



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 10:10 am GMT

PDB ID : 6YLY
EMDB ID : EMD-10842
Title : pre-60S State NE2 (TAP-Flag-Nop53)
Authors : Kater, L.; Beckmann, R.
Deposited on : 2020-04-07
Resolution : 3.80 Å(reported)
Based on initial models : 3JCT, 6N8J

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:

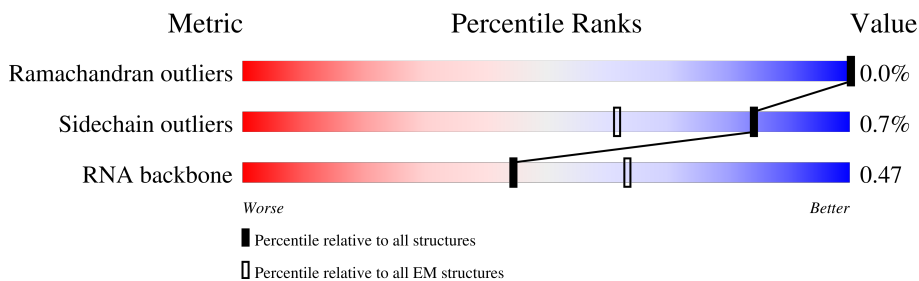
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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.



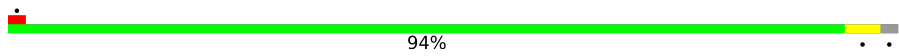
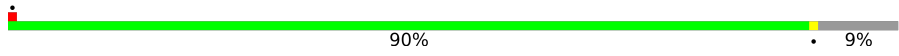
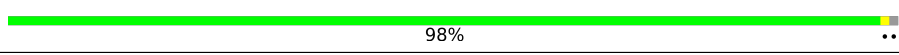
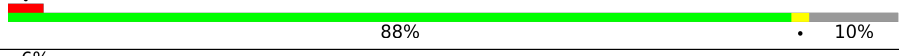
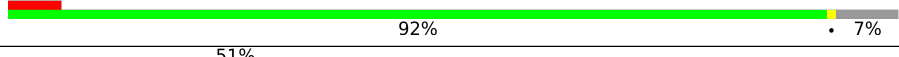

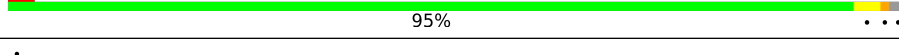
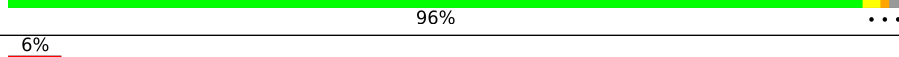
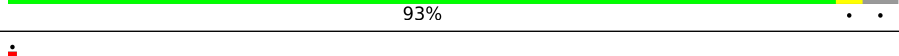
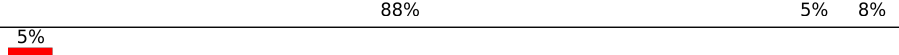
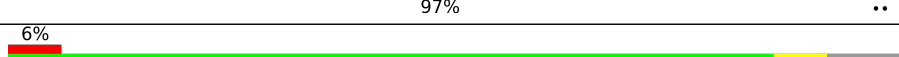
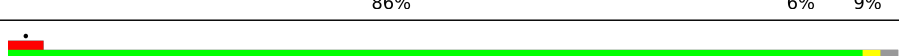
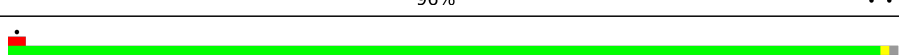
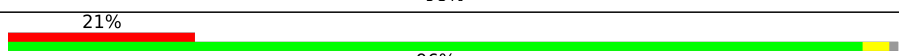
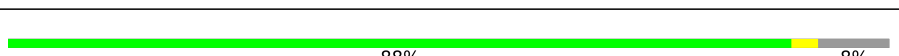
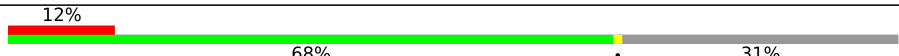
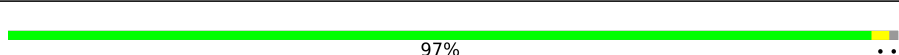
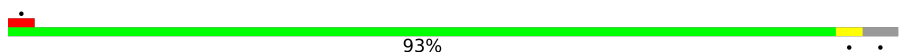



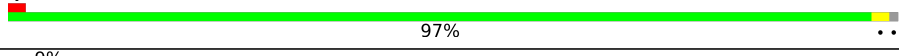

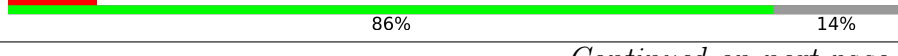

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	254	
2	a	149	
3	B	387	
4	b	647	
5	C	362	
6	c	105	
7	d	113	
8	E	176	

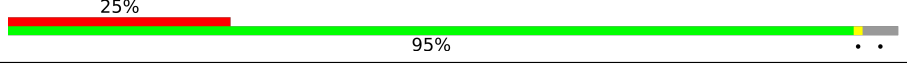

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	e	130	 94%
10	F	244	 90% 9%
11	f	107	 98%
12	G	256	 88% 10%
13	g	121	 6% 92% 7%
14	I	166	 51% 57% 42%
15	H	191	 95%
16	h	120	 96%
17	i	100	 6% 93% 7%
18	j	88	 88% 5% 8%
19	k	78	 5% 97%
20	L	199	 6% 86% 6% 9%
21	l	51	 96%
22	M	138	 98%
23	p	92	 21% 96%
24	N	204	 88% 8%
25	u	199	 12% 68% 31%
26	O	199	 97%
27	P	184	 93%
28	Q	186	 70% 28%
29	R	189	 5% 79% 19%
30	r	261	 24% 74%
31	S	172	 97%
32	T	160	 9% 33% 65%
33	U	121	 10% 86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	V	137	 7% 99%
35	W	236	 25% 95%
36	X	142	 99%
37	Y	127	 98%
38	y	245	 13% 92% 7%
39	Z	136	 98%
40	z	106	 22% 49% 50%
41	1	3396	 52% 24% 21%
42	3	158	 66% 28% 6%
43	K	376	 11% 66% 32%
44	n	605	 58% 39%
45	o	220	 55% 43%
46	q	455	 7% 30% 69%
47	t	322	 5% 85% 11%
48	6	232	 11% 17% 72%
49	s	520	 6% 93%

2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 120663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	180	1391	877	271	243	0	0

- Molecule 2 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	a	84	652	426	113	113	0	0

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	360	2866	1821	536	502	7	0	0

- Molecule 4 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	b	451	3651	2324	628	681	18	0	0

- Molecule 5 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	361	2749	1730	522	494	3	0	0

- Molecule 6 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	c	97	743	479	124	139	1	0	0

- Molecule 7 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	d	107	873	553	165	154	1	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	156	1239	800	222	216	1	0	0

- Molecule 9 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	e	127	1020	647	205	167	1	0	0

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	222	1784	1151	324	308	1	0	0

- Molecule 11 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	f	106	850	540	165	144	1	0	0

- Molecule 12 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	230	1798	1149	323	323	3	0	0

- Molecule 13 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	g	112	881	546	179	152	4	0	0

- Molecule 14 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	96	Total	C	N	O	S	0	0
			776	487	146	140	3		

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 16 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	118	Total	C	N	O	S	0	0
			964	612	185	166	1		

- Molecule 17 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	96	Total	C	N	O	S	0	0
			743	465	148	128	2		

- Molecule 18 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	81	Total	C	N	O	S	0	0
			646	394	141	106	5		

- Molecule 19 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 20 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	L	182	Total	C	N	O	0	0
			1451	902	299	250		

- Molecule 21 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 22 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 23 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 24 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	187	Total	C	N	O	S	0	0
			1607	1005	341	260	1		

- Molecule 25 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	u	137	Total	C	N	O	S	0	0
			1158	727	234	188	9		

- Molecule 26 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 27 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	P	176	Total	C	N	O	0	0
			1393	865	278	250		

- Molecule 28 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Q	134	1035	659	196	179	1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	R	154	1241	772	262	207		0	0

- Molecule 30 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	r	67	579	358	124	96	1	0	0

- Molecule 31 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	S	170	1425	916	265	241	3	0	0

- Molecule 32 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	T	56	434	268	86	79	1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	U	104	826	535	136	155		0	0

- Molecule 34 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	V	136	1003	628	189	179	7	0	0

- Molecule 35 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	W	227	1814	1149	310	350	5	0	0

- Molecule 36 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	X	141	1100	705	196	197	2	0	0

- Molecule 37 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	Y	126	993	625	192	176	0	0

- Molecule 38 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	y	227	1712	1062	298	346	6	0	0

- Molecule 39 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	Z	135	1092	710	202	180	0	0

- Molecule 40 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	z	53	430	264	85	81	0	0

- Molecule 41 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
41	1	2676	57244	25566	10318	18684	2676	0	0

- Molecule 42 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
42	3	158	3353	1500	586	1109	158	0	0

- Molecule 43 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	K	256	2064	1332	342	387	3	0	0

- Molecule 44 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n	371	3030	1963	523	534	10	0	0

- Molecule 45 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o	125	1046	676	188	178	4	0	0

- Molecule 46 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	q	141	1178	743	208	226	1	0	0

- Molecule 47 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	t	287	2306	1459	427	417	3	0	0

- Molecule 48 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	6	65	1370	614	228	463	65	0	0

- Molecule 49 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	s	36	301	184	69	46	2	0	0

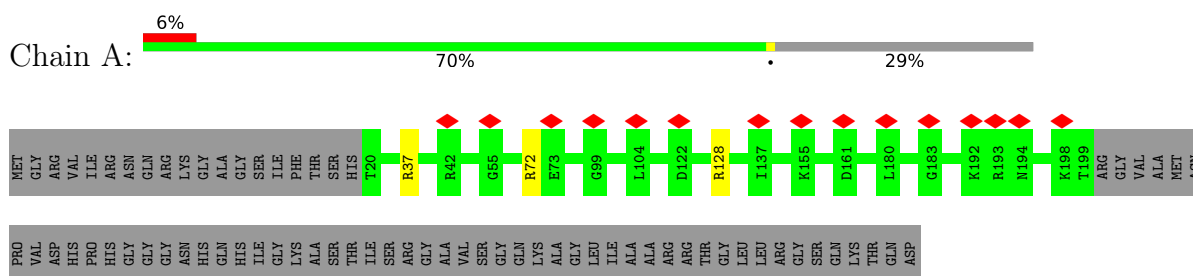
- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
50	j	1	Total	Zn	0
			1	1	
50	p	1	Total	Zn	0
			1	1	
50	u	1	Total	Zn	0
			1	1	

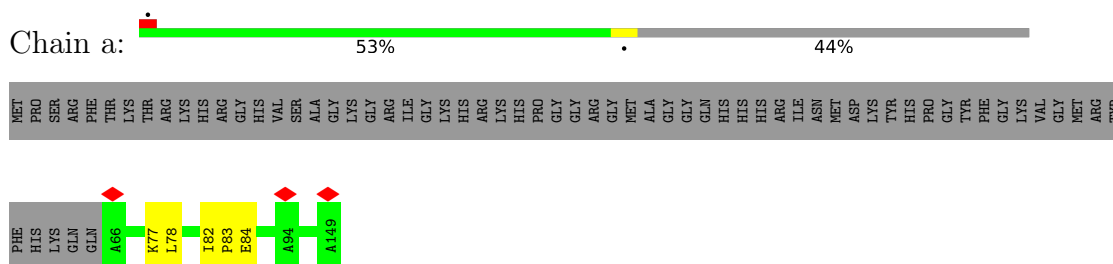
3 Residue-property plots [i](#)

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.

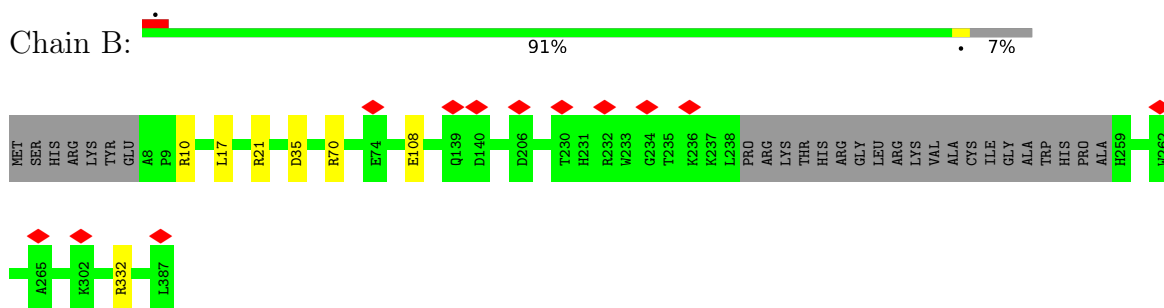
- Molecule 1: 60S ribosomal protein L2-A



- Molecule 2: 60S ribosomal protein L28

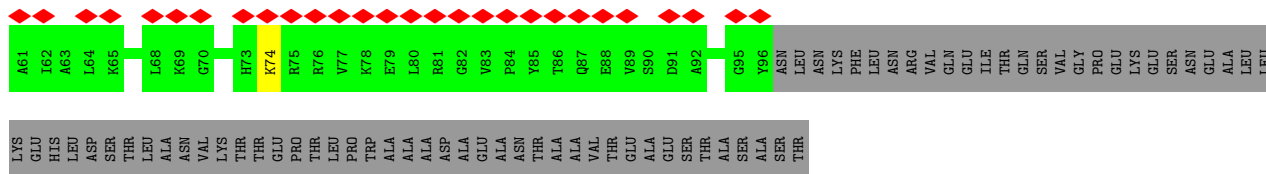


- Molecule 3: 60S ribosomal protein L3

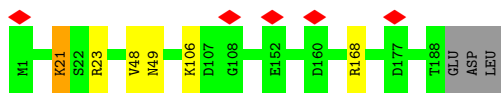


- Molecule 4: Nucleolar GTP-binding protein 1

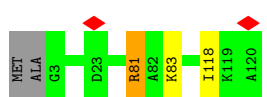




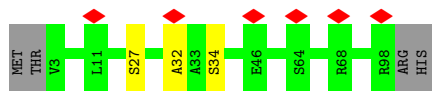
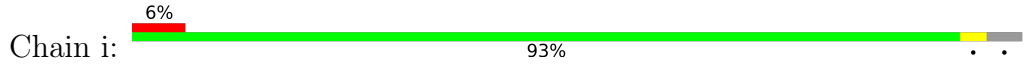
• Molecule 15: 60S ribosomal protein L9-A



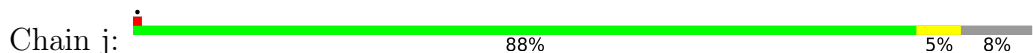
• Molecule 16: 60S ribosomal protein L35-A



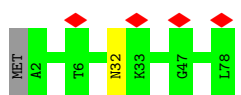
• Molecule 17: 60S ribosomal protein L36-A



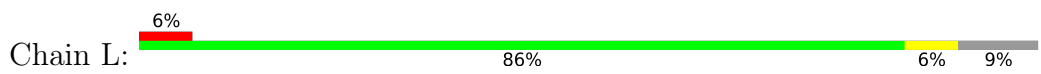
• Molecule 18: 60S ribosomal protein L37-A

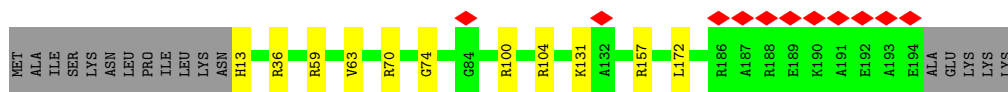


• Molecule 19: 60S ribosomal protein L38

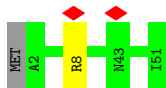


• Molecule 20: 60S ribosomal protein L13-A

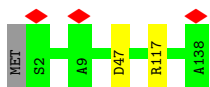




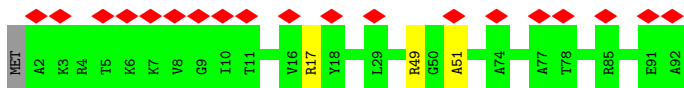
- Molecule 21: 60S ribosomal protein L39



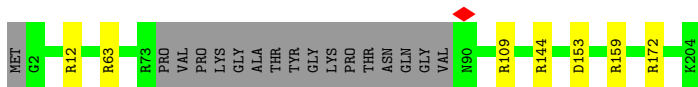
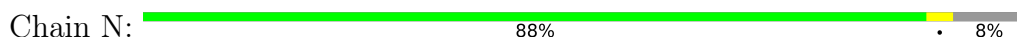
- Molecule 22: 60S ribosomal protein L14-A



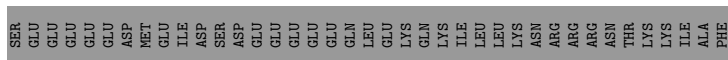
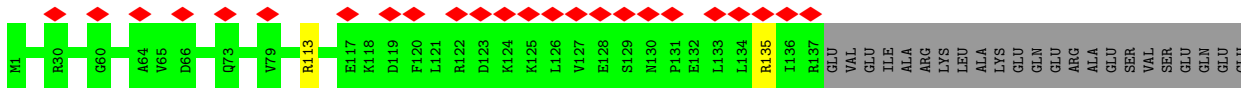
- Molecule 23: 60S ribosomal protein L43-A



- Molecule 24: 60S ribosomal protein L15-A

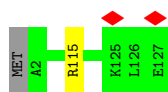


- Molecule 25: Ribosome biogenesis protein RLP24

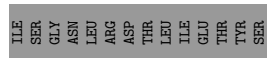
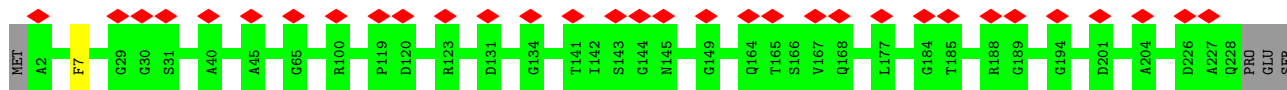
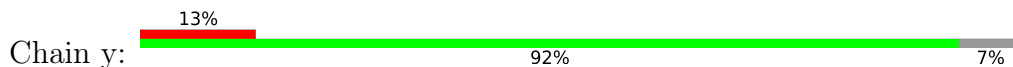


- Molecule 26: 60S ribosomal protein L16-A

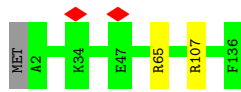




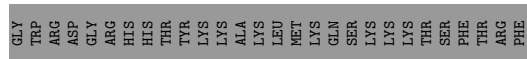
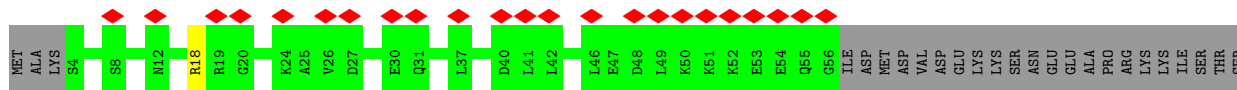
• Molecule 38: Eukaryotic translation initiation factor 6



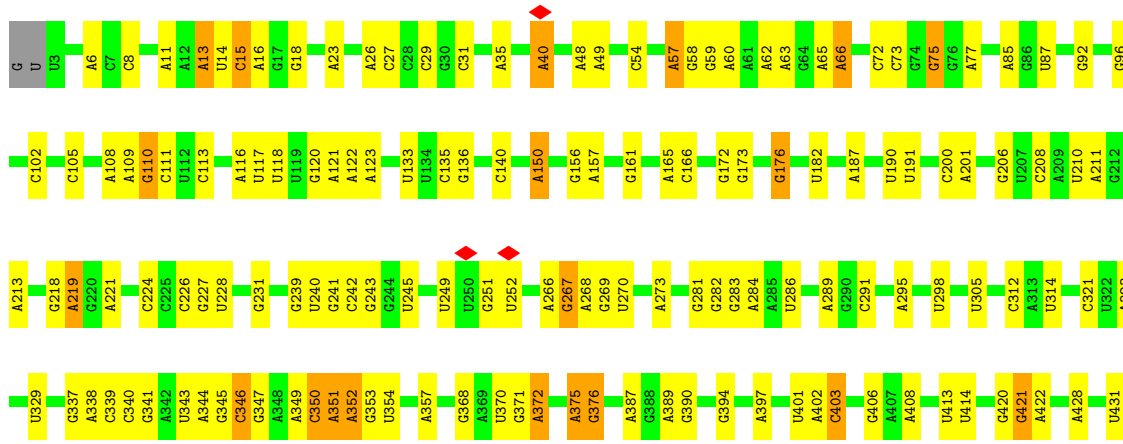
• Molecule 39: 60S ribosomal protein L27-A

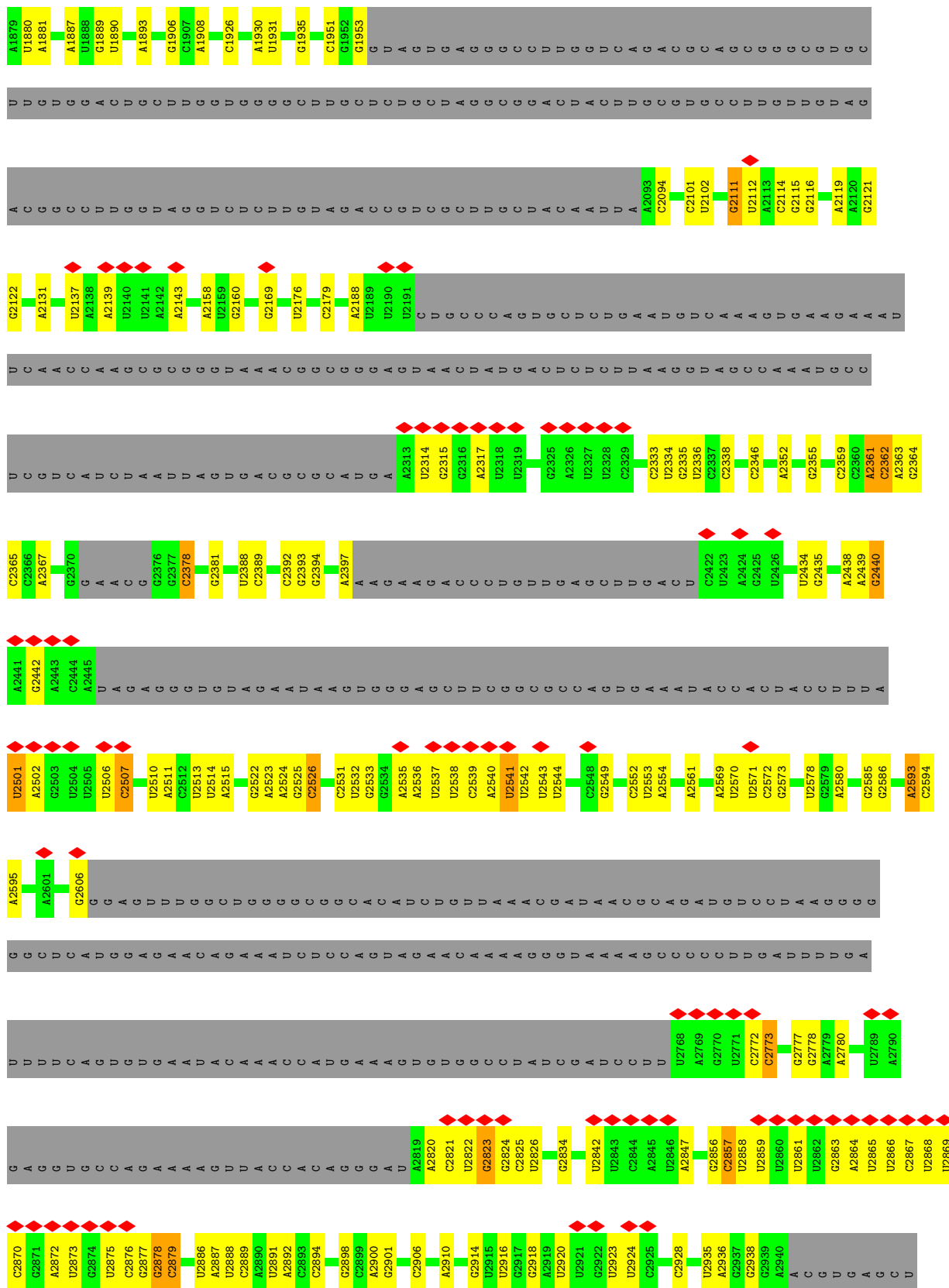


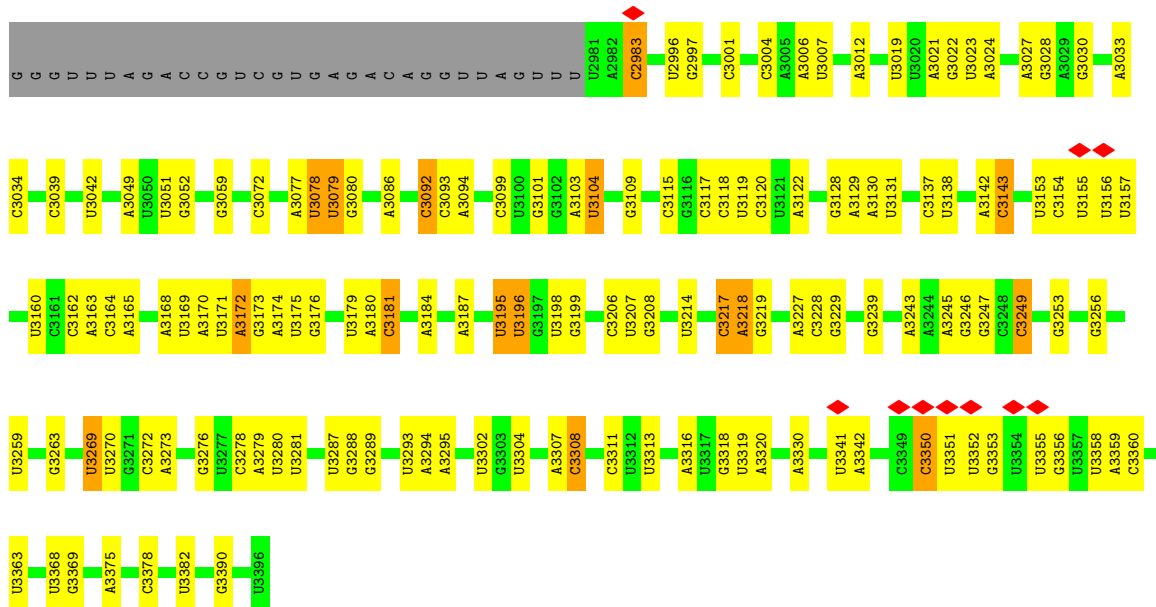
• Molecule 40: UPF0642 protein YBL028C



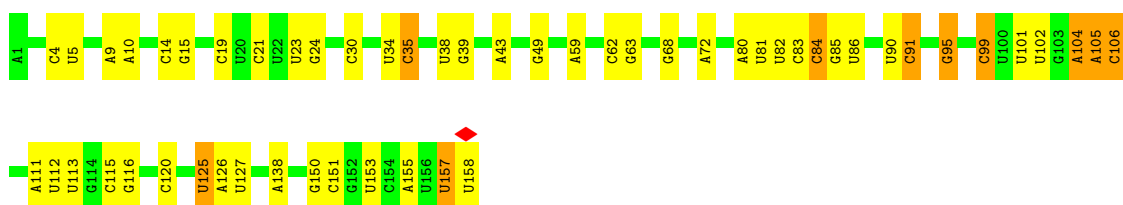
• Molecule 41: 25S rRNA



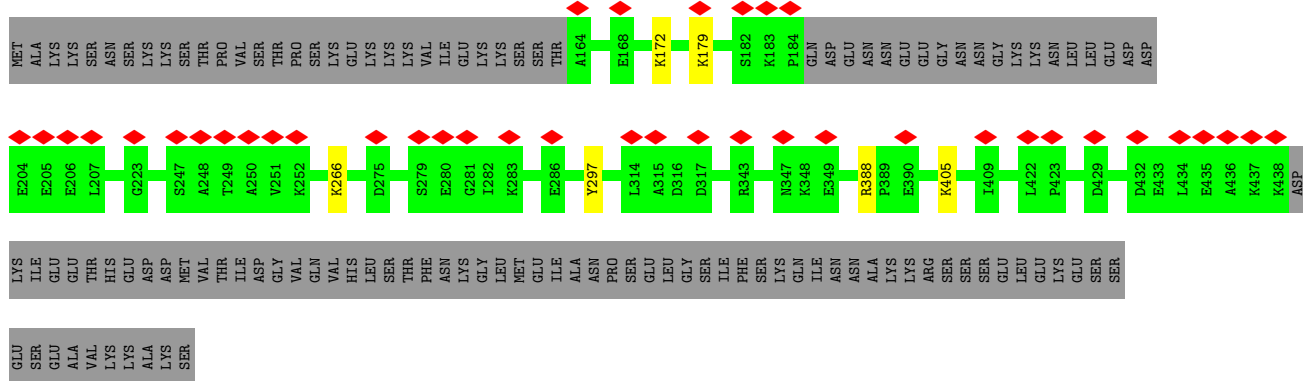




• Molecule 42: 5.8S rRNA



• Molecule 43: Proteasome-interacting protein CIC1



• Molecule 44: Pescadillo homolog



SER
GLU
TRP
SER
LYS
GLU
PHE
ASP
LEU
ASP
GLY
LEU
PHE
SER
SER
LEU
ASP
LYS
ALA
ILE
ASP
ALA
SER
LYS
ASP
GLN
ASP
THR
MET
MET
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30364	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.575	Depositor
Minimum map value	-0.352	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	416.25598, 416.25598, 416.25598	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/1417	0.79	5/1907 (0.3%)
2	a	0.52	0/665	0.71	0/900
3	B	0.57	0/2928	0.82	4/3936 (0.1%)
4	b	0.35	0/3720	0.67	1/5021 (0.0%)
5	C	0.75	0/2801	0.81	2/3792 (0.1%)
6	c	0.37	0/751	0.65	0/1008
7	d	0.54	0/887	0.84	3/1191 (0.3%)
8	E	0.52	0/1260	0.72	0/1694
9	e	0.78	0/1041	0.81	2/1394 (0.1%)
10	F	0.69	0/1821	0.77	2/2451 (0.1%)
11	f	0.93	0/868	0.88	1/1168 (0.1%)
12	G	0.62	0/1830	0.73	1/2469 (0.0%)
13	g	0.55	0/891	0.84	0/1191
14	I	0.37	0/789	0.73	1/1058 (0.1%)
15	H	0.41	0/1514	0.73	0/2039
16	h	0.67	0/973	0.79	1/1294 (0.1%)
17	i	0.44	0/749	0.76	0/995
18	j	0.86	0/661	0.97	4/876 (0.5%)
19	k	0.39	0/618	0.69	0/826
20	L	0.64	0/1475	0.89	5/1982 (0.3%)
21	l	0.50	0/443	0.93	2/588 (0.3%)
22	M	0.50	0/1074	0.71	1/1446 (0.1%)
23	p	0.37	0/701	0.77	1/934 (0.1%)
24	N	0.92	0/1639	0.93	6/2190 (0.3%)
25	u	0.42	0/1180	0.76	0/1569
26	O	0.79	0/1585	0.81	4/2128 (0.2%)
27	P	0.74	0/1415	0.81	2/1900 (0.1%)
28	Q	0.67	0/1050	0.84	3/1419 (0.2%)
29	R	0.46	0/1258	0.79	1/1679 (0.1%)
30	r	0.38	0/589	0.78	2/773 (0.3%)
31	S	0.50	0/1460	0.73	0/1962
32	T	0.36	0/440	0.78	0/594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	U	0.38	0/843	0.61	0/1143
34	V	0.40	0/1018	0.71	0/1369
35	W	0.32	0/1843	0.63	0/2483
36	X	0.71	0/1115	0.80	1/1500 (0.1%)
37	Y	0.67	0/1004	0.79	1/1341 (0.1%)
38	y	0.32	0/1733	0.66	0/2359
39	Z	0.39	0/1118	0.70	2/1497 (0.1%)
40	z	0.35	0/431	0.72	1/567 (0.2%)
41	1	1.73	75/64064 (0.1%)	1.38	559/99858 (0.6%)
42	3	1.35	9/3746 (0.2%)	1.49	50/5832 (0.9%)
43	K	0.36	0/2098	0.66	0/2830
44	n	0.48	0/3101	0.78	5/4187 (0.1%)
45	o	0.40	0/1067	0.73	0/1417
46	q	0.37	0/1197	0.73	2/1601 (0.1%)
47	t	0.39	0/2333	0.78	2/3128 (0.1%)
48	6	0.54	0/1527	1.17	7/2371 (0.3%)
49	s	2.83	10/301 (3.3%)	2.81	17/386 (4.4%)
All	All	1.30	94/129032 (0.1%)	1.17	701/188243 (0.4%)

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
2	a	0	4
3	B	1	1
4	b	0	2
5	C	0	4
7	d	0	1
9	e	0	3
10	F	0	1
12	G	0	4
15	H	0	3
16	h	0	2
17	i	0	3
19	k	0	1
20	L	0	2
22	M	0	1
23	p	0	1
27	P	0	2
28	Q	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
29	R	0	2
30	r	0	2
31	S	0	3
32	T	0	1
34	V	0	1
35	W	0	1
38	y	0	1
41	1	0	1
43	K	0	1
44	n	0	11
45	o	0	4
46	q	0	3
47	t	0	7
49	s	0	8
All	All	1	82

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	1200	A	N3-C4	213.88	2.63	1.34
41	1	1200	A	C2-N3	157.72	2.75	1.33
41	1	1200	A	C6-N1	137.77	2.31	1.35
41	1	1200	A	N1-C2	112.09	2.35	1.34
41	1	1200	A	C5-C4	88.28	2.00	1.38
41	1	1200	A	C5-C6	87.08	2.19	1.41
41	1	1200	A	N9-C4	58.35	1.72	1.37
41	1	1199	C	P-O5'	43.52	2.03	1.59
49	s	14	LYS	N-CA	31.39	2.09	1.46
41	1	1199	C	C5'-C4'	26.63	1.83	1.51
41	1	1199	C	C4'-C3'	25.81	1.81	1.53
41	1	1199	C	O5'-C5'	25.55	1.85	1.44
41	1	1200	A	C5'-C4'	24.21	1.80	1.51
41	1	1199	C	O3'-P	23.37	1.89	1.61
41	1	1200	A	P-O5'	23.33	1.83	1.59
41	1	1199	C	C3'-O3'	20.52	1.70	1.42
49	s	13	THR	C-N	17.86	1.75	1.34
41	1	1200	A	C1'-N9	17.55	1.75	1.48
49	s	16	LYS	CB-CG	16.94	1.98	1.52
49	s	15	LEU	CB-CG	15.38	1.97	1.52
41	1	1200	A	C8-N7	15.28	1.42	1.31
41	1	1200	A	O5'-C5'	13.65	1.66	1.44
41	1	1200	A	N9-C8	10.82	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	s	17	GLU	N-CA	10.30	1.67	1.46
41	1	1198	C	O3'-P	9.35	1.72	1.61
41	1	1200	A	C3'-C2'	9.16	1.63	1.52
49	s	17	GLU	C-N	8.36	1.48	1.33
41	1	1200	A	C4'-O4'	8.01	1.55	1.45
49	s	16	LYS	C-N	7.94	1.52	1.34
41	1	346	C	N1-C6	-7.43	1.32	1.37
41	1	1200	A	N7-C5	7.33	1.43	1.39
49	s	13	THR	C-O	7.32	1.37	1.23
41	1	1200	A	O4'-C1'	7.18	1.50	1.41
41	1	656	A	N7-C5	-6.95	1.35	1.39
49	s	17	GLU	CA-C	6.81	1.70	1.52
42	3	14	C	C4-C5	-6.76	1.37	1.43
41	1	27	C	C4-C5	-6.73	1.37	1.43
41	1	1198	C	C3'-O3'	6.42	1.51	1.42
41	1	16	A	N7-C5	-6.20	1.35	1.39
41	1	1416	C	N1-C6	-6.17	1.33	1.37
42	3	19	C	C4-C5	-6.14	1.38	1.43
41	1	1328	C	N1-C6	-6.09	1.33	1.37
41	1	1419	A	N9-C4	-6.06	1.34	1.37
41	1	29	C	C4-C5	-6.03	1.38	1.43
49	s	15	LEU	CA-CB	5.99	1.67	1.53
41	1	344	A	N7-C5	-5.86	1.35	1.39
41	1	349	A	N9-C4	-5.82	1.34	1.37
41	1	1496	C	C4-C5	-5.76	1.38	1.43
41	1	321	C	C4-C5	-5.76	1.38	1.43
41	1	16	A	C5-C6	-5.74	1.35	1.41
41	1	1333	C	C4-C5	-5.74	1.38	1.43
41	1	340	C	N1-C6	-5.72	1.33	1.37
41	1	1608	C	C4-C5	-5.70	1.38	1.43
41	1	1194	G	N7-C5	-5.69	1.35	1.39
41	1	1437	C	C4-C5	-5.68	1.38	1.43
41	1	660	A	N9-C4	-5.67	1.34	1.37
41	1	1422	G	N7-C5	-5.66	1.35	1.39
41	1	801	A	N7-C5	-5.64	1.35	1.39
42	3	35	C	C4-C5	-5.63	1.38	1.43
41	1	341	G	N7-C5	-5.57	1.35	1.39
41	1	656	A	C5-C6	-5.53	1.36	1.41
41	1	57	A	N9-C4	-5.44	1.34	1.37
41	1	1424	C	C4-C5	-5.35	1.38	1.43
41	1	13	A	N7-C5	-5.33	1.36	1.39
41	1	2352	A	N9-C4	-5.32	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	3	4	C	C4-C5	-5.29	1.38	1.43
41	1	341	G	N9-C8	-5.26	1.34	1.37
41	1	63	A	N9-C4	-5.26	1.34	1.37
41	1	8	C	C4-C5	-5.22	1.38	1.43
41	1	408	A	N9-C4	-5.22	1.34	1.37
42	3	105	A	N7-C5	-5.21	1.36	1.39
42	3	21	C	C4-C5	-5.18	1.38	1.43
41	1	1423	C	C4-C5	-5.17	1.38	1.43
41	1	1419	A	C5-C6	-5.17	1.36	1.41
41	1	1176	C	N1-C6	-5.17	1.34	1.37
41	1	35	A	N9-C4	-5.16	1.34	1.37
41	1	344	A	C5-C6	-5.14	1.36	1.41
41	1	31	C	C4-C5	-5.14	1.38	1.43
42	3	106	C	C4-C5	-5.13	1.38	1.43
41	1	340	C	N3-C4	-5.10	1.30	1.33
41	1	628	A	C6-N6	-5.09	1.29	1.33
41	1	1527	C	C4-C5	-5.08	1.38	1.43
41	1	656	A	N9-C8	-5.06	1.33	1.37
41	1	105	C	N1-C6	-5.06	1.34	1.37
41	1	403	C	N1-C6	-5.05	1.34	1.37
41	1	1332	A	N7-C5	-5.05	1.36	1.39
41	1	1419	A	C6-N6	-5.05	1.29	1.33
41	1	1435	A	N9-C4	-5.04	1.34	1.37
41	1	345	G	N7-C5	-5.03	1.36	1.39
41	1	638	C	C4-C5	-5.02	1.39	1.43
42	3	9	A	N7-C5	-5.01	1.36	1.39
41	1	54	C	C4-C5	-5.01	1.39	1.43
42	3	120	C	C4-C5	-5.01	1.39	1.43
41	1	927	C	C4-C5	-5.00	1.39	1.43

All (701) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1200	A	N1-C2-N3	-71.35	93.62	129.30
41	1	1200	A	C4-C5-N7	-48.99	86.20	110.70
41	1	1200	A	C8-N9-C4	-48.58	86.37	105.80
41	1	1200	A	N7-C8-N9	35.34	131.47	113.80
41	1	1200	A	C5-N7-C8	35.19	121.49	103.90
41	1	1200	A	C6-N1-C2	33.34	138.60	118.60
41	1	1200	A	C2-N3-C4	31.47	126.33	110.60
41	1	1199	C	P-O3'-C3'	23.34	147.71	119.70
41	1	1200	A	N9-C4-C5	21.59	114.44	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1199	C	P-O5'-C5'	21.36	155.07	120.90
41	1	1198	C	OP1-P-O3'	-20.74	59.58	105.20
41	1	1200	A	C6-C5-N7	20.40	146.58	132.30
41	1	1200	A	C4-C5-C6	20.40	127.20	117.00
49	s	15	LEU	CB-CG-CD1	20.15	145.25	111.00
49	s	16	LYS	CA-CB-CG	19.42	156.13	113.40
41	1	1200	A	O4'-C1'-N9	18.47	122.97	108.20
49	s	15	LEU	CA-CB-CG	18.36	157.52	115.30
41	1	1200	A	N3-C4-C5	-18.05	114.16	126.80
49	s	15	LEU	CB-CG-CD2	18.05	141.69	111.00
41	1	1198	C	P-O3'-C3'	17.34	140.51	119.70
41	1	1199	C	O5'-P-OP2	16.05	129.96	110.70
41	1	1200	A	C5'-C4'-O4'	15.59	127.81	109.10
41	1	1198	C	C6-N1-C2	-15.12	114.25	120.30
49	s	13	THR	C-N-CA	14.67	158.38	121.70
41	1	1200	A	C4-N9-C1'	13.83	151.19	126.30
49	s	16	LYS	C-N-CA	13.47	155.38	121.70
49	s	15	LEU	CD1-CG-CD2	-13.41	70.26	110.50
42	3	14	C	C5-C4-N4	-12.91	111.16	120.20
41	1	1198	C	C5-C6-N1	12.27	127.13	121.00
41	1	1199	C	O5'-P-OP1	12.05	125.16	110.70
41	1	1496	C	C6-N1-C2	-11.96	115.52	120.30
41	1	1199	C	C5'-C4'-C3'	11.88	135.00	116.00
41	1	1199	C	OP1-P-OP2	-11.58	102.23	119.60
41	1	1200	A	O5'-C5'-C4'	11.57	133.69	111.70
41	1	1198	C	O3'-P-O5'	11.41	125.68	104.00
41	1	1199	C	O5'-C5'-C4'	11.40	133.37	111.70
41	1	1200	A	P-O5'-C5'	11.20	138.82	120.90
49	s	14	LYS	C-N-CA	11.14	149.56	121.70
42	3	14	C	N3-C4-N4	11.09	125.76	118.00
49	s	16	LYS	N-CA-CB	-10.93	90.93	110.60
41	1	3278	C	N1-C2-O2	10.52	125.21	118.90
49	s	14	LYS	N-CA-CB	10.07	128.74	110.60
41	1	1255	C	N3-C2-O2	-9.88	114.98	121.90
41	1	1437	C	C6-N1-C2	-9.82	116.37	120.30
49	s	16	LYS	CB-CA-C	9.68	129.75	110.40
41	1	3023	U	C2-N1-C1'	9.64	129.27	117.70
41	1	1199	C	C4'-C3'-O3'	9.51	132.03	113.00
41	1	1496	C	C2-N1-C1'	9.40	129.14	118.80
41	1	1279	C	C6-N1-C2	-9.09	116.67	120.30
41	1	1671	C	N3-C2-O2	-8.92	115.66	121.90
41	1	1198	C	O4'-C1'-N1	8.81	115.25	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	2879	C	C6-N1-C2	-8.80	116.78	120.30
41	1	2773	C	C6-N1-C2	-8.74	116.80	120.30
41	1	341	G	C6-C5-N7	-8.73	125.16	130.40
41	1	922	U	C2-N1-C1'	8.73	128.17	117.70
41	1	3023	U	N3-C2-O2	-8.63	116.16	122.20
41	1	27	C	C6-N1-C2	-8.63	116.85	120.30
48	6	2	C	C6-N1-C2	-8.59	116.86	120.30
41	1	1194	G	C6-C5-N7	-8.57	125.26	130.40
41	1	1199	C	O3'-P-O5'	8.57	120.28	104.00
42	3	104	A	N1-C6-N6	-8.48	113.51	118.60
41	1	637	C	C6-N1-C2	-8.47	116.91	120.30
41	1	2362	C	N1-C2-O2	8.40	123.94	118.90
41	1	765	C	N1-C2-O2	8.40	123.94	118.90
41	1	16	A	C5-C6-N6	-8.40	116.98	123.70
41	1	656	A	N7-C8-N9	8.39	118.00	113.80
41	1	1527	C	N1-C2-O2	8.32	123.89	118.90
41	1	3278	C	C2-N1-C1'	8.21	127.83	118.80
41	1	1671	C	N1-C2-O2	8.18	123.81	118.90
41	1	1578	C	N1-C2-O2	8.15	123.79	118.90
41	1	1535	A	N1-C6-N6	-8.11	113.73	118.60
42	3	125	U	C2-N1-C1'	8.10	127.42	117.70
41	1	656	A	C5-N7-C8	-8.08	99.86	103.90
41	1	3308	C	C5-C4-N4	-7.90	114.67	120.20
42	3	9	A	N7-C8-N9	7.87	117.73	113.80
42	3	19	C	C5-C4-N4	-7.84	114.71	120.20
41	1	1255	C	N1-C2-O2	7.83	123.60	118.90
41	1	1194	G	C4-N9-C1'	7.79	136.62	126.50
41	1	16	A	C4-C5-N7	7.75	114.58	110.70
41	1	3023	U	C6-N1-C2	-7.75	116.35	121.00
41	1	1194	G	N7-C8-N9	7.71	116.95	113.10
49	s	16	LYS	CB-CG-CD	7.69	131.59	111.60
41	1	3162	C	C6-N1-C2	-7.68	117.23	120.30
41	1	1444	G	C6-C5-N7	-7.61	125.83	130.40
41	1	16	A	N9-C4-C5	-7.60	102.76	105.80
41	1	656	A	C5-C6-N6	-7.57	117.64	123.70
41	1	700	C	C6-N1-C2	-7.54	117.28	120.30
41	1	1608	C	C5-C4-N4	-7.54	114.92	120.20
41	1	3278	C	N3-C2-O2	-7.51	116.64	121.90
41	1	2362	C	N3-C2-O2	-7.44	116.69	121.90
41	1	1406	A	O5'-P-OP2	-7.43	99.01	105.70
42	3	21	C	N1-C2-O2	7.43	123.36	118.90
41	1	1496	C	N1-C2-O2	7.42	123.35	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1496	C	N3-C4-N4	7.39	123.17	118.00
41	1	700	C	N1-C2-O2	7.37	123.32	118.90
41	1	1432	C	N3-C4-C5	7.37	124.85	121.90
41	1	341	G	C4-N9-C1'	7.36	136.07	126.50
41	1	341	G	C8-N9-C1'	-7.32	117.48	127.00
41	1	2346	C	N1-C2-O2	7.32	123.29	118.90
41	1	321	C	C5-C4-N4	-7.30	115.09	120.20
41	1	1578	C	N3-C2-O2	-7.30	116.79	121.90
41	1	628	A	C4-C5-N7	7.30	114.35	110.70
41	1	2346	C	C2-N1-C1'	7.27	126.80	118.80
41	1	1496	C	C5-C6-N1	7.26	124.63	121.00
41	1	1597	C	C6-N1-C2	-7.24	117.41	120.30
41	1	3350	C	N3-C2-O2	-7.21	116.85	121.90
41	1	628	A	C5-C6-N6	-7.19	117.95	123.70
41	1	765	C	C2-N1-C1'	7.18	126.70	118.80
26	O	133	ARG	NE-CZ-NH1	7.17	123.89	120.30
41	1	1419	A	N9-C4-C5	-7.17	102.93	105.80
41	1	1444	G	C4-C5-N7	7.17	113.67	110.80
41	1	2823	G	N3-C2-N2	-7.17	114.88	119.90
41	1	1654	A	C5-C6-N6	-7.16	117.97	123.70
41	1	344	A	C5-C6-N6	-7.15	117.98	123.70
41	1	1333	C	C5-C4-N4	-7.15	115.20	120.20
41	1	1889	G	N3-C4-N9	7.12	130.27	126.00
41	1	3131	U	N3-C4-O4	7.10	124.37	119.40
41	1	113	C	C6-N1-C2	-7.08	117.47	120.30
41	1	1432	C	C5-C4-N4	-7.08	115.24	120.20
41	1	3311	C	C5-C4-N4	-7.05	115.27	120.20
49	s	13	THR	N-CA-C	7.04	130.02	111.00
41	1	1385	C	N1-C2-O2	7.03	123.12	118.90
41	1	820	A	C5-C6-N1	7.02	121.21	117.70
41	1	2137	U	C2-N1-C1'	7.01	126.12	117.70
41	1	656	A	C4-C5-N7	7.01	114.21	110.70
41	1	341	G	C4-C5-N7	7.00	113.60	110.80
41	1	1494	U	C5-C6-N1	7.00	126.20	122.70
41	1	1198	C	OP2-P-O3'	-6.98	89.85	105.20
41	1	823	C	C6-N1-C2	-6.95	117.52	120.30
41	1	979	U	P-O3'-C3'	6.94	128.02	119.70
1	A	128	ARG	NE-CZ-NH1	6.93	123.76	120.30
41	1	786	A	N1-C6-N6	-6.92	114.45	118.60
41	1	1198	C	C4'-C3'-O3'	6.91	126.82	113.00
41	1	1333	C	C6-N1-C2	-6.90	117.54	120.30
42	3	9	A	C5-N7-C8	-6.89	100.45	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1337	A	C5-C6-N6	-6.89	118.19	123.70
41	1	628	A	N9-C4-C5	-6.88	103.05	105.80
26	O	101	ARG	NE-CZ-NH1	6.87	123.73	120.30
41	1	3249	C	C6-N1-C2	-6.85	117.56	120.30
41	1	267	G	N1-C6-O6	-6.84	115.79	119.90
20	L	157	ARG	NE-CZ-NH1	6.84	123.72	120.30
42	3	19	C	N3-C4-N4	6.84	122.79	118.00
41	1	3131	U	C5-C6-N1	6.84	126.12	122.70
41	1	1866	C	C6-N1-C2	-6.83	117.57	120.30
41	1	658	G	C6-C5-N7	-6.82	126.31	130.40
41	1	628	A	C5-N7-C8	-6.82	100.49	103.90
41	1	1846	C	C6-N1-C2	-6.82	117.57	120.30
41	1	1525	G	C4-N9-C1'	6.81	135.36	126.50
41	1	62	A	N1-C6-N6	6.81	122.68	118.60
41	1	340	C	N1-C2-O2	6.80	122.98	118.90
41	1	341	G	N3-C4-N9	6.79	130.08	126.00
41	1	1535	A	C5-C6-N1	6.79	121.10	117.70
41	1	1594	A	C5-C6-N1	6.78	121.09	117.70
41	1	1189	C	C6-N1-C2	-6.77	117.59	120.30
41	1	16	A	N1-C6-N6	6.76	122.66	118.60
41	1	1527	C	N3-C2-O2	-6.74	117.18	121.90
41	1	341	G	N3-C2-N2	6.72	124.61	119.90
41	1	1169	A	C5-C6-N6	-6.70	118.34	123.70
41	1	500	C	C6-N1-C2	-6.69	117.62	120.30
41	1	376	G	O4'-C1'-N9	6.68	113.55	108.20
41	1	341	G	N1-C2-N2	-6.68	110.19	116.20
41	1	1194	G	C4-C5-N7	6.67	113.47	110.80
41	1	1194	G	N3-C4-N9	6.67	130.00	126.00
42	3	43	A	C5-C6-N6	-6.64	118.39	123.70
41	1	1496	C	N3-C2-O2	-6.62	117.26	121.90
41	1	1200	A	C5'-C4'-C3'	6.61	126.58	116.00
41	1	1334	U	C5-C4-O4	-6.60	121.94	125.90
41	1	3181	C	C2-N1-C1'	6.59	126.05	118.80
41	1	3007	U	C5-C6-N1	6.58	125.99	122.70
41	1	1333	C	N3-C4-N4	6.57	122.60	118.00
41	1	176	G	C6-C5-N7	-6.56	126.47	130.40
41	1	626	U	C5-C4-O4	-6.55	121.97	125.90
41	1	1437	C	C2-N1-C1'	6.55	126.00	118.80
41	1	1200	A	C3'-C2'-C1'	6.55	106.74	101.50
41	1	16	A	C6-C5-N7	-6.54	127.72	132.30
41	1	1494	U	C6-N1-C2	-6.54	117.08	121.00
41	1	341	G	N9-C4-C5	-6.54	102.79	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	765	C	N3-C2-O2	-6.54	117.33	121.90
42	3	15	G	N1-C2-N2	-6.51	110.34	116.20
18	j	21	ARG	NE-CZ-NH1	6.50	123.55	120.30
41	1	3131	U	C6-N1-C2	-6.50	117.10	121.00
41	1	3217	C	N1-C2-O2	6.49	122.80	118.90
41	1	1494	U	N3-C2-O2	-6.48	117.67	122.20
41	1	3311	C	N3-C4-C5	6.47	124.49	121.90
41	1	40	A	C4-N9-C1'	6.46	137.93	126.30
41	1	321	C	N1-C2-O2	6.45	122.77	118.90
41	1	344	A	C5-C6-N1	6.45	120.92	117.70
41	1	3023	U	N1-C2-O2	6.45	127.31	122.80
41	1	3131	U	C5-C4-O4	-6.45	122.03	125.90
41	1	1494	U	N1-C2-O2	6.44	127.31	122.80
41	1	700	C	N3-C2-O2	-6.44	117.39	121.90
42	3	19	C	C6-N1-C2	-6.43	117.73	120.30
41	1	1444	G	N9-C4-C5	-6.43	102.83	105.40
41	1	1327	C	N3-C2-O2	-6.42	117.40	121.90
41	1	40	A	O4'-C1'-N9	6.42	113.33	108.20
41	1	1363	A	N1-C6-N6	6.42	122.45	118.60
41	1	340	C	N3-C2-O2	-6.41	117.41	121.90
41	1	656	A	C6-C5-N7	-6.41	127.81	132.30
41	1	1141	C	N3-C2-O2	-6.40	117.42	121.90
41	1	803	C	C6-N1-C2	-6.38	117.75	120.30
41	1	1199	C	C2-N1-C1'	-6.38	111.78	118.80
41	1	1194	G	C8-N9-C1'	-6.38	118.71	127.00
41	1	628	A	C5-C6-N1	6.38	120.89	117.70
41	1	1836	C	N1-C2-O2	6.37	122.72	118.90
44	n	25	LEU	CB-CG-CD2	6.37	121.84	111.00
1	A	37	ARG	NE-CZ-NH2	6.37	123.48	120.30
3	B	17	LEU	CB-CA-C	6.36	122.29	110.20
41	1	1661	G	C6-C5-N7	-6.36	126.58	130.40
41	1	1598	G	N7-C8-N9	6.35	116.28	113.10
41	1	2094	C	N3-C2-O2	-6.34	117.46	121.90
41	1	13	A	C4-C5-N7	6.34	113.87	110.70
41	1	1277	C	C6-N1-C2	-6.34	117.77	120.30
41	1	1579	C	C6-N1-C2	-6.34	117.77	120.30
29	R	42	ARG	NE-CZ-NH1	6.33	123.47	120.30
41	1	1201	C	O4'-C1'-N1	6.32	113.26	108.20
41	1	23	A	C5-C6-N6	-6.31	118.66	123.70
41	1	2111	G	P-O3'-C3'	6.31	127.27	119.70
41	1	1595	U	C6-N1-C2	-6.30	117.22	121.00
41	1	345	G	N1-C2-N2	-6.30	110.53	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	176	G	N3-C4-N9	6.30	129.78	126.00
41	1	2389	C	C6-N1-C2	-6.29	117.78	120.30
41	1	655	C	C6-N1-C2	-6.29	117.79	120.30
41	1	1333	C	N1-C2-O2	6.29	122.67	118.90
42	3	115	C	N1-C2-O2	6.29	122.67	118.90
41	1	1889	G	C4-N9-C1'	6.28	134.66	126.50
41	1	1608	C	N3-C4-N4	6.27	122.39	118.00
3	B	21	ARG	NE-CZ-NH2	-6.27	117.16	120.30
41	1	3164	C	C6-N1-C2	-6.26	117.80	120.30
41	1	1561	G	C8-N9-C4	-6.26	103.90	106.40
41	1	3214	U	C2-N1-C1'	6.24	125.19	117.70
41	1	3181	C	N1-C2-O2	6.23	122.64	118.90
41	1	344	A	C4-C5-N7	6.23	113.81	110.70
42	3	4	C	C5-C4-N4	-6.22	115.85	120.20
41	1	1889	G	C6-C5-N7	-6.21	126.68	130.40
41	1	1328	C	N1-C2-O2	6.20	122.62	118.90
41	1	3278	C	C6-N1-C1'	-6.20	113.36	120.80
41	1	1199	C	C6-N1-C1'	6.19	128.23	120.80
41	1	1422	G	N7-C8-N9	6.19	116.19	113.10
49	s	14	LYS	CB-CA-C	-6.18	98.05	110.40
41	1	1661	G	N3-C4-N9	6.17	129.70	126.00
41	1	1338	C	N1-C2-O2	6.16	122.60	118.90
41	1	3004	C	C5-C4-N4	-6.15	115.89	120.20
41	1	1329	U	C5-C6-N1	6.15	125.77	122.70
41	1	922	U	N3-C2-O2	-6.14	117.90	122.20
42	3	112	U	N3-C2-O2	-6.14	117.90	122.20
24	N	63	ARG	NE-CZ-NH1	6.14	123.37	120.30
41	1	585	A	C5-C6-N1	6.14	120.77	117.70
41	1	3078	U	P-O3'-C3'	6.14	127.06	119.70
41	1	2857	C	N1-C2-O2	6.13	122.58	118.90
41	1	1615	C	N1-C2-O2	6.12	122.57	118.90
18	j	65	ARG	NE-CZ-NH1	6.11	123.36	120.30
41	1	1338	C	C6-N1-C2	-6.11	117.86	120.30
41	1	1419	A	C8-N9-C4	6.11	108.24	105.80
41	1	3131	U	C2-N1-C1'	6.11	125.03	117.70
41	1	1609	C	N1-C2-O2	6.10	122.56	118.90
41	1	8	C	C6-N1-C2	-6.09	117.86	120.30
41	1	729	C	C6-N1-C2	-6.09	117.87	120.30
42	3	91	C	N1-C2-O2	6.08	122.55	118.90
41	1	433	A	C5-C6-N1	6.08	120.74	117.70
42	3	9	A	C4-C5-N7	6.08	113.74	110.70
42	3	120	C	C5-C4-N4	-6.07	115.95	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	656	A	N1-C6-N6	6.07	122.24	118.60
41	1	500	C	N1-C2-O2	6.06	122.54	118.90
40	z	18	ARG	NE-CZ-NH1	6.05	123.33	120.30
41	1	1190	A	N9-C4-C5	-6.05	103.38	105.80
7	d	28	ARG	NE-CZ-NH1	6.04	123.32	120.30
41	1	793	C	C6-N1-C2	-6.04	117.88	120.30
41	1	8	C	N1-C2-O2	6.03	122.52	118.90
41	1	340	C	C2-N1-C1'	6.03	125.43	118.80
41	1	375	A	N1-C6-N6	-6.01	114.99	118.60
41	1	2333	C	N3-C2-O2	-6.01	117.69	121.90
48	6	2	C	N3-C2-O2	-6.00	117.70	121.90
24	N	172	ARG	NE-CZ-NH1	5.99	123.29	120.30
41	1	110	G	N9-C4-C5	-5.98	103.01	105.40
41	1	3051	U	C5-C6-N1	5.98	125.69	122.70
41	1	2333	C	N1-C2-O2	5.98	122.49	118.90
41	1	658	G	N3-C4-N9	5.97	129.59	126.00
41	1	1327	C	N1-C2-O2	5.97	122.48	118.90
42	3	9	A	C6-C5-N7	-5.97	128.12	132.30
41	1	227	G	N1-C2-N2	-5.97	110.83	116.20
42	3	120	C	N3-C4-N4	5.97	122.18	118.00
48	6	2	C	C2-N1-C1'	5.97	125.36	118.80
41	1	931	C	N1-C2-O2	5.97	122.48	118.90
41	1	1525	G	C8-N9-C1'	-5.96	119.25	127.00
41	1	2879	C	N3-C2-O2	-5.96	117.73	121.90
41	1	3217	C	N3-C2-O2	-5.95	117.73	121.90
41	1	632	G	C4-N9-C1'	5.95	134.23	126.50
41	1	1419	A	C4-C5-N7	5.95	113.67	110.70
41	1	102	C	C5-C4-N4	-5.94	116.04	120.20
41	1	952	A	N1-C6-N6	5.94	122.17	118.60
42	3	4	C	N3-C4-N4	5.94	122.16	118.00
41	1	140	C	C5-C4-N4	-5.94	116.04	120.20
24	N	159	ARG	NE-CZ-NH1	5.93	123.27	120.30
41	1	1390	A	N1-C6-N6	5.93	122.16	118.60
41	1	922	U	N1-C2-O2	5.91	126.94	122.80
28	Q	69	ARG	NE-CZ-NH1	5.91	123.25	120.30
41	1	1437	C	C5-C6-N1	5.91	123.95	121.00
41	1	23	A	C4-C5-N7	5.91	113.65	110.70
41	1	1527	C	C6-N1-C2	-5.90	117.94	120.30
41	1	1444	G	N3-C4-N9	5.89	129.54	126.00
44	n	216	ARG	NE-CZ-NH1	5.89	123.25	120.30
47	t	77	ARG	NE-CZ-NH2	5.89	123.25	120.30
41	1	586	C	N1-C2-O2	5.89	122.43	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1836	C	N3-C2-O2	-5.88	117.78	121.90
41	1	3143	C	N3-C2-O2	-5.87	117.79	121.90
41	1	628	A	N7-C8-N9	5.87	116.73	113.80
41	1	1460	A	C5-C6-N6	-5.87	119.00	123.70
22	M	117	ARG	NE-CZ-NH1	5.87	123.23	120.30
41	1	1190	A	C4-C5-N7	5.86	113.63	110.70
41	1	1423	C	C6-N1-C2	-5.86	117.96	120.30
41	1	1160	C	C5-C4-N4	-5.85	116.10	120.20
41	1	1660	C	C6-N1-C2	-5.84	117.96	120.30
41	1	3172	A	C5-C6-N1	5.84	120.62	117.70
41	1	1307	G	P-O3'-C3'	5.84	126.71	119.70
41	1	13	A	C6-C5-N7	-5.84	128.21	132.30
9	e	33	ARG	NE-CZ-NH1	5.83	123.22	120.30
41	1	351	A	C5-C6-N6	-5.83	119.03	123.70
42	3	153	U	C5-C4-O4	-5.83	122.40	125.90
41	1	433	A	C5-C6-N6	-5.83	119.04	123.70
41	1	1385	C	N3-C2-O2	-5.82	117.83	121.90
41	1	630	A	C4-C5-N7	5.81	113.61	110.70
41	1	3308	C	N3-C4-N4	5.81	122.07	118.00
39	Z	107	ARG	NE-CZ-NH1	5.81	123.21	120.30
41	1	637	C	N1-C2-O2	5.81	122.39	118.90
41	1	1199	C	N3-C4-N4	-5.81	113.94	118.00
41	1	1856	C	C5-C4-N4	-5.81	116.14	120.20
41	1	3007	U	N3-C4-O4	5.80	123.46	119.40
7	d	77	ARG	NE-CZ-NH1	5.79	123.20	120.30
41	1	1529	A	C5-C6-N6	-5.78	119.07	123.70
41	1	3162	C	C5-C6-N1	5.78	123.89	121.00
41	1	658	G	C4-N9-C1'	5.78	134.01	126.50
41	1	40	A	C8-N9-C1'	-5.78	117.31	127.70
41	1	1333	C	N3-C2-O2	-5.78	117.86	121.90
49	s	17	GLU	N-CA-C	5.77	126.59	111.00
41	1	1525	G	C6-C5-N7	-5.77	126.94	130.40
41	1	352	A	C5-C6-N1	5.77	120.58	117.70
41	1	811	U	N3-C4-O4	5.77	123.44	119.40
41	1	1618	G	C4-C5-N7	5.76	113.11	110.80
41	1	729	C	N1-C2-O2	5.76	122.36	118.90
41	1	658	G	C4-C5-N7	5.76	113.10	110.80
41	1	982	C	C6-N1-C2	-5.76	118.00	120.30
41	1	928	C	C6-N1-C2	-5.75	118.00	120.30
41	1	1169	A	C5-C6-N1	5.75	120.58	117.70
41	1	1363	A	C5-N7-C8	-5.75	101.03	103.90
41	1	1494	U	C2-N1-C1'	5.75	124.60	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1364	C	C5-C4-N4	-5.74	116.18	120.20
41	1	1857	C	N3-C2-O2	-5.74	117.88	121.90
20	L	59	ARG	NE-CZ-NH1	5.74	123.17	120.30
41	1	1598	G	C5-N7-C8	-5.73	101.43	104.30
36	X	138	ARG	NE-CZ-NH2	5.73	123.17	120.30
41	1	1419	A	C5-C6-N1	5.73	120.57	117.70
41	1	289	A	C4-C5-N7	5.73	113.56	110.70
41	1	351	A	N1-C6-N6	5.73	122.03	118.60
41	1	2773	C	C2-N1-C1'	5.73	125.10	118.80
41	1	630	A	N9-C4-C5	-5.72	103.51	105.80
41	1	938	C	N1-C2-O2	5.72	122.33	118.90
41	1	1424	C	C5-C4-N4	-5.71	116.20	120.20
41	1	23	A	N1-C6-N6	5.70	122.02	118.60
41	1	1352	A	P-O3'-C3'	5.70	126.53	119.70
46	q	393	ARG	NE-CZ-NH1	5.70	123.15	120.30
41	1	1198	C	C5'-C4'-C3'	5.69	125.10	116.00
41	1	637	C	C5-C6-N1	5.69	123.84	121.00
41	1	1561	G	N7-C8-N9	5.68	115.94	113.10
41	1	1598	G	C6-C5-N7	-5.68	126.99	130.40
41	1	2541	U	P-O3'-C3'	5.68	126.52	119.70
41	1	3143	C	N1-C2-O2	5.67	122.30	118.90
41	1	1586	G	C4-N9-C1'	5.67	133.87	126.50
41	1	312	C	C6-N1-C2	-5.67	118.03	120.30
41	1	1363	A	C5-C6-N6	-5.66	119.17	123.70
42	3	155	A	C5-C6-N6	-5.66	119.17	123.70
41	1	150	A	N1-C6-N6	5.66	122.00	118.60
21	l	8	ARG	NE-CZ-NH2	-5.65	117.47	120.30
11	f	18	ARG	NE-CZ-NH2	-5.64	117.48	120.30
37	Y	115	ARG	NE-CZ-NH1	5.64	123.12	120.30
41	1	13	A	C5-C6-N6	-5.64	119.19	123.70
41	1	16	A	C5-N7-C8	-5.64	101.08	103.90
21	l	8	ARG	NE-CZ-NH1	5.64	123.12	120.30
41	1	428	A	C5-C6-N1	5.63	120.52	117.70
41	1	929	A	N7-C8-N9	5.63	116.62	113.80
27	P	61	ARG	NE-CZ-NH1	5.63	123.12	120.30
41	1	2361	A	C5-C6-N6	-5.63	119.19	123.70
41	1	1190	A	C5-C6-N6	-5.63	119.20	123.70
41	1	1363	A	C4-C5-N7	5.63	113.51	110.70
41	1	1682	U	N3-C2-O2	-5.62	118.26	122.20
41	1	1437	C	N1-C2-O2	5.61	122.27	118.90
41	1	1889	G	C8-N9-C1'	-5.61	119.70	127.00
41	1	923	C	N1-C2-O2	5.61	122.27	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1169	A	C5-N7-C8	-5.61	101.10	103.90
47	t	33	ARG	NE-CZ-NH1	5.61	123.10	120.30
41	1	1598	G	C4-C5-N7	5.60	113.04	110.80
41	1	2983	C	C2-N1-C1'	5.60	124.96	118.80
41	1	66	A	C5-C6-N1	5.60	120.50	117.70
41	1	922	U	C6-N1-C1'	-5.59	113.37	121.20
41	1	1424	C	N3-C4-N4	5.59	121.92	118.00
42	3	105	A	O4'-C1'-N9	5.59	112.67	108.20
41	1	1337	A	C4-C5-N7	5.58	113.49	110.70
41	1	1608	C	N1-C2-O2	5.58	122.25	118.90
41	1	1200	A	P-O3'-C3'	5.58	126.39	119.70
41	1	683	U	C5-C6-N1	5.57	125.48	122.70
41	1	2355	G	N3-C2-N2	-5.56	116.01	119.90
41	1	2440	G	N3-C4-N9	5.56	129.34	126.00
7	d	28	ARG	NE-CZ-NH2	-5.56	117.52	120.30
41	1	663	C	N1-C2-O2	5.56	122.23	118.90
41	1	2094	C	N1-C2-O2	5.55	122.23	118.90
41	1	729	C	C5-C6-N1	5.55	123.78	121.00
41	1	1328	C	N3-C2-O2	-5.55	118.01	121.90
41	1	1316	C	N1-C2-O2	5.55	122.23	118.90
41	1	344	A	C5-N7-C8	-5.55	101.13	103.90
41	1	1337	A	C5-N7-C8	-5.55	101.13	103.90
41	1	1618	G	C6-C5-N7	-5.55	127.07	130.40
42	3	99	C	C5-C4-N4	-5.55	116.32	120.20
41	1	1420	C	N1-C2-O2	5.54	122.22	118.90
41	1	29	C	C5-C4-N4	-5.54	116.32	120.20
41	1	389	A	C4-C5-N7	5.54	113.47	110.70
42	3	106	C	N3-C4-C5	5.54	124.11	121.90
41	1	226	C	C5-C4-N4	-5.53	116.33	120.20
41	1	1141	C	N1-C2-O2	5.53	122.22	118.90
41	1	1437	C	N3-C2-O2	-5.53	118.03	121.90
41	1	394	G	C2-N3-C4	-5.52	109.14	111.90
41	1	1609	C	C6-N1-C2	-5.52	118.09	120.30
41	1	628	A	C6-C5-N7	-5.51	128.44	132.30
41	1	1337	A	N1-C6-N6	5.51	121.91	118.60
23	p	49	ARG	NE-CZ-NH1	5.51	123.06	120.30
42	3	68	G	N9-C4-C5	-5.51	103.20	105.40
41	1	1857	C	N1-C2-O2	5.51	122.20	118.90
1	A	128	ARG	NE-CZ-NH2	-5.50	117.55	120.30
5	C	195	ARG	NE-CZ-NH1	5.50	123.05	120.30
41	1	345	G	N3-C2-N2	5.50	123.75	119.90
41	1	1599	G	C4-C5-N7	5.50	113.00	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	979	U	C6-N1-C2	-5.50	117.70	121.00
41	1	2553	U	N3-C2-O2	-5.50	118.35	122.20
41	1	1428	A	C4-C5-N7	5.49	113.45	110.70
41	1	633	C	N3-C4-C5	5.49	124.10	121.90
41	1	1200	A	N9-C1'-C2'	5.49	121.14	114.00
4	b	215	ARG	NE-CZ-NH1	5.49	123.05	120.30
41	1	700	C	C5-C6-N1	5.48	123.74	121.00
41	1	27	C	C5-C6-N1	5.48	123.74	121.00
41	1	1338	C	N3-C2-O2	-5.48	118.06	121.90
41	1	1349	G	C4-N9-C1'	5.48	133.62	126.50
41	1	1424	C	C6-N1-C2	-5.48	118.11	120.30
41	1	1834	U	C6-N1-C2	-5.48	117.71	121.00
42	3	105	A	C5-C6-N1	5.48	120.44	117.70
41	1	1390	A	C5-N7-C8	-5.47	101.16	103.90
10	F	110	ARG	NE-CZ-NH2	5.47	123.04	120.30
41	1	350	C	C5-C4-N4	-5.47	116.37	120.20
41	1	1832	C	C5-C4-N4	-5.46	116.38	120.20
48	6	38	U	N3-C2-O2	-5.46	118.38	122.20
41	1	8	C	C5-C4-N4	-5.46	116.38	120.20
41	1	2346	C	N3-C2-O2	-5.46	118.08	121.90
41	1	700	C	C2-N1-C1'	5.46	124.80	118.80
41	1	634	C	N1-C2-O2	5.46	122.17	118.90
41	1	1201	C	O5'-P-OP1	5.45	117.24	110.70
41	1	1416	C	C5-C4-N4	-5.45	116.39	120.20
41	1	1561	G	O4'-C1'-N9	5.45	112.56	108.20
41	1	23	A	C5-N7-C8	-5.45	101.18	103.90
41	1	1889	G	N3-C4-C5	-5.44	125.88	128.60
41	1	406	G	O4'-C1'-N9	5.44	112.55	108.20
41	1	1279	C	C5-C6-N1	5.43	123.72	121.00
41	1	1496	C	C5-C4-N4	-5.43	116.40	120.20
42	3	5	U	C5-C6-N1	5.43	125.42	122.70
9	e	47	ARG	NE-CZ-NH1	5.43	123.02	120.30
41	1	150	A	C5-C6-N6	-5.43	119.36	123.70
5	C	220	ARG	NE-CZ-NH2	-5.43	117.59	120.30
42	3	125	U	C6-N1-C1'	-5.43	113.60	121.20
41	1	2857	C	N3-C2-O2	-5.42	118.10	121.90
24	N	12	ARG	NE-CZ-NH1	5.42	123.01	120.30
41	1	350	C	C6-N1-C2	-5.42	118.13	120.30
41	1	1428	A	N9-C4-C5	-5.42	103.63	105.80
41	1	3138	U	C5-C6-N1	5.42	125.41	122.70
41	1	3001	C	N1-C2-O2	5.41	122.15	118.90
42	3	19	C	N1-C2-O2	5.41	122.15	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	289	A	C5-N7-C8	-5.41	101.20	103.90
41	1	13	A	N7-C8-N9	5.41	116.50	113.80
41	1	58	G	C4-N9-C1'	5.40	133.53	126.50
41	1	314	U	C5-C6-N1	5.40	125.40	122.70
1	A	37	ARG	NE-CZ-NH1	-5.39	117.60	120.30
41	1	242	C	N1-C2-O2	5.39	122.14	118.90
41	1	1834	U	C5-C6-N1	5.39	125.40	122.70
41	1	3269	U	P-O3'-C3'	5.39	126.17	119.70
41	1	794	U	C5-C6-N1	5.39	125.39	122.70
41	1	1194	G	C8-N9-C4	-5.39	104.24	106.40
41	1	543	C	C6-N1-C2	-5.39	118.14	120.30
41	1	208	C	C5-C4-N4	-5.39	116.43	120.20
41	1	1201	C	C6-N1-C2	-5.38	118.15	120.30
41	1	347	G	N1-C2-N2	-5.38	111.36	116.20
41	1	2378	C	N1-C2-O2	5.38	122.13	118.90
41	1	3023	U	C5-C6-N1	5.38	125.39	122.70
42	3	68	G	C4-C5-N7	5.38	112.95	110.80
41	1	433	A	N9-C4-C5	-5.38	103.65	105.80
41	1	62	A	C5-C6-N6	-5.38	119.40	123.70
41	1	75	G	C4-C5-N7	5.37	112.95	110.80
41	1	3218	A	P-O3'-C3'	5.37	126.14	119.70
49	s	14	LYS	CA-C-N	-5.37	105.39	117.20
1	A	72	ARG	NE-CZ-NH1	5.36	122.98	120.30
41	1	1695	U	N3-C2-O2	-5.36	118.45	122.20
41	1	1525	G	C4-C5-N7	5.36	112.94	110.80
41	1	1615	C	C6-N1-C2	-5.35	118.16	120.30
41	1	13	A	C5-N7-C8	-5.34	101.23	103.90
41	1	2526	C	C6-N1-C2	-5.34	118.16	120.30
41	1	765	C	C6-N1-C1'	-5.34	114.39	120.80
41	1	977	C	C6-N1-C2	-5.34	118.16	120.30
41	1	1881	A	C5-C6-N6	-5.34	119.43	123.70
41	1	433	A	C4-C5-N7	5.34	113.37	110.70
41	1	1856	C	N1-C2-O2	5.33	122.10	118.90
41	1	2593	A	P-O3'-C3'	5.33	126.10	119.70
41	1	648	C	N3-C2-O2	-5.33	118.17	121.90
41	1	547	G	OP1-P-O3'	5.33	116.92	105.20
41	1	665	A	C5-C6-N1	5.32	120.36	117.70
41	1	1561	G	N3-C4-C5	-5.32	125.94	128.60
41	1	413	U	C5-C4-O4	-5.32	122.71	125.90
41	1	1640	G	C6-C5-N7	-5.32	127.21	130.40
12	G	249	ARG	NE-CZ-NH1	5.31	122.95	120.30
41	1	273	A	C5-C6-N1	5.31	120.35	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Q	69	ARG	NE-CZ-NH2	-5.31	117.65	120.30
48	6	7	C	O4'-C1'-N1	5.30	112.44	108.20
3	B	108	GLU	CB-CA-C	-5.30	99.80	110.40
41	1	1661	G	C4-N9-C1'	5.30	133.39	126.50
41	1	637	C	N3-C2-O2	-5.30	118.19	121.90
41	1	58	G	N7-C8-N9	5.29	115.75	113.10
48	6	38	U	N1-C2-O2	5.29	126.50	122.80
41	1	1586	G	C8-N9-C1'	-5.29	120.12	127.00
41	1	3162	C	N1-C2-O2	5.29	122.07	118.90
41	1	632	G	N7-C8-N9	5.29	115.74	113.10
41	1	2359	C	C5-C6-N1	5.29	123.64	121.00
41	1	6	A	C4-C5-N7	5.28	113.34	110.70
41	1	931	C	N3-C2-O2	-5.28	118.20	121.90
28	Q	38	ARG	NE-CZ-NH1	5.28	122.94	120.30
30	r	30	ARG	NE-CZ-NH2	5.28	122.94	120.30
41	1	1854	C	C6-N1-C2	-5.27	118.19	120.30
41	1	3350	C	N1-C2-O2	5.27	122.06	118.90
42	3	112	U	N1-C2-O2	5.27	126.49	122.80
41	1	1849	C	C5-C4-N4	-5.27	116.51	120.20
20	L	104	ARG	NE-CZ-NH1	5.27	122.93	120.30
41	1	3103	A	N9-C4-C5	-5.27	103.69	105.80
41	1	1144	U	C6-N1-C2	-5.26	117.84	121.00
41	1	1390	A	N9-C4-C5	-5.26	103.69	105.80
41	1	2114	C	C6-N1-C2	-5.26	118.20	120.30
41	1	2346	C	C6-N1-C2	-5.26	118.20	120.30
41	1	2338	C	N3-C2-O2	-5.26	118.22	121.90
41	1	15	C	C6-N1-C2	-5.25	118.20	120.30
24	N	109	ARG	NE-CZ-NH1	5.25	122.93	120.30
41	1	1426	C	C6-N1-C2	-5.25	118.20	120.30
42	3	84	C	N1-C2-O2	5.25	122.05	118.90
26	O	68	ARG	NE-CZ-NH1	5.25	122.92	120.30
41	1	291	C	C5-C4-N4	-5.25	116.53	120.20
41	1	952	A	C5-C6-N6	-5.25	119.50	123.70
41	1	1146	C	C6-N1-C2	-5.25	118.20	120.30
41	1	501	A	C5-C6-N1	5.25	120.32	117.70
42	3	15	G	N3-C2-N2	5.24	123.57	119.90
41	1	110	G	C4-C5-N7	5.24	112.90	110.80
41	1	803	C	C2-N1-C1'	5.24	124.56	118.80
41	1	2983	C	N1-C2-O2	5.24	122.05	118.90
41	1	29	C	N3-C4-N4	5.24	121.67	118.00
41	1	1160	C	N3-C4-N4	5.24	121.67	118.00
41	1	431	U	C5-C4-O4	-5.23	122.76	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1597	C	C5-C6-N1	5.23	123.62	121.00
41	1	3072	C	O4'-C1'-N1	5.23	112.39	108.20
41	1	1498	A	N7-C8-N9	5.23	116.42	113.80
41	1	1194	G	C5-N7-C8	-5.23	101.69	104.30
42	3	21	C	C6-N1-C2	-5.23	118.21	120.30
41	1	936	A	O4'-C1'-N9	5.23	112.38	108.20
41	1	228	U	N3-C2-O2	-5.22	118.54	122.20
41	1	371	G	C8-N9-C1'	-5.22	120.21	127.00
44	n	33	ARG	NE-CZ-NH1	5.22	122.91	120.30
41	1	1144	U	C5-C6-N1	5.22	125.31	122.70
44	n	369	ARG	NE-CZ-NH2	5.22	122.91	120.30
41	1	1064	A	P-O3'-C3'	5.21	125.96	119.70
41	1	1654	A	N1-C6-N6	5.21	121.73	118.60
41	1	2501	U	P-O3'-C3'	5.21	125.96	119.70
41	1	58	G	C5-N7-C8	-5.21	101.70	104.30
41	1	633	C	N1-C2-O2	5.21	122.02	118.90
41	1	1654	A	C5-C6-N1	5.21	120.30	117.70
41	1	1564	U	C6-N1-C2	-5.20	117.88	121.00
41	1	75	G	N9-C4-C5	-5.20	103.32	105.40
41	1	345	G	C2-N3-C4	-5.20	109.30	111.90
41	1	1498	A	C4-C5-N7	5.20	113.30	110.70
41	1	1147	G	C4-C5-N7	5.20	112.88	110.80
41	1	1460	A	C4-C5-N7	5.20	113.30	110.70
41	1	2346	C	C5-C4-N4	-5.19	116.56	120.20
42	3	105	A	C5-N7-C8	-5.19	101.30	103.90
41	1	8	C	C5-C6-N1	5.19	123.59	121.00
41	1	1390	A	C4-C5-N7	5.19	113.29	110.70
41	1	656	A	N9-C4-C5	-5.19	103.72	105.80
41	1	1131	G	C8-N9-C4	-5.18	104.33	106.40
41	1	628	A	N3-C4-N9	5.18	131.55	127.40
42	3	21	C	N3-C2-O2	-5.18	118.27	121.90
41	1	1423	C	C5-C4-N4	-5.18	116.57	120.20
41	1	414	U	C5-C4-O4	-5.18	122.79	125.90
41	1	3137	C	C5-C4-N4	-5.18	116.58	120.20
41	1	421	G	C4-N9-C1'	5.17	133.23	126.50
41	1	1872	C	C5-C4-N4	-5.17	116.58	120.20
41	1	1422	G	C6-C5-N7	-5.17	127.30	130.40
41	1	1462	A	C5-C6-N6	-5.17	119.56	123.70
41	1	289	A	C5-C6-N1	5.17	120.28	117.70
49	s	13	THR	CA-C-N	5.17	128.57	117.20
41	1	2878	G	O4'-C1'-N9	5.17	112.33	108.20
41	1	1851	G	C4-C5-N7	5.16	112.87	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1411	C	C6-N1-C2	-5.16	118.23	120.30
41	1	3092	C	C6-N1-C2	-5.16	118.24	120.30
41	1	3195	U	C2-N1-C1'	5.16	123.89	117.70
41	1	1400	G	N3-C4-N9	-5.16	122.91	126.00
41	1	3079	U	N1-C2-O2	5.16	126.41	122.80
41	1	16	A	N3-C4-N9	5.14	131.51	127.40
41	1	3079	U	N3-C2-O2	-5.14	118.60	122.20
41	1	648	C	N1-C2-O2	5.14	121.98	118.90
41	1	1460	A	N7-C8-N9	5.14	116.37	113.80
42	3	21	C	N3-C4-N4	5.14	121.60	118.00
41	1	820	A	C6-N1-C2	-5.14	115.52	118.60
41	1	1280	C	C6-N1-C2	-5.14	118.25	120.30
41	1	1169	A	C4-C5-N7	5.13	113.27	110.70
41	1	1390	A	C5-C6-N6	-5.13	119.60	123.70
41	1	1509	A	C5-N7-C8	-5.13	101.33	103.90
41	1	672	A	C5-C6-N6	-5.13	119.60	123.70
41	1	1412	G	N7-C8-N9	5.12	115.66	113.10
41	1	2824	G	C4-N9-C1'	5.12	133.16	126.50
41	1	1806	A	N1-C6-N6	5.12	121.67	118.60
48	6	2	C	N1-C2-O2	5.12	121.97	118.90
41	1	372	A	C5-C6-N6	-5.11	119.61	123.70
44	n	25	LEU	CB-CG-CD1	5.11	119.69	111.00
41	1	105	C	N1-C2-O2	5.11	121.97	118.90
41	1	1619	A	C4-C5-N7	5.11	113.26	110.70
3	B	21	ARG	NE-CZ-NH1	5.11	122.86	120.30
41	1	224	C	C5-C4-N4	-5.11	116.62	120.20
41	1	227	G	N3-C2-N2	5.11	123.48	119.90
41	1	2346	C	N3-C4-N4	5.11	121.58	118.00
41	1	1522	U	O4'-C1'-N1	5.10	112.28	108.20
41	1	886	C	C6-N1-C2	-5.10	118.26	120.30
42	3	157	U	O4'-C1'-N1	5.10	112.28	108.20
41	1	376	G	C8-N9-C4	-5.10	104.36	106.40
41	1	289	A	N9-C4-C5	-5.09	103.76	105.80
16	h	81	ARG	NE-CZ-NH1	5.09	122.84	120.30
41	1	632	G	C8-N9-C1'	-5.09	120.39	127.00
42	3	10	A	C4-C5-N7	5.09	113.24	110.70
41	1	1393	A	C5-C6-N1	5.08	120.24	117.70
41	1	345	G	N7-C8-N9	5.08	115.64	113.10
41	1	658	G	C8-N9-C1'	-5.08	120.39	127.00
41	1	1320	C	N1-C2-O2	5.08	121.95	118.90
42	3	91	C	C6-N1-C2	-5.08	118.27	120.30
41	1	291	C	N3-C4-N4	5.08	121.56	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1165	A	C5-C6-N1	5.08	120.24	117.70
41	1	1333	C	C2-N1-C1'	5.08	124.39	118.80
41	1	1115	G	C4-N9-C1'	5.08	133.10	126.50
41	1	2367	A	C5-C6-N1	5.07	120.24	117.70
41	1	1654	A	C4-C5-N7	5.07	113.23	110.70
42	3	101	U	N3-C4-O4	5.07	122.95	119.40
20	L	36	ARG	NE-CZ-NH1	5.07	122.83	120.30
41	1	435	C	C5-C4-N4	-5.07	116.65	120.20
42	3	150	G	N9-C4-C5	-5.07	103.37	105.40
41	1	543	C	N3-C2-O2	-5.06	118.36	121.90
41	1	1444	G	C8-N9-C1'	-5.06	120.42	127.00
18	j	63	ARG	NE-CZ-NH2	5.06	122.83	120.30
41	1	861	C	C6-N1-C2	-5.06	118.28	120.30
41	1	1498	A	C5-N7-C8	-5.06	101.37	103.90
41	1	3196	U	N1-C2-O2	5.06	126.34	122.80
42	3	30	C	N1-C2-O2	5.06	121.94	118.90
41	1	2879	C	N1-C2-O2	5.06	121.93	118.90
41	1	1566	A	C4-C5-N7	5.05	113.23	110.70
41	1	2507	C	C6-N1-C2	-5.05	118.28	120.30
27	P	171	ARG	NE-CZ-NH1	5.05	122.82	120.30
42	3	84	C	N3-C2-O2	-5.05	118.37	121.90
10	F	157	ASN	C-N-CA	5.05	134.32	121.70
41	1	40	A	N7-C8-N9	5.05	116.32	113.80
41	1	1740	U	C5-C6-N1	5.05	125.22	122.70
26	O	37	ARG	NE-CZ-NH1	5.04	122.82	120.30
41	1	1156	C	C5-C4-N4	-5.04	116.67	120.20
41	1	357	A	C5-C6-N1	5.04	120.22	117.70
41	1	811	U	C5-C4-O4	-5.04	122.88	125.90
41	1	3181	C	C6-N1-C1'	-5.04	114.75	120.80
30	r	9	ARG	NE-CZ-NH2	5.04	122.82	120.30
41	1	1214	U	C5-C4-O4	-5.04	122.88	125.90
41	1	2359	C	C6-N1-C2	-5.04	118.28	120.30
18	j	63	ARG	NE-CZ-NH1	-5.04	117.78	120.30
42	3	10	A	C5-N7-C8	-5.04	101.38	103.90
42	3	21	C	C5-C4-N4	-5.04	116.67	120.20
41	1	3104	U	C6-N1-C2	-5.03	117.98	121.00
24	N	144	ARG	NE-CZ-NH1	5.03	122.82	120.30
41	1	62	A	C5-N7-C8	-5.03	101.38	103.90
41	1	1194	G	N3-C2-N2	5.03	123.42	119.90
41	1	1423	C	N3-C4-N4	5.03	121.52	118.00
41	1	8	C	N3-C4-N4	5.03	121.52	118.00
41	1	58	G	C4-C5-N7	5.02	112.81	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1475	A	N1-C6-N6	5.02	121.61	118.60
41	1	626	U	N3-C4-O4	5.02	122.92	119.40
41	1	792	G	C6-C5-N7	-5.02	127.39	130.40
41	1	40	A	C6-C5-N7	-5.02	128.79	132.30
41	1	219	A	C5-C6-N1	5.02	120.21	117.70
41	1	1199	C	N3-C2-O2	-5.02	118.39	121.90
41	1	1234	G	C5-C6-O6	5.02	131.61	128.60
41	1	1413	G	C4-N9-C1'	5.02	133.02	126.50
41	1	3078	U	OP2-P-O3'	5.02	116.24	105.20
42	3	95	G	O5'-P-OP2	-5.02	101.19	105.70
39	Z	65	ARG	NE-CZ-NH1	5.01	122.81	120.30
41	1	1661	G	C4-C5-N7	5.01	112.81	110.80
41	1	2773	C	N3-C2-O2	-5.01	118.39	121.90
41	1	346	C	C6-N1-C1'	-5.01	114.79	120.80
41	1	1437	C	N3-C4-N4	5.01	121.50	118.00
42	3	9	A	C5-C6-N6	-5.01	119.69	123.70
14	I	46	LEU	CA-CB-CG	5.00	126.81	115.30
46	q	439	ARG	NE-CZ-NH1	5.00	122.80	120.30
20	L	70	ARG	NE-CZ-NH1	5.00	122.80	120.30
41	1	1498	A	C5-C6-N6	-5.00	119.70	123.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	17	LEU	CA

All (82) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	1	1200	A	Sidechain
3	B	35	ASP	Peptide
5	C	3	ARG	Peptide
5	C	317	PRO	Peptide
5	C	327	LEU	Peptide
5	C	338	LYS	Peptide
10	F	157	ASN	Peptide
12	G	133	LYS	Peptide
12	G	144	GLU	Peptide
12	G	30	THR	Peptide
12	G	76	ALA	Peptide
15	H	21	LYS	Peptide
15	H	48	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
15	H	49	ASN	Peptide
43	K	297	TYR	Peptide
20	L	131	LYS	Peptide
20	L	74	GLY	Peptide
22	M	47	ASP	Peptide
27	P	144	SER	Peptide
27	P	63	PHE	Peptide
28	Q	145	ASN	Peptide
29	R	130	ASN	Peptide
29	R	54	ALA	Peptide
31	S	167	ARG	Peptide
31	S	22	PRO	Peptide
31	S	23	LYS	Peptide
32	T	154	VAL	Peptide
34	V	89	ASP	Peptide
35	W	177	ALA	Peptide
2	a	77	LYS	Peptide
2	a	82	ILE	Peptide
2	a	83	PRO	Peptide
2	a	84	GLU	Peptide
4	b	368	ALA	Peptide
4	b	440	ASN	Peptide
7	d	84	ASP	Peptide
9	e	12	LYS	Peptide
9	e	121	ASN	Peptide
9	e	83	GLU	Peptide
16	h	118	ILE	Peptide
16	h	83	LYS	Peptide
17	i	27	SER	Peptide
17	i	32	ALA	Peptide
17	i	34	SER	Peptide
19	k	32	ASN	Peptide
44	n	1	MET	Peptide
44	n	123	PRO	Peptide
44	n	3	ILE	Peptide
44	n	375	ILE	Peptide
44	n	39	LYS	Peptide
44	n	4	LYS	Peptide
44	n	454	PRO	Peptide
44	n	5	LYS	Peptide
44	n	53	ASN	Peptide
44	n	54	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
44	n	55	GLY	Peptide
45	o	139	PHE	Peptide
45	o	140	VAL	Peptide
45	o	158	MET	Peptide
45	o	171	ALA	Peptide
23	p	51	ALA	Peptide
46	q	215	LYS	Peptide
46	q	225	LYS	Peptide
46	q	434	PRO	Peptide
30	r	2	PRO	Peptide
30	r	4	ASN	Peptide
49	s	12	SER	Peptide
49	s	14	LYS	Mainchain
49	s	15	LEU	Mainchain,Peptide
49	s	16	LYS	Mainchain,Peptide
49	s	17	GLU	Mainchain
49	s	20	LYS	Peptide
47	t	150	PRO	Peptide
47	t	152	ALA	Peptide
47	t	220	ASN	Peptide
47	t	223	GLU	Peptide
47	t	260	SER	Peptide
47	t	269	GLN	Peptide
47	t	280	PHE	Peptide
38	y	7	PHE	Peptide

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	
1	A	178/254 (70%)	178 (100%)	0	0	100	100
2	a	82/149 (55%)	78 (95%)	3 (4%)	1 (1%)	13	50
3	B	356/387 (92%)	344 (97%)	12 (3%)	0	100	100
4	b	447/647 (69%)	434 (97%)	13 (3%)	0	100	100
5	C	359/362 (99%)	347 (97%)	12 (3%)	0	100	100
6	c	95/105 (90%)	95 (100%)	0	0	100	100
7	d	105/113 (93%)	105 (100%)	0	0	100	100
8	E	152/176 (86%)	150 (99%)	2 (1%)	0	100	100
9	e	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
10	F	220/244 (90%)	210 (96%)	10 (4%)	0	100	100
11	f	104/107 (97%)	104 (100%)	0	0	100	100
12	G	228/256 (89%)	228 (100%)	0	0	100	100
13	g	110/121 (91%)	110 (100%)	0	0	100	100
14	I	94/166 (57%)	92 (98%)	2 (2%)	0	100	100
15	H	186/191 (97%)	182 (98%)	4 (2%)	0	100	100
16	h	116/120 (97%)	116 (100%)	0	0	100	100
17	i	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
18	j	79/88 (90%)	78 (99%)	1 (1%)	0	100	100
19	k	75/78 (96%)	75 (100%)	0	0	100	100
20	L	180/199 (90%)	172 (96%)	7 (4%)	1 (1%)	25	62
21	l	48/51 (94%)	48 (100%)	0	0	100	100
22	M	135/138 (98%)	134 (99%)	1 (1%)	0	100	100
23	p	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
24	N	183/204 (90%)	179 (98%)	4 (2%)	0	100	100
25	u	135/199 (68%)	133 (98%)	2 (2%)	0	100	100
26	O	195/199 (98%)	195 (100%)	0	0	100	100
27	P	172/184 (94%)	171 (99%)	1 (1%)	0	100	100
28	Q	132/186 (71%)	132 (100%)	0	0	100	100
29	R	152/189 (80%)	149 (98%)	3 (2%)	0	100	100
30	r	65/261 (25%)	57 (88%)	8 (12%)	0	100	100
31	S	168/172 (98%)	163 (97%)	5 (3%)	0	100	100
32	T	54/160 (34%)	50 (93%)	4 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	U	102/121 (84%)	101 (99%)	1 (1%)	0	100	100
34	V	134/137 (98%)	133 (99%)	1 (1%)	0	100	100
35	W	223/236 (94%)	221 (99%)	2 (1%)	0	100	100
36	X	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
37	Y	124/127 (98%)	124 (100%)	0	0	100	100
38	y	225/245 (92%)	223 (99%)	2 (1%)	0	100	100
39	Z	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
40	z	51/106 (48%)	51 (100%)	0	0	100	100
43	K	252/376 (67%)	245 (97%)	7 (3%)	0	100	100
44	n	365/605 (60%)	342 (94%)	23 (6%)	0	100	100
45	o	121/220 (55%)	117 (97%)	4 (3%)	0	100	100
46	q	137/455 (30%)	128 (93%)	9 (7%)	0	100	100
47	t	283/322 (88%)	264 (93%)	19 (7%)	0	100	100
49	s	34/520 (6%)	30 (88%)	4 (12%)	0	100	100
All	All	7234/9776 (74%)	7056 (98%)	176 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	78	LEU
20	L	63	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/196 (72%)	142 (100%)	0	100	100
2	a	68/119 (57%)	68 (100%)	0	100	100
3	B	301/323 (93%)	298 (99%)	3 (1%)	76	86
4	b	404/573 (70%)	401 (99%)	3 (1%)	84	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	288/289 (100%)	285 (99%)	3 (1%)	76	86
6	c	81/88 (92%)	81 (100%)	0	100	100
7	d	94/97 (97%)	94 (100%)	0	100	100
8	E	134/153 (88%)	134 (100%)	0	100	100
9	e	109/111 (98%)	109 (100%)	0	100	100
10	F	186/205 (91%)	185 (100%)	1 (0%)	88	94
11	f	90/91 (99%)	90 (100%)	0	100	100
12	G	189/208 (91%)	188 (100%)	1 (0%)	88	94
13	g	95/103 (92%)	94 (99%)	1 (1%)	73	85
14	I	83/141 (59%)	82 (99%)	1 (1%)	71	84
15	H	168/171 (98%)	164 (98%)	4 (2%)	49	71
16	h	104/105 (99%)	103 (99%)	1 (1%)	76	86
17	i	78/82 (95%)	78 (100%)	0	100	100
18	j	67/71 (94%)	66 (98%)	1 (2%)	65	81
19	k	68/69 (99%)	68 (100%)	0	100	100
20	L	142/159 (89%)	139 (98%)	3 (2%)	53	74
21	l	45/46 (98%)	45 (100%)	0	100	100
22	M	108/109 (99%)	108 (100%)	0	100	100
23	p	71/72 (99%)	70 (99%)	1 (1%)	67	81
24	N	163/176 (93%)	162 (99%)	1 (1%)	86	92
25	u	122/180 (68%)	120 (98%)	2 (2%)	62	79
26	O	160/162 (99%)	160 (100%)	0	100	100
27	P	141/146 (97%)	140 (99%)	1 (1%)	84	91
28	Q	110/151 (73%)	110 (100%)	0	100	100
29	R	127/154 (82%)	125 (98%)	2 (2%)	62	79
30	r	59/229 (26%)	59 (100%)	0	100	100
31	S	154/156 (99%)	154 (100%)	0	100	100
32	T	45/137 (33%)	43 (96%)	2 (4%)	28	57
33	U	91/107 (85%)	91 (100%)	0	100	100
34	V	104/105 (99%)	104 (100%)	0	100	100
35	W	201/213 (94%)	200 (100%)	1 (0%)	88	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	X	117/118 (99%)	117 (100%)	0	100	100
37	Y	109/110 (99%)	109 (100%)	0	100	100
38	y	193/211 (92%)	193 (100%)	0	100	100
39	Z	115/116 (99%)	115 (100%)	0	100	100
40	z	47/95 (50%)	47 (100%)	0	100	100
43	K	236/346 (68%)	231 (98%)	5 (2%)	53	74
44	n	334/548 (61%)	331 (99%)	3 (1%)	78	88
45	o	111/199 (56%)	110 (99%)	1 (1%)	78	88
46	q	131/420 (31%)	130 (99%)	1 (1%)	81	89
47	t	256/287 (89%)	253 (99%)	3 (1%)	71	84
49	s	32/445 (7%)	31 (97%)	1 (3%)	40	65
All	All	6273/8392 (75%)	6227 (99%)	46 (1%)	84	91

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	10	ARG
3	B	70	ARG
3	B	332	ARG
4	b	168	ARG
4	b	269	LYS
4	b	374	ARG
5	C	93	MET
5	C	120	TYR
5	C	197	ARG
10	F	34	LYS
12	G	227	ASP
13	g	106	LYS
14	I	74	LYS
15	H	21	LYS
15	H	23	ARG
15	H	106	LYS
15	H	168	ARG
16	h	81	ARG
18	j	75	LYS
20	L	13	HIS
20	L	100	ARG
20	L	172	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	p	17	ARG
24	N	153	ASP
25	u	113	ARG
25	u	135	ARG
27	P	120	ASN
29	R	8	LYS
29	R	71	ARG
32	T	102	ARG
32	T	110	LYS
35	W	174	LYS
43	K	172	LYS
43	K	179	LYS
43	K	266	LYS
43	K	388	ARG
43	K	405	LYS
44	n	13	ARG
44	n	251	LYS
44	n	254	LYS
45	o	213	LYS
46	q	257	LYS
47	t	22	LYS
47	t	130	ARG
47	t	198	LYS
49	s	15	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	140	ASN
3	B	182	GLN
4	b	26	GLN
4	b	415	ASN
5	C	328	ASN
12	G	95	ASN
14	I	73	HIS
15	H	100	ASN
15	H	102	ASN
15	H	116	ASN
15	H	156	GLN
15	H	163	GLN
16	h	59	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	j	76	ASN
20	L	120	GLN
21	l	50	ASN
24	N	70	ASN
25	u	37	HIS
25	u	110	ASN
26	O	31	GLN
27	P	96	GLN
27	P	145	HIS
31	S	62	ASN
31	S	65	ASN
34	V	81	GLN
36	X	85	GLN
43	K	358	ASN
45	o	154	ASN
45	o	163	GLN
47	t	53	ASN
47	t	88	ASN
47	t	265	ASN
47	t	274	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
41	1	2663/3396 (78%)	694 (26%)	43 (1%)
42	3	157/158 (99%)	36 (22%)	3 (1%)
48	6	63/232 (27%)	38 (60%)	0
All	All	2883/3786 (76%)	768 (26%)	46 (1%)

All (768) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
41	1	11	A
41	1	14	U
41	1	15	C
41	1	18	G
41	1	26	A
41	1	40	A
41	1	48	A
41	1	49	A
41	1	57	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	59	G
41	1	60	A
41	1	65	A
41	1	66	A
41	1	72	C
41	1	73	C
41	1	75	G
41	1	77	A
41	1	85	A
41	1	87	U
41	1	92	G
41	1	96	G
41	1	108	A
41	1	109	A
41	1	110	G
41	1	111	C
41	1	116	A
41	1	117	U
41	1	118	U
41	1	120	G
41	1	121	A
41	1	122	A
41	1	123	A
41	1	133	U
41	1	135	C
41	1	136	G
41	1	150	A
41	1	156	G
41	1	157	A
41	1	161	G
41	1	165	A
41	1	166	C
41	1	172	G
41	1	173	G
41	1	176	G
41	1	182	U
41	1	187	A
41	1	190	U
41	1	191	U
41	1	200	C
41	1	201	A
41	1	206	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	210	U
41	1	211	A
41	1	213	A
41	1	218	G
41	1	219	A
41	1	221	A
41	1	231	G
41	1	240	U
41	1	241	G
41	1	243	G
41	1	245	U
41	1	249	U
41	1	251	G
41	1	252	U
41	1	266	A
41	1	267	G
41	1	268	A
41	1	269	G
41	1	270	U
41	1	281	G
41	1	282	G
41	1	283	G
41	1	284	A
41	1	286	U
41	1	295	A
41	1	298	U
41	1	305	U
41	1	323	A
41	1	329	U
41	1	337	G
41	1	338	A
41	1	339	C
41	1	343	U
41	1	346	C
41	1	350	C
41	1	351	A
41	1	352	A
41	1	353	G
41	1	354	U
41	1	368	G
41	1	370	U
41	1	372	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	375	A
41	1	376	G
41	1	387	A
41	1	390	G
41	1	397	A
41	1	401	U
41	1	402	A
41	1	403	C
41	1	420	G
41	1	421	G
41	1	422	A
41	1	440	A
41	1	495	G
41	1	498	A
41	1	503	C
41	1	515	C
41	1	518	G
41	1	519	A
41	1	520	U
41	1	521	A
41	1	523	A
41	1	535	G
41	1	536	U
41	1	543	C
41	1	544	C
41	1	545	U
41	1	547	G
41	1	548	G
41	1	552	G
41	1	555	U
41	1	557	A
41	1	559	A
41	1	578	A
41	1	579	G
41	1	592	A
41	1	597	G
41	1	600	G
41	1	604	G
41	1	607	A
41	1	609	G
41	1	611	A
41	1	612	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	620	U
41	1	621	A
41	1	636	C
41	1	637	C
41	1	638	C
41	1	640	U
41	1	649	A
41	1	658	G
41	1	661	G
41	1	676	G
41	1	677	A
41	1	678	G
41	1	681	U
41	1	683	U
41	1	687	U
41	1	691	A
41	1	699	A
41	1	705	A
41	1	709	A
41	1	712	G
41	1	716	A
41	1	719	U
41	1	720	A
41	1	742	G
41	1	750	G
41	1	764	U
41	1	767	U
41	1	776	U
41	1	777	U
41	1	781	G
41	1	785	G
41	1	786	A
41	1	787	G
41	1	801	A
41	1	806	A
41	1	817	A
41	1	818	C
41	1	823	C
41	1	830	A
41	1	832	G
41	1	849	C
41	1	851	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	861	C
41	1	865	U
41	1	868	C
41	1	874	U
41	1	875	G
41	1	879	U
41	1	880	G
41	1	889	U
41	1	894	G
41	1	895	A
41	1	896	A
41	1	907	G
41	1	908	G
41	1	909	G
41	1	914	A
41	1	916	G
41	1	917	A
41	1	921	A
41	1	924	G
41	1	926	A
41	1	932	U
41	1	937	G
41	1	944	C
41	1	953	G
41	1	954	U
41	1	959	C
41	1	960	U
41	1	962	A
41	1	963	G
41	1	964	G
41	1	968	G
41	1	974	G
41	1	977	C
41	1	979	U
41	1	980	A
41	1	981	U
41	1	982	C
41	1	991	G
41	1	1063	G
41	1	1064	A
41	1	1065	A
41	1	1068	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	1093	A
41	1	1094	U
41	1	1095	U
41	1	1096	U
41	1	1097	G
41	1	1098	A
41	1	1103	A
41	1	1104	G
41	1	1117	G
41	1	1131	G
41	1	1132	C
41	1	1135	A
41	1	1141	C
41	1	1143	A
41	1	1151	U
41	1	1153	A
41	1	1159	A
41	1	1177	G
41	1	1178	G
41	1	1180	A
41	1	1181	U
41	1	1182	A
41	1	1186	G
41	1	1190	A
41	1	1191	U
41	1	1192	C
41	1	1193	A
41	1	1197	A
41	1	1198	C
41	1	1199	C
41	1	1200	A
41	1	1201	C
41	1	1202	A
41	1	1203	A
41	1	1205	A
41	1	1209	G
41	1	1213	G
41	1	1217	A
41	1	1221	A
41	1	1222	G
41	1	1232	C
41	1	1234	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	1235	U
41	1	1236	G
41	1	1238	C
41	1	1239	C
41	1	1241	U
41	1	1244	A
41	1	1245	A
41	1	1246	G
41	1	1247	U
41	1	1248	C
41	1	1252	A
41	1	1253	U
41	1	1254	C
41	1	1255	C
41	1	1258	U
41	1	1259	A
41	1	1262	G
41	1	1263	A
41	1	1264	G
41	1	1265	U
41	1	1269	U
41	1	1271	A
41	1	1272	C
41	1	1278	A
41	1	1279	C
41	1	1283	C
41	1	1284	C
41	1	1285	G
41	1	1286	A
41	1	1287	A
41	1	1303	A
41	1	1305	U
41	1	1307	G
41	1	1308	A
41	1	1309	U
41	1	1313	G
41	1	1318	A
41	1	1325	U
41	1	1330	A
41	1	1348	U
41	1	1349	G
41	1	1351	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	1352	A
41	1	1353	U
41	1	1355	A
41	1	1356	U
41	1	1357	G
41	1	1365	G
41	1	1375	G
41	1	1386	A
41	1	1390	A
41	1	1399	A
41	1	1400	G
41	1	1419	A
41	1	1428	A
41	1	1429	G
41	1	1434	G
41	1	1435	A
41	1	1436	U
41	1	1437	C
41	1	1446	A
41	1	1447	G
41	1	1451	C
41	1	1452	A
41	1	1455	U
41	1	1465	A
41	1	1470	U
41	1	1475	A
41	1	1477	A
41	1	1482	A
41	1	1483	G
41	1	1484	U
41	1	1487	G
41	1	1494	U
41	1	1503	A
41	1	1504	A
41	1	1507	G
41	1	1508	C
41	1	1511	U
41	1	1519	G
41	1	1523	U
41	1	1524	A
41	1	1527	C
41	1	1528	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	1530	U
41	1	1531	C
41	1	1541	G
41	1	1542	G
41	1	1544	G
41	1	1546	A
41	1	1556	C
41	1	1557	A
41	1	1560	G
41	1	1562	C
41	1	1563	C
41	1	1564	U
41	1	1565	G
41	1	1566	A
41	1	1576	G
41	1	1580	A
41	1	1582	C
41	1	1583	A
41	1	1587	A
41	1	1588	A
41	1	1589	A
41	1	1596	C
41	1	1605	A
41	1	1606	U
41	1	1607	U
41	1	1618	G
41	1	1619	A
41	1	1620	U
41	1	1629	U
41	1	1631	C
41	1	1632	A
41	1	1639	C
41	1	1642	A
41	1	1643	A
41	1	1644	C
41	1	1654	A
41	1	1656	A
41	1	1658	G
41	1	1683	A
41	1	1687	U
41	1	1717	U
41	1	1718	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	1722	U
41	1	1724	U
41	1	1725	C
41	1	1736	G
41	1	1741	A
41	1	1749	A
41	1	1750	A
41	1	1751	G
41	1	1759	C
41	1	1760	A
41	1	1762	C
41	1	1763	U
41	1	1765	U
41	1	1770	G
41	1	1773	C
41	1	1775	G
41	1	1780	G
41	1	1788	C
41	1	1797	A
41	1	1808	G
41	1	1814	A
41	1	1815	U
41	1	1816	A
41	1	1820	U
41	1	1821	U
41	1	1840	U
41	1	1841	A
41	1	1842	A
41	1	1846	C
41	1	1849	C
41	1	1850	A
41	1	1867	A
41	1	1878	G
41	1	1880	U
41	1	1887	A
41	1	1890	U
41	1	1893	A
41	1	1906	G
41	1	1908	A
41	1	1926	C
41	1	1930	A
41	1	1931	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	1935	G
41	1	1951	C
41	1	1953	G
41	1	2101	C
41	1	2102	U
41	1	2111	G
41	1	2112	U
41	1	2115	G
41	1	2116	G
41	1	2119	A
41	1	2121	G
41	1	2122	G
41	1	2131	A
41	1	2139	A
41	1	2143	A
41	1	2158	A
41	1	2160	G
41	1	2169	G
41	1	2176	U
41	1	2179	C
41	1	2188	A
41	1	2314	U
41	1	2315	G
41	1	2317	A
41	1	2334	U
41	1	2335	G
41	1	2336	U
41	1	2361	A
41	1	2363	A
41	1	2364	G
41	1	2365	C
41	1	2378	C
41	1	2381	G
41	1	2388	U
41	1	2393	G
41	1	2394	G
41	1	2397	A
41	1	2434	U
41	1	2435	G
41	1	2438	A
41	1	2439	A
41	1	2440	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	2442	G
41	1	2502	A
41	1	2506	U
41	1	2507	C
41	1	2510	U
41	1	2511	A
41	1	2514	U
41	1	2515	A
41	1	2522	G
41	1	2523	A
41	1	2524	A
41	1	2525	G
41	1	2526	C
41	1	2531	C
41	1	2532	U
41	1	2533	G
41	1	2535	A
41	1	2536	A
41	1	2537	U
41	1	2538	U
41	1	2539	C
41	1	2540	A
41	1	2541	U
41	1	2542	U
41	1	2543	U
41	1	2544	U
41	1	2549	G
41	1	2552	C
41	1	2554	A
41	1	2561	A
41	1	2569	A
41	1	2570	U
41	1	2571	U
41	1	2572	C
41	1	2573	G
41	1	2578	U
41	1	2580	A
41	1	2585	G
41	1	2586	G
41	1	2593	A
41	1	2594	C
41	1	2595	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	2606	G
41	1	2772	C
41	1	2773	C
41	1	2777	G
41	1	2778	G
41	1	2780	A
41	1	2820	A
41	1	2821	C
41	1	2822	U
41	1	2823	G
41	1	2825	C
41	1	2826	U
41	1	2834	G
41	1	2842	U
41	1	2847	A
41	1	2856	G
41	1	2857	C
41	1	2858	U
41	1	2859	U
41	1	2861	U
41	1	2863	G
41	1	2864	A
41	1	2865	U
41	1	2867	C
41	1	2868	U
41	1	2869	U
41	1	2870	C
41	1	2872	A
41	1	2873	U
41	1	2875	U
41	1	2876	C
41	1	2877	G
41	1	2878	G
41	1	2879	C
41	1	2887	A
41	1	2888	U
41	1	2889	C
41	1	2891	U
41	1	2892	A
41	1	2894	C
41	1	2898	G
41	1	2901	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	2906	C
41	1	2910	A
41	1	2914	G
41	1	2916	U
41	1	2918	G
41	1	2920	U
41	1	2923	U
41	1	2924	U
41	1	2928	C
41	1	2935	U
41	1	2936	A
41	1	2938	G
41	1	2983	C
41	1	2996	U
41	1	2997	G
41	1	3006	A
41	1	3012	A
41	1	3019	U
41	1	3021	A
41	1	3022	G
41	1	3024	A
41	1	3027	A
41	1	3028	G
41	1	3030	G
41	1	3033	A
41	1	3034	C
41	1	3039	C
41	1	3042	U
41	1	3049	A
41	1	3052	G
41	1	3059	G
41	1	3077	A
41	1	3078	U
41	1	3079	U
41	1	3080	G
41	1	3086	A
41	1	3092	C
41	1	3093	C
41	1	3094	A
41	1	3099	C
41	1	3101	G
41	1	3104	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	3109	G
41	1	3115	C
41	1	3117	C
41	1	3118	C
41	1	3119	U
41	1	3120	C
41	1	3122	A
41	1	3128	G
41	1	3129	A
41	1	3130	A
41	1	3142	A
41	1	3143	C
41	1	3153	U
41	1	3154	C
41	1	3155	U
41	1	3156	U
41	1	3157	U
41	1	3160	U
41	1	3163	A
41	1	3165	A
41	1	3168	A
41	1	3169	U
41	1	3170	A
41	1	3171	U
41	1	3172	A
41	1	3173	G
41	1	3174	A
41	1	3175	U
41	1	3176	G
41	1	3179	U
41	1	3180	A
41	1	3181	C
41	1	3184	A
41	1	3187	A
41	1	3195	U
41	1	3196	U
41	1	3198	U
41	1	3199	G
41	1	3206	C
41	1	3207	U
41	1	3208	G
41	1	3217	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	3218	A
41	1	3219	G
41	1	3227	A
41	1	3229	G
41	1	3239	G
41	1	3243	A
41	1	3245	A
41	1	3246	G
41	1	3247	G
41	1	3249	C
41	1	3253	G
41	1	3256	G
41	1	3259	U
41	1	3263	G
41	1	3269	U
41	1	3270	U
41	1	3272	C
41	1	3273	A
41	1	3276	G
41	1	3279	A
41	1	3280	U
41	1	3281	U
41	1	3287	U
41	1	3288	G
41	1	3289	G
41	1	3293	U
41	1	3294	A
41	1	3295	A
41	1	3302	U
41	1	3304	U
41	1	3307	A
41	1	3308	C
41	1	3313	U
41	1	3316	A
41	1	3318	G
41	1	3319	U
41	1	3320	A
41	1	3330	A
41	1	3341	U
41	1	3342	A
41	1	3350	C
41	1	3351	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	3352	U
41	1	3353	G
41	1	3355	U
41	1	3356	G
41	1	3359	A
41	1	3360	C
41	1	3363	U
41	1	3368	U
41	1	3369	G
41	1	3375	A
41	1	3378	C
41	1	3382	U
41	1	3390	G
42	3	23	U
42	3	24	G
42	3	34	U
42	3	35	C
42	3	38	U
42	3	39	G
42	3	49	G
42	3	59	A
42	3	62	C
42	3	63	G
42	3	72	A
42	3	80	A
42	3	81	U
42	3	82	U
42	3	83	C
42	3	84	C
42	3	85	G
42	3	86	U
42	3	90	U
42	3	91	C
42	3	95	G
42	3	99	C
42	3	102	U
42	3	104	A
42	3	105	A
42	3	106	C
42	3	111	A
42	3	113	U
42	3	116	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	3	125	U
42	3	126	A
42	3	127	U
42	3	138	A
42	3	151	C
42	3	157	U
42	3	158	U
48	6	4	U
48	6	5	C
48	6	6	U
48	6	7	C
48	6	8	A
48	6	9	A
48	6	14	U
48	6	15	C
48	6	16	U
48	6	17	G
48	6	23	U
48	6	24	A
48	6	25	G
48	6	26	U
48	6	27	G
48	6	29	G
48	6	33	U
48	6	34	A
48	6	36	U
48	6	39	U
48	6	40	U
48	6	41	G
48	6	42	G
48	6	43	A
48	6	47	A
48	6	49	C
48	6	52	G
48	6	53	A
48	6	54	A
48	6	56	U
48	6	57	U
48	6	58	G
48	6	59	C
48	6	65	U
48	6	66	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	6	230	A
48	6	231	A
48	6	232	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	1	13	A
41	1	65	A
41	1	239	G
41	1	282	G
41	1	338	A
41	1	439	C
41	1	547	G
41	1	637	C
41	1	763	G
41	1	916	G
41	1	979	U
41	1	1064	A
41	1	1097	G
41	1	1103	A
41	1	1199	C
41	1	1200	A
41	1	1307	G
41	1	1352	A
41	1	1355	A
41	1	1563	C
41	1	2101	C
41	1	2111	G
41	1	2362	C
41	1	2392	C
41	1	2501	U
41	1	2513	U
41	1	2525	G
41	1	2537	U
41	1	2541	U
41	1	2593	A
41	1	2857	C
41	1	2866	U
41	1	2886	U
41	1	2900	A
41	1	2996	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1	3078	U
41	1	3153	U
41	1	3218	A
41	1	3228	C
41	1	3269	U
41	1	3294	A
41	1	3350	C
41	1	3358	U
42	3	39	G
42	3	82	U
42	3	85	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	X	1
41	1	1
49	s	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	23:ALA	C	24:LEU	N	5.12
1	1	1199:C	O3'	1200:A	P	1.89
1	s	13:THR	C	14:LYS	N	1.75

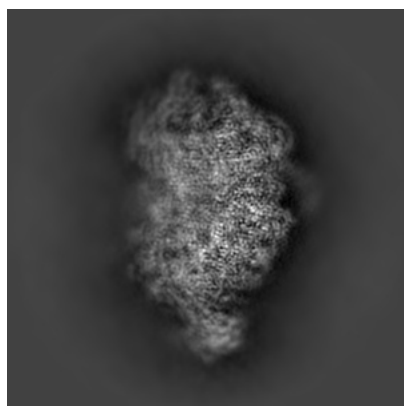
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10842. These allow visual inspection of the internal detail of the map and identification of artifacts.

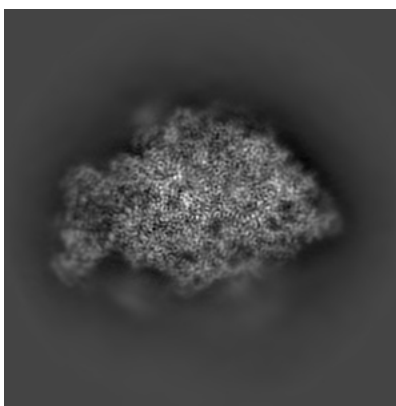
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

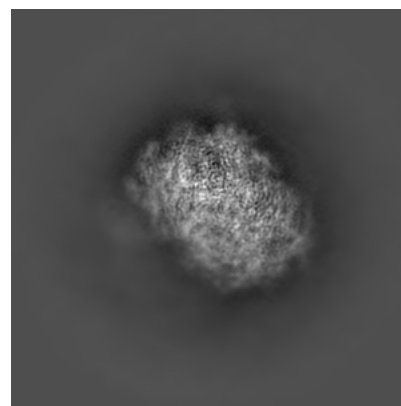
6.1.1 Primary map



X

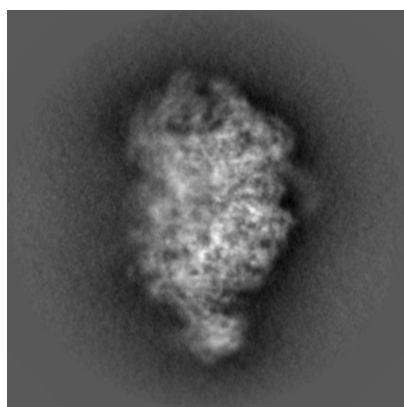


Y

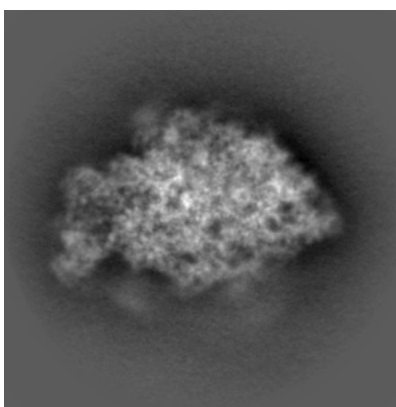


Z

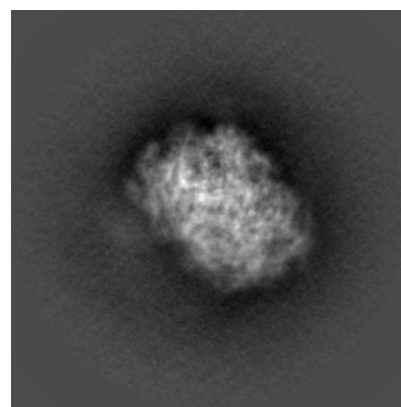
6.1.2 Raw map



X



Y

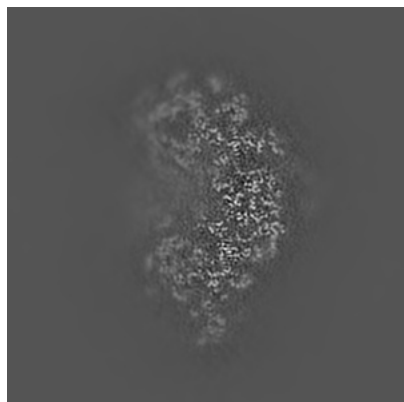


Z

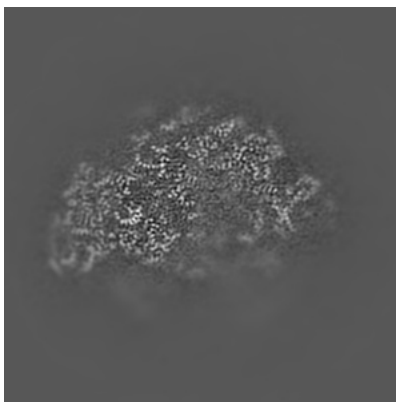
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

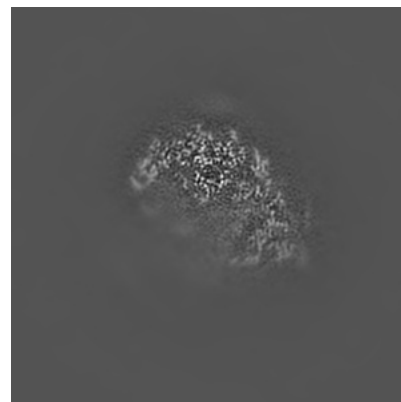
6.2.1 Primary map



X Index: 192

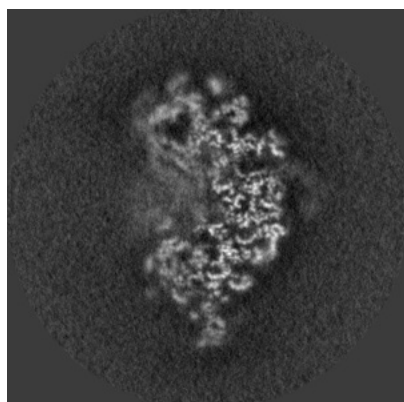


Y Index: 192

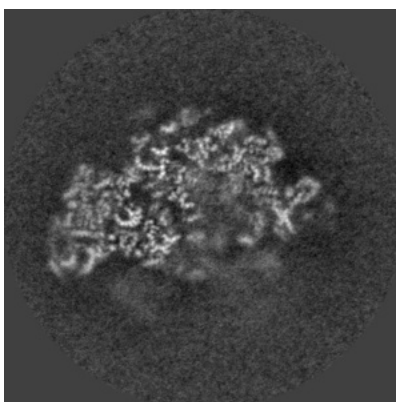


Z Index: 192

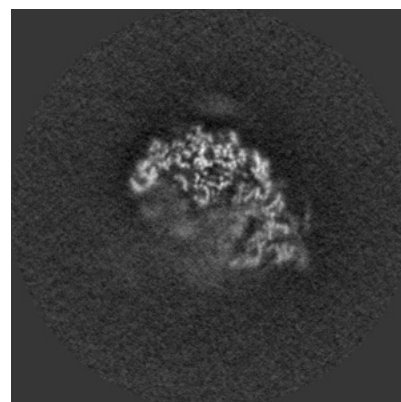
6.2.2 Raw map



X Index: 192



Y Index: 192

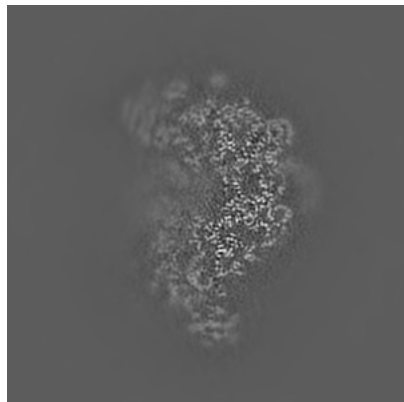


Z Index: 192

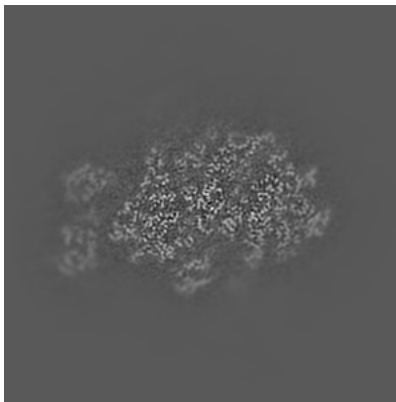
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

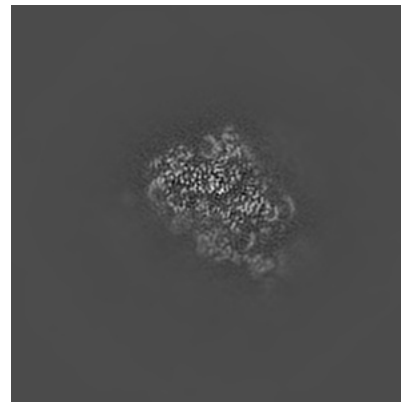
6.3.1 Primary map



X Index: 201

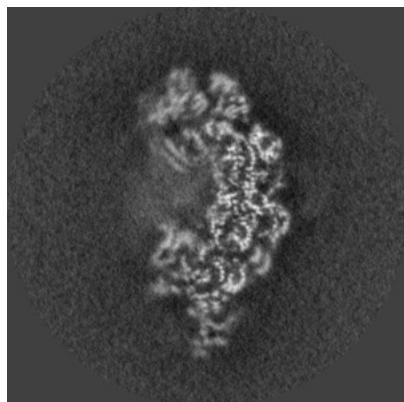


Y Index: 216

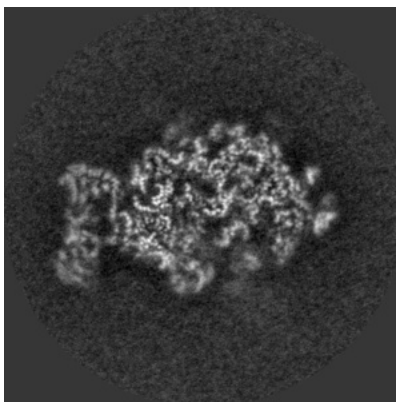


Z Index: 152

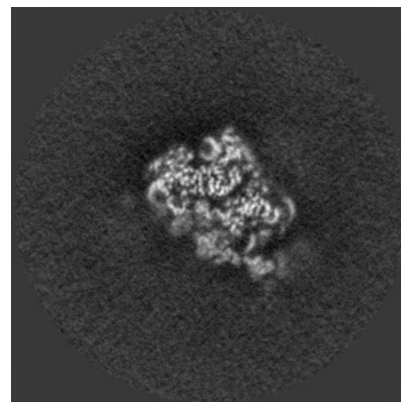
6.3.2 Raw map



X Index: 185



Y Index: 209



Z Index: 152

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

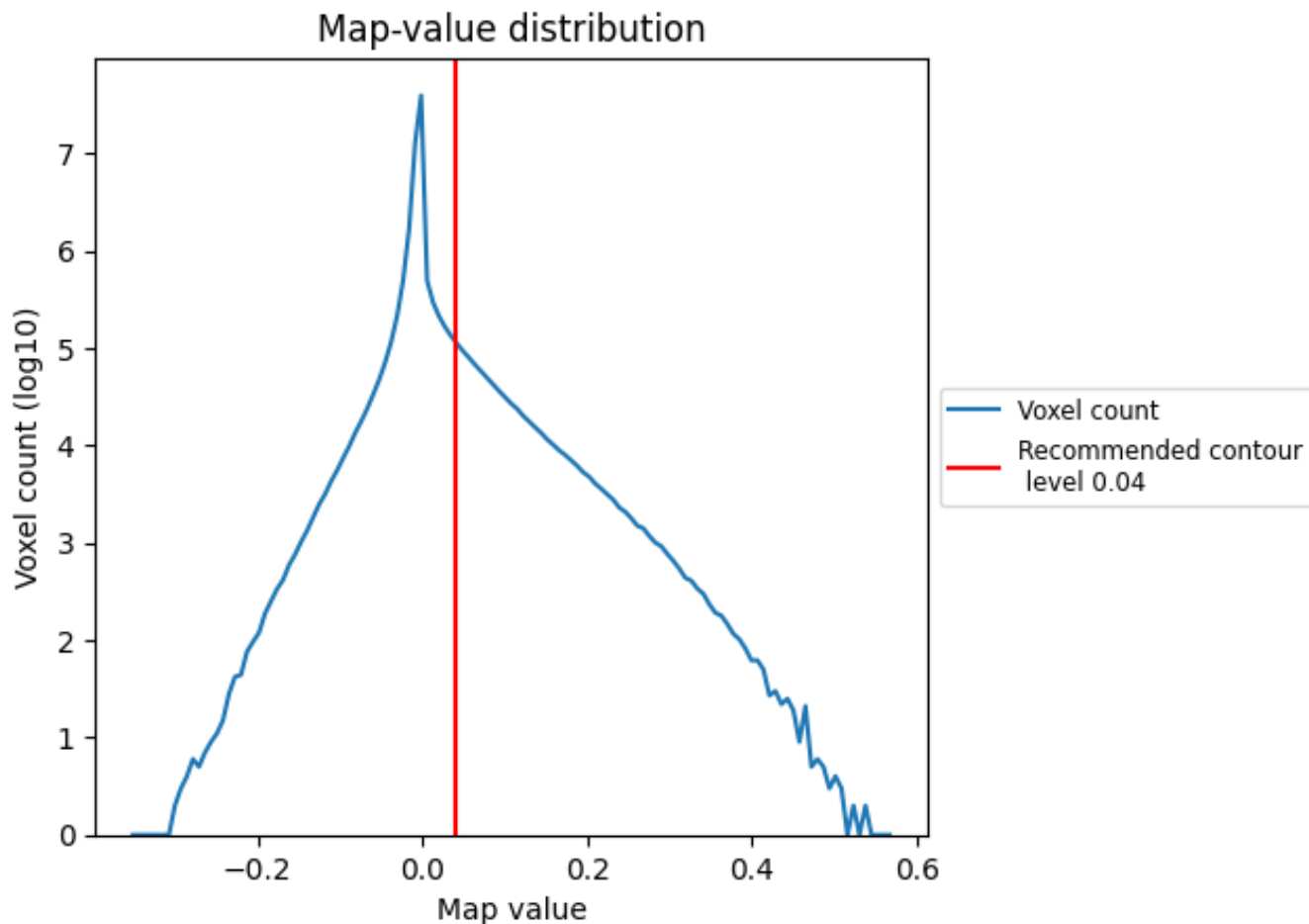
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

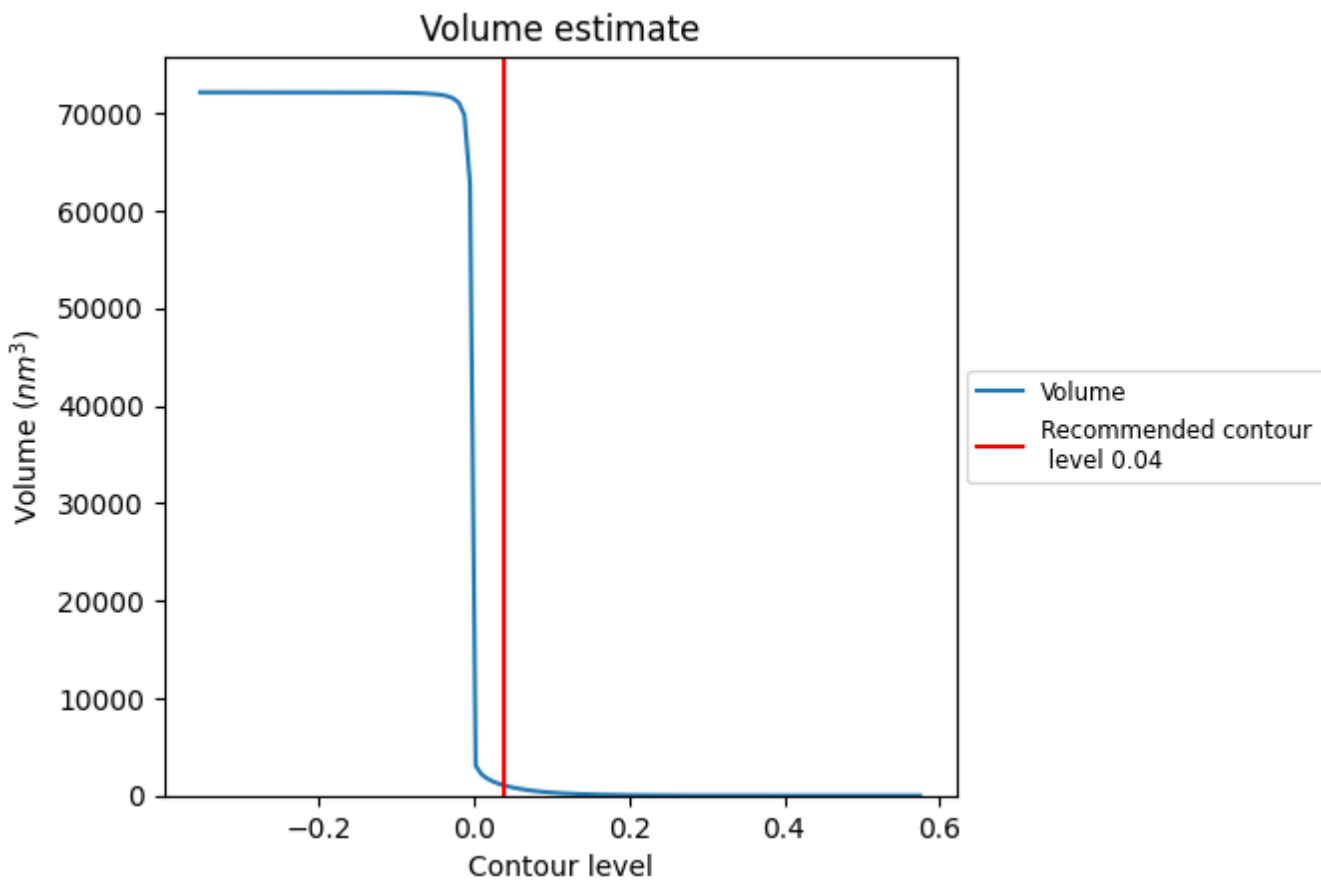
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

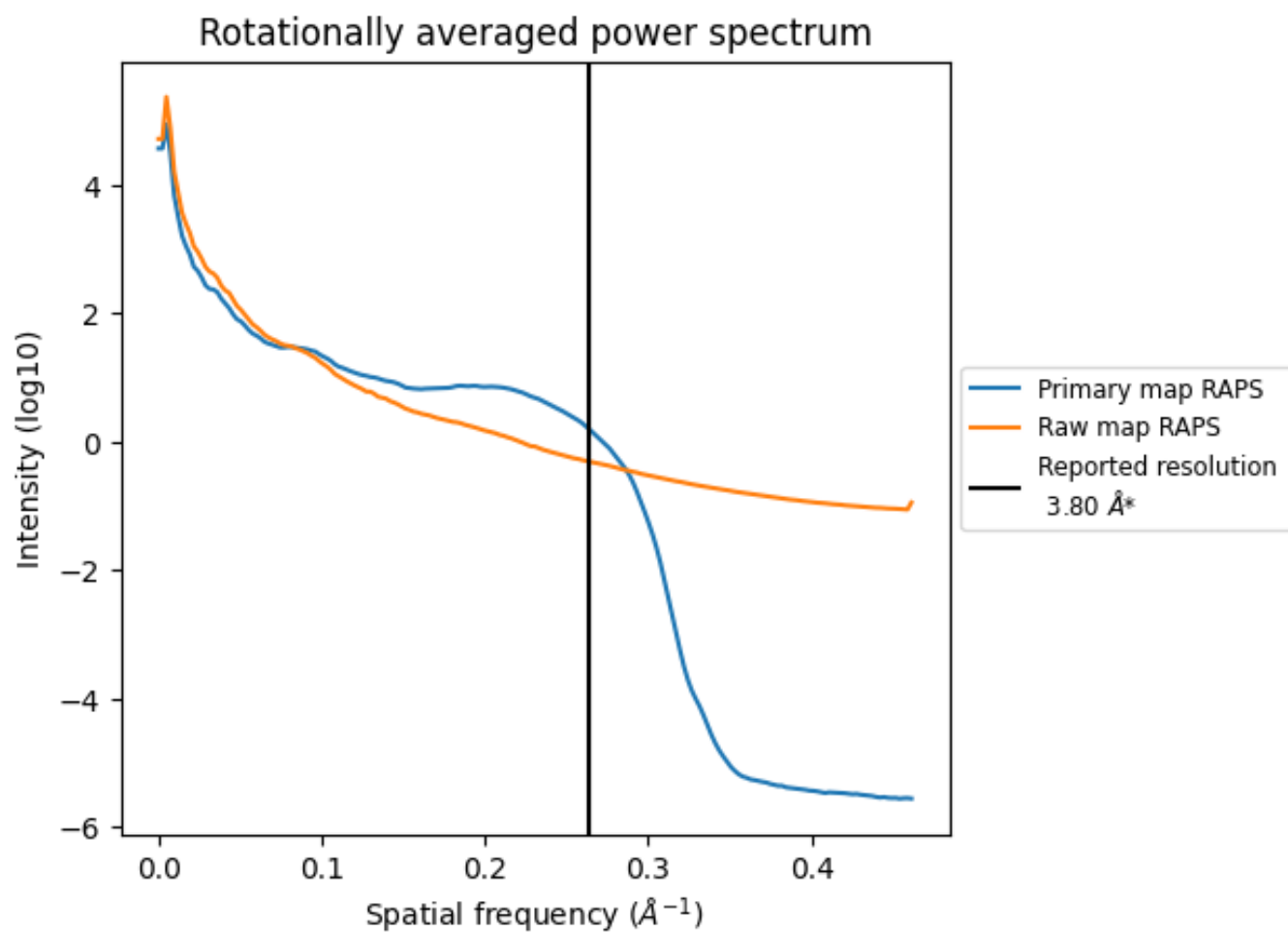
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1033 nm³; this corresponds to an approximate mass of 934 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

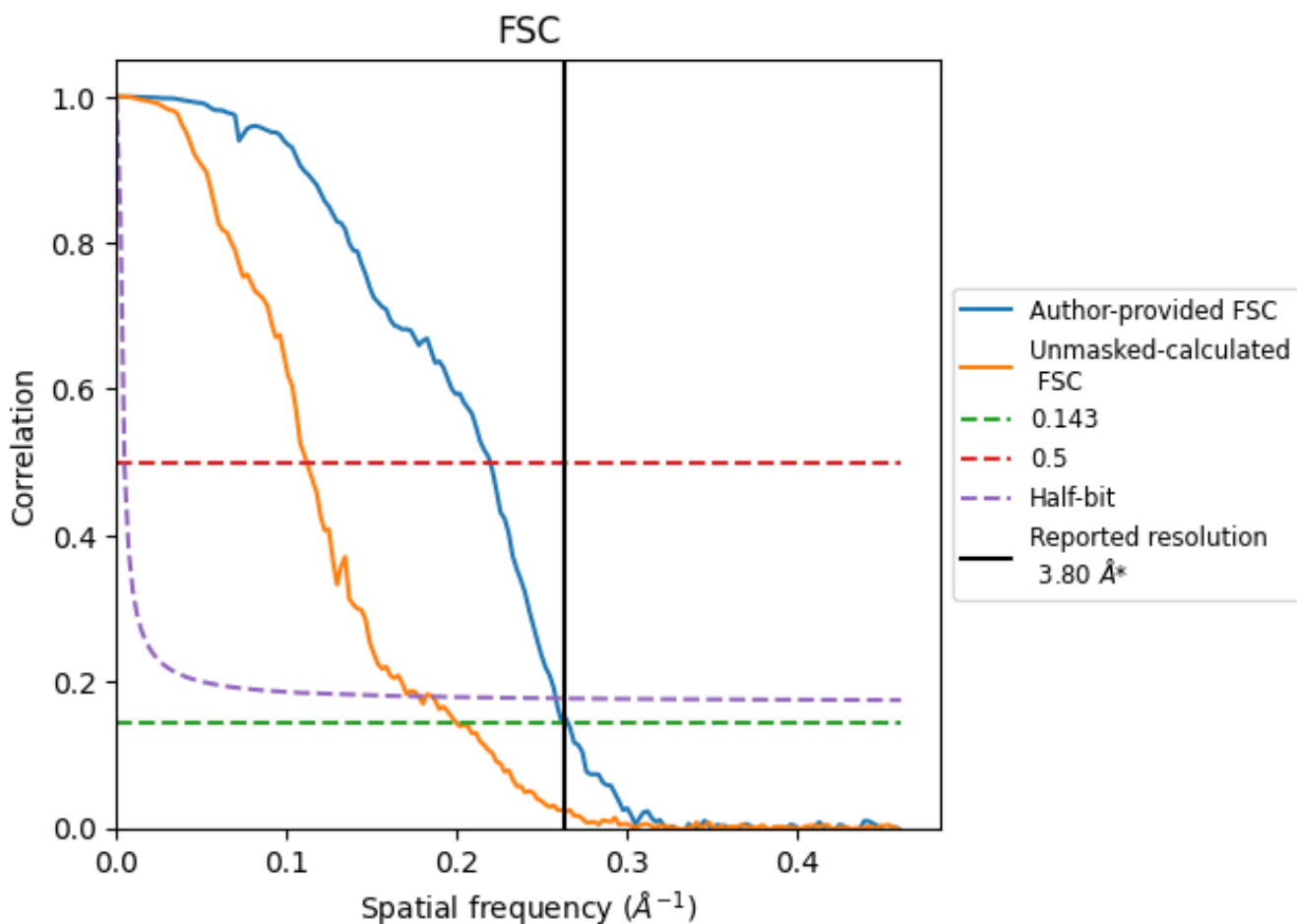


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

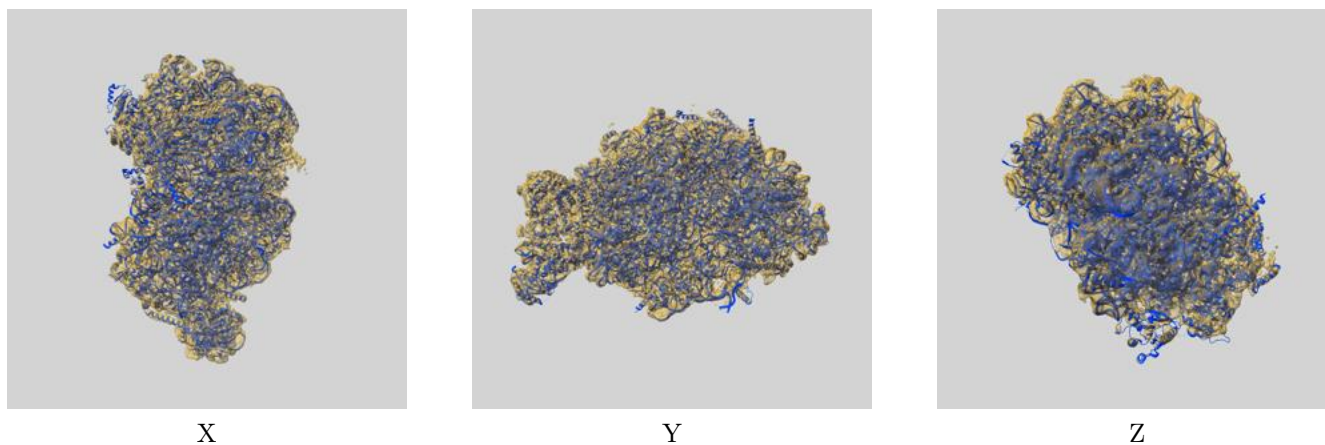
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.55	3.87
Unmasked-calculated*	5.00	8.94	5.62

*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 5.00 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

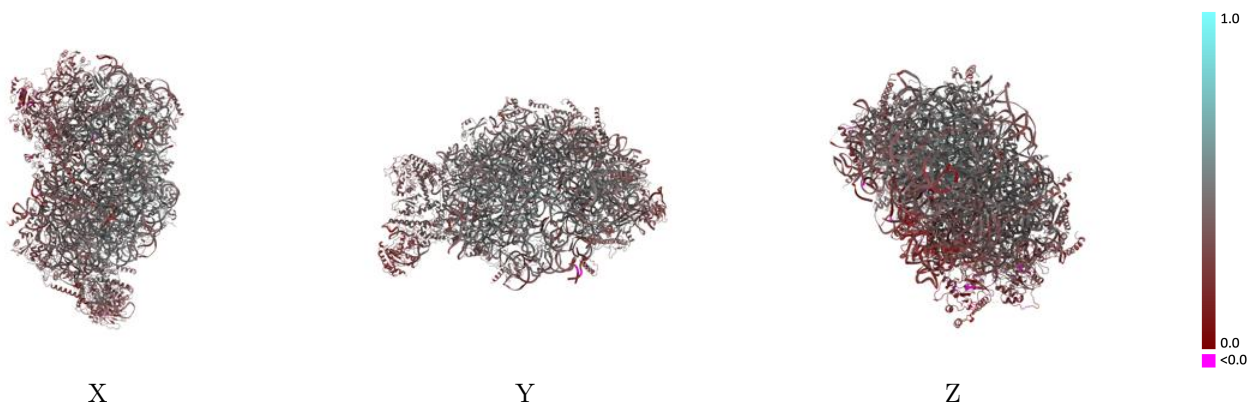
This section contains information regarding the fit between EMDB map EMD-10842 and PDB model 6YLY. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



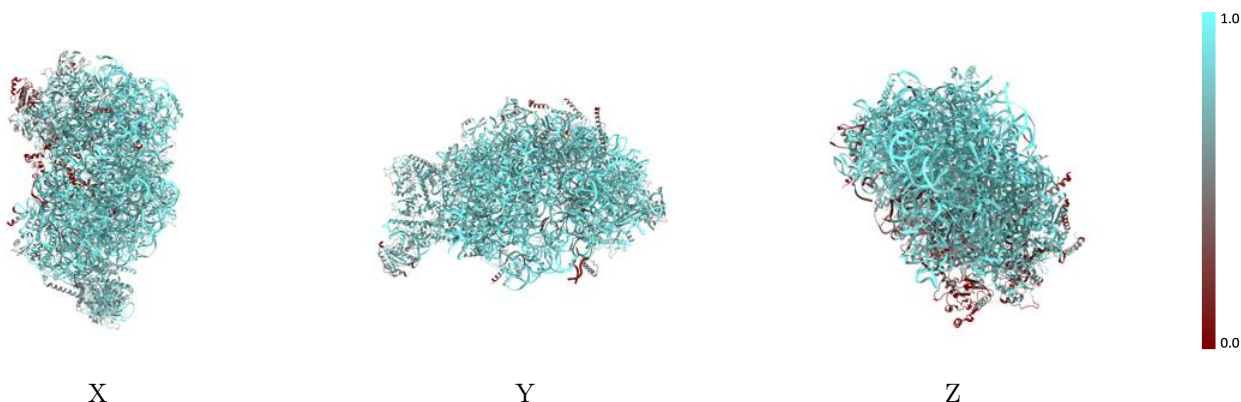
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



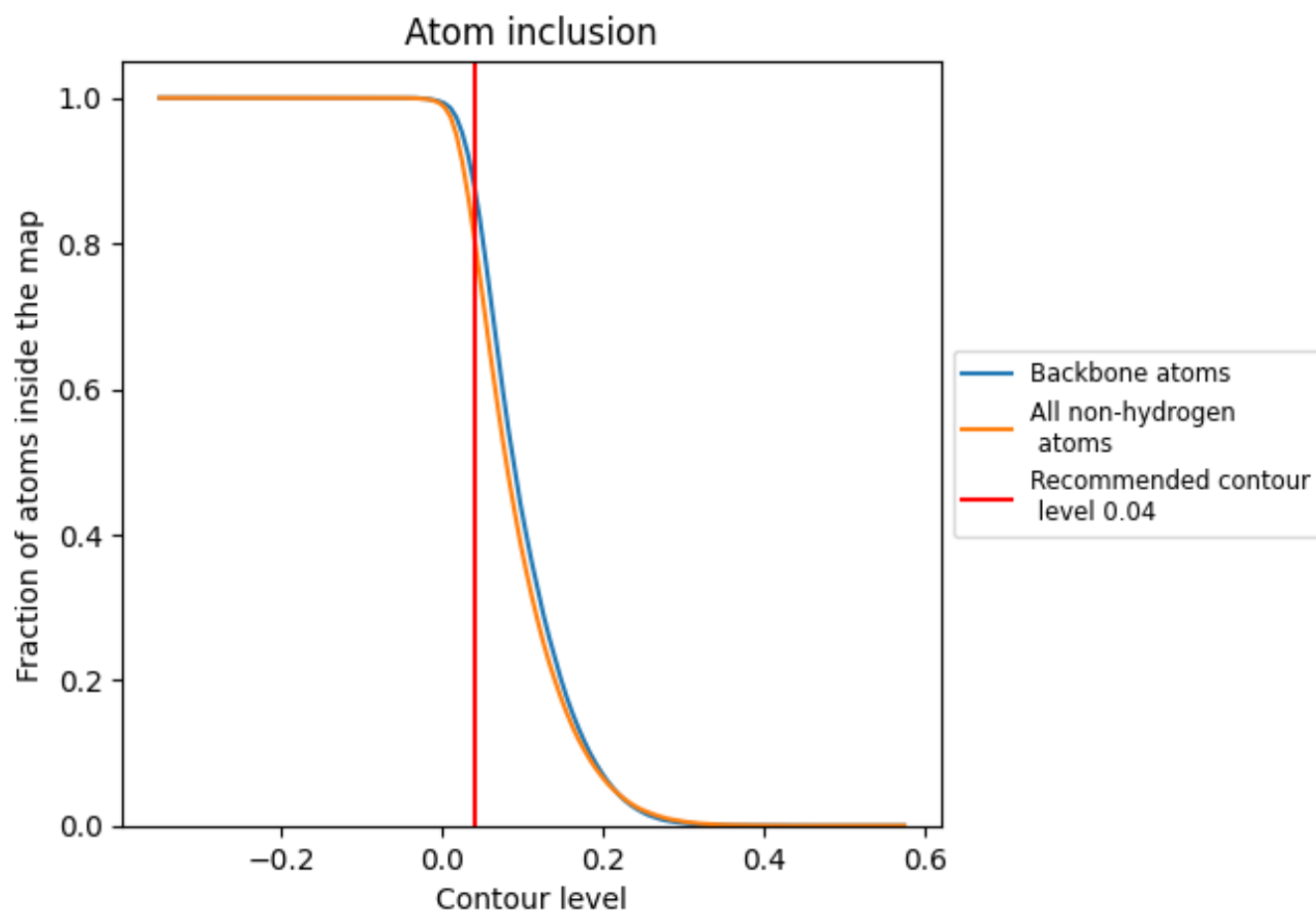
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8062	 0.3920
1	 0.8709	 0.3950
3	 0.9427	 0.4660
6	 0.8745	 0.3270
A	 0.7186	 0.3890
B	 0.8169	 0.4290
C	 0.8523	 0.4680
E	 0.8302	 0.4200
F	 0.8542	 0.4290
G	 0.7945	 0.4100
H	 0.7672	 0.3790
I	 0.1275	 0.3230
K	 0.6075	 0.2480
L	 0.8093	 0.4350
M	 0.8411	 0.4230
N	 0.8551	 0.4960
O	 0.8686	 0.4670
P	 0.8426	 0.4560
Q	 0.8560	 0.4510
R	 0.7582	 0.3970
S	 0.8308	 0.4330
T	 0.5629	 0.3010
U	 0.7217	 0.3520
V	 0.7140	 0.4080
W	 0.5474	 0.2400
X	 0.8571	 0.4680
Y	 0.8685	 0.4720
Z	 0.7740	 0.3700
a	 0.8406	 0.4200
b	 0.3954	 0.2420
c	 0.6566	 0.3000
d	 0.7993	 0.4370
e	 0.8451	 0.5010
f	 0.8879	 0.5020
g	 0.7688	 0.4370



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	 0.8689	 0.4650
i	 0.7955	 0.3940
j	 0.8551	 0.5000
k	 0.7295	 0.3980
l	 0.7181	 0.4520
n	 0.7579	 0.3690
o	 0.7002	 0.3010
p	 0.6045	 0.3380
q	 0.5957	 0.3320
r	 0.6810	 0.3290
s	 0.4118	 0.2620
t	 0.7131	 0.3390
u	 0.6439	 0.3560
y	 0.6684	 0.2980
z	 0.4810	 0.3480