



## Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 10:04 am GMT

PDB ID : 6ZMW  
EMDB ID : EMD-11302  
Title : Structure of a human 48S translational initiation complex  
Authors : Brito Querido, J.; Sokabe, M.; Kraatz, S.; Gordiyenko, Y.; Skehel, M.; Fraser, C.; Ramakrishnan, V.  
Deposited on : 2020-07-04  
Resolution : 3.70 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:

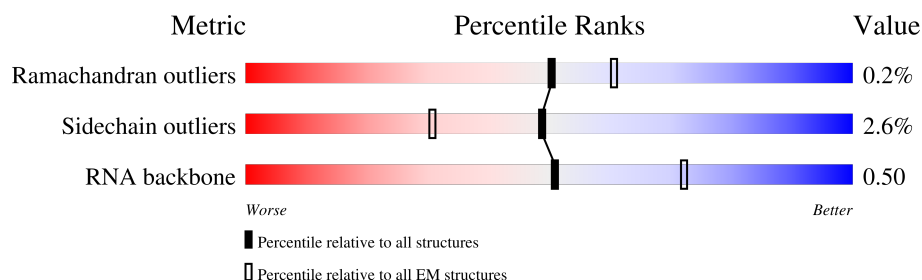
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
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	2	325	<p>82% 94% 6%</p>
2	1	814	<p>30% 71% 28%</p>
3	6	374	<p>17% 93% 6%</p>
4	4	357	<p>18% 71% 28%</p>
5	u	1382	<p>7% 50% 49%</p>
6	v	445	<p>7% 85% 14%</p>
7	S	249	<p>90% 8%</p>
8	y	913	<p>15% 75% 24%</p>

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Mol	Chain	Length	Quality of chain
9	8	352	
10	G	194	
11	H	84	
12	K	83	
13	L	293	
14	O	264	
15	N	295	
16	Q	115	
17	P	151	
18	I	151	
19	x	548	
20	3	218	
21	5	564	
22	7	28	
23	9	25	
24	A	1869	
25	B	158	
26	C	263	
27	D	194	
28	E	143	
29	F	59	
30	r	315	
31	J	130	
32	R	208	
33	T	133	

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Mol	Chain	Length	Quality of chain
34	V	204	
35	Y	146	
36	Z	243	
37	a	165	
38	b	145	
39	c	317	
40	d	145	
41	e	125	
42	f	152	
43	i	56	
44	k	156	
45	m	132	
46	n	69	
47	o	320	
48	p	113	
49	q	144	
50	z	258	
51	M	135	
52	h	119	
53	s	333	
54	w	75	
55	t	472	
56	j	406	
57	g	1310	

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 118155 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	304	Total	C	N	O	0	0
			1493	885	304	304		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	588	Total	C	N	O	S	0	0
			3258	1986	633	634	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	350	Total	C	N	O	S	0	0
			1917	1159	376	380	2		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	v	384	Total	C	N	O	S	0	0
			2635	1657	477	489	12		

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	y	697	Total	C	N	O	S	0	0
			5470	3437	980	1018	35		

- Molecule 9 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	317	Total	C	N	O	S	0	0
			1571	936	317	318			

- Molecule 10 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 11 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 12 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 13 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 14 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 16 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 17 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 18 is a protein called 40S ribosomal protein S13.

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

- Molecule 19 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	421	Total	C	N	O	S	0	0
			2831	1746	521	555	9		

- Molecule 20 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3	213	Total	C	N	O	S	0	0
			1057	631	213	213			

- Molecule 21 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	5	319	Total	C	N	O	0	0
			1581	943	319	319		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	7	28	Total	C	O	P	0	0
			336	140	168	28		

- Molecule 23 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 24 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	1719	Total	C	N	O	P	0	0
			36670	16380	6574	11998	1718		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 26 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 27 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
28	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 29 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	47	Total	C	N	O	S	0	0
			378	231	85	61	1		

- Molecule 30 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	r	275	Total	C	N	O	S	0	0
			2215	1398	387	418	12		

- Molecule 31 is a protein called 40S ribosomal protein S15a.

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

- Molecule 32 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 33 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 34 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	V	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 35 is a protein called 40S ribosomal protein S16.

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

- Molecule 36 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 37 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 38 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	110	Total	C	N	O	S	0	0
			913	580	168	158	7		

- Molecule 39 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 40 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 41 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	66	Total	C	N	O	S	0	0
			523	338	93	91	1		

- Molecule 42 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	142	Total	C	N	O	S	0	0
			1176	737	239	199	1		

- Molecule 43 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 44 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	53	Total	C	N	O	S	0	0
			435	276	82	70	7		

- Molecule 45 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 46 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
47	o	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	85	Total	C	N	O	S	0	0
			691	438	125	126	2		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	88	Total	C	N	O	S	0	0
			714	451	129	130	4		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	160	Total	C	N	O		0	0
			795	475	160	160			

- Molecule 51 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 52 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 53 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	138	Total	C	N	O	S	0	0
			1123	709	206	199	9		

- Molecule 54 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 55 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	t	356	Total	C	N	O	0	0
			1750	1038	356	356		

- Molecule 56 is a protein called Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	j	384	Total	C	N	O	S	0	0
			3073	1940	533	581	19		

- Molecule 57 is a protein called Eukaryotic translation initiation factor 4 gamma 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	g	224	Total	C	N	O	S	0	0
			1848	1168	324	341	15		

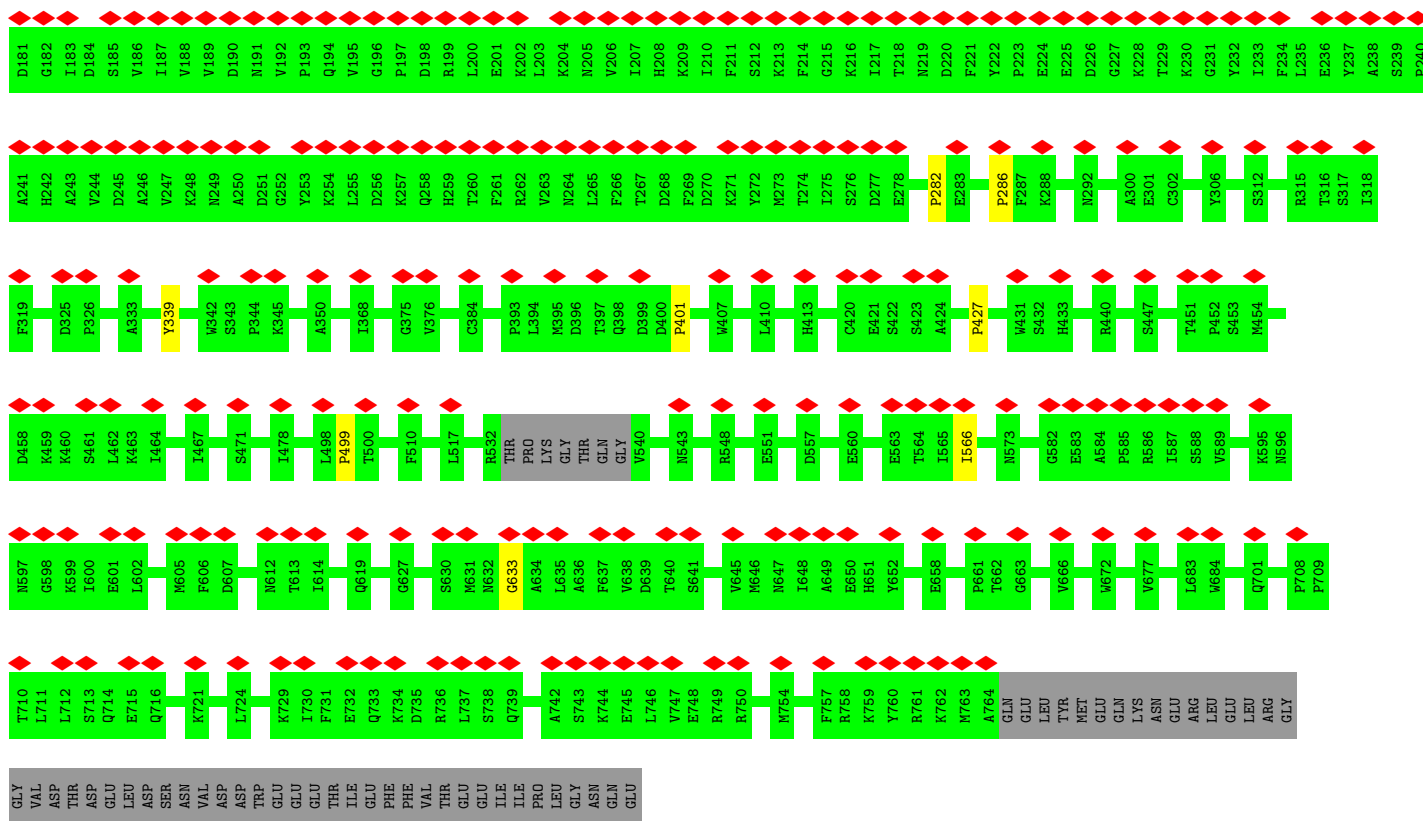
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
58	Q	1	Total	Zn	0
			1	1	
58	k	1	Total	Zn	0
			1	1	

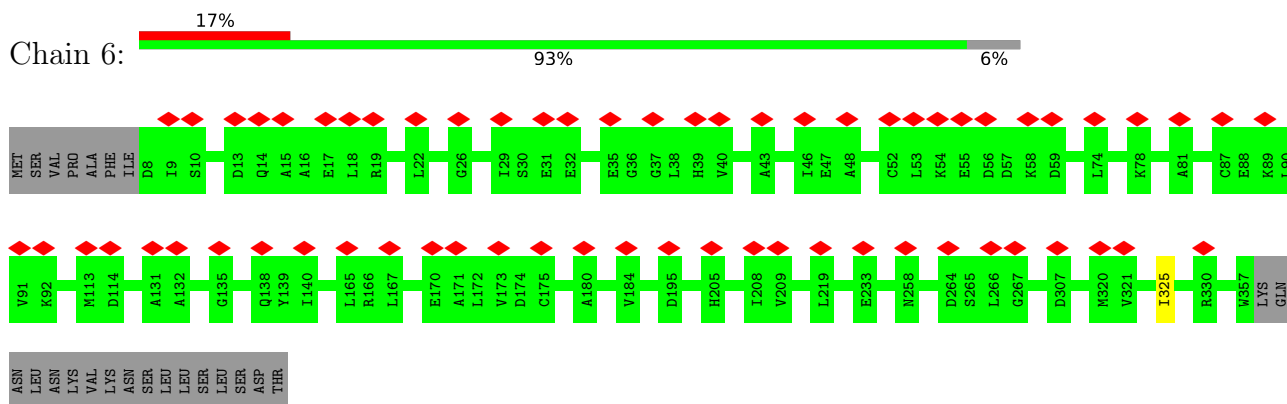
- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
59	A	87	Total	Mg	0
			87	87	
59	d	1	Total	Mg	0
			1	1	
59	f	1	Total	Mg	0
			1	1	

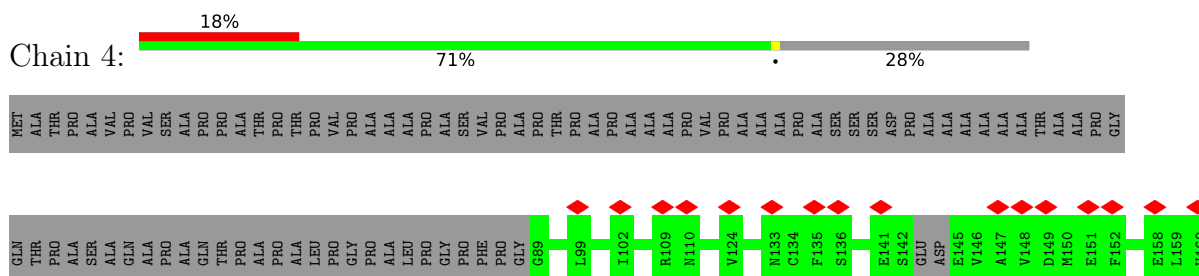


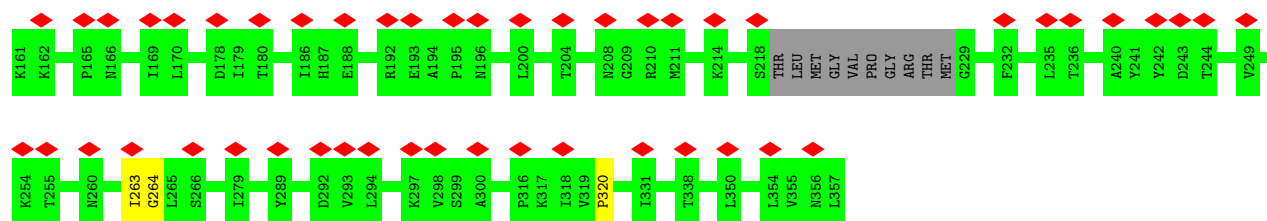


- Molecule 3: Eukaryotic translation initiation factor 3 subunit M

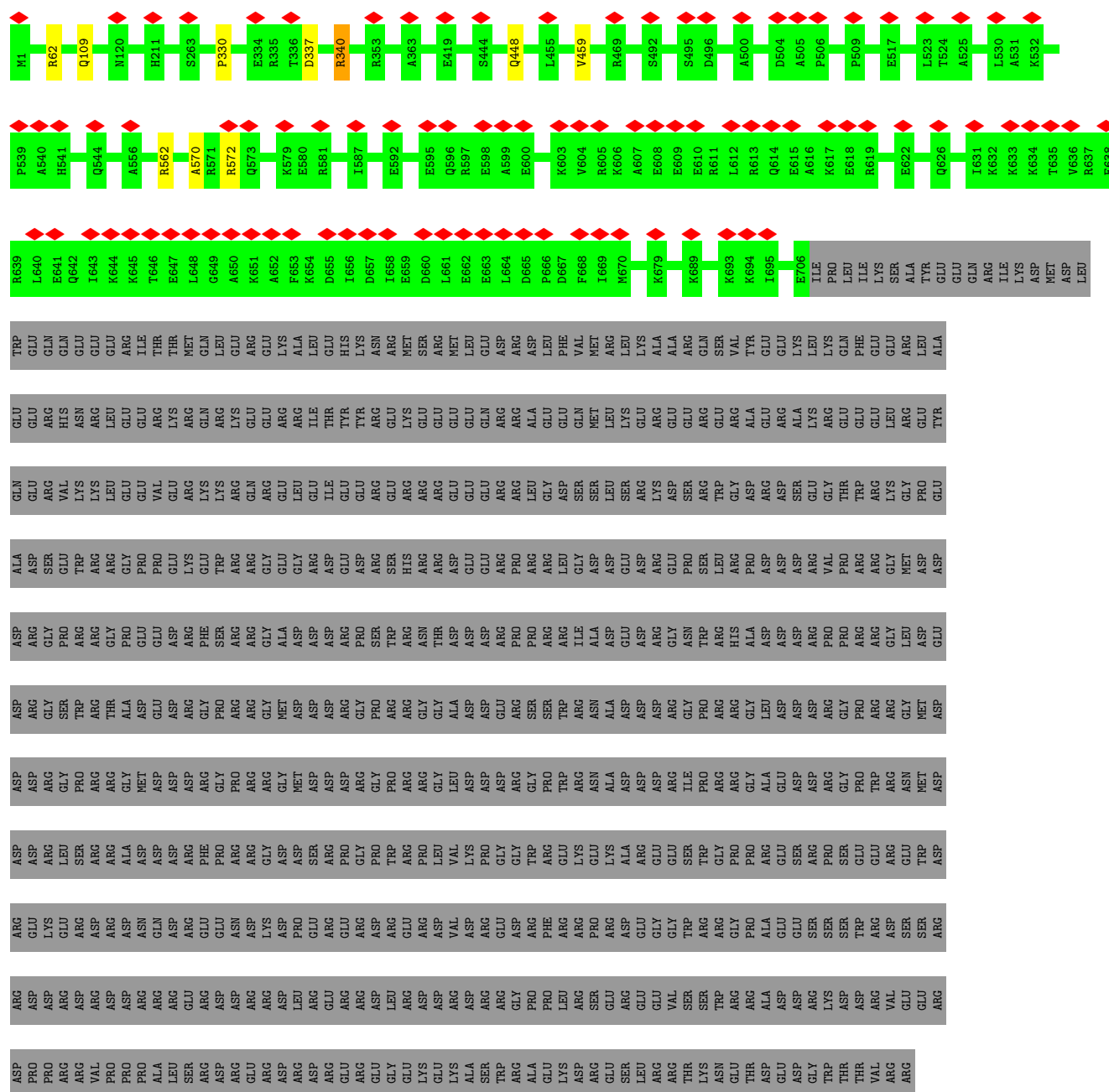


- Molecule 4: Eukaryotic translation initiation factor 3 subunit F



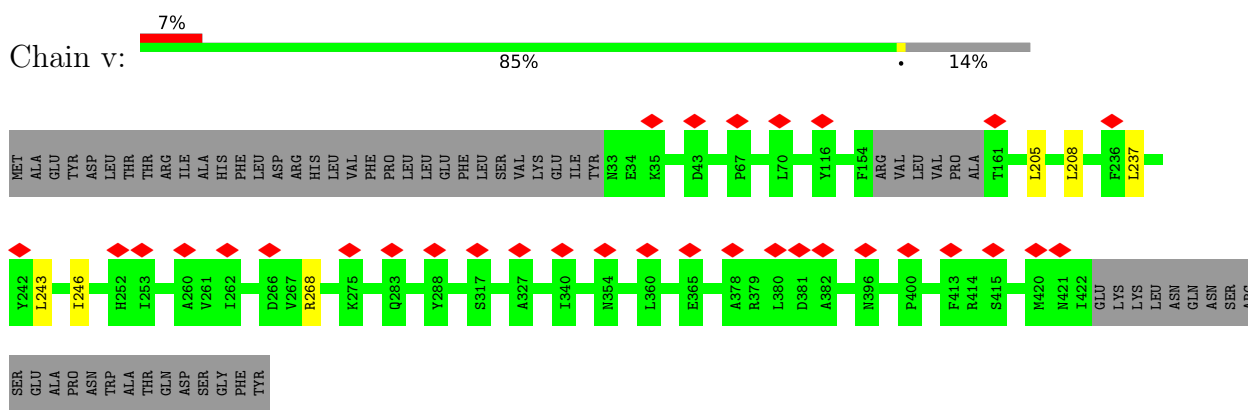


• Molecule 5: Eukaryotic translation initiation factor 3 subunit A

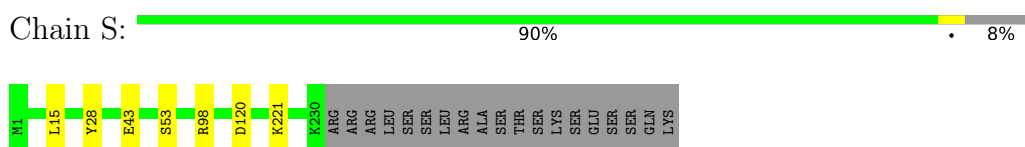


• Molecule 6: Eukaryotic translation initiation factor 3 subunit E

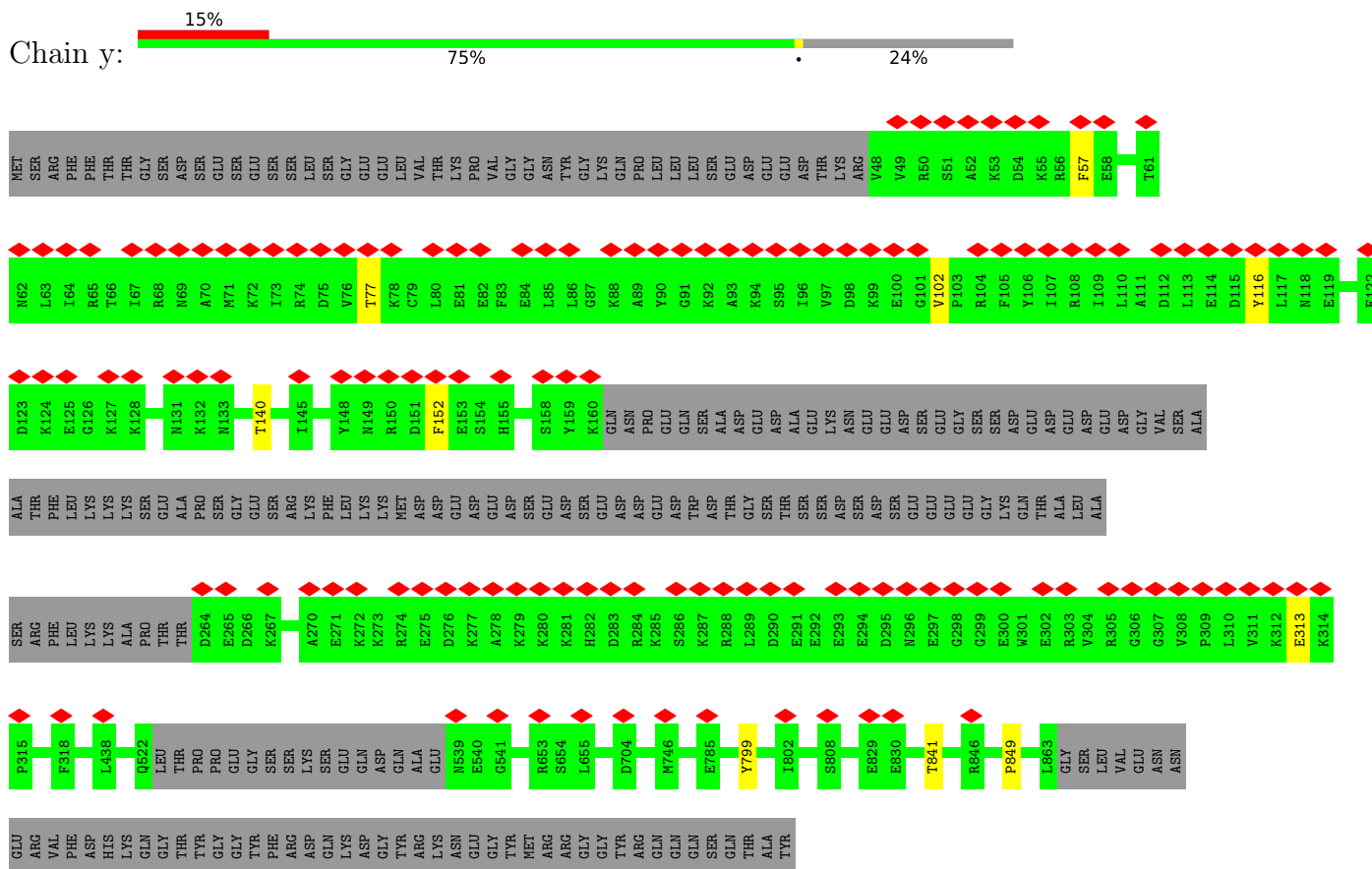




- Molecule 7: 40S ribosomal protein S6



- Molecule 8: Eukaryotic translation initiation factor 3 subunit C

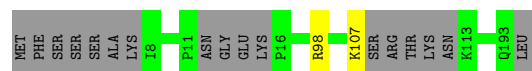


- Molecule 9: Eukaryotic translation initiation factor 3 subunit H



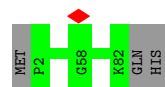
- Molecule 10: 40S ribosomal protein S7

Chain G:  90% . 9%



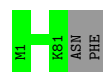
- Molecule 11: 40S ribosomal protein S27

Chain H:  96%



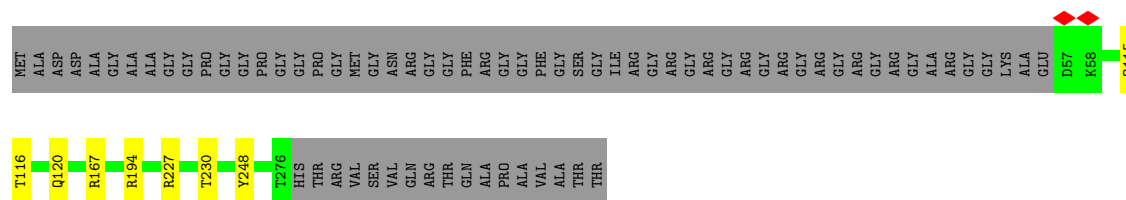
- Molecule 12: 40S ribosomal protein S21

Chain K:  98%

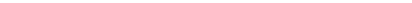


- Molecule 13: 40S ribosomal protein S2

Chain L:  72% 25%

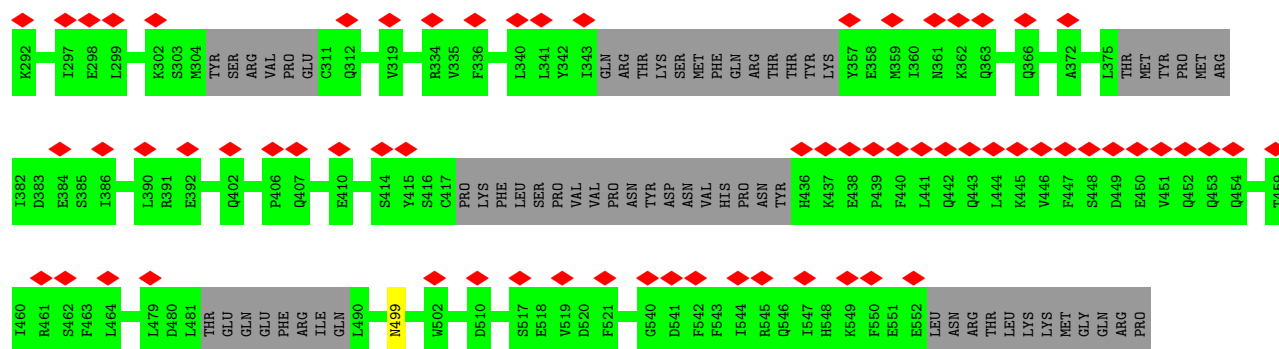


- Molecule 14: 40S ribosomal protein S3a

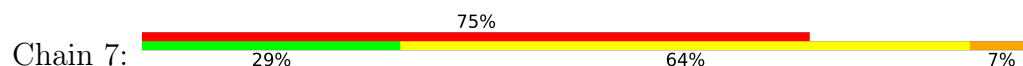
Chain 0:  80% 20%



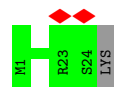




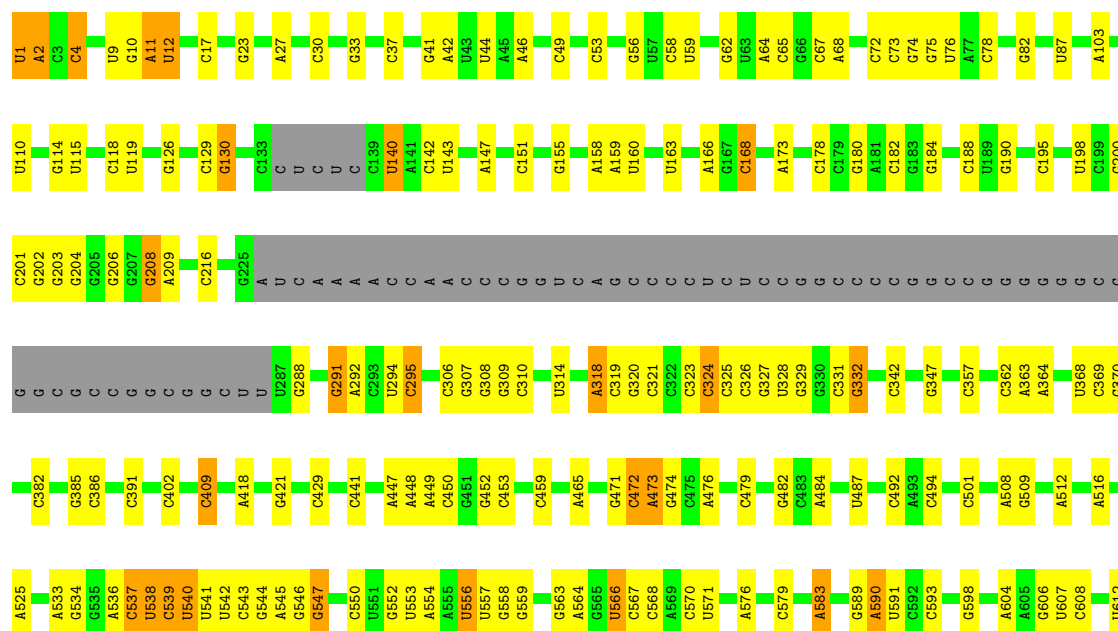
- Molecule 22: mRNA

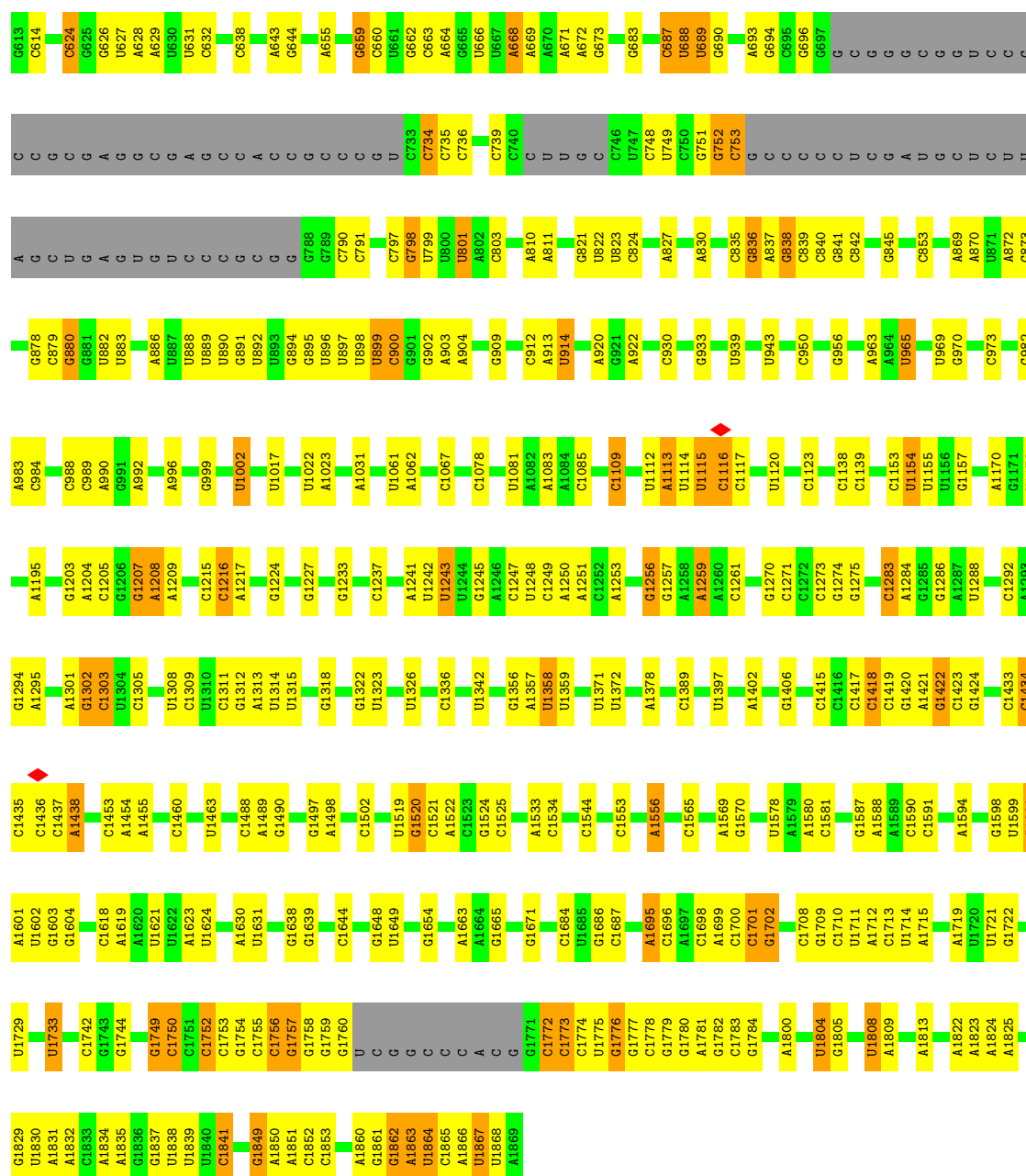


- Molecule 23: 60S ribosomal protein L41



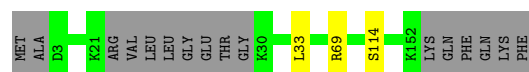
- Molecule 24: 18S rRNA





• Molecule 25: 40S ribosomal protein S11

Chain B: 88% 10%




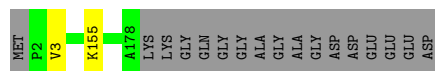
• Molecule 26: 40S ribosomal protein S4, X isoform

Chain C: 95% 10%



- Molecule 27: 40S ribosomal protein S9

Chain D:  90% 9%




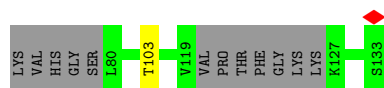
- Molecule 28: 40S ribosomal protein S23

Chain E:  97% ..




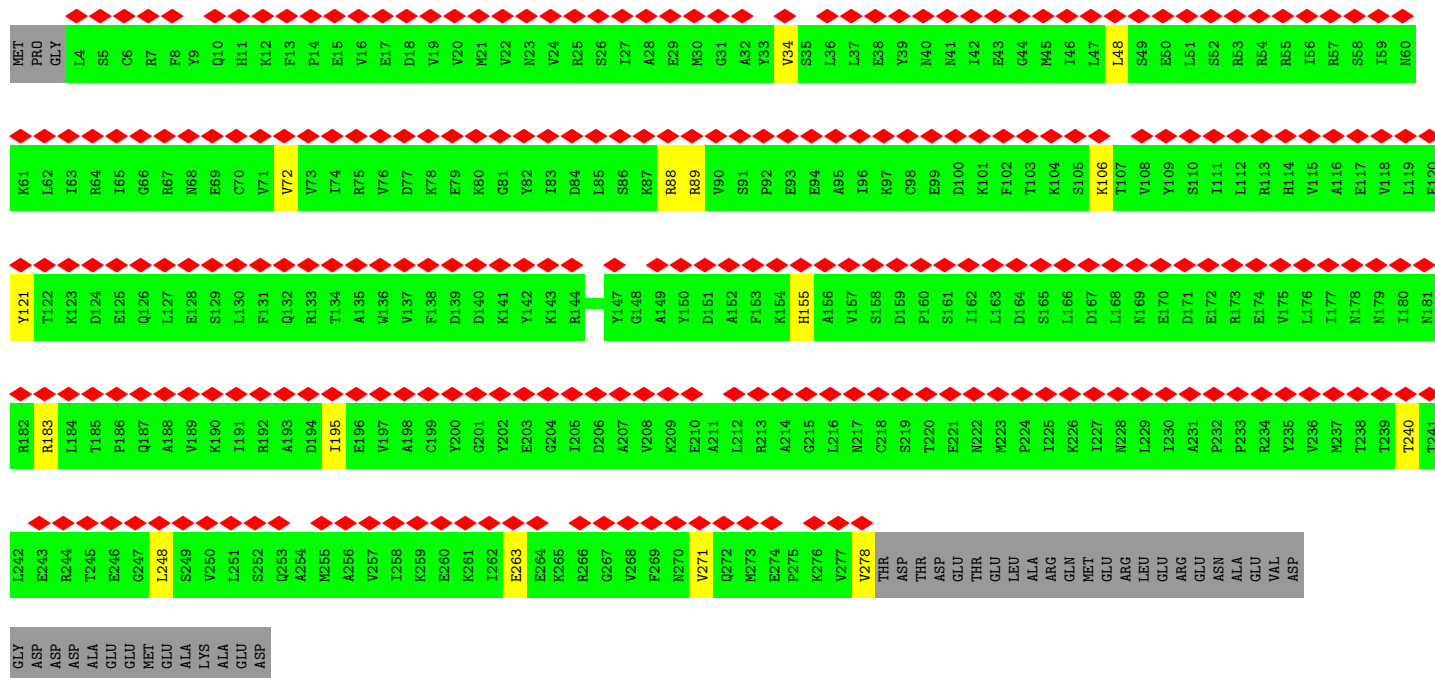
- Molecule 29: 40S ribosomal protein S30

Chain F:  78% 20%



- Molecule 30: Eukaryotic translation initiation factor 2 subunit 1

Chain r:  83% 5% 13%



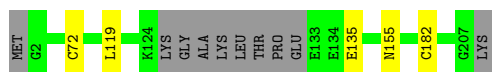
- Molecule 31: 40S ribosomal protein S15a

Chain J:  98% ..



- Molecule 32: 40S ribosomal protein S8

Chain R: 93% 5%



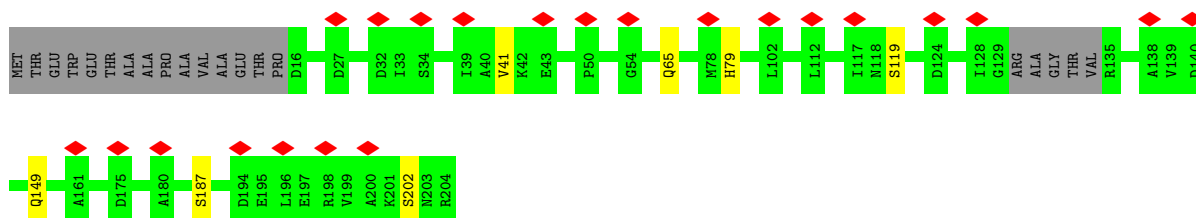
- Molecule 33: 40S ribosomal protein S24

Chain T: 91% 6%



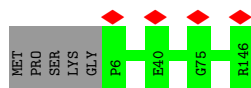
- Molecule 34: 40S ribosomal protein S5

Chain V: 11% 87% 10%



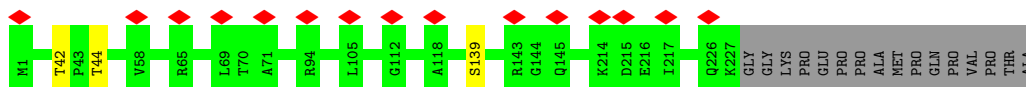
- Molecule 35: 40S ribosomal protein S16

Chain Y: 97%



- Molecule 36: 40S ribosomal protein S3

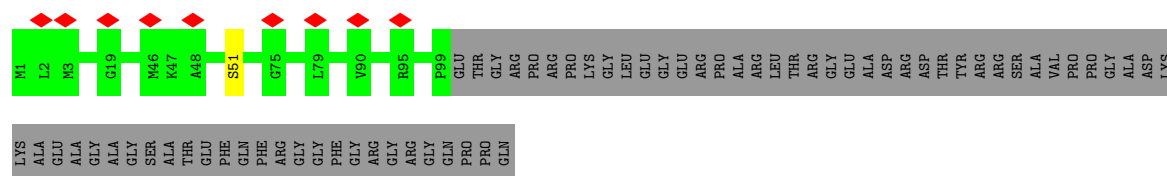
Chain Z: 6% 92% 7%



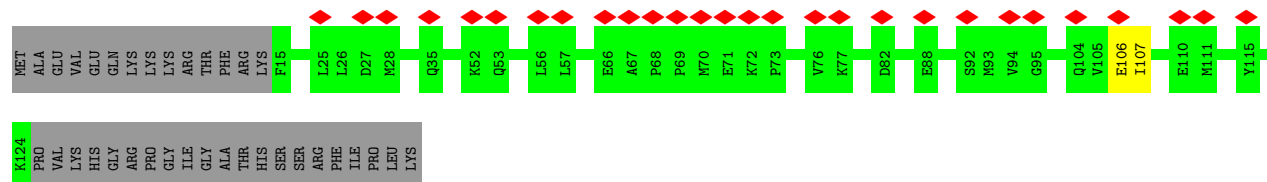
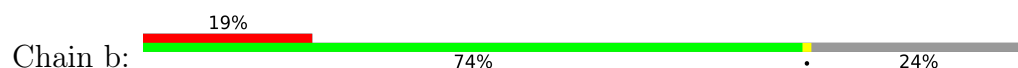
- Molecule 37: 40S ribosomal protein S10

Chain a: 5% 59% 40%

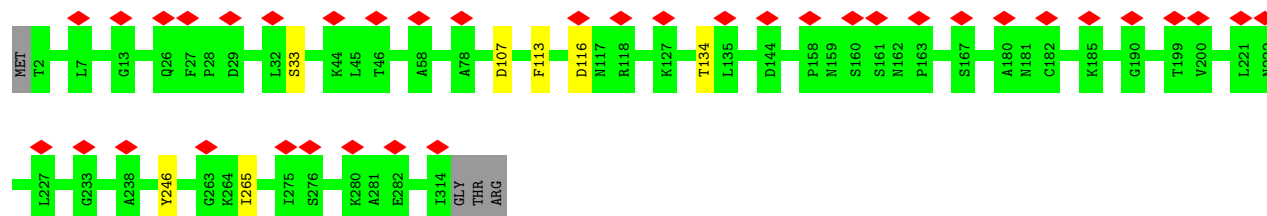




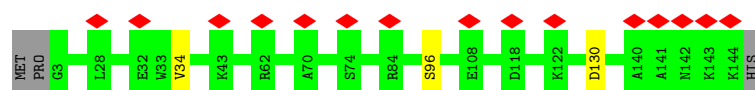
- Molecule 38: 40S ribosomal protein S15



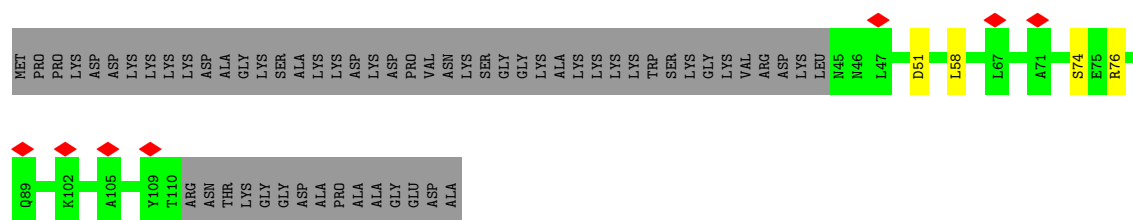
- Molecule 39: Receptor of activated protein C kinase 1



- Molecule 40: 40S ribosomal protein S19



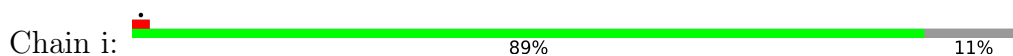
- Molecule 41: 40S ribosomal protein S25



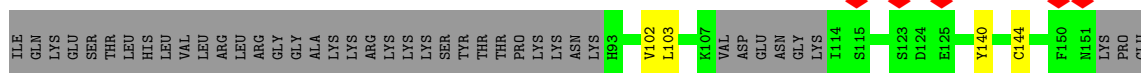
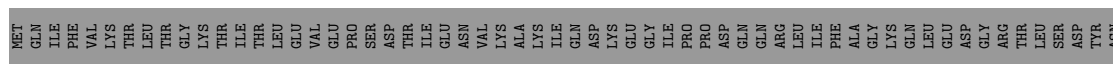
- Molecule 42: 40S ribosomal protein S18



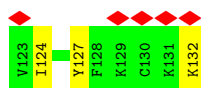
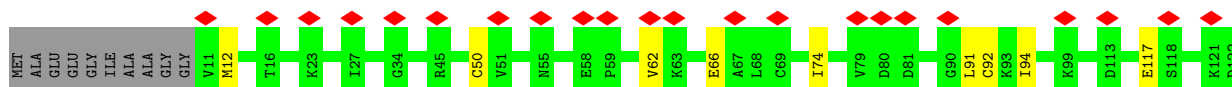
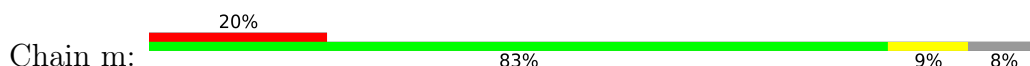
- Molecule 43: 40S ribosomal protein S29



- Molecule 44: Ubiquitin-40S ribosomal protein S27a



- Molecule 45: 40S ribosomal protein S12



- Molecule 46: 40S ribosomal protein S28



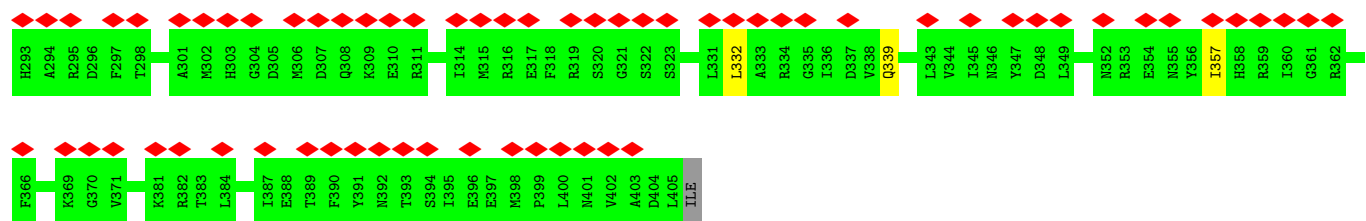
- Molecule 47: Eukaryotic translation initiation factor 3 subunit G





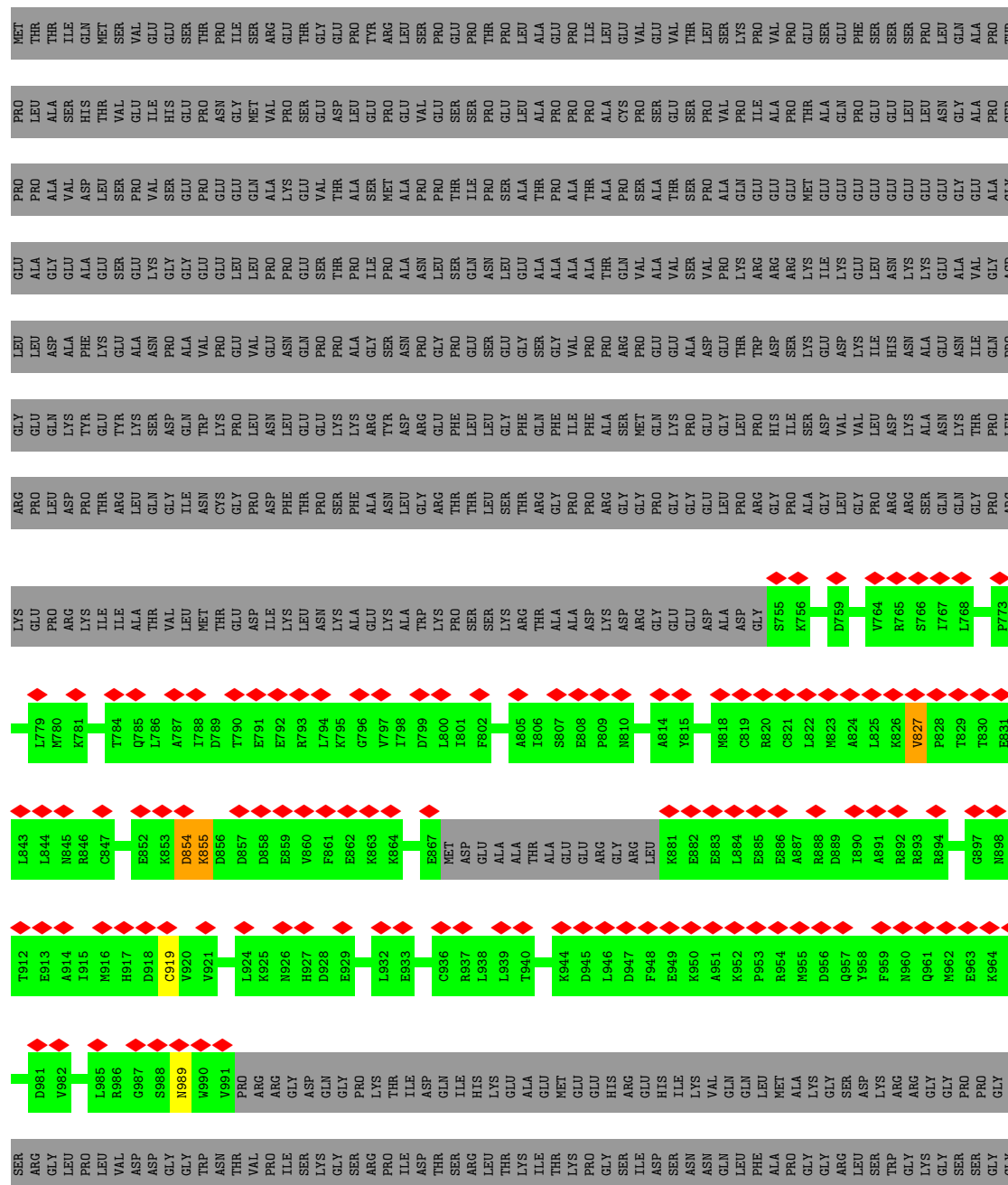






• Molecule 57: Eukaryotic translation initiation factor 4 gamma 1

Chain g: 11% 17% 83%



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	107	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.339	Depositor
Minimum map value	-0.216	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	537.0, 537.0, 537.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A2M, PSU, OMC, OMG, 5MC, JMH, MA6, UR3, 5MU, OMU, 6MZ, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	2	0.28	0/1491	0.71	0/2068
2	1	0.32	0/3279	0.69	1/4534 (0.0%)
3	6	0.29	0/1926	0.60	1/2669 (0.0%)
4	4	0.28	0/1269	0.63	0/1762
5	u	0.34	0/5475	0.63	1/7432 (0.0%)
6	v	0.32	0/2672	0.67	1/3647 (0.0%)
7	S	0.36	0/1885	0.63	0/2510
8	y	0.33	0/5557	0.60	0/7503
9	8	0.28	0/1569	0.63	0/2183
10	G	0.39	0/1451	0.68	1/1942 (0.1%)
11	H	0.41	0/644	0.67	0/864
12	K	0.43	0/623	0.61	0/833
13	L	0.49	0/1743	0.75	1/2354 (0.0%)
14	O	0.38	0/1742	0.61	0/2330
15	N	0.43	0/1670	0.62	0/2271
16	Q	0.49	0/805	0.75	2/1079 (0.2%)
17	P	0.41	0/1010	0.74	1/1353 (0.1%)
18	I	0.45	0/1232	0.67	0/1656
19	x	0.33	0/2874	0.71	2/3925 (0.1%)
20	3	0.27	0/1055	0.56	0/1469
21	5	0.27	0/1575	0.54	1/2187 (0.0%)
22	7	0.39	0/363	1.26	2/556 (0.4%)
23	9	0.32	0/231	0.55	0/294
24	A	0.79	5/40313 (0.0%)	1.28	418/62824 (0.7%)
25	B	0.44	0/1186	0.58	0/1585
26	C	0.40	0/2077	0.62	2/2796 (0.1%)
27	D	0.42	0/1502	0.58	0/2008
28	E	0.41	0/1105	0.61	0/1476
29	F	0.37	0/380	0.51	0/496
30	r	0.30	0/2247	0.63	0/3029
31	J	0.45	0/1051	0.60	0/1406
32	R	0.39	0/1654	0.61	1/2203 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	T	0.38	0/1032	0.54	0/1371
34	V	0.31	0/1481	0.66	1/1988 (0.1%)
35	Y	0.35	0/1142	0.68	0/1528
36	Z	0.34	0/1793	0.63	0/2414
37	a	0.34	0/859	0.63	0/1159
38	b	0.34	0/929	0.70	1/1241 (0.1%)
39	c	0.35	0/2493	0.71	0/3394
40	d	0.36	0/1123	0.65	0/1504
41	e	0.34	0/529	0.71	0/712
42	f	0.32	0/1194	0.69	0/1599
43	i	0.34	0/429	0.58	0/568
44	k	0.47	0/444	0.92	0/588
45	m	0.42	0/960	0.78	0/1286
46	n	0.38	0/500	0.72	0/669
47	o	0.37	0/628	0.77	0/846
48	p	0.34	0/701	0.79	0/936
49	q	0.32	0/722	0.74	1/963 (0.1%)
50	z	0.26	0/792	0.49	0/1101
51	M	0.37	0/1078	0.65	2/1447 (0.1%)
52	h	0.34	0/827	0.69	0/1110
53	s	0.33	0/1142	0.72	0/1534
54	w	0.43	0/1795	1.39	31/2798 (1.1%)
55	t	0.27	0/1745	0.61	0/2417
56	j	0.37	0/3119	0.74	0/4210
57	g	0.42	0/1869	0.80	1/2494 (0.0%)
All	All	0.54	5/122982 (0.0%)	0.95	472/175121 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	983	A	N9-C4	-8.08	1.33	1.37
24	A	1113	A	N9-C4	-5.84	1.34	1.37
24	A	1556	A	N9-C4	5.29	1.41	1.37
24	A	1438	A	N9-C4	-5.22	1.34	1.37
24	A	1520	G	N9-C4	5.07	1.42	1.38

All (472) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1701	C	N1-C2-O2	13.13	126.78	118.90
24	A	537	C	N1-C2-O2	12.91	126.64	118.90
24	A	1155	U	O5'-P-OP1	-12.82	94.16	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1756	C	N1-C2-O2	11.76	125.96	118.90
24	A	501	C	N1-C2-O2	11.75	125.95	118.90
24	A	1701	C	N3-C2-O2	-11.47	113.87	121.90
24	A	1453	C	N1-C2-O2	11.24	125.64	118.90
24	A	1578	U	N3-C2-O2	-11.10	114.43	122.20
24	A	1578	U	N1-C2-O2	10.96	130.47	122.80
24	A	501	C	C2-N1-C1'	10.95	130.85	118.80
24	A	537	C	N3-C2-O2	-10.92	114.26	121.90
24	A	996	A	O4'-C1'-N9	10.51	116.61	108.20
24	A	1273	C	O5'-P-OP2	-10.37	96.37	105.70
24	A	1756	C	C2-N1-C1'	9.97	129.77	118.80
24	A	1115	U	C2-N1-C1'	9.79	129.44	117.70
24	A	1756	C	N3-C2-O2	-9.73	115.09	121.90
24	A	1750	C	C5-C6-N1	9.65	125.83	121.00
24	A	1520	G	N3-C4-C5	-9.63	123.78	128.60
24	A	1205	C	C6-N1-C2	-9.55	116.48	120.30
24	A	1453	C	C2-N1-C1'	9.39	129.12	118.80
24	A	1752	C	C2-N1-C1'	9.25	128.97	118.80
24	A	1863	A	O5'-P-OP1	-9.24	97.38	105.70
24	A	1752	C	N1-C2-O2	9.22	124.43	118.90
24	A	552	G	C8-N9-C4	-9.16	102.74	106.40
24	A	1115	U	N1-C2-O2	9.10	129.17	122.80
24	A	1742	C	N1-C2-O2	9.06	124.33	118.90
24	A	501	C	N3-C2-O2	-8.99	115.60	121.90
24	A	76	U	C5-C6-N1	8.93	127.16	122.70
24	A	1776	G	N3-C4-C5	-8.92	124.14	128.60
24	A	402	C	C5-C6-N1	8.89	125.44	121.00
24	A	1115	U	N3-C2-O2	-8.85	116.00	122.20
24	A	1139	C	C2-N1-C1'	8.81	128.49	118.80
24	A	1520	G	N3-C4-N9	8.81	131.28	126.00
24	A	1852	C	N1-C2-O2	8.81	124.18	118.90
54	w	11	C	C5-C6-N1	8.48	125.24	121.00
24	A	1422	G	N3-C4-C5	-8.46	124.37	128.60
24	A	547	G	C4-N9-C1'	8.43	137.46	126.50
24	A	537	C	C2-N1-C1'	8.42	128.06	118.80
24	A	1701	C	C2-N1-C1'	8.41	128.06	118.80
24	A	1756	C	C6-N1-C2	-8.27	116.99	120.30
24	A	1271	C	C6-N1-C2	-8.26	117.00	120.30
24	A	1139	C	N3-C2-O2	-8.21	116.15	121.90
24	A	879	C	N1-C2-O2	8.20	123.82	118.90
22	7	20	A	O5'-P-OP2	8.20	120.54	110.70
24	A	1216	C	N1-C2-O2	8.18	123.81	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1283	C	C5-C6-N1	8.17	125.08	121.00
24	A	75	G	O4'-C1'-N9	-8.15	101.68	108.20
24	A	1302	G	O4'-C1'-N9	8.08	114.66	108.20
24	A	1123	C	N1-C2-O2	8.03	123.72	118.90
24	A	914	U	N3-C2-O2	-7.99	116.61	122.20
54	w	29	G	C5-C6-O6	-7.99	123.81	128.60
54	w	40	C	C6-N1-C2	-7.98	117.11	120.30
24	A	1804	U	C5-C6-N1	7.96	126.68	122.70
24	A	556	U	N3-C2-O2	-7.93	116.65	122.20
24	A	914	U	N1-C2-O2	7.88	128.31	122.80
24	A	1453	C	N3-C2-O2	-7.87	116.39	121.90
24	A	1750	C	C6-N1-C2	-7.86	117.16	120.30
24	A	1271	C	N1-C2-O2	7.84	123.61	118.90
24	A	1841	C	N1-C2-O2	7.83	123.60	118.90
54	w	11	C	N1-C2-O2	7.78	123.57	118.90
24	A	880	G	C2-N3-C4	7.78	115.79	111.90
24	A	1139	C	N1-C2-O2	7.76	123.56	118.90
24	A	1078	C	N1-C2-O2	7.75	123.55	118.90
24	A	402	C	C6-N1-C2	-7.73	117.21	120.30
19	x	480	ILE	CG1-CB-CG2	-7.72	94.41	111.40
24	A	1852	C	N3-C2-O2	-7.72	116.49	121.90
24	A	201	C	C6-N1-C2	-7.71	117.22	120.30
24	A	501	C	C6-N1-C1'	-7.70	111.56	120.80
24	A	1772	C	N1-C2-O2	7.69	123.51	118.90
24	A	632	C	N1-C2-O2	7.66	123.50	118.90
24	A	547	G	C6-C5-N7	-7.63	125.82	130.40
24	A	188	C	C6-N1-C2	-7.63	117.25	120.30
24	A	882	U	N1-C2-O2	7.62	128.14	122.80
54	w	29	G	C4-C5-N7	7.62	113.85	110.80
24	A	552	G	N7-C8-N9	7.55	116.87	113.10
24	A	1742	C	N3-C2-O2	-7.53	116.63	121.90
24	A	1772	C	C6-N1-C2	-7.52	117.29	120.30
24	A	1422	G	C4-N9-C1'	7.52	136.27	126.50
24	A	1752	C	N3-C2-O2	-7.51	116.64	121.90
24	A	168	C	N1-C2-O2	7.50	123.40	118.90
54	w	65	C	C6-N1-C2	-7.48	117.31	120.30
24	A	624	C	N1-C2-O2	7.48	123.39	118.90
24	A	1123	C	N3-C2-O2	-7.42	116.71	121.90
24	A	178	C	N1-C2-O2	7.41	123.35	118.90
24	A	739	C	C5-C6-N1	7.40	124.70	121.00
24	A	1808	U	N3-C2-O2	-7.35	117.05	122.20
24	A	1	U	OP1-P-O3'	7.33	121.33	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	547	G	C8-N9-C1'	-7.33	117.48	127.00
24	A	1808	U	N1-C2-O2	7.31	127.92	122.80
54	w	65	C	C5-C6-N1	7.30	124.65	121.00
24	A	1565	C	N1-C2-O2	7.29	123.28	118.90
24	A	836	G	C4-N9-C1'	7.29	135.97	126.50
24	A	1520	G	C4-N9-C1'	7.29	135.97	126.50
24	A	1422	G	N3-C4-N9	7.28	130.37	126.00
24	A	1863	A	N1-C6-N6	-7.27	114.24	118.60
24	A	1776	G	C2-N3-C4	7.26	115.53	111.90
24	A	1773	C	N1-C2-O2	7.20	123.22	118.90
24	A	1556	A	C2-N3-C4	7.20	114.20	110.60
54	w	73	C	C6-N1-C2	-7.11	117.45	120.30
24	A	836	G	N3-C4-C5	-7.10	125.05	128.60
24	A	1078	C	C2-N1-C1'	7.10	126.61	118.80
24	A	566	U	N1-C2-O2	7.09	127.76	122.80
24	A	1418	C	O4'-C1'-N1	7.07	113.86	108.20
24	A	4	C	N1-C2-O2	7.05	123.13	118.90
24	A	1709	G	O4'-C1'-N9	6.99	113.79	108.20
54	w	29	G	N1-C6-O6	6.96	124.08	119.90
24	A	130	G	N3-C4-N9	6.95	130.17	126.00
24	A	1752	C	C6-N1-C2	-6.93	117.53	120.30
24	A	1271	C	C2-N1-C1'	6.92	126.42	118.80
24	A	798	G	O5'-P-OP2	-6.92	99.47	105.70
24	A	1863	A	C2-N3-C4	6.91	114.06	110.60
24	A	1271	C	N3-C2-O2	-6.87	117.09	121.90
24	A	1	U	N1-C1'-C2'	6.85	122.90	114.00
24	A	879	C	C2-N1-C1'	6.84	126.33	118.80
24	A	1261	C	C2-N1-C1'	6.84	126.33	118.80
24	A	1600	G	P-O3'-C3'	6.84	127.91	119.70
24	A	1752	C	C6-N1-C1'	-6.83	112.60	120.80
24	A	1684	C	N1-C2-O2	6.82	122.99	118.90
24	A	118	C	N1-C2-O2	6.81	122.99	118.90
24	A	1776	G	N3-C4-N9	6.81	130.09	126.00
24	A	1772	C	N3-C2-O2	-6.81	117.13	121.90
24	A	1312	G	N3-C2-N2	-6.81	115.14	119.90
26	C	163	ASP	CB-CG-OD1	6.80	124.42	118.30
24	A	836	G	N3-C4-N9	6.80	130.08	126.00
24	A	537	C	C6-N1-C2	-6.80	117.58	120.30
24	A	501	C	C6-N1-C2	-6.78	117.59	120.30
24	A	1804	U	C6-N1-C2	-6.76	116.94	121.00
24	A	1520	G	C2-N3-C4	6.76	115.28	111.90
24	A	1261	C	C6-N1-C2	-6.75	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1078	C	C6-N1-C2	-6.75	117.60	120.30
24	A	1261	C	N1-C2-O2	6.75	122.95	118.90
24	A	1841	C	N3-C2-O2	-6.74	117.18	121.90
54	w	29	G	N9-C4-C5	-6.74	102.71	105.40
24	A	1453	C	C6-N1-C1'	-6.69	112.77	120.80
24	A	556	U	C2-N1-C1'	6.68	125.72	117.70
24	A	880	G	N3-C4-C5	-6.67	125.27	128.60
24	A	1249	C	C6-N1-C2	-6.67	117.63	120.30
24	A	1569	A	C8-N9-C4	-6.67	103.13	105.80
24	A	1591	C	C6-N1-C2	-6.65	117.64	120.30
24	A	1313	A	O4'-C1'-N9	-6.65	102.88	108.20
24	A	1702	G	N9-C1'-C2'	-6.65	104.69	112.00
24	A	1078	C	N3-C2-O2	-6.64	117.25	121.90
24	A	1207	G	C8-N9-C4	-6.64	103.74	106.40
24	A	494	C	N1-C2-O2	6.64	122.88	118.90
54	w	23	G	N7-C8-N9	6.63	116.41	113.10
24	A	130	G	N3-C4-C5	-6.62	125.29	128.60
24	A	566	U	N3-C2-O2	-6.62	117.57	122.20
24	A	1687	C	N1-C2-O2	6.61	122.87	118.90
24	A	1311	C	C5-C6-N1	6.60	124.30	121.00
24	A	632	C	N3-C2-O2	-6.59	117.29	121.90
24	A	130	G	C4-N9-C1'	6.59	135.06	126.50
24	A	983	A	C6-N1-C2	6.58	122.55	118.60
24	A	76	U	C6-N1-C2	-6.58	117.05	121.00
24	A	689	U	N3-C2-O2	-6.55	117.61	122.20
24	A	1261	C	C5-C6-N1	6.55	124.27	121.00
24	A	1569	A	N7-C8-N9	6.50	117.05	113.80
24	A	1701	C	C6-N1-C1'	-6.48	113.02	120.80
24	A	982	G	C8-N9-C4	-6.46	103.81	106.40
24	A	1216	C	N3-C2-O2	-6.46	117.38	121.90
24	A	402	C	C2-N3-C4	6.46	123.13	119.90
24	A	734	C	C6-N1-C2	-6.45	117.72	120.30
24	A	593	C	N1-C2-O2	6.44	122.76	118.90
24	A	1336	C	C6-N1-C2	-6.42	117.73	120.30
24	A	1022	U	N1-C2-O2	6.42	127.30	122.80
24	A	1115	U	C6-N1-C1'	-6.42	112.21	121.20
16	Q	15	ARG	NE-CZ-NH1	6.42	123.51	120.30
24	A	1757	G	C4-N9-C1'	6.41	134.83	126.50
24	A	1862	G	OP1-P-O3'	6.41	119.29	105.20
24	A	1776	G	C4-N9-C1'	6.40	134.82	126.50
24	A	1139	C	C6-N1-C1'	-6.39	113.13	120.80
24	A	1773	C	C6-N1-C2	-6.39	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	624	C	N3-C2-O2	-6.39	117.43	121.90
24	A	879	C	N3-C2-O2	-6.38	117.43	121.90
6	v	208	LEU	CA-CB-CG	6.38	129.97	115.30
24	A	1205	C	C5-C6-N1	6.37	124.19	121.00
24	A	1631	U	C5'-C4'-C3'	-6.37	105.81	116.00
24	A	538	U	C5-C6-N1	6.37	125.88	122.70
24	A	801	U	N3-C2-O2	-6.37	117.74	122.20
24	A	1237	C	C6-N1-C2	-6.36	117.76	120.30
24	A	1524	G	O4'-C1'-N9	6.35	113.28	108.20
24	A	1756	C	C6-N1-C1'	-6.35	113.19	120.80
54	w	33	C	N1-C2-O2	6.35	122.71	118.90
51	M	82	ASP	CB-CG-OD1	6.33	123.99	118.30
24	A	12	U	O4'-C1'-N1	6.32	113.25	108.20
24	A	1752	C	C5-C6-N1	6.30	124.15	121.00
24	A	1204	A	N9-C1'-C2'	-6.29	105.08	112.00
57	g	855	LYS	N-CA-CB	6.28	121.90	110.60
24	A	880	G	C8-N9-C4	-6.28	103.89	106.40
24	A	1157	G	N3-C4-N9	6.28	129.77	126.00
24	A	501	C	C5-C6-N1	6.27	124.14	121.00
24	A	632	C	C6-N1-C2	-6.26	117.80	120.30
24	A	547	G	C4-C5-N7	6.25	113.30	110.80
24	A	1389	C	N1-C2-O2	6.24	122.65	118.90
24	A	547	G	N7-C8-N9	6.24	116.22	113.10
24	A	1123	C	C6-N1-C2	-6.24	117.81	120.30
24	A	1259	A	C2-N3-C4	6.23	113.72	110.60
24	A	2	A	O5'-P-OP2	-6.21	100.11	105.70
24	A	1713	C	C6-N1-C2	-6.21	117.82	120.30
24	A	1359	U	O4'-C1'-N1	6.19	113.15	108.20
24	A	965	U	N3-C2-O2	-6.17	117.88	122.20
24	A	324	C	N1-C2-O2	6.16	122.59	118.90
24	A	1237	C	C5-C6-N1	6.16	124.08	121.00
24	A	1233	G	C4-C5-N7	6.16	113.26	110.80
24	A	1309	C	N1-C2-O2	6.15	122.59	118.90
24	A	49	C	N1-C2-O2	6.14	122.59	118.90
24	A	1422	G	C8-N9-C1'	-6.13	119.03	127.00
24	A	1696	C	N1-C2-O2	6.13	122.58	118.90
2	1	566	ILE	CG1-CB-CG2	-6.12	97.94	111.40
24	A	1591	C	N1-C2-O2	6.11	122.57	118.90
26	C	139	LEU	CA-CB-CG	6.11	129.36	115.30
24	A	1453	C	C5-C6-N1	6.11	124.06	121.00
24	A	1756	C	C5-C6-N1	6.11	124.05	121.00
24	A	688	U	P-O3'-C3'	6.10	127.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1422	G	C8-N9-C4	-6.10	103.96	106.40
24	A	739	C	C6-N1-C2	-6.09	117.86	120.30
24	A	1773	C	N3-C2-O2	-6.08	117.64	121.90
24	A	882	U	C2-N1-C1'	6.08	125.00	117.70
24	A	983	A	C5-N7-C8	-6.08	100.86	103.90
24	A	1773	C	C2-N1-C1'	6.07	125.47	118.80
5	u	570	ALA	N-CA-CB	6.06	118.58	110.10
54	w	22	C	C5-C6-N1	6.06	124.03	121.00
24	A	1271	C	C5-C6-N1	6.04	124.02	121.00
24	A	1207	G	C4-N9-C1'	6.04	134.36	126.50
24	A	882	U	N3-C2-O2	-6.04	117.97	122.20
24	A	538	U	C6-N1-C2	-6.04	117.38	121.00
24	A	836	G	C8-N9-C1'	-6.02	119.17	127.00
54	w	60	C	N1-C2-O2	6.01	122.50	118.90
54	w	11	C	C6-N1-C2	-6.01	117.90	120.30
54	w	29	G	C6-C5-N7	-6.01	126.80	130.40
24	A	53	C	C6-N1-C2	-5.99	117.90	120.30
24	A	178	C	N3-C2-O2	-5.99	117.71	121.90
24	A	1578	U	C2-N1-C1'	5.99	124.89	117.70
24	A	1710	C	C5-C6-N1	5.98	123.99	121.00
24	A	638	C	N1-C2-O2	5.97	122.48	118.90
24	A	1022	U	N3-C2-O2	-5.95	118.03	122.20
49	q	81	LEU	CA-CB-CG	5.95	128.99	115.30
24	A	659	G	C4-N9-C1'	5.95	134.23	126.50
24	A	216	C	C6-N1-C2	-5.93	117.93	120.30
24	A	168	C	N3-C2-O2	-5.92	117.75	121.90
24	A	1022	U	C2-N1-C1'	5.92	124.81	117.70
54	w	40	C	C5-C6-N1	5.91	123.95	121.00
24	A	1109	C	C6-N1-C2	-5.89	117.94	120.30
24	A	1067	C	N1-C2-O2	5.89	122.44	118.90
24	A	1729	U	N1-C2-O2	5.88	126.91	122.80
24	A	663	C	N1-C2-O2	5.87	122.42	118.90
24	A	965	U	N1-C2-O2	5.87	126.91	122.80
24	A	556	U	C6-N1-C2	-5.86	117.48	121.00
24	A	1113	A	N3-C4-N9	-5.86	122.71	127.40
54	w	11	C	C2-N1-C1'	5.85	125.23	118.80
24	A	1172	U	N1-C2-O2	5.84	126.89	122.80
24	A	1305	C	C5-C6-N1	5.82	123.91	121.00
24	A	899	U	O4'-C1'-N1	5.82	112.85	108.20
24	A	318	A	C2-N3-C4	5.81	113.50	110.60
24	A	1415	C	C6-N1-C2	-5.81	117.98	120.30
24	A	1520	G	C8-N9-C1'	-5.79	119.47	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1710	C	C6-N1-C2	-5.79	117.98	120.30
24	A	689	U	N1-C2-O2	5.78	126.84	122.80
24	A	752	G	C4-N9-C1'	5.78	134.01	126.50
24	A	30	C	C5-C6-N1	5.77	123.89	121.00
24	A	409	C	N1-C2-O2	5.77	122.36	118.90
24	A	638	C	N3-C2-O2	-5.77	117.86	121.90
24	A	1701	C	C6-N1-C2	-5.76	118.00	120.30
24	A	324	C	C2-N1-C1'	5.75	125.12	118.80
24	A	1749	G	O4'-C1'-N9	5.73	112.78	108.20
24	A	291	G	P-O3'-C3'	5.73	126.58	119.70
24	A	996	A	C4-N9-C1'	5.71	136.58	126.30
24	A	4	C	N3-C2-O2	-5.71	117.90	121.90
24	A	883	U	C6-N1-C2	-5.71	117.58	121.00
24	A	1116	C	N1-C2-O2	5.71	122.32	118.90
54	w	55	C	C6-N1-C2	-5.71	118.02	120.30
24	A	409	C	N3-C2-O2	-5.70	117.91	121.90
24	A	201	C	C5-C6-N1	5.69	123.84	121.00
24	A	1292	C	C6-N1-C2	-5.69	118.03	120.30
24	A	1249	C	C5-C6-N1	5.68	123.84	121.00
24	A	53	C	N1-C2-O2	5.68	122.31	118.90
51	M	73	LEU	CA-CB-CG	5.66	128.32	115.30
24	A	87	U	N3-C2-O2	-5.66	118.24	122.20
24	A	1556	A	N3-C4-C5	-5.66	122.84	126.80
24	A	4	C	C6-N1-C2	-5.66	118.04	120.30
24	A	566	U	C2-N1-C1'	5.64	124.47	117.70
54	w	55	C	N1-C2-O2	5.64	122.28	118.90
24	A	902	G	C4-N9-C1'	-5.63	119.19	126.50
24	A	1684	C	N3-C2-O2	-5.63	117.96	121.90
24	A	567	C	C6-N1-C2	-5.62	118.05	120.30
24	A	540	U	O4'-C1'-N1	5.62	112.70	108.20
24	A	1733	U	N1-C2-O2	5.61	126.73	122.80
24	A	1638	G	C4-N9-C1'	-5.61	119.21	126.50
24	A	1776	G	C8-N9-C4	-5.60	104.16	106.40
24	A	459	C	C6-N1-C2	-5.60	118.06	120.30
24	A	973	C	N1-C2-O2	5.59	122.26	118.90
54	w	73	C	N1-C2-O2	5.59	122.25	118.90
24	A	310	C	N1-C2-O2	5.59	122.25	118.90
24	A	1314	U	C2-N1-C1'	5.58	124.40	117.70
24	A	1256	G	N3-C4-N9	5.57	129.34	126.00
24	A	1556	A	N3-C4-N9	5.56	131.85	127.40
54	w	74	C	C6-N1-C2	-5.56	118.07	120.30
24	A	1841	C	C6-N1-C2	-5.56	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	151	C	N1-C2-O2	5.56	122.23	118.90
24	A	1695	A	O4'-C1'-N9	-5.56	103.75	108.20
24	A	208	G	C4-N9-C1'	5.55	133.72	126.50
24	A	734	C	C5-C6-N1	5.55	123.78	121.00
24	A	331	C	C6-N1-C2	-5.54	118.08	120.30
24	A	30	C	C6-N1-C2	-5.54	118.08	120.30
24	A	1590	C	C5-C6-N1	5.54	123.77	121.00
24	A	1604	G	C4-N9-C1'	5.54	133.70	126.50
24	A	1241	A	N9-C1'-C2'	-5.53	105.92	112.00
24	A	1804	U	N3-C2-O2	-5.52	118.34	122.20
24	A	983	A	N3-C4-N9	-5.51	122.99	127.40
24	A	1323	U	C5-C6-N1	5.51	125.45	122.70
24	A	1772	C	C5-C6-N1	5.50	123.75	121.00
24	A	1453	C	C6-N1-C2	-5.50	118.10	120.30
24	A	441	C	N1-C2-O2	5.48	122.19	118.90
24	A	1804	U	N1-C2-O2	5.48	126.64	122.80
24	A	130	G	C8-N9-C1'	-5.48	119.88	127.00
24	A	659	G	C8-N9-C1'	-5.48	119.88	127.00
24	A	1849	G	N9-C1'-C2'	-5.48	105.97	112.00
24	A	1591	C	N3-C2-O2	-5.47	118.07	121.90
24	A	1698	C	C6-N1-C2	5.47	122.49	120.30
54	w	22	C	C6-N1-C2	-5.47	118.11	120.30
24	A	835	C	N1-C2-O2	5.47	122.18	118.90
24	A	900	C	C6-N1-C2	-5.47	118.11	120.30
24	A	956	G	OP1-P-O3'	5.47	117.24	105.20
24	A	1733	U	N3-C2-O2	-5.47	118.37	122.20
24	A	1002	U	N1-C2-O2	5.47	126.63	122.80
24	A	1154	U	O4'-C1'-N1	5.47	112.57	108.20
24	A	140	U	N3-C2-O2	-5.46	118.38	122.20
24	A	209	A	C4-C5-N7	5.45	113.43	110.70
24	A	1315	U	N1-C2-O2	5.45	126.62	122.80
24	A	1565	C	C2-N1-C1'	5.45	124.79	118.80
24	A	880	G	N1-C6-O6	-5.45	116.63	119.90
24	A	459	C	N1-C2-O2	5.44	122.17	118.90
24	A	1708	C	N1-C2-O2	5.44	122.17	118.90
54	w	23	G	C6-C5-N7	-5.44	127.14	130.40
24	A	853	C	C6-N1-C2	-5.43	118.13	120.30
24	A	1590	C	C6-N1-C2	-5.43	118.13	120.30
24	A	1434	C	P-O3'-C3'	5.42	126.21	119.70
22	7	17	A	P-O3'-C3'	5.42	126.21	119.70
24	A	579	C	N1-C2-O2	5.42	122.15	118.90
24	A	1649	U	N1-C2-O2	5.42	126.59	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1696	C	N3-C2-O2	-5.42	118.11	121.90
24	A	201	C	N1-C2-O2	5.41	122.15	118.90
24	A	1631	U	O5'-P-OP1	-5.41	100.83	105.70
24	A	1772	C	C2-N1-C1'	5.41	124.75	118.80
24	A	996	A	C8-N9-C1'	-5.40	117.99	127.70
24	A	216	C	N3-C2-O2	-5.40	118.12	121.90
24	A	453	C	N1-C2-O2	5.39	122.14	118.90
24	A	1207	G	C8-N9-C1'	-5.39	120.00	127.00
54	w	73	C	C5-C6-N1	5.39	123.69	121.00
17	P	138	ASP	CB-CG-OD2	-5.39	113.45	118.30
24	A	537	C	C6-N1-C1'	-5.38	114.35	120.80
13	L	194	ARG	CG-CD-NE	5.37	123.07	111.80
24	A	1233	G	C5-N7-C8	-5.36	101.62	104.30
24	A	1358	U	N1-C2-O2	5.35	126.55	122.80
24	A	1808	U	C2-N1-C1'	5.35	124.12	117.70
21	5	499	ASN	C-N-CA	5.35	135.06	121.70
24	A	853	C	N1-C2-O2	5.34	122.11	118.90
24	A	1261	C	N3-C2-O2	-5.34	118.16	121.90
24	A	1078	C	C5-C6-N1	5.33	123.67	121.00
24	A	1233	G	C6-C5-N7	-5.33	127.20	130.40
38	b	107	ILE	C-N-CA	5.33	135.02	121.70
24	A	11	A	N9-C1'-C2'	-5.33	106.14	112.00
24	A	801	U	N1-C2-O2	5.32	126.53	122.80
24	A	547	G	C8-N9-C4	-5.32	104.27	106.40
24	A	593	C	N3-C2-O2	-5.32	118.18	121.90
24	A	902	G	N3-C4-C5	5.32	131.26	128.60
24	A	1203	G	N9-C1'-C2'	-5.31	106.16	112.00
24	A	4	C	C2-N1-C1'	5.31	124.64	118.80
24	A	324	C	N3-C2-O2	-5.31	118.18	121.90
54	w	10	G	C4-N9-C1'	5.31	133.41	126.50
24	A	1358	U	N1-C1'-C2'	-5.31	106.16	112.00
24	A	1687	C	N3-C2-O2	-5.31	118.18	121.90
54	w	55	C	N3-C2-O2	-5.31	118.18	121.90
24	A	1460	C	C6-N1-C2	-5.30	118.18	120.30
24	A	37	C	N3-C2-O2	-5.30	118.19	121.90
24	A	429	C	N1-C2-O2	5.29	122.08	118.90
24	A	879	C	C6-N1-C2	-5.29	118.18	120.30
24	A	118	C	N3-C2-O2	-5.29	118.20	121.90
24	A	1565	C	N3-C2-O2	-5.29	118.20	121.90
24	A	539	C	C6-N1-C2	-5.28	118.19	120.30
24	A	556	U	N1-C2-O2	5.28	126.50	122.80
24	A	696	G	C4-C5-N7	5.28	112.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1591	C	C5-C6-N1	5.27	123.64	121.00
24	A	1227	G	N3-C4-C5	-5.27	125.97	128.60
24	A	632	C	C5-C6-N1	5.26	123.63	121.00
24	A	1113	A	N3-C4-C5	5.25	130.48	126.80
24	A	735	C	N1-C2-O2	5.25	122.05	118.90
24	A	838	G	C4-N9-C1'	-5.24	119.68	126.50
24	A	332	G	O4'-C1'-N9	5.24	112.39	108.20
24	A	459	C	N3-C2-O2	-5.24	118.23	121.90
24	A	984	C	C6-N1-C2	-5.24	118.20	120.30
24	A	1256	G	C8-N9-C1'	-5.23	120.20	127.00
24	A	1256	G	C4-N9-C1'	5.23	133.30	126.50
24	A	188	C	C5-C6-N1	5.23	123.61	121.00
24	A	803	C	N1-C2-O2	5.23	122.04	118.90
24	A	571	U	N3-C2-O2	-5.22	118.54	122.20
24	A	1701	C	C3'-C2'-C1'	5.22	105.67	101.50
24	A	342	C	N1-C2-O2	5.21	122.03	118.90
24	A	1283	C	C5-C4-N4	-5.21	116.56	120.20
24	A	547	G	N9-C1'-C2'	-5.21	106.27	112.00
24	A	1630	A	O4'-C1'-N9	5.20	112.36	108.20
24	A	1157	G	N3-C4-C5	-5.20	126.00	128.60
24	A	1109	C	N1-C2-O2	5.20	122.02	118.90
24	A	1729	U	N3-C2-O2	-5.19	118.57	122.20
24	A	1864	U	N1-C2-O2	5.19	126.43	122.80
24	A	902	G	N3-C4-N9	-5.19	122.89	126.00
54	w	31	C	C6-N1-C2	-5.19	118.22	120.30
24	A	1311	C	C6-N1-C2	-5.18	118.23	120.30
24	A	570	C	N3-C2-O2	-5.18	118.27	121.90
24	A	1311	C	C5'-C4'-C3'	-5.18	107.72	116.00
24	A	1702	G	C3'-C2'-C1'	5.18	105.64	101.50
24	A	201	C	N3-C2-O2	-5.17	118.28	121.90
24	A	1247	C	N1-C2-O2	5.17	122.00	118.90
24	A	151	C	N3-C2-O2	-5.17	118.28	121.90
24	A	472	C	OP2-P-O3'	5.17	116.57	105.20
24	A	331	C	N3-C2-O2	-5.17	118.28	121.90
24	A	842	C	N1-C2-O2	5.16	122.00	118.90
34	V	65	GLN	C-N-CA	5.16	134.59	121.70
10	G	107	LYS	N-CA-C	-5.15	97.09	111.00
24	A	209	A	C5-N7-C8	-5.15	101.33	103.90
24	A	37	C	C6-N1-C2	-5.14	118.24	120.30
24	A	1581	C	C6-N1-C2	5.14	122.36	120.30
24	A	939	U	N1-C2-O2	5.14	126.40	122.80
24	A	216	C	N1-C2-O2	5.13	121.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	479	C	N1-C2-O2	5.13	121.98	118.90
24	A	1422	G	C2-N3-C4	5.13	114.47	111.90
24	A	1460	C	C5-C6-N1	5.13	123.57	121.00
24	A	583	A	N9-C1'-C2'	-5.13	106.36	112.00
24	A	1227	G	N3-C4-N9	5.13	129.08	126.00
24	A	1867	U	O4'-C1'-N1	5.13	112.30	108.20
54	w	31	C	N1-C2-O2	5.12	121.97	118.90
24	A	983	A	O4'-C1'-N9	-5.12	104.11	108.20
24	A	824	C	N1-C2-O2	5.11	121.97	118.90
24	A	357	C	N1-C2-O2	5.11	121.97	118.90
24	A	659	G	C6-C5-N7	-5.11	127.34	130.40
24	A	1714	U	C5-C6-N1	5.11	125.25	122.70
24	A	391	C	N1-C2-O2	5.11	121.96	118.90
32	R	119	LEU	CA-CB-CG	5.10	127.03	115.30
24	A	1139	C	C6-N1-C2	-5.09	118.26	120.30
24	A	53	C	N3-C2-O2	-5.09	118.34	121.90
24	A	357	C	N3-C2-O2	-5.09	118.34	121.90
24	A	1303	C	OP1-P-O3'	5.09	116.39	105.20
24	A	1270	G	N3-C2-N2	-5.08	116.34	119.90
24	A	473	A	OP2-P-O3'	5.08	116.38	105.20
24	A	1002	U	N3-C2-O2	-5.08	118.64	122.20
24	A	295	C	N1-C2-O2	5.08	121.95	118.90
3	6	325	ILE	CG1-CB-CG2	-5.07	100.24	111.40
24	A	687	C	P-O3'-C3'	5.07	125.78	119.70
24	A	1315	U	N3-C2-O2	-5.07	118.65	122.20
24	A	590	A	C2-N3-C4	5.06	113.13	110.60
24	A	1502	C	C6-N1-C2	-5.06	118.28	120.30
54	w	73	C	N3-C2-O2	-5.05	118.36	121.90
16	Q	15	ARG	CG-CD-NE	5.05	122.40	111.80
24	A	663	C	N3-C2-O2	-5.05	118.37	121.90
24	A	1757	G	N3-C4-C5	-5.04	126.08	128.60
24	A	1600	G	O4'-C1'-N9	5.04	112.23	108.20
24	A	666	U	N1-C2-O2	5.03	126.32	122.80
19	x	211	THR	C-N-CA	5.03	134.28	121.70
24	A	1208	A	C2-N3-C4	5.03	113.11	110.60
54	w	38	C	C6-N1-C2	-5.02	118.29	120.30
24	A	140	U	N1-C2-O2	5.02	126.31	122.80
24	A	753	C	N1-C2-O2	5.02	121.91	118.90
24	A	402	C	N1-C2-O2	5.02	121.91	118.90
24	A	1283	C	C6-N1-C2	-5.02	118.29	120.30
24	A	53	C	C5-C6-N1	5.01	123.51	121.00
24	A	494	C	N3-C2-O2	-5.01	118.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1204	A	C3'-C2'-C1'	5.01	105.51	101.50
24	A	1757	G	C8-N9-C1'	-5.01	120.49	127.00
24	A	1776	G	C8-N9-C1'	-5.01	120.49	127.00
24	A	195	C	C6-N1-C2	-5.01	118.30	120.30
24	A	666	U	N3-C2-O2	-5.01	118.70	122.20
24	A	1525	C	C5-C6-N1	5.00	123.50	121.00
24	A	539	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	300/325 (92%)	277 (92%)	23 (8%)	0	100	100
2	1	584/814 (72%)	541 (93%)	36 (6%)	7 (1%)	13	48
3	6	348/374 (93%)	296 (85%)	52 (15%)	0	100	100
4	4	251/357 (70%)	217 (86%)	31 (12%)	3 (1%)	13	48
5	u	705/1382 (51%)	656 (93%)	47 (7%)	2 (0%)	41	74
6	v	380/445 (85%)	331 (87%)	49 (13%)	0	100	100
7	S	228/249 (92%)	222 (97%)	6 (3%)	0	100	100
8	y	691/913 (76%)	645 (93%)	44 (6%)	2 (0%)	41	74
9	8	313/352 (89%)	264 (84%)	48 (15%)	1 (0%)	41	74
10	G	171/194 (88%)	158 (92%)	13 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	H	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
12	K	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
13	L	218/293 (74%)	205 (94%)	13 (6%)	0	100	100
14	O	209/264 (79%)	193 (92%)	16 (8%)	0	100	100
15	N	205/295 (70%)	189 (92%)	16 (8%)	0	100	100
16	Q	97/115 (84%)	92 (95%)	5 (5%)	0	100	100
17	P	131/151 (87%)	116 (88%)	15 (12%)	0	100	100
18	I	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
19	x	415/548 (76%)	373 (90%)	42 (10%)	0	100	100
20	3	209/218 (96%)	203 (97%)	5 (2%)	1 (0%)	29	66
21	5	307/564 (54%)	299 (97%)	8 (3%)	0	100	100
23	9	22/25 (88%)	22 (100%)	0	0	100	100
25	B	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
26	C	254/263 (97%)	250 (98%)	4 (2%)	0	100	100
27	D	175/194 (90%)	174 (99%)	1 (1%)	0	100	100
28	E	138/143 (96%)	133 (96%)	5 (4%)	0	100	100
29	F	43/59 (73%)	42 (98%)	1 (2%)	0	100	100
30	r	273/315 (87%)	250 (92%)	23 (8%)	0	100	100
31	J	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
32	R	194/208 (93%)	186 (96%)	8 (4%)	0	100	100
33	T	123/133 (92%)	122 (99%)	1 (1%)	0	100	100
34	V	180/204 (88%)	170 (94%)	10 (6%)	0	100	100
35	Y	139/146 (95%)	131 (94%)	8 (6%)	0	100	100
36	Z	225/243 (93%)	218 (97%)	7 (3%)	0	100	100
37	a	97/165 (59%)	93 (96%)	4 (4%)	0	100	100
38	b	108/145 (74%)	105 (97%)	3 (3%)	0	100	100
39	c	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
40	d	140/145 (97%)	133 (95%)	7 (5%)	0	100	100
41	e	64/125 (51%)	59 (92%)	5 (8%)	0	100	100
42	f	140/152 (92%)	136 (97%)	4 (3%)	0	100	100
43	i	48/56 (86%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	k	49/156 (31%)	43 (88%)	6 (12%)	0	100	100
45	m	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
46	n	61/69 (88%)	58 (95%)	3 (5%)	0	100	100
47	o	75/320 (23%)	72 (96%)	3 (4%)	0	100	100
48	p	83/113 (74%)	80 (96%)	3 (4%)	0	100	100
49	q	86/144 (60%)	76 (88%)	10 (12%)	0	100	100
50	z	154/258 (60%)	140 (91%)	14 (9%)	0	100	100
51	M	129/135 (96%)	121 (94%)	7 (5%)	1 (1%)	19	56
52	h	101/119 (85%)	94 (93%)	7 (7%)	0	100	100
53	s	136/333 (41%)	119 (88%)	17 (12%)	0	100	100
55	t	346/472 (73%)	334 (96%)	8 (2%)	4 (1%)	13	48
56	j	382/406 (94%)	365 (96%)	15 (4%)	2 (0%)	29	66
57	g	220/1310 (17%)	207 (94%)	9 (4%)	4 (2%)	8	41
All	All	10949/15464 (71%)	10216 (93%)	706 (6%)	27 (0%)	50	78

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	282	PRO
4	4	264	GLY
9	8	154	PRO
55	t	167	GLN
55	t	168	PRO
55	t	248	ARG
57	g	827	VAL
2	1	339	TYR
51	M	83	ASN
56	j	339	GLN
57	g	855	LYS
57	g	989	ASN
2	1	427	PRO
2	1	499	PRO
4	4	263	ILE
5	u	340	ARG
8	y	849	PRO
55	t	247	PRO
4	4	320	PRO

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Mol	Chain	Res	Type
8	y	313	GLU
57	g	854	ASP
2	1	286	PRO
2	1	401	PRO
5	u	330	PRO
20	3	206	ASP
2	1	633	GLY
56	j	173	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	
2	1	97/702 (14%)	97 (100%)	0	100	100
3	6	49/335 (15%)	49 (100%)	0	100	100
5	u	528/1259 (42%)	520 (98%)	8 (2%)	65	81
6	v	206/406 (51%)	201 (98%)	5 (2%)	49	71
7	S	200/218 (92%)	193 (96%)	7 (4%)	36	63
8	y	564/811 (70%)	556 (99%)	8 (1%)	67	82
10	G	159/174 (91%)	158 (99%)	1 (1%)	86	93
11	H	73/76 (96%)	73 (100%)	0	100	100
12	K	65/67 (97%)	65 (100%)	0	100	100
13	L	186/225 (83%)	179 (96%)	7 (4%)	33	61
14	O	192/231 (83%)	191 (100%)	1 (0%)	88	94
15	N	173/243 (71%)	173 (100%)	0	100	100
16	Q	86/98 (88%)	82 (95%)	4 (5%)	26	56
17	P	104/119 (87%)	102 (98%)	2 (2%)	57	76
18	I	130/131 (99%)	129 (99%)	1 (1%)	81	89
19	x	206/494 (42%)	196 (95%)	10 (5%)	25	56
23	9	23/24 (96%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	B	129/142 (91%)	126 (98%)	3 (2%)	50	71
26	C	220/225 (98%)	215 (98%)	5 (2%)	50	71
27	D	158/168 (94%)	156 (99%)	2 (1%)	69	83
28	E	112/115 (97%)	111 (99%)	1 (1%)	78	88
29	F	38/48 (79%)	37 (97%)	1 (3%)	46	69
30	r	247/280 (88%)	232 (94%)	15 (6%)	18	50
31	J	112/113 (99%)	110 (98%)	2 (2%)	59	77
32	R	172/180 (96%)	168 (98%)	4 (2%)	50	71
33	T	107/115 (93%)	103 (96%)	4 (4%)	34	61
34	V	156/170 (92%)	150 (96%)	6 (4%)	33	61
35	Y	117/121 (97%)	117 (100%)	0	100	100
36	Z	190/202 (94%)	187 (98%)	3 (2%)	62	80
37	a	90/136 (66%)	89 (99%)	1 (1%)	73	85
38	b	100/130 (77%)	99 (99%)	1 (1%)	76	86
39	c	272/275 (99%)	265 (97%)	7 (3%)	46	69
40	d	112/115 (97%)	109 (97%)	3 (3%)	44	68
41	e	58/103 (56%)	54 (93%)	4 (7%)	15	46
42	f	123/132 (93%)	121 (98%)	2 (2%)	62	80
43	i	44/49 (90%)	44 (100%)	0	100	100
44	k	47/140 (34%)	43 (92%)	4 (8%)	10	40
45	m	104/108 (96%)	92 (88%)	12 (12%)	5	27
46	n	56/62 (90%)	55 (98%)	1 (2%)	59	77
47	o	64/277 (23%)	61 (95%)	3 (5%)	26	56
48	p	74/96 (77%)	68 (92%)	6 (8%)	11	41
49	q	75/123 (61%)	65 (87%)	10 (13%)	4	22
51	M	119/122 (98%)	113 (95%)	6 (5%)	24	55
52	h	94/107 (88%)	94 (100%)	0	100	100
53	s	128/304 (42%)	116 (91%)	12 (9%)	8	35
56	j	339/357 (95%)	334 (98%)	5 (2%)	65	81
57	g	210/1121 (19%)	207 (99%)	3 (1%)	67	82
All	All	6908/11249 (61%)	6728 (97%)	180 (3%)	49	69

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	u	62	ARG
5	u	109	GLN
5	u	337	ASP
5	u	340	ARG
5	u	448	GLN
5	u	459	VAL
5	u	562	ARG
5	u	572	ARG
6	v	205	LEU
6	v	237	LEU
6	v	243	LEU
6	v	246	ILE
6	v	268	ARG
7	S	15	LEU
7	S	28	TYR
7	S	43	GLU
7	S	53	SER
7	S	98	ARG
7	S	120	ASP
7	S	221	LYS
8	y	57	PHE
8	y	77	THR
8	y	102	VAL
8	y	116	TYR
8	y	140	THR
8	y	152	PHE
8	y	799	TYR
8	y	841	THR
10	G	98	ARG
13	L	115	GLN
13	L	116	THR
13	L	120	GLN
13	L	167	ARG
13	L	227	ARG
13	L	230	THR
13	L	248	TYR
14	O	77	ASP
16	Q	12	LYS
16	Q	15	ARG
16	Q	86	ASN
16	Q	87	ARG
17	P	52	THR

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Mol	Chain	Res	Type
17	P	67	ASP
18	I	20	ARG
19	x	54	ARG
19	x	57	ASN
19	x	87	ARG
19	x	288	LEU
19	x	368	ASP
19	x	385	ASN
19	x	400	ASP
19	x	466	LEU
19	x	470	GLN
19	x	471	PHE
25	B	33	LEU
25	B	69	ARG
25	B	114	SER
26	C	12	VAL
26	C	54	TYR
26	C	69	PHE
26	C	139	LEU
26	C	171	ASP
27	D	3	VAL
27	D	155	LYS
28	E	105	PHE
29	F	103	THR
30	r	34	VAL
30	r	48	LEU
30	r	72	VAL
30	r	88	ARG
30	r	89	ARG
30	r	106	LYS
30	r	121	TYR
30	r	155	HIS
30	r	183	ARG
30	r	195	ILE
30	r	240	THR
30	r	248	LEU
30	r	263	GLU
30	r	271	VAL
30	r	278	VAL
31	J	30	CYS
31	J	80	ASP
32	R	72	CYS

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Mol	Chain	Res	Type
32	R	135	GLU
32	R	155	ASN
32	R	182	CYS
33	T	23	MET
33	T	80	ASP
33	T	100	LYS
33	T	113	ARG
34	V	41	VAL
34	V	79	HIS
34	V	119	SER
34	V	149	GLN
34	V	187	SER
34	V	202	SER
36	Z	42	THR
36	Z	44	THR
36	Z	139	SER
37	a	51	SER
38	b	106	GLU
39	c	33	SER
39	c	107	ASP
39	c	113	PHE
39	c	116	ASP
39	c	134	THR
39	c	246	TYR
39	c	265	ILE
40	d	34	VAL
40	d	96	SER
40	d	130	ASP
41	e	51	ASP
41	e	58	LEU
41	e	74	SER
41	e	76	ARG
42	f	83	PHE
42	f	112	GLU
44	k	102	VAL
44	k	103	LEU
44	k	140	TYR
44	k	144	CYS
45	m	12	MET
45	m	50	CYS
45	m	62	VAL
45	m	66	GLU

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Mol	Chain	Res	Type
45	m	74	ILE
45	m	91	LEU
45	m	92	CYS
45	m	94	ILE
45	m	117	GLU
45	m	124	ILE
45	m	127	TYR
45	m	132	LYS
46	n	46	VAL
47	o	240	THR
47	o	286	SER
47	o	313	GLU
48	p	41	ARG
48	p	59	LEU
48	p	60	VAL
48	p	85	LEU
48	p	102	LEU
48	p	108	LEU
49	q	28	PHE
49	q	39	ILE
49	q	51	CYS
49	q	53	ASP
49	q	55	VAL
49	q	68	LYS
49	q	73	THR
49	q	81	LEU
49	q	86	ASP
49	q	99	GLU
51	M	8	THR
51	M	66	VAL
51	M	71	ILE
51	M	73	LEU
51	M	75	GLU
51	M	81	ARG
53	s	179	LEU
53	s	187	MET
53	s	188	ARG
53	s	190	LYS
53	s	204	MET
53	s	219	PHE
53	s	227	LYS
53	s	228	LEU

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Mol	Chain	Res	Type
53	s	244	LEU
53	s	285	ARG
53	s	292	GLN
53	s	304	THR
56	j	58	ILE
56	j	112	LEU
56	j	169	ARG
56	j	332	LEU
56	j	357	ILE
57	g	827	VAL
57	g	854	ASP
57	g	919	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
5	u	236	GLN
5	u	442	GLN
5	u	477	HIS
6	v	377	ASN
19	x	57	ASN
19	x	470	GLN
19	x	479	GLN
25	B	112	HIS
32	R	64	ASN
34	V	36	GLN
57	g	980	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	7	27/28 (96%)	20 (74%)	0
24	A	1706/1869 (91%)	410 (24%)	42 (2%)
54	w	74/75 (98%)	33 (44%)	0
All	All	1807/1972 (91%)	463 (25%)	42 (2%)

All (463) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	7	4	A

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Mol	Chain	Res	Type
22	7	5	A
22	7	7	A
22	7	9	A
22	7	10	A
22	7	11	A
22	7	12	A
22	7	13	A
22	7	14	A
22	7	15	A
22	7	16	A
22	7	17	A
22	7	18	A
22	7	20	A
22	7	21	A
22	7	22	A
22	7	24	A
22	7	25	A
22	7	26	A
22	7	27	A
24	A	2	A
24	A	4	C
24	A	10	G
24	A	11	A
24	A	12	U
24	A	17	C
24	A	23	G
24	A	33	G
24	A	41	G
24	A	42	A
24	A	44	U
24	A	46	A
24	A	56	G
24	A	58	C
24	A	59	U
24	A	62	G
24	A	64	A
24	A	65	C
24	A	67	C
24	A	68	A
24	A	72	C
24	A	73	C
24	A	74	G

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Mol	Chain	Res	Type
24	A	78	C
24	A	82	G
24	A	103	A
24	A	110	U
24	A	114	G
24	A	115	U
24	A	126	G
24	A	129	C
24	A	130	G
24	A	140	U
24	A	142	C
24	A	143	U
24	A	147	A
24	A	155	G
24	A	158	A
24	A	160	U
24	A	163	U
24	A	168	C
24	A	173	A
24	A	180	G
24	A	182	C
24	A	184	G
24	A	190	G
24	A	198	U
24	A	200	G
24	A	202	G
24	A	203	G
24	A	204	G
24	A	206	G
24	A	208	G
24	A	288	G
24	A	291	G
24	A	292	A
24	A	294	U
24	A	295	C
24	A	306	C
24	A	307	G
24	A	308	G
24	A	309	G
24	A	314	U
24	A	318	A
24	A	319	C

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Mol	Chain	Res	Type
24	A	320	G
24	A	321	C
24	A	323	C
24	A	324	C
24	A	325	C
24	A	326	C
24	A	327	G
24	A	328	U
24	A	329	G
24	A	332	G
24	A	347	G
24	A	362	C
24	A	363	A
24	A	364	A
24	A	368	U
24	A	369	C
24	A	370	G
24	A	382	C
24	A	385	G
24	A	386	C
24	A	409	C
24	A	418	A
24	A	421	G
24	A	447	A
24	A	448	A
24	A	449	A
24	A	450	C
24	A	452	G
24	A	465	A
24	A	471	G
24	A	472	C
24	A	473	A
24	A	474	G
24	A	476	A
24	A	482	G
24	A	487	U
24	A	492	C
24	A	508	A
24	A	512	A
24	A	516	A
24	A	525	A
24	A	533	A

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Mol	Chain	Res	Type
24	A	534	G
24	A	536	A
24	A	537	C
24	A	538	U
24	A	539	C
24	A	540	U
24	A	541	U
24	A	542	U
24	A	543	C
24	A	544	G
24	A	545	A
24	A	546	G
24	A	547	G
24	A	550	C
24	A	553	U
24	A	554	A
24	A	556	U
24	A	557	U
24	A	558	G
24	A	559	G
24	A	563	G
24	A	564	A
24	A	566	U
24	A	568	C
24	A	576	A
24	A	583	A
24	A	589	G
24	A	590	A
24	A	591	U
24	A	598	G
24	A	604	A
24	A	606	G
24	A	607	U
24	A	608	C
24	A	614	C
24	A	624	C
24	A	626	G
24	A	627	U
24	A	628	A
24	A	629	A
24	A	631	U
24	A	643	A

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Mol	Chain	Res	Type
24	A	655	A
24	A	659	G
24	A	660	C
24	A	662	G
24	A	664	A
24	A	668	A2M
24	A	669	A
24	A	671	A
24	A	672	A
24	A	673	G
24	A	687	C
24	A	688	U
24	A	689	U
24	A	690	G
24	A	693	A
24	A	694	G
24	A	734	C
24	A	736	C
24	A	748	C
24	A	749	U
24	A	751	G
24	A	752	G
24	A	753	C
24	A	790	C
24	A	791	C
24	A	797	C
24	A	798	G
24	A	799	U
24	A	801	U
24	A	810	A
24	A	811	A
24	A	821	G
24	A	827	A
24	A	830	A
24	A	836	G
24	A	837	A
24	A	838	G
24	A	839	C
24	A	840	C
24	A	841	G
24	A	845	G
24	A	869	A

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Mol	Chain	Res	Type
24	A	870	A
24	A	872	A
24	A	873	G
24	A	878	G
24	A	880	G
24	A	886	A
24	A	888	U
24	A	889	U
24	A	890	U
24	A	891	G
24	A	892	U
24	A	894	G
24	A	895	G
24	A	896	U
24	A	897	U
24	A	898	U
24	A	899	U
24	A	900	C
24	A	903	A
24	A	904	A
24	A	909	G
24	A	912	C
24	A	913	A
24	A	914	U
24	A	920	A
24	A	922	A
24	A	930	C
24	A	933	G
24	A	943	U
24	A	950	C
24	A	963	A
24	A	965	U
24	A	969	U
24	A	970	G
24	A	989	C
24	A	990	A
24	A	992	A
24	A	999	G
24	A	1002	U
24	A	1017	U
24	A	1023	A
24	A	1061	U

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Mol	Chain	Res	Type
24	A	1062	A
24	A	1083	A
24	A	1085	C
24	A	1109	C
24	A	1112	U
24	A	1113	A
24	A	1114	U
24	A	1115	U
24	A	1116	C
24	A	1117	C
24	A	1120	U
24	A	1138	C
24	A	1153	C
24	A	1154	U
24	A	1170	A
24	A	1195	A
24	A	1207	G
24	A	1208	A
24	A	1209	A
24	A	1215	C
24	A	1216	C
24	A	1217	A
24	A	1224	G
24	A	1242	U
24	A	1243	PSU
24	A	1245	G
24	A	1248	U
24	A	1250	A
24	A	1251	A
24	A	1253	A
24	A	1256	G
24	A	1257	G
24	A	1259	A
24	A	1274	G
24	A	1275	G
24	A	1283	C
24	A	1284	A
24	A	1286	G
24	A	1288	U
24	A	1294	G
24	A	1295	A
24	A	1301	A

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Mol	Chain	Res	Type
24	A	1302	G
24	A	1303	C
24	A	1308	U
24	A	1318	G
24	A	1322	G
24	A	1326	U
24	A	1342	U
24	A	1356	G
24	A	1357	A
24	A	1358	U
24	A	1371	U
24	A	1372	U
24	A	1378	A
24	A	1397	U
24	A	1402	A
24	A	1406	G
24	A	1417	C
24	A	1418	C
24	A	1419	C
24	A	1420	G
24	A	1421	A
24	A	1422	G
24	A	1423	C
24	A	1424	G
24	A	1433	C
24	A	1435	C
24	A	1436	C
24	A	1437	C
24	A	1438	A
24	A	1454	A
24	A	1455	A
24	A	1463	U
24	A	1488	C
24	A	1489	A
24	A	1490	G
24	A	1497	G
24	A	1498	A
24	A	1519	U
24	A	1520	G
24	A	1521	C
24	A	1522	A
24	A	1533	A

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Mol	Chain	Res	Type
24	A	1534	C
24	A	1544	C
24	A	1553	C
24	A	1556	A
24	A	1570	G
24	A	1580	A
24	A	1587	G
24	A	1588	A
24	A	1594	A
24	A	1598	G
24	A	1599	U
24	A	1600	G
24	A	1601	A
24	A	1602	U
24	A	1618	C
24	A	1619	A
24	A	1621	U
24	A	1623	A
24	A	1624	U
24	A	1639	G
24	A	1644	C
24	A	1648	G
24	A	1654	G
24	A	1663	A
24	A	1665	G
24	A	1671	G
24	A	1686	G
24	A	1695	A
24	A	1699	A
24	A	1700	C
24	A	1701	C
24	A	1702	G
24	A	1711	U
24	A	1712	A
24	A	1715	A
24	A	1719	A
24	A	1721	U
24	A	1722	G
24	A	1733	U
24	A	1744	G
24	A	1749	G
24	A	1750	C

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Mol	Chain	Res	Type
24	A	1752	C
24	A	1753	C
24	A	1754	G
24	A	1755	C
24	A	1756	C
24	A	1757	G
24	A	1758	G
24	A	1759	G
24	A	1760	G
24	A	1772	C
24	A	1773	C
24	A	1774	C
24	A	1775	U
24	A	1776	G
24	A	1777	G
24	A	1778	C
24	A	1779	G
24	A	1780	G
24	A	1781	A
24	A	1782	G
24	A	1783	C
24	A	1784	G
24	A	1800	A
24	A	1804	U
24	A	1805	G
24	A	1808	U
24	A	1809	A
24	A	1813	A
24	A	1822	A
24	A	1823	A
24	A	1824	A
24	A	1825	A
24	A	1829	G
24	A	1831	A
24	A	1834	A
24	A	1835	A
24	A	1837	G
24	A	1838	U
24	A	1839	U
24	A	1841	C
24	A	1849	G
24	A	1853	C

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Mol	Chain	Res	Type
24	A	1860	A
24	A	1861	G
24	A	1862	G
24	A	1863	A
24	A	1864	U
24	A	1865	C
24	A	1866	A
24	A	1867	U
24	A	1868	U
54	w	2	G
54	w	6	A
54	w	7	G
54	w	8	U
54	w	9	G
54	w	10	G
54	w	14	A
54	w	15	G
54	w	16	C
54	w	17	G
54	w	18	G
54	w	19	A
54	w	20	A
54	w	42	G
54	w	43	A
54	w	44	G
54	w	45	G
54	w	46	U
54	w	51	G
54	w	52	G
54	w	54	U
54	w	55	C
54	w	56	G
54	w	57	A
54	w	58	A
54	w	60	C
54	w	63	U
54	w	64	C
54	w	71	U
54	w	72	A
54	w	73	C
54	w	74	C
54	w	75	A

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	1	U
24	A	9	U
24	A	291	G
24	A	368	U
24	A	370	G
24	A	687	C
24	A	688	U
24	A	689	U
24	A	797	C
24	A	798	G
24	A	912	C
24	A	913	A
24	A	988	C
24	A	989	C
24	A	990	A
24	A	1250	A
24	A	1357	A
24	A	1434	C
24	A	1519	U
24	A	1520	G
24	A	1521	C
24	A	1598	G
24	A	1599	U
24	A	1600	G
24	A	1601	A
24	A	1603	G
24	A	1699	A
24	A	1700	C
24	A	1701	C
24	A	1753	C
24	A	1759	G
24	A	1775	U
24	A	1781	A
24	A	1834	A
24	A	1860	A
24	A	1861	G
24	A	1862	G
24	A	1863	A
24	A	1864	U
24	A	1865	C
24	A	1866	A
24	A	1867	U

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

28 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$
24	PSU	A	1243	24	18,21,22	1.00	1 (5%)	22,30,33	0.70	0
24	A2M	A	668	59,24	18,25,26	0.66	0	18,36,39	0.83	1 (5%)
24	MA6	A	1850	24	19,26,27	0.85	1 (5%)	18,38,41	0.53	0
24	OMU	A	116	24	19,22,23	0.39	0	26,31,34	0.51	0
24	PSU	A	822	24	18,21,22	1.04	2 (11%)	22,30,33	0.84	1 (4%)
24	5MU	A	814	24	19,22,23	0.45	0	28,32,35	0.50	0
24	OMU	A	121	24	19,22,23	0.44	0	26,31,34	0.51	0
24	PSU	A	612	24	18,21,22	1.10	2 (11%)	22,30,33	0.75	1 (4%)
24	MA6	A	1851	24	19,26,27	0.82	1 (5%)	18,38,41	0.62	0
24	A2M	A	166	24	18,25,26	0.59	0	18,36,39	0.96	1 (5%)
24	A2M	A	1678	24	18,25,26	0.61	0	18,36,39	0.76	0
24	5MC	A	1374	24	18,22,23	0.44	0	26,32,35	0.61	0
24	OMC	A	174	59,24	19,22,23	0.43	0	26,31,34	0.44	0
24	JMH	A	1219	59,24	18,22,23	0.64	0	21,32,35	0.65	0
24	6MZ	A	1832	59,24	18,25,26	0.79	0	16,36,39	0.74	1 (6%)
24	OMG	A	683	24	18,26,27	1.06	3 (16%)	19,38,41	0.92	1 (5%)
24	A2M	A	27	59,24	18,25,26	0.63	0	18,36,39	0.77	1 (5%)
24	OMC	A	517	24	19,22,23	0.46	0	26,31,34	0.41	0
24	A2M	A	159	24	18,25,26	0.64	1 (5%)	18,36,39	0.76	1 (5%)
24	PSU	A	823	24	18,21,22	1.05	1 (5%)	22,30,33	0.68	0
24	PSU	A	119	24	18,21,22	0.97	1 (5%)	22,30,33	0.69	0
24	OMG	A	644	24	18,26,27	1.08	3 (16%)	19,38,41	0.74	1 (5%)
24	A2M	A	1031	24	18,25,26	0.61	0	18,36,39	0.91	1 (5%)
24	PSU	A	1081	24	18,21,22	1.04	2 (11%)	22,30,33	0.82	0
24	OMC	A	1703	24	19,22,23	0.44	0	26,31,34	0.49	0
24	UR3	A	1830	24	19,22,23	0.41	0	26,32,35	1.00	2 (7%)
24	OMG	A	509	59,24	18,26,27	1.09	3 (16%)	19,38,41	0.78	0
24	A2M	A	484	24	18,25,26	0.65	1 (5%)	18,36,39	0.76	1 (5%)

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
24	PSU	A	1243	24	-	0/7/25/26	0/2/2/2
24	A2M	A	668	59,24	-	2/5/27/28	0/3/3/3
24	MA6	A	1850	24	-	3/7/29/30	0/3/3/3
24	OMU	A	116	24	-	0/9/27/28	0/2/2/2
24	PSU	A	822	24	-	0/7/25/26	0/2/2/2
24	5MU	A	814	24	-	0/7/25/26	0/2/2/2
24	OMU	A	121	24	-	0/9/27/28	0/2/2/2
24	PSU	A	612	24	-	0/7/25/26	0/2/2/2
24	MA6	A	1851	24	-	5/7/29/30	0/3/3/3
24	A2M	A	166	24	-	0/5/27/28	0/3/3/3
24	A2M	A	1678	24	-	0/5/27/28	0/3/3/3
24	5MC	A	1374	24	-	0/7/25/26	0/2/2/2
24	OMC	A	174	59,24	-	0/9/27/28	0/2/2/2
24	JMH	A	1219	59,24	-	0/7/25/26	0/2/2/2
24	6MZ	A	1832	59,24	-	2/5/27/28	0/3/3/3
24	OMG	A	683	24	-	0/5/27/28	0/3/3/3
24	A2M	A	27	59,24	-	0/5/27/28	0/3/3/3
24	OMC	A	517	24	-	0/9/27/28	0/2/2/2
24	A2M	A	159	24	-	2/5/27/28	0/3/3/3
24	PSU	A	823	24	-	0/7/25/26	0/2/2/2
24	PSU	A	119	24	-	0/7/25/26	0/2/2/2
24	OMG	A	644	24	-	1/5/27/28	0/3/3/3
24	A2M	A	1031	24	-	0/5/27/28	0/3/3/3
24	PSU	A	1081	24	-	1/7/25/26	0/2/2/2
24	OMC	A	1703	24	-	0/9/27/28	0/2/2/2
24	UR3	A	1830	24	-	2/7/25/26	0/2/2/2
24	OMG	A	509	59,24	-	0/5/27/28	0/3/3/3
24	A2M	A	484	24	-	0/5/27/28	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1243	PSU	C6-C5	3.37	1.39	1.35
24	A	823	PSU	C6-C5	3.35	1.39	1.35
24	A	119	PSU	C6-C5	3.23	1.39	1.35
24	A	612	PSU	C6-C5	3.22	1.39	1.35
24	A	1081	PSU	C6-C5	3.20	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	822	PSU	C6-C5	3.14	1.39	1.35
24	A	683	OMG	C5-C6	-2.85	1.41	1.47
24	A	509	OMG	C5-C6	-2.84	1.41	1.47
24	A	644	OMG	C5-C6	-2.75	1.41	1.47
24	A	612	PSU	O4'-C1'	-2.52	1.40	1.43
24	A	1081	PSU	O4'-C1'	-2.31	1.40	1.43
24	A	822	PSU	O4'-C1'	-2.26	1.40	1.43
24	A	1850	MA6	C8-N7	-2.22	1.30	1.34
24	A	509	OMG	C8-N7	-2.15	1.31	1.35
24	A	683	OMG	C8-N7	-2.13	1.31	1.35
24	A	644	OMG	C8-N7	-2.10	1.31	1.35
24	A	484	A2M	C8-N7	-2.10	1.31	1.34
24	A	509	OMG	C5-C4	-2.09	1.37	1.43
24	A	644	OMG	C5-C4	-2.06	1.37	1.43
24	A	683	OMG	C5-C4	-2.06	1.37	1.43
24	A	159	A2M	C8-N7	-2.06	1.31	1.34
24	A	1851	MA6	C6-N1	2.02	1.36	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1832	6MZ	C2-N1-C6	2.44	118.68	116.59
24	A	668	A2M	C5-C6-N6	2.32	123.88	120.35
24	A	1031	A2M	C5-C6-N6	2.31	123.86	120.35
24	A	822	PSU	O4'-C1'-C2'	2.28	108.36	105.14
24	A	1830	UR3	C6-N1-C2	-2.25	119.77	121.79
24	A	166	A2M	C5-C6-N6	2.24	123.75	120.35
24	A	612	PSU	O4'-C1'-C2'	2.23	108.29	105.14
24	A	159	A2M	C5-C6-N6	2.20	123.69	120.35
24	A	1830	UR3	C1'-N1-C2	2.16	120.63	116.99
24	A	27	A2M	C5-C6-N6	2.11	123.56	120.35
24	A	644	OMG	O6-C6-C5	2.07	128.42	124.37
24	A	484	A2M	C5-C6-N6	2.05	123.47	120.35
24	A	683	OMG	O6-C6-C5	2.01	128.31	124.37

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1832	6MZ	N1-C6-N6-C9
24	A	1850	MA6	C5-C6-N6-C10
24	A	1850	MA6	N1-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
24	A	1851	MA6	O4'-C4'-C5'-O5'
24	A	1851	MA6	C5-C6-N6-C10
24	A	668	A2M	O4'-C4'-C5'-O5'
24	A	1851	MA6	C3'-C4'-C5'-O5'
24	A	668	A2M	C3'-C4'-C5'-O5'
24	A	1851	MA6	N1-C6-N6-C10
24	A	1830	UR3	O4'-C1'-N1-C2
24	A	159	A2M	C3'-C4'-C5'-O5'
24	A	1830	UR3	O4'-C1'-N1-C6
24	A	159	A2M	O4'-C4'-C5'-O5'
24	A	1850	MA6	C5-C6-N6-C9
24	A	1851	MA6	C5-C6-N6-C9
24	A	644	OMG	C4'-C5'-O5'-P
24	A	1081	PSU	C4'-C5'-O5'-P
24	A	1832	6MZ	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 91 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



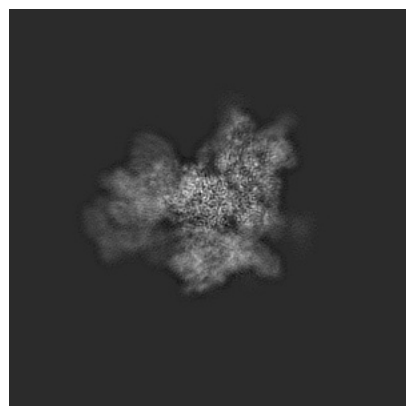
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11302. These allow visual inspection of the internal detail of the map and identification of artifacts.

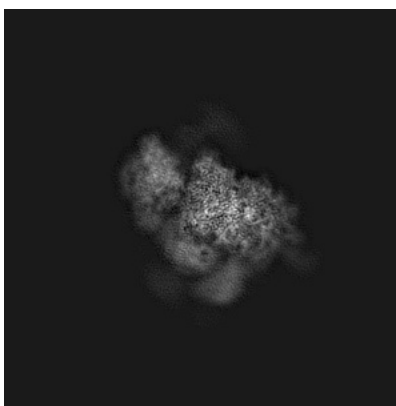
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

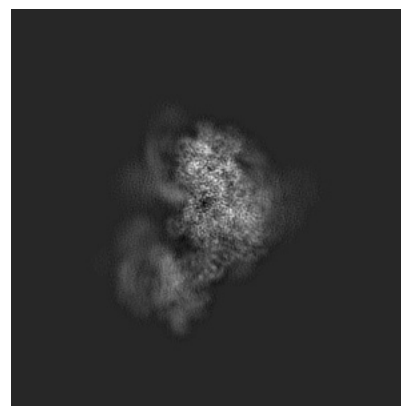
#### 6.1.1 Primary map



X

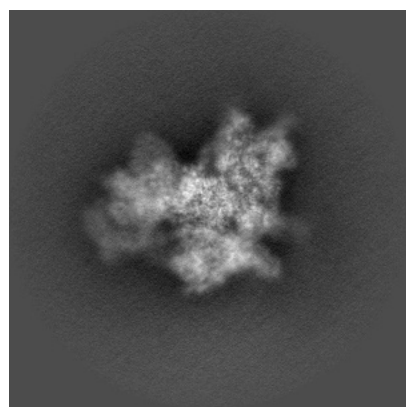


Y

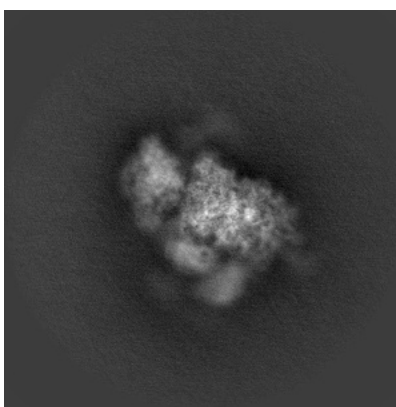


Z

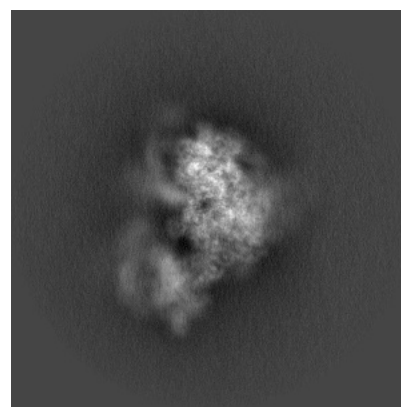
#### 6.1.2 Raw map



X



Y

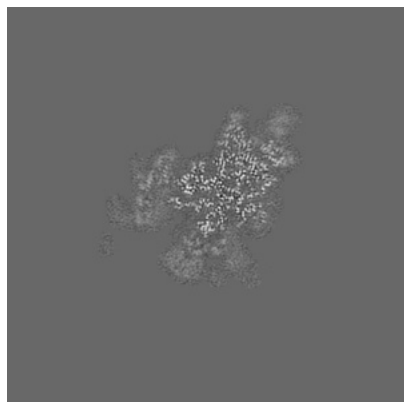


Z

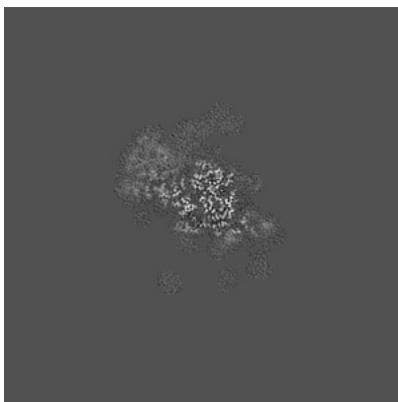
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

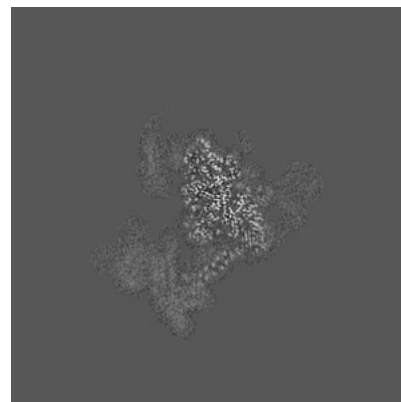
### 6.2.1 Primary map



X Index: 250

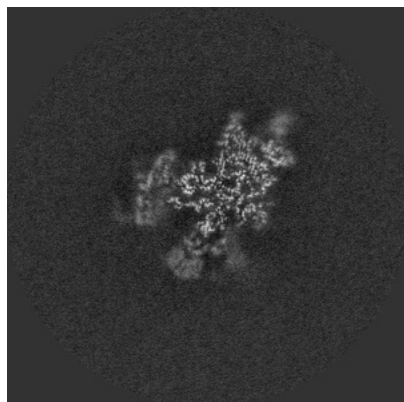


Y Index: 250

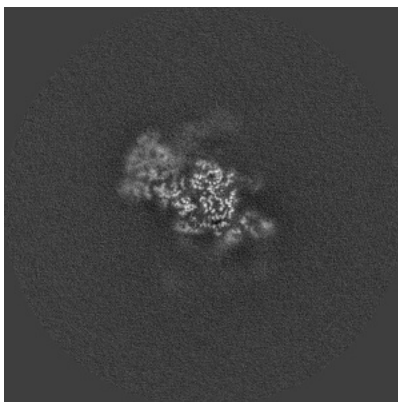


Z Index: 250

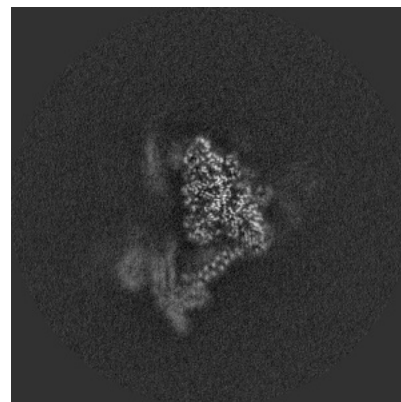
### 6.2.2 Raw map



X Index: 250



Y Index: 250

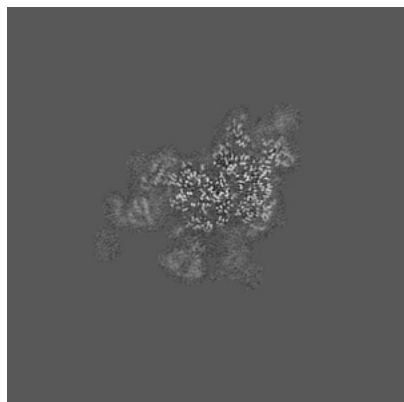


Z Index: 250

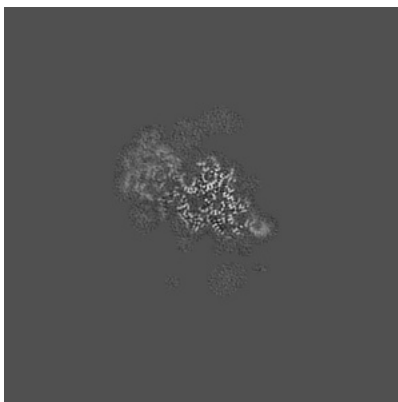
The images above show central slices of the map in three orthogonal directions.

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

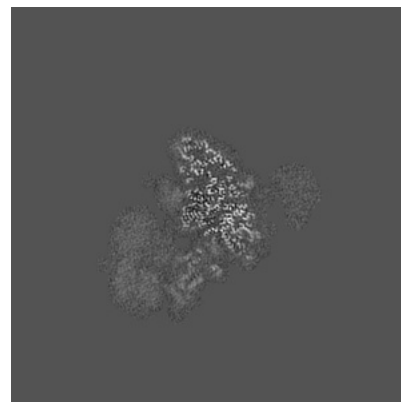
### 6.3.1 Primary map



X Index: 244

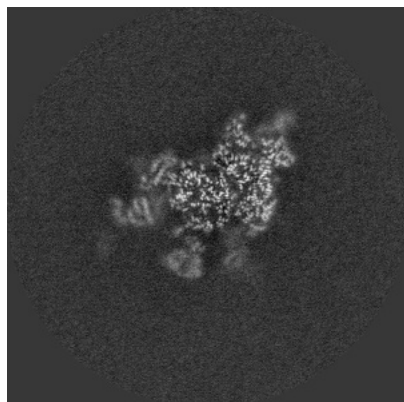


Y Index: 244

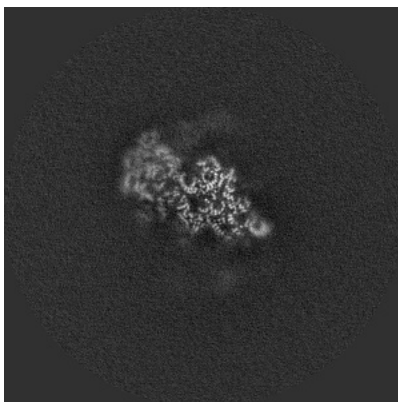


Z Index: 271

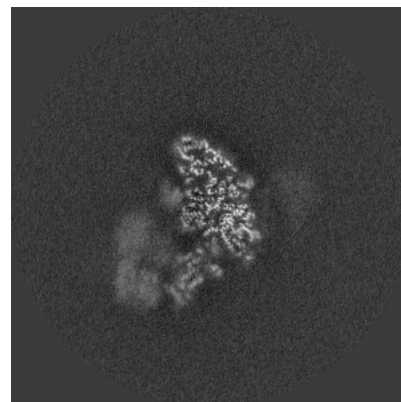
### 6.3.2 Raw map



X Index: 244



Y Index: 244

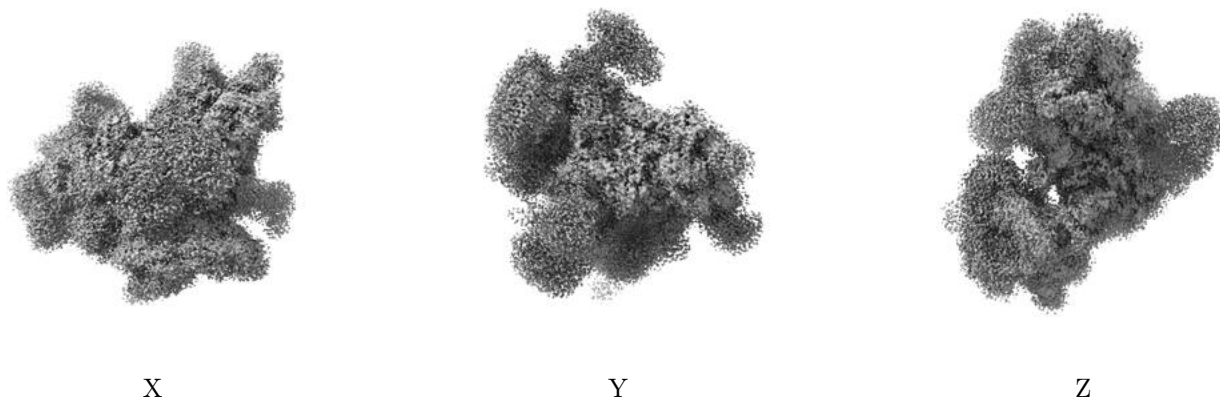


Z Index: 271

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

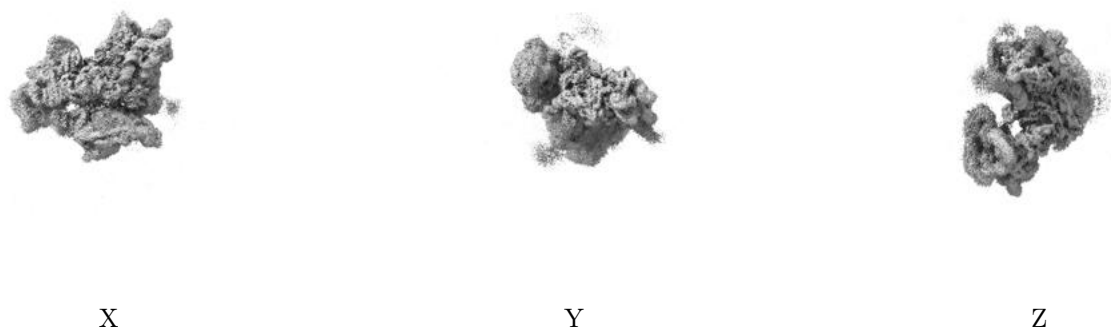
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

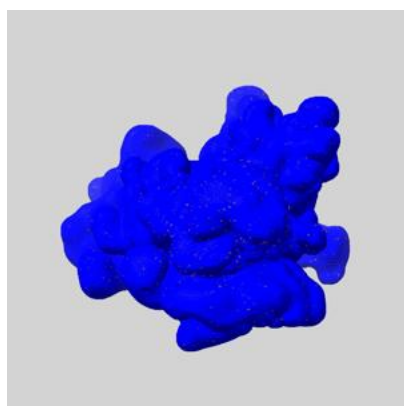
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

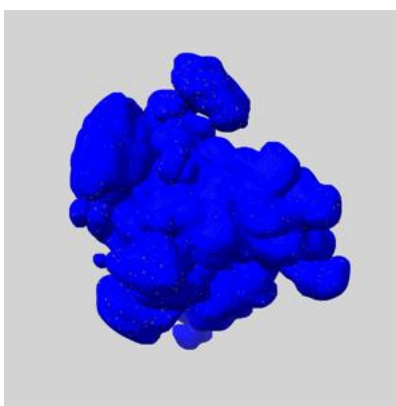
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

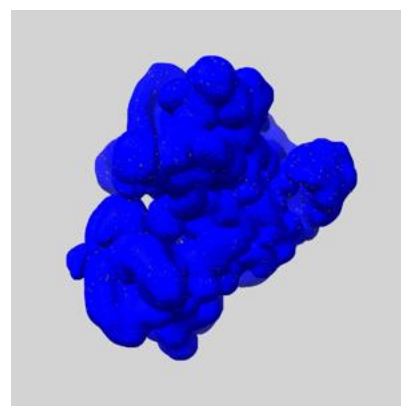
### 6.5.1 emd\_11302\_msk\_1.map [i](#)



X



Y

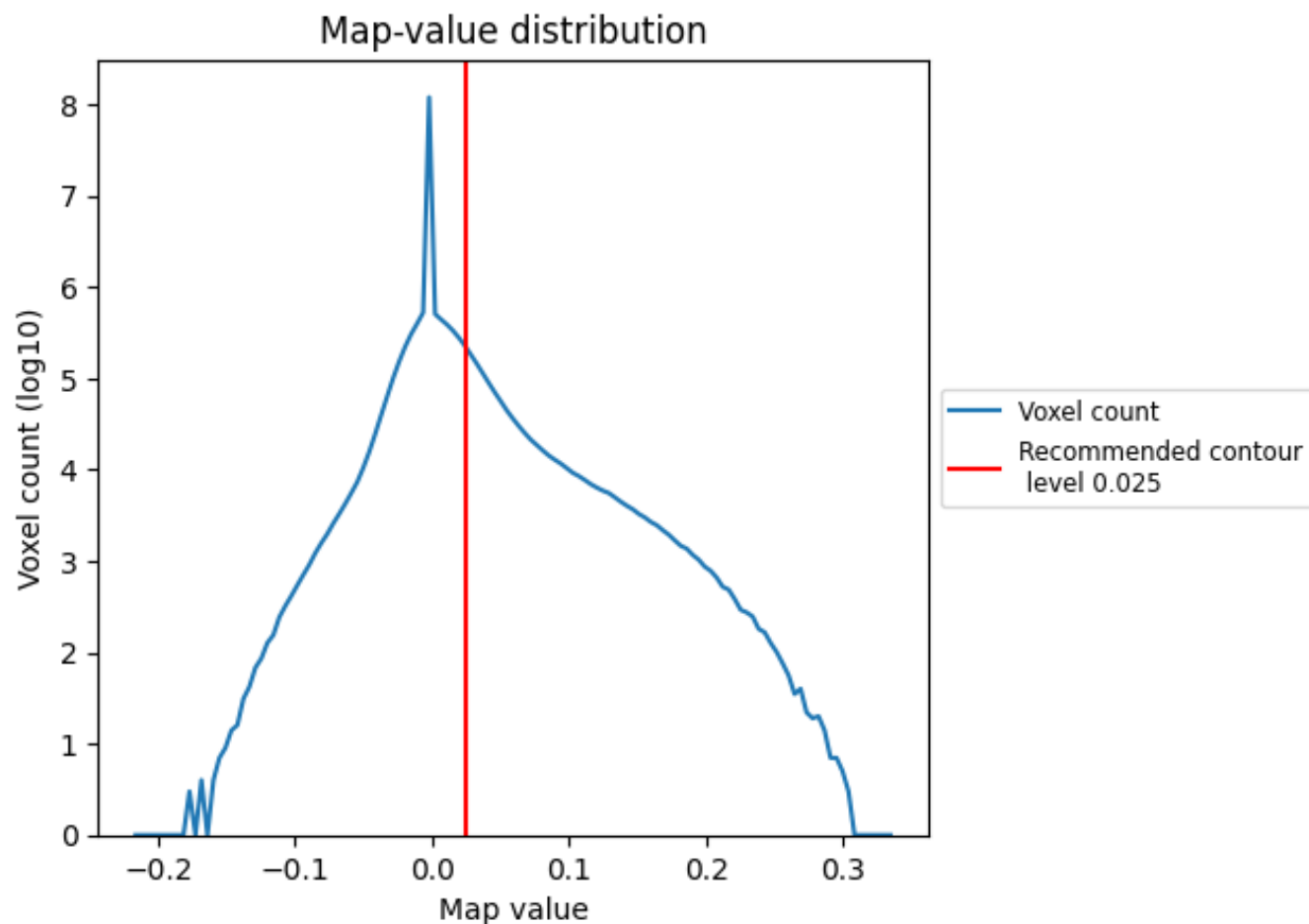


Z

## 7 Map analysis [i](#)

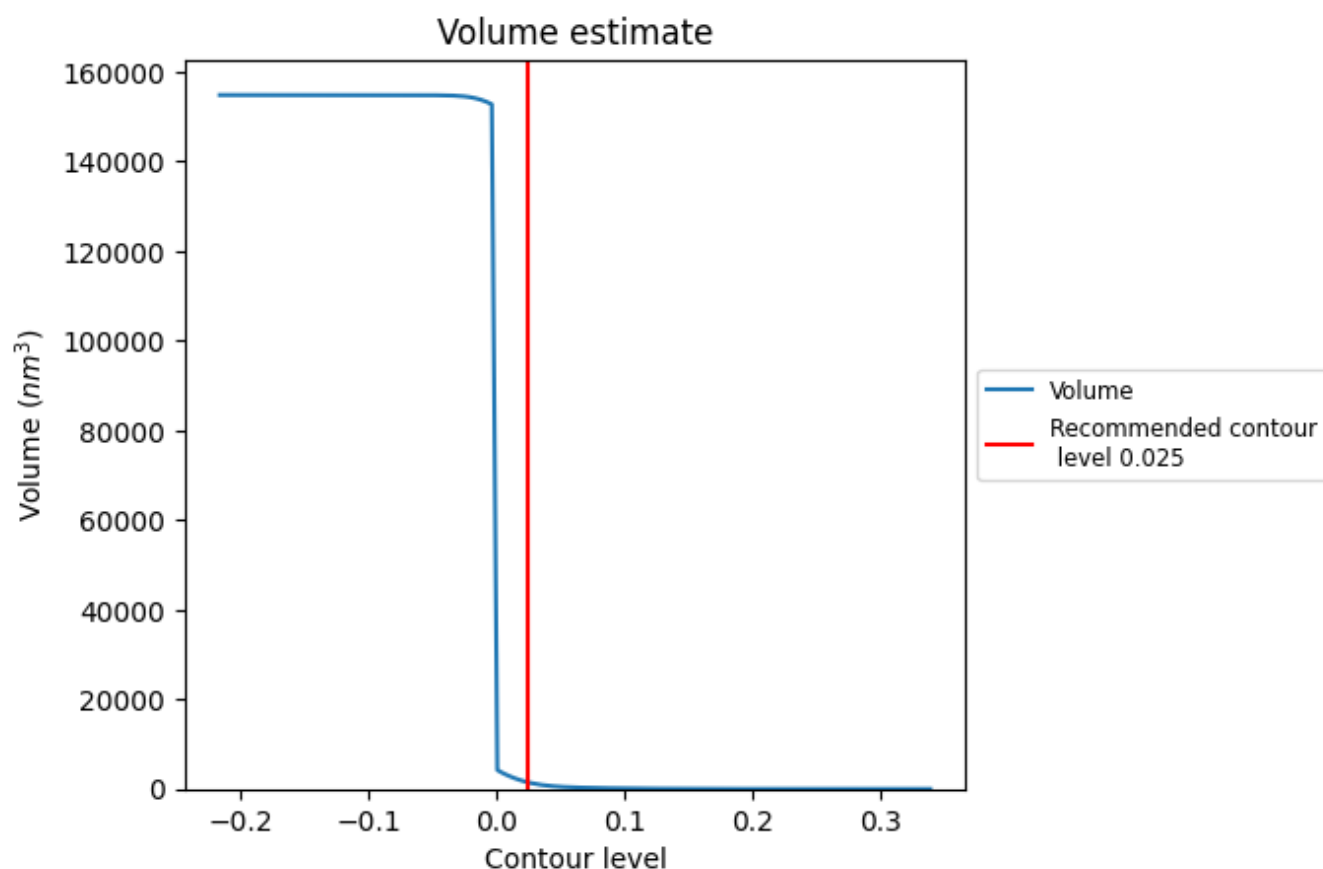
This section contains the results of statistical analysis of the map.

### 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.

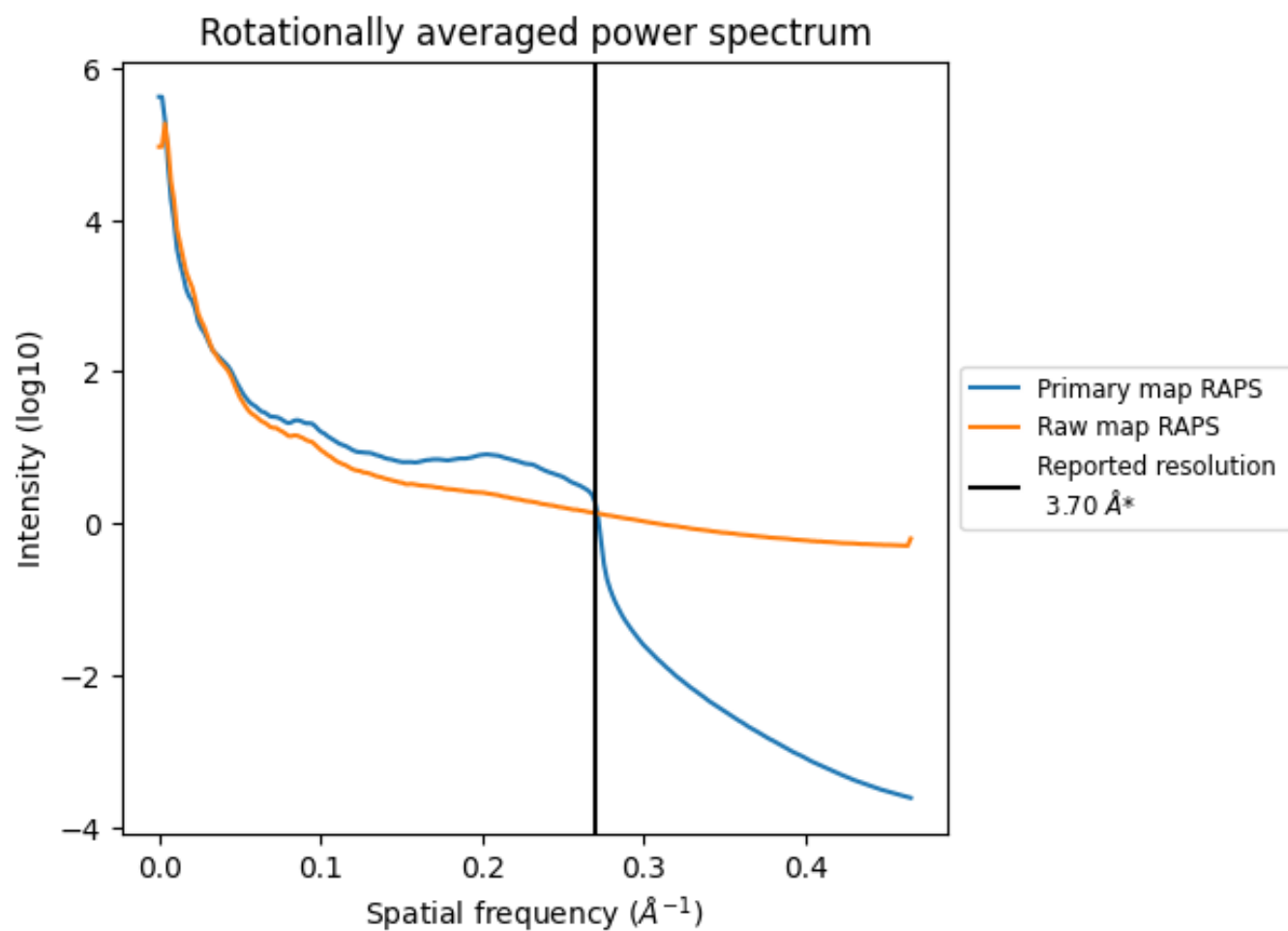
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1449 nm<sup>3</sup>; this corresponds to an approximate mass of 1309 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 ⓘ



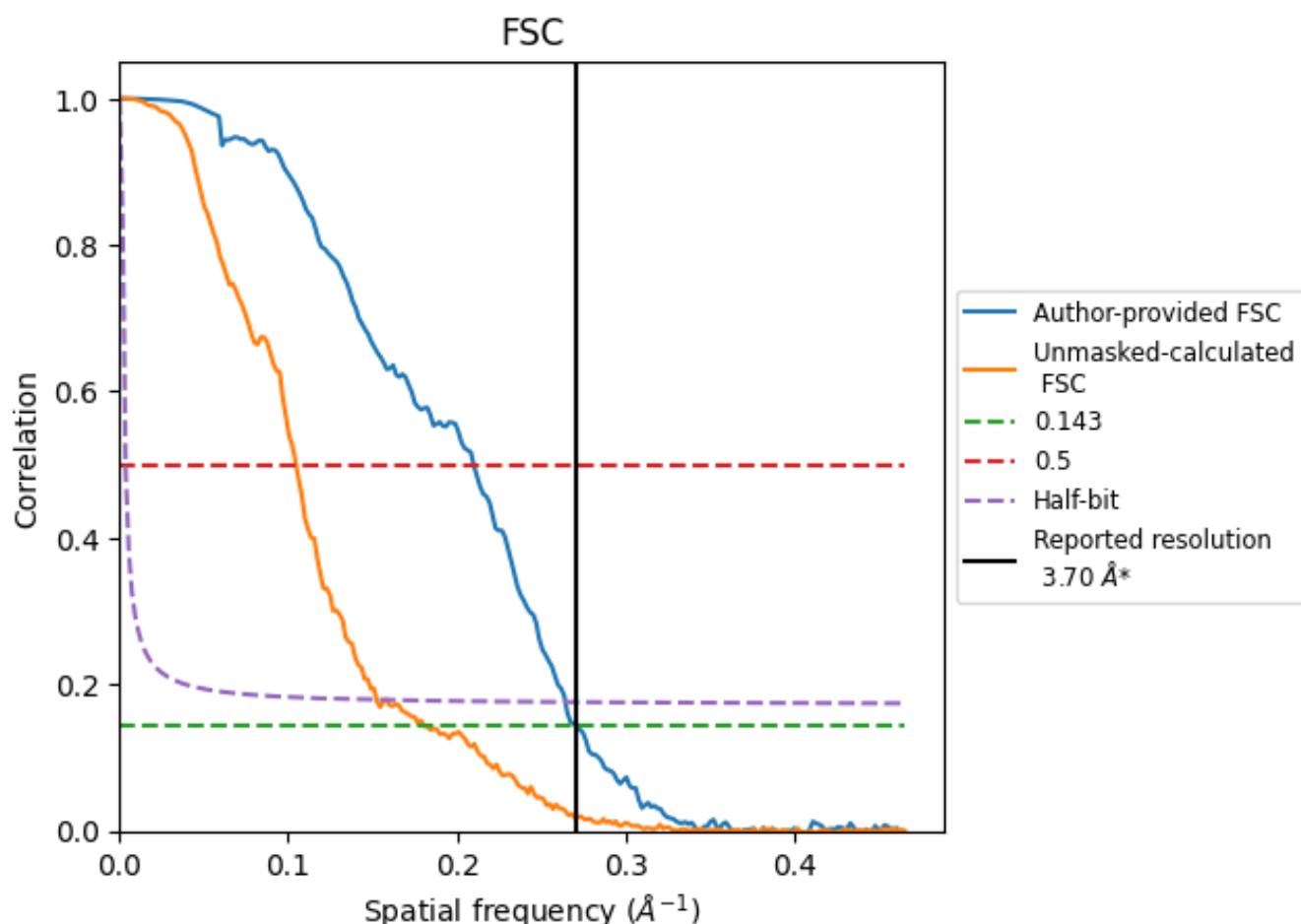
\*Reported resolution corresponds to spatial frequency of  $0.270 \text{ \AA}^{-1}$



## 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 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

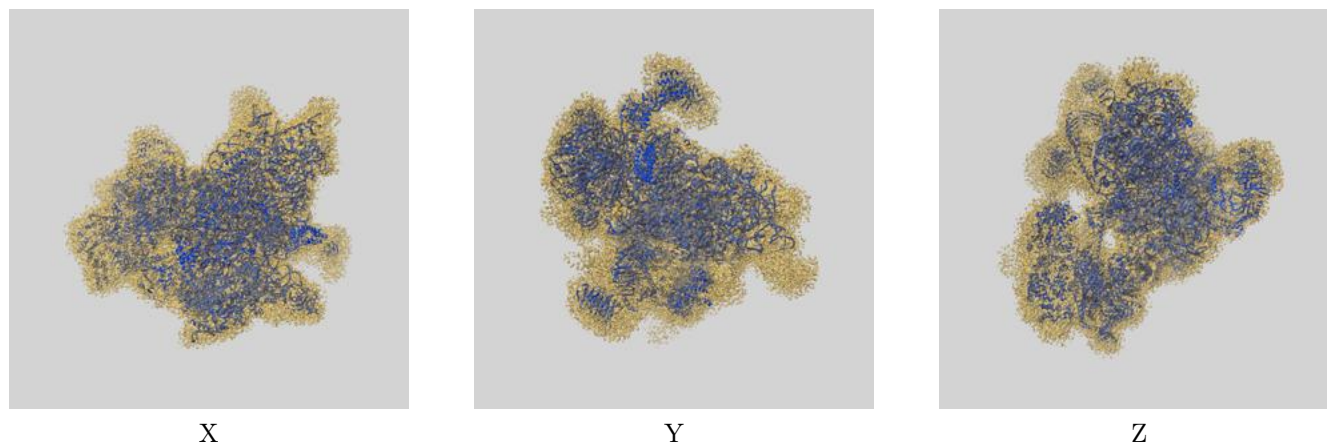
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.76	3.78
Unmasked-calculated*	5.54	9.55	6.56

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.54 differs from the reported value 3.7 by more than 10 %

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

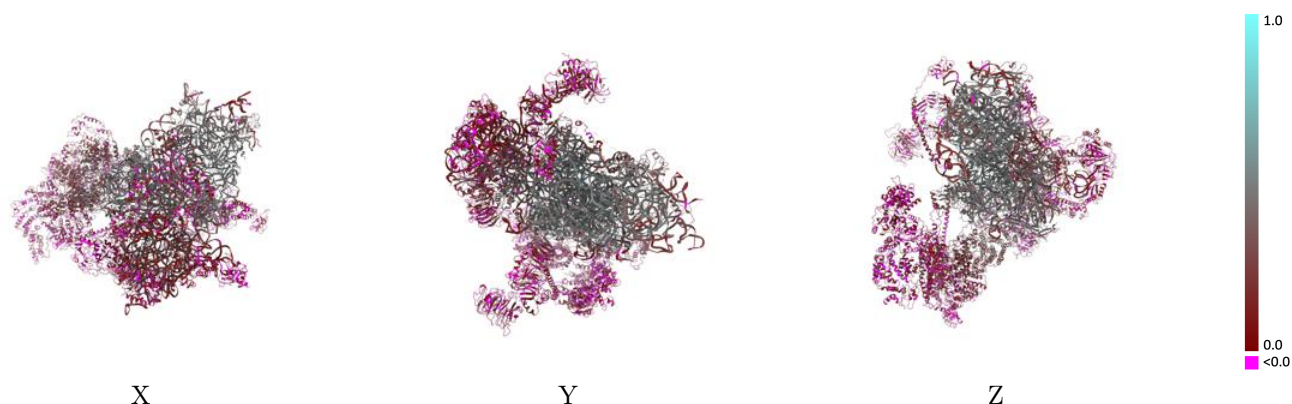
This section contains information regarding the fit between EMDB map EMD-11302 and PDB model 6ZMW. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

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



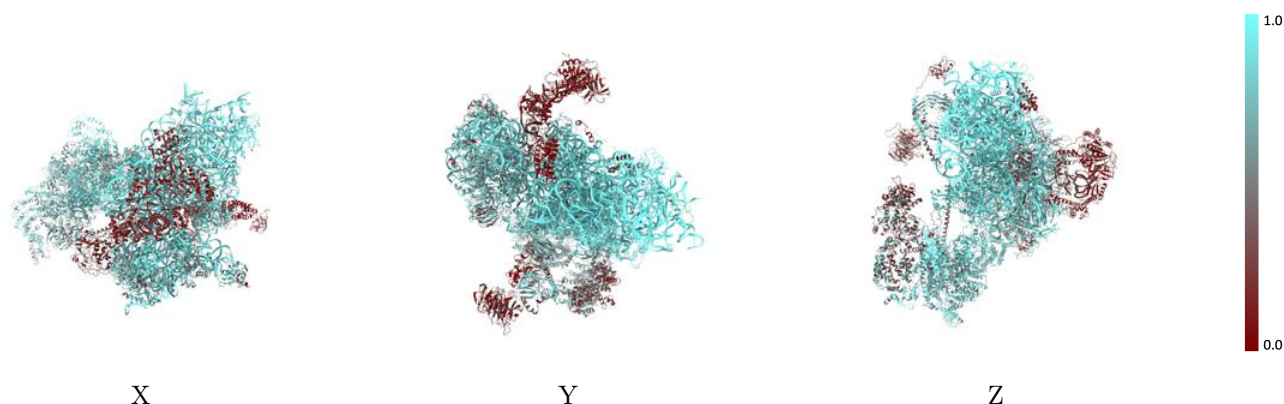
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



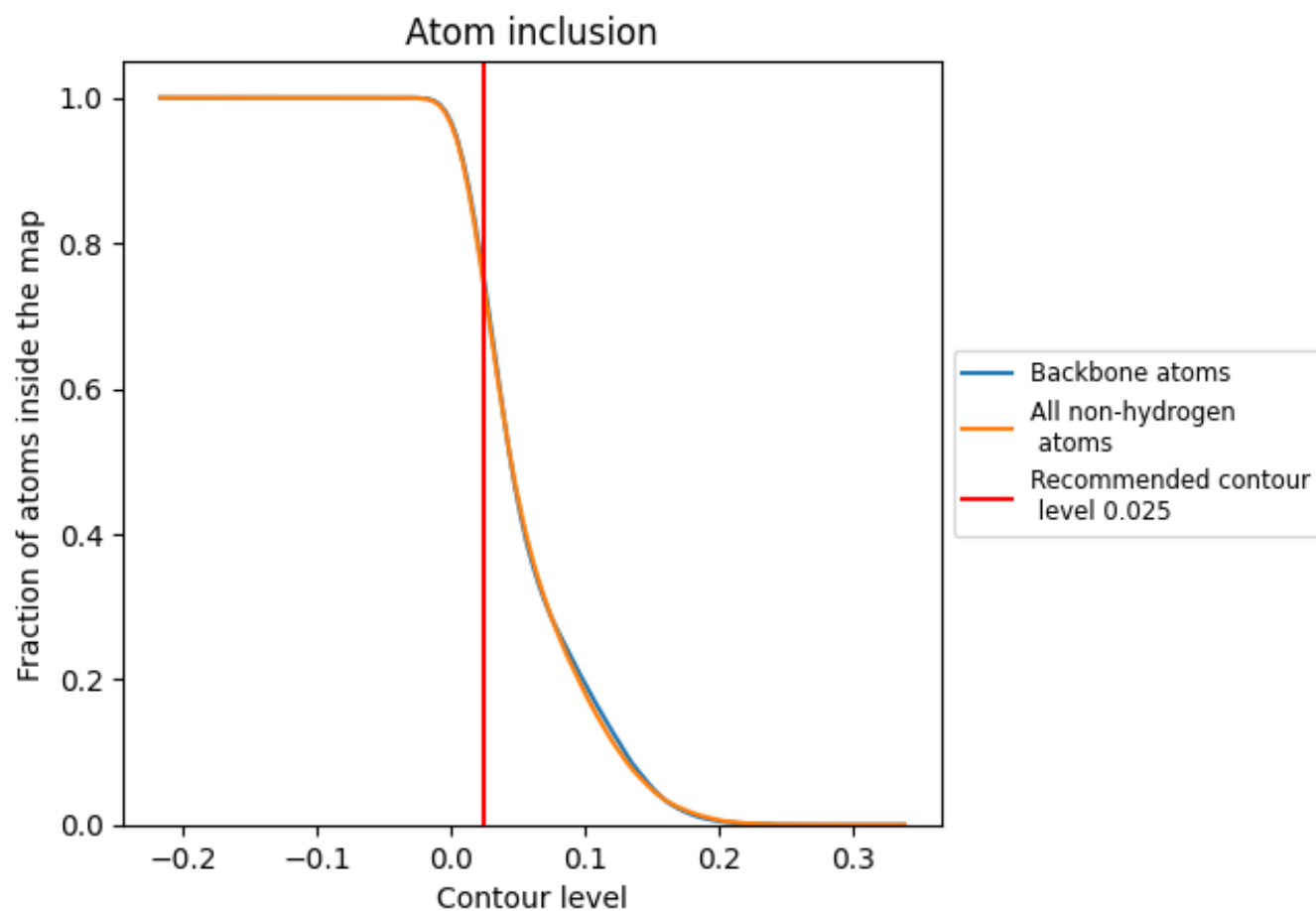
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7427	 0.2930
1	 0.5384	 0.1670
2	 0.1956	 0.1120
3	 0.6320	 0.1030
4	 0.6659	 0.1060
5	 0.6180	 0.1130
6	 0.7174	 0.1180
7	 0.2232	 0.1670
8	 0.6359	 0.1240
9	 0.8182	 0.4460
A	 0.9520	 0.3820
B	 0.9232	 0.4960
C	 0.9234	 0.5070
D	 0.9083	 0.4880
E	 0.9247	 0.5170
F	 0.9118	 0.4880
G	 0.8603	 0.4030
H	 0.8966	 0.4780
I	 0.9036	 0.4790
J	 0.9109	 0.5190
K	 0.8872	 0.4740
L	 0.8657	 0.4640
M	 0.8017	 0.3830
N	 0.9095	 0.4780
O	 0.8843	 0.4420
P	 0.8678	 0.4280
Q	 0.9068	 0.4850
R	 0.9177	 0.4460
S	 0.9228	 0.4040
T	 0.9259	 0.4690
V	 0.6709	 0.1900
Y	 0.7279	 0.2530
Z	 0.7387	 0.3100
a	 0.7032	 0.1760
b	 0.5819	 0.0970



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Chain	Atom inclusion	Q-score
c	 0.7181	 0.1900
d	 0.6887	 0.1350
e	 0.6250	 0.1070
f	 0.6537	 0.1310
g	 0.3188	 0.0700
h	 0.7651	 0.3260
i	 0.8130	 0.2940
j	 0.3685	 0.0680
k	 0.6611	 0.0570
m	 0.5897	 0.0640
n	 0.5544	 0.1890
o	 0.5359	 0.1060
p	 0.7191	 0.3500
q	 0.4403	 0.2350
r	 0.1024	 0.1310
s	 0.0939	 0.1190
t	 0.1423	 0.1150
u	 0.7293	 0.2270
v	 0.7641	 0.1550
w	 0.1864	 0.1340
x	 0.3490	 0.1270
y	 0.6921	 0.2760
z	 0.0805	 0.1120