



## wwPDB EM Validation Summary Report ⓘ

Jun 3, 2026 – 02:24 pm BST

PDB ID : 28ZU / pdb\_000028zu  
EMDB ID : EMD-57004  
Title : human 48S PIC with Kozak mRNA and eIF1A W70A mutant  
Authors : von Loeffelholz, O.; Barchet, C.; Klaholz, B.  
Deposited on : 2026-03-03  
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary 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:

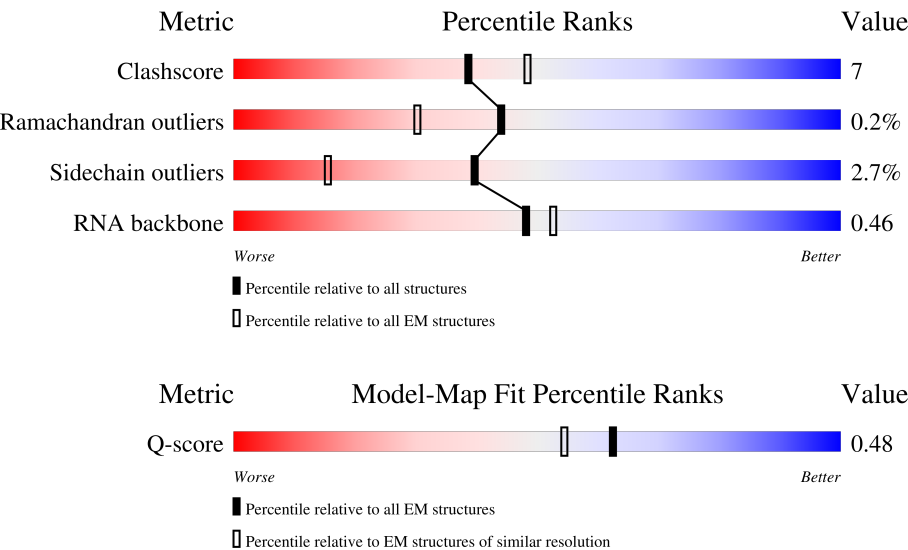
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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.









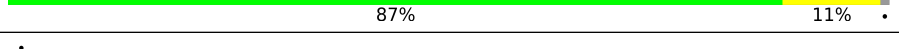
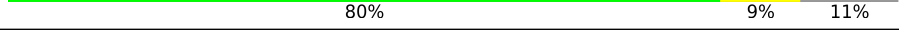
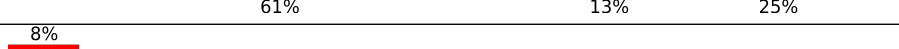
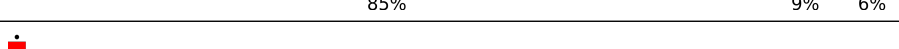
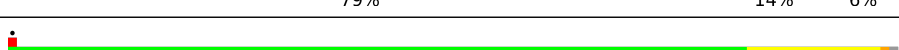

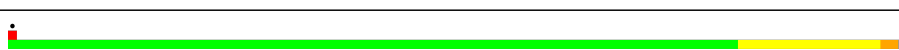

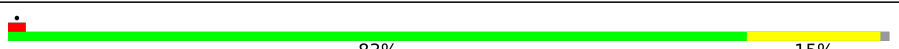





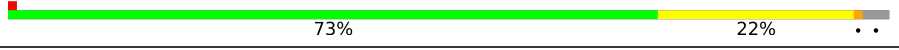
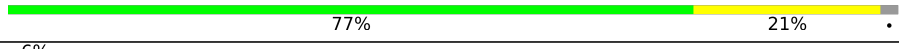



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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	S2	1869	
2	Ln	25	
3	SE	263	

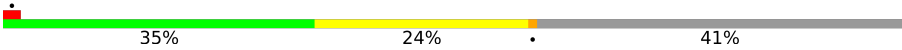

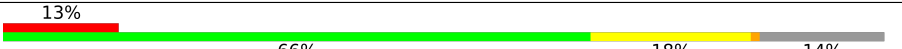
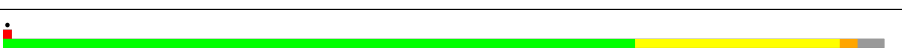
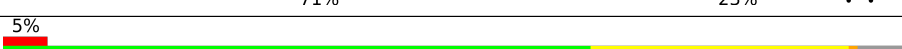
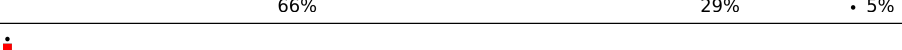
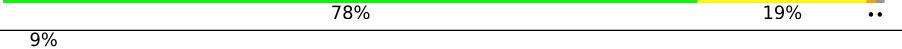

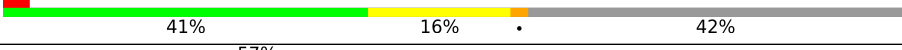

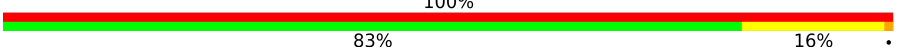

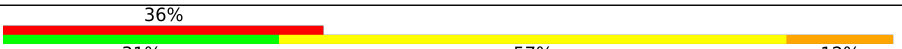
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Mol	Chain	Length	Quality of chain
4	SA	295	
5	SB	264	
6	SH	194	
7	SI	208	
8	SL	158	
9	SV	83	
10	SX	143	
11	Sa	115	
12	SC	293	
13	SG	249	
14	SJ	194	
15	SN	151	
16	SO	151	
17	SW	130	
18	SY	133	
19	Sb	84	
20	Se	133	
21	B	50	
22	SD	243	
23	SF	204	
24	Sf	156	
25	SR	135	
26	Sd	56	
27	Sg	317	
28	Sc	69	

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Mol	Chain	Length	Quality of chain
29	SK	165	
30	SM	132	
31	SU	119	
32	SQ	146	
33	SS	152	
34	ST	145	
35	SP	145	
36	SZ	125	
37	D	315	
38	E	472	
39	F	333	
40	G	75	
41	H	144	

## 2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 85890 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1740	Total	C	N	O	P	0	0
			36955	16511	6600	12105	1739		

- Molecule 2 is a protein called 60S ribosomal protein L41.

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

- Molecule 3 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SA	219	Total	C	N	O	S	0	0
			1727	1096	302	320	9		

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	215	Total	C	N	O	S	0	0
			1747	1109	312	312	14		

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SH	189	Total	C	N	O	S	0	0
			1523	972	280	270	1		

- Molecule 7 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 8 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SL	154	Total	C	N	O	S	0	0
			1258	802	235	215	6		

- Molecule 9 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 10 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 11 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 12 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SC	220	Total	C	N	O	S	0	0
			1709	1106	294	299	10		

- Molecule 13 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SG	234	Total	C	N	O	S	0	0
			1903	1188	384	324	7		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SJ	182	Total	C	N	O	S	0	0
			1512	962	303	245	2		

- Molecule 15 is a protein called 40S ribosomal protein S13.

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

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SO	138	IAS	ASP	conflict	UNP P62263

- Molecule 17 is a protein called 40S ribosomal protein S15a.

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

- Molecule 18 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SY	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 19 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 20 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Se	59	Total	C	N	O	S	0	0
			468	290	102	75	1		

- Molecule 21 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	28	Total	C	N	O	P	0	0
			594	267	109	190	28		

- Molecule 22 is a protein called 40S ribosomal protein S3.

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

- Molecule 23 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 24 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 25 is a protein called 40S ribosomal protein S17.

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

- Molecule 26 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 27 is a protein called Receptor of activated protein C kinase 1.



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

- Molecule 28 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 29 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SK	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 30 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SM	118	Total	C	N	O	S	0	0
			906	568	158	172	8		

- Molecule 31 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SU	102	Total	C	N	O	S	0	0
			811	508	154	145	4		

- Molecule 32 is a protein called 40S ribosomal protein S16.

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

- Molecule 33 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 34 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	ST	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 35 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SP	134	Total	C	N	O	S	0	0
			1103	703	208	185	7		

- Molecule 36 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SZ	73	Total	C	N	O	S	0	0
			585	374	108	102	1		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	D	292	Total	C	N	O	S	0	0
			2352	1477	411	451	13		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	E	472	Total	C	N	O	S	0	0
			3585	2272	628	667	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	F	16	Total	C	N	O	S	0	0
			143	91	25	26	1		

- Molecule 40 is a RNA chain called initiator tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	G	75	Total	C	N	O	P	1	0
			1623	728	299	521	75		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	H	115	Total	C	N	O	S	0	0
			918	568	177	169	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	70	ALA	TRP	conflict	UNP P47813

- Molecule 42 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
42	S2	17	Total	K	0
			17	17	
42	Sd	1	Total	K	0
			1	1	

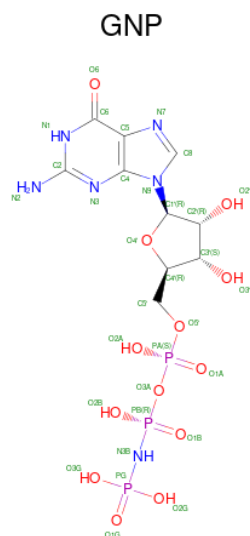
- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	S2	78	Total	Mg	0
			78	78	
43	SN	1	Total	Mg	0
			1	1	
43	B	4	Total	Mg	0
			4	4	

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

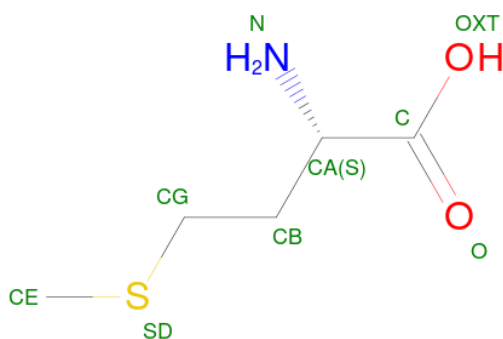
Mol	Chain	Residues	Atoms		AltConf
44	Sa	1	Total	Zn	0
			1	1	
44	Sf	1	Total	Zn	0
			1	1	
44	Sd	1	Total	Zn	0
			1	1	

- Molecule 45 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
45	E	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 46 is METHIONINE (CCD ID: MET) (formula:  $\text{C}_5\text{H}_{11}\text{NO}_2\text{S}$ ).

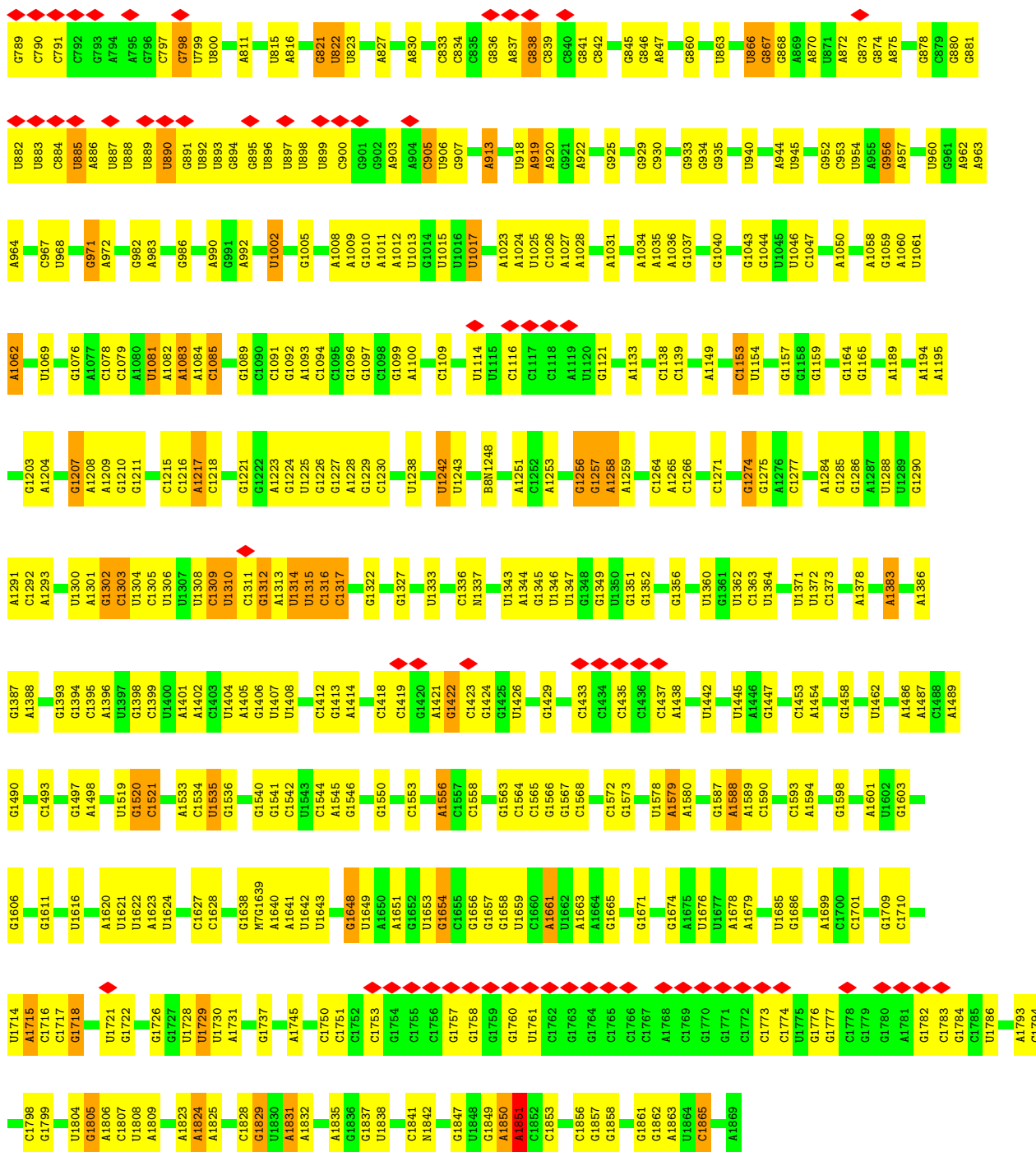


Mol	Chain	Residues	Atoms					AltConf
46	E	1	Total	C	N	O	S	0
			8	5	1	1	1	

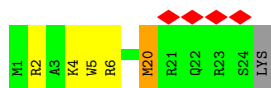
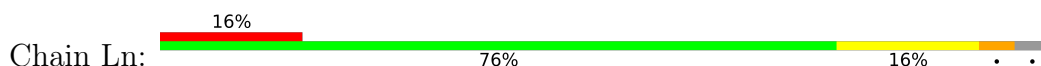
- Molecule 47 is water.

Mol	Chain	Residues	Atoms		AltConf
47	S2	349	Total 349	O 349	0
47	SE	2	Total 2	O 2	0
47	SL	2	Total 2	O 2	0
47	SX	1	Total 1	O 1	0
47	Sa	3	Total 3	O 3	0
47	SC	1	Total 1	O 1	0
47	SN	1	Total 1	O 1	0
47	SO	2	Total 2	O 2	0
47	SS	1	Total 1	O 1	0
47	ST	1	Total 1	O 1	0




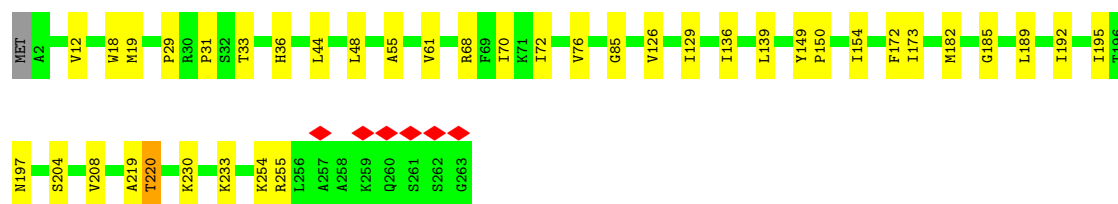


- Molecule 2: 60S ribosomal protein L41



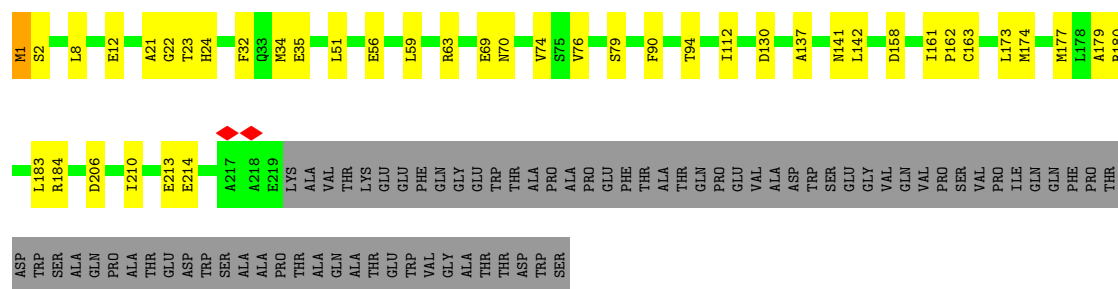
- Molecule 3: Small ribosomal subunit protein eS4, X isoform

Chain SE:  85% 14%



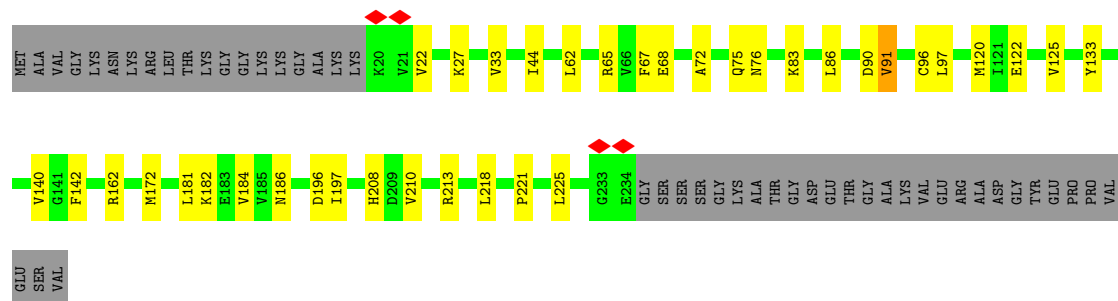
- Molecule 4: 40S ribosomal protein SA

Chain SA:  60% 14% 26%




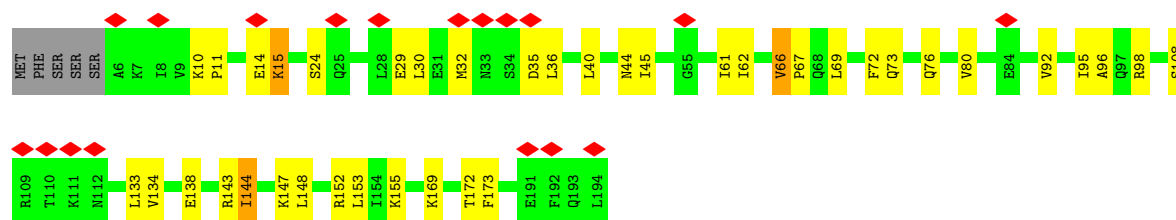
- Molecule 5: 40S ribosomal protein S3a

Chain SB:  67% 14% 19%




- Molecule 6: 40S ribosomal protein S7

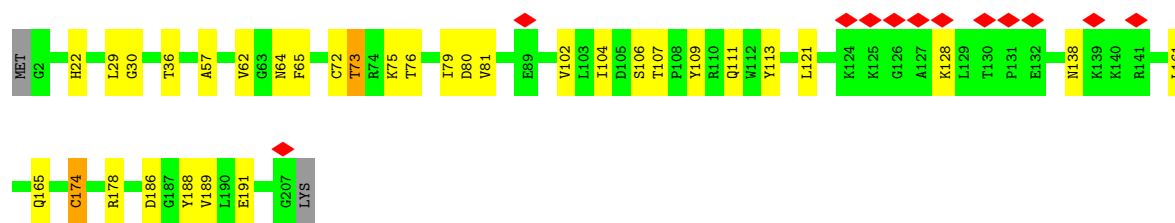
Chain SH:  9% 77% 19%



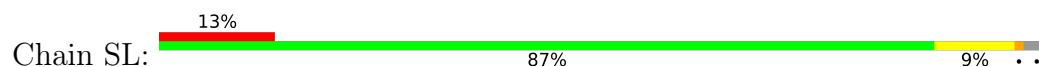
- Molecule 7: 40S ribosomal protein S8

Chain SI:  6% 83% 15%

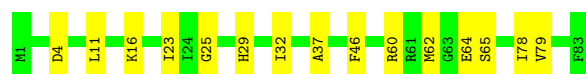
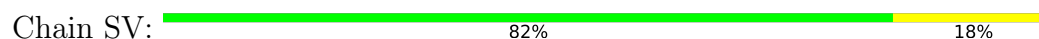




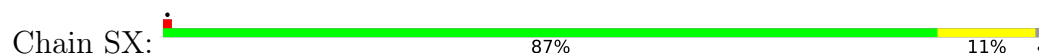
- Molecule 8: Small ribosomal subunit protein uS17



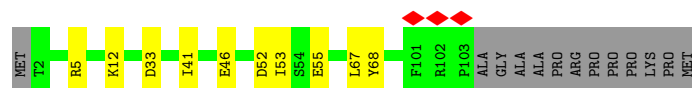
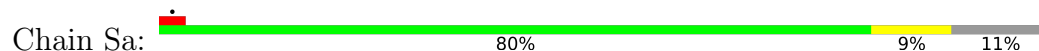
- Molecule 9: 40S ribosomal protein S21



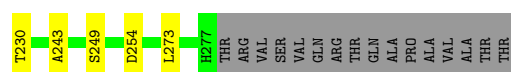
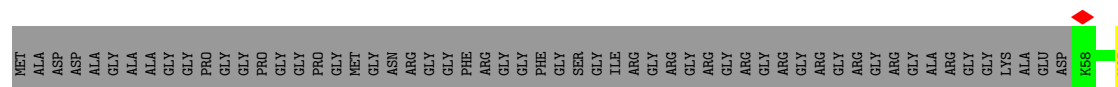
- Molecule 10: 40S ribosomal protein S23



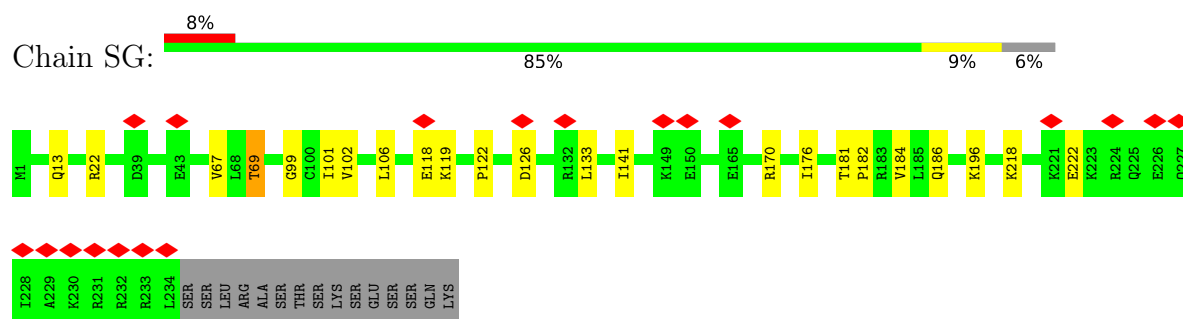
- Molecule 11: 40S ribosomal protein S26



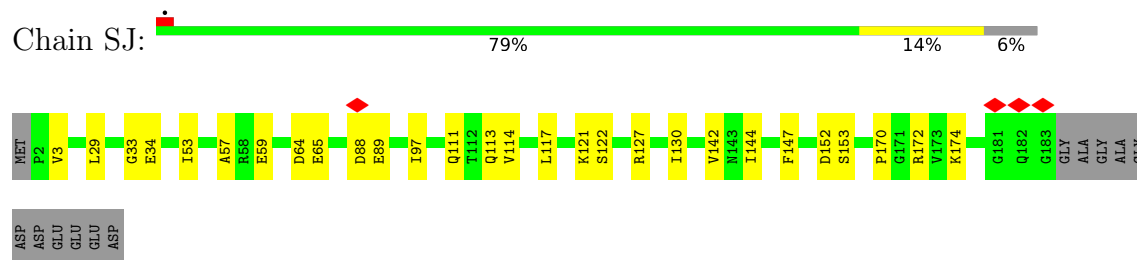
- Molecule 12: 40S ribosomal protein S2



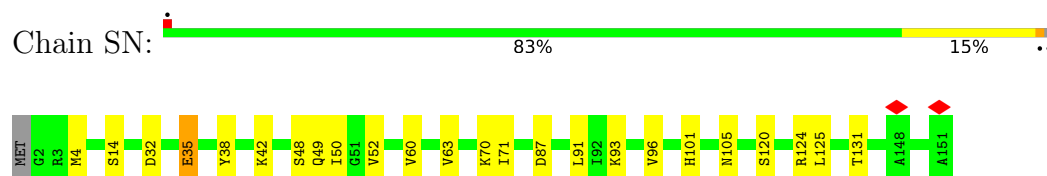
- Molecule 13: 40S ribosomal protein S6



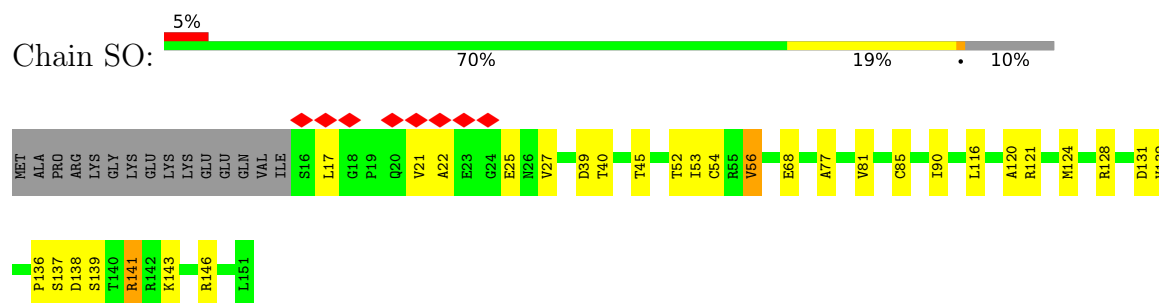
- Molecule 14: 40S ribosomal protein S9



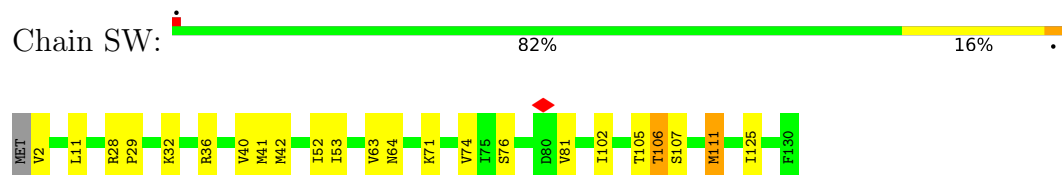
- Molecule 15: 40S ribosomal protein S13



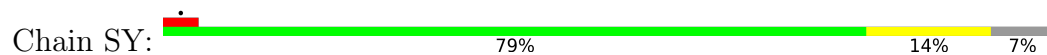
- Molecule 16: 40S ribosomal protein S14



- Molecule 17: 40S ribosomal protein S15a

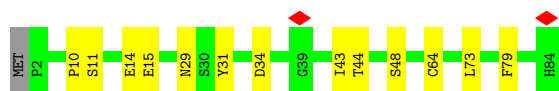
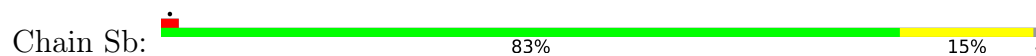


- Molecule 18: 40S ribosomal protein S24

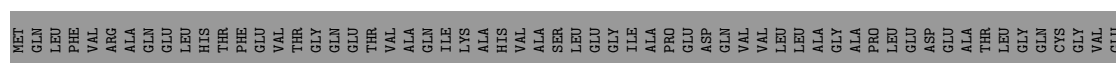
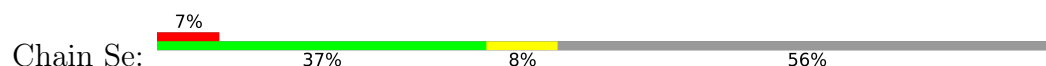




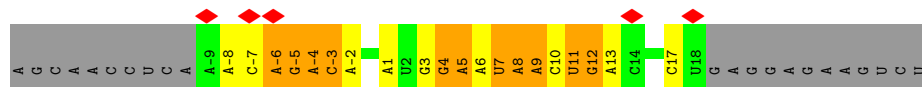
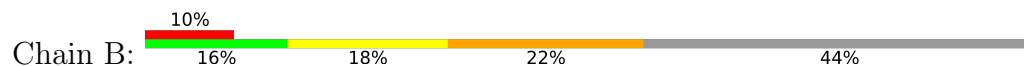
- Molecule 19: 40S ribosomal protein S27



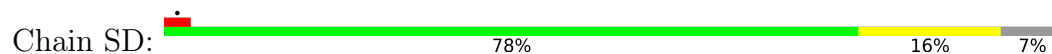
- Molecule 20: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



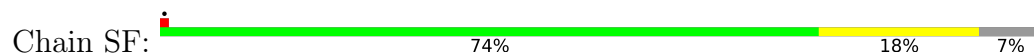
- Molecule 21: mRNA



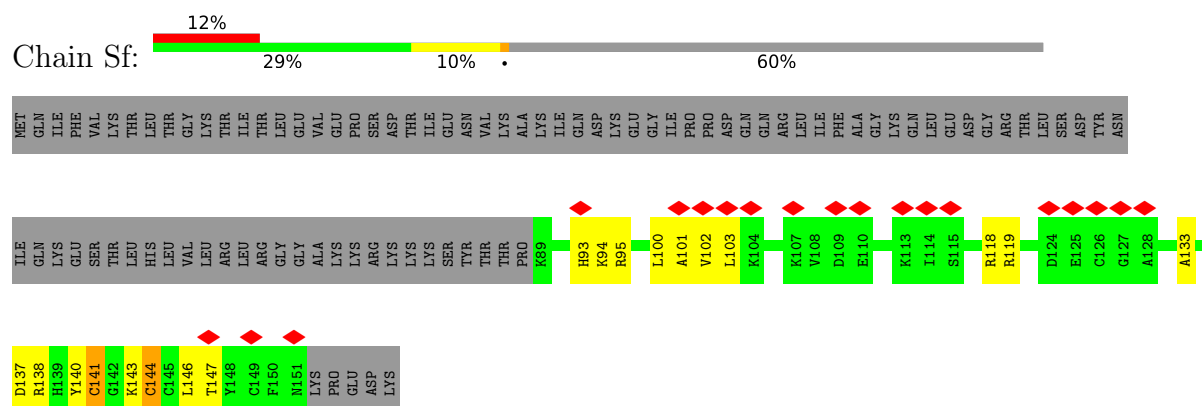
- Molecule 22: 40S ribosomal protein S3



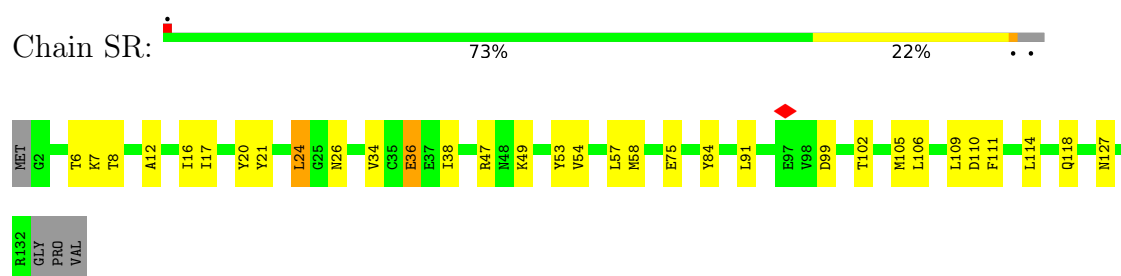
- Molecule 23: 40S ribosomal protein S5



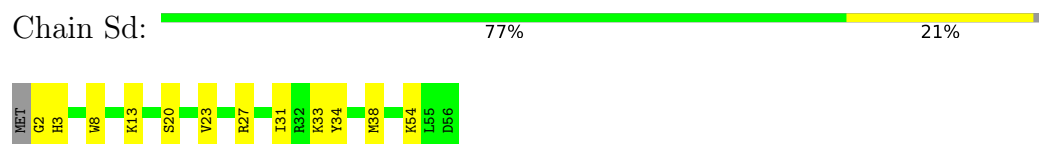
- Molecule 24: Ubiquitin



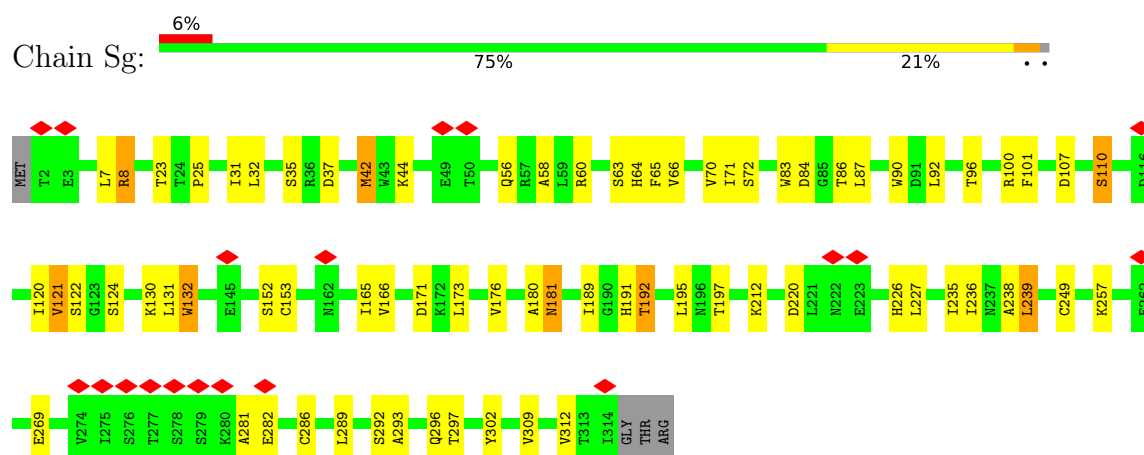
- Molecule 25: 40S ribosomal protein S17



- Molecule 26: 40S ribosomal protein S29



- Molecule 27: Receptor of activated protein C kinase 1

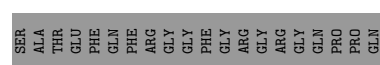
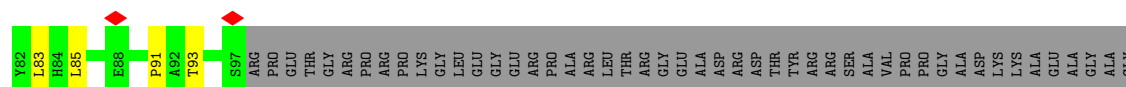
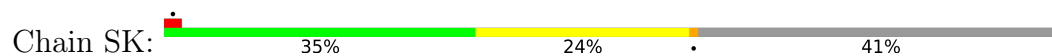


- Molecule 28: 40S ribosomal protein S28

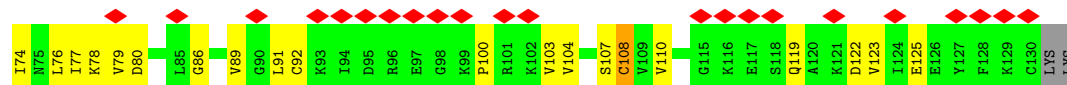
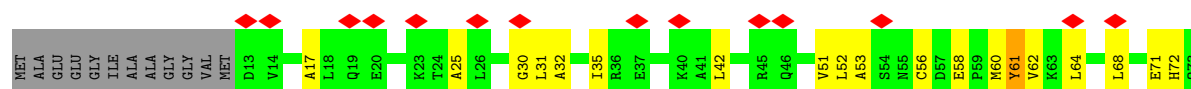




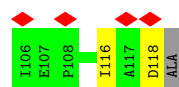
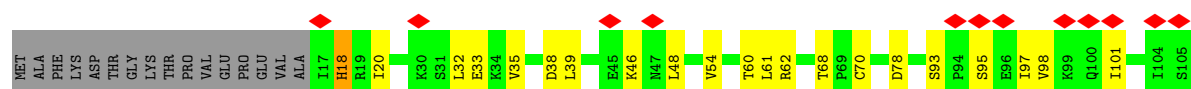
- Molecule 29: 40S ribosomal protein S10



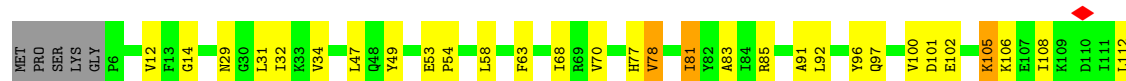
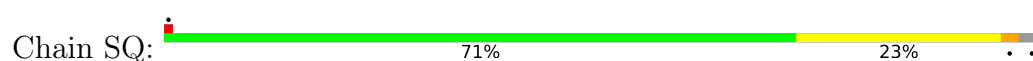
- Molecule 30: 40S ribosomal protein S12



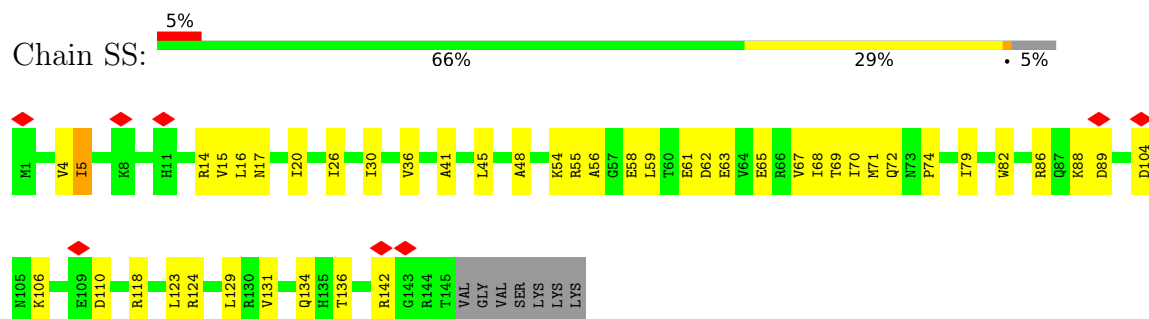
- Molecule 31: 40S ribosomal protein S20



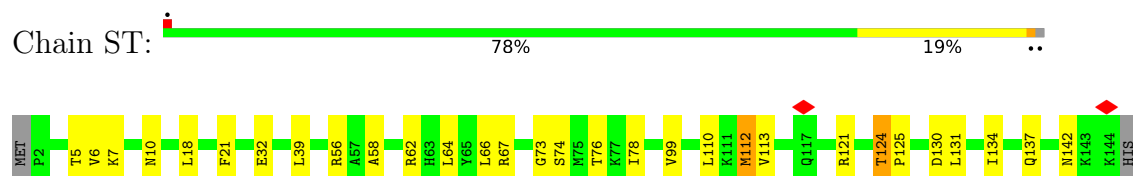
- Molecule 32: 40S ribosomal protein S16



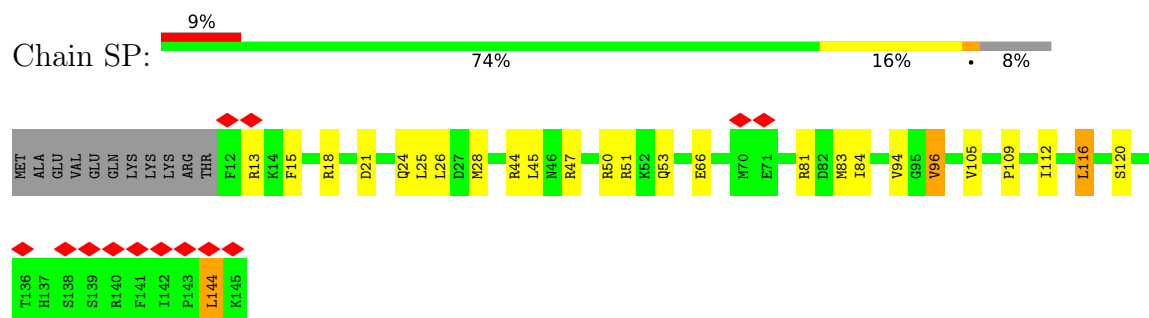
- Molecule 33: 40S ribosomal protein S18



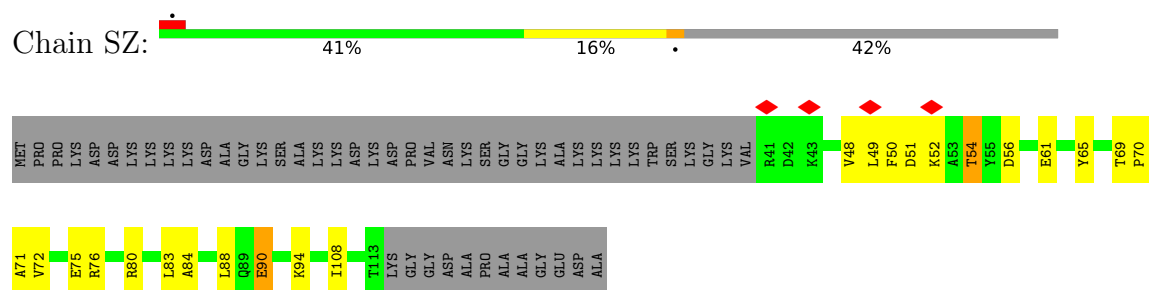
- Molecule 34: Small ribosomal subunit protein eS19



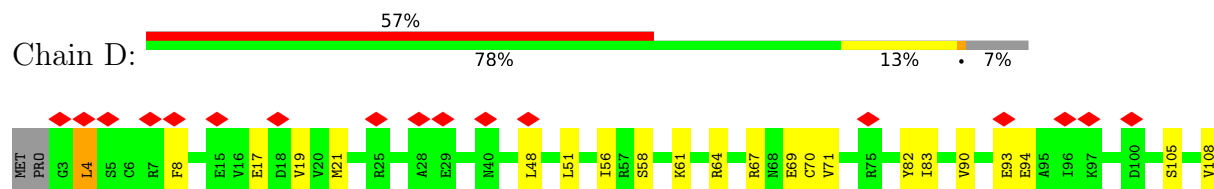
- Molecule 35: 40S ribosomal protein S15

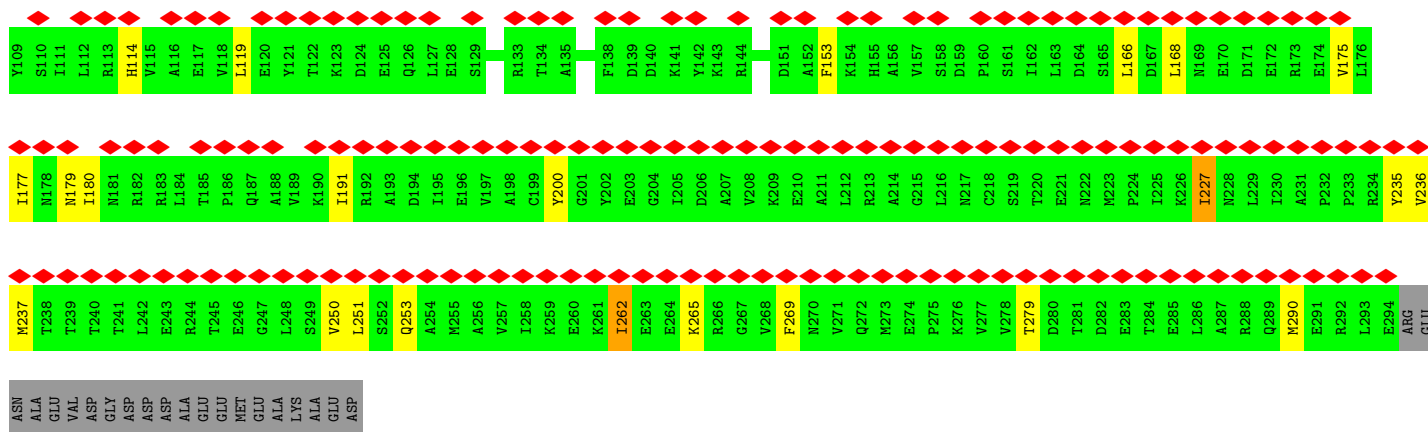


- Molecule 36: Small ribosomal subunit protein eS25

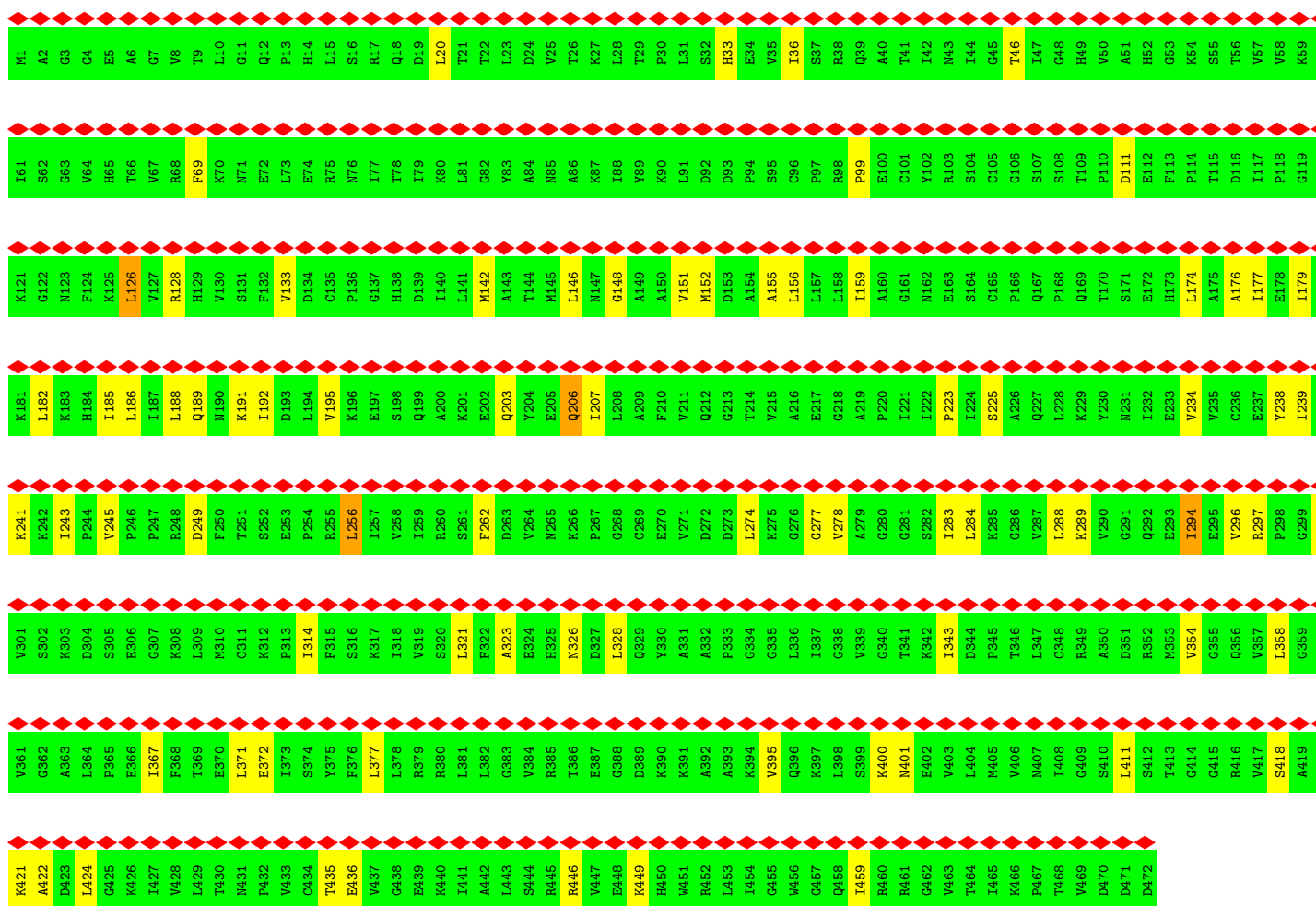
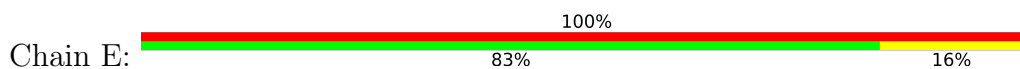


- Molecule 37: Eukaryotic translation initiation factor 2 subunit 1





• Molecule 38: Eukaryotic translation initiation factor 2 subunit 3



• Molecule 39: Eukaryotic translation initiation factor 2 subunit 2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30727	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	43.556	Depositor
Minimum map value	-18.915	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.307	Depositor
Recommended contour level	4.72	Depositor
Map size (Å)	374.40002, 374.40002, 374.40002	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72, 0.72, 0.72	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, 6MZ, OMU, T6A, GNP, H2U, ZN, IAS, NMM, UY1, MA6, MG, 4AC, 1MA, PSU, 1MG, OMG, OMC, K, 2MG, M7G, 5MC, A2M

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	S2	0.36	0/39125	0.32	0/60957
2	Ln	0.28	0/231	0.38	0/294
3	SE	0.29	0/2118	0.35	0/2849
4	SA	0.35	0/1764	0.43	0/2396
5	SB	0.30	0/1774	0.37	0/2373
6	SH	0.24	0/1546	0.40	0/2071
7	SI	0.28	0/1715	0.38	0/2287
8	SL	0.30	0/1280	0.37	0/1712
9	SV	0.32	0/643	0.36	0/860
10	SX	0.29	0/1116	0.35	0/1490
11	Sa	0.32	0/836	0.37	0/1121
12	SC	0.34	0/1746	0.37	0/2358
13	SG	0.24	0/1926	0.34	0/2563
14	SJ	0.30	0/1537	0.37	0/2052
15	SN	0.30	0/1232	0.38	0/1656
16	SO	0.34	0/1020	0.51	1/1366 (0.1%)
17	SW	0.35	0/1051	0.40	0/1406
18	SY	0.26	0/1031	0.35	0/1370
19	Sb	0.28	0/665	0.38	0/891
20	Se	0.28	0/474	0.39	0/623
21	B	0.26	0/664	0.40	0/1031
22	SD	0.29	0/1793	0.37	0/2414
23	SF	0.30	0/1516	0.40	0/2037
24	Sf	0.21	0/525	0.43	0/695
25	SR	0.30	0/1078	0.46	0/1447
26	Sd	0.33	0/470	0.43	0/623
27	Sg	0.27	0/2493	0.40	0/3394
28	Sc	0.31	0/508	0.36	0/680
29	SK	0.31	0/840	0.43	0/1133
30	SM	0.19	0/916	0.39	0/1233
31	SU	0.29	0/821	0.42	0/1103

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	SQ	0.32	0/1142	0.41	0/1528
33	SS	0.27	0/1216	0.39	0/1628
34	ST	0.28	0/1119	0.38	0/1498
35	SP	0.26	0/1126	0.37	0/1505
36	SZ	0.26	0/591	0.43	0/794
37	D	0.18	0/2384	0.34	0/3213
38	E	0.15	0/3643	0.33	0/4929
39	F	0.13	0/144	0.33	0/191
40	G	0.24	0/1600	0.30	0/2492
41	H	0.17	0/927	0.39	0/1230
All	All	0.32	0/88346	0.35	1/127493 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	SO	141	ARG	O-C-N	6.81	131.20	122.89

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36955	0	18673	379	0
2	Ln	230	0	276	4	0
3	SE	2076	0	2177	27	0
4	SA	1727	0	1729	44	0
5	SB	1747	0	1822	29	0
6	SH	1523	0	1622	37	0
7	SI	1686	0	1772	20	0
8	SL	1258	0	1332	9	0
9	SV	636	0	637	11	0
10	SX	1098	0	1167	10	0
11	Sa	821	0	870	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	SC	1709	0	1797	25	0
13	SG	1903	0	2068	15	0
14	SJ	1512	0	1629	20	0
15	SN	1208	0	1294	15	0
16	SO	1016	0	1038	29	0
17	SW	1034	0	1080	19	0
18	SY	1014	0	1082	14	0
19	Sb	651	0	672	9	0
20	Se	468	0	519	6	0
21	B	594	0	304	16	0
22	SD	1765	0	1865	36	0
23	SF	1495	0	1549	23	0
24	Sf	515	0	522	18	0
25	SR	1064	0	1118	29	0
26	Sd	459	0	448	10	0
27	Sg	2436	0	2393	45	0
28	Sc	506	0	536	21	0
29	SK	816	0	841	32	0
30	SM	906	0	921	31	0
31	SU	811	0	877	18	0
32	SQ	1124	0	1193	31	0
33	SS	1198	0	1261	34	0
34	ST	1113	0	1145	19	0
35	SP	1103	0	1156	17	0
36	SZ	585	0	640	17	0
37	D	2352	0	2392	30	0
38	E	3585	0	3736	50	0
39	F	143	0	144	2	0
40	G	1623	0	829	25	0
41	H	918	0	950	14	0
42	S2	17	0	0	0	0
42	Sd	1	0	0	0	0
43	B	4	0	0	0	0
43	S2	78	0	0	0	0
43	SN	1	0	0	0	0
44	Sa	1	0	0	0	0
44	Sd	1	0	0	0	0
44	Sf	1	0	0	0	0
45	E	32	0	13	0	0
46	E	8	0	8	0	0
47	S2	349	0	0	3	0
47	SC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	SE	2	0	0	0	0
47	SL	2	0	0	0	0
47	SN	1	0	0	0	0
47	SO	2	0	0	0	0
47	SS	1	0	0	0	0
47	ST	1	0	0	0	0
47	SX	1	0	0	0	0
47	Sa	3	0	0	0	0
All	All	85890	0	68097	1116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1116 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:670:A:P	47:S2:2006:HOH:O	2.20	0.98
1:S2:1519:U:P	47:S2:2005:HOH:O	2.33	0.85
37:D:56:ILE:HD12	37:D:56:ILE:O	1.76	0.85
38:E:156:LEU:HD12	38:E:188:LEU:HD21	1.63	0.80
2:Ln:20:MET:HA	2:Ln:20:MET:HE2	1.61	0.80

There are no symmetry-related clashes.

## 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	
2	Ln	22/25 (88%)	22 (100%)	0	0	100	100
3	SE	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
4	SA	217/295 (74%)	197 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SB	213/264 (81%)	200 (94%)	12 (6%)	1 (0%)	24	59
6	SH	187/194 (96%)	170 (91%)	16 (9%)	1 (0%)	24	59
7	SI	204/208 (98%)	188 (92%)	16 (8%)	0	100	100
8	SL	152/158 (96%)	135 (89%)	15 (10%)	2 (1%)	9	40
9	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
10	SX	139/143 (97%)	134 (96%)	5 (4%)	0	100	100
11	Sa	100/115 (87%)	91 (91%)	9 (9%)	0	100	100
12	SC	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
13	SG	232/249 (93%)	223 (96%)	9 (4%)	0	100	100
14	SJ	180/194 (93%)	170 (94%)	9 (5%)	1 (1%)	21	56
15	SN	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
16	SO	132/151 (87%)	116 (88%)	16 (12%)	0	100	100
17	SW	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
18	SY	122/133 (92%)	121 (99%)	1 (1%)	0	100	100
19	Sb	81/84 (96%)	71 (88%)	10 (12%)	0	100	100
20	Se	57/133 (43%)	49 (86%)	7 (12%)	1 (2%)	6	34
22	SD	225/243 (93%)	215 (96%)	10 (4%)	0	100	100
23	SF	187/204 (92%)	175 (94%)	11 (6%)	1 (0%)	24	59
24	Sf	61/156 (39%)	54 (88%)	7 (12%)	0	100	100
25	SR	129/135 (96%)	123 (95%)	6 (5%)	0	100	100
26	Sd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
27	Sg	311/317 (98%)	286 (92%)	25 (8%)	0	100	100
28	Sc	62/69 (90%)	53 (86%)	9 (14%)	0	100	100
29	SK	95/165 (58%)	88 (93%)	7 (7%)	0	100	100
30	SM	116/132 (88%)	106 (91%)	9 (8%)	1 (1%)	14	47
31	SU	100/119 (84%)	90 (90%)	10 (10%)	0	100	100
32	SQ	139/146 (95%)	129 (93%)	10 (7%)	0	100	100
33	SS	143/152 (94%)	135 (94%)	8 (6%)	0	100	100
34	ST	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
35	SP	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
36	SZ	71/125 (57%)	70 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	D	290/315 (92%)	276 (95%)	14 (5%)	0	100	100
38	E	470/472 (100%)	449 (96%)	20 (4%)	1 (0%)	43	73
39	F	14/333 (4%)	13 (93%)	1 (7%)	0	100	100
41	H	113/144 (78%)	94 (83%)	18 (16%)	1 (1%)	14	47
All	All	5723/6839 (84%)	5352 (94%)	361 (6%)	10 (0%)	44	73

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	SB	22	VAL
6	SH	15	LYS
20	Se	2	VAL
30	SM	80	ASP
41	H	84	TYR

### 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	Ln	23/24 (96%)	22 (96%)	1 (4%)	26	59
3	SE	224/225 (100%)	221 (99%)	3 (1%)	61	78
4	SA	182/243 (75%)	180 (99%)	2 (1%)	65	79
5	SB	196/231 (85%)	192 (98%)	4 (2%)	48	72
6	SH	169/174 (97%)	165 (98%)	4 (2%)	43	70
7	SI	178/180 (99%)	171 (96%)	7 (4%)	28	62
8	SL	138/142 (97%)	136 (99%)	2 (1%)	59	77
9	SV	67/67 (100%)	67 (100%)	0	100	100
10	SX	113/115 (98%)	112 (99%)	1 (1%)	70	81
11	Sa	89/98 (91%)	88 (99%)	1 (1%)	65	79
12	SC	186/225 (83%)	179 (96%)	7 (4%)	29	62
13	SG	204/218 (94%)	202 (99%)	2 (1%)	68	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	SJ	161/168 (96%)	159 (99%)	2 (1%)	63	79
15	SN	130/131 (99%)	126 (97%)	4 (3%)	35	66
16	SO	105/118 (89%)	103 (98%)	2 (2%)	50	73
17	SW	112/113 (99%)	108 (96%)	4 (4%)	31	63
18	SY	108/115 (94%)	105 (97%)	3 (3%)	38	68
19	Sb	75/76 (99%)	72 (96%)	3 (4%)	28	61
20	Se	48/104 (46%)	46 (96%)	2 (4%)	26	60
22	SD	190/202 (94%)	187 (98%)	3 (2%)	55	75
23	SF	159/170 (94%)	158 (99%)	1 (1%)	78	84
24	Sf	56/140 (40%)	51 (91%)	5 (9%)	9	34
25	SR	119/122 (98%)	115 (97%)	4 (3%)	32	64
26	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	71
27	Sg	272/275 (99%)	259 (95%)	13 (5%)	23	56
28	Sc	57/62 (92%)	56 (98%)	1 (2%)	51	74
29	SK	88/136 (65%)	84 (96%)	4 (4%)	24	58
30	SM	98/108 (91%)	95 (97%)	3 (3%)	35	66
31	SU	94/107 (88%)	93 (99%)	1 (1%)	65	79
32	SQ	117/121 (97%)	111 (95%)	6 (5%)	21	54
33	SS	126/132 (96%)	118 (94%)	8 (6%)	16	48
34	ST	112/114 (98%)	107 (96%)	5 (4%)	24	58
35	SP	120/130 (92%)	115 (96%)	5 (4%)	26	60
36	SZ	65/103 (63%)	60 (92%)	5 (8%)	12	41
37	D	262/280 (94%)	256 (98%)	6 (2%)	44	70
38	E	397/397 (100%)	388 (98%)	9 (2%)	44	70
39	F	16/304 (5%)	15 (94%)	1 (6%)	16	48
41	H	96/122 (79%)	96 (100%)	0	100	100
All	All	5000/5841 (86%)	4865 (97%)	135 (3%)	40	68

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	SZ	65	TYR
37	D	4	LEU

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Mol	Chain	Res	Type
38	E	256	LEU
18	SY	125	VAL
18	SY	68	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
36	SZ	64	ASN
37	D	23	ASN
38	E	33	HIS
12	SC	178	HIS
12	SC	120	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1713/1869 (91%)	337 (19%)	9 (0%)
21	B	27/50 (54%)	15 (55%)	2 (7%)
40	G	72/75 (96%)	27 (37%)	1 (1%)
All	All	1812/1994 (90%)	379 (20%)	12 (0%)

5 of 379 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	4	C
1	S2	17	C
1	S2	26	U
1	S2	33	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	1316	C
1	S2	1520	G
40	G	52	G
21	B	-5	G
1	S2	690	G

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

100 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	OMU	S2	121	1	19,22,23	0.38	0	26,31,34	0.52	0
1	PSU	S2	1186	1	18,21,22	0.61	0	22,30,33	0.60	0
1	PSU	S2	1596	1	18,21,22	0.60	0	22,30,33	0.55	0
1	PSU	S2	1367	1	18,21,22	0.62	0	22,30,33	0.58	0
1	PSU	S2	918	1	18,21,22	0.46	0	22,30,33	0.38	0
1	A2M	S2	27	1	22,25,26	0.14	0	31,36,39	0.28	0
1	PSU	S2	966	1	18,21,22	0.55	0	22,30,33	0.59	0
1	OMU	S2	428	1	19,22,23	0.31	0	26,31,34	0.42	0
1	OMG	S2	1328	42,1	23,26,27	0.35	0	33,38,41	0.37	0
1	PSU	S2	815	1	18,21,22	0.59	0	22,30,33	0.55	0
1	PSU	S2	801	1	18,21,22	0.62	0	22,30,33	0.62	0
1	PSU	S2	1174	1	18,21,22	0.61	0	22,30,33	0.61	0
1	OMG	S2	644	1	23,26,27	0.38	0	33,38,41	0.45	0
1	OMC	S2	1391	1	19,22,23	0.36	0	26,31,34	0.49	0
1	PSU	S2	105	1	18,21,22	0.58	0	22,30,33	0.60	0
1	PSU	S2	100	1	18,21,22	0.56	0	22,30,33	0.60	0
1	OMG	S2	509	43,1	23,26,27	0.43	0	33,38,41	0.51	0
1	OMC	S2	462	1	19,22,23	0.33	0	26,31,34	0.46	0
1	PSU	S2	651	1	18,21,22	0.62	0	22,30,33	0.56	0
1	PSU	S2	36	1	18,21,22	0.60	0	22,30,33	0.54	0
1	OMC	S2	517	1	19,22,23	0.35	0	26,31,34	0.47	0
1	B8N	S2	1248	1	24,29,30	0.66	1 (4%)	29,42,45	0.62	0
1	PSU	S2	1692	1	18,21,22	0.62	0	22,30,33	0.59	0
1	A2M	S2	576	1	22,25,26	0.13	0	31,36,39	0.43	0
1	PSU	S2	34	1	18,21,22	0.58	0	22,30,33	0.63	0
1	OMU	S2	116	1	19,22,23	0.33	0	26,31,34	0.48	0
1	PSU	S2	296	1	18,21,22	0.58	0	22,30,33	0.58	0
1	PSU	S2	300	1	18,21,22	0.53	0	22,30,33	0.59	0
1	PSU	S2	1177	1	18,21,22	0.58	0	22,30,33	0.65	0
1	PSU	S2	1643	43,1	18,21,22	0.68	1 (5%)	22,30,33	0.53	0
40	5MC	G	48	40	18,22,23	0.48	0	26,32,35	0.55	0
1	PSU	S2	406	1	18,21,22	0.58	0	22,30,33	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	S2	1003	1	18,21,22	0.62	0	22,30,33	0.56	0
1	PSU	S2	1056	1	18,21,22	0.64	0	22,30,33	0.59	0
1	OMG	S2	601	1	23,26,27	0.41	0	33,38,41	0.32	0
40	2MG	G	26	40	23,26,27	0.34	0	32,38,41	0.37	0
34	NMM	ST	67	34	9,11,12	0.61	0	6,12,14	2.04	2 (33%)
1	PSU	S2	93	1	18,21,22	0.65	0	22,30,33	0.53	0
40	1MG	G	10	40	22,26,27	0.30	0	33,39,42	0.60	1 (3%)
1	PSU	S2	681	1	18,21,22	0.67	0	22,30,33	0.51	0
1	OMC	S2	1272	1	19,22,23	0.37	0	26,31,34	0.41	0
1	4AC	S2	1842	1	21,24,25	0.39	0	29,34,37	0.39	0
1	OMU	S2	1288	1	19,22,23	0.34	0	26,31,34	0.44	0
1	PSU	S2	119	1	18,21,22	0.57	0	22,30,33	0.58	0
1	A2M	S2	468	1	22,25,26	0.12	0	31,36,39	0.42	0
1	PSU	S2	822	1	18,21,22	0.62	1 (5%)	22,30,33	0.56	0
1	PSU	S2	863	1	18,21,22	0.65	1 (5%)	22,30,33	0.51	0
1	OMG	S2	436	1	23,26,27	0.40	0	33,38,41	0.53	0
1	OMC	S2	174	1	19,22,23	0.34	0	26,31,34	0.40	0
1	OMU	S2	172	1	19,22,23	0.29	0	26,31,34	0.52	0
1	PSU	S2	218	1	18,21,22	0.56	0	22,30,33	0.56	0
1	A2M	S2	166	1	22,25,26	0.16	0	31,36,39	0.53	0
1	OMC	S2	1703	43,1	19,22,23	0.32	0	26,31,34	0.45	0
1	PSU	S2	649	1	18,21,22	0.59	0	22,30,33	0.65	0
1	PSU	S2	1625	1	18,21,22	0.58	0	22,30,33	0.63	0
1	PSU	S2	63	1	18,21,22	0.58	0	22,30,33	0.64	0
1	PSU	S2	866	1	18,21,22	0.48	0	22,30,33	0.76	0
1	PSU	S2	109	1	18,21,22	0.63	0	22,30,33	0.57	0
1	A2M	S2	484	1	22,25,26	0.11	0	31,36,39	0.18	0
1	PSU	S2	1045	1	18,21,22	0.55	0	22,30,33	0.65	0
1	PSU	S2	1232	1	18,21,22	0.60	0	22,30,33	0.65	0
40	1MA	G	58	40	21,25,26	0.48	0	31,37,40	0.74	1 (3%)
1	OMG	S2	683	1	23,26,27	0.42	0	33,38,41	0.48	0
1	A2M	S2	1678	1	22,25,26	0.13	0	31,36,39	0.32	0
1	OMG	S2	867	1	23,26,27	0.31	0	33,38,41	0.44	0
1	PSU	S2	1244	1	18,21,22	0.60	0	22,30,33	0.56	0
1	OMG	S2	1490	43,1	23,26,27	0.45	0	33,38,41	0.36	0
1	MA6	S2	1850	1	23,26,27	0.37	0	34,38,41	0.60	1 (2%)
1	PSU	S2	1360	42,1	18,21,22	0.74	1 (5%)	22,30,33	0.63	0
1	MA6	S2	1851	1	23,26,27	0.38	0	34,38,41	0.65	1 (2%)
40	H2U	G	47	40	18,21,22	0.35	0	21,30,33	0.46	0
1	OMG	S2	1447	1	23,26,27	0.39	0	33,38,41	0.43	0
1	PSU	S2	366	1	18,21,22	0.74	1 (5%)	22,30,33	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	S2	686	1	18,21,22	0.62	0	22,30,33	0.56	0
1	PSU	S2	1004	1	18,21,22	0.59	0	22,30,33	0.58	0
1	PSU	S2	609	1	18,21,22	0.59	0	22,30,33	0.60	0
1	A2M	S2	159	1	22,25,26	0.12	0	31,36,39	0.25	0
1	A2M	S2	99	43,1	22,25,26	0.13	0	31,36,39	0.47	0
1	PSU	S2	667	1	18,21,22	0.69	1 (5%)	22,30,33	0.55	0
1	UY1	S2	1326	43,1	19,22,23	0.46	0	22,31,34	0.47	0
1	PSU	S2	814	1	18,21,22	0.60	0	22,30,33	0.59	0
1	A2M	S2	1031	1	22,25,26	0.15	0	31,36,39	0.33	0
1	PSU	S2	1238	1	18,21,22	0.59	0	22,30,33	0.56	0
1	A2M	S2	668	1	22,25,26	0.18	0	31,36,39	0.33	0
1	PSU	S2	1046	1	18,21,22	0.62	1 (5%)	22,30,33	0.55	0
1	PSU	S2	1136	1	18,21,22	0.62	0	22,30,33	0.61	0
1	PSU	S2	572	1	18,21,22	0.64	1 (5%)	22,30,33	0.56	1 (4%)
16	IAS	SO	138	16	6,7,8	1.05	0	6,8,10	1.67	3 (50%)
40	T6A	G	37	40	31,34,35	0.48	0	44,49,52	0.45	0
1	4AC	S2	1337	1	21,24,25	0.41	0	29,34,37	0.41	0
1	OMU	S2	1442	43,1	19,22,23	0.35	0	26,31,34	0.40	0
1	A2M	S2	1383	1	22,25,26	0.19	0	31,36,39	0.59	1 (3%)
1	OMU	S2	1804	1	19,22,23	0.30	0	26,31,34	0.49	0
1	A2M	S2	590	1	22,25,26	0.14	0	31,36,39	0.28	0
1	PSU	S2	1445	1	18,21,22	0.66	1 (5%)	22,30,33	0.59	0
1	6MZ	S2	1832	42,43,1	22,25,26	0.17	0	30,36,39	0.29	0
1	A2M	S2	512	1	22,25,26	0.14	0	31,36,39	0.48	0
1	PSU	S2	1347	1	18,21,22	0.73	0	22,30,33	0.59	0
1	OMU	S2	354	1	19,22,23	0.35	0	26,31,34	0.72	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	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1186	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1596	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	918	1	-	2/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	966	1	-	1/7/25/26	0/2/2/2
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	S2	1328	42,1	-	0/9/27/28	0/3/3/3
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1174	1	-	1/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	2/9/27/28	0/3/3/3
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	100	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	43,1	-	0/9/27/28	0/3/3/3
1	OMC	S2	462	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	B8N	S2	1248	1	-	8/16/34/35	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	116	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	300	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1643	43,1	-	0/7/25/26	0/2/2/2
40	5MC	G	48	40	-	3/7/25/26	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1003	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
40	2MG	G	26	40	-	5/9/27/28	0/3/3/3
34	NMM	ST	67	34	-	2/9/11/13	-
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
40	1MG	G	10	40	-	1/7/25/26	0/3/3/3
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1272	1	-	0/9/27/28	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	OMU	S2	1288	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	436	1	-	3/9/27/28	0/3/3/3
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	2/9/27/28	0/3/3/3
1	OMC	S2	1703	43,1	-	0/9/27/28	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	63	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	4/7/25/26	0/2/2/2
1	PSU	S2	109	1	-	1/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1045	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
40	1MA	G	58	40	-	3/7/25/26	0/3/3/3
1	OMG	S2	683	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	OMG	S2	867	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1490	43,1	-	1/9/27/28	0/3/3/3
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
1	PSU	S2	1360	42,1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	2/11/29/30	0/3/3/3
40	H2U	G	47	40	-	5/7/38/39	0/2/2/2
1	OMG	S2	1447	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	366	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1004	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	159	1	-	2/9/27/28	0/3/3/3
1	A2M	S2	99	43,1	-	0/9/27/28	0/3/3/3
1	PSU	S2	667	1	-	2/7/25/26	0/2/2/2
1	UY1	S2	1326	43,1	-	4/9/27/28	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	668	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1046	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
16	IAS	SO	138	16	-	1/7/7/8	-
40	T6A	G	37	40	-	1/23/41/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	OMU	S2	1442	43,1	-	2/9/27/28	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
1	OMU	S2	1804	1	-	2/9/27/28	0/2/2/2
1	A2M	S2	590	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	6MZ	S2	1832	42,43,1	-	2/9/27/28	0/3/3/3
1	A2M	S2	512	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	366	PSU	O4'-C1'	-2.40	1.40	1.43
1	S2	667	PSU	O4'-C1'	-2.22	1.40	1.43
1	S2	1360	PSU	O4'-C1'	-2.22	1.40	1.43
1	S2	572	PSU	O4'-C1'	-2.15	1.40	1.43
1	S2	822	PSU	O4'-C1'	-2.13	1.40	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	ST	67	NMM	NE-CZ-NH2	-4.03	115.78	119.48
34	ST	67	NMM	NE-CZ-NH1	2.53	125.00	120.26
40	G	10	1MG	C6-C5-C4	-2.49	117.22	119.97
1	S2	1851	MA6	C2-N1-C6	2.36	117.33	111.75
1	S2	1850	MA6	C2-N1-C6	2.35	117.31	111.75

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	116	OMU	C1'-C2'-O2'-CM2
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	428	OMU	C2'-C1'-N1-C6
1	S2	468	A2M	C1'-C2'-O2'-CM'
1	S2	576	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

37 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	121	OMU	1	0
1	S2	918	PSU	1	0
1	S2	27	A2M	6	0
1	S2	428	OMU	1	0
1	S2	815	PSU	1	0
1	S2	644	OMG	1	0
1	S2	462	OMC	1	0
1	S2	576	A2M	4	0
1	S2	116	OMU	3	0
1	S2	93	PSU	1	0
40	G	10	1MG	3	0
1	S2	1842	4AC	3	0
1	S2	1288	OMU	2	0
1	S2	436	OMG	1	0
1	S2	866	PSU	2	0
1	S2	484	A2M	5	0
1	S2	1678	A2M	2	0
1	S2	867	OMG	5	0
1	S2	1850	MA6	3	0
1	S2	1851	MA6	3	0
40	G	47	H2U	1	0
1	S2	1447	OMG	1	0
1	S2	366	PSU	1	0
1	S2	609	PSU	1	0
1	S2	159	A2M	2	0
1	S2	99	A2M	1	0
1	S2	1031	A2M	1	0
1	S2	1238	PSU	1	0
1	S2	668	A2M	1	0
40	G	37	T6A	1	0
1	S2	1337	4AC	3	0
1	S2	1383	A2M	2	0
1	S2	1804	OMU	1	0
1	S2	1832	6MZ	2	0
1	S2	512	A2M	2	0
1	S2	1347	PSU	1	0
1	S2	354	OMU	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 106 ligands modelled in this entry, 104 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
45	GNP	E	501	-	33,34,34	2.21	5 (15%)	46,54,54	1.51	4 (8%)
46	MET	E	502	-	6,7,8	0.46	0	2,7,9	0.18	0

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
45	GNP	E	501	-	-	4/18/38/38	0/3/3/3
46	MET	E	502	-	-	1/5/6/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	E	501	GNP	PB-O3A	7.91	1.69	1.59
45	E	501	GNP	PG-N3B	6.51	1.80	1.63
45	E	501	GNP	PG-O1G	4.61	1.53	1.46
45	E	501	GNP	PB-O1B	3.11	1.51	1.46
45	E	501	GNP	PB-O2B	-2.11	1.51	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	E	501	GNP	O1G-PG-N3B	-7.51	100.72	111.77
45	E	501	GNP	O2B-PB-O1B	4.67	119.72	109.92
45	E	501	GNP	O2G-PG-O3G	2.31	113.79	107.64
45	E	501	GNP	O3A-PB-N3B	-2.23	100.40	106.59

There are no chirality outliers.

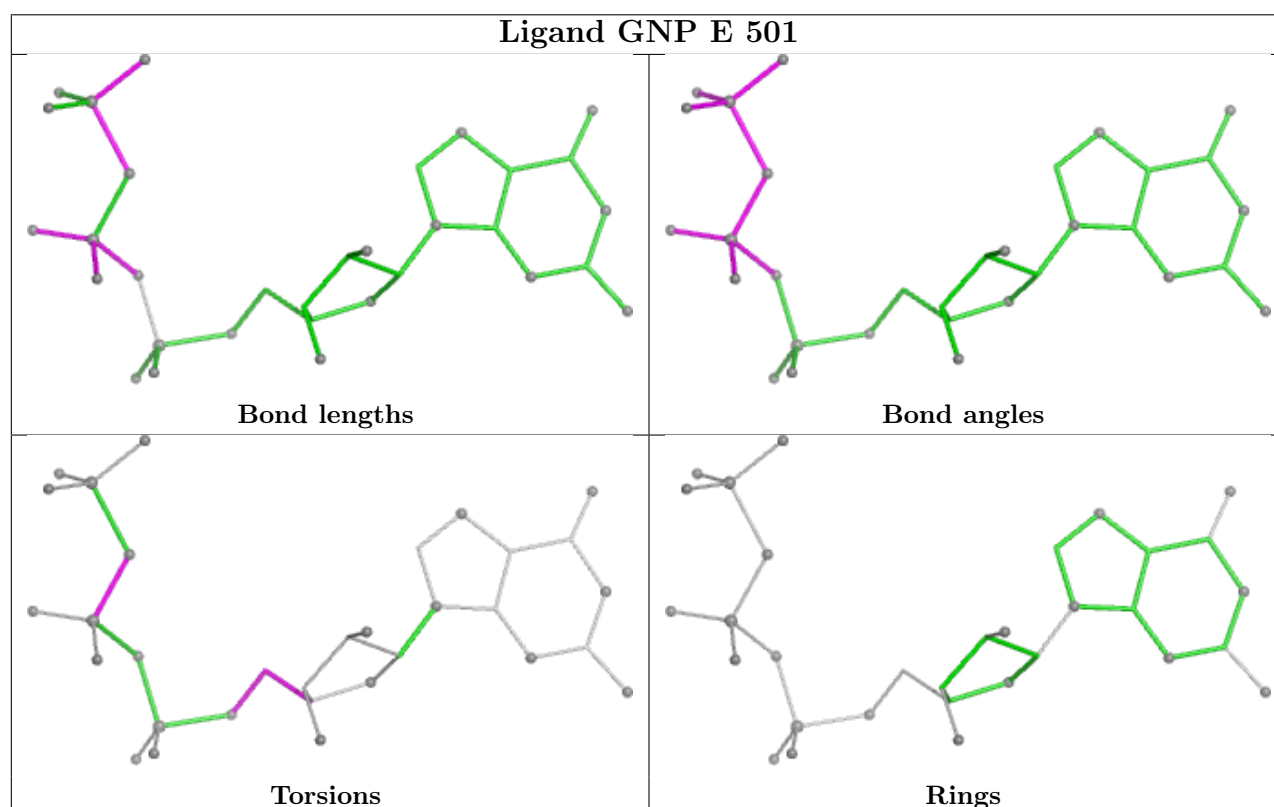
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	E	501	GNP	PG-N3B-PB-O1B
45	E	501	GNP	O4'-C4'-C5'-O5'
45	E	501	GNP	C3'-C4'-C5'-O5'
46	E	502	MET	CB-CG-SD-CE
45	E	501	GNP	C4'-C5'-O5'-PA

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	46:M7G	O3'	47:H2U	P	3.95

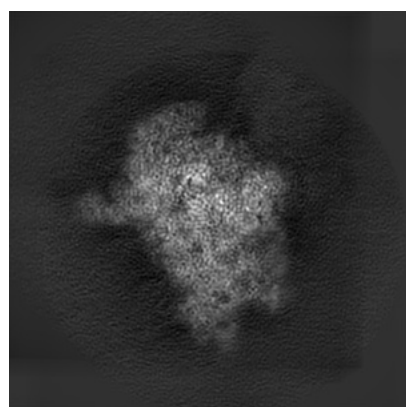
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57004. These allow visual inspection of the internal detail of the map and identification of artifacts.

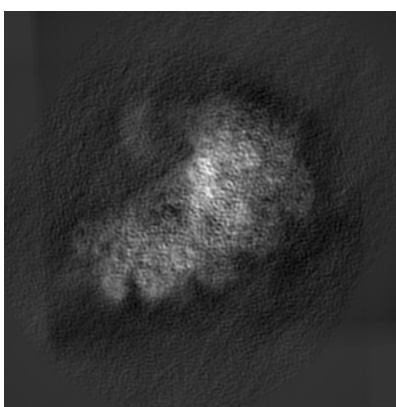
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

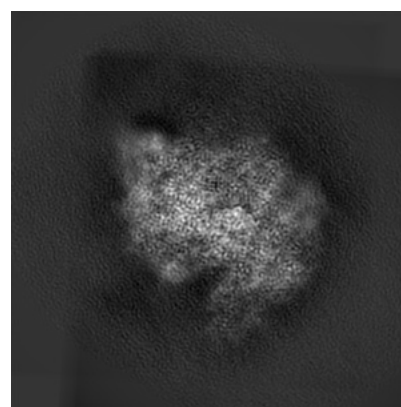
#### 6.1.1 Primary map



X



Y

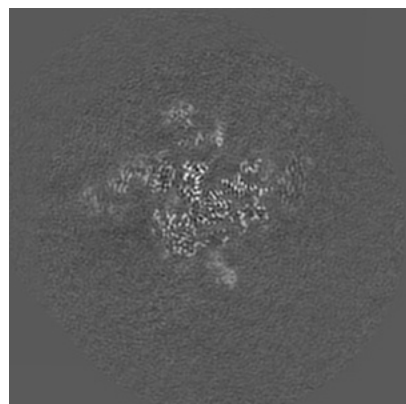


Z

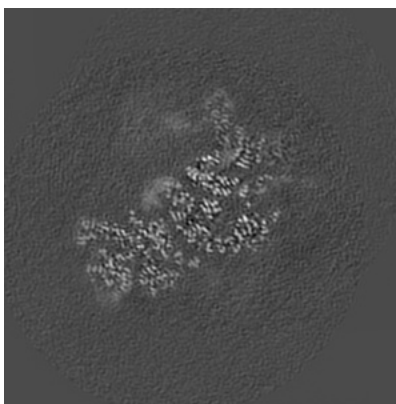
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

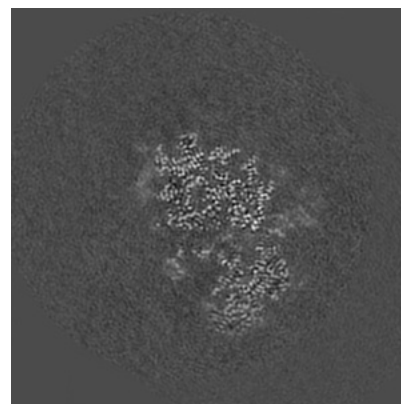
#### 6.2.1 Primary map



X Index: 260



Y Index: 260

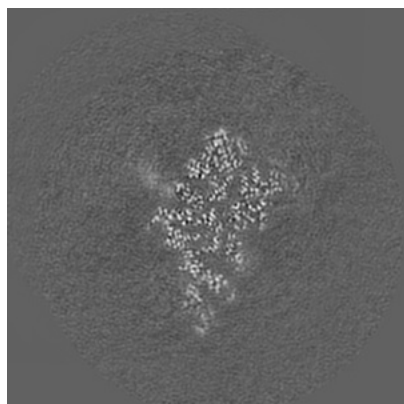


Z Index: 260

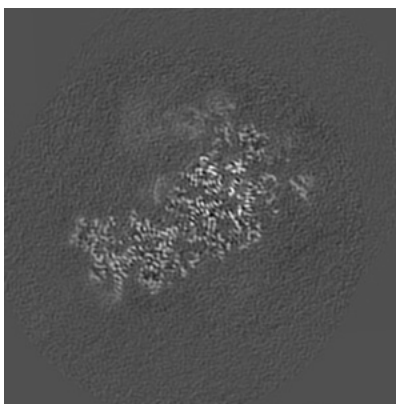
The images above show central slices of the map in three orthogonal directions.

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

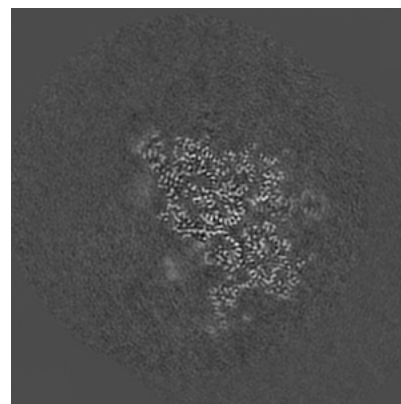
### 6.3.1 Primary map



X Index: 243



Y Index: 253

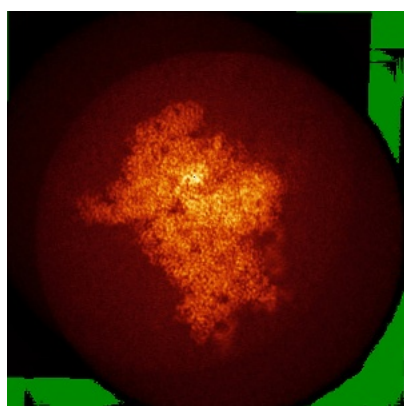


Z Index: 280

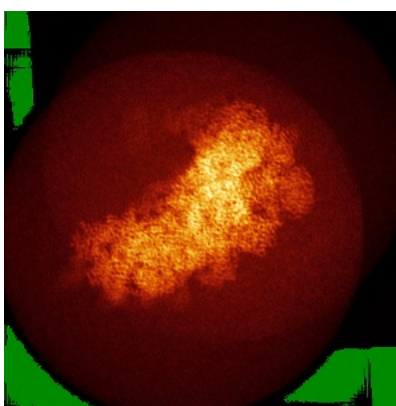
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

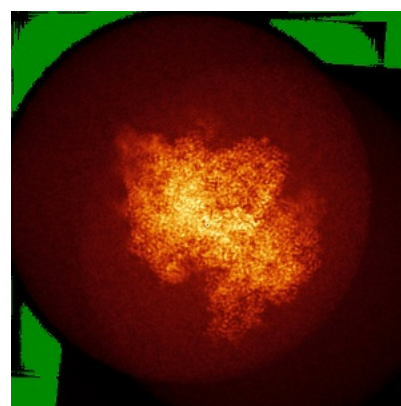
### 6.4.1 Primary map



X



Y

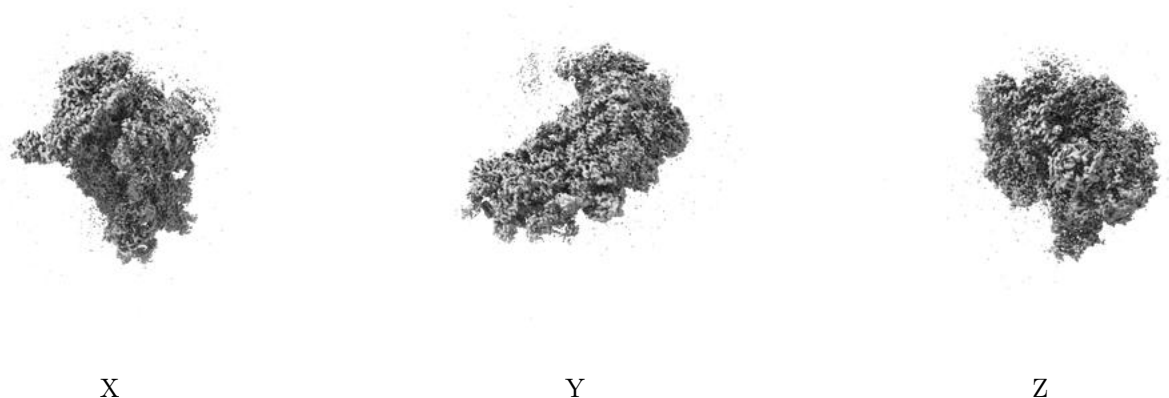


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.72. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

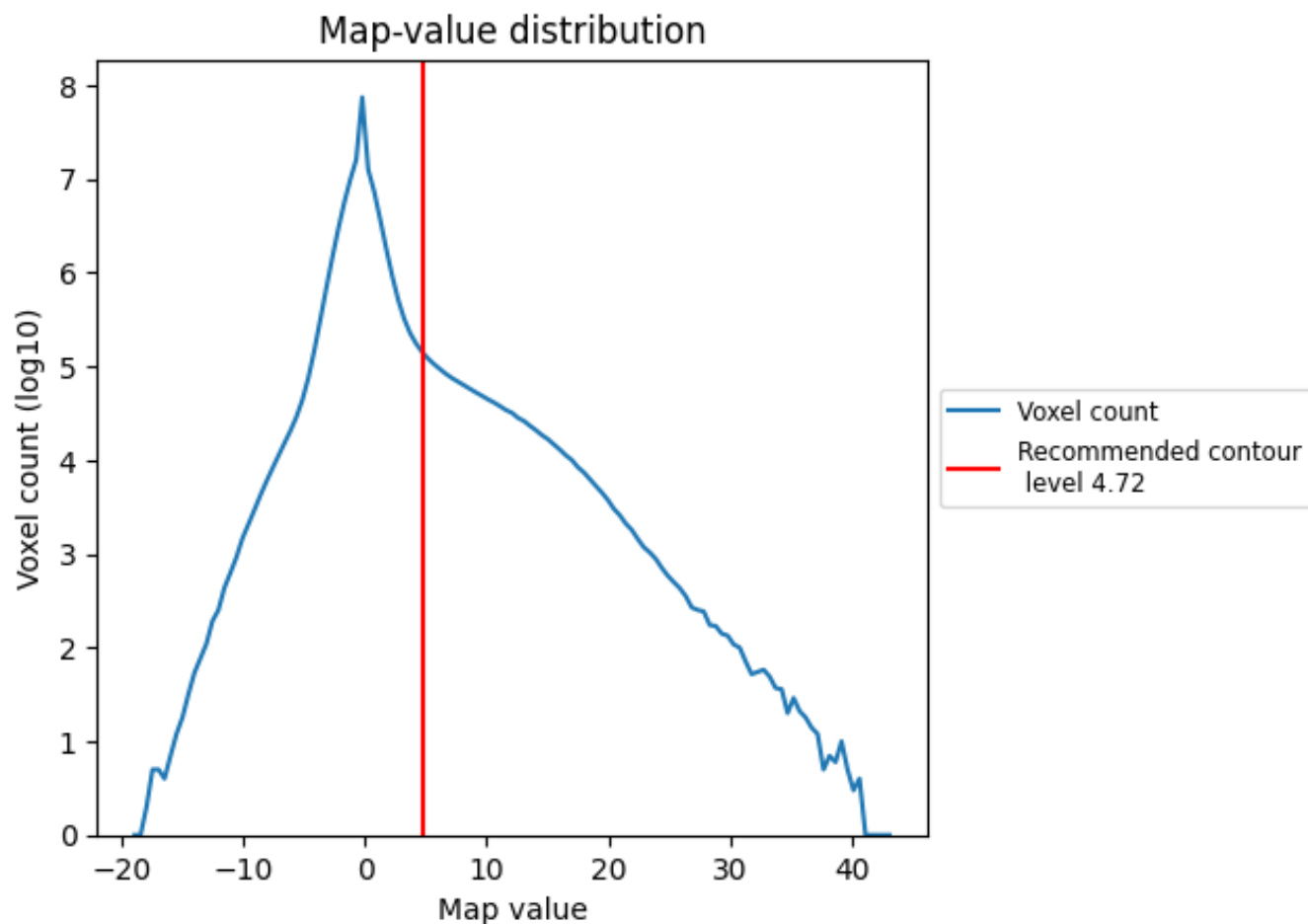
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

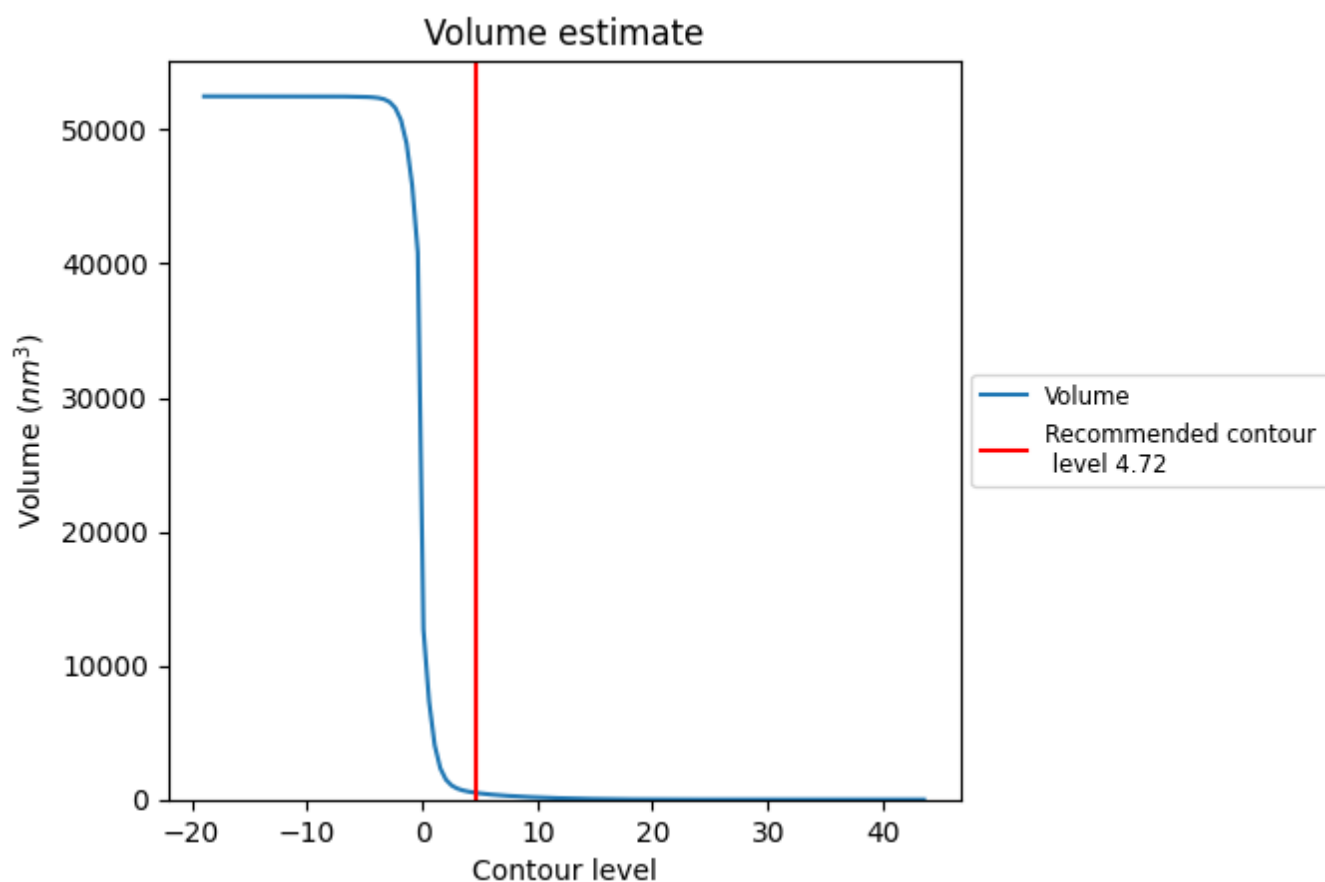
This section contains the results of statistical analysis of the map.

### 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](#)

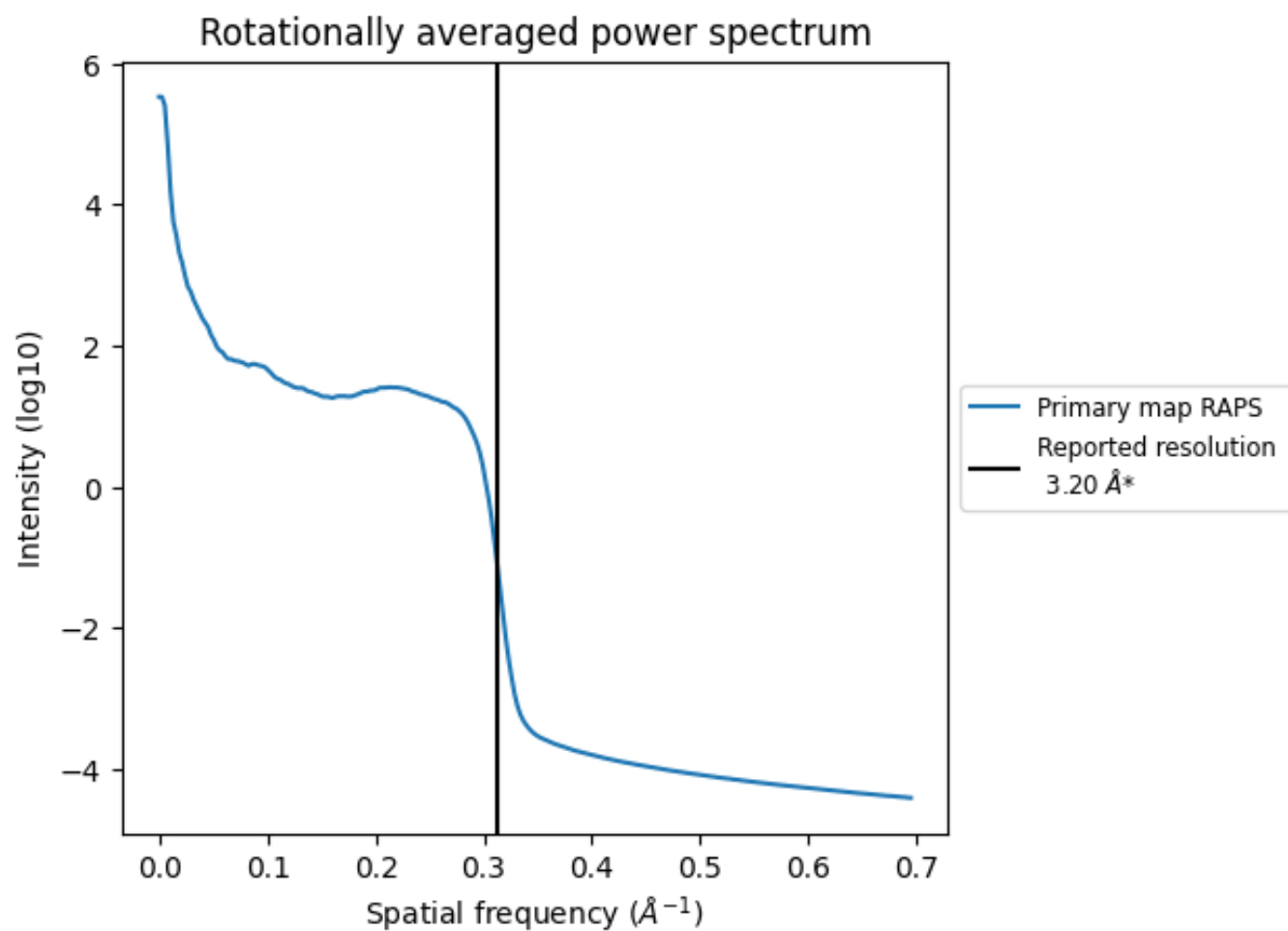


The volume at the recommended contour level is 498  $\text{nm}^3$ ; this corresponds to an approximate mass of 450 kDa.

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 0.312 Å<sup>-1</sup>

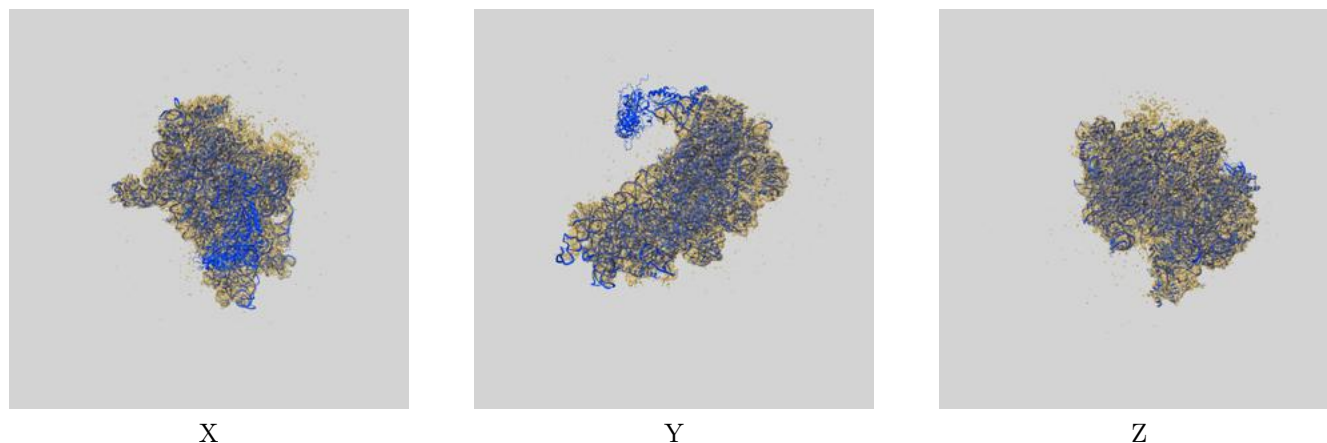
## 8 Fourier-Shell correlation ⓘ

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

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

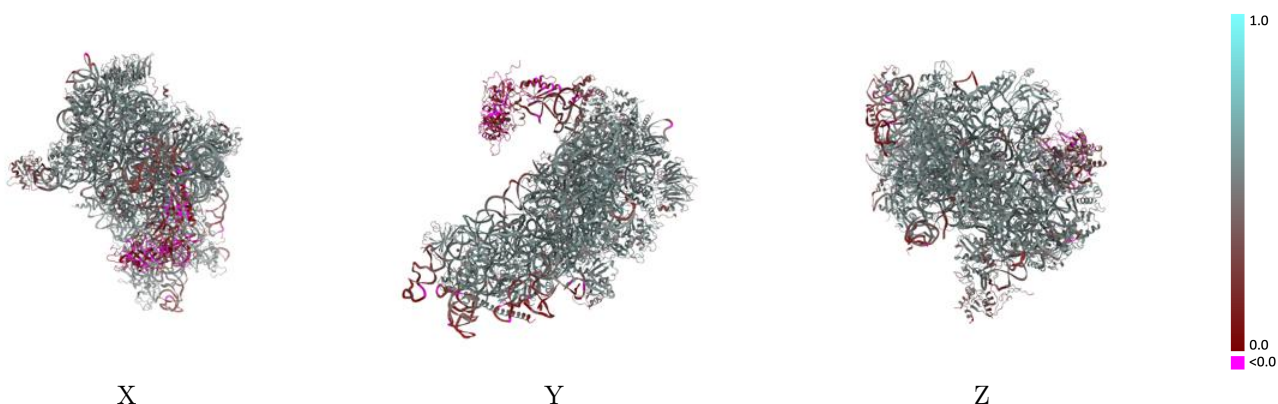
This section contains information regarding the fit between EMDB map EMD-57004 and PDB model 28ZU. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



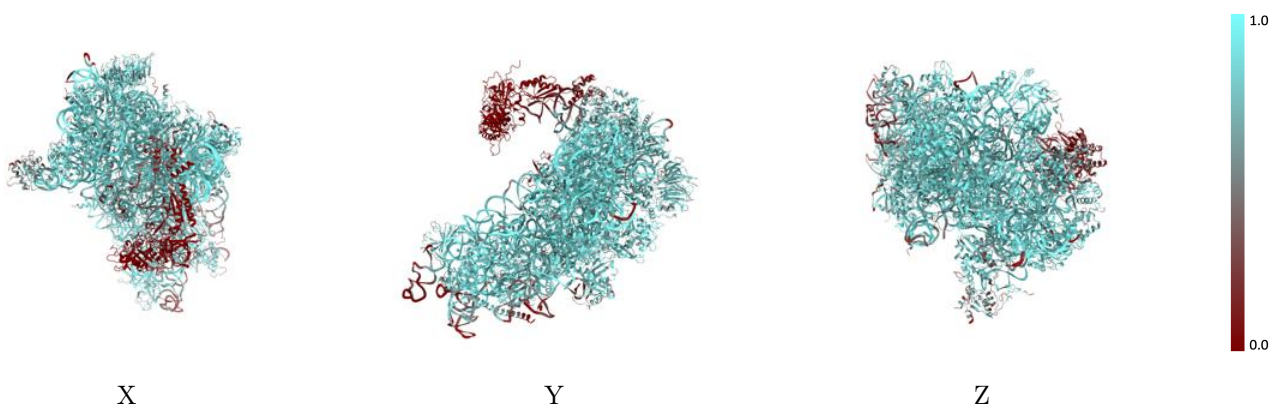
The images above show the 3D surface view of the map at the recommended contour level 4.72 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



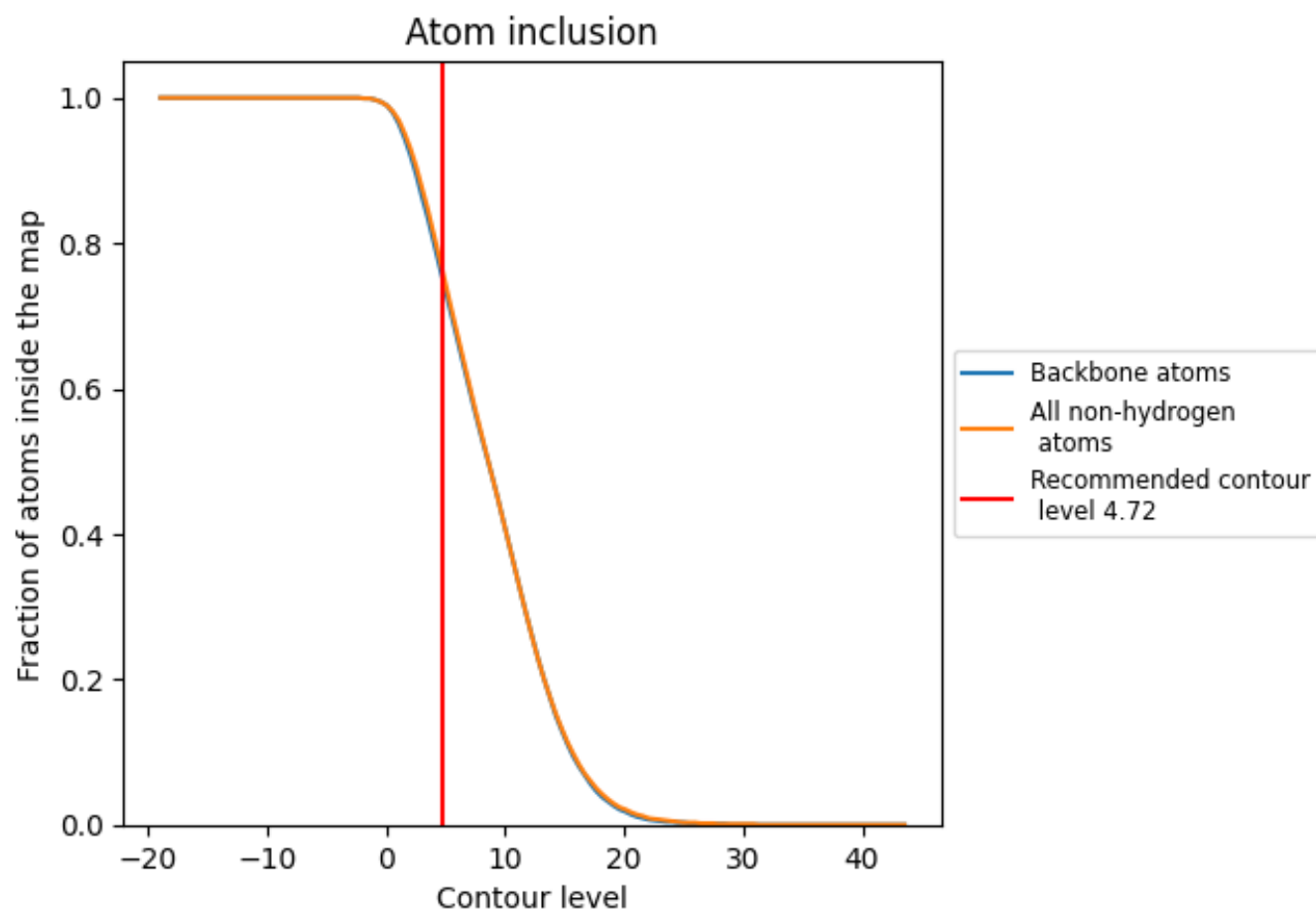
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.72).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 76% 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 (4.72) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7650	 0.4800
B	 0.6450	 0.3510
D	 0.3340	 0.3190
E	 0.0070	 0.1310
F	 0.0000	 0.1260
G	 0.5670	 0.3170
H	 0.4410	 0.4210
Ln	 0.7370	 0.5170
S2	 0.8580	 0.4890
SA	 0.8700	 0.5320
SB	 0.8400	 0.5400
SC	 0.8590	 0.5540
SD	 0.7980	 0.5220
SE	 0.8230	 0.5550
SF	 0.8400	 0.5410
SG	 0.7370	 0.4970
SH	 0.7240	 0.4970
SI	 0.8120	 0.5300
SJ	 0.8330	 0.5460
SK	 0.8080	 0.5160
SL	 0.7690	 0.5280
SM	 0.4990	 0.3690
SN	 0.8410	 0.5430
SO	 0.8450	 0.5280
SP	 0.7460	 0.5040
SQ	 0.8400	 0.5460
SR	 0.8060	 0.5260
SS	 0.7650	 0.5190
ST	 0.8110	 0.5270
SU	 0.7030	 0.4930
SV	 0.8680	 0.5530
SW	 0.8780	 0.5690
SX	 0.8410	 0.5580
SY	 0.8230	 0.5470
SZ	 0.7560	 0.5130



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Chain	Atom inclusion	Q-score
Sa	 0.8630	 0.5450
Sb	 0.8000	 0.5280
Sc	 0.8330	 0.5300
Sd	 0.8740	 0.5590
Se	 0.7040	 0.4940
Sf	 0.5620	 0.4000
Sg	 0.7660	 0.5070