



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 07:58 PM JST

PDB ID : 6LQM / pdb_00006lqm
EMDB ID : EMD-0948
Title : Cryo-EM structure of a pre-60S ribosomal subunit - state C
Authors : Liang, X.; Zuo, M.; Zhang, Y.; Li, N.; Ma, C.; Dong, M.; Gao, N.
Deposited on : 2020-01-14
Resolution : 3.09 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

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>.

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

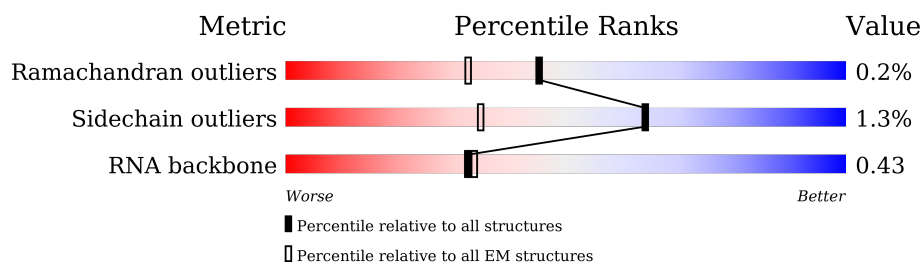
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 3.09 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.






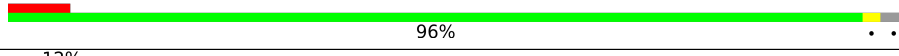
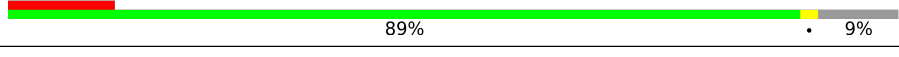
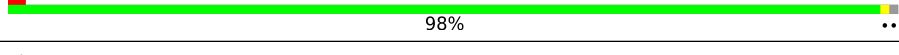
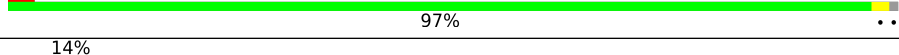

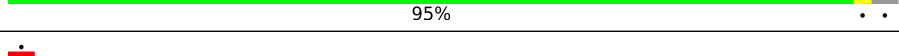
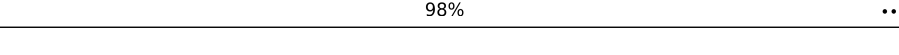
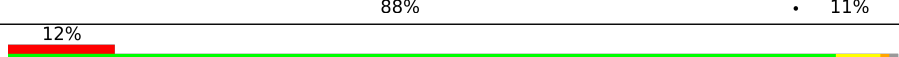
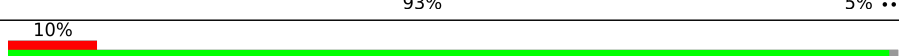
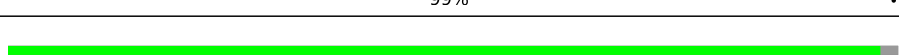
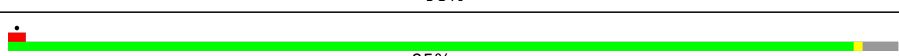

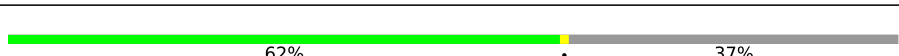

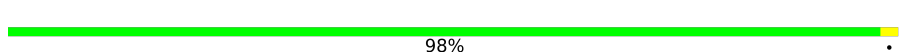
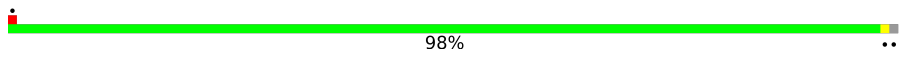
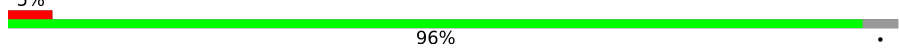
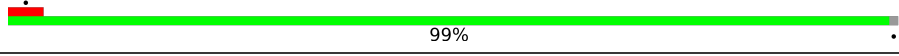
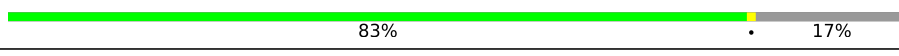
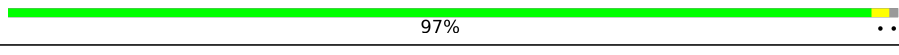
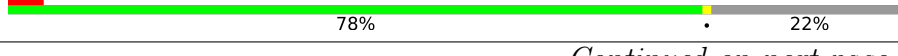

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 ≥ 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	0	477	
2	2	5070	
3	3	534	
4	5	120	
5	6	245	
6	8	156	
7	A	217	
8	B	403	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	C	159	
10	D	427	
11	E	115	
12	F	117	
13	G	266	
14	H	123	
15	I	192	
16	J	214	
17	K	105	
18	L	148	
19	M	97	
20	N	178	
21	O	70	
22	P	51	
23	Q	211	
24	R	128	
25	S	215	
26	T	125	
27	U	204	
28	V	203	
29	W	106	
30	X	92	
31	Y	184	
32	Z	188	
33	a	196	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	b	176	 98%
35	c	160	 97%
36	d	128	 9% 76% 21%
37	e	140	 92% 7%
38	f	157	 39% 61%
39	g	156	 74% 25%
40	h	145	 87% 10%
41	i	136	 99%
42	l	137	 87% 9%
43	m	257	 93%
44	r	297	 7% 98%
45	t	135	 93% 5%
46	u	110	 95% 5%
47	v	288	 10% 78% 18%
48	w	248	 90% 9%

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 139464 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 Zinc finger protein 622.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	66	Total	C	N	O	S	0	0
			555	347	111	89	8		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3532	Total	C	N	O	P	0	0
			75841	33834	13861	24615	3531		

- Molecule 3 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	254	Total	C	N	O	S	0	0
			2043	1297	357	372	17		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	504	GLY	-	expression tag	UNP Q96D46
3	505	SER	-	expression tag	UNP Q96D46
3	506	GLU	-	expression tag	UNP Q96D46
3	507	ASN	-	expression tag	UNP Q96D46
3	508	LEU	-	expression tag	UNP Q96D46
3	509	TYR	-	expression tag	UNP Q96D46
3	510	PHE	-	expression tag	UNP Q96D46
3	511	GLN	-	expression tag	UNP Q96D46
3	512	GLY	-	expression tag	UNP Q96D46
3	513	ASP	-	expression tag	UNP Q96D46
3	514	TYR	-	expression tag	UNP Q96D46
3	515	LYS	-	expression tag	UNP Q96D46
3	516	ASP	-	expression tag	UNP Q96D46
3	517	HIS	-	expression tag	UNP Q96D46
3	518	ASP	-	expression tag	UNP Q96D46

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3	519	GLY	-	expression tag	UNP Q96D46
3	520	ASP	-	expression tag	UNP Q96D46
3	521	TYR	-	expression tag	UNP Q96D46
3	522	LYS	-	expression tag	UNP Q96D46
3	523	ASP	-	expression tag	UNP Q96D46
3	524	HIS	-	expression tag	UNP Q96D46
3	525	ASP	-	expression tag	UNP Q96D46
3	526	ILE	-	expression tag	UNP Q96D46
3	527	ASP	-	expression tag	UNP Q96D46
3	528	TYR	-	expression tag	UNP Q96D46
3	529	LYS	-	expression tag	UNP Q96D46
3	530	ASP	-	expression tag	UNP Q96D46
3	531	ASP	-	expression tag	UNP Q96D46
3	532	ASP	-	expression tag	UNP Q96D46
3	533	ASP	-	expression tag	UNP Q96D46
3	534	LYS	-	expression tag	UNP Q96D46

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	220	Total	C	N	O	S	0	0
			1672	1040	288	333	11		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 7 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	212	Total	C	N	O	S	0	0
			1708	1092	308	300	8		

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 9 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	97	Total	C	N	O	S	0	0
			788	489	172	123	4		

- Molecule 10 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	358	Total	C	N	O	S	0	0
			2850	1794	569	473	14		

- Molecule 11 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 12 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 14 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 15 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 16 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	154	Total	C	N	O	S	0	0
			1249	795	233	212	9		

- Molecule 17 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 18 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 19 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 20 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 21 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 22 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 23 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	203	Total	C	N	O	S	0	0
			1640	1027	341	268	4		

- Molecule 24 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	47	Total	C	N	O	S	0	0
			387	237	83	61	6		

- Molecule 25 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 26 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 27 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 28 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 29 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	102	Total	C	N	O	S	1	0
			842	527	174	135	6		

- Molecule 30 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 31 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 32 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 33 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	153	Total	C	N	O	S	0	0
			1281	799	276	197	9		

- Molecule 34 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 35 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 36 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 37 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

- Molecule 38 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	61	Total	C	N	O	S	0	0
			515	330	100	82	3		

- Molecule 39 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	117	Total	C	N	O	S	0	0
			958	612	179	166	1		

- Molecule 40 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	131	Total	C	N	O	S	0	0
			1093	686	221	183	3		

- Molecule 41 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 42 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 43 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 44 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 45 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 46 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 47 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 48 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	2	245	Total	Mg	0
			245	245	
49	5	3	Total	Mg	0
			3	3	
49	B	1	Total	Mg	0
			1	1	

Continued on next page...

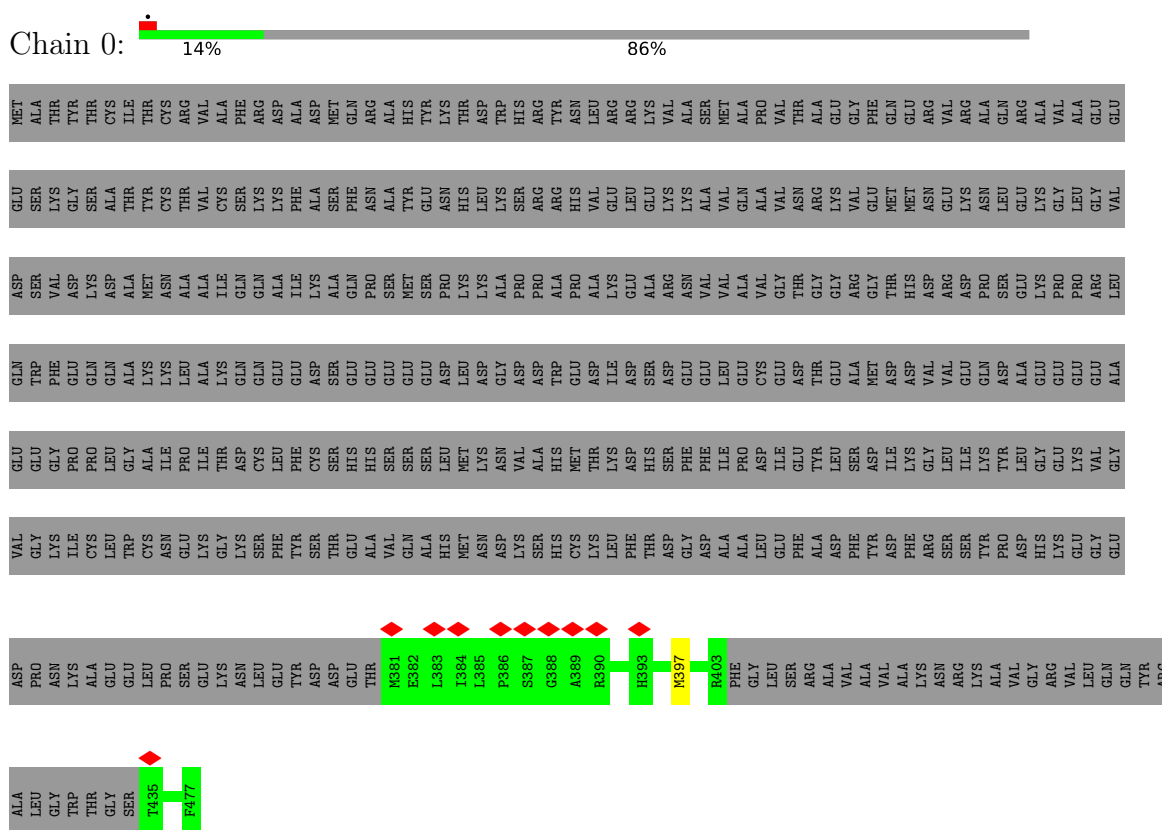
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
49	F	1	Total 1	Mg 1	0
49	m	1	Total 1	Mg 1	0

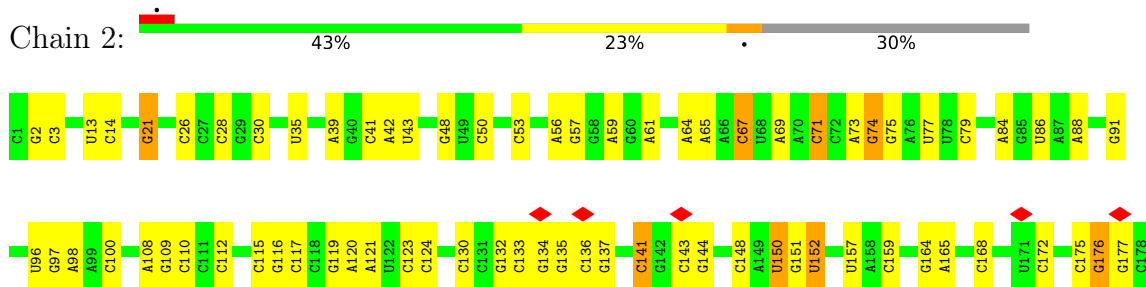
3 Residue-property plots

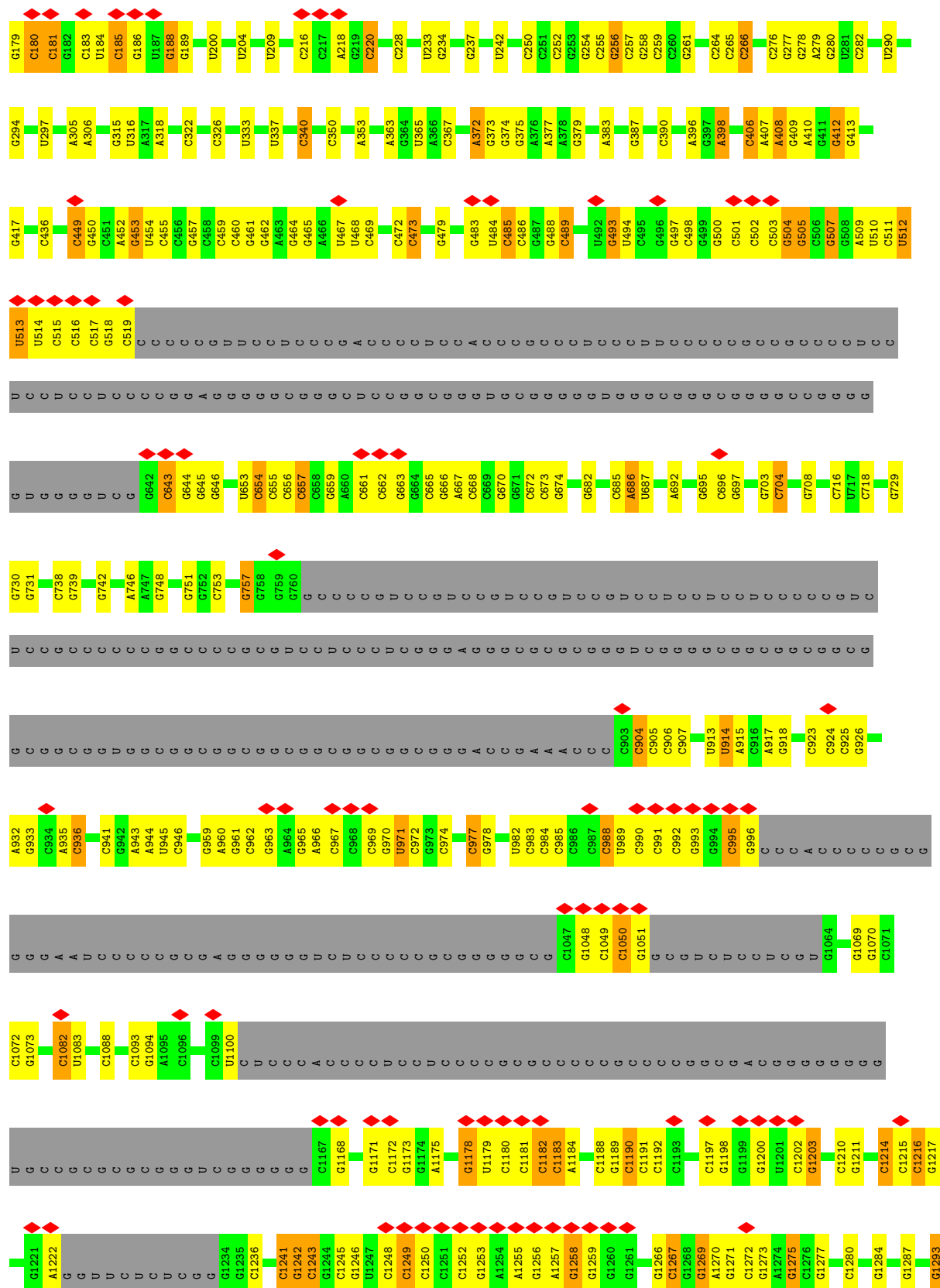
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Zinc finger protein 622



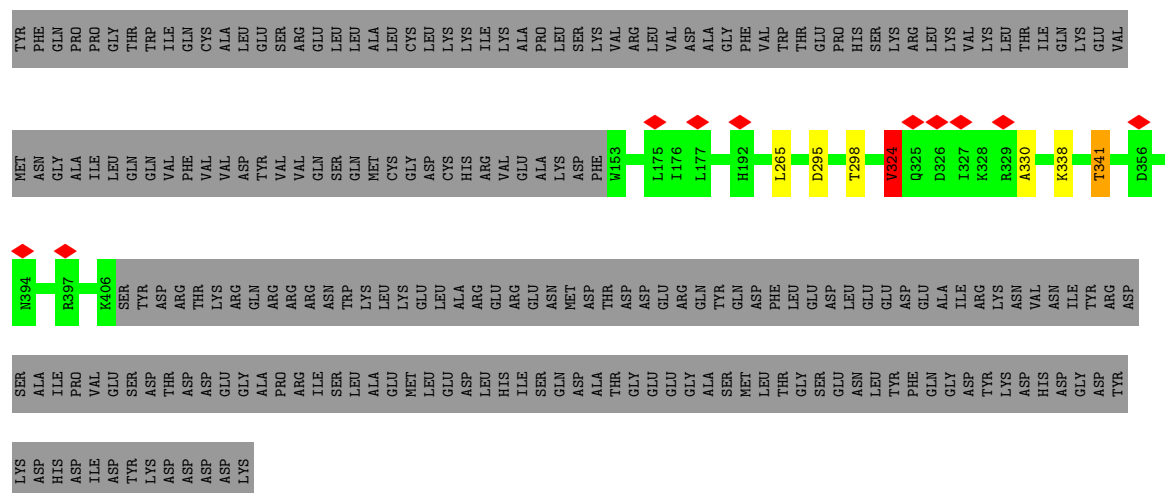
• Molecule 2: 28S rRNA



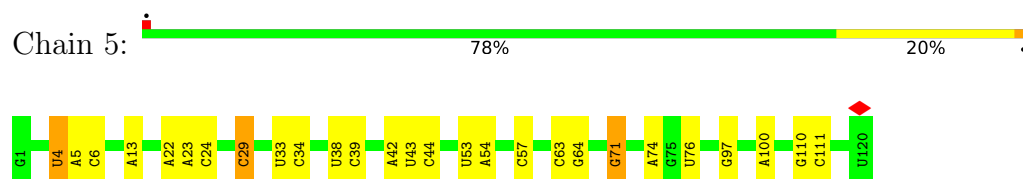




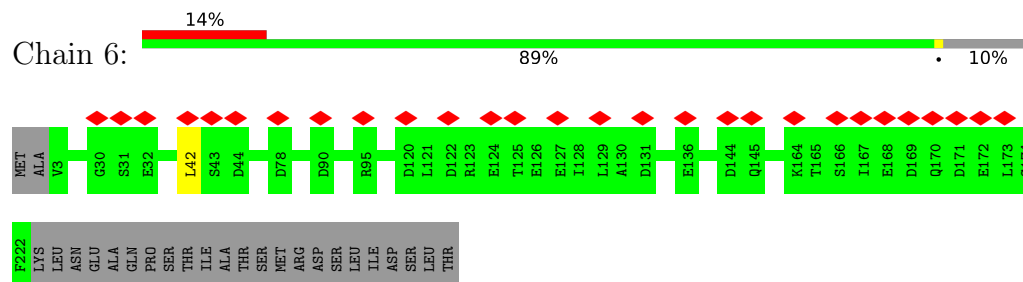




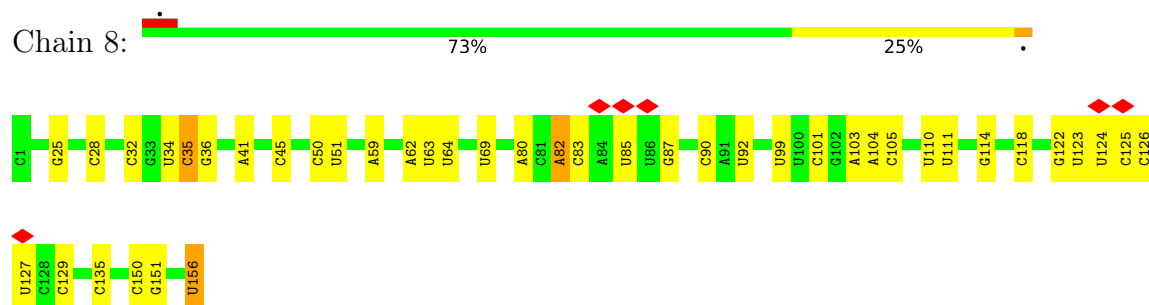
- Molecule 4: 5S rRNA



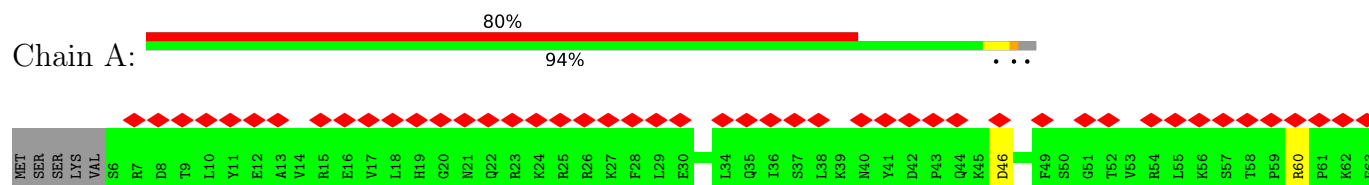
- Molecule 5: Eukaryotic translation initiation factor 6

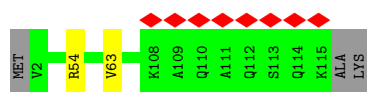


- Molecule 6: 5.8S rRNA

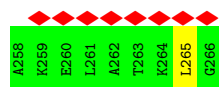
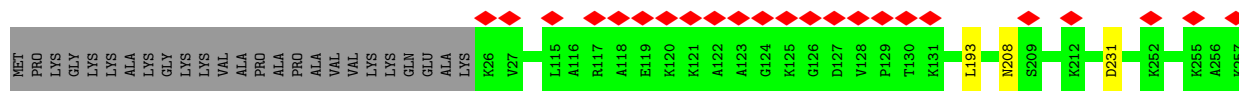
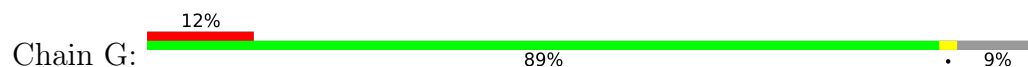


- Molecule 7: 60S ribosomal protein L10a

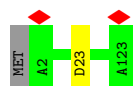




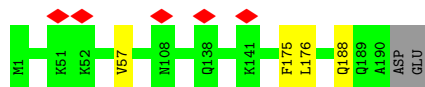
- Molecule 13: 60S ribosomal protein L7a



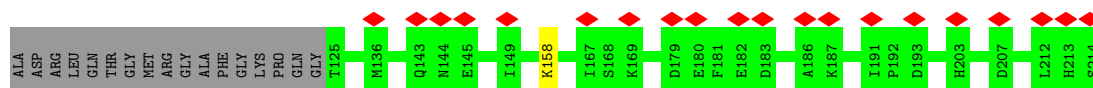
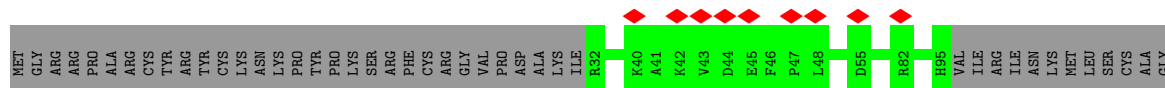
- Molecule 14: 60S ribosomal protein L35



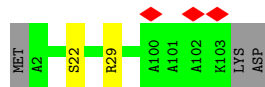
- Molecule 15: 60S ribosomal protein L9



- Molecule 16: 60S ribosomal protein L10-like



- Molecule 17: 60S ribosomal protein L36



- Molecule 18: 60S ribosomal protein L27a

- Chain M:  88% • 11%

MET T2 C22 K87 ARG ALA ALA VAL ALA ALA SER SER SER SER

- Chain N:  12% 93% 5%

NET	ALA	Q3	D4	Q5	G6	E7	K8	P11	V57	F60	R63	K78	E84	E91	Y92	E93	L94	R95	I113	D114	L115	G116	I117	K118	Y119	V132	D143	I173	P176	G177	K178
NET	ALA	Q3	D4	Q5	G6	E7	K8	P11	V57	F60	R63	K78	E84	E91	Y92	E93	L94	R95	I113	D114	L115	G116	I117	K118	Y119	V132	D143	I173	P176	G177	K178

- Chain O:  10% 99%

Diagram illustrating the 1000 Genomes Project sample structure. The samples are grouped into a single cluster, with a vertical bar labeled 'MET' indicating the reference population. The samples are labeled P2, D30, E51, E54, L60, P61, E68, L69, and K70, with red diamonds above each label.

- Chain P: 98%

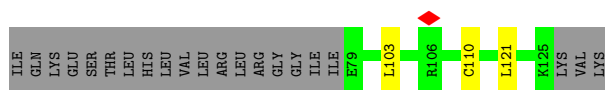
MET S2 L51

- Chain Q: 

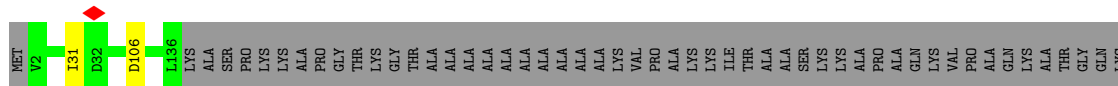
MET
 A2
 P62
 V70
 L124
 K130
 A133
 P134
 K135
 K145
 A203
 E204
 GLN
 ASP
 VAL
 GLU
 LYS
 LYS
 LYS

- Chain R: 34% 63%

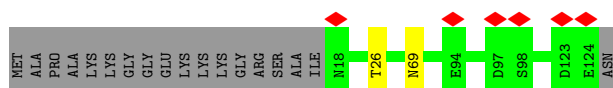
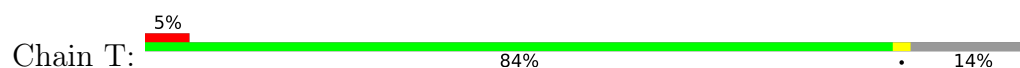
MET	GLN	ILE	PHE	VAL	LYS	THR	LEU	LEU	GLY	LYS	THR	ILE	THR	LEU	GLU	VAL	GLU	GLU	PRO	SER	ASP	THR	ILE	ILE	GLU	ASN	VAL	LYS	LYS	LYS	GLN	GLN	GLN	ARG	ILE	ILE	PHE	GLY	LYS	GLN	LEU	GLU	LEU	GLY	GLY	ARG	THR	LEU	SER	ASP	THR	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



- Molecule 25: 60S ribosomal protein L14



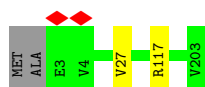
- Molecule 26: 60S ribosomal protein L31



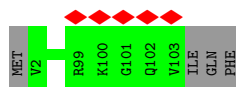
- Molecule 27: 60S ribosomal protein L15



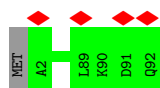
- Molecule 28: 60S ribosomal protein L13a




- Molecule 29: 60S ribosomal protein L36a

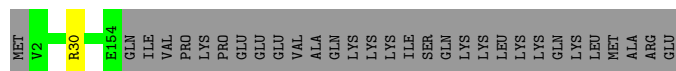


- Molecule 30: 60S ribosomal protein L37a



- Molecule 31: 60S ribosomal protein L17

Chain Y:  83% 17%




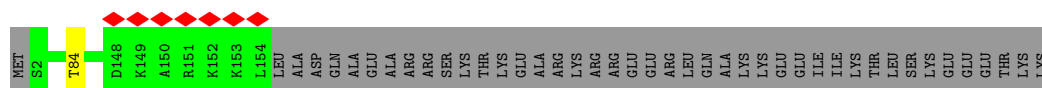
- Molecule 32: 60S ribosomal protein L18

Chain Z:  97%



- Molecule 33: 60S ribosomal protein L19

Chain a:  78% 22%



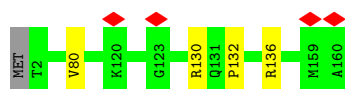
- Molecule 34: 60S ribosomal protein L18a

Chain b:  98%




- Molecule 35: 60S ribosomal protein L21

Chain c:  97%



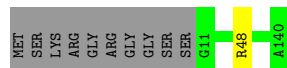
- Molecule 36: 60S ribosomal protein L22

Chain d:  9% 76% 21%



- Molecule 37: 60S ribosomal protein L23

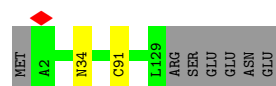
Chain e:  92% 7%



- Molecule 44: 60S ribosomal protein L5

MET	G2	F3	R23	D136	E213	E214	D217	N229	K256	P257	K258	K259	E260	V261	K262	K263	A281	F287	L288	R289	A290	Q291	E292	R293	A294	ALA	GLU	SFR
-----	----	----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

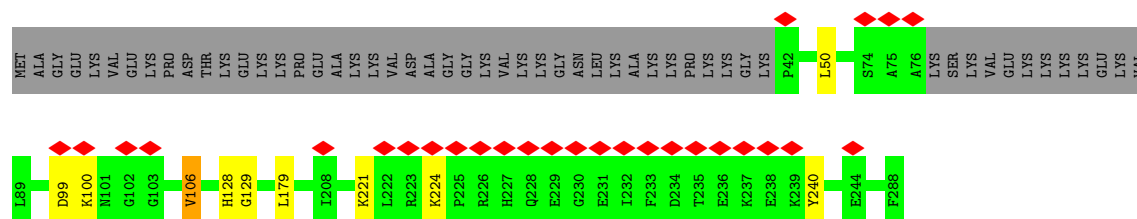
- Chain t:  93% • 5%



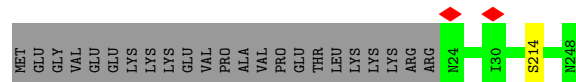
- Chain u: 95% 5%



- Chain v: 10% 78% 18%



- Chain w: 90% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21707	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.454	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	507.84, 507.84, 507.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, A2M, OMG, OMC, B8K, PSU, M7A, 6MZ, MHG, UR3, 2MG, 1MA, I4U, BGH, E6G, B9B, 5MU, B8H, MG, B8W, P4U, 5MC, E7G, B9H, B8T, B8Q, 7MG, P7G

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	0	0.40	0/563	0.59	0/742
2	2	1.68	62/82280 (0.1%)	1.37	1037/128277 (0.8%)
3	3	0.49	0/2086	0.67	1/2820 (0.0%)
4	5	1.23	0/2858	1.22	24/4455 (0.5%)
5	6	0.46	0/1696	0.67	1/2309 (0.0%)
6	8	1.45	2/3701 (0.1%)	1.26	33/5766 (0.6%)
7	A	0.46	2/1736 (0.1%)	0.81	5/2328 (0.2%)
8	B	0.67	0/3315	0.70	2/4435 (0.0%)
9	C	0.50	0/800	0.63	0/1055
10	D	0.73	1/2903 (0.0%)	0.70	3/3899 (0.1%)
11	E	0.56	0/742	0.72	1/996 (0.1%)
12	F	0.67	1/916 (0.1%)	0.64	0/1220
13	G	0.60	0/1960	0.70	2/2637 (0.1%)
14	H	0.60	0/1023	0.61	0/1351
15	I	0.59	0/1537	0.69	0/2066
16	J	0.39	0/1278	0.63	1/1708 (0.1%)
17	K	0.54	0/843	0.69	1/1115 (0.1%)
18	L	0.71	0/1191	0.69	0/1591
19	M	0.75	0/720	0.73	0/952
20	N	0.51	1/1433 (0.1%)	0.70	0/1915
21	O	0.55	0/575	0.65	0/761
22	P	0.67	0/454	0.65	0/599
23	Q	0.65	0/1671	0.68	1/2237 (0.0%)
24	R	0.52	1/393 (0.3%)	0.70	0/521
25	S	0.58	0/1133	0.63	0/1516
26	T	0.67	0/903	0.66	0/1216
27	U	0.76	0/1746	0.66	0/2338
28	V	0.68	0/1682	0.64	0/2250
29	W	0.69	0/858	0.66	0/1131
30	X	0.64	0/718	0.63	0/953
31	Y	0.71	0/1268	0.65	0/1701

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.74	1/1537 (0.1%)	0.71	0/2052
33	a	0.59	0/1297	0.63	0/1716
34	b	0.72	0/1493	0.61	0/2003
35	c	0.65	0/1326	0.66	0/1770
36	d	0.47	0/839	0.73	1/1126 (0.1%)
37	e	0.62	0/987	0.64	0/1324
38	f	0.64	0/528	0.59	0/703
39	g	0.61	0/975	0.64	0/1312
40	h	0.69	0/1110	0.65	0/1477
41	i	0.63	0/1130	0.61	0/1507
42	l	0.68	0/1017	0.62	0/1364
43	m	0.73	1/1936 (0.1%)	0.73	1/2596 (0.0%)
44	r	1.43	3/2428 (0.1%)	0.91	4/3252 (0.1%)
45	t	0.74	0/1071	0.65	0/1429
46	u	0.76	0/895	0.72	1/1198 (0.1%)
47	v	0.55	0/1935	0.71	2/2596 (0.1%)
48	w	0.69	1/1916 (0.1%)	0.68	0/2553
All	All	1.36	76/147402 (0.1%)	1.17	1121/216838 (0.5%)

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
3	3	0	4
7	A	0	3
11	E	0	1
13	G	0	1
15	I	0	2
18	L	0	1
20	N	0	1
34	b	0	1
35	c	0	3
42	l	0	2
43	m	0	1
45	t	0	2
46	u	0	2
47	v	0	1
All	All	0	25

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4280	A	N3-C4	148.71	2.24	1.34
2	2	4280	A	C6-N1	129.88	2.26	1.35
2	2	4280	A	N1-C2	98.61	2.23	1.34
2	2	4280	A	C2-N3	95.13	2.19	1.33
2	2	4280	A	C5-C4	93.78	2.04	1.38

The worst 5 of 1121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4280	A	N1-C2-N3	-64.44	97.08	129.30
2	2	4280	A	C2-N3-C4	49.77	135.48	110.60
2	2	4280	A	N7-C8-N9	28.07	127.84	113.80
2	2	4280	A	C6-N1-C2	27.68	135.21	118.60
44	r	23	ARG	CD-NE-CZ	27.05	161.47	123.60

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	324	VAL	Peptide
3	3	330	ALA	Peptide
3	3	338	LYS	Peptide
3	3	341	THR	Peptide
7	A	46	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [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	0	62/477 (13%)	58 (94%)	3 (5%)	1 (2%)	8	31
3	3	252/534 (47%)	220 (87%)	32 (13%)	0	100	100
5	6	218/245 (89%)	205 (94%)	13 (6%)	0	100	100
7	A	210/217 (97%)	179 (85%)	29 (14%)	2 (1%)	13	42
8	B	401/403 (100%)	380 (95%)	21 (5%)	0	100	100
9	C	93/159 (58%)	88 (95%)	5 (5%)	0	100	100
10	D	354/427 (83%)	327 (92%)	26 (7%)	1 (0%)	37	68
11	E	92/115 (80%)	87 (95%)	5 (5%)	0	100	100
12	F	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
13	G	239/266 (90%)	225 (94%)	14 (6%)	0	100	100
14	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
15	I	188/192 (98%)	173 (92%)	14 (7%)	1 (0%)	25	58
16	J	150/214 (70%)	135 (90%)	15 (10%)	0	100	100
17	K	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
18	L	145/148 (98%)	133 (92%)	11 (8%)	1 (1%)	19	51
19	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
20	N	174/178 (98%)	143 (82%)	29 (17%)	2 (1%)	12	39
21	O	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
22	P	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
23	Q	201/211 (95%)	184 (92%)	16 (8%)	1 (0%)	25	58
24	R	45/128 (35%)	38 (84%)	7 (16%)	0	100	100
25	S	133/215 (62%)	126 (95%)	7 (5%)	0	100	100
26	T	105/125 (84%)	98 (93%)	7 (7%)	0	100	100
27	U	201/204 (98%)	191 (95%)	9 (4%)	1 (0%)	25	58
28	V	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
29	W	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
30	X	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
31	Y	151/184 (82%)	140 (93%)	11 (7%)	0	100	100
32	Z	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
33	a	151/196 (77%)	145 (96%)	6 (4%)	0	100	100
34	b	173/176 (98%)	163 (94%)	9 (5%)	1 (1%)	22	53
35	c	157/160 (98%)	146 (93%)	11 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	d	99/128 (77%)	87 (88%)	12 (12%)	0	100	100
37	e	128/140 (91%)	120 (94%)	8 (6%)	0	100	100
38	f	59/157 (38%)	57 (97%)	2 (3%)	0	100	100
39	g	115/156 (74%)	108 (94%)	7 (6%)	0	100	100
40	h	129/145 (89%)	120 (93%)	9 (7%)	0	100	100
41	i	133/136 (98%)	115 (86%)	18 (14%)	0	100	100
42	l	123/137 (90%)	111 (90%)	12 (10%)	0	100	100
43	m	246/257 (96%)	221 (90%)	24 (10%)	1 (0%)	30	63
44	r	291/297 (98%)	267 (92%)	24 (8%)	0	100	100
45	t	126/135 (93%)	116 (92%)	10 (8%)	0	100	100
46	u	107/110 (97%)	100 (94%)	5 (5%)	2 (2%)	6	27
47	v	231/288 (80%)	209 (90%)	20 (9%)	2 (1%)	14	45
48	w	224/248 (90%)	208 (93%)	16 (7%)	0	100	100
All	All	7011/8660 (81%)	6475 (92%)	520 (7%)	16 (0%)	45	74

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	171	HIS
15	I	176	LEU
7	A	169	VAL
46	u	80	ASN
47	v	179	LEU

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	
1	0	58/404 (14%)	58 (100%)	0	100	100
3	3	234/485 (48%)	229 (98%)	5 (2%)	48	72
5	6	190/213 (89%)	189 (100%)	1 (0%)	86	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	A	191/196 (97%)	188 (98%)	3 (2%)	58	79
8	B	349/349 (100%)	346 (99%)	3 (1%)	75	88
9	C	80/126 (64%)	80 (100%)	0	100	100
10	D	298/348 (86%)	293 (98%)	5 (2%)	56	78
11	E	79/97 (81%)	78 (99%)	1 (1%)	65	82
12	F	98/100 (98%)	97 (99%)	1 (1%)	73	86
13	G	203/223 (91%)	202 (100%)	1 (0%)	86	92
14	H	109/110 (99%)	108 (99%)	1 (1%)	75	88
15	I	169/171 (99%)	168 (99%)	1 (1%)	84	91
16	J	133/181 (74%)	133 (100%)	0	100	100
17	K	86/89 (97%)	85 (99%)	1 (1%)	67	83
18	L	120/121 (99%)	120 (100%)	0	100	100
19	M	73/80 (91%)	72 (99%)	1 (1%)	62	81
20	N	148/149 (99%)	141 (95%)	7 (5%)	22	52
21	O	64/65 (98%)	64 (100%)	0	100	100
22	P	47/48 (98%)	47 (100%)	0	100	100
23	Q	169/177 (96%)	168 (99%)	1 (1%)	84	91
24	R	43/116 (37%)	41 (95%)	2 (5%)	22	52
25	S	115/161 (71%)	113 (98%)	2 (2%)	56	78
26	T	98/110 (89%)	96 (98%)	2 (2%)	50	74
27	U	171/172 (99%)	168 (98%)	3 (2%)	54	76
28	V	173/174 (99%)	171 (99%)	2 (1%)	67	83
29	W	91/94 (97%)	91 (100%)	0	100	100
30	X	74/75 (99%)	74 (100%)	0	100	100
31	Y	134/163 (82%)	133 (99%)	1 (1%)	81	90
32	Z	164/165 (99%)	161 (98%)	3 (2%)	54	76
33	a	137/175 (78%)	136 (99%)	1 (1%)	81	90
34	b	156/157 (99%)	155 (99%)	1 (1%)	84	91
35	c	139/140 (99%)	138 (99%)	1 (1%)	81	90
36	d	91/115 (79%)	88 (97%)	3 (3%)	33	62
37	e	100/107 (94%)	99 (99%)	1 (1%)	73	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	f	54/126 (43%)	54 (100%)	0	100	100
39	g	105/133 (79%)	103 (98%)	2 (2%)	52	75
40	h	122/135 (90%)	117 (96%)	5 (4%)	26	57
41	i	117/118 (99%)	116 (99%)	1 (1%)	75	88
42	l	109/121 (90%)	105 (96%)	4 (4%)	29	59
43	m	190/199 (96%)	185 (97%)	5 (3%)	41	68
44	r	246/250 (98%)	245 (100%)	1 (0%)	89	94
45	t	114/121 (94%)	114 (100%)	0	100	100
46	u	88/89 (99%)	88 (100%)	0	100	100
47	v	208/252 (82%)	202 (97%)	6 (3%)	37	65
48	w	195/215 (91%)	195 (100%)	0	100	100
All	All	6132/7415 (83%)	6054 (99%)	78 (1%)	64	82

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	h	55	VAL
44	r	217	ASP
40	h	78	TYR
42	l	105	ASP
47	v	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
20	N	98	ASN
41	i	40	HIS
27	U	196	ASN
39	g	151	ASN
44	r	225	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	3489/5070 (68%)	896 (25%)	27 (0%)
4	5	119/120 (99%)	18 (15%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	8	155/156 (99%)	24 (15%)	0
All	All	3763/5346 (70%)	938 (24%)	27 (0%)

5 of 938 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	2	G
2	2	13	U
2	2	21	G
2	2	30	C
2	2	39	A

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	2587	A
2	2	3614	G
2	2	4699	U
2	2	2760	G
2	2	3673	C

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

99 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	$\# Z > 2$
2	A2M	2	1534	49,2	18,25,26	4.17	8 (44%)	18,36,39	2.98	3 (16%)
2	E7G	2	2297	2	24,27,28	3.40	11 (45%)	30,40,43	2.25	11 (36%)
2	OMG	2	3792	2	18,26,27	2.31	6 (33%)	19,38,41	1.48	4 (21%)
2	5MU	2	4083	2	19,22,23	4.49	7 (36%)	28,32,35	3.87	9 (32%)
2	A2M	2	4571	2	18,25,26	4.20	9 (50%)	18,36,39	2.79	3 (16%)
2	OMC	2	3869	2	19,22,23	2.63	7 (36%)	26,31,34	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	2	3887	2	19,22,23	2.70	7 (36%)	26,31,34	0.97	0
2	OMG	2	2364	2	18,26,27	2.17	6 (33%)	19,38,41	1.65	4 (21%)
2	A2M	2	3723	2,17	18,25,26	4.22	6 (33%)	18,36,39	3.21	3 (16%)
2	PSU	2	3729	2	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
2	B8K	2	4690	2	24,28,29	4.42	15 (62%)	30,42,45	2.86	13 (43%)
2	5MC	2	4447	2	18,22,23	3.20	7 (38%)	26,32,35	1.67	5 (19%)
2	B9B	2	2754	2,41	21,28,29	5.61	8 (38%)	23,40,43	2.47	6 (26%)
2	OMG	2	1883	2	18,26,27	2.17	6 (33%)	19,38,41	1.90	5 (26%)
2	A2M	2	2401	2	18,25,26	4.16	9 (50%)	18,36,39	2.76	3 (16%)
2	OMC	2	3701	49,2	19,22,23	2.49	7 (36%)	26,31,34	0.83	0
2	A2M	2	1524	2	18,25,26	4.04	7 (38%)	18,36,39	3.13	4 (22%)
2	A2M	2	1326	2	18,25,26	4.06	7 (38%)	18,36,39	3.46	3 (16%)
2	A2M	2	1871	2	18,25,26	4.24	8 (44%)	18,36,39	2.99	4 (22%)
2	PSU	2	4636	2	18,21,22	1.27	3 (16%)	22,30,33	2.21	6 (27%)
2	1MA	2	1322	49,2	16,25,26	3.51	5 (31%)	18,37,40	1.86	3 (16%)
2	OMC	2	2861	2	19,22,23	2.75	7 (36%)	26,31,34	0.75	1 (3%)
2	OMC	2	2365	49,2	19,22,23	2.62	7 (36%)	26,31,34	0.86	1 (3%)
2	B8W	2	4129	2	18,26,27	6.07	8 (44%)	21,38,41	2.91	10 (47%)
2	PSU	2	4442	2	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
2	B8W	2	2380	2	18,26,27	6.11	8 (44%)	21,38,41	2.38	7 (33%)
2	MHG	2	4371	2	29,32,33	3.62	12 (41%)	34,46,49	2.59	12 (35%)
2	2MG	2	1517	2	18,26,27	2.13	6 (33%)	16,38,41	1.85	5 (31%)
2	P4U	2	1348	2	21,24,25	3.33	8 (38%)	27,33,36	1.13	1 (3%)
2	BGH	2	3899	2	25,29,30	3.97	16 (64%)	31,43,46	2.38	13 (41%)
2	I4U	2	1659	49,2	21,24,25	4.49	15 (71%)	27,34,37	1.80	7 (25%)
2	PSU	2	1677	2	18,21,22	1.40	3 (16%)	22,30,33	2.06	5 (22%)
2	OMG	2	4637	2	18,26,27	2.23	6 (33%)	19,38,41	1.59	4 (21%)
2	5MC	2	4335	2	18,22,23	3.18	7 (38%)	26,32,35	1.27	1 (3%)
2	PSU	2	4531	2	18,21,22	0.96	1 (5%)	22,30,33	1.77	4 (18%)
2	A2M	2	4523	49,2	18,25,26	3.99	8 (44%)	18,36,39	3.19	5 (27%)
2	OMC	2	3909	2	19,22,23	2.85	8 (42%)	26,31,34	1.46	4 (15%)
2	PSU	2	4403	2	18,21,22	1.05	1 (5%)	22,30,33	1.89	5 (22%)
2	PSU	2	4293	2	18,21,22	1.21	2 (11%)	22,30,33	1.94	4 (18%)
2	OMC	2	2422	49,2	19,22,23	2.69	7 (36%)	26,31,34	1.03	1 (3%)
2	B8W	2	4185	2	18,26,27	6.41	8 (44%)	21,38,41	2.52	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B8T	2	4671	2	19,22,23	3.13	8 (42%)	26,31,34	1.06	2 (7%)
2	P7G	2	3880	2	24,28,29	3.97	11 (45%)	27,41,44	2.12	3 (11%)
2	B9B	2	237	2	21,28,29	5.67	9 (42%)	23,40,43	2.41	6 (26%)
2	7MG	2	2522	2,12	22,26,27	3.13	10 (45%)	29,39,42	2.07	10 (34%)
2	B8H	2	1860	2	19,22,23	6.81	7 (36%)	22,32,35	2.48	5 (22%)
2	OMG	2	373	2,19	18,26,27	2.25	7 (38%)	19,38,41	1.76	5 (26%)
2	I4U	2	4194	2	21,24,25	4.65	16 (76%)	27,34,37	1.63	7 (25%)
2	B8T	2	4483	2	19,22,23	3.39	8 (42%)	26,31,34	0.87	2 (7%)
2	OMG	2	1316	49,2	18,26,27	2.24	6 (33%)	19,38,41	1.81	4 (21%)
2	PSU	2	2508	2	18,21,22	1.09	2 (11%)	22,30,33	1.86	4 (18%)
2	A2M	2	3718	2	18,25,26	4.25	7 (38%)	18,36,39	2.99	3 (16%)
2	UR3	2	4597	2	19,22,23	2.53	6 (31%)	26,32,35	1.32	4 (15%)
2	P7G	2	1909	2	24,28,29	4.18	11 (45%)	27,41,44	1.91	5 (18%)
2	A2M	2	3867	2	18,25,26	3.98	6 (33%)	18,36,39	2.97	4 (22%)
2	OMG	2	1625	49,2	18,26,27	2.25	7 (38%)	19,38,41	1.53	4 (21%)
2	OMG	2	4870	2	18,26,27	2.35	8 (44%)	19,38,41	1.61	4 (21%)
2	2MG	2	729	2,34	18,26,27	2.37	6 (33%)	16,38,41	1.63	3 (18%)
2	7MG	2	4550	2	22,26,27	2.99	10 (45%)	29,39,42	1.96	9 (31%)
2	OMG	2	2050	2	18,26,27	2.18	5 (27%)	19,38,41	1.63	5 (26%)
2	OMC	2	4536	2	19,22,23	2.60	7 (36%)	26,31,34	0.99	0
2	2MG	2	978	2	18,26,27	2.35	7 (38%)	16,38,41	1.42	4 (25%)
2	B8H	2	4296	2	19,22,23	6.90	6 (31%)	22,32,35	2.50	5 (22%)
2	6MZ	2	4220	2	18,25,26	1.92	4 (22%)	16,36,39	3.52	3 (18%)
2	OMG	2	4370	2,29	18,26,27	2.28	7 (38%)	19,38,41	1.63	5 (26%)
2	UR3	2	1866	2	19,22,23	2.77	5 (26%)	26,32,35	1.68	5 (19%)
2	OMG	2	2773	2	18,26,27	2.34	8 (44%)	19,38,41	1.66	4 (21%)
2	PSU	2	4450	49,2	18,21,22	1.06	2 (11%)	22,30,33	1.91	4 (18%)
2	B9H	2	2786	49,2	20,25,26	2.68	5 (25%)	22,35,38	3.46	7 (31%)
2	B9B	2	1574	2	21,28,29	5.63	9 (42%)	23,40,43	2.31	4 (17%)
2	PSU	2	4628	2	18,21,22	1.15	2 (11%)	22,30,33	1.89	5 (22%)
2	OMG	2	4623	2	18,26,27	2.22	6 (33%)	19,38,41	1.67	4 (21%)
2	OMU	2	4620	2	19,22,23	2.64	7 (36%)	26,31,34	1.84	5 (19%)
2	PSU	2	1582	2	18,21,22	1.18	3 (16%)	22,30,33	1.78	3 (13%)
2	OMG	2	1522	2	18,26,27	2.22	7 (38%)	19,38,41	1.51	3 (15%)
2	B8Q	2	1456	2	17,22,23	2.79	5 (29%)	22,32,35	2.35	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	2	2363	49,2	18,25,26	4.09	9 (50%)	18,36,39	3.03	3 (16%)
2	B8K	2	3897	2	24,28,29	4.12	16 (66%)	30,42,45	2.59	13 (43%)
2	B8W	2	4472	2	18,26,27	6.21	8 (44%)	21,38,41	2.50	8 (38%)
2	A2M	2	398	2	18,25,26	4.22	7 (38%)	18,36,39	2.96	3 (16%)
2	OMG	2	4196	49,2	18,26,27	2.33	8 (44%)	19,38,41	1.46	3 (15%)
2	PSU	2	3715	2	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
2	UR3	2	4530	2	19,22,23	2.84	6 (31%)	26,32,35	1.55	4 (15%)
2	E6G	2	4355	2	20,27,28	5.95	9 (45%)	22,39,42	2.74	9 (40%)
2	M7A	2	4564	2	20,25,26	1.91	4 (20%)	28,37,40	3.95	7 (25%)
2	5MC	2	3782	49,2	18,22,23	3.12	7 (38%)	26,32,35	1.22	3 (11%)
2	E7G	2	1797	2	24,27,28	3.57	11 (45%)	30,40,43	2.27	9 (30%)
2	A2M	2	3825	2	18,25,26	4.08	7 (38%)	18,36,39	3.04	3 (16%)
2	PSU	2	4500	2	18,21,22	1.19	3 (16%)	22,30,33	2.00	5 (22%)
2	2MG	2	4872	28,2,25	18,26,27	2.76	7 (38%)	16,38,41	1.62	3 (18%)
2	OMC	2	2804	2	19,22,23	2.56	7 (36%)	26,31,34	0.76	0
2	OMG	2	2424	49,2	18,26,27	2.27	7 (38%)	19,38,41	1.47	3 (15%)
2	7MG	2	1605	2	22,26,27	3.12	10 (45%)	29,39,42	2.08	8 (27%)
2	OMU	2	4306	2	19,22,23	2.68	7 (36%)	26,31,34	1.85	5 (19%)
2	A2M	2	3785	2	18,25,26	3.90	9 (50%)	18,36,39	3.04	3 (16%)
2	PSU	2	1683	2	18,21,22	1.24	2 (11%)	22,30,33	1.79	5 (22%)
2	OMG	2	4494	2	18,26,27	2.29	6 (33%)	19,38,41	1.57	5 (26%)
2	B8W	2	4529	49,2,3	18,26,27	6.03	7 (38%)	21,38,41	3.20	9 (42%)
2	1MA	2	4415	2	16,25,26	3.97	4 (25%)	18,37,40	1.72	3 (16%)

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
2	A2M	2	1534	49,2	-	2/5/27/28	0/3/3/3
2	E7G	2	2297	2	-	1/9/39/40	0/3/3/3
2	OMG	2	3792	2	-	0/5/27/28	0/3/3/3
2	5MU	2	4083	2	-	0/7/25/26	0/2/2/2
2	A2M	2	4571	2	-	0/5/27/28	0/3/3/3
2	OMC	2	3869	2	-	0/9/27/28	0/2/2/2
2	OMC	2	3887	2	-	1/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	2	2364	2	-	2/5/27/28	0/3/3/3
2	A2M	2	3723	2,17	-	0/5/27/28	0/3/3/3
2	PSU	2	3729	2	-	2/7/25/26	0/2/2/2
2	B8K	2	4690	2	-	0/11/41/42	0/3/3/3
2	5MC	2	4447	2	-	3/7/25/26	0/2/2/2
2	B9B	2	2754	2,41	-	4/7/29/30	0/3/3/3
2	OMG	2	1883	2	-	2/5/27/28	0/3/3/3
2	A2M	2	2401	2	-	2/5/27/28	0/3/3/3
2	OMC	2	3701	49,2	-	4/9/27/28	0/2/2/2
2	A2M	2	1524	2	-	0/5/27/28	0/3/3/3
2	A2M	2	1326	2	-	0/5/27/28	0/3/3/3
2	A2M	2	1871	2	-	0/5/27/28	0/3/3/3
2	PSU	2	4636	2	-	5/7/25/26	0/2/2/2
2	1MA	2	1322	49,2	-	0/3/25/26	0/3/3/3
2	OMC	2	2861	2	-	1/9/27/28	0/2/2/2
2	OMC	2	2365	49,2	-	0/9/27/28	0/2/2/2
2	B8W	2	4129	2	-	2/5/27/28	0/3/3/3
2	PSU	2	4442	2	-	0/7/25/26	0/2/2/2
2	B8W	2	2380	2	-	4/5/27/28	0/3/3/3
2	MHG	2	4371	2	-	7/16/46/47	0/3/3/3
2	2MG	2	1517	2	-	0/5/27/28	0/3/3/3
2	P4U	2	1348	2	-	2/10/29/30	0/2/2/2
2	BGH	2	3899	2	-	2/13/43/44	0/3/3/3
2	I4U	2	1659	49,2	-	1/9/29/30	0/2/2/2
2	PSU	2	1677	2	-	5/7/25/26	0/2/2/2
2	OMG	2	4637	2	-	2/5/27/28	0/3/3/3
2	5MC	2	4335	2	-	0/7/25/26	0/2/2/2
2	PSU	2	4531	2	-	0/7/25/26	0/2/2/2
2	A2M	2	4523	49,2	-	0/5/27/28	0/3/3/3
2	OMC	2	3909	2	-	1/9/27/28	0/2/2/2
2	PSU	2	4403	2	-	2/7/25/26	0/2/2/2
2	PSU	2	4293	2	-	0/7/25/26	0/2/2/2
2	OMC	2	2422	49,2	-	2/9/27/28	0/2/2/2
2	B8W	2	4185	2	-	3/5/27/28	0/3/3/3
2	B8T	2	4671	2	-	0/7/27/28	0/2/2/2
2	P7G	2	3880	2	-	5/10/40/41	0/3/3/3
2	B9B	2	237	2	-	6/7/29/30	0/3/3/3
2	7MG	2	2522	2,12	-	0/7/37/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8H	2	1860	2	-	2/7/25/26	0/2/2/2
2	OMG	2	373	2,19	-	0/5/27/28	0/3/3/3
2	I4U	2	4194	2	-	4/9/29/30	0/2/2/2
2	B8T	2	4483	2	-	0/7/27/28	0/2/2/2
2	OMG	2	1316	49,2	-	2/5/27/28	0/3/3/3
2	PSU	2	2508	2	-	0/7/25/26	0/2/2/2
2	A2M	2	3718	2	-	0/5/27/28	0/3/3/3
2	UR3	2	4597	2	-	0/7/25/26	0/2/2/2
2	P7G	2	1909	2	-	1/10/40/41	0/3/3/3
2	A2M	2	3867	2	-	2/5/27/28	0/3/3/3
2	OMG	2	1625	49,2	-	2/5/27/28	0/3/3/3
2	OMG	2	4870	2	-	3/5/27/28	0/3/3/3
2	2MG	2	729	2,34	-	1/5/27/28	0/3/3/3
2	7MG	2	4550	2	-	0/7/37/38	0/3/3/3
2	OMG	2	2050	2	-	0/5/27/28	0/3/3/3
2	OMC	2	4536	2	-	1/9/27/28	0/2/2/2
2	2MG	2	978	2	-	0/5/27/28	0/3/3/3
2	B8H	2	4296	2	-	4/7/25/26	0/2/2/2
2	6MZ	2	4220	2	-	0/5/27/28	0/3/3/3
2	OMG	2	4370	2,29	-	0/5/27/28	0/3/3/3
2	UR3	2	1866	2	-	0/7/25/26	0/2/2/2
2	OMG	2	2773	2	-	1/5/27/28	0/3/3/3
2	PSU	2	4450	49,2	-	1/7/25/26	0/2/2/2
2	B9H	2	2786	49,2	-	2/12/47/48	0/2/2/2
2	B9B	2	1574	2	-	3/7/29/30	0/3/3/3
2	PSU	2	4628	2	-	0/7/25/26	0/2/2/2
2	OMG	2	4623	2	-	0/5/27/28	0/3/3/3
2	OMU	2	4620	2	-	0/9/27/28	0/2/2/2
2	PSU	2	1582	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1522	2	-	0/5/27/28	0/3/3/3
2	B8Q	2	1456	2	-	0/7/42/43	0/2/2/2
2	A2M	2	2363	49,2	-	0/5/27/28	0/3/3/3
2	B8K	2	3897	2	-	3/11/41/42	0/3/3/3
2	B8W	2	4472	2	-	2/5/27/28	0/3/3/3
2	A2M	2	398	2	-	2/5/27/28	0/3/3/3
2	OMG	2	4196	49,2	-	1/5/27/28	0/3/3/3
2	PSU	2	3715	2	-	0/7/25/26	0/2/2/2
2	UR3	2	4530	2	-	2/7/25/26	0/2/2/2
2	E6G	2	4355	2	-	4/6/28/29	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M7A	2	4564	2	-	0/7/37/38	0/3/3/3
2	5MC	2	3782	49,2	-	0/7/25/26	0/2/2/2
2	E7G	2	1797	2	-	3/9/39/40	0/3/3/3
2	A2M	2	3825	2	-	0/5/27/28	0/3/3/3
2	PSU	2	4500	2	-	5/7/25/26	0/2/2/2
2	2MG	2	4872	28,2,25	-	2/5/27/28	0/3/3/3
2	OMC	2	2804	2	-	0/9/27/28	0/2/2/2
2	OMG	2	2424	49,2	-	0/5/27/28	0/3/3/3
2	7MG	2	1605	2	-	0/7/37/38	0/3/3/3
2	OMU	2	4306	2	-	0/9/27/28	0/2/2/2
2	A2M	2	3785	2	-	2/5/27/28	0/3/3/3
2	PSU	2	1683	2	-	1/7/25/26	0/2/2/2
2	OMG	2	4494	2	-	1/5/27/28	0/3/3/3
2	B8W	2	4529	49,2,3	-	2/5/27/28	0/3/3/3
2	1MA	2	4415	2	-	2/3/25/26	0/3/3/3

The worst 5 of 691 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4185	B8W	O4'-C1'	17.66	1.65	1.41
2	2	4472	B8W	O4'-C1'	17.39	1.65	1.41
2	2	2380	B8W	O4'-C1'	17.36	1.65	1.41
2	2	4129	B8W	O4'-C1'	17.34	1.65	1.41
2	2	4296	B8H	C6-C5	-17.27	1.10	1.34

The worst 5 of 468 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4564	M7A	C5-C6-N6	13.21	146.30	123.74
2	2	4083	5MU	C5-C4-N3	12.42	125.91	115.31
2	2	4220	6MZ	C1'-N9-C4	-12.33	104.98	126.64
2	2	4564	M7A	N6-C6-N1	-11.53	93.09	118.35
2	2	2786	B9H	C31-N3-C2	10.39	130.20	117.21

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	237	B9B	C5-C6-O6-C61
2	2	237	B9B	N1-C6-O6-C61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	2	237	B9B	C3'-C4'-C5'-O5'
2	2	237	B9B	C62-C61-O6-C6
2	2	398	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 251 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

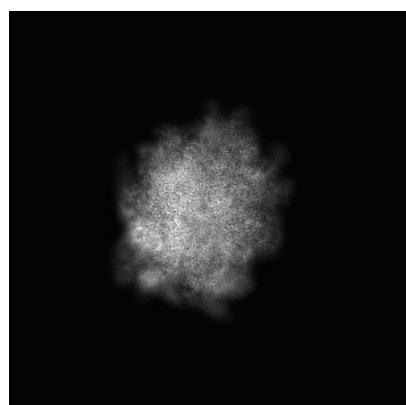
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0948. These allow visual inspection of the internal detail of the map and identification of artifacts.

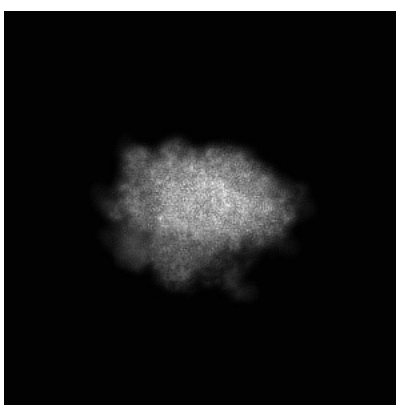
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

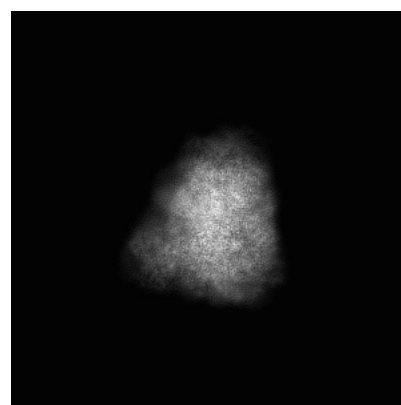
6.1.1 Primary map



X



Y

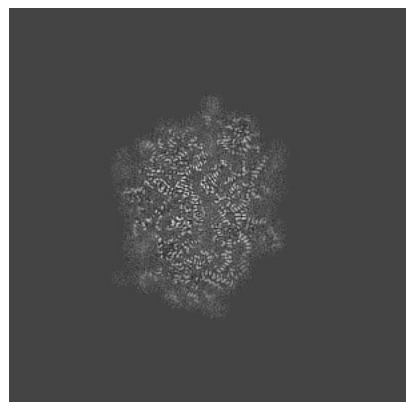


Z

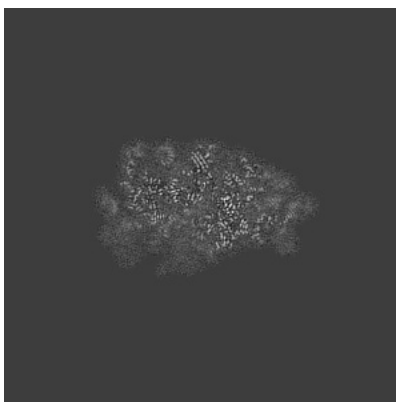
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

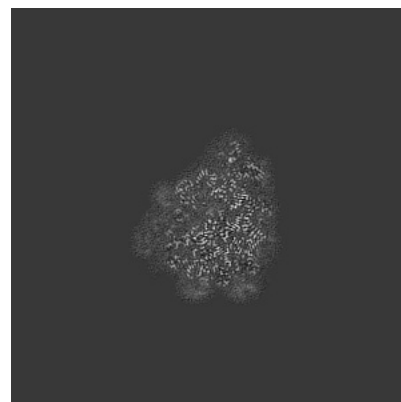
6.2.1 Primary map



X Index: 240



Y Index: 240

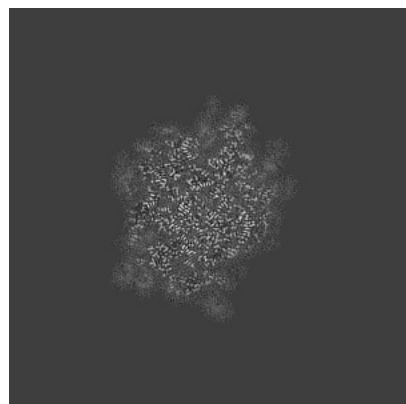


Z Index: 240

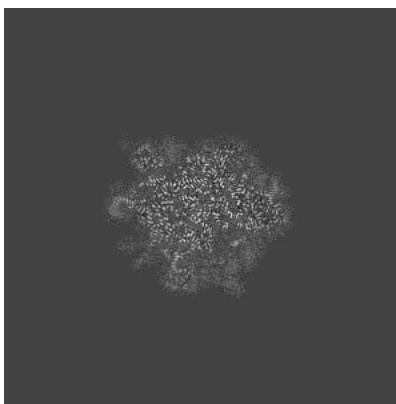
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

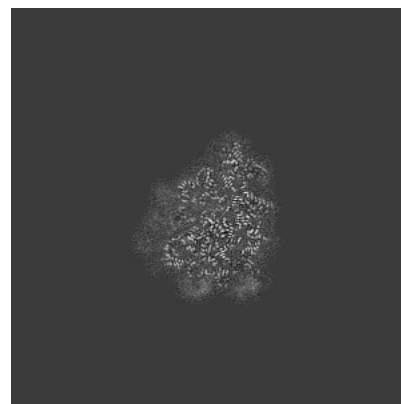
6.3.1 Primary map



X Index: 253



Y Index: 200

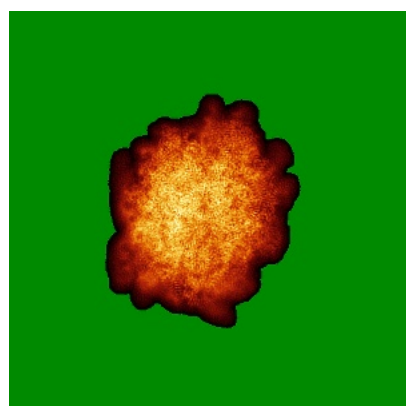


Z Index: 237

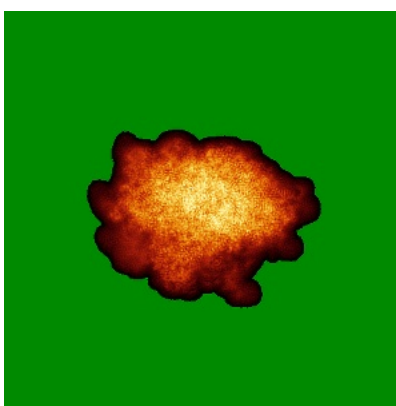
The images above show the largest variance slices of the map in three orthogonal directions.

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

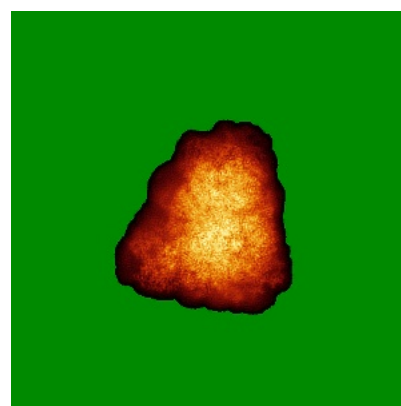
6.4.1 Primary map



X



Y

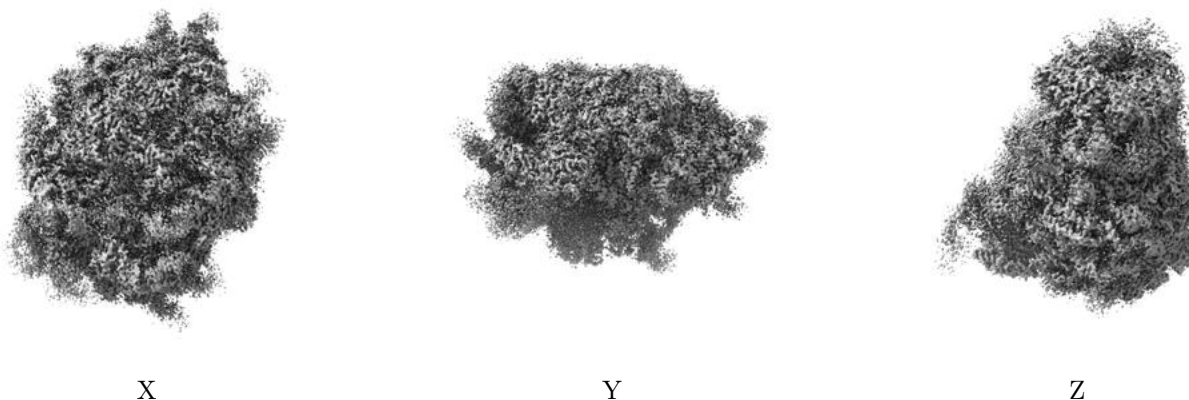


Z

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

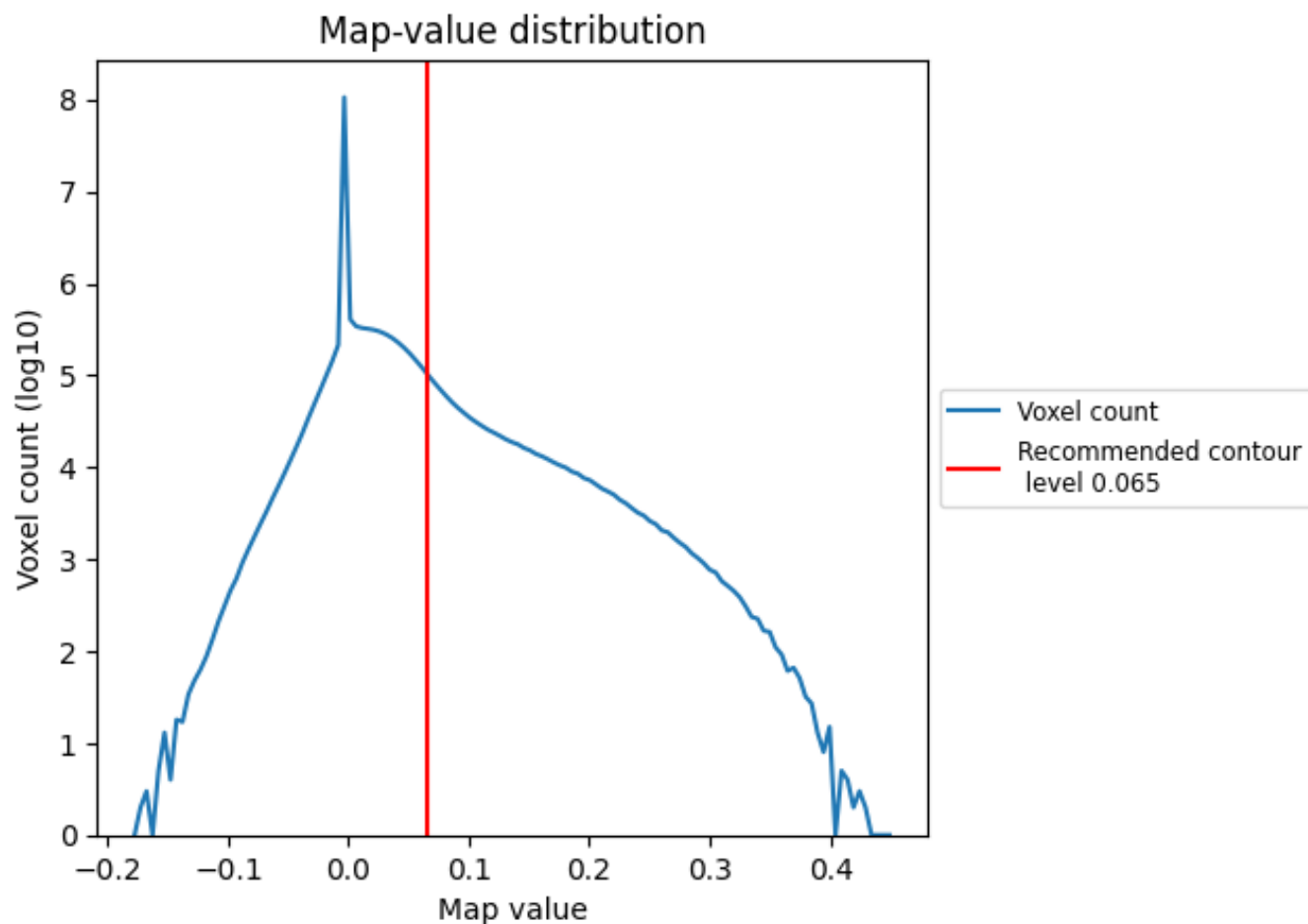
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

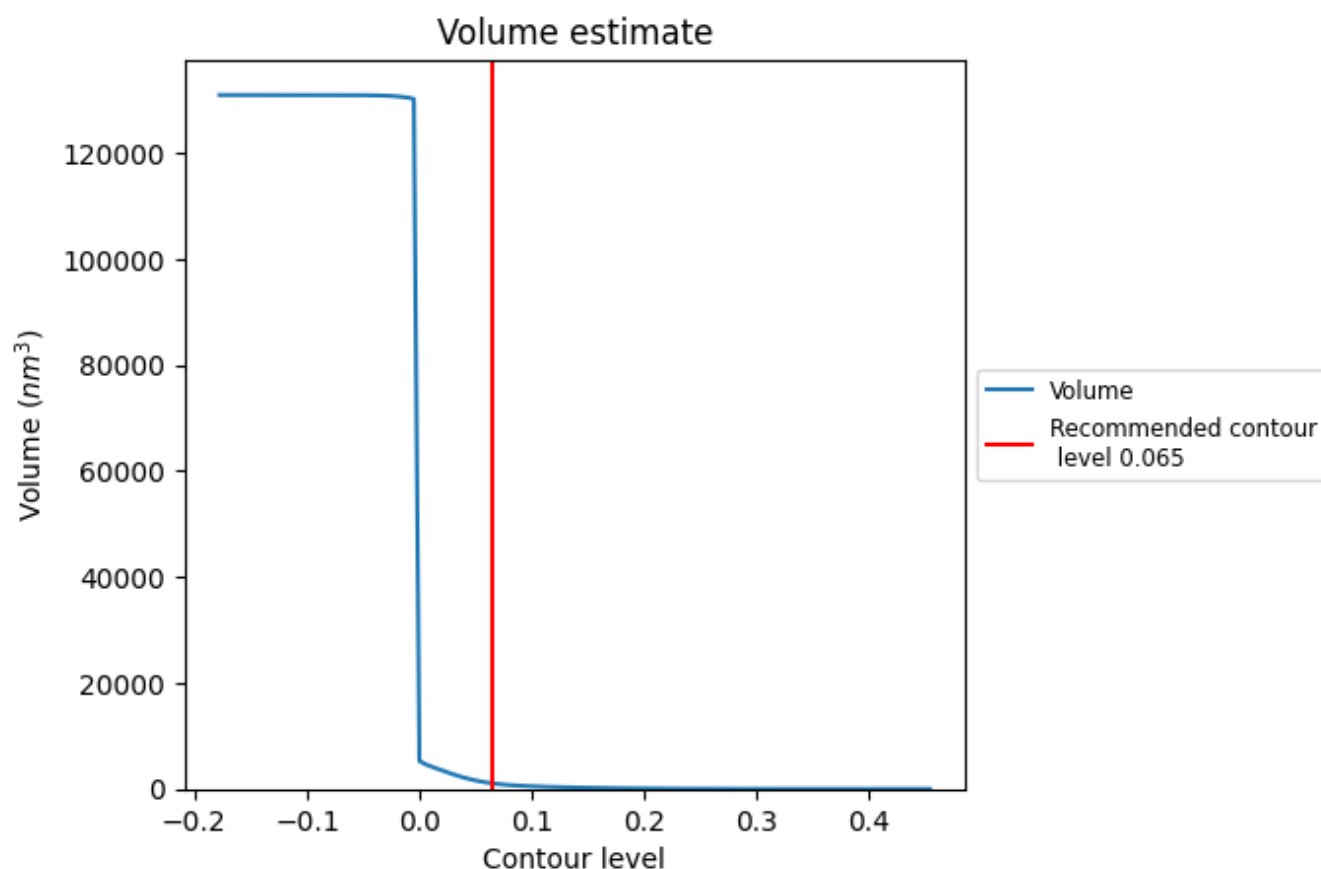
This section contains the results of statistical analysis of the map.

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.

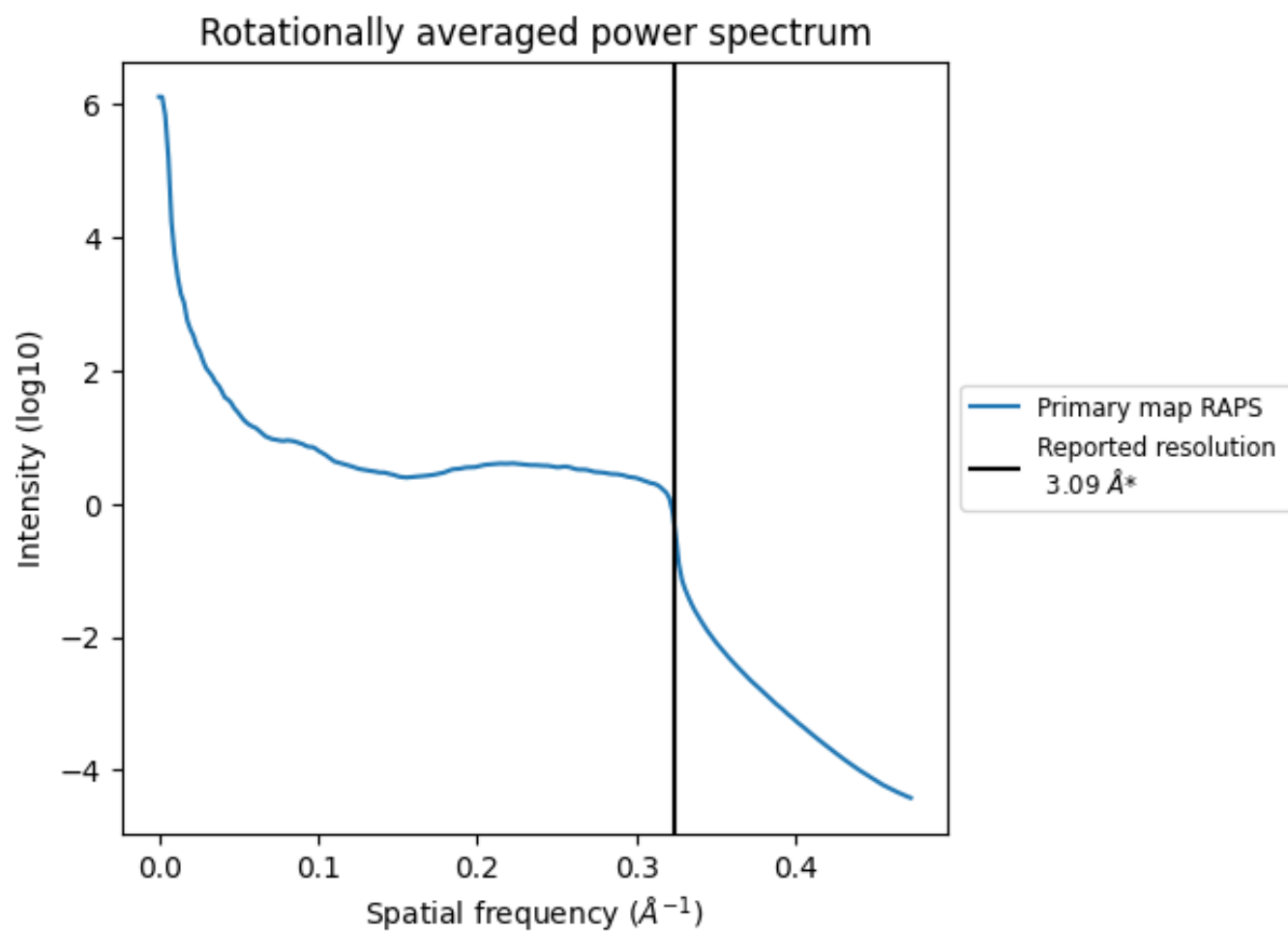
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1059 nm^3 ; this corresponds to an approximate mass of 957 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 0.324 Å⁻¹

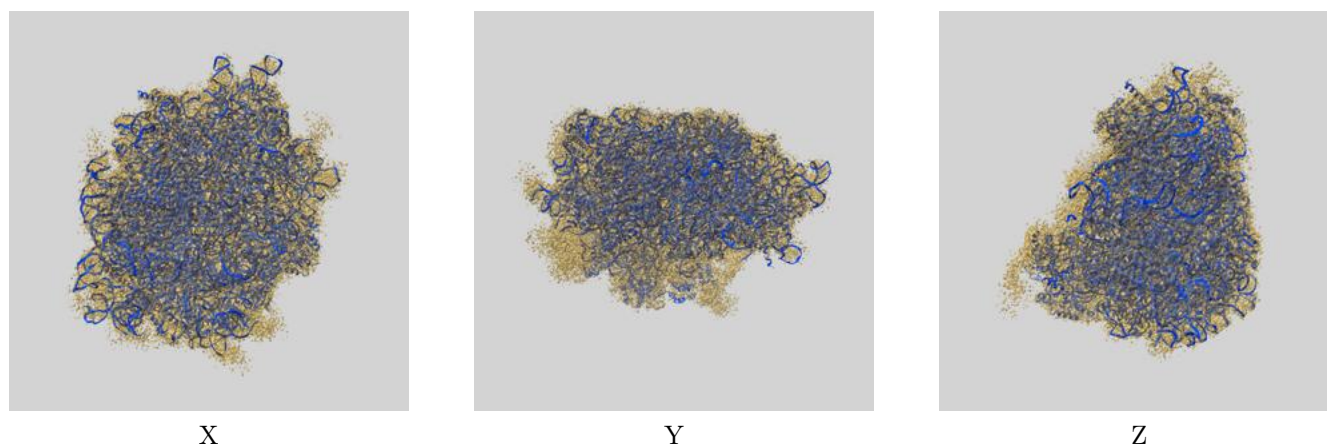
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

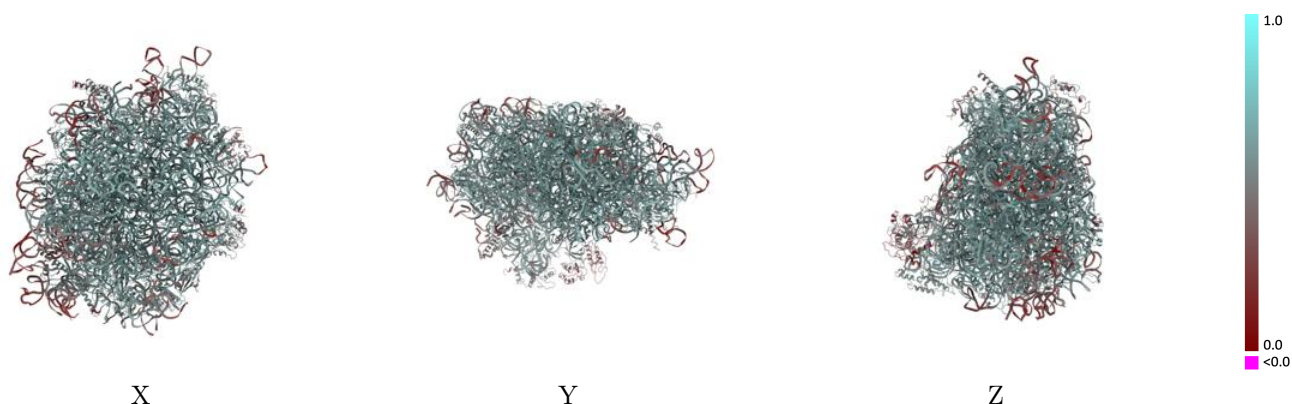
This section contains information regarding the fit between EMDB map EMD-0948 and PDB model 6LQM. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



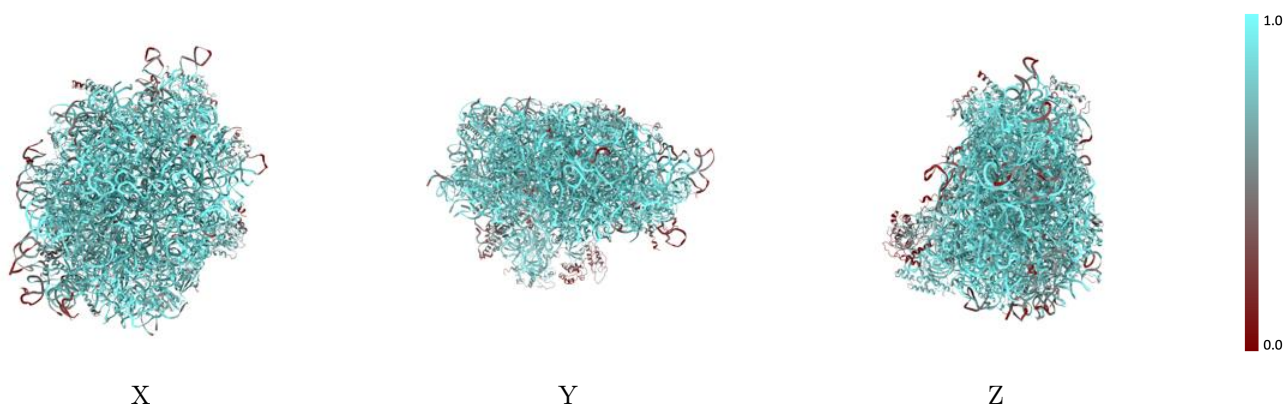
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



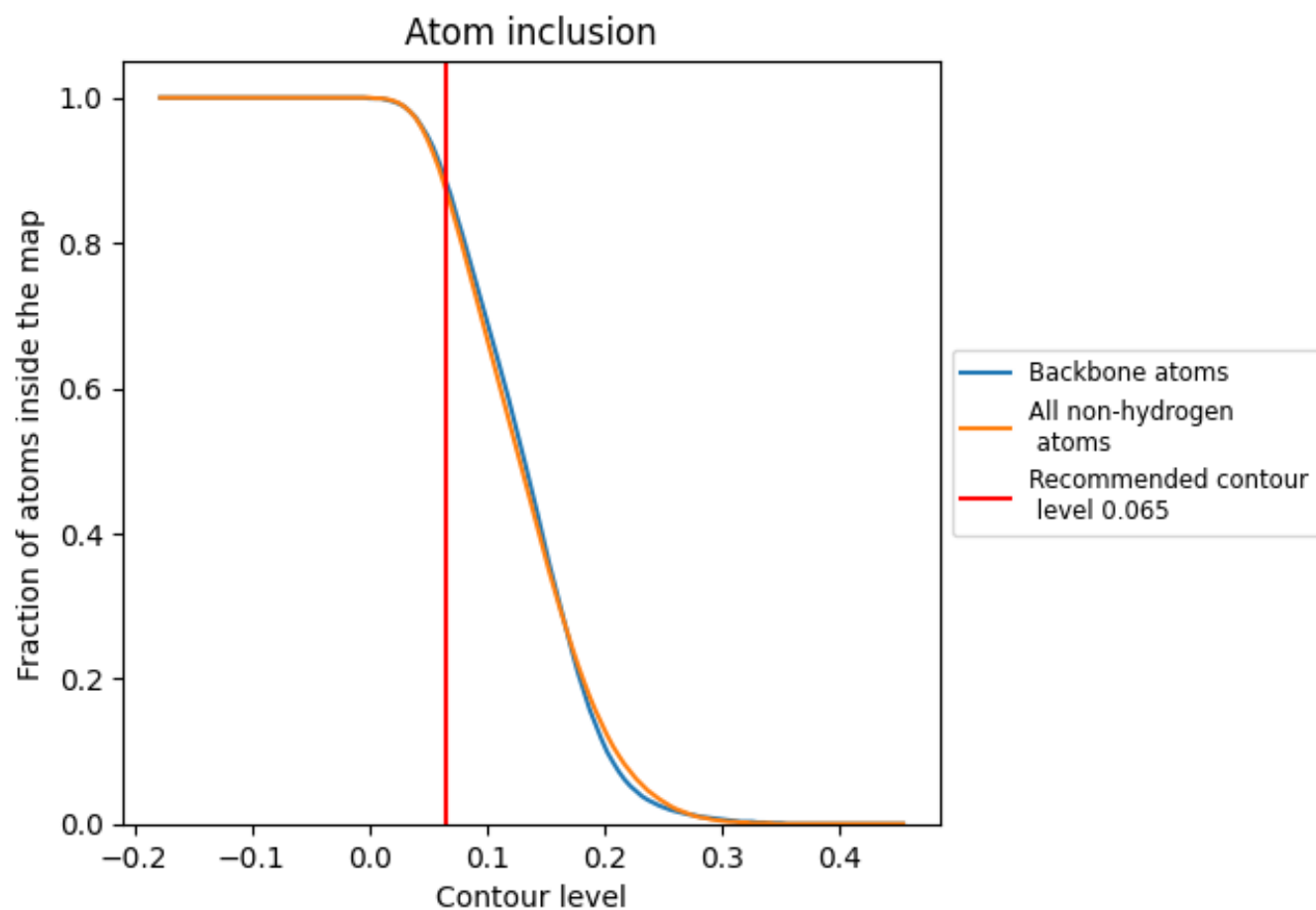
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5550
0	 0.6940	 0.4930
2	 0.8960	 0.5500
3	 0.7860	 0.5210
5	 0.9680	 0.5760
6	 0.6390	 0.5010
8	 0.9410	 0.5780
A	 0.2160	 0.2790
B	 0.8900	 0.5820
C	 0.8310	 0.5450
D	 0.9170	 0.5940
E	 0.7940	 0.5460
F	 0.8640	 0.5830
G	 0.7790	 0.5390
H	 0.8710	 0.5760
I	 0.8480	 0.5630
J	 0.6120	 0.5000
K	 0.8330	 0.5590
L	 0.9210	 0.6080
M	 0.9580	 0.6070
N	 0.6900	 0.4850
O	 0.7160	 0.5330
P	 0.9550	 0.5950
Q	 0.8780	 0.5790
R	 0.7610	 0.5280
S	 0.8930	 0.5770
T	 0.8480	 0.5760
U	 0.9720	 0.6150
V	 0.9150	 0.5950
W	 0.8820	 0.5730
X	 0.8610	 0.5810
Y	 0.9240	 0.6020
Z	 0.9520	 0.6100
a	 0.8660	 0.5700
b	 0.9420	 0.6010



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.8910	 0.5740
d	 0.6690	 0.4730
e	 0.9000	 0.5900
f	 0.8910	 0.5800
g	 0.8840	 0.5840
h	 0.8980	 0.5910
i	 0.8330	 0.5650
l	 0.9120	 0.5920
m	 0.9320	 0.6000
r	 0.7920	 0.5380
t	 0.9460	 0.6070
u	 0.9500	 0.6130
v	 0.7810	 0.5310
w	 0.9140	 0.5870