



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 07:52 AM EST

PDB ID : 4V7F
EMDB ID : EMD-2528
Title : Arx1 pre-60S particle.
Authors : Leidig, C.; Thoms, M.; Holdermann, I.; Bradatsch, B.; Berninghausen, O.;
Bange, G.; Sinning, I.; Hurt, E.; Beckmann, R.
Deposited on : 2013-12-10
Resolution : 8.70 Å(reported)
Based on initial model : 3U5D

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:

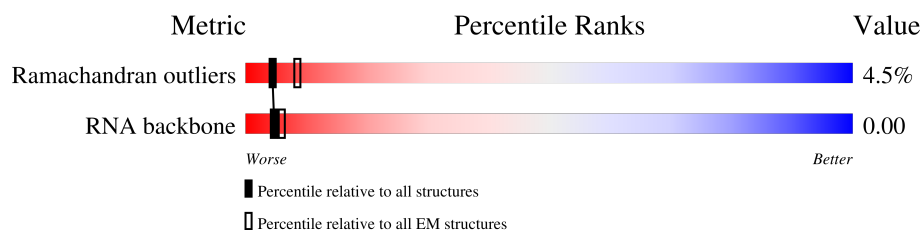
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 8.70 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
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	1	3396	
2	2	158	
3	3	121	
4	A	217	
5	B	254	
6	C	387	
7	D	362	
8	E	174	
9	F	191	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	G	176	
11	H	256	
12	I	165	
13	J	199	
14	K	199	
15	L	137	
16	M	138	
17	N	149	
18	O	204	
19	P	297	
20	Q	186	
21	R	189	
22	S	172	
23	T	160	
24	U	184	
25	V	121	
26	W	142	
27	X	127	
28	Y	136	
29	Z	120	
30	a	244	
31	b	105	
32	c	113	
33	d	130	
34	e	107	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
35	f	121	
36	g	100	
37	h	88	
38	i	78	
39	j	51	
40	k	92	
41	l	593	
42	m	245	
43	n	236	
44	o	647	
45	p	199	
46	q	515	
47	r	322	
47	s	322	

2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 47221 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	3394	Total	C	O	P	0	0
			20363	10182	6788	3393		

- Molecule 2 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	158	Total	C	O	P	0	0
			948	474	316	158		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	121	Total	C	O	P	0	0
			725	363	242	120		

- Molecule 4 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms			AltConf	Trace
4	A	217	Total	C	N	0	0
			651	434	217		

- Molecule 5 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms			AltConf	Trace
5	B	252	Total	C	N	0	0
			756	504	252		

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms			AltConf	Trace
6	C	386	Total	C	N	0	0
			1158	772	386		

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms			AltConf	Trace
7	D	361	Total	C	N	0	0
			1083	722	361		

- Molecule 8 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms			AltConf	Trace
8	E	169	Total	C	N	0	0
			507	338	169		

- Molecule 9 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms			AltConf	Trace
9	F	191	Total	C	N	0	0
			573	382	191		

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms			AltConf	Trace
10	G	175	Total	C	N	0	0
			525	350	175		

- Molecule 11 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms			AltConf	Trace
11	H	233	Total	C	N	0	0
			699	466	233		

- Molecule 12 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms			AltConf	Trace
12	I	127	Total	C	N	0	0
			381	254	127		

- Molecule 13 is a protein called 60S ribosomal protein L16.

Mol	Chain	Residues	Atoms			AltConf	Trace
13	J	197	Total	C	N	0	0
			591	394	197		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms			AltConf	Trace
14	K	193	Total	C	N	0	0
			579	386	193		

- Molecule 15 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms			AltConf	Trace
15	L	136	Total	C	N	0	0
			408	272	136		

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms			AltConf	Trace
16	M	136	Total	C	N	0	0
			408	272	136		

- Molecule 17 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms			AltConf	Trace
17	N	148	Total	C	N	0	0
			444	296	148		

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms			AltConf	Trace
18	O	203	Total	C	N	0	0
			609	406	203		

- Molecule 19 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms			AltConf	Trace
19	P	269	Total	C	N	0	0
			807	538	269		

- Molecule 20 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms			AltConf	Trace
20	Q	185	Total	C	N	0	0
			555	370	185		

- Molecule 21 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms			AltConf	Trace
21	R	188	Total	C	N	0	0
			564	376	188		

- Molecule 22 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms			AltConf	Trace
22	S	172	Total	C	N	0	0
			516	344	172		

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms			AltConf	Trace
23	T	159	Total	C	N	0	0
			477	318	159		

- Molecule 24 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms			AltConf	Trace
24	U	183	Total	C	N	0	0
			549	366	183		

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms			AltConf	Trace
25	V	100	Total	C	N	0	0
			300	200	100		

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms			AltConf	Trace
26	W	121	Total	C	N	0	0
			363	242	121		

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms			AltConf	Trace
27	X	126	Total	C	N	0	0
			378	252	126		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms			AltConf	Trace
28	Y	135	Total	C	N	0	0
			405	270	135		

- Molecule 29 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms			AltConf	Trace
29	Z	119	Total	C	N	0	0
			357	238	119		

- Molecule 30 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms			AltConf	Trace
30	a	222	Total	C	N	0	0
			666	444	222		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms			AltConf	Trace
31	b	97	Total	C	N	0	0
			291	194	97		

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms			AltConf	Trace
32	c	109	Total	C	N	0	0
			327	218	109		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms			AltConf	Trace
33	d	127	Total	C	N	0	0
			381	254	127		

- Molecule 34 is a protein called 60S ribosomal protein L33.

Mol	Chain	Residues	Atoms			AltConf	Trace
34	e	106	Total	C	N	0	0
			318	212	106		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms			AltConf	Trace
35	f	112	Total	C	N	0	0
			336	224	112		

- Molecule 36 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms			AltConf	Trace
36	g	99	Total	C	N	0	0
			297	198	99		

- Molecule 37 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms			AltConf	Trace
37	h	87	Total	C	N	0	0
			261	174	87		

- Molecule 38 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms			AltConf	Trace
38	i	77	Total	C	N	0	0
			231	154	77		

- Molecule 39 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms			AltConf	Trace
39	j	50	Total	C	N	0	0
			150	100	50		

- Molecule 40 is a protein called 60S ribosomal protein L43.

Mol	Chain	Residues	Atoms			AltConf	Trace
40	k	91	Total	C	N	0	0
			273	182	91		

- Molecule 41 is a protein called metalloprotease ARX1.

Mol	Chain	Residues	Atoms			AltConf	Trace
41	l	380	Total	C	N	0	0
			1140	760	380		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms			AltConf	Trace
42	m	224	Total	C	N	0	0
			672	448	224		

- Molecule 43 is a protein called mRNA turnover protein 4.

Mol	Chain	Residues	Atoms			AltConf	Trace
43	n	236	Total	C	N	0	0
			708	472	236		

- Molecule 44 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms			AltConf	Trace
44	o	347	Total	C	N	0	0
			1041	694	347		

- Molecule 45 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms			AltConf	Trace
45	p	63	Total	C	N	0	0
			189	126	63		

- Molecule 46 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms			AltConf	Trace
46	q	443	Total	C	N	0	0
			1329	886	443		

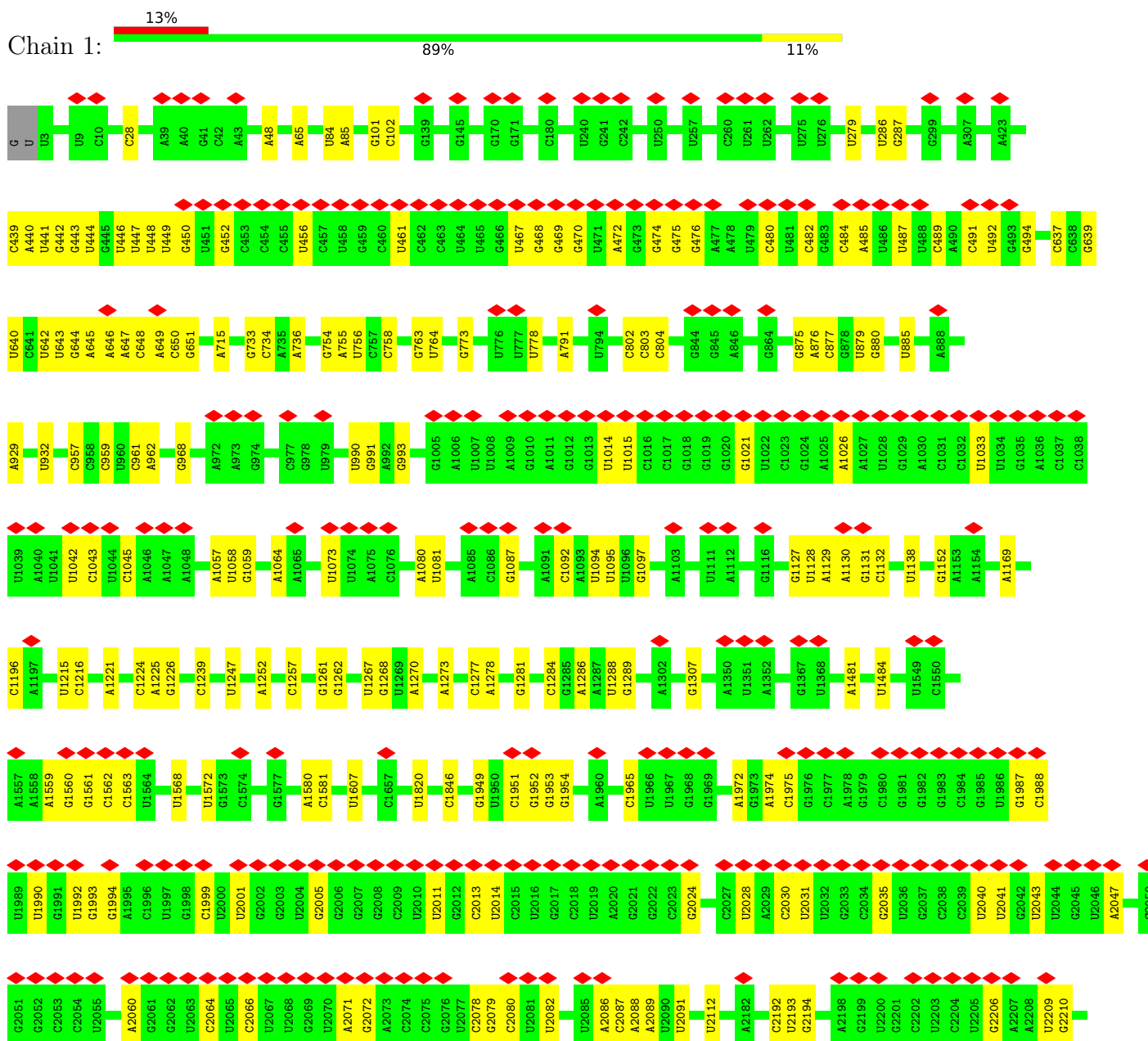
- Molecule 47 is a protein called Ribosome biogenesis protein RLP7.

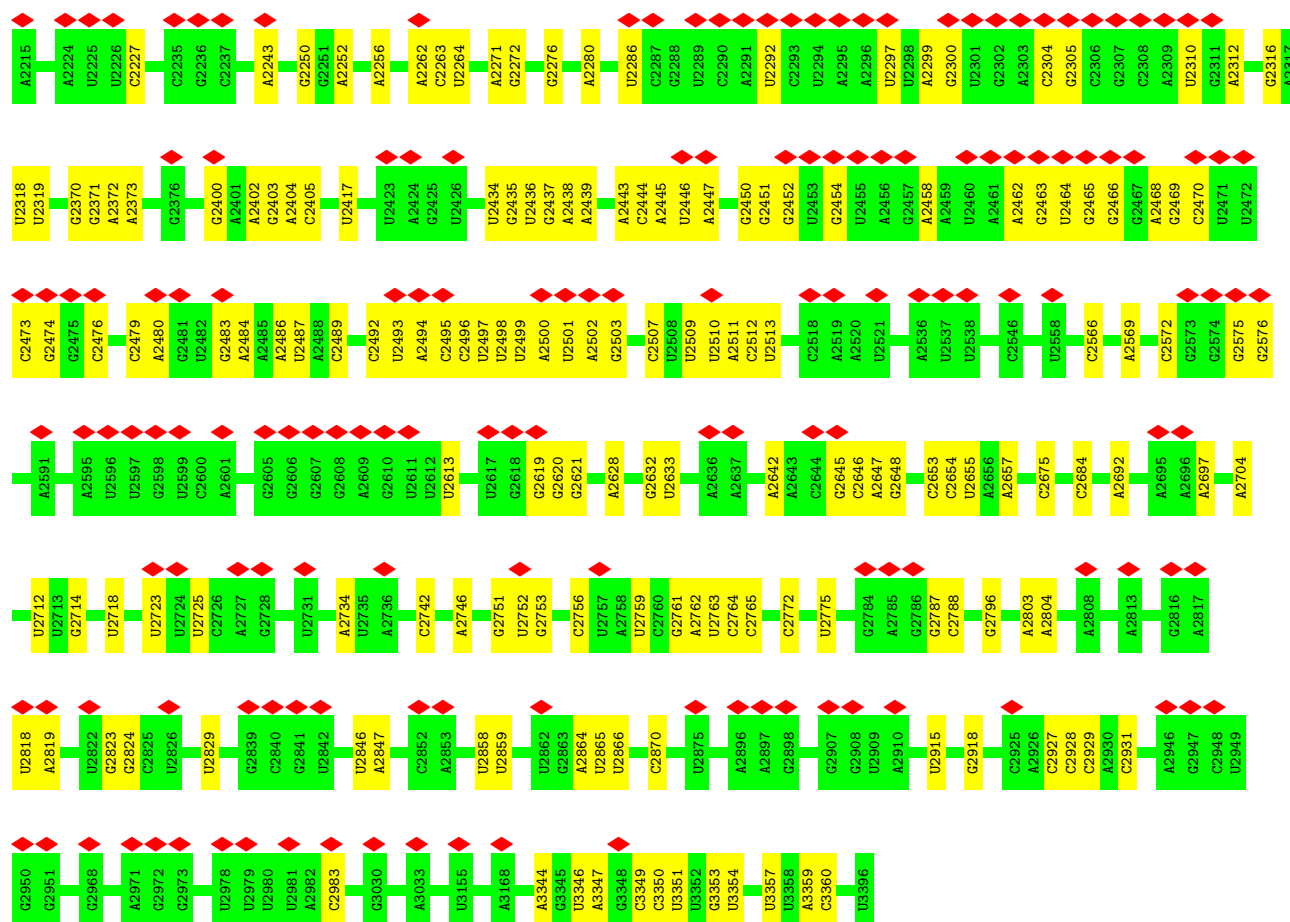
Mol	Chain	Residues	Atoms			AltConf	Trace
47	r	322	Total	C	N	0	0
			966	644	322		
47	s	322	Total	C	N	0	0
			966	644	322		

3 Residue-property plots

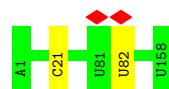
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 25S ribosomal RNA

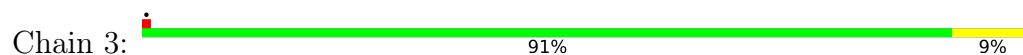




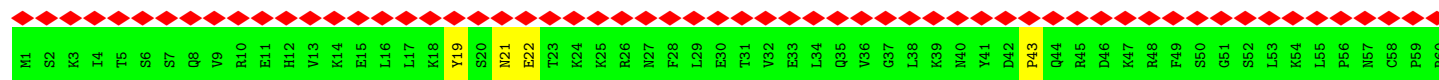
• Molecule 2: 5.8S ribosomal RNA



• Molecule 3: 5S ribosomal RNA

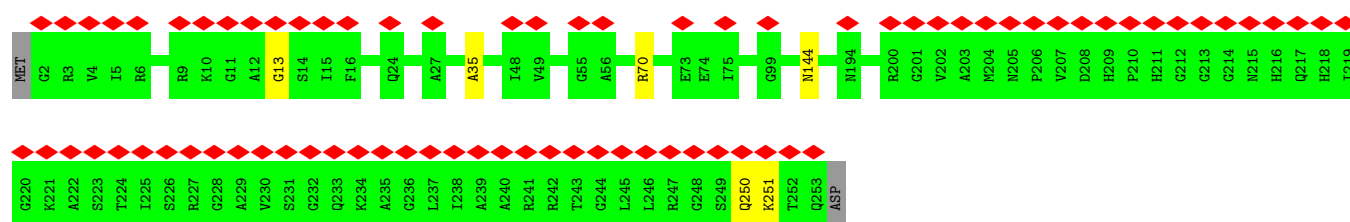


• Molecule 4: 60S ribosomal protein L1

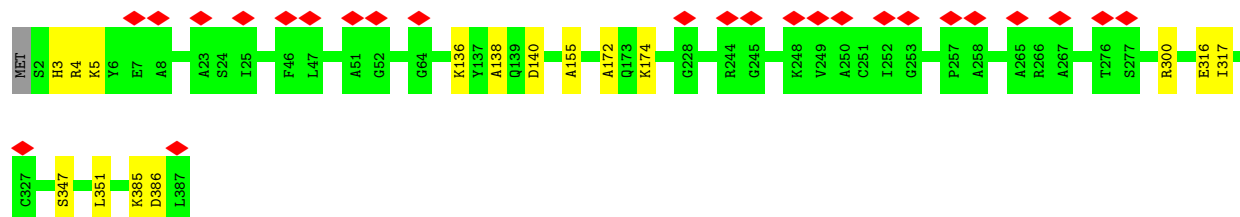




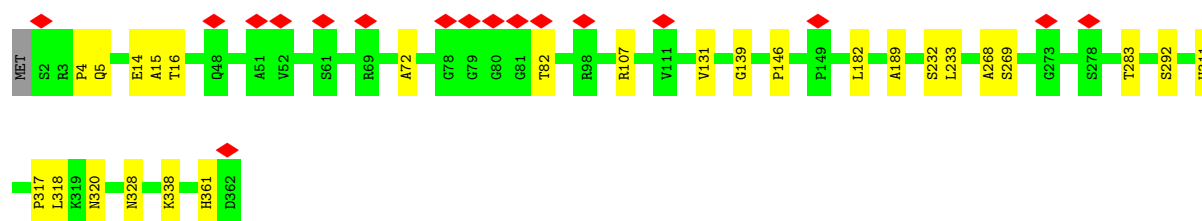
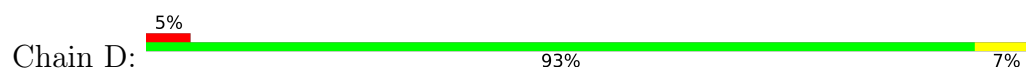
• Molecule 5: 60S ribosomal protein L2



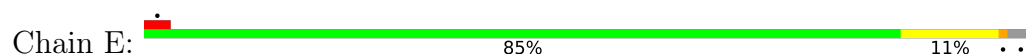
• Molecule 6: 60S ribosomal protein L3



• Molecule 7: 60S ribosomal protein L4

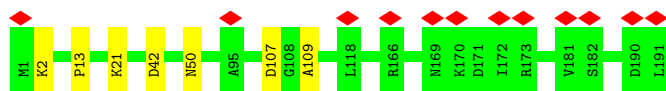


• Molecule 8: 60S ribosomal protein L11





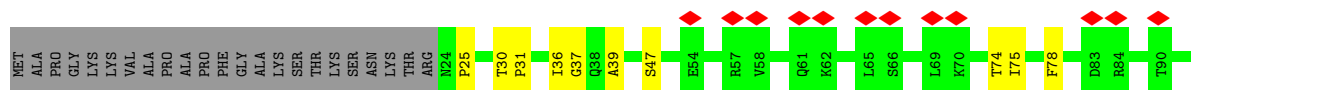
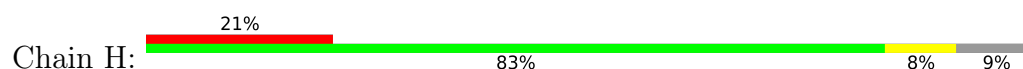
- Molecule 9: 60S ribosomal protein L9



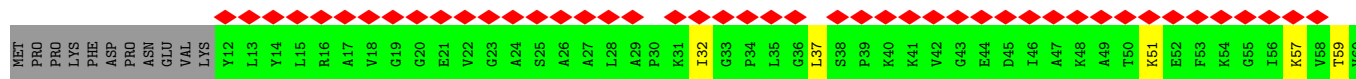
- Molecule 10: 60S ribosomal protein L6



- Molecule 11: 60S ribosomal protein L8

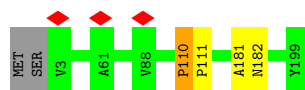


- Molecule 12: 60S ribosomal protein L12

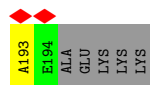
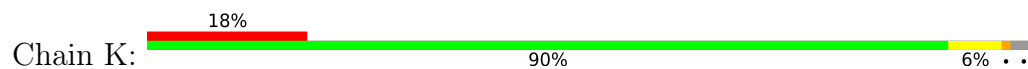


- Molecule 13: 60S ribosomal protein L16

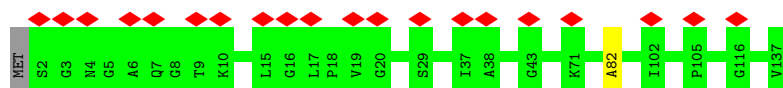




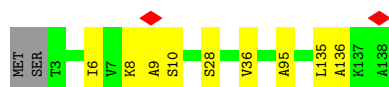
- Molecule 14: 60S ribosomal protein L13



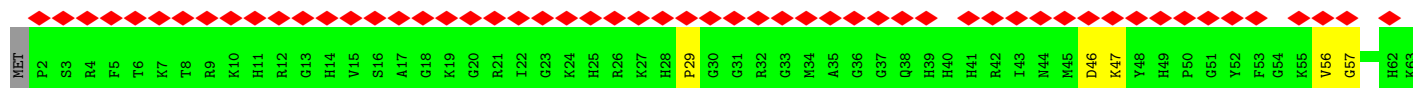
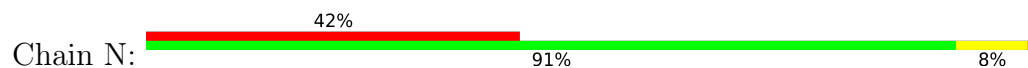
- Molecule 15: 60S ribosomal protein L23



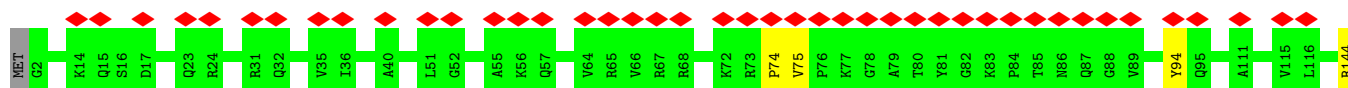
- Molecule 16: 60S ribosomal protein L14

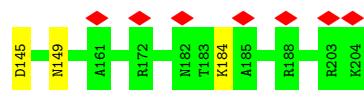


- Molecule 17: 60S ribosomal protein L28

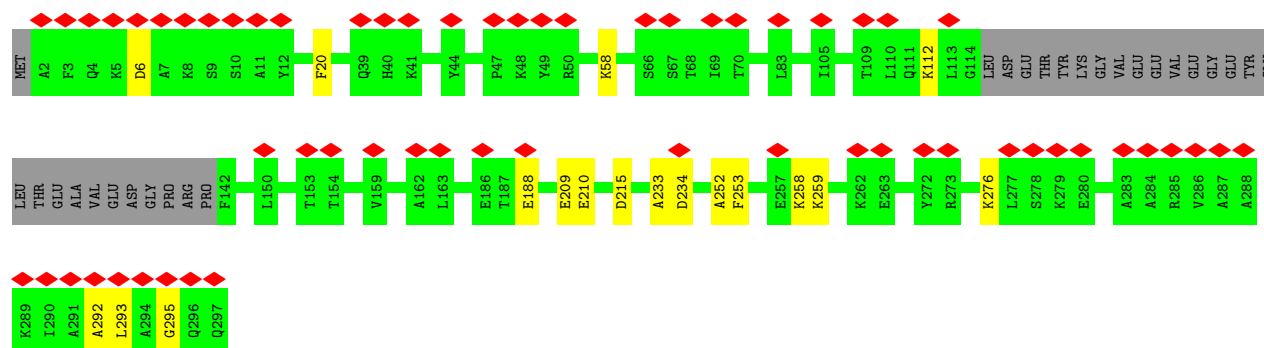
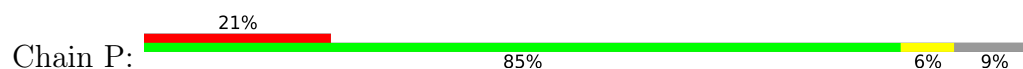


- Molecule 18: 60S ribosomal protein L15





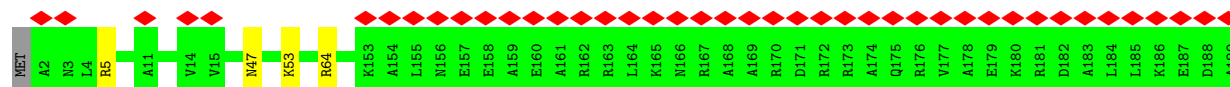
- Molecule 19: 60S ribosomal protein L5



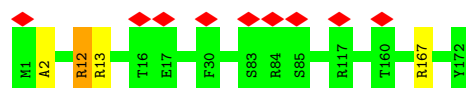
- Molecule 20: 60S ribosomal protein L18



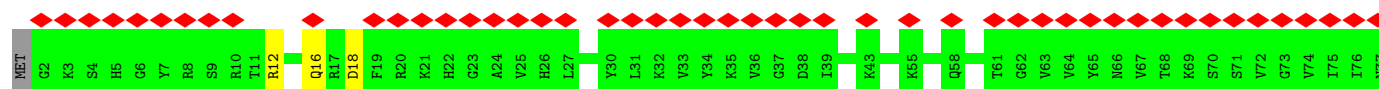
- Molecule 21: 60S ribosomal protein L19

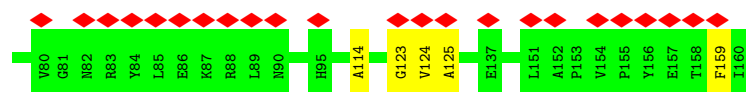


- Molecule 22: 60S ribosomal protein L20



- Molecule 23: 60S ribosomal protein L21

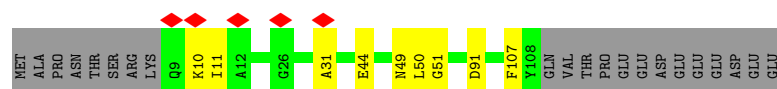




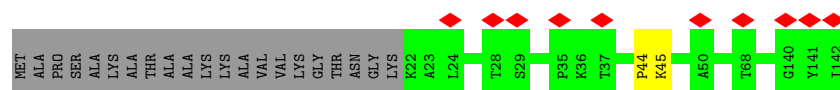
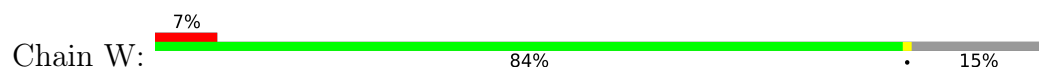
- Molecule 24: 60S ribosomal protein L17



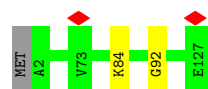
- Molecule 25: 60S ribosomal protein L22



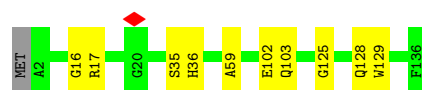
- Molecule 26: 60S ribosomal protein L25



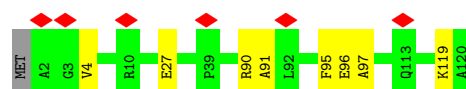
- Molecule 27: 60S ribosomal protein L26




- Molecule 28: 60S ribosomal protein L27

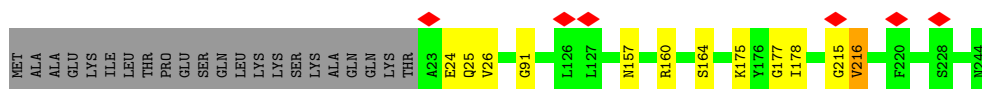


- Molecule 29: 60S ribosomal protein L35

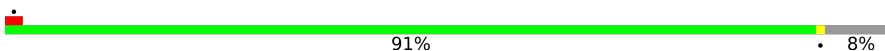


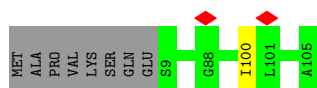
- Molecule 30: 60S ribosomal protein L7

Chain a: 



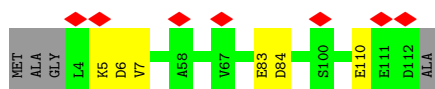
- Molecule 31: 60S ribosomal protein L30

Chain b: 



- Molecule 32: 60S ribosomal protein L31

Chain c: 



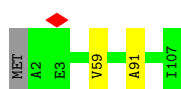
- Molecule 33: 60S ribosomal protein L32

Chain d: 



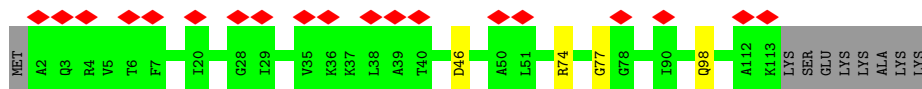
- Molecule 34: 60S ribosomal protein L33

Chain e: 




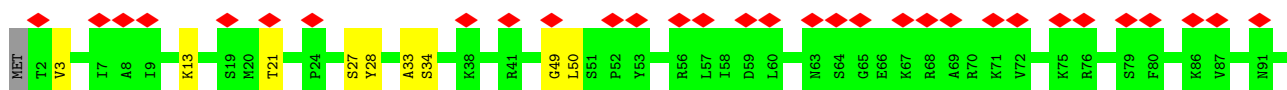
- Molecule 35: 60S ribosomal protein L34

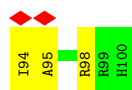
Chain f: 



- Molecule 36: 60S ribosomal protein L36

Chain g: 





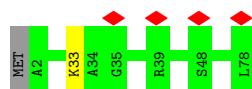
- Molecule 37: 60S ribosomal protein L37

Chain h: 95%



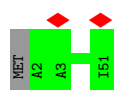
- Molecule 38: 60S ribosomal protein L38

Chain i: 97%



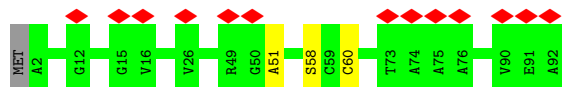
- Molecule 39: 60S ribosomal protein L39

Chain j: 98%



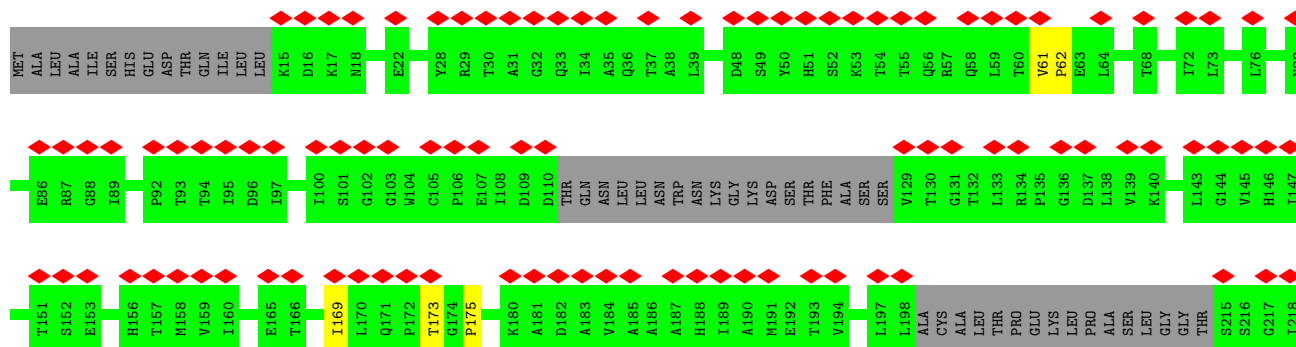
- Molecule 40: 60S ribosomal protein L43

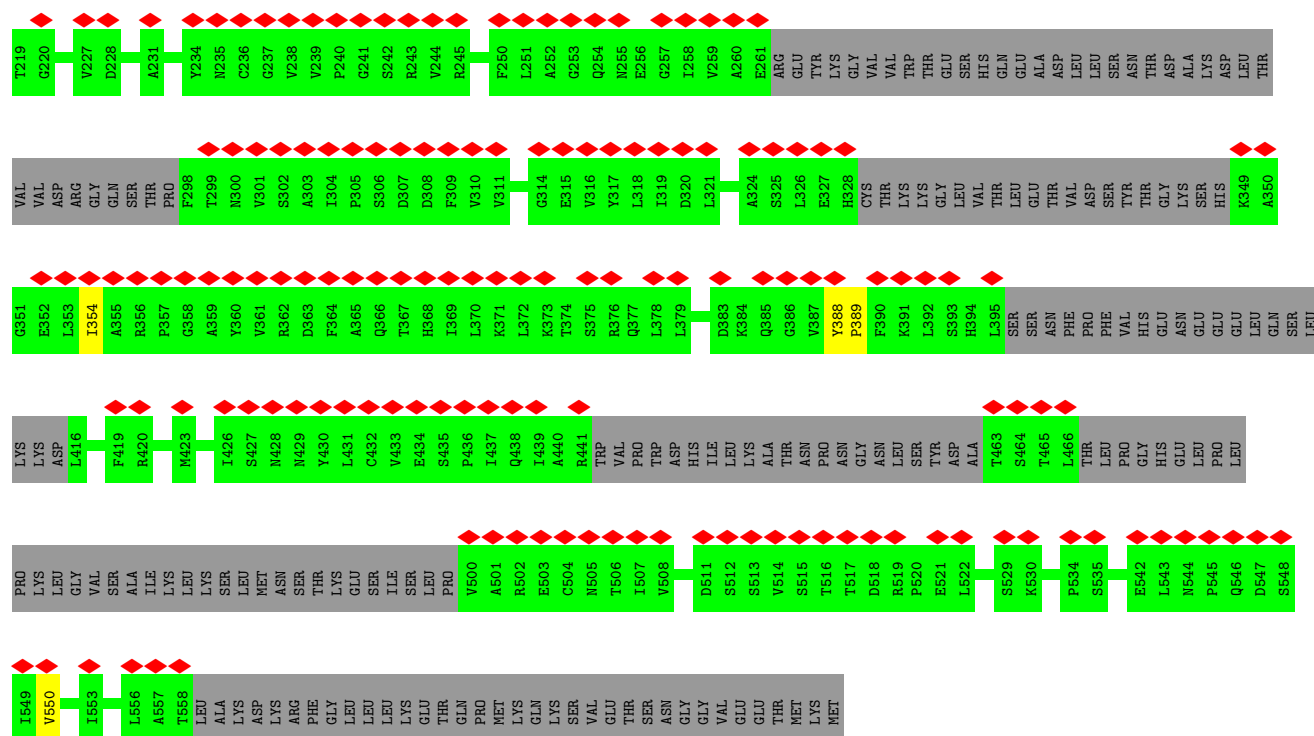
Chain k: 96%



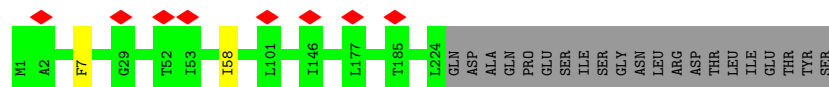
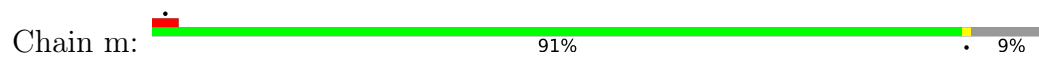
- Molecule 41: metalloprotease ARX1

Chain l: 63%





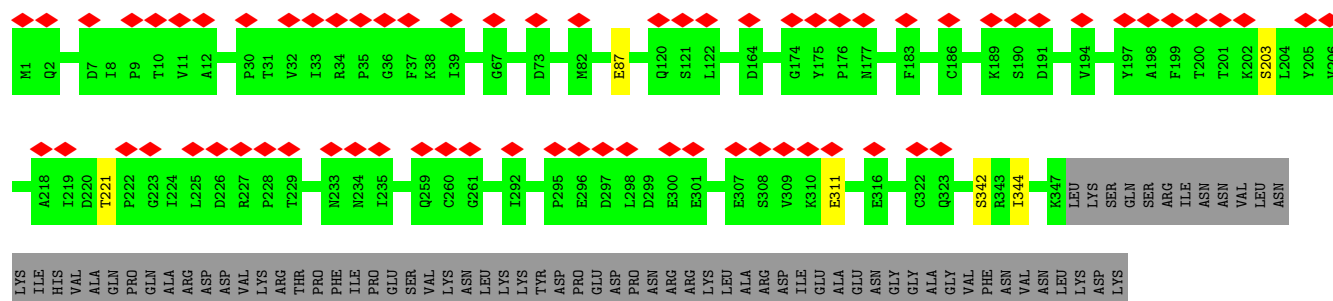
• Molecule 42: Eukaryotic translation initiation factor 6

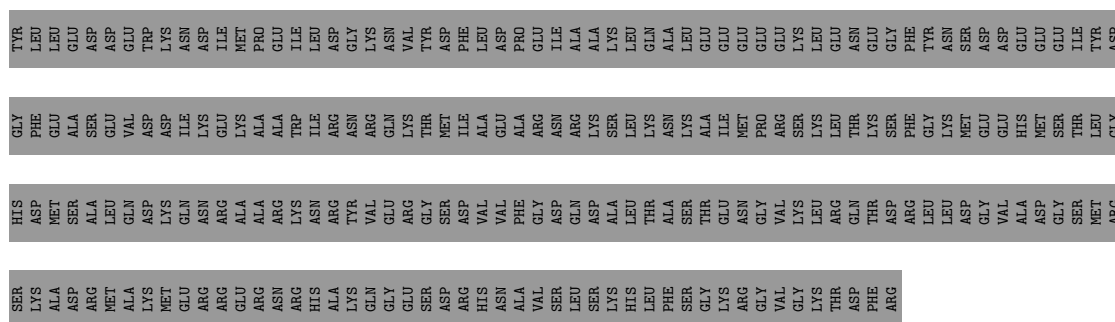


• Molecule 43: mRNA turnover protein 4

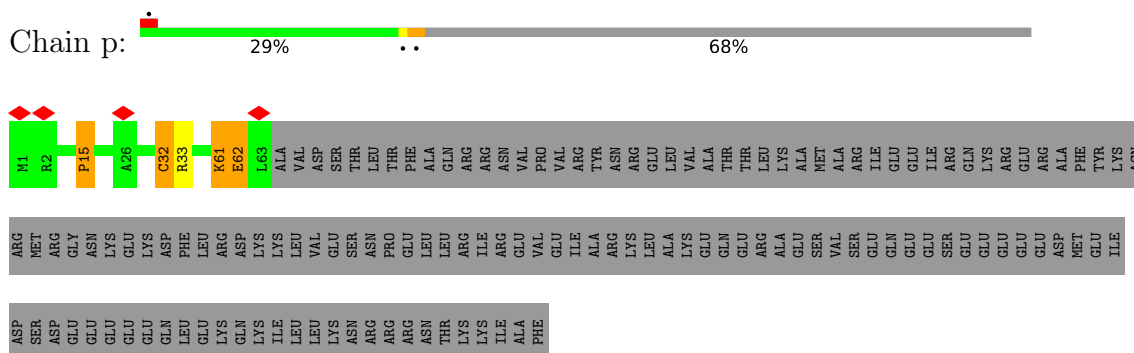


• Molecule 44: Nucleolar GTP-binding protein 1

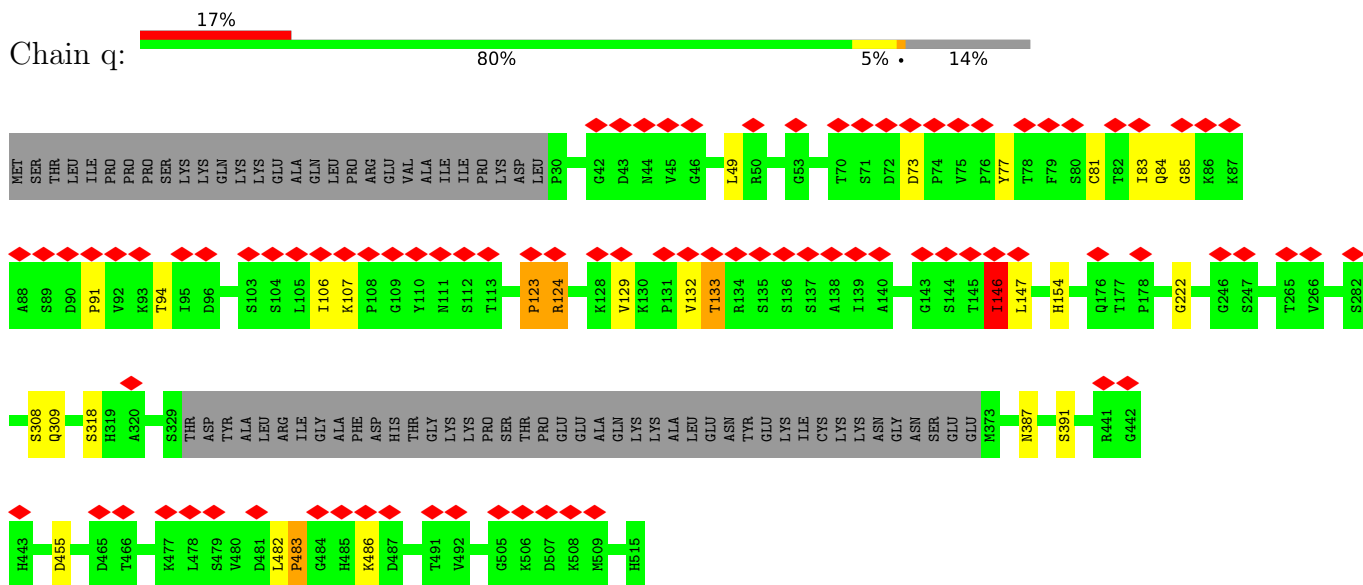




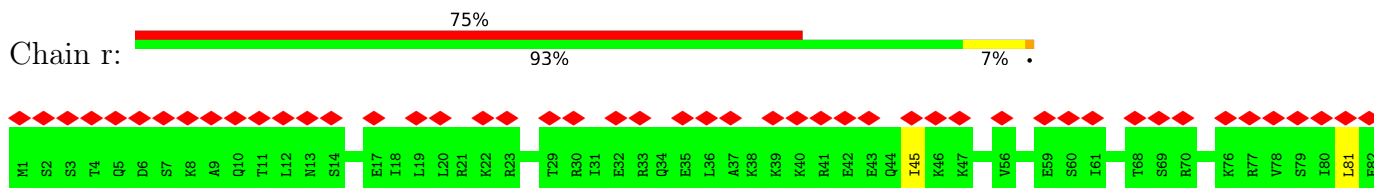
- Molecule 45: Ribosome biogenesis protein RLP24

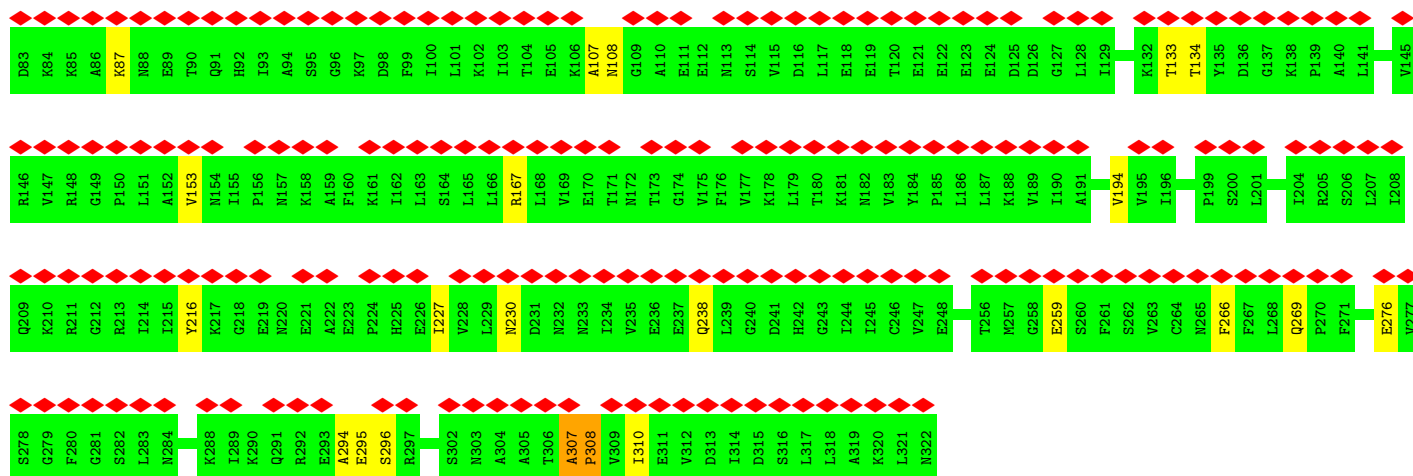


- Molecule 46: Ribosome assembly protein 4



- Molecule 47: Ribosome biogenesis protein RLP7





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75887	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	2.010	Depositor
Minimum map value	-0.822	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.45	Depositor
Map size (\AA)	439.047, 439.047, 439.047	wwPDB
Map dimensions	414, 414, 414	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0605, 1.0605, 1.0605	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.65	185/20361 (0.9%)	1.81	364/20359 (1.8%)
2	2	1.24	2/947 (0.2%)	0.67	0/946
3	3	1.97	7/724 (1.0%)	1.58	5/723 (0.7%)
4	A	1.38	1/650 (0.2%)	1.56	1/649 (0.2%)
5	B	0.63	0/755	1.00	0/754
6	C	0.68	0/1157	1.04	1/1156 (0.1%)
7	D	0.70	0/1082	1.14	4/1081 (0.4%)
8	E	0.55	0/506	0.93	0/505
9	F	0.56	0/572	0.91	0/571
10	G	0.69	0/524	1.13	1/523 (0.2%)
11	H	0.49	0/698	0.92	1/697 (0.1%)
12	I	1.82	5/380 (1.3%)	2.01	5/379 (1.3%)
13	J	0.48	0/590	0.76	0/589
14	K	0.66	0/578	1.07	2/577 (0.3%)
15	L	0.63	0/407	0.98	0/406
16	M	0.66	0/407	0.97	0/406
17	N	0.77	0/443	1.25	3/442 (0.7%)
18	O	0.68	0/608	1.03	0/607
19	P	0.54	0/805	0.91	0/803
20	Q	0.73	0/554	1.07	1/553 (0.2%)
21	R	0.56	0/563	0.91	0/562
22	S	0.73	0/515	1.03	1/514 (0.2%)
23	T	0.66	0/476	0.98	0/475
24	U	0.66	0/548	1.01	0/547
25	V	0.42	0/299	0.82	0/298
26	W	0.56	0/362	0.89	0/361
27	X	0.61	0/377	1.00	0/376
28	Y	0.46	0/404	0.94	0/403
29	Z	0.60	0/356	0.94	0/355
30	a	0.69	0/665	1.09	3/664 (0.5%)
31	b	0.42	0/290	0.79	0/289
32	c	0.59	0/326	0.92	0/325
33	d	0.70	0/380	1.01	0/379
34	e	0.76	0/317	1.01	0/316

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	f	0.57	0/335	0.92	0/334
36	g	0.62	0/296	1.05	1/295 (0.3%)
37	h	0.74	0/260	1.12	0/259
38	i	0.46	0/230	0.81	0/229
39	j	0.62	0/149	1.08	0/148
40	k	0.60	0/272	0.97	0/271
41	l	0.54	1/1138 (0.1%)	0.74	0/1136
42	m	0.29	0/671	0.84	1/670 (0.1%)
43	n	1.15	0/707	1.35	0/706
44	o	1.11	0/1040	1.20	0/1039
45	p	1.66	2/188 (1.1%)	1.86	4/187 (2.1%)
46	q	1.19	1/1327 (0.1%)	1.35	6/1325 (0.5%)
47	r	1.14	0/965	1.33	2/964 (0.2%)
47	s	1.14	0/965	1.33	2/964 (0.2%)
All	All	1.28	204/47169 (0.4%)	1.45	408/47117 (0.9%)

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
4	A	0	2
6	C	0	1
7	D	0	1
8	E	0	1
9	F	0	1
10	G	0	1
11	H	0	3
12	I	0	5
13	J	0	1
23	T	0	1
30	a	0	1
32	c	0	1
43	n	0	2
45	p	0	1
46	q	0	7
47	r	0	1
47	s	0	1
All	All	0	31

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	648	C	O5'-C5'	38.19	2.05	1.44
1	1	648	C	P-O5'	-26.01	1.33	1.59
1	1	2819	A	C5'-C4'	25.95	1.82	1.51
1	1	651	G	C5'-C4'	17.76	1.72	1.51
1	1	651	G	C4'-C3'	16.66	1.71	1.53
1	1	650	C	C4'-C3'	14.56	1.69	1.53
1	1	2818	U	O3'-P	-14.40	1.43	1.61
1	1	2372	A	P-O5'	-14.19	1.45	1.59
45	p	61	LYS	C-N	13.98	1.66	1.34
1	1	648	C	O3'-P	-13.39	1.45	1.61
1	1	644	G	C4'-C3'	-13.25	1.38	1.53
1	1	439	C	O3'-P	13.07	1.76	1.61
1	1	643	U	P-O5'	-12.55	1.47	1.59
1	1	2370	G	O3'-P	-11.66	1.47	1.61
1	1	642	U	C4'-C3'	-11.64	1.40	1.53
1	1	2373	A	O3'-P	-10.96	1.48	1.61
1	1	642	U	O3'-P	-10.79	1.48	1.61
1	1	2819	A	O5'-C5'	10.73	1.61	1.44
1	1	440	A	C5'-C4'	9.85	1.63	1.51
1	1	650	C	C5'-C4'	9.60	1.62	1.51
1	1	651	G	P-O5'	9.58	1.69	1.59
46	q	482	LEU	C-N	9.05	1.51	1.34
1	1	640	U	C5'-C4'	8.85	1.61	1.51
12	I	76	SER	N-CA	8.82	1.64	1.46
1	1	2319	U	P-O5'	-8.65	1.51	1.59
1	1	645	A	P-O5'	-8.62	1.51	1.59
1	1	639	G	C4'-C3'	8.60	1.62	1.53
1	1	440	A	C4'-C3'	8.16	1.62	1.53
1	1	644	G	O3'-P	-7.99	1.51	1.61
1	1	2417	U	O3'-P	-7.73	1.51	1.61
1	1	2264	U	P-O5'	-7.73	1.52	1.59
1	1	1129	A	C5'-C4'	7.70	1.60	1.51
1	1	1268	G	C5'-C4'	7.69	1.60	1.51
1	1	1267	U	P-O5'	-7.61	1.52	1.59
1	1	2371	G	P-O5'	-7.51	1.52	1.59
1	1	756	U	P-O5'	-7.29	1.52	1.59
1	1	2503	G	O3'-P	-7.28	1.52	1.61
1	1	1026	A	C5'-C4'	7.19	1.59	1.51
1	1	1988	C	O3'-P	-7.18	1.52	1.61
1	1	1021	G	C5'-C4'	7.14	1.59	1.51
1	1	1073	U	C5'-C4'	7.11	1.59	1.51
1	1	644	G	C5'-C4'	7.11	1.59	1.51
1	1	1278	A	C4'-C3'	7.11	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2372	A	C4'-C3'	7.09	1.60	1.53
3	3	75	G	P-O5'	-7.07	1.52	1.59
1	1	646	A	P-O5'	-7.01	1.52	1.59
1	1	2497	U	O3'-P	-6.93	1.52	1.61
1	1	494	G	C5'-C4'	6.92	1.59	1.51
1	1	2493	U	P-O5'	-6.86	1.52	1.59
1	1	1581	C	C4'-C3'	6.85	1.60	1.53
1	1	1993	G	C5'-C4'	6.85	1.59	1.51
1	1	2305	G	O3'-P	-6.74	1.53	1.61
1	1	648	C	C4'-C3'	-6.73	1.45	1.53
1	1	1560	G	P-O5'	-6.73	1.53	1.59
1	1	2271	A	O3'-P	-6.73	1.53	1.61
1	1	778	U	C3'-O3'	6.72	1.51	1.42
1	1	2299	A	O3'-P	-6.64	1.53	1.61
1	1	1128	U	C4'-C3'	6.64	1.60	1.53
3	3	7	G	P-O5'	-6.63	1.53	1.59
3	3	36	C	C5'-C4'	6.62	1.59	1.51
1	1	2404	A	C5'-C4'	6.61	1.59	1.51
1	1	651	G	C3'-O3'	6.54	1.51	1.42
1	1	2734	A	C5'-C4'	6.53	1.59	1.51
1	1	2858	U	P-O5'	-6.50	1.53	1.59
1	1	2014	U	P-O5'	-6.46	1.53	1.59
3	3	111	U	O3'-P	-6.39	1.53	1.61
1	1	2653	C	C5'-C4'	6.39	1.59	1.51
1	1	1152	G	P-O5'	-6.38	1.53	1.59
1	1	650	C	C3'-O3'	6.35	1.51	1.42
1	1	468	G	O3'-P	-6.33	1.53	1.61
1	1	2509	U	O3'-P	-6.30	1.53	1.61
1	1	639	G	C5'-C4'	6.29	1.58	1.51
1	1	85	A	O3'-P	-6.27	1.53	1.61
1	1	2276	G	C5'-C4'	6.26	1.58	1.51
1	1	2078	C	P-O5'	-6.23	1.53	1.59
1	1	1846	C	P-O5'	-6.21	1.53	1.59
1	1	2297	U	O3'-P	-6.21	1.53	1.61
1	1	715	A	C5'-C4'	6.20	1.58	1.51
1	1	2915	U	P-O5'	-6.18	1.53	1.59
2	2	82	U	P-O5'	6.17	1.66	1.59
1	1	1307	G	C3'-O3'	6.15	1.50	1.42
1	1	1042	U	P-O5'	-6.15	1.53	1.59
1	1	482	C	C5'-C4'	6.14	1.58	1.51
1	1	2451	G	P-O5'	-6.14	1.53	1.59
1	1	2436	U	O3'-P	-6.11	1.53	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1563	C	C5'-C4'	6.10	1.58	1.51
1	1	476	G	O3'-P	-6.10	1.53	1.61
1	1	2300	G	C4'-C3'	6.07	1.59	1.53
1	1	3347	A	C5'-C4'	6.06	1.58	1.51
3	3	48	U	O3'-P	-6.06	1.53	1.61
1	1	102	C	C5'-C4'	6.05	1.58	1.51
1	1	2788	C	C5'-C4'	6.02	1.58	1.51
3	3	8	G	C5'-C4'	5.99	1.58	1.51
1	1	449	U	C4'-C3'	5.91	1.59	1.53
1	1	1561	G	C5'-C4'	5.91	1.58	1.51
12	I	77	ALA	N-CA	5.91	1.58	1.46
1	1	2746	A	O3'-P	-5.90	1.54	1.61
1	1	1057	A	P-O5'	-5.90	1.53	1.59
1	1	1987	G	C5'-C4'	5.89	1.58	1.51
1	1	754	G	O3'-P	-5.89	1.54	1.61
1	1	1286	A	P-O5'	-5.89	1.53	1.59
1	1	1951	C	O3'-P	-5.88	1.54	1.61
1	1	2865	U	C5'-C4'	5.87	1.58	1.51
1	1	1033	U	P-O5'	-5.86	1.53	1.59
1	1	2492	C	P-O5'	5.86	1.65	1.59
1	1	1014	U	C4'-C3'	-5.85	1.46	1.52
12	I	75	PRO	N-CA	5.85	1.57	1.47
1	1	1138	U	O3'-P	-5.82	1.54	1.61
1	1	2001	U	C5'-C4'	5.81	1.58	1.51
1	1	2796	G	C5'-C4'	5.80	1.58	1.51
12	I	97	ASN	N-CA	-5.79	1.34	1.46
1	1	440	A	P-O5'	5.78	1.65	1.59
1	1	2454	G	C5'-C4'	5.77	1.58	1.51
1	1	1281	G	P-O5'	-5.77	1.53	1.59
1	1	2013	C	C5'-C4'	5.74	1.58	1.51
1	1	2746	A	P-O5'	-5.74	1.54	1.59
1	1	1994	G	O3'-P	-5.73	1.54	1.61
1	1	2507	C	O3'-P	-5.71	1.54	1.61
1	1	2697	A	C5'-C4'	5.70	1.58	1.51
1	1	491	C	O3'-P	-5.70	1.54	1.61
1	1	480	C	C5'-C4'	5.69	1.58	1.51
1	1	929	A	C5'-C4'	5.68	1.58	1.51
1	1	2272	G	C5'-C4'	5.67	1.58	1.51
1	1	962	A	P-O5'	5.67	1.65	1.59
1	1	286	U	O3'-P	-5.64	1.54	1.61
1	1	803	C	C5'-C4'	5.64	1.58	1.51
1	1	2772	C	O3'-P	-5.63	1.54	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	48	A	O3'-P	-5.61	1.54	1.61
1	1	3349	C	C5'-C4'	5.61	1.58	1.51
1	1	968	G	C5'-C4'	5.59	1.58	1.51
1	1	2657	A	C4'-C3'	5.56	1.59	1.53
1	1	1252	A	O3'-P	-5.54	1.54	1.61
1	1	2718	U	C5'-C4'	5.54	1.57	1.51
1	1	804	C	C5'-C4'	5.54	1.57	1.51
1	1	3351	U	C4'-C3'	5.53	1.59	1.53
1	1	2647	A	P-O5'	-5.52	1.54	1.59
1	1	2866	U	C5'-C4'	5.52	1.57	1.51
1	1	957	C	C4'-C3'	5.51	1.59	1.53
1	1	484	C	P-O5'	-5.43	1.54	1.59
1	1	2572	C	C5'-C4'	5.43	1.57	1.51
1	1	469	G	O3'-P	-5.43	1.54	1.61
1	1	485	A	C5'-C4'	5.43	1.57	1.51
1	1	1169	A	P-O5'	-5.42	1.54	1.59
1	1	2041	U	O3'-P	-5.42	1.54	1.61
1	1	2648	G	C5'-C4'	5.41	1.57	1.51
1	1	1288	U	O3'-P	-5.41	1.54	1.61
1	1	470	G	C4'-C3'	-5.40	1.47	1.52
1	1	2087	C	C4'-C3'	5.40	1.59	1.53
1	1	1257	C	O3'-P	-5.39	1.54	1.61
1	1	650	C	O3'-P	5.38	1.67	1.61
1	1	932	U	C5'-C4'	5.36	1.57	1.51
1	1	2280	A	C4'-C3'	5.36	1.59	1.53
1	1	651	G	O3'-P	5.35	1.67	1.61
1	1	2028	U	P-O5'	-5.35	1.54	1.59
45	p	62	GLU	N-CA	5.35	1.57	1.46
1	1	2576	G	C5'-C4'	5.33	1.57	1.51
1	1	2632	G	O3'-P	-5.32	1.54	1.61
1	1	2031	U	O3'-P	-5.31	1.54	1.61
1	1	791	A	P-O5'	-5.30	1.54	1.59
1	1	2064	C	C4'-C3'	5.30	1.58	1.53
1	1	2983	C	P-O5'	-5.28	1.54	1.59
1	1	2858	U	O3'-P	-5.28	1.54	1.61
1	1	647	A	C4'-C3'	5.26	1.58	1.53
3	3	33	U	C5'-C4'	5.26	1.57	1.51
1	1	1196	C	C5'-C4'	5.25	1.57	1.51
1	1	2927	C	C3'-O3'	5.24	1.49	1.42
1	1	449	U	C5'-C4'	5.24	1.57	1.51
1	1	2642	A	P-O5'	5.23	1.65	1.59
1	1	2043	U	C5'-C4'	5.23	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2714	G	C5'-C4'	5.23	1.57	1.51
1	1	2864	A	P-O5'	-5.22	1.54	1.59
1	1	993	G	P-O5'	-5.22	1.54	1.59
41	1	388	TYR	C-N	5.21	1.44	1.34
2	2	21	C	P-O5'	-5.21	1.54	1.59
12	I	57	LYS	CA-C	-5.20	1.39	1.52
1	1	2400	G	C5'-C4'	5.20	1.57	1.51
1	1	758	C	O3'-P	-5.18	1.54	1.61
1	1	1045	C	P-O5'	-5.18	1.54	1.59
1	1	2082	U	P-O5'	-5.17	1.54	1.59
1	1	2692	A	C5'-C4'	5.17	1.57	1.51
4	A	43	PRO	N-CA	-5.17	1.38	1.47
1	1	1999	C	C5'-C4'	5.16	1.57	1.51
1	1	2227	C	O3'-P	-5.13	1.54	1.61
1	1	1247	U	C4'-C3'	5.10	1.58	1.53
1	1	2312	A	C4'-C3'	5.09	1.58	1.53
1	1	443	G	P-O5'	-5.09	1.54	1.59
1	1	736	A	P-O5'	-5.09	1.54	1.59
1	1	1261	G	O3'-P	-5.08	1.55	1.61
1	1	1572	U	C3'-O3'	5.07	1.49	1.42
1	1	2439	A	O3'-P	-5.07	1.55	1.61
1	1	646	A	O3'-P	-5.06	1.55	1.61
1	1	1481	A	P-O5'	-5.06	1.54	1.59
1	1	1043	C	P-O5'	-5.06	1.54	1.59
1	1	1273	A	P-O5'	-5.06	1.54	1.59
1	1	1129	A	O3'-P	-5.06	1.55	1.61
1	1	287	G	C5'-C4'	5.06	1.57	1.51
1	1	734	C	C5'-C4'	5.04	1.57	1.51
1	1	773	G	C4'-C3'	5.03	1.58	1.53
1	1	2464	U	O3'-P	-5.03	1.55	1.61
1	1	2804	A	C5'-C4'	5.03	1.57	1.51
1	1	2193	U	C5'-C4'	5.02	1.57	1.51
1	1	2112	U	C3'-O3'	5.01	1.49	1.42
1	1	2761	G	C5'-C4'	5.01	1.57	1.51
1	1	2263	C	O3'-P	-5.00	1.55	1.61

All (408) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	885	U	P-O3'-C3'	44.33	172.90	119.70
1	1	649	A	P-O5'-C5'	31.07	170.61	120.90
1	1	648	C	P-O5'-C5'	-29.22	74.15	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2370	G	P-O3'-C3'	27.58	152.80	119.70
1	1	2509	U	P-O3'-C3'	27.15	152.28	119.70
1	1	2497	U	P-O3'-C3'	26.29	151.24	119.70
1	1	2819	A	O5'-C5'-C4'	25.63	160.39	111.70
1	1	2507	C	P-O3'-C3'	25.18	149.92	119.70
1	1	2503	G	P-O3'-C3'	22.24	146.39	119.70
1	1	2462	A	P-O3'-C3'	21.73	145.78	119.70
1	1	1138	U	P-O3'-C3'	21.21	145.16	119.70
1	1	2041	U	P-O3'-C3'	21.02	144.93	119.70
1	1	2500	A	P-O3'-C3'	21.00	144.90	119.70
1	1	647	A	O3'-P-O5'	-19.54	66.87	104.00
1	1	2030	C	P-O3'-C3'	19.48	143.08	119.70
1	1	440	A	C5'-C4'-C3'	19.34	146.95	116.00
1	1	651	G	C5'-C4'-C3'	19.26	146.82	116.00
1	1	2310	U	P-O3'-C3'	19.00	142.50	119.70
1	1	2489	C	P-O3'-C3'	18.96	142.46	119.70
1	1	2818	U	P-O3'-C3'	18.41	141.80	119.70
1	1	1288	U	P-O3'-C3'	18.39	141.76	119.70
1	1	1965	C	P-O3'-C3'	18.29	141.64	119.70
1	1	2439	A	P-O3'-C3'	18.00	141.30	119.70
1	1	456	U	P-O3'-C3'	17.98	141.28	119.70
1	1	2468	A	P-O3'-C3'	17.98	141.28	119.70
1	1	2194	G	P-O3'-C3'	17.98	141.27	119.70
1	1	2372	A	P-O5'-C5'	17.91	149.56	120.90
1	1	991	G	P-O5'-C5'	17.84	149.45	120.90
1	1	2697	A	P-O3'-C3'	17.74	140.99	119.70
1	1	2079	G	P-O3'-C3'	17.57	140.79	119.70
1	1	468	G	P-O3'-C3'	17.57	140.78	119.70
1	1	647	A	C5'-C4'-C3'	-17.36	88.22	116.00
1	1	648	C	O3'-P-O5'	-17.02	71.66	104.00
1	1	2080	C	P-O3'-C3'	16.72	139.76	119.70
1	1	2192	C	P-O3'-C3'	16.59	139.61	119.70
1	1	2483	G	P-O3'-C3'	16.16	139.09	119.70
1	1	880	G	P-O3'-C3'	16.01	138.91	119.70
1	1	876	A	C5'-C4'-C3'	15.77	141.24	116.00
1	1	2480	A	P-O3'-C3'	15.52	138.33	119.70
1	1	1580	A	P-O3'-C3'	15.51	138.31	119.70
1	1	494	G	P-O3'-C3'	15.48	138.28	119.70
1	1	2446	U	P-O3'-C3'	15.46	138.25	119.70
1	1	879	U	P-O3'-C3'	15.35	138.12	119.70
1	1	2499	U	P-O5'-C5'	15.23	145.26	120.90
1	1	2086	A	P-O3'-C3'	15.19	137.92	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2434	U	P-O3'-C3'	15.16	137.89	119.70
1	1	2450	G	P-O3'-C3'	15.05	137.76	119.70
1	1	1064	A	P-O3'-C3'	14.92	137.61	119.70
1	1	2297	U	P-O3'-C3'	14.86	137.53	119.70
1	1	2031	U	P-O3'-C3'	14.81	137.47	119.70
1	1	2654	C	P-O3'-C3'	14.81	137.47	119.70
1	1	2043	U	P-O3'-C3'	14.69	137.32	119.70
1	1	651	G	P-O5'-C5'	14.60	144.25	120.90
1	1	2803	A	P-O3'-C3'	14.49	137.09	119.70
1	1	491	C	P-O3'-C3'	14.09	136.61	119.70
1	1	2316	G	P-O3'-C3'	13.97	136.46	119.70
1	1	2445	A	P-O3'-C3'	13.94	136.42	119.70
10	G	128	LYS	CA-C-N	13.92	147.82	117.20
1	1	2463	G	P-O3'-C3'	13.92	136.40	119.70
1	1	959	C	P-O3'-C3'	13.88	136.36	119.70
1	1	2510	U	P-O5'-C5'	13.76	142.92	120.90
1	1	2501	U	P-O3'-C3'	13.72	136.16	119.70
1	1	472	A	P-O3'-C3'	13.61	136.03	119.70
1	1	2492	C	P-O3'-C3'	13.60	136.02	119.70
1	1	1058	U	P-O3'-C3'	13.58	136.00	119.70
1	1	2655	U	P-O3'-C3'	13.56	135.97	119.70
1	1	650	C	C5'-C4'-C3'	13.41	137.46	116.00
1	1	2403	G	P-O3'-C3'	13.35	135.72	119.70
1	1	2751	G	P-O3'-C3'	13.21	135.55	119.70
1	1	3350	C	P-O3'-C3'	13.08	135.40	119.70
1	1	2060	A	P-O3'-C3'	13.04	135.34	119.70
1	1	2071	A	P-O3'-C3'	13.02	135.33	119.70
1	1	2484	A	P-O3'-C3'	12.95	135.24	119.70
1	1	1221	A	P-O3'-C3'	12.94	135.22	119.70
1	1	2819	A	P-O5'-C5'	12.92	141.58	120.90
1	1	2437	G	P-O3'-C3'	12.70	134.93	119.70
1	1	442	G	P-O3'-C3'	12.69	134.92	119.70
1	1	763	G	P-O3'-C3'	12.65	134.88	119.70
1	1	2495	C	P-O3'-C3'	12.62	134.84	119.70
12	I	76	SER	N-CA-C	-12.61	76.96	111.00
1	1	1972	A	P-O3'-C3'	12.58	134.79	119.70
1	1	2373	A	P-O3'-C3'	12.48	134.68	119.70
1	1	715	A	P-O3'-C3'	12.45	134.64	119.70
1	1	2633	U	P-O3'-C3'	12.45	134.64	119.70
1	1	640	U	P-O5'-C5'	12.44	140.81	120.90
1	1	1094	U	P-O3'-C3'	12.15	134.28	119.70
1	1	2927	C	P-O3'-C3'	-12.10	105.18	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	645	A	O3'-P-O5'	-12.08	81.05	104.00
1	1	2829	U	P-O3'-C3'	11.98	134.08	119.70
1	1	448	U	P-O3'-C3'	11.92	134.00	119.70
1	1	1059	G	P-O3'-C3'	11.67	133.70	119.70
1	1	2494	A	P-O3'-C3'	11.54	133.55	119.70
1	1	2823	G	P-O3'-C3'	11.49	133.49	119.70
1	1	764	U	P-O3'-C3'	11.41	133.40	119.70
1	1	961	C	P-O3'-C3'	11.39	133.36	119.70
1	1	2040	U	P-O3'-C3'	11.38	133.36	119.70
1	1	439	C	P-O3'-C3'	-11.38	106.05	119.70
1	1	1988	C	P-O3'-C3'	11.30	133.27	119.70
1	1	1273	A	P-O3'-C3'	11.21	133.15	119.70
1	1	646	A	P-O3'-C3'	11.14	133.07	119.70
1	1	1562	C	P-O3'-C3'	11.13	133.06	119.70
1	1	474	G	P-O3'-C3'	10.96	132.85	119.70
1	1	650	C	O3'-P-O5'	10.95	124.80	104.00
1	1	1095	U	P-O3'-C3'	10.94	132.83	119.70
1	1	2072	G	P-O3'-C3'	10.81	132.67	119.70
1	1	2493	U	P-O3'-C3'	10.80	132.66	119.70
1	1	2511	A	P-O5'-C5'	10.69	138.01	120.90
1	1	2227	C	P-O3'-C3'	10.64	132.47	119.70
1	1	2753	G	P-O3'-C3'	10.62	132.44	119.70
1	1	2445	A	P-O5'-C5'	10.58	137.83	120.90
1	1	2066	C	P-O3'-C3'	10.48	132.28	119.70
46	q	123	PRO	C-N-CA	10.37	147.62	121.70
1	1	2870	C	P-O3'-C3'	10.30	132.06	119.70
1	1	2763	U	P-O3'-C3'	10.30	132.06	119.70
1	1	639	G	C5'-C4'-C3'	10.27	132.44	116.00
1	1	2404	A	P-O3'-C3'	10.15	131.88	119.70
1	1	2372	A	P-O3'-C3'	-10.01	107.69	119.70
1	1	651	G	O5'-C5'-C4'	9.95	130.61	111.70
1	1	2436	U	O3'-P-O5'	-9.94	85.11	104.00
1	1	649	A	O5'-C5'-C4'	9.93	130.57	111.70
1	1	1953	G	P-O3'-C3'	9.86	131.53	119.70
1	1	1277	C	P-O3'-C3'	9.78	131.44	119.70
1	1	1132	C	C5'-C4'-C3'	9.78	131.64	116.00
1	1	877	C	P-O5'-C5'	-9.76	105.29	120.90
1	1	1216	C	P-O3'-C3'	9.73	131.38	119.70
1	1	1994	G	P-O3'-C3'	9.68	131.31	119.70
1	1	645	A	P-O3'-C3'	9.67	131.30	119.70
1	1	2513	U	P-O3'-C3'	9.57	131.18	119.70
1	1	2451	G	P-O5'-C5'	9.54	136.17	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	p	61	LYS	C-N-CA	-9.54	97.86	121.70
1	1	2447	A	P-O3'-C3'	9.46	131.05	119.70
3	3	52	G	P-O3'-C3'	9.42	131.01	119.70
1	1	494	G	O3'-P-O5'	9.38	121.82	104.00
1	1	1128	U	C5'-C4'-C3'	9.33	130.93	116.00
45	p	62	GLU	N-CA-C	9.33	136.19	111.00
1	1	2493	U	P-O5'-C5'	9.28	135.75	120.90
1	1	1097	G	P-O3'-C3'	9.25	130.80	119.70
1	1	2469	G	C5'-C4'-C3'	9.12	130.60	116.00
1	1	2928	C	P-O3'-C3'	-9.07	108.82	119.70
1	1	2446	U	P-O5'-C5'	9.01	135.31	120.90
1	1	645	A	C5'-C4'-C3'	-8.98	101.62	116.00
1	1	441	U	P-O5'-C5'	8.98	135.27	120.90
1	1	2435	G	P-O3'-C3'	8.97	130.47	119.70
1	1	2613	U	P-O3'-C3'	8.97	130.46	119.70
1	1	1952	G	P-O3'-C3'	8.94	130.43	119.70
1	1	2509	U	O3'-P-O5'	-8.93	87.03	104.00
1	1	1215	U	P-O3'-C3'	8.89	130.38	119.70
1	1	2486	A	P-O3'-C3'	8.77	130.23	119.70
1	1	643	U	C5'-C4'-C3'	-8.64	102.18	116.00
1	1	2444	C	P-O3'-C3'	-8.62	109.36	119.70
1	1	2772	C	P-O3'-C3'	8.60	130.02	119.70
1	1	2819	A	C5'-C4'-C3'	8.52	129.63	116.00
47	r	308	PRO	N-CA-C	8.48	134.15	112.10
47	s	308	PRO	N-CA-C	8.47	134.13	112.10
1	1	2402	A	P-O3'-C3'	8.40	129.78	119.70
1	1	1581	C	P-O3'-C3'	8.38	129.76	119.70
1	1	3351	U	P-O3'-C3'	8.33	129.70	119.70
46	q	146	ILE	C-N-CA	8.32	142.50	121.70
1	1	640	U	C5'-C4'-C3'	8.32	129.31	116.00
1	1	1975	C	P-O5'-C5'	8.32	134.21	120.90
1	1	450	G	P-O3'-C3'	8.27	129.63	119.70
1	1	2292	U	P-O3'-C3'	8.22	129.57	119.70
1	1	2250	G	P-O5'-C5'	8.22	134.05	120.90
1	1	2370	G	O3'-P-O5'	-8.21	88.40	104.00
1	1	2372	A	O5'-C5'-C4'	-8.15	96.22	111.70
1	1	475	G	P-O3'-C3'	8.11	129.44	119.70
12	I	75	PRO	CA-C-N	7.97	134.74	117.20
1	1	2451	G	P-O3'-C3'	7.93	129.22	119.70
1	1	644	G	P-O3'-C3'	-7.91	110.21	119.70
1	1	2047	A	P-O3'-C3'	7.85	129.12	119.70
1	1	2866	U	P-O3'-C3'	7.81	129.08	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1972	A	C5'-C4'-C3'	7.77	128.44	116.00
46	q	147	LEU	N-CA-C	7.72	131.84	111.00
1	1	2859	U	P-O3'-C3'	7.67	128.90	119.70
1	1	639	G	O3'-P-O5'	7.65	118.54	104.00
1	1	2752	U	P-O3'-C3'	7.56	128.78	119.70
1	1	447	U	P-O3'-C3'	7.54	128.75	119.70
45	p	15	PRO	N-CA-C	7.54	131.71	112.10
1	1	650	C	P-O3'-C3'	7.53	128.74	119.70
1	1	2438	A	C5'-C4'-C3'	7.52	128.03	116.00
1	1	2299	A	P-O3'-C3'	7.50	128.70	119.70
12	I	77	ALA	C-N-CA	7.50	140.46	121.70
1	1	492	U	P-O3'-C3'	7.40	128.58	119.70
1	1	991	G	P-O3'-C3'	-7.37	110.86	119.70
1	1	1951	C	P-O3'-C3'	7.36	128.53	119.70
1	1	3344	A	P-O3'-C3'	7.36	128.53	119.70
1	1	2764	C	P-O3'-C3'	-7.30	110.94	119.70
1	1	990	U	O3'-P-O5'	-7.28	90.17	104.00
1	1	2089	A	P-O3'-C3'	7.28	128.44	119.70
1	1	1132	C	P-O3'-C3'	7.27	128.43	119.70
1	1	2684	C	P-O3'-C3'	-7.27	110.98	119.70
1	1	485	A	P-O3'-C3'	7.24	128.39	119.70
1	1	2575	G	P-O5'-C5'	7.23	132.47	120.90
1	1	646	A	O5'-C5'-C4'	-7.23	97.97	111.70
1	1	2469	G	P-O3'-C3'	7.22	128.36	119.70
1	1	1015	U	P-O5'-C5'	7.19	132.41	120.90
1	1	1131	G	C5'-C4'-C3'	7.19	127.50	116.00
1	1	2286	U	P-O3'-C3'	7.18	128.32	119.70
1	1	3360	C	P-O3'-C3'	7.14	128.27	119.70
1	1	2846	U	P-O3'-C3'	-7.12	111.15	119.70
1	1	1559	A	P-O3'-C3'	7.09	128.21	119.70
1	1	487	U	P-O5'-C5'	7.07	132.21	120.90
1	1	2452	G	P-O3'-C3'	7.06	128.18	119.70
1	1	1974	A	P-O3'-C3'	7.00	128.11	119.70
1	1	1130	A	P-O3'-C3'	6.96	128.05	119.70
1	1	2088	A	C5'-C4'-C3'	6.95	127.12	116.00
1	1	442	G	P-O5'-C5'	-6.87	109.91	120.90
1	1	3359	A	P-O3'-C3'	-6.86	111.47	119.70
1	1	1131	G	P-O5'-C5'	6.86	131.87	120.90
1	1	3353	G	P-O3'-C3'	6.83	127.90	119.70
1	1	2759	U	P-O3'-C3'	6.83	127.89	119.70
1	1	2210	G	P-O5'-C5'	6.81	131.80	120.90
1	1	1975	C	P-O3'-C3'	6.80	127.87	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2458	A	P-O3'-C3'	6.80	127.86	119.70
1	1	644	G	O3'-P-O5'	-6.79	91.09	104.00
1	1	1058	U	C5'-C4'-C3'	6.77	126.83	116.00
1	1	2469	G	O3'-P-O5'	-6.75	91.18	104.00
1	1	1560	G	P-O5'-C5'	6.71	131.63	120.90
1	1	1057	A	P-O5'-C5'	6.70	131.62	120.90
1	1	642	U	C5'-C4'-C3'	-6.68	105.31	116.00
1	1	2918	G	P-O3'-C3'	-6.64	111.73	119.70
1	1	2474	G	P-O3'-C3'	6.64	127.67	119.70
1	1	2931	C	P-O5'-C5'	6.64	131.53	120.90
1	1	1262	G	P-O3'-C3'	6.61	127.63	119.70
1	1	2502	A	P-O3'-C3'	6.60	127.62	119.70
30	a	216	VAL	N-CA-C	6.60	128.82	111.00
1	1	440	A	P-O5'-C5'	6.57	131.41	120.90
1	1	1129	A	P-O5'-C5'	-6.57	110.39	120.90
1	1	2492	C	O5'-C5'-C4'	6.57	124.18	111.70
1	1	2621	G	P-O3'-C3'	6.56	127.57	119.70
1	1	452	G	P-O3'-C3'	6.55	127.56	119.70
1	1	2479	C	P-O3'-C3'	-6.52	111.87	119.70
1	1	2759	U	C5'-C4'-C3'	6.50	126.40	116.00
1	1	1286	A	P-O3'-C3'	6.42	127.40	119.70
1	1	2470	C	P-O3'-C3'	6.39	127.37	119.70
1	1	2078	C	P-O3'-C3'	6.37	127.34	119.70
1	1	2466	G	P-O3'-C3'	6.36	127.33	119.70
1	1	2645	G	C5'-C4'-C3'	-6.36	105.83	116.00
3	3	111	U	P-O3'-C3'	6.33	127.29	119.70
1	1	2487	U	P-O3'-C3'	-6.31	112.12	119.70
1	1	2756	C	P-O3'-C3'	6.31	127.27	119.70
1	1	2464	U	P-O5'-C5'	-6.28	110.85	120.90
1	1	645	A	C4'-C3'-O3'	6.28	125.55	113.00
17	N	46	ASP	N-CA-C	-6.28	94.06	111.00
1	1	647	A	C4'-C3'-O3'	6.27	125.54	113.00
1	1	647	A	O5'-C5'-C4'	6.22	123.52	111.70
20	Q	99	THR	N-CA-C	6.21	127.76	111.00
1	1	2646	C	P-O3'-C3'	-6.20	112.26	119.70
1	1	1289	G	P-O3'-C3'	6.19	127.12	119.70
1	1	28	C	P-O3'-C3'	6.19	127.12	119.70
1	1	2628	A	C5'-C4'-C3'	6.18	125.89	116.00
1	1	84	U	P-O3'-C3'	6.17	127.11	119.70
1	1	2462	A	O3'-P-O5'	-6.17	92.27	104.00
1	1	2206	G	P-O5'-C5'	6.16	130.75	120.90
1	1	2927	C	P-O5'-C5'	6.16	130.75	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	22	GLU	N-CA-C	6.15	127.60	111.00
1	1	2024	G	P-O3'-C3'	6.15	127.08	119.70
1	1	2499	U	P-O3'-C3'	6.13	127.05	119.70
1	1	2818	U	O3'-P-O5'	6.12	115.63	104.00
11	H	158	ASP	N-CA-C	6.12	127.53	111.00
1	1	2371	G	P-O5'-C5'	6.10	130.66	120.90
1	1	2263	C	C5'-C4'-C3'	6.06	125.70	116.00
1	1	1820	U	P-O3'-C3'	6.05	126.96	119.70
1	1	1992	U	C5'-C4'-C3'	6.04	125.67	116.00
17	N	66	ALA	N-CA-C	-6.03	94.71	111.00
1	1	2262	A	O3'-P-O5'	-6.02	92.56	104.00
1	1	1092	C	P-O3'-C3'	6.01	126.91	119.70
1	1	644	G	O5'-C5'-C4'	6.00	123.11	111.70
1	1	1484	U	P-O3'-C3'	6.00	126.89	119.70
1	1	1239	C	P-O3'-C3'	-5.98	112.53	119.70
1	1	2035	G	P-O3'-C3'	5.97	126.86	119.70
1	1	1284	C	P-O3'-C3'	5.96	126.85	119.70
1	1	2443	A	P-O3'-C3'	5.96	126.85	119.70
1	1	2566	C	P-O3'-C3'	-5.96	112.55	119.70
1	1	2620	G	P-O3'-C3'	5.94	126.83	119.70
1	1	2373	A	P-O5'-C5'	-5.93	111.41	120.90
1	1	1278	A	P-O3'-C3'	5.93	126.81	119.70
7	D	189	ALA	C-N-CA	-5.92	109.87	122.30
1	1	2476	C	P-O3'-C3'	5.91	126.80	119.70
14	K	141	ALA	N-CA-C	-5.91	95.04	111.00
1	1	755	A	P-O5'-C5'	-5.90	111.46	120.90
1	1	1129	A	O5'-C5'-C4'	5.90	122.91	111.70
1	1	2465	G	P-O5'-C5'	-5.89	111.47	120.90
1	1	885	U	O3'-P-O5'	-5.88	92.83	104.00
1	1	1226	G	P-O5'-C5'	5.87	130.30	120.90
1	1	3357	U	P-O3'-C3'	-5.86	112.67	119.70
1	1	480	C	P-O3'-C3'	5.85	126.72	119.70
1	1	2438	A	P-O5'-C5'	-5.84	111.55	120.90
1	1	2280	A	P-O5'-C5'	-5.84	111.56	120.90
17	N	115	LYS	C-N-CA	-5.83	110.05	122.30
1	1	2192	C	P-O5'-C5'	5.81	130.19	120.90
30	a	215	GLY	N-CA-C	-5.80	98.61	113.10
1	1	2927	C	O3'-P-O5'	-5.79	92.99	104.00
1	1	2507	C	C5'-C4'-C3'	-5.79	106.74	116.00
7	D	139	GLY	N-CA-C	-5.78	98.66	113.10
1	1	650	C	C4'-C3'-O3'	5.77	124.54	113.00
1	1	876	A	O3'-P-O5'	-5.77	93.04	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2028	U	P-O5'-C5'	5.77	130.13	120.90
1	1	2765	C	P-O5'-C5'	5.77	130.12	120.90
1	1	443	G	C5'-C4'-C3'	-5.76	106.79	116.00
1	1	467	U	P-O3'-C3'	5.73	126.57	119.70
12	I	73	VAL	N-CA-C	-5.72	95.55	111.00
1	1	2438	A	P-O3'-C3'	5.72	126.56	119.70
1	1	444	U	P-O3'-C3'	5.70	126.54	119.70
1	1	1129	A	P-O3'-C3'	5.70	126.54	119.70
1	1	2675	C	P-O3'-C3'	5.70	126.54	119.70
1	1	2209	U	P-O3'-C3'	5.68	126.52	119.70
1	1	279	U	P-O5'-C5'	-5.67	111.83	120.90
1	1	2492	C	P-O5'-C5'	-5.66	111.84	120.90
1	1	875	G	P-O3'-C3'	5.64	126.47	119.70
1	1	2569	A	P-O3'-C3'	5.64	126.46	119.70
45	p	32	CYS	CA-C-N	5.63	129.59	117.20
1	1	1954	G	P-O3'-C3'	5.61	126.43	119.70
1	1	3354	U	P-O3'-C3'	-5.61	112.97	119.70
1	1	1081	U	P-O3'-C3'	5.61	126.43	119.70
1	1	2503	G	O3'-P-O5'	-5.60	93.35	104.00
1	1	991	G	C5'-C4'-C3'	5.58	124.93	116.00
1	1	1580	A	C5'-C4'-C3'	-5.58	107.07	116.00
6	C	316	GLU	N-CA-C	5.58	126.06	111.00
1	1	2493	U	C5'-C4'-C3'	5.56	124.90	116.00
1	1	65	A	P-O3'-C3'	5.56	126.37	119.70
1	1	802	C	P-O3'-C3'	5.56	126.37	119.70
1	1	2454	G	P-O3'-C3'	5.55	126.37	119.70
1	1	2371	G	P-O3'-C3'	-5.55	113.04	119.70
36	g	27	SER	N-CA-C	-5.53	96.06	111.00
46	q	222	GLY	N-CA-C	-5.53	99.27	113.10
1	1	2653	C	P-O3'-C3'	5.53	126.33	119.70
1	1	1949	G	P-O3'-C3'	5.52	126.32	119.70
1	1	2405	C	P-O3'-C3'	5.52	126.32	119.70
12	I	88	PRO	CA-C-N	5.51	132.54	117.10
1	1	446	U	P-O5'-C5'	5.51	129.72	120.90
1	1	2091	U	P-O5'-C5'	5.51	129.72	120.90
1	1	2473	C	P-O3'-C3'	5.50	126.31	119.70
47	r	266	PHE	N-CA-C	-5.50	96.14	111.00
47	s	266	PHE	N-CA-C	-5.50	96.14	111.00
1	1	2723	U	P-O3'-C3'	-5.49	113.11	119.70
1	1	990	U	P-O3'-C3'	-5.48	113.12	119.70
1	1	2243	A	P-O5'-C5'	-5.47	112.14	120.90
1	1	2498	U	C5'-C4'-C3'	-5.47	107.25	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2450	G	O3'-P-O5'	-5.47	93.61	104.00
1	1	1080	A	P-O5'-C5'	-5.45	112.18	120.90
1	1	1270	A	P-O3'-C3'	5.45	126.24	119.70
1	1	2512	C	P-O3'-C3'	5.45	126.24	119.70
1	1	1128	U	O3'-P-O5'	5.45	114.35	104.00
1	1	645	A	O5'-C5'-C4'	-5.44	101.36	111.70
3	3	93	C	P-O3'-C3'	-5.44	113.17	119.70
1	1	644	G	P-O5'-C5'	-5.43	112.21	120.90
1	1	2304	C	P-O3'-C3'	5.40	126.18	119.70
1	1	2479	C	C5'-C4'-C3'	5.40	124.63	116.00
1	1	1130	A	P-O5'-C5'	-5.39	112.28	120.90
1	1	2787	G	P-O3'-C3'	5.39	126.17	119.70
1	1	1990	U	P-O5'-C5'	5.38	129.51	120.90
1	1	2847	A	P-O5'-C5'	-5.38	112.29	120.90
46	q	147	LEU	CA-C-N	5.37	129.02	117.20
14	K	57	VAL	N-CA-C	-5.36	96.54	111.00
1	1	2256	A	P-O3'-C3'	5.35	126.12	119.70
1	1	2466	G	C5'-C4'-C3'	5.35	124.56	116.00
3	3	63	A	P-O5'-C5'	-5.35	112.34	120.90
1	1	440	A	P-O3'-C3'	5.34	126.11	119.70
1	1	1607	U	P-O3'-C3'	5.33	126.10	119.70
1	1	2742	C	C5'-C4'-C3'	-5.32	107.49	116.00
1	1	461	U	P-O3'-C3'	-5.30	113.33	119.70
1	1	2496	C	O3'-P-O5'	-5.29	93.95	104.00
1	1	2858	U	P-O3'-C3'	5.29	126.05	119.70
1	1	1087	G	P-O3'-C3'	-5.28	113.37	119.70
1	1	101	G	P-O3'-C3'	5.27	126.03	119.70
1	1	643	U	P-O3'-C3'	-5.26	113.39	119.70
1	1	2011	U	P-O5'-C5'	-5.26	112.48	120.90
1	1	1127	G	P-O5'-C5'	-5.24	112.51	120.90
1	1	2762	A	P-O3'-C3'	5.24	125.99	119.70
1	1	733	G	P-O5'-C5'	5.23	129.26	120.90
1	1	1224	C	P-O5'-C5'	5.22	129.26	120.90
1	1	639	G	C4'-C3'-O3'	5.22	123.44	113.00
1	1	3346	U	P-O5'-C5'	5.21	129.24	120.90
1	1	2718	U	P-O5'-C5'	5.19	129.21	120.90
1	1	2276	G	P-O5'-C5'	-5.18	112.61	120.90
46	q	483	PRO	N-CA-C	5.18	125.56	112.10
1	1	1224	C	P-O3'-C3'	-5.17	113.49	119.70
1	1	2252	A	P-O5'-C5'	-5.17	112.63	120.90
1	1	2657	A	P-O3'-C3'	5.17	125.90	119.70
1	1	1225	A	P-O3'-C3'	5.17	125.90	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2476	C	C5'-C4'-C3'	5.15	124.23	116.00
1	1	1568	U	P-O3'-C3'	5.14	125.87	119.70
7	D	82	THR	C-N-CA	-5.14	111.51	122.30
1	1	2318	U	P-O5'-C5'	-5.14	112.68	120.90
1	1	2263	C	P-O5'-C5'	-5.12	112.70	120.90
3	3	10	C	P-O5'-C5'	5.10	129.06	120.90
1	1	2775	U	P-O3'-C3'	-5.10	113.58	119.70
42	m	7	PHE	N-CA-C	-5.10	97.24	111.00
1	1	2373	A	C5'-C4'-C3'	5.09	124.15	116.00
1	1	2929	C	P-O3'-C3'	-5.08	113.60	119.70
1	1	2619	G	P-O3'-C3'	5.08	125.80	119.70
1	1	2507	C	P-O5'-C5'	-5.08	112.77	120.90
1	1	2824	G	P-O5'-C5'	-5.07	112.78	120.90
7	D	328	ASN	N-CA-C	5.07	124.70	111.00
22	S	12	ARG	N-CA-C	5.07	124.69	111.00
1	1	2725	U	P-O3'-C3'	-5.07	113.62	119.70
1	1	2417	U	P-O5'-C5'	-5.07	112.80	120.90
1	1	2500	A	O3'-P-O5'	-5.06	94.39	104.00
30	a	177	GLY	N-CA-C	-5.05	100.48	113.10
1	1	1131	G	O5'-C5'-C4'	-5.05	102.11	111.70
1	1	2492	C	C5'-C4'-C3'	5.05	124.08	116.00
1	1	2704	A	P-O3'-C3'	5.04	125.75	119.70
1	1	2005	G	P-O5'-C5'	-5.02	112.86	120.90
1	1	637	C	P-O3'-C3'	5.01	125.71	119.70
1	1	489	C	P-O5'-C5'	5.01	128.91	120.90
1	1	2712	U	P-O3'-C3'	5.01	125.71	119.70
1	1	1289	G	P-O5'-C5'	5.00	128.90	120.90

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	19	TYR	Peptide
4	A	210	MET	Peptide
6	C	172	ALA	Peptide
7	D	318	LEU	Peptide
8	E	8	PRO	Peptide
9	F	21	LYS	Peptide
10	G	51	ARG	Peptide
11	H	158	ASP	Peptide
11	H	30	THR	Peptide
11	H	74	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
12	I	121	PHE	Peptide
12	I	59	THR	Peptide
12	I	74	VAL	Peptide
12	I	75	PRO	Peptide
12	I	76	SER	Peptide
13	J	110	PRO	Peptide
23	T	16	GLN	Peptide
30	a	157	ASN	Peptide
32	c	110	GLU	Peptide
43	n	231	THR	Peptide
43	n	26	ILE	Peptide
45	p	32	CYS	Peptide
46	q	123	PRO	Peptide
46	q	124	ARG	Peptide
46	q	133	THR	Peptide
46	q	146	ILE	Peptide
46	q	81	CYS	Peptide
46	q	85	GLY	Peptide
46	q	94	THR	Peptide
47	r	307	ALA	Peptide
47	s	307	ALA	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	
4	A	215/217 (99%)	194 (90%)	11 (5%)	10 (5%)	2	21
5	B	250/254 (98%)	230 (92%)	14 (6%)	6 (2%)	6	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	384/387 (99%)	333 (87%)	37 (10%)	14 (4%)	3	25
7	D	359/362 (99%)	304 (85%)	34 (10%)	21 (6%)	1	18
8	E	167/174 (96%)	120 (72%)	26 (16%)	21 (13%)	0	5
9	F	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	4	26
10	G	173/176 (98%)	147 (85%)	16 (9%)	10 (6%)	1	18
11	H	231/256 (90%)	186 (80%)	26 (11%)	19 (8%)	1	12
12	I	125/165 (76%)	107 (86%)	11 (9%)	7 (6%)	2	19
13	J	195/199 (98%)	180 (92%)	11 (6%)	4 (2%)	7	36
14	K	191/199 (96%)	161 (84%)	18 (9%)	12 (6%)	1	17
15	L	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	22	63
16	M	134/138 (97%)	117 (87%)	8 (6%)	9 (7%)	1	15
17	N	146/149 (98%)	120 (82%)	15 (10%)	11 (8%)	1	13
18	O	201/204 (98%)	184 (92%)	10 (5%)	7 (4%)	3	25
19	P	265/297 (89%)	220 (83%)	27 (10%)	18 (7%)	1	15
20	Q	183/186 (98%)	163 (89%)	16 (9%)	4 (2%)	6	35
21	R	186/189 (98%)	170 (91%)	12 (6%)	4 (2%)	6	35
22	S	170/172 (99%)	154 (91%)	12 (7%)	4 (2%)	6	33
23	T	157/160 (98%)	140 (89%)	10 (6%)	7 (4%)	2	22
24	U	181/184 (98%)	155 (86%)	17 (9%)	9 (5%)	2	20
25	V	98/121 (81%)	75 (76%)	14 (14%)	9 (9%)	1	11
26	W	119/142 (84%)	106 (89%)	11 (9%)	2 (2%)	9	42
27	X	124/127 (98%)	107 (86%)	15 (12%)	2 (2%)	9	44
28	Y	133/136 (98%)	114 (86%)	9 (7%)	10 (8%)	1	13
29	Z	117/120 (98%)	99 (85%)	10 (8%)	8 (7%)	1	15
30	a	220/244 (90%)	200 (91%)	11 (5%)	9 (4%)	3	23
31	b	95/105 (90%)	86 (90%)	8 (8%)	1 (1%)	14	52
32	c	107/113 (95%)	94 (88%)	8 (8%)	5 (5%)	2	21
33	d	125/130 (96%)	111 (89%)	10 (8%)	4 (3%)	4	26
34	e	104/107 (97%)	100 (96%)	2 (2%)	2 (2%)	8	38
35	f	110/121 (91%)	97 (88%)	9 (8%)	4 (4%)	3	25
36	g	97/100 (97%)	75 (77%)	11 (11%)	11 (11%)	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	h	85/88 (97%)	71 (84%)	11 (13%)	3 (4%)	3	25
38	i	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	12	48
39	j	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
40	k	89/92 (97%)	77 (86%)	9 (10%)	3 (3%)	3	26
41	l	376/593 (63%)	354 (94%)	14 (4%)	8 (2%)	7	36
42	m	222/245 (91%)	208 (94%)	13 (6%)	1 (0%)	29	69
43	n	234/236 (99%)	219 (94%)	9 (4%)	6 (3%)	5	31
44	o	345/647 (53%)	330 (96%)	9 (3%)	6 (2%)	9	42
45	p	61/199 (31%)	53 (87%)	4 (7%)	4 (7%)	1	16
46	q	439/515 (85%)	377 (86%)	40 (9%)	22 (5%)	2	20
47	r	320/322 (99%)	266 (83%)	31 (10%)	23 (7%)	1	14
47	s	320/322 (99%)	266 (83%)	31 (10%)	23 (7%)	1	14
All	All	8299/9350 (89%)	7270 (88%)	658 (8%)	371 (4%)	4	22

All (371) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	21	ASN
4	A	74	VAL
4	A	135	PRO
4	A	151	VAL
5	B	144	ASN
6	C	3	HIS
6	C	5	LYS
6	C	140	ASP
6	C	174	LYS
6	C	300	ARG
6	C	347	SER
6	C	351	LEU
6	C	385	LYS
7	D	4	PRO
7	D	268	ALA
7	D	269	SER
7	D	283	THR
7	D	292	SER
7	D	320	ASN
7	D	338	LYS
7	D	361	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	E	8	PRO
8	E	11	ASP
8	E	12	LEU
8	E	74	PRO
8	E	94	ARG
8	E	165	GLN
9	F	50	ASN
9	F	109	ALA
10	G	6	ALA
10	G	98	VAL
10	G	121	LEU
10	G	122	PHE
11	H	25	PRO
11	H	31	PRO
11	H	36	ILE
11	H	37	GLY
11	H	156	ASP
12	I	37	LEU
12	I	51	LYS
12	I	75	PRO
12	I	76	SER
13	J	110	PRO
13	J	111	PRO
13	J	182	ASN
14	K	5	LYS
14	K	47	ALA
14	K	50	PRO
14	K	129	ASN
14	K	131	LYS
14	K	193	ALA
16	M	8	LYS
16	M	9	ALA
16	M	135	LEU
16	M	136	ALA
17	N	66	ALA
17	N	76	ASP
18	O	74	PRO
18	O	75	VAL
19	P	20	PHE
19	P	58	LYS
19	P	210	GLU
19	P	233	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	P	234	ASP
19	P	258	LYS
19	P	276	LYS
19	P	293	LEU
19	P	295	GLY
20	Q	99	THR
21	R	5	ARG
21	R	47	ASN
22	S	167	ARG
23	T	124	VAL
23	T	159	PHE
24	U	157	VAL
24	U	182	ILE
25	V	107	PHE
26	W	44	PRO
27	X	84	LYS
28	Y	17	ARG
28	Y	59	ALA
28	Y	125	GLY
28	Y	128	GLN
28	Y	129	TRP
29	Z	97	ALA
29	Z	119	LYS
30	a	25	GLN
30	a	26	VAL
30	a	216	VAL
31	b	100	ILE
32	c	5	LYS
32	c	6	ASP
32	c	7	VAL
32	c	83	GLU
32	c	84	ASP
33	d	12	LYS
33	d	27	ARG
33	d	123	LYS
36	g	13	LYS
36	g	33	ALA
37	h	85	LYS
41	l	62	PRO
41	l	169	ILE
43	n	18	LYS
43	n	25	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	n	133	LEU
44	o	203	SER
45	p	15	PRO
45	p	33	ARG
46	q	77	TYR
46	q	83	ILE
46	q	84	GLN
46	q	91	PRO
46	q	107	LYS
46	q	124	ARG
46	q	132	VAL
46	q	133	THR
46	q	391	SER
46	q	455	ASP
47	r	81	LEU
47	r	107	ALA
47	r	133	THR
47	r	134	THR
47	r	153	VAL
47	r	194	VAL
47	r	216	TYR
47	r	227	ILE
47	r	238	GLN
47	r	269	GLN
47	r	294	ALA
47	r	296	SER
47	r	308	PRO
47	s	81	LEU
47	s	107	ALA
47	s	133	THR
47	s	134	THR
47	s	153	VAL
47	s	194	VAL
47	s	216	TYR
47	s	227	ILE
47	s	238	GLN
47	s	269	GLN
47	s	294	ALA
47	s	296	SER
47	s	308	PRO
4	A	99	LEU
4	A	168	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	198	TRP
4	A	199	GLN
5	B	13	GLY
5	B	70	ARG
6	C	136	LYS
6	C	138	ALA
7	D	15	ALA
7	D	107	ARG
7	D	182	LEU
7	D	232	SER
7	D	311	HIS
7	D	317	PRO
8	E	9	MET
8	E	73	GLY
8	E	86	VAL
8	E	115	LYS
8	E	167	TYR
10	G	97	ASN
10	G	123	PRO
11	H	39	ALA
11	H	115	ALA
11	H	159	PRO
11	H	254	ASP
12	I	32	ILE
12	I	77	ALA
14	K	136	GLU
14	K	141	ALA
15	L	82	ALA
16	M	10	SER
17	N	47	LYS
17	N	57	GLY
17	N	121	VAL
18	O	144	ARG
18	O	184	LYS
19	P	188	GLU
19	P	209	GLU
19	P	215	ASP
19	P	292	ALA
20	Q	98	LYS
20	Q	183	GLY
22	S	2	ALA
22	S	12	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	S	13	ARG
23	T	125	ALA
24	U	164	LYS
25	V	11	ILE
25	V	50	LEU
25	V	51	GLY
25	V	91	ASP
26	W	45	LYS
27	X	92	GLY
29	Z	90	ARG
29	Z	95	PHE
29	Z	96	GLU
30	a	24	GLU
30	a	175	LYS
35	f	74	ARG
35	f	77	GLY
36	g	28	TYR
36	g	49	GLY
36	g	50	LEU
37	h	65	ARG
40	k	60	CYS
41	l	61	VAL
41	l	354	ILE
43	n	170	GLU
44	o	87	GLU
45	p	62	GLU
46	q	106	ILE
46	q	129	VAL
46	q	146	ILE
46	q	154	HIS
46	q	308	SER
46	q	309	GLN
46	q	318	SER
47	r	45	ILE
47	r	108	ASN
47	r	230	ASN
47	r	276	GLU
47	s	45	ILE
47	s	108	ASN
47	s	230	ASN
47	s	276	GLU
4	A	137	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	250	GLN
6	C	4	ARG
7	D	14	GLU
7	D	16	THR
8	E	140	ARG
8	E	169	ALA
8	E	173	ASP
9	F	42	ASP
11	H	78	PHE
11	H	122	LYS
14	K	134	GLU
14	K	166	ALA
16	M	28	SER
16	M	95	ALA
17	N	93	SER
18	O	145	ASP
19	P	112	LYS
21	R	53	LYS
21	R	64	ARG
23	T	114	ALA
24	U	160	ALA
25	V	10	LYS
25	V	44	GLU
28	Y	16	GLY
28	Y	35	SER
28	Y	102	GLU
29	Z	4	VAL
29	Z	91	ALA
35	f	46	ASP
35	f	98	GLN
36	g	34	SER
36	g	95	ALA
36	g	98	ARG
40	k	58	SER
41	l	173	THR
41	l	175	PRO
43	n	5	LYS
43	n	23	LYS
44	o	311	GLU
44	o	342	SER
45	p	61	LYS
46	q	486	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	r	259	GLU
47	s	259	GLU
6	C	386	ASP
7	D	146	PRO
7	D	233	LEU
8	E	95	ASN
8	E	108	GLU
8	E	114	ILE
8	E	117	ASP
9	F	13	PRO
10	G	95	GLY
10	G	129	GLU
11	H	157	VAL
11	H	253	SER
13	J	181	ALA
17	N	96	LYS
18	O	94	TYR
18	O	149	ASN
19	P	6	ASP
19	P	252	ALA
19	P	253	PHE
20	Q	162	ALA
23	T	12	ARG
24	U	158	ALA
24	U	161	ALA
24	U	163	LYS
25	V	31	ALA
25	V	49	ASN
28	Y	103	GLN
29	Z	27	GLU
30	a	160	ARG
33	d	40	SER
37	h	25	ARG
38	i	33	LYS
40	k	51	ALA
46	q	49	LEU
47	r	87	LYS
47	r	307	ALA
47	r	310	ILE
47	s	87	LYS
47	s	307	ALA
47	s	310	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	35	ALA
5	B	251	LYS
7	D	5	GLN
8	E	24	GLY
8	E	111	ASP
8	E	172	LEU
9	F	2	LYS
9	F	107	ASP
10	G	108	LYS
11	H	47	SER
12	I	95	ASP
14	K	130	GLY
14	K	133	PRO
16	M	6	ILE
16	M	36	VAL
17	N	56	VAL
17	N	117	ARG
23	T	18	ASP
30	a	178	ILE
34	e	59	VAL
36	g	3	VAL
47	r	167	ARG
47	r	295	GLU
47	s	167	ARG
47	s	295	GLU
4	A	134	PHE
6	C	155	ALA
6	C	317	ILE
7	D	72	ALA
10	G	130	ILE
11	H	75	ILE
17	N	91	LEU
19	P	259	LYS
24	U	162	GLU
30	a	164	SER
34	e	91	ALA
36	g	21	THR
36	g	94	ILE
44	o	221	THR
17	N	29	PRO
41	l	389	PRO
11	H	158	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	91	GLY
41	l	550	VAL
44	o	344	ILE
46	q	73	ASP
11	H	116	VAL
11	H	119	GLY
11	H	135	GLY
28	Y	36	HIS
7	D	131	VAL
24	U	84	PRO
42	m	58	ILE
46	q	387	ASN
46	q	483	PRO
23	T	123	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	0/3396	-	-
2	2	0/158	-	-
3	3	0/121	-	-
All	All	0/3675	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1
45	p	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	439:C	O3'	440:A	P	1.76
1	p	61:LYS	C	62:GLU	N	1.66

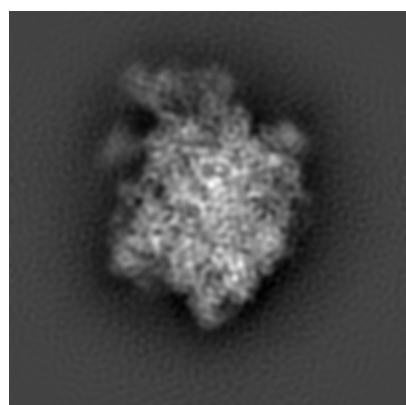
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2528. These allow visual inspection of the internal detail of the map and identification of artifacts.

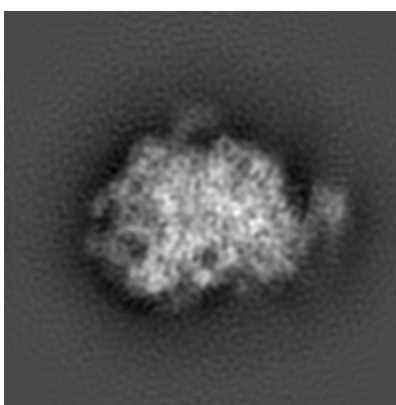
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

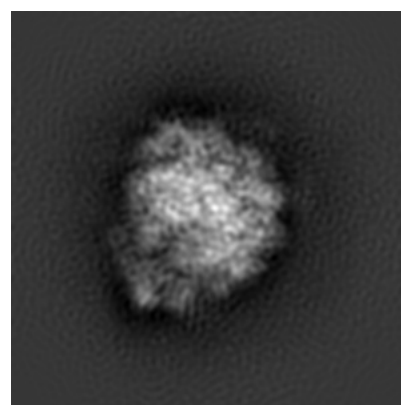
6.1.1 Primary map



X



Y

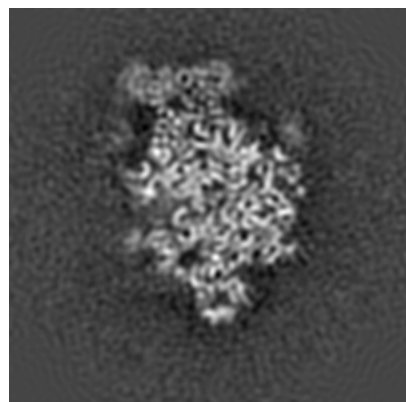


Z

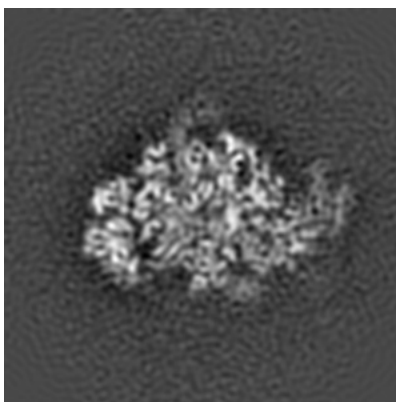
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

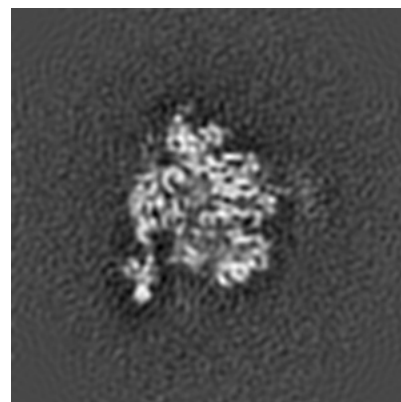
6.2.1 Primary map



X Index: 207



Y Index: 207

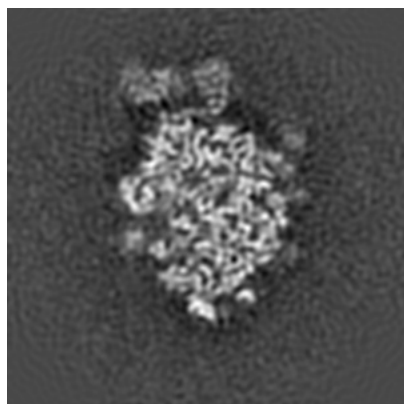


Z Index: 207

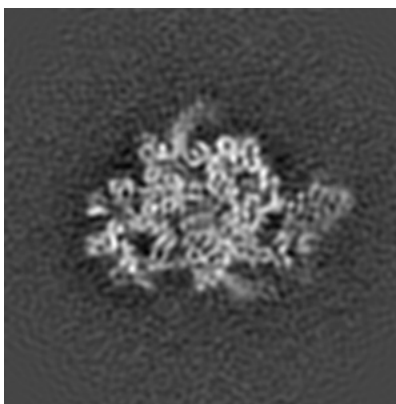
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

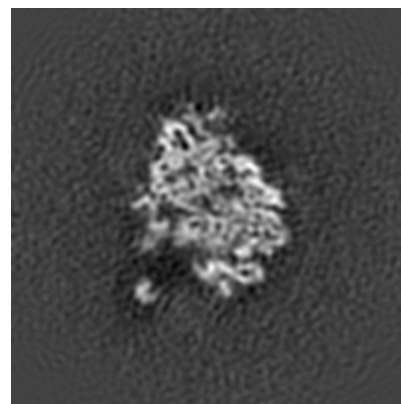
6.3.1 Primary map



X Index: 218



Y Index: 215

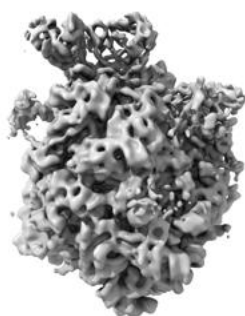


Z Index: 223

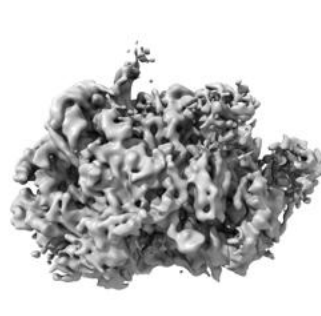
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

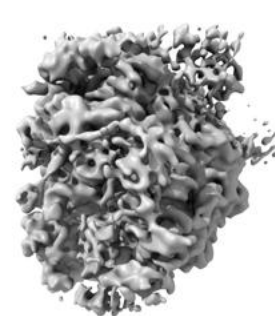
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

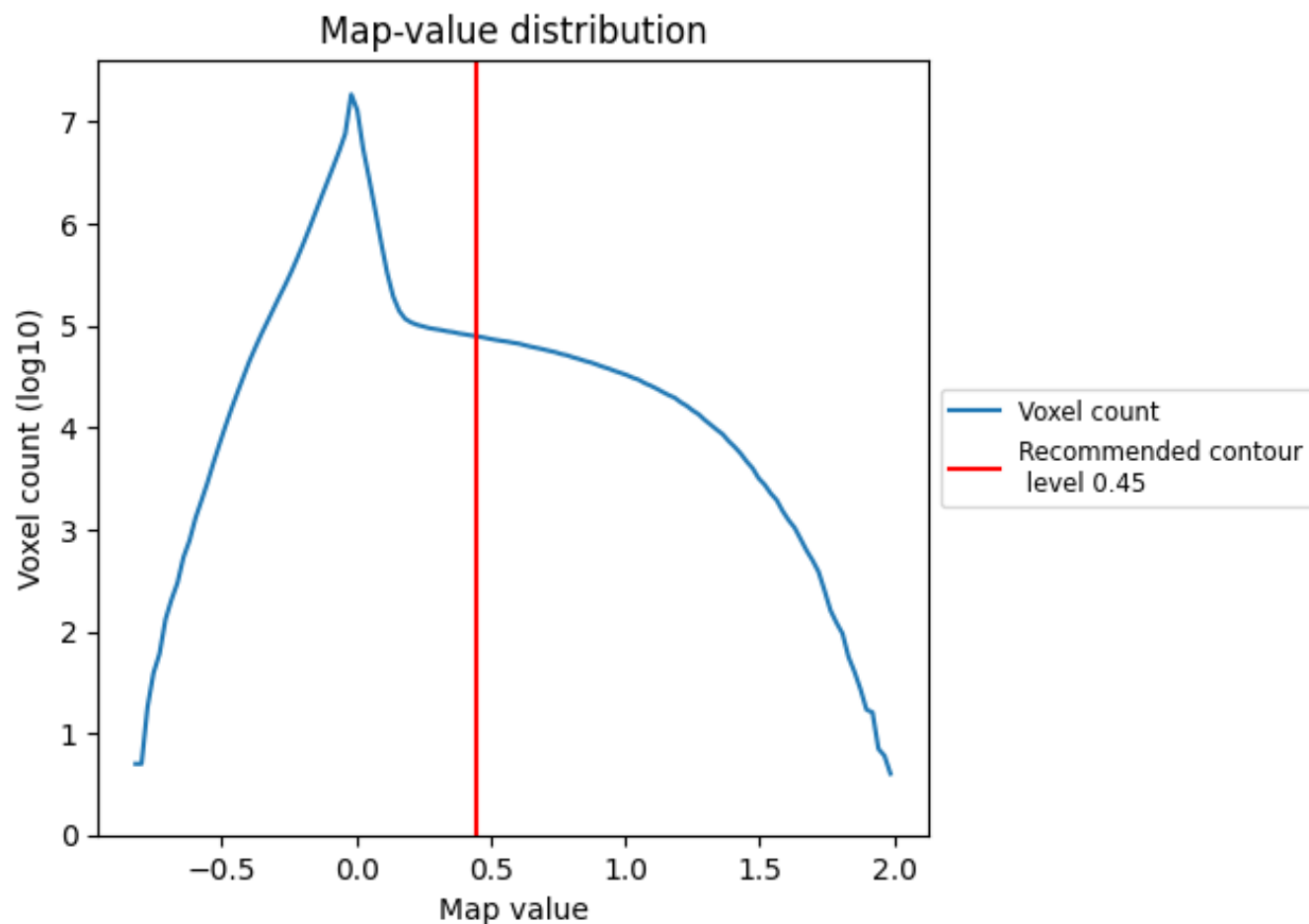
6.5 Mask visualisation

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

7 Map analysis [i](#)

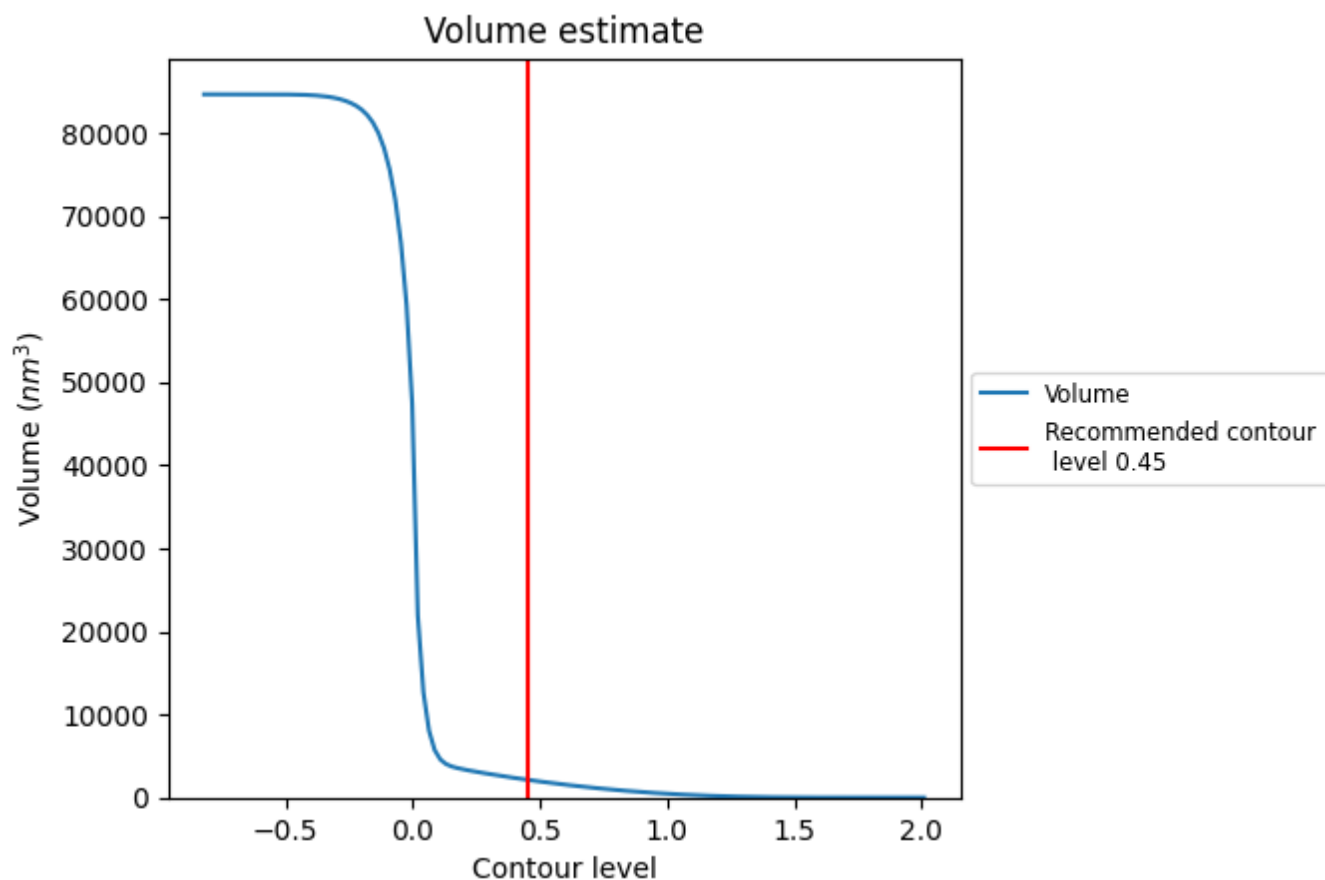
This section contains the results of statistical analysis of the map.

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.

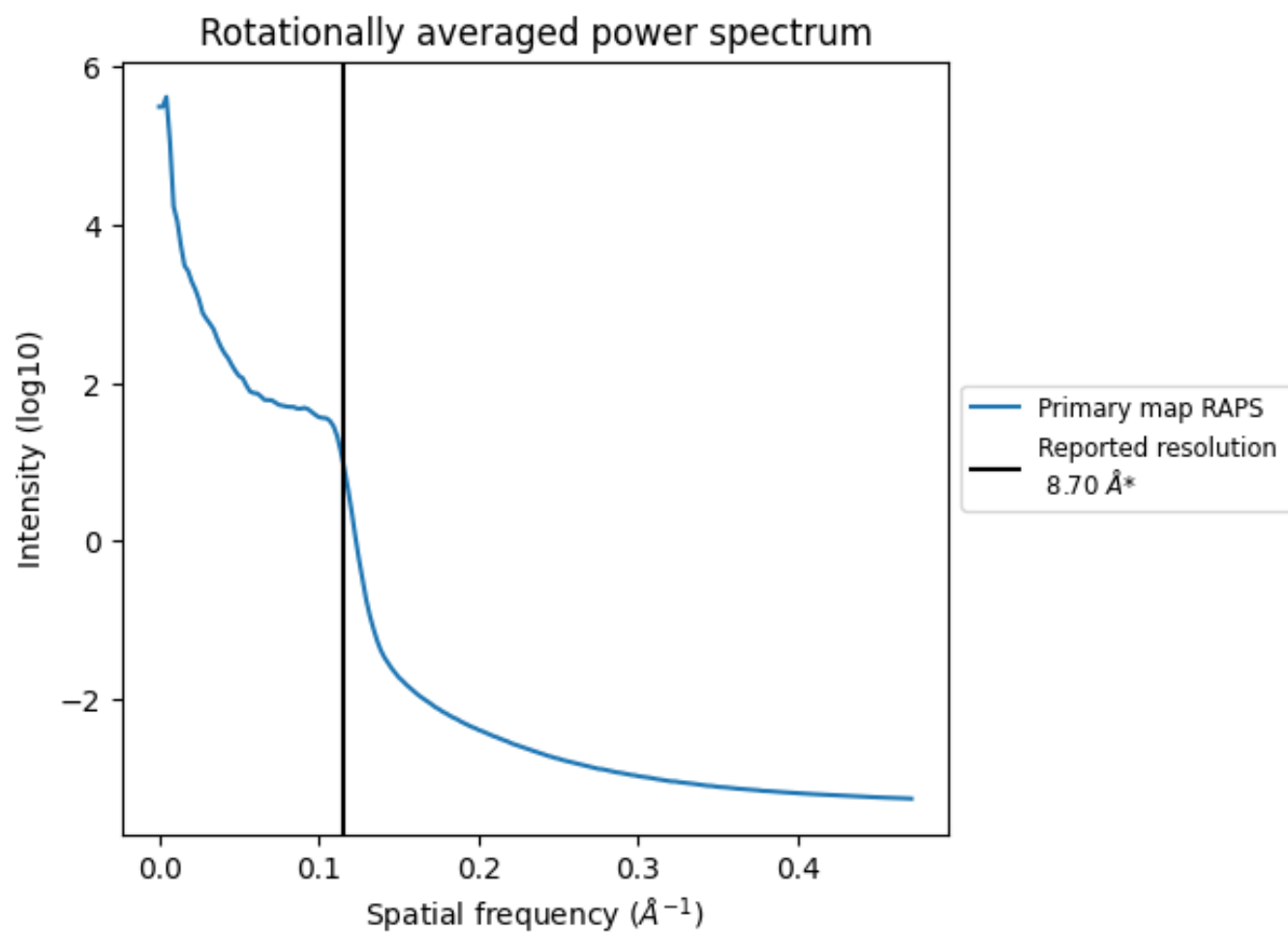
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2140 nm³; this corresponds to an approximate mass of 1933 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.115 \AA^{-1}

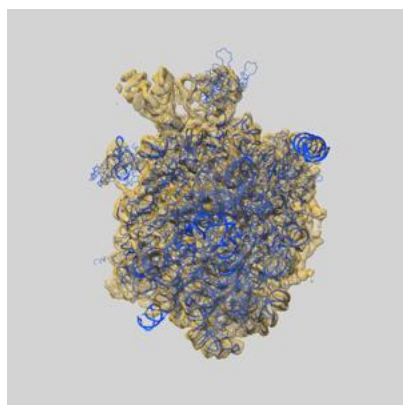
8 Fourier-Shell correlation ⓘ

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

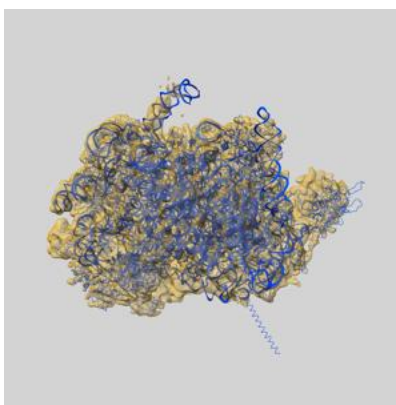
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2528 and PDB model 4V7F. Per-residue inclusion information can be found in section [3](#) on page [12](#).

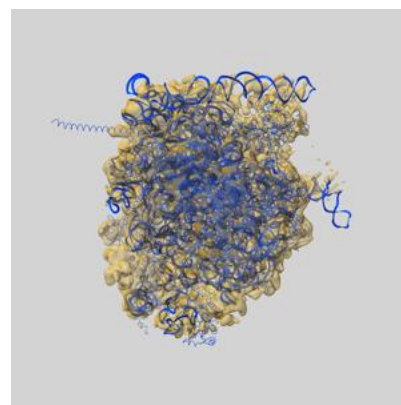
9.1 Map-model overlay [i](#)



X



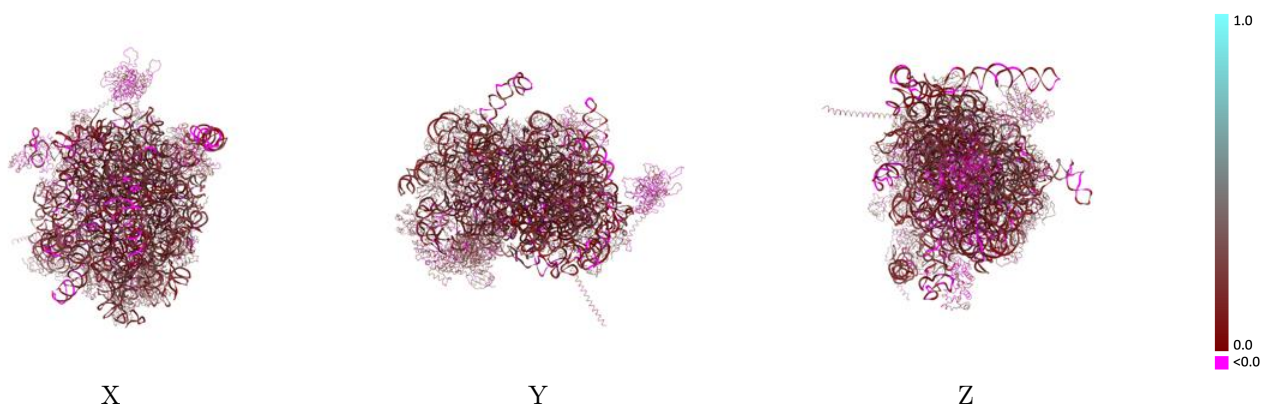
Y



Z

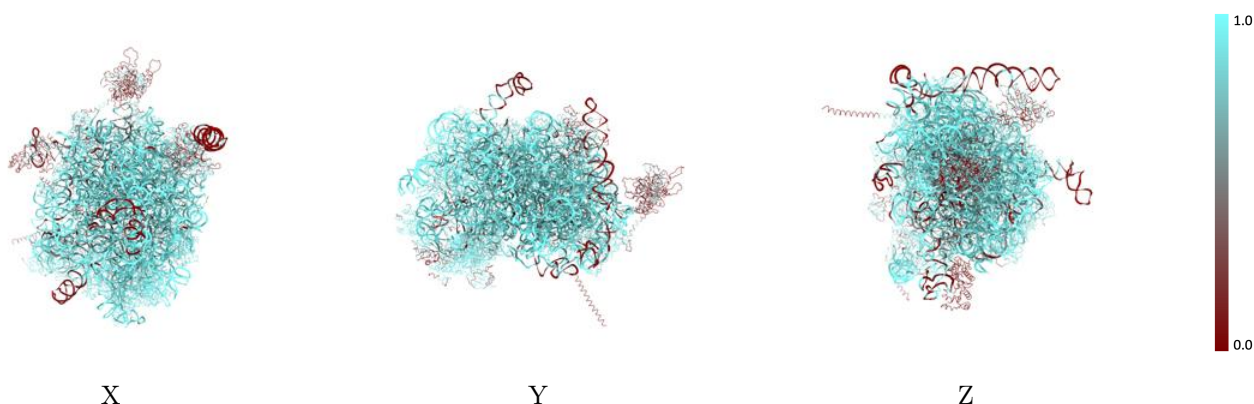
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



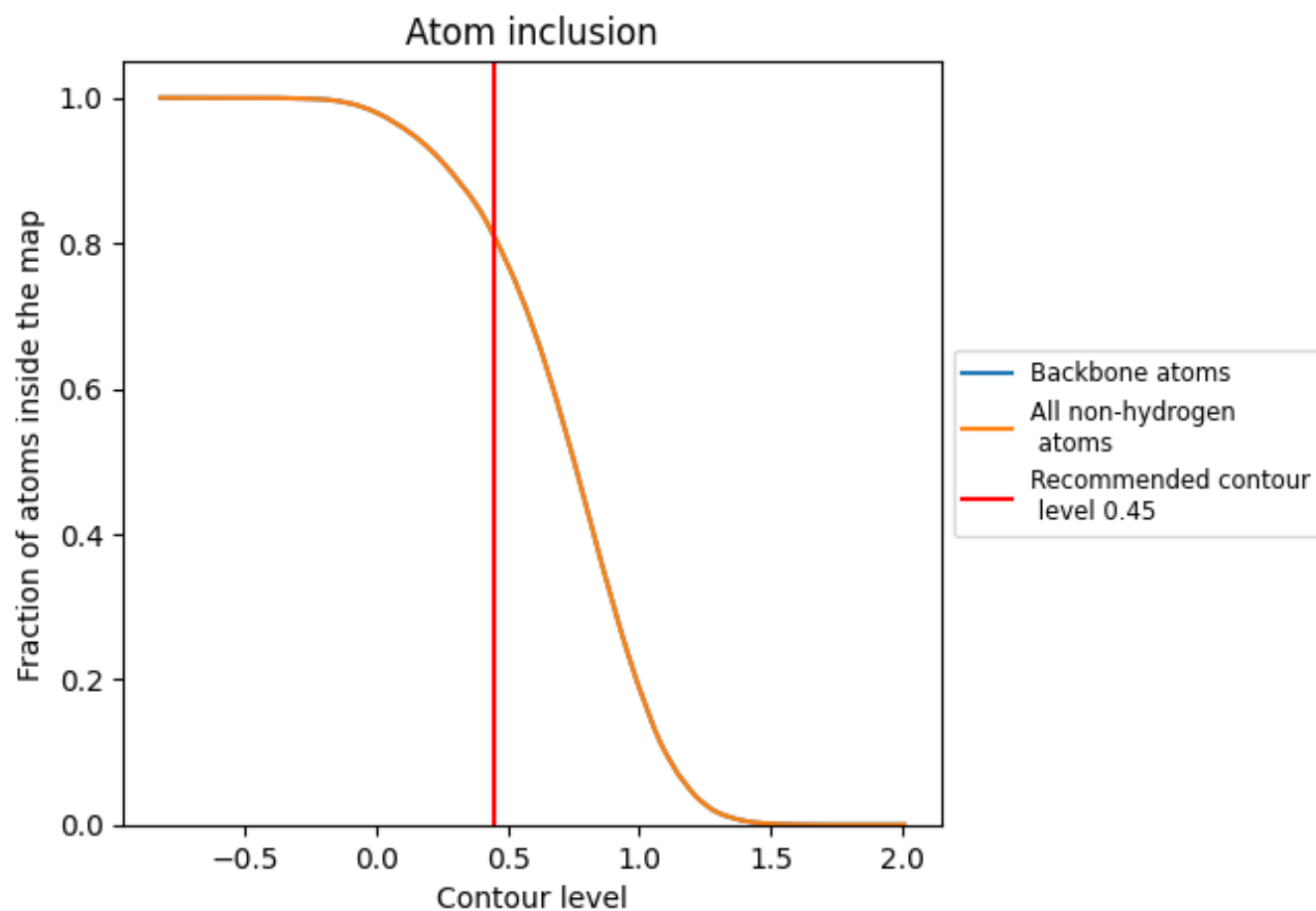
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8082	 0.1560
1	 0.8442	 0.1400
2	 0.9673	 0.1700
3	 0.9724	 0.1540
A	 0.0246	 0.0170
B	 0.6839	 0.1120
C	 0.9378	 0.1990
D	 0.9400	 0.2090
E	 0.9645	 0.1880
F	 0.9284	 0.2120
G	 0.9524	 0.2310
H	 0.7668	 0.1650
I	 0.3596	 0.0670
J	 0.9797	 0.2570
K	 0.8117	 0.1410
L	 0.8578	 0.1920
M	 0.9804	 0.2690
N	 0.5811	 0.0550
O	 0.7586	 0.1340
P	 0.7807	 0.1580
Q	 0.7874	 0.1820
R	 0.7730	 0.2020
S	 0.9419	 0.2150
T	 0.5409	 0.0560
U	 0.9490	 0.2170
V	 0.9400	 0.2290
W	 0.9008	 0.2300
X	 0.9815	 0.2090
Y	 0.9852	 0.2490
Z	 0.9608	 0.2350
a	 0.9760	 0.2420
b	 0.9828	 0.2430
c	 0.9358	 0.2360
d	 0.9265	 0.2230
e	 0.9843	 0.1910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.8274	 0.1640
g	 0.6700	 0.1370
h	 0.9425	 0.1650
i	 0.9567	 0.2660
j	 0.9667	 0.2520
k	 0.8498	 0.1810
l	 0.3632	 0.1410
m	 0.9628	 0.2360
n	 0.9449	 0.1950
o	 0.8012	 0.1900
p	 0.9418	 0.2080
q	 0.8126	 0.1440
r	 0.2474	 0.0310
s	 0.2277	 0.0010