'	7:A:1180:A:C5	2.55	0.41
7:A:1120:C:H2'	7:A:1121:U:C6	2.55	0.41
7:A:1227:C:H41	19:M:103:LYS:HG3	1.84	0.41
7:A:1510:C:C2'	7:A:1511:G:H5'	2.50	0.41
7:A:1511:G:HO2'	7:A:1512:C:H5	1.61	0.41
10:D:121:LYS:HG2	10:D:131:ASN:HB3	2.02	0.41
12:F:53:LYS:HE2	12:F:53:LYS:HB2	1.65	0.41
15:I:21:ILE:HD12	15:I:21:ILE:O	2.20	0.41
28:a:12:U:O2	28:a:2626:C:H4'	2.20	0.41
28:a:325:G:O6	56:a:6214:SPD:H32	2.20	0.41
28:a:575:A:OP2	28:a:2499:C:O2'	2.38	0.41
28:a:710:U:C2	28:a:711:G:C8	3.09	0.41
28:a:993:G:OP2	43:p:51:ARG:NH2	2.48	0.41
28:a:1499:C:C2	28:a:1500:G:C8	3.08	0.41
28:a:1506:U:H2'	28:a:1507:C:C6	2.55	0.41
28:a:2773:C:H2'	28:a:2774:C:H6	1.84	0.41
33:f:48:LYS:O	33:f:52:ASN:OD1	2.38	0.41
52:y:11:ARG:HB2	52:y:54:MET:HB2	2.01	0.41
7:A:105:G:N2	7:A:379:C:O3'	2.54	0.41
7:A:235:C:H2'	7:A:236:A:C8	2.55	0.41
7:A:468:A:N3	7:A:468:A:H2'	2.36	0.41
7:A:592:G:H2'	7:A:593:U:C6	2.55	0.41
7:A:635:A:H2'	7:A:636:U:C6	2.55	0.41
7:A:814:A:H4'	7:A:1512:C:H5'	2.01	0.41
9:C:47:LEU:HD11	9:C:87:LEU:HD21	2.02	0.41
12:F:19:PRO:O	12:F:23:GLU:HG2	2.21	0.41
15:I:41:ARG:O	15:I:45:ARG:NH1	2.54	0.41
15:I:94:LEU:HD12	15:I:94:LEU:HA	1.92	0.41
18:L:74:LEU:HD11	18:L:80:ILE:HG21	2.01	0.41
21:O:26:GLU:HG2	21:O:81:LEU:HD13	2.02	0.41
28:a:871:U:OP1	39:l:5:LYS:HG2	2.20	0.41
28:a:2567:G:H2'	28:a:2568:U:C6	2.55	0.41
7:A:258:A:H2'	7:A:259:G:C8	2.56	0.41
7:A:374:A:O2'	7:A:375:U:OP1	2.37	0.41
7:A:504:C:C2	7:A:542:G:N2	2.88	0.41
7:A:677:U:H3	7:A:713:G:H22	1.69	0.41
7:A:904:U:H2'	7:A:905:U:C6	2.56	0.41
7:A:1184:U:O2'	7:A:1186:G:OP2	2.38	0.41
9:C:111:LEU:O	9:C:204:LYS:NZ	2.52	0.41
10:D:4:TYR:OH	10:D:7:PRO:O	2.25	0.41
10:D:170:TRP:CD2	10:D:186:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:157:ARG:NH1	14:H:99:LEU:O	2.53	0.41
18:L:30:LYS:HE2	18:L:59:ASN:HD22	1.85	0.41
28:a:158:U:H2'	28:a:159:G:C8	2.55	0.41
28:a:304:U:H2'	28:a:305:C:C6	2.56	0.41
28:a:793:A:OP2	28:a:2071:A:O2'	2.36	0.41
28:a:819:A:H5"	28:a:973:A:N1	2.35	0.41
28:a:1268:A:H2'	28:a:1269:A:O4'	2.20	0.41
7:A:88:U:H2'	7:A:89:C:C6	2.55	0.41
7:A:414:A:C4	7:A:415:A:C8	3.09	0.41
7:A:663:A:H5'	7:A:836:G:OP1	2.20	0.41
7:A:1360:C:OP2	20:N:75:ARG:NH1	2.47	0.41
14:H:13:ARG:HD2	14:H:27:MET:HB3	2.03	0.41
26:T:26:SER:O	26:T:30:THR:HG22	2.21	0.41
26:T:28:MET:HE1	26:T:67:ILE:HG21	2.03	0.41
28:a:139:U:C4	46:s:1:MET:HE3	2.56	0.41
28:a:172:A:H2'	28:a:173:A:C8	2.56	0.41
28:a:286:U:C2	28:a:287:G:C8	3.09	0.41
28:a:1495:A:H2'	28:a:1496:A:C8	2.56	0.41
28:a:1682:G:OP2	28:a:1699:G:N2	2.49	0.41
28:a:1839:G:C2	28:a:1840:G:C8	3.08	0.41
28:a:2262:U:H2'	28:a:2263:C:H6	1.86	0.41
28:a:2303:G:O2'	33:f:121:SER:O	2.38	0.41
29:b:39:A:C2	29:b:44:G:C2	3.09	0.41
32:e:171:ASP:OD2	32:e:171:ASP:C	2.64	0.41
41:n:77:ALA:HB1	41:n:81:ARG:HH11	1.86	0.41
46:s:67:VAL:HG22	46:s:76:ARG:HD2	2.02	0.41
7:A:546:A:H4'	7:A:549:C:OP1	2.20	0.41
8:B:15:HIS:HB3	8:B:43:LEU:HD21	2.01	0.41
9:C:21:THR:O	9:C:21:THR:OG1	2.33	0.41
15:I:118:LEU:HD22	15:I:124:ARG:HG3	2.02	0.41
28:a:354:A:H2'	28:a:355:U:O4'	2.20	0.41
28:a:547:A:H4'	28:a:548:G:O4'	2.21	0.41
28:a:2700:A:H2'	28:a:2701:U:C6	2.56	0.41
34:g:94:TYR:HA	34:g:106:SER:O	2.21	0.41
37:j:63:VAL:HG12	37:j:107:LEU:HD21	2.03	0.41
7:A:767:A:O2'	7:A:1525:G:N3	2.48	0.41
7:A:1033:G:H2'	7:A:1034:G:O4'	2.21	0.41
7:A:1251:A:H2'	7:A:1252:G:C8	2.56	0.41
28:a:703:U:H2'	28:a:704:G:O4'	2.20	0.41
28:a:722:A:H2'	28:a:723:C:C6	2.56	0.41
28:a:1138:G:N2	36:i:108:MET:SD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2282:G:H4'	28:a:2389:G:O2'	2.20	0.41
28:a:2723:C:H2'	28:a:2724:U:O4'	2.21	0.41
56:a:6211:SPD:H72	56:a:6211:SPD:H41	1.82	0.41
29:b:45:A:C4	29:b:46:A:C8	3.09	0.41
33:f:4:LEU:HG	33:f:101:GLU:HB2	2.03	0.41
33:f:114:PHE:HZ	33:f:176:PRO:HB2	1.86	0.41
34:g:9:VAL:CG2	34:g:50:LEU:HB2	2.50	0.41
38:k:110:VAL:HB	38:k:127:VAL:HG22	2.02	0.41
7:A:62:U:OP1	7:A:385:C:O2'	2.38	0.41
7:A:461:A:H2'	7:A:462:G:H8	1.86	0.41
7:A:584:G:H2'	7:A:585:G:H8	1.86	0.41
7:A:751:U:H2'	7:A:752:G:O4'	2.20	0.41
7:A:764:C:N3	7:A:765:G:N7	2.68	0.41
7:A:920:U:H2'	7:A:921:U:C6	2.56	0.41
9:C:51:SER:O	9:C:51:SER:OG	2.31	0.41
10:D:105:MET:HG2	10:D:171:LEU:HD13	2.03	0.41
12:F:71:ILE:HD13	12:F:71:ILE:HA	1.87	0.41
15:I:24:GLY:N	15:I:60:LYS:O	2.38	0.41
16:J:48:ARG:HD3	20:N:101:TRP:CZ3	2.56	0.41
16:J:71:LEU:HD12	16:J:72:ARG:N	2.35	0.41
17:K:67:ALA:HB2	17:K:96:THR:HG23	2.02	0.41
17:K:81:ASN:HB3	17:K:106:ARG:HH21	1.84	0.41
17:K:126:LYS:HD3	17:K:126:LYS:HA	1.93	0.41
27:U:59:LYS:HE3	27:U:59:LYS:HB2	1.73	0.41
28:a:947:A:H2'	28:a:948:C:C6	2.56	0.41
28:a:1038:G:H2'	28:a:1039:A:C8	2.56	0.41
28:a:1874:C:H2'	28:a:1875:G:O4'	2.21	0.41
28:a:1932:A:H2'	28:a:1933:G:O4'	2.20	0.41
28:a:2896:C:H2'	28:a:2897:U:C6	2.56	0.41
34:g:89:LEU:HD11	34:g:96:ALA:HB2	2.03	0.41
40:m:54:LEU:HD23	40:m:66:ALA:HB2	2.02	0.41
41:n:79:ALA:O	41:n:83:LEU:HD22	2.21	0.41
45:r:41:LYS:HE3	53:z:22:LEU:HD11	2.02	0.41
48:u:51:GLN:HB2	48:u:57:TYR:OH	2.21	0.41
7:A:440:C:C2	7:A:441:A:C8	3.09	0.41
7:A:981:U:H2'	7:A:982:U:C5	2.56	0.41
7:A:1010:G:H2'	7:A:1011:C:H6	1.86	0.41
7:A:1033:G:N7	7:A:1034:G:H1'	2.35	0.41
7:A:1310:G:C6	7:A:1330:A:N1	2.89	0.41
10:D:70:ARG:HG2	10:D:70:ARG:NH1	2.35	0.41
10:D:105:MET:SD	10:D:180:GLY:HA3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:118:VAL:O	10:D:131:ASN:HA	2.20	0.41
10:D:168:PRO:HB3	10:D:170:TRP:CZ3	2.56	0.41
11:E:13:GLU:HB3	11:E:39:VAL:HG22	2.02	0.41
12:F:7:VAL:HG22	12:F:61:LEU:HG	2.03	0.41
13:G:50:LEU:HD23	13:G:50:LEU:HA	1.85	0.41
13:G:57:SER:OG	13:G:60:GLU:HB2	2.21	0.41
18:L:10:LYS:HA	18:L:11:PRO:HD3	1.90	0.41
19:M:83:LEU:HA	19:M:83:LEU:HD23	1.83	0.41
25:S:3:ARG:HH11	25:S:10:PHE:HB2	1.85	0.41
26:T:8:LYS:H	26:T:8:LYS:HG3	1.66	0.41
28:a:634:C:H2'	28:a:635:C:C6	2.55	0.41
28:a:721:A:H2'	28:a:722:A:C8	2.55	0.41
28:a:1328:A:O2'	28:a:1329:U:H2'	2.20	0.41
28:a:1928:A:H2'	28:a:1929:G:O4'	2.21	0.41
28:a:2644:G:O2'	28:a:2645:G:H5'	2.20	0.41
28:a:2676:C:P	37:j:31:ARG:HH22	2.42	0.41
35:h:34:GLY:C	35:h:36:ALA:H	2.28	0.41
37:j:90:ASN:OD1	37:j:90:ASN:N	2.53	0.41
52:y:3:LYS:HE3	52:y:3:LYS:HB2	1.73	0.41
7:A:174:A:C5	7:A:175:C:C5	3.09	0.40
7:A:363:A:C6	18:L:28:PRO:HD2	2.57	0.40
7:A:539:A:H2'	7:A:540:G:C8	2.56	0.40
7:A:859:G:H2'	7:A:860:A:H8	1.85	0.40
7:A:971:G:P	7:A:1232:G:H21	2.43	0.40
7:A:1245:G:H2'	7:A:1246:U:H6	1.86	0.40
7:A:1372:G:O3'	15:I:71:GLY:HA3	2.21	0.40
10:D:163:GLU:HA	10:D:163:GLU:OE2	2.20	0.40
28:a:207:A:H2'	28:a:208:C:O4'	2.21	0.40
28:a:579:G:H2'	28:a:580:U:C6	2.56	0.40
28:a:677:A:O2'	28:a:2071:A:H5'	2.21	0.40
28:a:686:U:H6	28:a:788:A:N1	2.19	0.40
28:a:1028:A:OP2	28:a:1126:A:N6	2.46	0.40
28:a:1301:A:H2	28:a:1626:A:H2	1.69	0.40
28:a:1734:G:C2	28:a:1735:A:C5	3.09	0.40
28:a:2514:U:H2'	28:a:2515:C:C6	2.56	0.40
28:a:2545:G:H2'	28:a:2546:U:O4'	2.20	0.40
7:A:79:G:H2'	7:A:80:G:C8	2.55	0.40
7:A:222:U:H2'	7:A:223:A:C8	2.55	0.40
7:A:458:U:H5'	7:A:459:U:OP2	2.21	0.40
7:A:908:A:H2'	7:A:909:A:C8	2.56	0.40
7:A:1512:C:H2'	7:A:1513:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:118:GLU:HG3	8:B:119:THR:N	2.34	0.40
9:C:86:LYS:HG2	9:C:86:LYS:H	1.75	0.40
9:C:189:ALA:HB3	9:C:196:ILE:HB	2.02	0.40
18:L:56:ARG:NE	18:L:62:GLU:OE2	2.52	0.40
28:a:39:G:H2'	28:a:40:U:C6	2.56	0.40
28:a:534:U:H2'	28:a:535:G:H8	1.86	0.40
28:a:541:A:H2'	28:a:542:C:C6	2.57	0.40
28:a:825:A:H2'	28:a:826:U:O4'	2.22	0.40
28:a:1181:U:H2'	28:a:1182:G:C8	2.56	0.40
28:a:1589:U:H2'	28:a:1590:A:H8	1.86	0.40
28:a:1685:C:H2'	28:a:1686:C:H6	1.86	0.40
47:t:14:LEU:O	47:t:19:LYS:HG3	2.21	0.40
7:A:40:C:C5	7:A:402:G:N2	2.85	0.40
12:F:14:GLN:N	12:F:14:GLN:OE1	2.54	0.40
17:K:123:PRO:HD2	27:U:38:TYR:CD1	2.57	0.40
19:M:55:THR:O	19:M:59:GLU:HG2	2.21	0.40
20:N:47:LYS:HD3	20:N:47:LYS:C	2.46	0.40
28:a:978:G:O4'	28:a:1001:A:H2	2.04	0.40
28:a:2743:U:O2'	34:g:153:ARG:NH1	2.55	0.40
28:a:2884:U:C2	53:z:50:ARG:HD3	2.56	0.40
30:c:16:VAL:HG22	30:c:206:GLY:HA3	2.03	0.40
36:i:135:GLN:CA	36:i:135:GLN:HE21	2.34	0.40
7:A:4:U:HO2'	7:A:5:U:P	2.41	0.40
7:A:81:A:O5'	7:A:81:A:H8	2.05	0.40
7:A:309:A:H2'	7:A:310:G:H8	1.87	0.40
7:A:925:G:C2	7:A:927:G:C8	3.10	0.40
7:A:979:C:O2	20:N:59:ARG:NH1	2.53	0.40
7:A:1033:G:N2	7:A:1033:G:OP2	2.52	0.40
7:A:1119:C:H2'	7:A:1120:C:H6	1.86	0.40
7:A:1309:U:OP2	19:M:98:ARG:HD2	2.21	0.40
7:A:1484:A:H2	28:a:1959:G:N3	2.20	0.40
11:E:26:LYS:HE2	11:E:26:LYS:HB3	1.85	0.40
12:F:10:VAL:HB	12:F:58:HIS:HB3	2.02	0.40
17:K:80:LYS:HE2	17:K:80:LYS:HB2	1.93	0.40
20:N:73:PHE:CZ	20:N:78:GLY:HA2	2.56	0.40
25:S:30:PRO:HA	25:S:48:THR:HG23	2.04	0.40
26:T:4:ILE:O	26:T:8:LYS:HG3	2.21	0.40
28:a:534:U:H2'	28:a:535:G:C8	2.57	0.40
28:a:881:G:H2'	28:a:882:G:H8	1.86	0.40
28:a:984:A:H2'	28:a:984:A:N3	2.37	0.40
28:a:1149:G:H2'	28:a:1150:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2508:G:O2'	28:a:2554:U:O2'	2.36	0.40
28:a:2532:G:N2	28:a:2663:G:O2'	2.54	0.40
28:a:2745:C:H2'	28:a:2746:U:C6	2.56	0.40
39:l:133:LYS:HB3	39:l:133:LYS:NZ	2.35	0.40
7:A:35:G:H2'	7:A:36:C:C6	2.56	0.40
7:A:406:G:H8	7:A:406:G:OP2	2.05	0.40
7:A:1411:A:H2'	7:A:1412:C:H6	1.86	0.40
10:D:124:MET:SD	10:D:146:ARG:HG3	2.61	0.40
12:F:29:ILE:HD13	12:F:64:VAL:CG1	2.51	0.40
19:M:24:GLY:O	19:M:29:ARG:NH1	2.48	0.40
28:a:236:C:H2'	28:a:237:C:H6	1.87	0.40
28:a:541:A:C6	28:a:553:G:C6	3.10	0.40
28:a:594:U:H2'	28:a:595:C:C6	2.56	0.40
28:a:1125:G:C6	28:a:1126:A:N6	2.89	0.40
28:a:1130:U:C2	28:a:2025:C:H5"	2.57	0.40
28:a:1270:C:H5"	28:a:1271:G:O5'	2.21	0.40
28:a:1786:A:H1'	28:a:1938:A:N6	2.36	0.40
28:a:2373:G:H2'	28:a:2374:C:C6	2.57	0.40
28:a:2834:G:H2'	28:a:2879:A:H61	1.87	0.40
36:i:4:PHE:O	43:p:64:ARG:NH2	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
8	B	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
9	C	204/233 (88%)	191 (94%)	11 (5%)	2 (1%)	12	45
10	D	203/206 (98%)	186 (92%)	17 (8%)	0	100	100
11	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
12	F	101/135 (75%)	94 (93%)	7 (7%)	0	100	100
13	G	151/179 (84%)	139 (92%)	12 (8%)	0	100	100
14	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
15	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
16	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	45
17	K	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
18	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
19	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
20	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
21	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
23	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
24	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
25	S	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
30	c	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
31	d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	59
32	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
33	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
34	g	174/177 (98%)	157 (90%)	16 (9%)	1 (1%)	21	56
35	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
36	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
37	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
38	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
39	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
41	n	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
42	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
43	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
44	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
45	r	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
46	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
47	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
48	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
49	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
50	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
51	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
52	y	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
53	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5483/5913 (93%)	5243 (96%)	235 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	81	GLY
31	d	149	ASN
16	J	57	VAL
34	g	47	ASP
9	C	80	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	43 (94%)	3 (6%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	67
5	4	55/62 (89%)	54 (98%)	1 (2%)	51	74
8	B	186/199 (94%)	180 (97%)	6 (3%)	34	65
9	C	170/190 (90%)	166 (98%)	4 (2%)	43	70
10	D	172/173 (99%)	169 (98%)	3 (2%)	53	75
11	E	119/126 (94%)	117 (98%)	2 (2%)	53	75
12	F	90/116 (78%)	83 (92%)	7 (8%)	11	41
13	G	126/147 (86%)	116 (92%)	10 (8%)	11	40
14	H	104/105 (99%)	103 (99%)	1 (1%)	68	80
15	I	105/107 (98%)	98 (93%)	7 (7%)	15	47
16	J	86/90 (96%)	83 (96%)	3 (4%)	32	64
17	K	90/99 (91%)	86 (96%)	4 (4%)	25	59
18	L	102/103 (99%)	100 (98%)	2 (2%)	48	72
19	M	93/96 (97%)	87 (94%)	6 (6%)	15	47
20	N	83/84 (99%)	79 (95%)	4 (5%)	23	56
21	O	76/77 (99%)	76 (100%)	0	100	100
22	P	65/65 (100%)	64 (98%)	1 (2%)	57	76
23	Q	73/78 (94%)	68 (93%)	5 (7%)	14	46
24	R	57/65 (88%)	54 (95%)	3 (5%)	20	53
25	S	72/79 (91%)	71 (99%)	1 (1%)	59	77
26	T	65/66 (98%)	61 (94%)	4 (6%)	16	49
27	U	60/61 (98%)	58 (97%)	2 (3%)	33	65
30	c	216/218 (99%)	208 (96%)	8 (4%)	30	63
31	d	163/163 (100%)	157 (96%)	6 (4%)	30	63
32	e	165/165 (100%)	163 (99%)	2 (1%)	63	79
33	f	148/150 (99%)	145 (98%)	3 (2%)	48	72
34	g	137/138 (99%)	129 (94%)	8 (6%)	18	51
35	h	32/114 (28%)	32 (100%)	0	100	100
36	i	116/116 (100%)	114 (98%)	2 (2%)	53	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	j	104/104 (100%)	98 (94%)	6 (6%)	18 51
38	k	103/103 (100%)	100 (97%)	3 (3%)	37 67
39	l	107/107 (100%)	105 (98%)	2 (2%)	50 73
40	m	98/103 (95%)	96 (98%)	2 (2%)	48 72
41	n	86/87 (99%)	86 (100%)	0	100 100
42	o	99/100 (99%)	98 (99%)	1 (1%)	68 80
43	p	89/90 (99%)	88 (99%)	1 (1%)	65 79
44	q	84/84 (100%)	79 (94%)	5 (6%)	17 50
45	r	93/93 (100%)	92 (99%)	1 (1%)	65 79
46	s	80/84 (95%)	77 (96%)	3 (4%)	29 62
47	t	83/85 (98%)	81 (98%)	2 (2%)	43 70
48	u	78/78 (100%)	75 (96%)	3 (4%)	29 62
49	v	58/63 (92%)	57 (98%)	1 (2%)	53 75
50	w	67/68 (98%)	67 (100%)	0	100 100
51	x	54/55 (98%)	52 (96%)	2 (4%)	30 63
52	y	48/49 (98%)	48 (100%)	0	100 100
53	z	47/48 (98%)	45 (96%)	2 (4%)	26 59
All	All	4573/4826 (95%)	4430 (97%)	143 (3%)	36 66

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	37	LYS
1	0	42	VAL
1	0	54	ILE
4	3	28	SER
5	4	34	LEU
8	B	8	ASP
8	B	44	GLU
8	B	117	LEU
8	B	118	GLU
8	B	159	ASP
8	B	205	ASP
9	C	5	VAL
9	C	14	ILE
9	C	52	VAL

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Mol	Chain	Res	Type
9	C	154	SER
10	D	68	LEU
10	D	179	GLU
10	D	184	ARG
11	E	22	SER
11	E	147	MET
12	F	2	ARG
12	F	36	ILE
12	F	70	VAL
12	F	82	ASP
12	F	92	THR
12	F	94	HIS
12	F	97	THR
13	G	6	VAL
13	G	15	ASP
13	G	31	MET
13	G	32	VAL
13	G	33	ASP
13	G	50	LEU
13	G	52	GLN
13	G	57	SER
13	G	75	VAL
13	G	116	MET
14	H	90	ASP
15	I	34	SER
15	I	58	VAL
15	I	87	LEU
15	I	88	MET
15	I	92	GLU
15	I	105	THR
15	I	111	VAL
16	J	80	THR
16	J	98	VAL
16	J	100	ILE
17	K	46	THR
17	K	85	MET
17	K	111	THR
17	K	114	THR
18	L	20	ASN
18	L	90	LEU
19	M	16	VAL
19	M	50	GLU

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Mol	Chain	Res	Type
19	M	73	ILE
19	M	89	LEU
19	M	93	ARG
19	M	104	THR
20	N	30	ILE
20	N	58	SER
20	N	82	ILE
20	N	97	LYS
22	P	63	GLN
23	Q	13	VAL
23	Q	26	GLU
23	Q	33	ILE
23	Q	42	THR
23	Q	68	SER
24	R	26	ILE
24	R	30	LYS
24	R	47	THR
25	S	13	LEU
26	T	3	ASN
26	T	28	MET
26	T	80	THR
26	T	85	LYS
27	U	4	ILE
27	U	42	THR
30	c	36	LYS
30	c	38	SER
30	c	39	LYS
30	c	72	ASP
30	c	146	MET
30	c	225	MET
30	c	251	GLN
30	c	257	THR
31	d	18	ASP
31	d	39	ASP
31	d	40	LEU
31	d	96	ILE
31	d	110	THR
31	d	186	LEU
32	e	110	SER
32	e	165	HIS
33	f	57	LEU
33	f	146	VAL

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Mol	Chain	Res	Type
33	f	152	LEU
34	g	10	VAL
34	g	36	THR
34	g	43	VAL
34	g	72	LEU
34	g	90	VAL
34	g	127	THR
34	g	169	VAL
34	g	176	LYS
36	i	17	VAL
36	i	135	GLN
37	j	13	ASN
37	j	45	GLU
37	j	47	ILE
37	j	58	LEU
37	j	76	VAL
37	j	104	THR
38	k	7	SER
38	k	42	SER
38	k	55	MET
39	l	7	THR
39	l	25	ASP
40	m	1	MET
40	m	98	LEU
42	o	73	VAL
43	p	51	ARG
44	q	1	MET
44	q	26	ASP
44	q	27	ILE
44	q	29	THR
44	q	72	VAL
45	r	86	MET
46	s	37	ASP
46	s	57	VAL
46	s	74	ILE
47	t	31	SER
47	t	83	VAL
48	u	7	GLU
48	u	62	THR
48	u	65	VAL
49	v	43	THR
51	x	30	MET

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Mol	Chain	Res	Type
51	x	58	ASN
53	z	9	THR
53	z	36	GLU

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

Mol	Chain	Res	Type
1	0	26	ASN
8	B	178	ASN
9	C	69	HIS
9	C	139	GLN
9	C	190	HIS
10	D	198	HIS
11	E	97	GLN
11	E	122	ASN
12	F	58	HIS
14	H	4	GLN
14	H	67	GLN
17	K	119	ASN
21	O	40	GLN
23	Q	9	GLN
26	T	13	GLN
26	T	52	ASN
30	c	25	HIS
30	c	53	HIS
30	c	90	ASN
31	d	173	GLN
32	e	136	GLN
33	f	5	HIS
34	g	73	ASN
35	h	11	ASN
36	i	135	GLN
38	k	104	GLN
39	l	3	GLN
41	n	104	GLN
47	t	45	HIS
48	u	49	ASN
50	w	36	HIS
51	x	31	GLN
52	y	20	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2748/2904 (94%)	324 (11%)	0
29	b	118/120 (98%)	13 (11%)	0
6	5	1/2 (50%)	1 (100%)	0
7	A	1517/1543 (98%)	310 (20%)	17 (1%)
All	All	4384/4569 (95%)	648 (14%)	17 (0%)

All (648) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
7	A	3	A
7	A	4	U
7	A	5	U
7	A	6	G
7	A	9	G
7	A	32	A
7	A	38	G
7	A	39	G
7	A	41	G
7	A	47	C
7	A	48	C
7	A	50	A
7	A	51	A
7	A	55	A
7	A	59	A
7	A	65	A
7	A	71	A
7	A	76	A
7	A	77	G
7	A	81	A
7	A	82	A
7	A	83	C
7	A	84	U
7	A	85	U
7	A	86	G
7	A	87	U
7	A	88	U
7	A	91	U
7	A	93	G
7	A	95	G
7	A	96	U

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Mol	Chain	Res	Type
7	A	100	G
7	A	121	U
7	A	130	A
7	A	131	A
7	A	136	C
7	A	142	G
7	A	143	A
7	A	144	G
7	A	149	A
7	A	167	G
7	A	168	G
7	A	173	U
7	A	177	G
7	A	181	A
7	A	182	A
7	A	183	C
7	A	187	G
7	A	194	C
7	A	197	A
7	A	204	G
7	A	215	C
7	A	220	G
7	A	240	G
7	A	245	U
7	A	247	G
7	A	251	G
7	A	266	G
7	A	267	C
7	A	280	C
7	A	289	G
7	A	295	C
7	A	319	G
7	A	321	A
7	A	328	C
7	A	344	A
7	A	351	G
7	A	352	C
7	A	354	G
7	A	356	A
7	A	363	A
7	A	365	U
7	A	367	U

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Mol	Chain	Res	Type
7	A	368	U
7	A	372	C
7	A	373	A
7	A	374	A
7	A	375	U
7	A	390	U
7	A	392	C
7	A	397	A
7	A	401	C
7	A	402	G
7	A	403	C
7	A	404	G
7	A	406	G
7	A	411	A
7	A	413	G
7	A	414	A
7	A	421	U
7	A	422	C
7	A	423	G
7	A	424	G
7	A	429	U
7	A	436	C
7	A	437	U
7	A	438	U
7	A	440	C
7	A	448	A
7	A	449	G
7	A	450	G
7	A	451	A
7	A	452	A
7	A	453	G
7	A	457	G
7	A	458	U
7	A	459	U
7	A	467	U
7	A	468	A
7	A	472	U
7	A	475	U
7	A	476	C
7	A	478	U
7	A	479	U
7	A	480	U

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Mol	Chain	Res	Type
7	A	481	G
7	A	484	G
7	A	486	U
7	A	487	A
7	A	489	C
7	A	496	A
7	A	497	G
7	A	499	A
7	A	501	C
7	A	509	A
7	A	511	C
7	A	512	U
7	A	518	C
7	A	521	G
7	A	524	G
7	A	527	G7M
7	A	530	G
7	A	531	U
7	A	532	A
7	A	539	A
7	A	543	U
7	A	545	C
7	A	547	A
7	A	549	C
7	A	559	A
7	A	564	C
7	A	572	A
7	A	573	A
7	A	576	C
7	A	577	G
7	A	578	C
7	A	588	G
7	A	602	A
7	A	607	A
7	A	610	G
7	A	614	U
7	A	621	A
7	A	626	A
7	A	628	G
7	A	633	G
7	A	650	G
7	A	653	A

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Mol	Chain	Res	Type
7	A	665	A
7	A	670	G
7	A	687	A
7	A	703	G
7	A	721	G
7	A	723	U
7	A	724	G
7	A	734	G
7	A	743	A
7	A	747	A
7	A	749	A
7	A	755	A
7	A	765	G
7	A	766	A
7	A	774	G
7	A	777	A
7	A	781	A
7	A	793	U
7	A	794	A
7	A	799	G
7	A	815	A
7	A	817	C
7	A	819	A
7	A	821	G
7	A	829	G
7	A	832	G
7	A	851	G
7	A	872	A
7	A	878	A
7	A	884	U
7	A	889	A
7	A	890	G
7	A	914	A
7	A	918	A
7	A	926	G
7	A	927	G
7	A	934	C
7	A	958	A
7	A	960	U
7	A	961	U
7	A	965	U
7	A	966	2MG

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Mol	Chain	Res	Type
7	A	969	A
7	A	975	A
7	A	976	G
7	A	977	A
7	A	984	C
7	A	992	U
7	A	993	G
7	A	994	A
7	A	1004	A
7	A	1008	U
7	A	1010	G
7	A	1017	C
7	A	1021	G
7	A	1027	C
7	A	1029	U
7	A	1030	U
7	A	1031	C
7	A	1032	G
7	A	1033	G
7	A	1034	G
7	A	1035	A
7	A	1036	G
7	A	1039	C
7	A	1042	A
7	A	1044	A
7	A	1065	U
7	A	1066	C
7	A	1067	A
7	A	1094	G
7	A	1095	U
7	A	1101	A
7	A	1122	U
7	A	1123	G
7	A	1124	U
7	A	1134	C
7	A	1136	U
7	A	1137	A
7	A	1138	A
7	A	1139	U
7	A	1140	G
7	A	1141	G
7	A	1160	U

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Mol	Chain	Res	Type
7	A	1169	U
7	A	1170	A
7	A	1172	A
7	A	1175	G
7	A	1182	G
7	A	1183	G
7	A	1185	G
7	A	1197	A
7	A	1198	A
7	A	1201	C
7	A	1214	A
7	A	1215	C
7	A	1228	A
7	A	1229	C
7	A	1237	A
7	A	1239	A
7	A	1242	G
7	A	1247	A
7	A	1248	U
7	A	1261	G
7	A	1271	G
7	A	1281	A
7	A	1286	A
7	A	1288	A
7	A	1298	G
7	A	1301	G
7	A	1303	C
7	A	1306	G
7	A	1313	G
7	A	1318	C
7	A	1321	C
7	A	1332	G
7	A	1333	A
7	A	1336	U
7	A	1337	C
7	A	1347	A
7	A	1354	G
7	A	1362	G
7	A	1364	A
7	A	1365	U
7	A	1371	G
7	A	1379	C

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Mol	Chain	Res	Type
7	A	1380	G
7	A	1392	U
7	A	1398	C
7	A	1405	C
7	A	1409	A
7	A	1420	G
7	A	1433	G
7	A	1442	A
7	A	1453	C
7	A	1454	G
7	A	1460	A
7	A	1488	G
7	A	1493	A
7	A	1495	G
7	A	1498	G
7	A	1507	U
7	A	1508	A
7	A	1511	G
7	A	1512	C
7	A	1518	G
7	A	1519	MA6
7	A	1520	MA6
7	A	1530	G
7	A	1531	G
7	A	1532	A
7	A	1534	C
7	A	1535	A
28	a	10	A
28	a	23	G
28	a	34	U
28	a	45	G
28	a	51	G
28	a	71	A
28	a	74	A
28	a	75	G
28	a	84	A
28	a	101	A
28	a	102	U
28	a	103	A
28	a	118	A
28	a	119	A
28	a	120	U

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Mol	Chain	Res	Type
28	a	125	A
28	a	139	U
28	a	142	A
28	a	163	C
28	a	164	C
28	a	181	A
28	a	196	A
28	a	199	A
28	a	216	A
28	a	222	A
28	a	223	A
28	a	248	G
28	a	264	C
28	a	265	A
28	a	272	A
28	a	274	C
28	a	278	A
28	a	282	A
28	a	285	G
28	a	289	G
28	a	294	A
28	a	311	A
28	a	329	G
28	a	330	A
28	a	345	A
28	a	361	G
28	a	362	A
28	a	386	G
28	a	396	G
28	a	405	U
28	a	411	G
28	a	412	A
28	a	435	C
28	a	481	G
28	a	491	G
28	a	504	A
28	a	505	A
28	a	509	C
28	a	529	A
28	a	530	G
28	a	532	A
28	a	545	U

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Mol	Chain	Res	Type
28	a	546	U
28	a	548	G
28	a	549	G
28	a	563	A
28	a	573	U
28	a	575	A
28	a	588	U
28	a	603	A
28	a	615	U
28	a	627	A
28	a	637	A
28	a	645	C
28	a	647	G
28	a	654	A
28	a	655	A
28	a	685	A
28	a	686	U
28	a	717	C
28	a	728	G
28	a	730	A
28	a	738	G
28	a	747	5MU
28	a	764	A
28	a	765	C
28	a	775	G
28	a	776	G
28	a	782	A
28	a	784	G
28	a	785	G
28	a	792	A
28	a	805	G
28	a	812	C
28	a	827	U
28	a	828	U
28	a	845	A
28	a	846	U
28	a	847	U
28	a	857	G
28	a	859	G
28	a	869	G
28	a	883	G
28	a	884	U

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Mol	Chain	Res	Type
28	a	888	C
28	a	890	C
28	a	891	G
28	a	895	U
28	a	896	A
28	a	897	C
28	a	898	C
28	a	907	G
28	a	910	A
28	a	931	U
28	a	946	C
28	a	961	C
28	a	973	A
28	a	974	G
28	a	983	A
28	a	989	G
28	a	996	A
28	a	1005	C
28	a	1012	U
28	a	1013	C
28	a	1025	G
28	a	1033	U
28	a	1045	C
28	a	1046	A
28	a	1047	G
28	a	1048	A
28	a	1108	U
28	a	1111	A
28	a	1112	G
28	a	1115	G
28	a	1116	G
28	a	1122	G
28	a	1128	G
28	a	1132	U
28	a	1133	A
28	a	1135	C
28	a	1142	A
28	a	1171	G
28	a	1206	G
28	a	1212	G
28	a	1236	G
28	a	1250	G

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Mol	Chain	Res	Type
28	a	1253	A
28	a	1256	G
28	a	1271	G
28	a	1272	A
28	a	1273	U
28	a	1300	G
28	a	1301	A
28	a	1343	G
28	a	1352	U
28	a	1365	A
28	a	1378	A
28	a	1379	U
28	a	1383	A
28	a	1386	C
28	a	1395	A
28	a	1403	A
28	a	1416	G
28	a	1417	C
28	a	1419	A
28	a	1427	A
28	a	1428	C
28	a	1452	G
28	a	1453	A
28	a	1482	G
28	a	1493	C
28	a	1497	U
28	a	1508	A
28	a	1510	G
28	a	1515	A
28	a	1524	G
28	a	1529	G
28	a	1534	U
28	a	1535	A
28	a	1536	C
28	a	1537	G
28	a	1566	A
28	a	1569	A
28	a	1578	U
28	a	1583	A
28	a	1584	U
28	a	1585	C
28	a	1608	A

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Mol	Chain	Res	Type
28	a	1613	G
28	a	1647	U
28	a	1648	U
28	a	1649	G
28	a	1674	G
28	a	1715	G
28	a	1729	U
28	a	1730	C
28	a	1732	C
28	a	1733	G
28	a	1738	G
28	a	1764	C
28	a	1773	A
28	a	1782	U
28	a	1800	C
28	a	1801	A
28	a	1808	A
28	a	1816	C
28	a	1829	A
28	a	1847	A
28	a	1848	A
28	a	1858	A
28	a	1870	C
28	a	1871	A
28	a	1872	A
28	a	1873	G
28	a	1905	C
28	a	1906	G
28	a	1907	G
28	a	1913	A
28	a	1914	C
28	a	1929	G
28	a	1930	G
28	a	1937	A
28	a	1955	U
28	a	1966	A
28	a	1967	C
28	a	1970	A
28	a	1971	U
28	a	1972	G
28	a	1991	U
28	a	1993	U

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Mol	Chain	Res	Type
28	a	2023	C
28	a	2031	A
28	a	2033	A
28	a	2043	C
28	a	2055	C
28	a	2056	G
28	a	2060	A
28	a	2061	G
28	a	2062	A
28	a	2069	G7M
28	a	2093	G
28	a	2198	A
28	a	2203	U
28	a	2204	G
28	a	2211	A
28	a	2225	A
28	a	2238	G
28	a	2239	G
28	a	2266	A
28	a	2279	G
28	a	2283	C
28	a	2287	A
28	a	2288	A
28	a	2305	U
28	a	2308	G
28	a	2319	G
28	a	2322	A
28	a	2325	G
28	a	2333	A
28	a	2334	U
28	a	2336	A
28	a	2345	G
28	a	2347	C
28	a	2361	G
28	a	2377	A
28	a	2383	G
28	a	2385	C
28	a	2402	U
28	a	2403	C
28	a	2406	A
28	a	2422	C
28	a	2425	A

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Mol	Chain	Res	Type
28	a	2429	G
28	a	2435	A
28	a	2440	C
28	a	2441	U
28	a	2445	2MG
28	a	2448	A
28	a	2469	A
28	a	2470	G
28	a	2476	A
28	a	2478	A
28	a	2491	U
28	a	2498	OMC
28	a	2502	G
28	a	2505	G
28	a	2518	A
28	a	2520	C
28	a	2529	G
28	a	2535	G
28	a	2547	A
28	a	2566	A
28	a	2567	G
28	a	2573	C
28	a	2585	U
28	a	2586	U
28	a	2602	A
28	a	2609	U
28	a	2613	U
28	a	2615	U
28	a	2629	U
28	a	2630	G
28	a	2661	G
28	a	2689	U
28	a	2690	U
28	a	2714	G
28	a	2726	A
28	a	2727	A
28	a	2732	G
28	a	2733	A
28	a	2744	G
28	a	2748	A
28	a	2752	C
28	a	2765	A

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Mol	Chain	Res	Type
28	a	2778	A
28	a	2780	G
28	a	2798	U
28	a	2818	U
28	a	2820	A
28	a	2821	A
28	a	2835	A
28	a	2836	U
28	a	2849	U
28	a	2861	U
28	a	2873	A
28	a	2883	A
28	a	2884	U
28	a	2891	U
28	a	2899	A
29	b	13	G
29	b	24	G
29	b	30	C
29	b	35	C
29	b	36	C
29	b	41	G
29	b	42	C
29	b	56	G
29	b	67	G
29	b	89	U
29	b	90	C
29	b	99	A
29	b	109	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	4	U
7	A	86	G
7	A	374	A
7	A	410	G
7	A	436	C
7	A	488	C
7	A	495	A
7	A	500	G
7	A	548	G
7	A	606	G

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Mol	Chain	Res	Type
7	A	722	G
7	A	765	G
7	A	960	U
7	A	1031	C
7	A	1035	A
7	A	1506	G
7	A	1533	U

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

39 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	$\#\|Z\| > 2$
31	MEQ	d	150	31	8,9,10	0.89	0	5,10,12	0.56	0
28	OMG	a	2251	28	23,26,27	0.85	2 (8%)	32,38,41	1.96	10 (31%)
28	G7M	a	2069	28	23,26,27	0.64	0	34,39,42	0.96	1 (2%)
28	OMU	a	2552	28	19,22,23	1.24	3 (15%)	25,31,34	1.98	6 (24%)
28	5MU	a	747	28	19,22,23	1.33	4 (21%)	27,32,35	2.24	7 (25%)
7	2MG	A	966	7	23,26,27	0.80	0	33,38,41	2.25	12 (36%)
28	2MA	a	2503	28,55	22,25,26	1.31	4 (18%)	32,37,40	2.02	7 (21%)
7	2MG	A	1208	7	23,26,27	0.80	0	33,38,41	2.16	9 (27%)
28	5MC	a	1962	28	19,22,23	1.55	2 (10%)	26,32,35	1.23	3 (11%)
7	5MC	A	1408	7	19,22,23	1.62	2 (10%)	26,32,35	1.10	3 (11%)
28	OMC	a	2498	28,55	19,22,23	1.11	1 (5%)	25,31,34	1.22	2 (8%)
28	PSU	a	2504	28	18,21,22	1.14	3 (16%)	21,30,33	2.03	4 (19%)
28	PSU	a	2605	28	18,21,22	1.26	3 (16%)	21,30,33	2.01	4 (19%)
28	PSU	a	2457	28	18,21,22	1.22	4 (22%)	21,30,33	2.17	5 (23%)
28	H2U	a	2449	28	18,21,22	0.64	0	19,30,33	1.11	1 (5%)
28	2MG	a	1835	28	23,26,27	0.87	1 (4%)	33,38,41	2.30	13 (39%)
7	G7M	A	527	7	23,26,27	0.58	0	34,39,42	0.95	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	5MC	A	967	7	19,22,23	1.41	2 (10%)	26,32,35	1.11	1 (3%)
7	PSU	A	516	7,55	18,21,22	1.16	3 (16%)	21,30,33	2.01	5 (23%)
28	PSU	a	1911	28	18,21,22	1.07	3 (16%)	21,30,33	2.03	4 (19%)
28	2MG	a	2445	28	23,26,27	0.93	2 (8%)	33,38,41	2.22	13 (39%)
28	3TD	a	1915	28	19,22,23	1.19	3 (15%)	23,32,35	1.92	3 (13%)
28	6MZ	a	1618	28	22,25,26	1.14	2 (9%)	29,36,39	2.28	9 (31%)
39	MS6	l	82	39	5,7,8	0.62	0	2,7,9	1.17	0
28	5MU	a	1939	28	19,22,23	1.33	4 (21%)	27,32,35	2.25	6 (22%)
28	PSU	a	2580	28	18,21,22	1.26	4 (22%)	21,30,33	2.12	5 (23%)
18	D2T	L	89	18	8,9,10	2.70	1 (12%)	6,11,13	1.43	1 (16%)
28	1MG	a	745	28	23,26,27	1.13	1 (4%)	33,39,42	1.81	6 (18%)
28	PSU	a	2604	28	18,21,22	1.20	3 (16%)	21,30,33	2.03	4 (19%)
7	MA6	A	1519	7	23,26,27	2.58	5 (21%)	33,38,41	2.84	7 (21%)
28	PSU	a	955	28	18,21,22	1.23	3 (16%)	21,30,33	2.03	4 (19%)
7	4OC	A	1403	7	20,23,24	2.35	4 (20%)	25,32,35	0.99	1 (4%)
28	PSU	a	746	28,55	18,21,22	1.13	3 (16%)	21,30,33	1.94	3 (14%)
28	PSU	a	1917	28	18,21,22	1.10	2 (11%)	21,30,33	1.91	4 (19%)
39	4D4	l	81	39	9,11,12	0.89	0	7,13,15	1.63	2 (28%)
7	MA6	A	1520	7	23,26,27	2.56	5 (21%)	33,38,41	2.81	7 (21%)
28	6MZ	a	2030	28	22,25,26	1.16	2 (9%)	29,36,39	2.37	10 (34%)
7	UR3	A	1499	7	19,22,23	3.79	6 (31%)	26,32,35	4.61	10 (38%)
7	2MG	A	1517	7	23,26,27	0.85	1 (4%)	33,38,41	2.28	12 (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
31	MEQ	d	150	31	-	2/8/9/11	-
28	OMG	a	2251	28	-	0/9/27/28	0/3/3/3
28	G7M	a	2069	28	-	0/7/25/26	0/3/3/3
28	OMU	a	2552	28	-	2/9/27/28	0/2/2/2
28	5MU	a	747	28	-	0/7/25/26	0/2/2/2
7	2MG	A	966	7	-	2/9/27/28	0/3/3/3
28	2MA	a	2503	28,55	-	1/7/25/26	0/3/3/3
7	2MG	A	1208	7	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	5MC	a	1962	28	-	0/7/25/26	0/2/2/2
7	5MC	A	1408	7	-	1/7/25/26	0/2/2/2
28	OMC	a	2498	28,55	-	0/9/27/28	0/2/2/2
28	PSU	a	2504	28	-	2/7/25/26	0/2/2/2
28	PSU	a	2605	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2457	28	-	0/7/25/26	0/2/2/2
28	H2U	a	2449	28	-	1/7/38/39	0/2/2/2
28	2MG	a	1835	28	-	2/9/27/28	0/3/3/3
7	G7M	A	527	7	-	2/7/25/26	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
7	PSU	A	516	7,55	-	0/7/25/26	0/2/2/2
28	PSU	a	1911	28	-	0/7/25/26	0/2/2/2
28	2MG	a	2445	28	-	2/9/27/28	0/3/3/3
28	3TD	a	1915	28	-	2/7/25/26	0/2/2/2
28	6MZ	a	1618	28	-	2/9/27/28	0/3/3/3
39	MS6	l	82	39	-	4/4/6/8	-
28	5MU	a	1939	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2580	28	-	2/7/25/26	0/2/2/2
18	D2T	L	89	18	-	1/7/12/14	-
28	1MG	a	745	28	-	0/7/25/26	0/3/3/3
28	PSU	a	2604	28	-	0/7/25/26	0/2/2/2
7	MA6	A	1519	7	-	0/11/29/30	0/3/3/3
28	PSU	a	955	28	-	0/7/25/26	0/2/2/2
7	4OC	A	1403	7	-	1/9/29/30	0/2/2/2
28	PSU	a	746	28,55	-	1/7/25/26	0/2/2/2
28	PSU	a	1917	28	-	0/7/25/26	0/2/2/2
39	4D4	l	81	39	-	2/11/12/14	-
7	MA6	A	1520	7	-	2/11/29/30	0/3/3/3
28	6MZ	a	2030	28	-	1/9/27/28	0/3/3/3
7	UR3	A	1499	7	-	0/7/25/26	0/2/2/2
7	2MG	A	1517	7	-	0/9/27/28	0/3/3/3

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1499	UR3	C2-N1	13.61	1.57	1.38
7	A	1403	4OC	O2-C2	8.31	1.39	1.23
7	A	1520	MA6	C5-N7	7.60	1.53	1.39
7	A	1519	MA6	C5-N7	7.57	1.52	1.39
18	L	89	D2T	CB-CA	-6.99	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1520	MA6	C8-N9	-5.92	1.27	1.37
7	A	1519	MA6	C8-N9	-5.88	1.27	1.37
7	A	1499	UR3	C6-N1	5.79	1.51	1.38
7	A	1519	MA6	C4-N9	-5.58	1.26	1.37
7	A	1408	5MC	C5-C4	-5.50	1.39	1.44
7	A	1520	MA6	C4-N9	-5.38	1.26	1.37
28	a	1962	5MC	C5-C4	-5.34	1.40	1.44
7	A	1499	UR3	C2-N3	5.21	1.49	1.39
7	A	967	5MC	C5-C4	-4.45	1.40	1.44
7	A	1403	4OC	C4-N4	4.24	1.44	1.36
28	a	2503	2MA	C6-N1	3.61	1.39	1.35
7	A	1403	4OC	C2-N3	3.52	1.43	1.36
7	A	1499	UR3	C6-C5	-3.49	1.27	1.35
28	a	1618	6MZ	C6-N6	3.36	1.38	1.34
28	a	2552	OMU	C2-N1	-3.29	1.33	1.38
28	a	2030	6MZ	C6-N6	3.20	1.37	1.34
28	a	1939	5MU	C2-N1	-3.18	1.33	1.38
28	a	747	5MU	C2-N1	-3.17	1.33	1.38
28	a	2503	2MA	C5-N7	-3.15	1.33	1.39
7	A	1519	MA6	C6-N6	3.12	1.45	1.36
7	A	1408	5MC	C2-N1	-3.11	1.33	1.40
28	a	745	1MG	C6-N1	-3.06	1.34	1.40
7	A	1519	MA6	C8-N7	3.05	1.37	1.31
7	A	1520	MA6	C6-N6	3.03	1.45	1.36
28	a	2498	OMC	C2-N1	-3.00	1.33	1.40
7	A	1520	MA6	C8-N7	2.93	1.37	1.31
7	A	967	5MC	C2-N1	-2.90	1.34	1.40
28	a	1962	5MC	C2-N1	-2.79	1.34	1.40
28	a	2580	PSU	O4'-C1'	-2.77	1.40	1.43
28	a	1915	3TD	C4-N3	-2.73	1.34	1.40
7	A	516	PSU	O4'-C1'	-2.65	1.40	1.43
28	a	2605	PSU	C2-N3	-2.62	1.33	1.37
28	a	747	5MU	C4-C5	-2.60	1.40	1.44
28	a	2605	PSU	C4-N3	-2.60	1.34	1.38
28	a	2552	OMU	C4-N3	-2.52	1.34	1.38
28	a	1939	5MU	C4-C5	-2.50	1.40	1.44
28	a	1939	5MU	C4-N3	-2.49	1.34	1.38
28	a	1915	3TD	C4-C5	-2.47	1.41	1.47
28	a	747	5MU	C4-N3	-2.47	1.34	1.38
28	a	2604	PSU	C4-N3	-2.46	1.34	1.38
28	a	2457	PSU	C4-N3	-2.45	1.34	1.38
28	a	955	PSU	C2-N1	-2.43	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2504	PSU	C4-N3	-2.41	1.34	1.38
28	a	1939	5MU	C2-N3	-2.38	1.33	1.38
28	a	955	PSU	C4-N3	-2.35	1.34	1.38
28	a	746	PSU	C4-N3	-2.34	1.34	1.38
28	a	2580	PSU	C4-N3	-2.32	1.34	1.38
28	a	747	5MU	C2-N3	-2.28	1.34	1.38
28	a	2580	PSU	C2-N1	-2.28	1.33	1.36
28	a	955	PSU	C2-N3	-2.27	1.33	1.37
7	A	1499	UR3	O4-C4	-2.27	1.18	1.23
28	a	1917	PSU	C2-N1	-2.27	1.33	1.36
28	a	2503	2MA	C5-C6	2.26	1.47	1.41
28	a	2605	PSU	C2-N1	-2.25	1.33	1.36
28	a	2552	OMU	C2-N3	-2.25	1.34	1.38
28	a	2604	PSU	C2-N3	-2.24	1.33	1.37
28	a	2457	PSU	C2-N1	-2.24	1.33	1.36
7	A	516	PSU	C4-N3	-2.24	1.34	1.38
28	a	2445	2MG	C6-N1	-2.23	1.34	1.38
28	a	2504	PSU	C2-N3	-2.22	1.33	1.37
7	A	1499	UR3	O2-C2	-2.22	1.18	1.22
28	a	1835	2MG	C6-N1	-2.22	1.34	1.38
28	a	2030	6MZ	C5-N7	-2.21	1.35	1.39
28	a	1618	6MZ	C5-N7	-2.21	1.35	1.39
28	a	2457	PSU	O4'-C1'	-2.17	1.40	1.43
28	a	746	PSU	O4'-C1'	-2.16	1.40	1.43
28	a	2604	PSU	C2-N1	-2.15	1.33	1.36
28	a	1911	PSU	C4-N3	-2.15	1.34	1.38
28	a	1917	PSU	C4-N3	-2.14	1.34	1.38
28	a	746	PSU	C2-N3	-2.13	1.34	1.37
7	A	1403	4OC	C6-C5	2.13	1.40	1.35
28	a	2580	PSU	C2-N3	-2.12	1.34	1.37
28	a	2504	PSU	C2-N1	-2.11	1.33	1.36
28	a	2457	PSU	C2-N3	-2.11	1.34	1.37
28	a	2445	2MG	C5-N7	-2.08	1.34	1.39
28	a	2251	OMG	C6-N1	-2.07	1.35	1.38
28	a	2251	OMG	C5-N7	-2.06	1.34	1.39
28	a	1915	3TD	C2-N1	-2.04	1.34	1.37
28	a	2503	2MA	C2-N3	-2.04	1.30	1.34
7	A	1517	2MG	C6-N1	-2.04	1.35	1.38
28	a	1911	PSU	C2-N3	-2.02	1.34	1.37
7	A	516	PSU	C2-N1	-2.01	1.34	1.36
28	a	1911	PSU	C2-N1	-2.00	1.34	1.36

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1499	UR3	C4-N3-C2	-14.64	112.80	124.58
7	A	1499	UR3	C6-N1-C2	-13.94	110.41	121.80
7	A	1519	MA6	C4-N9-C8	13.71	120.13	105.74
7	A	1520	MA6	C4-N9-C8	13.49	119.90	105.74
7	A	1499	UR3	C5-C4-N3	7.79	125.30	115.04
28	a	1835	2MG	C2-N3-C4	7.44	121.31	112.00
7	A	1517	2MG	C2-N3-C4	7.44	121.31	112.00
7	A	1208	2MG	C2-N3-C4	7.23	121.05	112.00
7	A	966	2MG	C2-N3-C4	7.14	120.93	112.00
28	a	2445	2MG	C2-N3-C4	6.95	120.69	112.00
28	a	1915	3TD	N1-C2-N3	6.86	121.12	116.13
28	a	2503	2MA	C5-C4-N3	-6.30	120.55	127.18
28	a	2457	PSU	N1-C2-N3	5.94	121.43	115.17
28	a	2580	PSU	N1-C2-N3	5.88	121.38	115.17
28	a	1939	5MU	C4-N3-C2	-5.80	119.74	127.34
28	a	745	1MG	C5-C4-N3	-5.77	119.20	128.39
28	a	2504	PSU	N1-C2-N3	5.74	121.22	115.17
28	a	1911	PSU	N1-C2-N3	5.67	121.15	115.17
28	a	747	5MU	C4-N3-C2	-5.66	119.92	127.34
28	a	955	PSU	N1-C2-N3	5.65	121.12	115.17
28	a	1618	6MZ	C5-C4-N3	-5.58	119.03	126.72
28	a	2251	OMG	C5-C4-N3	-5.51	119.61	128.39
28	a	2604	PSU	N1-C2-N3	5.51	120.98	115.17
28	a	1835	2MG	C5-C4-N3	-5.49	119.66	128.39
28	a	2605	PSU	N1-C2-N3	5.48	120.95	115.17
28	a	2030	6MZ	C9-N6-C6	-5.47	117.78	122.85
28	a	746	PSU	N1-C2-N3	5.41	120.88	115.17
7	A	1517	2MG	C5-C4-N3	-5.39	119.82	128.39
7	A	516	PSU	N1-C2-N3	5.38	120.85	115.17
7	A	1208	2MG	C5-C4-N3	-5.38	119.83	128.39
28	a	1917	PSU	N1-C2-N3	5.33	120.79	115.17
28	a	2552	OMU	C4-N3-C2	-5.30	120.03	126.61
28	a	2445	2MG	C5-C4-N3	-5.29	119.97	128.39
28	a	2030	6MZ	C5-C4-N3	-5.22	119.53	126.72
7	A	966	2MG	C5-C4-N3	-5.21	120.09	128.39
28	a	2251	OMG	C2-N3-C4	5.12	121.12	112.30
28	a	747	5MU	N3-C2-N1	5.10	121.53	114.89
28	a	2552	OMU	N3-C2-N1	5.09	121.52	114.89
28	a	1939	5MU	N3-C2-N1	5.04	121.46	114.89
28	a	1618	6MZ	C9-N6-C6	-4.91	118.30	122.85
28	a	2457	PSU	C4-N3-C2	-4.89	119.64	126.37
28	a	2503	2MA	N3-C4-N9	4.86	133.16	126.99
28	a	746	PSU	C4-N3-C2	-4.85	119.69	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	1939	5MU	C5-C4-N3	4.79	119.48	115.32
28	a	2605	PSU	C4-N3-C2	-4.71	119.88	126.37
28	a	1911	PSU	C4-N3-C2	-4.69	119.91	126.37
28	a	2504	PSU	C4-N3-C2	-4.63	120.00	126.37
28	a	1618	6MZ	N3-C4-N9	4.61	135.01	127.17
28	a	2604	PSU	C4-N3-C2	-4.59	120.04	126.37
28	a	2580	PSU	C4-N3-C2	-4.51	120.15	126.37
7	A	1499	UR3	C3U-N3-C4	4.51	124.12	117.87
28	a	955	PSU	C4-N3-C2	-4.47	120.21	126.37
7	A	516	PSU	C4-N3-C2	-4.39	120.33	126.37
28	a	747	5MU	C5-C4-N3	4.37	119.12	115.32
28	a	1939	5MU	O4-C4-C5	-4.34	119.95	124.92
28	a	747	5MU	O4-C4-C5	-4.32	119.97	124.92
7	A	1499	UR3	C1'-N1-C2	4.30	124.08	117.04
28	a	745	1MG	N9-C4-N3	4.26	134.47	125.95
28	a	1917	PSU	C4-N3-C2	-4.23	120.54	126.37
28	a	2030	6MZ	N3-C4-N9	4.20	134.32	127.17
28	a	745	1MG	C2-N3-C4	4.11	121.21	111.98
7	A	1519	MA6	N9-C8-N7	-4.09	108.14	113.94
28	a	1618	6MZ	N1-C2-N3	-4.08	122.40	128.58
7	A	1208	2MG	N9-C4-N3	4.07	134.09	125.95
28	a	2251	OMG	N9-C4-N3	4.06	134.08	125.95
28	a	2030	6MZ	C5-N7-C8	4.06	109.83	103.45
7	A	1520	MA6	N9-C8-N7	-4.06	108.18	113.94
28	a	1835	2MG	N9-C4-N3	3.99	133.94	125.95
7	A	1520	MA6	C4-C5-N7	-3.96	106.05	110.58
28	a	2445	2MG	N9-C4-N3	3.92	133.80	125.95
28	a	2030	6MZ	N1-C2-N3	-3.92	122.64	128.58
28	a	2445	2MG	C2-N1-C6	-3.90	119.84	124.55
28	a	2503	2MA	N6-C6-N1	3.89	122.28	117.03
28	a	1835	2MG	C2-N1-C6	-3.88	119.86	124.55
7	A	1517	2MG	N9-C4-N3	3.84	133.63	125.95
7	A	967	5MC	C5-C6-N1	-3.82	119.17	123.31
7	A	1519	MA6	C4-C5-N7	-3.81	106.22	110.58
7	A	1517	2MG	C2-N1-C6	-3.79	119.97	124.55
7	A	966	2MG	N9-C4-N3	3.77	133.50	125.95
7	A	966	2MG	C2-N1-C6	-3.75	120.01	124.55
28	a	1915	3TD	C4-N3-C2	-3.75	120.64	124.61
28	a	2503	2MA	C5-N7-C8	3.70	109.27	103.45
7	A	966	2MG	N1-C2-N2	3.69	120.32	116.56
28	a	1618	6MZ	C2-N3-C4	3.68	120.83	111.83
28	a	1939	5MU	C5-C6-N1	-3.68	119.32	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2457	PSU	O2-C2-N1	-3.65	119.03	122.79
28	a	2449	H2U	C5-C4-N3	-3.65	112.81	116.69
28	a	1962	5MC	C5-C6-N1	-3.63	119.37	123.31
28	a	1618	6MZ	C5-N7-C8	3.60	109.11	103.45
7	A	1517	2MG	N1-C2-N2	3.57	120.21	116.56
28	a	1835	2MG	N1-C2-N2	3.57	120.20	116.56
7	A	1520	MA6	C1'-N9-C8	-3.50	119.33	127.09
7	A	516	PSU	O2-C2-N1	-3.49	119.19	122.79
28	a	2030	6MZ	C2-N3-C4	3.45	120.27	111.83
28	a	2580	PSU	O2-C2-N1	-3.44	119.25	122.79
7	A	1408	5MC	C5-C6-N1	-3.43	119.59	123.31
7	A	1208	2MG	C2-N1-C6	-3.43	120.41	124.55
28	a	747	5MU	C5-C6-N1	-3.41	119.61	123.31
28	a	2030	6MZ	C4-C5-N7	-3.39	106.71	110.58
7	A	527	G7M	C8-N7-C5	-3.30	103.65	107.78
28	a	2498	OMC	CM2-O2'-C2'	-3.30	106.00	114.47
7	A	1499	UR3	C3U-N3-C2	3.30	123.08	117.33
28	a	2445	2MG	N1-C2-N2	3.29	119.92	116.56
28	a	2030	6MZ	N9-C8-N7	-3.28	109.29	113.94
28	a	955	PSU	O2-C2-N1	-3.23	119.45	122.79
7	A	1519	MA6	C1'-N9-C8	-3.23	119.93	127.09
28	a	2503	2MA	N9-C8-N7	-3.15	109.46	113.94
28	a	2552	OMU	C5-C4-N3	3.15	119.21	114.80
28	a	2604	PSU	O2-C2-N1	-3.15	119.54	122.79
28	a	1917	PSU	O2-C2-N1	-3.14	119.55	122.79
28	a	1911	PSU	O2-C2-N1	-3.12	119.57	122.79
39	l	81	4D4	NE-CZ-NH2	3.05	125.91	120.67
28	a	2552	OMU	CM2-O2'-C2'	-3.04	106.67	114.47
28	a	2069	G7M	C8-N7-C5	-3.03	104.00	107.78
28	a	2580	PSU	C6-N1-C2	-2.93	119.97	122.69
28	a	745	1MG	C8-N7-C5	2.91	109.45	104.26
28	a	2251	OMG	C2-N1-C6	-2.89	119.88	125.11
7	A	1519	MA6	C4-N9-C1'	-2.86	119.94	126.63
7	A	1520	MA6	C6-C5-N7	2.85	137.99	133.43
7	A	1519	MA6	C6-C5-N7	2.81	137.91	133.43
28	a	1915	3TD	C1'-C5-C4	2.79	121.85	117.61
28	a	1618	6MZ	C4-C5-N7	-2.79	107.39	110.58
28	a	955	PSU	C6-N1-C2	-2.79	120.11	122.69
28	a	2552	OMU	O4-C4-C5	-2.78	120.36	125.16
28	a	746	PSU	O2-C2-N1	-2.78	119.92	122.79
28	a	2445	2MG	C8-N7-C5	2.78	109.22	104.26
28	a	2498	OMC	O2-C2-N3	-2.78	117.94	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	966	2MG	C8-N7-C5	2.77	109.20	104.26
28	a	2552	OMU	O2-C2-N1	-2.77	119.19	122.80
28	a	1835	2MG	C8-N7-C5	2.76	109.17	104.26
28	a	1939	5MU	O2-C2-N1	-2.76	119.21	122.80
28	a	2251	OMG	CM2-O2'-C2'	-2.72	107.50	114.47
28	a	2251	OMG	C8-N7-C5	2.72	109.10	104.26
7	A	1519	MA6	C2-N1-C6	2.72	118.47	111.83
7	A	1208	2MG	C8-N7-C5	2.71	109.09	104.26
28	a	2445	2MG	CM2-N2-C2	-2.69	117.86	123.65
28	a	2605	PSU	O2-C2-N1	-2.68	120.02	122.79
28	a	2504	PSU	O2-C2-N1	-2.67	120.03	122.79
28	a	1618	6MZ	N9-C8-N7	-2.67	110.15	113.94
28	a	2503	2MA	C5-C6-N1	-2.66	114.76	118.90
7	A	1517	2MG	C8-N7-C5	2.66	108.99	104.26
28	a	2503	2MA	C4-C5-N7	-2.65	107.55	110.58
28	a	2030	6MZ	C6-C5-N7	2.64	135.31	132.43
28	a	747	5MU	O2-C2-N1	-2.63	119.37	122.80
7	A	1208	2MG	N1-C2-N2	2.60	119.22	116.56
7	A	1403	4OC	C6-C5-C4	2.59	120.12	117.00
28	a	1917	PSU	C6-N1-C2	-2.55	120.32	122.69
7	A	1499	UR3	O2-C2-N3	-2.54	117.81	121.33
7	A	1520	MA6	C4-N9-C1'	-2.51	120.76	126.63
28	a	2457	PSU	C6-N1-C2	-2.50	120.37	122.69
28	a	2504	PSU	C6-N1-C2	-2.47	120.40	122.69
7	A	1499	UR3	O4-C4-C5	-2.47	117.36	124.35
18	L	89	D2T	OD1-CG-CB	-2.44	117.34	122.44
7	A	1520	MA6	C2-N1-C6	2.42	117.75	111.83
7	A	516	PSU	C6-N1-C2	-2.42	120.45	122.69
7	A	966	2MG	CM2-N2-C2	-2.38	118.54	123.65
7	A	966	2MG	N2-C2-N3	-2.38	117.48	120.51
28	a	2445	2MG	O6-C6-C5	-2.32	120.40	126.53
7	A	1499	UR3	C6-C5-C4	2.32	125.17	120.73
28	a	1911	PSU	C6-N1-C2	-2.30	120.56	122.69
28	a	1835	2MG	CM2-N2-C2	-2.29	118.72	123.65
28	a	745	1MG	C4-C5-N7	-2.28	107.05	110.67
7	A	966	2MG	O6-C6-C5	-2.28	120.52	126.53
28	a	1835	2MG	O6-C6-C5	-2.27	120.54	126.53
28	a	2580	PSU	O4'-C1'-C2'	2.27	108.29	105.15
7	A	1517	2MG	C6-C5-N7	2.27	134.42	130.29
7	A	966	2MG	C6-C5-N7	2.26	134.40	130.29
28	a	2604	PSU	C6-N1-C2	-2.26	120.60	122.69
7	A	1517	2MG	CM2-N2-C2	-2.26	118.80	123.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	l	81	4D4	NH1-CZ-NE	-2.24	114.18	119.27
7	A	1408	5MC	C5-C4-N3	-2.24	119.46	121.75
7	A	1517	2MG	O6-C6-C5	-2.23	120.65	126.53
7	A	1208	2MG	O6-C6-C5	-2.22	120.67	126.53
7	A	516	PSU	O4'-C1'-C2'	2.22	108.22	105.15
7	A	1499	UR3	C1'-N1-C6	2.22	125.52	120.78
28	a	2251	OMG	O6-C6-C5	-2.21	120.69	126.53
28	a	745	1MG	C6-C5-N7	2.21	134.27	129.36
7	A	966	2MG	C4-C5-N7	-2.21	107.17	110.67
7	A	1517	2MG	C4-C5-N7	-2.18	107.22	110.67
28	a	1835	2MG	C4-C5-N7	-2.18	107.22	110.67
28	a	1835	2MG	C6-C5-N7	2.17	134.24	130.29
28	a	2445	2MG	N2-C2-N3	-2.17	117.75	120.51
28	a	2457	PSU	O4'-C1'-C2'	2.17	108.15	105.15
28	a	2030	6MZ	C4-N9-C8	2.16	108.00	105.74
28	a	1835	2MG	C5-C6-N1	2.14	118.70	113.25
7	A	1517	2MG	N2-C2-N3	-2.12	117.81	120.51
28	a	1962	5MC	O2-C2-N3	-2.11	119.00	122.33
28	a	2251	OMG	C4-C5-N7	-2.11	107.33	110.67
28	a	2445	2MG	C4-C5-N7	-2.10	107.34	110.67
7	A	1517	2MG	C5-C6-N1	2.08	118.56	113.25
28	a	1835	2MG	N2-C2-N3	-2.08	117.86	120.51
7	A	1408	5MC	O2-C2-N3	-2.08	119.06	122.33
28	a	2605	PSU	C6-N1-C2	-2.07	120.77	122.69
28	a	1962	5MC	C1'-N1-C6	-2.06	117.76	121.15
28	a	2445	2MG	N9-C8-N7	-2.05	109.61	113.40
28	a	2445	2MG	C5-C6-N1	2.04	118.45	113.25
7	A	966	2MG	N9-C8-N7	-2.03	109.63	113.40
28	a	1618	6MZ	C6-C5-N7	2.03	134.64	132.43
28	a	2251	OMG	C6-C5-N7	2.03	133.98	130.29
28	a	2251	OMG	C5-C6-N1	2.02	118.39	113.25
28	a	1835	2MG	N9-C8-N7	-2.01	109.67	113.40
28	a	747	5MU	C1'-N1-C2	2.01	121.21	117.59
7	A	1208	2MG	C6-C5-N7	2.01	133.95	130.29
7	A	527	G7M	C4-C5-N7	2.01	110.94	107.67
28	a	2445	2MG	C6-C5-N7	2.00	133.93	130.29
7	A	1208	2MG	C4-C5-N7	-2.00	107.50	110.67

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	966	2MG	O4'-C4'-C5'-O5'
7	A	1520	MA6	O4'-C4'-C5'-O5'
28	a	1915	3TD	O4'-C4'-C5'-O5'
39	l	82	MS6	CA-CB-CG-SD
7	A	527	G7M	C3'-C4'-C5'-O5'
28	a	1915	3TD	C3'-C4'-C5'-O5'
28	a	2445	2MG	C3'-C4'-C5'-O5'
28	a	2504	PSU	O4'-C4'-C5'-O5'
28	a	2445	2MG	O4'-C4'-C5'-O5'
28	a	2580	PSU	O4'-C4'-C5'-O5'
7	A	966	2MG	C3'-C4'-C5'-O5'
7	A	1520	MA6	C3'-C4'-C5'-O5'
31	d	150	MEQ	NE2-CD-CG-CB
31	d	150	MEQ	OE1-CD-CG-CB
7	A	527	G7M	O4'-C4'-C5'-O5'
28	a	2504	PSU	C3'-C4'-C5'-O5'
39	l	82	MS6	CB-CG-SD-CE
28	a	1835	2MG	O4'-C4'-C5'-O5'
28	a	1835	2MG	C3'-C4'-C5'-O5'
7	A	1403	4OC	O4'-C4'-C5'-O5'
39	l	82	MS6	N-CA-CB-CG
18	L	89	D2T	CG-CB-SB-CB1
28	a	1618	6MZ	N1-C6-N6-C9
39	l	81	4D4	NE-CD-CG-CB
28	a	2030	6MZ	O4'-C4'-C5'-O5'
7	A	1408	5MC	O4'-C4'-C5'-O5'
28	a	2503	2MA	O4'-C4'-C5'-O5'
39	l	81	4D4	CG-CD-NE-CZ
28	a	2552	OMU	C1'-C2'-O2'-CM2
28	a	2449	H2U	C4'-C5'-O5'-P
28	a	746	PSU	O4'-C1'-C5-C6
28	a	2552	OMU	C3'-C2'-O2'-CM2
28	a	2580	PSU	C3'-C4'-C5'-O5'
39	l	82	MS6	C-CA-CB-CG
28	a	1618	6MZ	C5-C6-N6-C9

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	d	150	MEQ	1	0
28	a	2251	OMG	1	0
28	a	2503	2MA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2445	2MG	1	0
28	a	1915	3TD	1	0
18	L	89	D2T	1	0
28	a	955	PSU	1	0
7	A	1403	4OC	1	0
28	a	2030	6MZ	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 327 ligands modelled in this entry, 310 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	SPD	a	6217	-	9,9,9	0.25	0	8,8,8	0.25	0
56	SPD	a	6220	-	9,9,9	0.28	0	8,8,8	0.32	0
56	SPD	a	6208	-	9,9,9	0.25	0	8,8,8	0.26	0
56	SPD	a	6212	-	9,9,9	0.28	0	8,8,8	0.29	0
56	SPD	a	6211	-	9,9,9	0.25	0	8,8,8	0.22	0
56	SPD	a	6213	-	9,9,9	0.25	0	8,8,8	0.26	0
56	SPD	a	6215	-	9,9,9	0.27	0	8,8,8	0.31	0
56	SPD	a	6214	-	9,9,9	0.28	0	8,8,8	0.24	0
56	SPD	a	6209	-	9,9,9	0.25	0	8,8,8	0.21	0
56	SPD	a	6218	-	9,9,9	0.26	0	8,8,8	0.43	0
56	SPD	a	6207	-	9,9,9	0.28	0	8,8,8	0.23	0
57	SPM	a	6221	-	13,13,13	0.35	0	12,12,12	0.94	0
56	SPD	a	6216	-	9,9,9	0.29	0	8,8,8	0.31	0
56	SPD	a	6219	-	9,9,9	0.27	0	8,8,8	0.34	0
56	SPD	a	6210	-	9,9,9	0.27	0	8,8,8	0.30	0
56	SPD	A	1691	-	9,9,9	0.25	0	8,8,8	0.26	0
56	SPD	A	1692	7	9,9,9	0.26	0	8,8,8	0.19	0

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
56	SPD	a	6217	-	-	2/7/7/7	-
56	SPD	a	6220	-	-	1/7/7/7	-
56	SPD	a	6208	-	-	3/7/7/7	-
56	SPD	a	6212	-	-	2/7/7/7	-
56	SPD	a	6211	-	-	4/7/7/7	-
56	SPD	a	6213	-	-	0/7/7/7	-
56	SPD	a	6215	-	-	4/7/7/7	-
56	SPD	a	6214	-	-	3/7/7/7	-
56	SPD	a	6209	-	-	2/7/7/7	-
56	SPD	a	6218	-	-	6/7/7/7	-
56	SPD	a	6207	-	-	4/7/7/7	-
57	SPM	a	6221	-	-	2/11/11/11	-
56	SPD	a	6216	-	-	3/7/7/7	-
56	SPD	a	6219	-	-	1/7/7/7	-
56	SPD	a	6210	-	-	1/7/7/7	-
56	SPD	A	1691	-	-	2/7/7/7	-
56	SPD	A	1692	7	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	A	1691	SPD	C3-C4-C5-N6
56	a	6207	SPD	C3-C4-C5-N6
56	a	6207	SPD	N6-C7-C8-C9
56	a	6208	SPD	N6-C7-C8-C9
56	a	6216	SPD	C3-C4-C5-N6
56	a	6209	SPD	C8-C7-N6-C5
56	a	6218	SPD	C4-C5-N6-C7
56	a	6218	SPD	C3-C4-C5-N6
56	A	1691	SPD	C2-C3-C4-C5
56	a	6216	SPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
56	a	6208	SPD	C7-C8-C9-N10
56	a	6210	SPD	C2-C3-C4-C5
56	a	6220	SPD	C2-C3-C4-C5
56	a	6218	SPD	N6-C7-C8-C9
56	a	6214	SPD	C8-C7-N6-C5
56	a	6217	SPD	C3-C4-C5-N6
56	a	6215	SPD	C4-C5-N6-C7
56	a	6214	SPD	N6-C7-C8-C9
56	a	6207	SPD	C7-C8-C9-N10
56	a	6207	SPD	N1-C2-C3-C4
56	a	6218	SPD	N1-C2-C3-C4
56	a	6216	SPD	C7-C8-C9-N10
56	a	6218	SPD	C7-C8-C9-N10
56	a	6212	SPD	N1-C2-C3-C4
56	A	1692	SPD	C8-C7-N6-C5
57	a	6221	SPM	C7-C6-N5-C4
56	a	6215	SPD	N6-C7-C8-C9
57	a	6221	SPM	C7-C8-C9-N10
56	a	6211	SPD	N6-C7-C8-C9
56	a	6214	SPD	N1-C2-C3-C4
56	a	6208	SPD	C4-C5-N6-C7
56	a	6215	SPD	C8-C7-N6-C5
56	a	6218	SPD	C8-C7-N6-C5
56	a	6211	SPD	C4-C5-N6-C7
56	A	1692	SPD	C4-C5-N6-C7
56	a	6211	SPD	C8-C7-N6-C5
56	a	6209	SPD	N6-C7-C8-C9
56	a	6217	SPD	C4-C5-N6-C7
56	a	6212	SPD	N6-C7-C8-C9
56	a	6219	SPD	C8-C7-N6-C5
56	a	6215	SPD	C3-C4-C5-N6
56	a	6211	SPD	C2-C3-C4-C5

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	a	6217	SPD	2	0
56	a	6208	SPD	3	0
56	a	6212	SPD	1	0
56	a	6211	SPD	2	0
56	a	6215	SPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	a	6214	SPD	3	0
56	a	6218	SPD	2	0
57	a	6221	SPM	1	0
56	a	6216	SPD	1	0
56	A	1691	SPD	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	A	3
28	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1914:C	O3'	1915:3TD	P	4.24
1	A	1402:G	O3'	1403:4OC	P	2.92
1	A	1498:G	O3'	1499:UR3	P	2.91
1	A	1518:G	O3'	1519:MA6	P	2.83

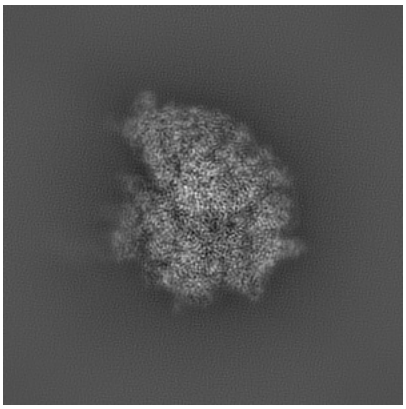
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-75650. These allow visual inspection of the internal detail of the map and identification of artifacts.

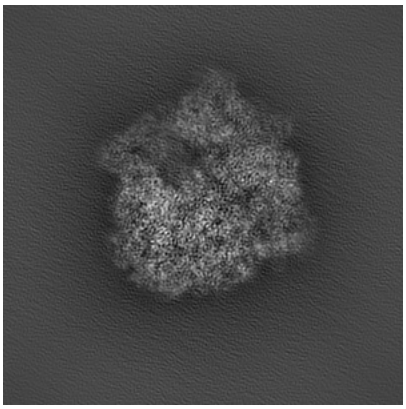
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

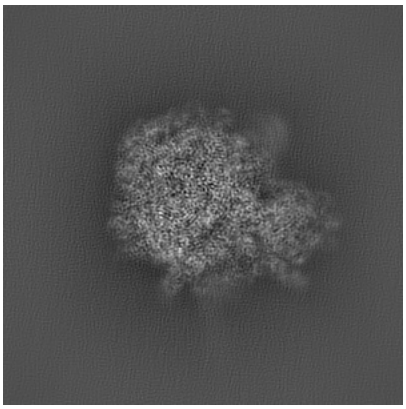
6.1.1 Primary map



X

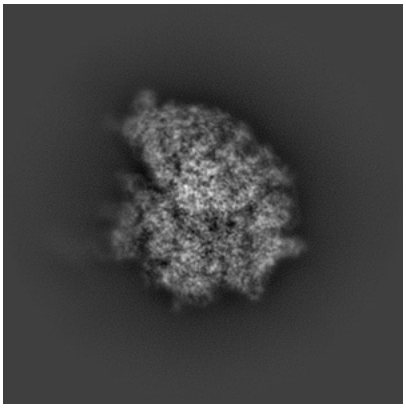


Y



Z

6.1.2 Raw map



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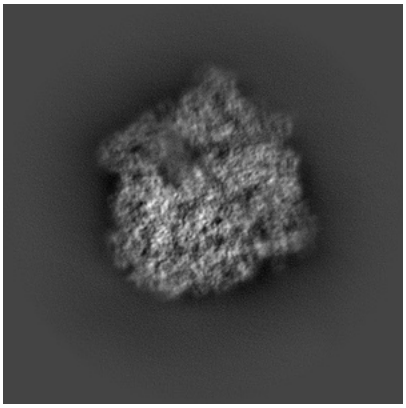
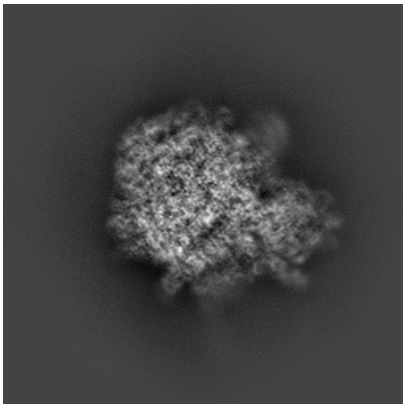


Y

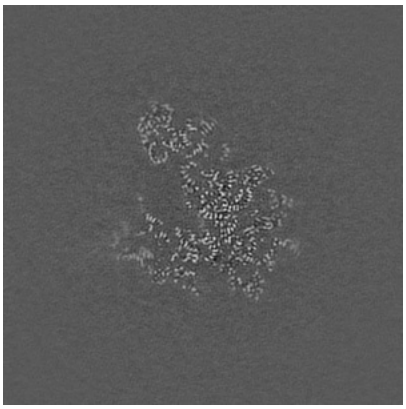


Z

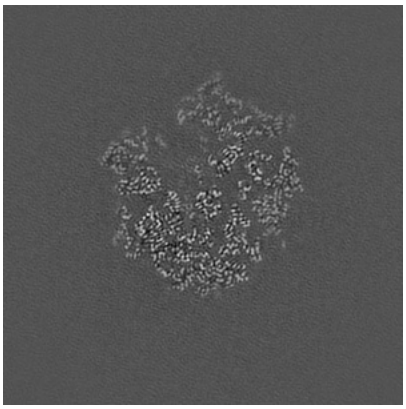
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

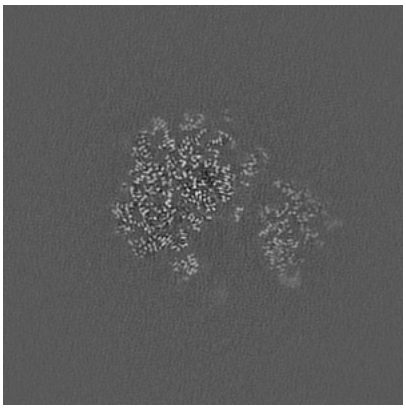
6.2.1 Primary map



X Index: 256

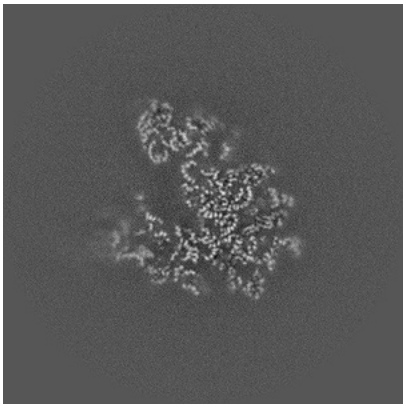


Y Index: 256



Z Index: 256

6.2.2 Raw map



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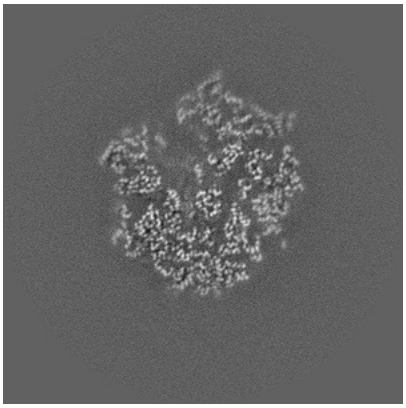
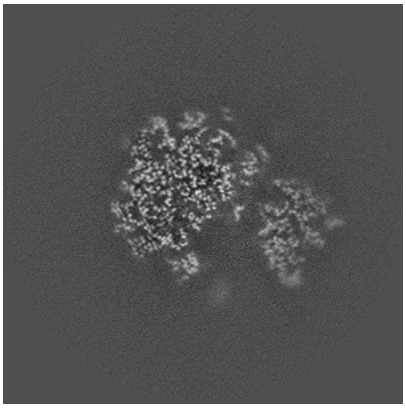


Y Index: 256

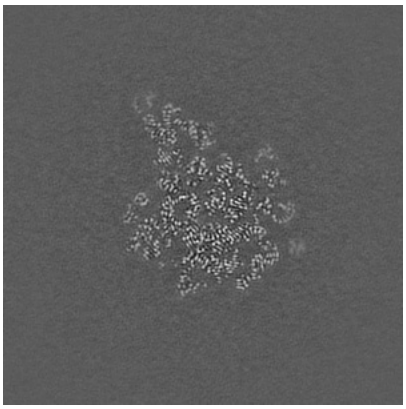


Z Index: 256

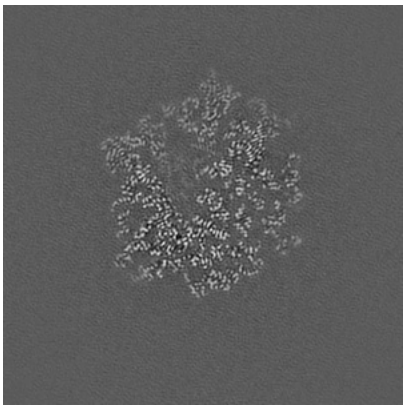
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

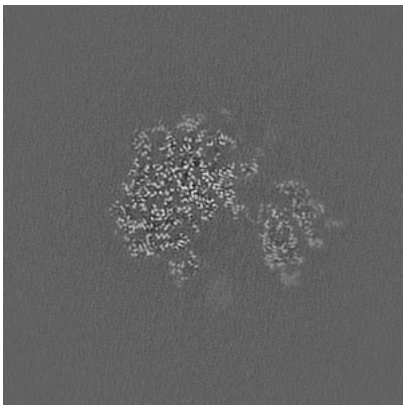
6.3.1 Primary map



X Index: 234

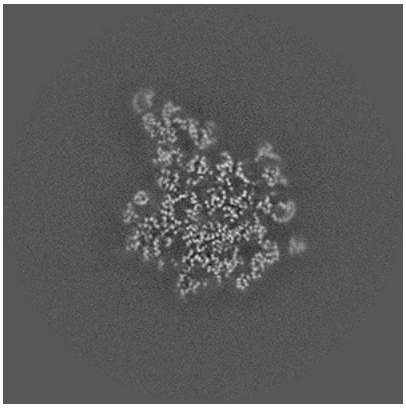


Y Index: 247

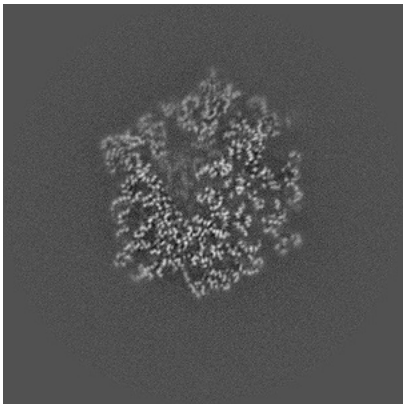


Z Index: 253

6.3.2 Raw map



X Index: 234



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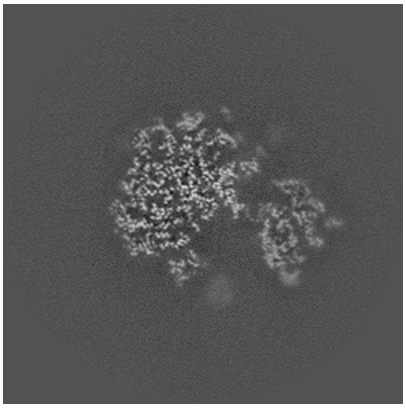
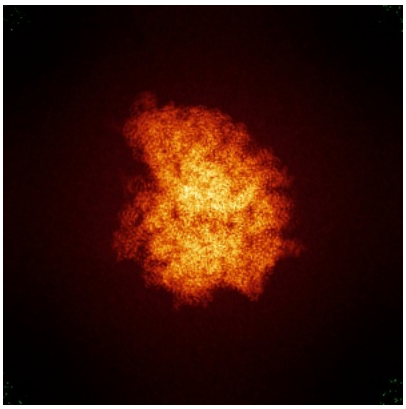


Z Index: 253

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



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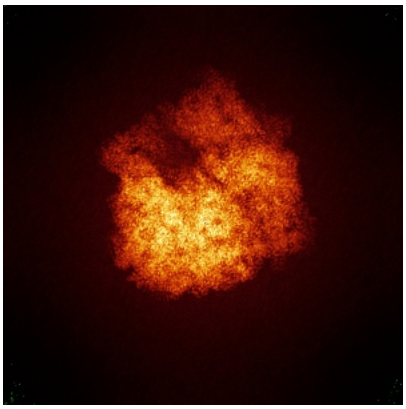

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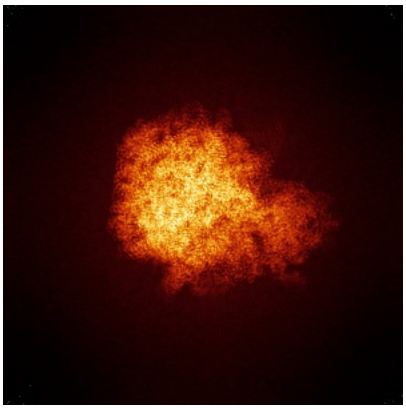
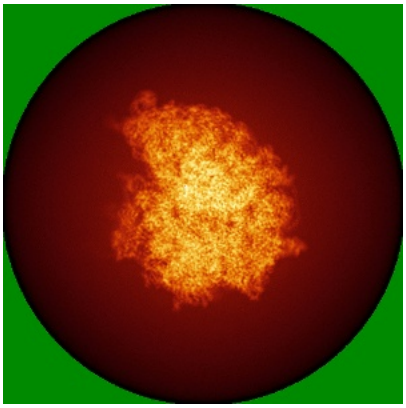
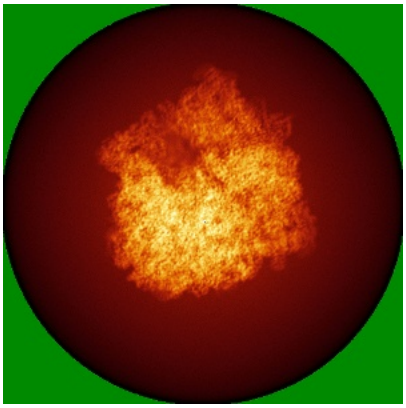


Z

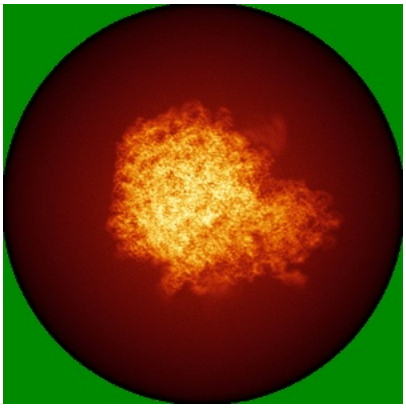
6.4.2 Raw map



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.

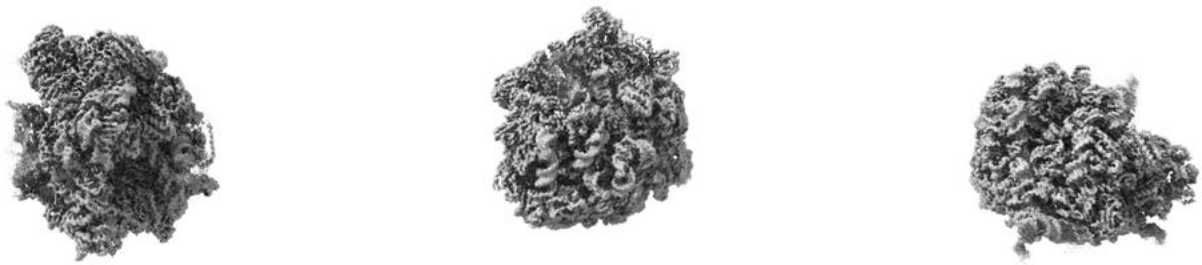
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. 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.

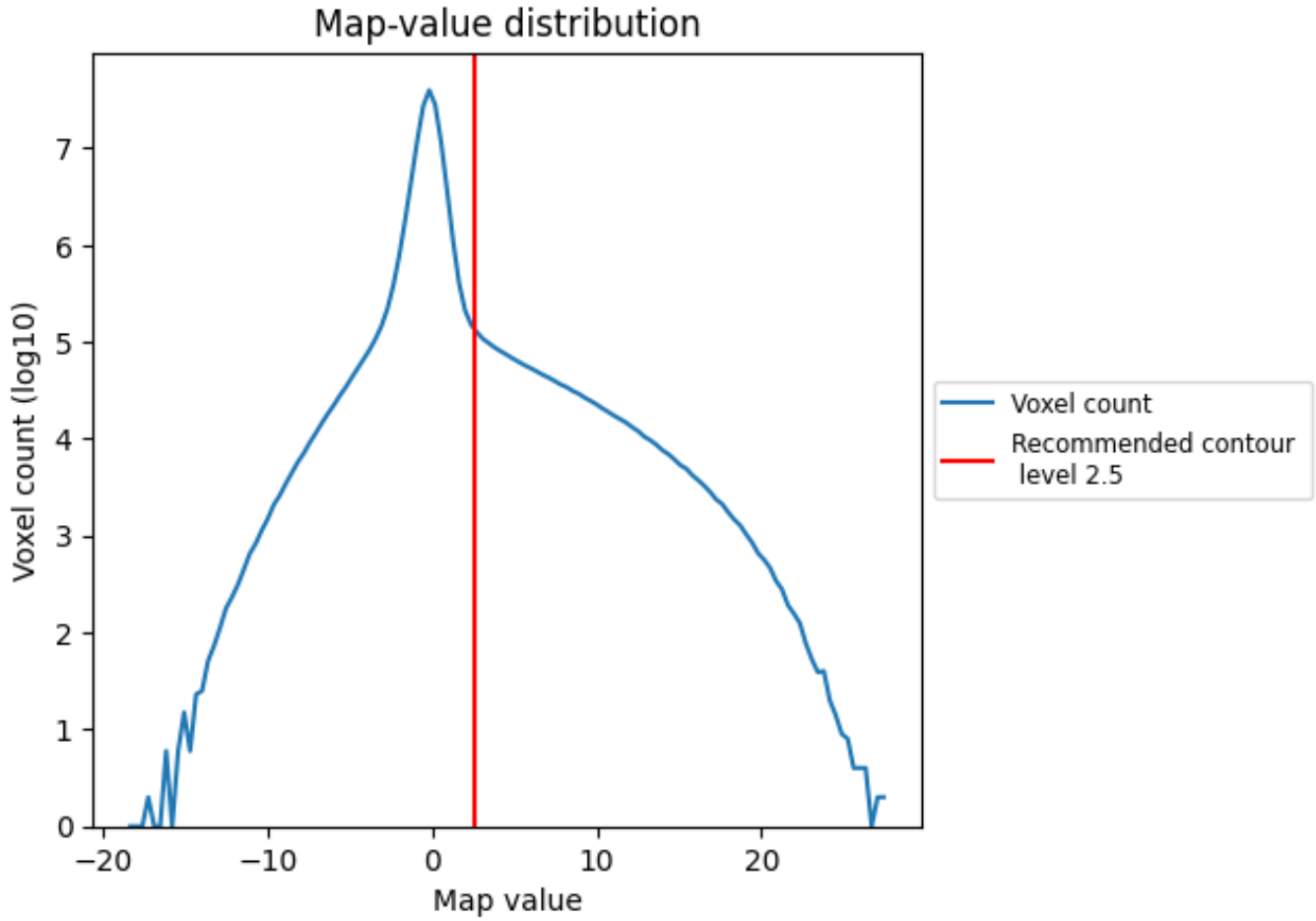
6.6 Mask visualisation (i)

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

7 Map analysis

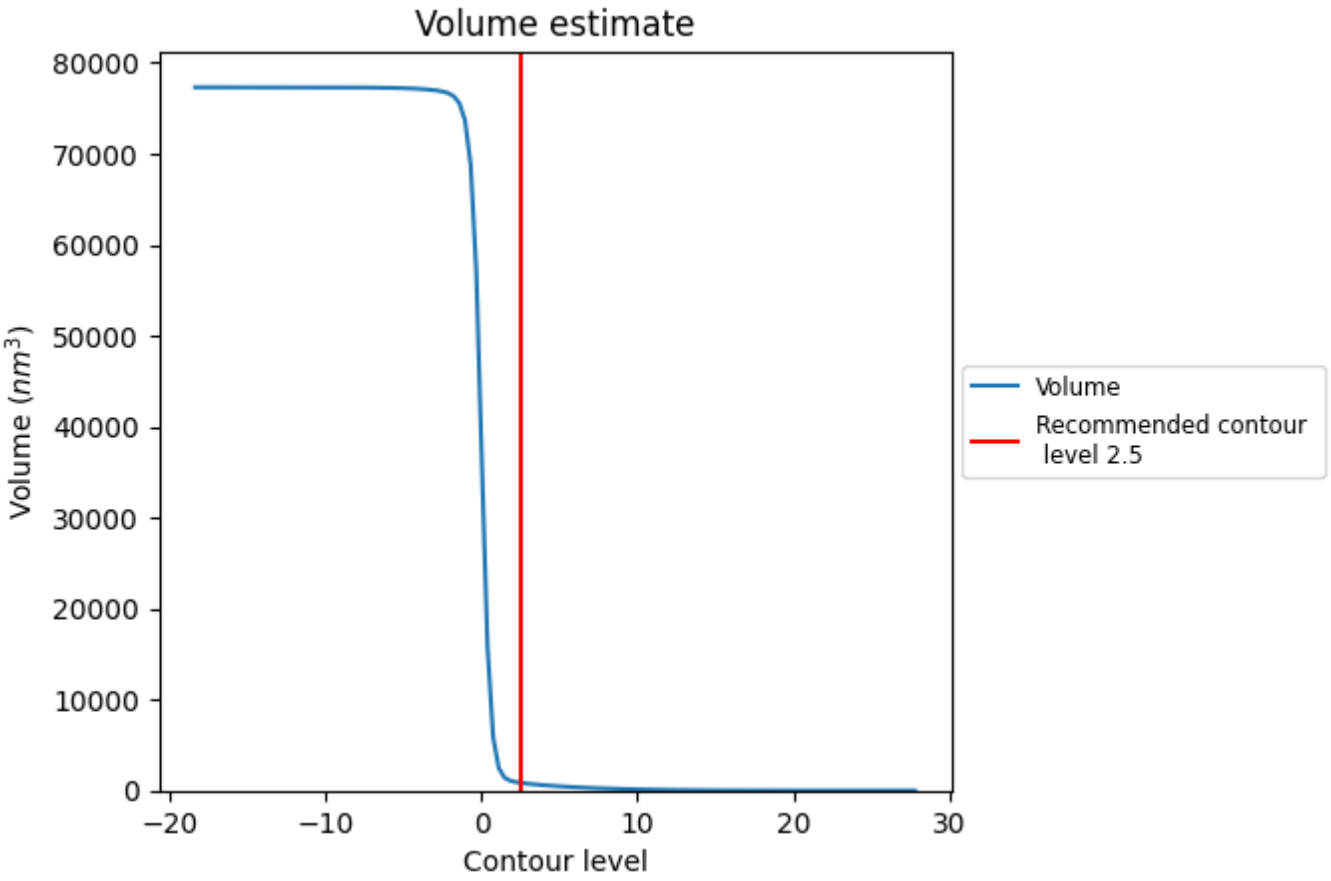
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

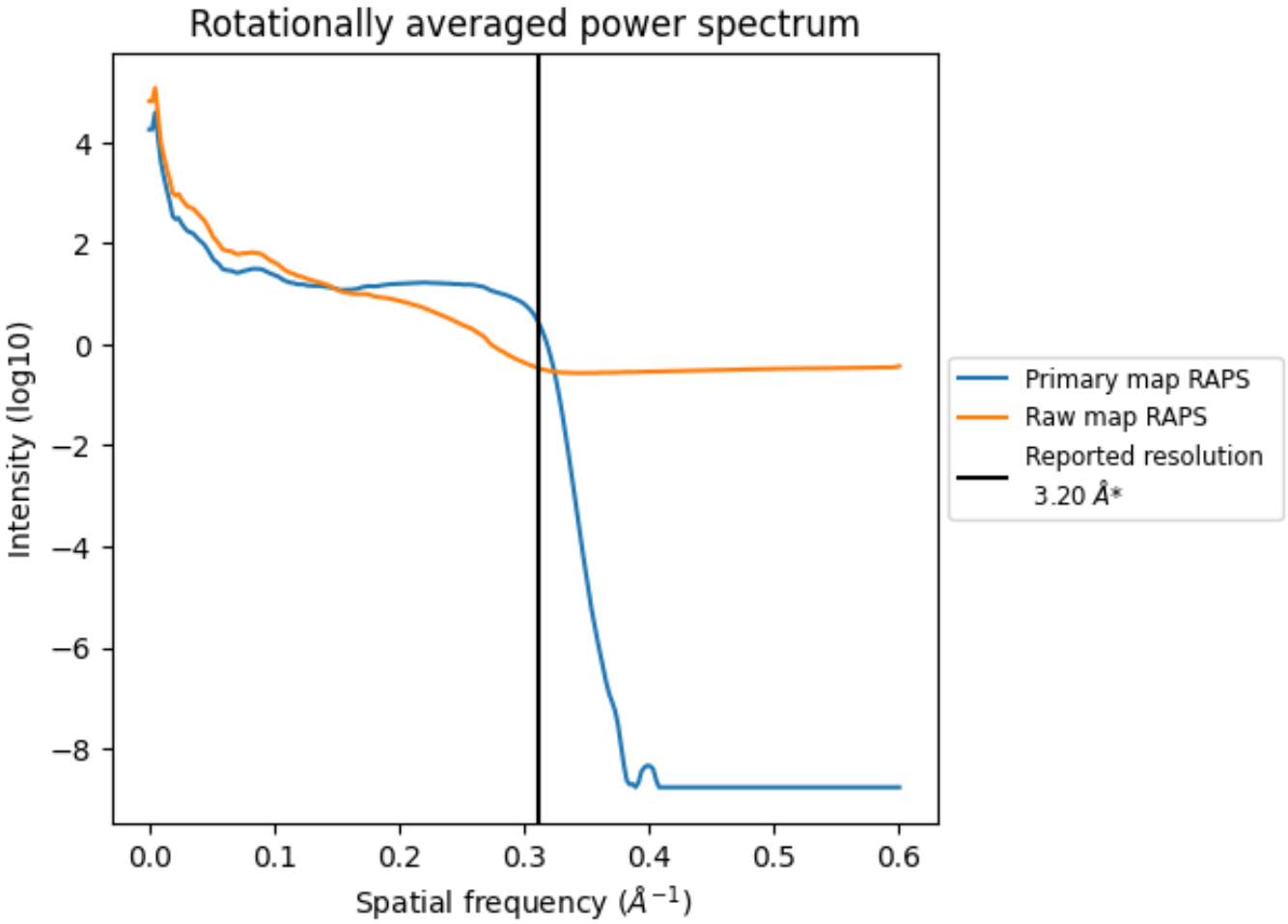
7.2 Volume estimate



The volume at the recommended contour level is 852 nm^3; this corresponds to an approximate mass of 769 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 (i)

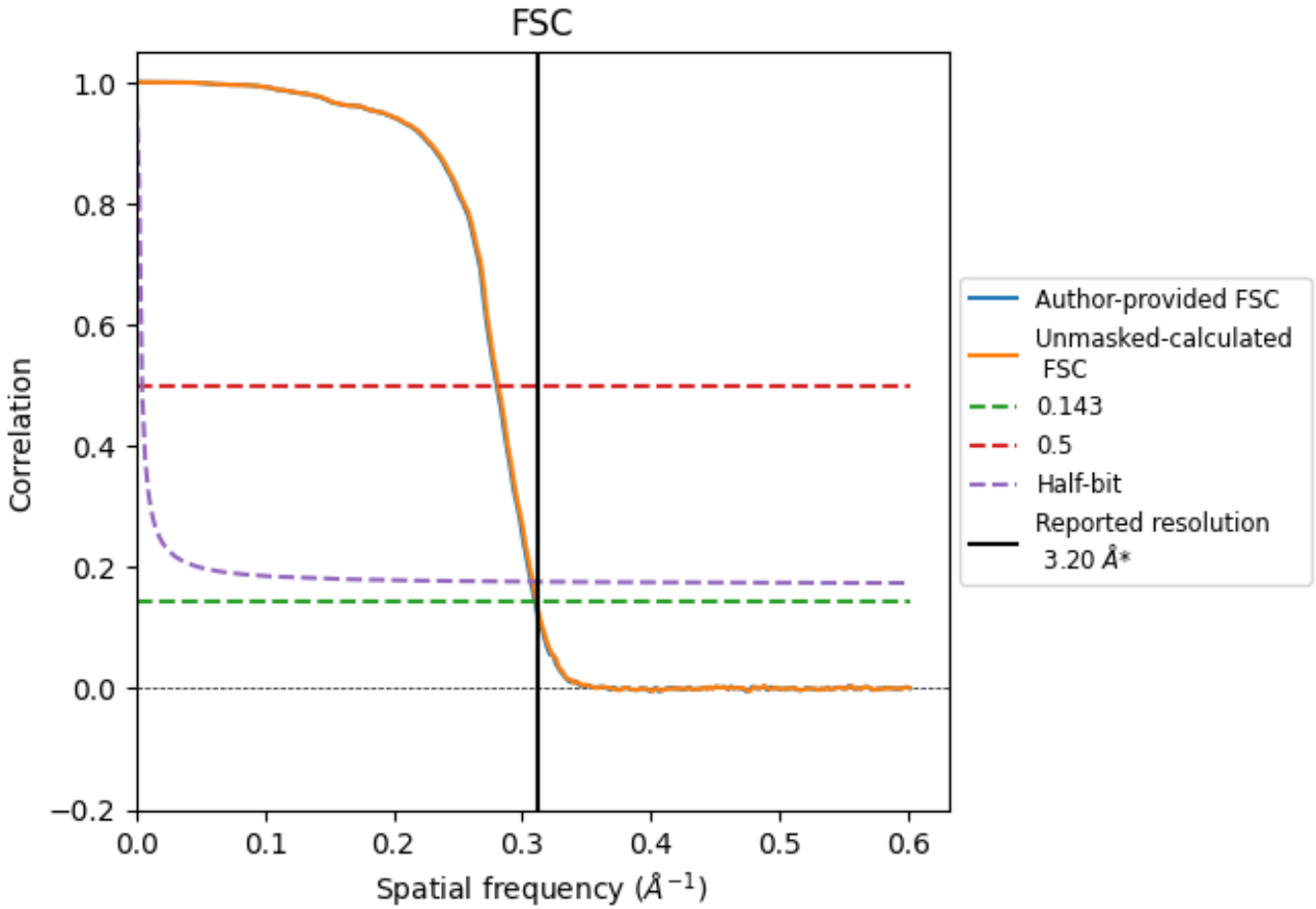


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

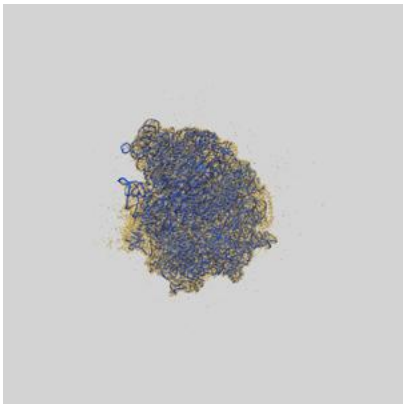
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.57	3.26
Unmasked-calculated*	3.21	3.55	3.25

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

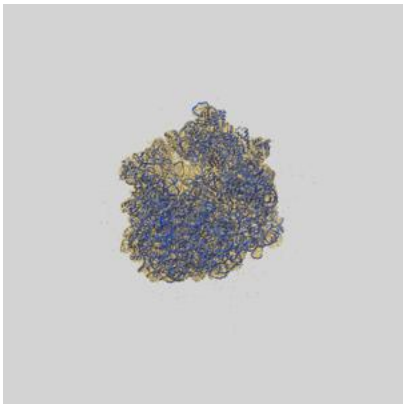
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-75650 and PDB model 11EL. Per-residue inclusion information can be found in section 3 on page 16.

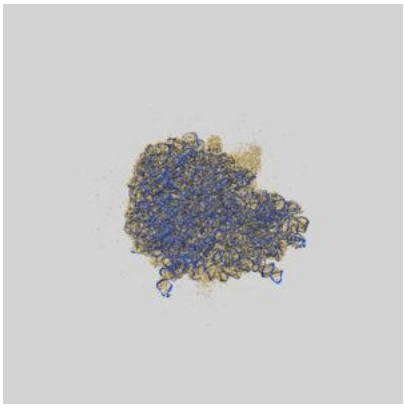
9.1 Map-model overlay



X



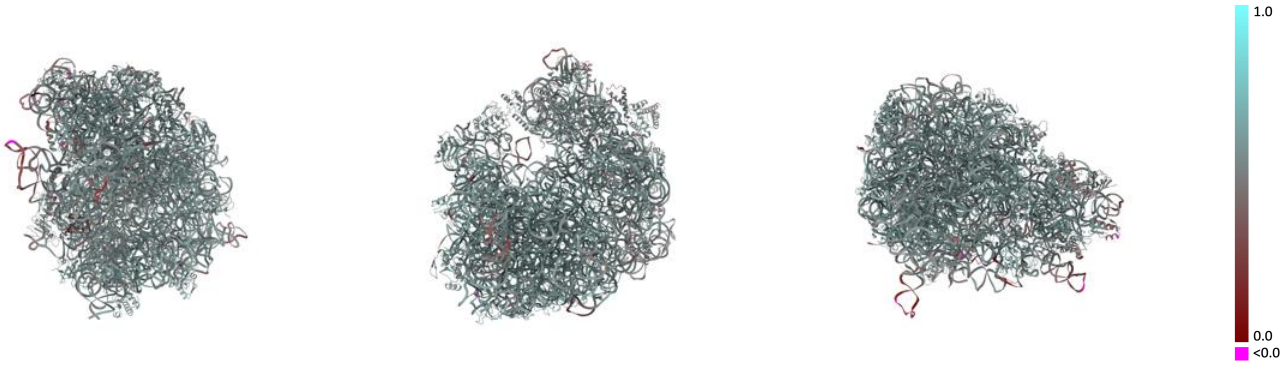
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

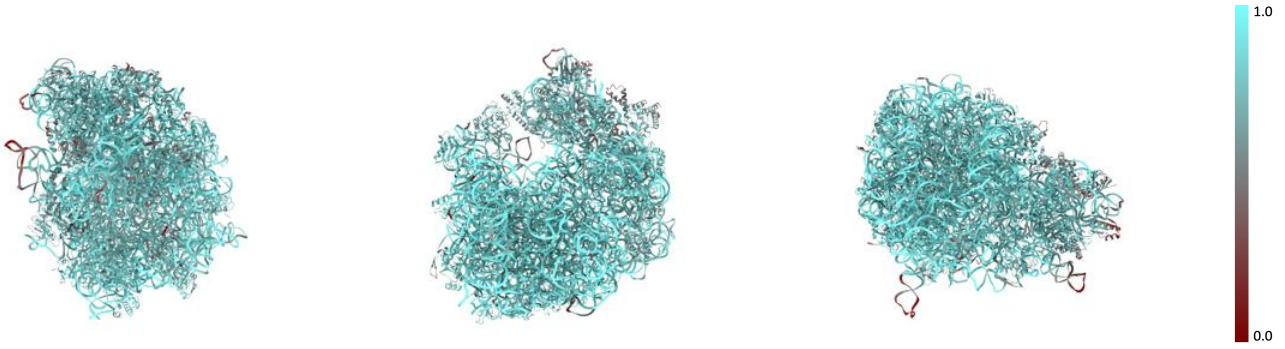
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

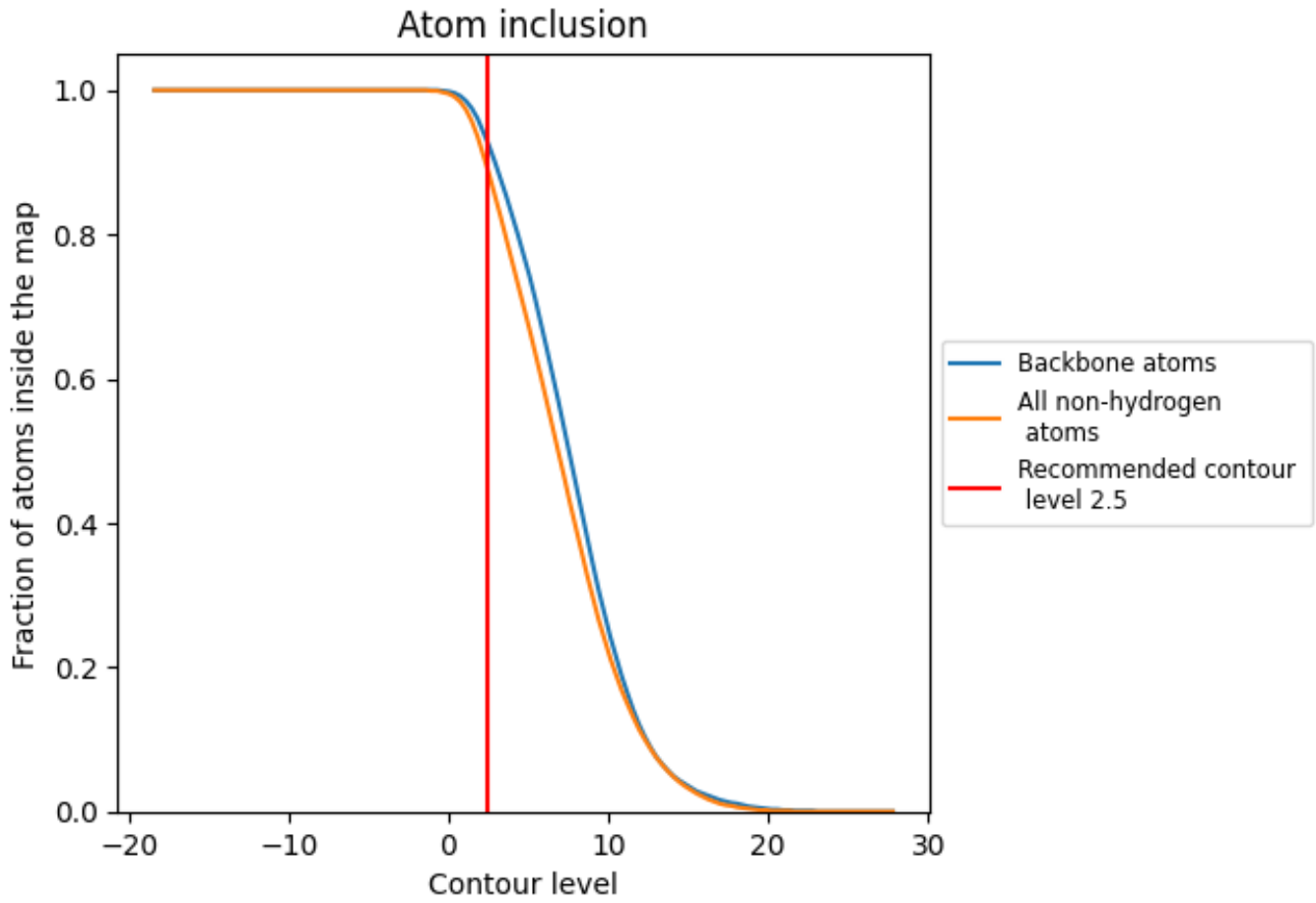
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.5560
0	0.6410	0.5560
1	0.9010	0.5960
2	0.9080	0.6030
3	0.8980	0.6060
4	0.7060	0.5010
5	0.0950	0.4890
A	0.8930	0.5350
B	0.6420	0.5180
C	0.7500	0.5470
D	0.7570	0.5480
E	0.8580	0.5740
F	0.8200	0.5440
G	0.6670	0.5000
H	0.8440	0.5760
I	0.6920	0.5260
J	0.5860	0.4920
K	0.8430	0.5570
L	0.8840	0.5780
M	0.7650	0.5410
N	0.7470	0.5370
O	0.8590	0.5700
P	0.6840	0.4320
Q	0.8160	0.5460
R	0.8300	0.5520
S	0.7640	0.5240
T	0.8260	0.5500
U	0.5080	0.4940
a	0.9370	0.5660
b	0.9170	0.5490
c	0.9250	0.5990
d	0.9050	0.5950
e	0.8200	0.5700
f	0.7500	0.5370
g	0.7800	0.5310

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Chain	Atom inclusion	Q-score
h	0.7370	0.5180
i	0.9050	0.5950
j	0.9010	0.5910
k	0.8790	0.5830
l	0.8880	0.5840
m	0.9010	0.5920
n	0.8300	0.5670
o	0.8910	0.5960
p	0.8930	0.5910
q	0.8700	0.5930
r	0.8640	0.5840
s	0.8410	0.5700
t	0.8200	0.5700
u	0.8540	0.5800
v	0.9000	0.5910
w	0.8950	0.5860
x	0.7950	0.5500
y	0.8580	0.5820
z	0.8880	0.5870