



# Full wwPDB EM Validation Report ⓘ

May 17, 2023 – 05:39 pm BST

PDB ID : 8CAH  
EMDB ID : EMD-16525  
Title : Cryo-EM structure of native Otu2-bound ubiquitinated 43S pre-initiation complex  
Authors : Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.  
Deposited on : 2023-01-24  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

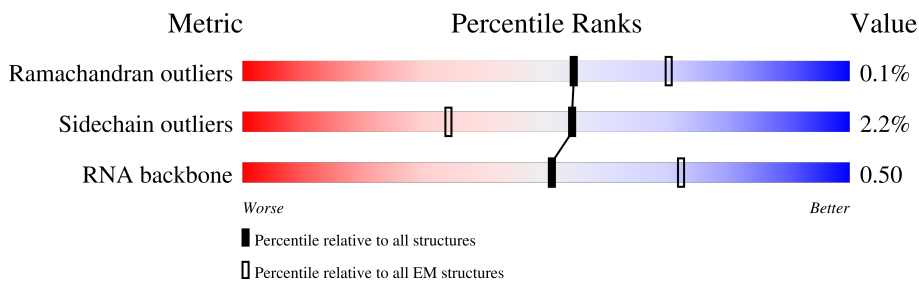
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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







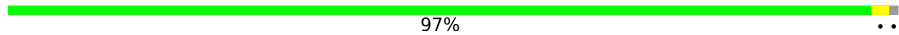
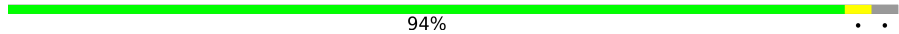
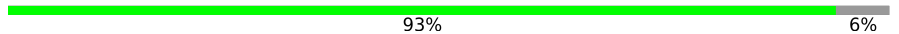


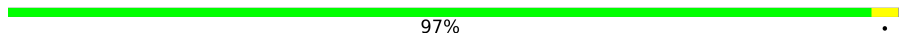

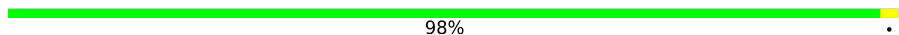
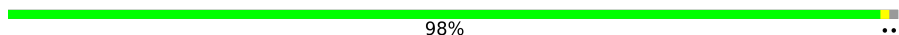
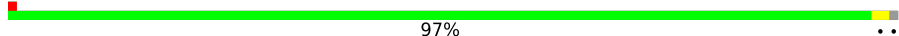


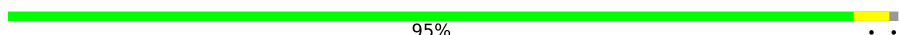
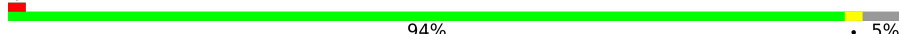





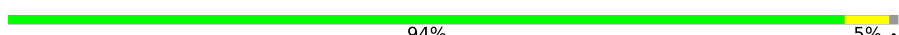

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	l	347	
2	r	274	
3	o	964	
4	p	763	
5	q	812	
6	i	153	
7	m	108	
8	j	77	

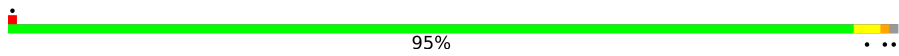
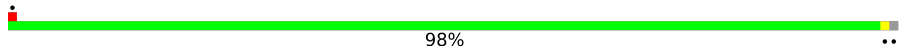

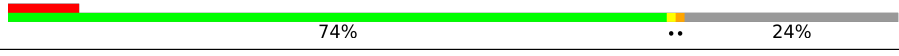
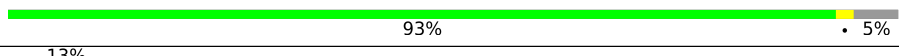
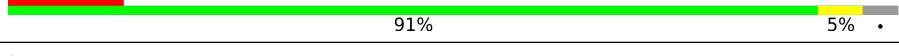
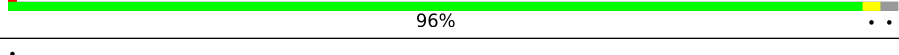
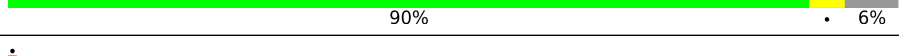
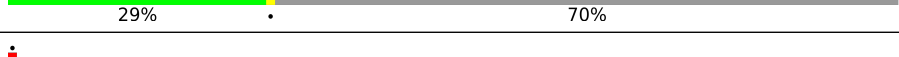
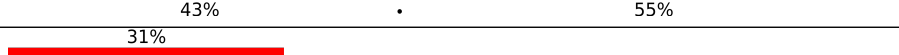
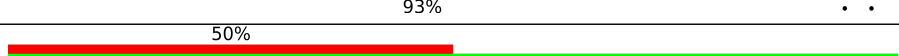
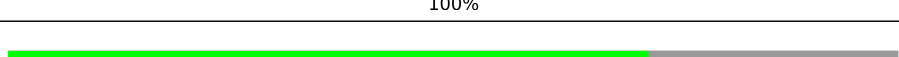

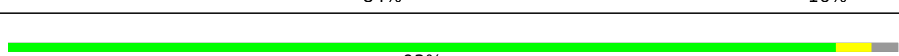
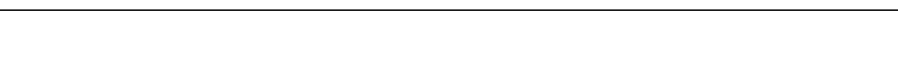
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Mol	Chain	Length	Quality of chain
9	2	1800	 67% 27%
10	P	252	 79% 18%
11	Q	255	 85% 11%
12	R	254	 83% 15%
13	S	261	 97%
14	T	236	 94%
15	V	200	 93% 6%
16	W	197	 90% 7%
17	X	156	 90% 9%
18	Y	151	 97%
19	Z	137	 91% 7%
20	a	87	 98%
21	b	130	 98%
22	c	145	 97%
23	d	135	 99%
24	e	119	 80% 18%
25	f	82	 95%
26	g	63	 94% 5%
27	E	142	 75% 7% 18%
28	A	240	 88% 5% 8%
29	B	225	 89% 8%
30	C	105	 83% 5% 12%
31	D	143	 6% 83% 15%
32	F	143	 94% 5%
33	H	136	 85% 11%

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Mol	Chain	Length	Quality of chain
34	I	146	 95%
35	J	144	 98%
36	K	121	 81% 17%
37	L	108	 8% 74% 24%
38	M	56	 93% 5%
39	N	76	 13% 91% 5%
40	O	319	 96%
41	h	67	 90% 6%
42	y	265	 29% 70%
42	z	265	 43% 55%
43	x	608	 31% 93%
44	k	76	 50% 100%
45	n	25	 72% 28%
46	G	307	 84% 16%
47	U	190	 93%

## 2 Entry composition [i](#)

There are 51 unique types of molecules in this entry. The entry contains 95563 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	l	330	1624	964	330	330	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	r	53	261	155	53	53	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	o	529	2631	1573	529	529	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	p	646	3201	1909	646	646	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	q	636	3169	1897	636	636	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	i	97	476	282	97	97	0	0

- Molecule 7 is a protein called SUI1 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	m	90	443	263	90	90	0	0

- Molecule 8 is a protein called RNA recognition motif (unknown).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	j	77	385	231	77	77	0	0

- Molecule 9 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	2	1745	37189	16626	6587	12231	1745	0	0

- Molecule 10 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	206	1603	1030	284	287	2	0	0

- Molecule 11 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	226	1798	1139	330	325	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R	216	1626	1042	287	295	2	0	0

- Molecule 13 is a protein called 40S ribosomal protein S4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S	258	2056	1308	387	358	3	0	0

- Molecule 14 is a protein called 40S ribosomal protein S6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	T	228	1815	1138	351	323	3	0	0

- Molecule 15 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	V	187	1476	916	295	263	2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	W	184	1479	935	285	258	1	0	0

- Molecule 17 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	X	142	1142	733	217	189	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Y	150	1192	759	224	207	2	0	0

- Molecule 19 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	127	923	568	185	167	3	0	0

- Molecule 20 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	a	87	673	415	125	131	2	0	0

- Molecule 21 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	b	129	1021	650	188	180	3	0	0

- Molecule 22 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	c	144	1121	708	220	191	2	0	0

- Molecule 23 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	d	134	1073	676	208	189	0	0

- Molecule 24 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	e	97	765	473	160	127	5	0	0

- Molecule 25 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	f	81	610	382	110	113	5	0	0

- Molecule 26 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	g	60	472	298	97	76	1	0	0

- Molecule 27 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	E	117	916	583	171	155	7	0	0

- Molecule 28 is a protein called 40S ribosomal protein S3.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	A	222	1729	1098	312	313	6	0	0

- Molecule 29 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	B	206	1605	1005	299	298	3	0	0

- Molecule 30 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	C	92	754	489	122	141	2	0	0

- Molecule 31 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	D	121	875	551	153	169	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	F	141	1105	708	203	194	0	0

- Molecule 33 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	H	121	948	596	179	171	2	0	0

- Molecule 34 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	I	145	1188	741	237	208	2	0	0

- Molecule 35 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	J	143	1112	694	208	208	2	0	0

- Molecule 36 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	K	100	797	506	144	146	1	0	0

- Molecule 37 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	L	82	651	416	123	112	0	0

- Molecule 38 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	M	53	442	274	92	72	4	0	0

- Molecule 39 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	N	73	560	355	106	95	4	0	0

- Molecule 40 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	O	312	2383	1514	409	452	8	0	0

- Molecule 41 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	h	63	491	303	96	91	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	z	120	Total	C	N	O	S	0	0
			896	556	172	166	2		
42	y	79	Total	C	N	O	S	0	0
			624	389	113	120	2		

- Molecule 43 is a protein called RLI1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	582	Total	C	N	O	S	0	0
			4607	2951	795	838	23		

- Molecule 44 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	k	76	Total	C	N	O	0	0
			374	222	76	76		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	19	PRO	SER	conflict	UNP P0CH08
k	24	GLU	ASP	conflict	UNP P0CH08
k	28	ALA	SER	conflict	UNP P0CH08

- Molecule 45 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	18	Total	C	N	O	S	0	0
			175	107	48	19	1		

- Molecule 46 is a protein called OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	G	259	Total	C	N	O	S	0	0
			1509	917	298	292	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	178	SER	CYS	conflict	UNP P38747

- Molecule 47 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
47	U	184	1473	946	263	264	0	0

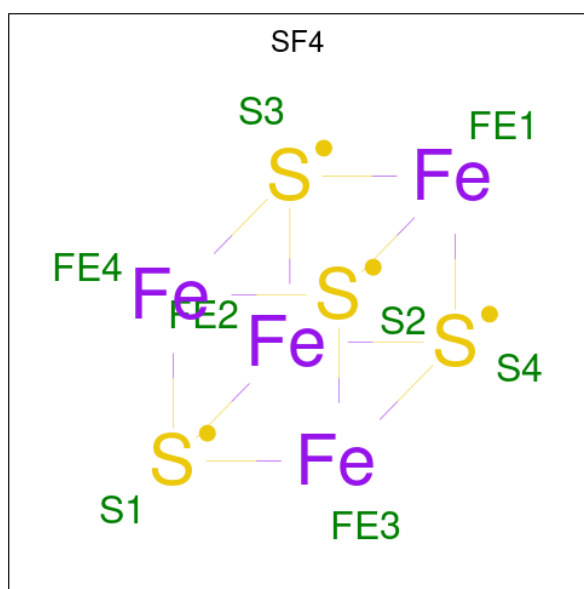
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	77	Total	Mg	0
			77	77	
48	S	1	Total	Mg	0
			1	1	
48	B	1	Total	Mg	0
			1	1	
48	x	1	Total	Mg	0
			1	1	

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

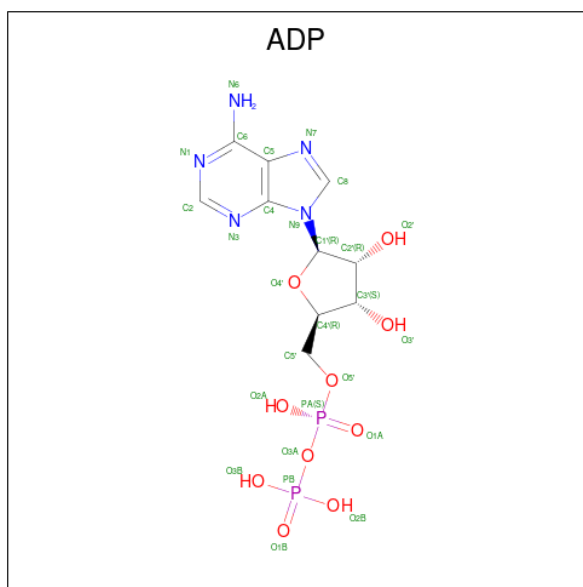
Mol	Chain	Residues	Atoms		AltConf
49	M	1	Total	Zn	0
			1	1	
49	N	1	Total	Zn	0
			1	1	

- Molecule 50 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
50	x	1	Total	Fe	S	0
			8	4	4	
50	x	1	Total	Fe	S	0
			8	4	4	

- Molecule 51 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

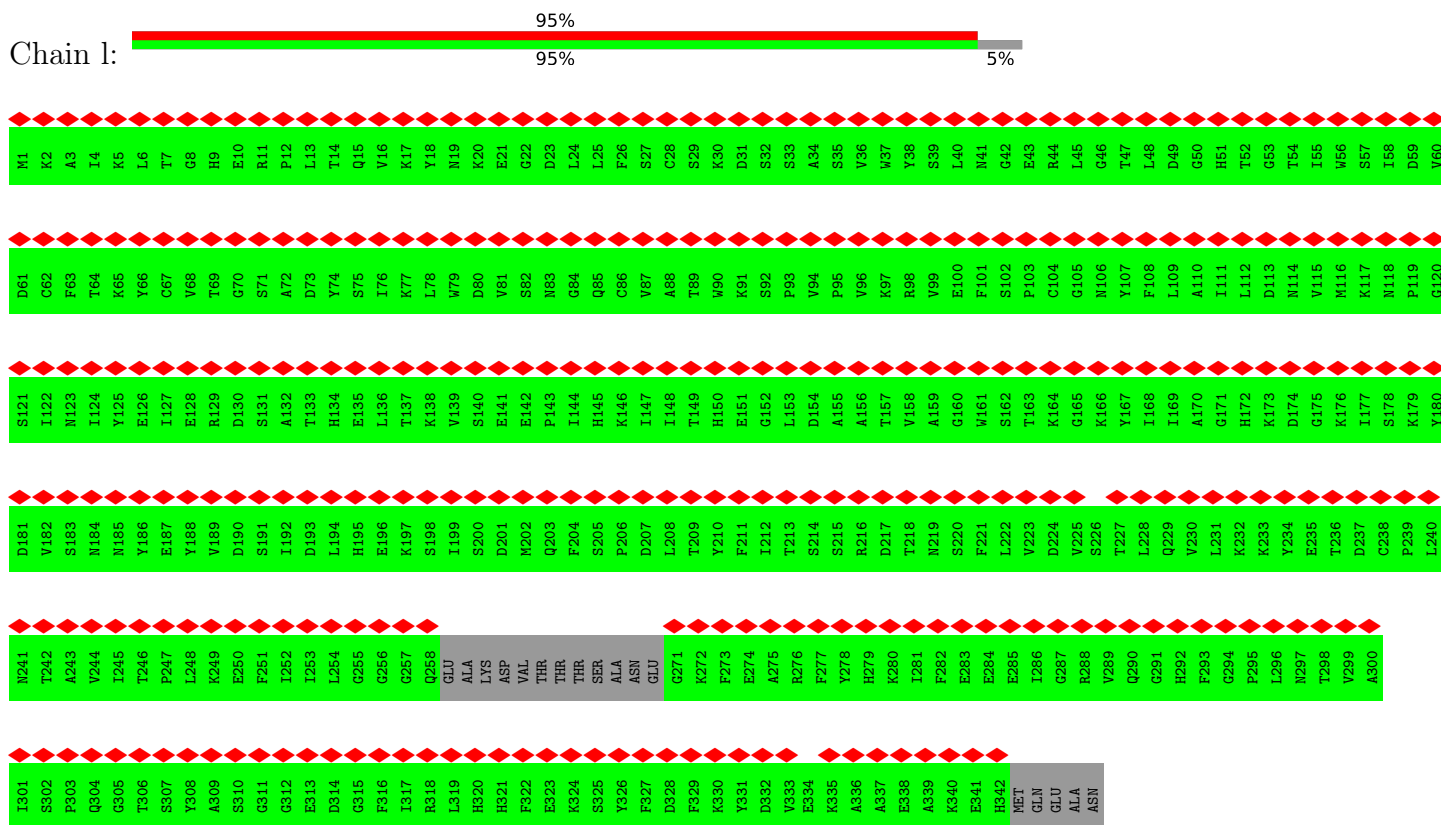


Mol	Chain	Residues	Atoms					AltConf
51	x	1	Total	C	N	O	P	0
			27	10	5	10	2	

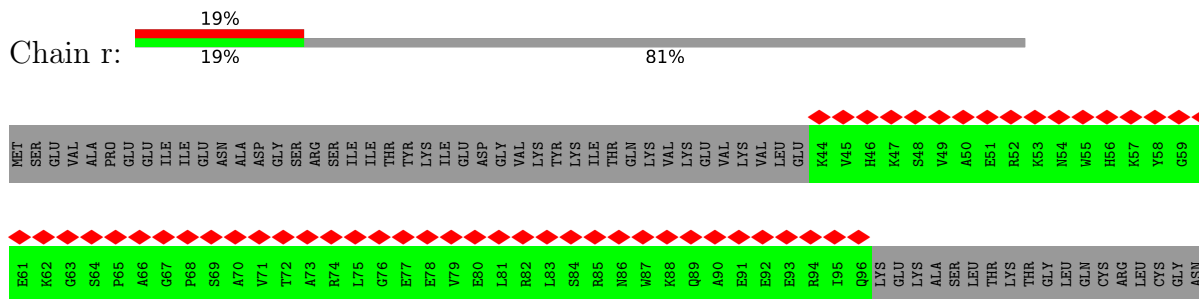
### 3 Residue-property plots

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: Eukaryotic translation initiation factor 3 subunit I

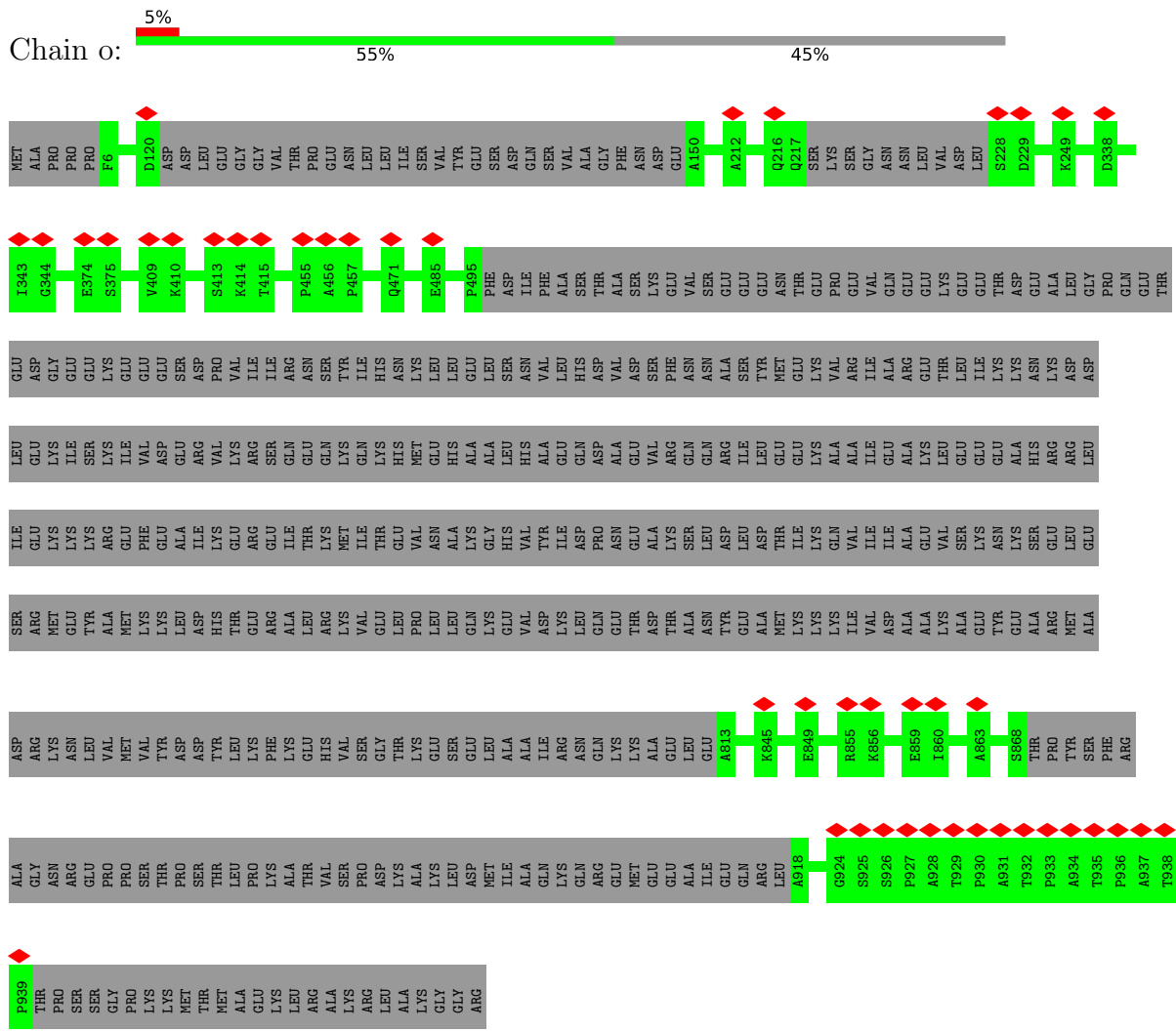


- Molecule 2: Eukaryotic translation initiation factor 3 subunit G

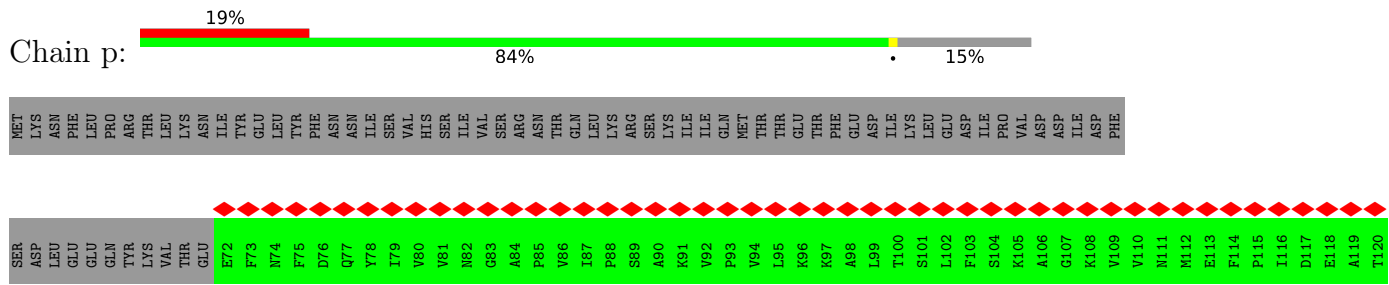


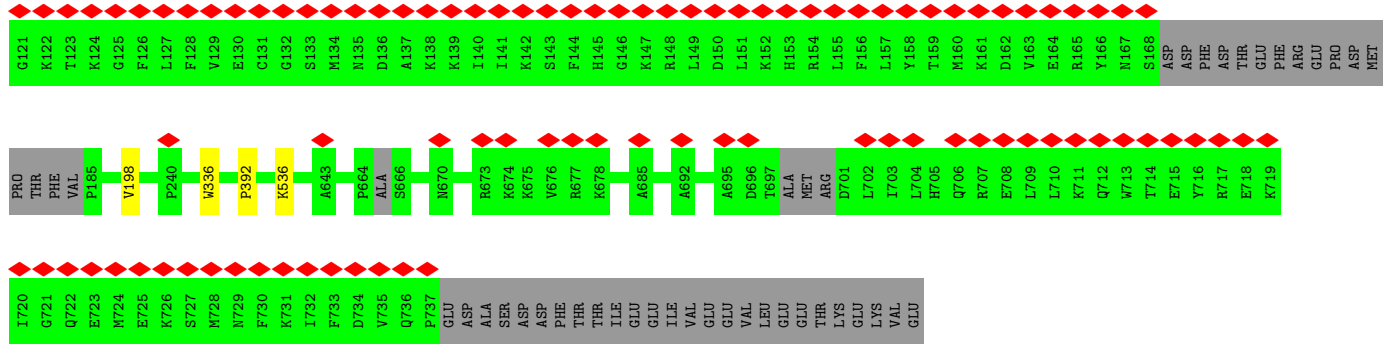
CYS PRO PHE LYS THR ILE LEU SER LEU ASP LEU PHE SER MET LEU ALA LEU LEU GLU ASP PRO ALA GLN SER TYR	TYR ARG ASP SER VAL GLU ARG ASP MET SER PHE THR LEU LEU GLY ILE MET PRO GLN VAL THR ASN ASN GLY GLY ASN LEU GLY ALA VAL ASP GLU GLY ALA ASN VAL SER ALA SER LEU PHE VAL PRO VAL GLY VAL GLY GLU GLY	SER SER GLU GLU PRO VAL ALA GLN SER LEU ASP PHE ARG LEU LEU ASP GLY SER TYR MET ASN ASN LEU LEU ILE ILE SER VAL VAL VAL TRP LYS PRO LYS LYS VAL LEU
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Molecule 3: Eukaryotic translation initiation factor 3 subunit A

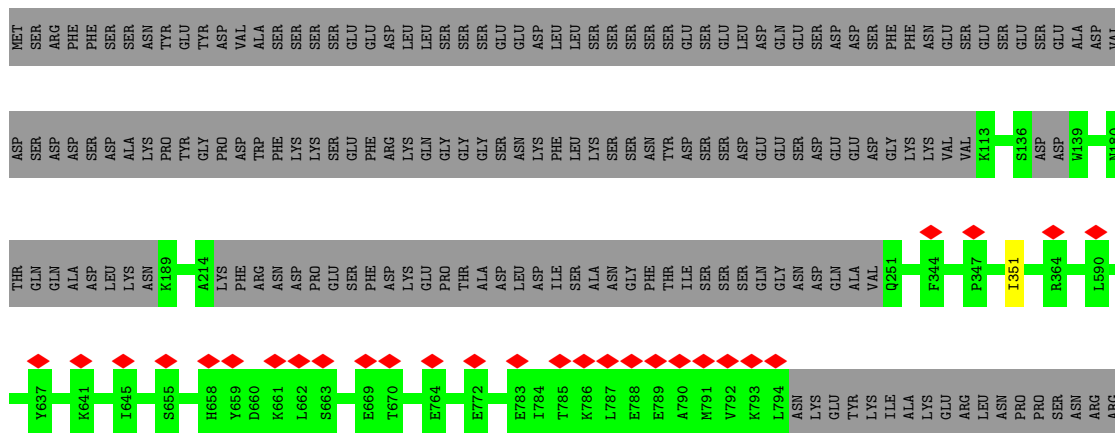
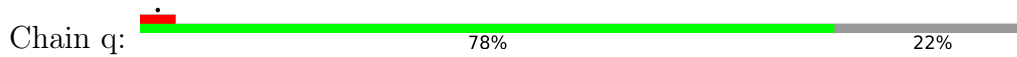


Molecule 4: Eukaryotic translation initiation factor 3 subunit B

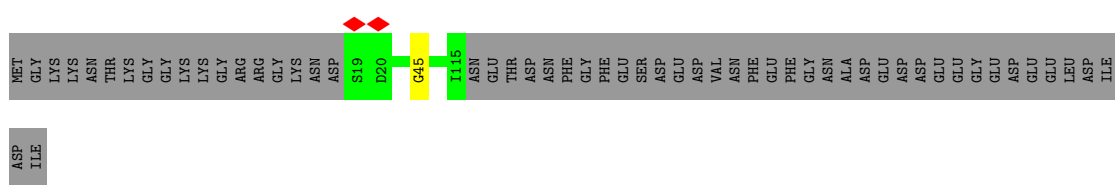




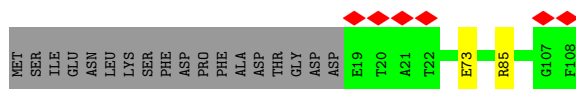
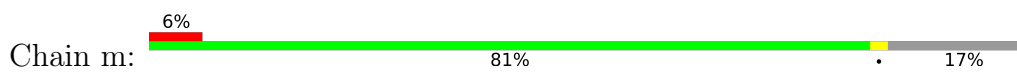
- Molecule 5: Eukaryotic translation initiation factor 3 subunit C



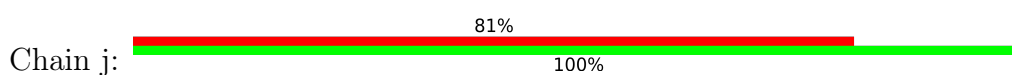
- Molecule 6: Eukaryotic translation initiation factor 4C



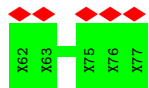
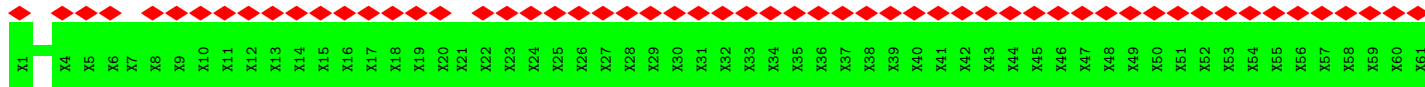
- Molecule 7: SUI1 isoform 1



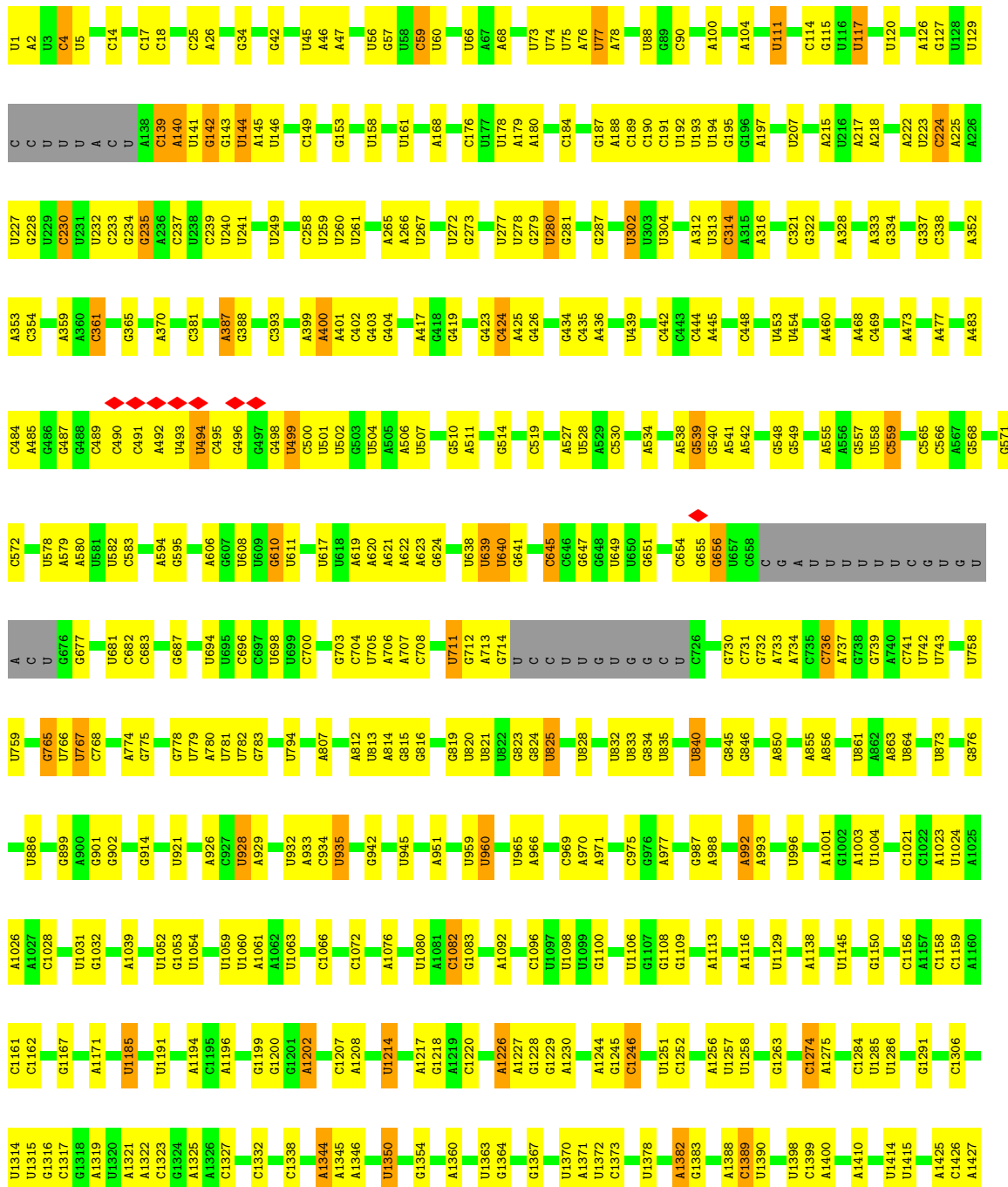
- Molecule 8: RNA recognition motif (unknown)

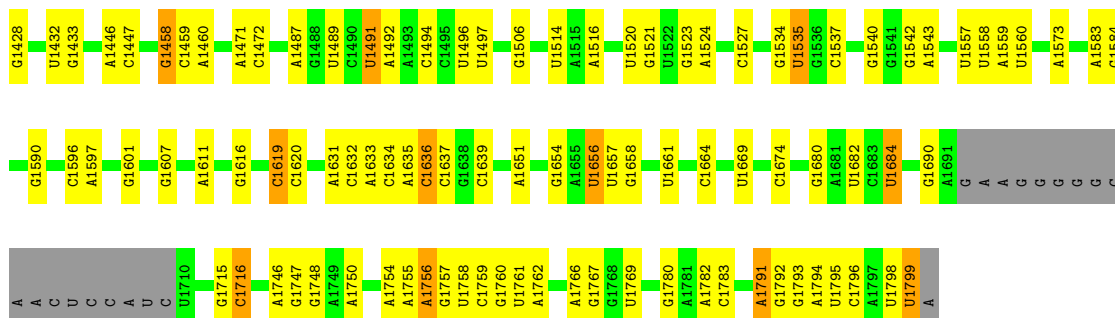




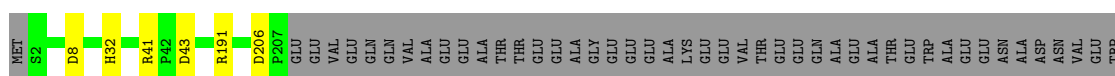
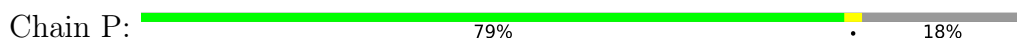


• Molecule 9: 18S ribosomal RNA

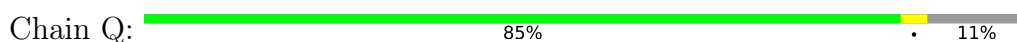




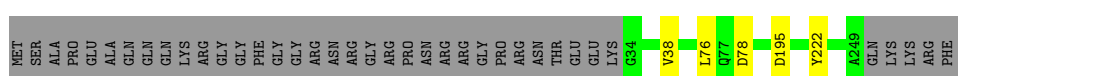
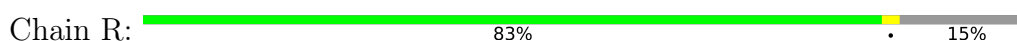
• Molecule 10: 40S ribosomal protein S0-A



• Molecule 11: 40S ribosomal protein S1-A



• Molecule 12: 40S ribosomal protein S2



• Molecule 13: 40S ribosomal protein S4-B

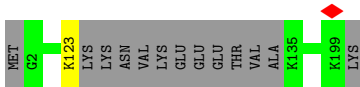


• Molecule 14: 40S ribosomal protein S6-B

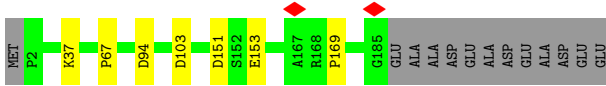
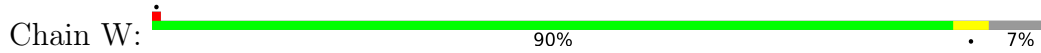


• Molecule 15: 40S ribosomal protein S8-A

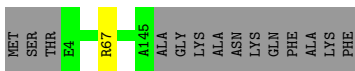
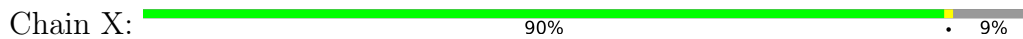




- Molecule 16: 40S ribosomal protein S9-A



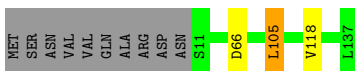
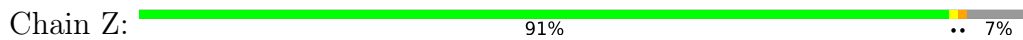
- Molecule 17: 40S ribosomal protein S11-A



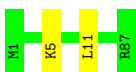
- Molecule 18: 40S ribosomal protein S13



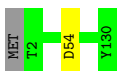
- Molecule 19: 40S ribosomal protein S14-A



- Molecule 20: 40S ribosomal protein S21-A



- Molecule 21: 40S ribosomal protein S22-A



- Molecule 22: 40S ribosomal protein S23-A

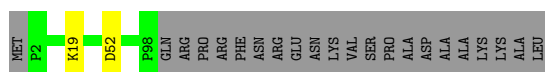
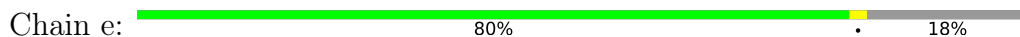




• Molecule 23: 40S ribosomal protein S24-A



• Molecule 24: 40S ribosomal protein S26-A



• Molecule 25: 40S ribosomal protein S27-A



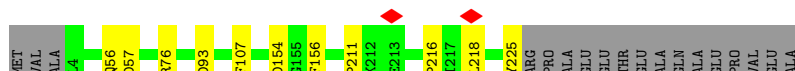
• Molecule 26: 40S ribosomal protein S30-A




• Molecule 27: RPS15 isoform 1

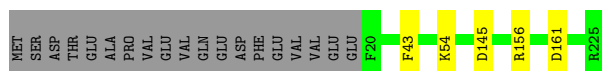


• Molecule 28: 40S ribosomal protein S3




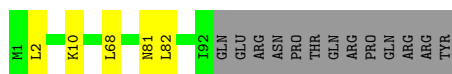
• Molecule 29: 40S ribosomal protein S5

Chain B:  89% 8%




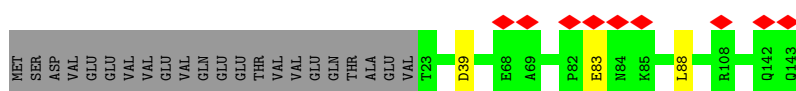
- Molecule 30: 40S ribosomal protein S10-A

Chain C:  83% 5% 12%



- Molecule 31: 40S ribosomal protein S12

Chain D:  6% 83% 15%




- Molecule 32: 40S ribosomal protein S16-A

Chain F:  94% 5%



- Molecule 33: 40S ribosomal protein S17-A

Chain H:  85% 11%



- Molecule 34: 40S ribosomal protein S18-A

Chain I:  95%

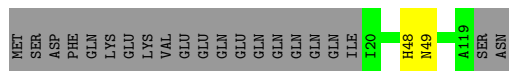
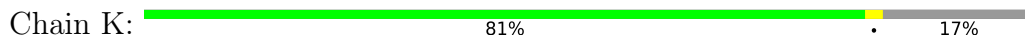


- Molecule 35: 40S ribosomal protein S19-A

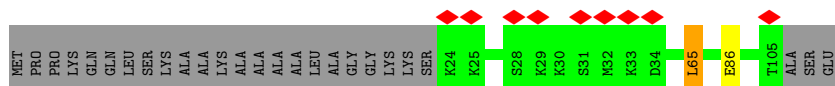
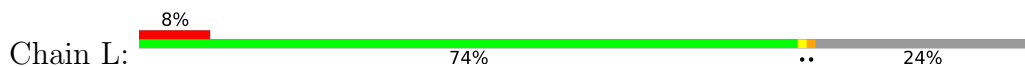
Chain J:  98%



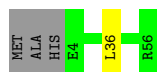
- Molecule 36: 40S ribosomal protein S20



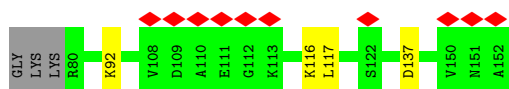
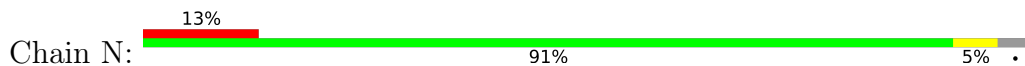
- Molecule 37: 40S ribosomal protein S25-A



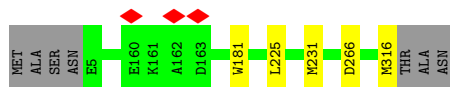
- Molecule 38: RPS29A isoform 1



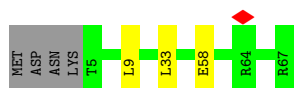
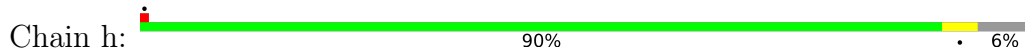
- Molecule 39: 40S ribosomal protein S31



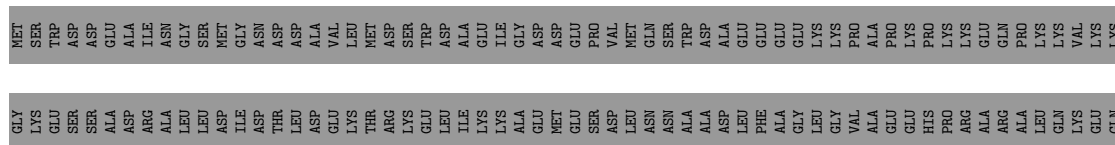
- Molecule 40: Guanine nucleotide-binding protein subunit beta-like protein



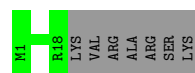
- Molecule 41: 40S ribosomal protein S28-A



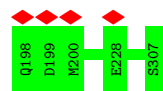
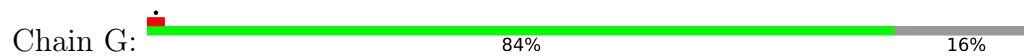
- Molecule 42: Eukaryotic translation initiation factor 3 subunit J







- Molecule 46: OTU domain-containing protein 2



- Molecule 47: 40S ribosomal protein S7-A





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18826	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.970	Depositor
Minimum map value	-1.905	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.25	Depositor
Map size ( $\text{\AA}$ )	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.045, 1.045, 1.045	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ZN, SF4

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	l	0.25	0/1622	0.49	0/2252
2	r	0.23	0/260	0.40	0/360
3	o	0.23	0/2626	0.33	0/3660
4	p	0.26	0/3197	0.46	0/4452
5	q	0.23	0/3165	0.35	0/4418
6	i	0.32	0/475	0.59	1/658 (0.2%)
7	m	0.25	0/442	0.45	0/613
9	2	0.83	2/41595 (0.0%)	1.15	291/64809 (0.4%)
10	P	0.43	0/1644	0.70	3/2249 (0.1%)
11	Q	0.39	0/1823	0.74	5/2447 (0.2%)
12	R	0.46	0/1656	0.70	3/2251 (0.1%)
13	S	0.47	0/2097	0.71	2/2823 (0.1%)
14	T	0.40	0/1839	0.74	3/2460 (0.1%)
15	V	0.47	0/1501	0.66	0/2006
16	W	0.44	0/1504	0.73	1/2016 (0.0%)
17	X	0.50	0/1168	0.63	0/1575
18	Y	0.47	0/1215	0.74	2/1638 (0.1%)
19	Z	0.42	0/934	0.77	2/1257 (0.2%)
20	a	0.47	0/682	0.76	0/921
21	b	0.47	0/1038	0.67	0/1395
22	c	0.48	0/1139	0.67	1/1518 (0.1%)
23	d	0.47	0/1087	0.67	0/1449
24	e	0.44	0/778	0.68	0/1042
25	f	0.45	0/620	0.80	1/838 (0.1%)
26	g	0.40	0/480	0.74	1/639 (0.2%)
27	E	0.33	0/936	0.89	7/1259 (0.6%)
28	A	0.44	1/1754 (0.1%)	0.79	5/2361 (0.2%)
29	B	0.30	0/1625	0.66	1/2197 (0.0%)
30	C	0.39	0/772	0.81	3/1044 (0.3%)
31	D	0.32	0/883	0.79	2/1199 (0.2%)
32	F	0.35	0/1125	0.65	1/1510 (0.1%)
33	H	0.35	0/957	0.75	0/1283

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
34	I	0.30	0/1207	0.70	2/1623 (0.1%)
35	J	0.30	0/1130	0.63	1/1517 (0.1%)
36	K	0.34	0/807	0.65	0/1091
37	L	0.28	0/661	0.72	1/888 (0.1%)
38	M	0.33	0/452	0.69	0/600
39	N	0.30	0/571	0.75	1/768 (0.1%)
40	O	0.28	0/2436	0.65	2/3318 (0.1%)
41	h	0.36	0/493	0.82	1/663 (0.2%)
42	y	0.48	0/631	1.00	2/851 (0.2%)
42	z	0.41	0/905	0.94	5/1213 (0.4%)
43	x	0.29	0/4694	0.63	5/6334 (0.1%)
44	k	0.24	0/373	0.48	0/517
45	n	0.34	0/176	0.78	0/225
46	G	0.26	0/1514	0.43	0/2075
47	U	0.39	0/1498	0.77	5/2019 (0.2%)
All	All	0.60	3/100187 (0.0%)	0.91	360/144301 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	p	0	1
21	b	0	1
42	z	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	211	PRO	CG-CD	-10.23	1.16	1.50
9	2	555	A	N7-C5	-5.27	1.36	1.39
9	2	142	G	C2-N3	-5.04	1.28	1.32

All (360) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	1756	A	O5'-P-OP2	-16.64	90.72	105.70
9	2	453	U	N1-C2-O2	13.03	131.92	122.80
9	2	1756	A	O5'-P-OP1	13.02	126.32	110.70
9	2	555	A	N7-C8-N9	12.72	120.16	113.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	453	U	C2-N1-C1'	12.53	132.74	117.70
28	A	211	PRO	N-CD-CG	-12.04	85.13	103.20
9	2	453	U	N3-C2-O2	-11.23	114.34	122.20
28	A	211	PRO	CA-N-CD	-11.03	96.05	111.50
42	z	180	LEU	CA-CB-CG	10.42	139.27	115.30
9	2	555	A	C8-N9-C4	-10.32	101.67	105.80
16	W	151	ASP	CB-CG-OD1	10.27	127.54	118.30
9	2	555	A	C5-N7-C8	-10.11	98.85	103.90
11	Q	59	ASP	CB-CG-OD2	10.09	127.38	118.30
9	2	767	U	N3-C2-O2	-10.05	115.16	122.20
9	2	1758	U	N3-C2-O2	-10.05	115.16	122.20
25	f	34	ASP	CB-CG-OD2	9.48	126.83	118.30
9	2	1639	C	C2-N1-C1'	9.41	129.16	118.80
9	2	1145	U	N3-C2-O2	-9.19	115.77	122.20
42	y	163	PRO	CA-N-CD	-9.11	98.74	111.50
9	2	1639	C	N1-C2-O2	9.10	124.36	118.90
9	2	453	U	C6-N1-C1'	-9.09	108.47	121.20
9	2	1389	C	C2-N1-C1'	9.07	128.78	118.80
9	2	1639	C	N3-C2-O2	-8.94	115.64	121.90
10	P	206	ASP	CB-CG-OD1	8.94	126.34	118.30
43	x	565	LEU	CA-CB-CG	8.79	135.52	115.30
40	O	266	ASP	CB-CG-OD1	8.76	126.18	118.30
14	T	20	ASP	CB-CG-OD1	8.75	126.17	118.30
34	I	73	MET	CA-CB-CG	8.72	128.12	113.30
9	2	1082	C	C2-N1-C1'	8.69	128.36	118.80
47	U	155	ASP	CB-CG-OD1	8.67	126.11	118.30
9	2	1162	C	N1-C2-O2	8.64	124.08	118.90
9	2	539	G	N3-C4-C5	-8.62	124.29	128.60
9	2	864	U	N3-C2-O2	-8.61	116.17	122.20
10	P	43	ASP	CB-CG-OD2	8.55	126.00	118.30
9	2	1258	U	N3-C2-O2	-8.53	116.23	122.20
9	2	736	C	N3-C2-O2	-8.53	115.93	121.90
9	2	1758	U	N1-C2-O2	8.49	128.74	122.80
9	2	144	U	C2-N1-C1'	8.26	127.62	117.70
9	2	864	U	C2-N1-C1'	8.26	127.61	117.70
9	2	1458	G	C4-N9-C1'	8.26	137.23	126.50
9	2	1560	U	C2-N1-C1'	8.21	127.55	117.70
9	2	142	G	N3-C2-N2	-8.18	114.17	119.90
9	2	1258	U	N1-C2-O2	8.14	128.50	122.80
9	2	864	U	N1-C2-O2	8.11	128.47	122.80
9	2	539	G	C8-N9-C4	-8.04	103.19	106.40
9	2	965	U	C2-N1-C1'	7.89	127.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	1286	U	N1-C2-O2	7.89	128.32	122.80
9	2	959	U	N3-C2-O2	-7.88	116.68	122.20
12	R	78	ASP	CB-CG-OD1	7.80	125.32	118.30
9	2	555	A	C2-N3-C4	-7.72	106.74	110.60
14	T	29	ASP	CB-CG-OD1	7.69	125.22	118.30
12	R	38	VAL	CG1-CB-CG2	-7.65	98.67	110.90
9	2	736	C	N1-C2-O2	7.62	123.47	118.90
9	2	1527	C	C2-N1-C1'	7.61	127.17	118.80
9	2	959	U	C5-C6-N1	7.58	126.49	122.70
9	2	1286	U	N3-C2-O2	-7.49	116.96	122.20
9	2	583	C	C6-N1-C2	-7.46	117.31	120.30
43	x	482	LEU	CA-CB-CG	7.41	132.35	115.30
9	2	1350	U	N1-C2-O2	7.34	127.94	122.80
9	2	767	U	N1-C2-O2	7.29	127.90	122.80
9	2	959	U	N1-C2-O2	7.29	127.90	122.80
9	2	1063	U	N1-C2-O2	7.29	127.90	122.80
9	2	610	G	C4-N9-C1'	7.27	135.95	126.50
9	2	224	C	N1-C2-O2	7.26	123.26	118.90
9	2	1258	U	C2-N1-C1'	7.26	126.41	117.70
9	2	959	U	C2-N1-C1'	7.23	126.37	117.70
9	2	1791	A	P-O3'-C3'	7.23	128.37	119.70
9	2	1755	A	P-O3'-C3'	7.21	128.36	119.70
9	2	1162	C	N3-C2-O2	-7.17	116.88	121.90
26	g	38	LEU	CA-CB-CG	7.14	131.73	115.30
9	2	1161	C	C5-C6-N1	7.13	124.56	121.00
47	U	158	ASP	CB-CG-OD2	7.11	124.70	118.30
9	2	832	U	N1-C2-O2	7.08	127.76	122.80
9	2	583	C	C2-N1-C1'	7.07	126.58	118.80
9	2	1145	U	C2-N1-C1'	7.07	126.19	117.70
13	S	38	LEU	CA-CB-CG	7.05	131.52	115.30
9	2	1458	G	C8-N9-C1'	-7.04	117.85	127.00
9	2	1129	U	N3-C2-O2	-7.03	117.28	122.20
9	2	1332	C	C2-N1-C1'	7.02	126.52	118.80
9	2	1458	G	N3-C4-N9	7.00	130.20	126.00
28	A	216	PRO	CA-N-CD	-7.00	101.69	111.50
9	2	1072	C	C6-N1-C2	-6.98	117.51	120.30
9	2	758	U	N3-C2-O2	-6.97	117.32	122.20
9	2	1024	U	N3-C2-O2	-6.97	117.32	122.20
9	2	1082	C	C6-N1-C2	-6.97	117.51	120.30
9	2	1758	U	C2-N1-C1'	6.97	126.06	117.70
9	2	144	U	N3-C2-O2	-6.96	117.33	122.20
39	N	137	ASP	CB-CG-OD1	6.96	124.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	77	U	P-O3'-C3'	6.96	128.05	119.70
9	2	1063	U	C2-N1-C1'	6.95	126.04	117.70
9	2	1286	U	C2-N1-C1'	6.91	126.00	117.70
9	2	1560	U	N3-C2-O2	-6.91	117.36	122.20
9	2	1350	U	N3-C2-O2	-6.90	117.37	122.20
9	2	1560	U	N1-C2-O2	6.90	127.63	122.80
30	C	2	LEU	CA-CB-CG	6.86	131.09	115.30
9	2	1639	C	C6-N1-C1'	-6.85	112.58	120.80
9	2	1063	U	N3-C2-O2	-6.84	117.41	122.20
9	2	1350	U	C2-N1-C1'	6.84	125.91	117.70
9	2	224	C	C2-N1-C1'	6.84	126.32	118.80
9	2	59	C	P-O3'-C3'	6.83	127.90	119.70
28	A	211	PRO	CA-CB-CG	-6.81	91.06	104.00
9	2	608	U	C2-N1-C1'	6.77	125.82	117.70
9	2	583	C	C5-C6-N1	6.76	124.38	121.00
9	2	18	C	C6-N1-C2	-6.72	117.61	120.30
9	2	190	C	C2-N1-C1'	6.72	126.19	118.80
9	2	1252	C	C5-C6-N1	6.72	124.36	121.00
9	2	230	C	N1-C2-O2	6.71	122.92	118.90
9	2	1596	C	C2-N1-C1'	6.68	126.15	118.80
9	2	1252	C	C2-N1-C1'	6.68	126.15	118.80
9	2	767	U	C2-N1-C1'	6.68	125.71	117.70
9	2	959	U	C6-N1-C2	-6.67	117.00	121.00
9	2	1162	C	C2-N1-C1'	6.65	126.11	118.80
27	E	26	LEU	CA-CB-CG	6.64	130.58	115.30
9	2	18	C	C5-C6-N1	6.64	124.32	121.00
9	2	861	U	C2-N1-C1'	6.64	125.67	117.70
9	2	1458	G	N3-C4-C5	-6.62	125.29	128.60
9	2	1620	C	N1-C2-O2	6.57	122.84	118.90
9	2	1274	C	P-O3'-C3'	6.56	127.57	119.70
9	2	142	G	N1-C2-N2	6.54	122.09	116.20
43	x	37	LEU	CA-CB-CG	6.54	130.35	115.30
9	2	711	U	P-O3'-C3'	6.53	127.53	119.70
6	i	45	GLY	N-CA-C	6.53	129.41	113.10
27	E	49	MET	CA-CB-CG	6.52	124.39	113.30
9	2	832	U	N3-C2-O2	-6.52	117.64	122.20
9	2	120	U	N3-C2-O2	-6.51	117.64	122.20
9	2	1674	C	C6-N1-C2	-6.50	117.70	120.30
9	2	1535	U	N1-C2-O2	6.49	127.34	122.80
30	C	10	LYS	CA-CB-CG	6.48	127.65	113.40
19	Z	118	VAL	CA-CB-CG1	6.45	120.58	110.90
9	2	639	U	P-O3'-C3'	6.45	127.44	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	530	C	N1-C2-O2	6.44	122.76	118.90
9	2	361	C	C6-N1-C2	-6.43	117.73	120.30
9	2	928	U	P-O3'-C3'	6.43	127.42	119.70
9	2	237	C	C2-N1-C1'	6.43	125.87	118.80
9	2	1317	C	C2-N1-C1'	6.43	125.87	118.80
9	2	184	C	C2-N1-C1'	6.43	125.87	118.80
9	2	1161	C	C6-N1-C2	-6.42	117.73	120.30
9	2	1066	C	C6-N1-C2	-6.40	117.74	120.30
9	2	1535	U	C2-N1-C1'	6.39	125.36	117.70
9	2	1759	C	C6-N1-C2	-6.37	117.75	120.30
9	2	237	C	N1-C2-O2	6.36	122.72	118.90
9	2	1327	C	C6-N1-C2	-6.36	117.76	120.30
27	E	25	LEU	CA-CB-CG	6.35	129.91	115.30
9	2	758	U	N1-C2-O2	6.34	127.24	122.80
9	2	1389	C	C6-N1-C1'	-6.34	113.19	120.80
31	D	88	LEU	CA-CB-CG	6.32	129.83	115.30
9	2	1382	A	P-O3'-C3'	6.31	127.28	119.70
9	2	258	C	N1-C2-O2	6.30	122.68	118.90
9	2	144	U	C5-C4-O4	-6.29	122.13	125.90
9	2	639	U	N3-C2-O2	-6.26	117.81	122.20
9	2	1021	C	C6-N1-C2	-6.24	117.80	120.30
9	2	1527	C	C6-N1-C2	-6.24	117.80	120.30
9	2	1755	A	N7-C8-N9	6.19	116.89	113.80
9	2	1214	U	N1-C2-O2	6.16	127.11	122.80
19	Z	105	LEU	CA-CB-CG	6.16	129.47	115.30
9	2	934	C	C2-N1-C1'	6.15	125.57	118.80
9	2	1082	C	O4'-C1'-N1	6.15	113.12	108.20
9	2	1129	U	N1-C2-O2	6.15	127.10	122.80
14	T	105	ASP	CB-CG-OD1	6.14	123.82	118.30
32	F	28	LEU	CA-CB-CG	6.14	129.41	115.30
9	2	1066	C	C2-N1-C1'	6.13	125.54	118.80
9	2	1145	U	N1-C2-O2	6.11	127.08	122.80
9	2	610	G	C8-N9-C1'	-6.11	119.06	127.00
34	I	73	MET	CB-CG-SD	6.08	130.64	112.40
9	2	1082	C	N1-C2-O2	6.08	122.55	118.90
9	2	965	U	N1-C2-O2	6.07	127.05	122.80
9	2	559	C	C2-N1-C1'	6.06	125.47	118.80
27	E	65	LEU	CA-CB-CG	6.05	129.21	115.30
9	2	768	C	C6-N1-C2	-6.04	117.89	120.30
9	2	1560	U	O4'-C1'-N1	6.03	113.02	108.20
9	2	1024	U	N1-C2-O2	6.02	127.02	122.80
40	O	225	LEU	CA-CB-CG	6.01	129.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	y	147	LYS	CA-CB-CG	6.01	126.63	113.40
18	Y	137	PRO	C-N-CA	6.00	136.71	121.70
9	2	1636	C	P-O3'-C3'	6.00	126.90	119.70
9	2	1799	U	N3-C2-O2	-5.99	118.00	122.20
9	2	144	U	C6-N1-C1'	-5.98	112.83	121.20
9	2	558	U	C2-N1-C1'	5.97	124.86	117.70
9	2	258	C	N3-C2-O2	-5.96	117.73	121.90
9	2	354	C	N1-C2-O2	5.94	122.47	118.90
9	2	1106	U	N3-C2-O2	-5.94	118.04	122.20
9	2	302	U	N3-C2-O2	-5.93	118.05	122.20
9	2	539	G	C4-N9-C1'	5.93	134.21	126.50
9	2	835	U	C2-N1-C1'	5.92	124.80	117.70
9	2	90	C	C6-N1-C2	-5.90	117.94	120.30
31	D	39	ASP	CB-CG-OD2	5.90	123.61	118.30
9	2	424	C	C5-C6-N1	5.90	123.95	121.00
9	2	1382	A	OP1-P-O3'	5.89	118.16	105.20
9	2	1535	U	N3-C2-O2	-5.89	118.08	122.20
9	2	1596	C	N1-C2-O2	5.88	122.43	118.90
9	2	489	C	C5-C6-N1	5.87	123.94	121.00
9	2	794	U	N1-C2-O2	5.87	126.91	122.80
9	2	1491	U	C2-N1-C1'	5.86	124.73	117.70
9	2	555	A	C5-C6-N1	-5.86	114.77	117.70
9	2	1214	U	C2-N1-C1'	5.86	124.73	117.70
9	2	1632	C	C2-N1-C1'	5.84	125.22	118.80
9	2	144	U	N3-C4-O4	5.82	123.48	119.40
37	L	65	LEU	CA-CB-CG	5.82	128.69	115.30
9	2	539	G	N3-C4-N9	5.82	129.49	126.00
9	2	1661	U	C2-N1-C1'	5.81	124.67	117.70
9	2	494	U	C2-N1-C1'	5.81	124.67	117.70
9	2	1162	C	C6-N1-C2	-5.81	117.98	120.30
9	2	442	C	C6-N1-C2	-5.80	117.98	120.30
9	2	1252	C	C6-N1-C2	-5.78	117.99	120.30
9	2	280	U	P-O3'-C3'	5.78	126.63	119.70
42	z	210	GLU	CA-CB-CG	5.77	126.09	113.40
9	2	1661	U	N1-C2-O2	5.76	126.83	122.80
9	2	530	C	N3-C2-O2	-5.76	117.87	121.90
9	2	828	U	C2-N1-C1'	5.76	124.61	117.70
9	2	230	C	C2-N1-C1'	5.75	125.13	118.80
9	2	267	U	N3-C2-O2	-5.74	118.18	122.20
43	x	215	LEU	CA-CB-CG	5.73	128.48	115.30
41	h	33	LEU	CA-CB-CG	5.73	128.47	115.30
9	2	120	U	N1-C2-O2	5.72	126.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	1489	U	C2-N1-C1'	5.71	124.56	117.70
9	2	1082	C	N3-C2-O2	-5.71	117.90	121.90
9	2	1389	C	C6-N1-C2	-5.71	118.02	120.30
9	2	794	U	N3-C2-O2	-5.71	118.20	122.20
9	2	144	U	N1-C2-O2	5.69	126.78	122.80
30	C	82	LEU	CA-CB-CG	5.69	128.39	115.30
18	Y	27	LYS	CB-CG-CD	5.68	126.36	111.60
9	2	1332	C	C6-N1-C2	-5.67	118.03	120.30
9	2	1082	C	C6-N1-C1'	-5.67	114.00	120.80
9	2	1527	C	C5-C6-N1	5.67	123.83	121.00
9	2	314	C	C6-N1-C2	-5.66	118.04	120.30
9	2	1799	U	N1-C2-O2	5.66	126.76	122.80
9	2	139	C	P-O3'-C3'	5.65	126.48	119.70
9	2	1214	U	N3-C2-O2	-5.63	118.26	122.20
13	S	212	ASP	CB-CG-OD2	5.63	123.36	118.30
9	2	539	G	N7-C8-N9	5.60	115.90	113.10
47	U	34	LEU	CA-CB-CG	5.60	128.18	115.30
9	2	224	C	N3-C2-O2	-5.59	117.98	121.90
22	c	133	LEU	CA-CB-CG	5.59	128.16	115.30
9	2	558	U	N1-C2-O2	5.58	126.71	122.80
42	z	170	LEU	CA-CB-CG	5.58	128.14	115.30
9	2	1596	C	N3-C2-O2	-5.58	118.00	121.90
9	2	400	A	P-O3'-C3'	5.57	126.39	119.70
9	2	361	C	C5-C6-N1	5.57	123.78	121.00
9	2	190	C	C6-N1-C2	-5.56	118.08	120.30
11	Q	184	LEU	CA-CB-CG	5.55	128.07	115.30
27	E	72	LYS	CA-CB-CG	5.55	125.61	113.40
9	2	1755	A	C8-N9-C4	-5.55	103.58	105.80
9	2	224	C	C6-N1-C2	-5.54	118.08	120.30
9	2	1389	C	C5-C6-N1	5.54	123.77	121.00
9	2	1664	C	C2-N1-C1'	5.52	124.87	118.80
9	2	354	C	C2-N3-C4	5.51	122.65	119.90
9	2	559	C	C6-N1-C2	-5.51	118.10	120.30
9	2	489	C	C6-N1-C2	-5.50	118.10	120.30
9	2	1527	C	N1-C2-O2	5.50	122.20	118.90
9	2	960	U	N1-C2-O2	5.50	126.65	122.80
9	2	768	C	N3-C2-O2	-5.49	118.06	121.90
9	2	142	G	N3-C4-N9	-5.49	122.70	126.00
47	U	18	LEU	CA-CB-CG	5.49	127.93	115.30
9	2	965	U	C6-N1-C1'	-5.48	113.53	121.20
9	2	149	C	C6-N1-C2	-5.48	118.11	120.30
9	2	1661	U	N3-C2-O2	-5.47	118.37	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	1756	A	N1-C6-N6	-5.47	115.32	118.60
9	2	794	U	C2-N1-C1'	5.47	124.26	117.70
12	R	76	LEU	CA-CB-CG	5.46	127.85	115.30
9	2	965	U	N3-C2-O2	-5.44	118.39	122.20
9	2	1491	U	N1-C2-O2	5.43	126.60	122.80
9	2	117	U	N3-C2-O2	-5.43	118.40	122.20
9	2	1108	G	O4'-C1'-N9	5.42	112.53	108.20
9	2	1389	C	N1-C2-O2	5.41	122.14	118.90
9	2	1161	C	C2-N1-C1'	5.40	124.74	118.80
10	P	206	ASP	C-N-CD	5.38	139.71	128.40
9	2	387	A	P-O3'-C3'	5.38	126.15	119.70
9	2	4	C	C6-N1-C2	-5.38	118.15	120.30
9	2	140	A	O5'-P-OP2	5.38	117.15	110.70
42	z	180	LEU	CB-CG-CD2	5.37	120.13	111.00
9	2	1491	U	N3-C2-O2	-5.37	118.44	122.20
9	2	224	C	C5-C6-N1	5.35	123.68	121.00
9	2	840	U	C2-N1-C1'	5.35	124.11	117.70
9	2	1756	A	C4-C5-C6	-5.35	114.33	117.00
9	2	1761	U	N3-C2-O2	-5.34	118.46	122.20
9	2	1633	A	C6-N1-C2	5.34	121.80	118.60
9	2	1	U	C5-C6-N1	5.34	125.37	122.70
9	2	302	U	N1-C2-O2	5.33	126.53	122.80
35	J	140	LEU	CA-CB-CG	5.33	127.57	115.30
9	2	864	U	C6-N1-C1'	-5.33	113.74	121.20
9	2	1632	C	C6-N1-C2	-5.33	118.17	120.30
9	2	1021	C	C2-N1-C1'	5.33	124.66	118.80
9	2	1246	C	N1-C2-O2	5.33	122.09	118.90
9	2	1656	U	N3-C2-O2	-5.33	118.47	122.20
9	2	992	A	O4'-C1'-N9	5.32	112.46	108.20
11	Q	59	ASP	CB-CG-OD1	-5.32	113.51	118.30
9	2	1066	C	C5-C6-N1	5.31	123.66	121.00
9	2	4	C	C2-N1-C1'	5.29	124.62	118.80
9	2	840	U	N1-C2-O2	5.29	126.50	122.80
9	2	1257	U	C2-N1-C1'	5.29	124.05	117.70
9	2	1274	C	N1-C2-O2	5.29	122.07	118.90
42	z	186	LYS	CB-CG-CD	5.29	125.34	111.60
9	2	935	U	N1-C2-O2	5.27	126.49	122.80
9	2	1497	U	N1-C2-O2	5.26	126.48	122.80
9	2	572	C	O5'-P-OP1	-5.24	100.98	105.70
9	2	14	C	C6-N1-C2	-5.23	118.21	120.30
9	2	640	U	P-O3'-C3'	5.23	125.98	119.70
11	Q	229	MET	CA-CB-CG	5.22	122.18	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	1	U	N1-C2-O2	5.22	126.45	122.80
9	2	825	U	N3-C2-O2	-5.22	118.55	122.20
9	2	1684	U	N1-C2-O2	5.22	126.45	122.80
9	2	1560	U	C6-N1-C1'	-5.22	113.90	121.20
9	2	1220	C	C6-N1-C2	-5.21	118.21	120.30
9	2	765	G	C4-N9-C1'	5.21	133.27	126.50
9	2	656	G	C4-N9-C1'	5.21	133.27	126.50
9	2	354	C	C5-C6-N1	5.20	123.60	121.00
9	2	88	U	N3-C2-O2	-5.20	118.56	122.20
9	2	645	C	C2-N1-C1'	5.20	124.51	118.80
47	U	9	LEU	CA-CB-CG	5.20	127.25	115.30
9	2	1716	C	N3-C2-O2	-5.19	118.27	121.90
9	2	558	U	N3-C2-O2	-5.18	118.57	122.20
9	2	617	U	C2-N1-C1'	5.18	123.92	117.70
9	2	189	C	C2-N1-C1'	5.17	124.49	118.80
9	2	494	U	N1-C2-O2	5.17	126.42	122.80
9	2	608	U	N3-C2-O2	-5.17	118.58	122.20
9	2	1619	C	N1-C2-O2	5.17	122.00	118.90
9	2	237	C	C6-N1-C2	-5.16	118.23	120.30
9	2	1220	C	C5-C6-N1	5.15	123.58	121.00
9	2	1497	U	N3-C2-O2	-5.15	118.59	122.20
9	2	1185	U	C2-N1-C1'	5.15	123.88	117.70
11	Q	55	LYS	CA-CB-CG	5.14	124.71	113.40
9	2	1669	U	N3-C2-O2	-5.14	118.60	122.20
9	2	184	C	C5-C6-N1	5.13	123.57	121.00
9	2	400	A	C8-N9-C4	-5.13	103.75	105.80
9	2	5	U	N3-C2-O2	-5.12	118.61	122.20
9	2	354	C	C6-N1-C2	-5.12	118.25	120.30
9	2	528	U	N3-C2-O2	-5.12	118.61	122.20
28	A	218	LEU	CA-CB-CG	5.12	127.08	115.30
9	2	1639	C	C6-N1-C2	-5.12	118.25	120.30
9	2	977	A	N1-C6-N6	-5.11	115.54	118.60
27	E	83	MET	CG-SD-CE	5.11	108.37	100.20
9	2	1063	U	C5-C6-N1	5.11	125.25	122.70
9	2	1226	A	P-O3'-C3'	5.10	125.82	119.70
9	2	687	G	N3-C2-N2	-5.10	116.33	119.90
9	2	1332	C	C5-C6-N1	5.10	123.55	121.00
9	2	149	C	C2-N1-C1'	5.10	124.41	118.80
9	2	759	U	N3-C2-O2	-5.09	118.64	122.20
9	2	235	G	N3-C2-N2	5.08	123.46	119.90
9	2	1145	U	C6-N1-C2	-5.07	117.96	121.00
9	2	1344	A	P-O3'-C3'	5.07	125.78	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	207	U	N3-C2-O2	-5.07	118.65	122.20
9	2	1664	C	N1-C2-O2	5.06	121.94	118.90
9	2	184	C	C6-N1-C2	-5.05	118.28	120.30
29	B	145	ASP	CB-CG-OD2	5.05	122.85	118.30
9	2	765	G	C4-C5-N7	5.05	112.82	110.80
9	2	1274	C	N3-C2-O2	-5.05	118.37	121.90
9	2	499	U	C5-C6-N1	5.04	125.22	122.70
9	2	1684	U	N3-C2-O2	-5.04	118.67	122.20
9	2	111	U	N1-C2-O2	5.04	126.33	122.80
27	E	83	MET	CB-CG-SD	5.04	127.50	112.40
9	2	765	G	N7-C8-N9	5.03	115.61	113.10
9	2	1656	U	N1-C2-O2	5.03	126.32	122.80
9	2	996	U	N1-C2-O2	5.02	126.31	122.80
9	2	975	C	C6-N1-C2	-5.02	118.29	120.30
9	2	1082	C	C5-C6-N1	5.02	123.51	121.00
9	2	381	C	C6-N1-C2	-5.02	118.29	120.30
43	x	443	LEU	CA-CB-CG	5.01	126.82	115.30
9	2	934	C	N1-C2-O2	5.01	121.90	118.90
9	2	1799	U	C2-N1-C1'	5.00	123.70	117.70
9	2	1202	A	C2-N3-C4	5.00	113.10	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	b	54	ASP	Peptide
4	p	336	TRP	Peptide
42	z	154	ARG	Sidechain

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

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

## 5.3 Torsion angles [\(i\)](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	l	326/347 (94%)	321 (98%)	5 (2%)	0	100	100
2	r	51/274 (19%)	49 (96%)	2 (4%)	0	100	100
3	o	519/964 (54%)	509 (98%)	10 (2%)	0	100	100
4	p	638/763 (84%)	604 (95%)	31 (5%)	3 (0%)	29	68
5	q	628/812 (77%)	601 (96%)	26 (4%)	1 (0%)	47	82
6	i	95/153 (62%)	87 (92%)	8 (8%)	0	100	100
7	m	88/108 (82%)	81 (92%)	5 (6%)	2 (2%)	6	30
10	P	204/252 (81%)	190 (93%)	14 (7%)	0	100	100
11	Q	222/255 (87%)	201 (90%)	21 (10%)	0	100	100
12	R	214/254 (84%)	202 (94%)	12 (6%)	0	100	100
13	S	256/261 (98%)	238 (93%)	18 (7%)	0	100	100
14	T	226/236 (96%)	217 (96%)	9 (4%)	0	100	100
15	V	183/200 (92%)	176 (96%)	7 (4%)	0	100	100
16	W	182/197 (92%)	172 (94%)	9 (5%)	1 (0%)	29	68
17	X	140/156 (90%)	134 (96%)	6 (4%)	0	100	100
18	Y	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
19	Z	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
20	a	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
21	b	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
22	c	142/145 (98%)	135 (95%)	6 (4%)	1 (1%)	22	60
23	d	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
24	e	95/119 (80%)	88 (93%)	7 (7%)	0	100	100
25	f	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
26	g	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
27	E	115/142 (81%)	110 (96%)	5 (4%)	0	100	100
28	A	220/240 (92%)	208 (94%)	12 (6%)	0	100	100
29	B	204/225 (91%)	194 (95%)	10 (5%)	0	100	100
30	C	90/105 (86%)	81 (90%)	9 (10%)	0	100	100
31	D	119/143 (83%)	103 (87%)	16 (13%)	0	100	100
32	F	139/143 (97%)	133 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	H	117/136 (86%)	111 (95%)	6 (5%)	0	100	100
34	I	143/146 (98%)	137 (96%)	5 (4%)	1 (1%)	22	60
35	J	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
36	K	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
37	L	80/108 (74%)	76 (95%)	4 (5%)	0	100	100
38	M	51/56 (91%)	51 (100%)	0	0	100	100
39	N	71/76 (93%)	60 (84%)	11 (16%)	0	100	100
40	O	310/319 (97%)	293 (94%)	17 (6%)	0	100	100
41	h	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
42	y	77/265 (29%)	71 (92%)	6 (8%)	0	100	100
42	z	118/265 (44%)	109 (92%)	9 (8%)	0	100	100
43	x	578/608 (95%)	549 (95%)	29 (5%)	0	100	100
44	k	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
45	n	16/25 (64%)	16 (100%)	0	0	100	100
46	G	253/307 (82%)	251 (99%)	2 (1%)	0	100	100
47	U	182/190 (96%)	171 (94%)	11 (6%)	0	100	100
All	All	8220/10188 (81%)	7788 (95%)	423 (5%)	9 (0%)	54	85

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	p	392	PRO
7	m	85	ARG
34	I	102	ALA
4	p	536	LYS
22	c	88	PRO
7	m	73	GLU
16	W	169	PRO
4	p	198	VAL
5	q	351	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	P	170/210 (81%)	166 (98%)	4 (2%)	49	79
11	Q	200/224 (89%)	194 (97%)	6 (3%)	41	75
12	R	175/205 (85%)	173 (99%)	2 (1%)	73	90
13	S	220/222 (99%)	216 (98%)	4 (2%)	59	85
14	T	189/201 (94%)	185 (98%)	4 (2%)	53	82
15	V	148/161 (92%)	147 (99%)	1 (1%)	84	94
16	W	156/166 (94%)	151 (97%)	5 (3%)	39	74
17	X	126/137 (92%)	125 (99%)	1 (1%)	81	93
18	Y	127/128 (99%)	125 (98%)	2 (2%)	62	86
19	Z	90/105 (86%)	88 (98%)	2 (2%)	52	81
20	a	71/74 (96%)	69 (97%)	2 (3%)	43	77
21	b	110/111 (99%)	110 (100%)	0	100	100
22	c	119/120 (99%)	118 (99%)	1 (1%)	81	93
23	d	112/113 (99%)	111 (99%)	1 (1%)	78	92
24	e	82/101 (81%)	80 (98%)	2 (2%)	49	79
25	f	70/71 (99%)	68 (97%)	2 (3%)	42	76
26	g	50/54 (93%)	50 (100%)	0	100	100
27	E	95/118 (80%)	91 (96%)	4 (4%)	30	66
28	A	182/195 (93%)	174 (96%)	8 (4%)	28	65
29	B	172/191 (90%)	168 (98%)	4 (2%)	50	80
30	C	78/98 (80%)	76 (97%)	2 (3%)	46	78
31	D	88/119 (74%)	87 (99%)	1 (1%)	73	90
32	F	117/119 (98%)	111 (95%)	6 (5%)	24	60
33	H	101/124 (82%)	96 (95%)	5 (5%)	24	60
34	I	127/129 (98%)	122 (96%)	5 (4%)	32	69
35	J	115/116 (99%)	114 (99%)	1 (1%)	78	92
36	K	93/114 (82%)	91 (98%)	2 (2%)	52	81
37	L	67/89 (75%)	65 (97%)	2 (3%)	41	75
38	M	47/49 (96%)	46 (98%)	1 (2%)	53	82
39	N	57/66 (86%)	54 (95%)	3 (5%)	22	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	O	250/262 (95%)	247 (99%)	3 (1%)	71	90
41	h	55/60 (92%)	53 (96%)	2 (4%)	35	70
42	y	69/221 (31%)	68 (99%)	1 (1%)	67	88
42	z	90/221 (41%)	87 (97%)	3 (3%)	38	73
43	x	516/537 (96%)	506 (98%)	10 (2%)	57	84
45	n	17/23 (74%)	17 (100%)	0	100	100
46	G	62/282 (22%)	62 (100%)	0	100	100
47	U	163/170 (96%)	160 (98%)	3 (2%)	59	85
All	All	4776/5706 (84%)	4671 (98%)	105 (2%)	54	81

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	P	8	ASP
10	P	32	HIS
10	P	41	ARG
10	P	191	ARG
11	Q	8	ARG
11	Q	59	ASP
11	Q	94	LYS
11	Q	108	ASP
11	Q	148	ASN
11	Q	205	PHE
12	R	195	ASP
12	R	222	TYR
13	S	11	ARG
13	S	77	ARG
13	S	182	TYR
13	S	197	HIS
14	T	22	HIS
14	T	23	ARG
14	T	25	ARG
14	T	37	ASP
15	V	123	LYS
16	W	37	LYS
16	W	67	PRO
16	W	94	ASP
16	W	103	ASP
16	W	153	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	X	67	ARG
18	Y	93	LYS
18	Y	140	LYS
19	Z	66	ASP
19	Z	105	LEU
20	a	5	LYS
20	a	11	LEU
22	c	107	PHE
23	d	34	ASN
24	e	19	LYS
24	e	52	ASP
25	f	56	CYS
25	f	78	SER
27	E	24	LYS
27	E	28	MET
27	E	59	LYS
27	E	86	VAL
28	A	56	GLN
28	A	57	ASP
28	A	76	ARG
28	A	93	ASP
28	A	107	PHE
28	A	154	ASP
28	A	156	PHE
28	A	225	TYR
29	B	43	PHE
29	B	54	LYS
29	B	156	ARG
29	B	161	ASP
30	C	68	LEU
30	C	81	ASN
31	D	83	GLU
32	F	6	SER
32	F	26	LYS
32	F	52	LEU
32	F	53	LEU
32	F	64	ASP
32	F	99	GLU
33	H	24	LEU
33	H	62	GLN
33	H	63	LYS
33	H	72	LYS

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Mol	Chain	Res	Type
33	H	84	TYR
34	I	40	ARG
34	I	73	MET
34	I	79	TYR
34	I	144	ARG
34	I	145	ARG
35	J	45	MET
36	K	48	HIS
36	K	49	ASN
37	L	65	LEU
37	L	86	GLU
38	M	36	LEU
39	N	92	LYS
39	N	116	LYS
39	N	117	LEU
40	O	181	TRP
40	O	231	MET
40	O	316	MET
41	h	9	LEU
41	h	58	GLU
42	z	167	LYS
42	z	186	LYS
42	z	206	ASP
42	y	209	ARG
43	x	205	TYR
43	x	216	LYS
43	x	383	MET
43	x	447	PHE
43	x	528	PHE
43	x	547	LYS
43	x	550	HIS
43	x	557	LEU
43	x	572	PHE
43	x	599	ASN
47	U	87	ASP
47	U	107	ARG
47	U	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
11	Q	92	GLN

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Mol	Chain	Res	Type
11	Q	95	ASN
28	A	111	ASN
36	K	36	ASN
42	z	165	ASN
43	x	315	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	2	1740/1800 (96%)	456 (26%)	16 (0%)

All (456) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	2	2	A
9	2	4	C
9	2	17	C
9	2	25	C
9	2	26	A
9	2	34	G
9	2	42	G
9	2	45	U
9	2	46	A
9	2	47	A
9	2	56	U
9	2	57	G
9	2	60	U
9	2	66	U
9	2	68	A
9	2	73	U
9	2	74	U
9	2	75	U
9	2	76	A
9	2	77	U
9	2	78	A
9	2	100	A
9	2	104	A
9	2	111	U
9	2	114	C
9	2	115	G
9	2	117	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	126	A
9	2	127	G
9	2	129	U
9	2	140	A
9	2	141	U
9	2	142	G
9	2	143	G
9	2	144	U
9	2	145	A
9	2	146	U
9	2	153	G
9	2	158	U
9	2	161	U
9	2	168	A
9	2	176	C
9	2	178	U
9	2	179	A
9	2	180	A
9	2	187	G
9	2	188	A
9	2	191	C
9	2	192	U
9	2	193	U
9	2	194	U
9	2	195	G
9	2	197	A
9	2	215	A
9	2	217	A
9	2	218	A
9	2	222	A
9	2	223	U
9	2	224	C
9	2	225	A
9	2	227	U
9	2	228	G
9	2	230	C
9	2	232	U
9	2	233	C
9	2	234	G
9	2	235	G
9	2	239	C
9	2	240	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	241	U
9	2	249	U
9	2	259	U
9	2	260	U
9	2	261	U
9	2	265	A
9	2	266	A
9	2	272	U
9	2	273	G
9	2	277	U
9	2	278	U
9	2	279	G
9	2	280	U
9	2	281	G
9	2	287	G
9	2	302	U
9	2	304	U
9	2	312	A
9	2	313	U
9	2	314	C
9	2	316	A
9	2	321	C
9	2	322	G
9	2	328	A
9	2	333	A
9	2	334	G
9	2	337	G
9	2	338	C
9	2	352	A
9	2	353	A
9	2	359	A
9	2	361	C
9	2	365	G
9	2	370	A
9	2	388	G
9	2	393	C
9	2	399	A
9	2	400	A
9	2	401	A
9	2	402	C
9	2	403	G
9	2	404	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	417	A
9	2	419	G
9	2	423	G
9	2	424	C
9	2	425	A
9	2	426	G
9	2	434	G
9	2	435	C
9	2	436	A
9	2	439	U
9	2	444	C
9	2	445	A
9	2	448	C
9	2	454	U
9	2	460	A
9	2	468	A
9	2	469	C
9	2	473	A
9	2	477	A
9	2	483	A
9	2	484	C
9	2	485	A
9	2	487	G
9	2	490	C
9	2	491	C
9	2	492	A
9	2	493	U
9	2	494	U
9	2	495	C
9	2	496	G
9	2	498	G
9	2	499	U
9	2	500	C
9	2	501	U
9	2	502	U
9	2	504	U
9	2	506	A
9	2	507	U
9	2	510	G
9	2	511	A
9	2	514	G
9	2	519	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	527	A
9	2	534	A
9	2	538	A
9	2	539	G
9	2	540	G
9	2	541	A
9	2	542	A
9	2	548	G
9	2	549	G
9	2	557	G
9	2	559	C
9	2	565	C
9	2	566	C
9	2	568	G
9	2	571	G
9	2	578	U
9	2	579	A
9	2	580	A
9	2	582	U
9	2	594	A
9	2	595	G
9	2	606	A
9	2	610	G
9	2	611	U
9	2	619	A
9	2	620	A
9	2	621	A
9	2	622	A
9	2	623	A
9	2	624	G
9	2	638	U
9	2	639	U
9	2	640	U
9	2	641	G
9	2	645	C
9	2	647	G
9	2	649	U
9	2	651	G
9	2	654	C
9	2	655	G
9	2	656	G
9	2	677	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	681	U
9	2	682	C
9	2	683	C
9	2	694	U
9	2	696	C
9	2	698	U
9	2	700	C
9	2	703	G
9	2	704	C
9	2	705	U
9	2	706	A
9	2	707	A
9	2	708	C
9	2	711	U
9	2	712	G
9	2	713	A
9	2	714	G
9	2	730	G
9	2	731	C
9	2	732	G
9	2	733	A
9	2	734	A
9	2	736	C
9	2	737	A
9	2	739	G
9	2	741	C
9	2	742	U
9	2	743	U
9	2	765	G
9	2	766	U
9	2	767	U
9	2	774	A
9	2	775	G
9	2	778	G
9	2	779	U
9	2	780	A
9	2	781	U
9	2	782	U
9	2	783	G
9	2	807	A
9	2	812	A
9	2	813	U

*Continued on next page...*



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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	814	A
9	2	815	G
9	2	816	G
9	2	819	G
9	2	820	U
9	2	821	U
9	2	823	G
9	2	824	G
9	2	825	U
9	2	833	U
9	2	834	G
9	2	840	U
9	2	845	G
9	2	846	G
9	2	850	A
9	2	855	A
9	2	856	A
9	2	863	A
9	2	873	U
9	2	876	G
9	2	886	U
9	2	899	G
9	2	901	G
9	2	902	G
9	2	914	G
9	2	921	U
9	2	926	A
9	2	929	A
9	2	932	U
9	2	933	A
9	2	935	U
9	2	942	G
9	2	945	U
9	2	951	A
9	2	960	U
9	2	966	A
9	2	969	C
9	2	970	A
9	2	971	A
9	2	987	G
9	2	988	A
9	2	992	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	993	A
9	2	1001	A
9	2	1003	A
9	2	1004	U
9	2	1023	A
9	2	1026	A
9	2	1028	C
9	2	1031	U
9	2	1032	G
9	2	1039	A
9	2	1052	U
9	2	1053	G
9	2	1054	U
9	2	1059	U
9	2	1060	U
9	2	1061	A
9	2	1076	A
9	2	1080	U
9	2	1082	C
9	2	1083	G
9	2	1092	A
9	2	1096	C
9	2	1098	U
9	2	1100	G
9	2	1109	G
9	2	1113	A
9	2	1116	A
9	2	1138	A
9	2	1150	G
9	2	1156	C
9	2	1158	C
9	2	1159	C
9	2	1167	G
9	2	1171	A
9	2	1185	U
9	2	1191	U
9	2	1194	A
9	2	1196	A
9	2	1199	G
9	2	1200	G
9	2	1202	A
9	2	1207	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	1208	A
9	2	1214	U
9	2	1217	A
9	2	1218	G
9	2	1227	A
9	2	1228	G
9	2	1229	G
9	2	1230	A
9	2	1244	A
9	2	1245	G
9	2	1246	C
9	2	1251	U
9	2	1256	A
9	2	1263	G
9	2	1274	C
9	2	1275	A
9	2	1284	C
9	2	1285	U
9	2	1291	G
9	2	1306	C
9	2	1314	U
9	2	1315	U
9	2	1316	G
9	2	1319	A
9	2	1321	A
9	2	1322	A
9	2	1323	C
9	2	1325	A
9	2	1338	C
9	2	1344	A
9	2	1345	A
9	2	1346	A
9	2	1350	U
9	2	1354	G
9	2	1360	A
9	2	1363	U
9	2	1364	G
9	2	1367	G
9	2	1370	U
9	2	1371	A
9	2	1372	U
9	2	1373	C

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	1378	U
9	2	1383	G
9	2	1388	A
9	2	1389	C
9	2	1390	U
9	2	1398	U
9	2	1399	C
9	2	1400	A
9	2	1410	A
9	2	1414	U
9	2	1415	U
9	2	1425	A
9	2	1426	C
9	2	1427	A
9	2	1428	G
9	2	1432	U
9	2	1433	G
9	2	1446	A
9	2	1447	C
9	2	1458	G
9	2	1459	C
9	2	1460	A
9	2	1471	A
9	2	1472	C
9	2	1487	A
9	2	1491	U
9	2	1492	A
9	2	1494	C
9	2	1496	U
9	2	1506	G
9	2	1514	U
9	2	1516	A
9	2	1520	U
9	2	1521	G
9	2	1523	G
9	2	1524	A
9	2	1534	G
9	2	1535	U
9	2	1537	C
9	2	1540	G
9	2	1542	G
9	2	1543	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2	1557	U
9	2	1558	U
9	2	1559	A
9	2	1573	A
9	2	1583	A
9	2	1584	G
9	2	1590	G
9	2	1597	A
9	2	1601	G
9	2	1607	G
9	2	1611	A
9	2	1616	G
9	2	1619	C
9	2	1631	A
9	2	1634	C
9	2	1635	A
9	2	1637	C
9	2	1651	A
9	2	1654	G
9	2	1656	U
9	2	1657	U
9	2	1658	G
9	2	1680	G
9	2	1682	U
9	2	1684	U
9	2	1690	G
9	2	1715	G
9	2	1716	C
9	2	1746	A
9	2	1747	G
9	2	1748	G
9	2	1750	A
9	2	1754	A
9	2	1756	A
9	2	1757	G
9	2	1760	G
9	2	1762	A
9	2	1766	A
9	2	1767	G
9	2	1769	U
9	2	1780	G
9	2	1782	A

*Continued on next page...*

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Mol	Chain	Res	Type
9	2	1783	C
9	2	1791	A
9	2	1792	G
9	2	1793	G
9	2	1794	A
9	2	1795	U
9	2	1796	C
9	2	1798	U
9	2	1799	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	2	59	C
9	2	77	U
9	2	139	C
9	2	280	U
9	2	387	A
9	2	400	A
9	2	639	U
9	2	640	U
9	2	711	U
9	2	928	U
9	2	1226	A
9	2	1274	C
9	2	1344	A
9	2	1382	A
9	2	1636	C
9	2	1791	A

#### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 82 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	SF4	x	702	43	0,12,12	-	-	-		
50	SF4	x	701	43	0,12,12	-	-	-		
51	ADP	x	703	43,48	24,29,29	0.93	1 (4%)	29,45,45	1.37	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	SF4	x	702	43	-	-	0/6/5/5
50	SF4	x	701	43	-	-	0/6/5/5
51	ADP	x	703	43,48	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	x	703	ADP	C5-C4	2.44	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	x	703	ADP	C3'-C2'-C1'	3.36	106.04	100.98
51	x	703	ADP	N3-C2-N1	-3.12	123.80	128.68
51	x	703	ADP	C4-C5-N7	-2.55	106.75	109.40
51	x	703	ADP	PA-O3A-PB	-2.09	125.67	132.83

There are no chirality outliers.

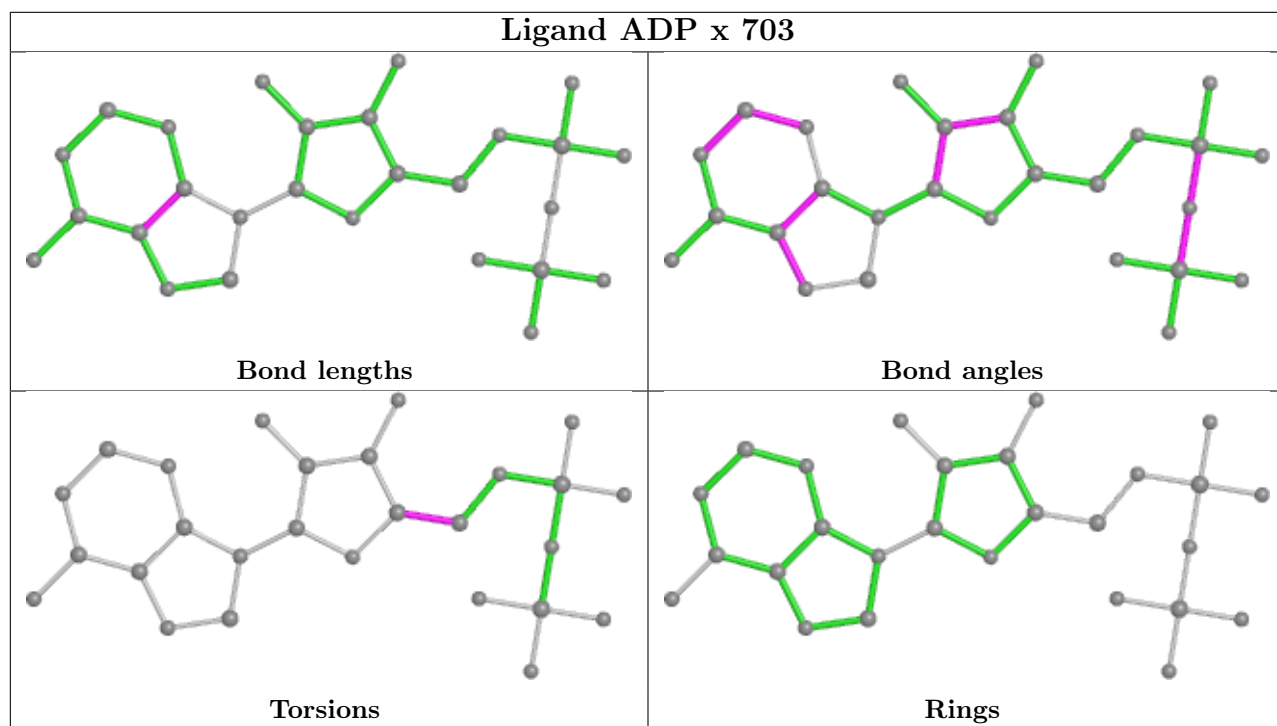
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	x	703	ADP	O4'-C4'-C5'-O5'
51	x	703	ADP	C3'-C4'-C5'-O5'

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

There are no chain breaks in this entry.

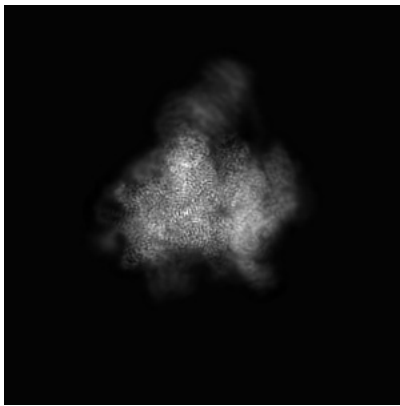
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16525. These allow visual inspection of the internal detail of the map and identification of artifacts.

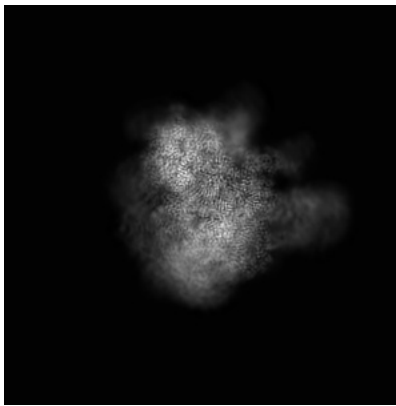
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

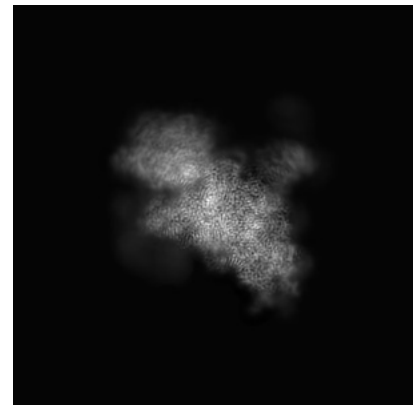
#### 6.1.1 Primary map



X

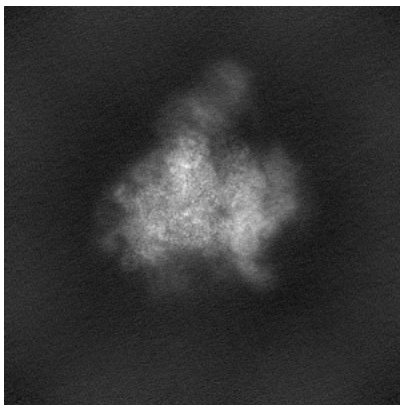


Y

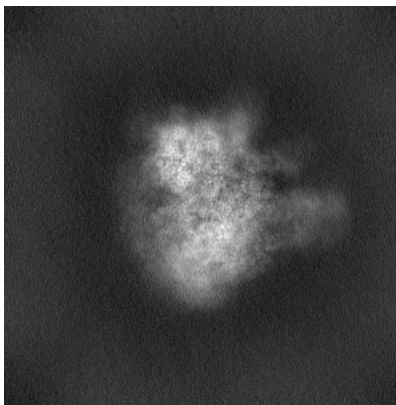


Z

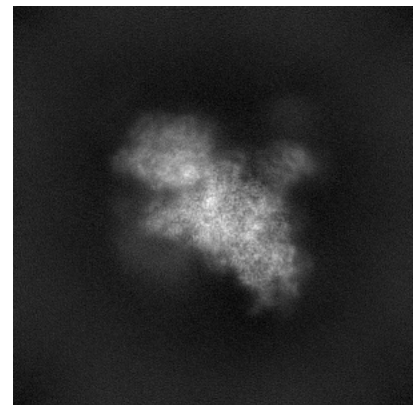
#### 6.1.2 Raw map



X



Y

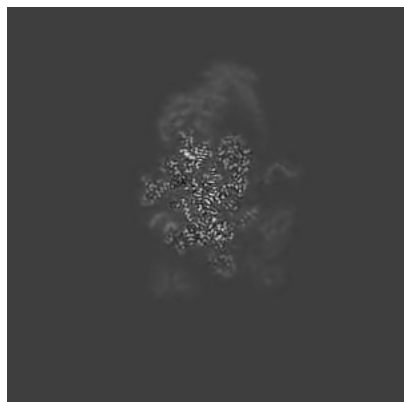


Z

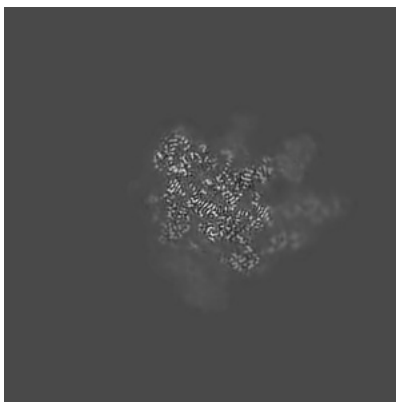
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

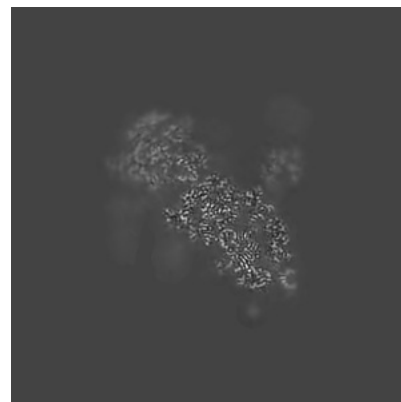
### 6.2.1 Primary map



X Index: 210

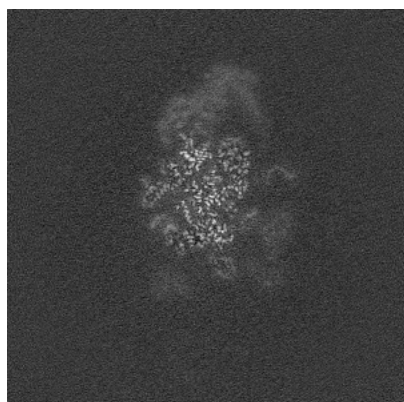


Y Index: 210

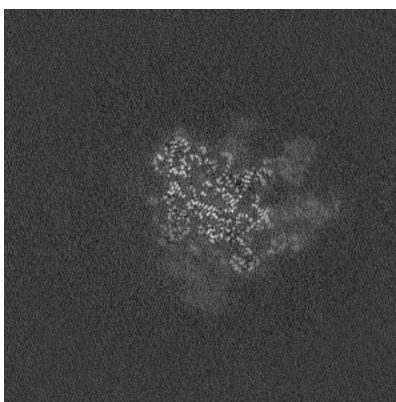


Z Index: 210

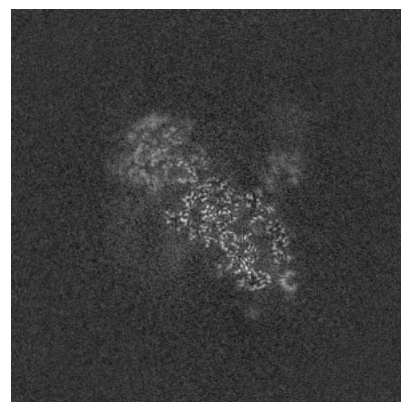
### 6.2.2 Raw map



X Index: 210



Y Index: 210

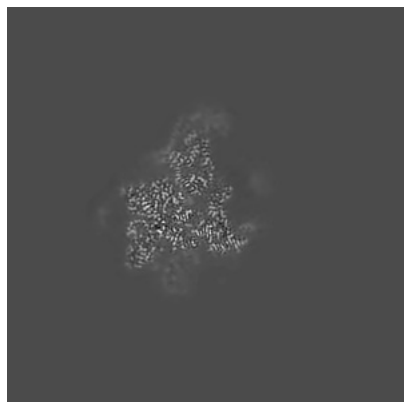


Z Index: 210

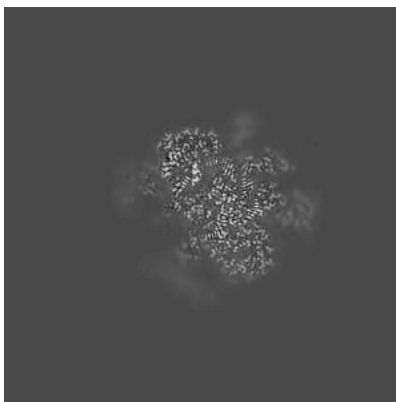
The images above show central slices of the map in three orthogonal directions.

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

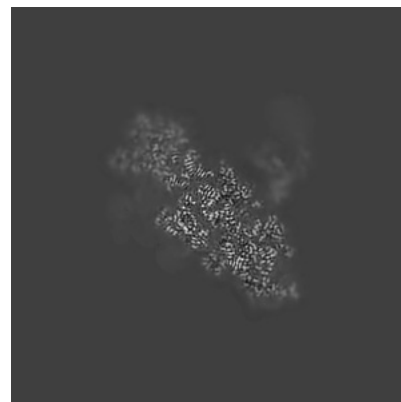
### 6.3.1 Primary map



X Index: 247

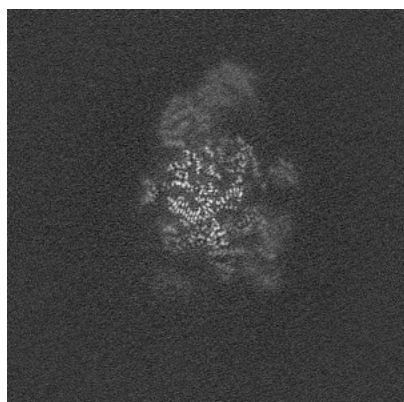


Y Index: 189

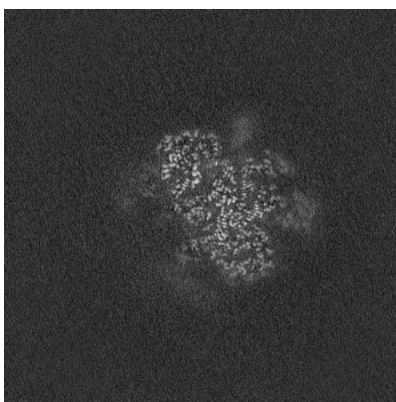


Z Index: 222

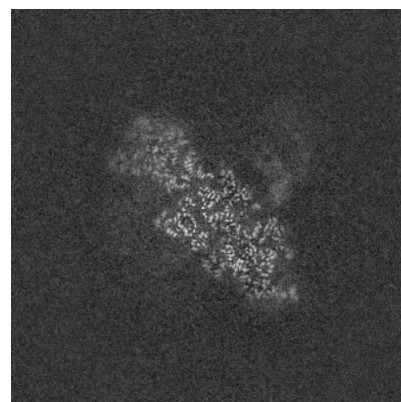
### 6.3.2 Raw map



X Index: 205



Y Index: 189

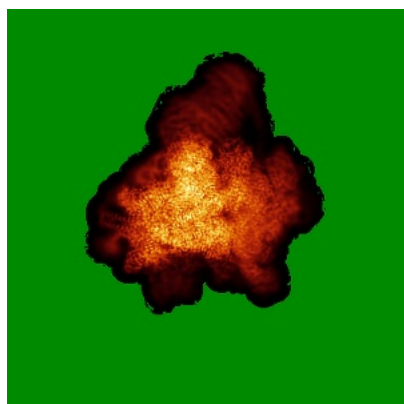


Z Index: 222

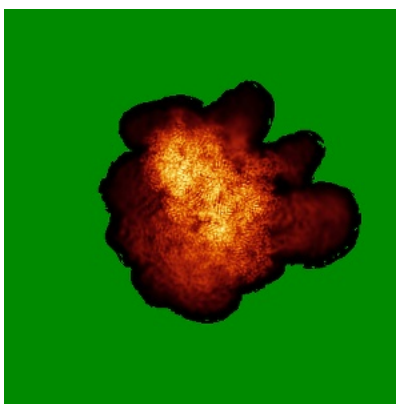
The images above show the largest variance slices of the map in three orthogonal directions.

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

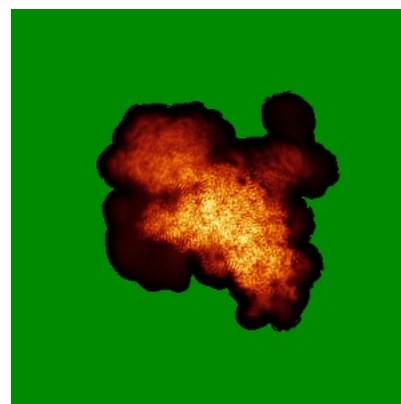
### 6.4.1 Primary map



X

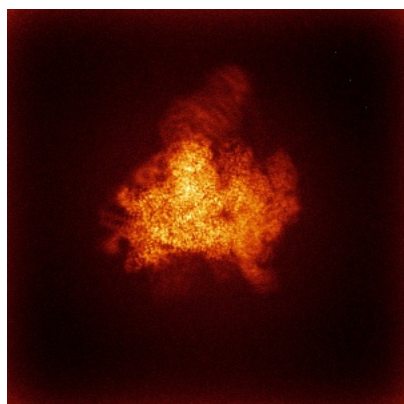


Y

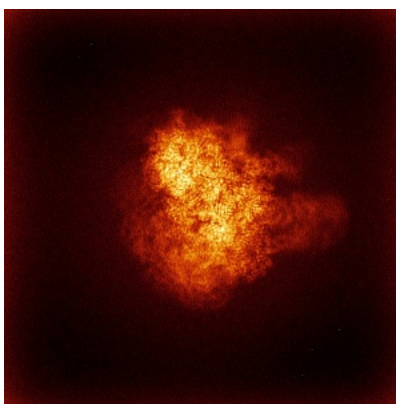


Z

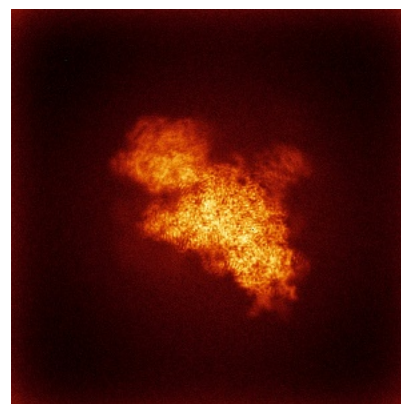
### 6.4.2 Raw map



X



Y

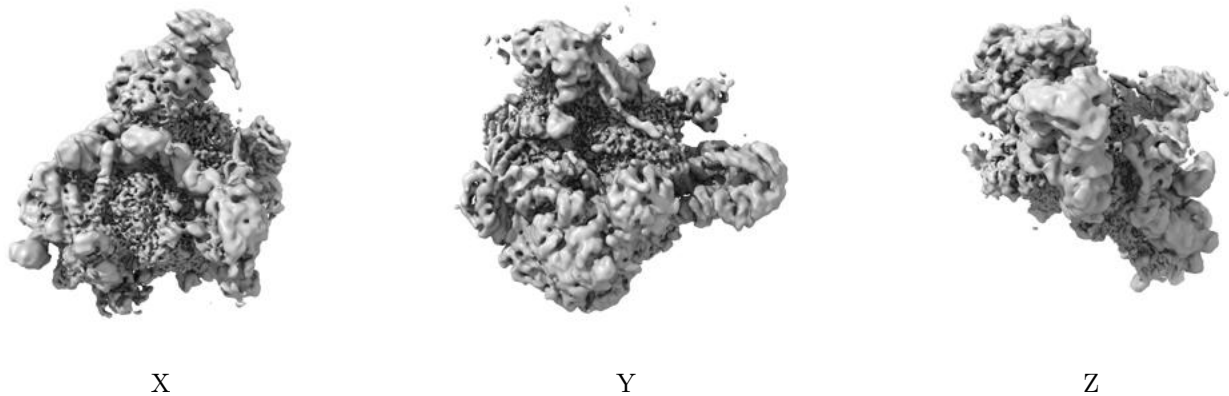


Z

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

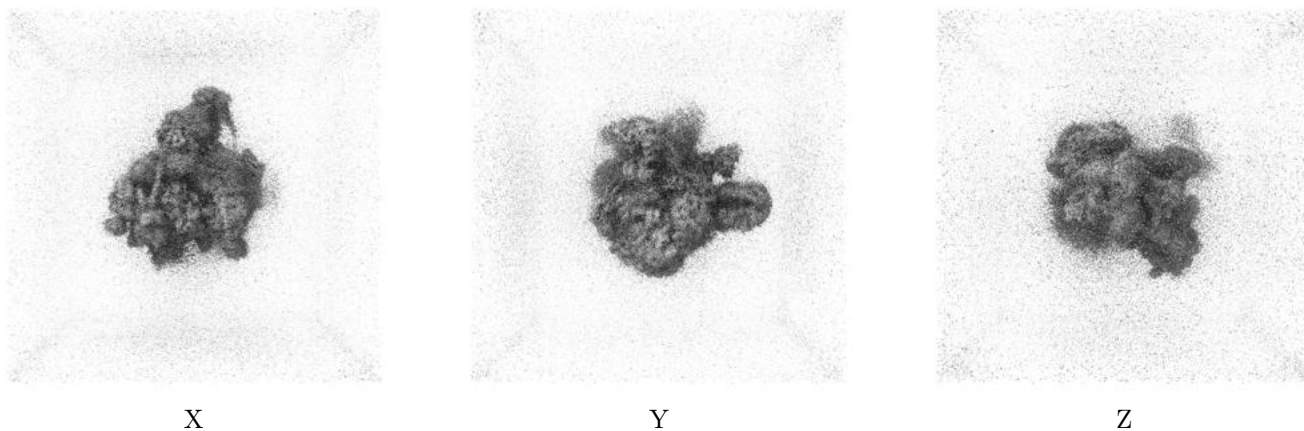
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

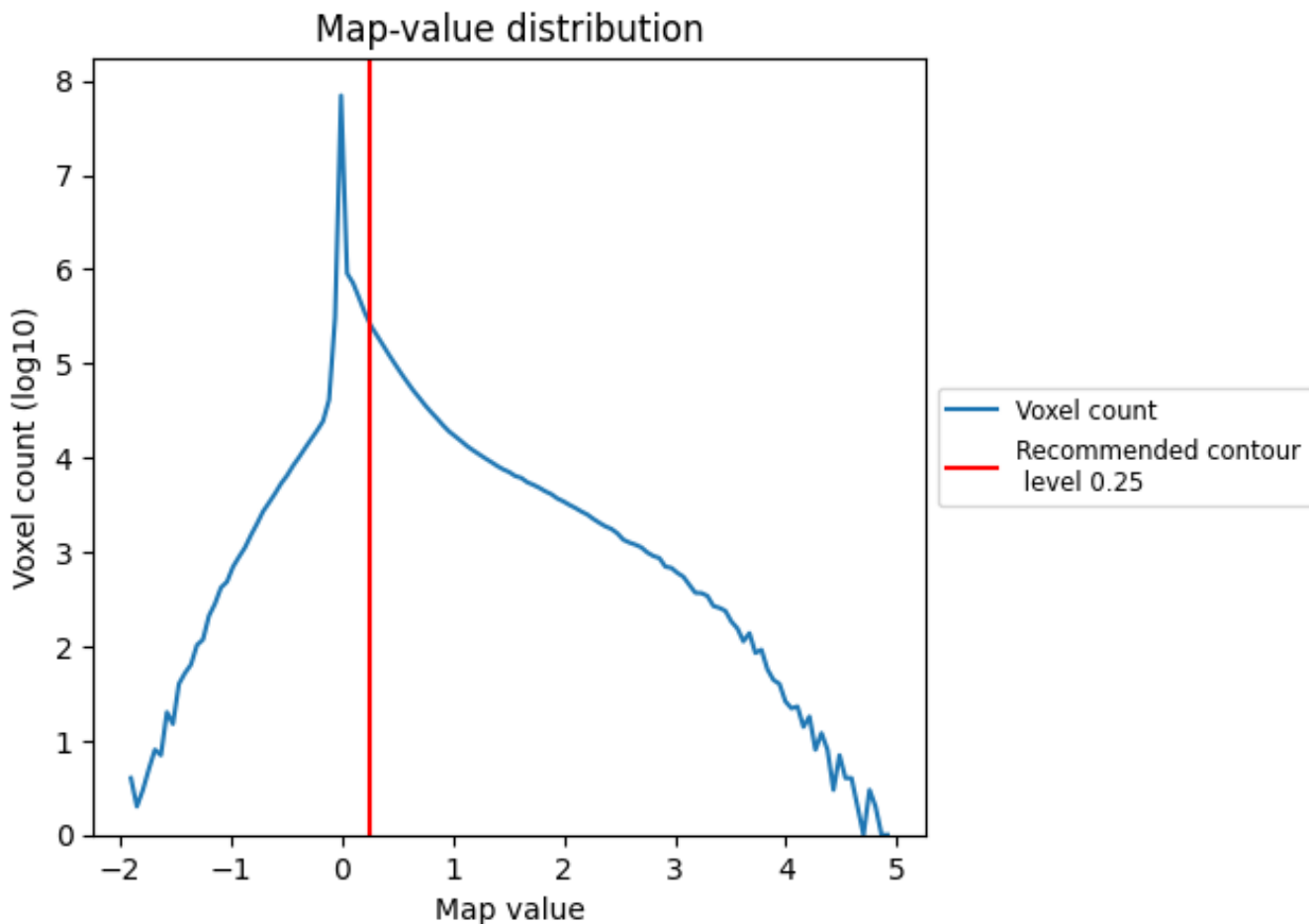
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

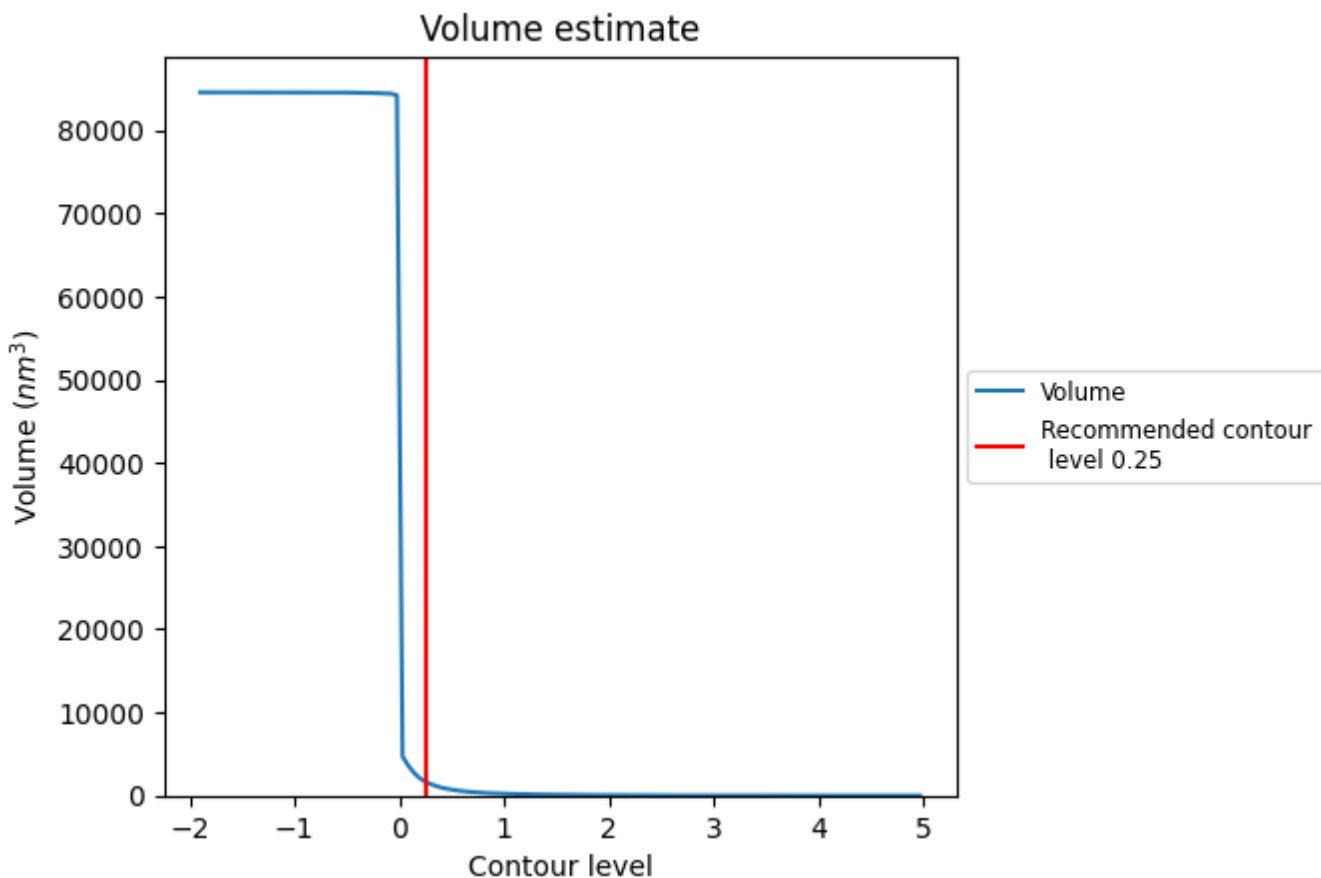
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

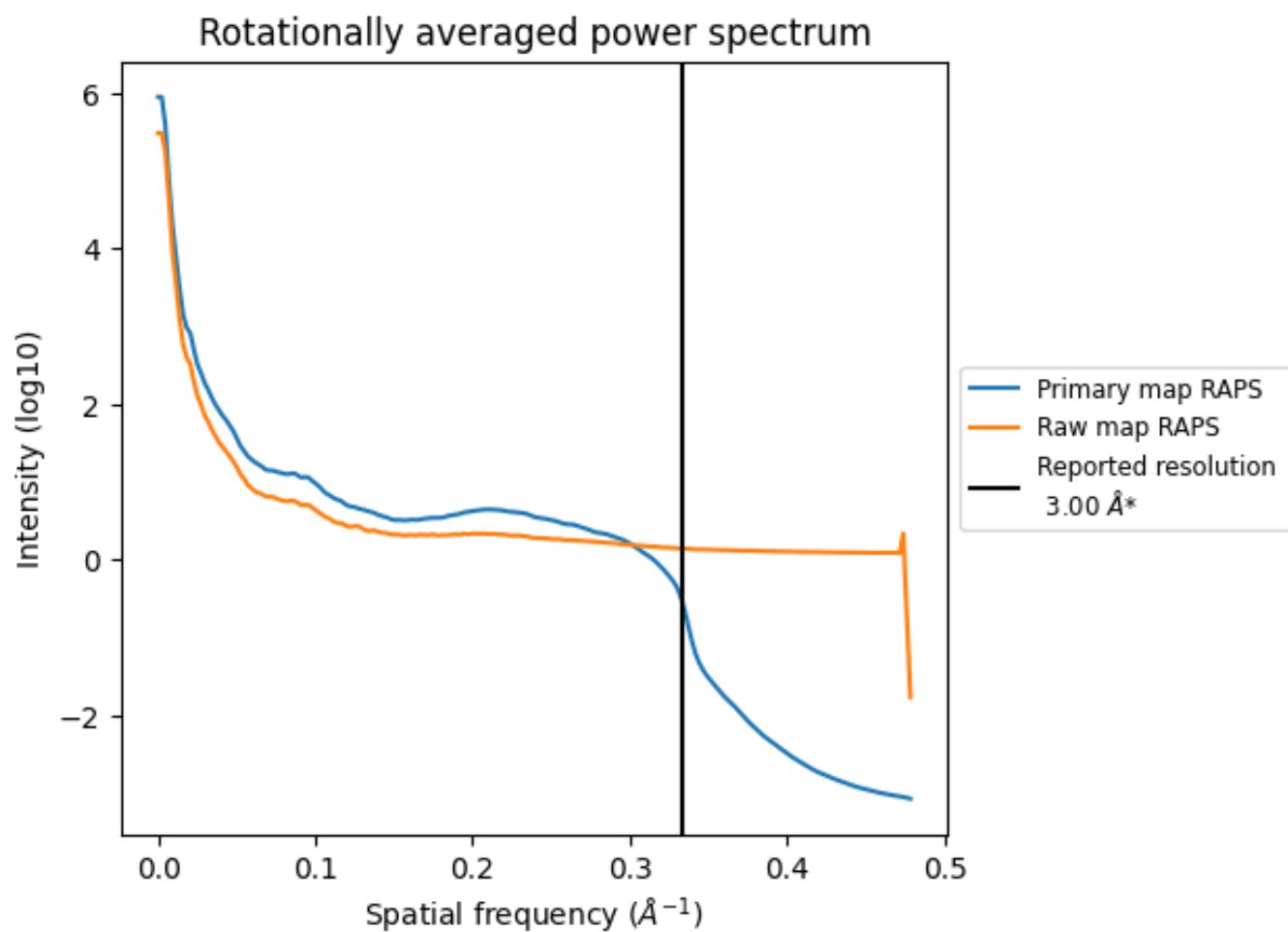


The volume at the recommended contour level is 1650 nm<sup>3</sup>; this corresponds to an approximate mass of 1491 kDa.

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



### 7.3 Rotationally averaged power spectrum i

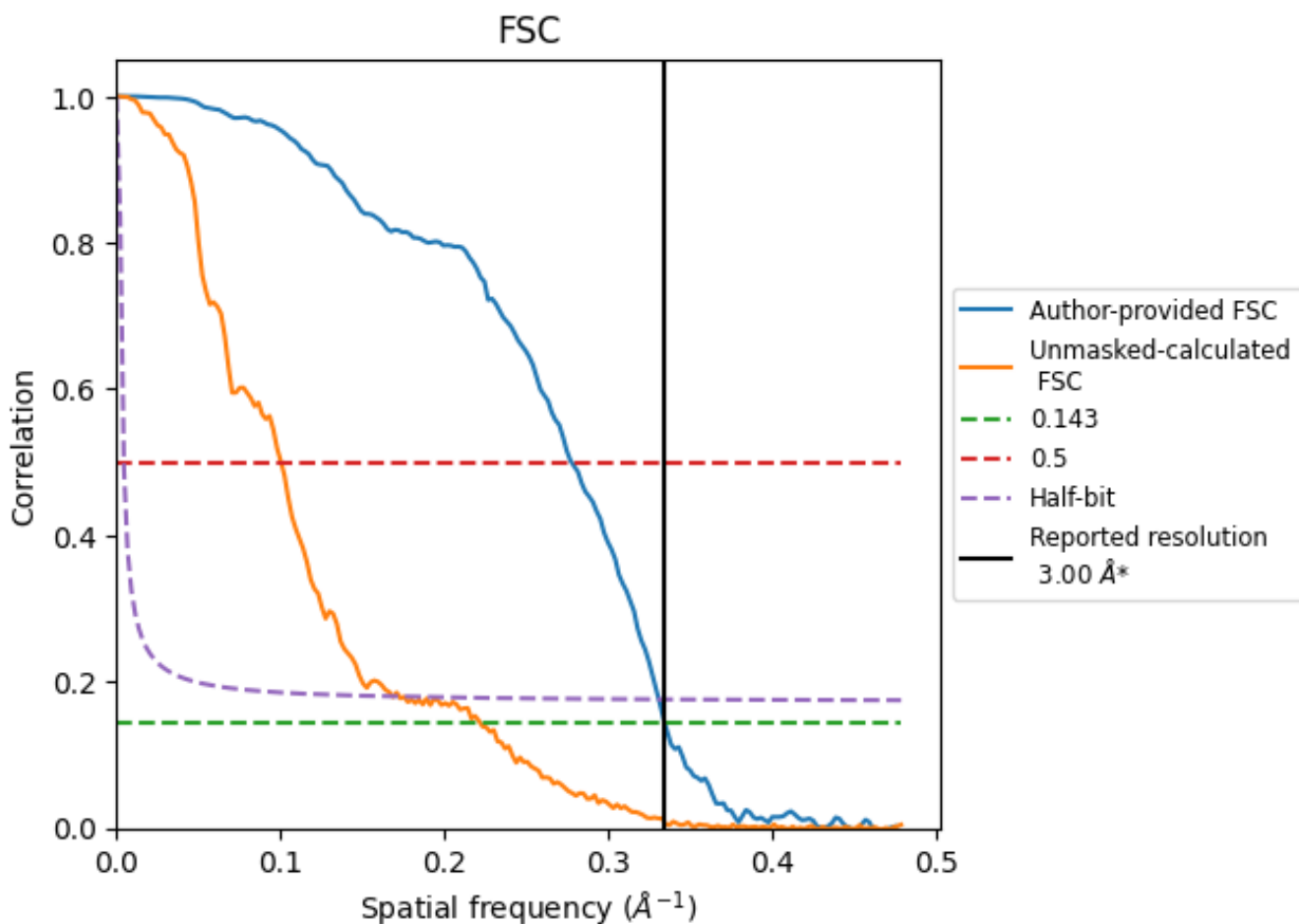


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

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

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

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

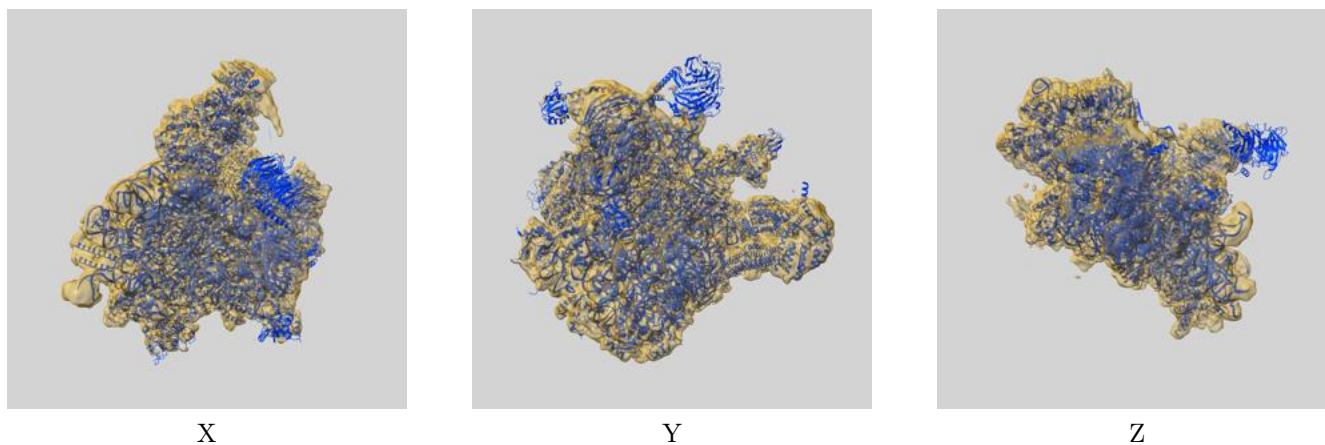
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.60	3.02
Unmasked-calculated*	4.50	9.97	5.94

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.0 by more than 10 %

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

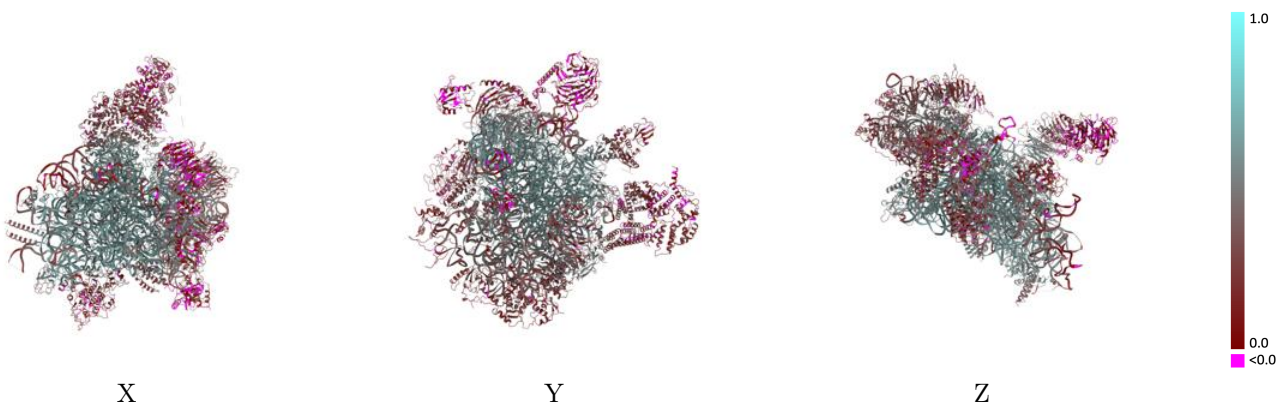
This section contains information regarding the fit between EMDB map EMD-16525 and PDB model 8CAH. Per-residue inclusion information can be found in section 3 on page 14.

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



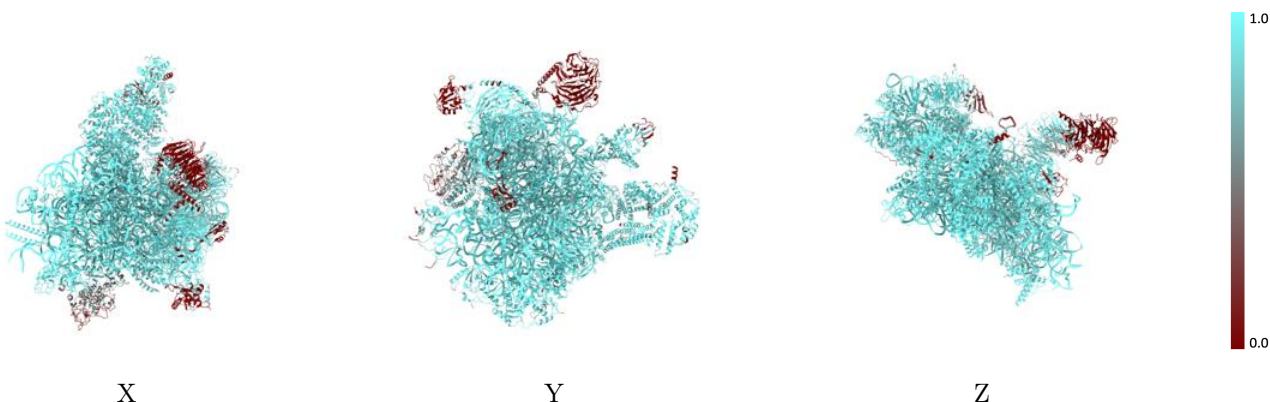
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



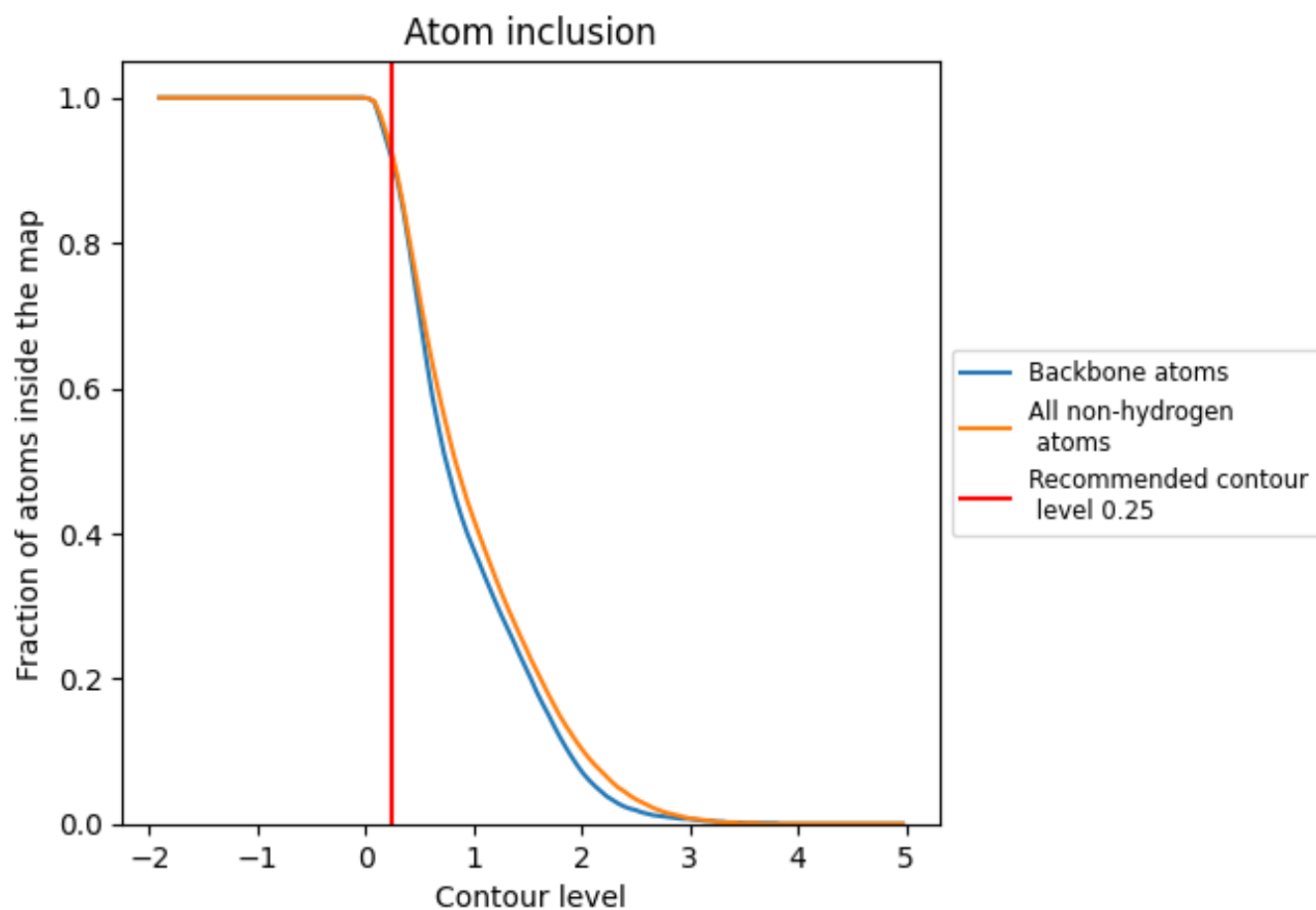
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





























The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9210	 0.4300
2	 0.9910	 0.5070
A	 0.9450	 0.4170
B	 0.9610	 0.3310
C	 0.9780	 0.3710
D	 0.8090	 0.1960
E	 0.9480	 0.2660
F	 0.9930	 0.3680
G	 0.9480	 0.3100
H	 0.9640	 0.4310
I	 0.9520	 0.2390
J	 0.9790	 0.2800
K	 0.9460	 0.3820
L	 0.8700	 0.1940
M	 1.0000	 0.4810
N	 0.8070	 0.1840
O	 0.9360	 0.2810
P	 0.9930	 0.5580
Q	 0.9810	 0.5110
R	 0.9940	 0.5820
S	 0.9960	 0.5850
T	 0.9830	 0.5030
U	 0.9770	 0.4820
V	 0.9940	 0.5700
W	 0.9820	 0.5760
X	 0.9870	 0.5920
Y	 0.9890	 0.5620
Z	 0.9870	 0.5350
a	 0.9890	 0.5720
b	 0.9990	 0.6120
c	 0.9930	 0.5910
d	 0.9880	 0.5540
e	 0.9910	 0.5710
f	 0.9780	 0.5400
g	 0.9360	 0.4980



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Chain	Atom inclusion	Q-score
h	 0.9370	 0.3410
i	 0.9500	 0.4380
j	 0.1950	 0.0630
k	 0.4920	 0.1840
l	 0.0110	 0.0720
m	 0.9320	 0.3930
n	 1.0000	 0.5870
o	 0.8920	 0.1950
p	 0.7640	 0.2750
q	 0.9420	 0.2330
r	 0.0000	 0.1080
x	 0.5460	 0.2130
y	 0.8360	 0.3210
z	 0.8890	 0.3550