



# wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 11:30 am BST

PDB ID : 28ZY / pdb\_000028zy  
EMDB ID : EMD-57010  
Title : human 48S PIC with mRNA (Kozak\_2)  
Authors : von Loeffelholz, O.; Barchet, C.; Klaholz, B.  
Deposited on : 2026-03-03  
Resolution : 3.00 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:

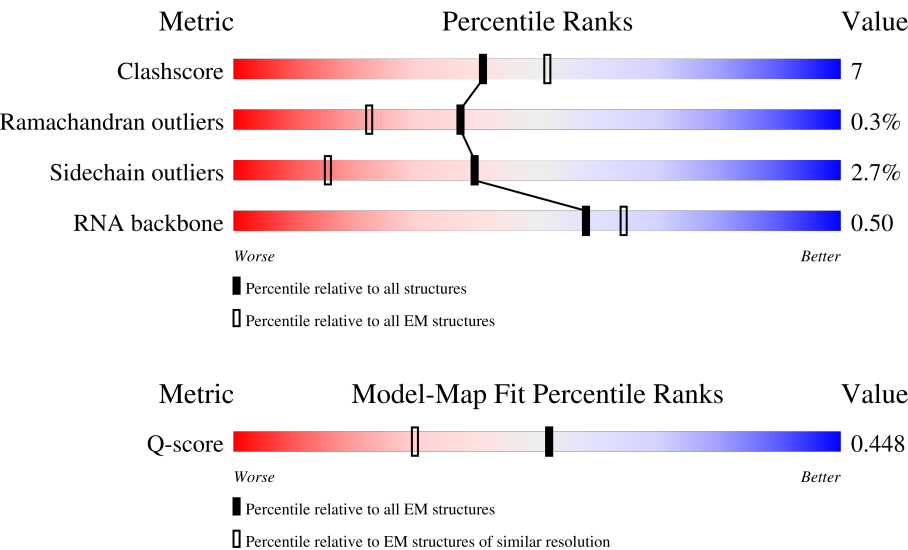
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 3.00 Å.

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









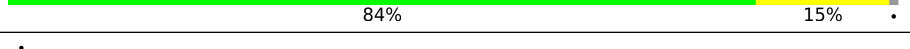
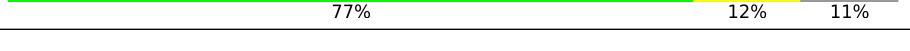
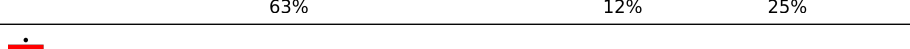
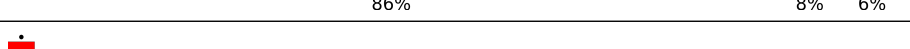
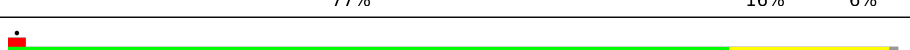

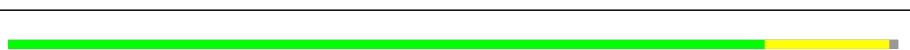

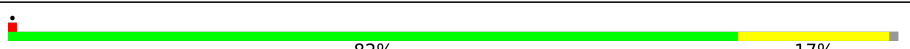





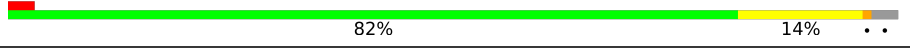
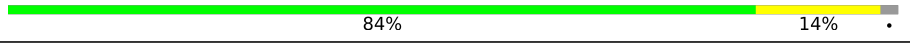



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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	

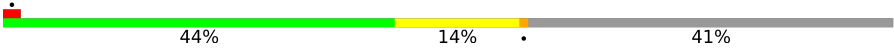





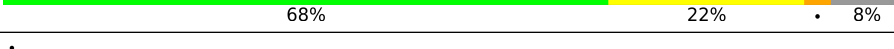
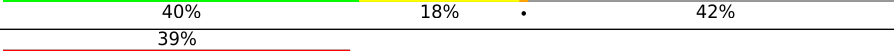
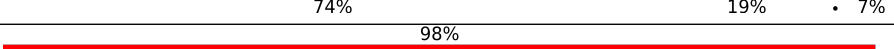
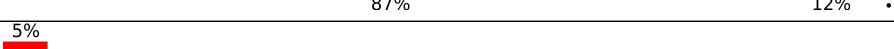
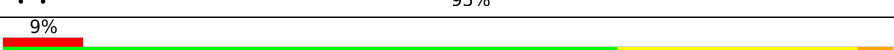

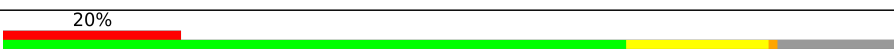

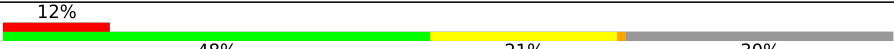




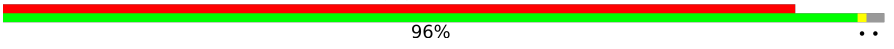
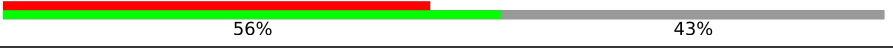

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Mol	Chain	Length	Quality of chain
4	SA	295	
5	SB	264	
6	SH	194	
7	SI	208	
8	SL	158	
9	SV	83	
10	SX	143	
11	Sa	115	
12	SC	293	
13	SG	249	
14	SJ	194	
15	SN	151	
16	SO	151	
17	SW	130	
18	SY	133	
19	Sb	84	
20	Se	133	
21	B	50	
22	SD	243	
23	SF	204	
24	Sf	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	
42	e	445	
43	d	548	
44	c	913	
45	a	1382	
46	3f	357	
47	m	374	
48	h	352	
49	k	218	
50	l	564	

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 108768 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	223	Total	C	N	O	S	0	0
			1806	1145	325	322	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	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sc	65	Total	C	N	O	S	0	0
			517	314	106	95	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	294	Total	C	N	O	S	0	0
			2367	1487	413	453	14		

- 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	111	Total	C	N	O	S	0	0
			895	556	170	164	5		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit E.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	414	Total	C	N	O	S	0	0
			2778	1714	511	544	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	c	642	Total	C	N	O	S	0	0
			5197	3274	925	963	35		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	a	589	Total	C	N	O	S	1	0
			4799	3029	865	882	23		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
46	3f	257	Total	C	N	O	0	0
			1272	757	257	258		

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

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

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	h	317	Total	C	N	O	0	0
			1571	936	317	318		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	k	213	Total	C	N	O	0	0
			1057	631	213	213		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	l	319	Total	C	N	O	0	0
			1581	943	319	319		

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

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

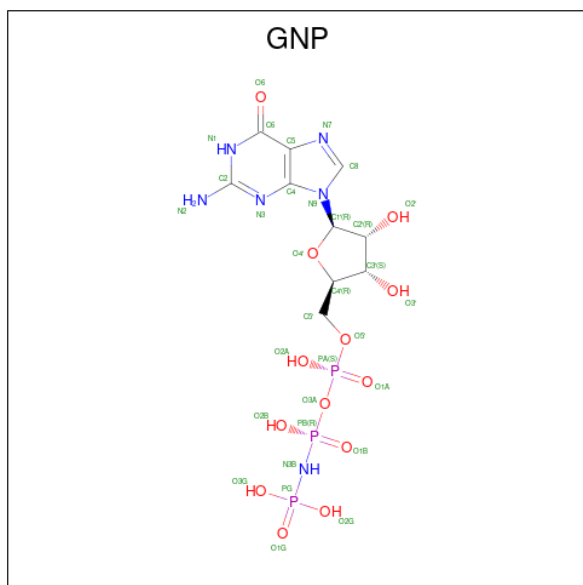
- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	S2	76	Total	Mg	0
			76	76	
52	SE	1	Total	Mg	0
			1	1	
52	SN	1	Total	Mg	0
			1	1	
52	SO	1	Total	Mg	0
			1	1	
52	B	7	Total	Mg	0
			7	7	
52	H	1	Total	Mg	0
			1	1	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

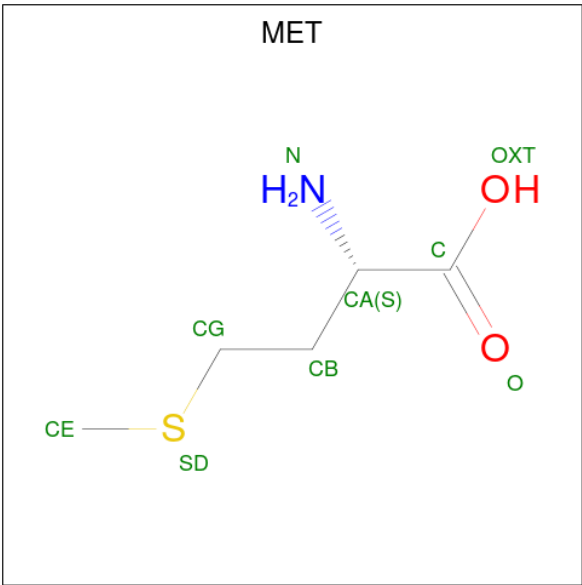
Mol	Chain	Residues	Atoms		AltConf
53	Sa	1	Total	Zn	0
			1	1	
53	Sf	1	Total	Zn	0
			1	1	
53	Sd	1	Total	Zn	0
			1	1	

- Molecule 54 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



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

- Molecule 55 is METHIONINE (CCD ID: MET) (formula:  $C_5H_{11}NO_2S$ ).



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

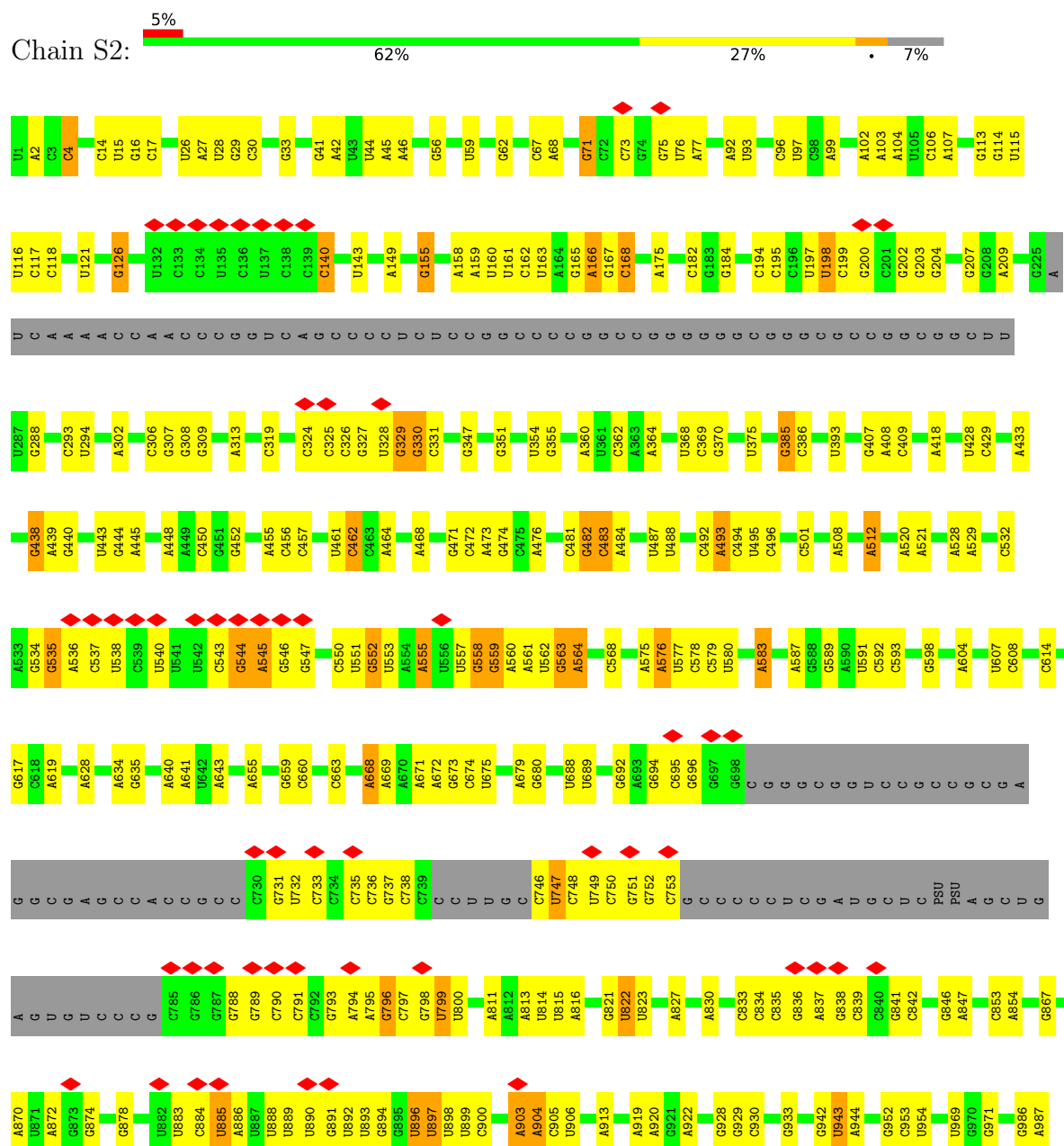
- Molecule 56 is water.

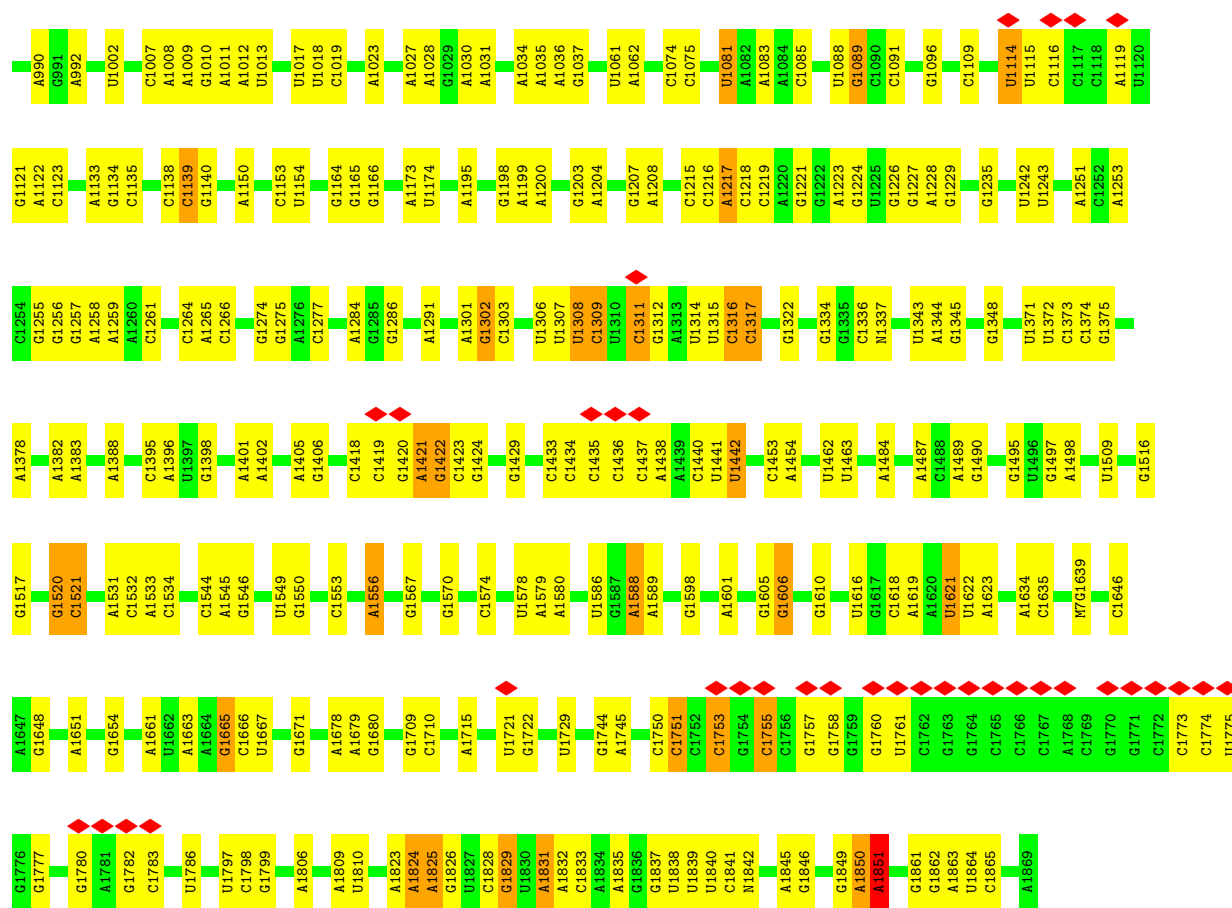
Mol	Chain	Residues	Atoms		AltConf
56	S2	349	Total	O	0
			349	349	
56	SE	1	Total	O	0
			1	1	
56	SB	1	Total	O	0
			1	1	
56	SL	2	Total	O	0
			2	2	
56	Sa	1	Total	O	0
			1	1	
56	SC	1	Total	O	0
			1	1	
56	SN	3	Total	O	0
			3	3	
56	SO	2	Total	O	0
			2	2	
56	SQ	1	Total	O	0
			1	1	
56	SS	1	Total	O	0
			1	1	
56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

### 3 Residue-property plots

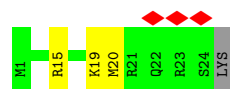
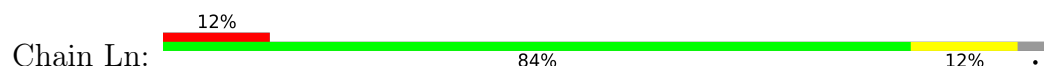
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 18S ribosomal RNA

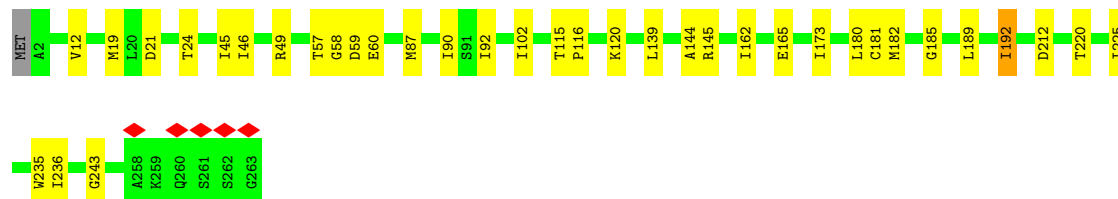
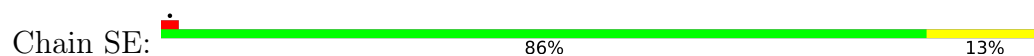




• Molecule 2: 60S ribosomal protein L41



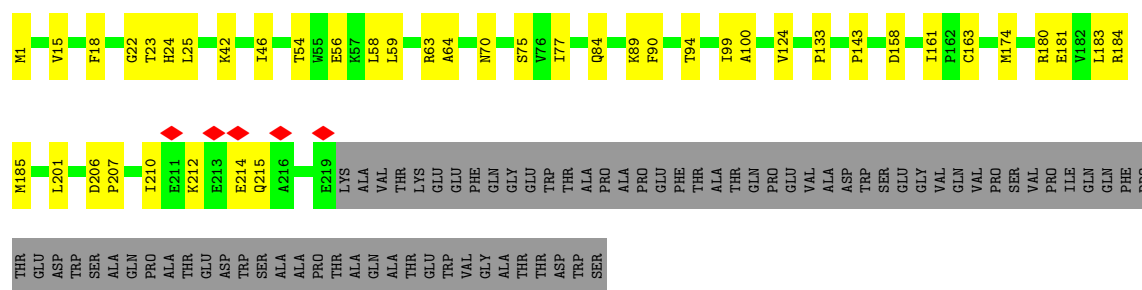
• Molecule 3: Small ribosomal subunit protein eS4, X isoform



• Molecule 4: 40S ribosomal protein SA

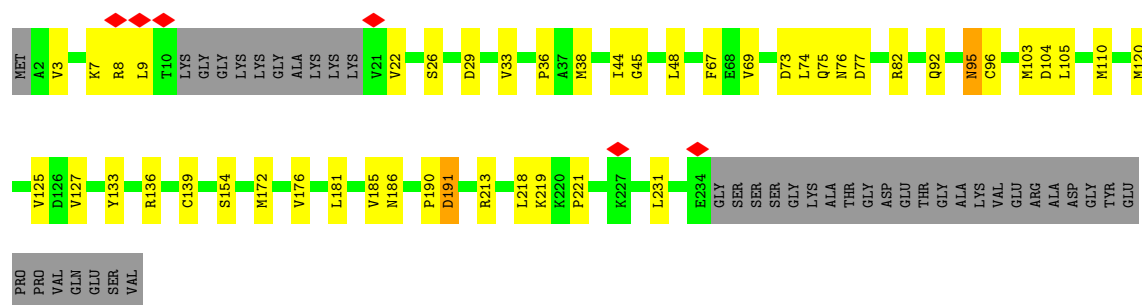






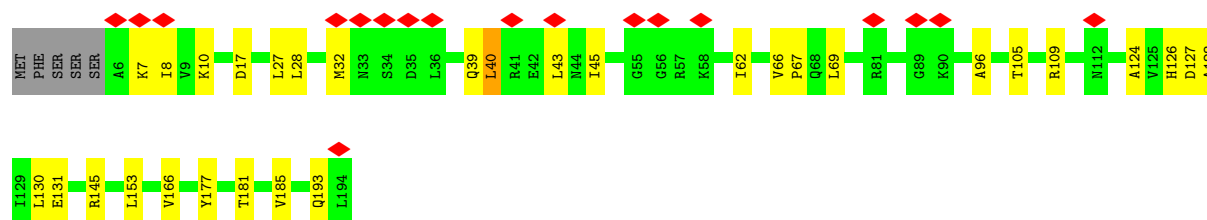
- Molecule 5: 40S ribosomal protein S3a

Chain SB: 67% 17% 16%



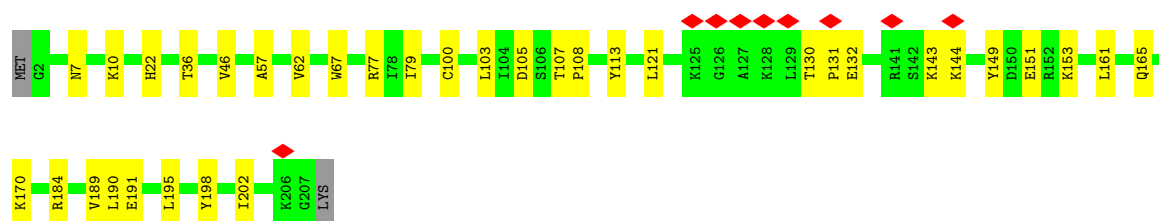
- Molecule 6: 40S ribosomal protein S7

Chain SH: 9% 81% 15%



- Molecule 7: 40S ribosomal protein S8

Chain SI: 82% 17%

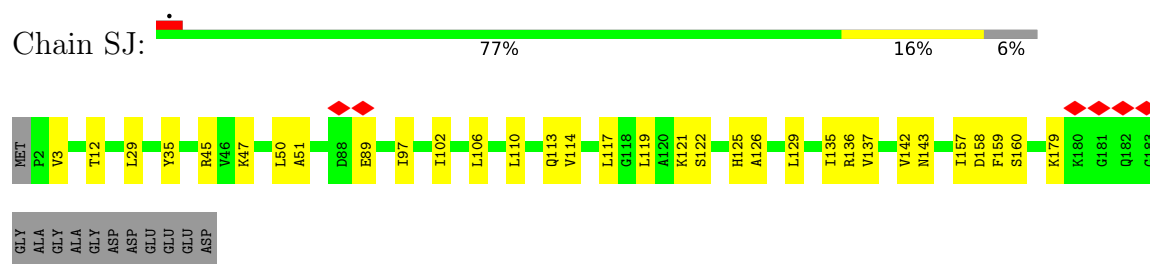


- Molecule 8: Small ribosomal subunit protein uS17

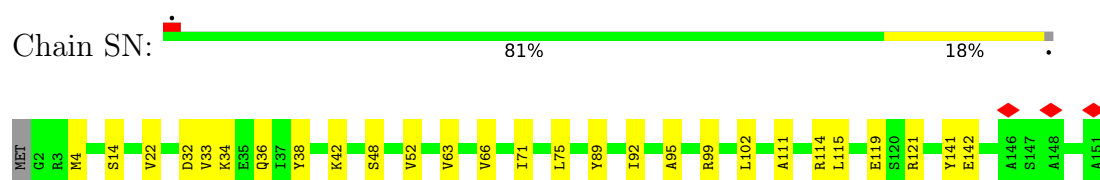
Chain SL: 9% 84% 13%



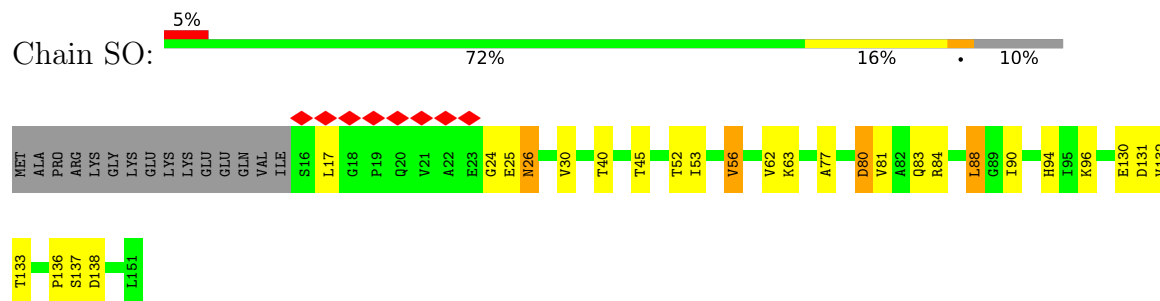
- Molecule 14: 40S ribosomal protein S9



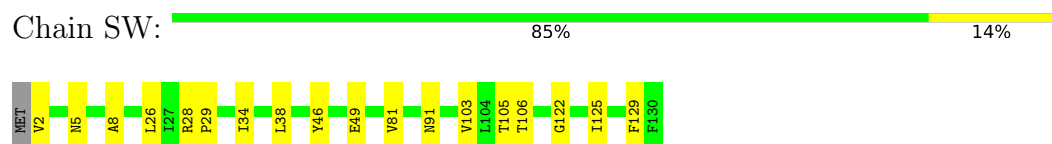
- Molecule 15: 40S ribosomal protein S13



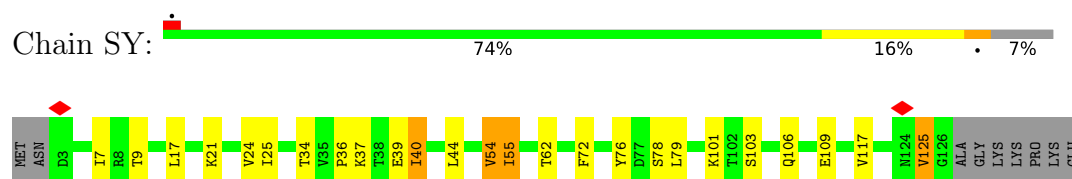
- Molecule 16: 40S ribosomal protein S14



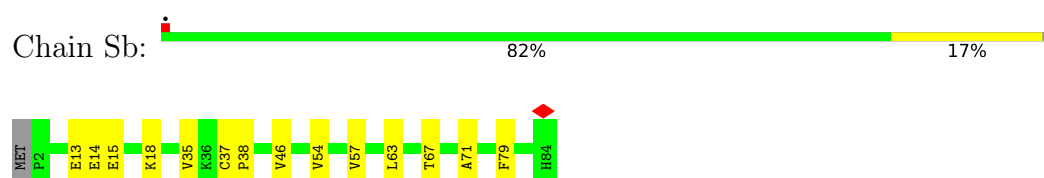
- Molecule 17: 40S ribosomal protein S15a



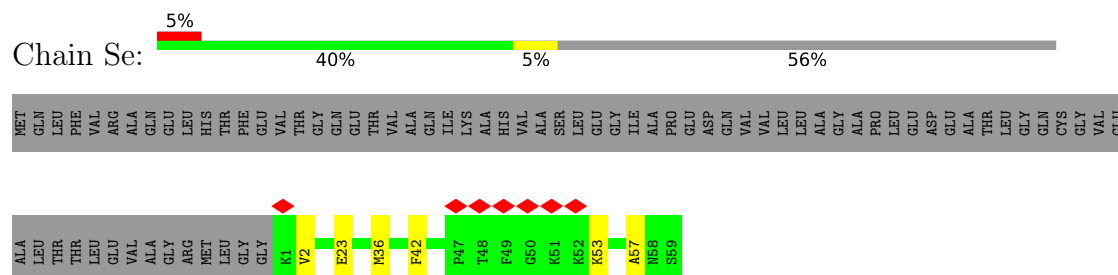
- Molecule 18: 40S ribosomal protein S24



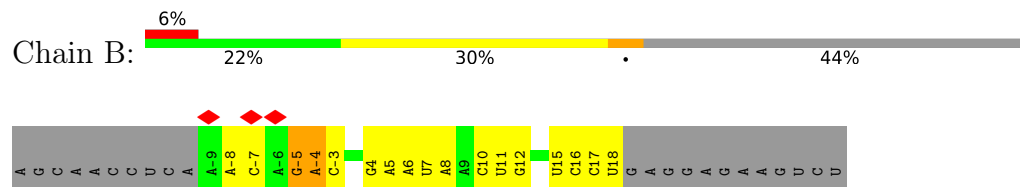
- Molecule 19: 40S ribosomal protein S27



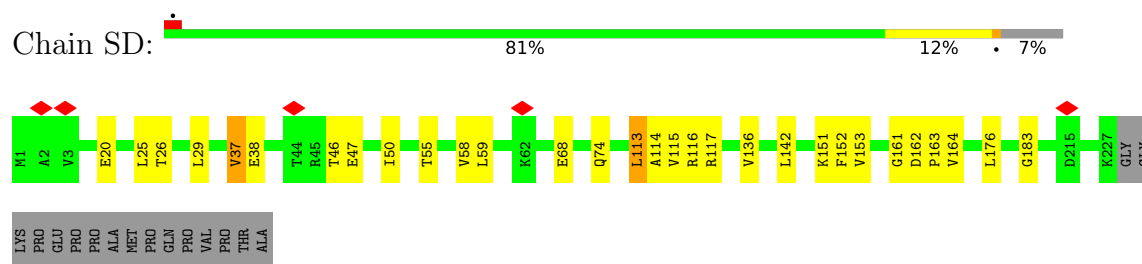
- Molecule 20: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



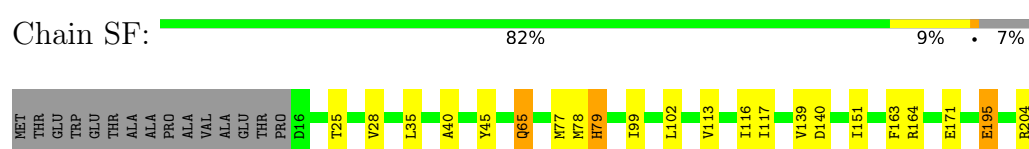
- Molecule 21: mRNA



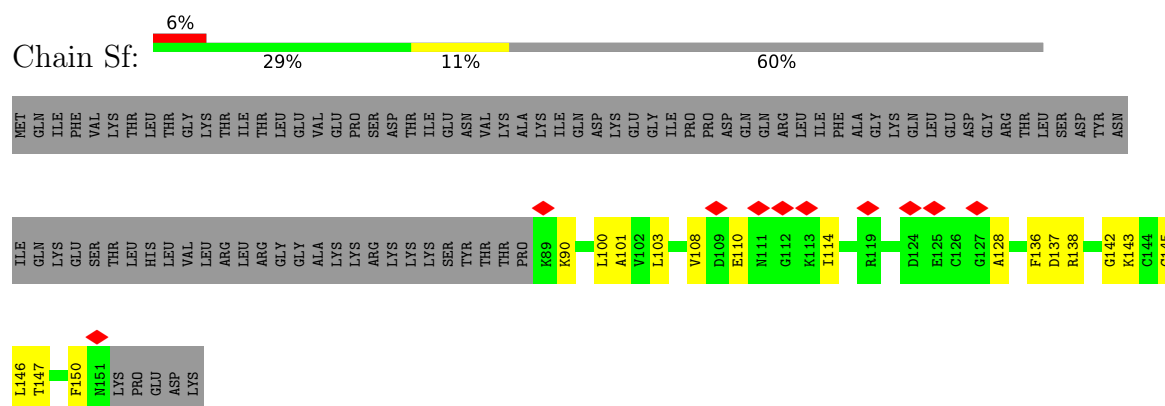
- Molecule 22: 40S ribosomal protein S3




- Molecule 23: 40S ribosomal protein S5

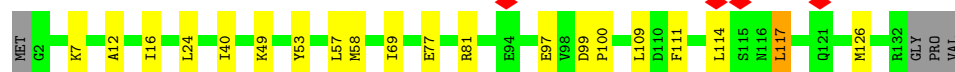


- Molecule 24: Ubiquitin




- Molecule 25: 40S ribosomal protein S17

Chain SR:  82% 14%




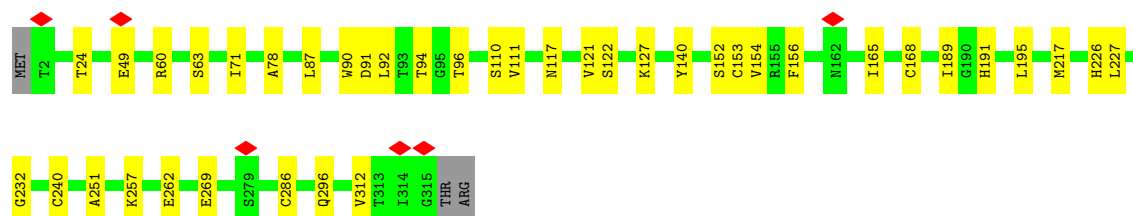
- Molecule 26: 40S ribosomal protein S29

Chain Sd:  84% 14%



- Molecule 27: Receptor of activated protein C kinase 1

Chain Sg:  86% 13%



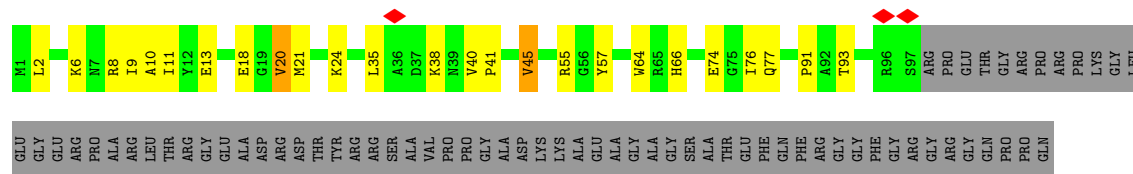
- Molecule 28: 40S ribosomal protein S28

Chain Sc:  75% 17% 6%



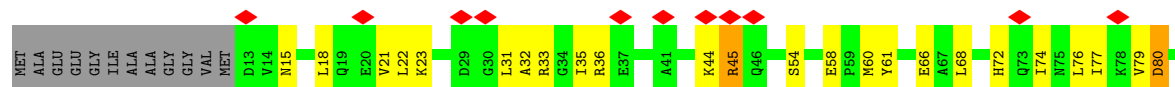
- Molecule 29: 40S ribosomal protein S10

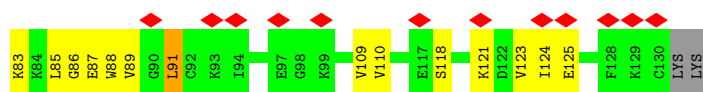
Chain SK:  44% 14% 41%



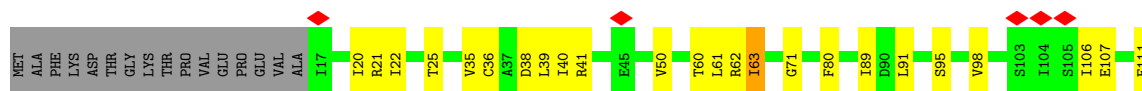
- Molecule 30: 40S ribosomal protein S12

Chain SM:  17% 61% 27% 11%

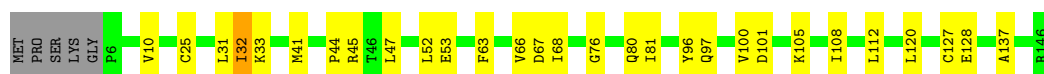
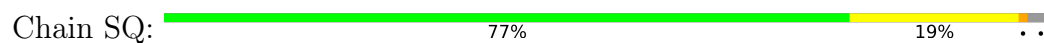




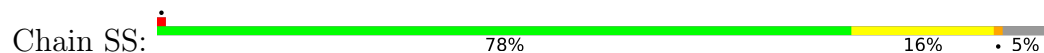
- Molecule 31: 40S ribosomal protein S20



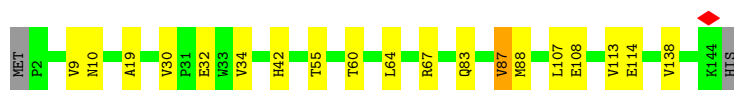
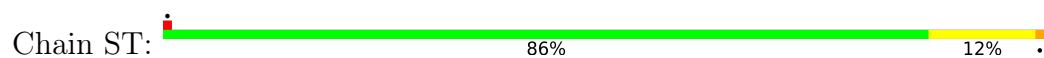
- Molecule 32: 40S ribosomal protein S16



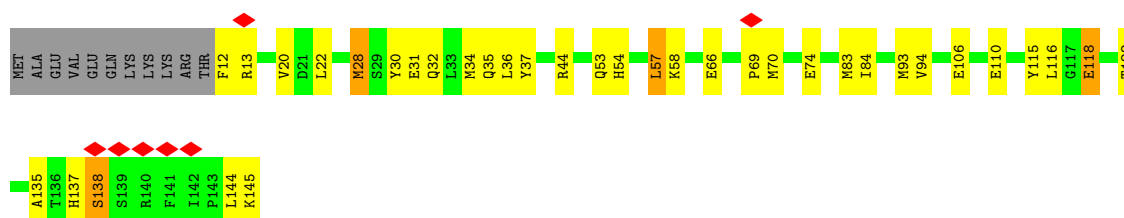
- Molecule 33: 40S ribosomal protein S18



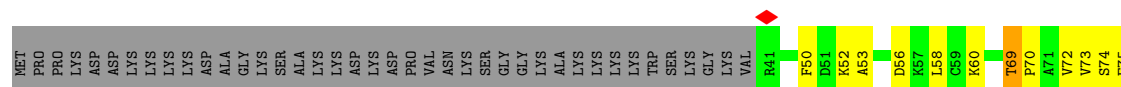
- Molecule 34: Small ribosomal subunit protein eS19



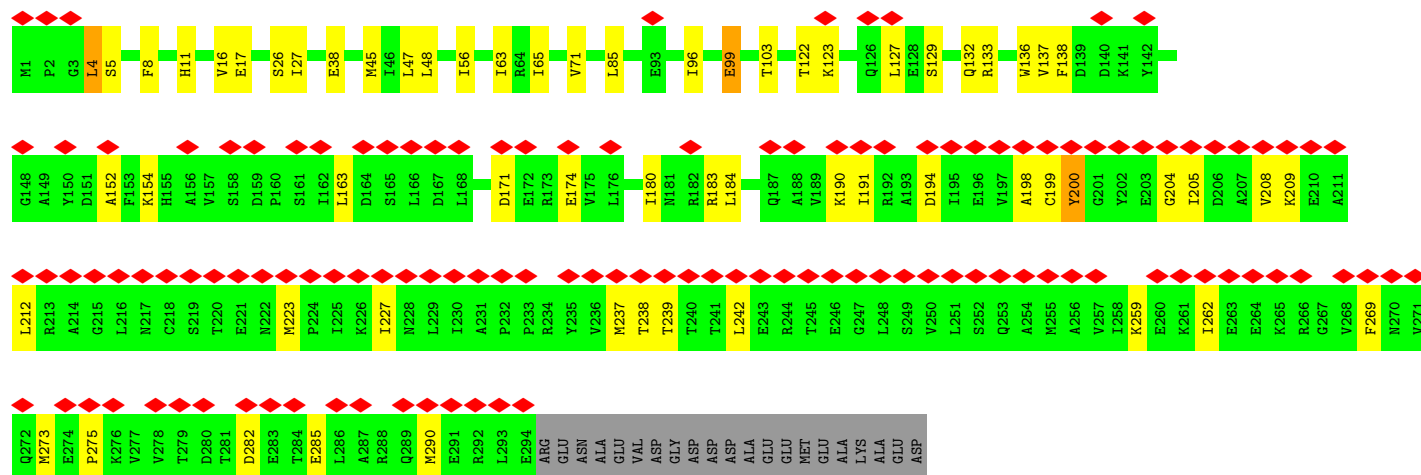
- Molecule 35: 40S ribosomal protein S15



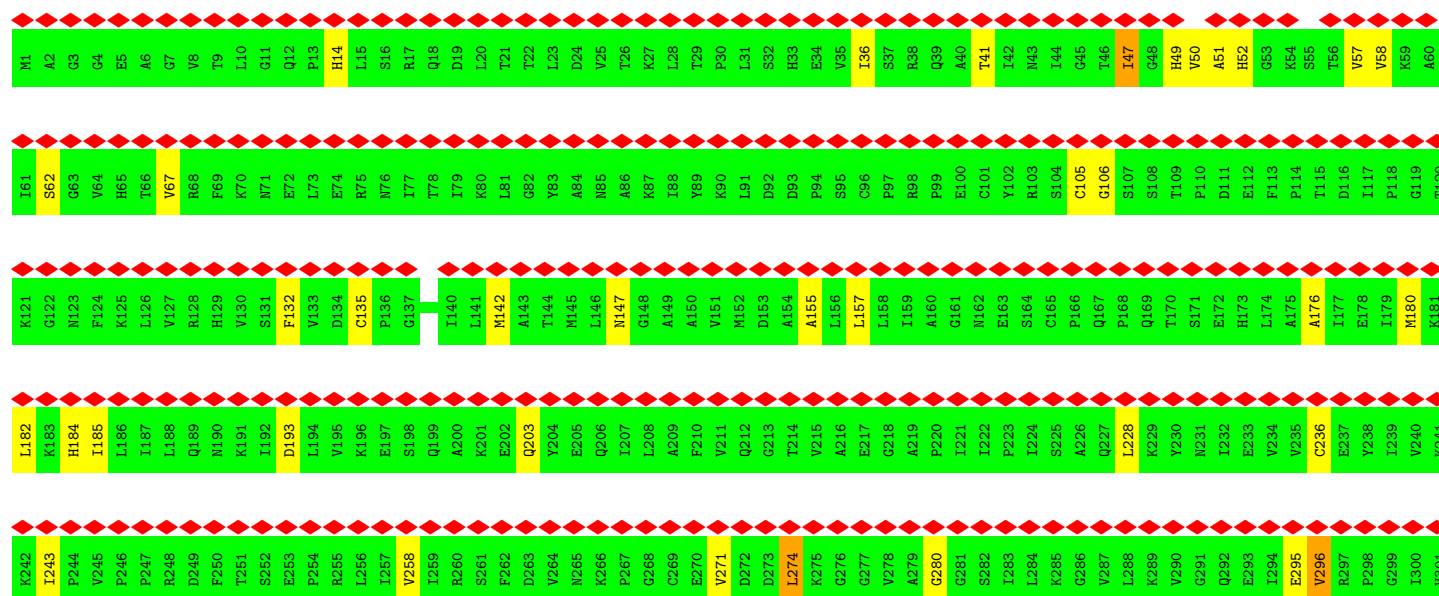
- Molecule 36: Small ribosomal subunit protein eS25

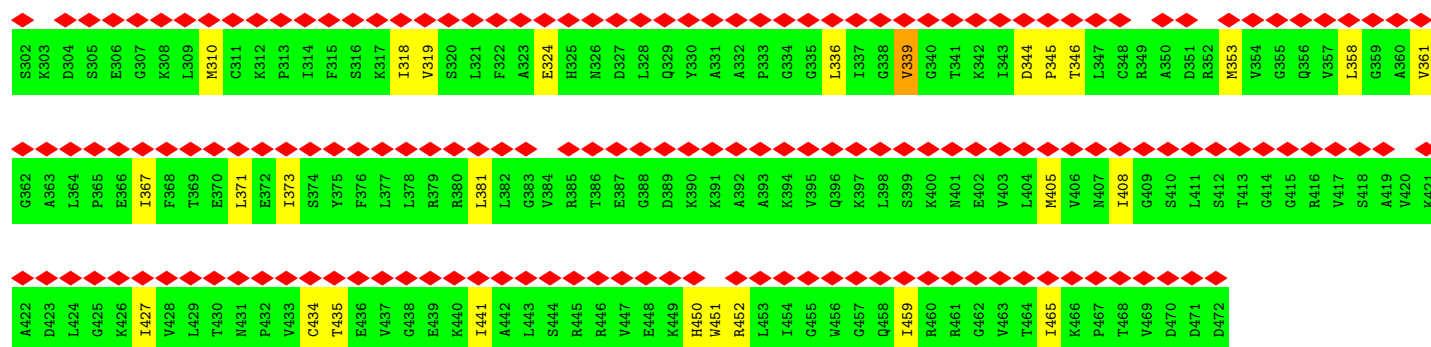


• Molecule 37: Eukaryotic translation initiation factor 2 subunit 1

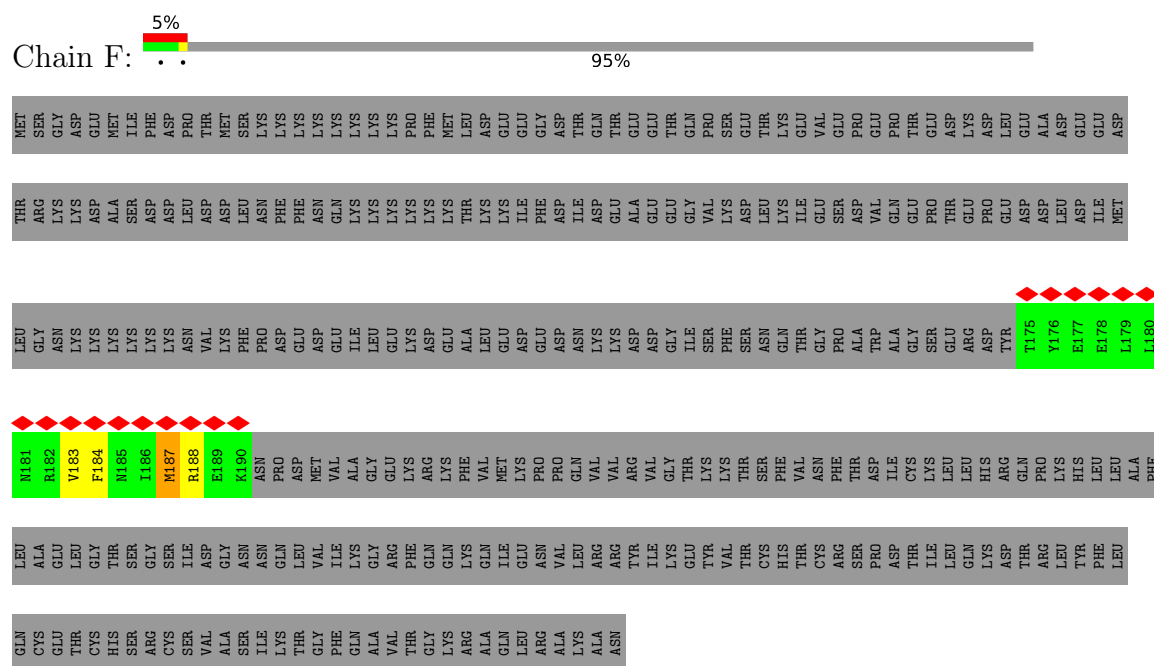


• Molecule 38: Eukaryotic translation initiation factor 2 subunit 3

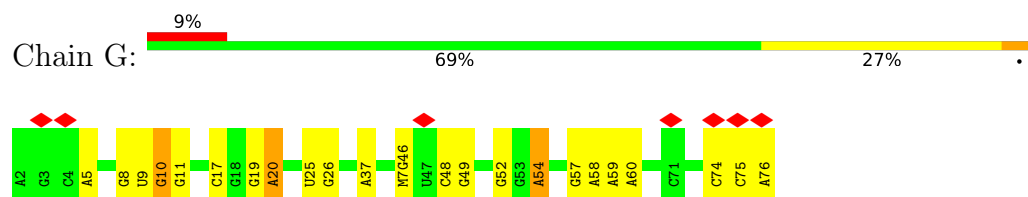




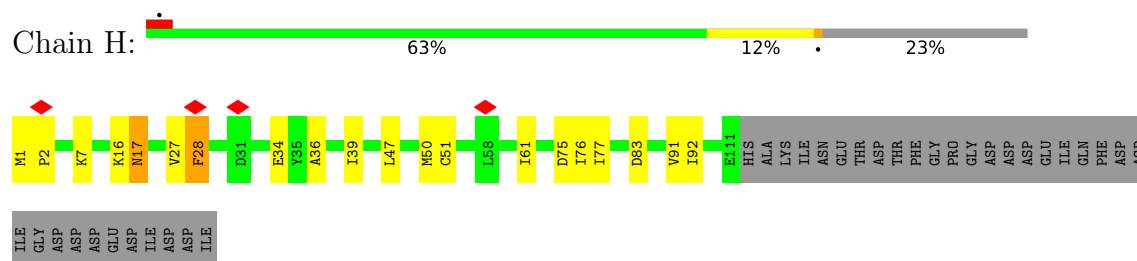
- Molecule 39: Eukaryotic translation initiation factor 2 subunit 2



- Molecule 40: initiator tRNA



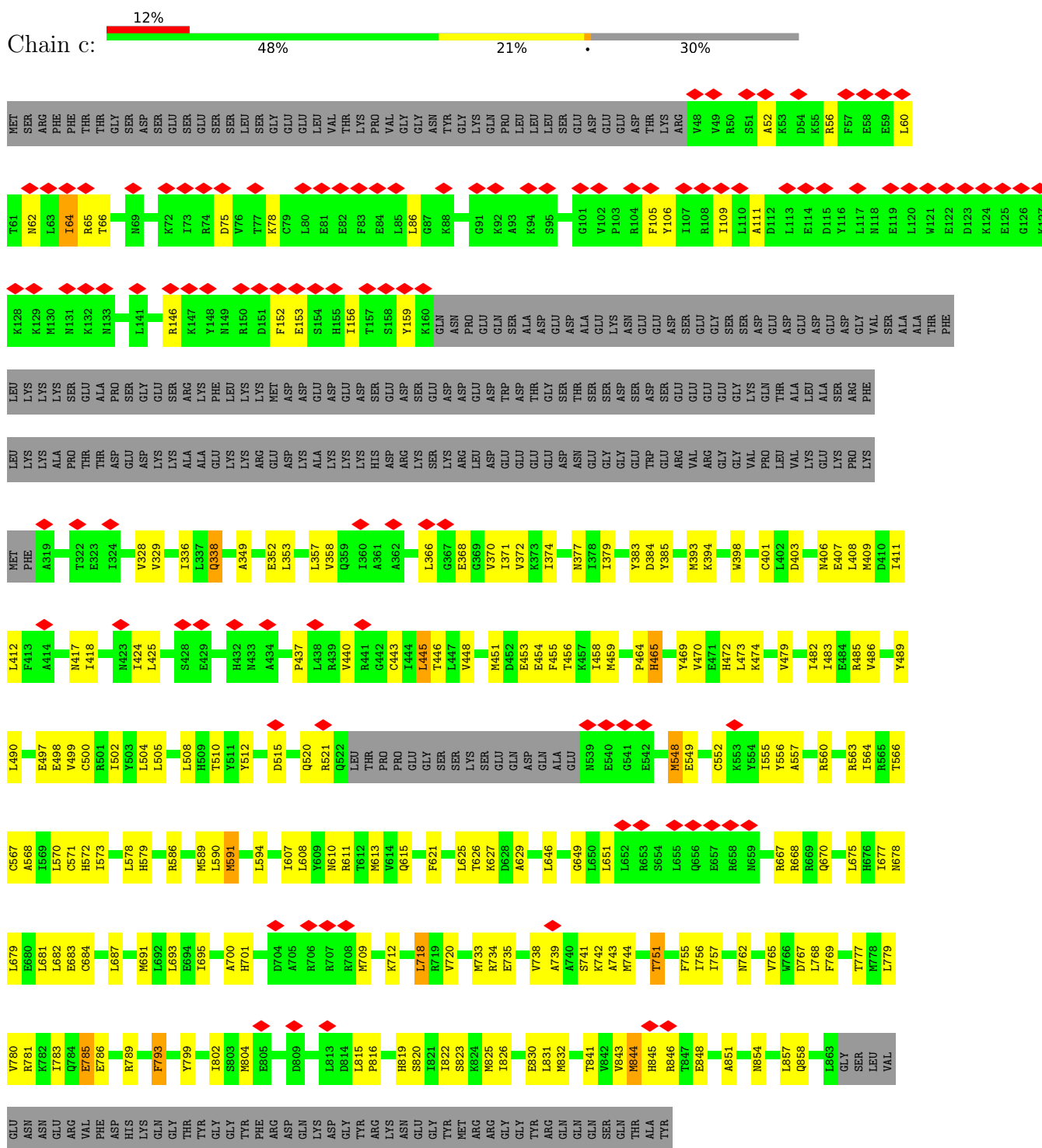
- Molecule 41: Eukaryotic translation initiation factor 1A, X-chromosomal



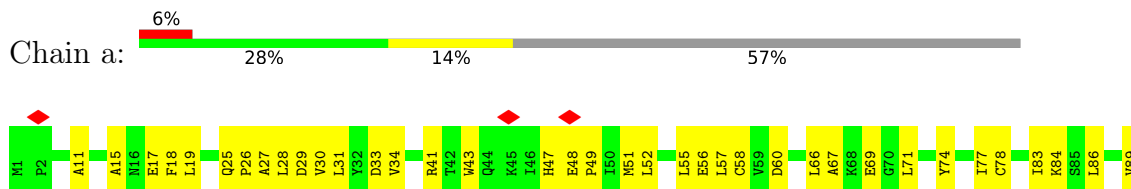
- Molecule 42: Eukaryotic translation initiation factor 3 subunit E







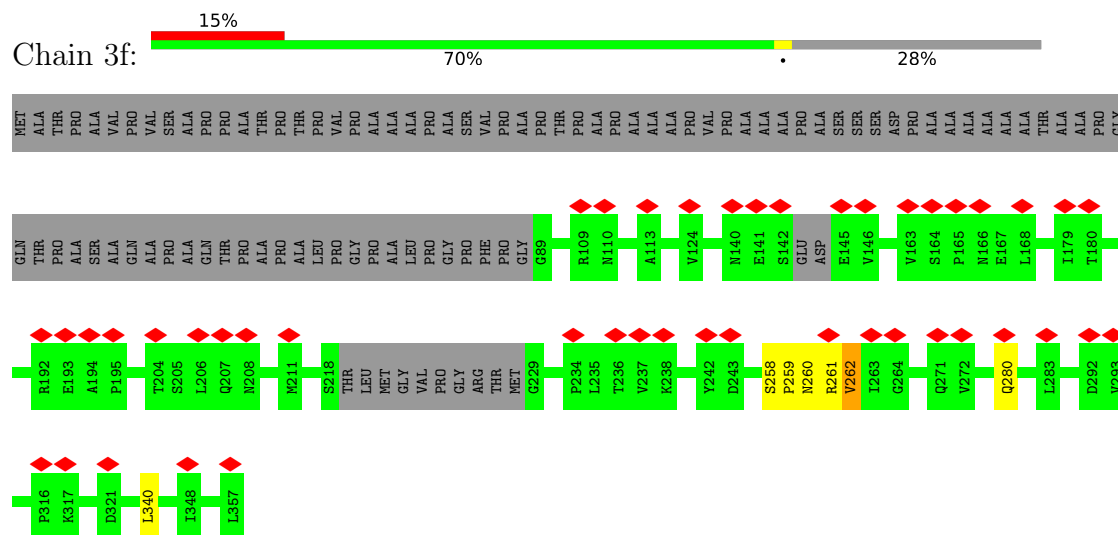
- Molecule 45: Eukaryotic translation initiation factor 3 subunit A



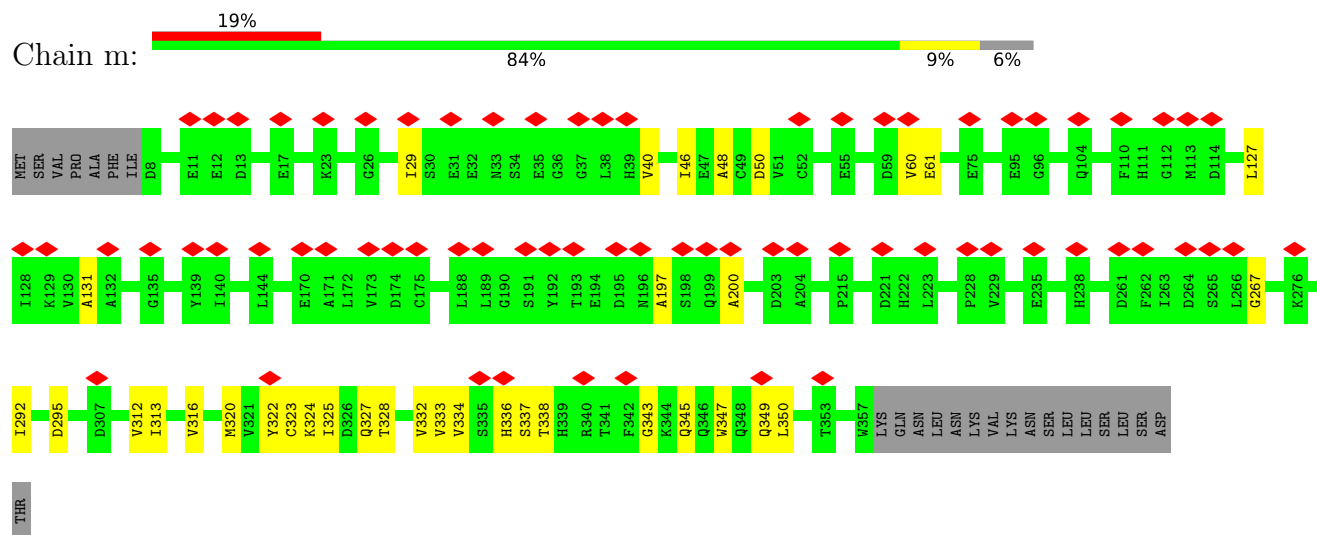


PRO ARG  
THR VAL  
ALA PRO  
PRO PRO  
ALA ALA  
LEU LEU  
SER ARG  
ASP ARG  
GLU ARG  
ASP ASP  
ARG ARG  
GLU ARG  
GLY GLY  
GLY LYS  
GLY LYS  
LYS LYS  
TRP TRP  
ARG ARG  
ALA ALA  
GLU LYS  
LYS ASP  
ARG ARG  
GLU SER  
LEU LEU  
ARG ARG  
THR THR  
LYS ASN  
GLU GLU  
THR THR  
ASP ASP  
GLU GLU  
ASP ASP  
GLY GLY  
TRP TRP  
THR THR  
VAL VAL  
ARG ARG

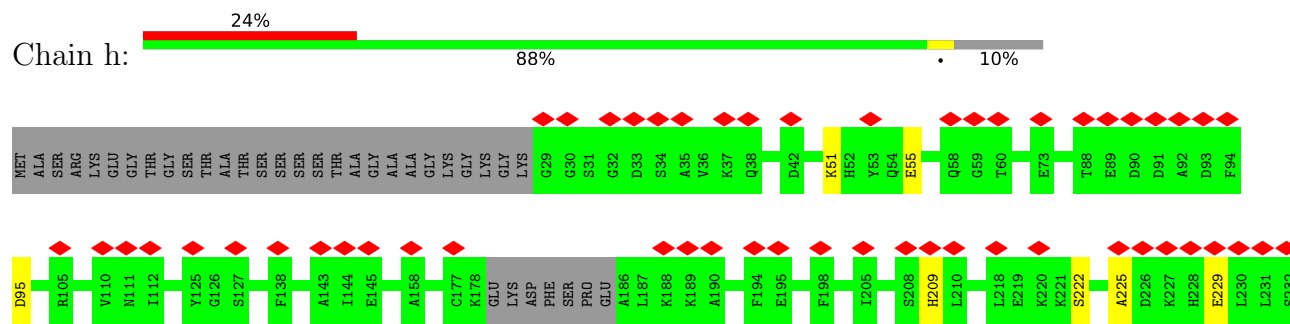
- Molecule 46: Eukaryotic translation initiation factor 3 subunit F

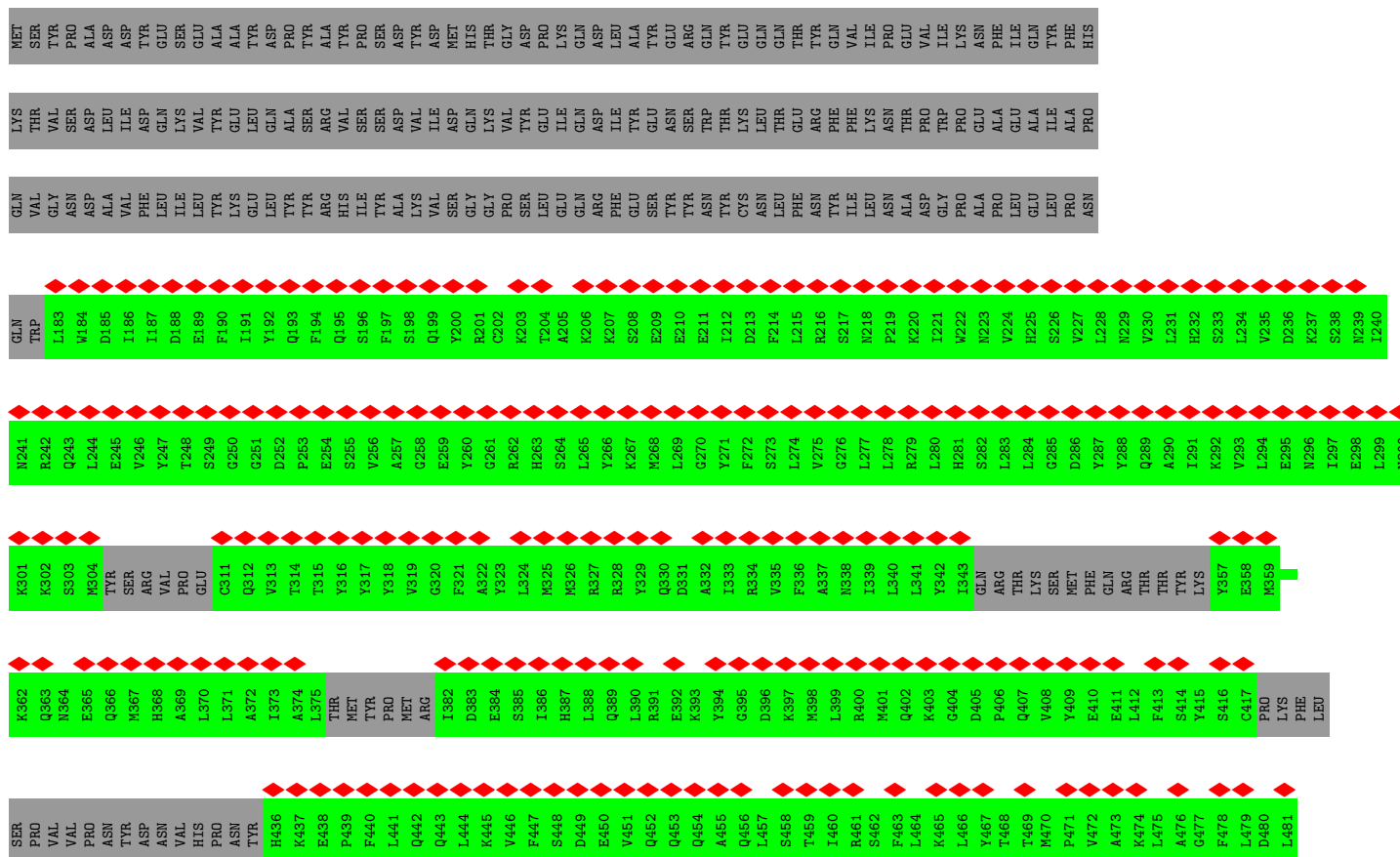


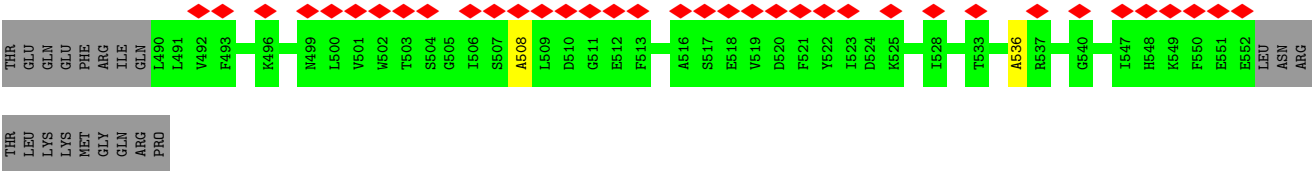
- Molecule 47: Eukaryotic translation initiation factor 3 subunit M



- Molecule 48: Eukaryotic translation initiation factor 3 subunit H







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36575	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	42.118	Depositor
Minimum map value	-17.754	Depositor
Average map value	0.052	Depositor
Map value standard deviation	1.246	Depositor
Recommended contour level	3.88	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, 1MA, 5MC, T6A, NMM, 4AC, OMU, PSU, OMC, M7G, K, A2M, 6MZ, GNP, 1MG, IAS, UY1, MG, OMG, 2MG, H2U, MA6, ZN

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	0.21	0/39125	0.26	0/60957
2	Ln	0.19	0/231	0.39	0/294
3	SE	0.18	0/2118	0.34	0/2849
4	SA	0.17	0/1764	0.36	0/2396
5	SB	0.17	0/1832	0.36	0/2449
6	SH	0.15	0/1546	0.35	0/2071
7	SI	0.16	0/1715	0.34	0/2287
8	SL	0.17	0/1280	0.32	0/1712
9	SV	0.18	0/643	0.30	0/860
10	SX	0.17	0/1116	0.35	0/1490
11	Sa	0.17	0/836	0.29	0/1121
12	SC	0.18	0/1746	0.33	0/2358
13	SG	0.16	0/1926	0.33	0/2563
14	SJ	0.15	0/1537	0.31	0/2052
15	SN	0.17	0/1232	0.33	0/1656
16	SO	0.46	1/1020 (0.1%)	0.38	0/1366
17	SW	0.19	0/1051	0.35	0/1406
18	SY	0.16	0/1031	0.37	0/1370
19	Sb	0.18	0/665	0.34	0/891
20	Se	0.16	0/474	0.33	0/623
21	B	0.13	0/664	0.27	0/1031
22	SD	0.16	0/1793	0.32	0/2414
23	SF	0.16	0/1516	0.29	0/2037
24	Sf	0.19	0/525	0.49	0/695
25	SR	0.19	0/1078	0.42	0/1447
26	Sd	0.19	0/470	0.35	0/623
27	Sg	0.16	0/2497	0.35	0/3399
28	Sc	0.17	0/519	0.33	0/694
29	SK	0.20	0/840	0.44	0/1133
30	SM	0.18	0/916	0.52	0/1233
31	SU	0.17	0/821	0.37	0/1103



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	SQ	0.18	0/1142	0.36	0/1528
33	SS	0.17	0/1216	0.34	0/1628
34	ST	0.16	0/1119	0.32	0/1498
35	SP	0.18	0/1126	0.46	0/1505
36	SZ	0.17	0/591	0.42	0/794
37	D	0.15	0/2400	0.37	0/3235
38	E	0.12	0/3643	0.31	0/4929
39	F	0.14	0/144	0.45	0/191
40	G	0.17	0/1600	0.22	0/2492
41	H	0.16	0/905	0.41	0/1202
42	e	0.16	0/2672	0.45	0/3647
43	d	0.14	0/2821	0.37	0/3852
44	c	0.19	0/5284	0.41	0/7123
45	a	0.19	0/4891	0.44	0/6615
46	3f	0.12	0/1269	0.30	0/1762
47	m	0.14	0/1926	0.39	0/2669
48	h	0.14	0/1569	0.39	0/2183
49	k	0.09	0/1055	0.25	0/1469
50	l	0.10	0/1575	0.27	0/2187
All	All	0.19	1/111475 (0.0%)	0.33	0/159089

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	SO	136	PRO	C-N	-13.20	1.14	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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	18671	232	0
2	Ln	230	0	276	2	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	SE	2076	0	2177	26	0
4	SA	1727	0	1729	40	0
5	SB	1806	0	1888	34	0
6	SH	1523	0	1622	22	0
7	SI	1686	0	1771	17	0
8	SL	1258	0	1332	16	0
9	SV	636	0	637	11	0
10	SX	1098	0	1167	14	0
11	Sa	821	0	870	7	0
12	SC	1709	0	1797	22	0
13	SG	1903	0	2068	12	0
14	SJ	1512	0	1629	27	0
15	SN	1208	0	1293	19	0
16	SO	1016	0	1037	20	0
17	SW	1034	0	1080	13	0
18	SY	1014	0	1082	18	0
19	Sb	651	0	672	9	0
20	Se	468	0	519	5	0
21	B	594	0	304	1	0
22	SD	1765	0	1865	20	0
23	SF	1495	0	1549	15	0
24	Sf	515	0	523	15	0
25	SR	1064	0	1118	18	0
26	Sd	459	0	448	6	0
27	Sg	2440	0	2396	26	0
28	Sc	517	0	549	11	0
29	SK	816	0	841	17	0
30	SM	906	0	921	33	0
31	SU	811	0	877	17	0
32	SQ	1124	0	1193	20	0
33	SS	1198	0	1261	18	0
34	ST	1113	0	1145	14	0
35	SP	1103	0	1156	33	0
36	SZ	585	0	640	16	0
37	D	2367	0	2411	45	0
38	E	3585	0	3736	41	0
39	F	143	0	144	5	0
40	G	1623	0	828	5	0
41	H	895	0	924	17	0
42	e	2635	0	2207	65	0
43	d	2778	0	2143	48	0
44	c	5197	0	5201	186	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	a	4799	0	4830	158	0
46	3f	1272	0	564	4	0
47	m	1917	0	1096	25	0
48	h	1571	0	683	4	0
49	k	1057	0	475	1	0
50	l	1581	0	689	3	0
51	S2	17	0	0	0	0
51	SX	1	0	0	0	0
51	Sd	1	0	0	0	0
52	B	7	0	0	0	0
52	H	1	0	0	0	0
52	S2	76	0	0	0	0
52	SE	1	0	0	0	0
52	SN	1	0	0	0	0
52	SO	1	0	0	0	0
53	Sa	1	0	0	0	0
53	Sd	1	0	0	0	0
53	Sf	1	0	0	0	0
54	E	32	0	13	0	0
55	E	8	0	8	1	0
56	S2	349	0	0	1	0
56	SB	1	0	0	0	0
56	SC	1	0	0	0	0
56	SE	1	0	0	0	0
56	SL	2	0	0	0	0
56	SN	3	0	0	0	0
56	SO	2	0	0	0	0
56	SQ	1	0	0	0	0
56	SS	1	0	0	0	0
56	ST	1	0	0	0	0
56	Sa	1	0	0	0	0
All	All	108768	0	86055	1346	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 1346 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)
45:a:11:ALA:HB2	45:a:34:VAL:HG21	1.48	0.96
44:c:371:ILE:HD11	44:c:411:ILE:HD13	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:e:215:ILE:HD12	42:e:232:ILE:HD12	1.56	0.88
43:d:28:MET:HE2	44:c:591:MET:HE1	1.61	0.82
7:SI:198:TYR:O	7:SI:202:ILE:HD12	1.81	0.81

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%)	251 (96%)	9 (4%)	0	100	100
4	SA	217/295 (74%)	211 (97%)	6 (3%)	0	100	100
5	SB	219/264 (83%)	207 (94%)	11 (5%)	1 (0%)	24	60
6	SH	187/194 (96%)	172 (92%)	15 (8%)	0	100	100
7	SI	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
8	SL	152/158 (96%)	141 (93%)	11 (7%)	0	100	100
9	SV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
10	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
11	Sa	100/115 (87%)	91 (91%)	9 (9%)	0	100	100
12	SC	218/293 (74%)	210 (96%)	8 (4%)	0	100	100
13	SG	232/249 (93%)	227 (98%)	5 (2%)	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%)	120 (91%)	12 (9%)	0	100	100
17	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
18	SY	122/133 (92%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
20	Se	57/133 (43%)	54 (95%)	3 (5%)	0	100	100
22	SD	225/243 (93%)	216 (96%)	9 (4%)	0	100	100
23	SF	187/204 (92%)	177 (95%)	9 (5%)	1 (0%)	24	60
24	Sf	61/156 (39%)	53 (87%)	7 (12%)	1 (2%)	7	34
25	SR	129/135 (96%)	124 (96%)	5 (4%)	0	100	100
26	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
27	Sg	312/317 (98%)	296 (95%)	16 (5%)	0	100	100
28	Sc	63/69 (91%)	55 (87%)	7 (11%)	1 (2%)	7	34
29	SK	95/165 (58%)	89 (94%)	6 (6%)	0	100	100
30	SM	116/132 (88%)	103 (89%)	11 (10%)	2 (2%)	7	32
31	SU	100/119 (84%)	94 (94%)	6 (6%)	0	100	100
32	SQ	139/146 (95%)	128 (92%)	11 (8%)	0	100	100
33	SS	143/152 (94%)	136 (95%)	7 (5%)	0	100	100
34	ST	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
35	SP	132/145 (91%)	122 (92%)	9 (7%)	1 (1%)	16	50
36	SZ	71/125 (57%)	68 (96%)	3 (4%)	0	100	100
37	D	292/315 (93%)	270 (92%)	20 (7%)	2 (1%)	18	53
38	E	470/472 (100%)	447 (95%)	21 (4%)	2 (0%)	30	65
39	F	14/333 (4%)	11 (79%)	3 (21%)	0	100	100
41	H	109/144 (76%)	96 (88%)	11 (10%)	2 (2%)	6	31
42	e	380/445 (85%)	338 (89%)	41 (11%)	1 (0%)	36	70
43	d	408/548 (74%)	369 (90%)	39 (10%)	0	100	100
44	c	636/913 (70%)	586 (92%)	50 (8%)	0	100	100
45	a	588/1382 (42%)	527 (90%)	61 (10%)	0	100	100
46	3f	251/357 (70%)	218 (87%)	29 (12%)	4 (2%)	7	34
47	m	348/374 (93%)	285 (82%)	58 (17%)	5 (1%)	9	36
48	h	313/352 (89%)	265 (85%)	46 (15%)	2 (1%)	21	56
49	k	209/218 (96%)	194 (93%)	13 (6%)	2 (1%)	12	45
50	l	307/564 (54%)	291 (95%)	16 (5%)	0	100	100
All	All	9169/11992 (76%)	8480 (92%)	661 (7%)	28 (0%)	37	70

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	SM	45	ARG
30	SM	80	ASP
35	SP	138	SER
37	D	200	TYR
41	H	17	ASN

### 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%)	23 (100%)	0	100	100
3	SE	224/225 (100%)	219 (98%)	5 (2%)	45	74
4	SA	182/243 (75%)	181 (100%)	1 (0%)	81	89
5	SB	202/231 (87%)	197 (98%)	5 (2%)	42	72
6	SH	169/174 (97%)	166 (98%)	3 (2%)	51	77
7	SI	178/180 (99%)	173 (97%)	5 (3%)	38	70
8	SL	138/142 (97%)	136 (99%)	2 (1%)	59	80
9	SV	67/67 (100%)	64 (96%)	3 (4%)	24	59
10	SX	113/115 (98%)	109 (96%)	4 (4%)	32	65
11	Sa	89/98 (91%)	86 (97%)	3 (3%)	32	66
12	SC	186/225 (83%)	183 (98%)	3 (2%)	55	79
13	SG	204/218 (94%)	201 (98%)	3 (2%)	57	80
14	SJ	161/168 (96%)	159 (99%)	2 (1%)	63	82
15	SN	130/131 (99%)	129 (99%)	1 (1%)	73	86
16	SO	105/118 (89%)	100 (95%)	5 (5%)	23	57
17	SW	112/113 (99%)	111 (99%)	1 (1%)	70	85
18	SY	108/115 (94%)	101 (94%)	7 (6%)	15	47
19	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	81
20	Se	48/104 (46%)	47 (98%)	1 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	SD	190/202 (94%)	183 (96%)	7 (4%)	30	64
23	SF	159/170 (94%)	157 (99%)	2 (1%)	61	81
24	Sf	56/140 (40%)	55 (98%)	1 (2%)	51	77
25	SR	119/122 (98%)	118 (99%)	1 (1%)	73	86
26	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	75
27	Sg	272/275 (99%)	264 (97%)	8 (3%)	37	70
28	Sc	58/62 (94%)	56 (97%)	2 (3%)	32	66
29	SK	88/136 (65%)	86 (98%)	2 (2%)	44	74
30	SM	98/108 (91%)	95 (97%)	3 (3%)	35	68
31	SU	94/107 (88%)	92 (98%)	2 (2%)	47	75
32	SQ	117/121 (97%)	113 (97%)	4 (3%)	32	66
33	SS	126/132 (96%)	121 (96%)	5 (4%)	28	62
34	ST	112/114 (98%)	111 (99%)	1 (1%)	70	85
35	SP	120/130 (92%)	115 (96%)	5 (4%)	26	61
36	SZ	65/103 (63%)	61 (94%)	4 (6%)	16	49
37	D	264/280 (94%)	259 (98%)	5 (2%)	50	76
38	E	397/397 (100%)	388 (98%)	9 (2%)	44	74
39	F	16/304 (5%)	15 (94%)	1 (6%)	16	48
41	H	94/123 (76%)	93 (99%)	1 (1%)	65	83
42	e	206/406 (51%)	198 (96%)	8 (4%)	28	62
43	d	200/494 (40%)	190 (95%)	10 (5%)	22	56
44	c	563/811 (69%)	540 (96%)	23 (4%)	27	61
45	a	528/1259 (42%)	514 (97%)	14 (3%)	39	71
47	m	49/335 (15%)	46 (94%)	3 (6%)	17	49
All	All	6553/9147 (72%)	6376 (97%)	177 (3%)	40	71

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	E	435	THR
44	c	465	HIS
42	e	231	ASN
43	d	318	TYR
44	c	741	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
35	SP	137	HIS
41	H	33	GLN
36	SZ	45	ASN
38	E	325	HIS
42	e	231	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1713/1869 (91%)	353 (20%)	9 (0%)
21	B	27/50 (54%)	17 (62%)	1 (3%)
40	G	72/75 (96%)	17 (23%)	0
All	All	1812/1994 (90%)	387 (21%)	10 (0%)

5 of 387 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	4	C
1	S2	17	C
1	S2	26	U
1	S2	33	G
1	S2	41	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	1520	G
1	S2	1824	A
21	B	-4	A
1	S2	1257	G
1	S2	1308	U

## 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	1288	1	19,22,23	0.33	0	26,31,34	0.42	0
1	PSU	S2	609	1	18,21,22	0.49	0	22,30,33	0.62	0
40	1MG	G	10	40	22,26,27	0.29	0	33,39,42	0.64	1 (3%)
1	OMU	S2	354	1	19,22,23	0.31	0	26,31,34	0.59	0
1	B8N	S2	1248	1	24,29,30	0.61	0	29,42,45	0.62	0
1	OMG	S2	644	1	23,26,27	0.30	0	33,38,41	0.41	0
1	PSU	S2	1186	1	18,21,22	0.50	0	22,30,33	0.59	0
1	PSU	S2	966	1	18,21,22	0.55	0	22,30,33	0.54	0
1	OMG	S2	1490	52,1	23,26,27	0.34	0	33,38,41	0.33	0
1	PSU	S2	1367	1	18,21,22	0.53	0	22,30,33	0.53	0
1	A2M	S2	576	1	22,25,26	0.09	0	31,36,39	0.29	0
1	PSU	S2	218	1	18,21,22	0.47	0	22,30,33	0.60	0
1	PSU	S2	1692	1	18,21,22	0.58	0	22,30,33	0.56	0
40	T6A	G	37	40	31,34,35	0.45	0	44,49,52	0.63	1 (2%)
1	PSU	S2	63	1	18,21,22	0.51	0	22,30,33	0.62	0
1	A2M	S2	1678	1	22,25,26	0.10	0	31,36,39	0.26	0
1	MA6	S2	1850	1	23,26,27	0.32	0	34,38,41	0.60	1 (2%)
40	2MG	G	26	40	23,26,27	0.34	0	32,38,41	0.37	0
1	PSU	S2	1004	1	18,21,22	0.50	0	22,30,33	0.57	0
1	PSU	S2	822	1	18,21,22	0.63	1 (5%)	22,30,33	0.50	0
1	PSU	S2	1643	52,1	18,21,22	0.59	0	22,30,33	0.56	0
1	PSU	S2	93	1	18,21,22	0.52	0	22,30,33	0.56	0
1	OMG	S2	509	52,1	23,26,27	0.34	0	33,38,41	0.46	0
1	PSU	S2	109	1	18,21,22	0.55	0	22,30,33	0.55	0
1	OMC	S2	517	1	19,22,23	0.31	0	26,31,34	0.43	0
1	PSU	S2	814	1	18,21,22	0.50	0	22,30,33	0.57	0
1	PSU	S2	296	1	18,21,22	0.54	0	22,30,33	0.54	0
1	UY1	S2	1326	52,1	19,22,23	0.43	0	22,31,34	0.43	0
1	PSU	S2	1046	1	18,21,22	0.53	0	22,30,33	0.53	0
1	A2M	S2	668	1	22,25,26	0.12	0	31,36,39	0.31	0
1	A2M	S2	159	1	22,25,26	0.11	0	31,36,39	0.23	0
1	4AC	S2	1842	1	21,24,25	0.32	0	29,34,37	0.29	0
1	PSU	S2	1596	1	18,21,22	0.55	0	22,30,33	0.52	0
1	PSU	S2	1360	51,1	18,21,22	0.57	0	22,30,33	0.63	0
1	PSU	S2	1244	1	18,21,22	0.53	0	22,30,33	0.55	0
1	PSU	S2	366	1	18,21,22	0.54	0	22,30,33	0.53	0
40	5MC	G	48	40	18,22,23	0.53	0	26,32,35	0.56	0
1	PSU	S2	119	1	18,21,22	0.52	0	22,30,33	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	S2	406	1	18,21,22	0.52	0	22,30,33	0.60	0
1	A2M	S2	590	1	22,25,26	0.11	0	31,36,39	0.31	0
1	OMG	S2	1328	51,1	23,26,27	0.32	0	33,38,41	0.40	0
1	A2M	S2	484	1	22,25,26	0.08	0	31,36,39	0.19	0
1	OMC	S2	1391	1	19,22,23	0.31	0	26,31,34	0.44	0
1	PSU	S2	572	1	18,21,22	0.54	0	22,30,33	0.54	0
1	OMU	S2	428	1	19,22,23	0.26	0	26,31,34	0.45	0
1	OMC	S2	462	1	19,22,23	0.29	0	26,31,34	0.41	0
1	PSU	S2	1625	1	18,21,22	0.54	0	22,30,33	0.58	0
1	A2M	S2	1031	1	22,25,26	0.10	0	31,36,39	0.23	0
1	A2M	S2	468	1	22,25,26	0.09	0	31,36,39	0.31	0
1	OMC	S2	1272	1	19,22,23	0.29	0	26,31,34	0.37	0
40	1MA	G	58	40	21,25,26	0.46	0	31,37,40	0.73	1 (3%)
1	PSU	S2	1056	1	18,21,22	0.54	0	22,30,33	0.55	0
1	4AC	S2	1337	1	21,24,25	0.33	0	29,34,37	0.35	0
1	PSU	S2	801	1	18,21,22	0.52	0	22,30,33	0.56	0
1	PSU	S2	918	1	18,21,22	0.46	0	22,30,33	0.37	0
1	PSU	S2	1445	1	18,21,22	0.55	0	22,30,33	0.56	0
1	PSU	S2	667	52,1	18,21,22	0.59	0	22,30,33	0.52	0
1	OMG	S2	601	1	23,26,27	0.32	0	33,38,41	0.32	0
1	A2M	S2	99	52,1	22,25,26	0.09	0	31,36,39	0.29	0
1	OMG	S2	683	1	23,26,27	0.32	0	33,38,41	0.46	0
1	OMU	S2	172	1	19,22,23	0.27	0	26,31,34	0.54	0
1	OMG	S2	867	1	23,26,27	0.31	0	33,38,41	0.31	0
1	PSU	S2	815	1	18,21,22	0.48	0	22,30,33	0.59	0
34	NMM	ST	67	34	9,11,12	0.64	0	6,12,14	1.75	2 (33%)
1	PSU	S2	1174	1	18,21,22	0.54	0	22,30,33	0.57	0
1	OMU	S2	1442	52,1	19,22,23	0.30	0	26,31,34	0.40	0
1	6MZ	S2	1832	52,51,1	22,25,26	0.13	0	30,36,39	0.28	0
1	PSU	S2	863	1	18,21,22	0.57	0	22,30,33	0.52	0
1	PSU	S2	649	1	18,21,22	0.53	0	22,30,33	0.64	0
1	PSU	S2	1232	1	18,21,22	0.54	0	22,30,33	0.54	0
1	PSU	S2	866	1	18,21,22	0.53	0	22,30,33	0.56	0
1	PSU	S2	100	1	18,21,22	0.49	0	22,30,33	0.58	0
1	OMG	S2	1447	1	23,26,27	0.30	0	33,38,41	0.41	0
1	PSU	S2	1347	1	18,21,22	0.56	0	22,30,33	0.55	0
1	OMC	S2	1703	52,1	19,22,23	0.29	0	26,31,34	0.51	0
1	PSU	S2	34	1	18,21,22	0.49	0	22,30,33	0.60	0
1	PSU	S2	651	1	18,21,22	0.53	0	22,30,33	0.58	0
1	PSU	S2	300	1	18,21,22	0.52	0	22,30,33	0.57	0
1	PSU	S2	1136	1	18,21,22	0.52	0	22,30,33	0.57	0
1	OMU	S2	1804	1	19,22,23	0.31	0	26,31,34	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	IAS	SO	138	16	6,7,8	1.05	0	6,8,10	1.66	3 (50%)
1	OMC	S2	174	1	19,22,23	0.29	0	26,31,34	0.42	0
1	PSU	S2	1045	1	18,21,22	0.49	0	22,30,33	0.62	0
1	OMU	S2	116	1	19,22,23	0.26	0	26,31,34	0.44	0
1	PSU	S2	36	1	18,21,22	0.53	0	22,30,33	0.53	0
1	PSU	S2	1177	1	18,21,22	0.54	0	22,30,33	0.56	0
1	PSU	S2	686	1	18,21,22	0.53	0	22,30,33	0.55	0
1	PSU	S2	105	1	18,21,22	0.49	0	22,30,33	0.58	0
1	A2M	S2	166	1	22,25,26	0.10	0	31,36,39	0.35	0
1	PSU	S2	681	1	18,21,22	0.55	0	22,30,33	0.55	0
1	A2M	S2	1383	1	22,25,26	0.08	0	31,36,39	0.48	0
1	A2M	S2	27	1	22,25,26	0.10	0	31,36,39	0.23	0
1	A2M	S2	512	1	22,25,26	0.09	0	31,36,39	0.50	1 (3%)
1	MA6	S2	1851	1	23,26,27	0.33	0	34,38,41	0.66	1 (2%)
1	PSU	S2	1003	1	18,21,22	0.54	0	22,30,33	0.54	0
1	PSU	S2	1238	1	18,21,22	0.53	0	22,30,33	0.55	0
40	H2U	G	47	40	18,21,22	0.31	0	21,30,33	0.45	0
1	OMU	S2	121	1	19,22,23	0.30	0	26,31,34	0.50	0
1	OMG	S2	436	1	23,26,27	0.35	0	33,38,41	0.48	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
1	OMU	S2	1288	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
40	1MG	G	10	40	-	2/7/25/26	0/3/3/3
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
1	B8N	S2	1248	1	-	2/16/34/35	0/2/2/2
1	OMG	S2	644	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1186	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1490	52,1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1367	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	218	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
40	T6A	G	37	40	-	0/23/41/42	0/3/3/3
1	PSU	S2	63	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
40	2MG	G	26	40	-	4/9/27/28	0/3/3/3
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	1643	52,1	-	0/7/25/26	0/2/2/2
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	52,1	-	0/9/27/28	0/3/3/3
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
1	UY1	S2	1326	52,1	-	2/9/27/28	0/2/2/2
1	PSU	S2	1046	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	668	1	-	3/9/27/28	0/3/3/3
1	A2M	S2	159	1	-	3/9/27/28	0/3/3/3
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	1596	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1360	51,1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	366	1	-	2/7/25/26	0/2/2/2
40	5MC	G	48	40	-	3/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	590	1	-	3/9/27/28	0/3/3/3
1	OMG	S2	1328	51,1	-	0/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
1	OMC	S2	462	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
1	OMC	S2	1272	1	-	0/9/27/28	0/2/2/2
40	1MA	G	58	40	-	0/7/25/26	0/3/3/3
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	918	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	667	52,1	-	2/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	99	52,1	-	0/9/27/28	0/3/3/3
1	OMG	S2	683	1	-	0/9/27/28	0/3/3/3
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	867	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
34	NMM	ST	67	34	-	0/9/11/13	-
1	PSU	S2	1174	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1442	52,1	-	1/9/27/28	0/2/2/2
1	6MZ	S2	1832	52,51,1	-	2/9/27/28	0/3/3/3
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	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	1447	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	52,1	-	0/9/27/28	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	651	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	1136	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	2/9/27/28	0/2/2/2
16	IAS	SO	138	16	-	1/7/7/8	-
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1045	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	36	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	686	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	512	1	-	1/9/27/28	0/3/3/3
1	MA6	S2	1851	1	-	3/11/29/30	0/3/3/3
1	PSU	S2	1003	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	H2U	G	47	40	-	3/7/38/39	0/2/2/2
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	822	PSU	O4'-C1'	-2.13	1.40	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	ST	67	NMM	NE-CZ-NH2	-3.23	116.52	119.48
40	G	10	1MG	C6-C5-C4	-2.67	117.02	119.97
40	G	37	T6A	C12-N11-C10	2.65	126.36	121.94
1	S2	1850	MA6	C2-N1-C6	2.40	117.42	111.75
1	S2	1851	MA6	C2-N1-C6	2.35	117.31	111.75

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	166	A2M	C1'-C2'-O2'-CM'
1	S2	428	OMU	C2'-C1'-N1-C2
1	S2	428	OMU	C2'-C1'-N1-C6
1	S2	468	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

28 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	354	OMU	1	0
1	S2	576	A2M	4	0
1	S2	1678	A2M	2	0
1	S2	1850	MA6	4	0
40	G	26	2MG	1	0
1	S2	93	PSU	1	0
1	S2	814	PSU	2	0
1	S2	668	A2M	3	0
1	S2	159	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1842	4AC	1	0
1	S2	484	A2M	3	0
1	S2	428	OMU	2	0
1	S2	462	OMC	1	0
1	S2	1031	A2M	1	0
1	S2	468	A2M	2	0
1	S2	1337	4AC	1	0
1	S2	99	A2M	1	0
1	S2	815	PSU	2	0
1	S2	1174	PSU	1	0
1	S2	1442	OMU	2	0
1	S2	1832	6MZ	4	0
1	S2	116	OMU	2	0
1	S2	166	A2M	6	0
1	S2	1383	A2M	1	0
1	S2	27	A2M	5	0
1	S2	512	A2M	3	0
1	S2	1851	MA6	3	0
1	S2	121	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 109 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	$\# Z  > 2$
55	MET	E	502	-	6,7,8	0.48	0	2,7,9	0.13	0
54	GNP	E	501	-	33,34,34	2.23	5 (15%)	46,54,54	1.48	3 (6%)

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
55	MET	E	502	-	-	2/5/6/8	-
54	GNP	E	501	-	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	E	501	GNP	PB-O3A	8.12	1.69	1.59
54	E	501	GNP	PG-N3B	6.53	1.80	1.63
54	E	501	GNP	PG-O1G	4.67	1.53	1.46
54	E	501	GNP	PB-O1B	3.10	1.51	1.46
54	E	501	GNP	PB-O2B	-2.15	1.51	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	E	501	GNP	O1G-PG-N3B	-7.18	101.20	111.77
54	E	501	GNP	O2B-PB-O1B	4.80	119.98	109.92
54	E	501	GNP	O2G-PG-O3G	2.30	113.77	107.64

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	E	501	GNP	PB-N3B-PG-O1G
54	E	501	GNP	PG-N3B-PB-O1B
54	E	501	GNP	C4'-C5'-O5'-PA
54	E	501	GNP	O4'-C4'-C5'-O5'
55	E	502	MET	C-CA-CB-CG

There are no ring outliers.

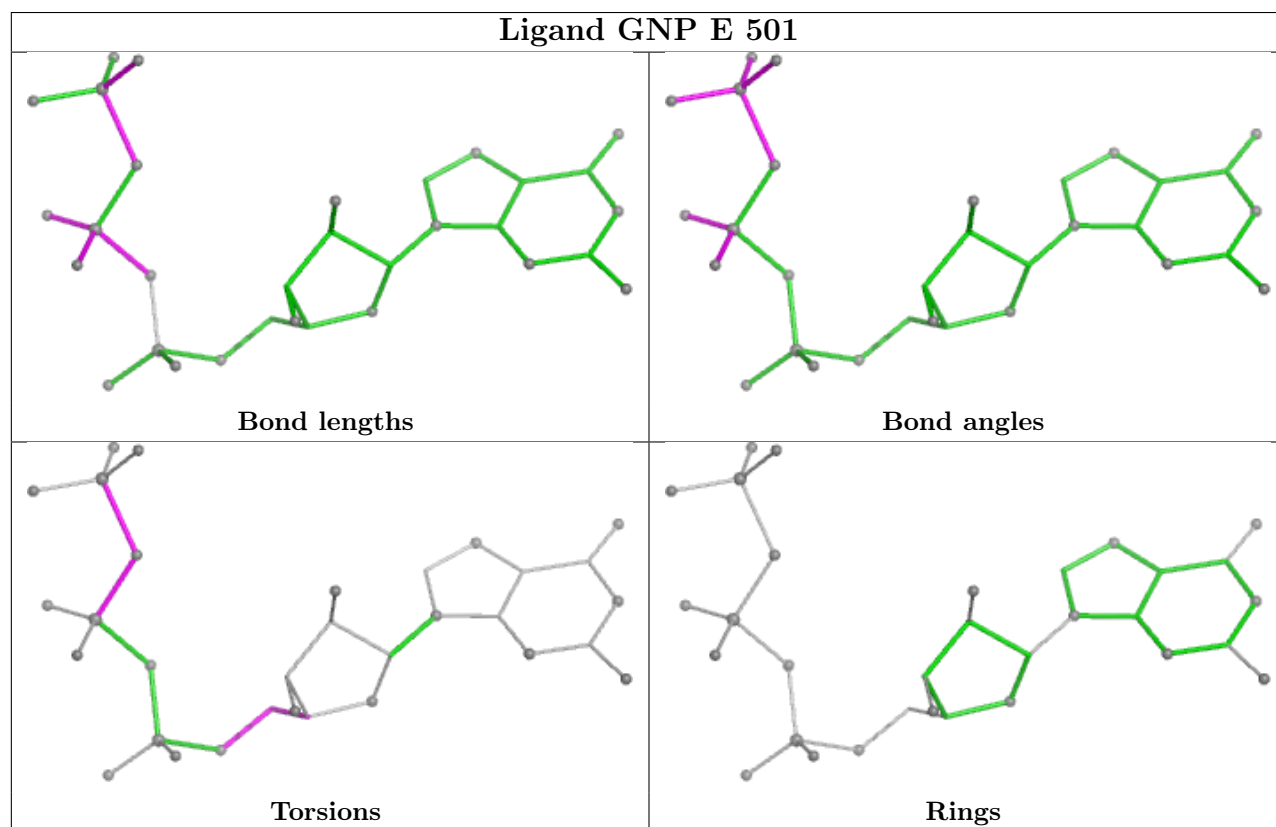
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	E	502	MET	1	0

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
16	SO	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SO	136:PRO	C	137:SER	N	1.14

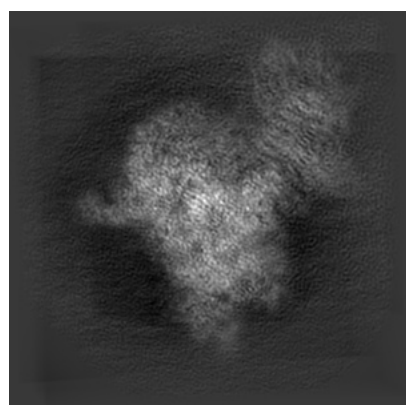
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57010. These allow visual inspection of the internal detail of the map and identification of artifacts.

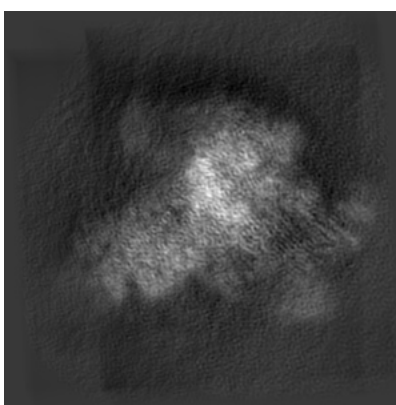
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

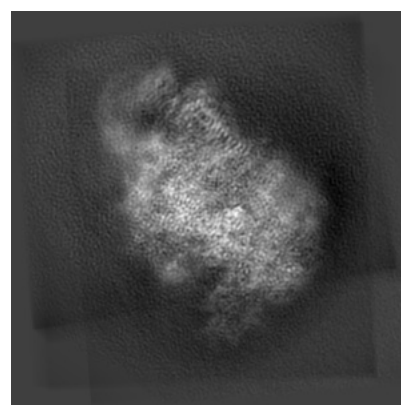
#### 6.1.1 Primary map



X



Y

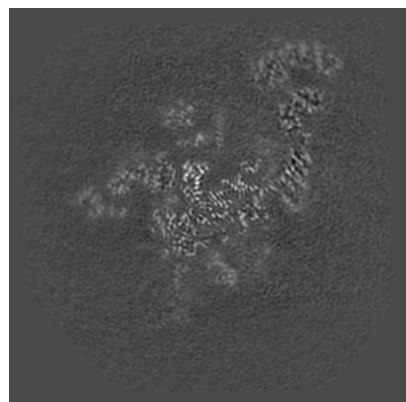


Z

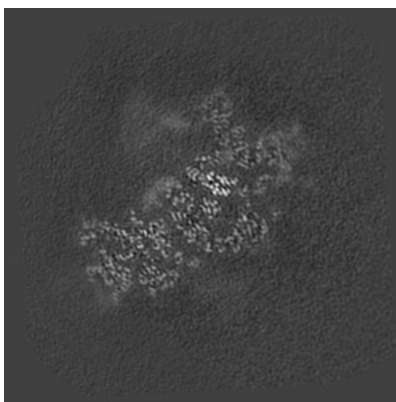
The images above show the map projected in three orthogonal directions.

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

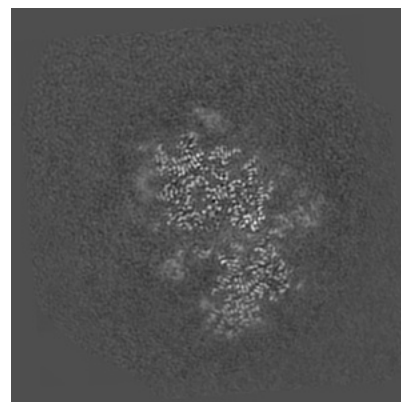
#### 6.2.1 Primary map



X Index: 260



Y Index: 260

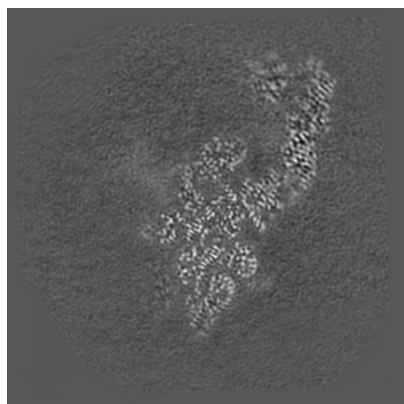


Z Index: 260

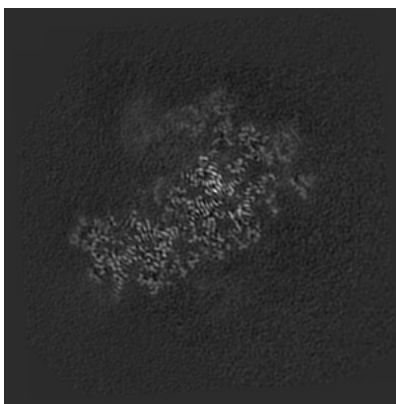
The images above show central slices of the map in three orthogonal directions.

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

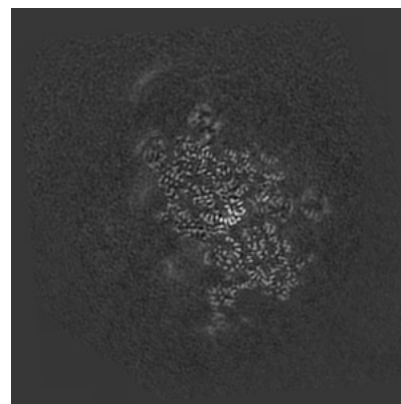
### 6.3.1 Primary map



X Index: 233



Y Index: 253

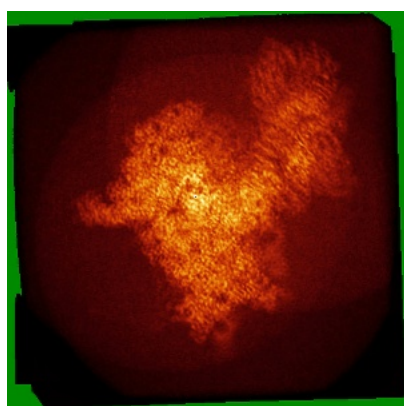


Z Index: 279

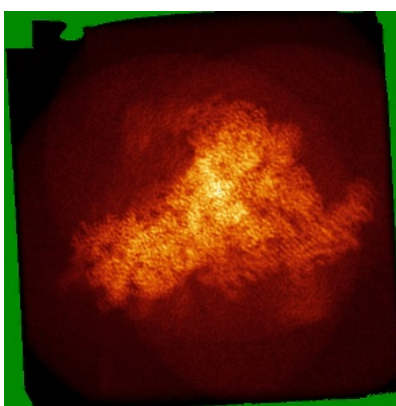
The images above show the largest variance slices of the map in three orthogonal directions.

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

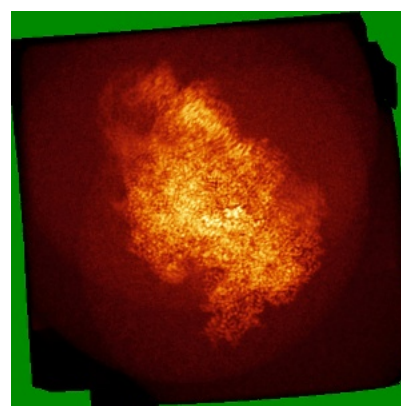
### 6.4.1 Primary map



X



Y

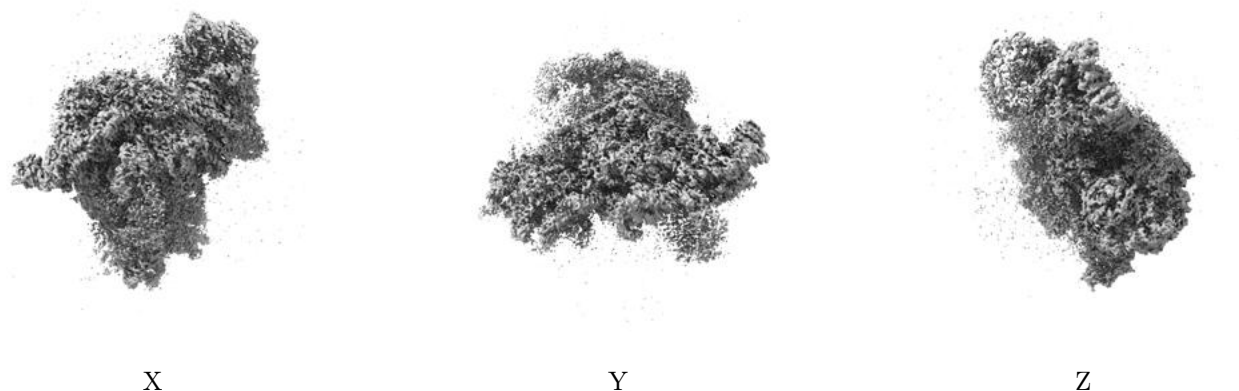


Z

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 3.88. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

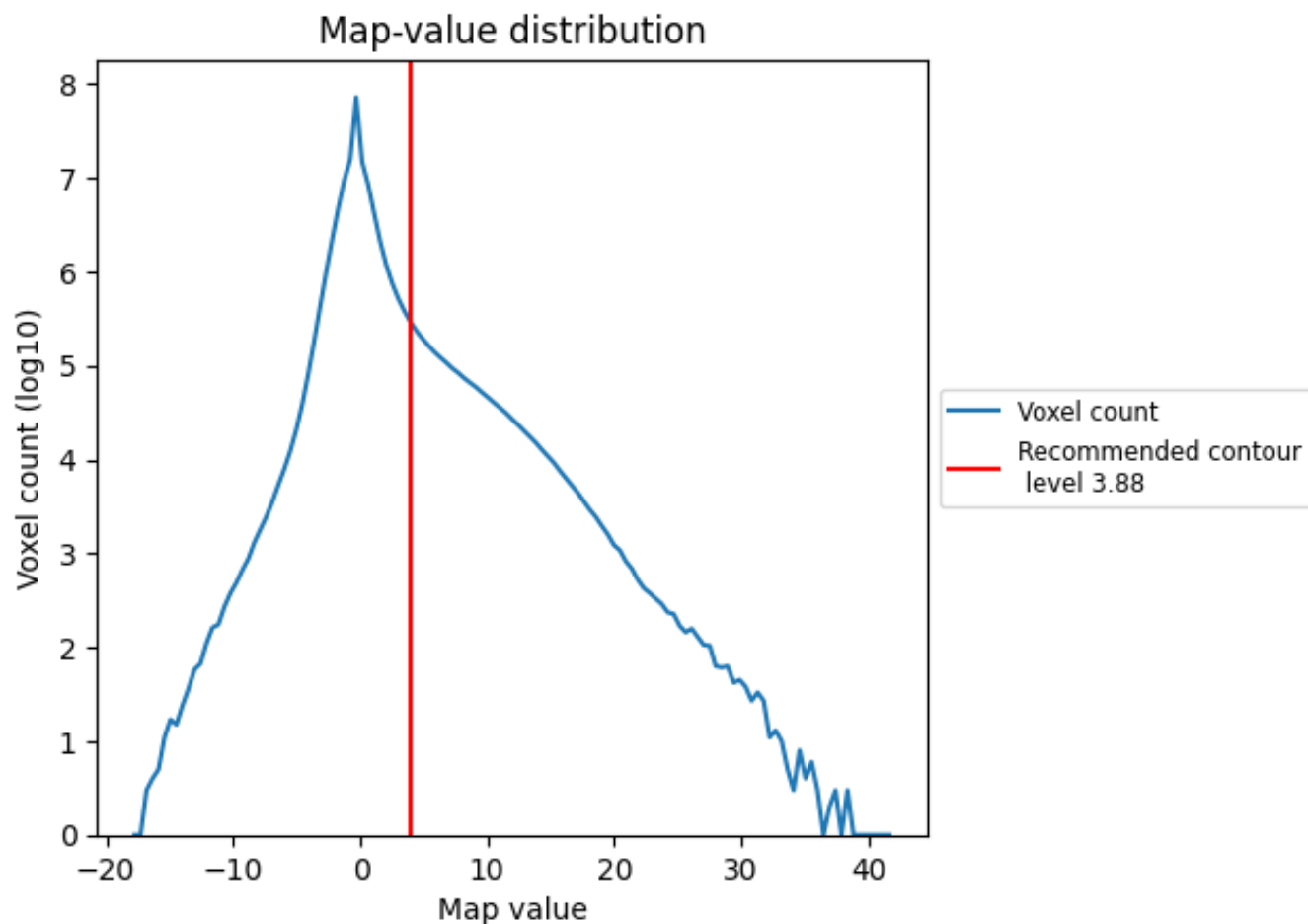
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

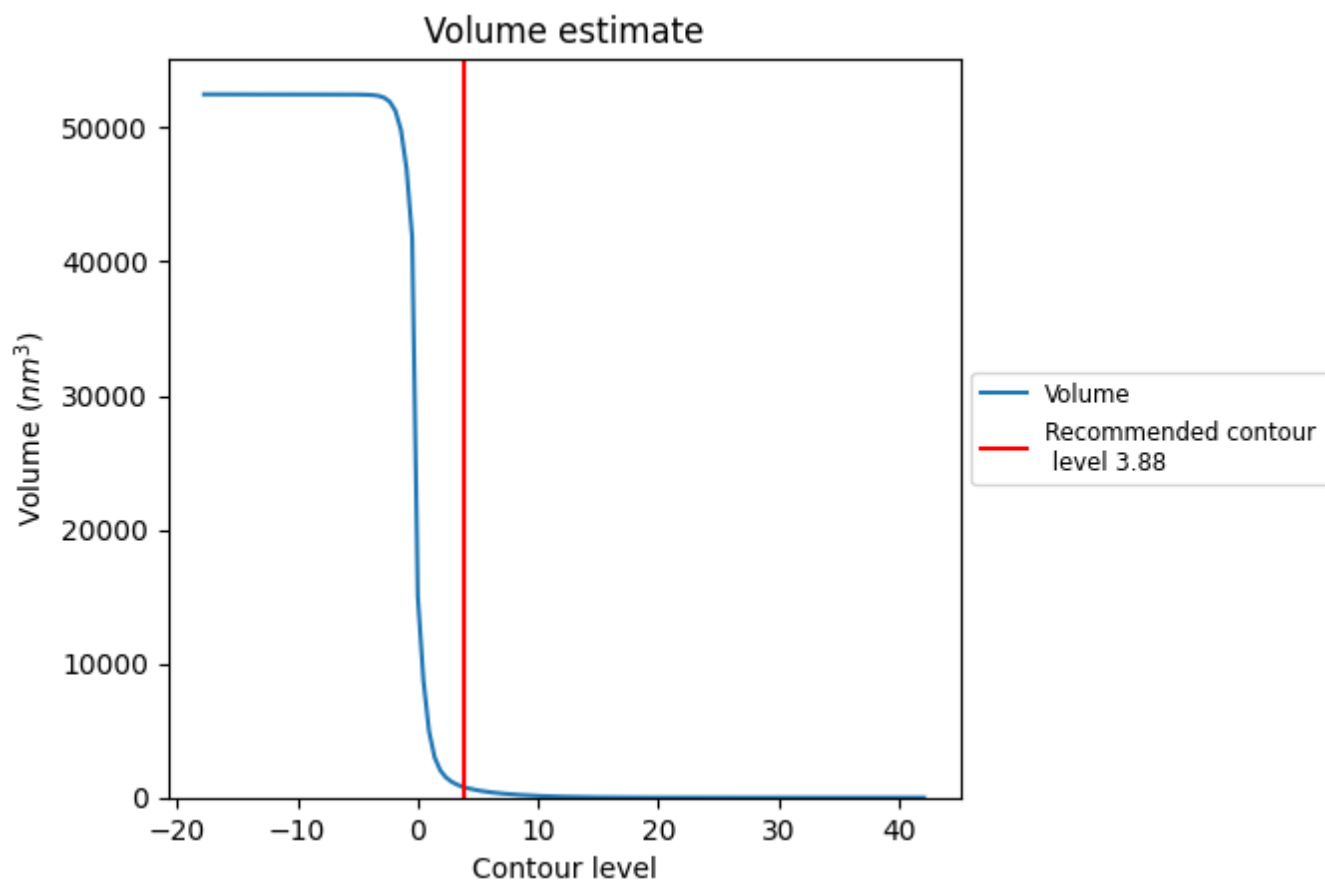
This section contains the results of statistical analysis of the map.

### 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.

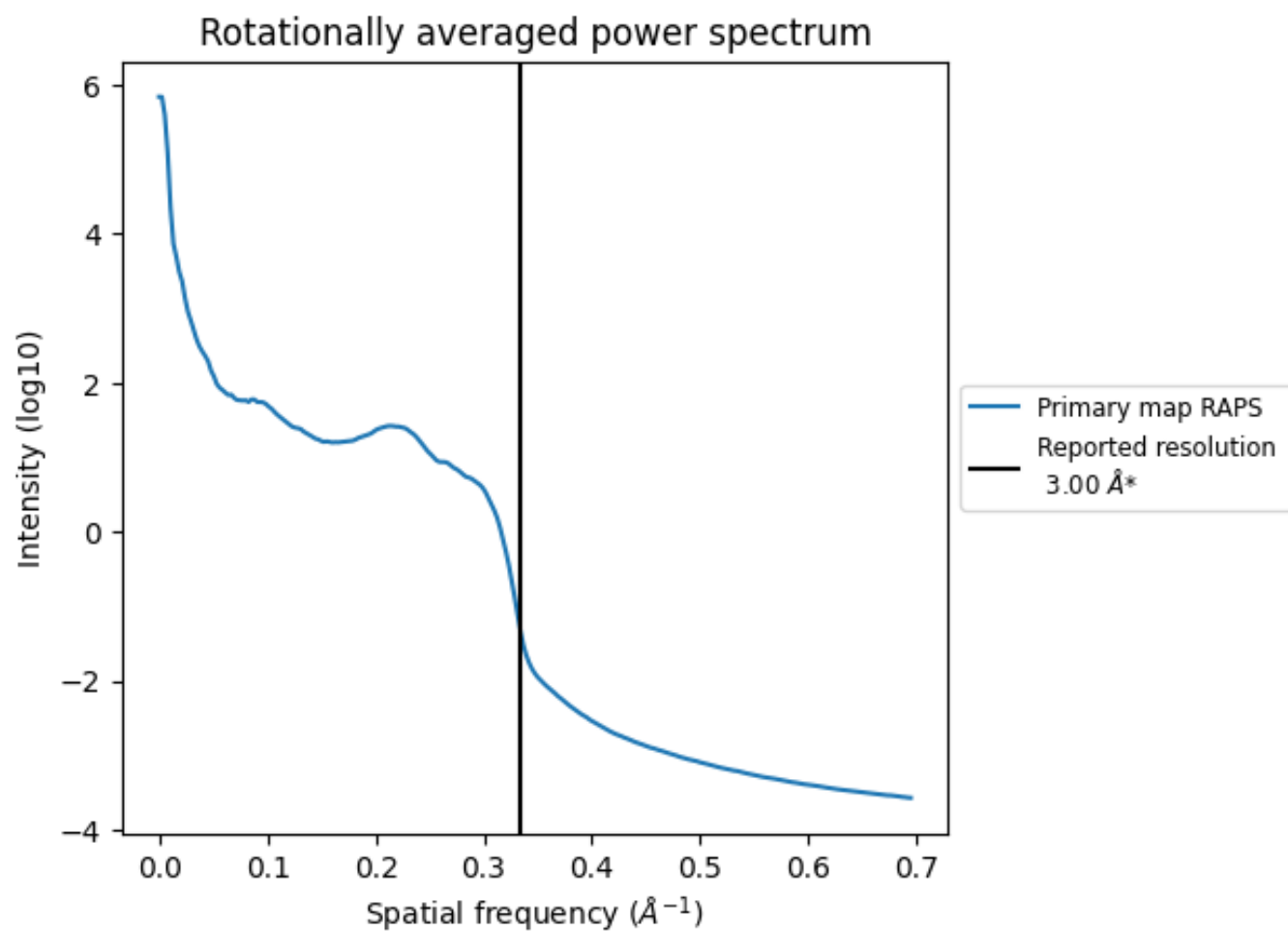
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 774 nm<sup>3</sup>; this corresponds to an approximate mass of 699 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 0.333 Å<sup>-1</sup>



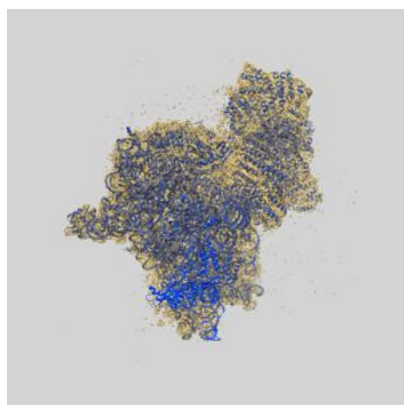
## 8 Fourier-Shell correlation

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

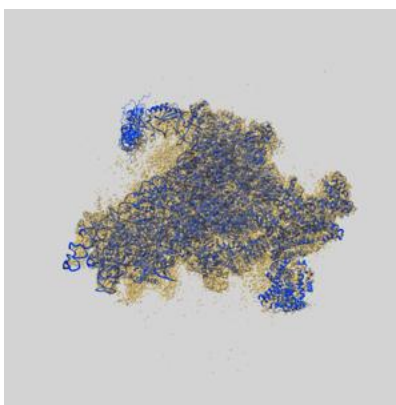
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57010 and PDB model 28ZY. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

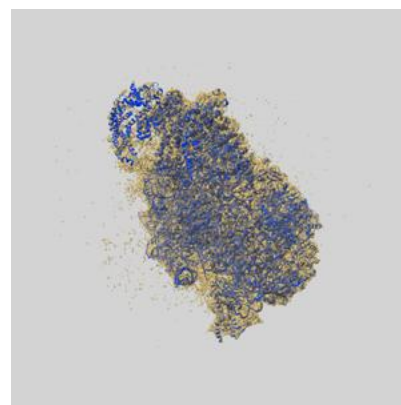
### 9.1 Map-model overlay [i](#)



X



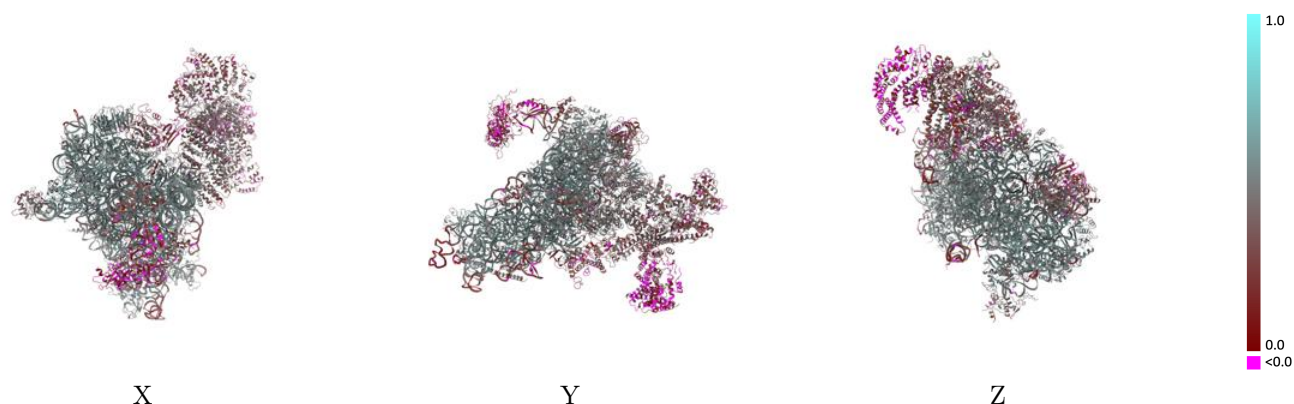
Y



Z

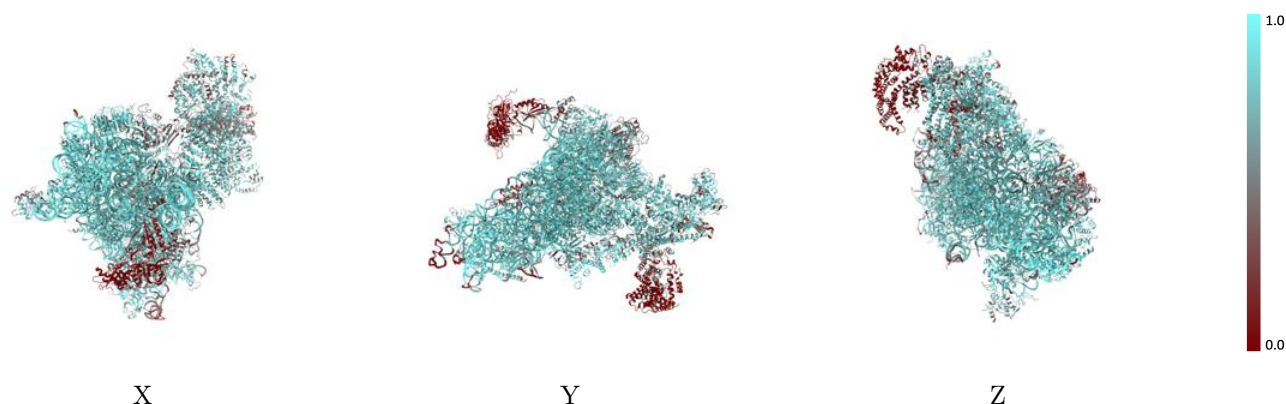
The images above show the 3D surface view of the map at the recommended contour level 3.88 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



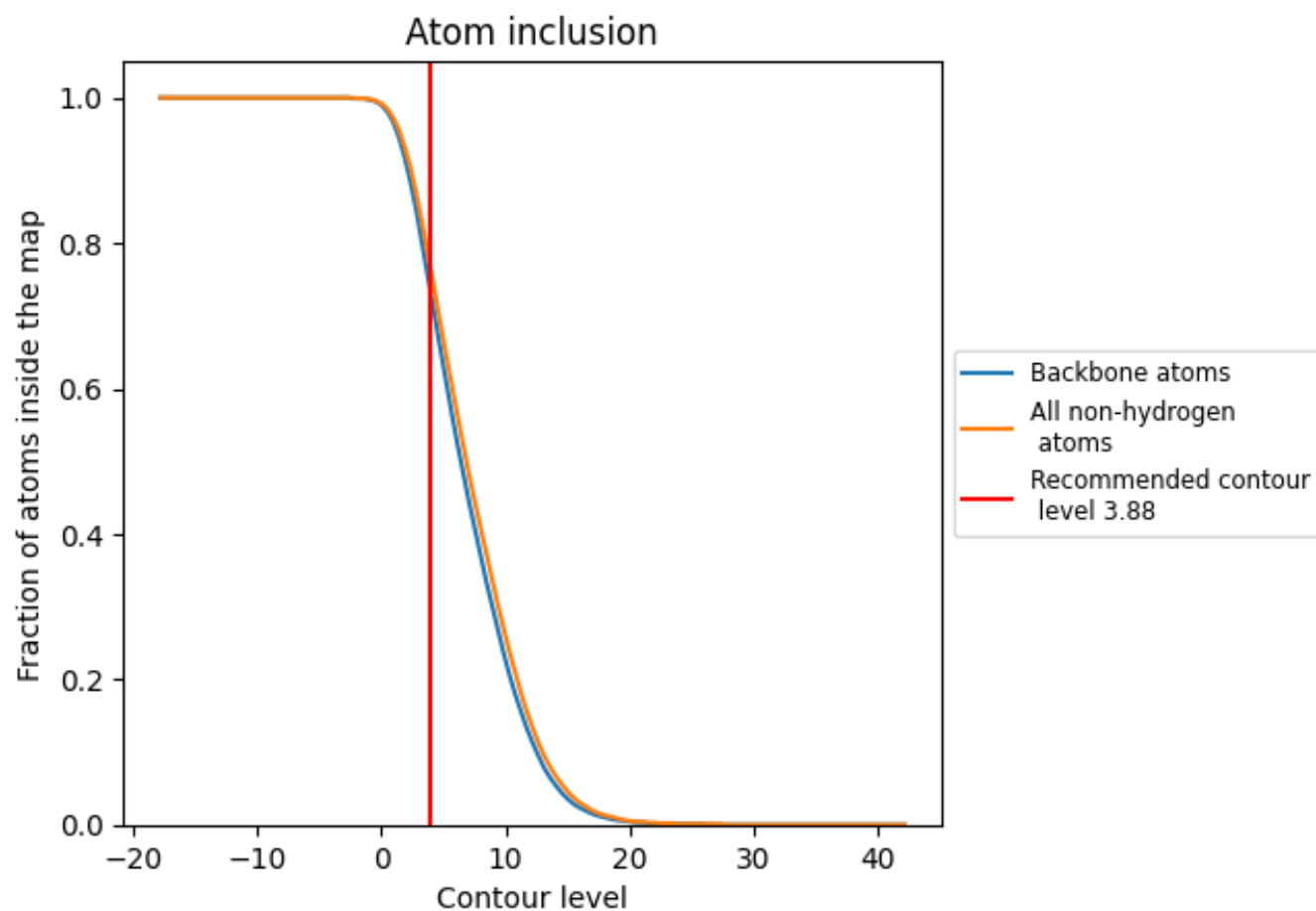
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.88).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 77% 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 (3.88) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.4480
3f	 0.6790	 0.3320
B	 0.7010	 0.3220
D	 0.4760	 0.3430
E	 0.0360	 0.1250
F	 0.0000	 0.0630
G	 0.7680	 0.3470
H	 0.8060	 0.4690
Ln	 0.8370	 0.5140
S2	 0.9050	 0.5050
SA	 0.8350	 0.5160
SB	 0.8420	 0.5070
SC	 0.8740	 0.5400
SD	 0.8460	 0.5190
SE	 0.8940	 0.5510
SF	 0.8830	 0.5450
SG	 0.8050	 0.5000
SH	 0.7360	 0.4660
SI	 0.8510	 0.5160
SJ	 0.8390	 0.5160
SK	 0.8510	 0.5250
SL	 0.8500	 0.5340
SM	 0.6070	 0.3850
SN	 0.8680	 0.5310
SO	 0.8460	 0.5160
SP	 0.8380	 0.5180
SQ	 0.8980	 0.5560
SR	 0.8130	 0.5110
SS	 0.8540	 0.5430
ST	 0.8740	 0.5390
SU	 0.7960	 0.5050
SV	 0.8360	 0.5220
SW	 0.9120	 0.5630
SX	 0.9090	 0.5530
SY	 0.8570	 0.5300



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Chain	Atom inclusion	Q-score
SZ	 0.8630	 0.5230
Sa	 0.8810	 0.5340
Sb	 0.8750	 0.5140
Sc	 0.8870	 0.5090
Sd	 0.9210	 0.5640
Se	 0.7480	 0.4980
Sf	 0.6870	 0.4100
Sg	 0.8410	 0.5140
a	 0.6960	 0.3620
c	 0.6890	 0.3710
d	 0.6050	 0.3170
e	 0.6550	 0.2820
h	 0.6380	 0.2950
k	 0.1180	 0.0820
l	 0.1890	 0.0980
m	 0.6780	 0.3070