Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:40 pm BST

PDB ID	:	6YLG / pdb_00006ylg
EMDB ID	:	EMD-10838
Title	:	Rix1-Rea1 pre-60S particle - 60S core, body 1 (rigid body refinement)
Authors	:	Kater, L.; Beckmann, R.
Deposited on	:	2020-04-07
Resolution	:	3.00 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:

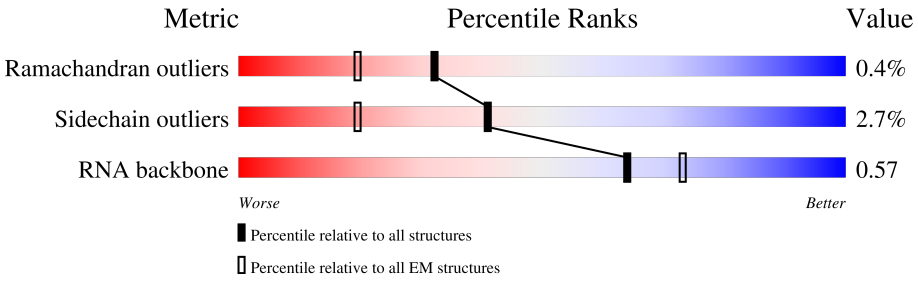
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.00 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	71% 18% 11%
2	2	158	80% 17%
3	3	121	80% 17%
4	4	593	22% 81% 14%
5	5	120	19% 61% 35%
6	A	254	94%
7	B	387	96%
8	C	362	98%

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Mol	Chain	Length	Quality of chain
9	D	297	23% 79% 18%
10	E	176	85% 11%
11	F	244	86% 11%
12	G	256	5% 85% 11%
13	H	191	96%
14	I	166	10% 71% 7% 22%
15	J	174	19% 93%
16	K	334	9% 67% 30%
17	L	199	88% 9%
18	M	138	94%
19	N	204	97%
20	O	199	97%
21	P	184	92% 7%
22	Q	186	76% 23%
23	R	189	79% 20%
24	S	172	5% 95%
25	T	160	21% 71% 6% 22%
26	U	121	80% 17%
27	V	137	6% 82% 12%
28	W	236	96%
29	X	142	10% 98%
30	Y	127	95%
31	Z	136	96%
32	a	149	60% 38%
33	b	647	12% 88% 6% 5%

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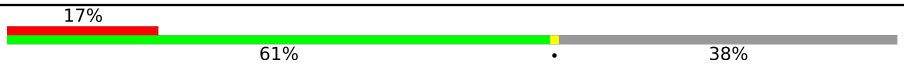
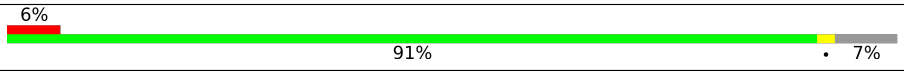
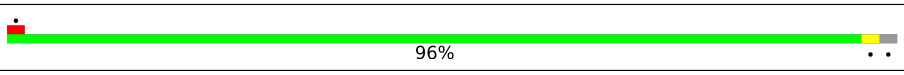
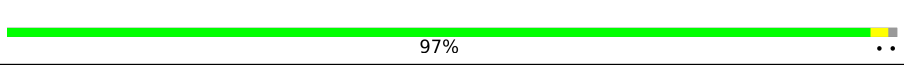
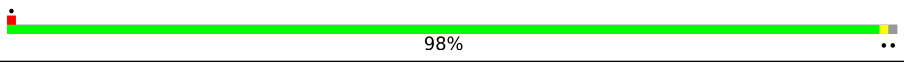
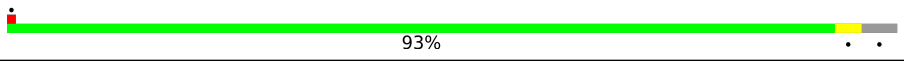
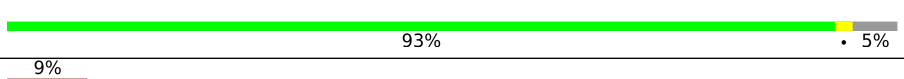
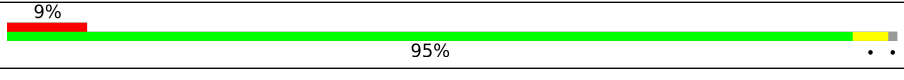
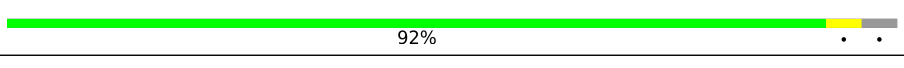
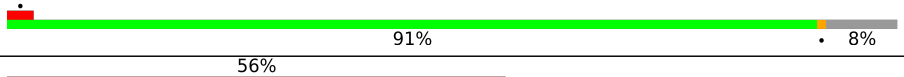
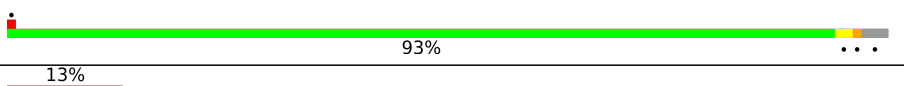
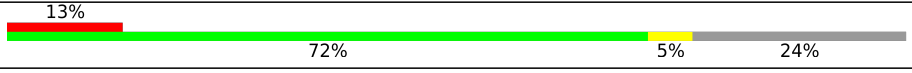
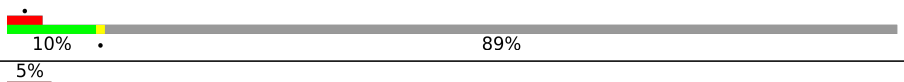
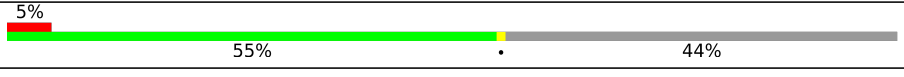
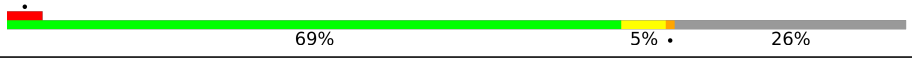
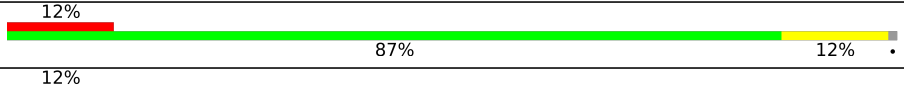
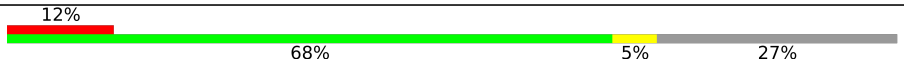
Mol	Chain	Length	Quality of chain
34	c	175	
35	d	113	
36	e	130	
37	f	107	
38	g	121	
39	h	120	
40	i	100	
41	j	88	
42	k	78	
43	l	51	
44	m	486	
45	n	105	
46	o	217	
47	p	92	
48	q	165	
49	r	261	
50	s	520	
51	t	767	
52	u	199	
53	x	515	
54	y	245	
55	z	106	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147190 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3039	65028	29041	11740	21208	3039	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	154	3273	1464	576	1079	154	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	117	2494	1114	446	817	117	0	0

- Molecule 4 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	509	3945	2503	673	754	15	0	0

- Molecule 5 is a protein called rRNA-processing protein CGR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	78	681	419	140	119	3	0	0

- Molecule 6 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	245	1863	1162	376	324	1	0	0

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 8 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	243	Total	C	N	O	S	0	0
			1969	1250	344	373	2		

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

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

- Molecule 11 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	216	Total	C	N	O	S	0	0
			1744	1127	317	299	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	228	Total	C	N	O	S	0	0
			1784	1142	320	319	3		

- Molecule 13 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	187	Total	C	N	O	S	0	0
			1486	944	270	268	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	130	Total	C	N	O	S	0	0
			1051	657	194	197	3		

- Molecule 15 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 16 is a protein called Pre-rRNA-processing protein IPI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	234	Total	C	N	O	S	0	0
			1875	1203	331	333	8		

- Molecule 17 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	L	181	Total	C	N	O	0	0
			1456	907	301	248		

- Molecule 18 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1040	666	196	176	2		

- Molecule 19 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 20 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 21 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	P	171	Total	C	N	O	0	0
			1360	845	272	243		

- Molecule 22 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	144	Total	C	N	O	S	0	0
			1110	704	213	192	1		

- Molecule 23 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	151	Total	C	N	O	0	0
			1219	757	258	204		

- Molecule 24 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 25 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	124	Total	C	N	O	S	0	0
			983	619	188	173	3		

- Molecule 26 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	101	Total	C	N	O	0	0
			800	518	131	151		

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 28 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	233	Total	C	N	O	S	0	0
			1877	1189	322	361	5		

- Molecule 29 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	140	Total	C	N	O	S	0	0
			1092	699	195	196	2		

- Molecule 30 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 31 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 33 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	613	Total	C	N	O	S	0	0
			4953	3110	892	926	25		

- Molecule 34 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	c	109	Total	C	N	O	0	0
			872	543	171	158		

- Molecule 35 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	105	Total	C	N	O	S	0	0
			856	544	163	148	1		

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	107	Total	C	N	O	S	0	0
			846	525	173	144	4		

- Molecule 39 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 40 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 41 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 42 is a protein called 60S ribosomal protein L38.

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

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	49	Total 428	C 266	N 96	O 64	S 2	0	0

- Molecule 44 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	439	Total 3546	C 2249	N 647	O 641	S 9	0	0

- Molecule 45 is a protein called 60S ribosomal protein L30.

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

- Molecule 46 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	o	177	Total 877	C 523	N 177	O 177	0	0

- Molecule 47 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	89	Total 680	C 421	N 136	O 117	S 6	0	0

- Molecule 48 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	126	Total 961	C 606	N 171	O 182	S 2	0	0

- Molecule 49 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	225	Total	C	N	O	S	0	0
			1818	1152	345	314	7		

- Molecule 50 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	56	Total	C	N	O	S	0	0
			463	291	94	77	1		

- Molecule 51 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	431	Total	C	N	O	S	0	0
			3395	2156	587	629	23		

- Molecule 52 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	148	Total	C	N	O	S	0	0
			1247	783	250	205	9		

- Molecule 53 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	388	Total	C	N	O	S	0	0
			3033	1900	549	564	20		

- Molecule 54 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	243	Total	C	N	O	S	0	0
			1841	1141	318	376	6		

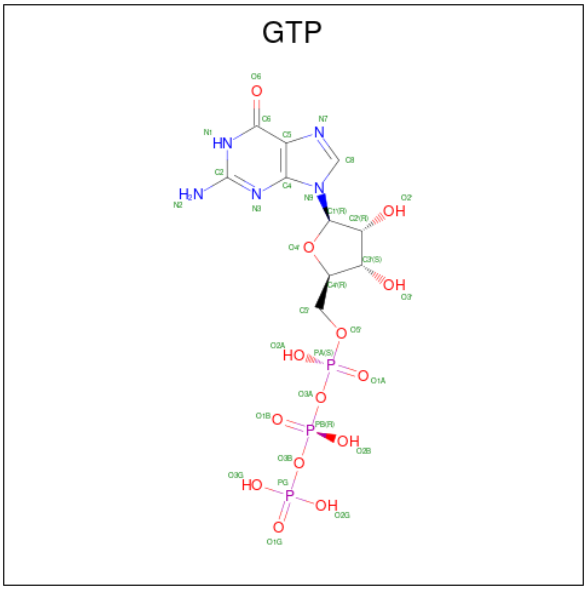
- Molecule 55 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	77	Total	C	N	O	S	0	0
			643	403	130	109	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	AltConf
57	b	1	Total C N O P 32 10 5 14 3	0
57	m	1	Total C N O P 32 10 5 14 3	0

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

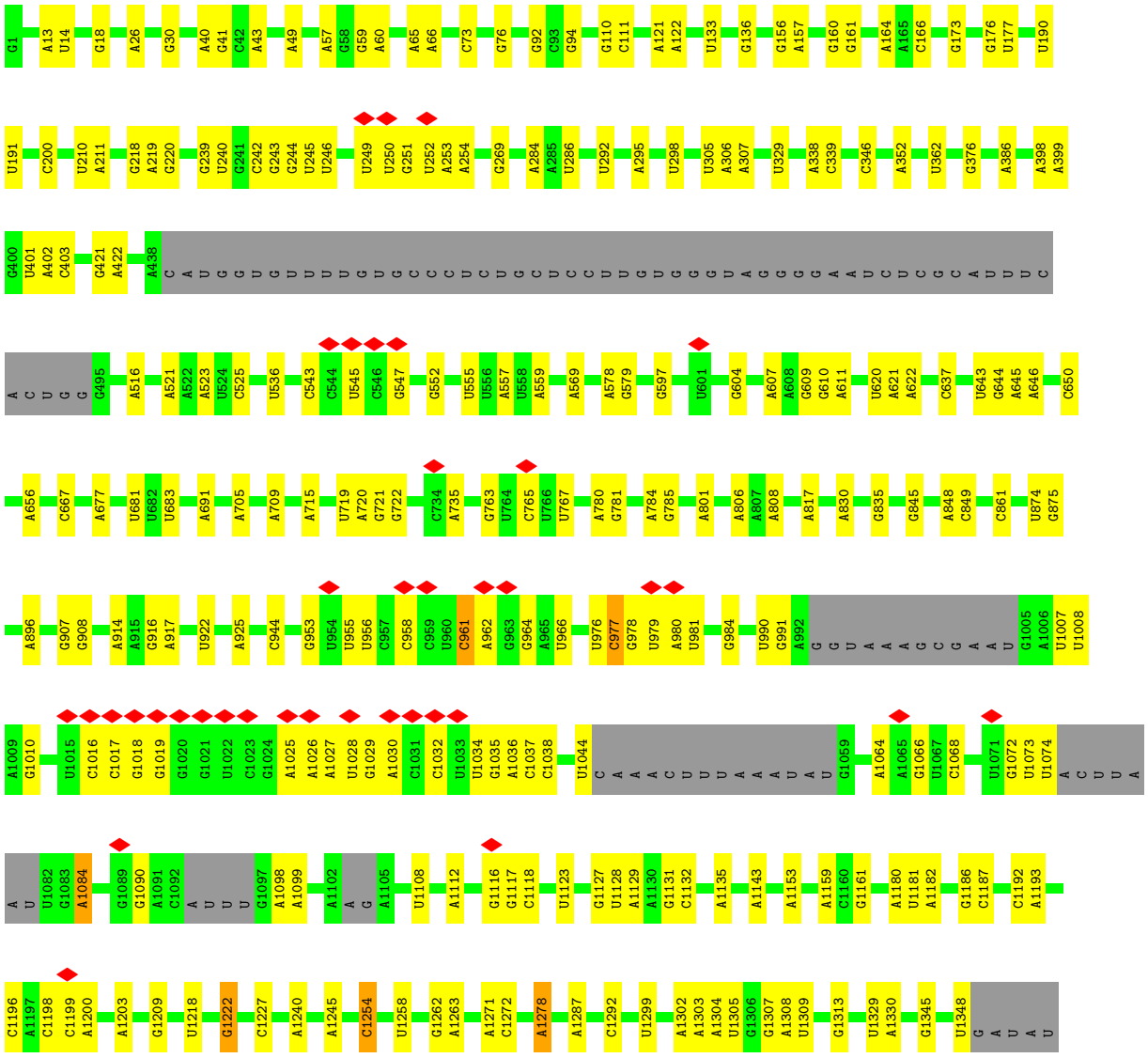
Mol	Chain	Residues	Atoms	AltConf
58	b	1	Total Mg 1 1	0
58	m	1	Total Mg 1 1	0

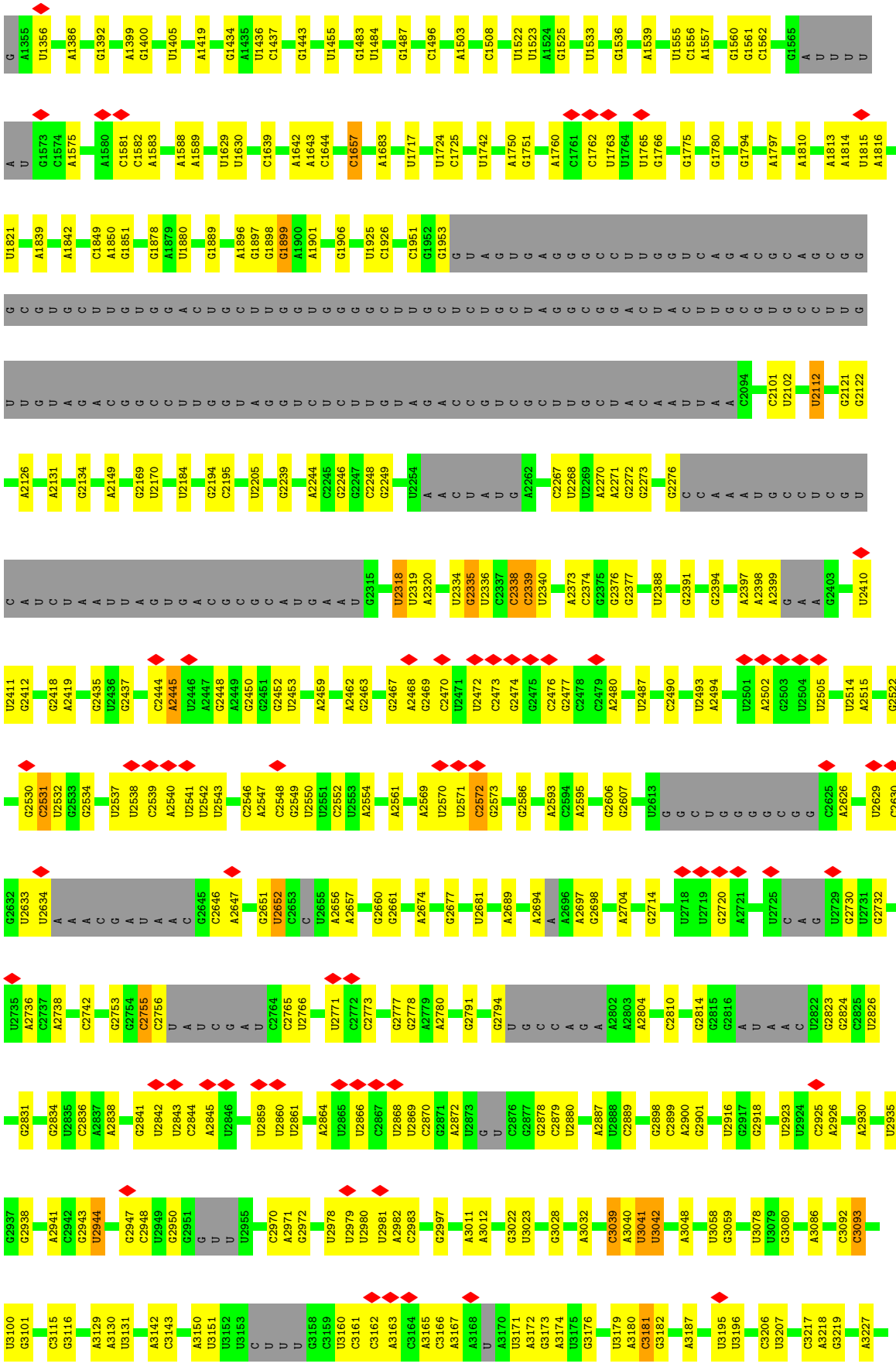
3 Residue-property plots (i)

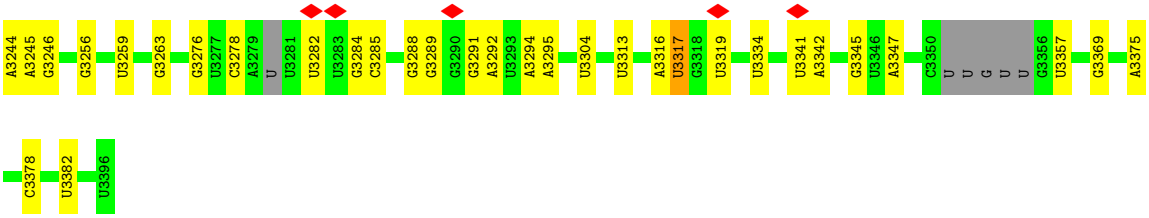
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 25S rRNA

Chain 1:

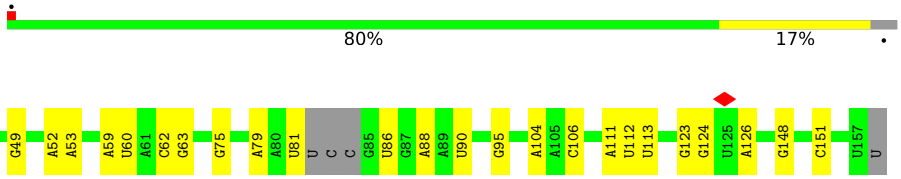






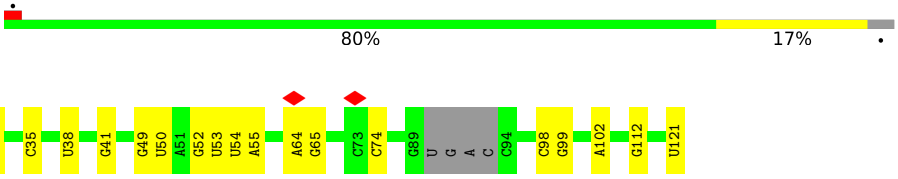
• Molecule 2: 5.8S rRNA

Chain 2:



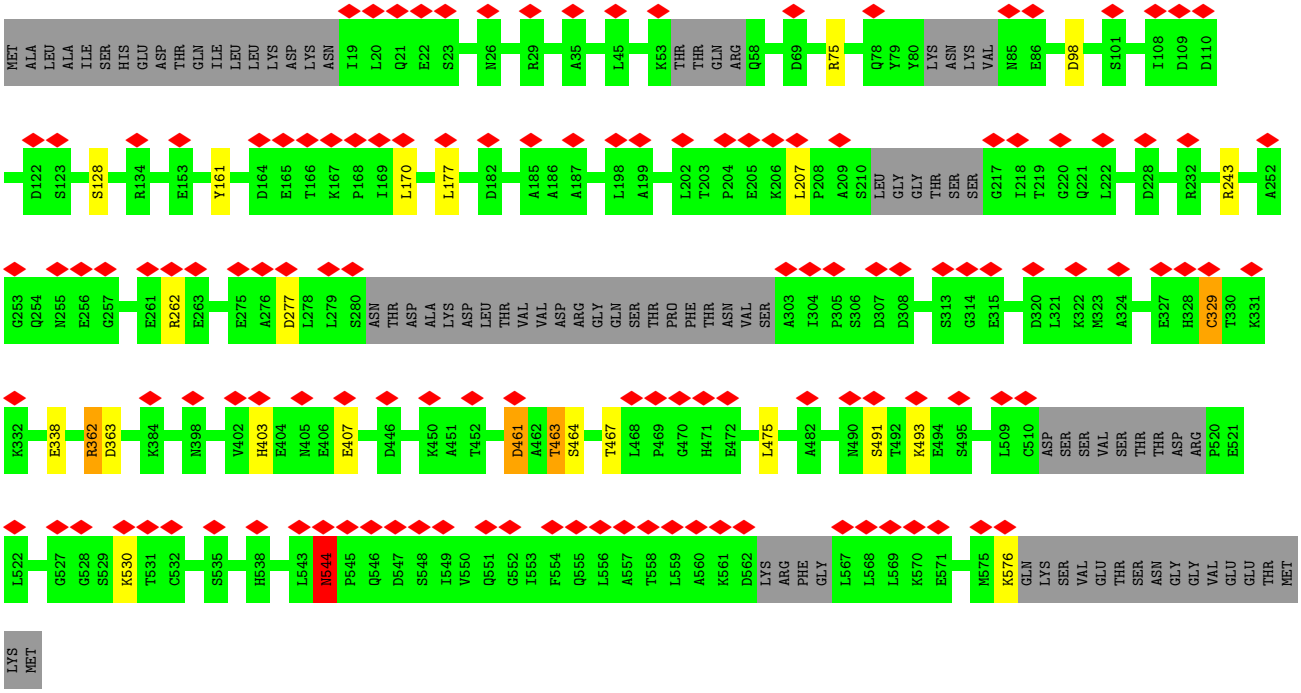
• Molecule 3: 5S rRNA

Chain 3:



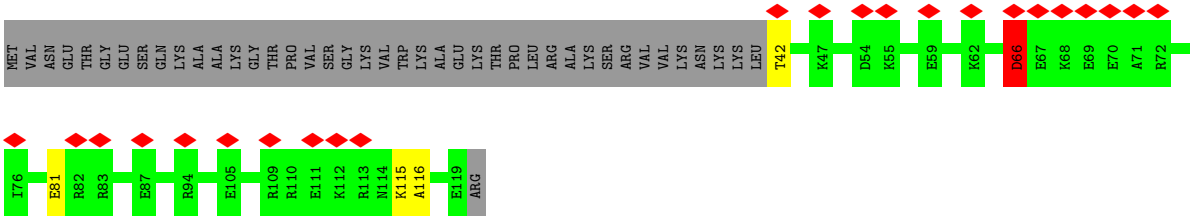
• Molecule 4: Probable metalloprotease ARX1

Chain 4:

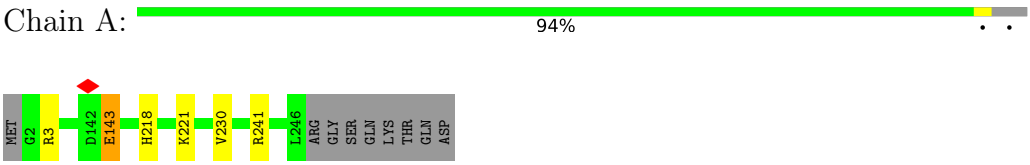


• Molecule 5: rRNA-processing protein CGR1

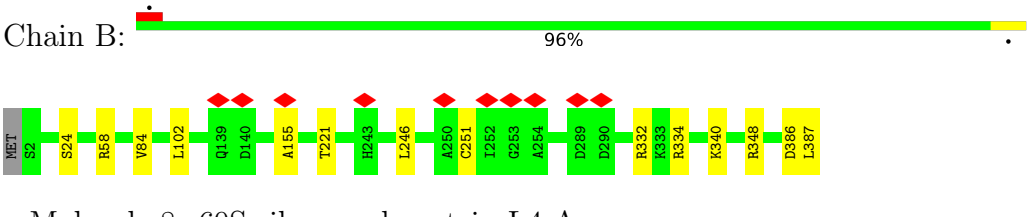
Chain 5:



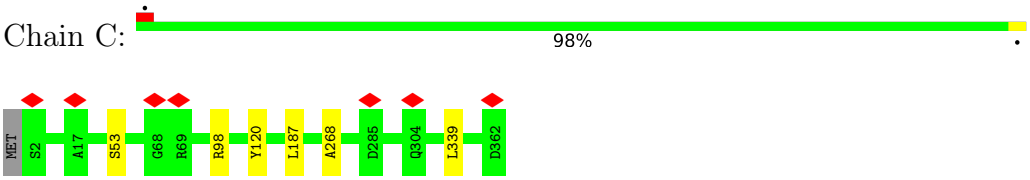
• Molecule 6: 60S ribosomal protein L2-A



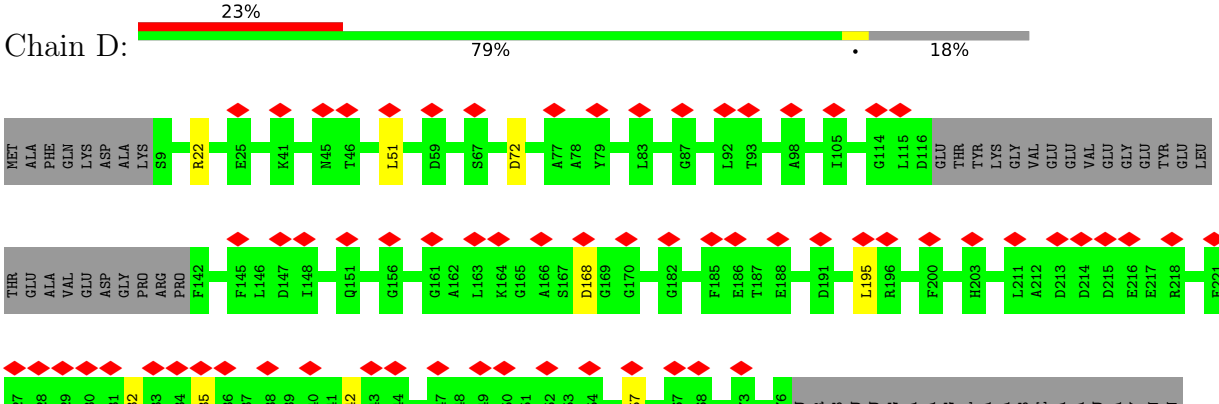
• Molecule 7: 60S ribosomal protein L3



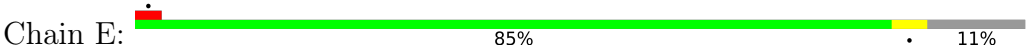
• Molecule 8: 60S ribosomal protein L4-A

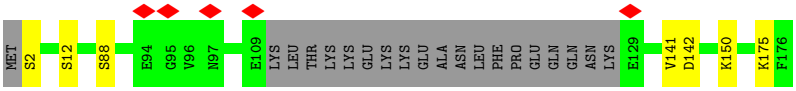


• Molecule 9: 60S ribosomal protein L5

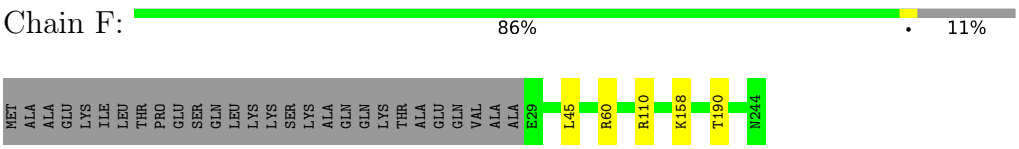


• Molecule 10: 60S ribosomal protein L6-A

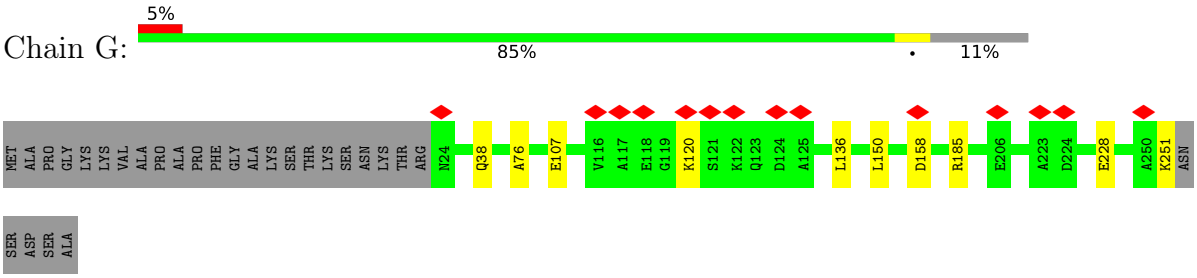




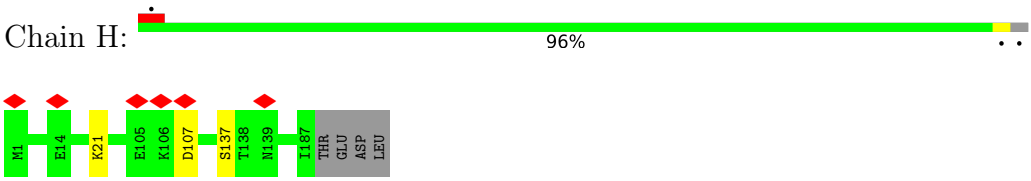
• Molecule 11: 60S ribosomal protein L7-A



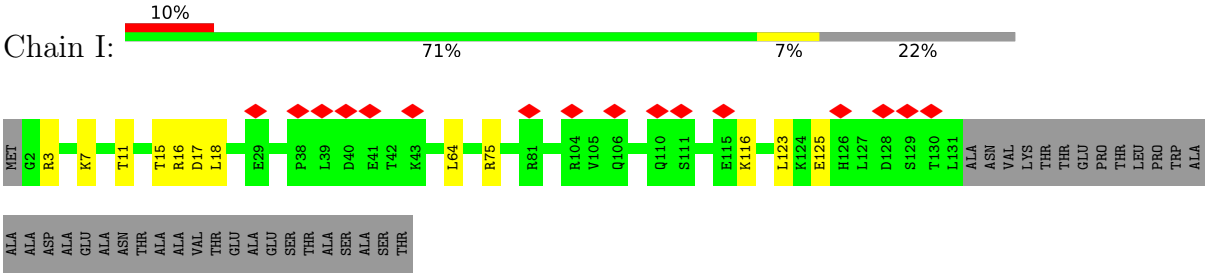
• Molecule 12: 60S ribosomal protein L8-A



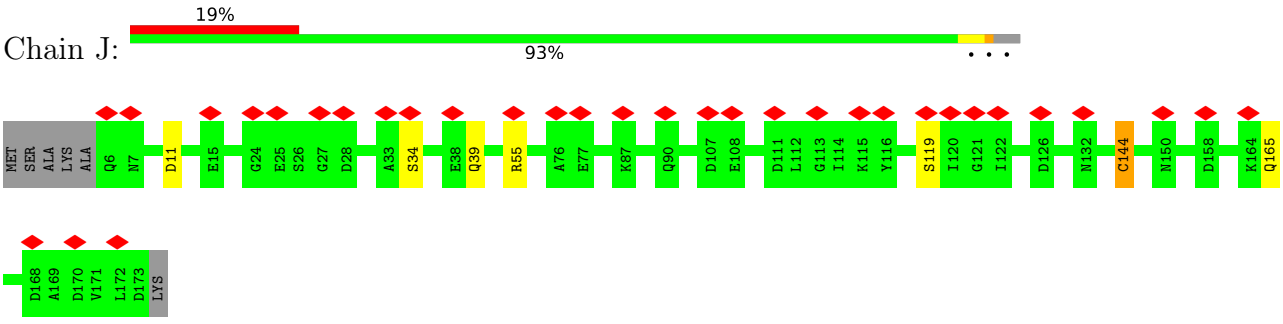
• Molecule 13: 60S ribosomal protein L9-A



• Molecule 14: Bud site selection protein 20

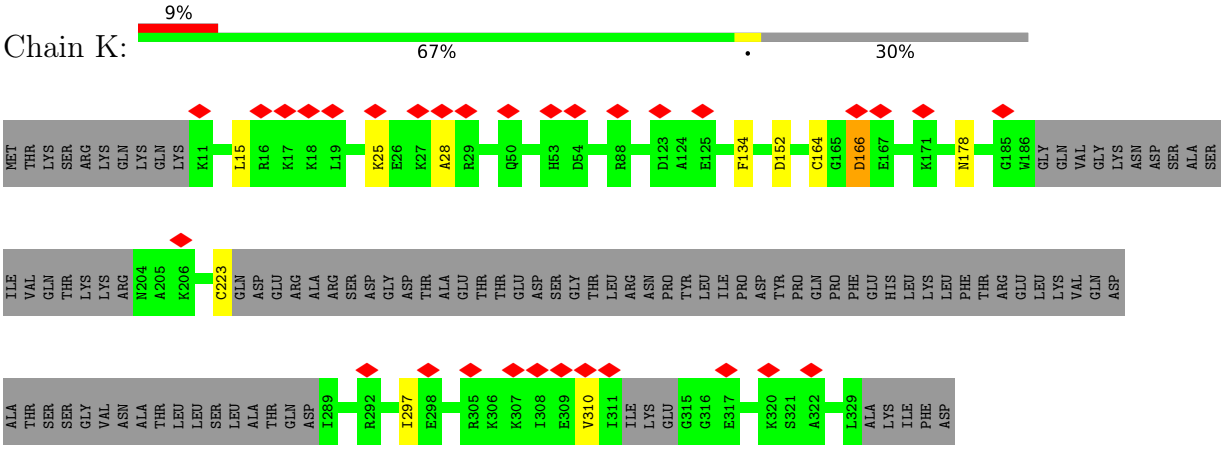


• Molecule 15: 60S ribosomal protein L11-A



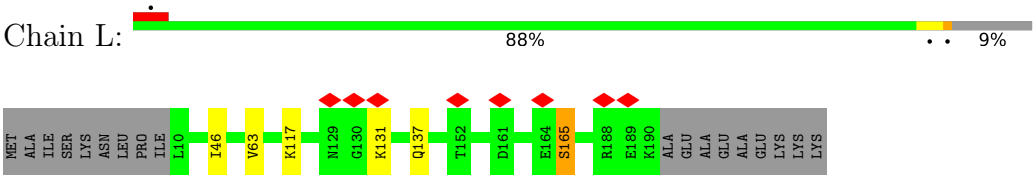
• Molecule 16: Pre-rRNA-processing protein IPI1

Chain K:



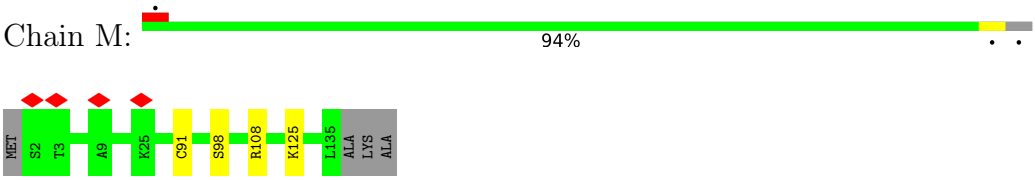
• Molecule 17: 60S ribosomal protein L13-A

Chain L:



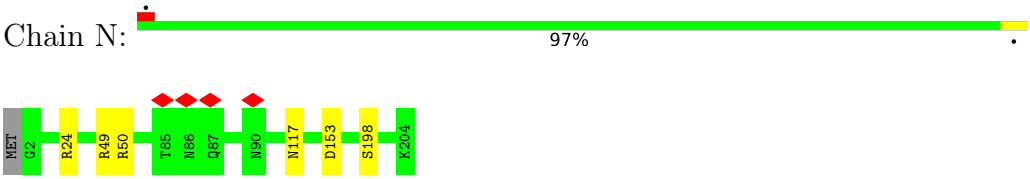
• Molecule 18: 60S ribosomal protein L14-A

Chain M:



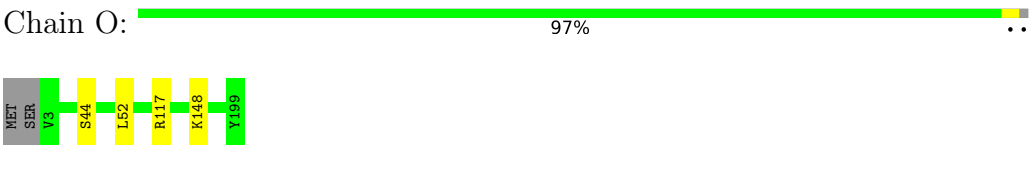
• Molecule 19: 60S ribosomal protein L15-A

Chain N:



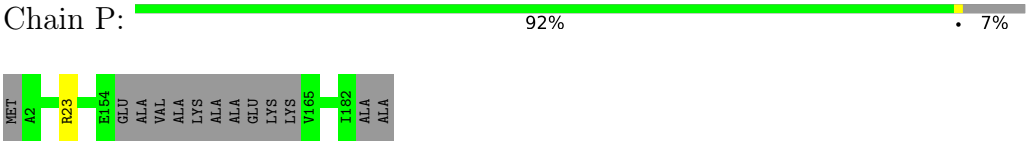
• Molecule 20: 60S ribosomal protein L16-A

Chain O:



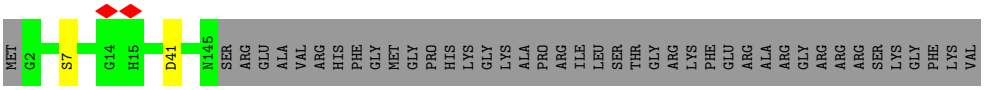
• Molecule 21: 60S ribosomal protein L17-A

Chain P:



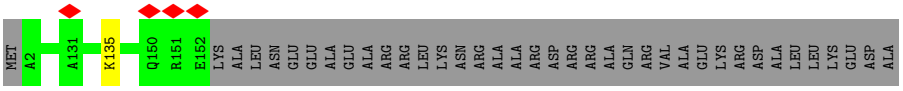
• Molecule 22: 60S ribosomal protein L18-A

Chain Q:



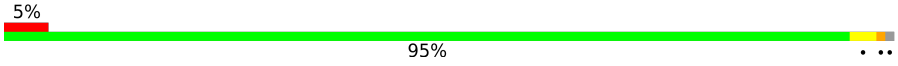
• Molecule 23: 60S ribosomal protein L19-A

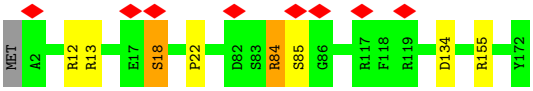
Chain R:



• Molecule 24: 60S ribosomal protein L20-A

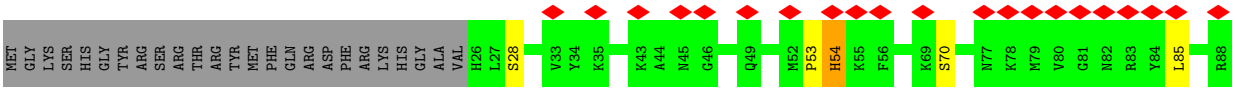
Chain S:

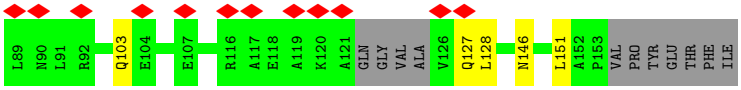




• Molecule 25: 60S ribosomal protein L21-A

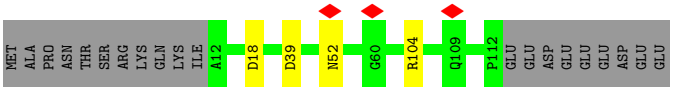
Chain T:





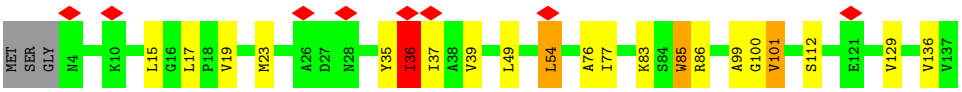
• Molecule 26: 60S ribosomal protein L22-A

Chain U:



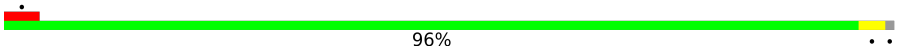
• Molecule 27: 60S ribosomal protein L23-A

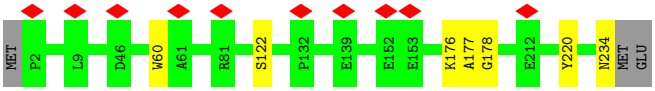
Chain V:



• Molecule 28: Ribosome assembly factor MRT4

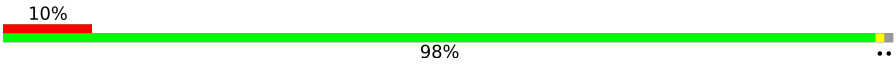
Chain W:

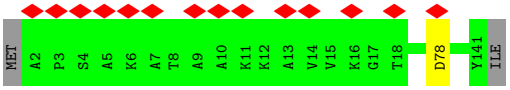




• Molecule 29: 60S ribosomal protein L25

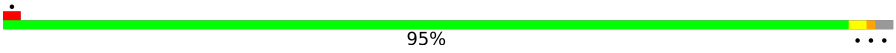
Chain X:

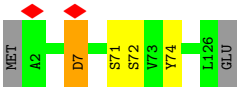




• Molecule 30: 60S ribosomal protein L26-A

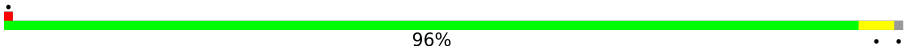
Chain Y:

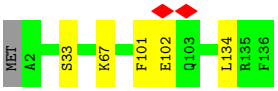




• Molecule 31: 60S ribosomal protein L27-A

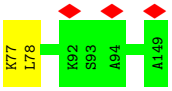
Chain Z:





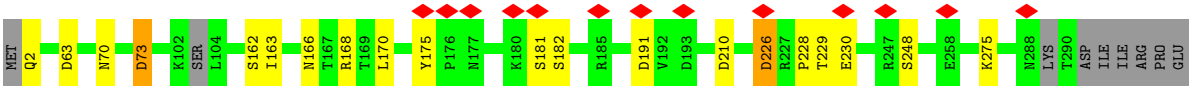
• Molecule 32: 60S ribosomal protein L28

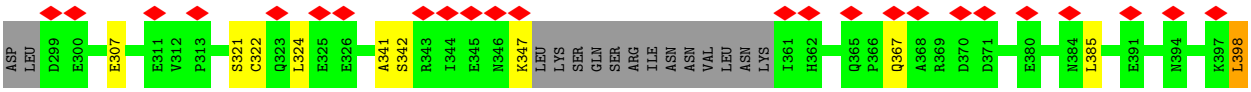
Chain a:

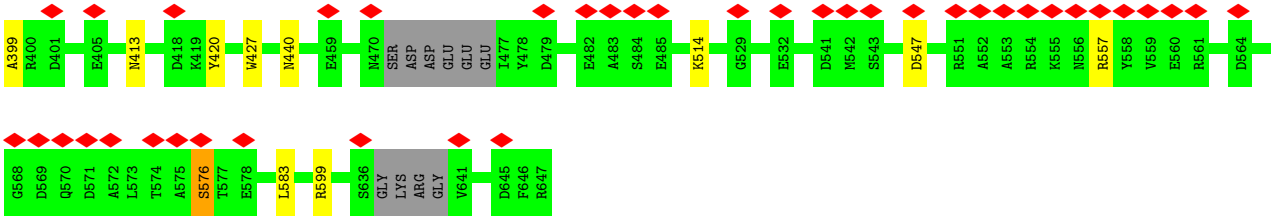


• Molecule 33: Nucleolar GTP-binding protein 1

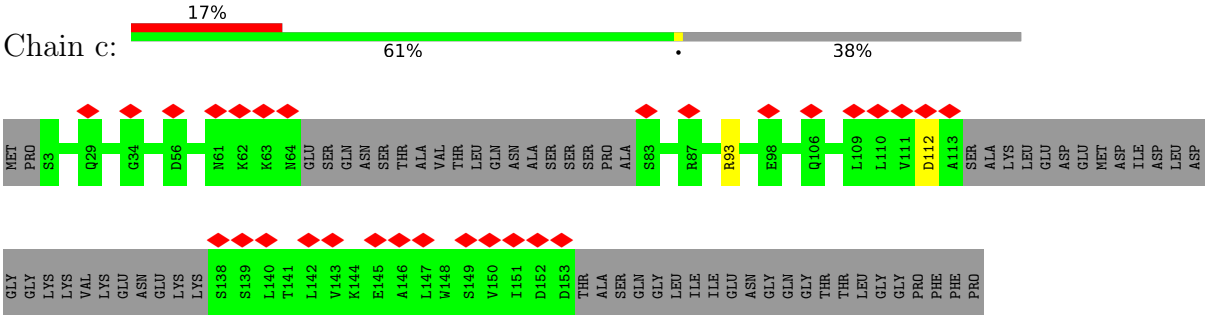
Chain b:



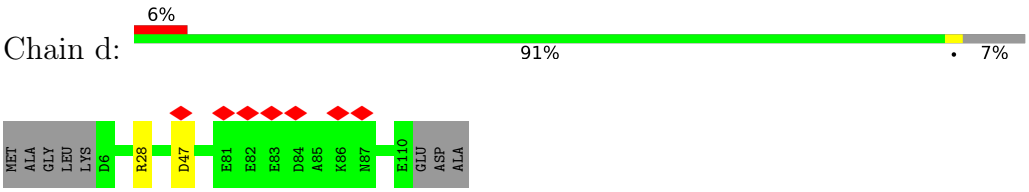




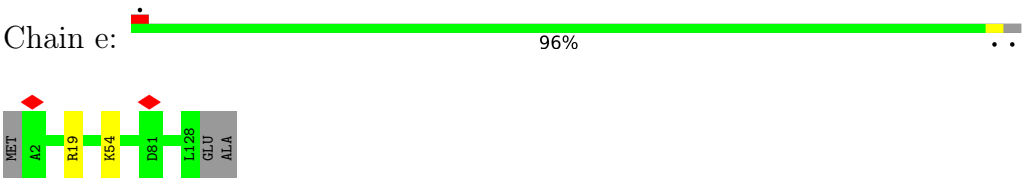
• Molecule 34: Ribosome biogenesis protein ALB1



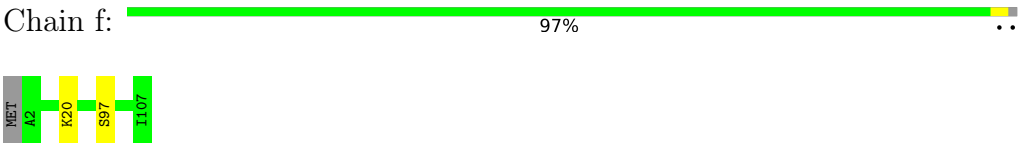
• Molecule 35: 60S ribosomal protein L31-A



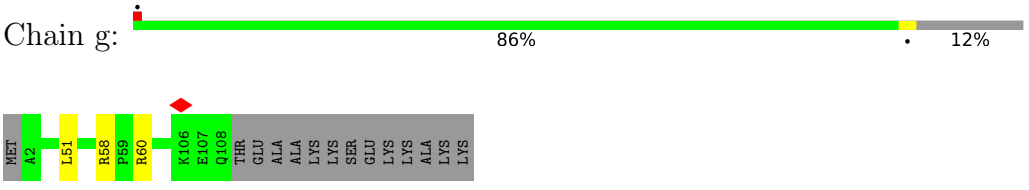
• Molecule 36: 60S ribosomal protein L32



• Molecule 37: 60S ribosomal protein L33-A

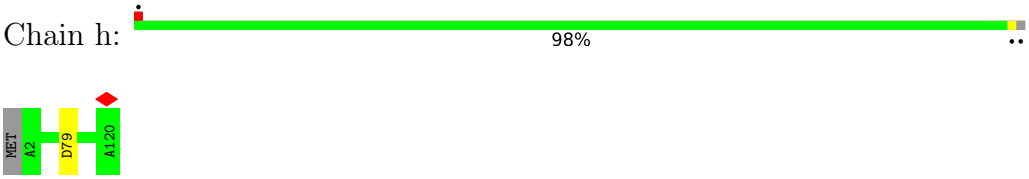


• Molecule 38: 60S ribosomal protein L34-A



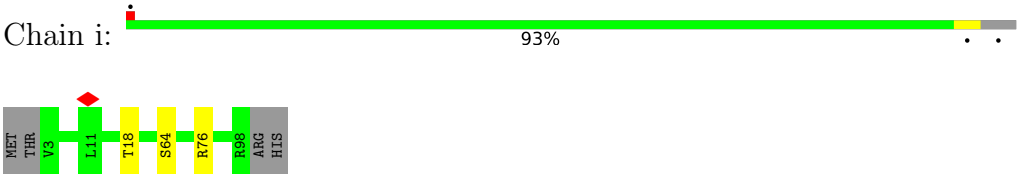
• Molecule 39: 60S ribosomal protein L35-A

Chain h:



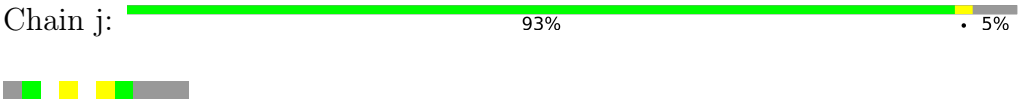
• Molecule 40: 60S ribosomal protein L36-A

Chain i:



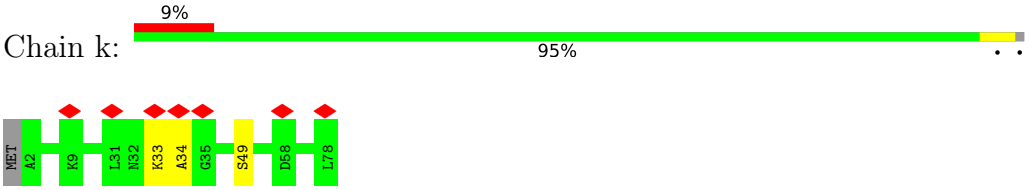
• Molecule 41: 60S ribosomal protein L37-A

Chain j:



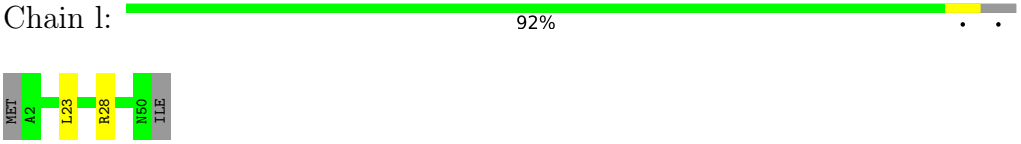
• Molecule 42: 60S ribosomal protein L38

Chain k:



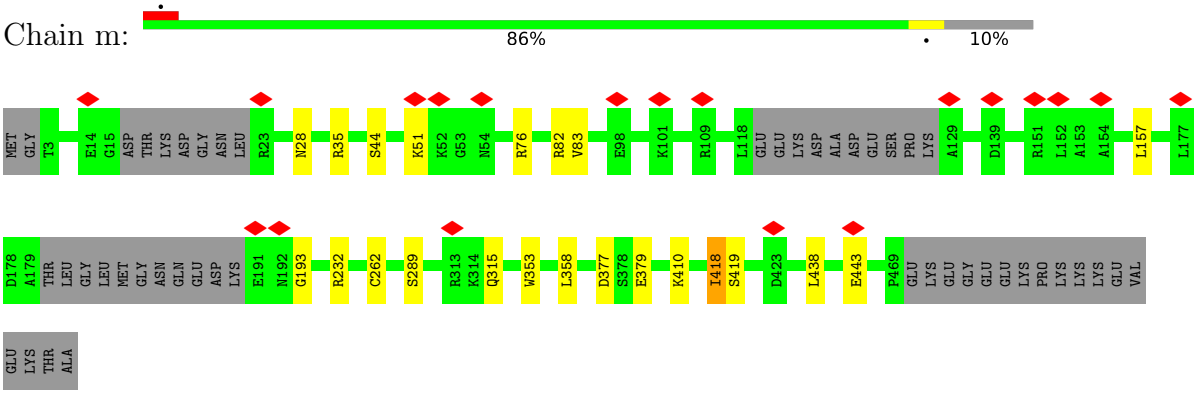
• Molecule 43: 60S ribosomal protein L39

Chain l:



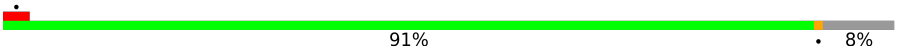
• Molecule 44: Nucleolar GTP-binding protein 2

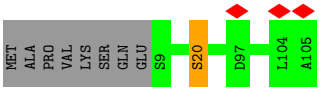
Chain m:



• Molecule 45: 60S ribosomal protein L30

Chain n:



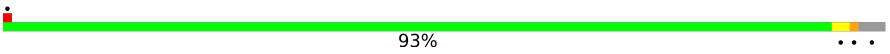


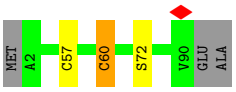
• Molecule 46: 60S ribosomal protein L1-A

Chain o:

• Molecule 47: 60S ribosomal protein L43-A

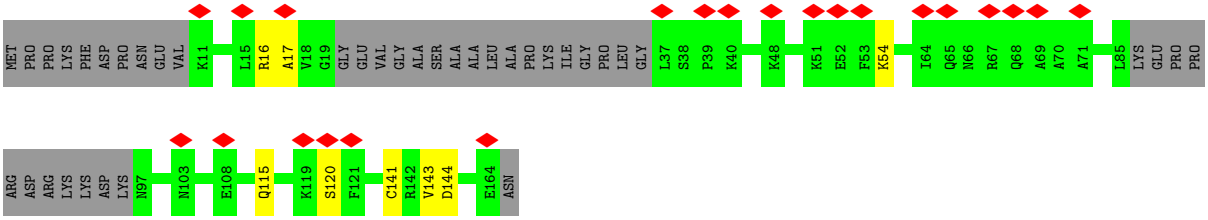
Chain p:





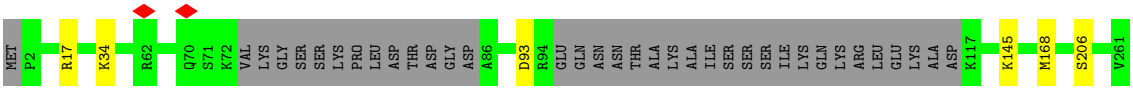
• Molecule 48: 60S ribosomal protein L12-A

Chain q:



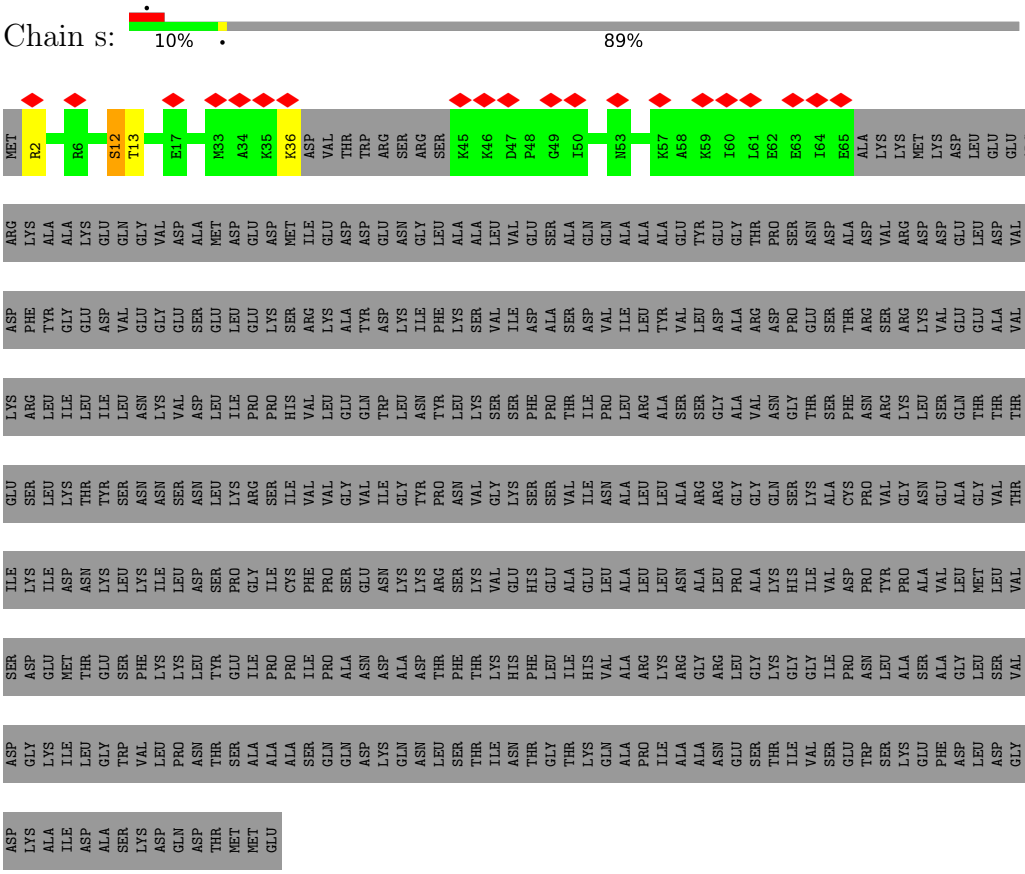
• Molecule 49: Ribosome biogenesis protein NSA2

Chain r:



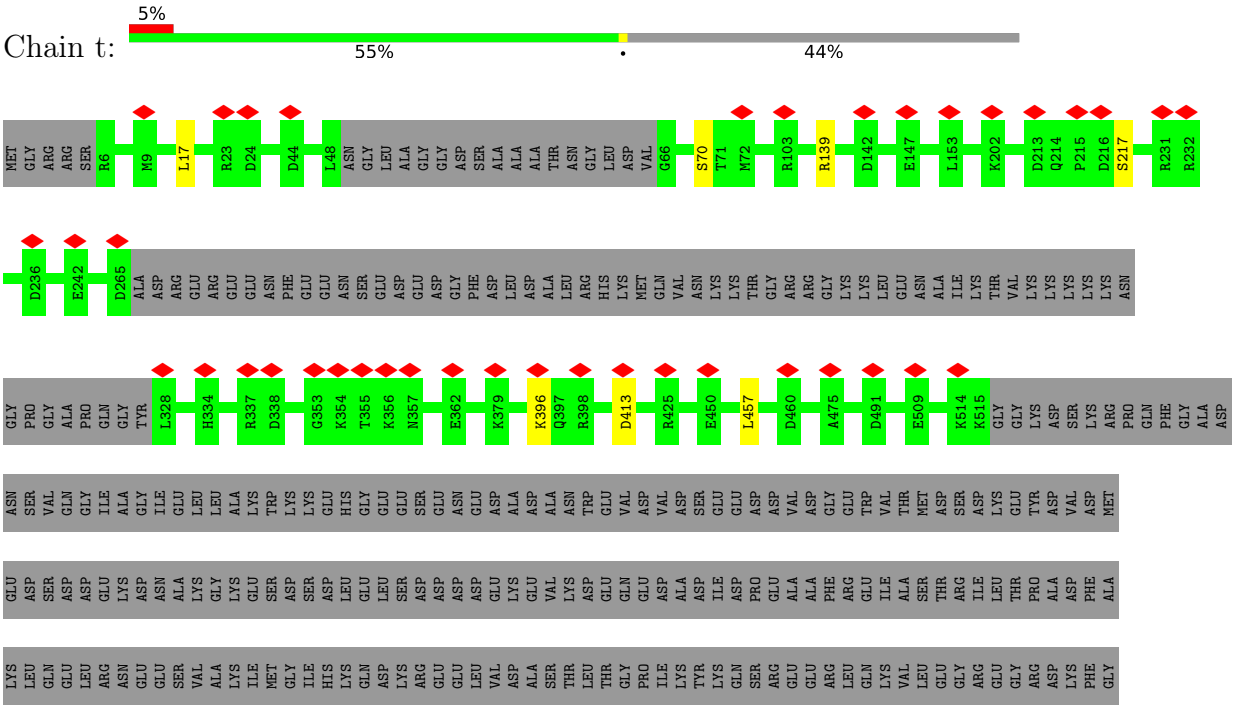
• Molecule 50: Nuclear GTP-binding protein NUG1

Chain s:

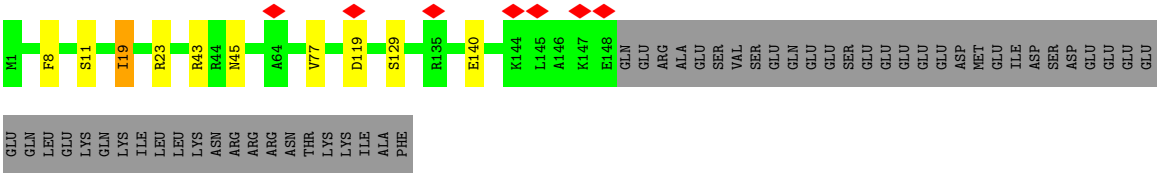


• Molecule 51: Protein SDA1

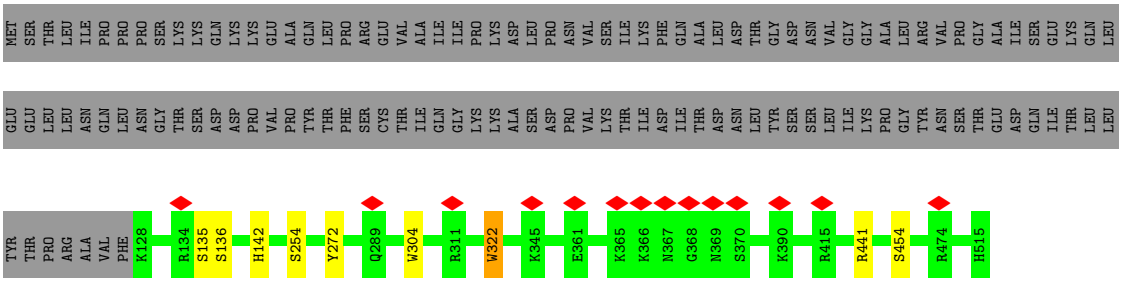
Chain t:



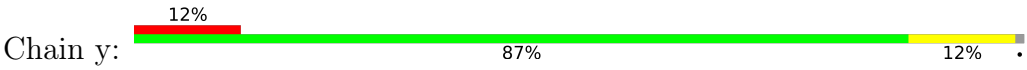
• Molecule 52: Ribosome biogenesis protein RLP24

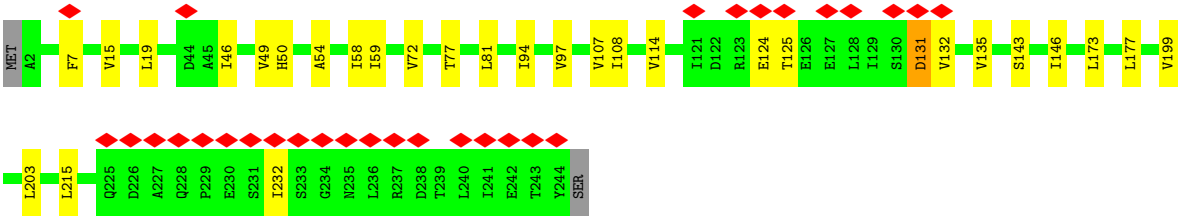


• Molecule 53: Ribosome assembly protein 4

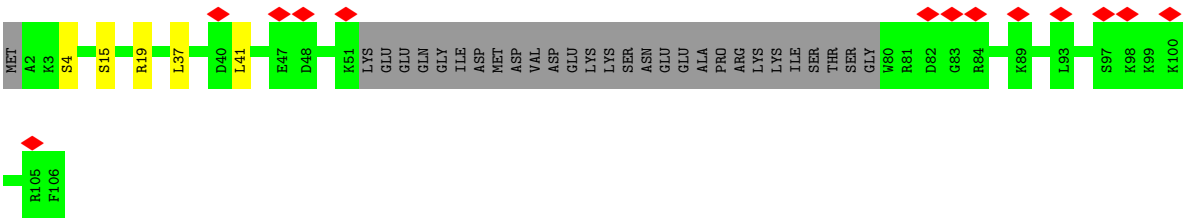


• Molecule 54: Eukaryotic translation initiation factor 6





• Molecule 55: UPF0642 protein YBL028C



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	114398	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 ($e^-/Å^2$)	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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: GTP, ZN, MG

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	0.37	5/72767 (0.0%)	0.91	87/113396 (0.1%)
2	2	0.36	0/3657	0.85	0/5692
3	3	0.27	0/2787	0.83	2/4339 (0.0%)
4	4	0.28	0/4015	0.63	3/5447 (0.1%)
5	5	0.31	0/685	0.69	1/895 (0.1%)
6	A	0.31	0/1897	0.65	1/2550 (0.0%)
7	B	0.31	0/3152	0.67	2/4239 (0.0%)
8	C	0.29	0/2801	0.58	0/3792
9	D	0.28	0/2013	0.62	0/2715
10	E	0.30	0/1260	0.63	1/1694 (0.1%)
11	F	0.31	0/1781	0.60	0/2396
12	G	0.31	0/1816	0.58	0/2450
13	H	0.29	0/1507	0.56	0/2029
14	I	0.28	0/1067	0.61	1/1433 (0.1%)
15	J	0.27	0/1365	0.66	1/1831 (0.1%)
16	K	0.27	0/1903	0.59	1/2561 (0.0%)
17	L	0.31	0/1480	0.69	2/1986 (0.1%)
18	M	0.28	0/1055	0.58	0/1421
19	N	0.32	0/1757	0.67	0/2354
20	O	0.31	0/1585	0.60	0/2128
21	P	0.32	0/1382	0.64	0/1856
22	Q	0.29	0/1127	0.63	0/1521
23	R	0.29	0/1236	0.66	0/1650
24	S	0.31	0/1473	0.63	1/1980 (0.1%)
25	T	0.29	0/997	0.67	1/1336 (0.1%)
26	U	0.30	0/817	0.52	0/1109
27	V	0.40	0/1008	1.18	18/1356 (1.3%)
28	W	0.28	0/1910	0.57	0/2575
29	X	0.29	0/1108	0.55	0/1492
30	Y	0.28	0/995	0.59	0/1329
31	Z	0.31	0/1118	0.61	0/1497
32	a	0.29	0/751	0.55	0/1013

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.29	0/5032	0.68	9/6756 (0.1%)
34	c	0.28	0/879	0.64	1/1171 (0.1%)
35	d	0.29	0/870	0.64	0/1168
36	e	0.28	0/1041	0.60	0/1394
37	f	0.31	0/868	0.58	0/1168
38	g	0.31	0/856	0.67	0/1144
39	h	0.30	0/978	0.56	0/1301
40	i	0.28	0/749	0.65	0/995
41	j	0.31	0/680	0.68	0/901
42	k	0.30	0/618	0.61	0/826
43	l	0.29	0/435	0.63	0/577
44	m	0.30	0/3617	0.63	1/4870 (0.0%)
45	n	0.28	0/751	0.63	2/1008 (0.2%)
46	o	0.24	0/872	0.70	2/1208 (0.2%)
47	p	0.31	0/687	0.65	0/915
48	q	0.27	0/969	0.59	0/1301
49	r	0.31	0/1850	0.62	0/2472
50	s	0.27	0/467	0.69	2/609 (0.3%)
51	t	0.27	0/3447	0.54	0/4643
52	u	0.31	0/1269	0.72	3/1687 (0.2%)
53	x	0.28	0/3111	0.61	2/4218 (0.0%)
54	y	0.34	0/1864	1.11	27/2538 (1.1%)
55	z	0.26	0/650	0.60	0/854
All	All	0.33	5/156832 (0.0%)	0.80	171/227786 (0.1%)

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	4	0	4
5	5	0	3
6	A	0	4
7	B	0	3
9	D	0	3
10	E	0	1
11	F	0	2
12	G	0	2
13	H	0	1
14	I	0	1
15	J	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	K	0	3
17	L	0	1
18	M	0	1
24	S	0	4
25	T	0	4
27	V	0	7
28	W	0	1
30	Y	0	1
31	Z	0	2
33	b	0	11
34	c	0	1
40	i	0	1
42	k	0	2
44	m	0	1
45	n	0	1
46	o	0	6
47	p	0	1
48	q	0	2
49	r	0	1
52	u	0	1
54	y	0	5
All	All	0	84

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	3093	C	C4-C5	10.73	1.51	1.43
1	1	3093	C	N1-C2	9.40	1.49	1.40
1	1	3093	C	N3-C4	9.07	1.40	1.33
1	1	3093	C	C2-N3	8.52	1.42	1.35
1	1	2318	U	C1'-N1	5.87	1.57	1.48

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3048	A	O4'-C1'-N9	12.94	118.55	108.20
1	1	3093	C	C5-C6-N1	10.67	126.34	121.00
1	1	2335	G	O4'-C1'-N9	10.03	116.22	108.20
1	1	3093	C	C6-N1-C2	-9.96	116.31	120.30
1	1	2531	C	C2-N1-C1'	9.73	129.51	118.80
54	y	54	ALA	C-N-CA	9.47	142.19	122.30
33	b	385	LEU	C-N-CA	9.22	144.75	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2531	C	N1-C2-O2	9.19	124.41	118.90
1	1	2339	C	O4'-C1'-N1	8.87	115.29	108.20
1	1	2531	C	N3-C2-O2	-8.73	115.79	121.90
1	1	1896	A	O4'-C1'-N9	8.71	115.16	108.20
1	1	3039	C	O4'-C1'-N1	8.38	114.90	108.20
1	1	2531	C	C6-N1-C2	-8.27	116.99	120.30
1	1	3161	C	C6-N1-C2	-8.11	117.06	120.30
7	B	348	ARG	CA-CB-CG	8.06	131.13	113.40
1	1	1897	G	O4'-C1'-N9	7.99	114.59	108.20
45	n	20	SER	O-C-N	-7.98	109.64	123.20
1	1	2339	C	N1-C1'-C2'	7.81	124.16	114.00
27	V	101	VAL	CG1-CB-CG2	7.53	122.94	110.90
52	u	23	ARG	C-N-CA	7.49	140.41	121.70
33	b	226	ASP	O-C-N	-7.36	110.92	122.70
1	1	3042	U	C5'-C4'-O4'	7.29	117.85	109.10
6	A	143	GLU	O-C-N	-7.29	111.03	122.70
1	1	2652	U	C2-N1-C1'	7.28	126.44	117.70
33	b	576	SER	O-C-N	-7.24	111.11	122.70
1	1	1898	G	C5'-C4'-O4'	7.24	117.79	109.10
1	1	2338	C	C2'-C3'-O3'	7.18	125.31	109.50
54	y	215	LEU	CB-CG-CD2	7.14	123.13	111.00
54	y	49	VAL	CG1-CB-CG2	7.06	122.20	110.90
52	u	77	VAL	CG1-CB-CG2	7.00	122.10	110.90
25	T	54	HIS	O-C-N	-6.99	111.52	122.70
44	m	193	GLY	C-N-CA	6.91	138.97	121.70
1	1	922	U	C2-N1-C1'	6.83	125.90	117.70
1	1	2880	U	C5'-C4'-O4'	6.82	117.29	109.10
1	1	2870	C	C6-N1-C2	-6.81	117.58	120.30
27	V	23	MET	C-N-CA	6.74	138.55	121.70
27	V	19	VAL	CG1-CB-CG2	6.73	121.66	110.90
27	V	129	VAL	CG1-CB-CG2	6.71	121.64	110.90
27	V	136	VAL	CG1-CB-CG2	6.71	121.63	110.90
27	V	39	VAL	CG1-CB-CG2	6.69	121.61	110.90
54	y	58	ILE	CG1-CB-CG2	6.69	126.12	111.40
1	1	1897	G	C5'-C4'-O4'	6.64	117.06	109.10
54	y	15	VAL	CG1-CB-CG2	6.60	121.47	110.90
54	y	97	VAL	CG1-CB-CG2	6.59	121.45	110.90
27	V	77	ILE	CG1-CB-CG2	6.58	125.87	111.40
1	1	2944	U	N3-C2-O2	-6.58	117.60	122.20
54	y	199	VAL	CG1-CB-CG2	6.57	121.41	110.90
54	y	72	VAL	CG1-CB-CG2	6.52	121.33	110.90
4	4	491	SER	O-C-N	-6.51	112.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3093	C	C2-N3-C4	-6.50	116.65	119.90
1	1	961	C	N1-C2-O2	6.50	122.80	118.90
1	1	1496	C	C6-N1-C2	-6.49	117.70	120.30
16	K	166	ASP	O-C-N	-6.48	112.33	122.70
54	y	114	VAL	CG1-CB-CG2	6.46	121.24	110.90
27	V	15	LEU	CB-CG-CD2	6.44	121.95	111.00
54	y	232	ILE	CG1-CB-CG2	6.41	125.51	111.40
54	y	173	LEU	CB-CG-CD1	6.41	121.90	111.00
52	u	19	ILE	CG1-CB-CG2	6.41	125.49	111.40
1	1	1108	U	N3-C2-O2	-6.36	117.75	122.20
54	y	177	LEU	CB-CG-CD2	6.33	121.77	111.00
54	y	46	ILE	CG1-CB-CG2	6.29	125.23	111.40
50	s	12	SER	CA-C-N	-6.26	103.44	117.20
1	1	2195	C	N1-C2-O2	6.22	122.63	118.90
1	1	3039	C	C5'-C4'-O4'	6.21	116.56	109.10
17	L	165	SER	O-C-N	6.21	132.63	122.70
1	1	2870	C	N1-C2-O2	6.20	122.62	118.90
54	y	94	ILE	CG1-CB-CG2	6.16	124.96	111.40
54	y	108	ILE	CG1-CB-CG2	6.16	124.95	111.40
1	1	2531	C	C6-N1-C1'	-6.14	113.43	120.80
1	1	961	C	N3-C2-O2	-6.14	117.61	121.90
1	1	1897	G	N9-C1'-C2'	6.09	121.92	114.00
1	1	2195	C	C2-N1-C1'	6.08	125.49	118.80
1	1	3041	U	C5'-C4'-O4'	6.08	116.39	109.10
1	1	2870	C	N3-C2-O2	-6.06	117.66	121.90
1	1	2374	C	C2-N1-C1'	6.05	125.46	118.80
1	1	292	U	C2-N1-C1'	6.04	124.95	117.70
4	4	544	ASN	O-C-N	-6.04	109.63	121.10
27	V	85	TRP	CA-CB-CG	6.02	125.13	113.70
1	1	2836	C	N3-C2-O2	-6.01	117.69	121.90
14	I	11	THR	CA-CB-CG2	5.99	120.78	112.40
1	1	2944	U	N1-C2-O2	5.99	126.99	122.80
54	y	107	VAL	CG1-CB-CG2	5.99	120.48	110.90
1	1	2652	U	N1-C2-O2	5.97	126.98	122.80
5	5	66	ASP	O-C-N	-5.96	113.16	122.70
50	s	12	SER	O-C-N	5.96	132.24	122.70
1	1	2836	C	N1-C2-O2	5.96	122.47	118.90
54	y	19	LEU	CB-CG-CD1	5.93	121.08	111.00
54	y	203	LEU	CB-CG-CD1	5.92	121.06	111.00
1	1	1108	U	N1-C2-O2	5.91	126.93	122.80
54	y	146	ILE	C-N-CA	5.91	136.47	121.70
1	1	1187	C	C2-N1-C1'	5.86	125.24	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	961	C	C6-N1-C2	-5.85	117.96	120.30
1	1	2652	U	N3-C2-O2	-5.84	118.11	122.20
1	1	2335	G	N9-C1'-C2'	5.84	121.59	114.00
45	n	20	SER	CA-C-N	5.79	127.78	116.20
1	1	2836	C	C2-N1-C1'	5.77	125.15	118.80
1	1	3048	A	N9-C1'-C2'	5.74	121.46	114.00
54	y	59	ILE	CG1-CB-CG2	5.72	124.00	111.40
1	1	3181	C	N1-C2-O2	5.72	122.33	118.90
1	1	1496	C	C2-N1-C1'	5.71	125.08	118.80
54	y	131	ASP	O-C-N	-5.67	113.62	122.70
1	1	835	G	O4'-C1'-N9	5.64	112.71	108.20
1	1	977	C	N1-C2-O2	5.64	122.28	118.90
1	1	1187	C	N1-C2-O2	5.64	122.28	118.90
54	y	81	LEU	CB-CG-CD1	5.63	120.57	111.00
27	V	36	ILE	CA-CB-CG1	5.60	121.64	111.00
1	1	1187	C	N3-C2-O2	-5.59	117.98	121.90
1	1	1896	A	N9-C1'-C2'	5.59	121.27	114.00
33	b	163	ILE	O-C-N	-5.59	113.76	122.70
1	1	2338	C	C5'-C4'-O4'	5.52	115.73	109.10
27	V	17	LEU	CB-CG-CD2	5.52	120.38	111.00
17	L	165	SER	CA-C-N	-5.52	105.06	117.20
27	V	49	LEU	CB-CG-CD2	5.51	120.37	111.00
53	x	135	SER	C-N-CA	5.51	135.47	121.70
54	y	77	THR	C-N-CA	5.50	135.44	121.70
53	x	322	TRP	CA-CB-CG	5.49	124.12	113.70
46	o	40	ASN	O-C-N	-5.48	113.93	122.70
1	1	292	U	N3-C2-O2	-5.47	118.37	122.20
33	b	229	THR	C-N-CA	-5.47	108.03	121.70
1	1	1299	U	C2-N1-C1'	5.44	124.22	117.70
4	4	461	ASP	O-C-N	-5.43	114.00	122.70
1	1	1657	C	C6-N1-C2	-5.43	118.13	120.30
1	1	3039	C	C5'-C4'-C3'	5.42	124.67	116.00
46	o	14	LYS	C-N-CA	-5.40	108.20	121.70
1	1	1278	A	C8-N9-C4	-5.39	103.64	105.80
15	J	144	CYS	O-C-N	-5.39	114.07	122.70
33	b	341	ALA	C-N-CA	-5.39	108.22	121.70
1	1	2445	A	O4'-C1'-N9	5.36	112.49	108.20
1	1	3023	U	N3-C2-O2	-5.35	118.45	122.20
1	1	1222	G	O4'-C1'-N9	5.33	112.47	108.20
33	b	73	ASP	O-C-N	-5.33	114.17	122.70
1	1	2755	C	C6-N1-C2	-5.33	118.17	120.30
1	1	1897	G	C5'-C4'-C3'	5.31	124.50	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2195	C	N3-C2-O2	-5.31	118.18	121.90
24	S	84	ARG	C-N-CA	5.30	134.95	121.70
3	3	98	C	C2-N1-C1'	5.29	124.61	118.80
1	1	1899	G	C5'-C4'-O4'	5.27	115.42	109.10
1	1	1898	G	C5'-C4'-C3'	5.26	124.42	116.00
1	1	2572	C	C6-N1-C2	-5.26	118.20	120.30
1	1	3039	C	N1-C1'-C2'	5.25	120.82	114.00
27	V	36	ILE	C-N-CA	5.24	134.81	121.70
7	B	58	ARG	C-N-CA	5.24	134.80	121.70
27	V	83	LYS	C-N-CA	5.24	134.80	121.70
1	1	3317	U	C2-N1-C1'	5.24	123.99	117.70
27	V	49	LEU	CB-CG-CD1	5.24	119.90	111.00
1	1	2339	C	C5'-C4'-C3'	5.22	124.36	116.00
1	1	1254	C	N3-C2-O2	-5.21	118.25	121.90
1	1	2831	G	N7-C8-N9	5.21	115.71	113.10
54	y	19	LEU	CB-CG-CD2	5.21	119.86	111.00
54	y	177	LEU	CB-CG-CD1	5.21	119.85	111.00
1	1	961	C	C2-N1-C1'	5.20	124.52	118.80
27	V	17	LEU	CB-CG-CD1	5.19	119.82	111.00
1	1	2490	C	N1-C2-O2	5.18	122.01	118.90
1	1	1084	A	N3-C4-N9	5.16	131.53	127.40
1	1	1525	G	C4-N9-C1'	5.16	133.20	126.50
27	V	54	LEU	CB-CG-CD2	5.16	119.77	111.00
1	1	3023	U	C2-N1-C1'	5.15	123.88	117.70
33	b	181	SER	C-N-CA	-5.14	108.86	121.70
33	b	398	LEU	O-C-N	5.10	130.86	122.70
54	y	15	VAL	CA-CB-CG2	5.10	118.55	110.90
1	1	2112	U	C2-N1-C1'	5.09	123.81	117.70
3	3	98	C	N3-C2-O2	-5.09	118.34	121.90
1	1	2550	U	C2-N1-C1'	5.08	123.80	117.70
1	1	1278	A	O4'-C1'-N9	5.07	112.26	108.20
54	y	124	GLU	C-N-CA	-5.06	109.06	121.70
10	E	141	VAL	C-N-CA	-5.05	109.07	121.70
34	c	93	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	1	3181	C	N3-C2-O2	-5.01	118.39	121.90
27	V	54	LEU	CB-CG-CD1	5.00	119.51	111.00
1	1	1084	A	C6-C5-N7	-5.00	128.80	132.30
1	1	656	A	N7-C8-N9	5.00	116.30	113.80

There are no chirality outliers.

All (84) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	329	CYS	Mainchain
4	4	362	ARG	Peptide
4	4	461	ASP	Mainchain
4	4	463	THR	Peptide
5	5	116	ALA	Peptide
5	5	42	THR	Mainchain
5	5	66	ASP	Mainchain
6	A	143	GLU	Mainchain,Peptide
6	A	221	LYS	Peptide
6	A	230	VAL	Peptide
7	B	155	ALA	Peptide
7	B	221	THR	Peptide
7	B	340	LYS	Peptide
9	D	168	ASP	Mainchain
9	D	235	SER	Mainchain
9	D	242	SER	Mainchain
10	E	142	ASP	Mainchain
11	F	158	LYS	Peptide
11	F	190	THR	Peptide
12	G	158	ASP	Mainchain
12	G	76	ALA	Peptide
13	H	21	LYS	Peptide
14	I	15	THR	Peptide
15	J	119	SER	Mainchain
15	J	144	CYS	Mainchain
15	J	34	SER	Mainchain
16	K	166	ASP	Mainchain
16	K	297	ILE	Mainchain
16	K	310	VAL	Mainchain
17	L	46	ILE	Peptide
18	M	98	SER	Mainchain
24	S	12	ARG	Peptide
24	S	155	ARG	Peptide
24	S	18	SER	Mainchain
24	S	22	PRO	Peptide
25	T	53	PRO	Peptide
25	T	54	HIS	Mainchain
25	T	70	SER	Mainchain,Peptide
27	V	100	GLY	Peptide
27	V	101	VAL	Peptide
27	V	35	TYR	Peptide
27	V	37	ILE	Mainchain,Peptide
27	V	76	ALA	Peptide

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Mol	Chain	Res	Type	Group
27	V	99	ALA	Peptide
28	W	176	LYS	Peptide
30	Y	7	ASP	Mainchain
31	Z	101	PHE	Peptide
31	Z	102	GLU	Peptide
33	b	182	SER	Mainchain
33	b	2	GLN	Peptide
33	b	226	ASP	Mainchain,Peptide
33	b	230	GLU	Mainchain
33	b	248	SER	Peptide
33	b	321	SER	Peptide
33	b	342	SER	Mainchain
33	b	367	GLN	Peptide
33	b	547	ASP	Mainchain
33	b	73	ASP	Mainchain
34	c	112	ASP	Mainchain
40	i	64	SER	Mainchain
42	k	33	LYS	Peptide
42	k	34	ALA	Peptide
44	m	418	ILE	Peptide
45	n	20	SER	Mainchain
46	o	104	SER	Mainchain
46	o	15	GLU	Mainchain
46	o	20	SER	Mainchain
46	o	40	ASN	Mainchain
46	o	80	CYS	Mainchain
46	o	88	ASP	Mainchain
47	p	60	CYS	Mainchain
48	q	143	VAL	Peptide
48	q	16	ARG	Peptide
49	r	145	LYS	Peptide
52	u	129	SER	Mainchain
54	y	125	THR	Mainchain
54	y	131	ASP	Mainchain
54	y	132	VAL	Mainchain
54	y	50	HIS	Peptide
54	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
4	4	495/593 (84%)	456 (92%)	34 (7%)	5 (1%)	13 46
5	5	76/120 (63%)	71 (93%)	5 (7%)	0	100 100
6	A	243/254 (96%)	227 (93%)	16 (7%)	0	100 100
7	B	384/387 (99%)	342 (89%)	41 (11%)	1 (0%)	37 70
8	C	359/362 (99%)	336 (94%)	21 (6%)	2 (1%)	22 57
9	D	239/297 (80%)	218 (91%)	21 (9%)	0	100 100
10	E	152/176 (86%)	148 (97%)	4 (3%)	0	100 100
11	F	214/244 (88%)	195 (91%)	19 (9%)	0	100 100
12	G	226/256 (88%)	209 (92%)	17 (8%)	0	100 100
13	H	185/191 (97%)	172 (93%)	13 (7%)	0	100 100
14	I	128/166 (77%)	113 (88%)	13 (10%)	2 (2%)	8 34
15	J	166/174 (95%)	145 (87%)	20 (12%)	1 (1%)	22 57
16	K	226/334 (68%)	210 (93%)	14 (6%)	2 (1%)	14 49
17	L	179/199 (90%)	165 (92%)	12 (7%)	2 (1%)	12 44
18	M	132/138 (96%)	126 (96%)	6 (4%)	0	100 100
19	N	201/204 (98%)	187 (93%)	14 (7%)	0	100 100
20	O	195/199 (98%)	194 (100%)	1 (0%)	0	100 100
21	P	167/184 (91%)	155 (93%)	12 (7%)	0	100 100
22	Q	142/186 (76%)	131 (92%)	11 (8%)	0	100 100
23	R	149/189 (79%)	142 (95%)	7 (5%)	0	100 100
24	S	169/172 (98%)	156 (92%)	10 (6%)	3 (2%)	7 32
25	T	120/160 (75%)	115 (96%)	5 (4%)	0	100 100
26	U	99/121 (82%)	95 (96%)	4 (4%)	0	100 100
27	V	132/137 (96%)	120 (91%)	10 (8%)	2 (2%)	8 36
28	W	231/236 (98%)	225 (97%)	4 (2%)	2 (1%)	14 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	X	138/142 (97%)	130 (94%)	8 (6%)	0	100	100
30	Y	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
31	Z	133/136 (98%)	118 (89%)	15 (11%)	0	100	100
32	a	91/149 (61%)	84 (92%)	5 (6%)	2 (2%)	5	27
33	b	600/647 (93%)	538 (90%)	58 (10%)	4 (1%)	19	54
34	c	103/175 (59%)	99 (96%)	4 (4%)	0	100	100
35	d	103/113 (91%)	100 (97%)	3 (3%)	0	100	100
36	e	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
37	f	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
38	g	105/121 (87%)	104 (99%)	1 (1%)	0	100	100
39	h	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
40	i	94/100 (94%)	85 (90%)	8 (8%)	1 (1%)	12	44
41	j	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
42	k	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
43	l	47/51 (92%)	44 (94%)	3 (6%)	0	100	100
44	m	431/486 (89%)	390 (90%)	38 (9%)	3 (1%)	19	54
45	n	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
46	o	167/217 (77%)	145 (87%)	22 (13%)	0	100	100
47	p	87/92 (95%)	84 (97%)	2 (2%)	1 (1%)	12	44
48	q	120/165 (73%)	101 (84%)	16 (13%)	3 (2%)	4	24
49	r	219/261 (84%)	197 (90%)	20 (9%)	2 (1%)	14	49
50	s	52/520 (10%)	47 (90%)	3 (6%)	2 (4%)	2	15
51	t	425/767 (55%)	399 (94%)	26 (6%)	0	100	100
52	u	146/199 (73%)	139 (95%)	7 (5%)	0	100	100
53	x	386/515 (75%)	364 (94%)	22 (6%)	0	100	100
54	y	241/245 (98%)	220 (91%)	20 (8%)	1 (0%)	30	66
55	z	73/106 (69%)	67 (92%)	6 (8%)	0	100	100
All	All	9491/11641 (82%)	8808 (93%)	642 (7%)	41 (0%)	32	66

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	339	LEU

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Mol	Chain	Res	Type
28	W	177	ALA
33	b	398	LEU
33	b	399	ALA
4	4	329	CYS
4	4	363	ASP
7	B	386	ASP
17	L	63	VAL
17	L	165	SER
27	V	54	LEU
32	a	78	LEU
44	m	419	SER
49	r	17	ARG
50	s	12	SER
4	4	463	THR
4	4	467	THR
14	I	18	LEU
15	J	165	GLN
24	S	13	ARG
24	S	18	SER
24	S	85	SER
28	W	178	GLY
47	p	60	CYS
50	s	13	THR
14	I	17	ASP
32	a	77	LYS
33	b	576	SER
8	C	268	ALA
16	K	25	LYS
16	K	28	ALA
48	q	120	SER
48	q	144	ASP
4	4	544	ASN
40	i	18	THR
44	m	157	LEU
48	q	17	ALA
49	r	206	SER
44	m	418	ILE
27	V	36	ILE
33	b	228	PRO
54	y	135	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
4	4	445/520 (86%)	425 (96%)	20 (4%)	23 57
5	5	70/106 (66%)	67 (96%)	3 (4%)	25 58
6	A	188/196 (96%)	185 (98%)	3 (2%)	58 82
7	B	322/323 (100%)	314 (98%)	8 (2%)	42 73
8	C	288/289 (100%)	284 (99%)	4 (1%)	62 83
9	D	205/245 (84%)	199 (97%)	6 (3%)	37 70
10	E	134/153 (88%)	129 (96%)	5 (4%)	29 63
11	F	183/205 (89%)	180 (98%)	3 (2%)	58 82
12	G	187/208 (90%)	179 (96%)	8 (4%)	25 58
13	H	167/171 (98%)	165 (99%)	2 (1%)	67 86
14	I	116/141 (82%)	108 (93%)	8 (7%)	13 42
15	J	146/150 (97%)	143 (98%)	3 (2%)	48 77
16	K	214/302 (71%)	208 (97%)	6 (3%)	38 70
17	L	145/159 (91%)	142 (98%)	3 (2%)	48 77
18	M	107/109 (98%)	104 (97%)	3 (3%)	38 70
19	N	175/176 (99%)	169 (97%)	6 (3%)	32 66
20	O	160/162 (99%)	156 (98%)	4 (2%)	42 73
21	P	139/146 (95%)	138 (99%)	1 (1%)	81 91
22	Q	118/151 (78%)	116 (98%)	2 (2%)	56 81
23	R	125/154 (81%)	124 (99%)	1 (1%)	79 90
24	S	155/156 (99%)	153 (99%)	2 (1%)	65 85
25	T	107/137 (78%)	100 (94%)	7 (6%)	14 43
26	U	88/107 (82%)	84 (96%)	4 (4%)	23 57
27	V	103/105 (98%)	99 (96%)	4 (4%)	27 61
28	W	210/213 (99%)	206 (98%)	4 (2%)	52 79
29	X	116/118 (98%)	115 (99%)	1 (1%)	75 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	Y	108/110 (98%)	104 (96%)	4 (4%)	29 63
31	Z	115/116 (99%)	112 (97%)	3 (3%)	41 72
32	a	76/119 (64%)	75 (99%)	1 (1%)	65 85
33	b	541/573 (94%)	519 (96%)	22 (4%)	26 60
34	c	99/153 (65%)	99 (100%)	0	100 100
35	d	92/97 (95%)	90 (98%)	2 (2%)	47 76
36	e	109/111 (98%)	107 (98%)	2 (2%)	54 80
37	f	90/91 (99%)	88 (98%)	2 (2%)	47 76
38	g	92/103 (89%)	89 (97%)	3 (3%)	33 67
39	h	104/105 (99%)	103 (99%)	1 (1%)	73 88
40	i	78/82 (95%)	77 (99%)	1 (1%)	65 85
41	j	69/71 (97%)	67 (97%)	2 (3%)	37 70
42	k	68/69 (99%)	67 (98%)	1 (2%)	60 83
43	l	44/46 (96%)	42 (96%)	2 (4%)	23 57
44	m	388/428 (91%)	370 (95%)	18 (5%)	23 56
45	n	81/88 (92%)	81 (100%)	0	100 100
47	p	70/72 (97%)	68 (97%)	2 (3%)	37 70
48	q	105/136 (77%)	102 (97%)	3 (3%)	37 70
49	r	198/229 (86%)	195 (98%)	3 (2%)	60 83
50	s	50/445 (11%)	48 (96%)	2 (4%)	27 61
51	t	379/665 (57%)	372 (98%)	7 (2%)	54 80
52	u	131/180 (73%)	124 (95%)	7 (5%)	19 51
53	x	338/451 (75%)	330 (98%)	8 (2%)	44 74
54	y	209/211 (99%)	208 (100%)	1 (0%)	86 94
55	z	69/95 (73%)	64 (93%)	5 (7%)	12 39
All	All	8116/9748 (83%)	7893 (97%)	223 (3%)	41 71

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	75	ARG
4	4	98	ASP
4	4	128	SER

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Mol	Chain	Res	Type
4	4	161	TYR
4	4	170	LEU
4	4	177	LEU
4	4	207	LEU
4	4	243	ARG
4	4	262	ARG
4	4	277	ASP
4	4	338	GLU
4	4	362	ARG
4	4	403	HIS
4	4	407	GLU
4	4	464	SER
4	4	475	LEU
4	4	493	LYS
4	4	530	LYS
4	4	544	ASN
4	4	576	LYS
5	5	66	ASP
5	5	81	GLU
5	5	115	LYS
6	A	3	ARG
6	A	218	HIS
6	A	241	ARG
7	B	24	SER
7	B	84	VAL
7	B	102	LEU
7	B	246	LEU
7	B	251	CYS
7	B	332	ARG
7	B	334	ARG
7	B	387	LEU
8	C	53	SER
8	C	98	ARG
8	C	120	TYR
8	C	187	LEU
9	D	22	ARG
9	D	51	LEU
9	D	72	ASP
9	D	195	LEU
9	D	232	ASP
9	D	257	GLU
10	E	2	SER

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Mol	Chain	Res	Type
10	E	12	SER
10	E	88	SER
10	E	150	LYS
10	E	175	LYS
11	F	45	LEU
11	F	60	ARG
11	F	110	ARG
12	G	38	GLN
12	G	107	GLU
12	G	120	LYS
12	G	136	LEU
12	G	150	LEU
12	G	185	ARG
12	G	228	GLU
12	G	251	LYS
13	H	107	ASP
13	H	137	SER
14	I	3	ARG
14	I	7	LYS
14	I	16	ARG
14	I	64	LEU
14	I	75	ARG
14	I	116	LYS
14	I	123	LEU
14	I	125	GLU
15	J	11	ASP
15	J	39	GLN
15	J	55	ARG
16	K	15	LEU
16	K	134	PHE
16	K	152	ASP
16	K	164	CYS
16	K	178	ASN
16	K	223	CYS
17	L	117	LYS
17	L	131	LYS
17	L	137	GLN
18	M	91	CYS
18	M	108	ARG
18	M	125	LYS
19	N	24	ARG
19	N	49	ARG

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Mol	Chain	Res	Type
19	N	50	ARG
19	N	117	ASN
19	N	153	ASP
19	N	198	SER
20	O	44	SER
20	O	52	LEU
20	O	117	ARG
20	O	148	LYS
21	P	23	ARG
22	Q	7	SER
22	Q	41	ASP
23	R	135	LYS
24	S	84	ARG
24	S	134	ASP
25	T	28	SER
25	T	85	LEU
25	T	103	GLN
25	T	127	GLN
25	T	128	LEU
25	T	146	ASN
25	T	151	LEU
26	U	18	ASP
26	U	39	ASP
26	U	52	ASN
26	U	104	ARG
27	V	36	ILE
27	V	85	TRP
27	V	86	ARG
27	V	112	SER
28	W	60	TRP
28	W	122	SER
28	W	220	TYR
28	W	234	ASN
29	X	78	ASP
30	Y	7	ASP
30	Y	71	SER
30	Y	72	SER
30	Y	74	TYR
31	Z	33	SER
31	Z	67	LYS
31	Z	134	LEU
32	a	60	TYR

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Mol	Chain	Res	Type
33	b	63	ASP
33	b	70	ASN
33	b	162	SER
33	b	166	ASN
33	b	168	ARG
33	b	170	LEU
33	b	175	TYR
33	b	191	ASP
33	b	210	ASP
33	b	275	LYS
33	b	307	GLU
33	b	322	CYS
33	b	324	LEU
33	b	347	LYS
33	b	413	ASN
33	b	420	TYR
33	b	427	TRP
33	b	440	ASN
33	b	514	LYS
33	b	557	ARG
33	b	583	LEU
33	b	599	ARG
35	d	28	ARG
35	d	47	ASP
36	e	19	ARG
36	e	54	LYS
37	f	20	LYS
37	f	97	SER
38	g	51	LEU
38	g	58	ARG
38	g	60	ARG
39	h	79	ASP
40	i	76	ARG
41	j	36	SER
41	j	84	SER
42	k	49	SER
43	l	23	LEU
43	l	28	ARG
44	m	28	ASN
44	m	35	ARG
44	m	44	SER
44	m	51	LYS

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Mol	Chain	Res	Type
44	m	76	ARG
44	m	82	ARG
44	m	83	VAL
44	m	232	ARG
44	m	262	CYS
44	m	289	SER
44	m	315	GLN
44	m	353	TRP
44	m	358	LEU
44	m	377	ASP
44	m	379	GLU
44	m	410	LYS
44	m	438	LEU
44	m	443	GLU
47	p	57	CYS
47	p	72	SER
48	q	54	LYS
48	q	115	GLN
48	q	141	CYS
49	r	34	LYS
49	r	93	ASP
49	r	168	MET
50	s	2	ARG
50	s	36	LYS
51	t	17	LEU
51	t	70	SER
51	t	139	ARG
51	t	217	SER
51	t	396	LYS
51	t	413	ASP
51	t	457	LEU
52	u	8	PHE
52	u	11	SER
52	u	19	ILE
52	u	43	ARG
52	u	45	ASN
52	u	119	ASP
52	u	140	GLU
53	x	136	SER
53	x	142	HIS
53	x	254	SER
53	x	272	TYR

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Mol	Chain	Res	Type
53	x	304	TRP
53	x	322	TRP
53	x	441	ARG
53	x	454	SER
54	y	143	SER
55	z	4	SER
55	z	15	SER
55	z	19	ARG
55	z	37	LEU
55	z	41	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	85	ASN
4	4	235	ASN
4	4	273	HIS
4	4	274	GLN
4	4	544	ASN
8	C	48	GLN
8	C	196	ASN
8	C	304	GLN
11	F	186	HIS
12	G	77	GLN
12	G	232	HIS
13	H	49	ASN
13	H	59	ASN
16	K	213	ASN
18	M	41	GLN
19	N	195	ASN
20	O	55	HIS
24	S	8	GLN
25	T	103	GLN
26	U	49	ASN
26	U	52	ASN
27	V	132	ASN
28	W	44	HIS
33	b	217	GLN
33	b	384	ASN
33	b	509	ASN
33	b	579	ASN
34	c	44	ASN

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Mol	Chain	Res	Type
34	c	61	ASN
34	c	64	ASN
41	j	30	GLN
42	k	40	GLN
43	l	20	ASN
51	t	29	GLN
51	t	421	ASN
52	u	110	ASN
53	x	176	GLN
53	x	424	ASN
54	y	9	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3010/3396 (88%)	598 (19%)	26 (0%)
2	2	152/158 (96%)	27 (17%)	1 (0%)
3	3	115/121 (95%)	19 (16%)	1 (0%)
All	All	3277/3675 (89%)	644 (19%)	28 (0%)

All (644) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	14	U
1	1	18	G
1	1	26	A
1	1	30	G
1	1	40	A
1	1	41	G
1	1	43	A
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	73	C
1	1	76	G
1	1	92	G
1	1	94	G

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Mol	Chain	Res	Type
1	1	110	G
1	1	111	C
1	1	121	A
1	1	122	A
1	1	133	U
1	1	136	G
1	1	156	G
1	1	157	A
1	1	161	G
1	1	164	A
1	1	166	C
1	1	173	G
1	1	176	G
1	1	177	U
1	1	190	U
1	1	191	U
1	1	200	C
1	1	210	U
1	1	211	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	240	U
1	1	242	C
1	1	243	G
1	1	244	G
1	1	245	U
1	1	246	U
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	253	A
1	1	254	A
1	1	269	G
1	1	284	A
1	1	286	U
1	1	295	A
1	1	298	U
1	1	305	U
1	1	306	A
1	1	307	A

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Mol	Chain	Res	Type
1	1	329	U
1	1	338	A
1	1	339	C
1	1	346	C
1	1	352	A
1	1	362	U
1	1	376	G
1	1	386	A
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	421	G
1	1	422	A
1	1	516	A
1	1	521	A
1	1	523	A
1	1	525	C
1	1	536	U
1	1	543	C
1	1	545	U
1	1	547	G
1	1	552	G
1	1	555	U
1	1	557	A
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	597	G
1	1	604	G
1	1	607	A
1	1	609	G
1	1	610	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	622	A
1	1	637	C
1	1	643	U
1	1	644	G

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Mol	Chain	Res	Type
1	1	645	A
1	1	646	A
1	1	650	C
1	1	667	C
1	1	677	A
1	1	681	U
1	1	683	U
1	1	691	A
1	1	705	A
1	1	709	A
1	1	715	A
1	1	719	U
1	1	720	A
1	1	721	G
1	1	722	G
1	1	735	A
1	1	763	G
1	1	765	C
1	1	767	U
1	1	780	A
1	1	781	G
1	1	784	A
1	1	785	G
1	1	801	A
1	1	806	A
1	1	808	A
1	1	817	A
1	1	830	A
1	1	845	G
1	1	848	A
1	1	849	C
1	1	861	C
1	1	874	U
1	1	875	G
1	1	896	A
1	1	907	G
1	1	908	G
1	1	914	A
1	1	916	G
1	1	917	A
1	1	925	A
1	1	944	C

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Mol	Chain	Res	Type
1	1	953	G
1	1	955	U
1	1	956	U
1	1	958	C
1	1	961	C
1	1	962	A
1	1	964	G
1	1	966	U
1	1	976	U
1	1	977	C
1	1	978	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	984	G
1	1	991	G
1	1	1007	U
1	1	1008	U
1	1	1010	G
1	1	1016	C
1	1	1017	C
1	1	1018	G
1	1	1019	G
1	1	1025	A
1	1	1026	A
1	1	1027	A
1	1	1028	U
1	1	1029	G
1	1	1030	A
1	1	1032	C
1	1	1034	U
1	1	1035	G
1	1	1036	A
1	1	1037	C
1	1	1038	C
1	1	1044	U
1	1	1064	A
1	1	1066	G
1	1	1068	C
1	1	1072	G
1	1	1073	U
1	1	1074	U

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Mol	Chain	Res	Type
1	1	1084	A
1	1	1090	G
1	1	1098	A
1	1	1099	A
1	1	1112	A
1	1	1116	G
1	1	1117	G
1	1	1118	C
1	1	1123	U
1	1	1127	G
1	1	1128	U
1	1	1129	A
1	1	1131	G
1	1	1132	C
1	1	1135	A
1	1	1143	A
1	1	1153	A
1	1	1159	A
1	1	1161	G
1	1	1180	A
1	1	1181	U
1	1	1182	A
1	1	1186	G
1	1	1192	C
1	1	1193	A
1	1	1196	C
1	1	1198	C
1	1	1199	C
1	1	1200	A
1	1	1203	A
1	1	1209	G
1	1	1218	U
1	1	1222	G
1	1	1227	C
1	1	1240	A
1	1	1245	A
1	1	1254	C
1	1	1258	U
1	1	1262	G
1	1	1263	A
1	1	1271	A
1	1	1272	C

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Mol	Chain	Res	Type
1	1	1278	A
1	1	1287	A
1	1	1292	C
1	1	1302	A
1	1	1303	A
1	1	1304	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1330	A
1	1	1345	G
1	1	1348	U
1	1	1356	U
1	1	1386	A
1	1	1392	G
1	1	1399	A
1	1	1400	G
1	1	1405	U
1	1	1419	A
1	1	1434	G
1	1	1436	U
1	1	1437	C
1	1	1443	G
1	1	1455	U
1	1	1483	G
1	1	1484	U
1	1	1487	G
1	1	1503	A
1	1	1508	C
1	1	1522	U
1	1	1523	U
1	1	1533	U
1	1	1536	G
1	1	1539	A
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1560	G
1	1	1561	G
1	1	1562	C

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Mol	Chain	Res	Type
1	1	1575	A
1	1	1581	C
1	1	1582	C
1	1	1583	A
1	1	1588	A
1	1	1589	A
1	1	1629	U
1	1	1630	U
1	1	1639	C
1	1	1642	A
1	1	1643	A
1	1	1644	C
1	1	1657	C
1	1	1683	A
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1742	U
1	1	1750	A
1	1	1751	G
1	1	1760	A
1	1	1762	C
1	1	1763	U
1	1	1765	U
1	1	1766	G
1	1	1775	G
1	1	1780	G
1	1	1794	G
1	1	1797	A
1	1	1810	A
1	1	1813	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1821	U
1	1	1839	A
1	1	1842	A
1	1	1849	C
1	1	1850	A
1	1	1851	G
1	1	1878	G
1	1	1880	U

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Mol	Chain	Res	Type
1	1	1889	G
1	1	1901	A
1	1	1906	G
1	1	1925	U
1	1	1926	C
1	1	1951	C
1	1	1953	G
1	1	2102	U
1	1	2112	U
1	1	2121	G
1	1	2122	G
1	1	2126	A
1	1	2131	A
1	1	2134	G
1	1	2149	A
1	1	2169	G
1	1	2170	U
1	1	2184	U
1	1	2194	G
1	1	2205	U
1	1	2239	G
1	1	2244	A
1	1	2246	G
1	1	2249	G
1	1	2267	C
1	1	2268	U
1	1	2270	A
1	1	2271	A
1	1	2272	G
1	1	2273	G
1	1	2276	G
1	1	2319	U
1	1	2320	A
1	1	2334	U
1	1	2335	G
1	1	2336	U
1	1	2338	C
1	1	2339	C
1	1	2340	U
1	1	2373	A
1	1	2376	G
1	1	2377	G

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Mol	Chain	Res	Type
1	1	2388	U
1	1	2391	G
1	1	2394	G
1	1	2397	A
1	1	2398	A
1	1	2399	A
1	1	2410	U
1	1	2411	U
1	1	2412	G
1	1	2418	G
1	1	2419	A
1	1	2435	G
1	1	2437	G
1	1	2444	C
1	1	2445	A
1	1	2448	G
1	1	2450	G
1	1	2452	G
1	1	2453	U
1	1	2459	A
1	1	2462	A
1	1	2463	G
1	1	2467	G
1	1	2468	A
1	1	2469	G
1	1	2470	C
1	1	2472	U
1	1	2473	C
1	1	2474	G
1	1	2476	C
1	1	2477	G
1	1	2480	A
1	1	2487	U
1	1	2493	U
1	1	2494	A
1	1	2502	A
1	1	2505	U
1	1	2514	U
1	1	2515	A
1	1	2522	G
1	1	2524	A
1	1	2530	G

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Mol	Chain	Res	Type
1	1	2531	C
1	1	2532	U
1	1	2534	G
1	1	2537	U
1	1	2538	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2546	C
1	1	2547	A
1	1	2548	C
1	1	2549	G
1	1	2552	C
1	1	2554	A
1	1	2561	A
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2586	G
1	1	2593	A
1	1	2595	A
1	1	2606	G
1	1	2607	G
1	1	2626	A
1	1	2629	U
1	1	2630	C
1	1	2631	U
1	1	2633	U
1	1	2634	U
1	1	2646	C
1	1	2647	A
1	1	2651	G
1	1	2652	U
1	1	2656	A
1	1	2657	A
1	1	2660	G
1	1	2661	G
1	1	2674	A

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Mol	Chain	Res	Type
1	1	2677	G
1	1	2681	U
1	1	2689	A
1	1	2694	A
1	1	2697	A
1	1	2698	G
1	1	2704	A
1	1	2714	G
1	1	2720	G
1	1	2730	G
1	1	2732	G
1	1	2736	A
1	1	2738	A
1	1	2742	C
1	1	2753	G
1	1	2755	C
1	1	2756	C
1	1	2765	C
1	1	2766	U
1	1	2771	U
1	1	2773	C
1	1	2777	G
1	1	2778	G
1	1	2780	A
1	1	2791	G
1	1	2794	G
1	1	2804	A
1	1	2810	C
1	1	2814	G
1	1	2823	G
1	1	2824	G
1	1	2826	U
1	1	2834	G
1	1	2838	A
1	1	2841	G
1	1	2842	U
1	1	2843	U
1	1	2844	C
1	1	2845	A
1	1	2859	U
1	1	2860	U
1	1	2861	U

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Mol	Chain	Res	Type
1	1	2864	A
1	1	2866	U
1	1	2868	U
1	1	2869	U
1	1	2872	A
1	1	2878	G
1	1	2879	C
1	1	2887	A
1	1	2889	C
1	1	2898	G
1	1	2899	C
1	1	2901	G
1	1	2916	U
1	1	2918	G
1	1	2923	U
1	1	2925	C
1	1	2926	A
1	1	2930	A
1	1	2935	U
1	1	2936	A
1	1	2938	G
1	1	2941	A
1	1	2943	G
1	1	2944	U
1	1	2947	G
1	1	2948	C
1	1	2950	G
1	1	2970	C
1	1	2971	A
1	1	2972	G
1	1	2978	U
1	1	2979	U
1	1	2980	U
1	1	2981	U
1	1	2982	A
1	1	2983	C
1	1	2997	G
1	1	3011	A
1	1	3012	A
1	1	3022	G
1	1	3028	G
1	1	3032	A

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Mol	Chain	Res	Type
1	1	3039	C
1	1	3040	A
1	1	3042	U
1	1	3058	U
1	1	3059	G
1	1	3078	U
1	1	3080	G
1	1	3086	A
1	1	3092	C
1	1	3093	C
1	1	3100	U
1	1	3101	G
1	1	3115	C
1	1	3116	G
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3150	A
1	1	3151	U
1	1	3160	U
1	1	3162	C
1	1	3163	A
1	1	3165	A
1	1	3167	A
1	1	3171	U
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3182	G
1	1	3187	A
1	1	3195	U
1	1	3196	U
1	1	3206	C
1	1	3207	U
1	1	3217	C
1	1	3218	A

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Mol	Chain	Res	Type
1	1	3219	G
1	1	3227	A
1	1	3244	A
1	1	3245	A
1	1	3246	G
1	1	3256	G
1	1	3259	U
1	1	3263	G
1	1	3276	G
1	1	3278	C
1	1	3282	U
1	1	3284	G
1	1	3285	C
1	1	3288	G
1	1	3289	G
1	1	3291	G
1	1	3292	A
1	1	3294	A
1	1	3295	A
1	1	3304	U
1	1	3313	U
1	1	3316	A
1	1	3317	U
1	1	3319	U
1	1	3334	U
1	1	3341	U
1	1	3342	A
1	1	3345	G
1	1	3347	A
1	1	3357	U
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3382	U
2	2	25	G
2	2	34	U
2	2	35	C
2	2	49	G
2	2	52	A
2	2	53	A
2	2	59	A
2	2	60	U

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Mol	Chain	Res	Type
2	2	62	C
2	2	63	G
2	2	75	G
2	2	79	A
2	2	81	U
2	2	86	U
2	2	88	A
2	2	90	U
2	2	95	G
2	2	104	A
2	2	106	C
2	2	111	A
2	2	112	U
2	2	113	U
2	2	123	G
2	2	124	G
2	2	126	A
2	2	148	G
2	2	151	C
3	3	7	G
3	3	11	A
3	3	22	A
3	3	35	C
3	3	38	U
3	3	41	G
3	3	49	G
3	3	50	U
3	3	52	G
3	3	53	U
3	3	54	U
3	3	55	A
3	3	64	A
3	3	65	G
3	3	74	C
3	3	99	G
3	3	102	A
3	3	112	G
3	3	121	U

All (28) RNA pucker outliers are listed below:

Continued on next page...

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Mol	Chain	Res	Type
1	1	13	A
1	1	40	A
1	1	160	G
1	1	239	G
1	1	784	A
1	1	916	G
1	1	990	U
1	1	1128	U
1	1	1302	A
1	1	1307	G
1	1	1329	U
1	1	1899	G
1	1	2101	C
1	1	2248	C
1	1	2318	U
1	1	2338	C
1	1	2339	C
1	1	2444	C
1	1	2472	U
1	1	2537	U
1	1	2541	U
1	1	2651	G
1	1	2900	A
1	1	3041	U
1	1	3042	U
1	1	3166	C
2	2	123	G
3	3	52	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	GTP	b	701	33,58	26,34,34	1.14	2 (7%)	32,54,54	1.70	7 (21%)
57	GTP	m	501	58	26,34,34	1.14	1 (3%)	32,54,54	1.59	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	GTP	b	701	33,58	-	2/18/38/38	0/3/3/3
57	GTP	m	501	58	-	6/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	b	701	GTP	C5-C6	-4.09	1.39	1.47
57	m	501	GTP	C5-C6	-4.06	1.39	1.47
57	b	701	GTP	C2-N3	2.28	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	b	701	GTP	PA-O3A-PB	-4.29	118.11	132.83
57	m	501	GTP	PA-O3A-PB	-3.93	119.34	132.83
57	m	501	GTP	PB-O3B-PG	-3.63	120.36	132.83
57	b	701	GTP	PB-O3B-PG	-3.53	120.70	132.83
57	b	701	GTP	C5-C6-N1	3.37	119.91	113.95
57	m	501	GTP	C5-C6-N1	3.18	119.57	113.95
57	b	701	GTP	C2-N1-C6	-3.11	119.38	125.10
57	m	501	GTP	C8-N7-C5	3.10	108.89	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	b	701	GTP	C8-N7-C5	3.08	108.86	102.99
57	m	501	GTP	C2-N1-C6	-2.97	119.63	125.10
57	b	701	GTP	C3'-C2'-C1'	2.80	105.20	100.98
57	b	701	GTP	O6-C6-C5	-2.55	119.40	124.37
57	m	501	GTP	C3'-C2'-C1'	2.50	104.75	100.98
57	m	501	GTP	O6-C6-C5	-2.07	120.34	124.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

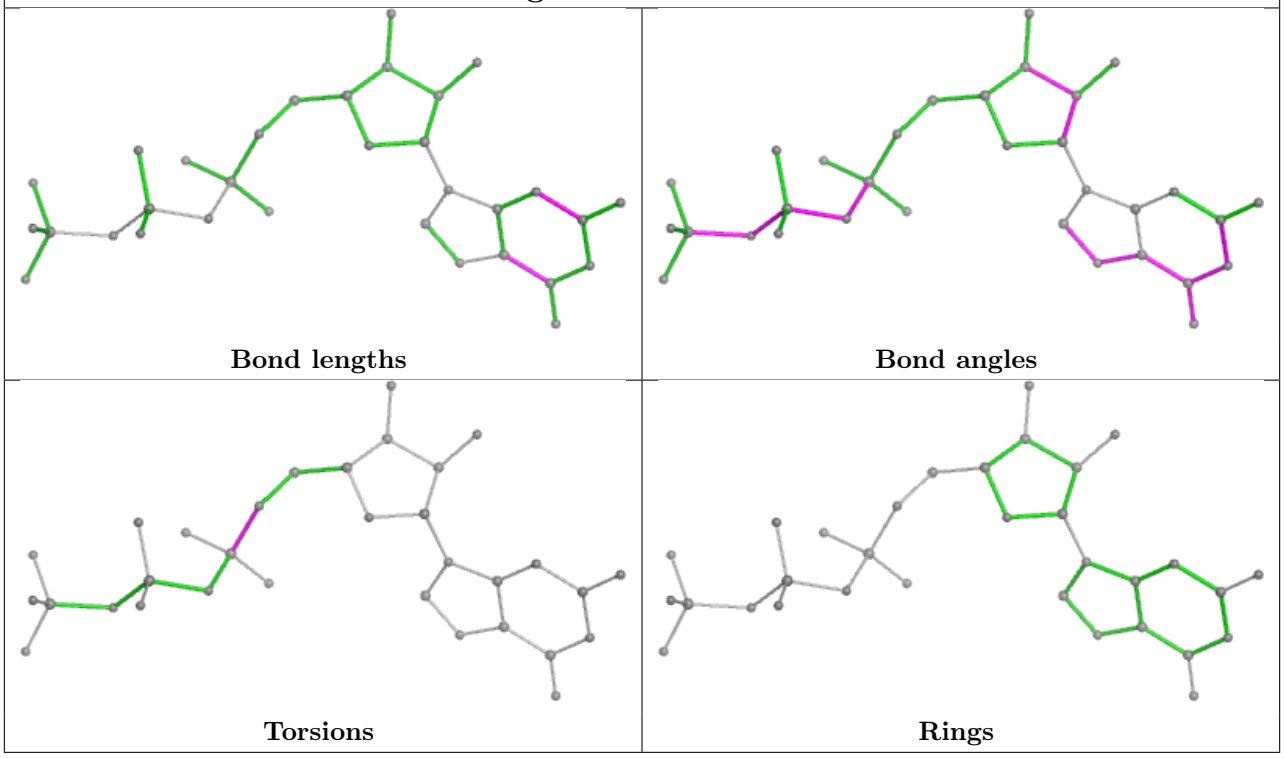
Mol	Chain	Res	Type	Atoms
57	b	701	GTP	C5'-O5'-PA-O1A
57	m	501	GTP	C5'-O5'-PA-O3A
57	m	501	GTP	C5'-O5'-PA-O2A
57	m	501	GTP	O4'-C4'-C5'-O5'
57	m	501	GTP	C4'-C5'-O5'-PA
57	m	501	GTP	C3'-C4'-C5'-O5'
57	m	501	GTP	PB-O3A-PA-O1A
57	b	701	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

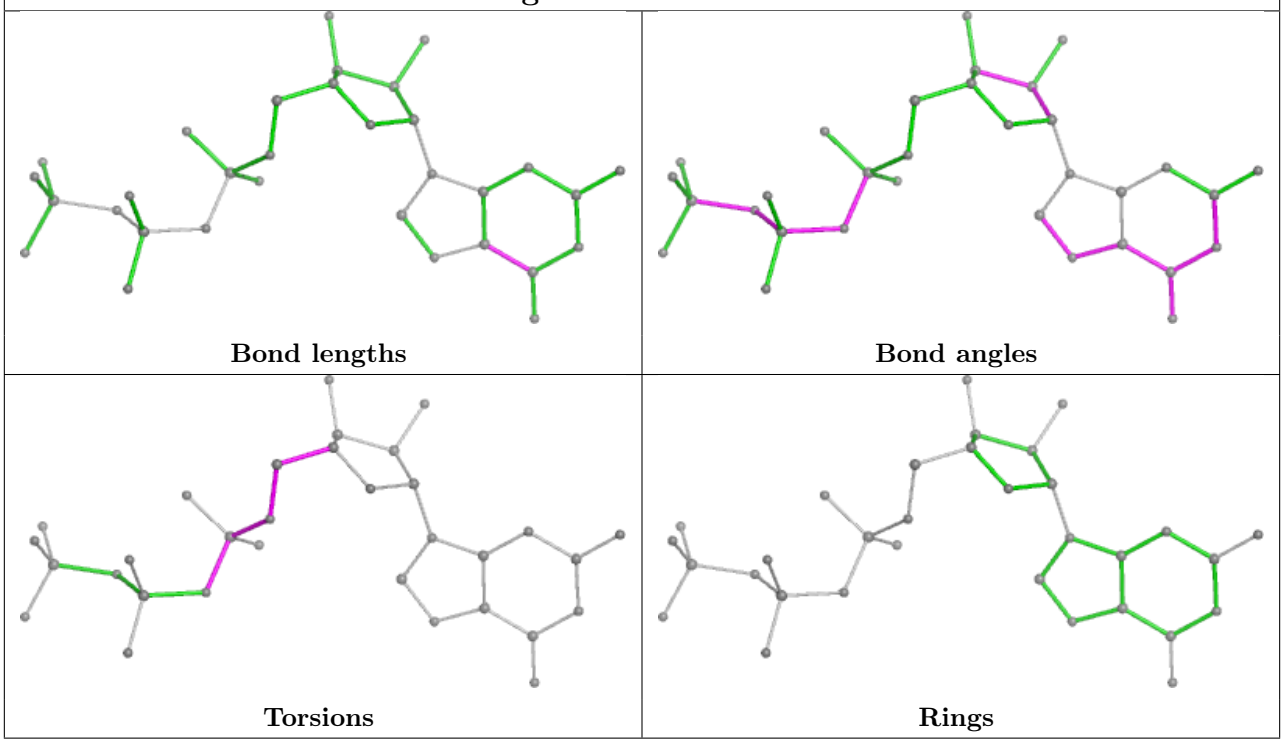
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP b 701



Ligand GTP m 501



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	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	3167:A	O3'	3168:A	P	4.92
1	1	1012:G	O3'	1013:G	P	3.13
1	1	1039:U	O3'	1040:A	P	3.07

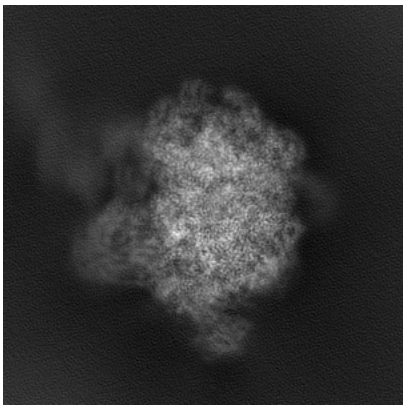
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10838. These allow visual inspection of the internal detail of the map and identification of artifacts.

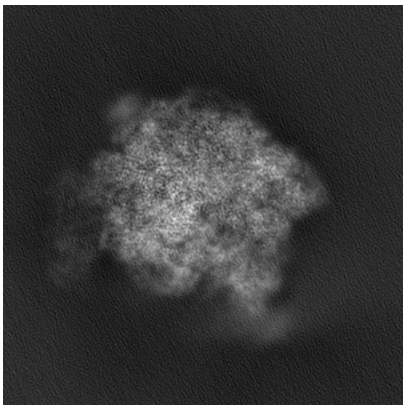
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

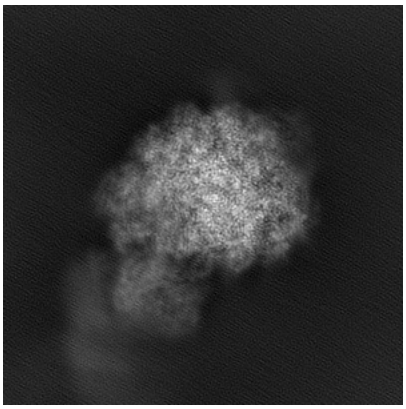
6.1.1 Primary map



X

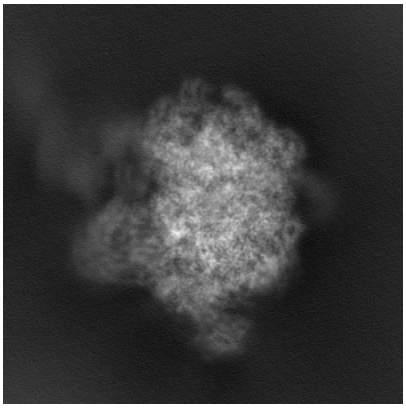


Y

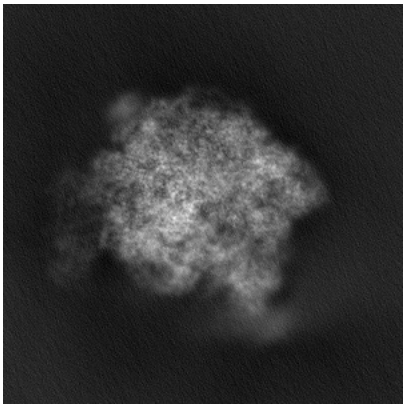


Z

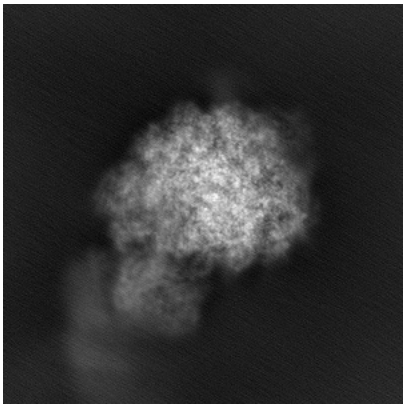
6.1.2 Raw map



X



Y

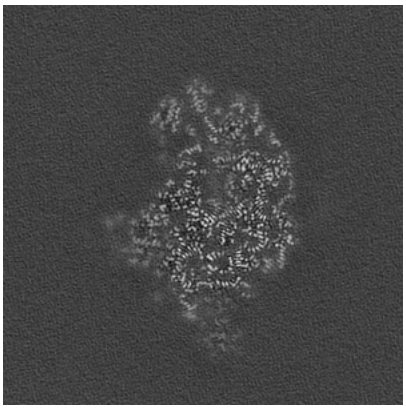


Z

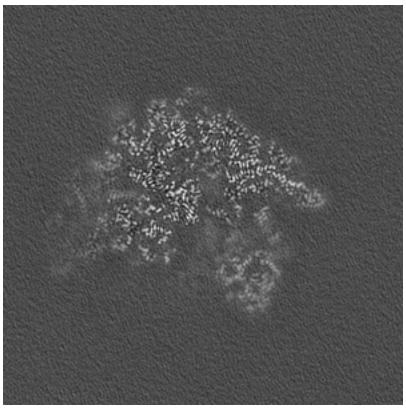
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

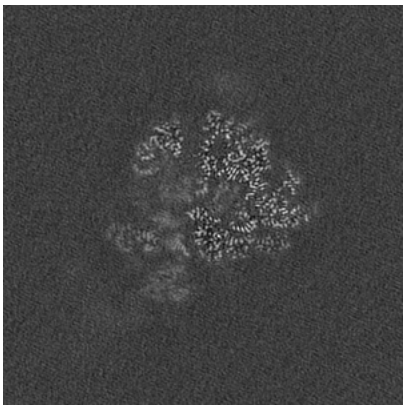
6.2.1 Primary map



X Index: 200

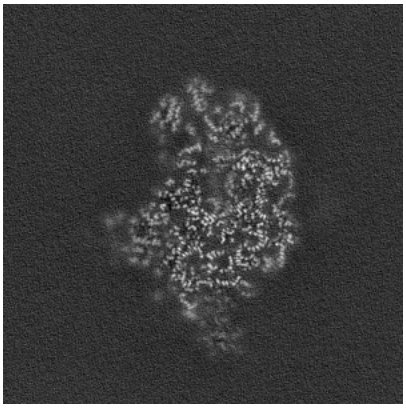


Y Index: 200

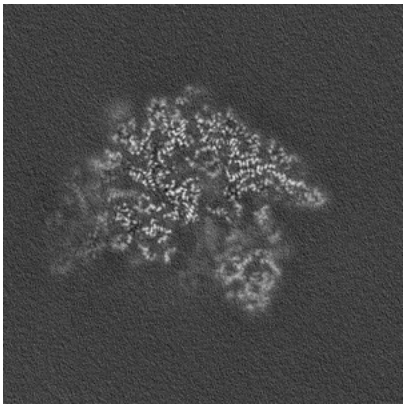


Z Index: 200

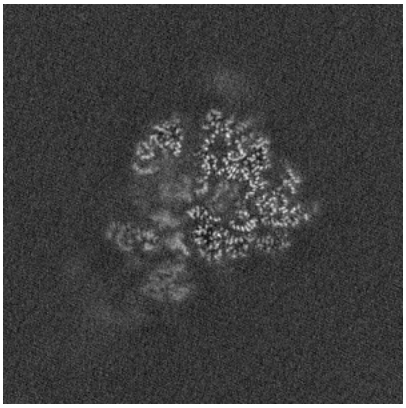
6.2.2 Raw map



X Index: 200



Y Index: 200

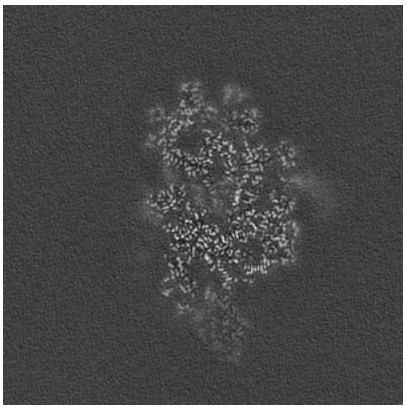


Z Index: 200

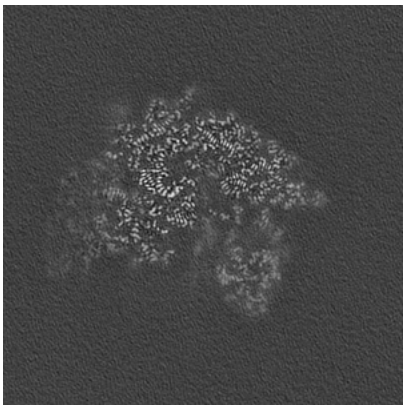
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

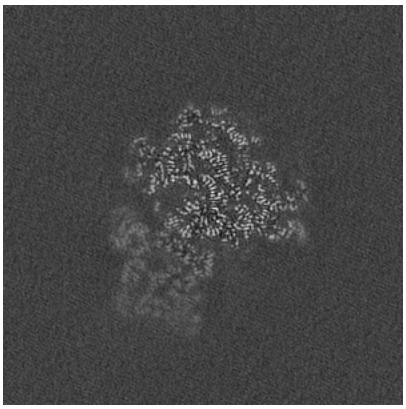
6.3.1 Primary map



X Index: 216

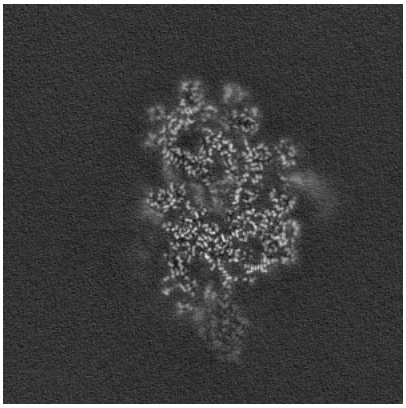


Y Index: 203

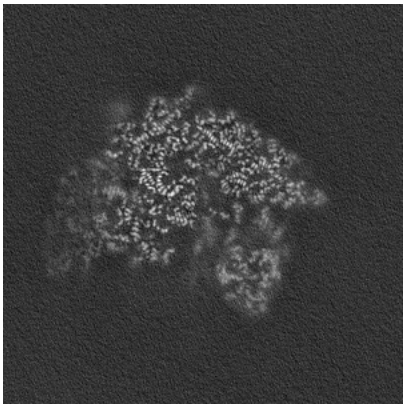


Z Index: 171

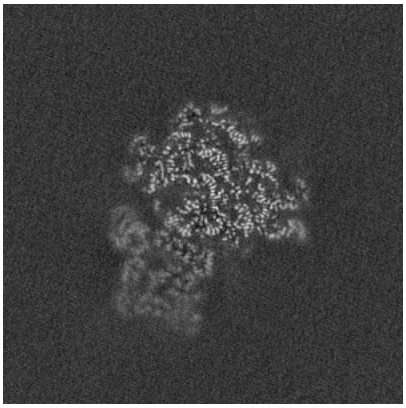
6.3.2 Raw map



X Index: 216



Y Index: 203

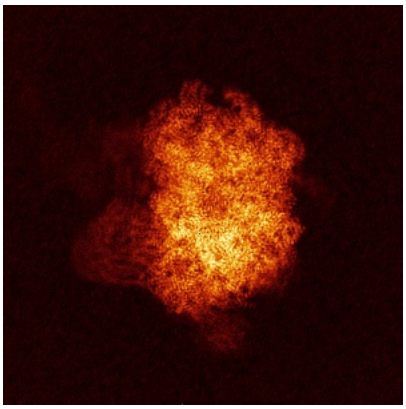


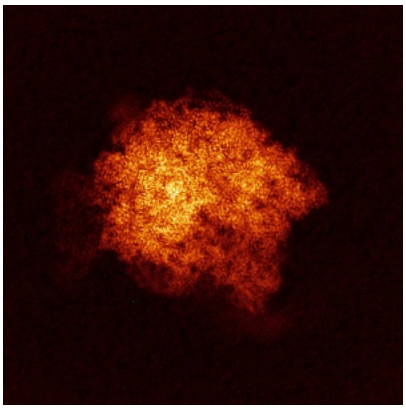
Z Index: 171

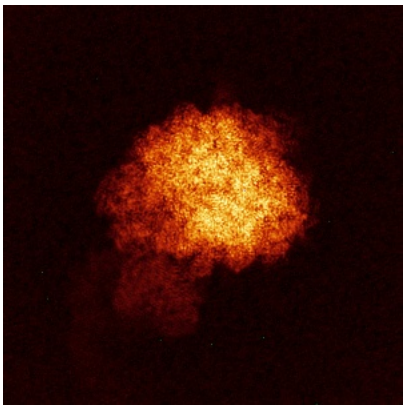
The images above show the largest variance slices of the map in three orthogonal directions.

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

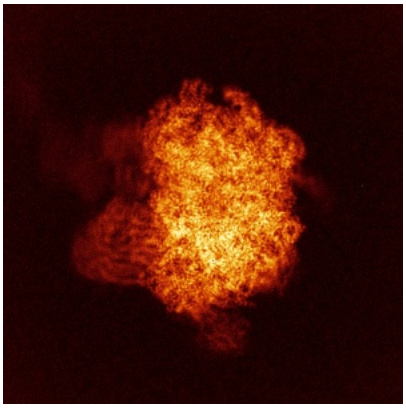
6.4.1 Primary map

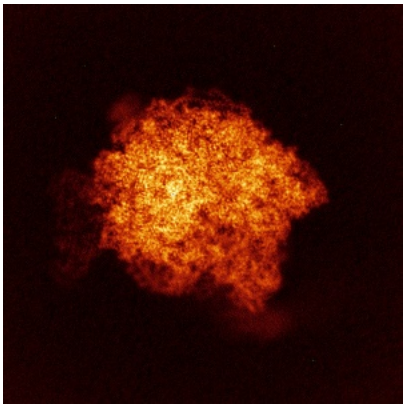

X

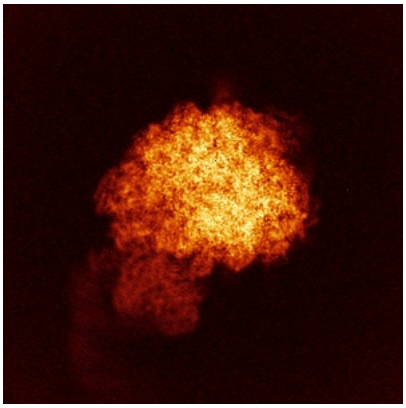

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

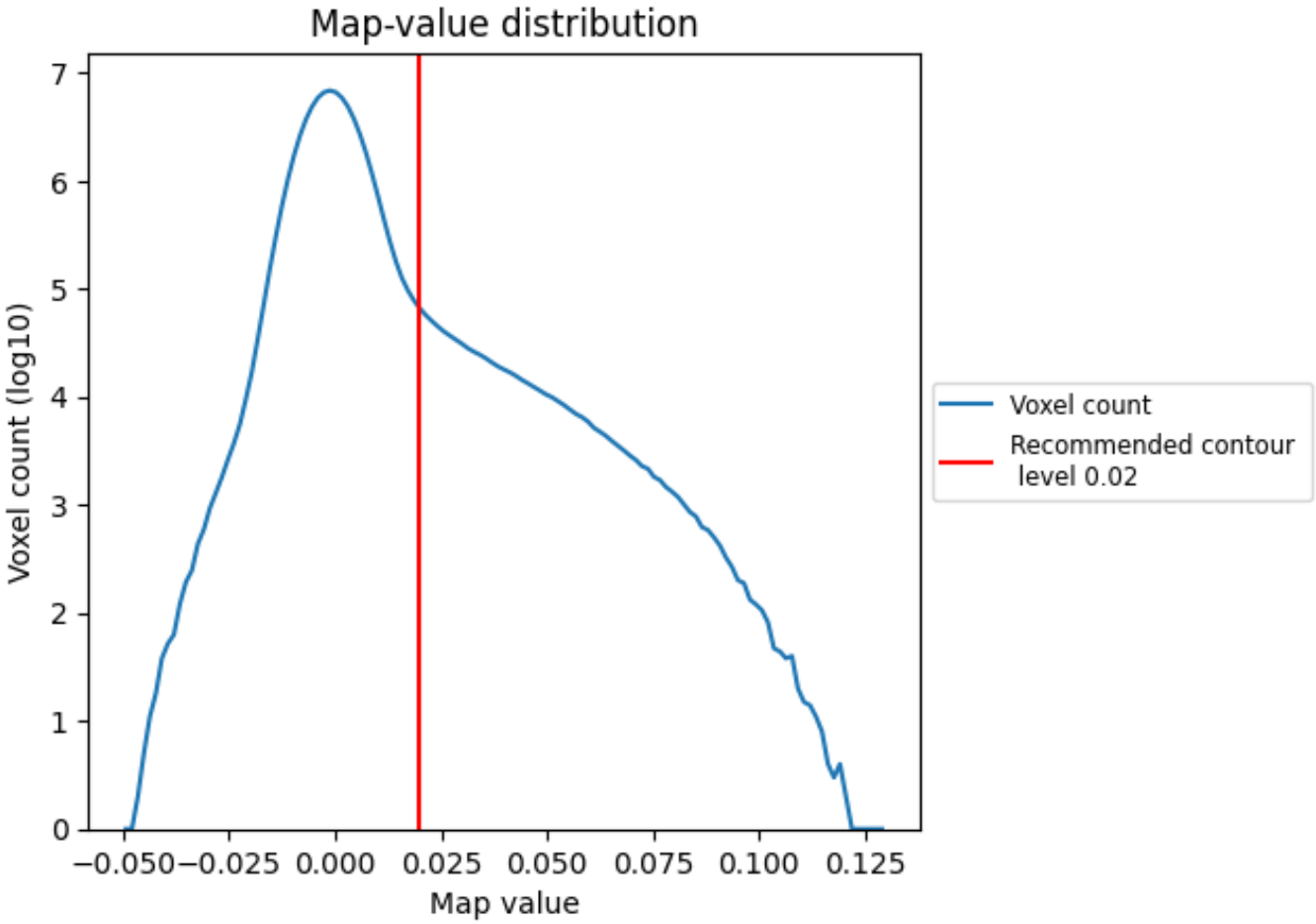
6.6 Mask visualisation (i)

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

7 Map analysis

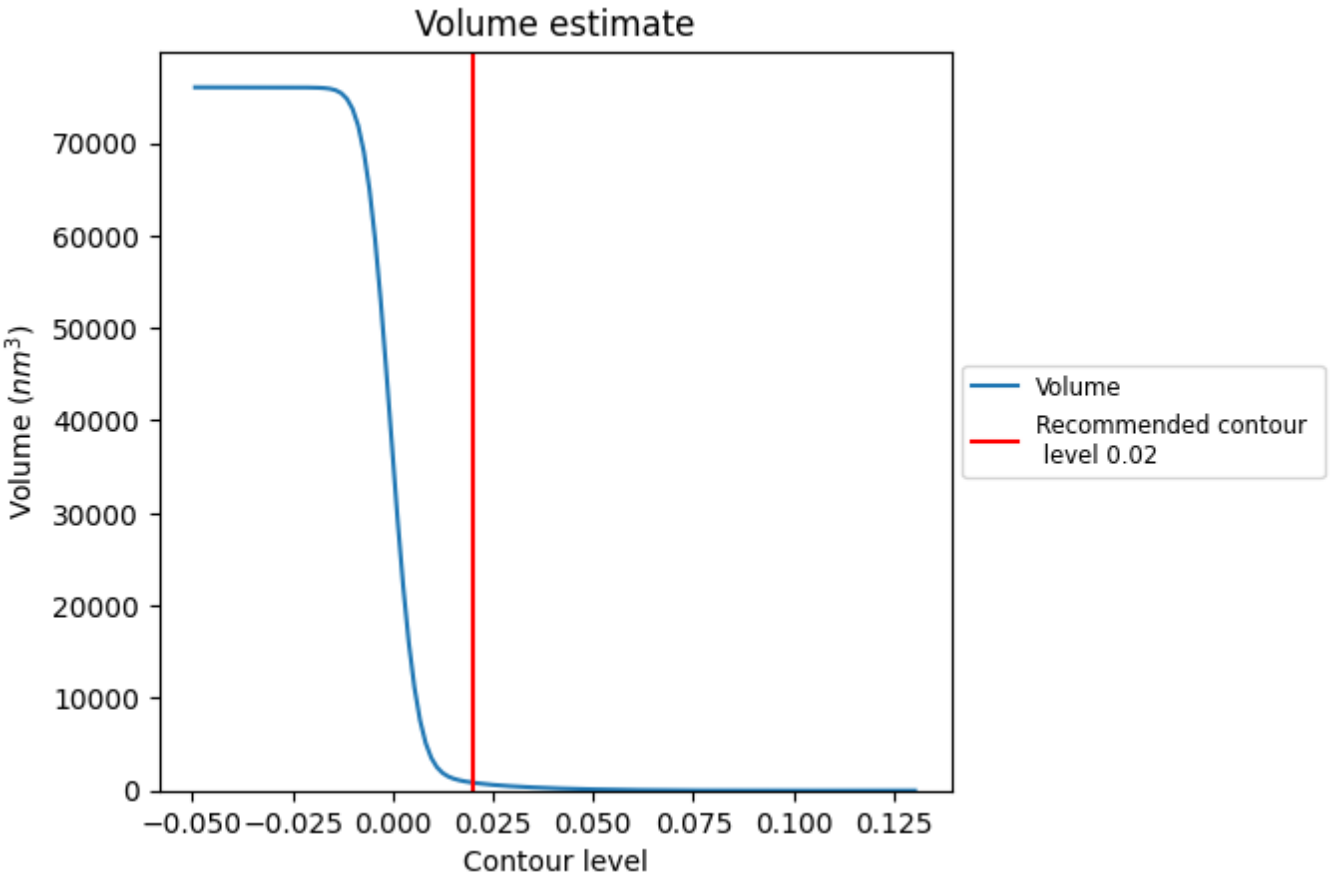
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

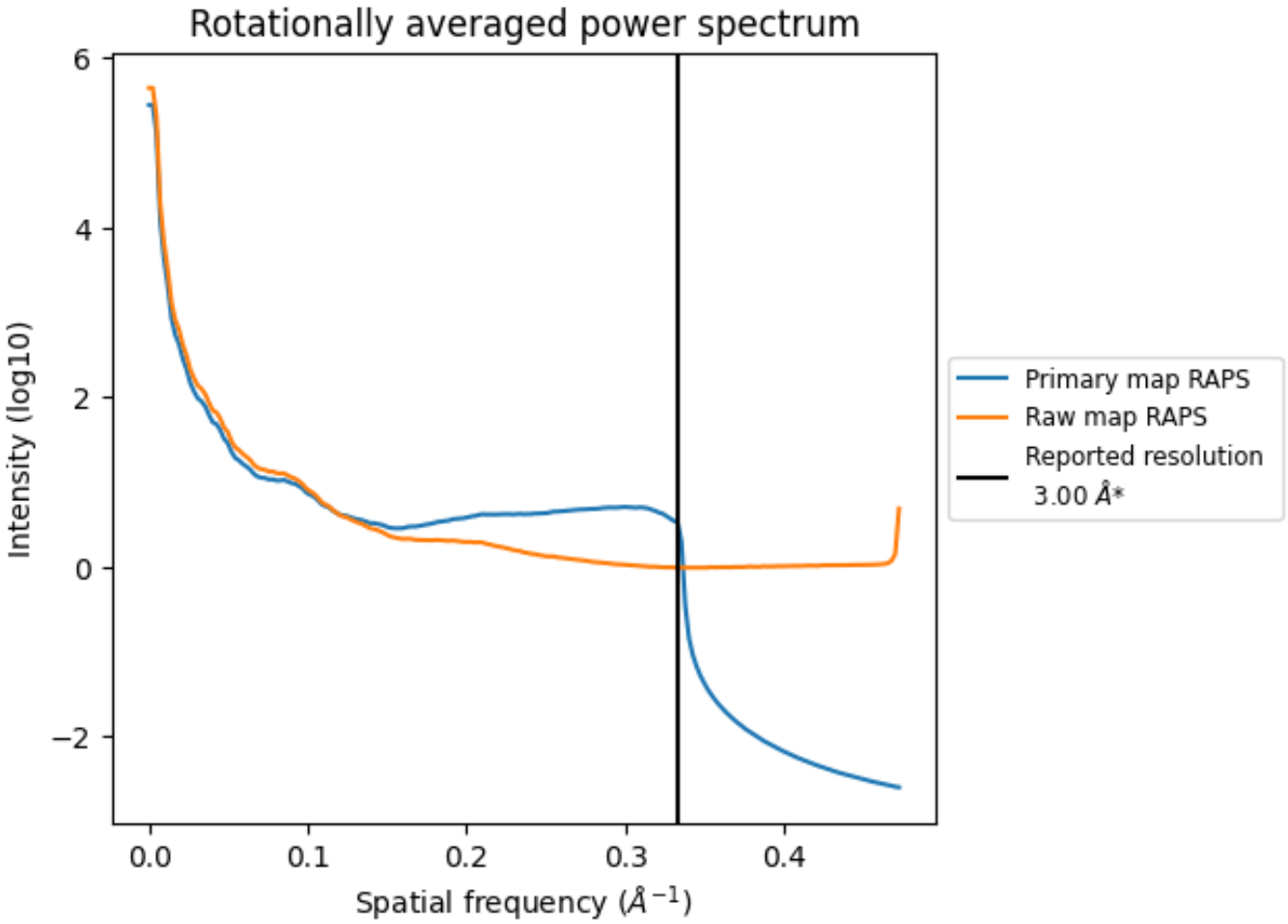
7.2 Volume estimate



The volume at the recommended contour level is 856 nm^3; this corresponds to an approximate mass of 773 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)

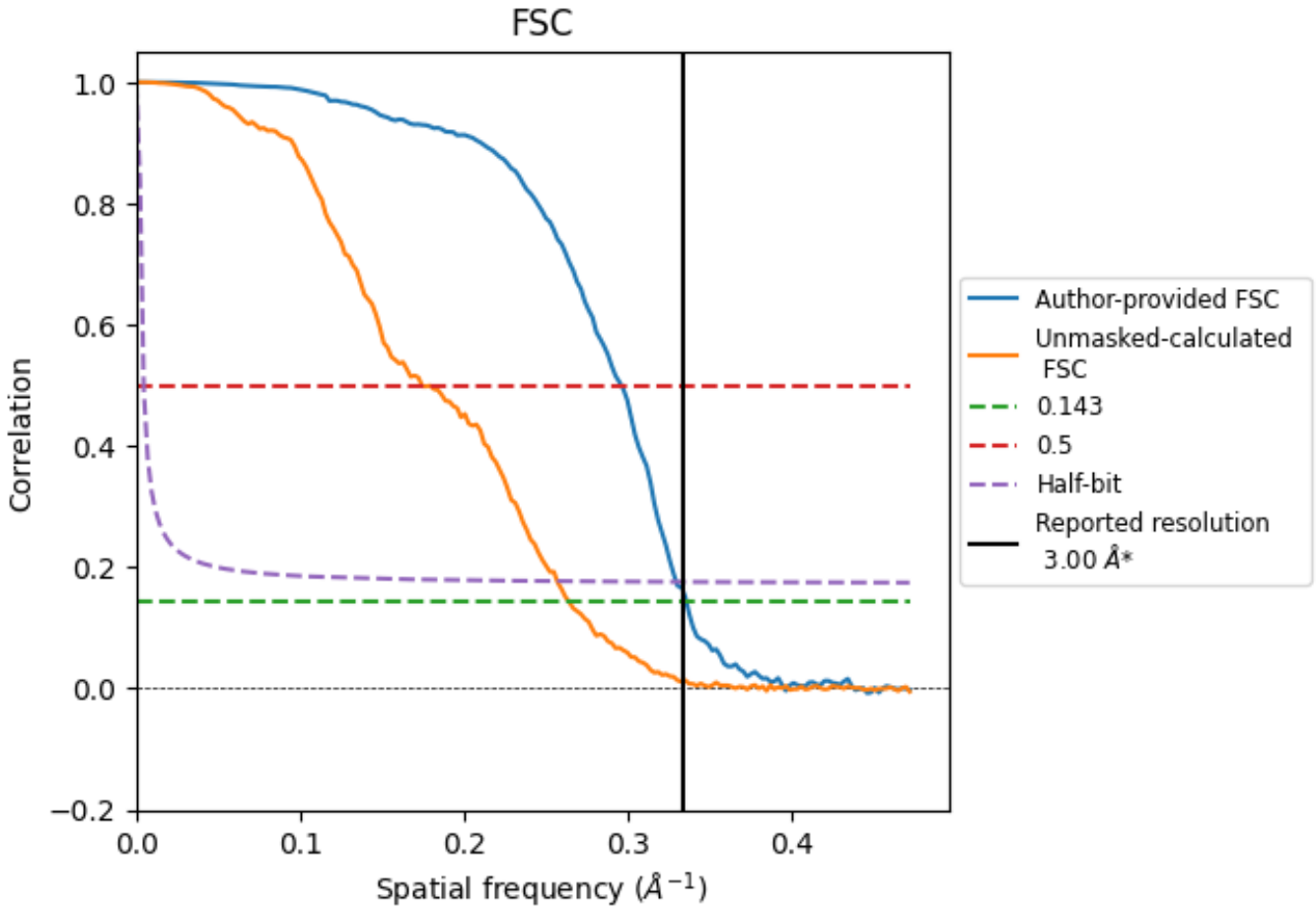


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

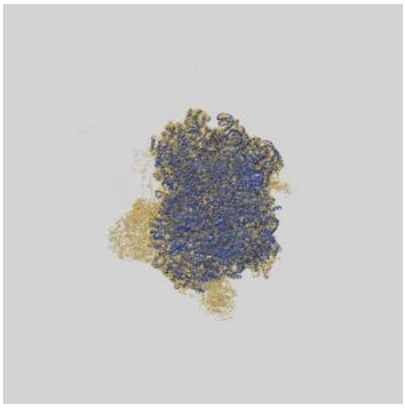
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.38	3.03
Unmasked-calculated*	3.79	5.73	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.0 by more than 10 %

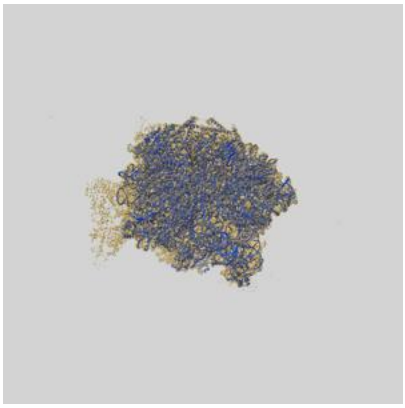
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10838 and PDB model 6YLG. Per-residue inclusion information can be found in section 3 on page 14.

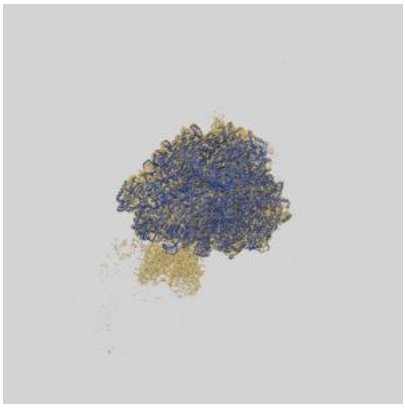
9.1 Map-model overlay



X



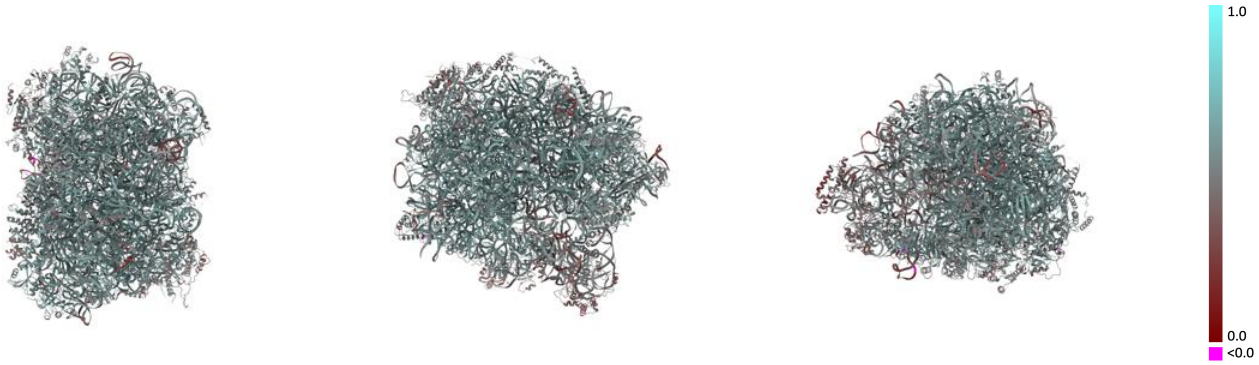
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

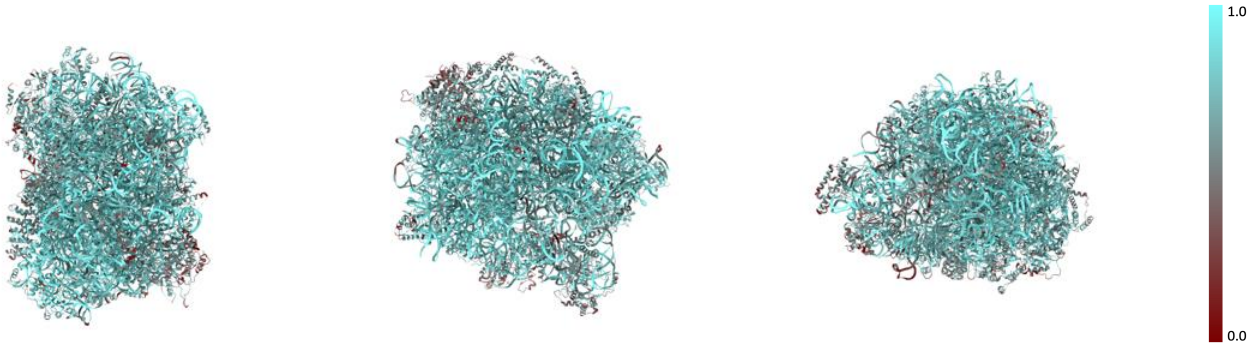
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

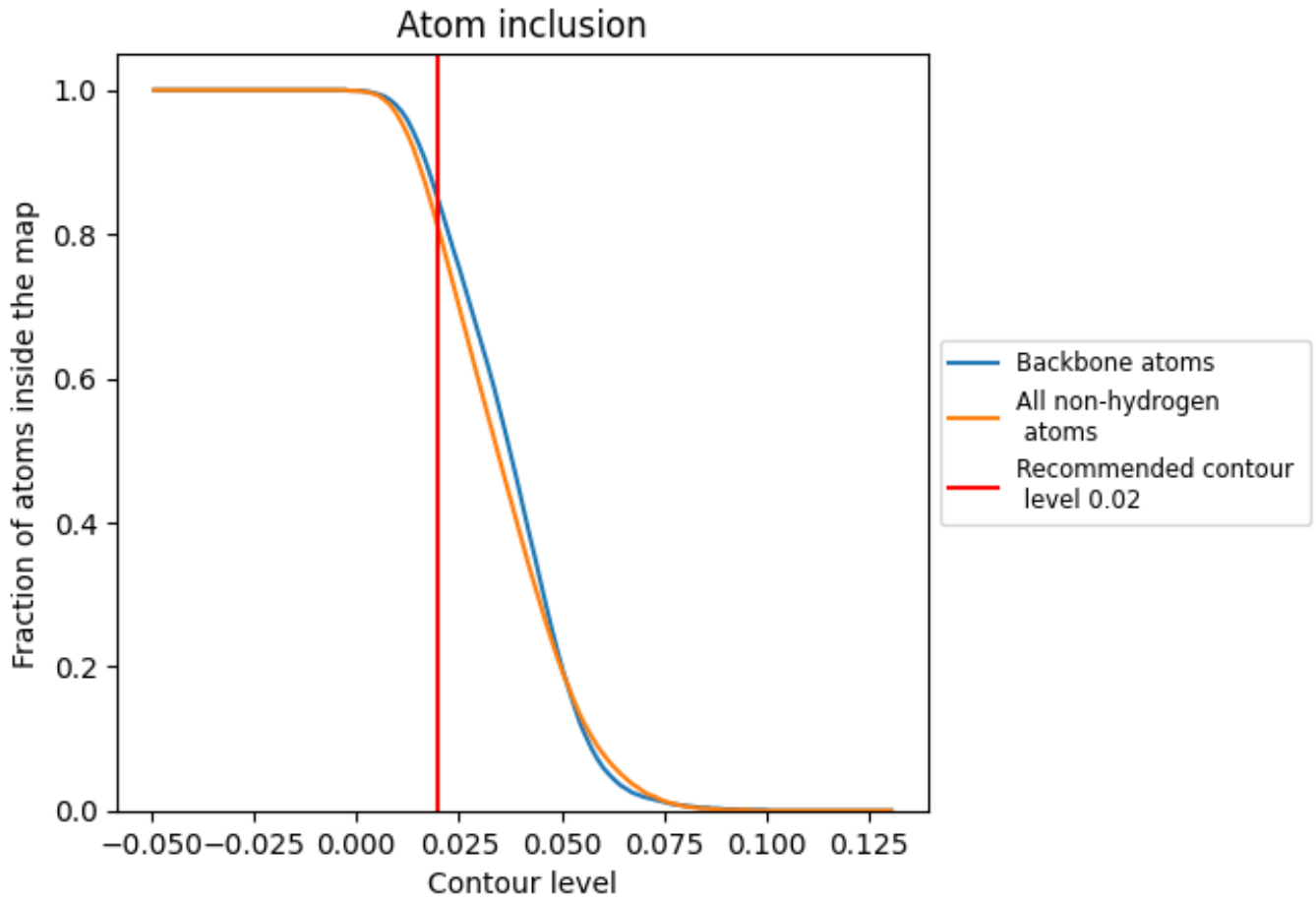
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 85% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.5450
1	0.8930	0.5550
2	0.9410	0.5890
3	0.8600	0.4940
4	0.5350	0.4960
5	0.5110	0.4530
A	0.8680	0.6000
B	0.8140	0.5750
C	0.8000	0.5680
D	0.5290	0.4160
E	0.7600	0.5430
F	0.7970	0.5550
G	0.7490	0.5330
H	0.7890	0.5620
I	0.6210	0.5320
J	0.6060	0.4570
K	0.6130	0.4870
L	0.7890	0.5520
M	0.8070	0.5580
N	0.8530	0.5920
O	0.8290	0.5790
P	0.8210	0.5800
Q	0.7790	0.5570
R	0.8060	0.5610
S	0.7420	0.5420
T	0.5150	0.4710
U	0.7730	0.5390
V	0.7460	0.5110
W	0.7110	0.5050
X	0.7670	0.5720
Y	0.7970	0.5690
Z	0.7860	0.5410
a	0.8120	0.5640
b	0.6590	0.5160
c	0.5520	0.5410

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Chain	Atom inclusion	Q-score
d	0.7870	0.5720
e	0.8070	0.5820
f	0.8540	0.6020
g	0.8070	0.5760
h	0.8040	0.5690
i	0.7500	0.5420
j	0.8830	0.6000
k	0.6910	0.5320
l	0.8530	0.6010
m	0.7500	0.5510
n	0.7850	0.5390
o	0.3630	0.3880
p	0.8140	0.5820
q	0.6040	0.4710
r	0.7920	0.5720
s	0.4980	0.5050
t	0.6360	0.5100
u	0.7590	0.5460
x	0.7530	0.5360
y	0.6930	0.5060
z	0.6190	0.5340