Full wwPDB EM Validation Report

Apr 17, 2024 – 08:46 am BST

PDB ID	:	8P03
EMDB ID	:	EMD-17329
Title	:	48S late-stage initiation complex with m6A mRNA
Authors	:	Guca, E.; Lima, L.H.F.; Boissier, F.; Hashem, Y.
Deposited on	:	2023-05-09
Resolution	:	3.04 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:

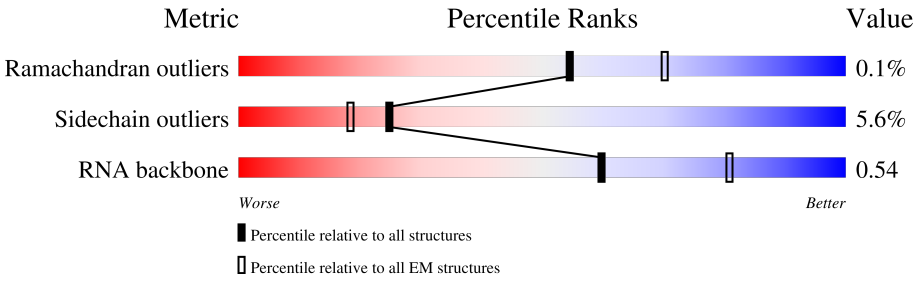
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.04 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1	75	37% 52% 35% 13%
2	2	1863	8% 60% 27% 6% · 6%
3	3	9	33% 22% 56% 22%
4	A	284	61% 86% 8% 6%
5	C	207	· 93% 7%
6	D	215	· 97% ·
7	E	270	· 78% 5% 16%
8	F	227	6% 94% 5%

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Mol	Chain	Length	Quality of chain
9	G	263	97%
10	H	191	92% 5%
11	I	237	9% 95% 5%
12	J	190	42% 94% 6%
13	K	206	10% 91% 9%
14	L	194	6% 93%
15	M	98	7% 94% 6%
16	N	158	16% 96%
17	O	132	40% 86% 8% 6%
18	P	150	94% 5%
19	Q	151	83% 7% 10%
20	R	145	14% 86% 9%
21	S	141	91% 9%
22	T	135	15% 87% 6% 7%
23	U	152	6% 89% 7% 5%
24	V	141	95% 5%
25	W	119	8% 82% 6% 13%
26	X	83	94% 6%
27	Y	130	95% 5%
28	Z	143	95%
29	a	133	5% 89% 5% 5%
30	b	115	78% 8% 14%
31	c	84	7% 94% 6%
32	d	69	84% 9% 7%
33	e	56	80% 14% 5%

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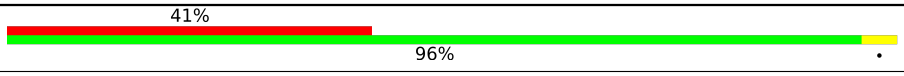
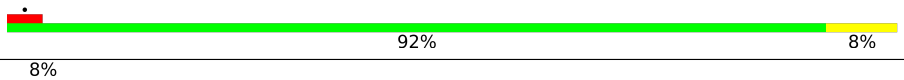
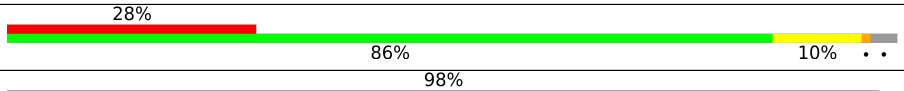
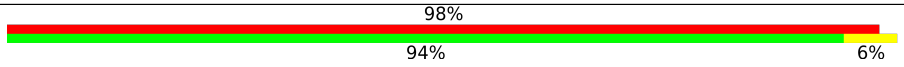
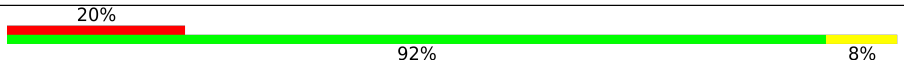
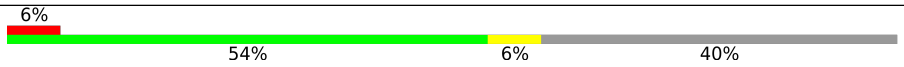
Mol	Chain	Length	Quality of chain
34	f	71	
35	g	313	
36	i	133	
37	j	111	
38	k	595	
39	l	25	
40	n	124	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 86276 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 initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1614	722	299	519	74		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1743	Total	C	N	O	P	0	0
			37193	16605	6660	12186	1742		

- Molecule 3 is a RNA chain called m6A-methylated mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	9	Total	C	N	O	P	0	0
			193	87	36	61	9		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	266	Total	C	N	O	S	0	0
			2146	1354	376	405	11		

- Molecule 5 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	207	Total	C	N	O	S	0	0
			1637	1042	288	299	8		

- Molecule 6 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	215	Total	C	N	O	S	0	0
			1741	1107	309	310	15		

- Molecule 7 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	226	Total	C	N	O	S	0	0
			1754	1139	298	310	7		

- Molecule 8 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	227	Total	C	N	O	S	0	0
			1764	1124	317	315	8		

- Molecule 9 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 10 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	187	Total	C	N	O	S	0	0
			1482	928	279	268	7		

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	237	Total	C	N	O	S	0	0
			1924	1199	387	331	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	130	THR	PRO	conflict	UNP A0A5K1UJS7

- Molecule 12 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 13 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	188	Total	C	N	O	S	0	0
			1542	979	309	251	3		

- Molecule 15 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 16 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 18 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 19 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 20 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	140	Total	C	N	O	S	0	0
			1154	733	219	195	7		

- Molecule 21 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 22 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	126	Total	C	N	O	S	0	0
			1019	639	188	187	5		

- Molecule 23 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	145	Total	C	N	O	S	0	0
			1194	747	243	203	1		

- Molecule 24 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	141	Total	C	N	O	S	0	0
			1113	701	213	196	3		

- Molecule 25 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 26 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 27 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 28 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	142	Total	C	N	O	S	0	0
			1106	698	220	184	4		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	126	Total	C	N	O	S	0	0
			1021	645	198	173	5		

- Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	99	Total	C	N	O	S	0	0
			789	491	162	130	6		

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	53	Total	C	N	O	S	0	0
			444	278	90	71	5		

- Molecule 34 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 35 is a protein called Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 36 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	58	Total	C	N	O	S	0	0
			464	287	102	74	1		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	108	Total	C	N	O	S	0	0
			874	543	166	161	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	39	ILE	VAL	conflict	UNP G1SYS4
j	76	ILE	VAL	conflict	UNP G1SYS4

- Molecule 38 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	595	Total	C	N	O	S	0	0
			4693	2995	802	865	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	538	ILE	VAL	conflict	UNP G1SG72

- Molecule 39 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	25	Total 240	C 145	N 64	O 28	S 3	0	0

- Molecule 40 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	75	Total 598	C 382	N 111	O 104	S 1	0	0

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

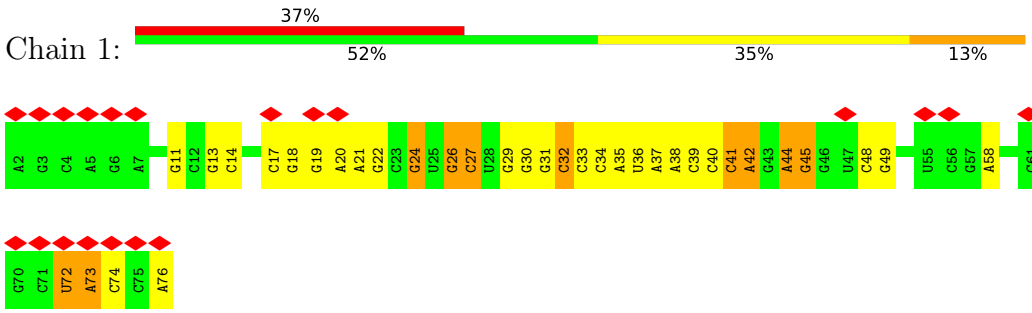
Mol	Chain	Residues	Atoms		AltConf
41	2	175	Total 175	Mg 175	0
41	3	1	Total 1	Mg 1	0
41	I	1	Total 1	Mg 1	0
41	Z	1	Total 1	Mg 1	0

3 Residue-property plots (i)

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

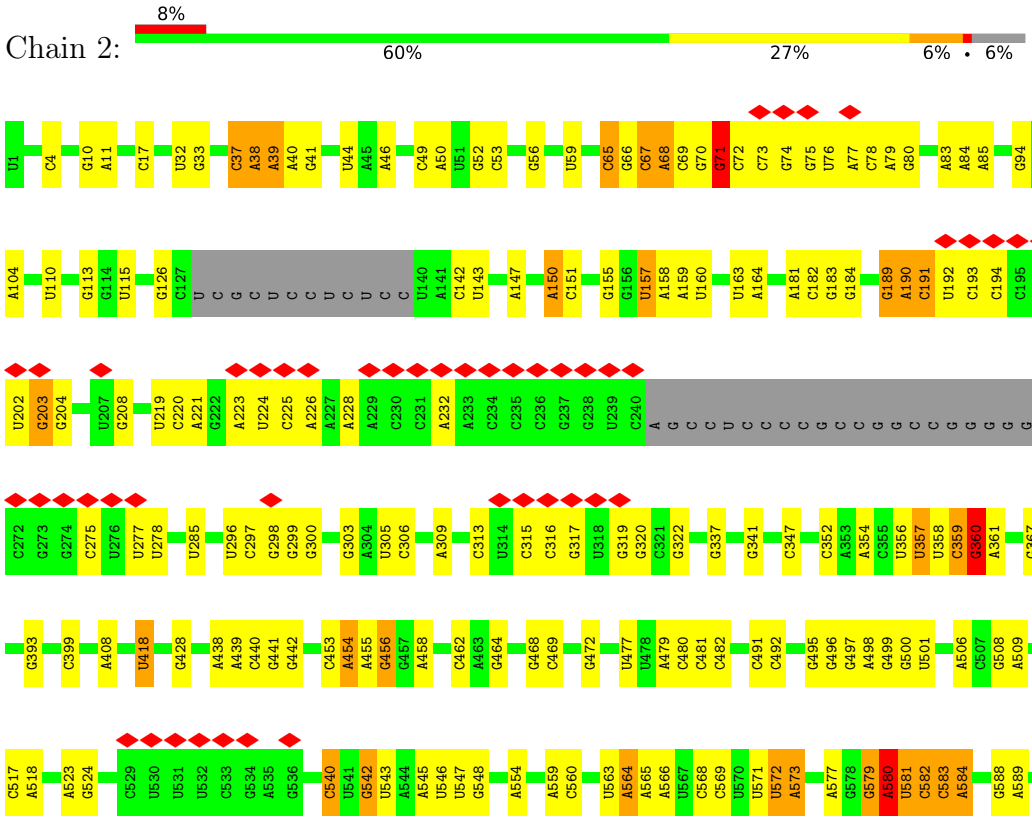
• Molecule 1: initiator methionylated tRNA

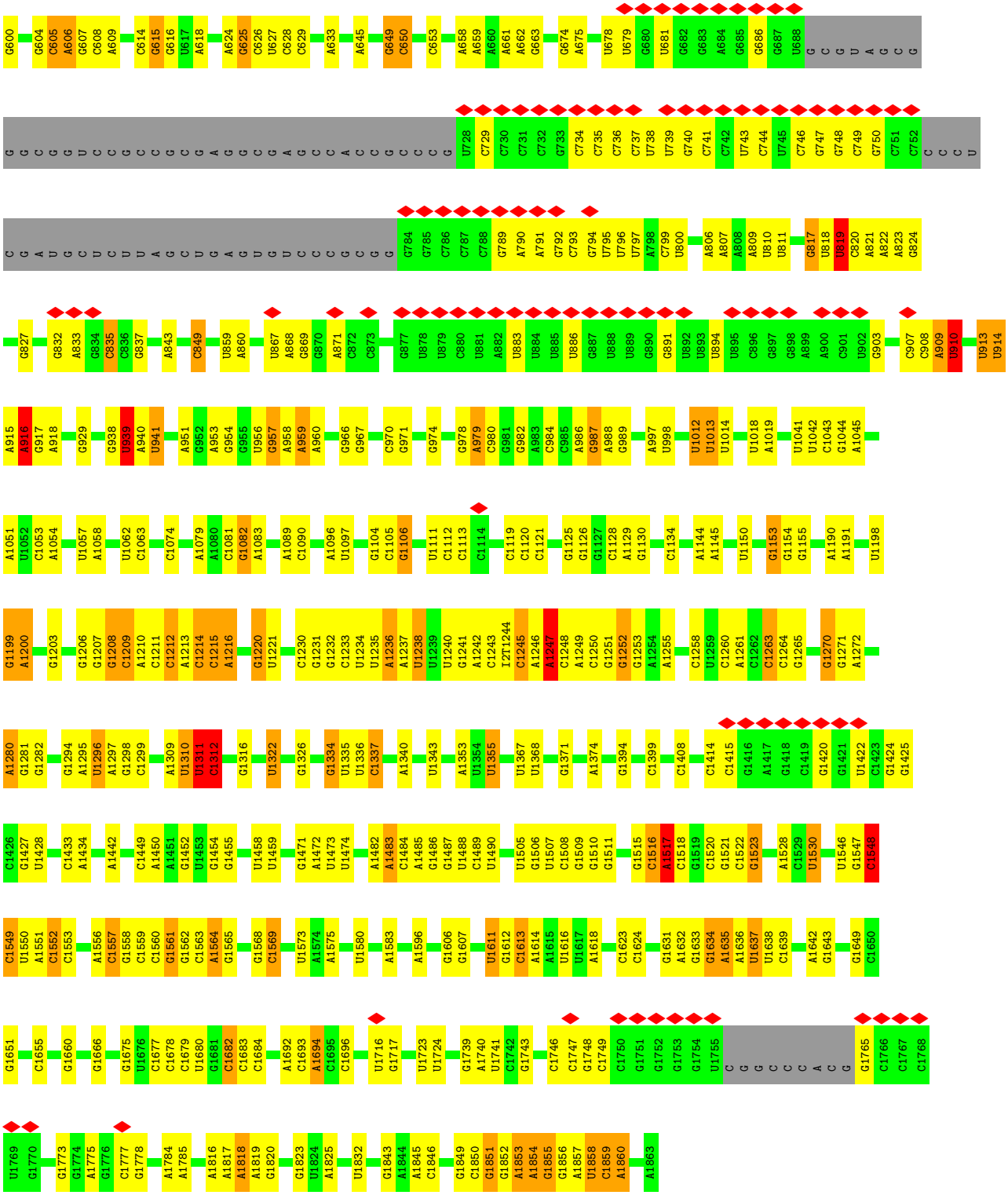
Chain 1:



• Molecule 2: 18S ribosomal RNA

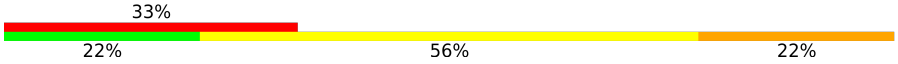
Chain 2:

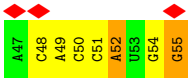




• Molecule 3: m6A-methylated mRNA

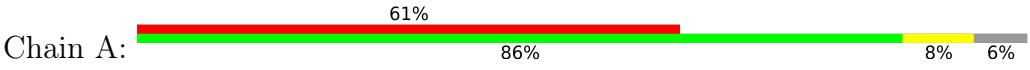
Chain 3:

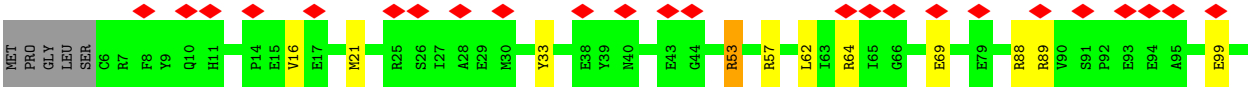


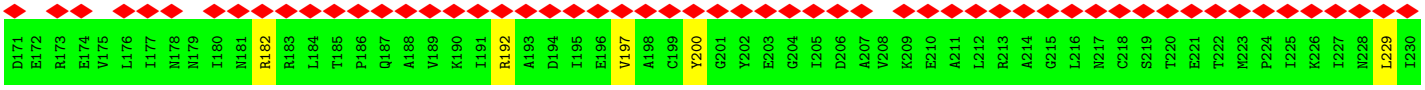


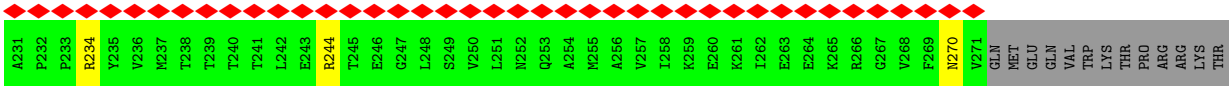
• Molecule 4: Eukaryotic translation initiation factor 2 subunit 1

Chain A:



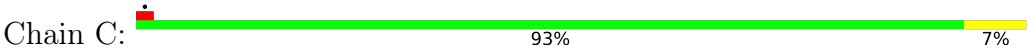


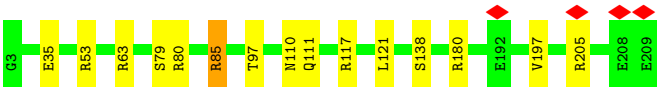




• Molecule 5: 40S ribosomal protein SA

Chain C:



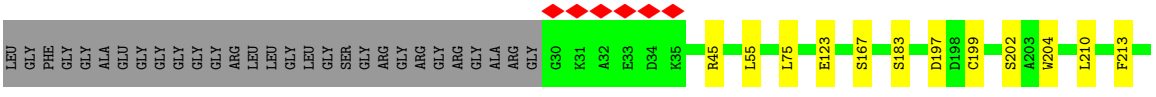


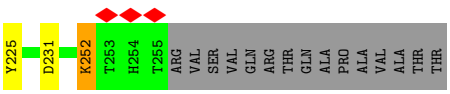
• Molecule 6: ribosomal protein eS1

Chain D:

• Molecule 7: 40S ribosomal protein S2

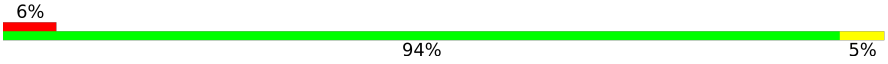
Chain E:

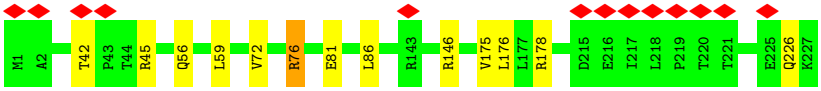




• Molecule 8: Ribosomal protein S3

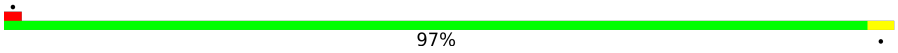
Chain F:





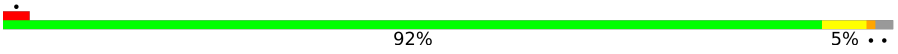
• Molecule 9: 40S ribosomal protein S4

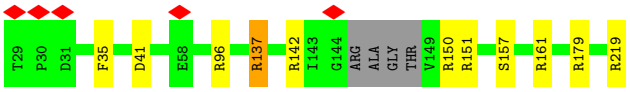
Chain G:



• Molecule 10: Ribosomal protein S5

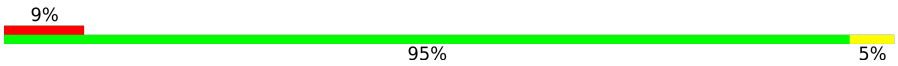
Chain H:

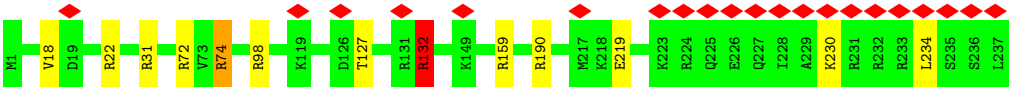




• Molecule 11: 40S ribosomal protein S6

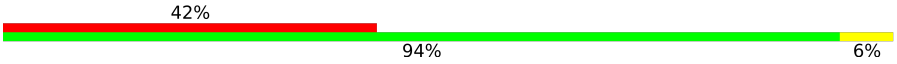
Chain I:

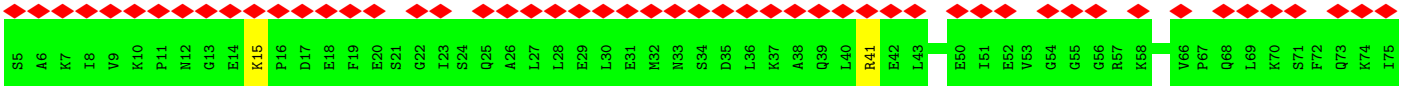


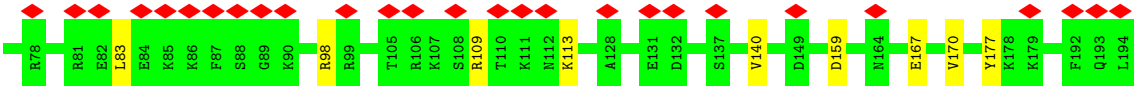


• Molecule 12: ribosomal protein eS7

Chain J:

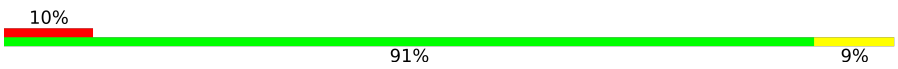


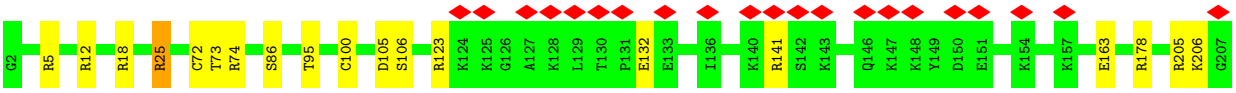




• Molecule 13: 40S ribosomal protein S8

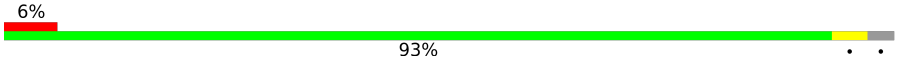
Chain K:

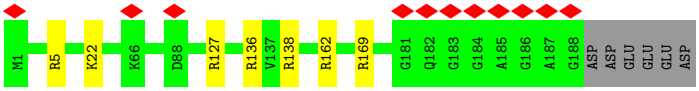




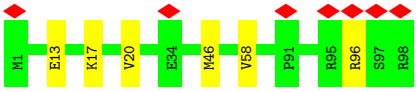
• Molecule 14: 40S ribosomal protein S9

Chain L:

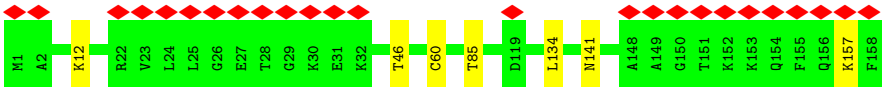




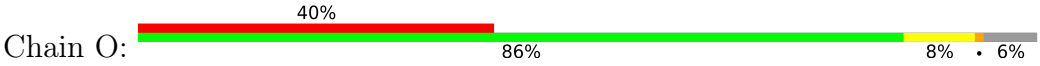
• Molecule 15: 40S ribosomal protein eS10

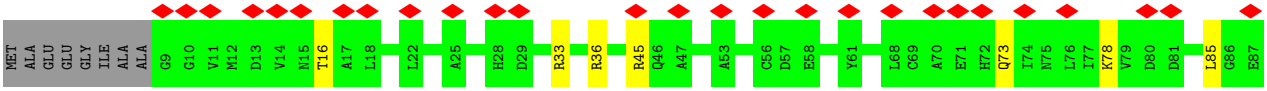


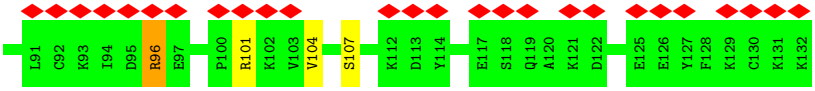
• Molecule 16: 40S ribosomal protein S11



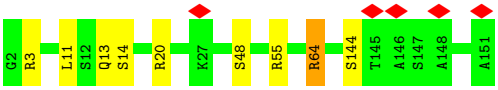
• Molecule 17: 40S ribosomal protein S12



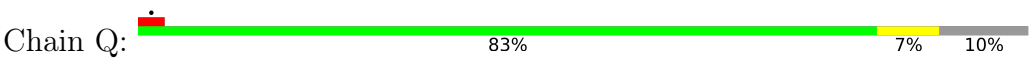


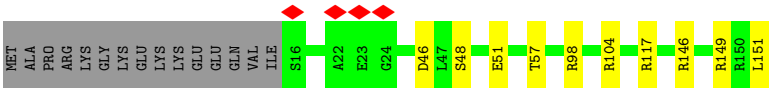


• Molecule 18: ribosomal protein uS15

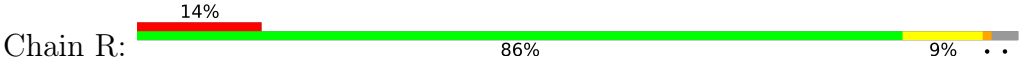


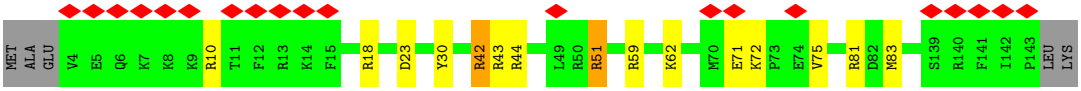
• Molecule 19: 40S ribosomal protein uS11



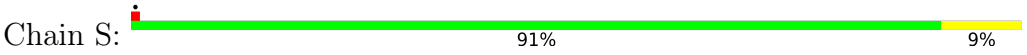


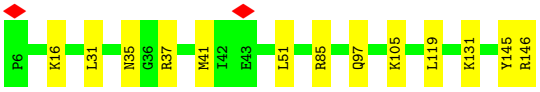
• Molecule 20: 40S ribosomal protein uS19



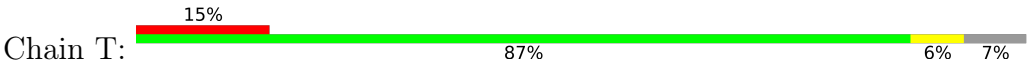


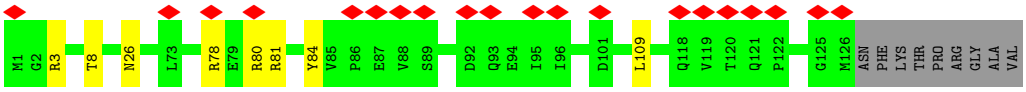
• Molecule 21: 40S ribosomal protein uS9



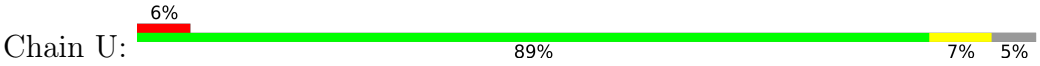


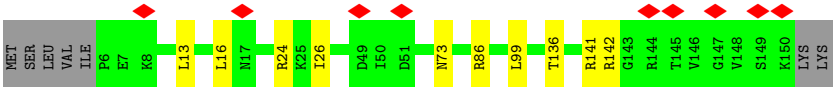
• Molecule 22: 40S ribosomal protein eS17





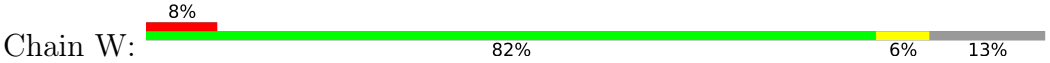
• Molecule 23: 40S ribosomal protein uS13

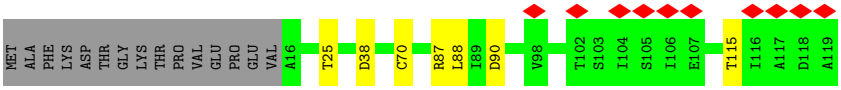




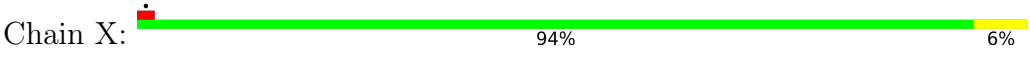
• Molecule 24: 40S ribosomal protein eS19

• Molecule 25: 40S ribosomal protein uS10



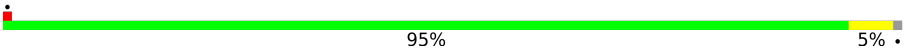


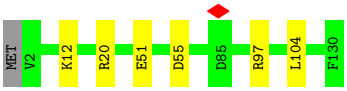
• Molecule 26: 40S ribosomal protein S21



• Molecule 27: Ribosomal protein S15a

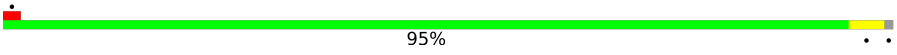
Chain Y:

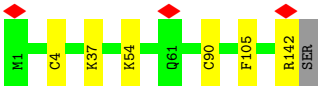




• Molecule 28: 40S ribosomal protein S23

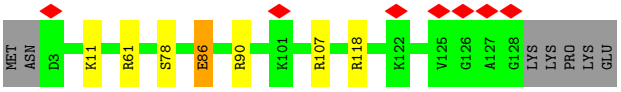
Chain Z:





• Molecule 29: 40S ribosomal protein S24

Chain a:

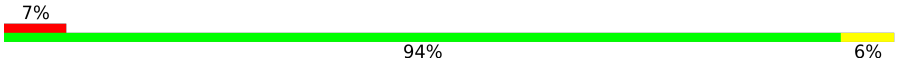


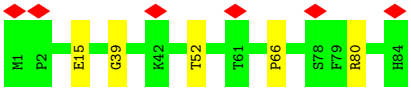
• Molecule 30: 40S ribosomal protein S26

Chain b:

• Molecule 31: 40S ribosomal protein S27

Chain c:



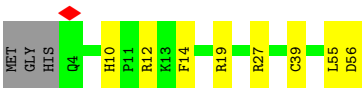


• Molecule 32: 40S ribosomal protein S28

Chain d:

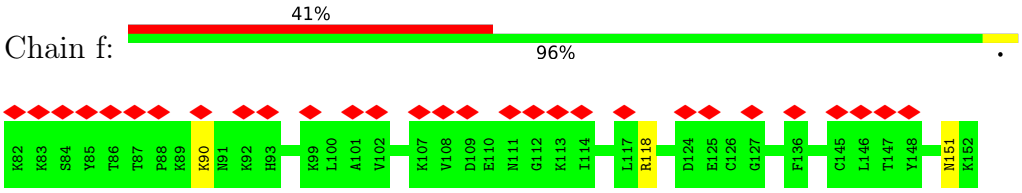
• Molecule 33: 40S ribosomal protein S29

Chain e:



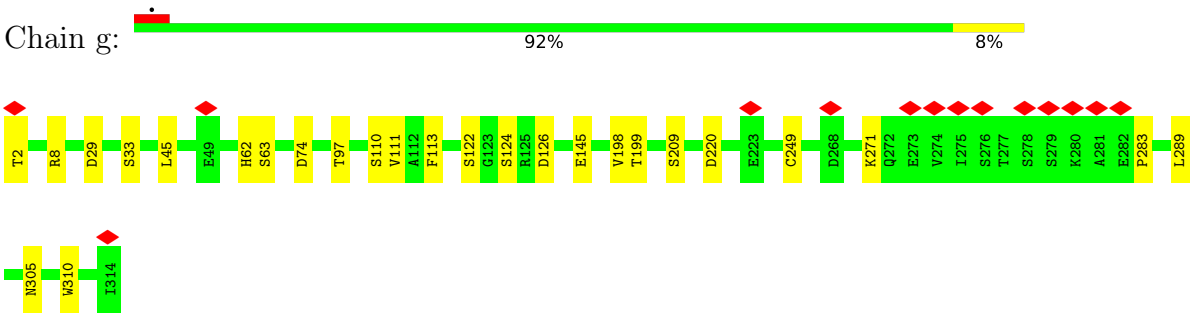
• Molecule 34: ribosomal protein eS31

Chain f:



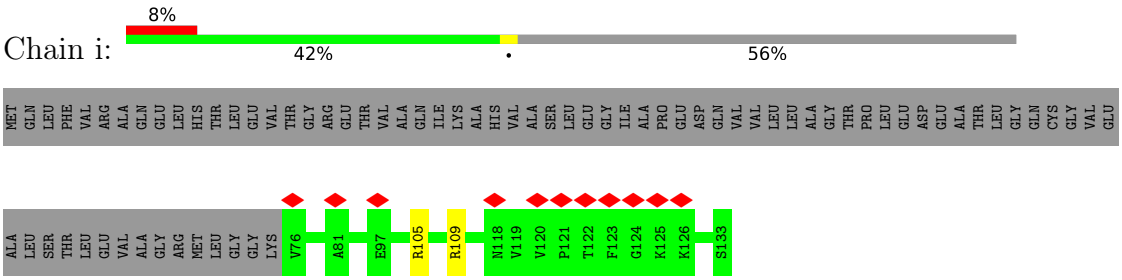
• Molecule 35: Ribosomal protein RACK1

Chain g:



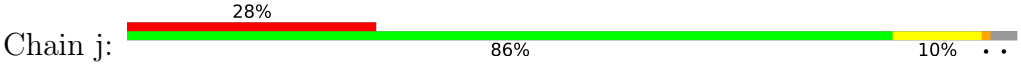
• Molecule 36: 40S ribosomal protein S30

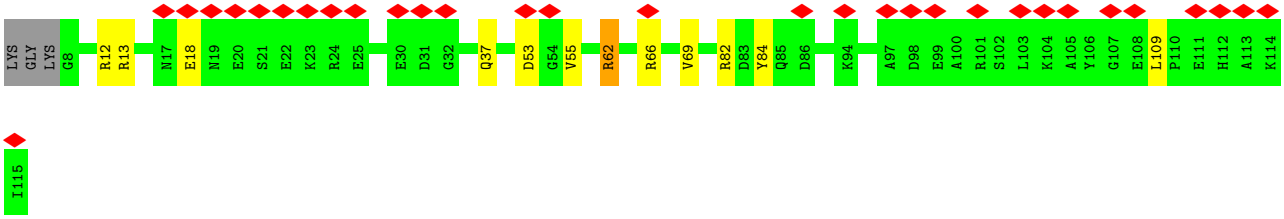
Chain i:



• Molecule 37: Eukaryotic translation initiation factor 4C

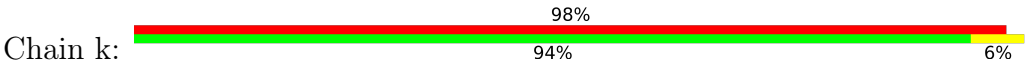
Chain j:

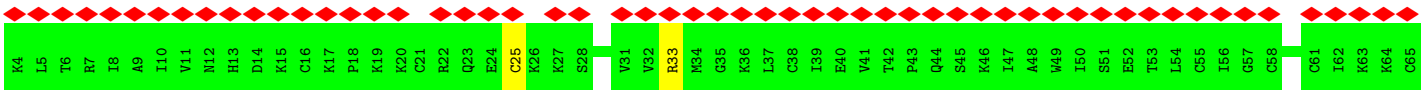


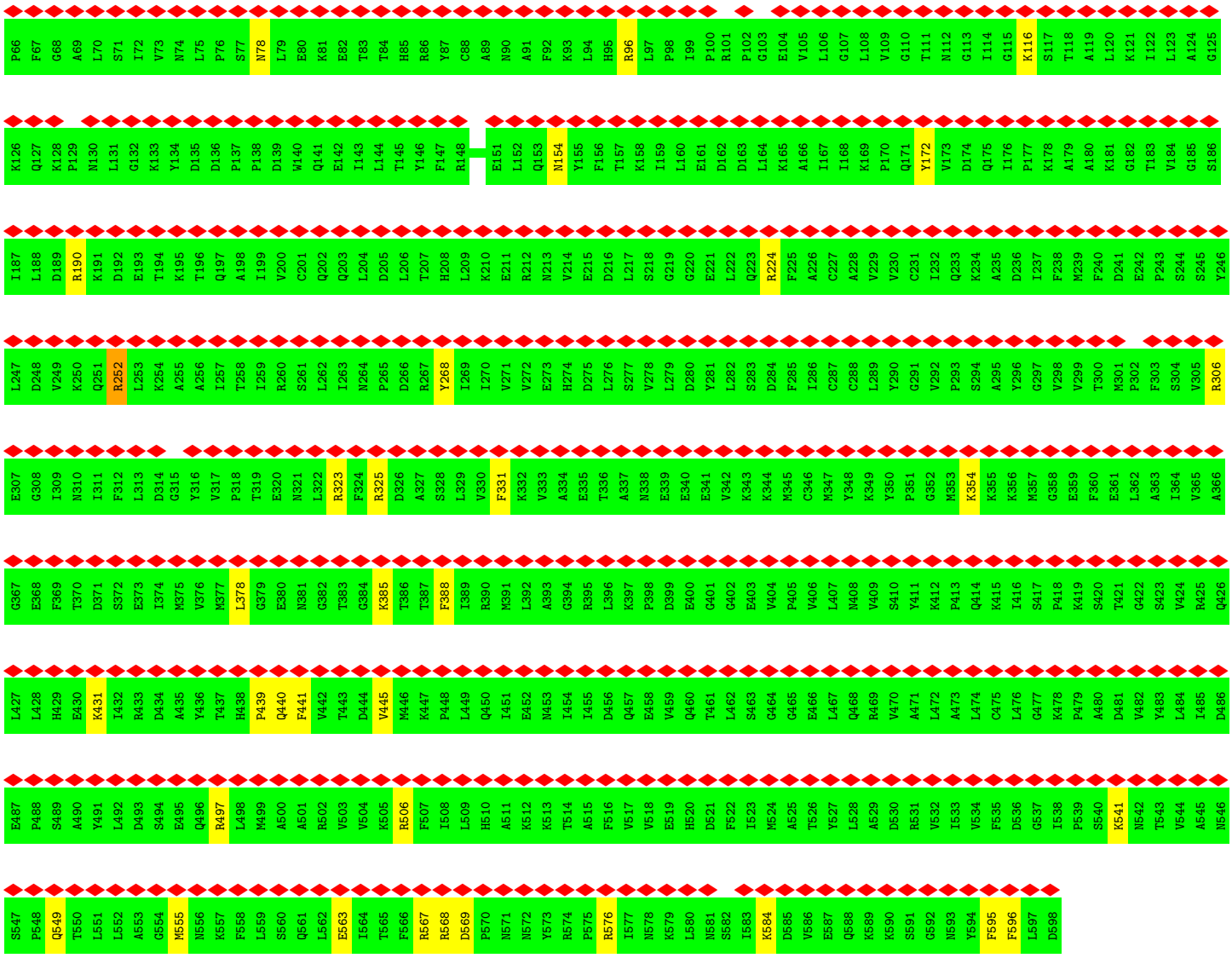


• Molecule 38: ATP binding cassette subfamily E member 1

Chain k:

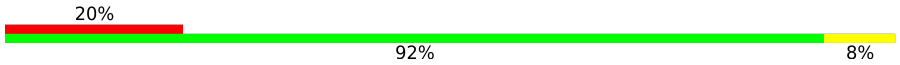


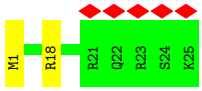




- Molecule 39: 60S ribosomal protein L41

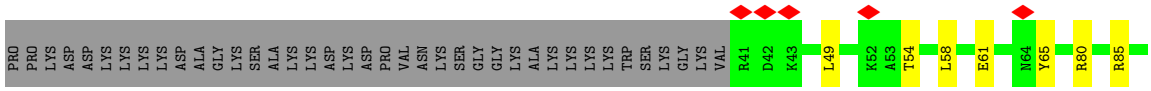
Chain l:

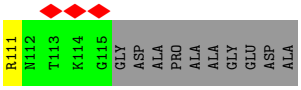




- Molecule 40: 40S ribosomal protein S25

Chain n:




R111
N112
T113
K114
G115
GLY
ASP
ALA
PRO
ALA
ALA
GLY
GLU
ASP
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.080	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, MG, MA6, I2T

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	1.02	2/1770 (0.1%)	1.68	37/2759 (1.3%)
2	2	0.87	75/41554 (0.2%)	1.33	662/64761 (1.0%)
3	3	1.28	0/188	1.98	10/288 (3.5%)
4	A	0.47	0/2177	0.85	9/2935 (0.3%)
5	C	0.52	0/1674	0.88	7/2275 (0.3%)
6	D	0.36	0/1769	0.61	0/2367
7	E	0.38	0/1794	0.61	1/2430 (0.0%)
8	F	0.31	0/1792	0.51	1/2412 (0.0%)
9	G	0.28	0/2125	0.50	0/2856
10	H	0.42	0/1503	0.73	6/2020 (0.3%)
11	I	0.39	0/1946	0.69	5/2588 (0.2%)
12	J	0.34	0/1553	0.61	1/2079 (0.0%)
13	K	0.49	0/1709	0.82	5/2278 (0.2%)
14	L	0.45	0/1567	0.76	4/2092 (0.2%)
15	M	0.45	0/852	0.77	1/1147 (0.1%)
16	N	0.39	0/1319	0.59	0/1761
17	O	0.51	0/968	0.84	3/1296 (0.2%)
18	P	0.42	0/1232	0.72	3/1656 (0.2%)
19	Q	0.53	0/1029	0.91	3/1380 (0.2%)
20	R	0.65	0/1177	1.09	9/1571 (0.6%)
21	S	0.39	0/1142	0.63	3/1528 (0.2%)
22	T	0.44	0/1031	0.81	3/1383 (0.2%)
23	U	0.38	0/1212	0.64	1/1621 (0.1%)
24	V	0.49	0/1133	0.82	3/1517 (0.2%)
25	W	0.28	0/832	0.51	0/1117
26	X	0.37	0/643	0.60	0/860
27	Y	0.47	0/1051	0.80	0/1406
28	Z	0.36	0/1124	0.59	0/1500
29	a	0.59	0/1038	0.96	4/1380 (0.3%)
30	b	0.54	0/802	0.91	6/1076 (0.6%)
31	c	0.46	0/673	0.82	1/902 (0.1%)
32	d	0.32	0/508	0.58	0/680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.54	0/454	0.96	4/603 (0.7%)
34	f	0.41	0/594	0.66	0/786
35	g	0.37	0/2494	0.67	0/3394
36	i	0.62	0/469	0.96	1/617 (0.2%)
37	j	0.39	0/884	0.71	4/1175 (0.3%)
38	k	0.52	0/4780	0.81	10/6452 (0.2%)
39	l	0.25	0/241	0.39	0/305
40	n	0.45	0/604	0.80	3/810 (0.4%)
All	All	0.69	77/91407 (0.1%)	1.10	810/132063 (0.6%)

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
1	1	0	9
2	2	0	94
3	3	0	1
4	A	0	1
5	C	0	1
10	H	0	1
11	I	0	2
13	K	0	2
14	L	0	1
18	P	0	1
19	Q	0	1
20	R	0	3
22	T	0	1
36	i	0	1
37	j	0	2
38	k	0	3
All	All	0	124

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	72	U	O3'-P	-15.85	1.42	1.61
2	2	1245	C	O3'-P	-10.77	1.48	1.61
2	2	270	G	P-OP1	7.37	1.61	1.49
2	2	1724	U	P-OP1	7.35	1.61	1.49
2	2	1765	G	P-OP1	7.34	1.61	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	270	G	P-OP2	7.33	1.61	1.49
2	2	1097	U	P-OP1	7.32	1.61	1.49
2	2	1765	G	P-OP2	7.30	1.61	1.49
2	2	1557	C	C4-N4	-6.38	1.28	1.33
2	2	481	C	C4-N4	-6.09	1.28	1.33
2	2	809	A	C5-C4	-6.00	1.34	1.38
2	2	1083	A	C5-C4	-5.98	1.34	1.38
2	2	595	A	C5-C4	-5.98	1.34	1.38
2	2	598	C	C4-N4	-5.94	1.28	1.33
2	2	1216	A	C5-C4	-5.91	1.34	1.38
2	2	1089	A	C5-C4	-5.88	1.34	1.38
2	2	606	A	C5-C4	-5.84	1.34	1.38
2	2	39	A	C5-C4	-5.83	1.34	1.38
2	2	1614	A	C5-C4	-5.71	1.34	1.38
2	2	1190	A	C5-C4	-5.67	1.34	1.38
2	2	1309	A	C5-C4	-5.64	1.34	1.38
2	2	918	A	C5-C4	-5.63	1.34	1.38
2	2	480	C	C4-N4	-5.60	1.28	1.33
2	2	1678	C	C4-N4	-5.59	1.28	1.33
2	2	953	A	C5-C4	-5.54	1.34	1.38
2	2	1853	A	C5-C4	-5.54	1.34	1.38
2	2	50	A	C5-C4	-5.52	1.34	1.38
2	2	38	A	C5-C4	-5.52	1.34	1.38
2	2	1209	C	N3-C4	-5.50	1.30	1.33
2	2	104	A	C5-C4	-5.48	1.34	1.38
2	2	675	A	C5-C4	-5.46	1.34	1.38
2	2	509	A	C5-C4	-5.44	1.34	1.38
2	2	564	A	C5-C4	-5.42	1.34	1.38
2	2	916	A	C5-C4	-5.39	1.34	1.38
2	2	1129	A	C5-C4	-5.38	1.34	1.38
2	2	1516	C	C4-N4	-5.34	1.29	1.33
2	2	1860	A	C5-C4	-5.33	1.35	1.38
2	2	989	G	C2-N2	-5.32	1.29	1.34
2	2	980	C	C4-N4	-5.31	1.29	1.33
2	2	650	C	N3-C4	-5.31	1.30	1.33
2	2	1522	C	C4-N4	-5.30	1.29	1.33
2	2	940	A	C5-C4	-5.28	1.35	1.38
2	2	498	A	C5-C4	-5.28	1.35	1.38
2	2	102	A	C5-C4	-5.27	1.35	1.38
2	2	799	C	C4-N4	-5.26	1.29	1.33
2	2	1684	C	C4-N4	-5.25	1.29	1.33
2	2	495	G	C2-N2	-5.25	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1209	C	C4-N4	-5.23	1.29	1.33
2	2	104	A	C6-N1	-5.22	1.31	1.35
2	2	1784	A	C5-C4	-5.21	1.35	1.38
2	2	1855	G	C2-N2	-5.21	1.29	1.34
2	2	607	G	C2-N2	-5.19	1.29	1.34
2	2	822	A	C5-C4	-5.16	1.35	1.38
2	2	1119	C	C4-N4	-5.16	1.29	1.33
2	2	83	A	C5-C4	-5.15	1.35	1.38
2	2	1854	A	C5-C4	-5.15	1.35	1.38
2	2	979	A	C5-C4	-5.15	1.35	1.38
2	2	1849	G	N1-C2	-5.14	1.33	1.37
2	2	624	A	C5-C4	-5.12	1.35	1.38
2	2	1623	C	C4-N4	-5.11	1.29	1.33
2	2	1312	C	C4-N4	-5.10	1.29	1.33
2	2	96	C	C4-N4	-5.09	1.29	1.33
2	2	85	A	C5-C4	-5.09	1.35	1.38
2	2	1556	A	C5-C4	-5.08	1.35	1.38
2	2	508	G	C2-N2	-5.07	1.29	1.34
2	2	1272	A	C5-C4	-5.06	1.35	1.38
2	2	1295	A	C5-C4	-5.06	1.35	1.38
2	2	614	C	C4-N4	-5.06	1.29	1.33
1	1	41	C	C4-N4	-5.04	1.29	1.33
2	2	1214	C	C4-N4	-5.04	1.29	1.33
2	2	823	A	C5-C4	-5.04	1.35	1.38
2	2	614	C	N3-C4	-5.03	1.30	1.33
2	2	1090	C	C4-N4	-5.03	1.29	1.33
2	2	1851	G	C2-N2	-5.02	1.29	1.34
2	2	1564	A	C5-C4	-5.01	1.35	1.38
2	2	37	C	C4-N4	-5.01	1.29	1.33
2	2	809	A	C6-N1	-5.01	1.32	1.35

All (810) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	72	U	OP2-P-O3'	-38.61	20.25	105.20
2	2	71	G	O4'-C1'-N9	12.55	118.24	108.20
1	1	72	U	OP1-P-O3'	12.43	132.54	105.20
2	2	498	A	N1-C6-N6	-12.32	111.21	118.60
2	2	581	U	O4'-C1'-N1	12.25	118.00	108.20
2	2	104	A	N1-C6-N6	-11.40	111.76	118.60
1	1	35	A	N1-C6-N6	-11.16	111.91	118.60
2	2	915	A	O4'-C1'-N9	11.02	117.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1740	A	N1-C6-N6	-11.00	112.00	118.60
2	2	159	A	N1-C6-N6	-10.92	112.05	118.60
2	2	150	A	N1-C6-N6	-10.87	112.08	118.60
22	T	78	ARG	NE-CZ-NH2	10.84	125.72	120.30
2	2	1562	G	O4'-C1'-N9	10.83	116.86	108.20
2	2	103	A	N1-C6-N6	-10.70	112.18	118.60
2	2	1089	A	N1-C6-N6	-10.69	112.19	118.60
2	2	1785	A	N1-C6-N6	-10.64	112.22	118.60
2	2	1053	C	O4'-C1'-N1	10.63	116.70	108.20
2	2	1818	A	N1-C6-N6	-10.52	112.29	118.60
2	2	50	A	N1-C6-N6	-10.50	112.30	118.60
2	2	916	A	N1-C6-N6	-10.49	112.30	118.60
2	2	1694	A	N1-C6-N6	-10.48	112.31	118.60
2	2	606	A	N1-C6-N6	-10.41	112.36	118.60
2	2	85	A	N1-C6-N6	-10.33	112.40	118.60
2	2	1483	A	N1-C6-N6	-10.23	112.46	118.60
2	2	822	A	N1-C6-N6	-9.94	112.63	118.60
2	2	38	A	N1-C6-N6	-9.88	112.67	118.60
2	2	84	A	N1-C6-N6	-9.88	112.67	118.60
2	2	1245	C	OP1-P-O3'	9.88	126.94	105.20
5	C	205	ARG	NE-CZ-NH2	9.88	125.24	120.30
20	R	18	ARG	NE-CZ-NH2	9.87	125.24	120.30
2	2	1482	A	N1-C6-N6	-9.80	112.72	118.60
2	2	584	A	N1-C6-N6	-9.76	112.75	118.60
2	2	1053	C	N3-C2-O2	-9.72	115.09	121.90
2	2	83	A	N1-C6-N6	-9.70	112.78	118.60
2	2	954	G	O4'-C1'-N9	9.67	115.94	108.20
2	2	190	A	N1-C6-N6	-9.66	112.80	118.60
2	2	958	A	N1-C6-N6	-9.65	112.81	118.60
2	2	1237	A	N1-C6-N6	-9.61	112.83	118.60
2	2	1280	A	N1-C6-N6	-9.49	112.90	118.60
2	2	1295	A	N1-C6-N6	-9.49	112.91	118.60
2	2	909	A	O4'-C1'-N9	9.47	115.78	108.20
2	2	67	C	N3-C2-O2	-9.44	115.29	121.90
2	2	579	G	O4'-C1'-N9	9.44	115.75	108.20
2	2	1819	A	N1-C6-N6	-9.43	112.94	118.60
2	2	960	A	N1-C6-N6	-9.42	112.95	118.60
2	2	1246	A	N1-C6-N6	-9.40	112.96	118.60
2	2	1190	A	N1-C6-N6	-9.39	112.97	118.60
2	2	515	A	N1-C6-N6	-9.32	113.01	118.60
2	2	68	A	N1-C6-N6	-9.31	113.01	118.60
2	2	1216	A	N1-C6-N6	-9.28	113.03	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	P	55	ARG	NE-CZ-NH2	9.28	124.94	120.30
2	2	819	U	O4'-C1'-N1	9.26	115.61	108.20
2	2	1614	A	N1-C6-N6	-9.25	113.05	118.60
2	2	953	A	N1-C6-N6	-9.24	113.05	118.60
2	2	809	A	N1-C6-N6	-9.21	113.07	118.60
2	2	1692	A	N1-C6-N6	-9.18	113.09	118.60
2	2	491	C	C2-N1-C1'	9.16	128.88	118.80
2	2	580	A	N1-C6-N6	-9.12	113.13	118.60
2	2	1051	A	N1-C6-N6	-9.07	113.16	118.60
1	1	42	A	N1-C6-N6	-9.07	113.16	118.60
2	2	940	A	N1-C6-N6	-9.07	113.16	118.60
2	2	200	U	O4'-C1'-N1	9.06	115.45	108.20
2	2	102	A	N1-C6-N6	-9.02	113.19	118.60
2	2	835	C	C2-N1-C1'	8.96	128.66	118.80
2	2	860	A	N1-C6-N6	-8.95	113.23	118.60
2	2	675	A	N1-C6-N6	-8.95	113.23	118.60
2	2	1216	A	C5-C6-N1	8.89	122.14	117.70
2	2	39	A	N1-C6-N6	-8.85	113.29	118.60
2	2	491	C	N1-C2-O2	8.85	124.21	118.90
2	2	515	A	C5-C6-N1	8.81	122.10	117.70
2	2	270	G	P-O5'-C5'	-8.79	106.84	120.90
2	2	1765	G	P-O5'-C5'	-8.78	106.85	120.90
2	2	454	A	N1-C6-N6	-8.68	113.39	118.60
2	2	1247	A	N1-C6-N6	-8.62	113.42	118.60
2	2	595	A	N1-C6-N6	-8.61	113.44	118.60
2	2	458	A	N1-C6-N6	-8.56	113.46	118.60
4	A	234	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	1	44	A	N1-C6-N6	-8.49	113.50	118.60
2	2	1089	A	C5-C6-N1	8.49	121.94	117.70
2	2	1309	A	N1-C6-N6	-8.47	113.52	118.60
2	2	953	A	C5-C6-N1	8.46	121.93	117.70
2	2	1083	A	N1-C6-N6	-8.46	113.53	118.60
2	2	158	A	N1-C6-N6	-8.46	113.53	118.60
2	2	1213	A	N1-C6-N6	-8.45	113.53	118.60
36	i	109	ARG	NE-CZ-NH2	8.44	124.52	120.30
20	R	44	ARG	NE-CZ-NH2	8.43	124.52	120.30
10	H	219	ARG	NE-CZ-NH2	8.40	124.50	120.30
2	2	1083	A	C5-C6-N1	8.40	121.90	117.70
21	S	146	ARG	NE-CZ-NH2	8.39	124.49	120.30
2	2	1692	A	C5-C6-N1	8.38	121.89	117.70
2	2	606	A	C5-C6-N1	8.37	121.89	117.70
38	k	306	ARG	NE-CZ-NH2	8.34	124.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	835	C	N1-C2-O2	8.33	123.90	118.90
2	2	959	A	N1-C6-N6	-8.33	113.60	118.60
2	2	38	A	C5-C6-N1	8.33	121.86	117.70
2	2	1340	A	C5-C6-N1	8.32	121.86	117.70
2	2	564	A	C5-C6-N1	8.30	121.85	117.70
21	S	146	ARG	NE-CZ-NH1	8.27	124.44	120.30
2	2	916	A	C5-C6-N1	8.27	121.83	117.70
2	2	221	A	N1-C6-N6	-8.26	113.64	118.60
2	2	1818	A	C5-C6-N1	8.26	121.83	117.70
2	2	1614	A	C5-C6-N1	8.22	121.81	117.70
2	2	580	A	O4'-C1'-N9	8.20	114.76	108.20
4	A	64	ARG	NE-CZ-NH2	8.20	124.40	120.30
2	2	523	A	N1-C6-N6	-8.20	113.68	118.60
2	2	1636	A	N1-C6-N6	-8.19	113.69	118.60
2	2	103	A	C5-C6-N1	8.18	121.79	117.70
2	2	1817	A	C5-C6-N1	8.17	121.78	117.70
2	2	85	A	C5-C6-N1	8.16	121.78	117.70
2	2	1564	A	N1-C6-N6	-8.16	113.70	118.60
2	2	498	A	C5-C6-N1	8.15	121.78	117.70
2	2	960	A	C5-C6-N1	8.14	121.77	117.70
2	2	516	A	N1-C6-N6	-8.12	113.73	118.60
2	2	595	A	C5-C6-N1	8.12	121.76	117.70
2	2	1517	A	N1-C6-N6	-8.08	113.75	118.60
2	2	164	A	N1-C6-N6	-8.05	113.77	118.60
2	2	573	A	N1-C6-N6	-8.04	113.77	118.60
2	2	1054	A	O4'-C1'-N9	8.03	114.62	108.20
2	2	509	A	N1-C6-N6	-8.01	113.79	118.60
2	2	823	A	N1-C6-N6	-8.01	113.80	118.60
2	2	1054	A	N1-C6-N6	-8.00	113.80	118.60
2	2	822	A	C5-C6-N1	7.99	121.69	117.70
1	1	34	C	N3-C2-O2	-7.99	116.31	121.90
30	b	6	ARG	NE-CZ-NH2	7.99	124.29	120.30
2	2	40	A	N1-C6-N6	-7.94	113.83	118.60
2	2	67	C	N1-C2-O2	7.94	123.66	118.90
2	2	614	C	N3-C2-O2	-7.92	116.35	121.90
2	2	11	A	N1-C6-N6	-7.92	113.85	118.60
2	2	1090	C	N3-C2-O2	-7.90	116.37	121.90
2	2	624	A	N1-C6-N6	-7.88	113.87	118.60
2	2	159	A	C5-C6-N1	7.87	121.64	117.70
3	3	52	A	N1-C6-N6	-7.87	113.88	118.60
11	I	98	ARG	NE-CZ-NH2	7.87	124.24	120.30
2	2	102	A	C5-C6-N1	7.86	121.63	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1854	A	C5-C6-N1	7.86	121.63	117.70
2	2	1817	A	N1-C6-N6	-7.85	113.89	118.60
2	2	559	A	C5-C6-N1	7.85	121.62	117.70
2	2	1210	A	N1-C6-N6	-7.84	113.89	118.60
2	2	1556	A	N1-C6-N6	-7.84	113.90	118.60
2	2	1819	A	C5-C6-N1	7.82	121.61	117.70
2	2	1129	A	N1-C6-N6	-7.82	113.91	118.60
2	2	959	A	C5-C6-N1	7.81	121.60	117.70
2	2	1213	A	C5-C6-N1	7.81	121.60	117.70
2	2	518	A	C5-C6-N1	7.81	121.60	117.70
2	2	1236	A	N1-C6-N6	-7.80	113.92	118.60
20	R	10	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	2	609	A	N1-C6-N6	-7.79	113.93	118.60
2	2	589	A	C5-C6-N1	7.78	121.59	117.70
2	2	158	A	C5-C6-N1	7.77	121.59	117.70
2	2	1853	A	N1-C6-N6	-7.76	113.94	118.60
2	2	83	A	C5-C6-N1	7.75	121.58	117.70
2	2	1051	A	C5-C6-N1	7.74	121.57	117.70
2	2	418	U	N3-C2-O2	-7.73	116.79	122.20
2	2	1353	A	C5-C6-N1	7.72	121.56	117.70
2	2	809	A	C5-C6-N1	7.71	121.56	117.70
2	2	1564	A	C5-C6-N1	7.71	121.55	117.70
2	2	1784	A	N1-C6-N6	-7.71	113.97	118.60
2	2	39	A	C5-C6-N1	7.70	121.55	117.70
13	K	123	ARG	NE-CZ-NH2	7.69	124.15	120.30
2	2	918	A	N1-C6-N6	-7.69	113.99	118.60
2	2	1482	A	C5-C6-N1	7.66	121.53	117.70
2	2	219	U	O4'-C1'-N1	7.64	114.31	108.20
2	2	589	A	N1-C6-N6	-7.64	114.02	118.60
10	H	161	ARG	NE-CZ-NH2	7.64	124.12	120.30
2	2	1853	A	C5-C6-N1	7.62	121.51	117.70
1	1	35	A	C4-C5-C6	-7.62	113.19	117.00
2	2	518	A	N1-C6-N6	-7.61	114.03	118.60
2	2	1784	A	C5-C6-N1	7.61	121.50	117.70
2	2	675	A	C5-C6-N1	7.60	121.50	117.70
2	2	359	C	P-O3'-C3'	7.59	128.81	119.70
2	2	584	A	C5-C6-N1	7.59	121.49	117.70
2	2	361	A	N1-C6-N6	-7.57	114.06	118.60
21	S	146	ARG	NH1-CZ-NH2	-7.57	111.07	119.40
2	2	580	A	C5-C6-N1	7.56	121.48	117.70
1	1	35	A	C5-C6-N1	7.55	121.48	117.70
2	2	1636	A	C5-C6-N1	7.54	121.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1246	A	C5-C6-N1	7.54	121.47	117.70
4	A	244	ARG	NE-CZ-NH2	7.54	124.07	120.30
2	2	958	A	C5-C6-N1	7.54	121.47	117.70
2	2	582	C	P-O3'-C3'	7.53	128.74	119.70
2	2	84	A	C5-C6-N1	7.53	121.46	117.70
2	2	1816	A	N1-C6-N6	-7.53	114.08	118.60
2	2	819	U	N3-C2-O2	-7.52	116.94	122.20
2	2	1696	C	N3-C2-O2	-7.50	116.65	121.90
2	2	799	C	N3-C2-O2	-7.50	116.65	121.90
2	2	565	A	C5-C6-N1	7.49	121.45	117.70
2	2	1854	A	N1-C6-N6	-7.48	114.11	118.60
2	2	598	C	N3-C2-O2	-7.48	116.66	121.90
2	2	1247	A	C5-C6-N1	7.48	121.44	117.70
2	2	479	A	N1-C6-N6	-7.47	114.12	118.60
2	2	221	A	C5-C6-N1	7.47	121.43	117.70
2	2	909	A	C5-C6-N1	7.46	121.43	117.70
2	2	50	A	C5-C6-N1	7.46	121.43	117.70
2	2	150	A	C5-C6-N1	7.45	121.42	117.70
5	C	85	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	2	1089	A	C4-C5-C6	-7.41	113.30	117.00
2	2	1557	C	O4'-C1'-N1	7.41	114.13	108.20
2	2	1043	C	N3-C2-O2	-7.40	116.72	121.90
2	2	823	A	C5-C6-N1	7.40	121.40	117.70
2	2	1335	U	O4'-C1'-N1	7.40	114.12	108.20
37	j	12	ARG	NE-CZ-NH2	7.39	124.00	120.30
2	2	1242	A	C5-C6-N1	7.39	121.39	117.70
2	2	958	A	C4-C5-C6	-7.36	113.32	117.00
2	2	1242	A	N1-C6-N6	-7.35	114.19	118.60
2	2	1517	A	C5-C6-N1	7.35	121.37	117.70
2	2	1483	A	C5-C6-N1	7.34	121.37	117.70
2	2	1816	A	O4'-C1'-N9	7.33	114.07	108.20
13	K	5	ARG	NE-CZ-NH2	7.33	123.97	120.30
2	2	458	A	C5-C6-N1	7.33	121.36	117.70
3	3	52	A	C5-C6-N1	7.33	121.36	117.70
22	T	80	ARG	NE-CZ-NH2	7.29	123.95	120.30
30	b	15	ARG	NE-CZ-NH2	7.29	123.94	120.30
2	2	479	A	C5-C6-N1	7.28	121.34	117.70
2	2	1237	A	C5-C6-N1	7.27	121.34	117.70
2	2	979	A	N1-C6-N6	-7.27	114.24	118.60
2	2	68	A	C4-C5-C6	-7.27	113.37	117.00
2	2	1200	A	C5-C6-N1	7.26	121.33	117.70
2	2	160	U	O4'-C1'-N1	7.26	114.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	164	A	C5-C6-N1	7.26	121.33	117.70
2	2	1209	C	N3-C2-O2	-7.26	116.82	121.90
2	2	1190	A	C4-C5-C6	-7.25	113.37	117.00
2	2	860	A	C5-C6-N1	7.25	121.33	117.70
1	1	44	A	C5-C6-N1	7.25	121.32	117.70
1	1	42	A	C5-C6-N1	7.24	121.32	117.70
2	2	1484	C	N3-C2-O2	-7.24	116.83	121.90
2	2	1816	A	C5-C6-N1	7.24	121.32	117.70
2	2	1054	A	C5-C6-N1	7.24	121.32	117.70
2	2	624	A	C5-C6-N1	7.23	121.32	117.70
2	2	626	C	N3-C2-O2	-7.22	116.85	121.90
24	V	121	ARG	NE-CZ-NH2	7.22	123.91	120.30
2	2	565	A	N1-C6-N6	-7.22	114.27	118.60
2	2	1785	A	C5-C6-N1	7.21	121.31	117.70
37	j	18	GLU	OE1-CD-OE2	-7.20	114.66	123.30
2	2	1694	A	C5-C6-N1	7.19	121.30	117.70
2	2	1280	A	C5-C6-N1	7.19	121.30	117.70
2	2	1340	A	N1-C6-N6	-7.19	114.28	118.60
2	2	1309	A	O4'-C1'-N9	7.18	113.94	108.20
2	2	1190	A	C5-C6-N1	7.17	121.28	117.70
2	2	1210	A	C5-C6-N1	7.17	121.29	117.70
2	2	940	A	C5-C6-N1	7.16	121.28	117.70
2	2	1120	C	N3-C2-O2	-7.16	116.89	121.90
2	2	1129	A	C5-C6-N1	7.16	121.28	117.70
2	2	1855	G	O4'-C1'-N9	7.15	113.92	108.20
2	2	69	C	N3-C2-O2	-7.14	116.90	121.90
2	2	1309	A	C5-C6-N1	7.12	121.26	117.70
2	2	954	G	C3'-C2'-C1'	7.12	107.19	101.50
2	2	1353	A	N1-C6-N6	-7.11	114.33	118.60
2	2	609	A	C5-C6-N1	7.11	121.25	117.70
2	2	1482	A	C4-C5-C6	-7.11	113.45	117.00
8	F	76	ARG	NE-CZ-NH2	7.11	123.85	120.30
2	2	1516	C	N3-C2-O2	-7.09	116.94	121.90
2	2	1635	A	N1-C6-N6	-7.09	114.35	118.60
2	2	909	A	N1-C6-N6	-7.08	114.36	118.60
2	2	1518	C	N3-C2-O2	-7.08	116.95	121.90
2	2	1250	C	N3-C2-O2	-7.04	116.97	121.90
2	2	40	A	C5-C6-N1	7.04	121.22	117.70
2	2	454	A	C5-C6-N1	7.03	121.22	117.70
2	2	1860	A	C5-C6-N1	7.03	121.22	117.70
2	2	605	C	N3-C2-O2	-7.02	116.99	121.90
2	2	1280	A	C4-C5-C6	-7.02	113.49	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1849	G	N1-C6-O6	-7.02	115.69	119.90
2	2	491	C	N3-C2-O2	-7.01	116.99	121.90
2	2	509	A	C5-C6-N1	7.00	121.20	117.70
2	2	545	A	N1-C6-N6	-6.99	114.41	118.60
2	2	49	C	N3-C2-O2	-6.98	117.01	121.90
2	2	1043	C	O4'-C1'-N1	6.97	113.78	108.20
2	2	1295	A	C5-C6-N1	6.96	121.18	117.70
2	2	37	C	O4'-C1'-N1	6.96	113.77	108.20
1	1	27	C	N3-C2-O2	-6.95	117.03	121.90
2	2	11	A	C4-C5-C6	-6.95	113.53	117.00
2	2	102	A	O4'-C1'-N9	6.95	113.76	108.20
2	2	1272	A	C5-C6-N1	6.94	121.17	117.70
2	2	190	A	C5-C6-N1	6.94	121.17	117.70
2	2	1860	A	N1-C6-N6	-6.93	114.44	118.60
2	2	159	A	C4-C5-C6	-6.93	113.53	117.00
2	2	1682	C	N3-C2-O2	-6.93	117.05	121.90
1	1	44	A	C4-C5-C6	-6.92	113.54	117.00
19	Q	146	ARG	NE-CZ-NH2	6.91	123.76	120.30
2	2	68	A	C5-C6-N1	6.91	121.16	117.70
2	2	1560	C	N3-C2-O2	-6.91	117.06	121.90
2	2	1552	C	N1-C2-O2	6.91	123.04	118.90
2	2	103	A	C4-C5-C6	-6.90	113.55	117.00
2	2	1200	A	N1-C6-N6	-6.87	114.48	118.60
2	2	1624	C	N3-C2-O2	-6.87	117.09	121.90
2	2	918	A	C5-C6-N1	6.86	121.13	117.70
2	2	11	A	C5-C6-N1	6.84	121.12	117.70
2	2	1818	A	C4-C5-C6	-6.84	113.58	117.00
2	2	1053	C	N1-C2-O2	6.82	122.99	118.90
2	2	545	A	C5-C6-N1	6.82	121.11	117.70
2	2	1449	C	C2-N1-C1'	6.81	126.29	118.80
3	3	51	C	N3-C2-O2	-6.81	117.13	121.90
2	2	1251	G	N1-C6-O6	-6.80	115.82	119.90
2	2	835	C	N3-C2-O2	-6.80	117.14	121.90
2	2	1724	U	OP1-P-OP2	-6.80	109.41	119.60
2	2	517	C	N3-C2-O2	-6.79	117.15	121.90
2	2	1097	U	OP1-P-OP2	-6.79	109.41	119.60
2	2	979	A	C5-C6-N1	6.79	121.09	117.70
2	2	67	C	O4'-C1'-C2'	-6.78	99.02	105.80
2	2	595	A	C4-C5-C6	-6.77	113.61	117.00
2	2	1765	G	OP1-P-OP2	-6.77	109.45	119.60
2	2	270	G	OP1-P-OP2	-6.75	109.47	119.60
2	2	1119	C	N3-C2-O2	-6.74	117.18	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	615	G	N1-C6-O6	-6.74	115.86	119.90
2	2	469	C	N3-C2-O2	-6.73	117.19	121.90
2	2	203	G	N1-C6-O6	-6.73	115.86	119.90
2	2	1231	G	N1-C6-O6	-6.72	115.87	119.90
2	2	70	G	N1-C6-O6	-6.72	115.87	119.90
30	b	10	ARG	NE-CZ-NH2	6.72	123.66	120.30
2	2	1557	C	N3-C2-O2	-6.72	117.20	121.90
2	2	564	A	N1-C6-N6	-6.71	114.57	118.60
2	2	150	A	C4-C5-C6	-6.71	113.64	117.00
2	2	1684	C	N3-C2-O2	-6.70	117.21	121.90
12	J	98	ARG	NE-CZ-NH2	6.69	123.64	120.30
2	2	1233	C	N3-C2-O2	-6.69	117.22	121.90
2	2	573	A	C5-C6-N1	6.68	121.04	117.70
2	2	1090	C	O4'-C1'-N1	6.68	113.54	108.20
2	2	85	A	C4'-C3'-C2'	-6.67	95.93	102.60
2	2	1635	A	C5-C6-N1	6.67	121.03	117.70
2	2	583	C	O4'-C1'-N1	6.66	113.53	108.20
2	2	1522	C	O4'-C1'-N1	6.65	113.52	108.20
2	2	1515	G	C5'-C4'-O4'	6.64	117.08	109.10
2	2	104	A	C5-C6-N1	6.63	121.01	117.70
2	2	1106	G	C5'-C4'-C3'	-6.62	105.40	116.00
1	1	38	A	N1-C6-N6	-6.61	114.64	118.60
2	2	916	A	O4'-C1'-N9	6.60	113.48	108.20
2	2	491	C	C6-N1-C1'	-6.60	112.88	120.80
2	2	569	C	N3-C2-O2	-6.60	117.28	121.90
2	2	1082	G	O4'-C1'-N9	6.59	113.47	108.20
2	2	970	C	N3-C2-O2	-6.59	117.29	121.90
2	2	1614	A	C4-C5-C6	-6.59	113.71	117.00
2	2	1309	A	C4-C5-C6	-6.58	113.71	117.00
1	1	41	C	N3-C2-O2	-6.58	117.29	121.90
2	2	83	A	C4-C5-C6	-6.58	113.71	117.00
2	2	1520	C	N3-C2-O2	-6.58	117.30	121.90
2	2	1483	A	C4-C5-C6	-6.57	113.72	117.00
2	2	1221	U	O4'-C1'-N1	6.57	113.45	108.20
2	2	980	C	N3-C2-O2	-6.54	117.32	121.90
2	2	579	G	C5'-C4'-O4'	6.54	116.95	109.10
2	2	1556	A	C4-C5-C6	-6.53	113.73	117.00
2	2	1683	C	N3-C2-O2	-6.53	117.33	121.90
2	2	1552	C	C2-N1-C1'	6.52	125.97	118.80
2	2	606	A	C4-C5-C6	-6.52	113.74	117.00
2	2	1121	C	N3-C2-O2	-6.52	117.34	121.90
2	2	10	G	N1-C6-O6	-6.50	116.00	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1130	G	N1-C6-O6	-6.50	116.00	119.90
40	n	85	ARG	NE-CZ-NH2	6.49	123.55	120.30
2	2	1859	C	N3-C2-O2	-6.49	117.36	121.90
2	2	589	A	C4-C5-C6	-6.48	113.76	117.00
11	I	72	ARG	NE-CZ-NH2	6.48	123.54	120.30
3	3	52	A	C4-C5-C6	-6.48	113.76	117.00
2	2	523	A	C5-C6-N1	6.47	120.93	117.70
2	2	1238	U	N3-C2-O2	-6.46	117.68	122.20
2	2	1819	A	C4-C5-C6	-6.45	113.78	117.00
2	2	377	C	N3-C2-O2	-6.44	117.39	121.90
10	H	150	ARG	NE-CZ-NH2	6.44	123.52	120.30
2	2	1854	A	O4'-C1'-N9	6.44	113.35	108.20
22	T	81	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	1	38	A	C5-C6-N1	6.40	120.90	117.70
2	2	987	G	C3'-C2'-C1'	6.40	106.62	101.50
29	a	107	ARG	NE-CZ-NH2	6.40	123.50	120.30
5	C	180	ARG	NE-CZ-NH2	6.40	123.50	120.30
2	2	628	C	N3-C2-O2	-6.40	117.42	121.90
2	2	822	A	C4-C5-C6	-6.40	113.80	117.00
2	2	1488	U	N3-C2-O2	-6.40	117.72	122.20
2	2	559	A	N1-C6-N6	-6.39	114.76	118.60
13	K	25	ARG	NE-CZ-NH2	6.39	123.50	120.30
2	2	608	C	N3-C2-O2	-6.39	117.43	121.90
2	2	1515	G	O4'-C1'-N9	-6.38	103.09	108.20
2	2	1018	U	C2-N1-C1'	6.37	125.34	117.70
2	2	1337	C	N3-C2-O2	-6.37	117.44	121.90
2	2	1155	G	N1-C6-O6	-6.36	116.08	119.90
2	2	523	A	C4-C5-C6	-6.36	113.82	117.00
2	2	860	A	C4-C5-C6	-6.36	113.82	117.00
2	2	1230	C	N3-C2-O2	-6.35	117.45	121.90
2	2	191	C	N3-C2-O2	-6.35	117.45	121.90
2	2	71	G	N3-C2-N2	-6.35	115.45	119.90
2	2	915	A	C5-C6-N1	6.35	120.88	117.70
18	P	64	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	2	1561	G	C5-C6-N1	6.34	114.67	111.50
2	2	1233	C	O4'-C1'-N1	6.33	113.27	108.20
2	2	481	C	N3-C2-O2	-6.33	117.47	121.90
2	2	1853	A	C4-C5-C6	-6.33	113.83	117.00
1	1	32	C	O4'-C1'-N1	6.33	113.26	108.20
2	2	583	C	C3'-C2'-C1'	6.33	106.56	101.50
20	R	43	ARG	NE-CZ-NH2	6.33	123.46	120.30
2	2	71	G	P-O3'-C3'	6.33	127.29	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	629	C	N3-C2-O2	-6.32	117.47	121.90
2	2	1212	C	N3-C2-O2	-6.32	117.48	121.90
2	2	38	A	O4'-C1'-N9	6.32	113.25	108.20
2	2	515	A	C4-C5-C6	-6.32	113.84	117.00
2	2	1858	U	O4'-C1'-N1	6.32	113.25	108.20
2	2	1312	C	N3-C2-O2	-6.31	117.48	121.90
2	2	1678	C	N3-C2-O2	-6.31	117.48	121.90
2	2	624	A	C4-C5-C6	-6.30	113.85	117.00
2	2	614	C	C5'-C4'-C3'	-6.30	105.92	116.00
2	2	53	C	N3-C2-O2	-6.30	117.49	121.90
1	1	40	C	N3-C2-O2	-6.30	117.49	121.90
2	2	1740	A	C5-C6-N1	6.28	120.84	117.70
2	2	909	A	C4-C5-C6	-6.27	113.86	117.00
4	A	88	ARG	NE-CZ-NH2	6.25	123.43	120.30
2	2	524	G	N1-C6-O6	-6.24	116.15	119.90
2	2	583	C	N3-C2-O2	-6.24	117.53	121.90
31	c	80	ARG	NE-CZ-NH2	6.24	123.42	120.30
2	2	1556	A	C5-C6-N1	6.22	120.81	117.70
2	2	1639	C	N3-C2-O2	-6.22	117.55	121.90
2	2	1295	A	C4-C5-C6	-6.22	113.89	117.00
37	j	62	ARG	NE-CZ-NH2	6.22	123.41	120.30
2	2	597	U	O4'-C1'-N1	6.21	113.17	108.20
2	2	1490	U	O4'-C1'-N1	6.21	113.17	108.20
2	2	498	A	C4-C5-C6	-6.19	113.90	117.00
2	2	1693	C	N3-C2-O2	-6.19	117.57	121.90
2	2	1521	G	N1-C6-O6	-6.19	116.19	119.90
2	2	480	C	N3-C2-O2	-6.19	117.57	121.90
2	2	361	A	C5-C6-N1	6.18	120.79	117.70
2	2	1559	C	N3-C2-O2	-6.17	117.58	121.90
2	2	341	G	N1-C6-O6	-6.17	116.20	119.90
2	2	1210	A	C4-C5-C6	-6.17	113.92	117.00
2	2	1042	U	O4'-C1'-N1	6.15	113.12	108.20
2	2	835	C	C6-N1-C1'	-6.15	113.42	120.80
2	2	1264	C	N3-C2-O2	-6.14	117.60	121.90
2	2	953	A	C4-C5-C6	-6.14	113.93	117.00
2	2	1515	G	P-O3'-C3'	6.14	127.06	119.70
2	2	809	A	C4-C5-C6	-6.14	113.93	117.00
38	k	224	ARG	NE-CZ-NH2	6.13	123.36	120.30
2	2	1636	A	C4-C5-C6	-6.12	113.94	117.00
2	2	497	G	N1-C6-O6	-6.12	116.23	119.90
2	2	201	G	N3-C2-N2	-6.12	115.62	119.90
14	L	136	ARG	NE-CZ-NH2	6.12	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1557	C	C3'-C2'-C1'	6.10	106.38	101.50
2	2	65	C	N3-C2-O2	-6.10	117.63	121.90
2	2	1247	A	C4-C5-C6	-6.10	113.95	117.00
20	R	18	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
10	H	142	ARG	NE-CZ-NH2	6.09	123.34	120.30
2	2	823	A	C4-C5-C6	-6.08	113.96	117.00
2	2	835	C	C6-N1-C2	-6.08	117.87	120.30
2	2	1530	U	N1-C2-O2	6.08	127.06	122.80
2	2	393	G	N1-C6-O6	-6.07	116.26	119.90
2	2	456	G	C5-C6-N1	6.07	114.53	111.50
2	2	220	C	N3-C2-O2	-6.07	117.65	121.90
2	2	37	C	N3-C2-O2	-6.07	117.65	121.90
2	2	516	A	C4-C5-C6	-6.06	113.97	117.00
2	2	1637	U	O4'-C1'-N1	6.06	113.05	108.20
2	2	52	G	N1-C6-O6	-6.04	116.28	119.90
2	2	516	A	C5-C6-N1	6.04	120.72	117.70
2	2	479	A	C4-C5-C6	-6.02	113.99	117.00
4	A	53	ARG	NE-CZ-NH2	6.02	123.31	120.30
2	2	1215	C	N3-C2-O2	-6.02	117.69	121.90
2	2	1322	U	N3-C2-O2	-6.01	117.99	122.20
2	2	1611	U	N3-C2-O2	-6.00	118.00	122.20
2	2	509	A	C4-C5-C6	-6.00	114.00	117.00
2	2	1243	C	N3-C2-O2	-6.00	117.70	121.90
2	2	1236	A	C5-C6-N1	5.99	120.69	117.70
13	K	12	ARG	NE-CZ-NH2	5.97	123.29	120.30
2	2	1270	G	N1-C6-O6	-5.97	116.32	119.90
2	2	1129	A	C4-C5-C6	-5.97	114.02	117.00
2	2	609	A	C4-C5-C6	-5.95	114.02	117.00
2	2	151	C	N3-C2-O2	-5.95	117.74	121.90
38	k	325	ARG	NE-CZ-NH2	5.94	123.27	120.30
2	2	959	A	C4-C5-C6	-5.94	114.03	117.00
2	2	1634	G	N1-C6-O6	-5.94	116.34	119.90
2	2	1258	C	N3-C2-O2	-5.94	117.74	121.90
2	2	1104	G	N1-C6-O6	-5.93	116.34	119.90
2	2	675	A	C4-C5-C6	-5.93	114.04	117.00
2	2	1530	U	C2-N1-C1'	5.93	124.81	117.70
2	2	158	A	C4-C5-C6	-5.92	114.04	117.00
2	2	1548	C	N3-C2-O2	-5.92	117.75	121.90
2	2	1855	G	N1-C6-O6	-5.92	116.35	119.90
2	2	1635	A	C4-C5-C6	-5.92	114.04	117.00
2	2	1154	G	N1-C6-O6	-5.92	116.35	119.90
2	2	614	C	C5'-C4'-O4'	5.91	116.20	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	k	252	ARG	NE-CZ-NH2	5.91	123.26	120.30
2	2	800	U	C4'-C3'-C2'	-5.91	96.69	102.60
14	L	127	ARG	NE-CZ-NH2	5.90	123.25	120.30
2	2	1816	A	C5'-C4'-C3'	-5.89	106.58	116.00
2	2	374	U	O4'-C1'-N1	5.88	112.91	108.20
2	2	453	C	N3-C2-O2	-5.88	117.78	121.90
2	2	1817	A	C4-C5-C6	-5.88	114.06	117.00
2	2	1623	C	N3-C2-O2	-5.87	117.79	121.90
2	2	85	A	C4-C5-C6	-5.87	114.06	117.00
1	1	42	A	C4-C5-C6	-5.87	114.07	117.00
2	2	625	G	N1-C6-O6	-5.87	116.38	119.90
2	2	579	G	N1-C6-O6	-5.86	116.38	119.90
2	2	1054	A	C3'-C2'-C1'	5.86	106.19	101.50
2	2	1677	C	N3-C2-O2	-5.85	117.81	121.90
2	2	1552	C	N3-C2-O2	-5.84	117.81	121.90
2	2	1563	C	N3-C2-O2	-5.84	117.81	121.90
2	2	1153	G	N1-C6-O6	-5.84	116.40	119.90
2	2	377	C	O4'-C1'-N1	5.84	112.87	108.20
2	2	1692	A	C4-C5-C6	-5.83	114.08	117.00
2	2	817	G	N1-C6-O6	-5.83	116.40	119.90
2	2	1258	C	O4'-C1'-N1	5.83	112.86	108.20
2	2	221	A	C4-C5-C6	-5.82	114.09	117.00
2	2	938	G	N1-C6-O6	-5.81	116.41	119.90
2	2	469	C	O4'-C1'-N1	5.81	112.84	108.20
2	2	824	G	N1-C6-O6	-5.80	116.42	119.90
2	2	1199	G	N1-C6-O6	-5.79	116.43	119.90
2	2	940	A	C4-C5-C6	-5.79	114.11	117.00
2	2	1238	U	O4'-C1'-N1	5.79	112.83	108.20
2	2	190	A	C4-C5-C6	-5.78	114.11	117.00
2	2	1517	A	C4-C5-C6	-5.78	114.11	117.00
30	b	95	ARG	NE-CZ-NH2	5.77	123.19	120.30
2	2	1062	U	O4'-C1'-N1	5.76	112.81	108.20
2	2	565	A	C4-C5-C6	-5.76	114.12	117.00
13	K	141	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	2	916	A	C4-C5-C6	-5.75	114.13	117.00
2	2	1083	A	C4-C5-C6	-5.74	114.13	117.00
2	2	1633	G	P-O3'-C3'	5.74	126.59	119.70
15	M	46	MET	O-C-N	-5.74	113.52	122.70
11	I	132	ARG	NE-CZ-NH2	5.74	123.17	120.30
19	Q	149	ARG	NE-CZ-NH2	5.73	123.16	120.30
2	2	458	A	C4-C5-C6	-5.72	114.14	117.00
2	2	1569	C	N3-C2-O2	-5.72	117.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	498	A	C5'-C4'-C3'	-5.72	106.84	116.00
2	2	1051	A	C4-C5-C6	-5.72	114.14	117.00
2	2	1334	G	N1-C6-O6	-5.72	116.47	119.90
2	2	1694	A	C4-C5-C6	-5.72	114.14	117.00
2	2	1310	U	N3-C2-O2	-5.71	118.20	122.20
2	2	1449	C	N1-C2-O2	5.71	122.33	118.90
20	R	81	ARG	NE-CZ-NH2	5.71	123.16	120.30
2	2	605	C	C3'-C2'-C1'	5.71	106.07	101.50
2	2	978	G	O4'-C1'-N9	5.71	112.76	108.20
1	1	68	C	C2-N1-C1'	5.70	125.07	118.80
2	2	1014	U	N3-C2-O2	-5.70	118.21	122.20
2	2	1607	G	C4'-C3'-C2'	-5.69	96.91	102.60
2	2	1207	G	N1-C6-O6	-5.69	116.49	119.90
40	n	111	ARG	NE-CZ-NH2	5.69	123.15	120.30
2	2	341	G	C5-C6-N1	5.68	114.34	111.50
2	2	1311	U	N3-C2-O2	-5.68	118.22	122.20
2	2	1213	A	C4-C5-C6	-5.67	114.16	117.00
2	2	454	A	C4-C5-C6	-5.67	114.17	117.00
2	2	1240	U	O4'-C1'-N1	5.67	112.74	108.20
10	H	151	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	1	32	C	N3-C2-O2	-5.66	117.94	121.90
2	2	650	C	C1'-O4'-C4'	5.66	114.42	109.90
14	L	162	ARG	NE-CZ-NH2	5.65	123.13	120.30
2	2	1343	U	O4'-C1'-N1	5.65	112.72	108.20
2	2	1220	G	C5-C6-N1	5.64	114.32	111.50
2	2	810	U	N1-C2-N3	5.64	118.28	114.90
2	2	1850	C	N3-C2-O2	-5.63	117.96	121.90
2	2	1153	G	N3-C4-C5	-5.63	125.78	128.60
2	2	629	C	C4'-C3'-C2'	-5.63	96.97	102.60
3	3	50	C	N3-C2-O2	-5.62	117.96	121.90
2	2	518	A	C4-C5-C6	-5.62	114.19	117.00
2	2	1530	U	N3-C2-O2	-5.62	118.27	122.20
2	2	571	U	C5-C6-N1	-5.61	119.90	122.70
2	2	1126	G	N3-C4-N9	-5.60	122.64	126.00
2	2	909	A	C4'-C3'-C2'	-5.60	97.00	102.60
2	2	1128	C	N3-C2-O2	-5.60	117.98	121.90
2	2	568	C	N3-C2-O2	-5.60	117.98	121.90
3	3	50	C	O4'-C1'-N1	5.60	112.68	108.20
2	2	1208	G	N1-C6-O6	-5.59	116.54	119.90
2	2	1245	C	OP2-P-O3'	-5.59	92.89	105.20
2	2	598	C	N1-C2-O2	5.59	122.25	118.90
2	2	508	G	N3-C2-N2	-5.59	115.99	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1153	G	C5-C6-N1	5.59	114.29	111.50
2	2	84	A	C4-C5-C6	-5.58	114.21	117.00
2	2	626	C	N1-C2-O2	5.58	122.25	118.90
2	2	1054	A	C4-C5-C6	-5.58	114.21	117.00
2	2	1246	A	C4-C5-C6	-5.58	114.21	117.00
2	2	1855	G	O4'-C1'-C2'	-5.58	100.22	105.80
1	1	35	A	C6-C5-N7	5.58	136.21	132.30
17	O	96	ARG	NE-CZ-NH2	5.58	123.09	120.30
2	2	1230	C	O4'-C1'-N1	5.57	112.66	108.20
2	2	1784	A	C4-C5-C6	-5.57	114.21	117.00
2	2	1523	G	N1-C6-O6	-5.57	116.56	119.90
40	n	65	TYR	CB-CG-CD2	-5.56	117.67	121.00
2	2	1044	G	N3-C4-C5	-5.55	125.82	128.60
5	C	53	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	1	73	A	C2-N3-C4	5.55	113.38	110.60
2	2	811	U	N3-C2-O2	-5.55	118.32	122.20
2	2	1852	G	N1-C6-O6	-5.55	116.57	119.90
2	2	1693	C	O4'-C1'-N1	5.54	112.63	108.20
2	2	468	G	N1-C6-O6	-5.54	116.58	119.90
38	k	323	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	2	1723	U	OP1-P-O3'	5.53	117.37	105.20
2	2	102	A	C4-C5-C6	-5.53	114.23	117.00
2	2	1209	C	N3-C4-N4	-5.53	114.13	118.00
2	2	915	A	N1-C6-N6	-5.53	115.28	118.60
2	2	1509	G	N1-C6-O6	-5.53	116.58	119.90
2	2	564	A	C4-C5-C6	-5.52	114.24	117.00
2	2	1212	C	C4'-C3'-C2'	-5.52	97.08	102.60
2	2	1237	A	C4-C5-C6	-5.52	114.24	117.00
2	2	598	C	N3-C4-C5	5.52	124.11	121.90
2	2	1785	A	C4-C5-C6	-5.51	114.25	117.00
2	2	1232	G	N1-C6-O6	-5.51	116.60	119.90
2	2	319	G	N3-C4-N9	5.50	129.30	126.00
2	2	960	A	C4-C5-C6	-5.50	114.25	117.00
2	2	819	U	N1-C2-N3	5.50	118.20	114.90
2	2	71	G	C3'-C2'-C1'	-5.49	97.11	101.50
2	2	1564	A	C4-C5-C6	-5.49	114.25	117.00
2	2	376	C	N3-C2-O2	-5.49	118.06	121.90
5	C	80	ARG	NE-CZ-NH2	5.49	123.05	120.30
4	A	57	ARG	NE-CZ-NH2	5.49	123.04	120.30
2	2	1353	A	C4-C5-C6	-5.49	114.26	117.00
2	2	915	A	C3'-C2'-C1'	-5.48	97.11	101.50
3	3	54	G	C5'-C4'-C3'	-5.48	107.23	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	373	G	N1-C6-O6	-5.47	116.61	119.90
2	2	917	G	O4'-C1'-N9	5.47	112.58	108.20
2	2	649	G	C4-N9-C1'	5.46	133.60	126.50
2	2	941	U	O4'-C1'-N1	5.46	112.57	108.20
2	2	1041	U	N1-C2-N3	5.46	118.18	114.90
2	2	1090	C	C4'-C3'-C2'	-5.46	97.14	102.60
2	2	1235	U	N1-C2-N3	5.46	118.17	114.90
1	1	26	G	N3-C2-N2	-5.45	116.08	119.90
2	2	96	C	N3-C2-O2	-5.45	118.08	121.90
2	2	1237	A	C4'-C3'-C2'	-5.45	97.15	102.60
20	R	59	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	2	1340	A	C4-C5-C6	-5.44	114.28	117.00
2	2	908	C	P-O3'-C3'	-5.44	113.17	119.70
2	2	39	A	C4-C5-C6	-5.44	114.28	117.00
2	2	1041	U	O4'-C1'-N1	5.44	112.55	108.20
2	2	360	G	C5-C6-N1	5.44	114.22	111.50
1	1	34	C	N1-C2-O2	5.43	122.16	118.90
2	2	1849	G	C5-C6-N1	5.43	114.22	111.50
2	2	957	G	C4'-C3'-C2'	-5.43	97.17	102.60
33	e	12	ARG	NE-CZ-NH2	5.43	123.01	120.30
2	2	38	A	C4-C5-C6	-5.42	114.29	117.00
2	2	1613	C	N3-C2-O2	-5.42	118.10	121.90
1	1	27	C	N1-C2-O2	5.42	122.15	118.90
2	2	1606	G	N1-C6-O6	-5.42	116.65	119.90
2	2	597	U	N3-C2-O2	-5.42	118.41	122.20
29	a	118	ARG	NE-CZ-NH2	5.42	123.01	120.30
29	a	61	ARG	NE-CZ-NH2	5.41	123.01	120.30
2	2	1549	C	N3-C2-O2	-5.41	118.11	121.90
2	2	67	C	N1-C1'-C2'	5.41	121.03	114.00
24	V	94	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	2	954	G	C5-C6-N1	5.39	114.20	111.50
38	k	306	ARG	CD-NE-CZ	5.38	131.14	123.60
2	2	1263	C	N3-C2-O2	-5.38	118.13	121.90
2	2	481	C	N3-C4-C5	5.38	124.05	121.90
2	2	1487	G	N1-C6-O6	-5.38	116.67	119.90
2	2	357	U	C3'-C2'-C1'	5.38	105.80	101.50
2	2	94	G	N1-C6-O6	-5.37	116.68	119.90
2	2	674	G	N1-C6-O6	-5.37	116.68	119.90
2	2	918	A	C4-C5-C6	-5.37	114.31	117.00
2	2	954	G	C8-N9-C4	-5.37	104.25	106.40
2	2	1231	G	C5-C6-N1	5.37	114.18	111.50
2	2	913	U	O4'-C1'-N1	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1484	C	N1-C2-O2	5.36	122.12	118.90
2	2	1851	G	N1-C6-O6	-5.36	116.68	119.90
2	2	909	A	C3'-C2'-C1'	-5.36	97.21	101.50
2	2	1560	C	N1-C2-O2	5.36	122.12	118.90
2	2	939	U	N1-C2-N3	5.36	118.11	114.90
2	2	849	C	C2-N1-C1'	5.36	124.69	118.80
2	2	1014	U	O4'-C1'-N1	5.36	112.48	108.20
2	2	1209	C	O4'-C1'-N1	5.36	112.48	108.20
38	k	567	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	1	11	G	C5-C6-N1	5.35	114.18	111.50
2	2	1214	C	N3-C2-O2	-5.35	118.15	121.90
2	2	581	U	C5-C6-N1	-5.34	120.03	122.70
2	2	1126	G	N3-C2-N2	-5.34	116.16	119.90
33	e	19	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	2	1236	A	C4-C5-C6	-5.34	114.33	117.00
2	2	1816	A	C4-C5-C6	-5.34	114.33	117.00
2	2	915	A	P-O3'-C3'	5.33	126.10	119.70
2	2	1041	U	C4'-C3'-C2'	-5.33	97.27	102.60
29	a	90	ARG	NE-CZ-NH2	5.33	122.97	120.30
38	k	190	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	1	45	G	C4'-C3'-C2'	-5.33	97.27	102.60
2	2	1234	U	O4'-C1'-N1	5.32	112.46	108.20
2	2	542	G	N3-C2-N2	-5.32	116.18	119.90
2	2	66	G	N1-C6-O6	-5.32	116.71	119.90
2	2	1425	G	N1-C6-O6	-5.31	116.72	119.90
17	O	33	ARG	NE-CZ-NH2	5.31	122.95	120.30
2	2	469	C	C4'-C3'-C2'	-5.30	97.30	102.60
2	2	1558	G	N1-C6-O6	-5.29	116.72	119.90
2	2	1624	C	N1-C2-O2	5.29	122.07	118.90
2	2	155	G	C5-C6-N1	5.29	114.14	111.50
2	2	1265	G	N1-C6-O6	-5.29	116.73	119.90
1	1	34	C	C6-N1-C2	-5.29	118.19	120.30
24	V	67	ARG	NE-CZ-NH2	5.29	122.94	120.30
33	e	27	ARG	NE-CZ-NH2	5.29	122.94	120.30
2	2	1248	C	O4'-C1'-N1	5.28	112.43	108.20
2	2	1155	G	C4'-C3'-C2'	-5.28	97.32	102.60
1	1	31	G	N1-C6-O6	-5.28	116.73	119.90
2	2	157	U	C5-C6-N1	-5.28	120.06	122.70
2	2	67	C	C2-N1-C1'	5.28	124.60	118.80
2	2	987	G	N1-C6-O6	-5.28	116.73	119.90
2	2	1041	U	C5-C6-N1	-5.27	120.06	122.70
2	2	1200	A	C8-N9-C4	-5.27	103.69	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1511	G	N1-C6-O6	-5.27	116.74	119.90
2	2	10	G	C5-C6-N1	5.27	114.14	111.50
2	2	1634	G	C5-C6-N1	5.27	114.13	111.50
2	2	1639	C	C4'-C3'-C2'	-5.27	97.33	102.60
1	1	36	U	O4'-C1'-N1	5.25	112.40	108.20
2	2	1206	G	N1-C6-O6	-5.25	116.75	119.90
18	P	20	ARG	NE-CZ-NH2	5.25	122.92	120.30
2	2	356	U	N3-C2-O2	-5.24	118.53	122.20
38	k	576	ARG	NE-CZ-NH2	5.23	122.92	120.30
5	C	205	ARG	NE-CZ-NH1	-5.23	117.69	120.30
5	C	63	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	2	956	U	N1-C2-N3	5.22	118.03	114.90
2	2	1568	G	N1-C6-O6	-5.22	116.77	119.90
2	2	496	G	N1-C6-O6	-5.22	116.77	119.90
2	2	560	C	C4'-C3'-C2'	-5.22	97.38	102.60
2	2	1089	A	C6-C5-N7	5.22	135.95	132.30
2	2	497	G	C5-C6-N1	5.22	114.11	111.50
2	2	572	U	C5-C6-N1	-5.22	120.09	122.70
2	2	1200	A	N7-C8-N9	5.21	116.41	113.80
1	1	39	C	N3-C2-O2	-5.21	118.25	121.90
2	2	1270	G	C5'-C4'-C3'	-5.21	107.67	116.00
2	2	496	G	N3-C4-C5	-5.21	126.00	128.60
1	1	11	G	N1-C6-O6	-5.21	116.78	119.90
2	2	580	A	C4-C5-C6	-5.20	114.40	117.00
1	1	33	C	N3-C2-O2	-5.20	118.26	121.90
2	2	1130	G	C5-C6-N1	5.20	114.10	111.50
2	2	1265	G	C5-C6-N1	5.19	114.10	111.50
23	U	86	ARG	NE-CZ-NH2	5.19	122.90	120.30
2	2	1523	G	C5-C6-N1	5.19	114.10	111.50
1	1	30	G	C5'-C4'-C3'	-5.19	107.70	116.00
2	2	501	U	O4'-C1'-N1	5.19	112.35	108.20
2	2	375	G	N3-C4-C5	-5.18	126.01	128.60
2	2	987	G	N3-C4-C5	-5.18	126.01	128.60
2	2	53	C	O4'-C1'-N1	5.18	112.35	108.20
2	2	1312	C	C4'-C3'-C2'	-5.18	97.42	102.60
37	j	13	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	2	1216	A	C2-N3-C4	5.18	113.19	110.60
3	3	54	G	N1-C6-O6	-5.18	116.80	119.90
2	2	1855	G	N3-C2-N2	-5.17	116.28	119.90
2	2	373	G	C4'-C3'-C2'	-5.17	97.43	102.60
2	2	1216	A	C4-C5-C6	-5.17	114.42	117.00
2	2	491	C	C6-N1-C2	-5.16	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1522	C	N3-C2-O2	-5.16	118.29	121.90
2	2	69	C	N1-C2-O2	5.15	121.99	118.90
2	2	1454	G	N1-C6-O6	-5.15	116.81	119.90
2	2	1198	U	N3-C2-O2	-5.15	118.59	122.20
2	2	97	U	O4'-C1'-N1	5.15	112.32	108.20
2	2	989	G	N1-C6-O6	-5.15	116.81	119.90
2	2	559	A	C4-C5-C6	-5.15	114.43	117.00
1	1	24	G	O4'-C1'-N9	5.15	112.32	108.20
2	2	1677	C	O4'-C1'-N1	5.15	112.32	108.20
2	2	954	G	C4'-C3'-C2'	-5.14	97.46	102.60
20	R	51	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	2	1206	G	C5-C6-N1	5.14	114.07	111.50
2	2	1041	U	N3-C2-O2	-5.14	118.61	122.20
2	2	194	C	N1-C2-O2	5.13	121.98	118.90
2	2	584	A	O4'-C1'-N9	5.13	112.30	108.20
4	A	57	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	2	1260	C	N3-C4-C5	5.12	123.95	121.90
2	2	821	A	P-O3'-C3'	5.12	125.85	119.70
2	2	1510	G	N1-C6-O6	-5.12	116.83	119.90
2	2	1611	U	N1-C2-N3	5.12	117.97	114.90
2	2	495	G	N1-C6-O6	-5.12	116.83	119.90
2	2	1455	G	N1-C6-O6	-5.12	116.83	119.90
2	2	1296	U	C5'-C4'-C3'	-5.12	107.82	116.00
3	3	55	G	N1-C6-O6	-5.12	116.83	119.90
1	1	24	G	N1-C6-O6	-5.11	116.83	119.90
2	2	1558	G	N3-C4-C5	-5.11	126.04	128.60
2	2	1612	G	N1-C6-O6	-5.11	116.83	119.90
4	A	192	ARG	NE-CZ-NH2	5.11	122.86	120.30
2	2	375	G	C5-C6-N1	5.11	114.05	111.50
2	2	52	G	C8-N9-C4	-5.11	104.36	106.40
2	2	1153	G	C2-N3-C4	5.10	114.45	111.90
2	2	938	G	C3'-C2'-C1'	5.09	105.58	101.50
2	2	910	U	N1-C2-N3	5.09	117.96	114.90
2	2	1557	C	N1-C2-O2	5.09	121.95	118.90
2	2	597	U	C3'-C2'-C1'	5.09	105.57	101.50
2	2	629	C	C6-N1-C2	-5.09	118.27	120.30
2	2	1241	G	N1-C6-O6	-5.09	116.85	119.90
17	O	101	ARG	NE-CZ-NH2	5.09	122.84	120.30
2	2	1515	G	N3-C4-C5	-5.09	126.06	128.60
2	2	164	A	C4-C5-C6	-5.08	114.46	117.00
2	2	1638	U	O4'-C1'-N1	5.08	112.27	108.20
2	2	1296	U	O4'-C1'-N1	5.08	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	987	G	C5-C6-N1	5.08	114.04	111.50
2	2	377	C	C4'-C3'-C2'	-5.07	97.53	102.60
19	Q	104	ARG	NE-CZ-NH2	5.07	122.84	120.30
2	2	1220	G	C4'-C3'-C2'	-5.07	97.53	102.60
10	H	219	ARG	NE-CZ-NH1	-5.07	117.76	120.30
2	2	1355	U	N3-C2-O2	-5.07	118.65	122.20
2	2	579	G	N3-C4-C5	-5.07	126.07	128.60
2	2	1484	C	N3-C4-C5	5.07	123.93	121.90
2	2	1252	G	N3-C4-C5	-5.06	126.07	128.60
2	2	1243	C	N1-C2-O2	5.06	121.94	118.90
11	I	74	ARG	NE-CZ-NH2	5.06	122.83	120.30
2	2	501	U	C4'-C3'-C2'	-5.06	97.54	102.60
2	2	971	G	N1-C6-O6	-5.05	116.87	119.90
2	2	1454	G	C5-C6-N1	5.05	114.03	111.50
2	2	540	C	O4'-C1'-N1	5.05	112.24	108.20
2	2	1515	G	N9-C1'-C2'	5.05	120.56	114.00
2	2	1483	A	C6-C5-N7	5.05	135.83	132.30
3	3	54	G	O4'-C1'-N9	5.05	112.24	108.20
2	2	584	A	C4-C5-C6	-5.05	114.48	117.00
11	I	159	ARG	NE-CZ-NH2	5.05	122.82	120.30
2	2	1096	A	OP1-P-O3'	5.04	116.29	105.20
2	2	1242	A	C4-C5-C6	-5.04	114.48	117.00
7	E	45	ARG	NE-CZ-NH2	5.04	122.82	120.30
30	b	22	ARG	NE-CZ-NH2	5.04	122.82	120.30
2	2	979	A	C4-C5-C6	-5.04	114.48	117.00
2	2	1484	C	O4'-C1'-N1	5.04	112.23	108.20
2	2	859	U	O4'-C1'-N1	5.03	112.23	108.20
2	2	1679	C	N3-C2-O2	-5.03	118.38	121.90
14	L	138	ARG	NE-CZ-NH2	5.03	122.81	120.30
2	2	458	A	C4'-C3'-C2'	-5.03	97.57	102.60
2	2	1121	C	N3-C4-C5	5.03	123.91	121.90
2	2	1236	A	C3'-C2'-C1'	5.03	105.52	101.50
38	k	96	ARG	NE-CZ-NH2	5.03	122.81	120.30
2	2	958	A	C6-C5-N7	5.02	135.82	132.30
2	2	800	U	N3-C2-O2	-5.02	118.69	122.20
4	A	182	ARG	NE-CZ-NH2	5.02	122.81	120.30
2	2	1215	C	N3-C4-N4	-5.02	114.49	118.00
33	e	19	ARG	NE-CZ-NH2	5.02	122.81	120.30
2	2	1199	G	N9-C4-C5	5.01	107.40	105.40
2	2	1623	C	C4'-C3'-C2'	-5.01	97.59	102.60
20	R	42	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	1	73	A	N3-C4-N9	5.01	131.41	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1234	U	N1-C2-N3	5.01	117.91	114.90
2	2	1154	G	C5-C6-N1	5.01	114.00	111.50
2	2	1198	U	N1-C2-N3	5.01	117.90	114.90
30	b	42	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (124) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	24	G	Sidechain
1	1	26	G	Sidechain
1	1	27	C	Sidechain
1	1	29	G	Sidechain
1	1	32	C	Sidechain
1	1	41	C	Sidechain
1	1	42	A	Sidechain
1	1	44	A	Sidechain
1	1	45	G	Sidechain
2	2	1012	U	Sidechain
2	2	1013	U	Sidechain
2	2	1082	G	Sidechain
2	2	1105	C	Sidechain
2	2	1106	G	Sidechain
2	2	1153	G	Sidechain
2	2	1199	G	Sidechain
2	2	1200	A	Sidechain
2	2	1208	G	Sidechain
2	2	1209	C	Sidechain
2	2	1212	C	Sidechain
2	2	1214	C	Sidechain
2	2	1215	C	Sidechain
2	2	1216	A	Sidechain
2	2	1236	A	Sidechain
2	2	1245	C	Sidechain
2	2	1247	A	Sidechain
2	2	1263	C	Sidechain
2	2	1296	U	Sidechain
2	2	1310	U	Sidechain
2	2	1311	U	Sidechain
2	2	1312	C	Sidechain
2	2	1322	U	Sidechain
2	2	1334	G	Sidechain

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Mol	Chain	Res	Type	Group
2	2	1336	U	Sidechain
2	2	1355	U	Sidechain
2	2	1452	G	Sidechain
2	2	1483	A	Sidechain
2	2	150	A	Sidechain
2	2	1517	A	Sidechain
2	2	1523	G	Sidechain
2	2	1548	C	Sidechain
2	2	1557	C	Sidechain
2	2	1561	G	Sidechain
2	2	1564	A	Sidechain
2	2	1565	G	Sidechain
2	2	1569	C	Sidechain
2	2	157	U	Sidechain
2	2	1611	U	Sidechain
2	2	1613	C	Sidechain
2	2	163	U	Sidechain
2	2	1635	A	Sidechain
2	2	1637	U	Sidechain
2	2	1675	G	Sidechain
2	2	1680	U	Sidechain
2	2	1682	C	Sidechain
2	2	1694	A	Sidechain
2	2	1818	A	Sidechain
2	2	1851	G	Sidechain
2	2	1853	A	Sidechain
2	2	1854	A	Sidechain
2	2	1860	A	Sidechain
2	2	189	G	Sidechain
2	2	190	A	Sidechain
2	2	192	U	Sidechain
2	2	201	G	Sidechain
2	2	203	G	Sidechain
2	2	204	G	Sidechain
2	2	357	U	Sidechain
2	2	360	G	Sidechain
2	2	37	C	Sidechain
2	2	374	U	Sidechain
2	2	38	A	Sidechain
2	2	39	A	Sidechain
2	2	456	G	Sidechain
2	2	499	G	Sidechain

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Mol	Chain	Res	Type	Group
2	2	500	G	Sidechain
2	2	515	A	Sidechain
2	2	540	C	Sidechain
2	2	542	G	Sidechain
2	2	563	U	Sidechain
2	2	564	A	Sidechain
2	2	572	U	Sidechain
2	2	580	A	Sidechain
2	2	581	U	Sidechain
2	2	604	G	Sidechain
2	2	605	C	Sidechain
2	2	606	A	Sidechain
2	2	615	G	Sidechain
2	2	625	G	Sidechain
2	2	627	U	Sidechain
2	2	65	C	Sidechain
2	2	71	G	Sidechain
2	2	819	U	Sidechain
2	2	910	U	Sidechain
2	2	914	U	Sidechain
2	2	916	A	Sidechain
2	2	939	U	Sidechain
2	2	941	U	Sidechain
2	2	957	G	Sidechain
2	2	959	A	Sidechain
2	2	97	U	Sidechain
2	2	979	A	Sidechain
2	2	982	G	Sidechain
3	3	52	A	Sidechain
4	A	89	ARG	Sidechain
5	C	85	ARG	Sidechain
10	H	137	ARG	Sidechain
11	I	132	ARG	Sidechain
11	I	74	ARG	Sidechain
13	K	18	ARG	Sidechain
13	K	25	ARG	Sidechain
14	L	5	ARG	Sidechain
18	P	64	ARG	Sidechain
19	Q	98	ARG	Sidechain
20	R	30	TYR	Sidechain
20	R	42	ARG	Sidechain
20	R	51	ARG	Sidechain

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Mol	Chain	Res	Type	Group
22	T	84	TYR	Sidechain
36	i	105	ARG	Sidechain
37	j	62	ARG	Sidechain
37	j	66	ARG	Sidechain
38	k	172	TYR	Sidechain
38	k	252	ARG	Sidechain
38	k	497	ARG	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
4	A	264/284 (93%)	237 (90%)	27 (10%)	0	100	100
5	C	205/207 (99%)	184 (90%)	21 (10%)	0	100	100
6	D	213/215 (99%)	188 (88%)	25 (12%)	0	100	100
7	E	224/270 (83%)	209 (93%)	14 (6%)	1 (0%)	34	69
8	F	225/227 (99%)	206 (92%)	19 (8%)	0	100	100
9	G	261/263 (99%)	241 (92%)	20 (8%)	0	100	100
10	H	183/191 (96%)	169 (92%)	14 (8%)	0	100	100
11	I	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
12	J	188/190 (99%)	162 (86%)	26 (14%)	0	100	100
13	K	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
14	L	186/194 (96%)	174 (94%)	12 (6%)	0	100	100
15	M	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
16	N	156/158 (99%)	150 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	O	122/132 (92%)	98 (80%)	24 (20%)	0	100	100
18	P	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
19	Q	134/151 (89%)	118 (88%)	16 (12%)	0	100	100
20	R	138/145 (95%)	122 (88%)	16 (12%)	0	100	100
21	S	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
22	T	124/135 (92%)	110 (89%)	14 (11%)	0	100	100
23	U	143/152 (94%)	131 (92%)	12 (8%)	0	100	100
24	V	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
25	W	102/119 (86%)	97 (95%)	5 (5%)	0	100	100
26	X	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
27	Y	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
28	Z	140/143 (98%)	127 (91%)	13 (9%)	0	100	100
29	a	124/133 (93%)	107 (86%)	16 (13%)	1 (1%)	19	54
30	b	97/115 (84%)	91 (94%)	6 (6%)	0	100	100
31	c	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	13	44
32	d	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
33	e	51/56 (91%)	48 (94%)	3 (6%)	0	100	100
34	f	69/71 (97%)	56 (81%)	13 (19%)	0	100	100
35	g	311/313 (99%)	284 (91%)	26 (8%)	1 (0%)	41	74
36	i	56/133 (42%)	49 (88%)	7 (12%)	0	100	100
37	j	106/111 (96%)	98 (92%)	8 (8%)	0	100	100
38	k	593/595 (100%)	516 (87%)	76 (13%)	1 (0%)	47	80
39	l	23/25 (92%)	23 (100%)	0	0	100	100
40	n	73/124 (59%)	68 (93%)	5 (7%)	0	100	100
All	All	5824/6191 (94%)	5286 (91%)	533 (9%)	5 (0%)	54	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	E	252	LYS
38	k	439	PRO
35	g	283	PRO
29	a	86	GLU
31	c	39	GLY

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
4	A	238/255 (93%)	223 (94%)	15 (6%)	18 49
5	C	173/173 (100%)	164 (95%)	9 (5%)	23 57
6	D	196/196 (100%)	190 (97%)	6 (3%)	40 73
7	E	190/214 (89%)	176 (93%)	14 (7%)	13 42
8	F	190/190 (100%)	177 (93%)	13 (7%)	16 46
9	G	225/225 (100%)	216 (96%)	9 (4%)	31 66
10	H	159/161 (99%)	153 (96%)	6 (4%)	33 67
11	I	207/207 (100%)	198 (96%)	9 (4%)	29 63
12	J	170/170 (100%)	160 (94%)	10 (6%)	19 51
13	K	177/177 (100%)	164 (93%)	13 (7%)	14 42
14	L	162/168 (96%)	160 (99%)	2 (1%)	71 89
15	M	89/89 (100%)	84 (94%)	5 (6%)	21 54
16	N	142/142 (100%)	135 (95%)	7 (5%)	25 59
17	O	104/108 (96%)	95 (91%)	9 (9%)	10 34
18	P	130/130 (100%)	124 (95%)	6 (5%)	27 61
19	Q	106/119 (89%)	100 (94%)	6 (6%)	20 53
20	R	126/130 (97%)	120 (95%)	6 (5%)	25 60
21	S	117/117 (100%)	105 (90%)	12 (10%)	7 26
22	T	114/121 (94%)	110 (96%)	4 (4%)	36 69
23	U	125/132 (95%)	116 (93%)	9 (7%)	14 43
24	V	113/113 (100%)	109 (96%)	4 (4%)	36 69
25	W	94/107 (88%)	87 (93%)	7 (7%)	13 42
26	X	67/67 (100%)	62 (92%)	5 (8%)	13 41
27	Y	112/113 (99%)	106 (95%)	6 (5%)	22 55
28	Z	114/115 (99%)	108 (95%)	6 (5%)	22 56
29	a	108/115 (94%)	105 (97%)	3 (3%)	43 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	b	87/99 (88%)	84 (97%)	3 (3%)	37 70
31	c	76/76 (100%)	73 (96%)	3 (4%)	32 66
32	d	57/62 (92%)	51 (90%)	6 (10%)	7 25
33	e	47/49 (96%)	42 (89%)	5 (11%)	6 24
34	f	64/64 (100%)	61 (95%)	3 (5%)	26 61
35	g	272/272 (100%)	247 (91%)	25 (9%)	9 31
36	i	48/106 (45%)	48 (100%)	0	100 100
37	j	91/93 (98%)	84 (92%)	7 (8%)	13 40
38	k	523/523 (100%)	498 (95%)	25 (5%)	25 60
39	l	24/24 (100%)	22 (92%)	2 (8%)	11 37
40	n	66/102 (65%)	61 (92%)	5 (8%)	13 41
All	All	5103/5324 (96%)	4818 (94%)	285 (6%)	25 54

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	16	VAL
4	A	21	MET
4	A	33	TYR
4	A	53	ARG
4	A	62	LEU
4	A	69	GLU
4	A	99	GLU
4	A	119	LEU
4	A	126	GLN
4	A	130	LEU
4	A	144	ARG
4	A	197	VAL
4	A	200	TYR
4	A	229	LEU
4	A	270	ASN
5	C	35	GLU
5	C	79	SER
5	C	97	THR
5	C	110	ASN
5	C	111	GLN
5	C	117	ARG
5	C	121	LEU

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Mol	Chain	Res	Type
5	C	138	SER
5	C	197	VAL
6	D	78	GLU
6	D	146	CYS
6	D	149	GLN
6	D	170	GLU
6	D	191	ASP
6	D	209	ASP
7	E	55	LEU
7	E	75	LEU
7	E	123	GLU
7	E	167	SER
7	E	183	SER
7	E	197	ASP
7	E	199	CYS
7	E	202	SER
7	E	204	TRP
7	E	210	LEU
7	E	213	PHE
7	E	225	TYR
7	E	231	ASP
7	E	252	LYS
8	F	42	THR
8	F	45	ARG
8	F	56	GLN
8	F	59	LEU
8	F	72	VAL
8	F	76	ARG
8	F	81	GLU
8	F	86	LEU
8	F	146	ARG
8	F	175	VAL
8	F	176	LEU
8	F	178	ARG
8	F	226	GLN
9	G	1	MET
9	G	19	MET
9	G	26	VAL
9	G	134	LYS
9	G	181	CYS
9	G	198	ARG
9	G	232	ASN

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Mol	Chain	Res	Type
9	G	240	ARG
9	G	246	LEU
10	H	35	PHE
10	H	41	ASP
10	H	96	ARG
10	H	137	ARG
10	H	157	SER
10	H	179	ARG
11	I	18	VAL
11	I	22	ARG
11	I	31	ARG
11	I	127	THR
11	I	132	ARG
11	I	190	ARG
11	I	219	GLU
11	I	230	LYS
11	I	234	LEU
12	J	15	LYS
12	J	41	ARG
12	J	83	LEU
12	J	109	ARG
12	J	113	LYS
12	J	140	VAL
12	J	159	ASP
12	J	167	GLU
12	J	170	VAL
12	J	177	TYR
13	K	72	CYS
13	K	73	THR
13	K	74	ARG
13	K	86	SER
13	K	95	THR
13	K	100	CYS
13	K	105	ASP
13	K	106	SER
13	K	132	GLU
13	K	163	GLU
13	K	178	ARG
13	K	205	ARG
13	K	206	LYS
14	L	22	LYS
14	L	169	ARG

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Mol	Chain	Res	Type
15	M	13	GLU
15	M	17	LYS
15	M	20	VAL
15	M	58	VAL
15	M	96	ARG
16	N	12	LYS
16	N	46	THR
16	N	60	CYS
16	N	85	THR
16	N	134	LEU
16	N	141	ASN
16	N	157	LYS
17	O	16	THR
17	O	36	ARG
17	O	45	ARG
17	O	73	GLN
17	O	78	LYS
17	O	85	LEU
17	O	96	ARG
17	O	104	VAL
17	O	107	SER
18	P	3	ARG
18	P	11	LEU
18	P	13	GLN
18	P	14	SER
18	P	48	SER
18	P	144	SER
19	Q	46	ASP
19	Q	48	SER
19	Q	51	GLU
19	Q	57	THR
19	Q	117	ARG
19	Q	151	LEU
20	R	23	ASP
20	R	62	LYS
20	R	71	GLU
20	R	72	LYS
20	R	75	VAL
20	R	83	MET
21	S	16	LYS
21	S	31	LEU
21	S	35	ASN

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Mol	Chain	Res	Type
21	S	37	ARG
21	S	41	MET
21	S	51	LEU
21	S	85	ARG
21	S	97	GLN
21	S	105	LYS
21	S	119	LEU
21	S	131	LYS
21	S	145	TYR
22	T	3	ARG
22	T	8	THR
22	T	26	ASN
22	T	109	LEU
23	U	13	LEU
23	U	16	LEU
23	U	24	ARG
23	U	26	ILE
23	U	73	ASN
23	U	99	LEU
23	U	136	THR
23	U	141	ARG
23	U	142	ARG
24	V	5	THR
24	V	29	LYS
24	V	36	THR
24	V	87	VAL
25	W	25	THR
25	W	38	ASP
25	W	70	CYS
25	W	87	ARG
25	W	88	LEU
25	W	90	ASP
25	W	115	THR
26	X	10	ASP
26	X	21	ASN
26	X	35	ASN
26	X	50	PHE
26	X	67	ASP
27	Y	12	LYS
27	Y	20	ARG
27	Y	51	GLU
27	Y	55	ASP

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Mol	Chain	Res	Type
27	Y	97	ARG
27	Y	104	LEU
28	Z	4	CYS
28	Z	37	LYS
28	Z	54	LYS
28	Z	90	CYS
28	Z	105	PHE
28	Z	142	ARG
29	a	11	LYS
29	a	78	SER
29	a	86	GLU
30	b	26	CYS
30	b	46	GLU
30	b	76	SER
31	c	15	GLU
31	c	52	THR
31	c	66	PRO
32	d	5	ARG
32	d	17	VAL
32	d	30	VAL
32	d	33	GLU
32	d	38	THR
32	d	67	ARG
33	e	10	HIS
33	e	14	PHE
33	e	39	CYS
33	e	55	LEU
33	e	56	ASP
34	f	90	LYS
34	f	118	ARG
34	f	151	ASN
35	g	2	THR
35	g	8	ARG
35	g	29	ASP
35	g	33	SER
35	g	45	LEU
35	g	62	HIS
35	g	63	SER
35	g	74	ASP
35	g	97	THR
35	g	110	SER
35	g	111	VAL

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Mol	Chain	Res	Type
35	g	113	PHE
35	g	122	SER
35	g	124	SER
35	g	126	ASP
35	g	145	GLU
35	g	198	VAL
35	g	199	THR
35	g	209	SER
35	g	220	ASP
35	g	249	CYS
35	g	271	LYS
35	g	289	LEU
35	g	305	ASN
35	g	310	TRP
37	j	37	GLN
37	j	53	ASP
37	j	55	VAL
37	j	69	VAL
37	j	82	ARG
37	j	84	TYR
37	j	109	LEU
38	k	25	CYS
38	k	33	ARG
38	k	78	ASN
38	k	116	LYS
38	k	154	ASN
38	k	268	TYR
38	k	331	PHE
38	k	354	LYS
38	k	378	LEU
38	k	385	LYS
38	k	388	PHE
38	k	431	LYS
38	k	440	GLN
38	k	441	PHE
38	k	445	VAL
38	k	506	ARG
38	k	541	LYS
38	k	549	GLN
38	k	555	MET
38	k	563	GLU
38	k	568	ARG

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Mol	Chain	Res	Type
38	k	569	ASP
38	k	584	LYS
38	k	595	PHE
38	k	596	PHE
39	l	1	MET
39	l	18	ARG
40	n	49	LEU
40	n	54	THR
40	n	58	LEU
40	n	61	GLU
40	n	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	23	ASN
4	A	68	ASN
4	A	132	GLN
5	C	110	ASN
5	C	132	GLN
6	D	208	HIS
7	E	113	HIS
8	F	56	GLN
8	F	74	GLN
9	G	8	HIS
9	G	138	HIS
9	G	142	HIS
9	G	214	ASN
10	H	66	HIS
10	H	89	ASN
10	H	97	ASN
10	H	125	GLN
10	H	129	ASN
11	I	4	ASN
11	I	13	GLN
12	J	25	GLN
12	J	39	GLN
12	J	157	HIS
13	K	35	ASN
13	K	52	ASN
13	K	165	GLN
16	N	11	GLN

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Mol	Chain	Res	Type
16	N	83	GLN
16	N	121	GLN
17	O	72	HIS
19	Q	79	GLN
21	S	35	ASN
21	S	77	HIS
21	S	80	GLN
21	S	86	GLN
22	T	48	ASN
23	U	42	HIS
24	V	11	GLN
24	V	12	GLN
26	X	49	GLN
27	Y	15	ASN
28	Z	26	GLN
28	Z	77	ASN
28	Z	92	ASN
29	a	89	HIS
30	b	43	ASN
31	c	49	HIS
31	c	51	GLN
33	e	5	GLN
34	f	91	ASN
35	g	20	GLN
35	g	76	GLN
35	g	117	ASN
35	g	187	ASN
37	j	19	ASN
37	j	37	GLN
38	k	414	GLN
38	k	429	HIS
38	k	510	HIS
38	k	549	GLN
38	k	572	ASN
40	n	46	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	15 (20%)	1 (1%)
2	2	1735/1863 (93%)	319 (18%)	20 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	3	7/9 (77%)	2 (28%)	0
All	All	1816/1947 (93%)	336 (18%)	21 (1%)

All (336) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	13	G
1	1	14	C
1	1	17	C
1	1	18	G
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	48	C
1	1	49	G
1	1	58	A
1	1	72	U
1	1	73	A
1	1	74	C
1	1	76	A
2	2	4	C
2	2	17	C
2	2	32	U
2	2	33	G
2	2	41	G
2	2	44	U
2	2	46	A
2	2	56	G
2	2	59	U
2	2	67	C
2	2	68	A
2	2	72	C
2	2	73	C
2	2	74	G
2	2	75	G
2	2	76	U
2	2	77	A
2	2	78	C
2	2	79	A
2	2	80	G
2	2	103	A

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Mol	Chain	Res	Type
2	2	110	U
2	2	113	G
2	2	115	U
2	2	126	G
2	2	142	C
2	2	143	U
2	2	147	A
2	2	181	A
2	2	182	C
2	2	183	G
2	2	184	G
2	2	191	C
2	2	193	C
2	2	197	U
2	2	198	U
2	2	202	U
2	2	208	G
2	2	223	A
2	2	224	U
2	2	225	C
2	2	226	A
2	2	228	A
2	2	232	A
2	2	275	C
2	2	277	U
2	2	278	U
2	2	285	U
2	2	296	U
2	2	297	C
2	2	298	G
2	2	299	G
2	2	300	G
2	2	303	G
2	2	305	U
2	2	306	C
2	2	309	A
2	2	313	C
2	2	315	C
2	2	316	C
2	2	317	G
2	2	320	G
2	2	322	G

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Mol	Chain	Res	Type
2	2	337	G
2	2	347	C
2	2	352	C
2	2	354	A
2	2	358	U
2	2	359	C
2	2	360	G
2	2	367	G
2	2	375	G
2	2	376	C
2	2	388	A
2	2	399	C
2	2	408	A
2	2	418	U
2	2	428	G
2	2	438	A
2	2	439	A
2	2	440	C
2	2	441	G
2	2	442	G
2	2	454	A
2	2	455	A
2	2	462	C
2	2	464	G
2	2	472	G
2	2	477	U
2	2	482	C
2	2	492	C
2	2	506	A
2	2	513	A
2	2	515	A
2	2	516	A
2	2	543	U
2	2	546	U
2	2	547	U
2	2	548	G
2	2	554	A
2	2	566	A
2	2	573	A
2	2	577	A
2	2	580	A
2	2	582	C

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Mol	Chain	Res	Type
2	2	583	C
2	2	584	A
2	2	588	G
2	2	594	A
2	2	596	G
2	2	597	U
2	2	598	C
2	2	600	G
2	2	616	G
2	2	618	A
2	2	633	A
2	2	645	A
2	2	649	G
2	2	650	C
2	2	653	C
2	2	658	A
2	2	659	A
2	2	661	A
2	2	662	A
2	2	663	G
2	2	678	U
2	2	679	U
2	2	681	U
2	2	686	G
2	2	729	C
2	2	734	C
2	2	735	C
2	2	736	C
2	2	737	C
2	2	738	U
2	2	739	U
2	2	740	G
2	2	741	C
2	2	743	U
2	2	744	C
2	2	746	C
2	2	747	G
2	2	748	G
2	2	749	C
2	2	750	G
2	2	789	G
2	2	790	A

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Mol	Chain	Res	Type
2	2	791	A
2	2	792	G
2	2	793	C
2	2	794	G
2	2	795	U
2	2	796	U
2	2	797	U
2	2	806	A
2	2	807	A
2	2	817	G
2	2	818	U
2	2	819	U
2	2	820	C
2	2	827	G
2	2	832	G
2	2	833	A
2	2	835	C
2	2	837	G
2	2	843	A
2	2	849	C
2	2	867	U
2	2	868	A
2	2	869	G
2	2	871	A
2	2	883	U
2	2	886	U
2	2	891	G
2	2	894	U
2	2	903	G
2	2	907	C
2	2	909	A
2	2	910	U
2	2	913	U
2	2	914	U
2	2	916	A
2	2	929	G
2	2	939	U
2	2	951	A
2	2	966	G
2	2	967	G
2	2	974	G
2	2	984	C

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Mol	Chain	Res	Type
2	2	986	A
2	2	987	G
2	2	988	A
2	2	997	A
2	2	998	U
2	2	1013	U
2	2	1019	A
2	2	1045	A
2	2	1057	U
2	2	1058	A
2	2	1063	C
2	2	1074	C
2	2	1079	A
2	2	1081	C
2	2	1111	U
2	2	1112	C
2	2	1113	C
2	2	1125	G
2	2	1134	C
2	2	1144	A
2	2	1145	A
2	2	1150	U
2	2	1191	A
2	2	1203	G
2	2	1211	C
2	2	1220	G
2	2	1238	U
2	2	1247	A
2	2	1249	A
2	2	1252	G
2	2	1253	G
2	2	1255	A
2	2	1261	A
2	2	1270	G
2	2	1271	G
2	2	1280	A
2	2	1281	G
2	2	1282	G
2	2	1294	G
2	2	1297	A
2	2	1298	G
2	2	1299	C

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Mol	Chain	Res	Type
2	2	1311	U
2	2	1312	C
2	2	1316	G
2	2	1326	G
2	2	1337	C
2	2	1367	U
2	2	1368	U
2	2	1371	G
2	2	1374	A
2	2	1394	G
2	2	1399	C
2	2	1408	C
2	2	1414	C
2	2	1415	C
2	2	1420	G
2	2	1422	U
2	2	1424	G
2	2	1428	U
2	2	1433	C
2	2	1434	A
2	2	1442	A
2	2	1450	A
2	2	1458	U
2	2	1459	U
2	2	1472	A
2	2	1473	U
2	2	1474	U
2	2	1485	A
2	2	1486	G
2	2	1489	C
2	2	1505	U
2	2	1506	G
2	2	1507	U
2	2	1508	C
2	2	1516	C
2	2	1517	A
2	2	1528	A
2	2	1530	U
2	2	1546	U
2	2	1547	G
2	2	1548	C
2	2	1549	C

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Mol	Chain	Res	Type
2	2	1550	U
2	2	1551	A
2	2	1552	C
2	2	1553	C
2	2	1573	U
2	2	1575	A
2	2	1580	U
2	2	1583	A
2	2	1596	A
2	2	1616	U
2	2	1618	A
2	2	1631	G
2	2	1632	A
2	2	1634	G
2	2	1642	A
2	2	1643	G
2	2	1649	G
2	2	1651	G
2	2	1655	C
2	2	1660	G
2	2	1666	G
2	2	1716	U
2	2	1717	G
2	2	1739	G
2	2	1741	U
2	2	1743	G
2	2	1746	C
2	2	1747	C
2	2	1748	G
2	2	1749	C
2	2	1773	G
2	2	1775	A
2	2	1777	C
2	2	1778	G
2	2	1820	G
2	2	1823	G
2	2	1825	A
2	2	1832	U
2	2	1843	G
2	2	1845	A
2	2	1846	C
2	2	1855	G

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Mol	Chain	Res	Type
2	2	1856	G
2	2	1857	A
2	2	1858	U
2	2	1859	C
3	3	48	C
3	3	55	G

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	72	U
2	2	71	G
2	2	189	G
2	2	360	G
2	2	579	G
2	2	583	C
2	2	596	G
2	2	747	G
2	2	817	G
2	2	909	A
2	2	987	G
2	2	1012	U
2	2	1270	G
2	2	1311	U
2	2	1427	G
2	2	1433	C
2	2	1471	G
2	2	1472	A
2	2	1548	C
2	2	1550	U
2	2	1855	G

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	T6A	1	37	1	27,34,35	1.28	3 (11%)	29,49,52	1.85	6 (20%)
2	I2T	2	1244	2	24,29,30	0.87	1 (4%)	29,42,45	1.16	2 (6%)
3	MA6	3	49	3	18,25,27	0.96	1 (5%)	16,36,41	1.52	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	T6A	1	37	1	-	5/19/41/42	0/3/3/3
2	I2T	2	1244	2	-	0/16/34/35	0/2/2/2
3	MA6	3	49	3	-	2/5/27/30	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	37	T6A	ODA-C13	4.70	1.36	1.22
2	2	1244	I2T	O36-C34	-2.58	1.22	1.30
1	1	37	T6A	ODB-C13	-2.30	1.23	1.30
3	3	49	MA6	C8-N7	-2.25	1.30	1.34
1	1	37	T6A	C8-N7	-2.20	1.30	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	37	T6A	C12-N11-C10	5.27	130.72	121.94
1	1	37	T6A	C2-N1-C6	4.27	120.25	116.59
3	3	49	MA6	C10-N6-C6	4.14	126.44	122.87
2	2	1244	I2T	C3'-C2'-C1'	3.41	105.61	101.64
3	3	49	MA6	C2-N1-C6	3.15	119.29	116.59
1	1	37	T6A	O10-C10-N6	-3.09	118.39	123.62
1	1	37	T6A	ODB-C13-C12	2.86	124.31	114.21
1	1	37	T6A	N6-C10-N11	2.65	117.46	113.76
2	2	1244	I2T	O2'-C2'-C3'	-2.60	103.42	111.82
1	1	37	T6A	C1'-N9-C4	-2.15	122.87	126.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	37	T6A	O10-C10-N6-C6
3	3	49	MA6	O4'-C4'-C5'-O5'
3	3	49	MA6	C3'-C4'-C5'-O5'
1	1	37	T6A	C14-C12-N11-C10
1	1	37	T6A	N11-C10-N6-C6
1	1	37	T6A	N11-C12-C13-ODA
1	1	37	T6A	N11-C12-C13-ODB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 178 ligands modelled in this entry, 178 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	9.48

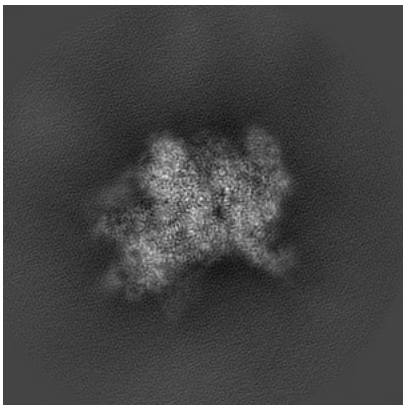
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17329. These allow visual inspection of the internal detail of the map and identification of artifacts.

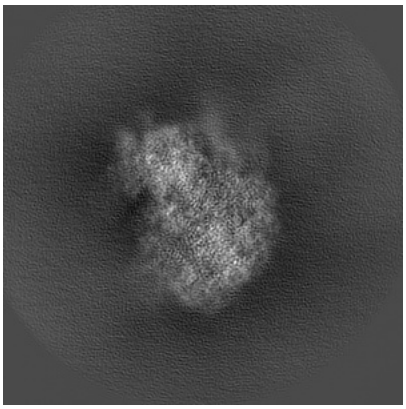
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

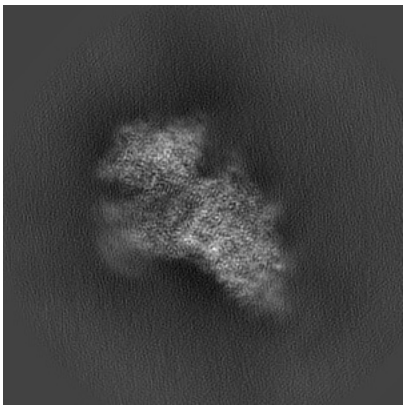
6.1.1 Primary map



X

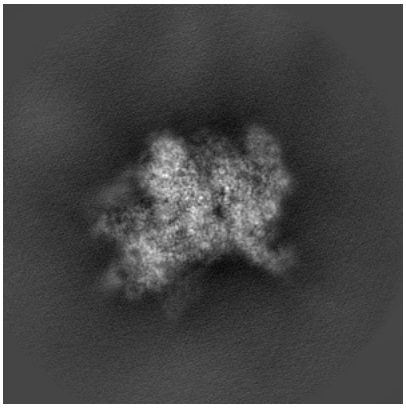


Y

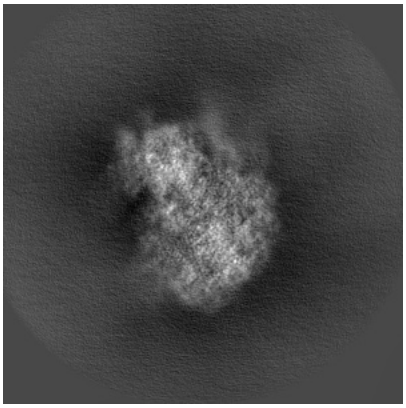


Z

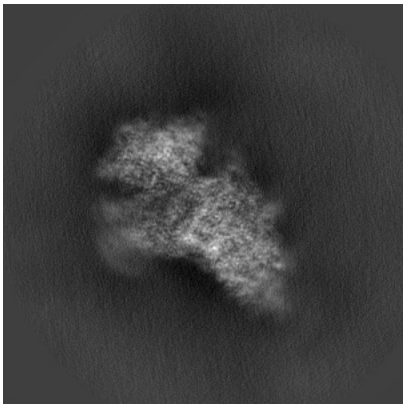
6.1.2 Raw map



X



Y

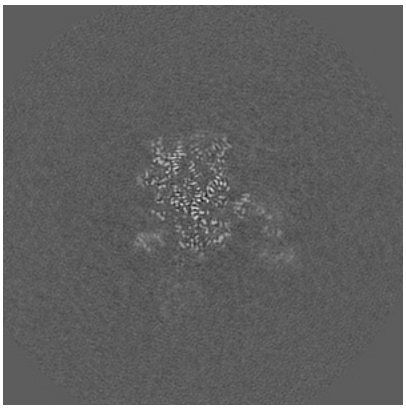


Z

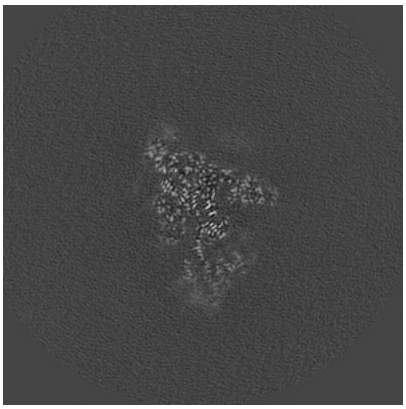
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

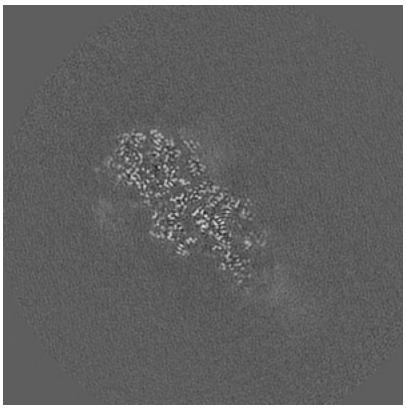
6.2.1 Primary map



X Index: 192

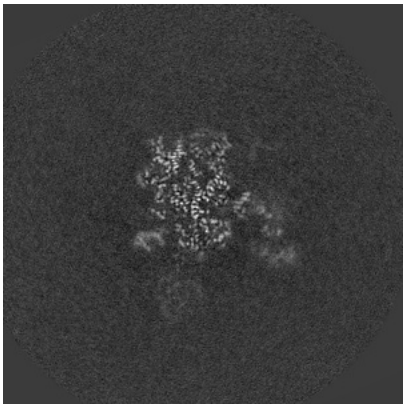


Y Index: 192

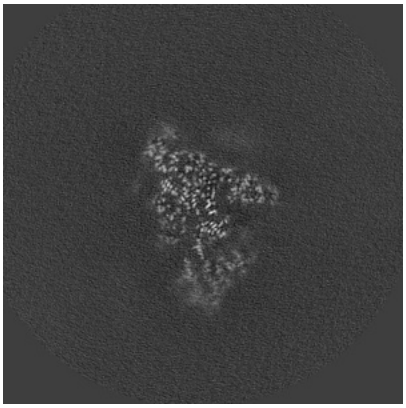


Z Index: 192

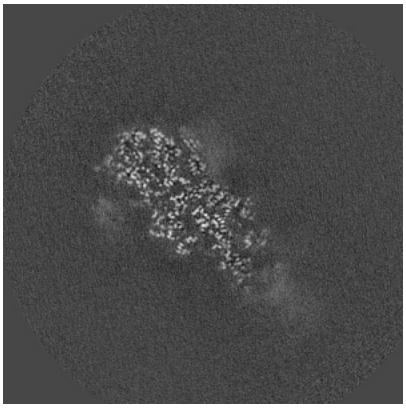
6.2.2 Raw map



X Index: 192



Y Index: 192

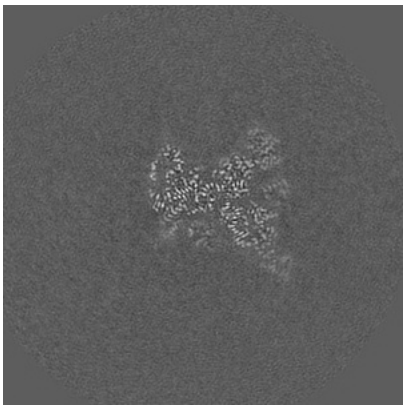


Z Index: 192

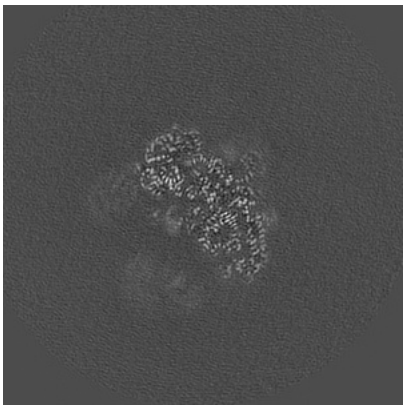
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

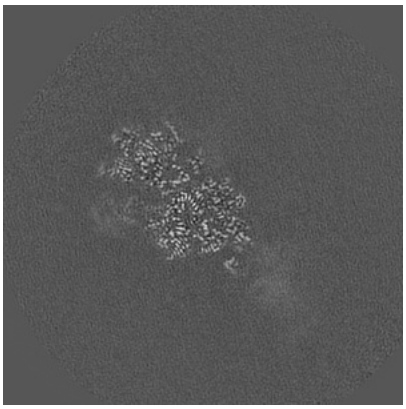
6.3.1 Primary map



X Index: 170

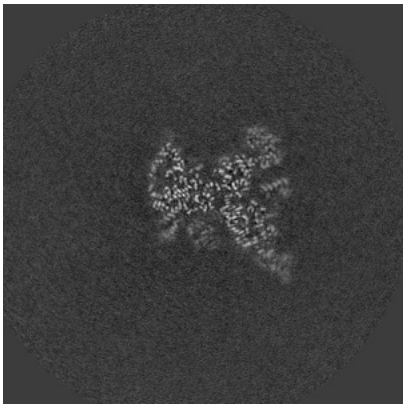


Y Index: 160

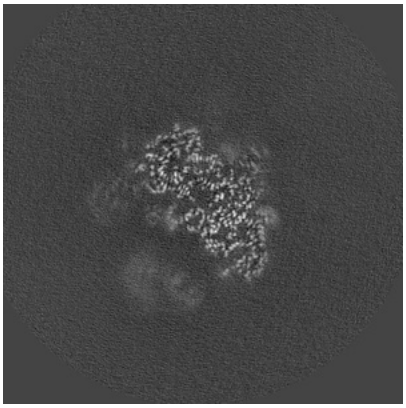


Z Index: 199

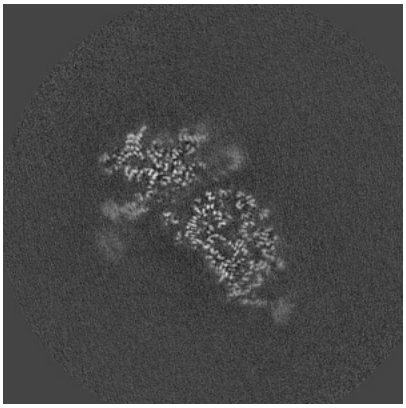
6.3.2 Raw map



X Index: 169



Y Index: 158

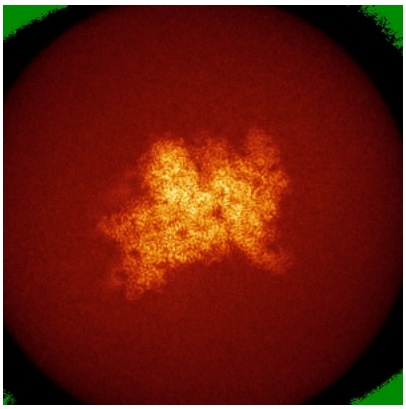


Z Index: 180

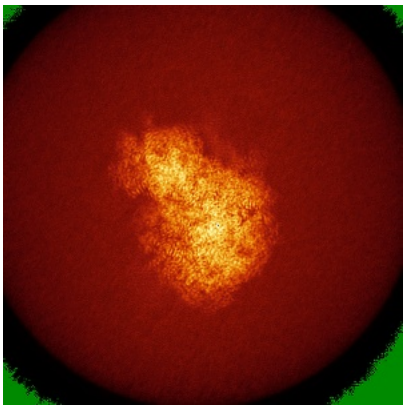
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

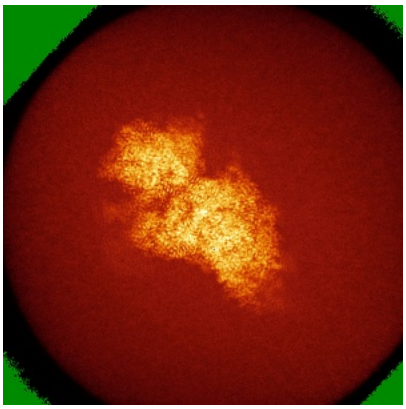
6.4.1 Primary map



X

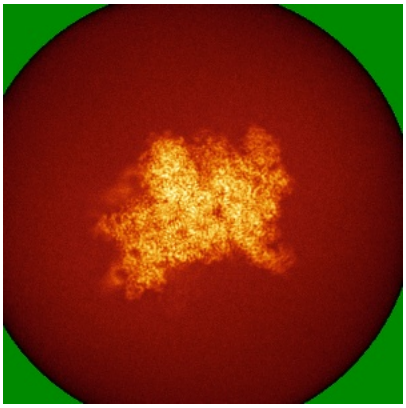


Y

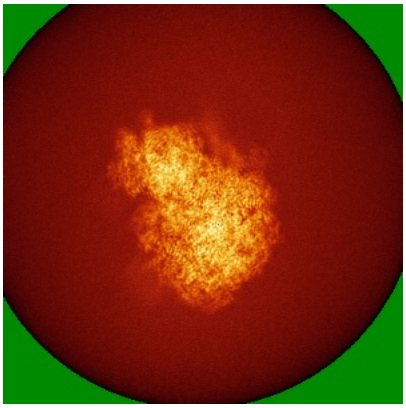


Z

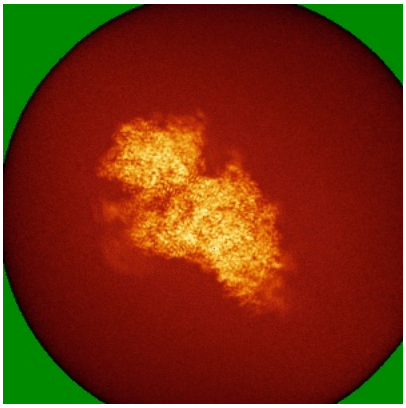
6.4.2 Raw map



X



Y

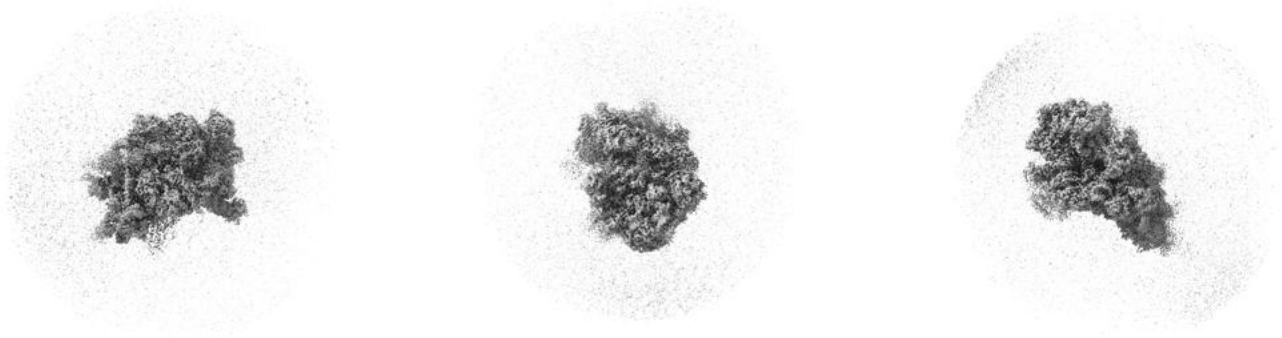


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

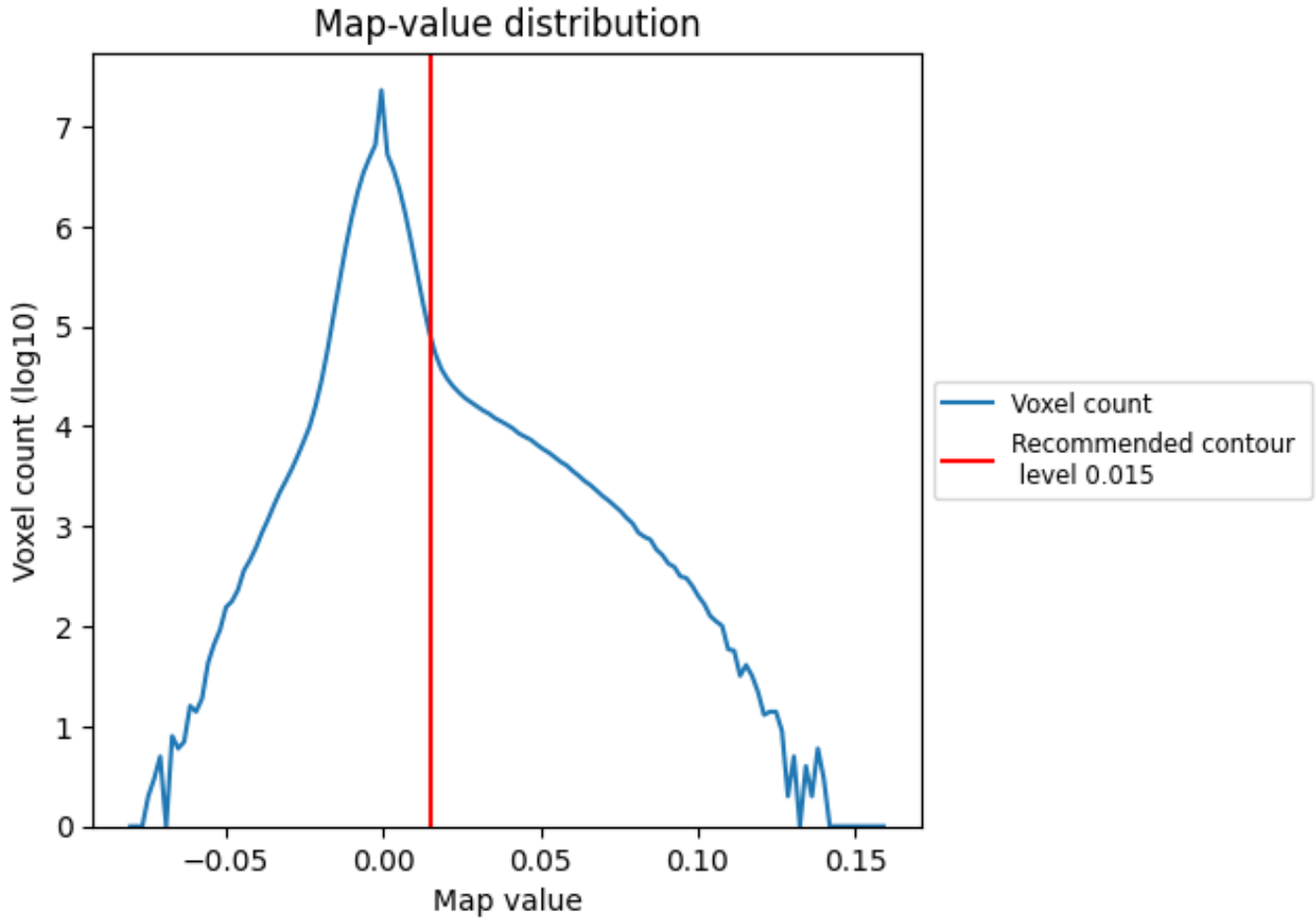
6.6 Mask visualisation (i)

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

7 Map analysis

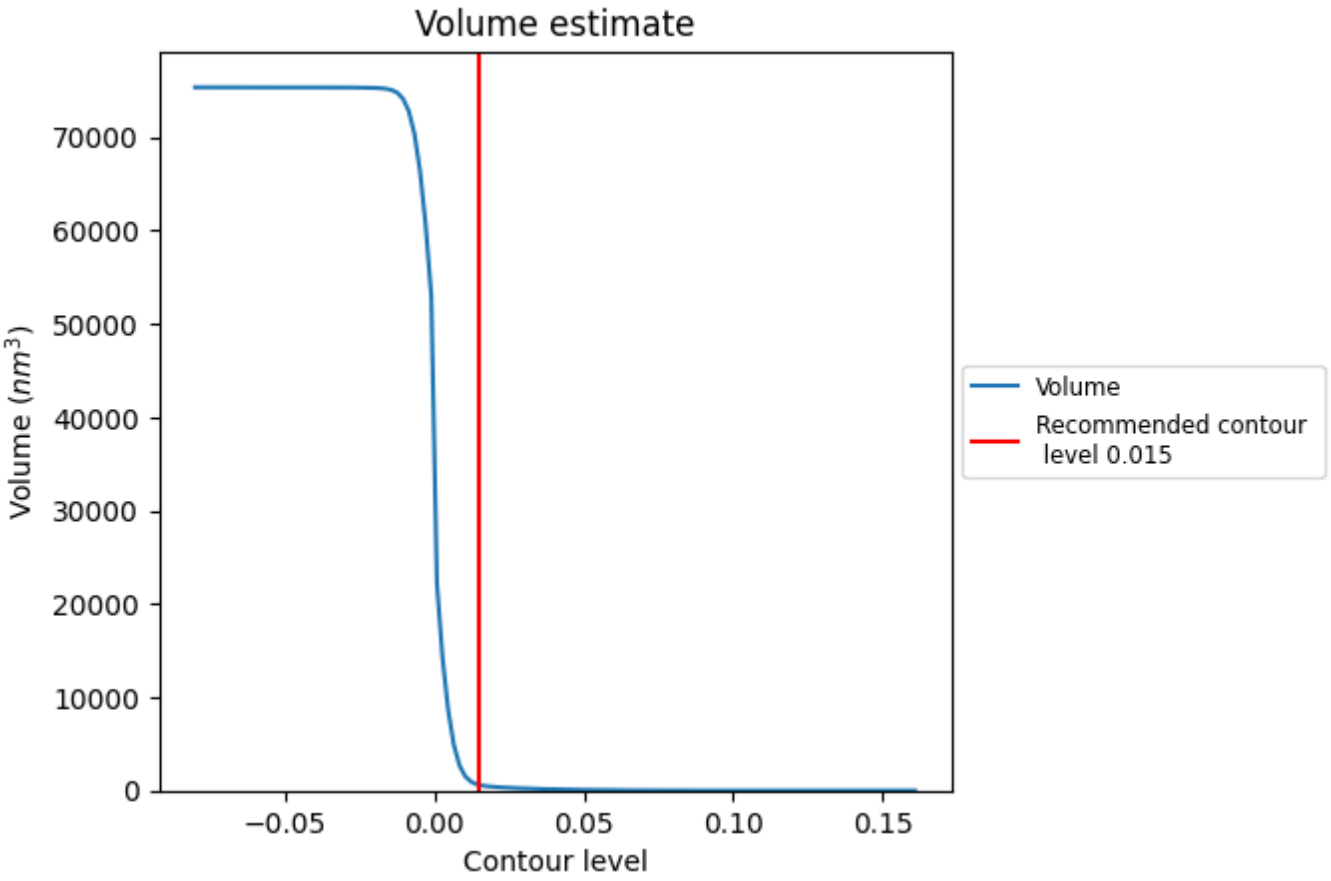
This section contains the results of statistical analysis of the map.

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.

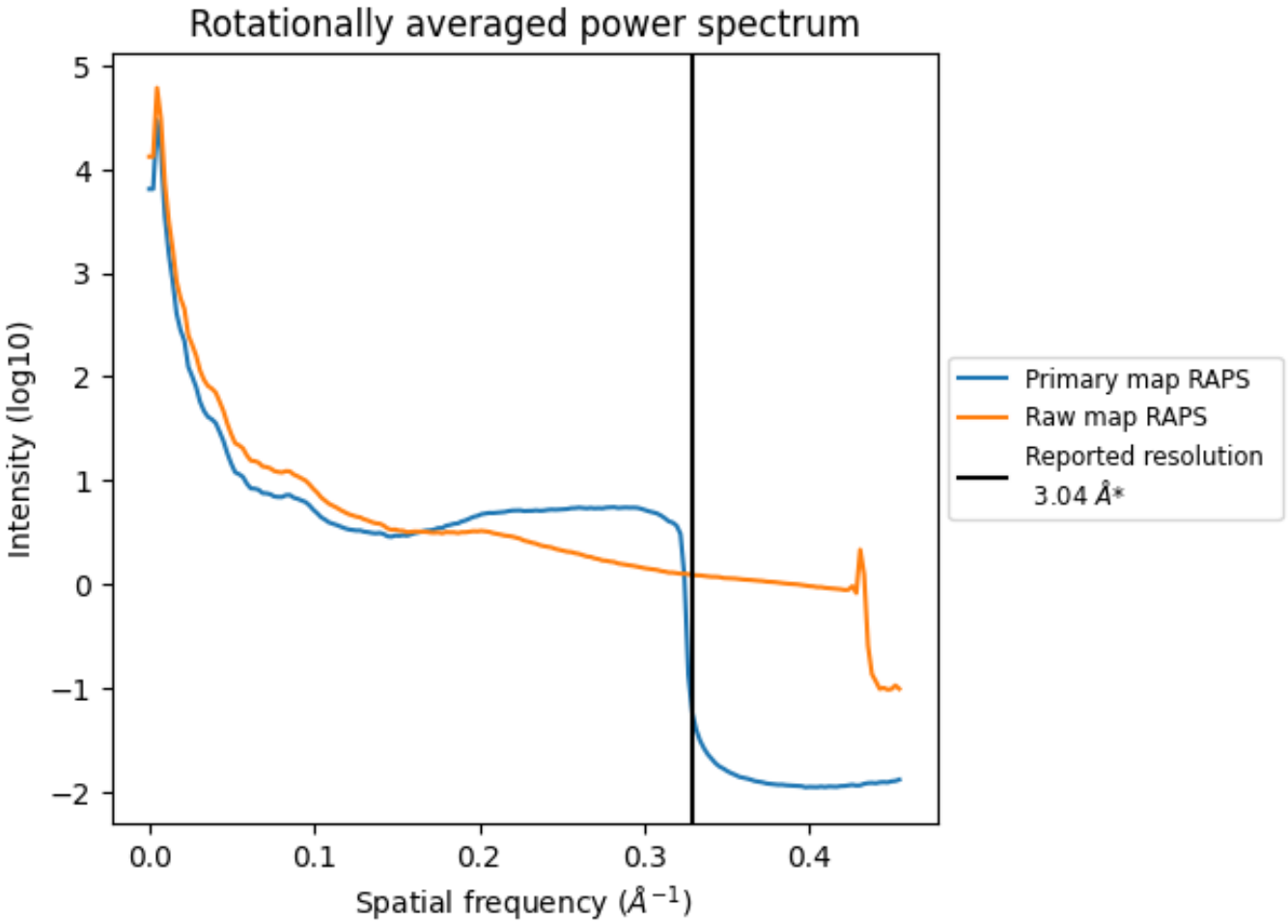
7.2 Volume estimate



The volume at the recommended contour level is 603 nm^3; this corresponds to an approximate mass of 544 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)

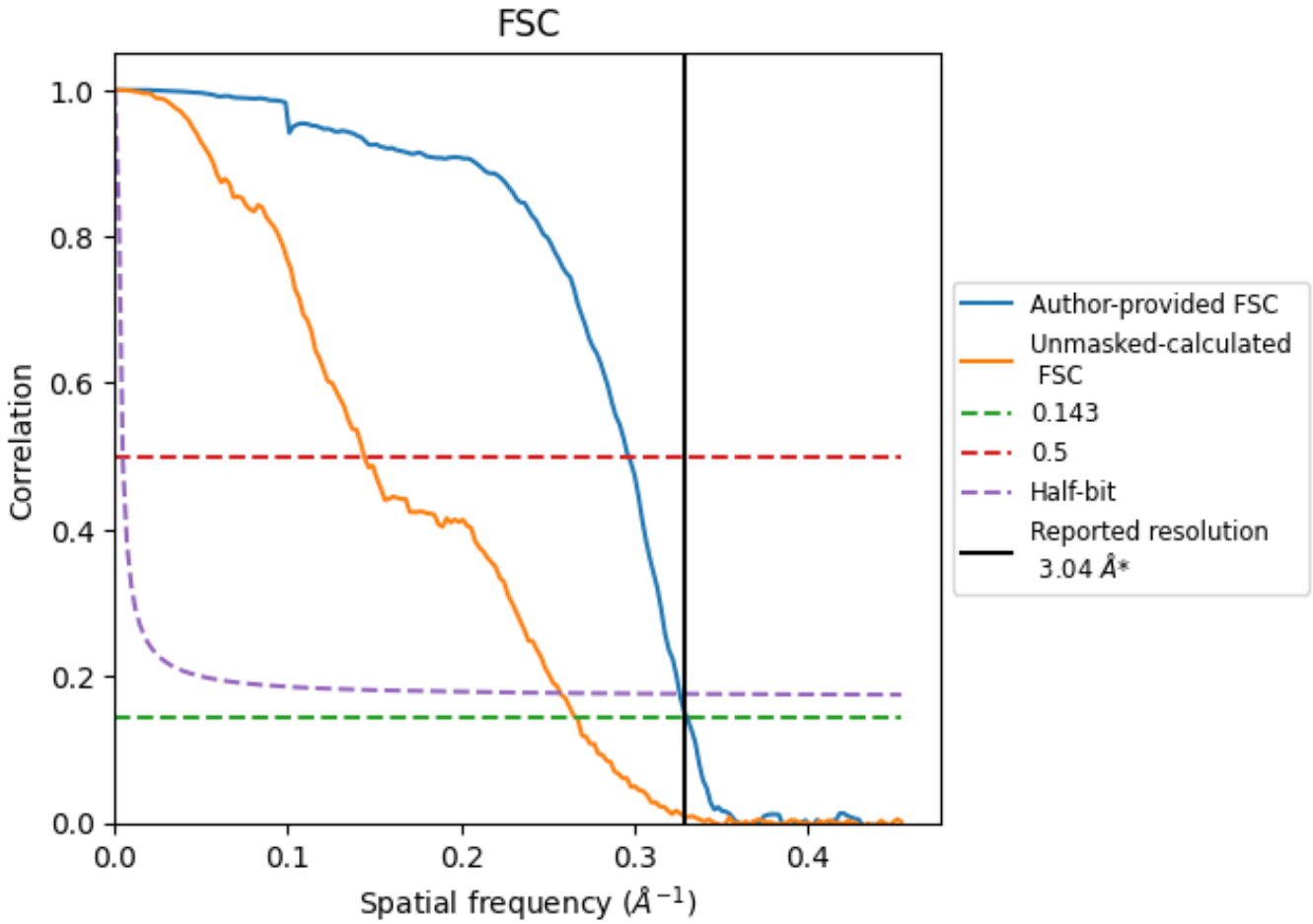


*Reported resolution corresponds to spatial frequency of 0.329 $Å^{-1}$

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 0.329 Å^{-1}

8.2 Resolution estimates (i)

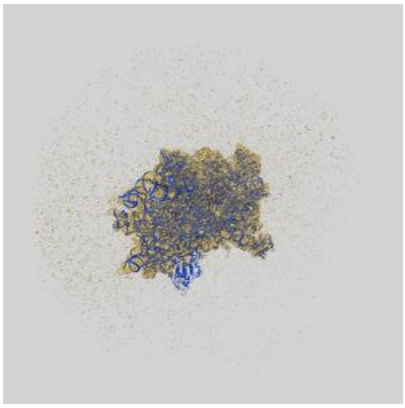
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.02	3.37	3.06
Unmasked-calculated*	3.75	6.94	3.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.04 by more than 10 %

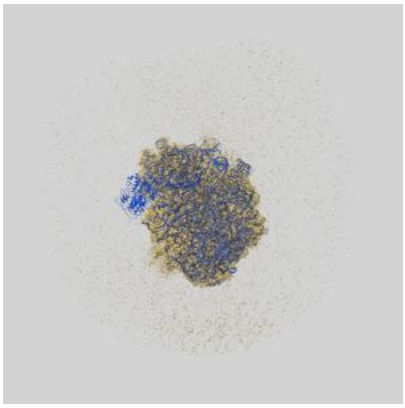
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17329 and PDB model 8P03. Per-residue inclusion information can be found in section 3 on page 12.

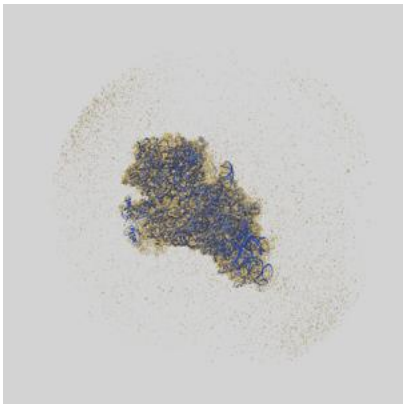
9.1 Map-model overlay



X



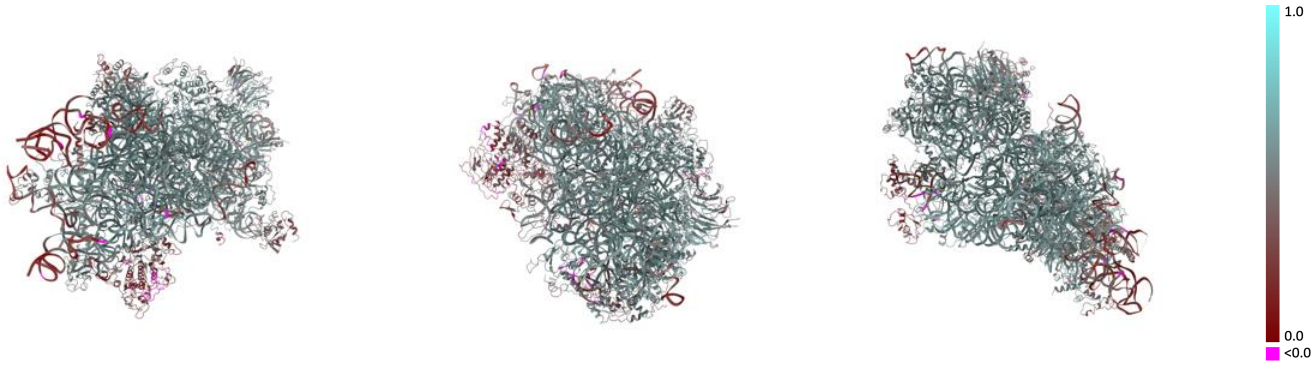
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

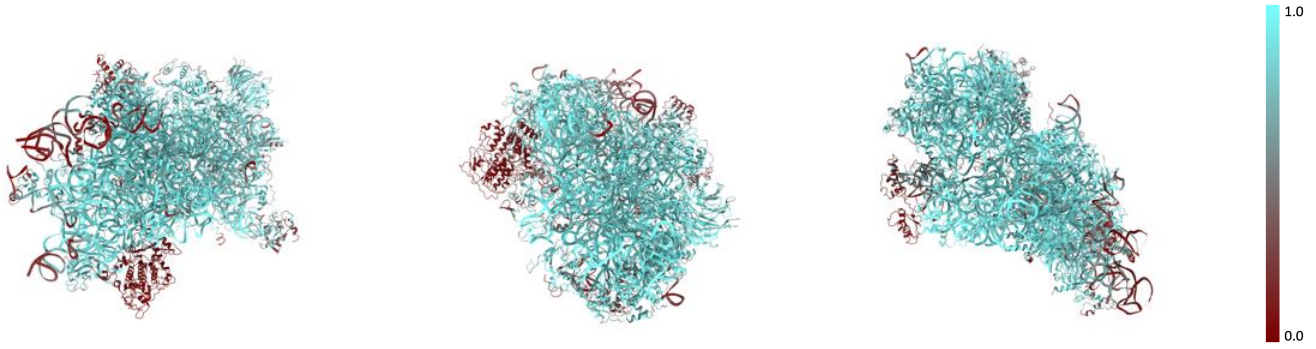
9.2 Q-score mapped to coordinate model (i)



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.

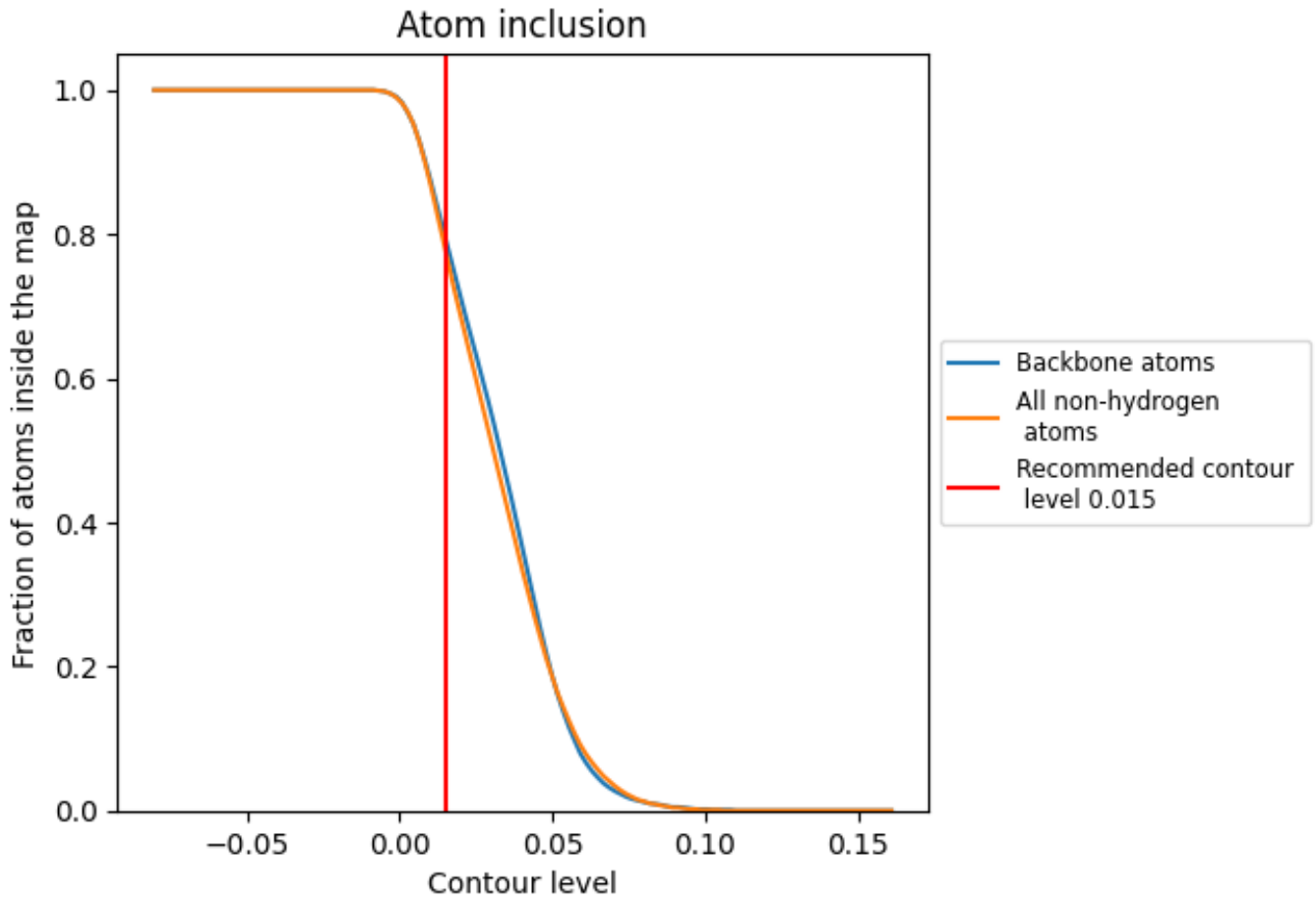
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.5090
1	0.5590	0.2840
2	0.8780	0.5300
3	0.6750	0.4840
A	0.2870	0.3460
C	0.8770	0.5660
D	0.8720	0.5610
E	0.8640	0.5720
F	0.7900	0.5310
G	0.8780	0.5760
H	0.8550	0.5580
I	0.7760	0.5120
J	0.4800	0.4390
K	0.8050	0.5290
L	0.8560	0.5610
M	0.8420	0.5300
N	0.7750	0.5430
O	0.4710	0.3690
P	0.8740	0.5650
Q	0.8770	0.5660
R	0.7490	0.5100
S	0.9030	0.5800
T	0.7090	0.4990
U	0.8020	0.5310
V	0.8780	0.5570
W	0.7530	0.5290
X	0.8730	0.5670
Y	0.9100	0.6000
Z	0.8700	0.5880
a	0.8420	0.5330
b	0.8990	0.5840
c	0.8080	0.5320
d	0.8000	0.5620
e	0.9110	0.5780
f	0.5290	0.3770

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	0.8190	0.5210
i	0.7030	0.5160
j	0.5350	0.4920
k	0.0650	0.2560
l	0.7170	0.5250
n	0.7310	0.5130