



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:39 am GMT

PDB ID : 6FYY  
EMDB ID : EMD-4328  
Title : Structure of a partial yeast 48S preinitiation complex with eIF5 N-terminal domain (model C2)  
Authors : Llacer, J.L.; Hussain, T.; Gordiyenko, Y.; Ramakrishnan, V.  
Deposited on : 2018-03-12  
Resolution : 3.05 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

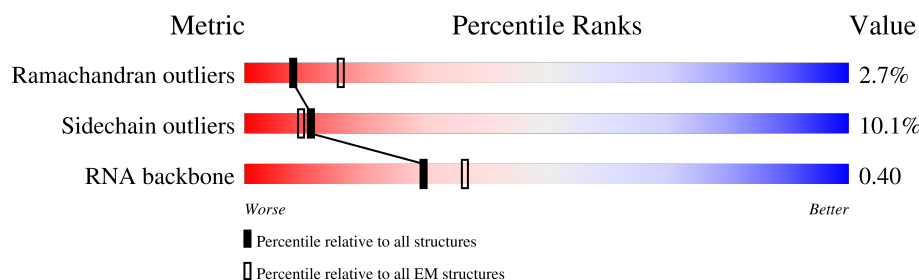
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	76	<div> <div>62%</div> <div>55%</div> <div>30%</div> <div>13%</div> <div>.</div> </div>
2	2	1798	<div> <div>12%</div> <div>61%</div> <div>37%</div> <div>..</div> </div>
3	3	49	<div> <div>49%</div> <div>27%</div> <div>37%</div> <div>37%</div> </div>
4	A	254	<div> <div>6%</div> <div>72%</div> <div>14%</div> <div>14%</div> </div>
5	B	255	<div> <div>13%</div> <div>76%</div> <div>11%</div> <div>.</div> <div>12%</div> </div>
6	C	259	<div> <div>74%</div> <div>11%</div> <div>15%</div> </div>
7	D	237	<div> <div>7%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
8	E	261	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	

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Mol	Chain	Length	Quality of chain
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	405	
43	o	964	
44	p	763	
45	q	812	
46	r	274	
47	s	347	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C4J	2	1190	X	-	-	-

## 2 Entry composition [i](#)

There are 51 unique types of molecules in this entry. The entry contains 104316 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 tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1780	Total	C	N	O	P	0	0
			37812	16904	6659	12469	1780		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	G	U	conflict	GB 49642208
2	678	U	G	conflict	GB 49642208
2	1190	C4J	U	conflict	GB 49642208

- Molecule 3 is a RNA chain called mRNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	31	Total	C	N	O	P	4	0
			719	324	108	252	35		

- Molecule 4 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 5 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	225	Total	C	N	O	S	0	0
			1797	1135	330	329	3		

- Molecule 6 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	220	Total	C	N	O	S	0	0
			1648	1053	291	300	4		

- Molecule 7 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	227	Total	C	N	O	S	0	0
			1774	1126	320	323	5		

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	230	Total	C	N	O	S	0	0
			1832	1146	352	330	4		

- Molecule 11 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	M	117	Total	C	N	O	0	0
			885	553	161	171		

- Molecule 17 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	151	Total	C	N	O	S	0	0
			1195	761	224	207	3		

- Molecule 18 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	129	Total	C	N	O	S	0	0
			955	585	191	176	3		

- Molecule 19 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	117	Total	C	N	O	S	0	0
			923	592	165	161	5		

- Molecule 20 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Q	141	Total	C	N	O	0	0
			1105	709	204	192		

- Molecule 21 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	130	Total	C	N	O	S	0	0
			1033	643	194	193	3		

- Molecule 22 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1189	739	239	209	2		

- Molecule 23 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 24 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called KLLA0B11231p.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 29 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	78	Total	C	N	O	S	0	0
			594	376	111	106	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	103	Total	C	N	O	S	0	0
			812	500	173	134	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	64	Total	C	N	O	S	0	0
			499	308	99	91	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	55	Total	C	N	O	S	0	0
			461	289	93	78	1		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	60	Total	C	N	O	S	0	0
			472	295	96	80	1		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	74	Total	C	N	O	S	0	0
			584	374	111	95	4		

- Molecule 36 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	320	Total	C	N	O	S	0	0
			2469	1561	432	471	5		

- Molecule 37 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	121	Total	C	N	O	S	0	0
			958	587	183	183	5		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	147	Total	C	N	O	S	0	0
			1140	724	201	208	7		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	529	Total	C	N	O	S	0	0
			4070	2597	697	769	7		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	647	Total	C	N	O	S	0	0
			5114	3274	880	942	18		

- Molecule 45 is a protein called eIF3c, Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	621	Total	C	N	O	S	0	0
			4827	3076	813	926	12		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	r	49	Total	C	N	O	0	0
			392	240	76	76		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	330	Total	C	N	O	S	0	0
			2606	1661	429	507	9		

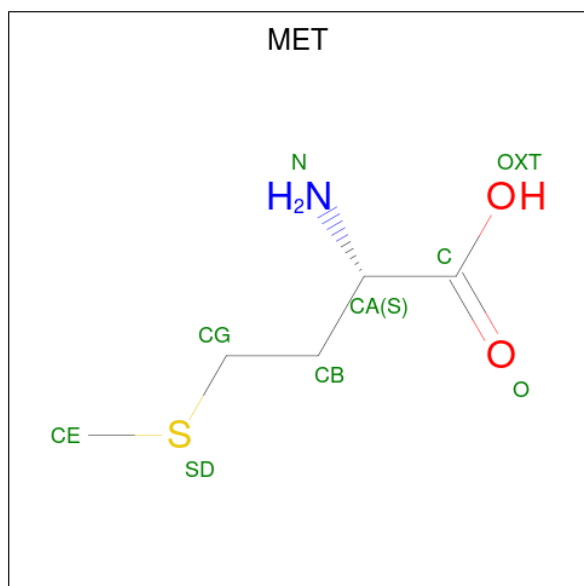
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	116	Total	Mg	0
			116	116	
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

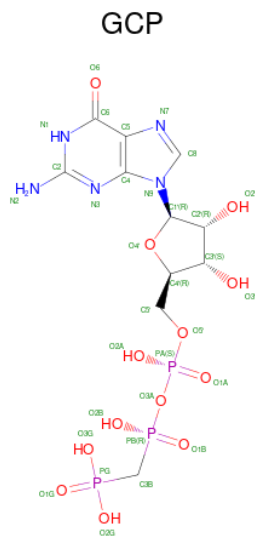
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	m	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

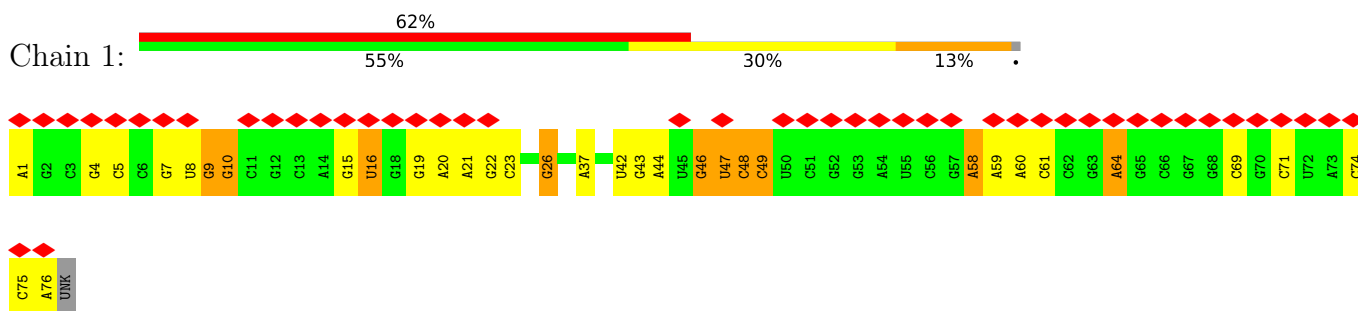


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

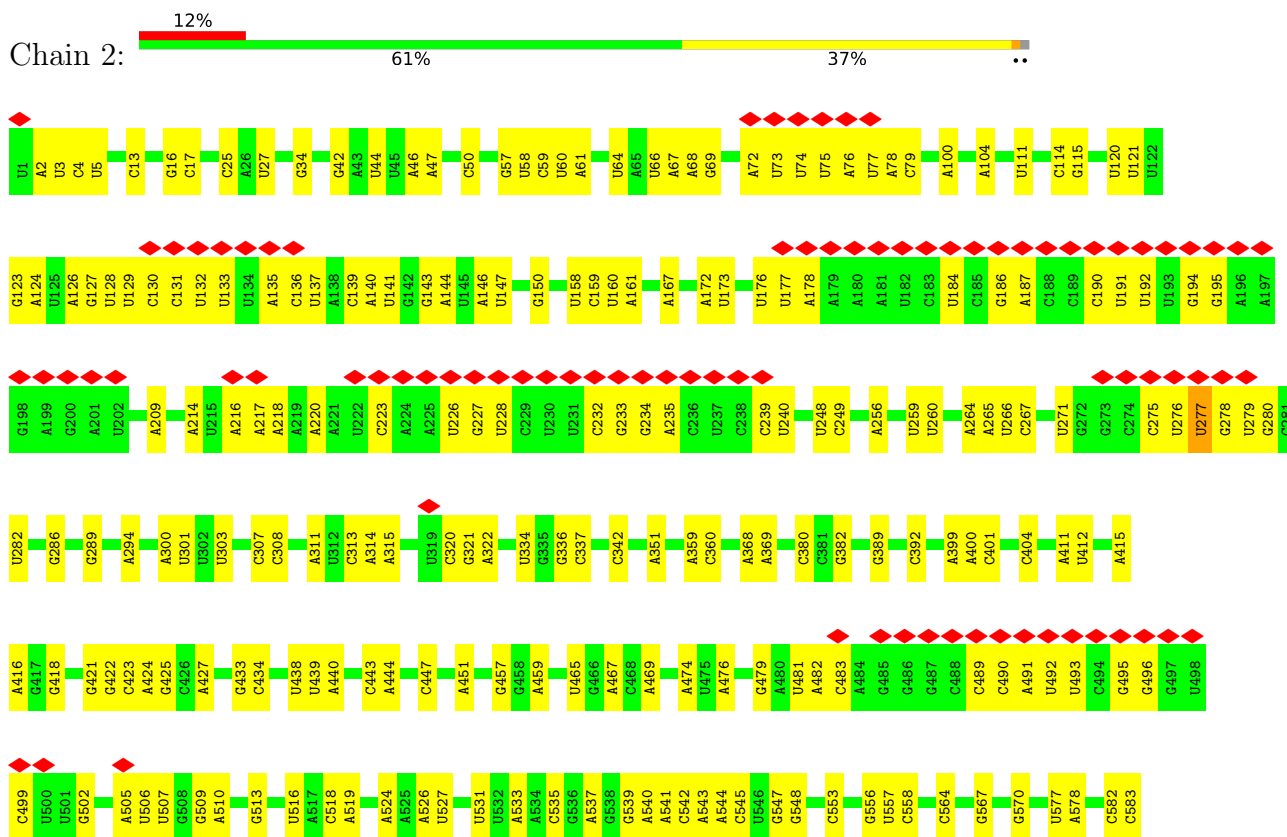
### 3 Residue-property plots

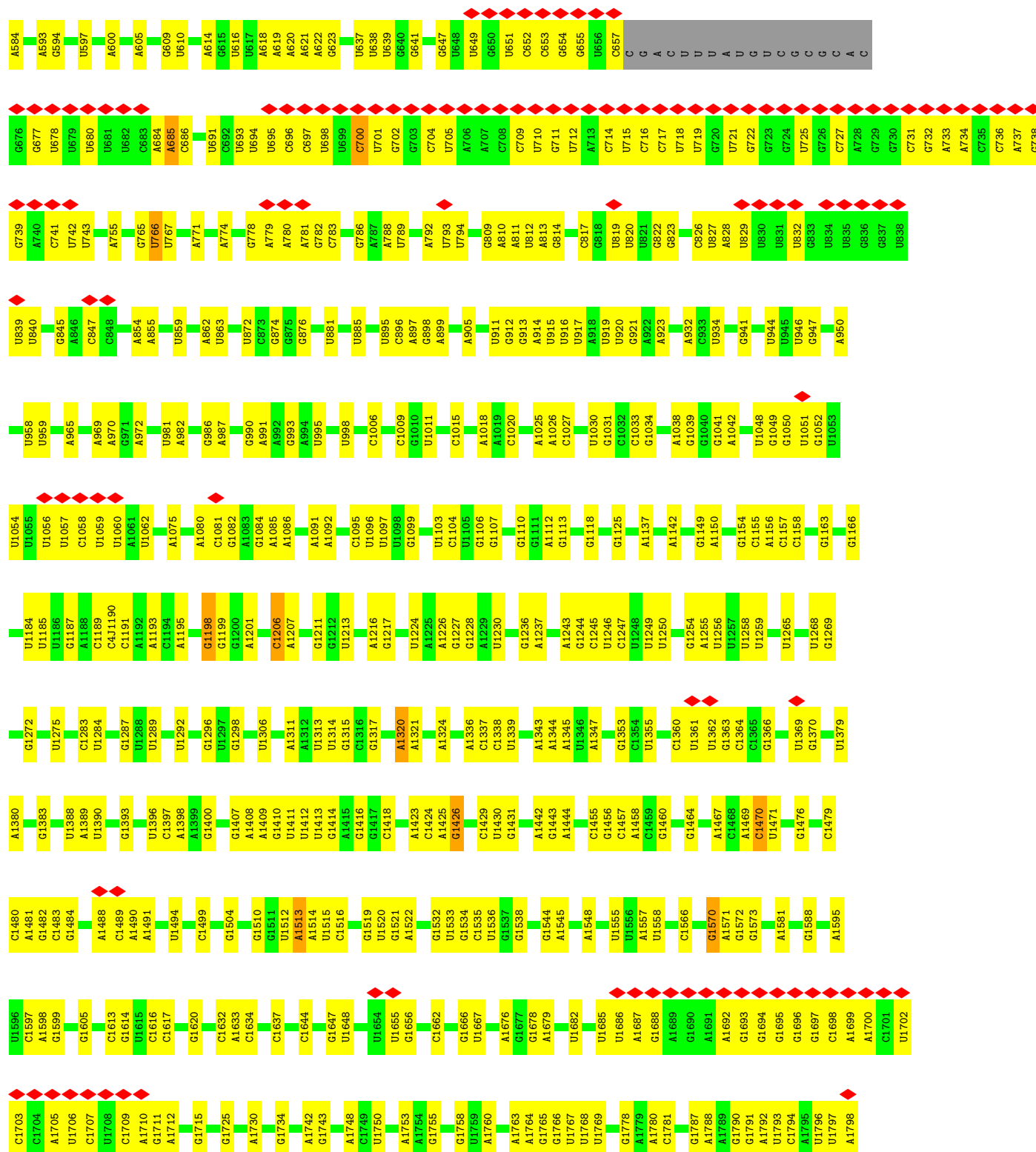
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: tRNAi

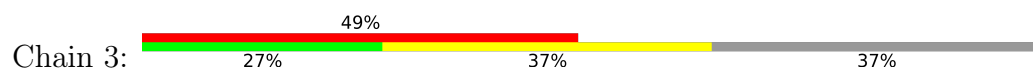


#### • Molecule 2: 18S ribosomal RNA






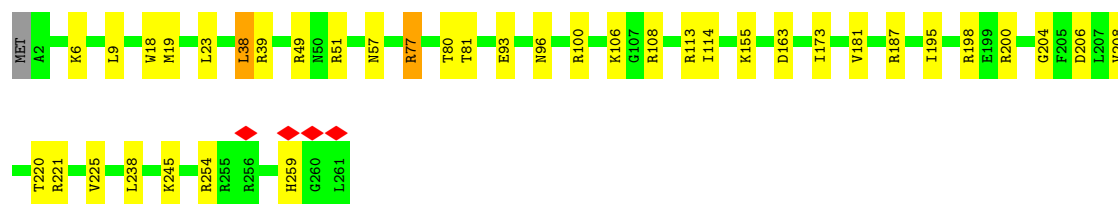
• Molecule 3: mRNA (31-MER)






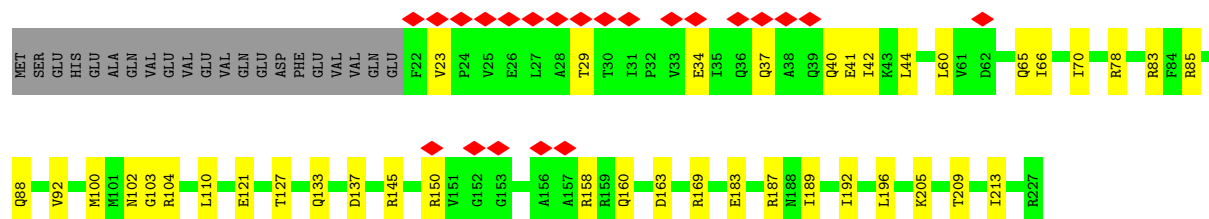


Chain E: 




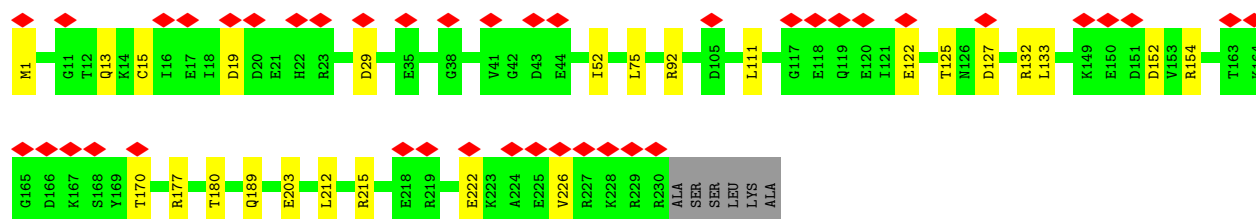
• Molecule 9: KLLA0D10659p

Chain F: 




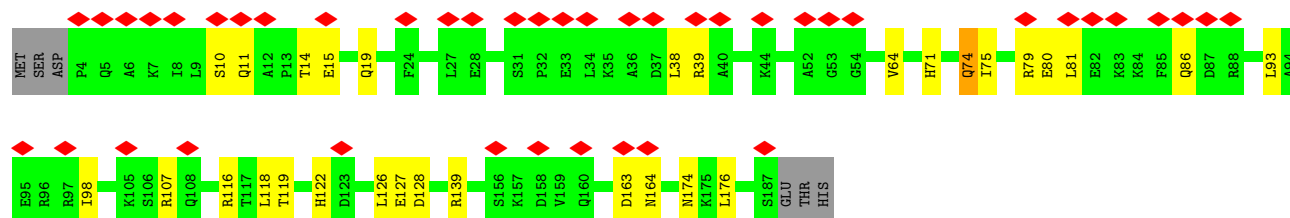
• Molecule 10: 40S ribosomal protein S6

Chain G: 




• Molecule 11: 40S ribosomal protein S7

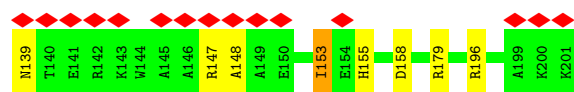
Chain H: 



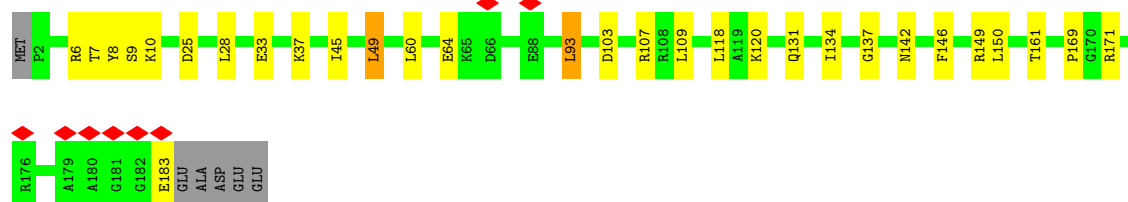
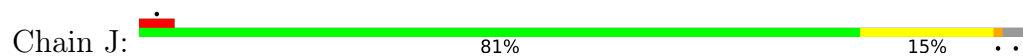
• Molecule 12: 40S ribosomal protein S8

Chain I: 

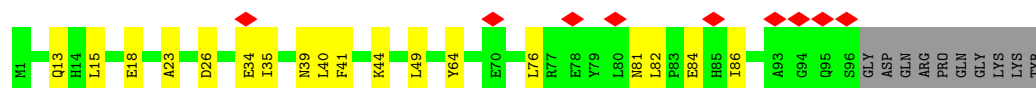
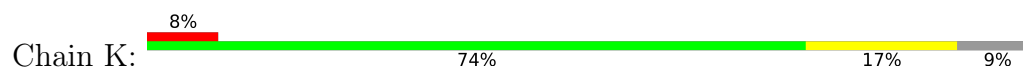




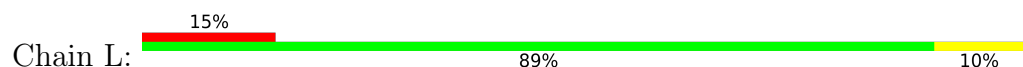
• Molecule 13: KLLA0E23673p



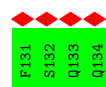
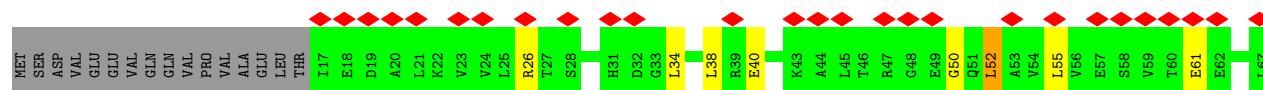
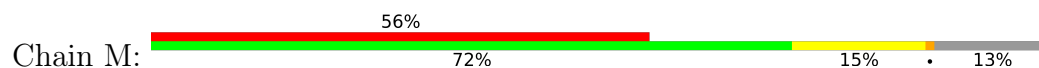
• Molecule 14: KLLA0B08173p



• Molecule 15: KLLA0A10483p



• Molecule 16: 40S ribosomal protein S12

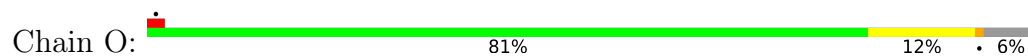


• Molecule 17: KLLA0F18040p

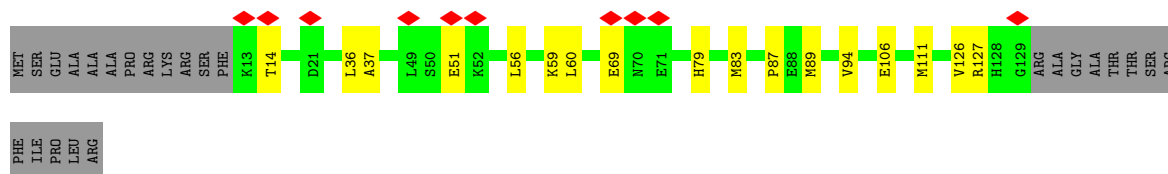




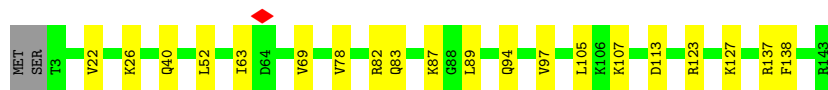
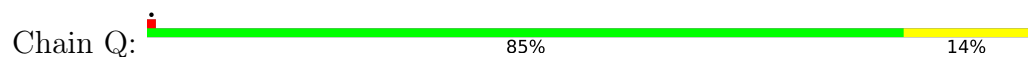
- Molecule 18: 40S ribosomal protein S14



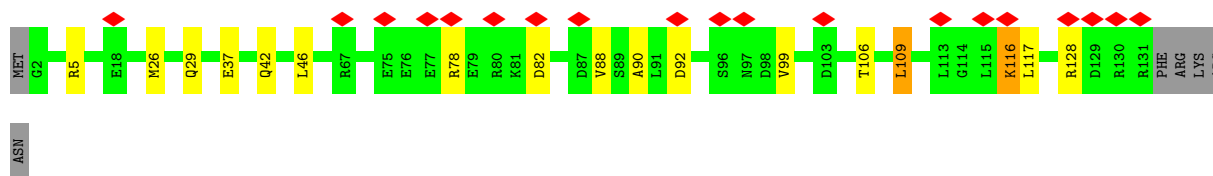
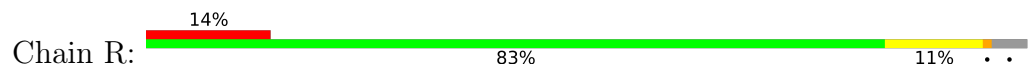
- Molecule 19: KLLA0F07843p



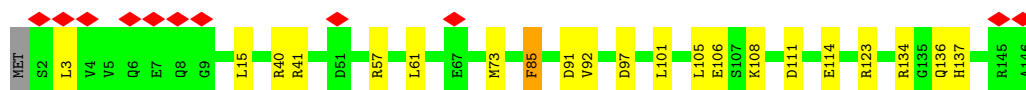
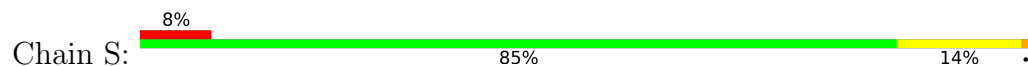
- Molecule 20: 40S ribosomal protein S16



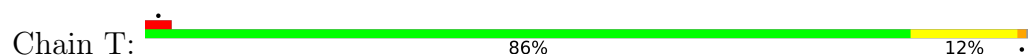
- Molecule 21: KLLA0B01474p

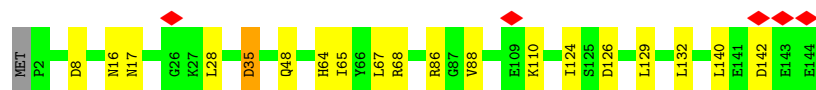


- Molecule 22: KLLA0B01562p

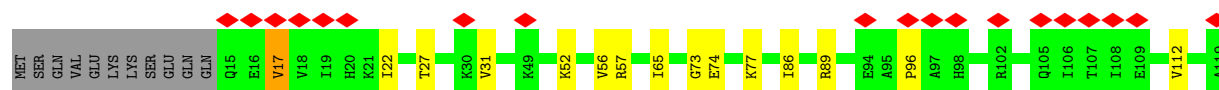
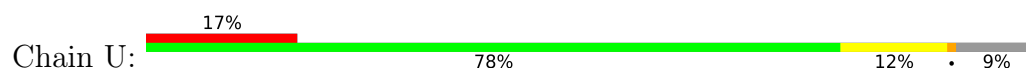


- Molecule 23: KLLA0A07194p

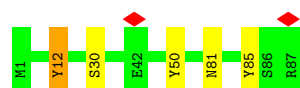




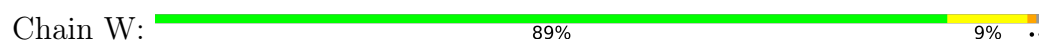
- Molecule 24: KLLA0F25542p



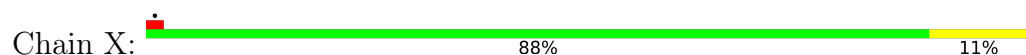
- Molecule 25: 40S ribosomal protein S21



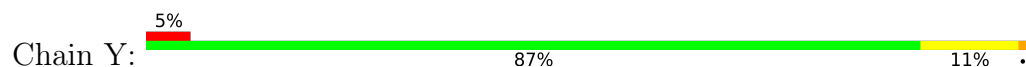
- Molecule 26: 40S ribosomal protein S22



- Molecule 27: KLLA0B11231p

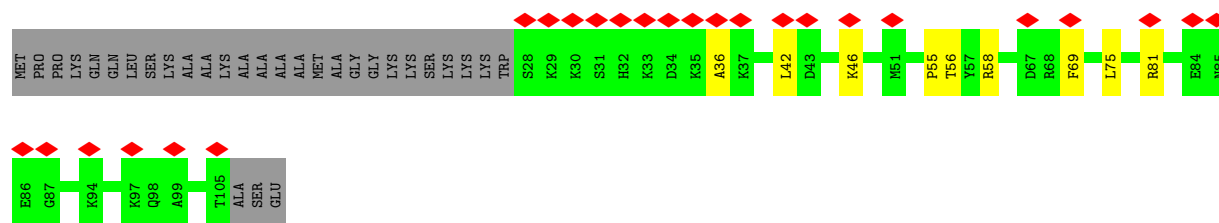


- Molecule 28: 40S ribosomal protein S24

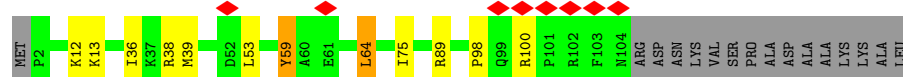
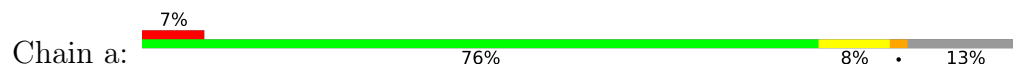


- Molecule 29: KLLA0B06182p

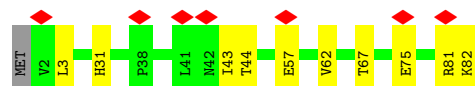
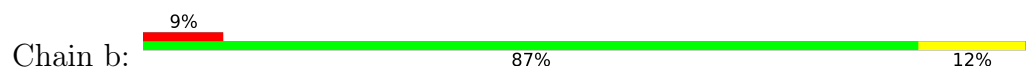




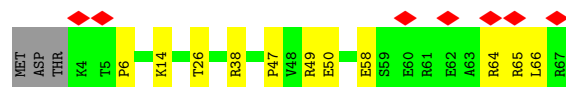
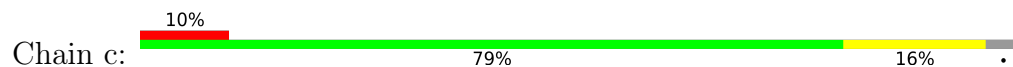
- Molecule 30: 40S ribosomal protein S26



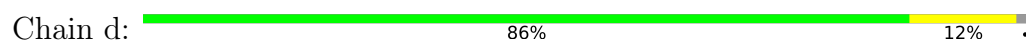
- Molecule 31: 40S ribosomal protein S27



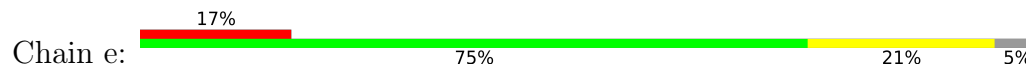
- Molecule 32: 40S ribosomal protein S28



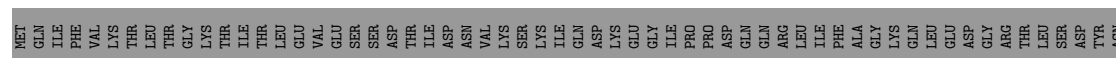
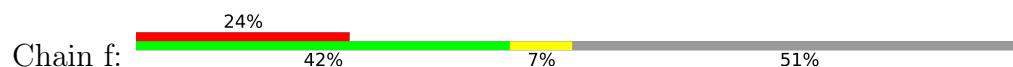
- Molecule 33: 40S ribosomal protein S29

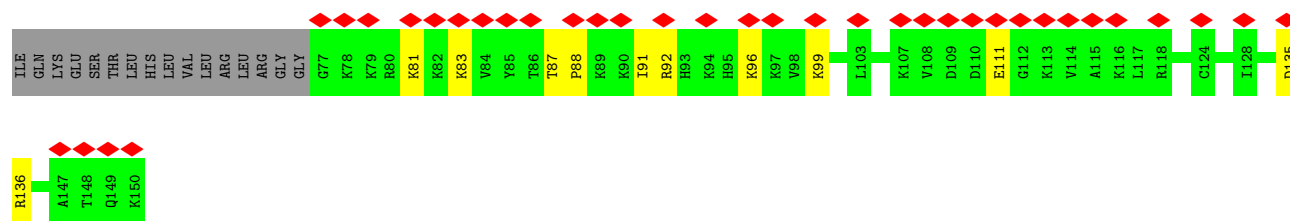


- Molecule 34: 40S ribosomal protein S30

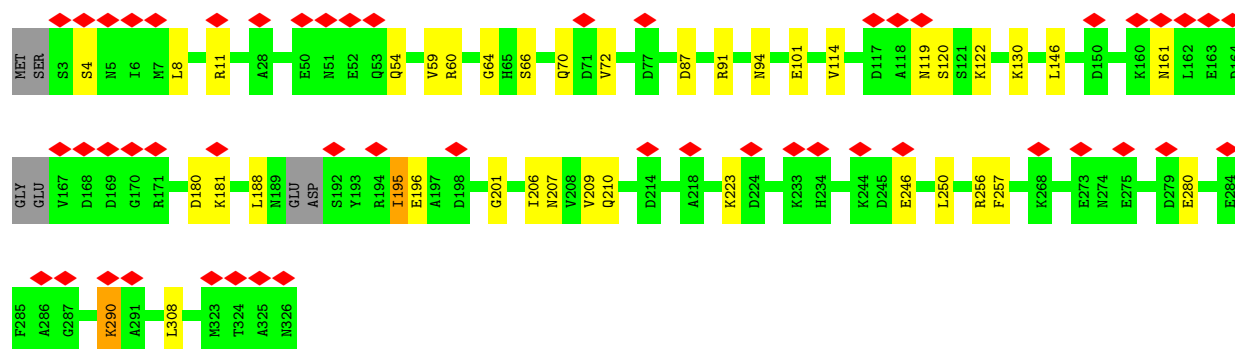
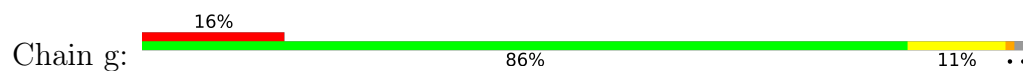


- Molecule 35: Ubiquitin-40S ribosomal protein S27a





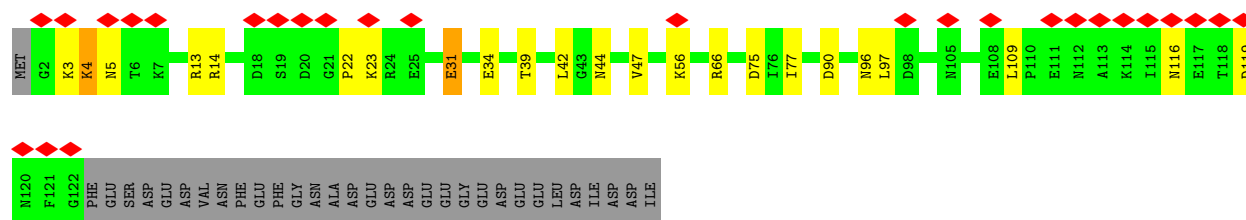
• Molecule 36: KLLA0E12277p



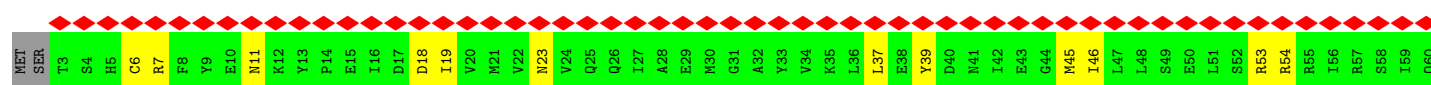
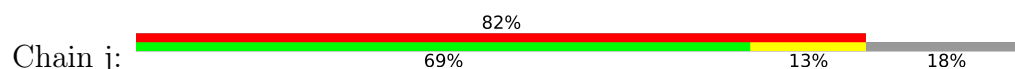
• Molecule 37: 60S ribosomal protein L41-A



• Molecule 38: Eukaryotic translation initiation factor 1A



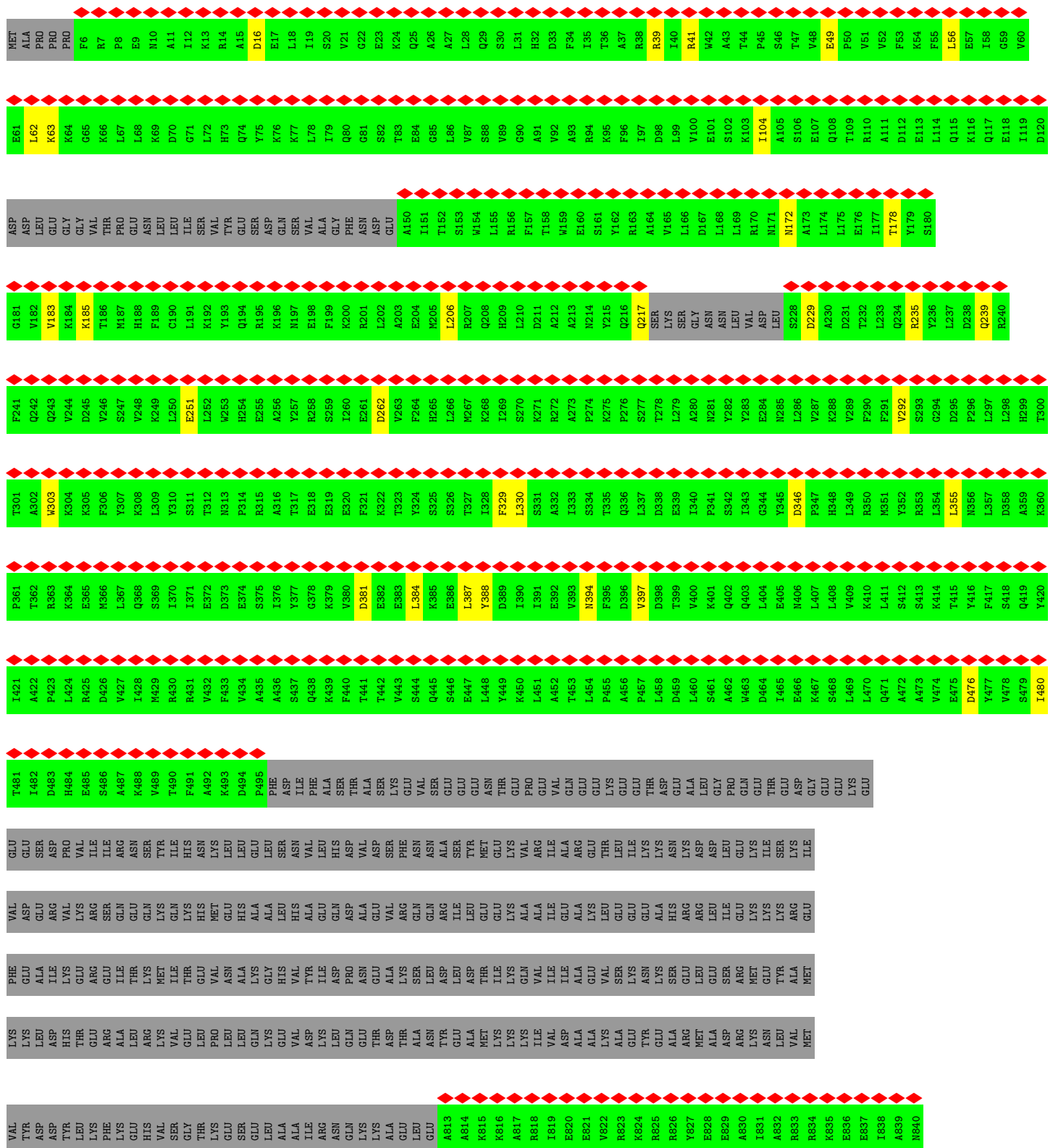
• Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha



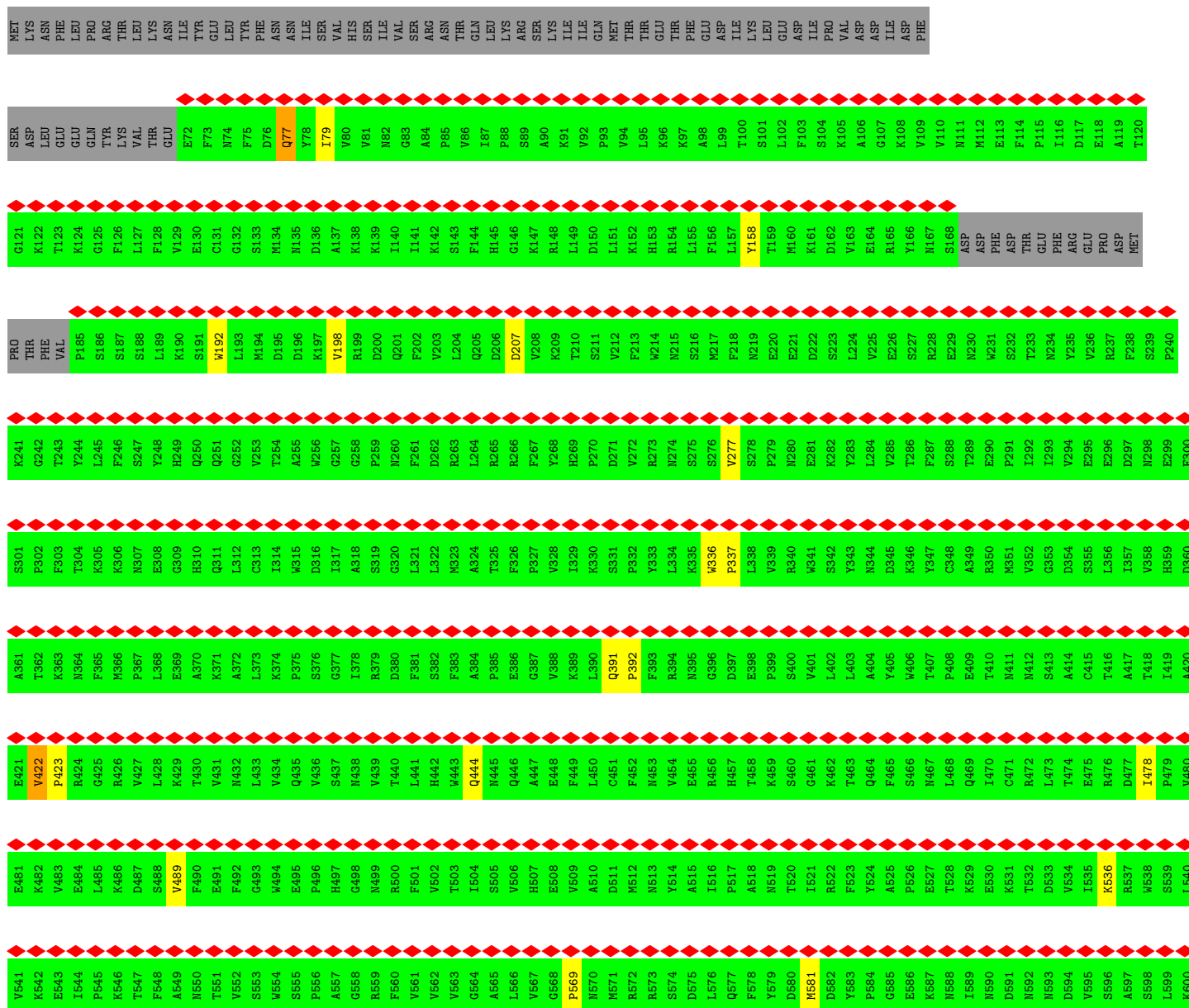
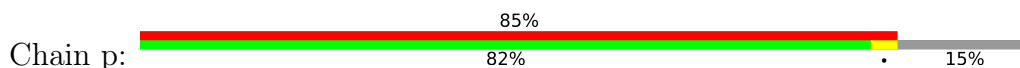




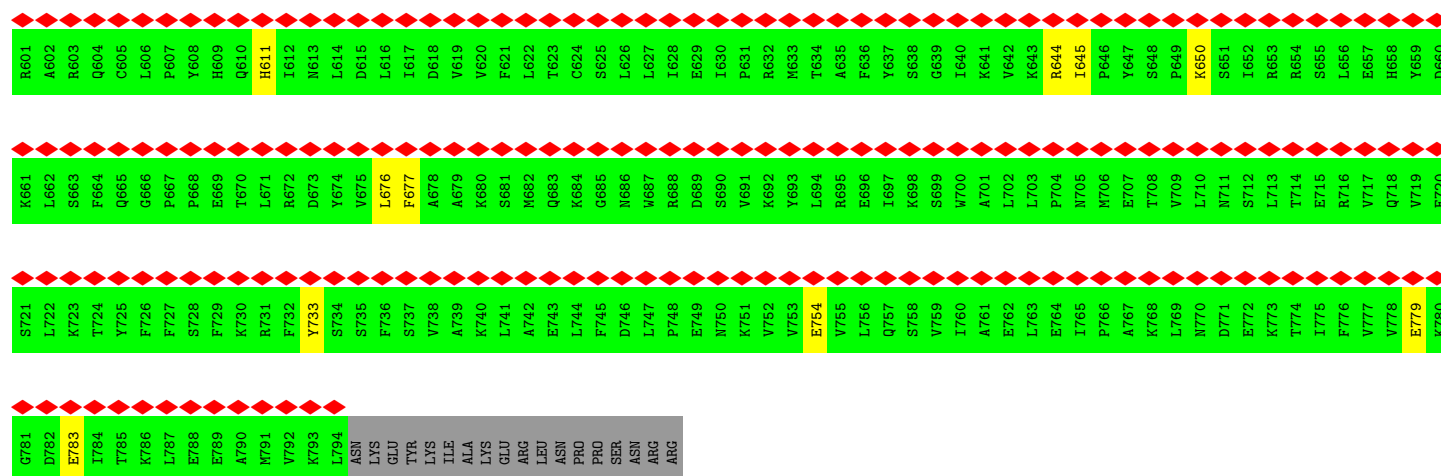




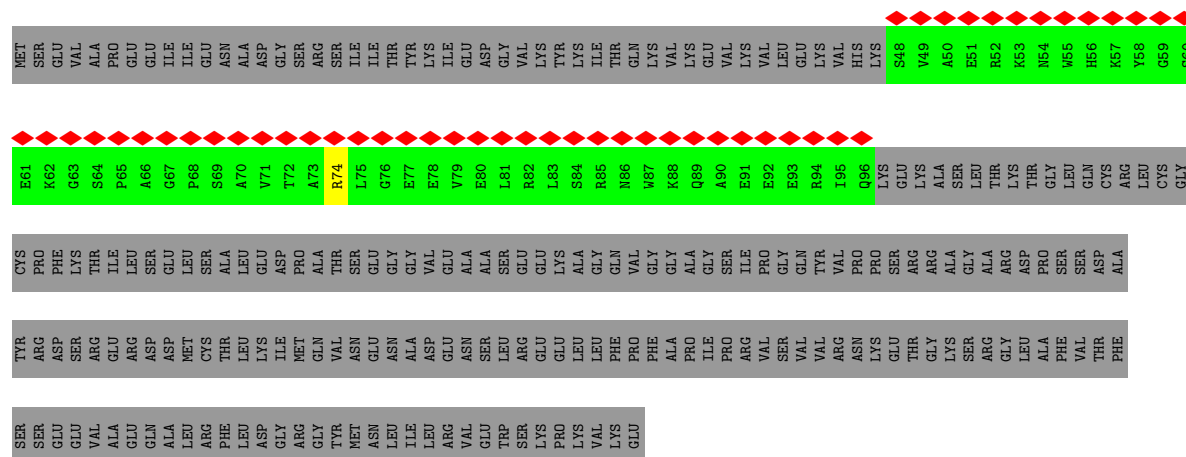
- Molecule 44: Eukaryotic translation initiation factor 3 subunit B



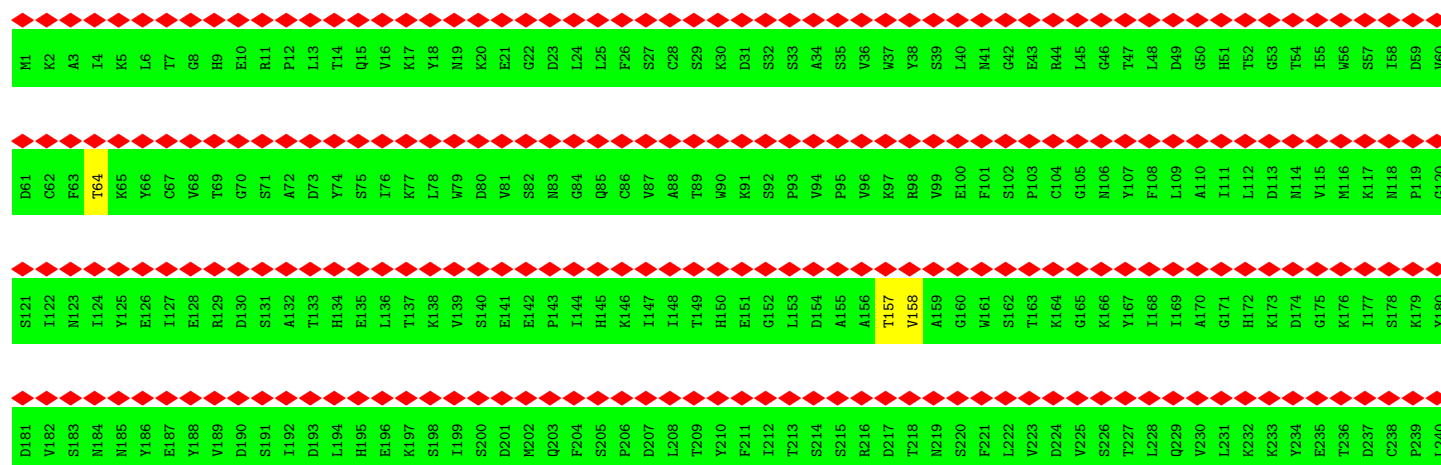




• Molecule 46: Eukaryotic translation initiation factor 3 subunit G



• Molecule 47: Eukaryotic translation initiation factor 3 subunit I



N241	T242	A243	V244	I245	T246	P247	L248	K249	E250	F251	I252	I253	L254	G255	G256	G257	Q258	GLU	ALA	LYS	ASP	VAL	THR	THR	SER	ALA	ASN	GLU	G271	K272	F273	E274	A275	R276	F277	Y278	H279	K280	I281	F282	E283	E284	E285	I286	G287	R288	V289	Q290	G291	H292	F293	G294	P295	L296	N297	T298	V299	A300
I301	S302	P303	Q304	G305	T306	S307	Y308	A309	S310	G311	G312	E313	D314	G315	F316	I317	R318	L319	H320	H321	F322	E323	K324	S325	Y326	F327	D328	F329	K330	Y331	D332	V333	E334	K335	A336	A337	E338	A339	K340	E341	H342	MET	GLN	GLU	ALA	ASN												

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.157	Depositor
Minimum map value	-0.645	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: T6A, 1MA, C4J, 2MG, MG, MA6, M2G, PSU, 1MG, GCP, AYA, ZN, H2U, RIA, 5MC, 7MG

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	0.36	1/1529 (0.1%)	0.71	0/2376
2	2	0.29	0/41987	0.70	9/65416 (0.0%)
3	3	0.39	0/797	0.81	2/1233 (0.2%)
4	A	0.40	0/1742	0.72	1/2383 (0.0%)
5	B	0.37	0/1813	0.73	2/2438 (0.1%)
6	C	0.39	0/1678	0.71	0/2277
7	D	0.40	0/1800	0.73	0/2421
8	E	0.38	0/2122	0.71	1/2861 (0.0%)
9	F	0.39	0/1628	0.75	0/2198
10	G	0.38	0/1855	0.70	0/2479
11	H	0.40	0/1507	0.73	1/2028 (0.0%)
12	I	0.38	0/1515	0.72	0/2029
13	J	0.40	0/1495	0.78	1/2001 (0.0%)
14	K	0.46	0/831	0.76	1/1123 (0.1%)
15	L	0.40	0/1276	0.64	0/1718
16	M	0.42	0/891	0.75	1/1201 (0.1%)
17	N	0.40	0/1218	0.72	0/1638
18	O	0.39	0/966	0.74	0/1297
19	P	0.38	0/942	0.67	0/1269
20	Q	0.39	0/1125	0.73	0/1510
21	R	0.42	0/1044	0.78	1/1402 (0.1%)
22	S	0.39	0/1208	0.74	0/1624
23	T	0.39	0/1129	0.72	0/1520
24	U	0.38	0/857	0.72	0/1158
25	V	0.37	0/696	0.68	0/938
26	W	0.39	0/1039	0.74	0/1399
27	X	0.41	0/1137	0.71	0/1516
28	Y	0.38	0/1075	0.65	0/1433
29	Z	0.38	0/603	0.68	1/814 (0.1%)
30	a	0.37	0/825	0.68	0/1106
31	b	0.36	0/619	0.63	0/837
32	c	0.35	0/501	0.70	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	d	0.38	0/473	0.66	0/629
34	e	0.39	0/480	0.69	0/640
35	f	0.41	0/597	0.61	0/795
36	g	0.37	0/2523	0.65	0/3434
37	h	0.33	0/234	0.70	0/300
38	i	0.38	0/969	0.68	0/1287
39	j	0.42	0/2034	0.63	0/2737
40	k	0.39	0/3079	0.60	0/4157
41	l	0.42	0/1051	0.59	0/1402
42	m	0.40	0/1164	0.64	0/1575
43	o	0.42	0/4140	0.64	6/5608 (0.1%)
44	p	0.43	0/5245	0.59	0/7115
45	q	0.44	0/4523	0.61	0/6114
46	r	0.40	0/399	0.54	0/535
47	s	0.43	0/2669	0.59	0/3611
All	All	0.36	1/109030 (0.0%)	0.69	27/156255 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	1	0
20	Q	0	1
44	p	0	2
All	All	1	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-10.07	1.49	1.61

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	18[A]	U	P-O3'-C3'	8.96	130.45	119.70
3	3	18[B]	U	P-O3'-C3'	8.96	130.45	119.70
2	2	685	A	C2'-C3'-O3'	7.20	125.34	109.50
5	B	181	LEU	CA-CB-CG	6.82	130.97	115.30
2	2	616	U	N1-C1'-C2'	6.17	122.03	114.00
43	o	933	PRO	N-CA-CB	6.06	110.58	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	o	939	PRO	N-CA-CB	6.05	110.56	103.30
2	2	700	C	C2'-C3'-O3'	6.03	123.35	113.70
2	2	1470	C	C2'-C3'-O3'	6.02	123.33	113.70
43	o	930	PRO	N-CA-CB	5.99	110.49	103.30
21	R	109	LEU	CA-CB-CG	5.87	128.79	115.30
43	o	936	PRO	N-CA-CB	5.85	110.32	103.30
2	2	1206	C	C2'-C3'-O3'	5.80	122.98	113.70
16	M	52	LEU	CA-CB-CG	5.70	128.41	115.30
43	o	927	PRO	N-CA-CB	5.63	110.06	103.30
29	Z	42	LEU	CA-CB-CG	5.59	128.15	115.30
4	A	120	LEU	CA-CB-CG	5.47	127.89	115.30
5	B	120	LEU	CA-CB-CG	5.43	127.79	115.30
2	2	1198	G	C2'-C3'-O3'	5.43	122.38	113.70
8	E	38	LEU	CA-CB-CG	5.42	127.78	115.30
14	K	41	PHE	N-CA-CB	5.24	120.04	110.60
2	2	277	U	C2'-C3'-O3'	5.19	122.01	113.70
2	2	1320	A	N9-C1'-C2'	5.15	120.70	114.00
11	H	118	LEU	CA-CB-CG	5.12	127.07	115.30
13	J	49	LEU	CA-CB-CG	5.10	127.02	115.30
2	2	1513	A	C2'-C3'-O3'	5.03	121.75	113.70
43	o	387	LEU	CA-CB-CG	5.02	126.84	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	1190	C4J	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	Q	40	GLN	Peptide
44	p	336	TRP	Peptide
44	p	391	GLN	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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	217/254 (85%)	192 (88%)	16 (7%)	9 (4%)	3	14
5	B	220/255 (86%)	191 (87%)	19 (9%)	10 (4%)	2	12
6	C	218/259 (84%)	197 (90%)	16 (7%)	5 (2%)	6	24
7	D	225/237 (95%)	211 (94%)	8 (4%)	6 (3%)	5	21
8	E	258/261 (99%)	233 (90%)	21 (8%)	4 (2%)	9	33
9	F	204/227 (90%)	173 (85%)	21 (10%)	10 (5%)	2	11
10	G	228/236 (97%)	211 (92%)	15 (7%)	2 (1%)	17	47
11	H	182/190 (96%)	161 (88%)	14 (8%)	7 (4%)	3	15
12	I	184/201 (92%)	162 (88%)	12 (6%)	10 (5%)	2	9
13	J	180/188 (96%)	152 (84%)	20 (11%)	8 (4%)	2	12
14	K	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	18
15	L	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	5	22
16	M	113/134 (84%)	85 (75%)	20 (18%)	8 (7%)	1	5
17	N	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	22	52
18	O	127/137 (93%)	107 (84%)	13 (10%)	7 (6%)	2	9
19	P	115/142 (81%)	98 (85%)	11 (10%)	6 (5%)	2	10
20	Q	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	6	25
21	R	128/136 (94%)	110 (86%)	11 (9%)	7 (6%)	2	9
22	S	143/146 (98%)	127 (89%)	13 (9%)	3 (2%)	7	26
23	T	141/144 (98%)	132 (94%)	7 (5%)	2 (1%)	11	36
24	U	104/117 (89%)	90 (86%)	9 (9%)	5 (5%)	2	11
25	V	85/87 (98%)	80 (94%)	2 (2%)	3 (4%)	3	17
26	W	127/130 (98%)	115 (91%)	7 (6%)	5 (4%)	3	15
27	X	142/145 (98%)	126 (89%)	12 (8%)	4 (3%)	5	21
28	Y	132/135 (98%)	123 (93%)	5 (4%)	4 (3%)	4	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Z	76/108 (70%)	62 (82%)	10 (13%)	4 (5%)	2	10
30	a	101/119 (85%)	84 (83%)	11 (11%)	6 (6%)	1	8
31	b	79/82 (96%)	68 (86%)	9 (11%)	2 (2%)	5	22
32	c	62/67 (92%)	55 (89%)	5 (8%)	2 (3%)	4	18
33	d	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
34	e	58/63 (92%)	44 (76%)	9 (16%)	5 (9%)	1	3
35	f	72/150 (48%)	57 (79%)	13 (18%)	2 (3%)	5	21
36	g	314/326 (96%)	276 (88%)	29 (9%)	9 (3%)	4	20
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	119/153 (78%)	102 (86%)	11 (9%)	6 (5%)	2	11
39	j	243/304 (80%)	213 (88%)	25 (10%)	5 (2%)	7	26
40	k	388/527 (74%)	333 (86%)	47 (12%)	8 (2%)	7	26
41	l	120/285 (42%)	109 (91%)	11 (9%)	0	100	100
42	m	145/405 (36%)	126 (87%)	17 (12%)	2 (1%)	11	36
43	o	519/964 (54%)	483 (93%)	30 (6%)	6 (1%)	13	40
44	p	637/763 (84%)	583 (92%)	43 (7%)	11 (2%)	9	32
45	q	538/812 (66%)	490 (91%)	39 (7%)	9 (2%)	9	32
46	r	47/274 (17%)	43 (92%)	4 (8%)	0	100	100
47	s	326/347 (94%)	311 (95%)	15 (5%)	0	100	100
All	All	7928/10147 (78%)	7065 (89%)	650 (8%)	213 (3%)	8	21

All (213) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	141	VAL
7	D	220	PRO
9	F	104	ARG
11	H	64	VAL
11	H	74	GLN
12	I	22	ARG
12	I	153	ILE
13	J	169	PRO
16	M	82	VAL
16	M	84	ASP
18	O	91	SER

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Mol	Chain	Res	Type
18	O	124	ASP
19	P	36	LEU
24	U	17	VAL
24	U	96	PRO
25	V	30	SER
26	W	58	SER
27	X	63	GLN
30	a	36	ILE
34	e	54	ARG
38	i	31	GLU
38	i	66	ARG
38	i	116	ASN
44	p	337	PRO
44	p	392	PRO
4	A	206	ASN
5	B	19	ARG
5	B	214	LYS
7	D	221	SER
9	F	44	LEU
9	F	103	GLY
10	G	122	GLU
11	H	163	ASP
12	I	40	THR
12	I	147	ARG
13	J	118	LEU
15	L	3	THR
15	L	55	ASP
16	M	110	SER
17	N	3	ARG
18	O	51	ASP
18	O	114	ARG
19	P	89	MET
20	Q	138	PHE
21	R	99	VAL
21	R	117	LEU
22	S	85	PHE
25	V	12	TYR
27	X	3	LYS
28	Y	4	ALA
29	Z	55	PRO
29	Z	56	THR
34	e	47	VAL

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Mol	Chain	Res	Type
34	e	48	THR
36	g	4	SER
36	g	195	ILE
38	i	4	LYS
39	j	81	GLY
40	k	122	GLY
42	m	12	PRO
44	p	423	PRO
4	A	26	ALA
4	A	202	TYR
5	B	51	SER
5	B	131	ASP
5	B	148	ASN
7	D	197	SER
9	F	37	GLN
9	F	127	THR
11	H	10	SER
12	I	94	ASN
13	J	146	PHE
13	J	171	ARG
14	K	64	TYR
16	M	50	GLY
16	M	98	ASP
18	O	40	ALA
18	O	126	THR
19	P	69	GLU
20	Q	97	VAL
21	R	5	ARG
21	R	92	ASP
26	W	29	PRO
26	W	72	CYS
30	a	13	LYS
30	a	59	TYR
32	c	6	PRO
36	g	64	GLY
36	g	119	ASN
36	g	146	LEU
38	i	22	PRO
39	j	64	ARG
40	k	127	ARG
40	k	497	GLU
40	k	507	LYS

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Mol	Chain	Res	Type
43	o	62	LEU
43	o	63	LYS
43	o	251	GLU
44	p	77	GLN
45	q	460	PRO
45	q	468	THR
45	q	536	ASP
45	q	558	CYS
4	A	158	VAL
4	A	195	TRP
4	A	207	PRO
6	C	151	THR
6	C	253	THR
8	E	77	ARG
8	E	245	LYS
9	F	205	LYS
11	H	14	THR
11	H	98	ILE
12	I	99	ALA
12	I	120	SER
13	J	93	LEU
14	K	23	ALA
16	M	77	VAL
16	M	81	LYS
16	M	122	GLN
19	P	87	PRO
20	Q	113	ASP
21	R	90	ALA
21	R	116	LYS
23	T	28	LEU
23	T	35	ASP
24	U	77	LYS
25	V	81	ASN
27	X	41	SER
30	a	100	ARG
31	b	75	GLU
34	e	11	ALA
34	e	52	GLY
36	g	120	SER
36	g	161	ASN
36	g	290	LYS
38	i	97	LEU

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Mol	Chain	Res	Type
44	p	634	GLU
45	q	645	ILE
45	q	650	LYS
4	A	93	THR
5	B	54	LEU
5	B	221	PRO
5	B	224	ASP
6	C	40	TRP
8	E	195	ILE
10	G	152	ASP
12	I	52	ASN
12	I	148	ALA
13	J	134	ILE
14	K	26	ASP
15	L	4	GLU
15	L	7	VAL
18	O	42	VAL
21	R	88	VAL
22	S	91	ASP
24	U	73	GLY
24	U	89	ARG
26	W	30	SER
28	Y	36	SER
29	Z	36	ALA
30	a	64	LEU
35	f	111	GLU
40	k	383	GLU
40	k	408	ARG
42	m	5	ILE
43	o	49	GLU
43	o	394	ASN
44	p	207	ASP
44	p	569	PRO
45	q	514	LYS
45	q	779	GLU
4	A	68	PRO
5	B	207	LEU
6	C	155	GLN
7	D	219	GLU
9	F	42	ILE
9	F	66	ILE
9	F	102	ASN

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Mol	Chain	Res	Type
12	I	58	LEU
13	J	120	LYS
13	J	137	GLY
19	P	14	THR
28	Y	5	ILE
29	Z	69	PHE
31	b	62	VAL
39	j	6	CYS
39	j	197	GLY
44	p	198	VAL
44	p	536	LYS
45	q	351	ILE
5	B	206	PRO
27	X	4	GLY
36	g	201	GLY
40	k	225	PRO
43	o	933	PRO
44	p	422	VAL
4	A	103	THR
9	F	23	VAL
22	S	92	VAL
30	a	98	PRO
32	c	47	PRO
35	f	88	PRO
7	D	43	PRO
44	p	478	ILE
7	D	4	ILE
19	P	37	ALA
26	W	83	ILE
39	j	226	PRO
8	E	204	GLY
11	H	75	ILE
28	Y	35	VAL
40	k	282	PRO

### 5.3.2 Protein sidechains ⓘ

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	180/211 (85%)	152 (84%)	28 (16%)	2	10
5	B	201/228 (88%)	180 (90%)	21 (10%)	7	24
6	C	177/203 (87%)	152 (86%)	25 (14%)	3	13
7	D	188/196 (96%)	161 (86%)	27 (14%)	3	12
8	E	223/224 (100%)	188 (84%)	35 (16%)	2	10
9	F	174/194 (90%)	144 (83%)	30 (17%)	2	7
10	G	192/200 (96%)	169 (88%)	23 (12%)	5	18
11	H	164/170 (96%)	141 (86%)	23 (14%)	3	13
12	I	147/159 (92%)	124 (84%)	23 (16%)	2	10
13	J	153/158 (97%)	130 (85%)	23 (15%)	3	11
14	K	88/96 (92%)	74 (84%)	14 (16%)	2	9
15	L	136/137 (99%)	124 (91%)	12 (9%)	10	32
16	M	93/109 (85%)	80 (86%)	13 (14%)	3	13
17	N	128/128 (100%)	120 (94%)	8 (6%)	18	45
18	O	97/104 (93%)	84 (87%)	13 (13%)	4	14
19	P	99/119 (83%)	88 (89%)	11 (11%)	6	21
20	Q	117/119 (98%)	101 (86%)	16 (14%)	3	14
21	R	116/124 (94%)	105 (90%)	11 (10%)	8	28
22	S	127/129 (98%)	108 (85%)	19 (15%)	3	11
23	T	117/118 (99%)	99 (85%)	18 (15%)	2	10
24	U	96/107 (90%)	85 (88%)	11 (12%)	5	20
25	V	73/73 (100%)	70 (96%)	3 (4%)	30	61
26	W	110/111 (99%)	101 (92%)	9 (8%)	11	35
27	X	119/120 (99%)	107 (90%)	12 (10%)	7	25
28	Y	108/109 (99%)	95 (88%)	13 (12%)	5	18
29	Z	59/88 (67%)	55 (93%)	4 (7%)	16	42
30	a	85/100 (85%)	77 (91%)	8 (9%)	8	28
31	b	71/72 (99%)	63 (89%)	8 (11%)	6	21
32	c	55/59 (93%)	46 (84%)	9 (16%)	2	9
33	d	47/48 (98%)	40 (85%)	7 (15%)	3	11
34	e	51/55 (93%)	43 (84%)	8 (16%)	2	10
35	f	60/133 (45%)	51 (85%)	9 (15%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	g	264/272 (97%)	232 (88%)	32 (12%)	5	17
37	h	23/23 (100%)	21 (91%)	2 (9%)	10	33
38	i	100/130 (77%)	81 (81%)	19 (19%)	1	5
39	j	224/274 (82%)	189 (84%)	35 (16%)	2	10
40	k	332/449 (74%)	318 (96%)	14 (4%)	30	60
41	l	119/246 (48%)	115 (97%)	4 (3%)	37	67
42	m	125/352 (36%)	106 (85%)	19 (15%)	3	10
43	o	406/846 (48%)	379 (93%)	27 (7%)	16	43
44	p	544/693 (78%)	532 (98%)	12 (2%)	52	76
45	q	506/523 (97%)	485 (96%)	21 (4%)	30	60
46	r	40/232 (17%)	39 (98%)	1 (2%)	47	74
47	s	287/301 (95%)	281 (98%)	6 (2%)	53	77
All	All	6821/8542 (80%)	6135 (90%)	686 (10%)	11	25

All (686) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	LEU
4	A	6	THR
4	A	17	LEU
4	A	24	LEU
4	A	33	GLN
4	A	34	GLU
4	A	54	TRP
4	A	55	GLU
4	A	58	VAL
4	A	79	ARG
4	A	80	THR
4	A	86	VAL
4	A	93	THR
4	A	108	THR
4	A	109	ASN
4	A	111	ILE
4	A	116	LYS
4	A	121	VAL
4	A	127	ARG
4	A	157	ASP
4	A	162	CYS

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Mol	Chain	Res	Type
4	A	165	ARG
4	A	168	HIS
4	A	172	LEU
4	A	182	LEU
4	A	185	ARG
4	A	191	ARG
4	A	212	GLN
5	B	26	ARG
5	B	37	THR
5	B	72	ASP
5	B	78	ASP
5	B	82	ARG
5	B	89	ASP
5	B	103	MET
5	B	105	PHE
5	B	107	THR
5	B	110	LEU
5	B	111	ARG
5	B	120	LEU
5	B	127	VAL
5	B	132	ASP
5	B	140	ILE
5	B	152	ARG
5	B	160	HIS
5	B	177	GLN
5	B	178	ASN
5	B	181	LEU
5	B	213	ARG
6	C	58	ILE
6	C	63	LEU
6	C	68	VAL
6	C	72	GLN
6	C	83	ASP
6	C	86	MET
6	C	99	GLN
6	C	102	ARG
6	C	109	VAL
6	C	116	VAL
6	C	118	LEU
6	C	131	ARG
6	C	145	ARG
6	C	146	ARG

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Mol	Chain	Res	Type
6	C	153	LEU
6	C	155	GLN
6	C	159	LEU
6	C	173	ARG
6	C	206	THR
6	C	223	ILE
6	C	227	TYR
6	C	230	LEU
6	C	233	ASN
6	C	238	GLN
6	C	241	THR
7	D	11	LEU
7	D	12	VAL
7	D	27	ARG
7	D	41	VAL
7	D	51	ARG
7	D	62	ASN
7	D	66	ILE
7	D	70	THR
7	D	71	LEU
7	D	75	LYS
7	D	81	ARG
7	D	84	ILE
7	D	91	VAL
7	D	103	GLU
7	D	110	LEU
7	D	117	ARG
7	D	120	TYR
7	D	123	VAL
7	D	143	ARG
7	D	162	GLN
7	D	164	VAL
7	D	173	ARG
7	D	176	LEU
7	D	178	ARG
7	D	214	GLU
7	D	226	ARG
7	D	228	THR
8	E	6	LYS
8	E	9	LEU
8	E	18	TRP
8	E	19	MET

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Mol	Chain	Res	Type
8	E	23	LEU
8	E	38	LEU
8	E	39	ARG
8	E	49	ARG
8	E	51	ARG
8	E	57	ASN
8	E	77	ARG
8	E	80	THR
8	E	81	THR
8	E	93	GLU
8	E	96	ASN
8	E	100	ARG
8	E	106	LYS
8	E	108	ARG
8	E	113	ARG
8	E	114	ILE
8	E	155	LYS
8	E	163	ASP
8	E	173	ILE
8	E	181	VAL
8	E	187	ARG
8	E	198	ARG
8	E	200	ARG
8	E	206	ASP
8	E	208	VAL
8	E	220	THR
8	E	221	ARG
8	E	225	VAL
8	E	238	LEU
8	E	254	ARG
8	E	259	HIS
9	F	29	THR
9	F	34	GLU
9	F	40	GLN
9	F	41	GLU
9	F	60	LEU
9	F	65	GLN
9	F	70	ILE
9	F	78	ARG
9	F	83	ARG
9	F	85	ARG
9	F	88	GLN

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Mol	Chain	Res	Type
9	F	92	VAL
9	F	100	MET
9	F	110	LEU
9	F	121	GLU
9	F	133	GLN
9	F	137	ASP
9	F	145	ARG
9	F	150	ARG
9	F	158	ARG
9	F	160	GLN
9	F	163	ASP
9	F	169	ARG
9	F	183	GLU
9	F	187	ARG
9	F	189	ILE
9	F	192	ILE
9	F	196	LEU
9	F	209	THR
9	F	213	ILE
10	G	1	MET
10	G	13	GLN
10	G	15	CYS
10	G	19	ASP
10	G	29	ASP
10	G	52	ILE
10	G	75	LEU
10	G	92	ARG
10	G	111	LEU
10	G	125	THR
10	G	127	ASP
10	G	132	ARG
10	G	133	LEU
10	G	154	ARG
10	G	170	THR
10	G	177	ARG
10	G	180	THR
10	G	189	GLN
10	G	203	GLU
10	G	212	LEU
10	G	215	ARG
10	G	222	GLU
10	G	226	VAL

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Mol	Chain	Res	Type
11	H	11	GLN
11	H	15	GLU
11	H	19	GLN
11	H	38	LEU
11	H	39	ARG
11	H	71	HIS
11	H	74	GLN
11	H	79	ARG
11	H	80	GLU
11	H	81	LEU
11	H	86	GLN
11	H	93	LEU
11	H	107	ARG
11	H	116	ARG
11	H	119	THR
11	H	122	HIS
11	H	126	LEU
11	H	127	GLU
11	H	128	ASP
11	H	139	ARG
11	H	164	ASN
11	H	174	ASN
11	H	176	LEU
12	I	5	ARG
12	I	8	ARG
12	I	20	GLN
12	I	22	ARG
12	I	23	LYS
12	I	24	LYS
12	I	25	ARG
12	I	29	LEU
12	I	32	GLN
12	I	35	ASN
12	I	46	VAL
12	I	47	ARG
12	I	58	LEU
12	I	72	VAL
12	I	77	ARG
12	I	92	ARG
12	I	96	LEU
12	I	139	ASN
12	I	153	ILE

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Mol	Chain	Res	Type
12	I	155	HIS
12	I	158	ASP
12	I	179	ARG
12	I	196	ARG
13	J	6	ARG
13	J	7	THR
13	J	8	TYR
13	J	9	SER
13	J	10	LYS
13	J	25	ASP
13	J	28	LEU
13	J	33	GLU
13	J	37	LYS
13	J	45	ILE
13	J	49	LEU
13	J	60	LEU
13	J	64	GLU
13	J	93	LEU
13	J	103	ASP
13	J	107	ARG
13	J	109	LEU
13	J	131	GLN
13	J	142	ASN
13	J	149	ARG
13	J	150	LEU
13	J	161	THR
13	J	183	GLU
14	K	13	GLN
14	K	15	LEU
14	K	18	GLU
14	K	34	GLU
14	K	35	ILE
14	K	39	ASN
14	K	40	LEU
14	K	44	LYS
14	K	49	LEU
14	K	76	LEU
14	K	81	ASN
14	K	82	LEU
14	K	84	GLU
14	K	86	ILE
15	L	10	GLU

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Mol	Chain	Res	Type
15	L	36	LYS
15	L	56	LYS
15	L	67	ARG
15	L	69	LYS
15	L	70	ILE
15	L	79	ARG
15	L	84	ILE
15	L	111	VAL
15	L	117	VAL
15	L	125	VAL
15	L	136	ARG
16	M	26	ARG
16	M	34	LEU
16	M	38	LEU
16	M	40	GLU
16	M	52	LEU
16	M	55	LEU
16	M	61	GLU
16	M	79	LEU
16	M	88	LEU
16	M	91	TRP
16	M	97	ILE
16	M	100	ASP
16	M	106	VAL
17	N	3	ARG
17	N	9	LYS
17	N	83	GLU
17	N	88	LEU
17	N	99	ARG
17	N	107	LYS
17	N	116	ILE
17	N	121	ARG
18	O	24	ASN
18	O	37	GLU
18	O	47	LYS
18	O	48	VAL
18	O	49	LYS
18	O	52	ARG
18	O	65	GLN
18	O	66	ASP
18	O	72	LYS
18	O	102	LEU

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Mol	Chain	Res	Type
18	O	124	ASP
18	O	126	THR
18	O	137	LEU
19	P	51	GLU
19	P	56	LEU
19	P	59	LYS
19	P	60	LEU
19	P	79	HIS
19	P	83	MET
19	P	94	VAL
19	P	106	GLU
19	P	111	MET
19	P	126	VAL
19	P	127	ARG
20	Q	22	VAL
20	Q	26	LYS
20	Q	52	LEU
20	Q	63	ILE
20	Q	69	VAL
20	Q	78	VAL
20	Q	82	ARG
20	Q	83	GLN
20	Q	87	LYS
20	Q	89	LEU
20	Q	94	GLN
20	Q	105	LEU
20	Q	107	LYS
20	Q	123	ARG
20	Q	127	LYS
20	Q	137	ARG
21	R	26	MET
21	R	29	GLN
21	R	37	GLU
21	R	42	GLN
21	R	46	LEU
21	R	78	ARG
21	R	82	ASP
21	R	106	THR
21	R	109	LEU
21	R	116	LYS
21	R	128	ARG
22	S	3	LEU

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Mol	Chain	Res	Type
22	S	15	LEU
22	S	40	ARG
22	S	41	ARG
22	S	57	ARG
22	S	61	LEU
22	S	73	MET
22	S	85	PHE
22	S	97	ASP
22	S	101	LEU
22	S	105	LEU
22	S	106	GLU
22	S	108	LYS
22	S	111	ASP
22	S	114	GLU
22	S	123	ARG
22	S	134	ARG
22	S	136	GLN
22	S	137	HIS
23	T	8	ASP
23	T	16	ASN
23	T	17	ASN
23	T	35	ASP
23	T	48	GLN
23	T	64	HIS
23	T	65	ILE
23	T	67	LEU
23	T	68	ARG
23	T	86	ARG
23	T	88	VAL
23	T	110	LYS
23	T	124	ILE
23	T	126	ASP
23	T	129	LEU
23	T	132	LEU
23	T	140	LEU
23	T	142	ASP
24	U	17	VAL
24	U	22	ILE
24	U	27	THR
24	U	31	VAL
24	U	52	LYS
24	U	56	VAL

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Mol	Chain	Res	Type
24	U	57	ARG
24	U	65	ILE
24	U	74	GLU
24	U	86	ILE
24	U	112	VAL
25	V	12	TYR
25	V	50	TYR
25	V	85	TYR
26	W	7	LEU
26	W	24	GLN
26	W	25	VAL
26	W	28	ARG
26	W	47	ILE
26	W	83	ILE
26	W	88	LYS
26	W	104	LEU
26	W	129	VAL
27	X	14	LYS
27	X	16	ARG
27	X	64	PRO
27	X	72	VAL
27	X	79	ASN
27	X	90	ASP
27	X	94	ASN
27	X	100	ASP
27	X	107	PHE
27	X	127	VAL
27	X	141	GLU
27	X	144	ARG
28	Y	8	ARG
28	Y	20	ARG
28	Y	34	ASN
28	Y	35	VAL
28	Y	74	LEU
28	Y	84	LYS
28	Y	105	ARG
28	Y	106	GLN
28	Y	111	ARG
28	Y	112	LYS
28	Y	117	LYS
28	Y	121	THR
28	Y	128	LYS

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Mol	Chain	Res	Type
29	Z	46	LYS
29	Z	58	ARG
29	Z	75	LEU
29	Z	81	ARG
30	a	12	LYS
30	a	38	ARG
30	a	39	MET
30	a	53	LEU
30	a	59	TYR
30	a	64	LEU
30	a	75	ILE
30	a	89	ARG
31	b	3	LEU
31	b	31	HIS
31	b	43	ILE
31	b	44	THR
31	b	57	GLU
31	b	67	THR
31	b	81	ARG
31	b	82	LYS
32	c	14	LYS
32	c	26	THR
32	c	38	ARG
32	c	49	ARG
32	c	50	GLU
32	c	58	GLU
32	c	64	ARG
32	c	65	ARG
32	c	66	LEU
33	d	19	ARG
33	d	20	GLN
33	d	30	LEU
33	d	38	ILE
33	d	39	ASP
33	d	41	GLN
33	d	49	ASP
34	e	10	ARG
34	e	17	GLN
34	e	24	GLN
34	e	26	LYS
34	e	36	LYS
34	e	37	ARG

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Mol	Chain	Res	Type
34	e	53	LYS
34	e	55	LYS
35	f	81	LYS
35	f	83	LYS
35	f	87	THR
35	f	91	ILE
35	f	92	ARG
35	f	96	LYS
35	f	99	LYS
35	f	135	ASP
35	f	136	ARG
36	g	8	LEU
36	g	11	ARG
36	g	54	GLN
36	g	59	VAL
36	g	60	ARG
36	g	66	SER
36	g	70	GLN
36	g	72	VAL
36	g	87	ASP
36	g	91	ARG
36	g	94	ASN
36	g	101	GLU
36	g	114	VAL
36	g	122	LYS
36	g	130	LYS
36	g	180	ASP
36	g	181	LYS
36	g	188	LEU
36	g	195	ILE
36	g	196	GLU
36	g	206	ILE
36	g	207	ASN
36	g	209	VAL
36	g	210	GLN
36	g	223	LYS
36	g	246	GLU
36	g	250	LEU
36	g	256	ARG
36	g	257	PHE
36	g	280	GLU
36	g	290	LYS

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Mol	Chain	Res	Type
36	g	308	LEU
37	h	13	LEU
37	h	16	LYS
38	i	3	LYS
38	i	4	LYS
38	i	5	ASN
38	i	13	ARG
38	i	14	ARG
38	i	23	LYS
38	i	31	GLU
38	i	34	GLU
38	i	39	THR
38	i	42	LEU
38	i	44	ASN
38	i	47	VAL
38	i	56	LYS
38	i	75	ASP
38	i	77	ILE
38	i	90	ASP
38	i	96	ASN
38	i	109	LEU
38	i	119	ASP
39	j	7	ARG
39	j	11	ASN
39	j	18	ASP
39	j	19	ILE
39	j	23	ASN
39	j	37	LEU
39	j	39	TYR
39	j	45	MET
39	j	46	ILE
39	j	53	ARG
39	j	54	ARG
39	j	62	LEU
39	j	63	ILE
39	j	69	ASP
39	j	79	GLU
39	j	80	LYS
39	j	84	ASP
39	j	87	LYS
39	j	97	LYS
39	j	119	PHE

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Mol	Chain	Res	Type
39	j	124	GLU
39	j	126	LEU
39	j	163	LYS
39	j	169	LEU
39	j	185	ARG
39	j	187	ASP
39	j	195	TYR
39	j	198	ILE
39	j	203	ASP
39	j	230	LEU
39	j	235	LEU
39	j	244	LEU
39	j	251	ILE
39	j	255	ILE
39	j	258	TYR
40	k	136	ILE
40	k	311	ILE
40	k	315	LEU
40	k	318	ILE
40	k	352	GLU
40	k	359	ILE
40	k	395	LEU
40	k	403	ASP
40	k	406	LEU
40	k	426	ILE
40	k	432	ILE
40	k	494	GLU
40	k	508	HIS
40	k	510	ARG
41	l	180	ILE
41	l	191	LEU
41	l	211	LEU
41	l	213	ILE
42	m	5	ILE
42	m	8	ASP
42	m	15	ARG
42	m	24	LYS
42	m	25	VAL
42	m	34	THR
42	m	41	ASP
42	m	48	ARG
42	m	53	ILE

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Mol	Chain	Res	Type
42	m	70	ASP
42	m	71	LYS
42	m	111	ILE
42	m	113	LYS
42	m	114	ASP
42	m	117	LEU
42	m	118	VAL
42	m	120	ASP
42	m	131	ASP
42	m	132	LEU
43	o	16	ASP
43	o	39	ARG
43	o	41	ARG
43	o	56	LEU
43	o	104	ILE
43	o	172	ASN
43	o	178	THR
43	o	183	VAL
43	o	185	LYS
43	o	206	LEU
43	o	217	GLN
43	o	229	ASP
43	o	235	ARG
43	o	239	GLN
43	o	262	ASP
43	o	292	VAL
43	o	303	TRP
43	o	329	PHE
43	o	330	LEU
43	o	346	ASP
43	o	355	LEU
43	o	381	ASP
43	o	384	LEU
43	o	388	TYR
43	o	397	VAL
43	o	476	ASP
43	o	480	ILE
44	p	77	GLN
44	p	79	ILE
44	p	158	TYR
44	p	192	TRP
44	p	277	VAL

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Mol	Chain	Res	Type
44	p	422	VAL
44	p	444	GLN
44	p	489	VAL
44	p	581	MET
44	p	616	ASP
44	p	631	HIS
44	p	678	LYS
45	q	273	GLN
45	q	305	ASP
45	q	315	ILE
45	q	324	ASP
45	q	335	THR
45	q	336	ILE
45	q	352	GLU
45	q	406	ASN
45	q	407	LEU
45	q	438	ASP
45	q	490	LEU
45	q	532	ILE
45	q	567	LEU
45	q	577	ARG
45	q	611	HIS
45	q	644	ARG
45	q	676	LEU
45	q	677	PHE
45	q	733	TYR
45	q	754	GLU
45	q	783	GLU
46	r	74	ARG
47	s	64	THR
47	s	157	THR
47	s	158	VAL
47	s	308	TYR
47	s	313	GLU
47	s	328	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	83	GLN
4	A	109	ASN
5	B	101	HIS

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Mol	Chain	Res	Type
5	B	124	ASN
6	C	64	HIS
6	C	99	GLN
6	C	152	ASN
6	C	233	ASN
7	D	159	HIS
7	D	179	GLN
8	E	50	ASN
8	E	57	ASN
8	E	112	HIS
8	E	130	GLN
8	E	216	ASN
9	F	65	GLN
9	F	102	ASN
9	F	188	ASN
10	G	10	ASN
10	G	13	GLN
10	G	139	ASN
11	H	29	ASN
11	H	74	GLN
11	H	110	GLN
11	H	150	GLN
11	H	170	GLN
12	I	64	ASN
13	J	38	ASN
13	J	110	GLN
13	J	142	ASN
13	J	155	HIS
14	K	39	ASN
14	K	81	ASN
14	K	85	HIS
15	L	8	GLN
15	L	138	ASN
17	N	49	GLN
17	N	62	GLN
17	N	105	ASN
18	O	99	GLN
19	P	104	GLN
20	Q	83	GLN
21	R	105	GLN
22	S	87	ASN
22	S	99	HIS

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Mol	Chain	Res	Type
22	S	136	GLN
23	T	12	GLN
23	T	43	ASN
23	T	64	HIS
25	V	21	ASN
25	V	33	GLN
26	W	24	GLN
26	W	80	ASN
26	W	92	ASN
27	X	79	ASN
28	Y	15	ASN
28	Y	22	GLN
28	Y	29	HIS
30	a	17	HIS
30	a	80	HIS
31	b	26	GLN
31	b	42	ASN
32	c	43	ASN
33	d	37	ASN
33	d	41	GLN
34	e	46	ASN
35	f	95	HIS
36	g	51	ASN
36	g	94	ASN
36	g	203	ASN
36	g	321	GLN
38	i	5	ASN
38	i	85	GLN
39	j	60	GLN
39	j	103	GLN
39	j	109	HIS
40	k	124	GLN
40	k	344	ASN
40	k	415	GLN
40	k	465	ASN
42	m	64	GLN
42	m	94	ASN
42	m	134	HIS
43	o	194	GLN
43	o	216	GLN
43	o	243	GLN
43	o	299	HIS

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Mol	Chain	Res	Type
43	o	394	ASN
43	o	403	GLN
44	p	467	ASN
44	p	592	ASN
44	p	712	GLN
45	q	340	GLN
45	q	386	ASN
45	q	406	ASN
45	q	495	ASN
45	q	540	GLN
45	q	582	GLN
45	q	610	GLN
47	s	145	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	72/76 (94%)	29 (40%)	8 (11%)
2	2	1775/1798 (98%)	654 (36%)	72 (4%)
3	3	27/49 (55%)	16 (59%)	4 (14%)
All	All	1874/1923 (97%)	699 (37%)	84 (4%)

All (699) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	5	C
1	1	8	U
1	1	9	1MG
1	1	10	2MG
1	1	15	G
1	1	16	H2U
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	23	C
1	1	26	M2G
1	1	42	U
1	1	44	A
1	1	46	7MG

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Mol	Chain	Res	Type
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	58	1MA
1	1	59	A
1	1	60	A
1	1	61	C
1	1	64	RIA
1	1	69	C
1	1	71	C
1	1	74	C
1	1	75	C
1	1	76	A
2	2	2	A
2	2	3	U
2	2	4	C
2	2	5	U
2	2	13	C
2	2	16	G
2	2	17	C
2	2	25	C
2	2	27	U
2	2	34	G
2	2	42	G
2	2	46	A
2	2	47	A
2	2	50	C
2	2	57	G
2	2	58	U
2	2	59	C
2	2	60	U
2	2	61	A
2	2	64	U
2	2	66	U
2	2	67	A
2	2	68	A
2	2	69	G
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A

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Mol	Chain	Res	Type
2	2	77	U
2	2	78	A
2	2	79	C
2	2	100	A
2	2	104	A
2	2	111	U
2	2	114	C
2	2	115	G
2	2	121	U
2	2	123	G
2	2	124	A
2	2	126	A
2	2	127	G
2	2	128	U
2	2	129	U
2	2	130	C
2	2	131	C
2	2	132	U
2	2	133	U
2	2	135	A
2	2	136	C
2	2	137	U
2	2	139	C
2	2	140	A
2	2	141	U
2	2	143	G
2	2	144	A
2	2	146	A
2	2	147	U
2	2	150	G
2	2	158	U
2	2	159	C
2	2	160	U
2	2	161	A
2	2	167	A
2	2	172	A
2	2	173	U
2	2	176	U
2	2	177	U
2	2	178	A
2	2	184	U
2	2	186	G

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Mol	Chain	Res	Type
2	2	187	A
2	2	190	C
2	2	191	U
2	2	192	U
2	2	194	G
2	2	195	G
2	2	209	A
2	2	214	A
2	2	217	A
2	2	218	A
2	2	220	A
2	2	223	C
2	2	226	U
2	2	227	G
2	2	228	U
2	2	232	C
2	2	233	G
2	2	234	G
2	2	235	A
2	2	239	C
2	2	240	U
2	2	248	U
2	2	249	C
2	2	256	A
2	2	259	U
2	2	260	U
2	2	264	A
2	2	265	A
2	2	266	U
2	2	267	C
2	2	271	U
2	2	275	C
2	2	276	U
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	282	U
2	2	286	G
2	2	289	G
2	2	294	A
2	2	300	A

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Mol	Chain	Res	Type
2	2	301	U
2	2	303	U
2	2	307	C
2	2	308	C
2	2	311	A
2	2	313	C
2	2	314	A
2	2	315	A
2	2	320	C
2	2	321	G
2	2	322	A
2	2	334	U
2	2	336	G
2	2	337	C
2	2	342	C
2	2	351	A
2	2	359	A
2	2	360	C
2	2	368	A
2	2	369	A
2	2	380	C
2	2	382	G
2	2	389	G
2	2	392	C
2	2	399	A
2	2	400	A
2	2	401	C
2	2	404	C
2	2	411	A
2	2	412	U
2	2	415	A
2	2	416	A
2	2	418	G
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	427	A
2	2	433	G
2	2	434	C
2	2	438	U

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Mol	Chain	Res	Type
2	2	439	U
2	2	440	A
2	2	443	C
2	2	444	A
2	2	447	C
2	2	457	G
2	2	459	A
2	2	469	A
2	2	474	A
2	2	476	A
2	2	479	G
2	2	481	U
2	2	482	A
2	2	483	C
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	499	C
2	2	502	G
2	2	505	A
2	2	506	U
2	2	507	U
2	2	509	G
2	2	510	A
2	2	513	G
2	2	516	U
2	2	518	C
2	2	519	A
2	2	524	A
2	2	526	A
2	2	527	U
2	2	531	U
2	2	533	A
2	2	535	C
2	2	537	A
2	2	539	G
2	2	540	A
2	2	541	A

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Mol	Chain	Res	Type
2	2	542	C
2	2	543	A
2	2	544	A
2	2	545	C
2	2	547	G
2	2	548	G
2	2	553	C
2	2	556	G
2	2	557	U
2	2	558	C
2	2	564	C
2	2	567	G
2	2	570	G
2	2	577	U
2	2	578	A
2	2	582	C
2	2	583	C
2	2	584	A
2	2	593	A
2	2	594	G
2	2	597	U
2	2	600	A
2	2	605	A
2	2	609	G
2	2	610	U
2	2	614	A
2	2	618	A
2	2	619	A
2	2	620	A
2	2	621	A
2	2	622	A
2	2	623	G
2	2	637	U
2	2	638	U
2	2	639	U
2	2	641	G
2	2	647	G
2	2	649	U
2	2	651	U
2	2	652	C
2	2	653	C
2	2	654	G

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Mol	Chain	Res	Type
2	2	655	G
2	2	657	C
2	2	677	G
2	2	678	U
2	2	680	U
2	2	684	A
2	2	686	C
2	2	691	U
2	2	693	U
2	2	694	U
2	2	695	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	701	U
2	2	702	G
2	2	704	C
2	2	705	U
2	2	709	C
2	2	710	U
2	2	711	G
2	2	712	U
2	2	714	C
2	2	715	U
2	2	716	C
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	725	U
2	2	727	C
2	2	731	C
2	2	732	G
2	2	733	A
2	2	734	A
2	2	736	C
2	2	737	A
2	2	738	G
2	2	739	G
2	2	741	C
2	2	742	U

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Mol	Chain	Res	Type
2	2	743	U
2	2	755	A
2	2	765	G
2	2	766	PSU
2	2	767	U
2	2	771	A
2	2	774	A
2	2	778	G
2	2	779	A
2	2	780	A
2	2	781	A
2	2	782	G
2	2	783	C
2	2	786	G
2	2	788	A
2	2	789	U
2	2	792	A
2	2	793	U
2	2	794	U
2	2	809	G
2	2	811	A
2	2	812	U
2	2	813	A
2	2	814	G
2	2	817	C
2	2	819	U
2	2	820	U
2	2	822	G
2	2	823	G
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	832	U
2	2	839	U
2	2	840	U
2	2	845	G
2	2	847	C
2	2	854	A
2	2	855	A
2	2	859	U
2	2	862	A

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Mol	Chain	Res	Type
2	2	863	U
2	2	872	U
2	2	874	G
2	2	876	G
2	2	881	U
2	2	885	U
2	2	895	U
2	2	896	C
2	2	897	A
2	2	898	G
2	2	899	A
2	2	905	A
2	2	911	U
2	2	912	G
2	2	913	G
2	2	914	A
2	2	915	U
2	2	916	U
2	2	917	U
2	2	919	U
2	2	920	U
2	2	921	G
2	2	923	A
2	2	932	A
2	2	934	U
2	2	941	G
2	2	944	U
2	2	947	G
2	2	950	A
2	2	958	U
2	2	959	U
2	2	965	A
2	2	969	A
2	2	970	A
2	2	972	A
2	2	981	U
2	2	982	A
2	2	986	G
2	2	987	A
2	2	990	G
2	2	991	A
2	2	993	G

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Mol	Chain	Res	Type
2	2	995	U
2	2	1009	C
2	2	1011	U
2	2	1015	C
2	2	1018	A
2	2	1020	C
2	2	1025	A
2	2	1026	A
2	2	1027	C
2	2	1030	U
2	2	1031	G
2	2	1033	C
2	2	1034	G
2	2	1038	A
2	2	1039	G
2	2	1041	G
2	2	1042	A
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1060	U
2	2	1062	U
2	2	1075	A
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1085	A
2	2	1086	A
2	2	1091	A
2	2	1092	A
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1099	G
2	2	1103	U

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Mol	Chain	Res	Type
2	2	1104	C
2	2	1106	G
2	2	1110	G
2	2	1112	A
2	2	1113	G
2	2	1118	G
2	2	1125	G
2	2	1137	A
2	2	1142	A
2	2	1149	G
2	2	1150	A
2	2	1154	G
2	2	1155	C
2	2	1156	A
2	2	1157	C
2	2	1158	C
2	2	1163	G
2	2	1166	G
2	2	1184	U
2	2	1185	U
2	2	1187	G
2	2	1189	C
2	2	1191	C
2	2	1193	A
2	2	1195	A
2	2	1198	G
2	2	1199	G
2	2	1201	A
2	2	1206	C
2	2	1207	A
2	2	1211	G
2	2	1213	U
2	2	1216	A
2	2	1217	G
2	2	1224	U
2	2	1226	A
2	2	1227	G
2	2	1228	G
2	2	1230	U
2	2	1236	G
2	2	1237	A
2	2	1243	A

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Mol	Chain	Res	Type
2	2	1244	G
2	2	1245	C
2	2	1246	U
2	2	1247	C
2	2	1249	U
2	2	1250	U
2	2	1254	G
2	2	1255	A
2	2	1256	U
2	2	1258	U
2	2	1259	U
2	2	1265	U
2	2	1268	U
2	2	1269	G
2	2	1272	G
2	2	1275	U
2	2	1283	C
2	2	1284	U
2	2	1287	G
2	2	1292	U
2	2	1296	G
2	2	1298	G
2	2	1306	U
2	2	1311	A
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1317	G
2	2	1320	A
2	2	1321	A
2	2	1324	A
2	2	1336	A
2	2	1337	C
2	2	1338	C
2	2	1339	U
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1347	A
2	2	1353	G
2	2	1355	U
2	2	1360	C

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Mol	Chain	Res	Type
2	2	1361	U
2	2	1362	U
2	2	1363	G
2	2	1364	C
2	2	1366	G
2	2	1369	U
2	2	1370	G
2	2	1379	U
2	2	1380	A
2	2	1383	G
2	2	1388	U
2	2	1389	A
2	2	1390	U
2	2	1393	G
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1407	G
2	2	1408	A
2	2	1409	A
2	2	1410	G
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1414	G
2	2	1416	G
2	2	1418	C
2	2	1423	A
2	2	1424	C
2	2	1425	A
2	2	1426	2MG
2	2	1429	C
2	2	1430	U
2	2	1431	G
2	2	1442	A
2	2	1443	G
2	2	1444	A
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1458	A

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Mol	Chain	Res	Type
2	2	1460	G
2	2	1464	G
2	2	1467	A
2	2	1469	A
2	2	1471	U
2	2	1476	G
2	2	1480	C
2	2	1481	A
2	2	1482	G
2	2	1483	C
2	2	1484	G
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1494	U
2	2	1499	C
2	2	1504	G
2	2	1510	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1520	U
2	2	1521	G
2	2	1522	A
2	2	1532	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1536	U
2	2	1538	G
2	2	1544	G
2	2	1548	A
2	2	1555	U
2	2	1557	A
2	2	1558	U
2	2	1566	C
2	2	1570	2MG
2	2	1571	A

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Mol	Chain	Res	Type
2	2	1572	G
2	2	1581	A
2	2	1588	G
2	2	1595	A
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1605	G
2	2	1614	G
2	2	1616	C
2	2	1617	C
2	2	1620	G
2	2	1632	C
2	2	1633	A
2	2	1634	C
2	2	1644	C
2	2	1647	G
2	2	1648	U
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1666	G
2	2	1667	U
2	2	1676	A
2	2	1678	G
2	2	1679	A
2	2	1682	U
2	2	1685	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1699	A
2	2	1700	A
2	2	1702	U
2	2	1703	C

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Mol	Chain	Res	Type
2	2	1705	A
2	2	1706	U
2	2	1707	C
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1715	G
2	2	1725	G
2	2	1730	A
2	2	1734	G
2	2	1742	A
2	2	1743	G
2	2	1748	A
2	2	1750	U
2	2	1753	A
2	2	1755	G
2	2	1758	G
2	2	1760	A
2	2	1763	A
2	2	1764	A
2	2	1766	G
2	2	1767	U
2	2	1768	U
2	2	1769	U
2	2	1778	G
2	2	1781	C
2	2	1787	G
2	2	1788	A
2	2	1790	G
2	2	1791	G
2	2	1792	A
2	2	1793	U
2	2	1794	C
2	2	1796	U
2	2	1797	U
2	2	1798	A
3	3	19	A
3	3	20	A
3	3	22	U
3	3	23	A
3	3	24	U

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Mol	Chain	Res	Type
3	3	25	A
3	3	26	A
3	3	33	C
3	3	34	U
3	3	36	U
3	3	38	C
3	3	39	U
3	3	40	C
3	3	43	U
3	3	44	C
3	3	45	U

All (84) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	7	G
1	1	8	U
1	1	43	G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	58	1MA
1	1	74	C
2	2	3	U
2	2	16	G
2	2	44	U
2	2	66	U
2	2	74	U
2	2	126	A
2	2	128	U
2	2	130	C
2	2	131	C
2	2	176	U
2	2	190	C
2	2	216	A
2	2	217	A
2	2	239	C
2	2	275	C
2	2	277	U
2	2	279	U
2	2	321	G
2	2	336	G

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Mol	Chain	Res	Type
2	2	399	A
2	2	451	A
2	2	467	A
2	2	542	C
2	2	544	A
2	2	597	U
2	2	685	A
2	2	693	U
2	2	695	U
2	2	700	C
2	2	710	U
2	2	721	U
2	2	780	A
2	2	781	A
2	2	810	A
2	2	826	C
2	2	828	A
2	2	854	A
2	2	896	C
2	2	912	G
2	2	914	A
2	2	946	U
2	2	1057	U
2	2	1058	C
2	2	1080	A
2	2	1107	G
2	2	1198	G
2	2	1206	C
2	2	1226	A
2	2	1284	U
2	2	1320	A
2	2	1338	C
2	2	1343	A
2	2	1430	U
2	2	1455	C
2	2	1456	G
2	2	1470	C
2	2	1479	C
2	2	1513	A
2	2	1515	U
2	2	1533	U
2	2	1545	A

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Mol	Chain	Res	Type
2	2	1570	2MG
2	2	1571	A
2	2	1599	G
2	2	1613	C
2	2	1648	U
2	2	1655	U
2	2	1678	G
2	2	1765	G
2	2	1766	G
2	2	1796	U
2	2	1797	U
3	3	22	U
3	3	33	C
3	3	35	C
3	3	38	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	7MG	1	46	1	22,26,27	1.44	4 (18%)	29,39,42	2.62	10 (34%)
5	AYA	B	2	-	6,7,8	0.65	0	5,8,10	0.72	0
2	5MC	2	1637	2	18,22,23	1.03	1 (5%)	26,32,35	1.36	6 (23%)
1	1MG	1	9	1	18,26,27	1.02	0	19,39,42	1.58	4 (21%)
2	PSU	2	120	2	18,21,22	1.40	2 (11%)	22,30,33	1.93	4 (18%)
1	M2G	1	26	1	20,27,28	1.74	3 (15%)	22,40,43	1.34	4 (18%)
2	5MC	2	1006	2	18,22,23	0.96	1 (5%)	26,32,35	1.66	6 (23%)
1	H2U	1	47	1	18,21,22	0.85	0	21,30,33	1.38	3 (14%)
2	MA6	2	1780	2	19,26,27	1.11	2 (10%)	18,38,41	1.77	4 (22%)
1	2MG	1	10	1	18,26,27	0.98	1 (5%)	16,38,41	1.08	2 (12%)
1	5MC	1	48	1	18,22,23	1.03	1 (5%)	26,32,35	1.26	3 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PSU	2	766	2	18,21,22	1.37	2 (11%)	22,30,33	2.12	5 (22%)
1	H2U	1	16	1	18,21,22	0.83	0	21,30,33	1.67	4 (19%)
2	2MG	2	1570	2	18,26,27	0.94	0	16,38,41	1.42	3 (18%)
2	PSU	2	465	2	18,21,22	1.51	3 (16%)	22,30,33	1.89	5 (22%)
1	RIA	1	64	1	31,38,39	0.51	0	39,57,60	0.71	1 (2%)
2	7MG	2	1573	1,2	22,26,27	1.55	7 (31%)	29,39,42	2.63	6 (20%)
2	2MG	2	1426	2,48	18,26,27	0.95	0	16,38,41	1.40	4 (25%)
2	PSU	2	1289	2	18,21,22	1.48	3 (16%)	22,30,33	1.89	3 (13%)
2	PSU	2	998	2	18,21,22	1.41	3 (16%)	22,30,33	1.92	4 (18%)
1	5MC	1	49	1	18,22,23	1.10	1 (5%)	26,32,35	1.34	4 (15%)
1	1MA	1	58	1	16,25,26	1.86	4 (25%)	18,37,40	1.48	3 (16%)
1	T6A	1	37	1	27,34,35	1.04	2 (7%)	29,49,52	2.71	10 (34%)
2	C4J	2	1190	2	24,29,30	0.52	0	29,42,45	1.00	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	7MG	1	46	1	-	1/7/37/38	0/3/3/3
5	AYA	B	2	-	-	0/4/6/8	-
2	5MC	2	1637	2	-	1/7/25/26	0/2/2/2
1	1MG	1	9	1	-	3/3/25/26	0/3/3/3
2	PSU	2	120	2	-	0/7/25/26	0/2/2/2
1	M2G	1	26	1	-	2/7/29/30	0/3/3/3
2	5MC	2	1006	2	-	0/7/25/26	0/2/2/2
1	H2U	1	47	1	-	4/7/38/39	0/2/2/2
2	MA6	2	1780	2	-	5/7/29/30	0/3/3/3
1	2MG	1	10	1	-	2/5/27/28	0/3/3/3
1	5MC	1	48	1	-	3/7/25/26	0/2/2/2
2	PSU	2	766	2	-	1/7/25/26	0/2/2/2
1	H2U	1	16	1	-	2/7/38/39	0/2/2/2
2	2MG	2	1570	2	-	0/5/27/28	0/3/3/3
2	PSU	2	465	2	-	0/7/25/26	0/2/2/2
1	RIA	1	64	1	-	3/13/51/52	0/4/4/4
2	7MG	2	1573	1,2	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MG	2	1426	2,48	-	3/5/27/28	0/3/3/3
2	PSU	2	1289	2	-	0/7/25/26	0/2/2/2
2	PSU	2	998	2	-	0/7/25/26	0/2/2/2
1	5MC	1	49	1	-	2/7/25/26	0/2/2/2
1	1MA	1	58	1	-	0/3/25/26	0/3/3/3
1	T6A	1	37	1	-	5/19/41/42	0/3/3/3
2	C4J	2	1190	2	1/1/7/7	0/16/34/35	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	1MA	C2-N3	5.71	1.35	1.29
1	1	26	M2G	C2-N3	5.61	1.37	1.30
2	2	465	PSU	C6-C5	4.22	1.40	1.35
2	2	1289	PSU	C6-C5	4.21	1.40	1.35
2	2	120	PSU	C6-C5	3.89	1.39	1.35
2	2	998	PSU	C6-C5	3.88	1.39	1.35
2	2	766	PSU	C6-C5	3.74	1.39	1.35
1	1	26	M2G	C2-N2	3.74	1.42	1.35
1	1	58	1MA	C6-N6	3.44	1.36	1.27
1	1	49	5MC	C6-C5	3.32	1.40	1.34
2	2	1637	5MC	C6-C5	3.29	1.40	1.34
1	1	46	7MG	C5-C4	3.21	1.48	1.38
1	1	48	5MC	C6-C5	3.07	1.39	1.34
2	2	1573	7MG	C5-C4	3.04	1.48	1.38
2	2	1573	7MG	C8-N9	2.98	1.47	1.46
2	2	1573	7MG	C4-N9	-2.77	1.34	1.37
2	2	465	PSU	C4-N3	-2.74	1.33	1.38
1	1	46	7MG	C8-N9	2.68	1.47	1.46
2	2	1289	PSU	C4-N3	-2.65	1.33	1.38
1	1	46	7MG	C4-N9	-2.63	1.34	1.37
2	2	766	PSU	C4-N3	-2.61	1.34	1.38
2	2	1780	MA6	C5-C4	2.55	1.47	1.40
2	2	1006	5MC	C6-N1	-2.54	1.33	1.38
1	1	37	T6A	C5-C4	2.49	1.47	1.40
2	2	998	PSU	C4-N3	-2.31	1.34	1.38
2	2	465	PSU	C2-N3	-2.29	1.33	1.37
2	2	1573	7MG	C5-N7	-2.28	1.33	1.35
2	2	1573	7MG	C6-N1	-2.22	1.34	1.38
1	1	46	7MG	C5-C6	2.22	1.49	1.43
2	2	120	PSU	C4-N3	-2.20	1.34	1.38
2	2	1573	7MG	C1'-N9	2.17	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	998	PSU	C4-C5	2.14	1.50	1.44
1	1	58	1MA	C5-C4	2.13	1.48	1.43
1	1	10	2MG	O4'-C1'	2.12	1.44	1.41
1	1	37	T6A	O4'-C1'	2.11	1.44	1.41
2	2	1780	MA6	C6-N1	2.08	1.36	1.33
1	1	26	M2G	O4'-C1'	2.08	1.44	1.41
2	2	1573	7MG	C5-C6	2.06	1.48	1.43
1	1	58	1MA	O4'-C1'	2.05	1.43	1.41
2	2	1289	PSU	C4-C5	2.04	1.50	1.44

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1573	7MG	N9-C4-N3	8.85	138.71	125.47
1	1	46	7MG	N9-C4-N3	8.73	138.53	125.47
1	1	37	T6A	C12-N11-C10	8.59	136.24	121.94
1	1	37	T6A	C2-N1-C6	7.43	122.96	116.59
2	2	1289	PSU	N1-C2-N3	6.10	122.04	115.13
2	2	465	PSU	N1-C2-N3	5.93	121.85	115.13
2	2	998	PSU	N1-C2-N3	5.93	121.85	115.13
2	2	766	PSU	N1-C2-N3	5.92	121.84	115.13
2	2	1573	7MG	C5-C4-N3	-5.77	117.14	128.13
2	2	120	PSU	N1-C2-N3	5.56	121.42	115.13
1	1	46	7MG	C5-C4-N3	-5.39	117.85	128.13
1	1	16	H2U	O4'-C1'-N1	5.03	116.15	109.30
1	1	37	T6A	C14-C12-C13	5.00	118.72	110.19
2	2	1573	7MG	N9-C8-N7	-4.99	96.24	103.38
1	1	46	7MG	N9-C8-N7	-4.91	96.35	103.38
1	1	46	7MG	C2-N3-C4	4.68	120.64	112.30
2	2	1573	7MG	C2-N3-C4	4.63	120.55	112.30
2	2	766	PSU	C4-N3-C2	-4.07	120.47	126.34
2	2	1780	MA6	C4-C5-N7	-4.07	105.16	109.40
1	1	58	1MA	C3'-C2'-C1'	3.84	106.76	100.98
1	1	37	T6A	N3-C2-N1	-3.78	122.77	128.68
2	2	120	PSU	C4-N3-C2	-3.77	120.91	126.34
2	2	1289	PSU	C4-N3-C2	-3.75	120.94	126.34
2	2	1006	5MC	C5-C4-N3	-3.75	117.63	121.67
2	2	1573	7MG	O4'-C1'-N9	3.73	114.38	109.30
2	2	998	PSU	C4-N3-C2	-3.72	120.98	126.34
2	2	1006	5MC	CM5-C5-C6	-3.64	117.99	122.85
2	2	120	PSU	O2-C2-N1	-3.53	118.91	122.79
2	2	1780	MA6	N3-C2-N1	-3.46	123.27	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	465	PSU	C4-N3-C2	-3.43	121.40	126.34
2	2	766	PSU	O2-C2-N1	-3.40	119.05	122.79
2	2	1190	C4J	C4-N3-C2	-3.39	121.17	125.46
2	2	998	PSU	O2-C2-N1	-3.34	119.12	122.79
1	1	47	H2U	C3'-C2'-C1'	3.23	107.56	101.43
1	1	9	1MG	O6-C6-C5	-3.17	118.58	124.19
2	2	1780	MA6	C10-N6-C6	-3.15	109.98	119.51
1	1	9	1MG	C5-C6-N1	3.11	118.58	113.90
1	1	26	M2G	N1-C2-N2	3.06	120.65	118.04
1	1	49	5MC	O2-C2-N3	-3.06	117.36	122.33
2	2	465	PSU	C6-C5-C4	-3.05	116.06	118.20
1	1	46	7MG	C5-C6-N1	2.99	116.26	110.99
1	1	48	5MC	O2-C2-N3	-2.91	117.60	122.33
1	1	37	T6A	N6-C6-N1	2.90	122.61	118.72
2	2	766	PSU	C3'-C2'-C1'	2.89	105.01	101.64
1	1	49	5MC	C5-C4-N3	-2.89	118.56	121.67
2	2	1637	5MC	C5-C4-N3	-2.88	118.57	121.67
2	2	1780	MA6	C10-N6-C9	-2.82	107.03	116.12
2	2	1426	2MG	C5-C6-N1	2.78	118.86	113.95
2	2	1573	7MG	C5-C6-N1	2.77	115.88	110.99
2	2	1570	2MG	C3'-C2'-C1'	2.75	105.11	100.98
1	1	46	7MG	O4'-C1'-N9	2.74	113.03	109.30
2	2	1289	PSU	O2-C2-N1	-2.74	119.78	122.79
1	1	48	5MC	C5-C6-N1	-2.73	120.53	123.34
1	1	26	M2G	C5-C6-N1	2.68	118.69	113.95
2	2	1637	5MC	O4'-C1'-N1	2.67	114.47	108.36
1	1	26	M2G	O6-C6-C5	-2.67	119.16	124.37
2	2	1006	5MC	O2-C2-N3	-2.66	118.01	122.33
2	2	1006	5MC	C5-C6-N1	-2.63	120.63	123.34
1	1	16	H2U	C5-C4-N3	2.62	119.59	116.65
2	2	1637	5MC	C5-C6-N1	-2.62	120.65	123.34
1	1	37	T6A	C4-C5-N7	-2.59	106.70	109.40
2	2	1426	2MG	C8-N7-C5	2.57	107.89	102.99
2	2	766	PSU	C6-C5-C4	-2.56	116.41	118.20
2	2	998	PSU	C6-C5-C4	-2.56	116.41	118.20
2	2	1637	5MC	O2-C2-N3	-2.53	118.21	122.33
1	1	48	5MC	O4'-C1'-N1	2.49	114.07	108.36
1	1	16	H2U	C4-N3-C2	-2.47	123.74	125.79
2	2	1570	2MG	C5-C6-N1	2.45	118.28	113.95
1	1	49	5MC	O4'-C1'-N1	2.41	113.87	108.36
2	2	465	PSU	O2-C2-N1	-2.41	120.14	122.79
2	2	1426	2MG	O6-C6-C5	-2.39	119.70	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	O10-C10-N6	-2.36	119.62	123.62
1	1	47	H2U	C4-N3-C2	-2.36	123.84	125.79
2	2	120	PSU	C6-C5-C4	-2.33	116.57	118.20
2	2	1006	5MC	N4-C4-N3	2.33	122.73	118.48
1	1	58	1MA	C8-N7-C5	2.32	107.42	102.99
1	1	9	1MG	C3'-C2'-C1'	2.31	104.46	100.98
2	2	1426	2MG	CM2-N2-C2	2.31	128.97	123.86
1	1	37	T6A	C14-C12-N11	2.30	117.60	111.72
1	1	9	1MG	C8-N7-C5	2.27	107.32	102.99
2	2	1570	2MG	C8-N7-C5	2.26	107.29	102.99
2	2	1006	5MC	C2'-C1'-N1	-2.23	106.89	113.22
1	1	46	7MG	CM7-N7-C5	2.22	132.13	126.40
1	1	47	H2U	C5-C4-N3	2.22	119.14	116.65
2	2	1637	5MC	CM5-C5-C6	-2.20	119.91	122.85
1	1	10	2MG	C8-N7-C5	2.17	107.13	102.99
1	1	26	M2G	C8-N7-C5	2.17	107.13	102.99
2	2	1637	5MC	N1-C2-N3	2.13	122.68	118.81
1	1	10	2MG	C5-C6-N1	2.11	117.68	113.95
1	1	46	7MG	C5-C4-N9	-2.10	103.62	106.35
1	1	16	H2U	C4'-O4'-C1'	-2.09	104.85	109.47
1	1	37	T6A	C3'-C2'-C1'	2.07	104.10	100.98
1	1	58	1MA	C5-C6-N1	2.05	116.95	113.90
1	1	37	T6A	C15-C14-C12	2.04	116.41	112.29
1	1	46	7MG	O3'-C3'-C4'	-2.03	105.17	111.05
1	1	64	RIA	C5-C6-N6	2.03	123.44	120.35
1	1	49	5MC	C3'-C2'-C1'	2.02	105.27	101.43
2	2	465	PSU	O2-C2-N3	-2.02	118.00	121.82
1	1	46	7MG	O6-C6-C5	-2.02	122.59	127.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	1190	C4J	C4'

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	1780	MA6	O4'-C4'-C5'-O5'
2	2	1780	MA6	C5-C6-N6-C10
2	2	1780	MA6	N1-C6-N6-C10
1	1	9	1MG	O4'-C4'-C5'-O5'
1	1	9	1MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	10	2MG	O4'-C4'-C5'-O5'
1	1	16	H2U	C4'-C5'-O5'-P
1	1	26	M2G	C3'-C4'-C5'-O5'
1	1	37	T6A	C14-C12-N11-C10
1	1	37	T6A	N11-C12-C14-O14
1	1	47	H2U	O4'-C4'-C5'-O5'
1	1	47	H2U	C3'-C4'-C5'-O5'
1	1	48	5MC	C4'-C5'-O5'-P
1	1	64	RIA	C3'-C4'-C5'-O5'
2	2	1780	MA6	C3'-C4'-C5'-O5'
1	1	10	2MG	C3'-C4'-C5'-O5'
1	1	48	5MC	O4'-C4'-C5'-O5'
1	1	48	5MC	C3'-C4'-C5'-O5'
1	1	47	H2U	C2'-C1'-N1-C2
2	2	1426	2MG	O4'-C4'-C5'-O5'
1	1	26	M2G	O4'-C4'-C5'-O5'
1	1	64	RIA	O1'-C4'-C5'-O5'
1	1	47	H2U	C2'-C1'-N1-C6
1	1	37	T6A	N11-C12-C14-C15
1	1	37	T6A	N11-C12-C13-ODA
2	2	1573	7MG	O4'-C4'-C5'-O5'
2	2	1573	7MG	C3'-C4'-C5'-O5'
1	1	49	5MC	O4'-C4'-C5'-O5'
1	1	37	T6A	N11-C12-C13-ODB
1	1	46	7MG	C4'-C5'-O5'-P
1	1	64	RIA	C4A-C5A-O5A-P
1	1	9	1MG	C4'-C5'-O5'-P
2	2	1426	2MG	C4'-C5'-O5'-P
2	2	1780	MA6	C4'-C5'-O5'-P
2	2	766	PSU	C3'-C4'-C5'-O5'
2	2	1426	2MG	C3'-C4'-C5'-O5'
1	1	49	5MC	C3'-C4'-C5'-O5'
2	2	1637	5MC	O4'-C4'-C5'-O5'
1	1	16	H2U	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 124 ligands modelled in this entry, 122 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$
50	MET	k	601	-	6,7,8	0.47	0	2,7,9	0.12	0
51	GCP	k	603	-	27,34,34	1.91	7 (25%)	34,54,54	1.94	8 (23%)

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
50	MET	k	601	-	-	1/5/6/8	-
51	GCP	k	603	-	-	1/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.35	1.61	1.50
51	k	603	GCP	C5-C6	4.61	1.49	1.41
51	k	603	GCP	PB-O3A	2.98	1.61	1.58
51	k	603	GCP	PG-O3G	-2.84	1.48	1.54
51	k	603	GCP	PG-O2G	2.83	1.61	1.54
51	k	603	GCP	C5-C4	2.77	1.48	1.40
51	k	603	GCP	PB-O2B	2.18	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C2-N3-C4	5.27	121.38	115.36
51	k	603	GCP	C2-N1-C6	4.05	122.36	115.93
51	k	603	GCP	C5-C6-N1	-3.83	118.19	123.43
51	k	603	GCP	C4-C5-C6	-3.77	117.20	120.80
51	k	603	GCP	N3-C2-N1	-3.51	122.55	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C3'-C2'-C1'	3.13	105.69	100.98
51	k	603	GCP	PB-O3A-PA	-3.04	122.93	132.56
51	k	603	GCP	C4-C5-N7	-2.69	106.60	109.40

There are no chirality outliers.

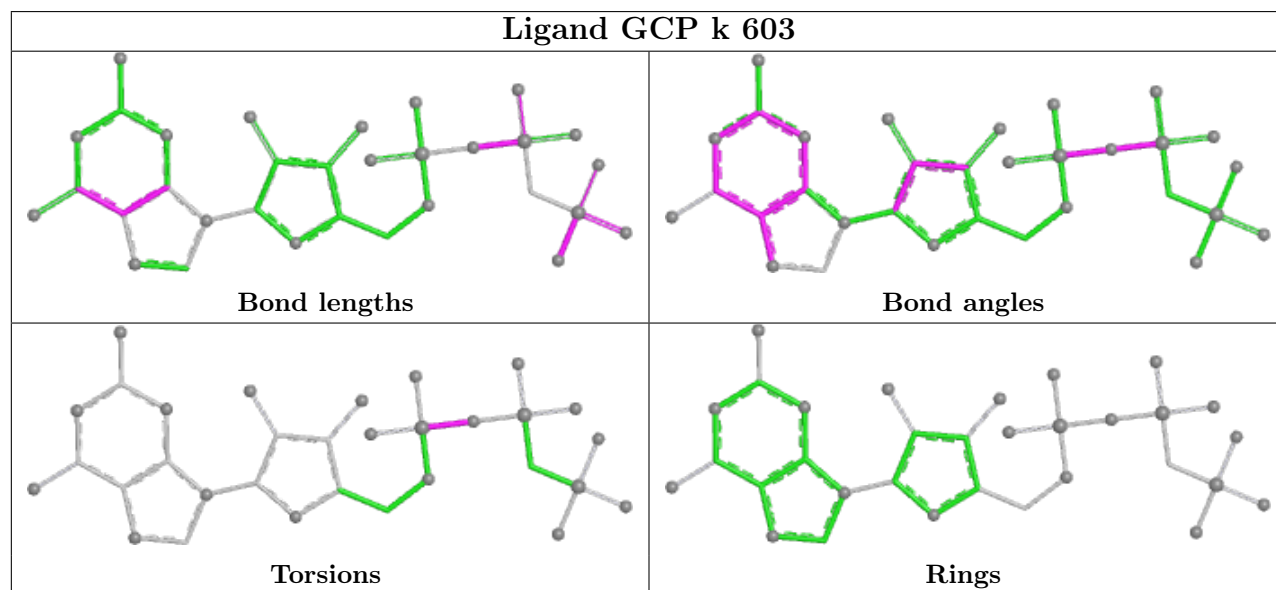
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	k	601	MET	CA-CB-CG-SD
51	k	603	GCP	PB-O3A-PA-O1A

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 than 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.





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	q	8
2	2	1
1	1	1
44	p	1
5	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	214:UNK	C	251:GLN	N	50.55
1	q	158:UNK	C	166:UNK	N	17.71
1	q	181:UNK	C	190:UNK	N	14.31
1	q	135:UNK	C	139:UNK	N	7.79
1	q	203:UNK	C	207:UNK	N	6.84
1	2	224:A	O3'	225:A	P	4.58
1	1	16:H2U	O3'	18:G	P	4.54
1	q	582:GLN	C	583:GLN	N	3.87
1	q	148:UNK	C	150:UNK	N	3.60
1	q	605:CYS	C	606:LEU	N	3.34
1	p	688:GLU	C	689:GLU	N	3.29
1	B	2:AYA	C	3:VAL	N	3.09

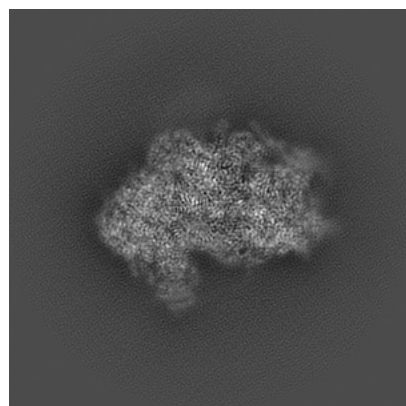
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4328. These allow visual inspection of the internal detail of the map and identification of artifacts.

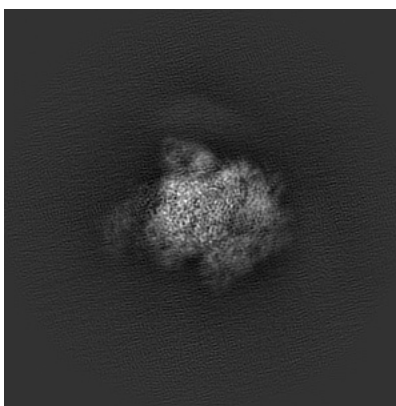
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

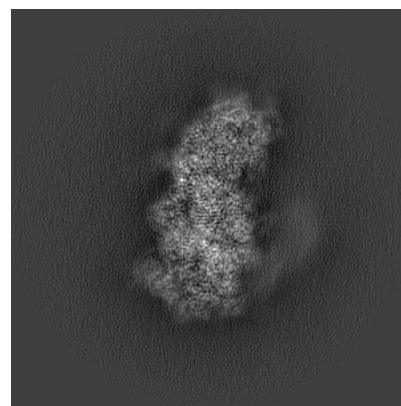
#### 6.1.1 Primary map



X

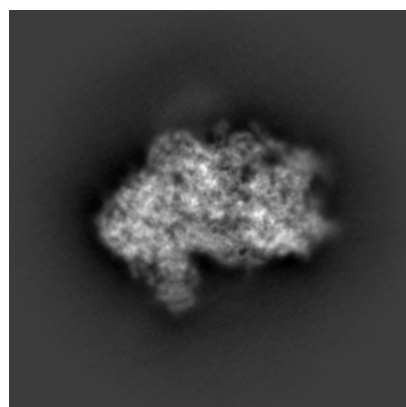


Y

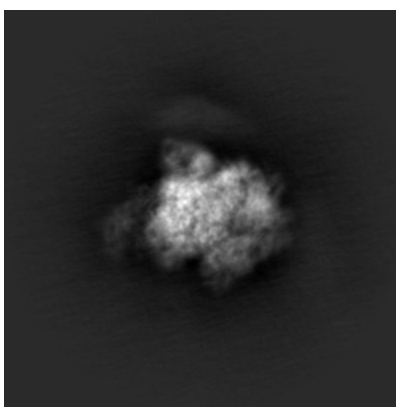


Z

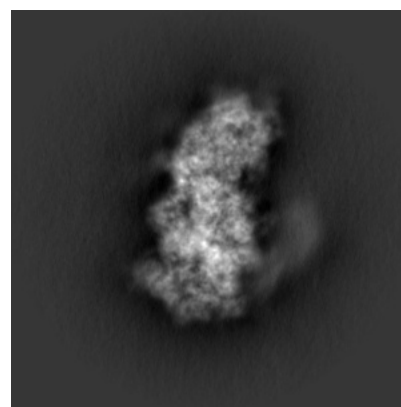
#### 6.1.2 Raw map



X



Y

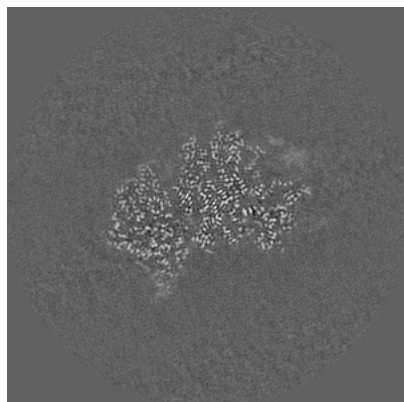


Z

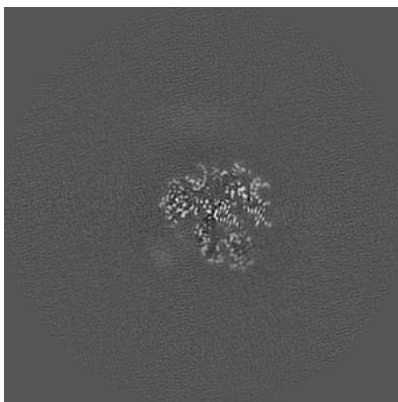
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

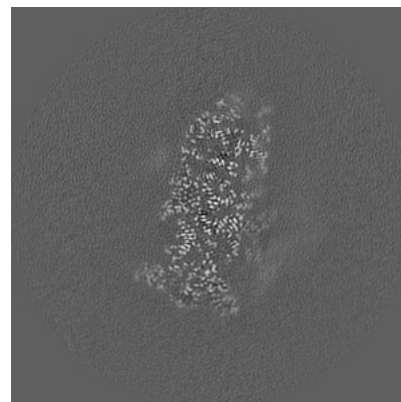
### 6.2.1 Primary map



X Index: 150

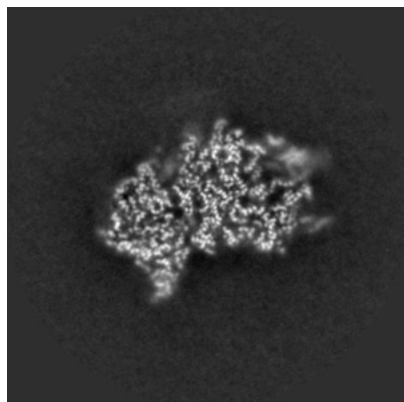


Y Index: 150

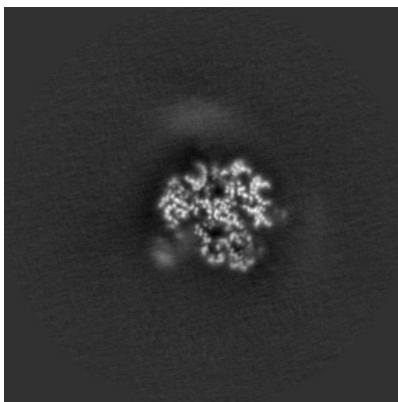


Z Index: 150

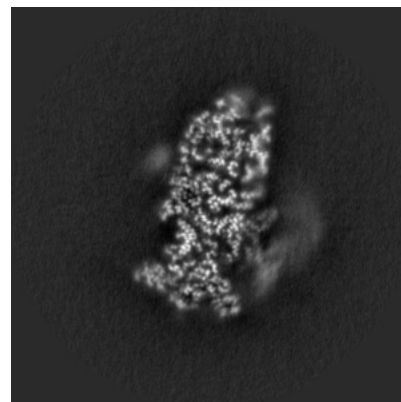
### 6.2.2 Raw map



X Index: 150



Y Index: 150

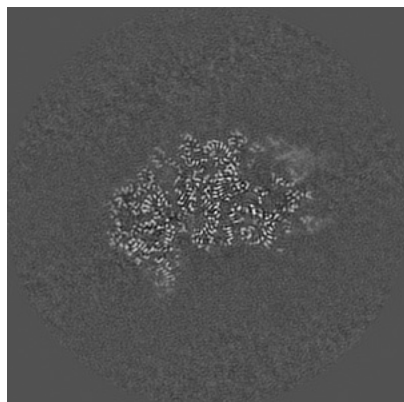


Z Index: 150

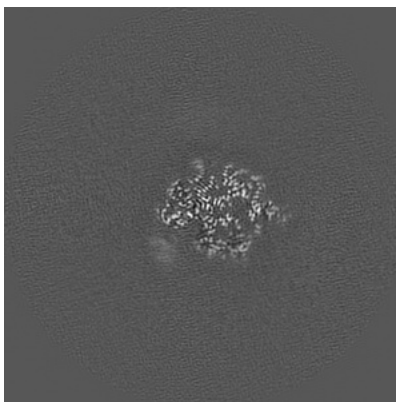
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

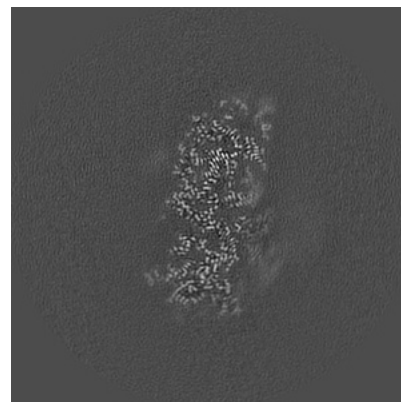
### 6.3.1 Primary map



X Index: 152

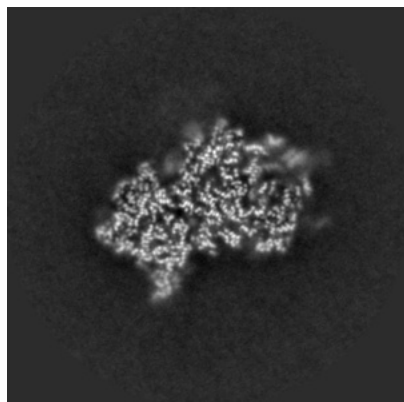


Y Index: 155

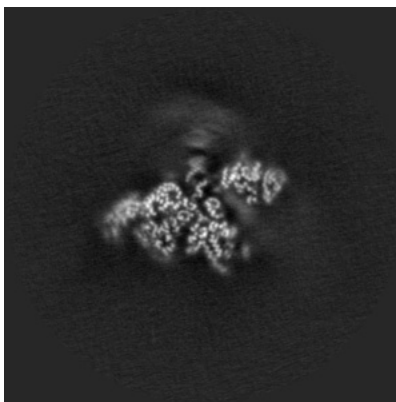


Z Index: 147

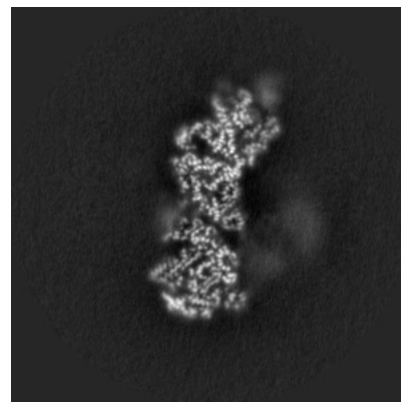
### 6.3.2 Raw map



X Index: 148



Y Index: 119

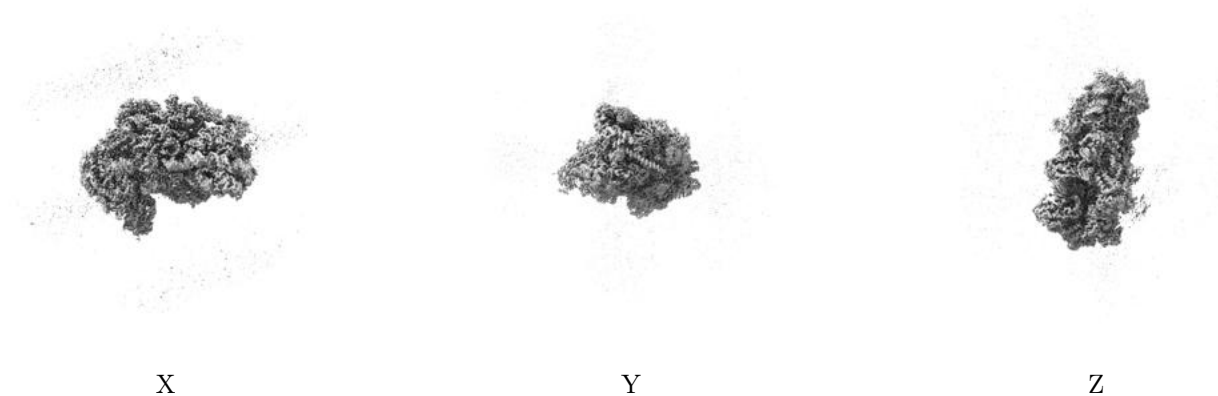


Z Index: 132

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

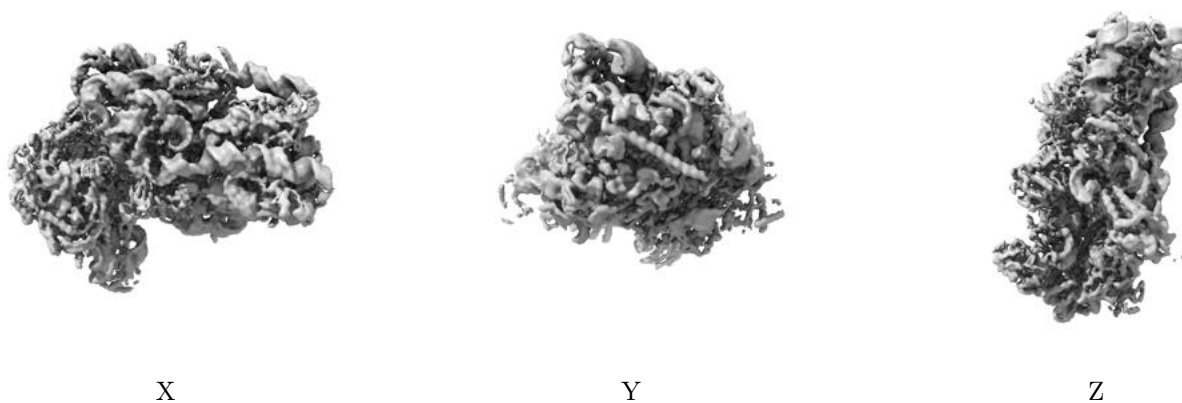
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

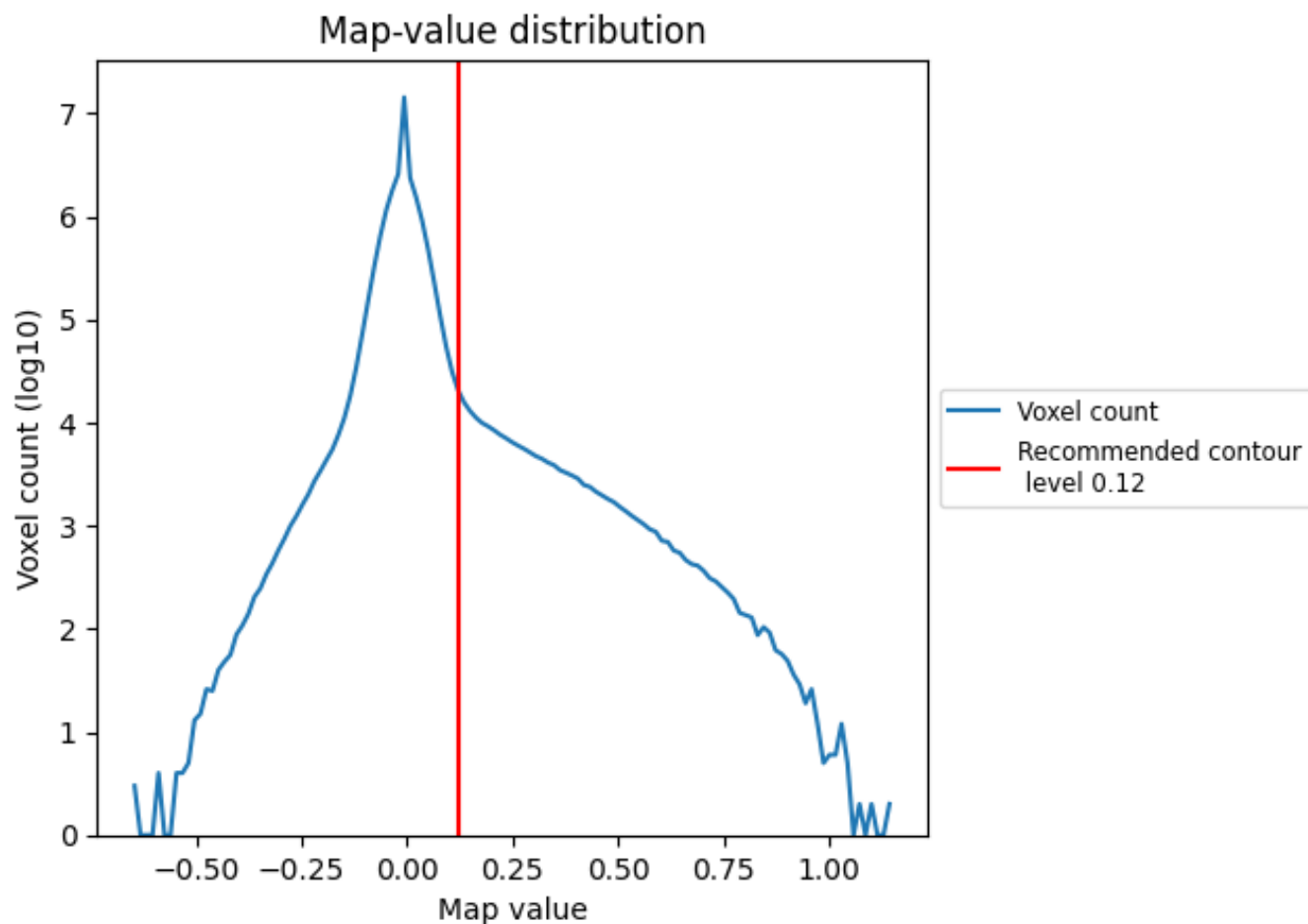
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

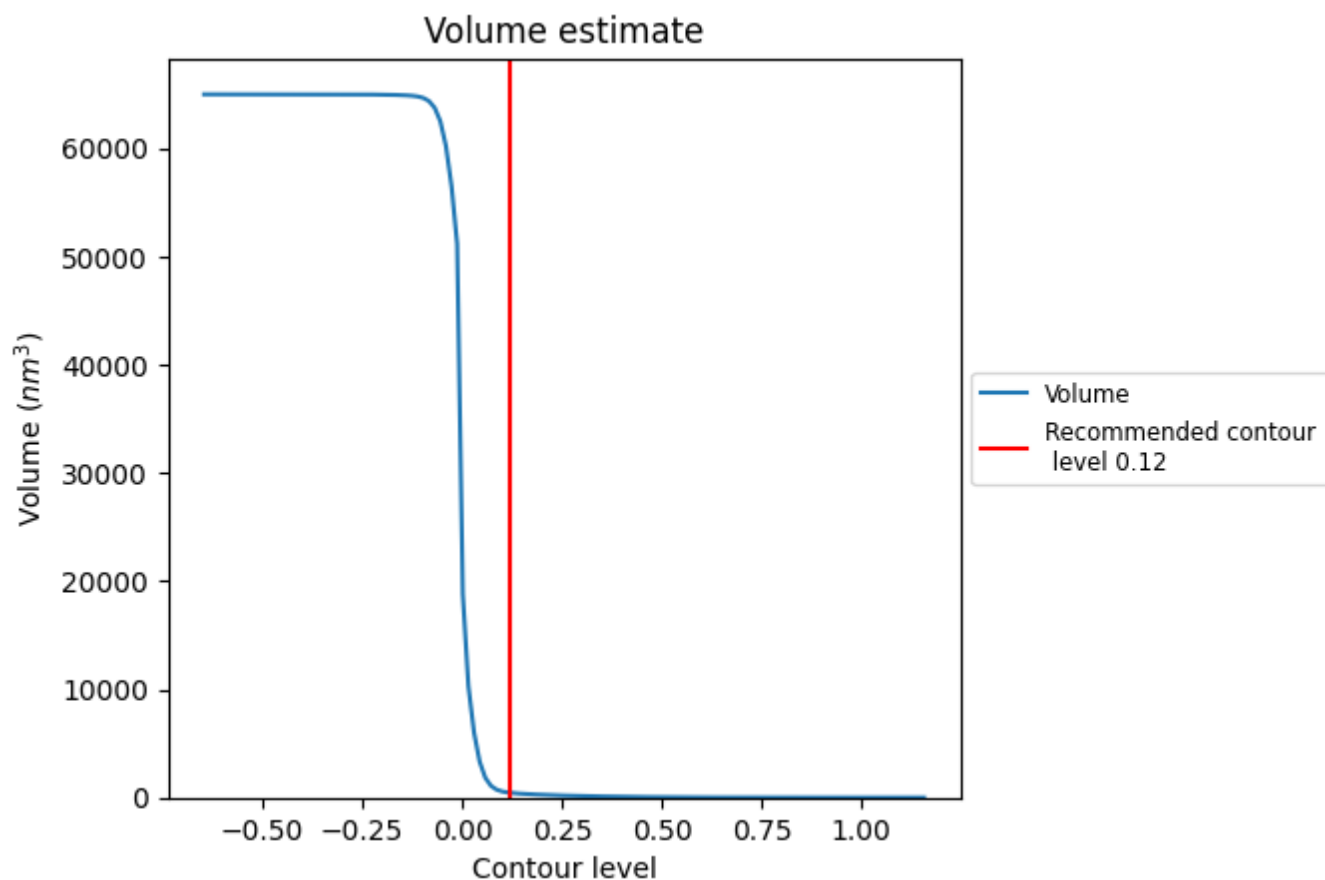
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

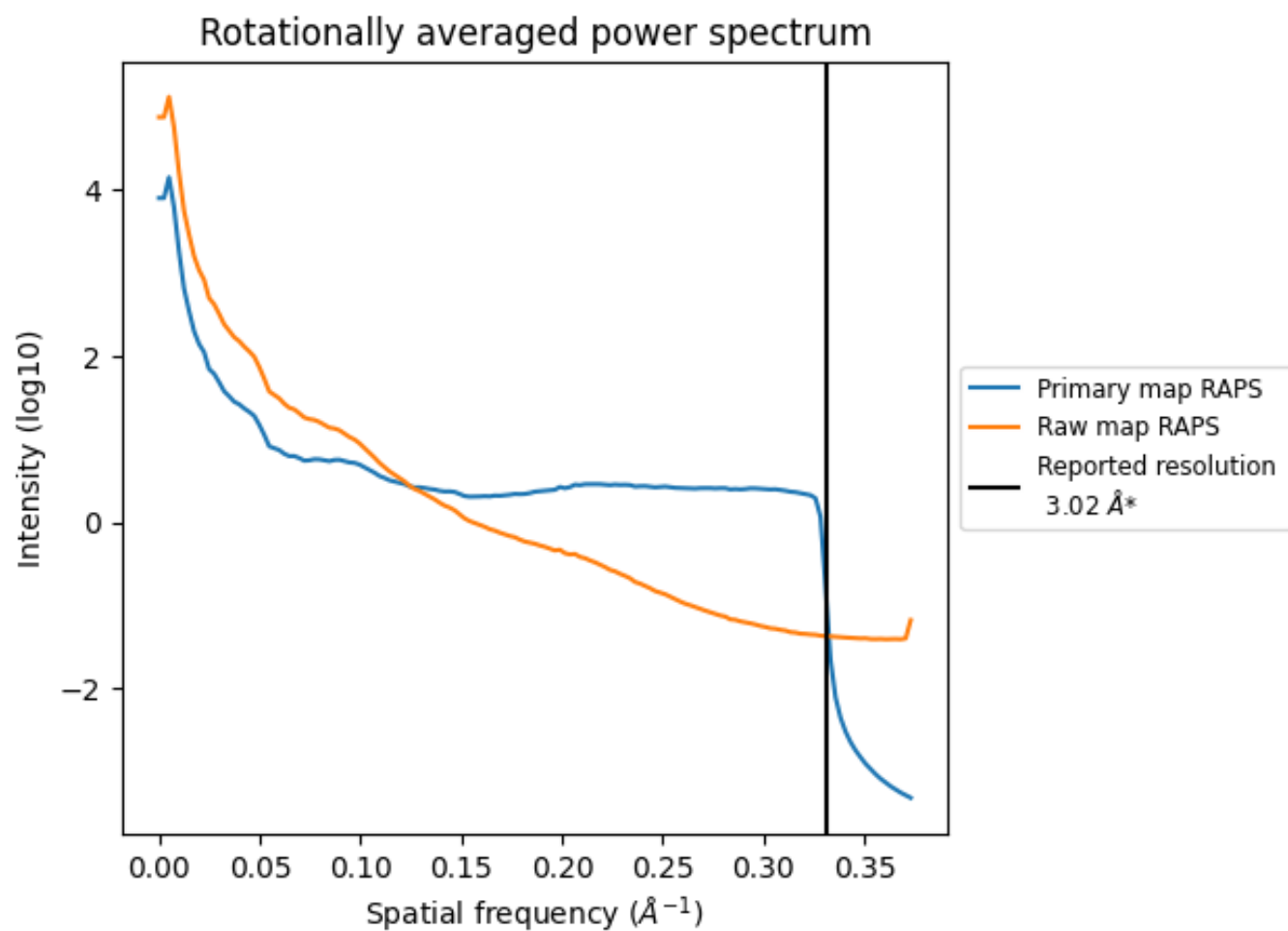
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm<sup>3</sup>; this corresponds to an approximate mass of 404 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



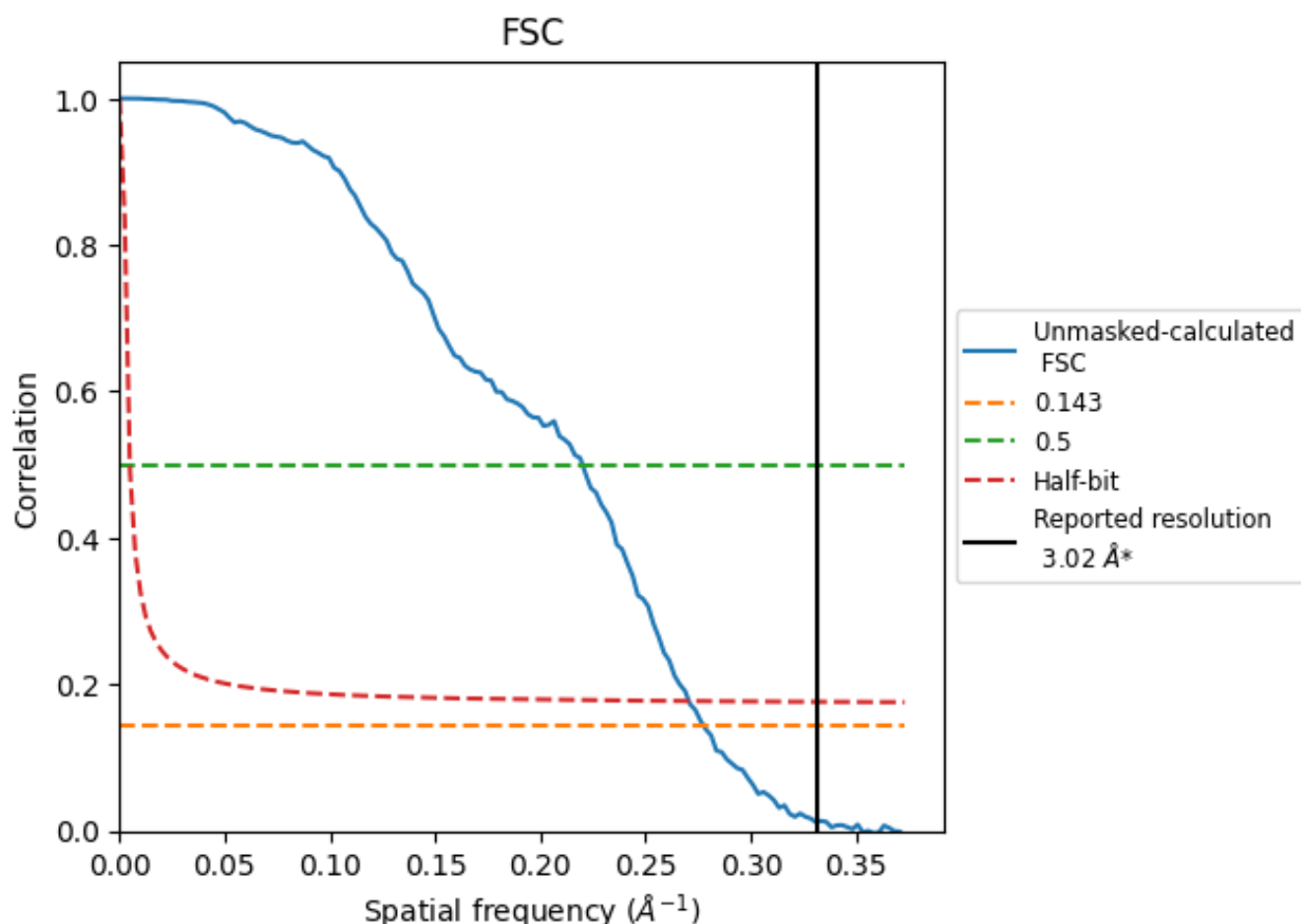
\*Reported resolution corresponds to spatial frequency of 0.331  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.331  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

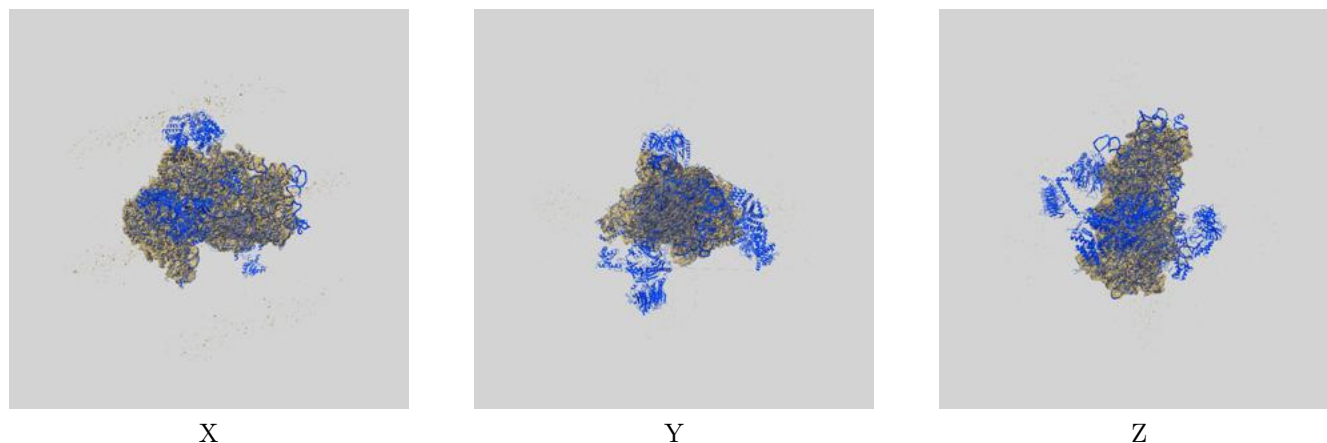
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.60	4.55	3.70

\*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 3.60 differs from the reported value 3.02 by more than 10 %

## 9 Map-model fit [i](#)

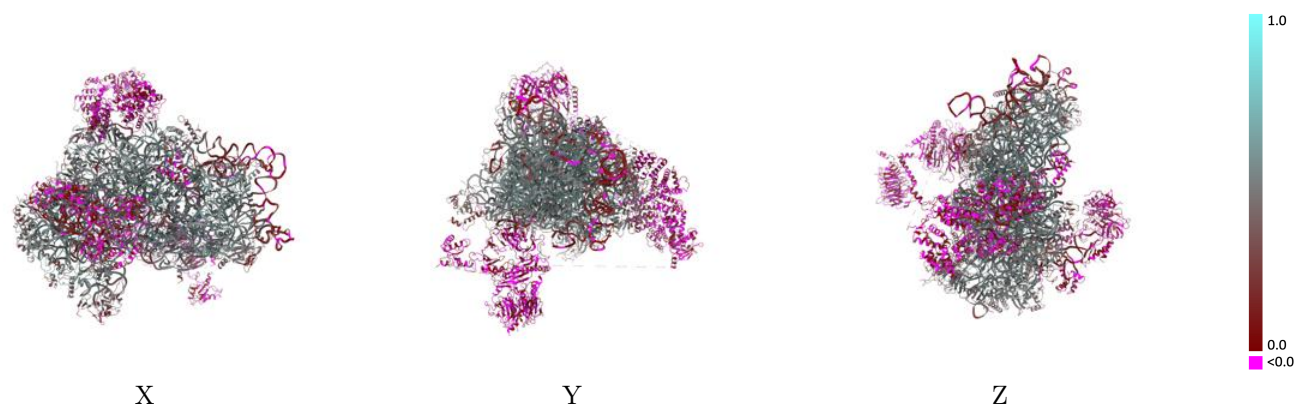
This section contains information regarding the fit between EMDB map EMD-4328 and PDB model 6FYY. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



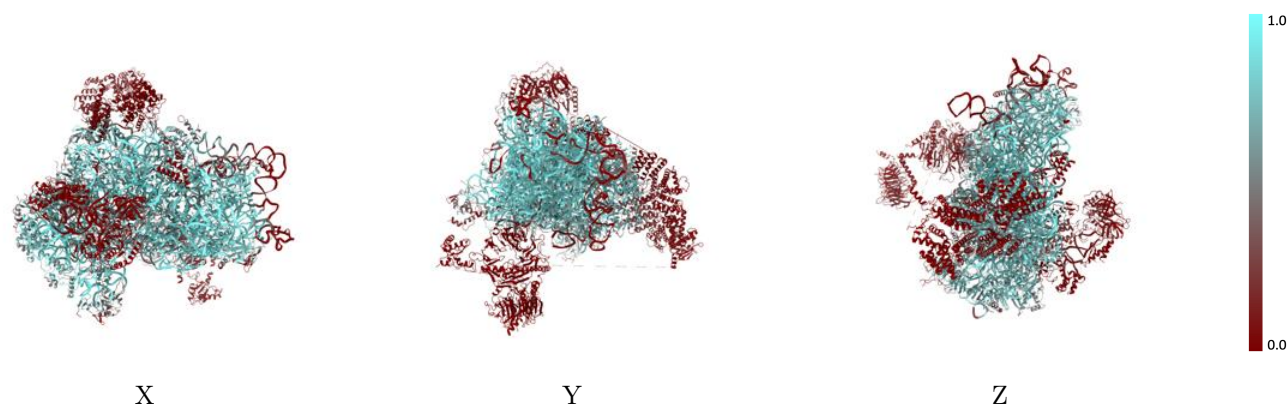
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



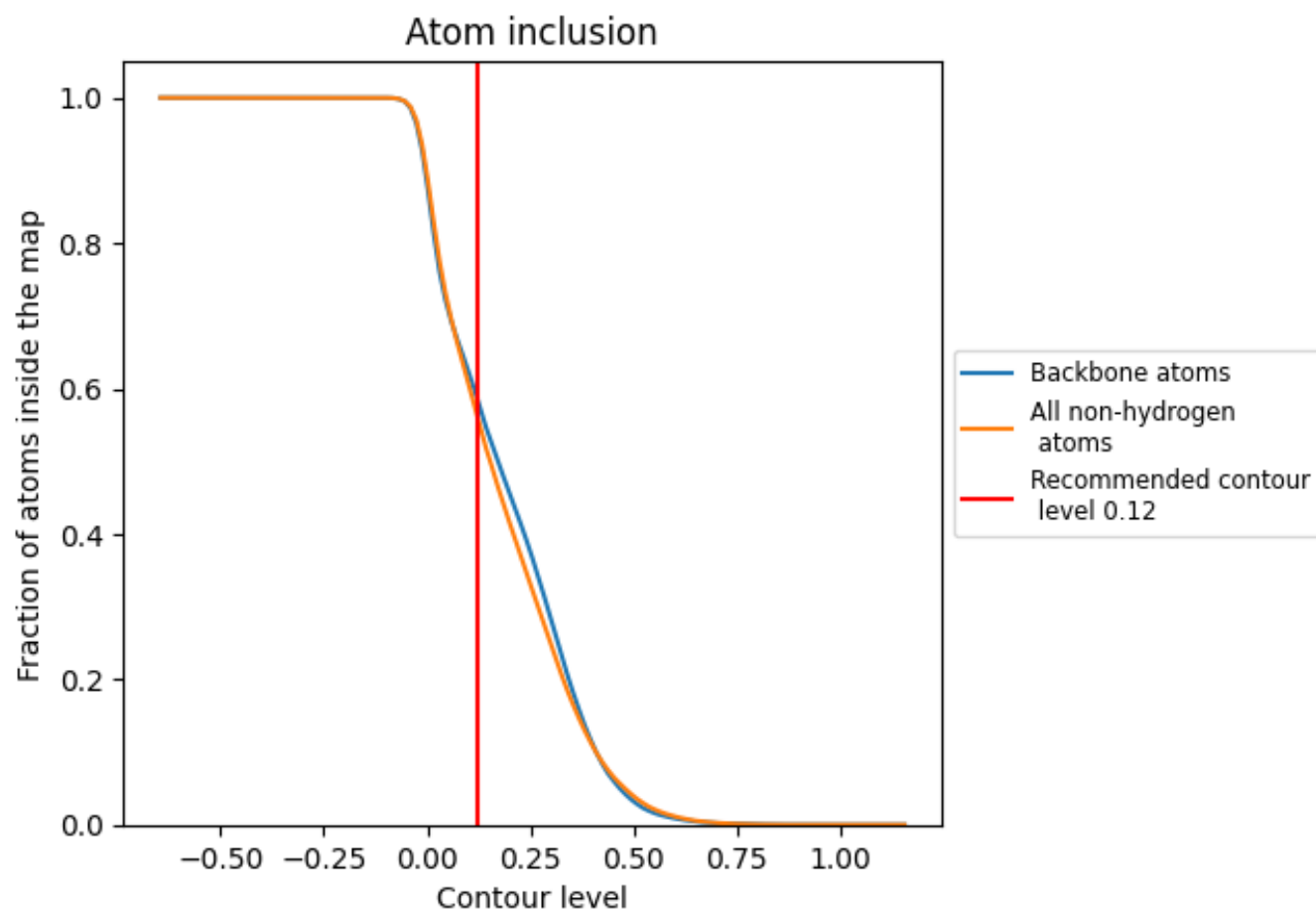
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 57% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5662	 0.3780
1	 0.3118	 0.2600
2	 0.8103	 0.4820
3	 0.2567	 0.2510
A	 0.7071	 0.4840
B	 0.6635	 0.4590
C	 0.7642	 0.5220
D	 0.6755	 0.4700
E	 0.7961	 0.5310
F	 0.6622	 0.4770
G	 0.6329	 0.4360
H	 0.5626	 0.4250
I	 0.7197	 0.4870
J	 0.7648	 0.5110
K	 0.6910	 0.4620
L	 0.6963	 0.4930
M	 0.2854	 0.2570
N	 0.7519	 0.5110
O	 0.7403	 0.5100
P	 0.7044	 0.4800
Q	 0.7481	 0.5120
R	 0.6328	 0.4600
S	 0.6997	 0.4680
T	 0.7694	 0.5010
U	 0.5916	 0.4170
V	 0.7361	 0.5000
W	 0.8000	 0.5420
X	 0.8049	 0.5470
Y	 0.7549	 0.5010
Z	 0.4991	 0.3820
a	 0.7568	 0.5150
b	 0.6894	 0.4940
c	 0.6618	 0.4980
d	 0.8575	 0.5620
e	 0.6790	 0.4730



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Chain	Atom inclusion	Q-score
f	 0.4188	 0.3750
g	 0.6164	 0.4590
h	 0.4717	 0.4180
i	 0.6143	 0.4750
j	 0.0031	 0.1410
k	 0.0007	 0.0430
l	 0.0010	 0.0530
m	 0.2219	 0.3860
o	 0.0003	 0.0240
p	 0.0000	 0.0450
q	 0.0008	 0.0430
r	 0.0000	 0.0090
s	 0.0004	 0.0250