



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 11:11 pm GMT

PDB ID : 9GUS
EMDB ID : EMD-51618
Title : 30S mRNA delivery complex TEC resolved (30S only)
Authors : Rahil, H.; Weixlbaumer, A.; Webster, M.W.
Deposited on : 2024-09-20
Resolution : 3.50 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:

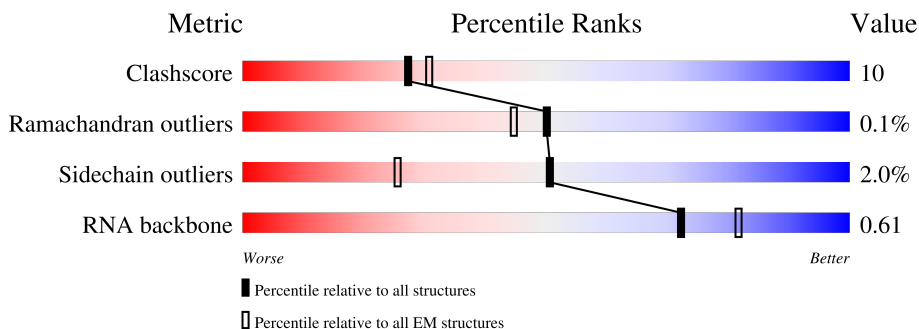
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













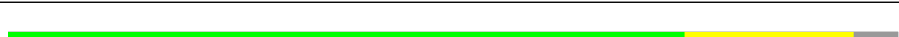


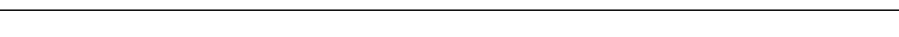
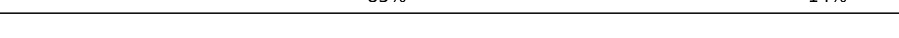
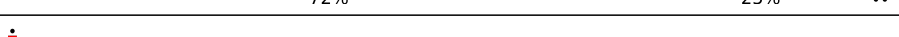

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1541	47% (green), 46% (yellow), 7% (orange)
2	B	557	24% (green), 6% (yellow), 69% (grey)
3	C	241	78% (green), 15% (yellow), 6% (grey)
4	D	233	77% (green), 13% (yellow), 9% (grey)
5	E	206	84% (green), 15% (yellow)
6	F	156	83% (green), 17% (yellow)
7	G	131	61% (green), 18% (yellow), 21% (grey)

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Mol	Chain	Length	Quality of chain
8	H	156	 76% 21% ..
9	I	130	 90% 8% ..
10	J	130	 73% 25% ..
11	K	103	 75% 22% ..
12	L	129	 64% 27% 9%
13	M	124	 77% 20% ..
14	N	118	 75% 21% ..
15	O	101	 86% 13% .
16	P	89	 90% 8% ..
17	Q	82	 85% 15%
18	R	84	 76% 19% 5%
19	S	75	 65% 24% 11%
20	T	92	 71% 20% 10%
21	U	87	 85% 14% .
22	V	71	 72% 25% ..
23	W	77	 23% 64% 13%
24	X	53	 11% 11% 11% 66%

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 55373 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1539	33023	14736	6046	10702	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	174	1100	674	197	228	1	0	0

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	226	1764	1116	316	324	8	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	211	1653	1046	310	293	4	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 6 is a protein called 30S ribosomal protein S5.

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

- Molecule 7 is a protein called Small ribosomal subunit protein bS6.

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

- Molecule 8 is a protein called 30S ribosomal protein S7.

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

- Molecule 9 is a protein called 30S ribosomal protein S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	128	1031	639	207	182	3	0	0

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	808	504	155	148	1	0	0

- Molecule 12 is a protein called 30S ribosomal protein S11.

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

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	122	951	588	195	163	5	0	0

- Molecule 14 is a protein called 30S ribosomal protein S13.

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

- Molecule 15 is a protein called 30S ribosomal protein S14.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 17 is a protein called 30S ribosomal protein S16.

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

- Molecule 18 is a protein called 30S ribosomal protein S17.

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

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	67	554	350	104	99	1	0	0

- Molecule 20 is a protein called 30S ribosomal protein S19.

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

- Molecule 21 is a protein called 30S ribosomal protein S20.

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

- Molecule 22 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	W	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	18	Total	C	N	O	P	0	0
			387	173	70	126	18		

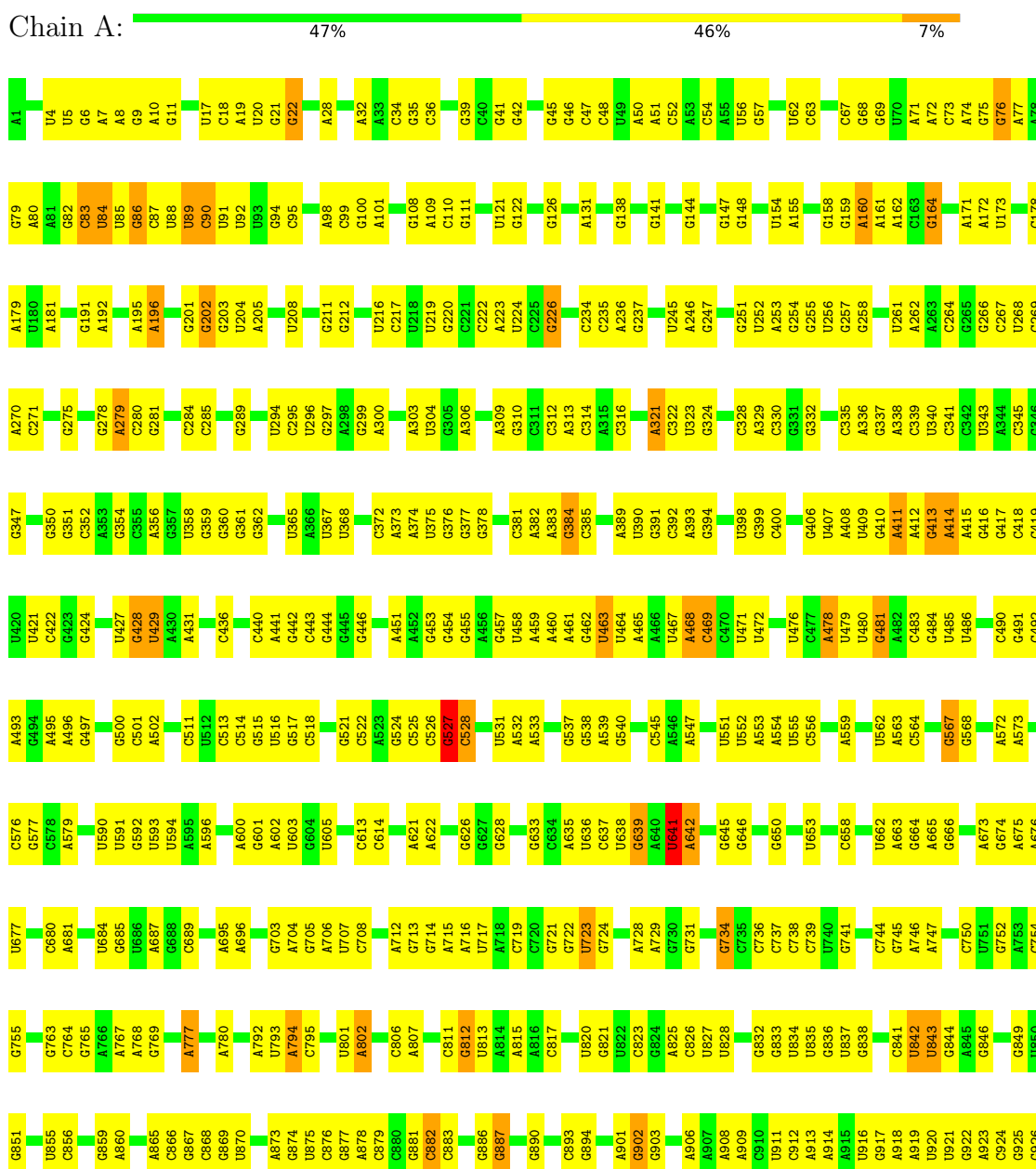
- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

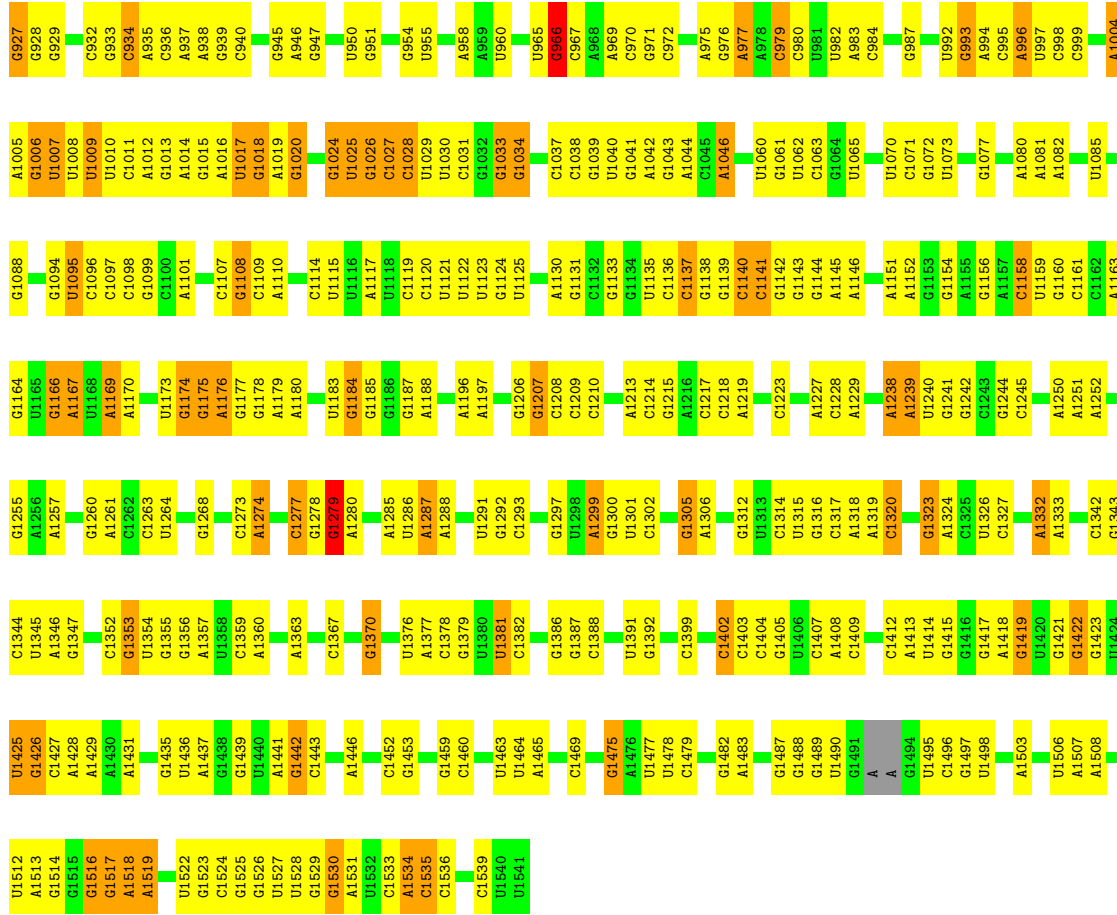
Mol	Chain	Residues	Atoms		AltConf
25	A	124	Total	Mg	0
			124	124	
25	M	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA






● Molecule 2: 30S ribosomal protein S1

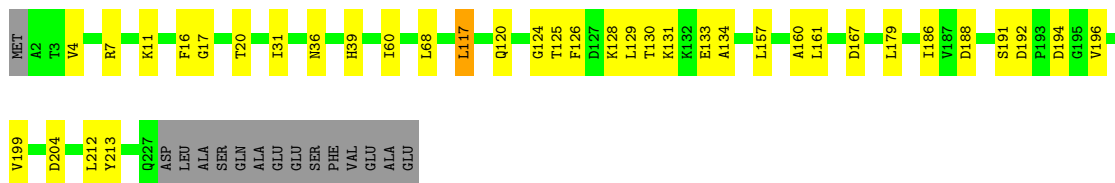


H1	V122	ASP	GLY	ILE	GLY	ASP
S4	A129	MET	ARG	SER	GLU	ALA
Q7	R142	TRP	VAL	GLY	ALA	LYS
T18	V166	LYS	ASN	LEU	VAL	ALA
A30	S169	ARG	THR	LEU	ARG	THR
L37	R170	HIS	ASP	LYS	THR	LYS
V38	R171	PRO	THR	ALA	LYS	ALA
D39	I174	GLY	ASP	ASN	GLY	ASP
A40	I174	VAL	ILE	TRP	VAL	VAL
G41	G41	ASN	ILE	GLN	ALA	ALA
L42	L42	VAL	ILE	PHE	GLY	TYR
R43	R43	GLY	VAL	ALA	LEU	LEU
S46	S46	ASP	VAL	GLY	VAL	ALA
A50	A50	GLU	ILE	THR	LEU	ALA
F53	F53	THR	THR	ASN	GLN	SER
K54	K54	VAL	THR	GLY	VAL	ALA
R55	R55	LEU	THR	ASP	GLU	ARG
G58	G58	LYS	THR	VAL	ARG	ARG
E61	E61	PHE	THR	GLY	ARG	VAL
Q63	Q63	LEU	THR	GLY	ASP	VAL
D66	D66	LEU	THR	ILE	LEU	VAL
D69	D69	VAL	VAL	PHE	PRO	GLU
V70	V70	VAL	VAL	ILE	ASN	LEU
A71	A71	LEU	VAL	GLY	ASN	ALA
L72	L72	LEU	VAL	ASP	VAL	PHE
D73	D73	LEU	VAL	ILE	LEU	VAL
V75	V75	GLN	VAL	ILE	ASN	VAL
E76	E76	LEU	VAL	GLY	LEU	GLY
F79	F79	GLY	VAL	ASP	ASN	VAL
T82	T82	PRO	VAL	GLY	TRP	THR
L83	L83	ASP	VAL	ILE	ALA	VAL
L84	L84	TRP	VAL	VAL	ALA	VAL
S85	S85	ALA	VAL	VAL	ASP	VAL
R86	R86	LEU	VAL	VAL	ASP	VAL
A89	A89	ARG	VAL	HIS	GLY	VAL
K90	K90	GLY	VAL	LEU	LEU	VAL
A101	A101	TYR	VAL	ASP	GLY	VAL
A105	A105	GLY	VAL	ASP	GLY	VAL
I112	I112	THR	VAL	THR	THR	THR
		THR	THR	THR	THR	THR


LYS ASP GLU ALA ASP GLU LYS ASP ALA ALA ILE THR VAL ASN LYS GLN GLU ASP ALA ASN PHE SER ASN ASN MET ALA ALA PHE PHE LYS ALA ALA LYS GLY GLU

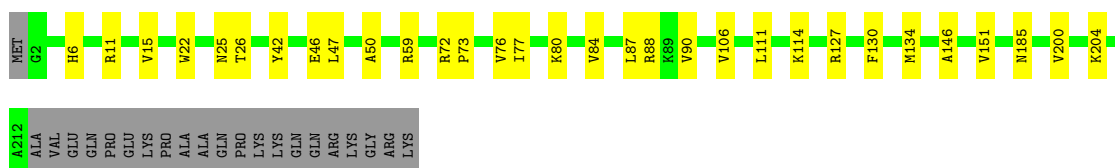
• Molecule 3: 30S ribosomal protein S2

Chain C:  78% 15% 6%




• Molecule 4: Small ribosomal subunit protein uS3

Chain D:  77% 13% 9%

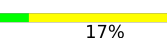


• Molecule 5: Small ribosomal subunit protein uS4

Chain E:  84% 15%



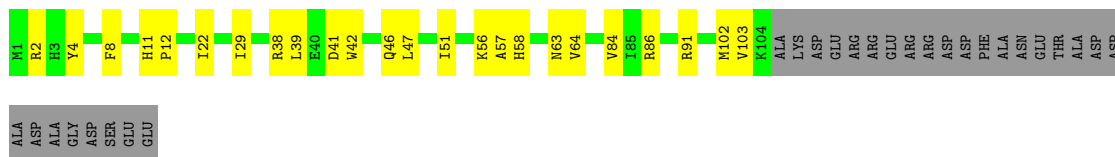
• Molecule 6: 30S ribosomal protein S5

Chain F:  83% 17%



• Molecule 7: Small ribosomal subunit protein bS6

Chain G: 61% 18% 21%



• Molecule 8: 30S ribosomal protein S7

Chain H: 76% 21%



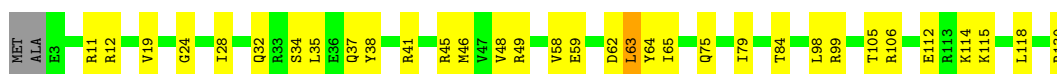
- Molecule 9: 30S ribosomal protein S8

Chain I: 90% 8% ..



- Molecule 10: 30S ribosomal protein S9

Chain J: 73% 25% ..



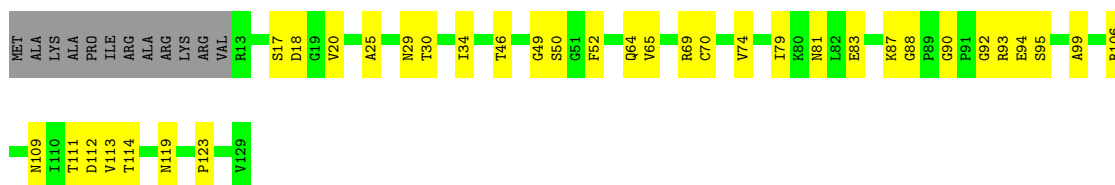
- Molecule 11: 30S ribosomal protein S10

Chain K: 75% 22% ..



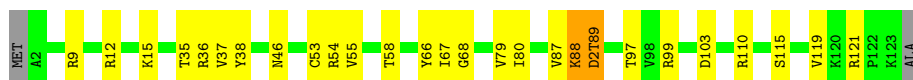
- Molecule 12: 30S ribosomal protein S11

Chain L: 64% 27% 9%



- Molecule 13: 30S ribosomal protein S12

Chain M: 77% 20% ..




- Molecule 14: 30S ribosomal protein S13

Chain N: 75% 21% ..




- Molecule 15: 30S ribosomal protein S14

Chain O:  86% 13%




- Molecule 16: Small ribosomal subunit protein uS15

Chain P:  90% 8%



- Molecule 17: 30S ribosomal protein S16

Chain Q:  85% 15%



- Molecule 18: 30S ribosomal protein S17

Chain R:  76% 19% 5%



- Molecule 19: 30S ribosomal protein S18

Chain S:  65% 24% 11%




- Molecule 20: 30S ribosomal protein S19

Chain T:  71% 20% 10%



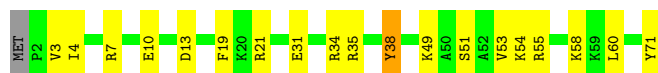
- Molecule 21: 30S ribosomal protein S20

Chain U:  85% 14%



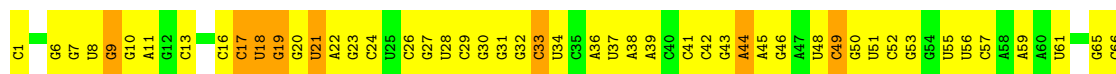
- Molecule 22: 30S ribosomal protein S21

Chain V:  72% 25% ..



- Molecule 23: tRNA(fmet) P-site

Chain W:  23% 64% 13%



- Molecule 24: mRNA

Chain X:  11% 11% 11% 66%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.95	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	4.336	Depositor
Minimum map value	-1.468	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	0.159	Depositor
Map size (\AA)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84, 0.84, 0.84	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, G7M, MG, D2T, 5MC, MA6, 4OC, PSU, 2MG, H2U, 5MU, UR3, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/36692	0.84	14/57230 (0.0%)
2	B	0.29	0/1105	0.52	1/1505 (0.1%)
3	C	0.30	0/1795	0.50	0/2418
4	D	0.32	0/1680	0.53	0/2263
5	E	0.29	0/1665	0.52	0/2227
6	F	0.30	0/1165	0.52	0/1568
7	G	0.32	0/867	0.54	0/1171
8	H	0.28	0/1219	0.55	0/1635
9	I	0.28	0/989	0.49	0/1326
10	J	0.32	0/1043	0.58	0/1387
11	K	0.30	0/818	0.59	0/1105
12	L	0.27	0/893	0.53	0/1205
13	M	0.30	0/954	0.57	0/1279
14	N	0.27	0/900	0.57	0/1204
15	O	0.31	0/817	0.55	0/1088
16	P	0.27	0/722	0.53	0/964
17	Q	0.29	0/659	0.56	0/884
18	R	0.27	0/657	0.52	0/881
19	S	0.30	0/563	0.54	0/754
20	T	0.32	0/680	0.51	0/915
21	U	0.30	0/676	0.47	0/895
22	V	0.28	0/598	0.59	0/792
23	W	0.37	1/1725 (0.1%)	0.83	0/2687
24	X	0.39	0/433	0.98	3/673 (0.4%)
All	All	0.40	1/59315 (0.0%)	0.76	18/88056 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	1	C	OP3-P	-10.49	1.48	1.61

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	882	C	N3-C2-O2	-8.07	116.25	121.90
2	B	43	LYS	CD-CE-NZ	-6.69	96.32	111.70
1	A	812	G	O4'-C1'-N9	6.57	113.45	108.20
1	A	1158	C	C2-N1-C1'	5.92	125.31	118.80
1	A	979	C	C2-N1-C1'	5.85	125.23	118.80
24	X	18	G	C2-N3-C4	-5.81	108.99	111.90
1	A	979	C	N1-C2-O2	5.64	122.28	118.90
1	A	641	U	P-O3'-C3'	5.57	126.38	119.70
1	A	1007	U	C2-N1-C1'	5.36	124.13	117.70
1	A	882	C	N1-C2-O2	5.33	122.10	118.90
1	A	1279	G	N7-C8-N9	5.24	115.72	113.10
1	A	754	C	C2-N1-C1'	5.17	124.49	118.80
1	A	567	G	C6-N1-C2	-5.12	122.03	125.10
1	A	641	U	OP2-P-O3'	5.12	116.46	105.20
1	A	563	A	C4-N9-C1'	5.11	135.49	126.30
24	X	18	G	N1-C2-N3	5.08	126.95	123.90
24	X	18	G	C6-C5-N7	-5.06	127.36	130.40
1	A	496	A	O4'-C1'-N9	5.03	112.22	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33023	0	16643	575	0
2	B	1100	0	880	26	0
3	C	1764	0	1788	22	0
4	D	1653	0	1727	17	0
5	E	1643	0	1707	24	0
6	F	1152	0	1194	15	0
7	G	848	0	846	12	0
8	H	1203	0	1254	22	0
9	I	979	0	1031	8	0
10	J	1031	0	1076	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	808	0	845	12	0
12	L	877	0	887	26	0
13	M	951	0	1012	19	0
14	N	891	0	952	16	0
15	O	805	0	844	10	0
16	P	714	0	734	8	0
17	Q	649	0	666	8	0
18	R	648	0	691	12	0
19	S	554	0	573	12	0
20	T	663	0	688	15	0
21	U	670	0	719	10	0
22	V	590	0	629	13	0
23	W	1645	0	841	51	0
24	X	387	0	193	10	0
25	A	124	0	0	0	0
25	M	1	0	0	0	0
All	All	55373	0	38420	885	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 10.

All (885) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1425:U:H3	1:A:1475:G:H1	1.02	0.99
23:W:51:U:H3	23:W:65:G:H1	0.93	0.93
1:A:664:G:H22	1:A:741:G:H1	1.21	0.87
1:A:1422:G:H1	1:A:1478:U:H3	1.21	0.87
1:A:713:G:H2'	1:A:714:G:C8	2.13	0.82
1:A:859:G:H2'	1:A:860:A:H8	1.45	0.81
1:A:744:C:H2'	1:A:745:G:H8	1.46	0.81
1:A:1130:A:H2'	1:A:1131:G:H8	1.46	0.80
1:A:1261:A:N6	1:A:1274:A:O2'	2.17	0.78
1:A:1530:G:H2'	1:A:1531:A:H8	1.48	0.77
1:A:859:G:H2'	1:A:860:A:C8	2.21	0.76
15:O:6:MET:SD	15:O:9:ARG:NH2	2.59	0.76
1:A:823:C:HO2'	9:I:2:SER:N	1.84	0.75
1:A:958:A:OP1	20:T:55:ARG:NH1	2.19	0.75
1:A:1009:U:O4	1:A:1020:G:O6	2.04	0.75
1:A:1009:U:H3	1:A:1020:G:H1	1.32	0.75
1:A:1239:A:H62	1:A:1299:A:H62	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:G:H5'	13:M:121:ARG:HH12	1.51	0.75
1:A:1251:A:H2'	1:A:1252:A:C8	2.22	0.74
1:A:1005:A:N6	1:A:1024:G:O2'	2.20	0.74
10:J:112:GLU:OE2	10:J:115:LYS:NZ	2.21	0.74
1:A:1391:U:H2'	1:A:1392:G:C8	2.23	0.74
6:F:105:ILE:HD11	6:F:112:ARG:HA	1.70	0.74
1:A:714:G:H2'	1:A:715:A:C8	2.24	0.73
1:A:1386:G:H2'	1:A:1387:G:H8	1.52	0.73
1:A:1011:C:H2'	1:A:1012:A:H8	1.54	0.72
1:A:1011:C:H2'	1:A:1012:A:C8	2.25	0.72
8:H:5:ARG:HD2	8:H:7:ILE:H	1.54	0.72
9:I:28:PRO:O	9:I:33:LYS:NZ	2.22	0.72
1:A:1530:G:H2'	1:A:1531:A:C8	2.24	0.72
12:L:88:GLY:H	12:L:114:THR:HG22	1.55	0.71
4:D:47:LEU:HB3	4:D:50:ALA:HB3	1.73	0.71
1:A:875:U:O2'	9:I:15:ARG:NH1	2.23	0.70
1:A:87:C:H2'	1:A:88:U:C6	2.26	0.70
1:A:1229:A:OP2	14:N:113:ARG:NH1	2.24	0.70
2:B:43:LYS:HZ2	3:C:16:PHE:HB3	1.55	0.70
15:O:3:LYS:HB2	15:O:6:MET:HG2	1.74	0.70
1:A:736:C:OP1	19:S:61:ARG:NH1	2.26	0.68
1:A:1439:G:OP1	21:U:33:LYS:NZ	2.27	0.68
1:A:600:A:OP2	9:I:88:ARG:NH1	2.26	0.68
1:A:1130:A:H2'	1:A:1131:G:C8	2.29	0.68
1:A:219:U:H2'	1:A:220:G:H8	1.59	0.68
7:G:46:GLN:H	7:G:56:LYS:HA	1.58	0.68
1:A:56:U:H2'	1:A:57:G:H8	1.58	0.68
1:A:235:C:H2'	1:A:236:A:H8	1.58	0.67
1:A:1250:A:H2'	1:A:1251:A:C8	2.29	0.67
1:A:877:G:C2	1:A:878:A:N7	2.62	0.67
1:A:946:A:H2'	1:A:947:G:H8	1.60	0.67
1:A:750:C:O2'	16:P:21:ASP:OD1	2.12	0.67
1:A:1478:U:H2'	1:A:1479:C:C6	2.30	0.67
1:A:970:C:N4	10:J:130:ARG:O	2.28	0.67
1:A:1318:A:H5''	20:T:3:ARG:HH12	1.60	0.66
22:V:54:LYS:HE3	22:V:58:LYS:HE3	1.76	0.66
1:A:1218:C:H2'	1:A:1219:A:C8	2.29	0.66
12:L:64:GLN:HG3	12:L:99:ALA:HB2	1.76	0.66
17:Q:15:PRO:HD2	17:Q:42:ILE:HD11	1.77	0.66
4:D:46:GLU:HG2	4:D:87:LEU:HD21	1.78	0.66
1:A:744:C:H2'	1:A:745:G:C8	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:ALA:HB2	6:F:124:LEU:HG	1.77	0.66
1:A:1098:C:O2'	22:V:71:TYR:OXT	2.10	0.66
20:T:3:ARG:HH21	20:T:7:LYS:HB3	1.61	0.66
1:A:126:G:OP1	1:A:605:U:O2'	2.14	0.66
19:S:9:LYS:N	24:X:13:U:HO2'	1.94	0.66
1:A:745:G:H2'	1:A:746:A:H8	1.60	0.66
1:A:1355:G:H2'	1:A:1356:G:H8	1.61	0.66
1:A:1391:U:H2'	1:A:1392:G:H8	1.58	0.66
1:A:83:C:O2'	1:A:86:G:N2	2.27	0.65
1:A:1297:G:O2'	8:H:114:LYS:NZ	2.28	0.65
1:A:1176:A:H2'	1:A:1177:G:C8	2.31	0.65
1:A:1251:A:H2'	1:A:1252:A:H8	1.61	0.65
1:A:745:G:H2'	1:A:746:A:C8	2.32	0.65
1:A:1464:U:H2'	1:A:1465:A:H8	1.61	0.65
1:A:946:A:H2'	1:A:947:G:C8	2.32	0.64
1:A:1255:G:OP2	11:K:45:ARG:NH2	2.30	0.64
8:H:113:ASP:HB2	8:H:119:ARG:HG3	1.77	0.64
1:A:677:U:H3	1:A:713:G:H22	1.43	0.64
14:N:9:ILE:HG23	14:N:18:ALA:HB1	1.79	0.64
1:A:411:A:H4'	1:A:412:A:H5'	1.80	0.64
1:A:501:C:H2'	1:A:502:A:H8	1.63	0.64
1:A:21:G:H2'	1:A:22:G:C8	2.33	0.64
1:A:362:G:OP1	13:M:58:THR:OG1	2.16	0.64
1:A:1516:2MG:N2	1:A:1519:MA6:OP2	2.31	0.64
1:A:1071:C:H2'	1:A:1072:G:H8	1.63	0.64
1:A:1522:U:H2'	1:A:1523:G:H8	1.63	0.63
23:W:16:C:H5'	23:W:18:U:H5	1.63	0.63
20:T:50:ALA:HB1	20:T:57:HIS:HB3	1.81	0.63
1:A:17:U:H2'	1:A:18:C:C6	2.33	0.63
1:A:1081:A:OP2	6:F:52:LYS:NZ	2.30	0.63
18:R:79:VAL:HG22	18:R:80:GLU:HG3	1.80	0.63
11:K:36:VAL:HG13	11:K:76:ILE:HG12	1.81	0.63
7:G:47:LEU:HD21	7:G:57:ALA:HB3	1.80	0.62
3:C:126:PHE:O	3:C:128:LYS:NZ	2.28	0.62
1:A:876:C:H2'	1:A:877:G:H8	1.65	0.62
1:A:1323:G:H2'	1:A:1324:A:H8	1.65	0.62
1:A:674:G:H2'	1:A:675:A:C8	2.34	0.62
1:A:1404:C:H2'	1:A:1405:G:C8	2.34	0.62
1:A:202:G:HO2'	1:A:468:A:H8	1.46	0.61
1:A:1088:G:H21	1:A:1167:A:H62	1.49	0.61
8:H:22:LEU:HD21	8:H:66:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:G:H2'	1:A:148:G:C8	2.35	0.61
1:A:980:C:O2'	15:O:13:ARG:NH1	2.34	0.61
12:L:46:THR:HG23	12:L:49:GLY:H	1.66	0.61
1:A:1323:G:H2'	1:A:1324:A:C8	2.35	0.61
1:A:811:C:O2'	1:A:901:A:N1	2.33	0.61
1:A:923:A:O2'	1:A:1399:C:OP2	2.19	0.61
1:A:958:A:C6	20:T:55:ARG:HB2	2.35	0.61
1:A:1025:U:H4'	1:A:1026:G:H5'	1.83	0.61
1:A:56:U:H2'	1:A:57:G:C8	2.36	0.60
8:H:113:ASP:OD2	8:H:122:ASN:ND2	2.34	0.60
1:A:1239:A:H62	1:A:1299:A:N6	1.98	0.60
2:B:55:ASN:ND2	2:B:61:GLU:OE2	2.34	0.60
18:R:64:CYS:HG	18:R:74:THR:HG1	1.49	0.60
4:D:151:VAL:HG12	4:D:200:VAL:HG22	1.82	0.60
24:X:8:A:H2'	24:X:9:G:C8	2.37	0.60
1:A:1425:U:H2'	1:A:1426:G:H8	1.66	0.60
7:G:29:ILE:HD13	7:G:64:VAL:HG11	1.84	0.60
12:L:17:SER:HA	12:L:79:ILE:HA	1.83	0.60
17:Q:39:PHE:HD1	17:Q:50:THR:HG22	1.65	0.60
1:A:1010:U:H2'	1:A:1011:C:C6	2.36	0.60
12:L:87:LYS:HB2	12:L:113:VAL:HG23	1.83	0.60
1:A:28:A:O2'	1:A:296:U:OP1	2.18	0.59
10:J:84:THR:HG23	10:J:98:LEU:HD13	1.83	0.59
1:A:1287:A:H2'	1:A:1288:A:C8	2.37	0.59
5:E:192:SER:OG	5:E:194:ASP:OD1	2.15	0.59
11:K:8:ILE:HG23	11:K:100:ILE:HG12	1.83	0.59
14:N:7:ILE:HD11	14:N:22:ILE:HG12	1.84	0.59
1:A:714:G:H2'	1:A:715:A:H8	1.66	0.59
1:A:1277:C:O2'	1:A:1279:G:H8	1.84	0.59
1:A:1314:C:H2'	1:A:1315:U:C6	2.38	0.59
6:F:88:VAL:HG23	6:F:93:ARG:HG2	1.85	0.59
6:F:57:PRO:HG3	23:W:57:C:O2'	2.03	0.58
1:A:626:G:OP1	17:Q:35:ARG:NH2	2.36	0.58
1:A:707:U:H2'	1:A:708:C:H6	1.68	0.58
1:A:89:U:H2'	1:A:90:C:C6	2.39	0.58
1:A:275:G:H5'	18:R:16:LYS:HD2	1.85	0.58
5:E:170:TRP:CD2	5:E:186:PRO:HB3	2.38	0.58
12:L:25:ALA:HB1	12:L:90:GLY:HA3	1.86	0.58
1:A:335:C:H2'	1:A:336:A:H8	1.69	0.58
11:K:25:ILE:HD11	11:K:92:LEU:HD11	1.84	0.58
15:O:46:LEU:HB3	20:T:13:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1299:A:O2'	1:A:1301:U:O4'	2.20	0.58
1:A:1077:G:N2	1:A:1080:A:OP2	2.33	0.58
14:N:4:ILE:HD13	14:N:9:ILE:HD12	1.84	0.58
1:A:235:C:H2'	1:A:236:A:C8	2.38	0.58
1:A:501:C:H2'	1:A:502:A:C8	2.38	0.58
17:Q:12:LYS:HG2	17:Q:13:LYS:HG2	1.84	0.58
1:A:500:G:H2'	1:A:501:C:C6	2.39	0.57
3:C:68:LEU:HB3	3:C:161:LEU:HD12	1.85	0.57
1:A:997:U:H2'	1:A:998:C:H6	1.69	0.57
8:H:68:ASN:O	8:H:138:ARG:NH1	2.38	0.57
1:A:1318:A:H5''	20:T:3:ARG:NH1	2.18	0.57
4:D:50:ALA:HB1	4:D:76:VAL:HG22	1.86	0.57
23:W:34:U:N3	23:W:37:U:OP2	2.37	0.57
8:H:58:GLU:N	8:H:58:GLU:OE1	2.36	0.57
1:A:358:U:H2'	1:A:359:G:H8	1.69	0.57
1:A:1218:C:H2'	1:A:1219:A:H8	1.69	0.57
1:A:256:U:H2'	1:A:257:G:H8	1.70	0.57
1:A:932:C:H2'	1:A:933:G:C8	2.40	0.57
1:A:1513:A:H2'	1:A:1514:G:H8	1.68	0.57
1:A:339:C:H2'	1:A:340:U:C6	2.40	0.57
1:A:866:C:C4	1:A:867:G:H1'	2.40	0.57
1:A:1240:U:O4	8:H:109:ARG:NH1	2.34	0.57
2:B:46:SER:OG	2:B:82:THR:OG1	2.22	0.57
23:W:9:G:H1'	23:W:46:G:H2'	1.87	0.57
1:A:1027:C:C2	1:A:1028:C:C5	2.93	0.57
12:L:20:VAL:HG13	12:L:83:GLU:HG3	1.86	0.57
23:W:32:G:H2'	23:W:33:OMC:O4'	2.04	0.57
1:A:309:A:H2'	1:A:310:G:H8	1.70	0.57
1:A:1314:C:H2'	1:A:1315:U:H6	1.70	0.57
1:A:256:U:H2'	1:A:257:G:C8	2.40	0.56
5:E:19:LEU:HB2	5:E:21:LEU:HG	1.87	0.56
6:F:80:THR:HA	6:F:120:VAL:HG13	1.88	0.56
12:L:119:ASN:OD1	22:V:35:ARG:NH2	2.28	0.56
19:S:34:THR:HG23	19:S:36:SER:H	1.70	0.56
24:X:11:U:H4'	24:X:12:A:O5'	2.05	0.56
1:A:1342:C:H2'	1:A:1343:G:C8	2.41	0.56
1:A:1518:MA6:H2'	1:A:1519:MA6:H8	1.88	0.56
11:K:4:GLN:OE1	11:K:4:GLN:N	2.37	0.56
23:W:29:C:H2'	23:W:30:G:H8	1.70	0.56
19:S:42:SER:HA	19:S:45:THR:HG22	1.86	0.56
22:V:13:ASP:OD1	22:V:13:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:G:H2'	1:A:1188:A:C8	2.40	0.56
1:A:34:C:H2'	1:A:35:G:H8	1.69	0.56
1:A:269:C:H2'	1:A:270:A:H8	1.71	0.56
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.56
1:A:911:U:H2'	1:A:912:C:C6	2.41	0.56
8:H:51:ALA:HB2	8:H:58:GLU:HG3	1.87	0.56
10:J:32:GLN:NE2	10:J:64:TYR:OH	2.39	0.56
1:A:1412:C:H2'	1:A:1413:A:C8	2.41	0.56
5:E:171:LEU:HD23	5:E:182:PHE:HA	1.88	0.56
1:A:297:G:N2	1:A:300:A:OP2	2.31	0.56
1:A:979:C:O2	15:O:59:ARG:NH1	2.39	0.56
1:A:539:A:H2'	1:A:540:G:C8	2.41	0.55
1:A:1183:U:O2'	1:A:1185:G:OP2	2.24	0.55
1:A:1418:A:N6	1:A:1482:G:O2'	2.39	0.55
1:A:216:U:H2'	1:A:217:C:C6	2.42	0.55
1:A:689:C:OP1	12:L:29:ASN:ND2	2.39	0.55
1:A:707:U:H2'	1:A:708:C:C6	2.41	0.55
1:A:878:A:C2	1:A:879:C:C2	2.94	0.55
1:A:362:G:N2	1:A:365:U:OP2	2.40	0.55
1:A:390:U:H2'	1:A:391:G:H8	1.72	0.55
1:A:1347:G:O6	10:J:12:ARG:NH2	2.40	0.55
1:A:1377:A:OP1	8:H:92:ARG:NH2	2.40	0.55
23:W:59:A:O2'	23:W:61:U:OP2	2.19	0.55
23:W:65:G:H2'	23:W:66:C:C6	2.41	0.55
1:A:704:A:C4	1:A:705:G:C8	2.95	0.55
23:W:29:C:H2'	23:W:30:G:C8	2.41	0.55
1:A:375:U:OP1	17:Q:70:ARG:NH1	2.39	0.55
1:A:440:C:C2	1:A:441:A:C8	2.95	0.55
2:B:73:ASP:HB2	2:B:83:LEU:HB3	1.89	0.55
1:A:1018:G:H2'	1:A:1019:A:C8	2.41	0.55
10:J:45:ARG:O	10:J:49:ARG:HG2	2.07	0.55
23:W:70:C:H2'	23:W:71:G:C8	2.42	0.55
1:A:492:C:H2'	1:A:493:A:C8	2.42	0.55
1:A:662:U:H2'	1:A:663:A:C8	2.42	0.55
1:A:1463:U:H2'	1:A:1464:U:C6	2.42	0.55
16:P:18:ASP:OD1	16:P:18:ASP:N	2.40	0.54
1:A:1018:G:H2'	1:A:1019:A:H8	1.72	0.54
1:A:1096:C:H2'	1:A:1097:C:H6	1.71	0.54
1:A:1356:G:H2'	1:A:1357:A:C8	2.42	0.54
1:A:1507:A:H2'	1:A:1508:A:C8	2.42	0.54
14:N:75:MET:HA	14:N:78:LYS:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:A:H2'	1:A:1164:G:H8	1.72	0.54
1:A:1535:C:H2'	1:A:1536:C:C6	2.42	0.54
7:G:38:ARG:NH2	7:G:63:ASN:OD1	2.38	0.54
3:C:129:LEU:HB3	3:C:133:GLU:HB2	1.89	0.54
21:U:17:ALA:O	21:U:21:ASN:ND2	2.37	0.54
1:A:19:A:H2'	1:A:20:U:C6	2.43	0.54
1:A:1004:A:C6	1:A:1026:G:HI'	2.43	0.54
1:A:75:G:H2'	1:A:76:G:O4'	2.07	0.54
1:A:339:C:H2'	1:A:340:U:H6	1.73	0.54
1:A:350:G:H2'	1:A:351:G:C8	2.43	0.54
1:A:1137:C:O2	1:A:1138:G:N1	2.41	0.54
12:L:114:THR:O	19:S:73:ARG:NH1	2.40	0.54
1:A:1513:A:H2'	1:A:1514:G:C8	2.43	0.54
1:A:555:U:H2'	1:A:556:C:C6	2.43	0.54
1:A:337:G:H2'	1:A:338:A:C8	2.43	0.54
1:A:514:C:H2'	1:A:515:G:H8	1.72	0.54
1:A:932:C:H5''	8:H:4:ARG:HH11	1.73	0.54
1:A:950:U:H2'	1:A:951:G:H8	1.73	0.54
1:A:1355:G:H2'	1:A:1356:G:C8	2.41	0.54
1:A:1431:A:H2	1:A:1469:C:H41	1.56	0.54
1:A:270:A:H2'	1:A:271:C:C6	2.43	0.53
1:A:993:G:H2'	1:A:995:C:H41	1.73	0.53
1:A:1223:C:P	20:T:78:ARG:HH21	2.31	0.53
1:A:384:G:H2'	1:A:385:C:C6	2.43	0.53
1:A:236:A:H2'	1:A:237:G:H8	1.73	0.53
1:A:408:A:H2'	1:A:409:U:C6	2.44	0.53
1:A:1062:U:H2'	1:A:1063:C:C6	2.44	0.53
1:A:1518:MA6:O5'	1:A:1518:MA6:H8	2.08	0.53
1:A:673:A:H2'	1:A:674:G:C8	2.43	0.53
1:A:993:G:O2'	1:A:994:A:N7	2.41	0.53
1:A:1187:G:H2'	1:A:1188:A:H8	1.73	0.53
4:D:77:ILE:HG23	4:D:84:VAL:HG23	1.90	0.53
9:I:11:LEU:HD22	9:I:75:ILE:HD11	1.90	0.53
1:A:938:A:N3	1:A:1376:U:O2'	2.38	0.53
1:A:1417:G:O2'	1:A:1483:A:N6	2.41	0.53
23:W:37:U:H2'	23:W:38:A:H8	1.74	0.53
1:A:8:A:N7	5:E:206:LYS:HA	2.24	0.53
1:A:322:C:H2'	1:A:323:U:C6	2.43	0.53
1:A:936:C:C2	1:A:937:A:C8	2.97	0.53
2:B:43:LYS:NZ	3:C:17:GLY:O	2.34	0.53
1:A:820:U:H4'	1:A:821:G:OP2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:G:OP1	8:H:35:LYS:NZ	2.41	0.53
1:A:1354:U:H2'	1:A:1355:G:H8	1.73	0.53
1:A:1427:C:H2'	1:A:1428:A:H8	1.74	0.53
1:A:108:G:H5'	1:A:109:A:H5''	1.91	0.53
1:A:752:G:H5''	16:P:73:LYS:NZ	2.24	0.53
1:A:1169:A:H2'	1:A:1170:A:C8	2.44	0.52
5:E:100:ASN:OD1	5:E:111:ARG:NH1	2.33	0.52
1:A:1071:C:H2'	1:A:1072:G:C8	2.44	0.52
2:B:46:SER:OG	2:B:82:THR:O	2.26	0.52
5:E:65:TYR:OH	5:E:95:GLU:OE2	2.21	0.52
1:A:376:G:H2'	1:A:377:G:H8	1.73	0.52
1:A:1305:G:HO2'	1:A:1306:A:H8	1.57	0.52
12:L:111:THR:HG23	22:V:3:VAL:HG22	1.92	0.52
14:N:23:TYR:HB3	14:N:66:GLU:HB3	1.91	0.52
16:P:17:ARG:NH1	16:P:18:ASP:OD1	2.43	0.52
1:A:255:G:H2'	1:A:256:U:C6	2.45	0.52
1:A:1016:A:O2'	1:A:1217:C:O2'	2.25	0.52
1:A:261:U:OP2	21:U:74:ARG:NH1	2.39	0.52
1:A:451:A:H61	1:A:481:G:H5'	1.75	0.52
23:W:70:C:H2'	23:W:71:G:H8	1.73	0.52
1:A:41:G:H2'	1:A:42:G:H8	1.74	0.52
9:I:30:SER:HB2	9:I:33:LYS:HG3	1.92	0.52
1:A:312:C:H2'	1:A:313:A:H8	1.75	0.52
1:A:524:G:H2'	1:A:525:C:C6	2.45	0.52
1:A:1037:C:H2'	1:A:1038:C:C6	2.45	0.52
1:A:794:A:H2'	1:A:795:C:C6	2.44	0.52
1:A:1041:G:H2'	1:A:1042:A:C8	2.45	0.52
1:A:1425:U:O4	1:A:1475:G:O6	2.28	0.52
1:A:1488:G:H2'	1:A:1489:G:H8	1.75	0.52
7:G:11:HIS:HD2	7:G:12:PRO:HD2	1.75	0.52
1:A:178:C:C2	1:A:179:A:C8	2.98	0.52
1:A:635:A:H2'	1:A:636:U:C6	2.45	0.52
1:A:695:A:H2'	1:A:696:A:C8	2.45	0.51
1:A:868:C:H2'	1:A:869:G:O4'	2.10	0.51
1:A:1386:G:H2'	1:A:1387:G:C8	2.40	0.51
1:A:459:A:H2'	1:A:460:A:C8	2.45	0.51
2:B:18:THR:OG1	3:C:36:ASN:ND2	2.43	0.51
1:A:236:A:H2'	1:A:237:G:C8	2.44	0.51
1:A:1436:U:C2	1:A:1437:A:C8	2.98	0.51
1:A:638:U:C2	1:A:639:G:C8	2.99	0.51
1:A:223:A:H2'	1:A:224:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:A:N1	1:A:278:G:O2'	2.37	0.51
1:A:551:U:H2'	1:A:552:U:H6	1.75	0.51
1:A:264:C:O2'	18:R:66:PRO:O	2.28	0.51
1:A:1292:G:H2'	1:A:1293:C:H6	1.76	0.51
1:A:1343:G:H2'	1:A:1344:C:C6	2.46	0.51
2:B:40:ALA:HB3	2:B:42:LEU:HD11	1.93	0.51
1:A:356:A:N3	1:A:368:U:O2'	2.36	0.51
1:A:460:A:H2'	1:A:461:A:C8	2.46	0.51
1:A:806:C:H2'	1:A:807:A:H8	1.75	0.51
12:L:18:ASP:HB3	12:L:81:ASN:HB2	1.93	0.51
1:A:1117:A:N6	1:A:1156:G:H22	2.09	0.51
2:B:70:VAL:HG11	2:B:84:LEU:HB3	1.93	0.51
23:W:9:G:O2'	23:W:46:G:N3	2.33	0.51
1:A:500:G:H5''	13:M:121:ARG:NH1	2.25	0.51
1:A:945:G:C2	1:A:946:A:C8	2.98	0.51
23:W:37:U:H2'	23:W:38:A:C8	2.46	0.51
1:A:413:G:O2'	1:A:428:G:N2	2.44	0.51
1:A:676:A:H2'	1:A:677:U:H6	1.76	0.51
1:A:728:A:H2'	1:A:729:A:C8	2.45	0.51
1:A:728:A:H2'	1:A:729:A:H8	1.76	0.51
1:A:877:G:C2	1:A:878:A:C8	2.98	0.51
1:A:1261:A:N6	1:A:1274:A:HO2'	2.09	0.51
1:A:1524:C:H2'	1:A:1525:G:C8	2.46	0.51
2:B:71:ALA:N	2:B:89:ALA:HB2	2.26	0.51
11:K:6:ILE:HG22	11:K:102:LEU:HB3	1.93	0.51
23:W:72:C:H2'	23:W:73:A:H5'	1.92	0.51
1:A:312:C:H2'	1:A:313:A:C8	2.46	0.50
1:A:902:G:H2'	1:A:903:G:H8	1.75	0.50
1:A:1273:C:H2'	1:A:1274:A:O4'	2.10	0.50
1:A:1305:G:H21	1:A:1332:A:H2	1.58	0.50
2:B:54:LYS:HB3	2:B:58:GLY:HA2	1.92	0.50
2:B:71:ALA:H	2:B:89:ALA:HB2	1.75	0.50
3:C:4:VAL:HG11	3:C:212:LEU:HD21	1.93	0.50
1:A:358:U:H2'	1:A:359:G:C8	2.45	0.50
1:A:1175:G:N3	1:A:1176:A:C8	2.79	0.50
7:G:51:ILE:HD13	7:G:86:ARG:HH11	1.76	0.50
1:A:279:A:H5''	1:A:280:C:H3'	1.93	0.50
1:A:1037:C:H2'	1:A:1038:C:H6	1.76	0.50
1:A:1477:U:H2'	1:A:1478:U:C6	2.46	0.50
11:K:7:ARG:HG2	11:K:73:LEU:HD11	1.93	0.50
12:L:52:PHE:HE1	12:L:65:VAL:HG11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:U:H2'	1:A:591:U:H6	1.76	0.50
1:A:1120:C:H2'	1:A:1121:U:H6	1.77	0.50
19:S:10:PHE:HB3	24:X:14:U:H4'	1.93	0.50
1:A:159:G:N2	1:A:162:A:OP2	2.43	0.50
1:A:673:A:C6	1:A:734:G:C6	3.00	0.50
1:A:636:U:OP1	18:R:6:ARG:NH2	2.44	0.50
1:A:834:U:H2'	1:A:835:U:C6	2.47	0.50
1:A:1107:C:C4	1:A:1108:G:C8	2.99	0.50
1:A:1119:C:H2'	1:A:1120:C:H6	1.76	0.50
1:A:1345:U:C2	1:A:1377:A:C2	3.00	0.50
23:W:10:G:H2'	23:W:11:A:H8	1.77	0.50
23:W:32:G:N1	23:W:41:C:N3	2.59	0.50
1:A:390:U:H2'	1:A:391:G:C8	2.47	0.49
1:A:1096:C:H2'	1:A:1097:C:C6	2.48	0.49
1:A:1342:C:H2'	1:A:1343:G:H8	1.76	0.49
3:C:192:ASP:OD1	3:C:192:ASP:N	2.45	0.49
5:E:188:ARG:NH1	5:E:192:SER:O	2.34	0.49
23:W:67:C:H2'	23:W:68:C:O4'	2.12	0.49
1:A:636:U:P	18:R:6:ARG:HH21	2.35	0.49
1:A:765:G:N2	1:A:813:U:OP2	2.45	0.49
1:A:1039:G:H2'	1:A:1040:U:C6	2.46	0.49
7:G:2:ARG:HB3	7:G:91:ARG:HH11	1.76	0.49
1:A:323:U:H2'	1:A:324:G:O4'	2.12	0.49
1:A:500:G:H2'	1:A:501:C:H6	1.77	0.49
1:A:591:U:H2'	1:A:592:G:H8	1.77	0.49
1:A:1166:G:O2'	1:A:1167:A:OP1	2.26	0.49
1:A:1177:G:H2'	1:A:1178:G:O4'	2.12	0.49
2:B:66:ASP:N	2:B:66:ASP:OD1	2.44	0.49
5:E:55:LEU:O	5:E:59:GLN:HG2	2.12	0.49
1:A:997:U:O2'	1:A:998:C:H5'	2.12	0.49
1:A:1137:C:H1'	1:A:1138:G:N2	2.27	0.49
1:A:996:A:H2'	1:A:997:U:C6	2.48	0.49
13:M:36:ARG:HG2	13:M:38:TYR:HD1	1.78	0.49
14:N:86:TYR:O	14:N:90:ARG:HG2	2.13	0.49
23:W:51:U:O2	23:W:65:G:N2	2.32	0.49
1:A:792:A:H1'	1:A:794:A:N7	2.28	0.49
1:A:1027:C:N3	1:A:1028:C:N4	2.60	0.49
4:D:114:LYS:HD3	4:D:185:ASN:ND2	2.28	0.49
1:A:545:C:H5'	5:E:69:GLU:HB2	1.94	0.49
1:A:932:C:H2'	1:A:933:G:H8	1.78	0.49
1:A:1436:U:H2'	1:A:1437:A:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:10:G:N2	23:W:27:G:H1'	2.28	0.49
1:A:373:A:C2	1:A:374:A:C8	3.01	0.49
1:A:590:U:H2'	1:A:591:U:C6	2.48	0.48
2:B:39:ASP:OD1	2:B:40:ALA:N	2.46	0.48
14:N:17:ILE:O	14:N:20:THR:HG22	2.13	0.48
1:A:79:G:H2'	1:A:80:A:O4'	2.13	0.48
1:A:746:A:H2'	1:A:747:A:C8	2.47	0.48
1:A:255:G:P	18:R:71:LYS:HZ3	2.36	0.48
1:A:299:G:H2'	1:A:300:A:C8	2.48	0.48
1:A:407:U:H2'	1:A:408:A:C8	2.48	0.48
1:A:635:A:H2'	1:A:636:U:H6	1.78	0.48
1:A:912:C:H2'	1:A:913:A:C8	2.48	0.48
19:S:36:SER:HA	19:S:72:ASP:HB2	1.95	0.48
1:A:837:U:H2'	1:A:838:G:H8	1.77	0.48
1:A:923:A:H2'	1:A:924:C:C6	2.48	0.48
6:F:89:HIS:CE1	6:F:138:ARG:HD2	2.48	0.48
1:A:460:A:H2'	1:A:461:A:H8	1.78	0.48
1:A:641:U:H1'	1:A:642:A:OP2	2.14	0.48
1:A:1060:U:H2'	1:A:1061:G:H8	1.78	0.48
1:A:1109:C:C2	1:A:1110:A:C8	3.02	0.48
1:A:1178:G:H3'	10:J:99:ARG:NH2	2.28	0.48
1:A:1404:C:H2'	1:A:1405:G:H8	1.79	0.48
1:A:715:A:H2'	1:A:716:A:C8	2.48	0.48
1:A:763:G:H2'	1:A:764:C:C6	2.48	0.48
1:A:1173:U:C2	1:A:1174:G:C8	3.02	0.48
1:A:1292:G:H2'	1:A:1293:C:C6	2.49	0.48
1:A:1524:C:H2'	1:A:1525:G:H8	1.79	0.48
20:T:80:TYR:CZ	20:T:82:GLY:HA2	2.49	0.48
23:W:44:A:H2'	23:W:45:A:C8	2.49	0.48
1:A:712:A:H2'	1:A:713:G:C8	2.49	0.48
1:A:715:A:H2'	1:A:716:A:H8	1.79	0.48
1:A:928:G:H2'	1:A:929:G:C8	2.49	0.48
18:R:26:GLU:HA	18:R:41:THR:HA	1.95	0.48
1:A:160:A:H2'	1:A:161:A:O4'	2.13	0.48
1:A:399:G:H2'	1:A:400:C:C6	2.48	0.48
1:A:658:C:O4'	16:P:22:THR:HG21	2.13	0.48
5:E:139:PRO:HA	5:E:182:PHE:HD2	1.78	0.48
9:I:39:VAL:HG21	9:I:110:VAL:HG12	1.95	0.48
11:K:53:ILE:HD11	11:K:61:ALA:HB1	1.96	0.48
22:V:4:ILE:HD13	22:V:19:PHE:HD1	1.77	0.48
23:W:34:U:O2	23:W:36:A:H3'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:C:H2'	1:A:419:C:C6	2.49	0.48
1:A:996:A:N7	1:A:1046:A:O2'	2.47	0.48
23:W:37:U:C2	23:W:38:A:C8	3.01	0.48
1:A:21:G:H2'	1:A:22:G:H8	1.77	0.48
2:B:50:ALA:HA	2:B:53:PHE:HD1	1.78	0.48
3:C:31:ILE:HD13	3:C:39:HIS:CD2	2.49	0.48
1:A:950:U:H2'	1:A:951:G:C8	2.49	0.47
1:A:1095:U:H2'	1:A:1096:C:C6	2.49	0.47
1:A:1435:G:H2'	1:A:1436:U:C6	2.49	0.47
9:I:112:THR:HG23	9:I:115:ALA:H	1.78	0.47
15:O:64:CYS:HB3	15:O:68:GLY:H	1.79	0.47
24:X:11:U:H1'	24:X:12:A:OP2	2.14	0.47
1:A:335:C:C2	1:A:336:A:C8	3.02	0.47
1:A:1495:U:H2'	1:A:1496:C:H6	1.79	0.47
10:J:65:ILE:HD13	10:J:79:ILE:HG23	1.96	0.47
1:A:939:G:H2'	1:A:940:C:C6	2.49	0.47
2:B:129:ALA:HA	2:B:166:VAL:O	2.13	0.47
3:C:124:GLY:O	3:C:126:PHE:N	2.45	0.47
10:J:34:SER:HB2	10:J:37:GLN:HG3	1.95	0.47
12:L:123:PRO:HD2	22:V:38:TYR:HB2	1.95	0.47
24:X:7:G:H2'	24:X:8:A:C8	2.49	0.47
1:A:928:G:H2'	1:A:929:G:H8	1.79	0.47
1:A:996:A:C4	1:A:997:U:C5	3.02	0.47
22:V:51:SER:O	22:V:55:ARG:HG3	2.15	0.47
1:A:312:C:C2	1:A:313:A:C8	3.03	0.47
1:A:335:C:H2'	1:A:336:A:C8	2.49	0.47
1:A:996:A:H2'	1:A:997:U:H6	1.79	0.47
2:B:30:ALA:HB3	2:B:37:LEU:HB2	1.96	0.47
6:F:110:ALA:HB1	6:F:137:VAL:HG23	1.95	0.47
8:H:5:ARG:HH11	8:H:7:ILE:HB	1.79	0.47
1:A:98:A:H2'	1:A:99:C:C6	2.50	0.47
1:A:100:G:C4	1:A:101:A:C8	3.02	0.47
1:A:410:G:N1	1:A:431:A:OP2	2.37	0.47
1:A:736:C:H2'	1:A:737:C:C6	2.49	0.47
1:A:745:G:C2	1:A:746:A:C5	3.03	0.47
1:A:874:G:C6	1:A:875:U:C4	3.03	0.47
1:A:918:A:H2'	1:A:919:A:C8	2.49	0.47
1:A:1140:C:O2'	1:A:1141:C:H6	1.97	0.47
4:D:73:PRO:O	4:D:77:ILE:HG13	2.13	0.47
23:W:51:U:H2'	23:W:52:C:C6	2.49	0.47
1:A:17:U:H2'	1:A:18:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:A:H2'	1:A:172:A:C8	2.50	0.47
1:A:201:G:HO2'	1:A:469:C:HO2'	1.61	0.47
1:A:389:A:H3'	1:A:390:U:H6	1.78	0.47
1:A:552:U:C2	1:A:553:A:C8	3.03	0.47
1:A:882:C:O2'	1:A:883:C:H5'	2.14	0.47
1:A:1163:A:H2'	1:A:1164:G:C8	2.49	0.47
1:A:1241:G:H2'	1:A:1242:G:H8	1.79	0.47
1:A:1425:U:H2'	1:A:1426:G:C8	2.48	0.47
3:C:196:VAL:HB	3:C:199:VAL:HG23	1.96	0.47
8:H:72:THR:OG1	8:H:142:HIS:NE2	2.33	0.47
11:K:59:LYS:HE2	11:K:62:ARG:NH2	2.30	0.47
12:L:29:ASN:OD1	12:L:30:THR:N	2.48	0.47
20:T:36:ARG:NH2	20:T:75:ALA:O	2.47	0.47
23:W:6:G:H2'	23:W:7:G:C8	2.50	0.47
1:A:398:U:H2'	1:A:399:G:H8	1.78	0.47
1:A:1518:MA6:H2'	1:A:1519:MA6:C8	2.45	0.47
8:H:65:ALA:O	8:H:69:VAL:HG23	2.14	0.47
13:M:79:VAL:O	13:M:103:ASP:HB2	2.14	0.47
23:W:28:U:C2	23:W:29:C:C5	3.03	0.47
1:A:407:U:H2'	1:A:408:A:H8	1.79	0.47
1:A:203:G:O2'	1:A:465:A:N1	2.47	0.47
1:A:219:U:H2'	1:A:220:G:C8	2.44	0.47
1:A:983:A:H5'	1:A:984:C:OP2	2.14	0.47
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.97	0.47
1:A:1489:G:H2'	1:A:1490:U:C6	2.50	0.47
3:C:188:ASP:HB2	3:C:204:ASP:OD2	2.15	0.47
5:E:8:LYS:HB3	5:E:21:LEU:HB3	1.97	0.47
1:A:526:C:OP2	13:M:88:LYS:HE2	2.16	0.46
1:A:1263:C:H2'	1:A:1264:U:H6	1.80	0.46
1:A:1315:U:O2	1:A:1360:A:H2	1.96	0.46
19:S:29:LEU:HB3	19:S:68:LEU:HD11	1.97	0.46
23:W:65:G:H2'	23:W:66:C:H6	1.79	0.46
1:A:88:U:H2'	1:A:89:U:H5'	1.97	0.46
1:A:1208:C:H2'	1:A:1209:C:H6	1.80	0.46
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.46
2:B:73:ASP:OD1	2:B:73:ASP:N	2.47	0.46
1:A:415:A:C4	1:A:416:G:C8	3.04	0.46
1:A:1250:A:N3	1:A:1370:G:O2'	2.47	0.46
1:A:427:U:OP2	1:A:428:G:O2'	2.26	0.46
1:A:602:A:H2'	1:A:603:U:C6	2.51	0.46
1:A:645:G:C2	1:A:646:G:C8	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:C:H2'	1:A:738:C:C6	2.51	0.46
4:D:42:TYR:CZ	4:D:90:VAL:HG11	2.51	0.46
12:L:83:GLU:HB2	12:L:109:ASN:HB2	1.96	0.46
14:N:83:LEU:HD11	20:T:65:GLU:HB3	1.95	0.46
1:A:62:U:H2'	1:A:63:C:C6	2.51	0.46
1:A:881:G:OP1	13:M:9:ARG:NH2	2.48	0.46
18:R:17:MET:HG3	18:R:20:SER:HB2	1.97	0.46
23:W:29:C:C2	23:W:30:G:C8	3.04	0.46
1:A:763:G:H2'	1:A:764:C:H6	1.81	0.46
1:A:1004:A:H2'	1:A:1005:A:O4'	2.16	0.46
1:A:1319:A:C8	1:A:1323:G:C5	3.03	0.46
1:A:1426:G:C6	1:A:1475:G:C6	3.04	0.46
10:J:115:LYS:HB2	10:J:118:LEU:HD12	1.97	0.46
1:A:110:C:H2'	1:A:111:G:O4'	2.16	0.46
1:A:538:G:H2'	1:A:539:A:H8	1.81	0.46
1:A:621:A:H2'	1:A:622:A:C8	2.51	0.46
1:A:705:G:C5	1:A:706:A:C8	3.04	0.46
1:A:1013:G:N2	1:A:1016:A:OP2	2.25	0.46
1:A:1184:G:C2	1:A:1185:G:C8	3.04	0.46
1:A:1352:C:H2'	1:A:1353:G:C8	2.50	0.46
1:A:381:C:H2'	1:A:382:A:O4'	2.16	0.46
1:A:593:U:H2'	1:A:594:U:C6	2.51	0.46
1:A:934:C:C4	1:A:1345:U:C5	3.04	0.46
5:E:9:LEU:HD13	5:E:32:CYS:HB3	1.97	0.46
23:W:28:U:H2'	23:W:29:C:H6	1.81	0.46
1:A:768:A:H4'	1:A:1523:G:N2	2.31	0.46
13:M:46:ASN:ND2	13:M:89:D2T:OD2	2.49	0.46
1:A:202:G:O2'	1:A:468:A:H8	1.98	0.46
1:A:253:A:H2'	1:A:254:G:C8	2.51	0.46
1:A:471:U:H2'	1:A:472:U:C6	2.51	0.46
1:A:567:G:H2'	1:A:568:G:O4'	2.16	0.46
24:X:19:U:H2'	24:X:20:U:O4'	2.16	0.46
1:A:826:C:H2'	1:A:827:U:C6	2.52	0.45
1:A:908:A:H2'	1:A:909:A:C8	2.50	0.45
1:A:1121:U:H2'	1:A:1122:U:H6	1.81	0.45
5:E:174:ASP:OD2	5:E:177:LYS:NZ	2.32	0.45
8:H:110:LYS:HB2	8:H:110:LYS:HE3	1.70	0.45
23:W:51:U:H2'	23:W:52:C:H6	1.80	0.45
1:A:600:A:H2'	1:A:601:G:H8	1.81	0.45
1:A:636:U:H2'	1:A:637:C:H6	1.80	0.45
1:A:954:G:H2'	1:A:955:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:U:H2'	1:A:1496:C:C6	2.51	0.45
2:B:75:VAL:O	2:B:82:THR:HG22	2.17	0.45
23:W:52:C:H2'	23:W:53:G:O4'	2.17	0.45
1:A:1072:G:H2'	1:A:1073:U:C6	2.51	0.45
1:A:1387:G:H2'	1:A:1388:C:H6	1.81	0.45
10:J:58:VAL:HG13	10:J:59:GLU:HG2	1.98	0.45
23:W:28:U:H2'	23:W:29:C:C6	2.52	0.45
1:A:201:G:O2'	1:A:469:C:O2'	2.29	0.45
1:A:429:U:H3'	5:E:9:LEU:HD12	1.99	0.45
1:A:490:C:H2'	1:A:491:G:H8	1.81	0.45
1:A:1209:C:C2	1:A:1210:C:C5	3.05	0.45
1:A:1512:U:H2'	1:A:1513:A:H8	1.82	0.45
1:A:444:G:C6	1:A:491:G:C6	3.04	0.45
1:A:551:U:H2'	1:A:552:U:C6	2.51	0.45
1:A:602:A:H2'	1:A:603:U:H6	1.81	0.45
1:A:689:C:OP1	12:L:46:THR:OG1	2.21	0.45
1:A:707:U:C2	1:A:708:C:C5	3.05	0.45
1:A:923:A:H2'	1:A:924:C:H6	1.81	0.45
1:A:1033:G:H2'	1:A:1034:G:O4'	2.17	0.45
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.17	0.45
3:C:117:LEU:HD12	3:C:120:GLN:NE2	2.32	0.45
1:A:237:G:H5''	18:R:27:ARG:NH2	2.32	0.45
2:B:69:ASP:OD1	2:B:69:ASP:N	2.49	0.45
14:N:11:ASP:HA	14:N:45:ILE:HB	1.99	0.45
14:N:81:MET:SD	14:N:92:ARG:HB3	2.57	0.45
1:A:481:G:O2'	1:A:483:C:N4	2.50	0.45
1:A:539:A:H2'	1:A:540:G:H8	1.80	0.45
1:A:674:G:N2	1:A:717:U:O2	2.44	0.45
1:A:855:U:H2'	1:A:856:C:H6	1.82	0.45
1:A:1488:G:H2'	1:A:1489:G:C8	2.52	0.45
19:S:30:LYS:HA	19:S:33:ILE:HG12	1.99	0.45
1:A:377:G:H2'	1:A:378:G:H8	1.82	0.45
1:A:920:U:H2'	1:A:921:U:C6	2.52	0.45
1:A:925:G:C2	1:A:927:G:C8	3.05	0.45
1:A:1517:G:H3'	1:A:1518:MA6:H8	1.99	0.45
15:O:54:ASP:HA	15:O:59:ARG:HD3	1.99	0.45
1:A:562:U:H1'	13:M:12:ARG:HB3	1.99	0.45
1:A:736:C:H2'	1:A:737:C:H6	1.82	0.45
1:A:780:A:N6	1:A:801:U:OP2	2.47	0.45
1:A:1442:G:H2'	1:A:1443:C:C6	2.52	0.45
10:J:28:ILE:HG13	10:J:63:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:A:H5'	1:A:281:G:O4'	2.17	0.44
1:A:833:G:H2'	1:A:834:U:C6	2.52	0.44
19:S:74:HIS:O	19:S:75:GLN:HG3	2.17	0.44
23:W:49:C:H4'	23:W:50:G:H5''	2.00	0.44
1:A:513:C:H2'	1:A:514:C:C6	2.52	0.44
1:A:722:G:H5'	1:A:723:U:OP1	2.17	0.44
1:A:890:G:O2'	1:A:906:A:N6	2.51	0.44
1:A:965:U:H5''	1:A:966:2MG:OP1	2.17	0.44
1:A:1014:A:N3	1:A:1219:A:H1'	2.33	0.44
1:A:1319:A:C8	1:A:1323:G:C6	3.05	0.44
6:F:81:LEU:HG	6:F:147:MET:SD	2.58	0.44
1:A:253:A:H2'	1:A:254:G:H8	1.83	0.44
1:A:338:A:H2'	1:A:339:C:H6	1.82	0.44
1:A:417:G:H2'	1:A:418:C:C6	2.52	0.44
1:A:552:U:H2'	1:A:553:A:H8	1.81	0.44
6:F:150:PRO:HA	6:F:153:VAL:HG22	2.00	0.44
1:A:303:A:H2'	1:A:304:U:O4'	2.18	0.44
1:A:1088:G:H21	1:A:1167:A:N6	2.15	0.44
1:A:1179:A:H2'	1:A:1180:A:O4'	2.17	0.44
1:A:1238:A:H2	1:A:1241:G:N3	2.15	0.44
1:A:1512:U:H2'	1:A:1513:A:C8	2.52	0.44
4:D:130:PHE:O	4:D:134:MET:HG2	2.17	0.44
1:A:613:C:H2'	1:A:614:C:C6	2.53	0.44
1:A:684:U:H2'	1:A:685:G:O4'	2.18	0.44
1:A:842:U:H5'	1:A:843:U:OP2	2.18	0.44
1:A:855:U:H2'	1:A:856:C:C6	2.53	0.44
1:A:1418:A:C4	1:A:1419:G:H1'	2.53	0.44
12:L:88:GLY:O	12:L:93:ARG:NH1	2.50	0.44
13:M:80:ILE:HD12	13:M:97:THR:HG22	2.00	0.44
1:A:35:G:H2'	1:A:36:C:C6	2.52	0.44
1:A:89:U:H2'	1:A:90:C:C5	2.53	0.44
1:A:1422:G:N2	1:A:1478:U:O2	2.30	0.44
15:O:73:PHE:CZ	15:O:78:GLY:HA2	2.52	0.44
22:V:31:GLU:OE1	22:V:34:ARG:NE	2.50	0.44
1:A:41:G:H2'	1:A:42:G:C8	2.52	0.44
1:A:268:U:H2'	1:A:269:C:C6	2.53	0.44
1:A:676:A:H2'	1:A:677:U:C6	2.53	0.44
1:A:719:C:O2'	19:S:38:LYS:HB3	2.17	0.44
1:A:801:U:C2	1:A:802:A:C8	3.06	0.44
1:A:825:A:H2'	1:A:826:C:H6	1.82	0.44
23:W:17:C:H2'	23:W:18:U:C5	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:U:H2'	1:A:21:G:O4'	2.17	0.44
1:A:525:C:H2'	1:A:526:C:C6	2.53	0.44
12:L:18:ASP:HA	12:L:81:ASN:O	2.18	0.44
18:R:64:CYS:SG	18:R:74:THR:OG1	2.64	0.44
1:A:45:G:H2'	1:A:46:G:C8	2.52	0.44
1:A:739:C:O2'	16:P:42:HIS:ND1	2.49	0.44
1:A:1263:C:H2'	1:A:1264:U:C6	2.53	0.44
1:A:1315:U:H2'	1:A:1316:G:O4'	2.18	0.44
1:A:1381:U:C2	1:A:1382:C:C6	3.06	0.44
1:A:82:G:N1	1:A:88:U:N3	2.66	0.43
1:A:284:C:H2'	1:A:285:C:H6	1.84	0.43
1:A:384:G:H2'	1:A:385:C:H6	1.81	0.43
1:A:1417:G:N2	1:A:1482:G:H2'	2.32	0.43
6:F:90:THR:HB	6:F:135:ASN:ND2	2.33	0.43
23:W:68:C:C2	23:W:69:C:C5	3.06	0.43
1:A:591:U:C2	1:A:592:G:C8	3.07	0.43
1:A:920:U:H2'	1:A:921:U:H6	1.83	0.43
1:A:1123:U:O2'	1:A:1124:G:H5'	2.18	0.43
1:A:1178:G:H3'	10:J:99:ARG:HH22	1.83	0.43
23:W:32:G:C2	23:W:41:C:C2	3.06	0.43
24:X:17:U:H2'	24:X:18:G:O4'	2.18	0.43
1:A:382:A:H2'	1:A:383:A:C8	2.53	0.43
1:A:902:G:N3	1:A:903:G:C8	2.86	0.43
5:E:56:ARG:HH12	5:E:63:ARG:HH21	1.65	0.43
10:J:24:GLY:HA3	10:J:62:ASP:OD2	2.18	0.43
10:J:38:TYR:OH	10:J:75:GLN:NE2	2.50	0.43
1:A:360:G:H2'	1:A:361:G:C8	2.53	0.43
1:A:1120:C:H2'	1:A:1121:U:C6	2.53	0.43
4:D:111:LEU:HD22	4:D:146:ALA:HB2	1.99	0.43
4:D:204:LYS:HB3	4:D:204:LYS:HE2	1.61	0.43
8:H:40:GLU:OE2	10:J:41:ARG:NH1	2.51	0.43
17:Q:44:SER:OG	17:Q:45:GLU:N	2.51	0.43
1:A:255:G:H2'	1:A:256:U:H6	1.82	0.43
12:L:81:ASN:HD21	12:L:106:ARG:NH2	2.16	0.43
23:W:23:G:H2'	23:W:24:C:H6	1.83	0.43
23:W:27:G:C2	23:W:28:U:C6	3.07	0.43
23:W:52:C:C2	23:W:65:G:C2	3.06	0.43
1:A:338:A:H2'	1:A:339:C:C6	2.54	0.43
1:A:1422:G:C2	1:A:1423:G:C5	3.07	0.43
2:B:4:SER:HB3	2:B:7:GLN:HG3	1.99	0.43
4:D:22:TRP:HB3	4:D:59:ARG:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:ASN:OD1	4:D:26:THR:N	2.51	0.43
1:A:664:G:H2'	1:A:666:G:OP1	2.19	0.43
1:A:922:G:H2'	1:A:923:A:C8	2.53	0.43
3:C:7:ARG:O	3:C:11:LYS:HG2	2.19	0.43
5:E:27:ALA:HB3	5:E:30:THR:HG23	2.01	0.43
7:G:8:PHE:HB2	7:G:84:VAL:HG21	2.00	0.43
1:A:19:A:H2'	1:A:20:U:H6	1.84	0.43
1:A:408:A:H2'	1:A:409:U:H6	1.82	0.43
1:A:938:A:H2	1:A:1376:U:H1'	1.84	0.43
1:A:1160:G:C2	1:A:1161:C:C6	3.07	0.43
1:A:1268:G:H1'	1:A:1326:U:O2'	2.19	0.43
1:A:1417:G:H2'	1:A:1482:G:N2	2.34	0.43
1:A:1495:U:C2	1:A:1496:C:C5	3.07	0.43
4:D:72:ARG:O	4:D:76:VAL:HG23	2.19	0.43
5:E:190:ASP:OD1	5:E:190:ASP:N	2.52	0.43
20:T:21:LYS:HB2	20:T:21:LYS:HE3	1.81	0.43
24:X:8:A:H2'	24:X:9:G:H8	1.82	0.43
1:A:859:G:OP2	1:A:869:G:N1	2.38	0.43
1:A:893:C:H2'	1:A:894:G:C8	2.54	0.43
1:A:1436:U:H2'	1:A:1437:A:C8	2.53	0.43
2:B:86:ARG:HH21	2:B:90:LYS:HE2	1.84	0.43
14:N:40:ALA:HB3	14:N:43:VAL:HG13	1.99	0.43
1:A:138:G:C6	1:A:226:G:C6	3.07	0.43
12:L:34:ILE:HB	12:L:74:VAL:HG21	2.01	0.43
21:U:51:PHE:HA	21:U:54:MET:HG2	2.01	0.43
23:W:45:A:H2'	23:W:46:G:O4'	2.19	0.43
1:A:411:A:C6	1:A:429:U:C4	3.07	0.42
1:A:562:U:C5	13:M:15:LYS:HD2	2.54	0.42
1:A:1459:G:H2'	1:A:1460:C:C6	2.54	0.42
2:B:86:ARG:O	2:B:90:LYS:HG3	2.18	0.42
5:E:170:TRP:CE2	5:E:186:PRO:HB3	2.53	0.42
11:K:20:GLN:O	11:K:24:GLU:HG2	2.18	0.42
23:W:33:OMC:C2	23:W:39:A:N6	2.87	0.42
1:A:45:G:H2'	1:A:46:G:H8	1.84	0.42
1:A:321:A:H2'	1:A:322:C:C6	2.54	0.42
1:A:685:G:N2	1:A:704:A:OP2	2.45	0.42
1:A:737:C:H2'	1:A:738:C:H6	1.83	0.42
1:A:842:U:H3'	1:A:843:U:H5''	2.00	0.42
1:A:1525:G:H2'	1:A:1526:G:H8	1.84	0.42
3:C:20:THR:HG22	3:C:39:HIS:CE1	2.54	0.42
4:D:84:VAL:O	4:D:88:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:44:SER:N	17:Q:47:GLU:OE1	2.50	0.42
24:X:18:G:O5'	24:X:18:G:H8	2.01	0.42
1:A:343:U:H2'	1:A:345:C:C5	2.55	0.42
1:A:680:C:H2'	1:A:681:A:H8	1.84	0.42
1:A:1206:G:C4	1:A:1207:2MG:C8	3.08	0.42
1:A:1320:C:N3	20:T:36:ARG:NH1	2.67	0.42
1:A:1326:U:H2'	1:A:1327:C:C6	2.54	0.42
13:M:35:THR:N	13:M:54:ARG:O	2.51	0.42
21:U:34:LYS:HB3	21:U:34:LYS:HE2	1.85	0.42
22:V:7:ARG:HB3	22:V:10:GLU:HB2	2.01	0.42
1:A:866:C:H42	1:A:873:A:H2	1.67	0.42
3:C:167:ASP:HB2	3:C:191:SER:HA	2.01	0.42
6:F:38:VAL:HG11	6:F:114:VAL:HG22	1.99	0.42
1:A:154:U:H2'	1:A:155:A:H8	1.85	0.42
1:A:222:C:H2'	1:A:223:A:H8	1.83	0.42
1:A:636:U:H2'	1:A:637:C:C6	2.55	0.42
1:A:752:G:H5''	16:P:73:LYS:HZ1	1.85	0.42
21:U:44:LYS:HB3	21:U:44:LYS:HE2	1.82	0.42
1:A:84:U:O4	1:A:87:C:O2'	2.36	0.42
1:A:294:U:H2'	1:A:295:C:C6	2.54	0.42
1:A:865:A:H2'	1:A:866:C:O4'	2.20	0.42
1:A:917:G:H2'	1:A:918:A:C8	2.54	0.42
1:A:1316:G:N1	1:A:1319:A:OP2	2.49	0.42
7:G:22:ILE:HG23	7:G:39:LEU:HD21	2.02	0.42
23:W:71:G:C2	23:W:72:C:C2	3.08	0.42
1:A:392:C:C2	1:A:393:A:C8	3.08	0.42
1:A:886:G:C6	1:A:887:G:C5	3.08	0.42
1:A:1426:G:H2'	1:A:1427:C:H6	1.85	0.42
2:B:169:SER:O	2:B:171:ARG:N	2.52	0.42
5:E:104:ARG:HH12	5:E:111:ARG:NH2	2.18	0.42
11:K:3:ASN:ND2	11:K:79:PRO:O	2.52	0.42
21:U:35:VAL:HG21	21:U:54:MET:SD	2.60	0.42
1:A:462:G:H2'	1:A:463:U:O4'	2.19	0.42
1:A:1005:A:OP2	1:A:1024:G:N2	2.51	0.42
1:A:1019:A:H2'	1:A:1020:G:O4'	2.19	0.42
1:A:1122:U:H2'	1:A:1123:U:C6	2.54	0.42
3:C:120:GLN:HB2	3:C:126:PHE:HE2	1.85	0.42
14:N:77:ILE:O	14:N:81:MET:HG2	2.19	0.42
1:A:234:C:H2'	1:A:235:C:H6	1.85	0.42
1:A:252:U:N3	1:A:253:A:N7	2.68	0.42
1:A:769:G:H4'	1:A:1513:A:H4'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:A:H1'	1:A:982:U:O4	2.20	0.42
1:A:1006:G:C6	1:A:1024:G:H1'	2.55	0.42
5:E:56:ARG:HA	5:E:56:ARG:HD3	1.64	0.42
11:K:39:PRO:HB3	11:K:74:VAL:HG22	2.01	0.42
23:W:10:G:H2'	23:W:11:A:C8	2.55	0.42
1:A:459:A:H2'	1:A:460:A:H8	1.84	0.41
1:A:936:C:C4	1:A:937:A:N7	2.88	0.41
3:C:60:ILE:HD13	3:C:160:ALA:HB2	2.02	0.41
3:C:131:LYS:HA	3:C:134:ALA:HB3	2.02	0.41
3:C:194:ASP:OD1	3:C:194:ASP:N	2.52	0.41
6:F:133:PRO:HA	6:F:136:VAL:HG12	2.01	0.41
8:H:111:ARG:NH2	8:H:113:ASP:OD1	2.53	0.41
12:L:70:CYS:O	12:L:74:VAL:HG23	2.20	0.41
14:N:49:SER:H	14:N:52:GLN:NE2	2.18	0.41
1:A:264:C:O3'	18:R:65:ARG:NH1	2.53	0.41
1:A:538:G:H2'	1:A:539:A:C8	2.55	0.41
1:A:946:A:O2'	1:A:1333:A:N3	2.47	0.41
1:A:1291:U:H2'	1:A:1292:G:H8	1.85	0.41
1:A:1527:U:H2'	1:A:1528:U:C6	2.55	0.41
10:J:35:LEU:HD11	10:J:48:VAL:HG11	2.01	0.41
12:L:50:SER:HA	12:L:69:ARG:NH1	2.34	0.41
13:M:68:GLY:O	13:M:99:ARG:NH1	2.50	0.41
1:A:195:A:O2'	1:A:196:A:H5'	2.19	0.41
1:A:765:G:H3'	1:A:812:G:H22	1.84	0.41
1:A:767:A:H2'	1:A:768:A:H8	1.86	0.41
1:A:1008:U:H2'	1:A:1009:U:O4'	2.19	0.41
1:A:1143:G:H2'	1:A:1144:G:H8	1.85	0.41
1:A:1174:G:C2'	1:A:1175:G:H5'	2.50	0.41
1:A:1244:G:H2'	1:A:1245:C:H6	1.85	0.41
1:A:1408:A:H2'	1:A:1409:C:C6	2.55	0.41
23:W:26:C:C4	23:W:27:G:C8	3.08	0.41
1:A:34:C:H2'	1:A:35:G:C8	2.53	0.41
1:A:284:C:H2'	1:A:285:C:C6	2.54	0.41
1:A:442:G:C6	1:A:443:C:C4	3.09	0.41
1:A:677:U:O2	1:A:777:A:O2'	2.36	0.41
1:A:1017:U:O2'	1:A:1018:G:O4'	2.38	0.41
4:D:11:ARG:HB3	4:D:15:VAL:HG12	2.02	0.41
7:G:41:ASP:OD2	7:G:58:HIS:NE2	2.47	0.41
7:G:42:TRP:CD1	7:G:103:VAL:HG23	2.56	0.41
12:L:93:ARG:NH2	12:L:112:ASP:OD2	2.53	0.41
21:U:67:ILE:HD12	21:U:67:ILE:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:C:H2'	1:A:68:G:C8	2.56	0.41
1:A:158:G:C6	1:A:164:G:C5	3.09	0.41
1:A:414:A:C4	1:A:415:A:C8	3.08	0.41
1:A:471:U:H2'	1:A:472:U:H6	1.85	0.41
1:A:1013:G:N2	1:A:1015:G:H3'	2.36	0.41
1:A:1534:A:O4'	22:V:58:LYS:NZ	2.46	0.41
1:A:191:G:H2'	1:A:192:A:C8	2.55	0.41
1:A:374:A:C6	1:A:375:U:C4	3.09	0.41
1:A:522:C:OP2	13:M:66:TYR:OH	2.33	0.41
1:A:1417:G:H2'	1:A:1482:G:H22	1.85	0.41
8:H:58:GLU:H	8:H:58:GLU:CD	2.20	0.41
12:L:92:GLY:C	12:L:94:GLU:H	2.24	0.41
13:M:37:VAL:HG22	13:M:53:CYS:SG	2.61	0.41
1:A:10:A:H2'	1:A:11:G:H8	1.86	0.41
1:A:376:G:H5''	17:Q:5:ARG:HB2	2.03	0.41
1:A:1326:U:H2'	1:A:1327:C:H6	1.83	0.41
3:C:157:LEU:HD13	3:C:179:LEU:HD13	2.03	0.41
6:F:62:LYS:HB2	6:F:62:LYS:HE3	1.73	0.41
20:T:19:VAL:HG11	20:T:44:MET:HG2	2.02	0.41
1:A:340:U:H2'	1:A:341:C:H6	1.86	0.41
1:A:393:A:C2	1:A:394:G:C8	3.09	0.41
1:A:893:C:H2'	1:A:894:G:H8	1.85	0.41
1:A:1240:U:OP1	8:H:116:MET:HB2	2.21	0.41
1:A:1426:G:H2'	1:A:1427:C:C6	2.56	0.41
1:A:1534:A:C2'	1:A:1535:C:H5'	2.51	0.41
8:H:74:GLU:HG2	8:H:75:VAL:H	1.86	0.41
19:S:11:CYS:SG	19:S:48:ARG:HG2	2.60	0.41
23:W:17:C:H5''	23:W:18:U:C6	2.55	0.41
1:A:91:U:C2	1:A:92:U:C5	3.09	0.41
1:A:204:U:H2'	1:A:205:A:C8	2.56	0.41
1:A:313:A:H2'	1:A:314:C:C6	2.56	0.41
1:A:358:U:C2	1:A:359:G:C8	3.08	0.41
1:A:721:G:H4'	1:A:722:G:O4'	2.21	0.41
1:A:842:U:H3'	1:A:843:U:C5'	2.51	0.41
1:A:951:G:OP2	14:N:101:ARG:NH2	2.53	0.41
1:A:1081:A:C4	1:A:1082:A:C8	3.09	0.41
1:A:1114:C:H2'	1:A:1115:U:C6	2.56	0.41
1:A:1124:G:N2	1:A:1125:U:O4	2.41	0.41
1:A:1174:G:H2'	1:A:1175:G:H5'	2.03	0.41
1:A:1175:G:C4	1:A:1176:A:C8	3.09	0.41
1:A:1367:C:P	10:J:114:LYS:HZ1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ALA:O	2:B:105:ALA:N	2.52	0.41
5:E:170:TRP:CD1	5:E:171:LEU:HG	2.56	0.41
13:M:53:CYS:SG	13:M:67:ILE:HD11	2.61	0.41
23:W:51:U:O4	23:W:65:G:O6	2.39	0.41
1:A:6:G:O2'	1:A:7:A:H8	2.03	0.41
1:A:86:G:H2'	1:A:87:C:C5	2.56	0.41
1:A:455:G:C2	1:A:478:A:C2	3.09	0.41
1:A:527:G7M:H2'	1:A:528:C:H5'	2.02	0.41
1:A:1179:A:OP2	10:J:99:ARG:NH2	2.54	0.41
14:N:34:LEU:HA	14:N:34:LEU:HD23	1.83	0.41
1:A:35:G:N3	13:M:115:SER:OG	2.53	0.40
1:A:827:U:H2'	1:A:870:U:O4	2.20	0.40
1:A:1539:C:P	22:V:21:ARG:HH22	2.44	0.40
4:D:6:HIS:HB2	15:O:89:MET:CE	2.50	0.40
16:P:67:LEU:HD23	16:P:67:LEU:HA	1.89	0.40
23:W:71:G:C6	23:W:72:C:C4	3.09	0.40
1:A:161:A:H2'	1:A:162:A:C8	2.56	0.40
1:A:418:C:H2'	1:A:419:C:H6	1.86	0.40
1:A:1121:U:C2	1:A:1122:U:C5	3.09	0.40
1:A:1143:G:N3	1:A:1144:G:C8	2.90	0.40
5:E:10:LYS:HE3	5:E:10:LYS:HB2	1.88	0.40
6:F:111:MET:HE2	6:F:111:MET:HB3	1.94	0.40
10:J:11:ARG:O	10:J:106:ARG:NE	2.54	0.40
12:L:64:GLN:HB2	12:L:95:SER:OG	2.22	0.40
1:A:453:G:C4	1:A:454:G:C8	3.09	0.40
1:A:927:G:C2	1:A:928:G:C8	3.09	0.40
1:A:1061:G:H2'	1:A:1062:U:C6	2.56	0.40
1:A:1427:C:H2'	1:A:1428:A:C8	2.55	0.40
7:G:2:ARG:HB2	7:G:4:TYR:CE2	2.56	0.40
21:U:79:LEU:HD23	21:U:79:LEU:HA	1.90	0.40
23:W:17:C:H5'	23:W:19:G:OP2	2.20	0.40
1:A:554:A:H2'	1:A:555:U:C6	2.57	0.40
1:A:999:C:N4	1:A:1042:A:H61	2.18	0.40
1:A:1359:C:OP2	15:O:75:ARG:NE	2.54	0.40
3:C:186:ILE:HD13	3:C:213:TYR:CD2	2.56	0.40
5:E:33:LYS:HE2	5:E:33:LYS:HB3	1.85	0.40
8:H:50:LEU:HD22	8:H:124:LEU:HB3	2.02	0.40
13:M:55:VAL:HG21	13:M:80:ILE:HD11	2.04	0.40
22:V:49:LYS:O	22:V:53:VAL:HG23	2.21	0.40
23:W:30:G:H2'	23:W:31:G:H8	1.86	0.40
1:A:73:C:C2	1:A:74:A:C8	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:A:H2'	1:A:909:A:H8	1.85	0.40
1:A:1119:C:H2'	1:A:1120:C:C6	2.55	0.40
2:B:112:ILE:HA	2:B:122:VAL:HA	2.03	0.40
13:M:110:ARG:HB2	13:M:119:VAL:HG21	2.03	0.40
20:T:32:ARG:HH21	20:T:34:TRP:HH2	1.69	0.40
21:U:24:ARG:HD3	21:U:24:ARG:HA	1.90	0.40
23:W:41:C:H2'	23:W:42:C:H6	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	172/557 (31%)	162 (94%)	10 (6%)	0	100	100
3	C	224/241 (93%)	211 (94%)	13 (6%)	0	100	100
4	D	209/233 (90%)	202 (97%)	6 (3%)	1 (0%)	25	59
5	E	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
6	F	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
7	G	102/131 (78%)	95 (93%)	7 (7%)	0	100	100
8	H	151/156 (97%)	146 (97%)	5 (3%)	0	100	100
9	I	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
10	J	126/130 (97%)	120 (95%)	6 (5%)	0	100	100
11	K	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
12	L	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
13	M	119/124 (96%)	113 (95%)	5 (4%)	1 (1%)	16	51
14	N	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
15	O	98/101 (97%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
17	Q	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
18	R	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
19	S	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
20	T	81/92 (88%)	81 (100%)	0	0	100	100
21	U	84/87 (97%)	84 (100%)	0	0	100	100
22	V	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	2554/3095 (82%)	2463 (96%)	89 (4%)	2 (0%)	50	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	80	LYS
13	M	88	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	
2	B	75/461 (16%)	68 (91%)	7 (9%)	7	29
3	C	187/199 (94%)	184 (98%)	3 (2%)	58	76
4	D	172/190 (90%)	170 (99%)	2 (1%)	67	82
5	E	172/173 (99%)	172 (100%)	0	100	100
6	F	119/119 (100%)	117 (98%)	2 (2%)	56	75
7	G	91/112 (81%)	90 (99%)	1 (1%)	70	83
8	H	126/129 (98%)	118 (94%)	8 (6%)	15	42
9	I	104/105 (99%)	103 (99%)	1 (1%)	73	84
10	J	106/107 (99%)	102 (96%)	4 (4%)	28	57
11	K	88/90 (98%)	85 (97%)	3 (3%)	32	60
12	L	90/99 (91%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	102/103 (99%)	101 (99%)	1 (1%)	73	84
14	N	93/96 (97%)	90 (97%)	3 (3%)	34	62
15	O	83/84 (99%)	83 (100%)	0	100	100
16	P	76/77 (99%)	74 (97%)	2 (3%)	41	66
17	Q	65/65 (100%)	65 (100%)	0	100	100
18	R	74/78 (95%)	72 (97%)	2 (3%)	40	65
19	S	58/65 (89%)	58 (100%)	0	100	100
20	T	72/79 (91%)	71 (99%)	1 (1%)	62	79
21	U	65/66 (98%)	65 (100%)	0	100	100
22	V	60/61 (98%)	58 (97%)	2 (3%)	33	61
All	All	2078/2558 (81%)	2036 (98%)	42 (2%)	50	72

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1	MET
2	B	42	LEU
2	B	63	GLN
2	B	66	ASP
2	B	73	ASP
2	B	76	GLU
2	B	79	PHE
3	C	117	LEU
3	C	125	THR
3	C	130	THR
4	D	106	VAL
4	D	127	ARG
6	F	105	ILE
6	F	123	VAL
7	G	102	MET
8	H	6	VAL
8	H	7	ILE
8	H	36	LYS
8	H	57	SER
8	H	58	GLU
8	H	80	VAL
8	H	120	LEU
8	H	154	TYR

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Mol	Chain	Res	Type
9	I	88	ARG
10	J	19	VAL
10	J	46	MET
10	J	63	LEU
10	J	105	THR
11	K	18	ILE
11	K	36	VAL
11	K	50	THR
13	M	87	VAL
14	N	11	ASP
14	N	20	THR
14	N	64	VAL
16	P	18	ASP
16	P	40	GLN
18	R	25	ILE
18	R	50	ASN
20	T	63	THR
22	V	38	TYR
22	V	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	39	HIS
3	C	122	GLN
4	D	41	GLN
4	D	69	HIS
4	D	185	ASN
5	E	40	GLN
5	E	59	GLN
5	E	74	ASN
5	E	116	GLN
5	E	136	GLN
5	E	198	HIS
6	F	83	HIS
7	G	11	HIS
10	J	32	GLN
10	J	37	GLN
10	J	75	GLN
10	J	110	GLN
12	L	81	ASN

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Mol	Chain	Res	Type
14	N	52	GLN
16	P	46	HIS
16	P	80	GLN
17	Q	18	GLN
20	T	57	HIS
21	U	48	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1534/1541 (99%)	264 (17%)	5 (0%)
23	W	76/77 (98%)	17 (22%)	1 (1%)
24	X	17/53 (32%)	6 (35%)	1 (5%)
All	All	1627/1671 (97%)	287 (17%)	7 (0%)

All (287) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	52	C
1	A	54	C
1	A	69	G
1	A	71	A
1	A	72	A
1	A	76	G
1	A	77	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	89	U
1	A	90	C

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Mol	Chain	Res	Type
1	A	94	G
1	A	95	C
1	A	121	U
1	A	122	G
1	A	131	A
1	A	141	G
1	A	144	G
1	A	160	A
1	A	164	G
1	A	173	U
1	A	181	A
1	A	196	A
1	A	202	G
1	A	208	U
1	A	211	G
1	A	212	G
1	A	226	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	258	G
1	A	262	A
1	A	266	G
1	A	267	C
1	A	279	A
1	A	289	G
1	A	306	A
1	A	316	C
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	384	G
1	A	406	G
1	A	411	A
1	A	413	G

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Mol	Chain	Res	Type
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	436	C
1	A	446	G
1	A	457	G
1	A	458	U
1	A	463	U
1	A	464	U
1	A	467	U
1	A	468	A
1	A	469	C
1	A	476	U
1	A	478	A
1	A	479	U
1	A	480	U
1	A	481	G
1	A	484	G
1	A	485	U
1	A	486	U
1	A	495	A
1	A	497	G
1	A	511	C
1	A	517	G
1	A	518	C
1	A	521	G
1	A	527	G7M
1	A	528	C
1	A	531	U
1	A	532	A
1	A	533	A
1	A	537	G
1	A	547	A
1	A	559	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A

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Mol	Chain	Res	Type
1	A	596	A
1	A	628	G
1	A	633	G
1	A	639	G
1	A	642	A
1	A	650	G
1	A	653	U
1	A	665	A
1	A	687	A
1	A	703	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	802	A
1	A	815	A
1	A	817	C
1	A	828	U
1	A	832	G
1	A	836	G
1	A	841	C
1	A	842	U
1	A	843	U
1	A	844	G
1	A	846	G
1	A	849	G
1	A	851	G
1	A	887	G
1	A	902	G
1	A	914	A
1	A	916	U
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A

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Mol	Chain	Res	Type
1	A	971	G
1	A	972	C
1	A	975	A
1	A	976	G
1	A	977	A
1	A	987	G
1	A	992	U
1	A	993	G
1	A	996	A
1	A	1004	A
1	A	1006	G
1	A	1007	U
1	A	1009	U
1	A	1017	U
1	A	1018	G
1	A	1020	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1043	G
1	A	1044	A
1	A	1046	A
1	A	1065	U
1	A	1070	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1099	G
1	A	1101	A
1	A	1108	G
1	A	1133	G
1	A	1135	U
1	A	1136	C
1	A	1137	C
1	A	1139	G

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Mol	Chain	Res	Type
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1145	A
1	A	1146	A
1	A	1151	A
1	A	1152	A
1	A	1154	G
1	A	1158	C
1	A	1159	U
1	A	1167	A
1	A	1169	A
1	A	1174	G
1	A	1175	G
1	A	1176	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1239	A
1	A	1257	A
1	A	1260	G
1	A	1274	A
1	A	1277	C
1	A	1278	G
1	A	1279	G
1	A	1280	A
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1320	C

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Mol	Chain	Res	Type
1	A	1323	G
1	A	1332	A
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1419	G
1	A	1421	G
1	A	1422	G
1	A	1425	U
1	A	1426	G
1	A	1429	A
1	A	1441	A
1	A	1442	G
1	A	1446	A
1	A	1452	C
1	A	1453	G
1	A	1475	G
1	A	1487	G
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
1	A	1535	C
23	W	9	G
23	W	13	C
23	W	17	C
23	W	18	U
23	W	19	G
23	W	20	G
23	W	21	H2U
23	W	22	A
23	W	43	G
23	W	44	A
23	W	48	U

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Mol	Chain	Res	Type
23	W	49	C
23	W	68	C
23	W	73	A
23	W	75	C
23	W	76	C
23	W	77	A
24	X	11	U
24	X	12	A
24	X	13	U
24	X	14	U
24	X	15	C
24	X	17	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	428	G
1	A	641	U
1	A	843	U
1	A	1166	G
1	A	1214	C
23	W	48	U
24	X	11	U

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

17 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
23	5MU	W	55	23	19,22,23	1.40	5 (26%)	28,32,35	2.01	6 (21%)
1	4OC	A	1402	1	20,23,24	3.50	9 (45%)	26,32,35	0.86	0
1	5MC	A	967	1	18,22,23	4.01	7 (38%)	26,32,35	1.04	2 (7%)
13	D2T	M	89	13	7,9,10	1.05	0	6,11,13	2.36	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	1207	1	18,26,27	2.38	7 (38%)	16,38,41	1.48	4 (25%)
23	OMC	W	33	23	19,22,23	3.06	8 (42%)	26,31,34	0.77	0
1	5MC	A	1407	1	18,22,23	4.05	7 (38%)	26,32,35	0.96	1 (3%)
1	MA6	A	1518	1	18,26,27	1.28	3 (16%)	19,38,41	3.80	2 (10%)
23	H2U	W	21	23	18,21,22	3.00	5 (27%)	21,30,33	1.52	4 (19%)
23	PSU	W	56	23	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
1	PSU	A	516	1	18,21,22	1.05	2 (11%)	22,30,33	1.83	5 (22%)
1	UR3	A	1498	1	19,22,23	2.74	7 (36%)	26,32,35	1.26	1 (3%)
1	MA6	A	1519	1	18,26,27	1.33	3 (16%)	19,38,41	4.18	2 (10%)
1	G7M	A	527	1	20,26,27	2.47	7 (35%)	17,39,42	1.15	2 (11%)
1	2MG	A	1516	1	18,26,27	2.32	7 (38%)	16,38,41	1.47	4 (25%)
23	4SU	W	8	23	18,21,22	4.21	8 (44%)	26,30,33	2.21	4 (15%)
1	2MG	A	966	1	18,26,27	2.34	7 (38%)	16,38,41	1.35	3 (18%)

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
23	5MU	W	55	23	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
1	5MC	A	967	1	-	1/7/25/26	0/2/2/2
13	D2T	M	89	13	-	1/7/12/14	-
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
23	OMC	W	33	23	-	1/9/27/28	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	3/7/29/30	0/3/3/3
23	H2U	W	21	23	-	5/7/38/39	0/2/2/2
23	PSU	W	56	23	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	7/7/29/30	0/3/3/3
1	G7M	A	527	1	-	3/3/25/26	0/3/3/3
1	2MG	A	1516	1	-	1/5/27/28	0/3/3/3
23	4SU	W	8	23	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/5/27/28	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C6-C5	10.11	1.51	1.34
1	A	967	5MC	C6-C5	10.03	1.51	1.34
23	W	8	4SU	C4-N3	9.56	1.47	1.37
23	W	21	H2U	C2-N1	8.93	1.48	1.35
23	W	8	4SU	C2-N1	7.93	1.51	1.38
1	A	967	5MC	C4-N3	7.47	1.46	1.34
1	A	1402	4OC	C4-N3	7.43	1.45	1.32
1	A	1407	5MC	C4-N3	7.42	1.46	1.34
1	A	1498	UR3	C2-N1	7.01	1.48	1.38
1	A	1407	5MC	C2-N3	6.81	1.50	1.36
1	A	967	5MC	C2-N3	6.80	1.50	1.36
23	W	8	4SU	C2-N3	6.63	1.49	1.38
1	A	1402	4OC	C6-C5	6.46	1.50	1.35
23	W	33	OMC	C2-N3	6.43	1.49	1.36
23	W	33	OMC	C6-C5	6.20	1.49	1.35
23	W	8	4SU	C6-C5	6.18	1.49	1.35
1	A	1498	UR3	C6-C5	6.14	1.49	1.35
1	A	1402	4OC	C2-N3	6.08	1.48	1.36
23	W	21	H2U	C2-N3	6.05	1.48	1.38
23	W	8	4SU	C5-C4	5.74	1.50	1.42
23	W	21	H2U	C4-N3	5.60	1.47	1.37
1	A	1407	5MC	C4-N4	5.47	1.48	1.34
1	A	1407	5MC	C6-N1	5.39	1.47	1.38
23	W	8	4SU	C4-S4	-5.34	1.58	1.68
1	A	967	5MC	C4-N4	5.33	1.48	1.34
1	A	967	5MC	C6-N1	5.26	1.47	1.38
1	A	527	G7M	C2-N3	5.23	1.45	1.33
23	W	33	OMC	C4-N3	5.20	1.45	1.34
1	A	1402	4OC	C4-N4	5.12	1.46	1.35
1	A	1498	UR3	C2-N3	5.11	1.48	1.39
1	A	527	G7M	C4-N3	5.08	1.49	1.37
23	W	33	OMC	C4-N4	4.94	1.45	1.33
1	A	966	2MG	C2-N2	4.85	1.44	1.33
1	A	1407	5MC	C2-N1	4.85	1.50	1.40
1	A	527	G7M	C2-N2	4.83	1.45	1.34
1	A	1207	2MG	C2-N2	4.74	1.43	1.33
1	A	1516	2MG	C2-N2	4.63	1.43	1.33
1	A	967	5MC	C2-N1	4.61	1.50	1.40
1	A	1402	4OC	O2-C2	-4.60	1.15	1.23
1	A	1402	4OC	C5-C4	4.40	1.50	1.40
23	W	33	OMC	C2-N1	4.36	1.49	1.40
1	A	1402	4OC	C2-N1	4.34	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	966	2MG	C4-N3	4.33	1.47	1.37
1	A	1207	2MG	C6-N1	4.25	1.44	1.37
1	A	1207	2MG	C2-N1	4.22	1.43	1.36
1	A	1516	2MG	C4-N3	4.14	1.47	1.37
1	A	966	2MG	C2-N1	4.10	1.43	1.36
1	A	1516	2MG	C2-N1	4.06	1.43	1.36
1	A	1207	2MG	C4-N3	4.05	1.47	1.37
1	A	1516	2MG	C6-N1	3.97	1.43	1.37
1	A	966	2MG	C6-N1	3.86	1.43	1.37
1	A	1402	4OC	CM4-N4	3.75	1.52	1.45
23	W	33	OMC	C6-N1	3.39	1.46	1.38
23	W	56	PSU	C6-C5	3.38	1.39	1.35
1	A	1519	MA6	C2-N3	3.36	1.37	1.32
1	A	527	G7M	C5-C6	3.27	1.53	1.45
1	A	527	G7M	C6-N1	3.25	1.42	1.37
23	W	8	4SU	C6-N1	3.25	1.45	1.38
1	A	1207	2MG	O6-C6	-3.23	1.16	1.23
1	A	966	2MG	O6-C6	-3.19	1.16	1.23
1	A	1402	4OC	C6-N1	3.18	1.45	1.38
1	A	1516	2MG	O6-C6	-3.17	1.16	1.23
1	A	1518	MA6	C2-N3	3.06	1.37	1.32
1	A	1498	UR3	C6-N1	3.01	1.45	1.38
1	A	1518	MA6	C10-N6	3.01	1.52	1.45
23	W	8	4SU	O2-C2	-3.00	1.17	1.23
1	A	516	PSU	C6-C5	2.99	1.38	1.35
1	A	1516	2MG	C5-C6	2.89	1.53	1.47
1	A	966	2MG	C5-C6	2.85	1.53	1.47
1	A	527	G7M	O6-C6	-2.79	1.17	1.23
23	W	55	5MU	C6-C5	2.78	1.39	1.34
1	A	1519	MA6	C10-N6	2.74	1.52	1.45
1	A	1207	2MG	C5-C6	2.73	1.52	1.47
1	A	527	G7M	C2-N1	2.72	1.44	1.37
23	W	55	5MU	C4-N3	-2.64	1.33	1.38
1	A	1207	2MG	C5-C4	-2.62	1.36	1.43
23	W	33	OMC	O2-C2	-2.61	1.18	1.23
23	W	33	OMC	C5-C4	2.58	1.48	1.42
1	A	967	5MC	O2-C2	-2.39	1.19	1.23
1	A	1407	5MC	O2-C2	-2.37	1.19	1.23
1	A	1519	MA6	C5-C4	-2.34	1.34	1.40
1	A	1516	2MG	C5-C4	-2.33	1.37	1.43
1	A	1518	MA6	C5-C4	-2.30	1.34	1.40
1	A	1498	UR3	C5-C4	2.28	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	55	5MU	C6-N1	-2.24	1.34	1.38
23	W	55	5MU	C2-N3	-2.23	1.34	1.38
1	A	1498	UR3	O4-C4	-2.21	1.18	1.23
23	W	21	H2U	O4-C4	-2.19	1.18	1.23
23	W	21	H2U	O2-C2	-2.17	1.19	1.23
23	W	55	5MU	C4-C5	2.16	1.48	1.44
1	A	966	2MG	C5-C4	-2.16	1.37	1.43
1	A	1498	UR3	C4-N3	2.12	1.45	1.40
1	A	516	PSU	O4'-C1'	-2.05	1.41	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	N1-C6-N6	-17.14	99.02	117.06
1	A	1518	MA6	N1-C6-N6	-15.24	101.02	117.06
23	W	8	4SU	C4-N3-C2	-7.77	119.79	127.34
1	A	1518	MA6	N3-C2-N1	-5.93	119.41	128.68
23	W	8	4SU	C5-C4-N3	5.56	119.85	114.69
1	A	1519	MA6	N3-C2-N1	-5.46	120.15	128.68
23	W	55	5MU	C4-N3-C2	-4.97	120.92	127.35
1	A	1498	UR3	C4-N3-C2	-4.83	120.02	124.56
23	W	55	5MU	C5-C4-N3	4.72	119.34	115.31
23	W	55	5MU	N3-C2-N1	4.56	120.94	114.89
1	A	516	PSU	N1-C2-N3	4.50	120.23	115.13
23	W	56	PSU	C4-N3-C2	-4.48	119.89	126.34
1	A	516	PSU	C4-N3-C2	-4.44	119.94	126.34
23	W	56	PSU	N1-C2-N3	4.29	119.99	115.13
23	W	55	5MU	O4-C4-C5	-4.18	120.06	124.90
13	M	89	D2T	CB1-SB-CB	3.98	109.64	102.44
23	W	21	H2U	C4-N3-C2	-3.85	122.60	125.79
23	W	55	5MU	C5-C6-N1	-3.77	119.46	123.34
1	A	967	5MC	C5-C6-N1	-3.76	119.47	123.34
23	W	8	4SU	N3-C2-N1	3.74	119.86	114.89
23	W	21	H2U	C5-C6-N1	3.54	123.28	111.61
1	A	1516	2MG	C5-C6-N1	3.41	119.98	113.95
1	A	1207	2MG	C5-C6-N1	3.37	119.91	113.95
23	W	8	4SU	C5-C4-S4	-3.31	120.20	124.47
1	A	966	2MG	C5-C6-N1	3.29	119.77	113.95
1	A	516	PSU	O2-C2-N1	-3.05	119.44	122.79
13	M	89	D2T	OD2-CG-CB	3.04	119.71	113.15
1	A	1407	5MC	C5-C6-N1	-2.79	120.47	123.34
1	A	1207	2MG	C8-N7-C5	2.68	108.09	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	21	H2U	C5-C4-N3	2.65	119.62	116.65
1	A	527	G7M	C2-N1-C6	-2.58	120.34	125.10
1	A	1516	2MG	CM2-N2-C2	-2.56	118.21	123.86
1	A	1516	2MG	C8-N7-C5	2.54	107.83	102.99
1	A	516	PSU	C6-N1-C2	-2.49	120.13	122.68
1	A	1207	2MG	O6-C6-C5	-2.46	119.58	124.37
1	A	516	PSU	O4'-C1'-C2'	2.42	108.56	105.14
1	A	966	2MG	C8-N7-C5	2.34	107.45	102.99
23	W	21	H2U	O2-C2-N1	-2.27	120.25	123.11
1	A	1516	2MG	O6-C6-C5	-2.23	120.02	124.37
23	W	56	PSU	C6-C5-C4	2.19	119.73	118.20
1	A	966	2MG	O6-C6-C5	-2.16	120.15	124.37
1	A	1207	2MG	CM2-N2-C2	-2.14	119.14	123.86
23	W	56	PSU	O2-C2-N1	-2.12	120.46	122.79
1	A	967	5MC	CM5-C5-C6	-2.12	120.02	122.85
23	W	55	5MU	O2-C2-N1	-2.04	120.07	122.79
1	A	527	G7M	CN7-N7-C8	-2.03	115.67	125.43

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	C5-C6-N6-C9
1	A	1518	MA6	C5-C6-N6-C10
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C10
23	W	21	H2U	O4'-C1'-N1-C6
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	1518	MA6	N1-C6-N6-C10
1	A	966	2MG	C3'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	1519	MA6	C4'-C5'-O5'-P
23	W	33	OMC	C3'-C2'-O2'-CM2
1	A	527	G7M	C4'-C5'-O5'-P
1	A	1519	MA6	N1-C6-N6-C9
23	W	21	H2U	C4'-C5'-O5'-P
1	A	967	5MC	O4'-C4'-C5'-O5'
23	W	21	H2U	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
13	M	89	D2T	CG-CB-SB-CB1
23	W	21	H2U	O4'-C1'-N1-C2
23	W	21	H2U	C2'-C1'-N1-C2
1	A	1516	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
13	M	89	D2T	1	0
1	A	1207	2MG	2	0
23	W	33	OMC	2	0
1	A	1518	MA6	4	0
1	A	1519	MA6	3	0
1	A	527	G7M	1	0
1	A	1516	2MG	1	0
1	A	966	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 125 ligands modelled in this entry, 125 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

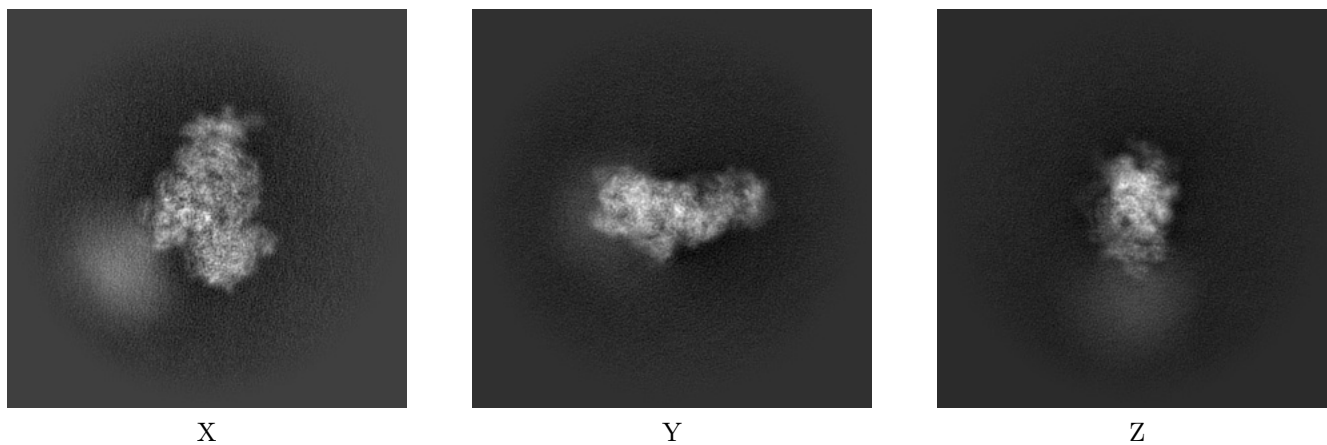
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51618. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

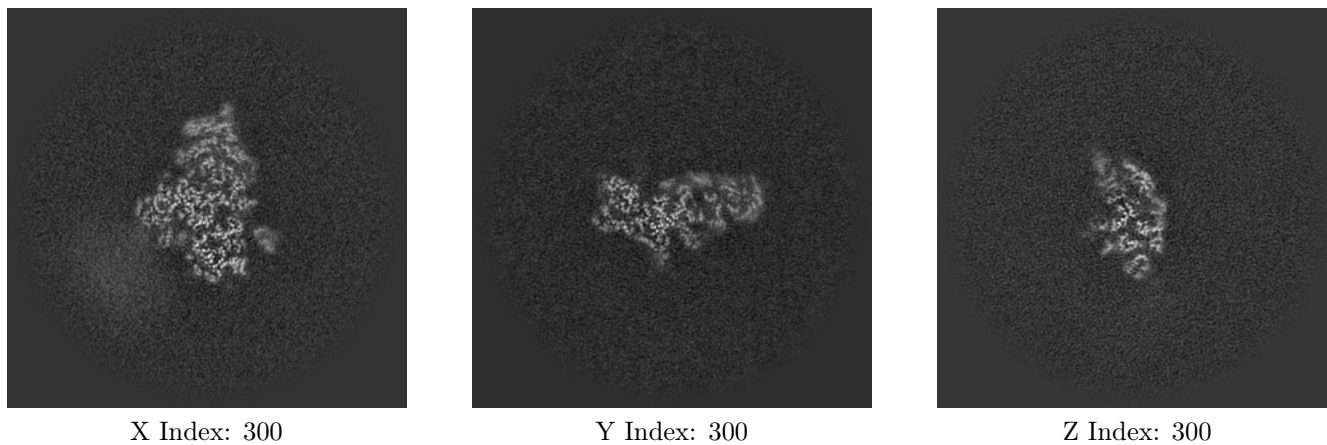
6.1.1 Primary map



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

6.2 Central slices [i](#)

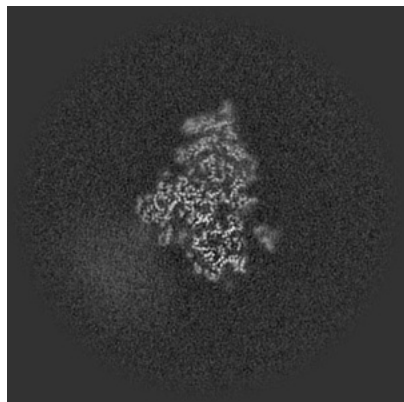
6.2.1 Primary map



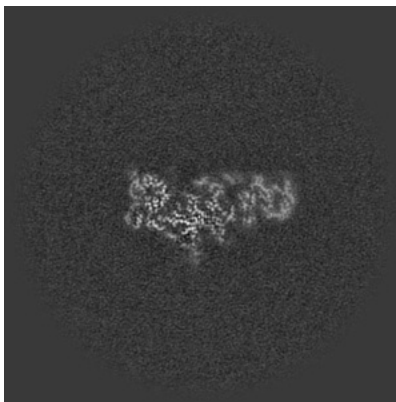
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

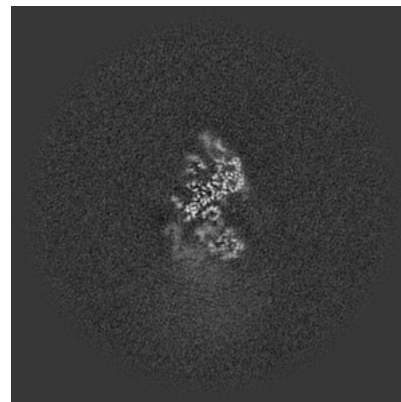
6.3.1 Primary map



X Index: 299



Y Index: 303

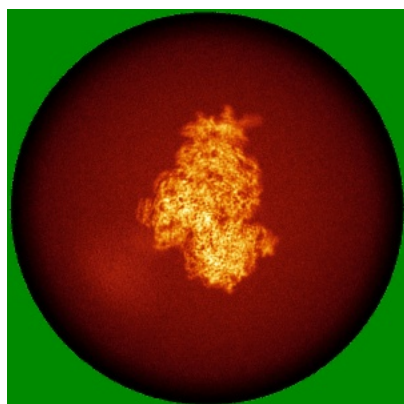


Z Index: 256

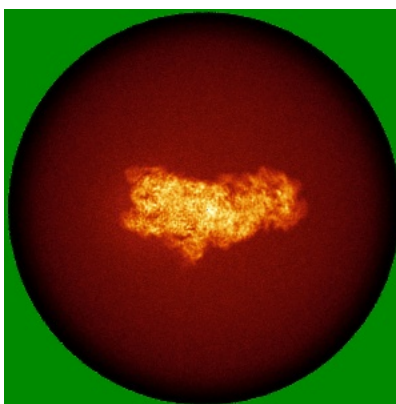
The images above show the largest variance slices of the map in three orthogonal directions.

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

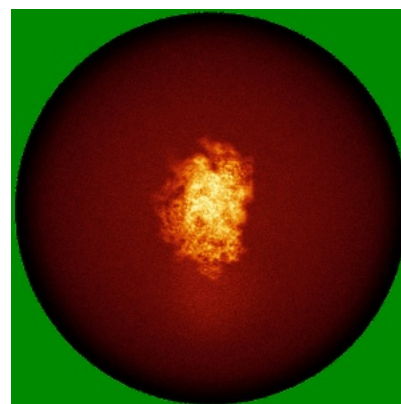
6.4.1 Primary map



X



Y

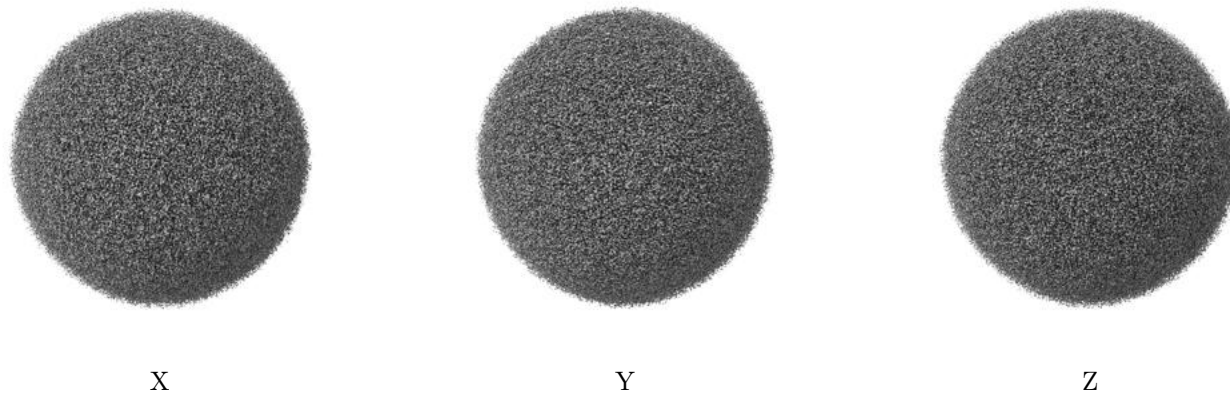


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.159. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

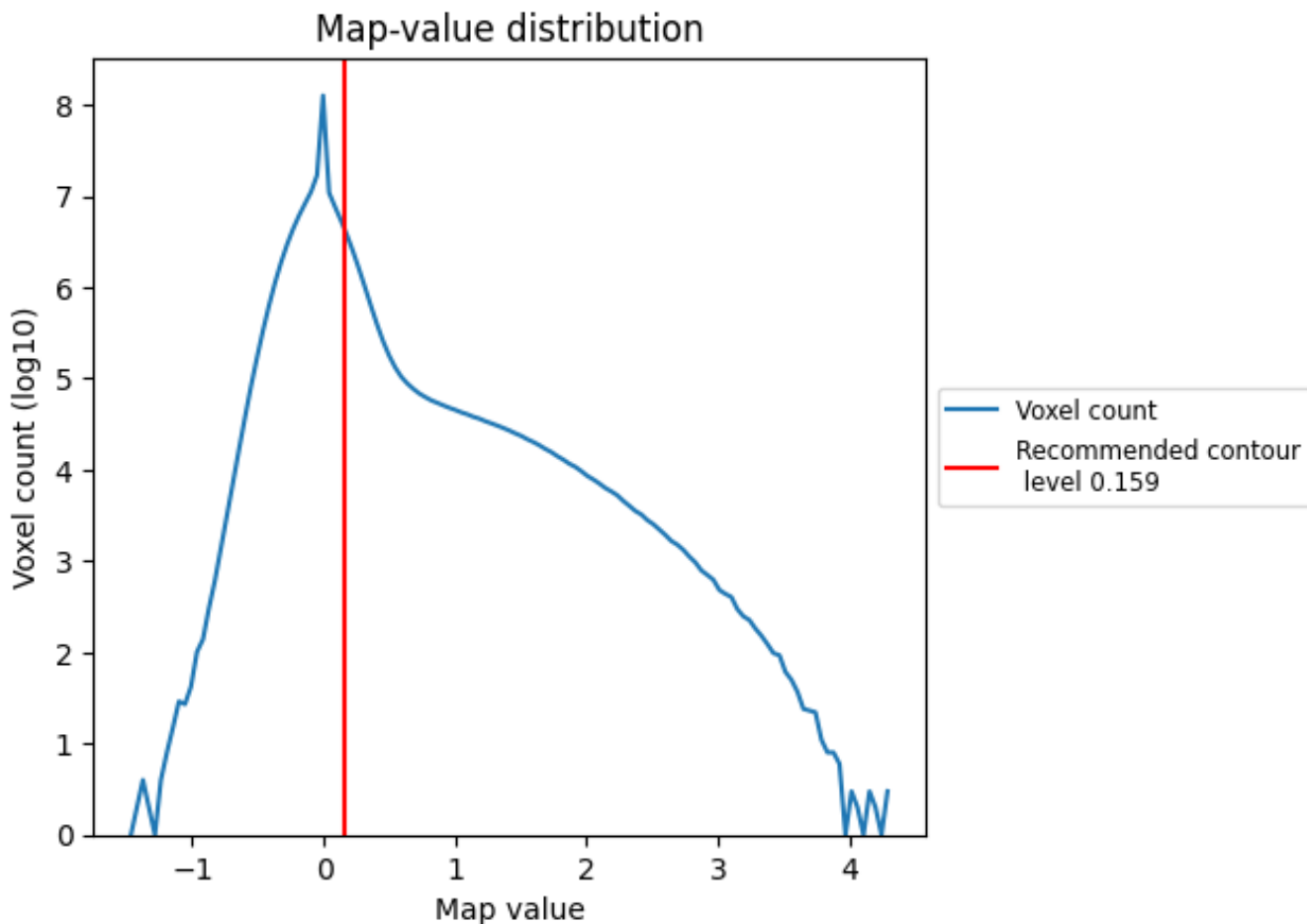
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

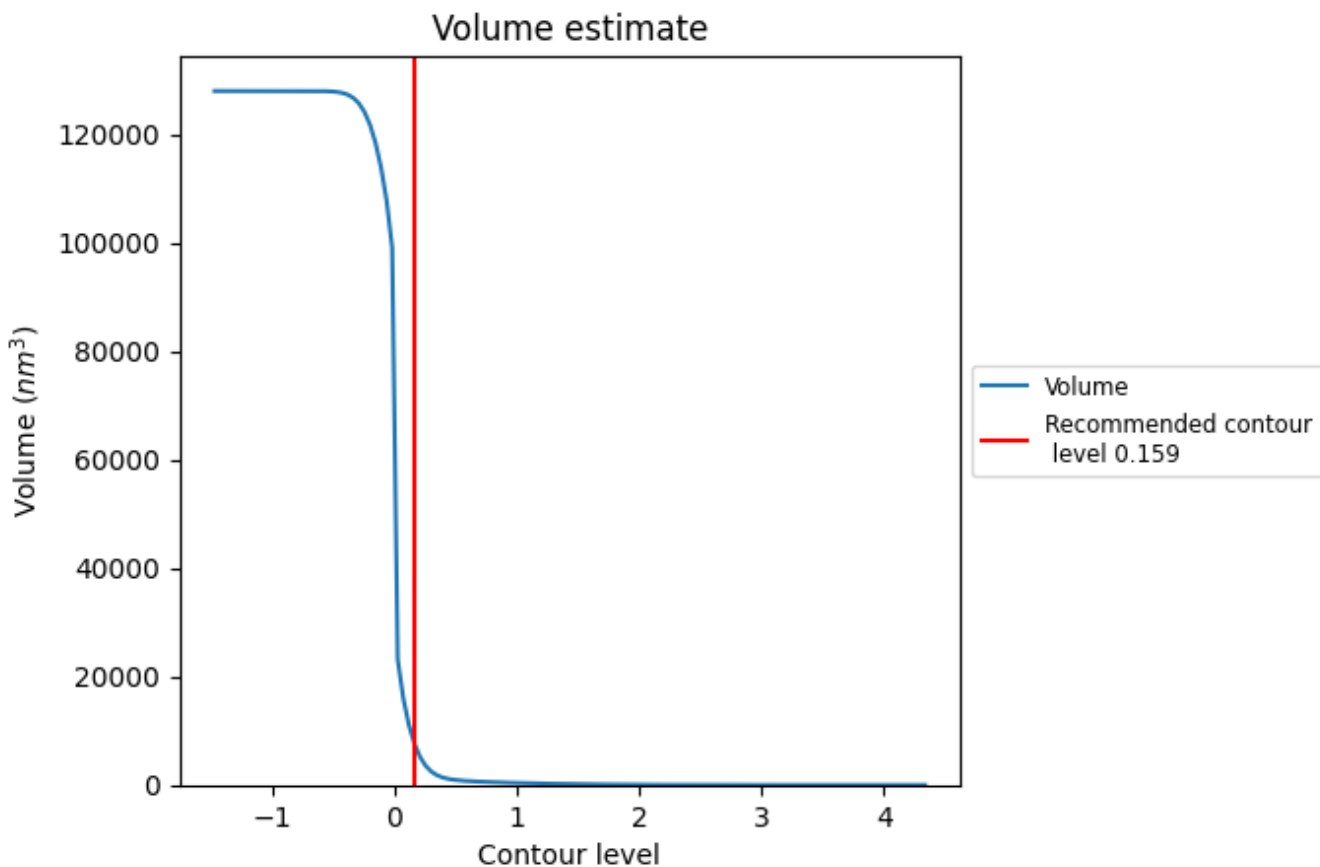
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

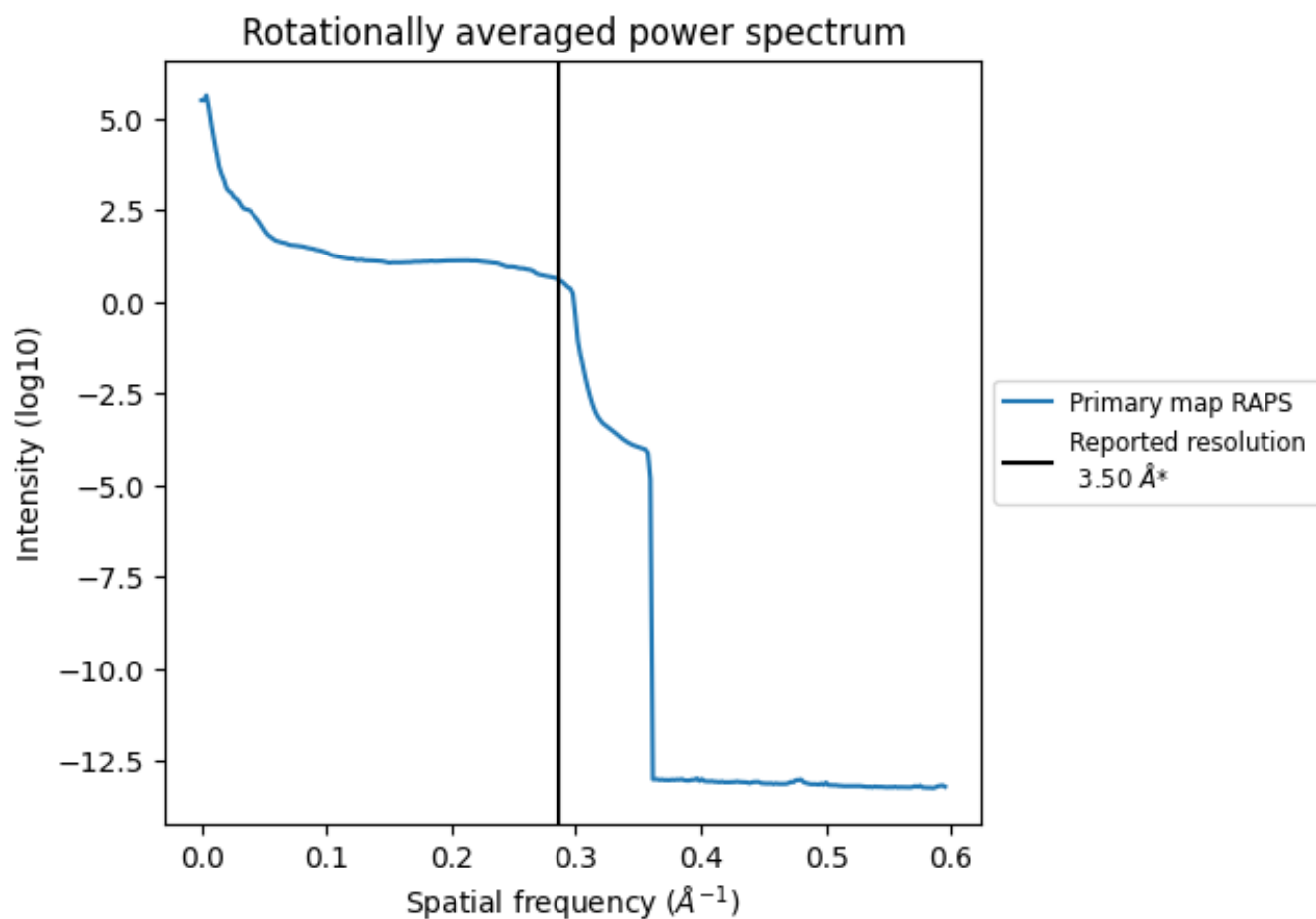
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 8075 nm^3 ; this corresponds to an approximate mass of 7295 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 0.286 Å⁻¹

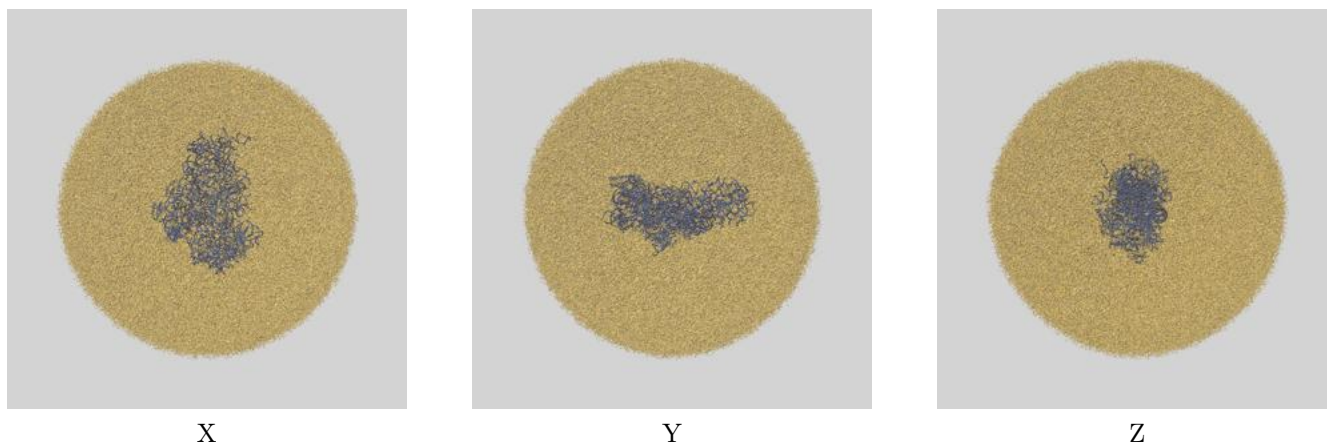
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

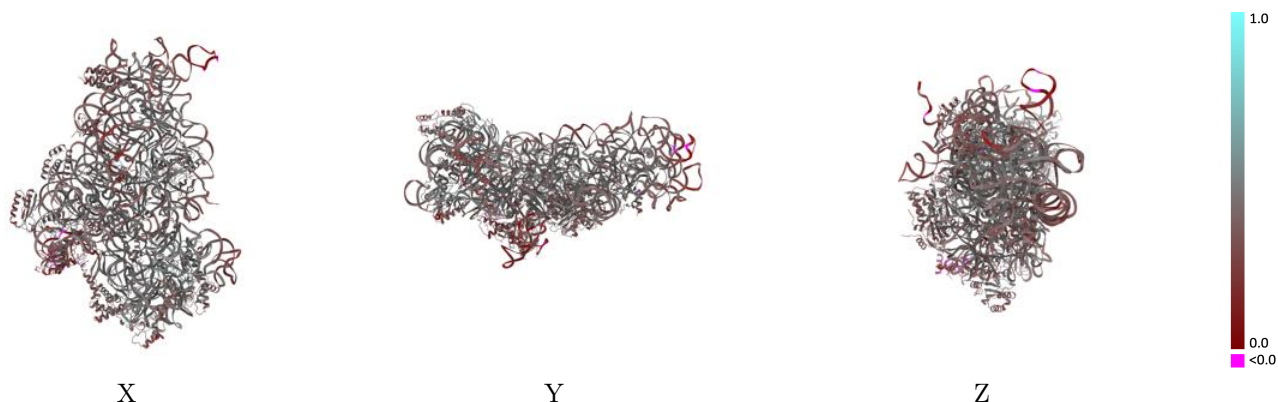
This section contains information regarding the fit between EMDB map EMD-51618 and PDB model 9GUS. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



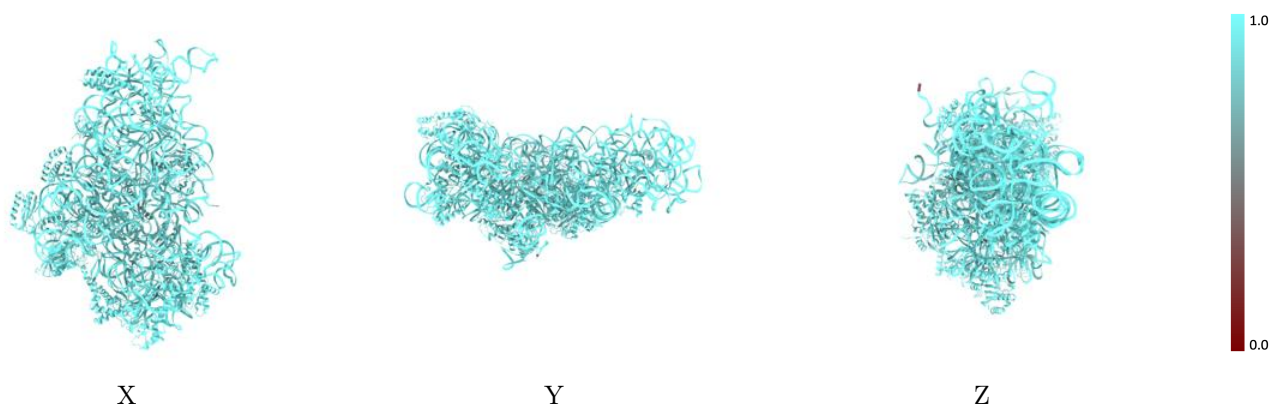
The images above show the 3D surface view of the map at the recommended contour level 0.159 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



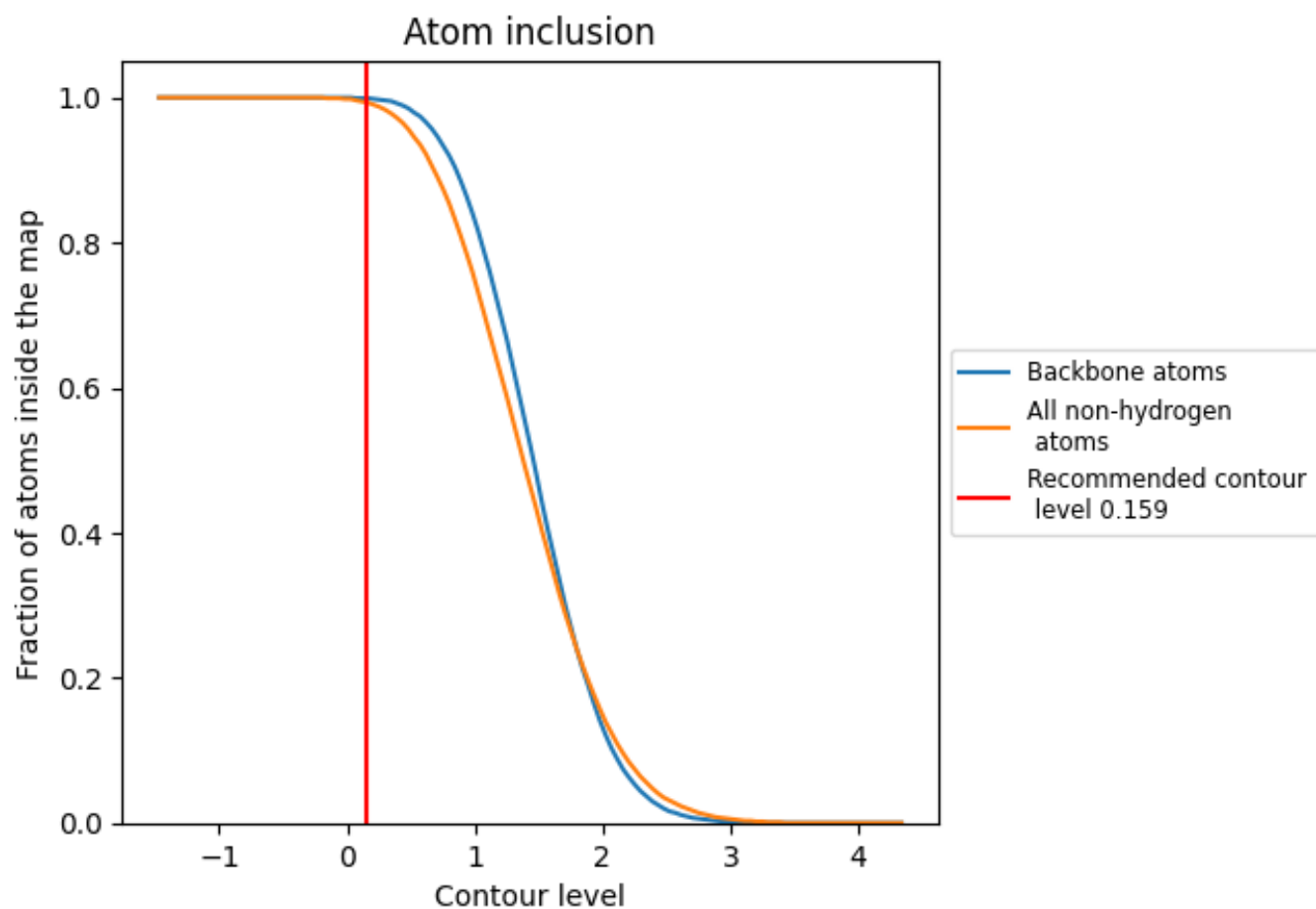
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.159).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.159) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9930	 0.4010
A	 1.0000	 0.4180
B	 0.9910	 0.2370
C	 0.9700	 0.3570
D	 0.9810	 0.4440
E	 0.9820	 0.3900
F	 0.9740	 0.4310
G	 0.9880	 0.3690
H	 0.9740	 0.3740
I	 0.9820	 0.4180
J	 0.9910	 0.4390
K	 0.9830	 0.4150
L	 0.9790	 0.3320
M	 0.9940	 0.4400
N	 0.9950	 0.3980
O	 0.9920	 0.4500
P	 0.9900	 0.3840
Q	 0.9890	 0.4350
R	 0.9920	 0.3850
S	 0.9790	 0.3810
T	 0.9920	 0.4480
U	 0.9910	 0.3810
V	 0.9660	 0.3260
W	 0.9820	 0.2320
X	 0.9790	 0.1360

