



# wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 01:25 PM EDT

PDB ID : 8FLB / pdb\_00008flb  
EMDB ID : EMD-29273  
Title : Human nuclear pre-60S ribosomal subunit (State K2)  
Authors : Vanden Broeck, A.; Klinge, S.  
Deposited on : 2022-12-21  
Resolution : 2.55 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

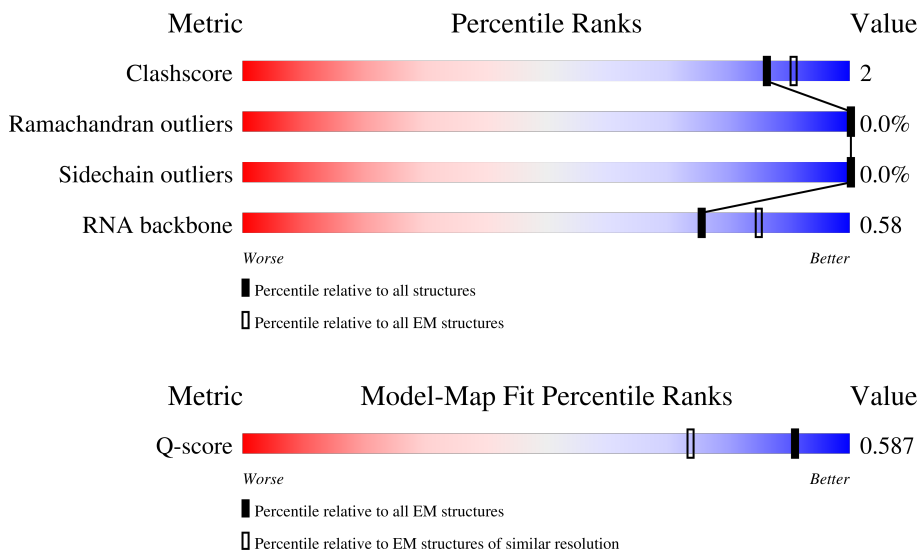
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7475 ( 2.05 - 3.05 )

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	BA	165	
2	L1	157	
3	L3	5070	

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Mol	Chain	Length	Quality of chain
4	L4	121	85% 13%
5	L5	178	89% 6% 6%
6	L6	211	8% 94% 5%
7	L7	203	95%
8	L8	215	60% 37%
9	L9	204	93% 6%
10	LA	184	78% 5% 17%
11	LB	188	95% 5%
12	LC	176	93% 7%
13	LD	196	74% 5% 21%
14	LE	160	92%
15	LF	128	73% 7% 20%
16	LG	140	98%
17	LH	156	89% 8%
18	LI	145	85% 8% 8%
19	LJ	136	89% 10%
20	LK	148	93% 6%
21	LL	137	86% 5% 9%
22	LM	159	9% 52% 5% 43%
23	LN	403	92% 7%
24	LO	115	6% 81% 17%
25	LP	125	82% 15%
26	LQ	135	90% 5% 5%
27	LR	117	90% 6%
28	LS	123	96%

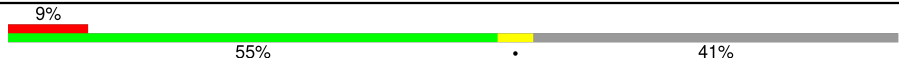
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Mol	Chain	Length	Quality of chain
29	LT	110	97%
30	LU	105	7% 90% 7%
31	LV	106	97%
32	LW	97	81% 7% 11%
33	LX	92	92% 7%
34	LY	70	6% 90% 9%
35	LZ	51	86% 12%
36	NK	129	14% 50% 48%
37	NL	478	52% 45%
38	NP	134	5% 71% 7% 22%
39	NR	203	69% 5% 25%
40	SA	427	78% 5% 16%
41	SB	297	88% 7%
42	SC	288	6% 67% 8% 25%
43	SD	248	87% 9%
44	SE	266	7% 82% 5% 13%
45	SF	257	88% 7% 5%
46	SG	192	91% 8%
47	SH	293	5% 28% 68%
48	SI	255	8% 87% 8%
49	SK	245	91% 9%
50	SM	588	64% 32%
51	SQ	239	17% 52% 47%
52	SR	634	7% 89% 6% 5%
53	SV	163	80% 6% 15%

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Mol	Chain	Length	Quality of chain
54	VB	99	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '9%', a green segment in the middle labeled '55%', and a grey segment on the right labeled '41%'. A small black dot is located on the green segment.</p>

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149034 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 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	BA	91	449	267	91	91	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L1	154	3278	1463	581	1080	154	0	0

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L3	3420	73423	32721	13453	23829	3420	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L4	120	2561	1141	456	844	120	0	0

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L5	168	1349	853	251	239	6	0	0

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L6	210	1701	1064	352	281	4	0	0

- Molecule 7 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L7	201	1650	1063	321	261	5	0	0

- Molecule 8 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L8	135	1111	713	213	178	7	0	0

- Molecule 9 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L9	203	1701	1072	359	266	4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L17.

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

- Molecule 11 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LB	187	1512	944	314	249	5	0	0

- Molecule 12 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LC	176	1461	930	284	236	11	0	0

- Molecule 13 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LD	154	1289	805	277	198	9	0	0

- Molecule 14 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LE	154	Total	C	N	O	S	0	0
			1264	803	246	210	5		

- Molecule 15 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LF	103	Total	C	N	O	S	0	0
			842	538	148	154	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LG	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 17 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LH	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 18 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LI	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 19 is a protein called 60S ribosomal protein L27.

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

- Molecule 20 is a protein called 60S ribosomal protein L27a.

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

- Molecule 21 is a protein called 60S ribosomal protein L28.

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

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LM	91	Total	C	N	O	S	0	0
			751	469	165	113	4		

- Molecule 23 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LN	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 24 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LO	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 25 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LP	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 26 is a protein called 60S ribosomal protein L32.

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

- Molecule 27 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LR	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 28 is a protein called 60S ribosomal protein L35.

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

- Molecule 29 is a protein called 60S ribosomal protein L35a.

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

- Molecule 30 is a protein called 60S ribosomal protein L36.

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

- Molecule 31 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LV	104	851	533	174	138	6	0	0

- Molecule 32 is a protein called 60S ribosomal protein L37.

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

- Molecule 33 is a protein called 60S ribosomal protein L37a.

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

- Molecule 34 is a protein called 60S ribosomal protein L38.

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

- Molecule 35 is a protein called 60S ribosomal protein L39.

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

- Molecule 36 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NK	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 37 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NL	263	Total	C	N	O	S	0	0
			2175	1347	433	393	2		

- Molecule 38 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NP	104	Total	C	N	O	S	0	0
			847	520	178	145	4		

- Molecule 39 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
39	NR	152	Total	C	N	O	P	S	1	0
			1299	809	249	235	1	5		

- Molecule 40 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 41 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SB	275	Total	C	N	O	S	0	0
			2243	1419	406	404	14		

- Molecule 42 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SC	217	Total	C	N	O	S	0	0
			1747	1124	332	287	4		

- Molecule 43 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SD	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 44 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SE	231	Total	C	N	O	S	1	0
			1869	1191	361	313	4		

- Molecule 45 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SF	245	Total	C	N	O	S	0	0
			1876	1177	383	310	6		

- Molecule 46 is a protein called 60S ribosomal protein L9.

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

- Molecule 47 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SH	93	Total	C	N	O	S	0	0
			773	501	130	139	3		

- Molecule 48 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SI	234	Total	C	N	O	S	3	0
			1952	1267	365	316	4		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 50 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SM	399	Total	C	N	O	S	0	0
			3278	2120	576	571	11		

- Molecule 51 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	SQ	127	Total	C	N	O	0	0
			650	388	132	130		

- Molecule 52 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SR	601	Total	C	N	O	S	0	0
			4932	3105	899	902	26		

- Molecule 53 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SV	139	Total	C	N	O	S	0	0
			1184	754	229	191	10		

- Molecule 54 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	VB	58	Total	C	N	O	S	0	0
			455	285	95	74	1		

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	L1	4	Total	Mg	0
			4	4	
55	L3	74	Total	Mg	0
			74	74	
55	L4	3	Total	Mg	0
			3	3	

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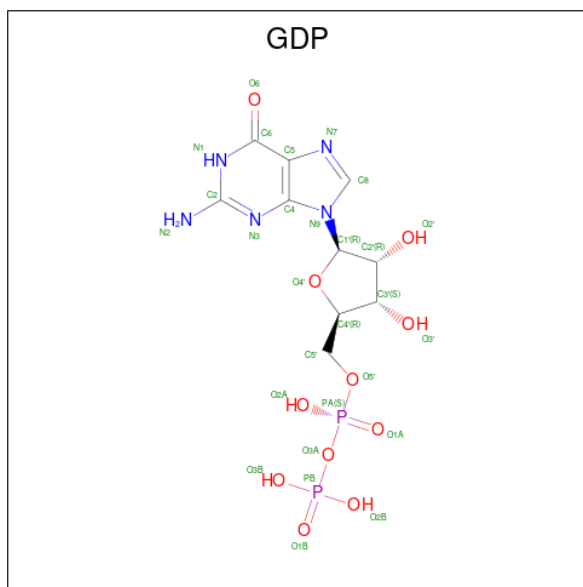
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Mol	Chain	Residues	Atoms		AltConf
55	LG	1	Total 1	Mg 1	0
55	LN	1	Total 1	Mg 1	0
55	LQ	1	Total 1	Mg 1	0
55	LR	1	Total 1	Mg 1	0
55	LT	1	Total 1	Mg 1	0
55	SF	1	Total 1	Mg 1	0
55	SR	1	Total 1	Mg 1	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	LR	1	Total 1	Zn 1	0
56	LV	1	Total 1	Zn 1	0
56	LW	1	Total 1	Zn 1	0
56	LX	1	Total 1	Zn 1	0
56	NP	1	Total 1	Zn 1	0
56	SV	1	Total 1	Zn 1	0

- Molecule 57 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	SR	1	28	10	5	11	2	0

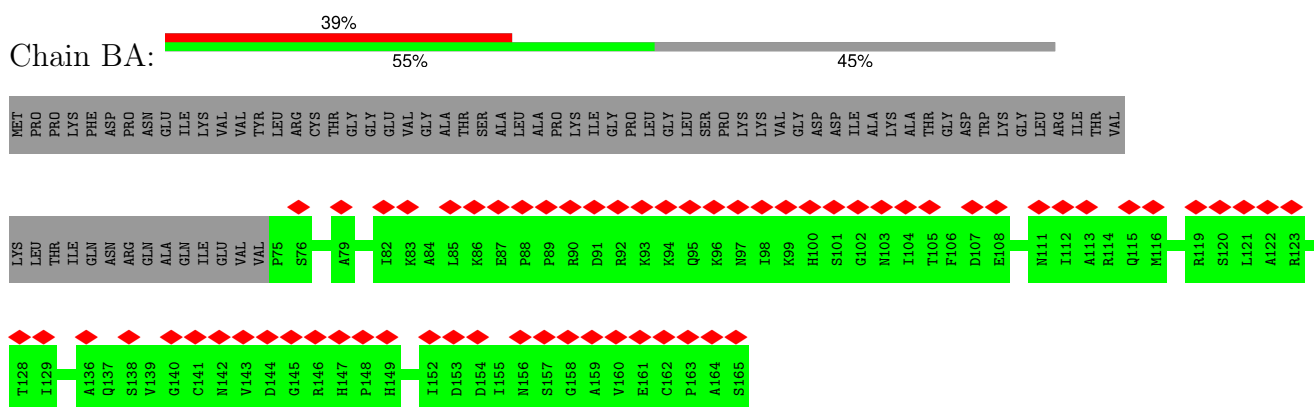
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
58	SR	1	1	1	0

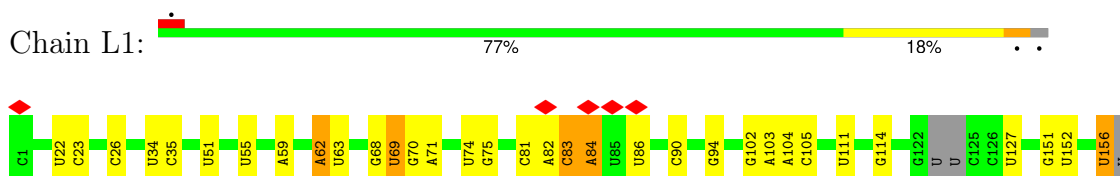
### 3 Residue-property plots [i](#)

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.

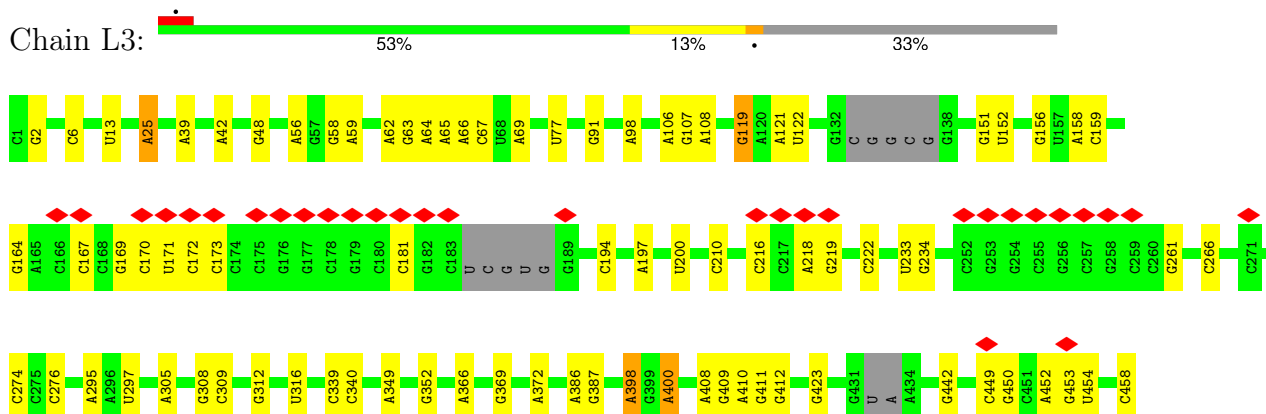
- Molecule 1: 60S ribosomal protein L12

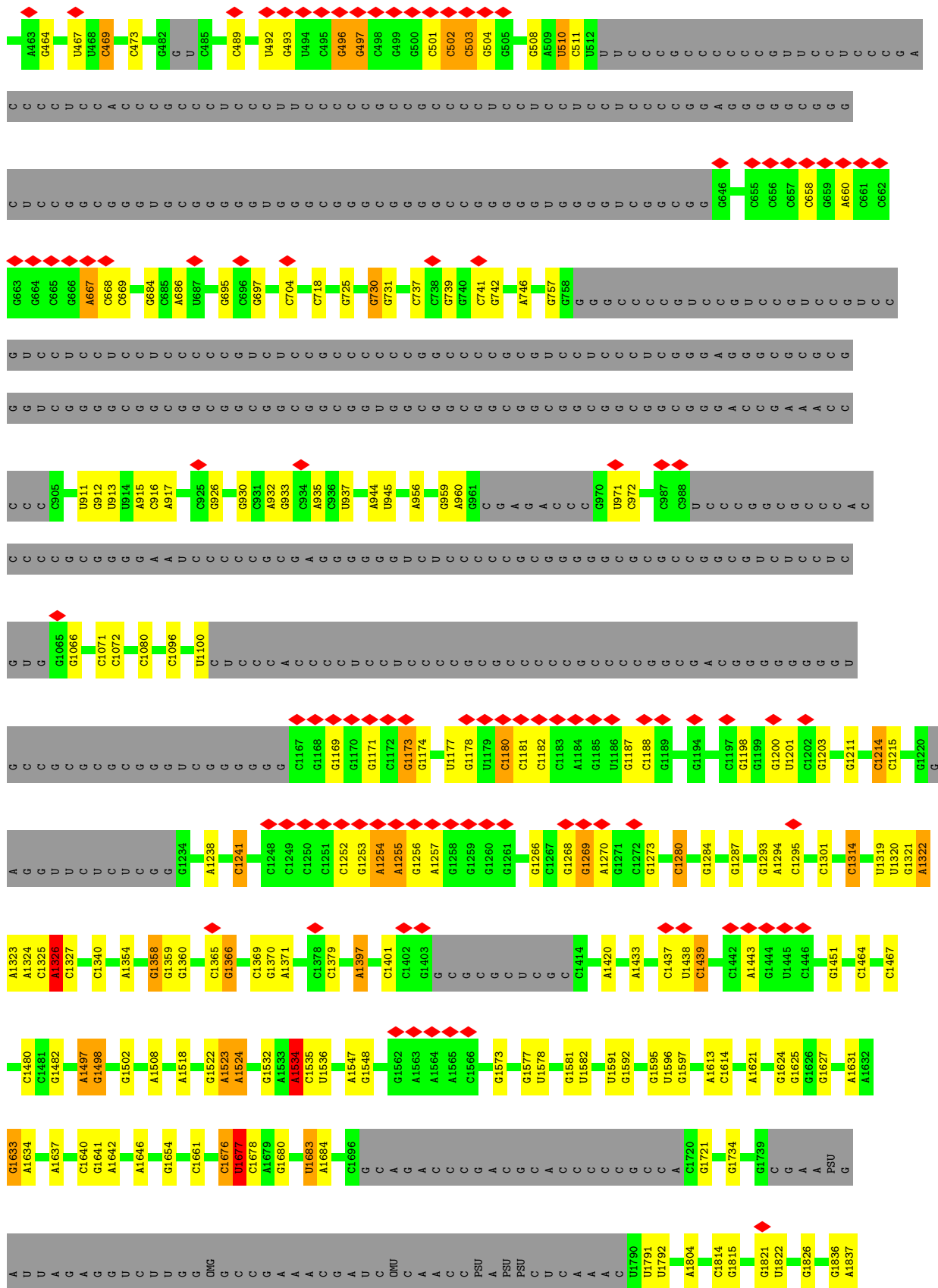


- Molecule 2: 5.8S rRNA

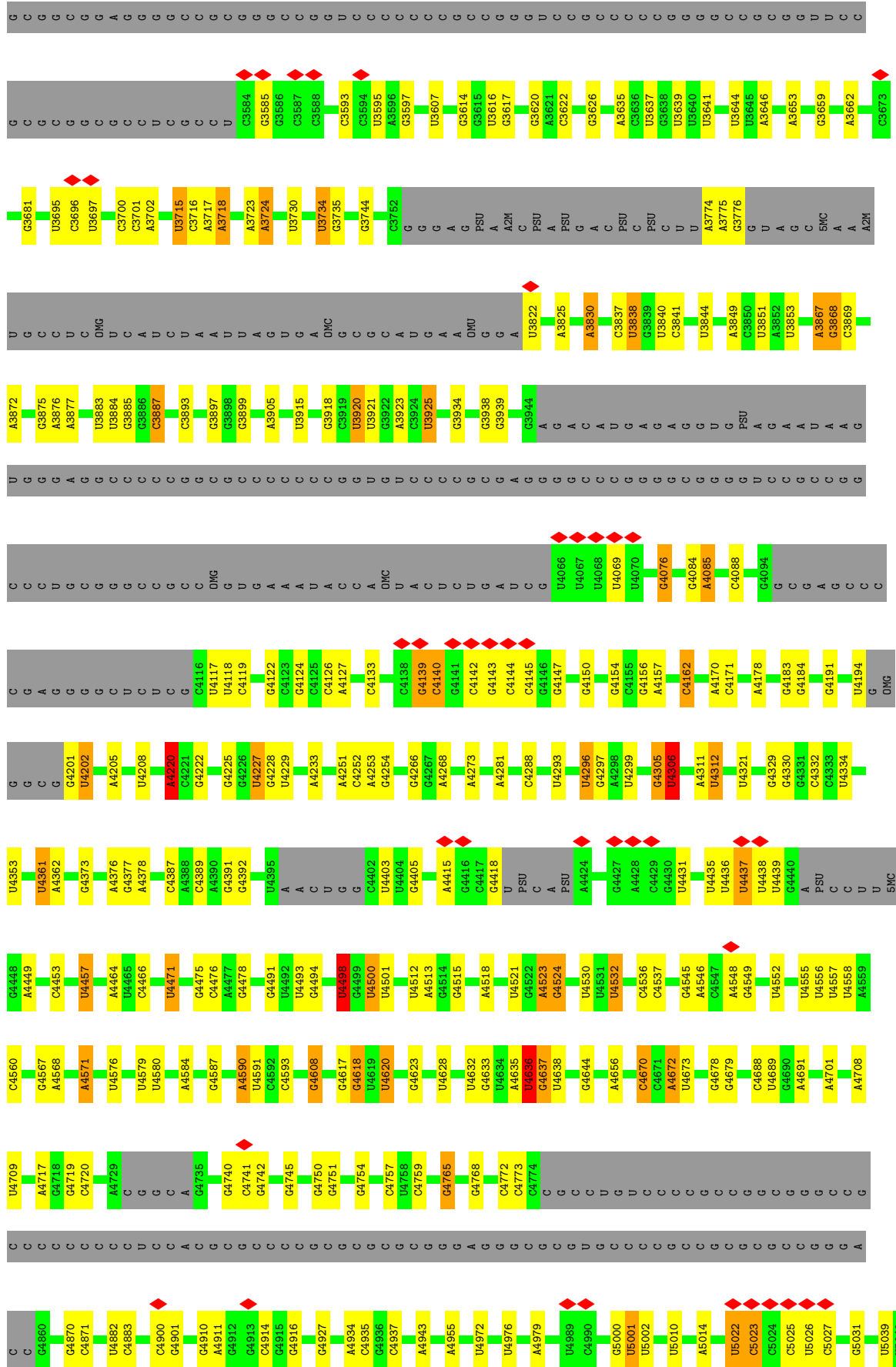


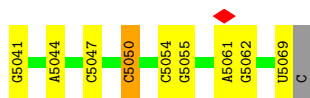
- Molecule 3: 28S rRNA



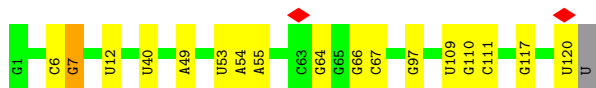
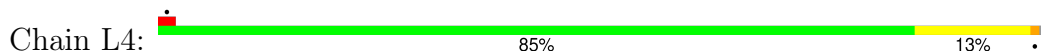








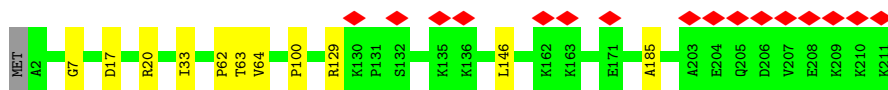
• Molecule 4: 5S rRNA



• Molecule 5: 60S ribosomal protein L11



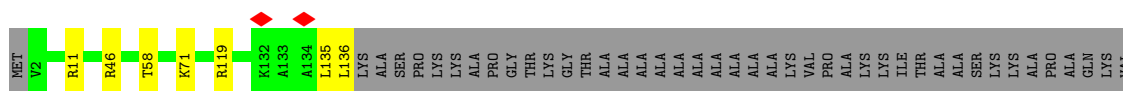
• Molecule 6: 60S ribosomal protein L13



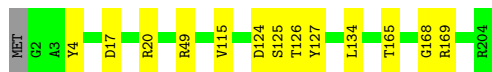
• Molecule 7: 60S ribosomal protein L13a



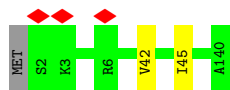
• Molecule 8: 60S ribosomal protein L14



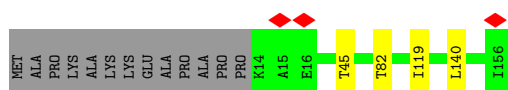
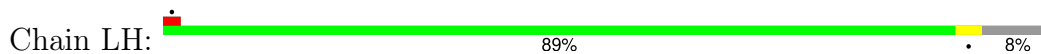
• Molecule 9: 60S ribosomal protein L15



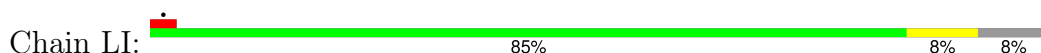




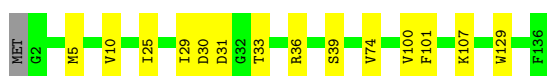
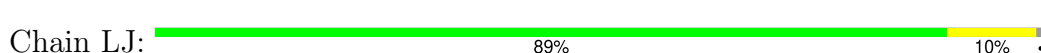
• Molecule 17: 60S ribosomal protein L23a



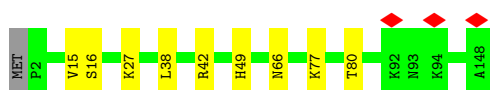
• Molecule 18: 60S ribosomal protein L26



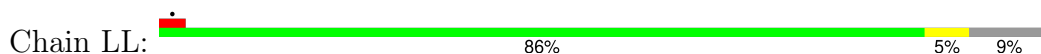
• Molecule 19: 60S ribosomal protein L27



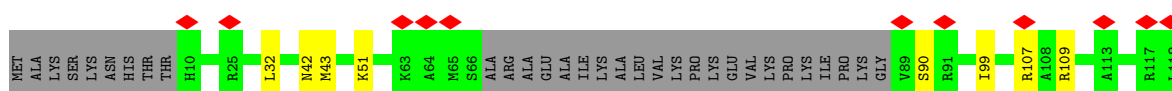
• Molecule 20: 60S ribosomal protein L27a

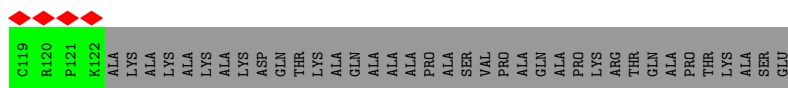


• Molecule 21: 60S ribosomal protein L28

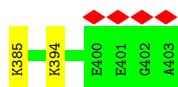


• Molecule 22: 60S ribosomal protein L29

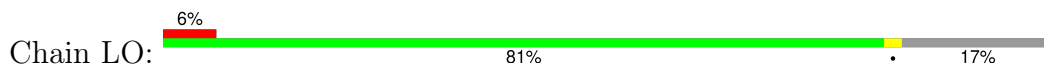




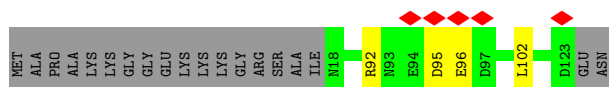
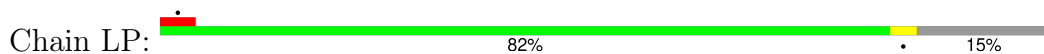
- Molecule 23: 60S ribosomal protein L3



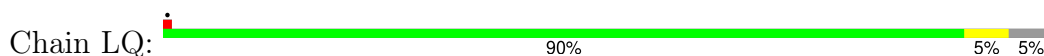
- Molecule 24: 60S ribosomal protein L30



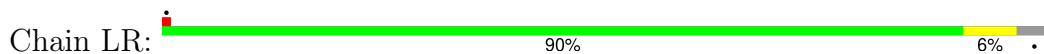
- Molecule 25: 60S ribosomal protein L31



- Molecule 26: 60S ribosomal protein L32

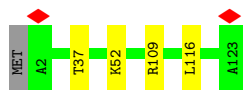


- Molecule 27: 60S ribosomal protein L34



- Molecule 28: 60S ribosomal protein L35

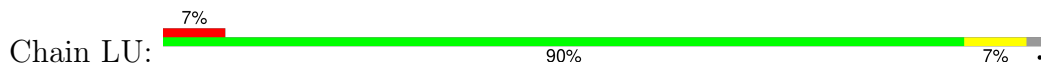




- Molecule 29: 60S ribosomal protein L35a



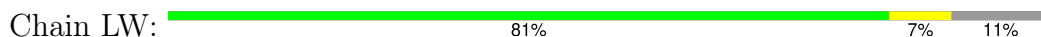
- Molecule 30: 60S ribosomal protein L36



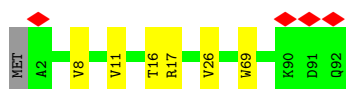
- Molecule 31: 60S ribosomal protein L36a



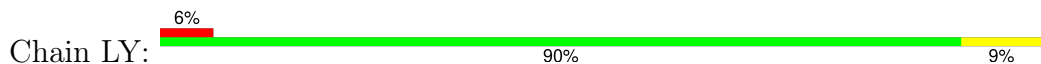
- Molecule 32: 60S ribosomal protein L37



- Molecule 33: 60S ribosomal protein L37a



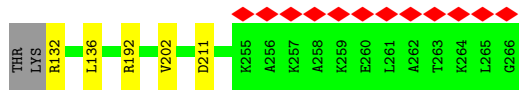
- Molecule 34: 60S ribosomal protein L38



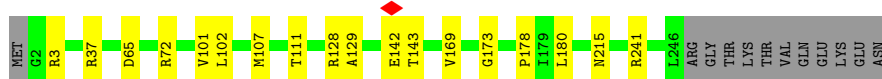
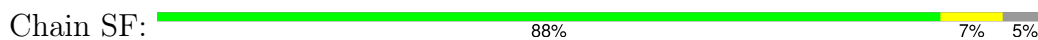
- Molecule 35: 60S ribosomal protein L39







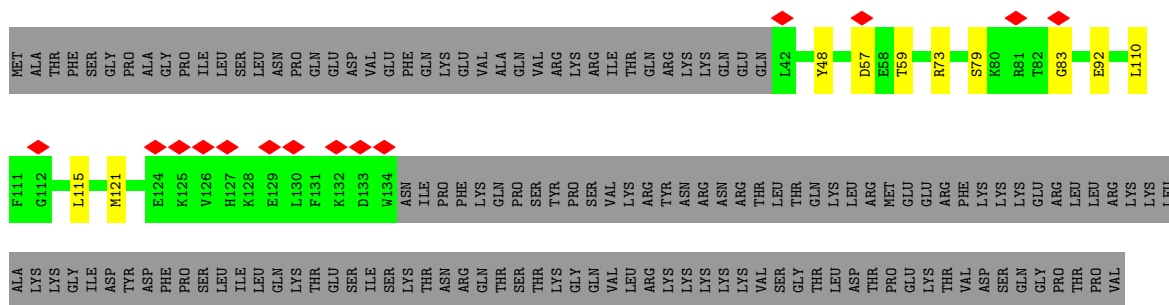
• Molecule 45: 60S ribosomal protein L8



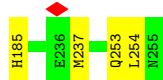
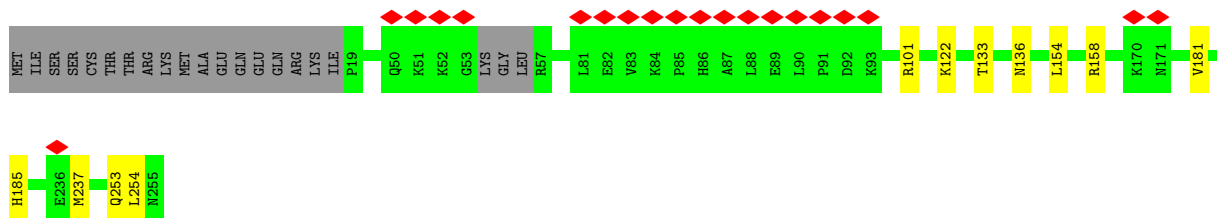
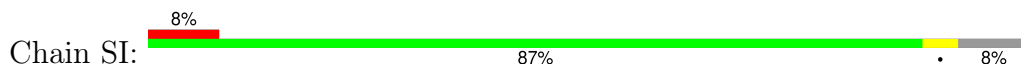
• Molecule 46: 60S ribosomal protein L9



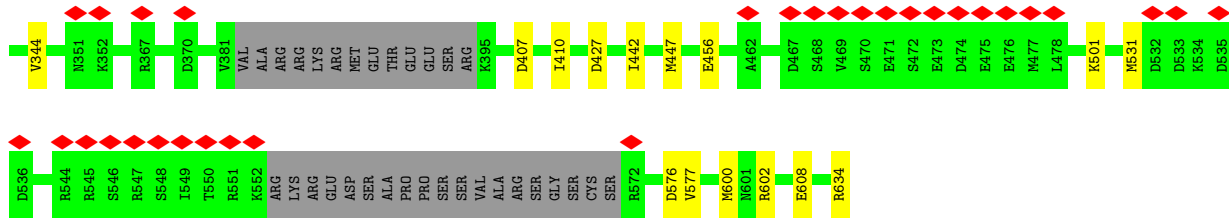
• Molecule 47: MKI67 FHA domain-interacting nucleolar phosphoprotein



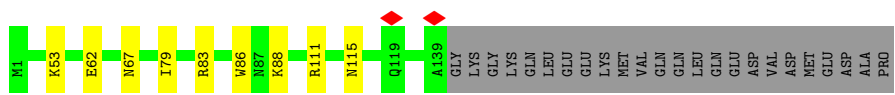
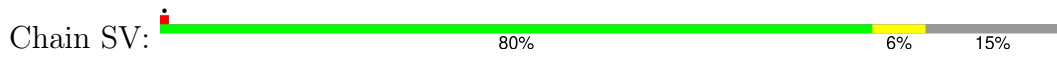
• Molecule 48: 60S ribosomal protein L7-like 1



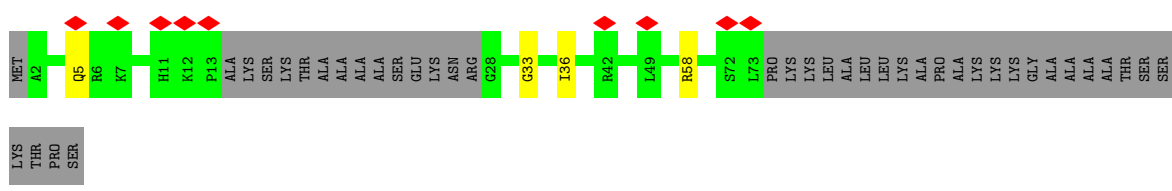




• Molecule 53: Probable ribosome biogenesis protein RLP24



• Molecule 54: Leydig cell tumor 10 kDa protein homolog



LYS  
THR  
PRO  
SER

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66157	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.877	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.055	Depositor
Map value standard deviation	0.194	Depositor
Recommended contour level	0.85	Depositor
Map size ( $\text{\AA}$ )	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.072, 1.072, 1.072	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, HIC, A2M, PTR, OMG, OMU, 1MA, 6MZ, UR3, GDP, ZN, MG, K, PSU

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	BA	0.11	0/448	0.26	0/622
2	L1	0.20	0/3589	0.26	0/5589
3	L3	0.20	0/79642	0.28	0/124218
4	L4	0.24	0/2861	0.29	0/4459
5	L5	0.16	0/1372	0.29	0/1836
6	L6	0.15	0/1732	0.28	0/2315
7	L7	0.17	0/1682	0.30	0/2250
8	L8	0.15	0/1133	0.27	0/1516
9	L9	0.18	0/1746	0.31	0/2338
10	LA	0.15	0/1268	0.32	0/1701
11	LB	0.18	0/1536	0.33	0/2052
12	LC	0.18	0/1501	0.32	0/2013
13	LD	0.14	0/1305	0.24	0/1727
14	LE	0.20	0/1291	0.34	0/1724
15	LF	0.13	0/856	0.28	0/1149
16	LG	0.17	0/1048	0.31	0/1402
17	LH	0.14	0/1175	0.28	0/1572
18	LI	0.16	0/1132	0.29	0/1504
19	LJ	0.16	0/1130	0.26	0/1507
20	LK	0.16	0/1191	0.29	0/1591
21	LL	0.15	0/1017	0.28	0/1364
22	LM	0.16	0/763	0.30	0/1005
23	LN	0.16	0/3294	0.31	0/4406
24	LO	0.11	0/748	0.23	0/1004
25	LP	0.17	0/894	0.30	0/1204
26	LQ	0.16	0/1071	0.28	0/1429
27	LR	0.15	0/898	0.29	0/1197
28	LS	0.13	0/1023	0.24	0/1351
29	LT	0.16	0/895	0.30	0/1198
30	LU	0.13	0/843	0.29	0/1115
31	LV	0.18	0/864	0.33	0/1140
32	LW	0.17	0/720	0.37	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	LX	0.13	0/718	0.28	0/953
34	LY	0.12	0/575	0.24	0/761
35	LZ	0.17	0/454	0.29	0/599
36	NK	0.12	0/587	0.25	0/767
37	NL	0.12	0/2207	0.25	0/2955
38	NP	0.14	0/864	0.29	0/1154
39	NR	0.12	0/1306	0.26	0/1740
40	SA	0.17	0/2907	0.30	0/3905
41	SB	0.17	0/2287	0.30	0/3065
42	SC	0.14	0/1781	0.28	0/2388
43	SD	0.16	0/1905	0.29	0/2539
44	SE	0.16	0/1903	0.31	0/2559
45	SF	0.16	0/1914	0.31	0/2567
46	SG	0.15	0/1537	0.28	0/2066
47	SH	0.12	0/794	0.26	0/1071
48	SI	0.13	0/2003	0.26	0/2688
49	SK	0.14	0/1877	0.31	0/2554
50	SM	0.15	0/3357	0.27	0/4529
51	SQ	0.11	0/648	0.29	0/894
52	SR	0.14	0/5014	0.29	0/6727
53	SV	0.18	0/1207	0.31	0/1600
54	VB	0.11	0/459	0.28	0/605
All	All	0.18	0/156972	0.28	0/229136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	449	0	207	0	0
2	L1	3278	0	1665	17	0
3	L3	73423	0	37192	281	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L4	2561	0	1295	7	0
5	L5	1349	0	1383	6	0
6	L6	1701	0	1818	12	0
7	L7	1650	0	1794	7	0
8	L8	1111	0	1174	8	0
9	L9	1701	0	1749	10	0
10	LA	1242	0	1269	7	0
11	LB	1512	0	1628	7	0
12	LC	1461	0	1502	8	0
13	LD	1289	0	1429	8	0
14	LE	1264	0	1328	6	0
15	LF	842	0	864	5	0
16	LG	1034	0	1097	3	0
17	LH	1156	0	1268	5	0
18	LI	1115	0	1205	10	0
19	LJ	1107	0	1182	8	0
20	LK	1162	0	1213	7	0
21	LL	1002	0	1068	6	0
22	LM	751	0	820	8	0
23	LN	3239	0	3377	24	0
24	LO	738	0	774	1	0
25	LP	879	0	924	2	0
26	LQ	1053	0	1147	6	0
27	LR	888	0	977	4	0
28	LS	1015	0	1148	4	0
29	LT	876	0	912	2	0
30	LU	832	0	917	7	0
31	LV	851	0	920	1	0
32	LW	705	0	737	5	0
33	LX	708	0	756	6	0
34	LY	569	0	637	4	0
35	LZ	444	0	483	5	0
36	NK	581	0	656	2	0
37	NL	2175	0	2235	14	0
38	NP	847	0	854	7	0
39	NR	1299	0	1318	7	0
40	SA	2853	0	3028	24	0
41	SB	2243	0	2268	9	0
42	SC	1747	0	1897	17	0
43	SD	1870	0	1996	8	0
44	SE	1869	0	2014	11	0
45	SF	1876	0	1970	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	SG	1518	0	1601	10	0
47	SH	773	0	755	5	0
48	SI	1952	0	2086	7	0
49	SK	1852	0	1828	11	0
50	SM	3278	0	3332	20	0
51	SQ	650	0	308	1	0
52	SR	4932	0	5071	26	0
53	SV	1184	0	1248	8	0
54	VB	455	0	504	4	0
55	L1	4	0	0	0	0
55	L3	74	0	0	0	0
55	L4	3	0	0	0	0
55	LG	1	0	0	0	0
55	LN	1	0	0	0	0
55	LQ	1	0	0	0	0
55	LR	1	0	0	0	0
55	LT	1	0	0	0	0
55	SF	1	0	0	0	0
55	SR	1	0	0	0	0
56	LR	1	0	0	0	0
56	LV	1	0	0	0	0
56	LW	1	0	0	0	0
56	LX	1	0	0	0	0
56	NP	1	0	0	0	0
56	SV	1	0	0	0	0
57	SR	28	0	12	0	0
58	SR	1	0	0	0	0
All	All	149034	0	112840	529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 529 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:SA:109:ARG:O	40:SA:109:ARG:HG2	1.76	0.86
3:L3:4156:G:OP2	3:L3:4157:A:O2'	1.97	0.82
3:L3:1322:1MA:O2'	3:L3:1323:A:O4'	1.94	0.82
3:L3:1480:C:O2'	3:L3:1482:G:OP2	1.98	0.81
4:L4:40:U:O2	5:L5:75:ARG:NH1	2.13	0.81

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	89/165 (54%)	89 (100%)	0	0	100	100
5	L5	166/178 (93%)	165 (99%)	1 (1%)	0	100	100
6	L6	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
7	L7	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
8	L8	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
9	L9	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
10	LA	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
11	LB	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
12	LC	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
13	LD	152/196 (78%)	150 (99%)	2 (1%)	0	100	100
14	LE	150/160 (94%)	145 (97%)	5 (3%)	0	100	100
15	LF	101/128 (79%)	99 (98%)	2 (2%)	0	100	100
16	LG	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
17	LH	141/156 (90%)	141 (100%)	0	0	100	100
18	LI	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
19	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
20	LK	145/148 (98%)	143 (99%)	2 (1%)	0	100	100
21	LL	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
22	LM	87/159 (55%)	86 (99%)	1 (1%)	0	100	100
23	LN	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
24	LO	93/115 (81%)	93 (100%)	0	0	100	100
25	LP	104/125 (83%)	102 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LQ	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
27	LR	110/117 (94%)	110 (100%)	0	0	100	100
28	LS	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
29	LT	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
30	LU	100/105 (95%)	100 (100%)	0	0	100	100
31	LV	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
32	LW	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
33	LX	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
34	LY	67/70 (96%)	67 (100%)	0	0	100	100
35	LZ	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
36	NK	63/129 (49%)	62 (98%)	1 (2%)	0	100	100
37	NL	259/478 (54%)	258 (100%)	1 (0%)	0	100	100
38	NP	100/134 (75%)	100 (100%)	0	0	100	100
39	NR	150/203 (74%)	147 (98%)	3 (2%)	0	100	100
40	SA	356/427 (83%)	352 (99%)	4 (1%)	0	100	100
41	SB	273/297 (92%)	269 (98%)	4 (2%)	0	100	100
42	SC	211/288 (73%)	204 (97%)	7 (3%)	0	100	100
43	SD	223/248 (90%)	218 (98%)	5 (2%)	0	100	100
44	SE	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
45	SF	243/257 (95%)	236 (97%)	7 (3%)	0	100	100
46	SG	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
47	SH	91/293 (31%)	90 (99%)	1 (1%)	0	100	100
48	SI	233/255 (91%)	230 (99%)	3 (1%)	0	100	100
49	SK	242/245 (99%)	237 (98%)	5 (2%)	0	100	100
50	SM	393/588 (67%)	388 (99%)	5 (1%)	0	100	100
51	SQ	121/239 (51%)	119 (98%)	2 (2%)	0	100	100
52	SR	595/634 (94%)	587 (99%)	7 (1%)	1 (0%)	43	56
53	SV	137/163 (84%)	136 (99%)	1 (1%)	0	100	100
54	VB	54/99 (54%)	54 (100%)	0	0	100	100
All	All	8516/10313 (83%)	8390 (98%)	125 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	SR	88	ASP

### 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	
5	L5	142/149 (95%)	142 (100%)	0	100	100
6	L6	176/177 (99%)	176 (100%)	0	100	100
7	L7	173/174 (99%)	173 (100%)	0	100	100
8	L8	115/161 (71%)	115 (100%)	0	100	100
9	L9	171/172 (99%)	171 (100%)	0	100	100
10	LA	134/163 (82%)	134 (100%)	0	100	100
11	LB	164/165 (99%)	164 (100%)	0	100	100
12	LC	157/157 (100%)	157 (100%)	0	100	100
13	LD	138/175 (79%)	138 (100%)	0	100	100
14	LE	136/140 (97%)	136 (100%)	0	100	100
15	LF	93/115 (81%)	93 (100%)	0	100	100
16	LG	106/107 (99%)	106 (100%)	0	100	100
17	LH	124/133 (93%)	124 (100%)	0	100	100
18	LI	124/135 (92%)	124 (100%)	0	100	100
19	LJ	117/118 (99%)	117 (100%)	0	100	100
20	LK	120/121 (99%)	120 (100%)	0	100	100
21	LL	109/121 (90%)	109 (100%)	0	100	100
22	LM	77/126 (61%)	77 (100%)	0	100	100
23	LN	347/348 (100%)	347 (100%)	0	100	100
24	LO	80/97 (82%)	80 (100%)	0	100	100
25	LP	97/110 (88%)	97 (100%)	0	100	100
26	LQ	114/121 (94%)	114 (100%)	0	100	100
27	LR	96/100 (96%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	LS	109/110 (99%)	109 (100%)	0	100	100
29	LT	88/89 (99%)	88 (100%)	0	100	100
30	LU	86/89 (97%)	86 (100%)	0	100	100
31	LV	92/94 (98%)	92 (100%)	0	100	100
32	LW	73/80 (91%)	73 (100%)	0	100	100
33	LX	74/75 (99%)	74 (100%)	0	100	100
34	LY	64/65 (98%)	64 (100%)	0	100	100
35	LZ	47/48 (98%)	47 (100%)	0	100	100
36	NK	61/115 (53%)	61 (100%)	0	100	100
37	NL	227/402 (56%)	227 (100%)	0	100	100
38	NP	88/114 (77%)	88 (100%)	0	100	100
39	NR	140/183 (76%)	140 (100%)	0	100	100
40	SA	298/348 (86%)	297 (100%)	1 (0%)	86	92
41	SB	234/250 (94%)	234 (100%)	0	100	100
42	SC	192/252 (76%)	192 (100%)	0	100	100
43	SD	194/215 (90%)	194 (100%)	0	100	100
44	SE	198/223 (89%)	198 (100%)	0	100	100
45	SF	188/199 (94%)	188 (100%)	0	100	100
46	SG	169/171 (99%)	169 (100%)	0	100	100
47	SH	85/274 (31%)	85 (100%)	0	100	100
48	SI	212/228 (93%)	212 (100%)	0	100	100
49	SK	212/213 (100%)	212 (100%)	0	100	100
50	SM	354/509 (70%)	354 (100%)	0	100	100
51	SQ	6/214 (3%)	6 (100%)	0	100	100
52	SR	545/574 (95%)	545 (100%)	0	100	100
53	SV	128/149 (86%)	128 (100%)	0	100	100
54	VB	48/76 (63%)	48 (100%)	0	100	100
All	All	7322/8744 (84%)	7321 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	SA	109	ARG

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

Mol	Chain	Res	Type
29	LT	99	HIS
50	SM	211	HIS
39	NR	102	GLN
50	SM	50	HIS
52	SR	209	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	18 (11%)	0
3	L3	3390/5070 (66%)	431 (12%)	8 (0%)
4	L4	119/121 (98%)	10 (8%)	0
All	All	3661/5348 (68%)	459 (12%)	8 (0%)

5 of 459 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	23	C
2	L1	34	U
2	L1	35	C
2	L1	59	A
2	L1	62	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L3	3616	U
3	L3	2095	A
3	L3	1625	OMG
3	L3	1324	A
3	L3	1853	G

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

109 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
3	A2M	L3	1326	3	22,25,26	0.89	0	30,36,39	2.04	7 (23%)
3	PSU	L3	4576	3	18,21,22	1.09	1 (5%)	21,30,33	1.92	6 (28%)
3	OMG	L3	4228	3	23,26,27	0.56	0	32,38,41	0.59	0
3	PSU	L3	4299	3	18,21,22	1.03	2 (11%)	21,30,33	2.04	5 (23%)
3	OMU	L3	3925	3	19,22,23	1.99	6 (31%)	25,31,34	1.89	5 (20%)
3	PSU	L3	4500	3	18,21,22	1.03	1 (5%)	21,30,33	1.98	5 (23%)
3	PSU	L3	4673	3	18,21,22	1.10	2 (11%)	21,30,33	1.95	4 (19%)
3	A2M	L3	1524	3	22,25,26	0.87	0	30,36,39	2.16	8 (26%)
3	PSU	L3	3851	3	18,21,22	1.10	1 (5%)	21,30,33	1.95	4 (19%)
3	PSU	L3	4403	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	6 (28%)
3	OMG	L3	4499	3	23,26,27	0.46	0	32,38,41	0.46	0
3	PSU	L3	4293	3	18,21,22	1.01	1 (5%)	21,30,33	1.79	4 (19%)
3	A2M	L3	3867	3	22,25,26	0.87	0	30,36,39	2.08	7 (23%)
3	PSU	L3	4361	3	18,21,22	1.05	2 (11%)	21,30,33	2.00	4 (19%)
3	PSU	L3	4353	3	18,21,22	1.07	1 (5%)	21,30,33	2.05	6 (28%)
3	A2M	L3	2401	3	22,25,26	0.88	0	30,36,39	2.12	8 (26%)
3	OMC	L3	4456	3	19,22,23	0.54	0	25,31,34	0.66	0
3	PSU	L3	3637	3	18,21,22	1.05	1 (5%)	21,30,33	1.98	5 (23%)
3	PSU	L3	4493	3	18,21,22	1.07	1 (5%)	21,30,33	1.94	4 (19%)
3	A2M	L3	398	3	22,25,26	0.89	0	30,36,39	2.10	8 (26%)
3	PSU	L3	3734	3	18,21,22	1.11	1 (5%)	21,30,33	1.96	6 (28%)
2	PSU	L1	55	2	18,21,22	1.09	2 (11%)	21,30,33	1.92	5 (23%)
3	PSU	L3	2632	3	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
3	A2M	L3	2787	3	22,25,26	0.90	1 (4%)	30,36,39	2.10	7 (23%)
3	OMC	L3	2824	3	19,22,23	0.56	0	25,31,34	0.70	0
3	OMG	L3	3899	3	23,26,27	0.54	0	32,38,41	0.54	0
3	OMC	L3	2351	55,3	19,22,23	0.64	0	25,31,34	0.88	2 (8%)
3	OMG	L3	4618	3	23,26,27	0.51	0	32,38,41	0.52	0
3	OMC	L3	3701	3	19,22,23	0.52	0	25,31,34	0.57	0
39	PTR	NR	127	39	15,16,17	1.25	1 (6%)	17,22,24	0.61	0
3	PSU	L3	4471	3	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
3	OMC	L3	3887	3	19,22,23	0.55	0	25,31,34	0.65	0
3	PSU	L3	3695	3	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMG	L1	75	2	23,26,27	0.50	0	32,38,41	0.47	0
3	PSU	L3	3884	3	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
3	OMG	L3	1316	3	23,26,27	0.53	0	32,38,41	0.50	0
3	PSU	L3	1677	3	18,21,22	1.01	1 (5%)	21,30,33	1.89	5 (23%)
3	PSU	L3	4972	3	18,21,22	1.08	1 (5%)	21,30,33	1.95	5 (23%)
3	OMC	L3	3869	3	19,22,23	0.58	0	25,31,34	0.68	0
3	PSU	L3	4431	3	18,21,22	1.15	1 (5%)	21,30,33	1.94	5 (23%)
3	OMG	L3	2364	3	23,26,27	0.51	0	32,38,41	0.50	0
3	PSU	L3	3822	3	18,21,22	1.15	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L3	1860	3	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
3	A2M	L3	1534	55,3	22,25,26	0.92	1 (4%)	30,36,39	2.05	7 (23%)
3	OMG	L3	1522	3	23,26,27	0.53	0	32,38,41	0.61	0
3	OMC	L3	3841	3	19,22,23	0.55	0	25,31,34	0.64	0
3	PSU	L3	4532	3	18,21,22	1.09	1 (5%)	21,30,33	2.00	5 (23%)
3	OMC	L3	4536	3	19,22,23	0.57	0	25,31,34	0.67	0
3	OMG	L3	4637	3	23,26,27	0.51	0	32,38,41	0.49	0
3	A2M	L3	4590	3	22,25,26	0.91	0	30,36,39	2.01	8 (26%)
3	1MA	L3	1322	3	21,25,26	0.49	0	30,37,40	0.84	1 (3%)
3	OMG	L3	4392	3	23,26,27	0.53	0	32,38,41	0.49	0
3	PSU	L3	4689	3	18,21,22	1.07	1 (5%)	21,30,33	1.97	5 (23%)
3	OMU	L3	2415	3	19,22,23	2.04	7 (36%)	25,31,34	1.84	5 (20%)
3	A2M	L3	4523	3	22,25,26	0.88	0	30,36,39	2.08	7 (23%)
3	A2M	L3	1871	3	22,25,26	0.86	0	30,36,39	2.18	8 (26%)
3	OMU	L3	2837	3	19,22,23	2.05	7 (36%)	25,31,34	1.89	5 (20%)
3	PSU	L3	3920	55,3	18,21,22	1.08	2 (11%)	21,30,33	1.90	5 (23%)
3	OMG	L3	4370	3	23,26,27	0.56	0	32,38,41	0.55	0
3	A2M	L3	2815	3	22,25,26	0.89	0	30,36,39	2.10	7 (23%)
3	OMG	L3	3744	3	23,26,27	0.48	0	32,38,41	0.48	0
3	PSU	L3	4296	3	18,21,22	1.07	2 (11%)	21,30,33	1.97	5 (23%)
3	PSU	L3	4457	3	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
3	OMG	L3	4494	3	23,26,27	0.53	0	32,38,41	0.52	0
2	PSU	L1	69	2	18,21,22	1.10	1 (5%)	21,30,33	2.01	6 (28%)
3	A2M	L3	3718	3	22,25,26	0.93	1 (4%)	30,36,39	1.95	7 (23%)
3	PSU	L3	4636	3	18,21,22	1.11	1 (5%)	21,30,33	2.06	6 (28%)
3	OMC	L3	2365	3	19,22,23	0.55	0	25,31,34	0.71	0
3	PSU	L3	5010	3	18,21,22	1.09	1 (5%)	21,30,33	1.92	5 (23%)
3	OMC	L3	1340	3	19,22,23	0.60	0	25,31,34	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	L3	4552	3	18,21,22	1.05	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L3	1683	3	18,21,22	1.07	2 (11%)	21,30,33	2.04	5 (23%)
3	A2M	L3	2363	55,3	22,25,26	0.89	1 (4%)	30,36,39	2.01	7 (23%)
3	PSU	L3	4628	3	18,21,22	1.06	2 (11%)	21,30,33	1.93	6 (28%)
3	OMU	L3	4498	3	19,22,23	2.11	7 (36%)	25,31,34	1.79	5 (20%)
3	OMC	L3	2861	3	19,22,23	0.54	0	25,31,34	0.69	1 (4%)
3	OMG	L3	2424	3	23,26,27	0.52	0	32,38,41	0.44	0
3	PSU	L3	3715	3	18,21,22	1.12	1 (5%)	21,30,33	1.97	6 (28%)
3	PSU	L3	3844	3	18,21,22	1.13	1 (5%)	21,30,33	1.97	5 (23%)
3	OMU	L3	4227	3	19,22,23	1.99	6 (31%)	25,31,34	1.86	4 (16%)
3	A2M	L3	3830	3	22,25,26	0.89	0	30,36,39	2.06	7 (23%)
3	A2M	L3	400	3	22,25,26	0.86	0	30,36,39	2.04	7 (23%)
3	A2M	L3	3825	3	22,25,26	0.88	0	30,36,39	2.10	7 (23%)
3	PSU	L3	4579	3	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
3	OMU	L3	4306	3	19,22,23	2.00	6 (31%)	25,31,34	1.91	4 (16%)
3	OMC	L3	2804	3	19,22,23	0.58	0	25,31,34	0.66	0
3	PSU	L3	1862	3	18,21,22	1.10	2 (11%)	21,30,33	1.98	5 (23%)
3	PSU	L3	3639	3	18,21,22	1.05	1 (5%)	21,30,33	1.95	5 (23%)
23	HIC	LN	245	23	10,11,12	1.49	1 (10%)	9,14,16	1.22	1 (11%)
3	A2M	L3	3724	3	22,25,26	0.88	0	30,36,39	2.05	7 (23%)
3	A2M	L3	4571	3	22,25,26	0.86	0	30,36,39	2.00	7 (23%)
3	PSU	L3	4521	3	18,21,22	1.06	1 (5%)	21,30,33	1.94	4 (19%)
3	OMG	L3	3627	3	23,26,27	0.50	0	32,38,41	0.58	0
3	PSU	L3	3730	3	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L3	1792	3	18,21,22	1.06	1 (5%)	21,30,33	1.92	5 (23%)
3	OMG	L3	1625	3	23,26,27	0.52	0	32,38,41	0.48	0
3	OMG	L3	2876	3	23,26,27	0.48	0	32,38,41	0.45	0
3	OMC	L3	2422	55,3	19,22,23	0.55	0	25,31,34	0.68	0
3	UR3	L3	4530	3	19,22,23	1.15	3 (15%)	26,32,35	1.53	2 (7%)
3	PSU	L3	1536	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
3	6MZ	L3	4220	3	22,25,26	1.17	2 (9%)	29,36,39	2.19	9 (31%)
3	PSU	L3	3853	3	18,21,22	1.04	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L3	2508	3	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L3	1582	3	18,21,22	1.06	1 (5%)	21,30,33	2.00	5 (23%)
3	PSU	L3	2839	3	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
3	OMU	L3	4620	3	19,22,23	1.95	6 (31%)	25,31,34	1.64	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	L3	4312	3	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
3	PSU	L3	5001	3	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
3	OMG	L3	4623	3	23,26,27	0.49	0	32,38,41	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L3	1326	3	-	3/9/27/28	0/3/3/3
3	PSU	L3	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4228	3	-	2/9/27/28	0/3/3/3
3	PSU	L3	4299	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	3925	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4500	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4673	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	1524	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	3851	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4403	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4499	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3867	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4353	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2401	3	-	2/9/27/28	0/3/3/3
3	OMC	L3	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	3637	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4493	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	398	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	3734	3	-	0/7/25/26	0/2/2/2
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
3	PSU	L3	2632	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2787	3	-	5/9/27/28	0/3/3/3
3	OMC	L3	2824	3	-	0/9/27/28	0/2/2/2
3	OMG	L3	3899	3	-	1/9/27/28	0/3/3/3
3	OMC	L3	2351	55,3	-	2/9/27/28	0/2/2/2
3	OMG	L3	4618	3	-	3/9/27/28	0/3/3/3
3	OMC	L3	3701	3	-	7/9/27/28	0/2/2/2
39	PTR	NR	127	39	-	1/10/11/13	0/1/1/1
3	PSU	L3	4471	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L3	3887	3	-	2/9/27/28	0/2/2/2
3	PSU	L3	3695	3	-	0/7/25/26	0/2/2/2
2	OMG	L1	75	2	-	1/9/27/28	0/3/3/3
3	PSU	L3	3884	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	1316	3	-	2/9/27/28	0/3/3/3
3	PSU	L3	1677	3	-	3/7/25/26	0/2/2/2
3	PSU	L3	4972	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	3869	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4431	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	2364	3	-	3/9/27/28	0/3/3/3
3	PSU	L3	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1860	3	-	2/7/25/26	0/2/2/2
3	A2M	L3	1534	55,3	-	1/9/27/28	0/3/3/3
3	OMG	L3	1522	3	-	0/9/27/28	0/3/3/3
3	OMC	L3	3841	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4532	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	4536	3	-	0/9/27/28	0/2/2/2
3	OMG	L3	4637	3	-	2/9/27/28	0/3/3/3
3	A2M	L3	4590	3	-	3/9/27/28	0/3/3/3
3	1MA	L3	1322	3	-	0/7/25/26	0/3/3/3
3	OMG	L3	4392	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4689	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	2415	3	-	0/9/27/28	0/2/2/2
3	A2M	L3	4523	3	-	2/9/27/28	0/3/3/3
3	A2M	L3	1871	3	-	1/9/27/28	0/3/3/3
3	OMU	L3	2837	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	3920	55,3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4370	3	-	0/9/27/28	0/3/3/3
3	A2M	L3	2815	3	-	1/9/27/28	0/3/3/3
3	OMG	L3	3744	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4457	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4494	3	-	0/9/27/28	0/3/3/3
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
3	A2M	L3	3718	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4636	3	-	1/7/25/26	0/2/2/2
3	OMC	L3	2365	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	5010	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4552	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	1683	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2363	55,3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4628	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	4498	3	-	2/9/27/28	0/2/2/2
3	OMC	L3	2861	3	-	1/9/27/28	0/2/2/2
3	OMG	L3	2424	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3844	3	-	1/7/25/26	0/2/2/2
3	OMU	L3	4227	3	-	1/9/27/28	0/2/2/2
3	A2M	L3	3830	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	400	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	3825	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	4579	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	4306	3	-	4/9/27/28	0/2/2/2
3	OMC	L3	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3639	3	-	0/7/25/26	0/2/2/2
23	HIC	LN	245	23	-	2/5/6/8	0/1/1/1
3	A2M	L3	3724	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	4571	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4521	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	3730	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1792	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	1625	3	-	2/9/27/28	0/3/3/3
3	OMG	L3	2876	3	-	2/9/27/28	0/3/3/3
3	OMC	L3	2422	55,3	-	0/9/27/28	0/2/2/2
3	UR3	L3	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1536	3	-	0/7/25/26	0/2/2/2
3	6MZ	L3	4220	3	-	3/9/27/28	0/3/3/3
3	PSU	L3	3853	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	2839	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	5001	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4623	3	-	0/9/27/28	0/3/3/3

The worst 5 of 113 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	4498	OMU	C6-N1	4.88	1.49	1.38
3	L3	2415	OMU	C6-N1	4.66	1.49	1.38
3	L3	2837	OMU	C6-N1	4.66	1.49	1.38
3	L3	4306	OMU	C6-N1	4.64	1.49	1.38
3	L3	4620	OMU	C6-N1	4.57	1.49	1.38

The worst 5 of 411 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4220	6MZ	C5-C4-N3	-5.86	118.65	126.72
3	L3	2815	A2M	C5-C4-N3	-5.77	118.77	126.72
3	L3	3825	A2M	C5-C4-N3	-5.71	118.85	126.72
3	L3	3925	OMU	C4-N3-C2	-5.69	119.55	126.61
3	L3	2787	A2M	C5-C4-N3	-5.66	118.92	126.72

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	75	OMG	C1'-C2'-O2'-CM2
3	L3	398	A2M	C1'-C2'-O2'-CM'
3	L3	1316	OMG	C1'-C2'-O2'-CM2
3	L3	1326	A2M	O4'-C4'-C5'-O5'
3	L3	1326	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

57 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	1326	A2M	2	0
3	L3	3925	OMU	1	0
3	L3	4500	PSU	1	0
3	L3	1524	A2M	1	0
3	L3	3867	A2M	1	0
3	L3	4361	PSU	1	0
3	L3	398	A2M	2	0
3	L3	3734	PSU	1	0
3	L3	2632	PSU	1	0
3	L3	2824	OMC	1	0
3	L3	3899	OMG	1	0
3	L3	2351	OMC	2	0
3	L3	4618	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	3701	OMC	1	0
3	L3	4471	PSU	1	0
3	L3	3887	OMC	1	0
2	L1	75	OMG	2	0
3	L3	1677	PSU	3	0
3	L3	3869	OMC	1	0
3	L3	2364	OMG	1	0
3	L3	1534	A2M	3	0
3	L3	1522	OMG	1	0
3	L3	3841	OMC	1	0
3	L3	4536	OMC	1	0
3	L3	4637	OMG	1	0
3	L3	1322	1MA	3	0
3	L3	4392	OMG	1	0
3	L3	2415	OMU	1	0
3	L3	2837	OMU	1	0
3	L3	3920	PSU	1	0
3	L3	2815	A2M	1	0
3	L3	3744	OMG	1	0
3	L3	4296	PSU	1	0
3	L3	4457	PSU	1	0
3	L3	4494	OMG	1	0
2	L1	69	PSU	2	0
3	L3	3718	A2M	2	0
3	L3	4636	PSU	1	0
3	L3	1340	OMC	1	0
3	L3	1683	PSU	1	0
3	L3	2363	A2M	3	0
3	L3	4498	OMU	1	0
3	L3	2861	OMC	1	0
3	L3	2424	OMG	1	0
3	L3	3715	PSU	1	0
3	L3	4227	OMU	1	0
3	L3	3830	A2M	1	0
3	L3	400	A2M	2	0
3	L3	4306	OMU	2	0
3	L3	3724	A2M	2	0
3	L3	4571	A2M	1	0
3	L3	2876	OMG	2	0
3	L3	4220	6MZ	3	0
3	L3	4620	OMU	1	0
3	L3	4312	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	5001	PSU	1	0
3	L3	4623	OMG	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 95 are monoatomic - leaving 1 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
57	GDP	SR	1001	58,55	29,30,30	3.03	12 (41%)	45,47,47	2.70	17 (37%)

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
57	GDP	SR	1001	58,55	-	0/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	SR	1001	GDP	O6-C6	8.79	1.40	1.23
57	SR	1001	GDP	C5-N7	6.54	1.52	1.39
57	SR	1001	GDP	PA-O3A	4.98	1.64	1.59
57	SR	1001	GDP	C2-N2	4.84	1.45	1.34
57	SR	1001	GDP	C8-N9	-4.04	1.28	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	SR	1001	GDP	C8-N9-C4	7.78	120.61	106.03
57	SR	1001	GDP	C5-C4-N3	-6.77	117.61	128.39
57	SR	1001	GDP	N9-C4-N3	6.71	139.36	125.95
57	SR	1001	GDP	C2-N3-C4	5.38	121.56	112.30
57	SR	1001	GDP	C6-C5-N7	4.82	139.06	130.29

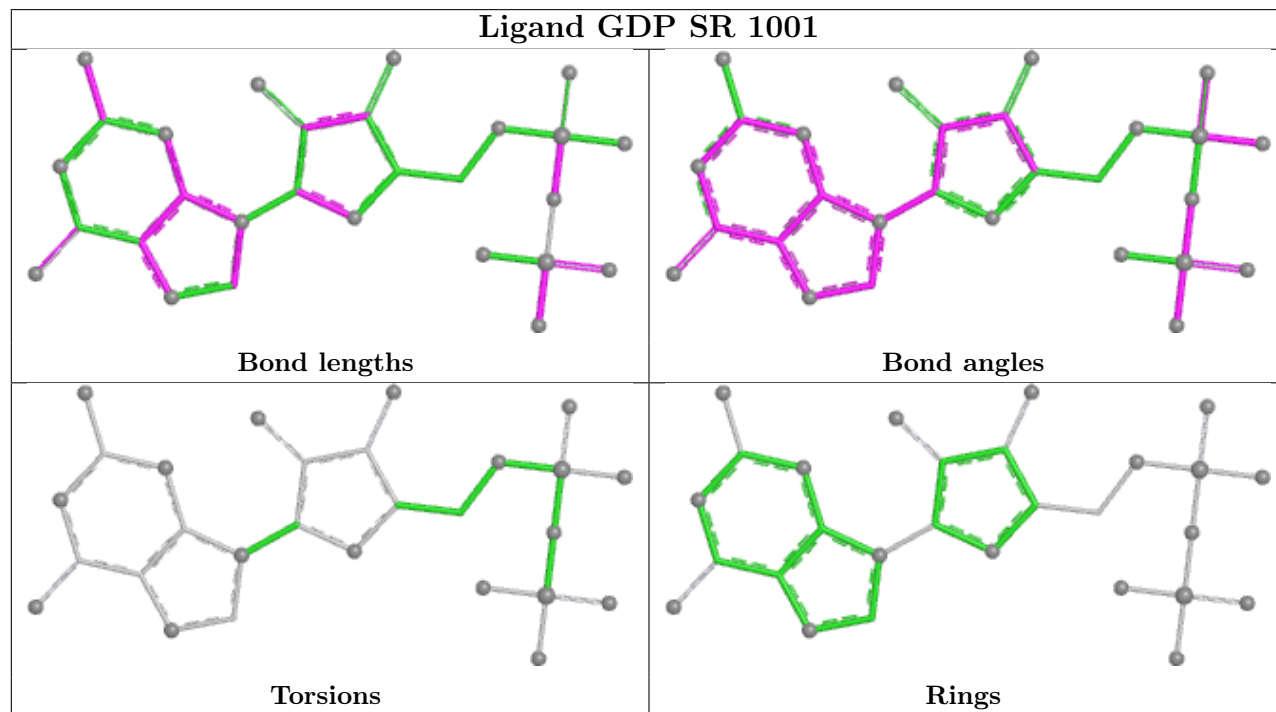
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

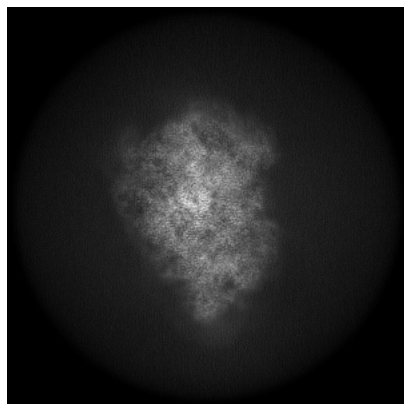
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29273. These allow visual inspection of the internal detail of the map and identification of artifacts.

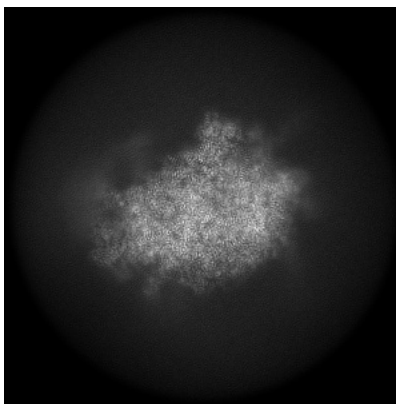
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

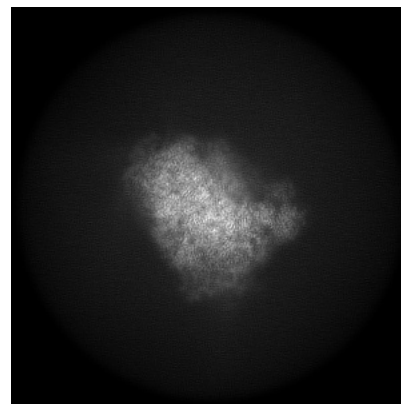
#### 6.1.1 Primary map



X

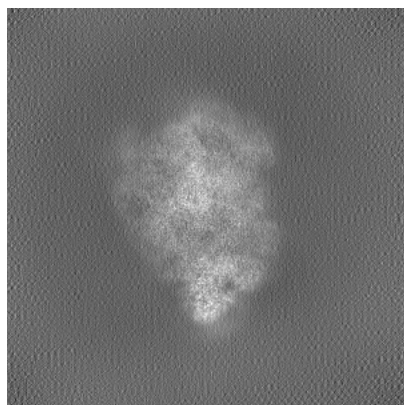


Y

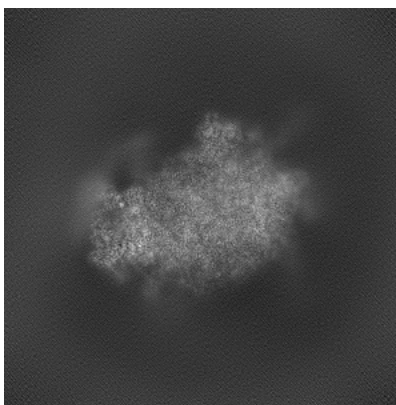


Z

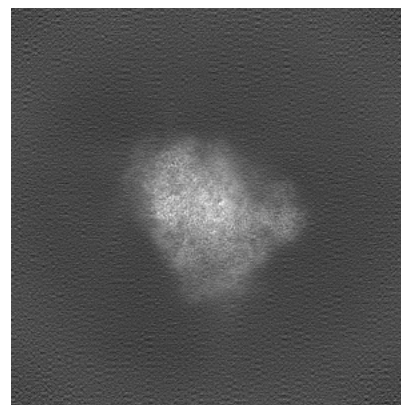
#### 6.1.2 Raw map



X



Y

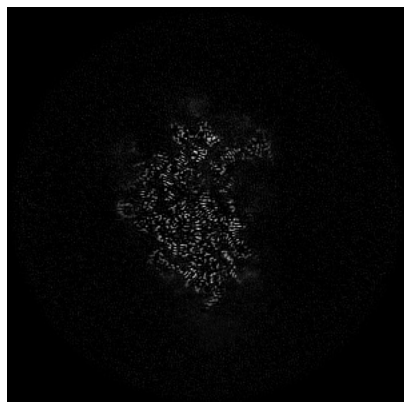


Z

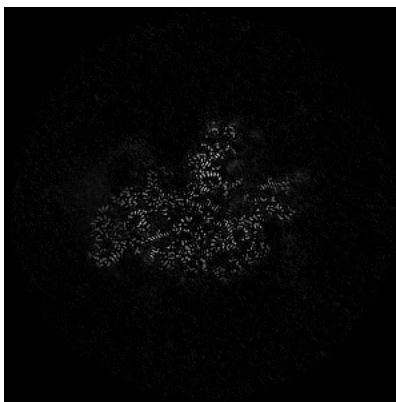
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

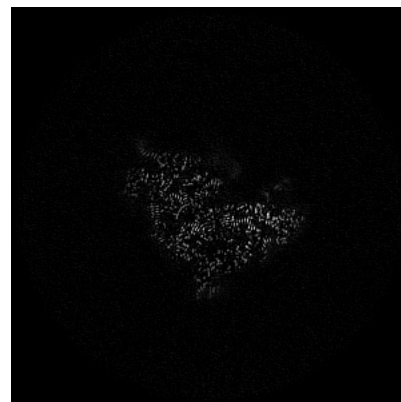
### 6.2.1 Primary map



X Index: 240

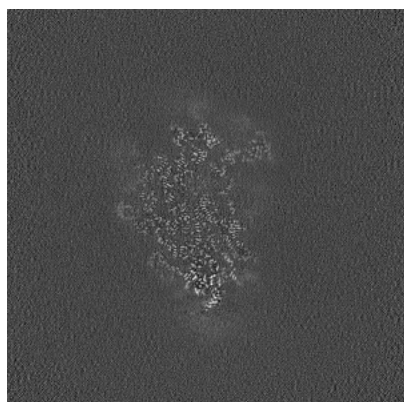


Y Index: 240

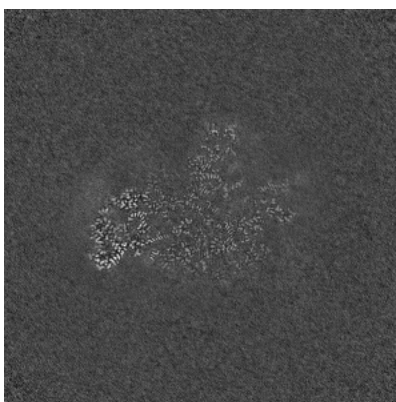


Z Index: 240

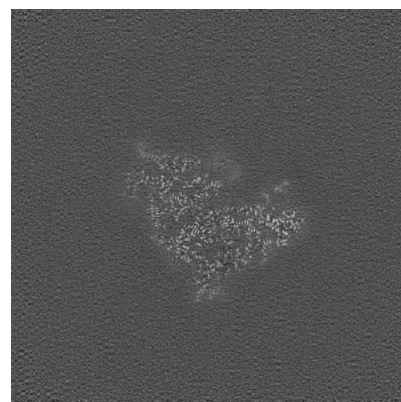
### 6.2.2 Raw map



X Index: 240



Y Index: 240

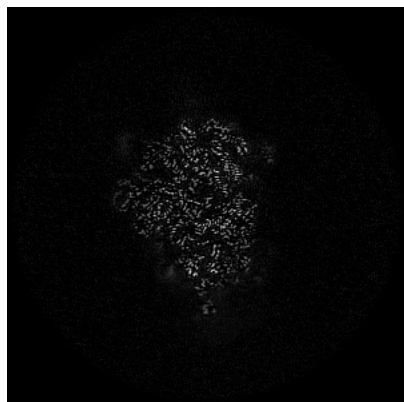


Z Index: 240

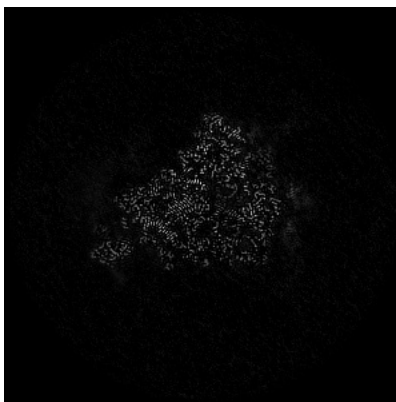
The images above show central slices of the map in three orthogonal directions.

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

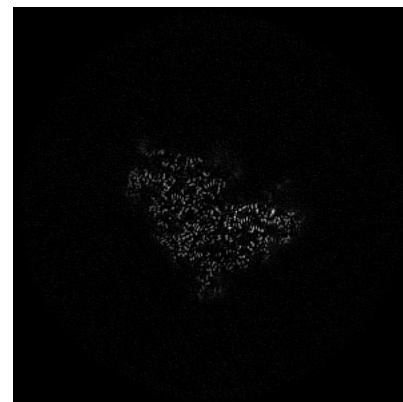
### 6.3.1 Primary map



X Index: 226

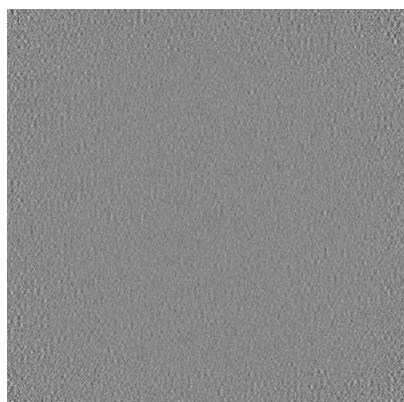


Y Index: 227

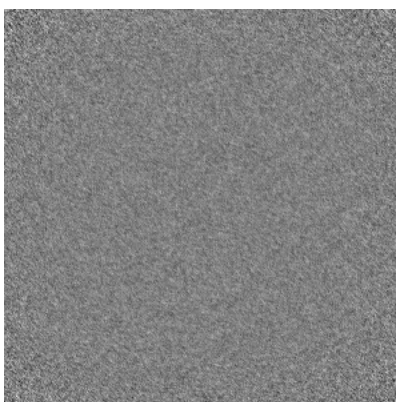


Z Index: 239

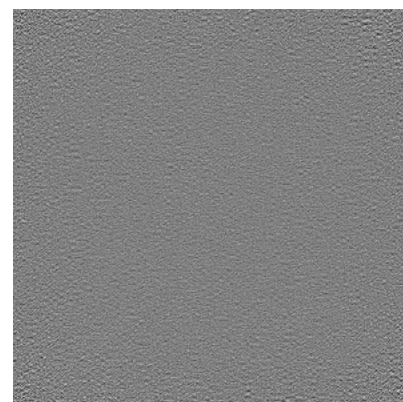
### 6.3.2 Raw map



X Index: 0



Y Index: 0

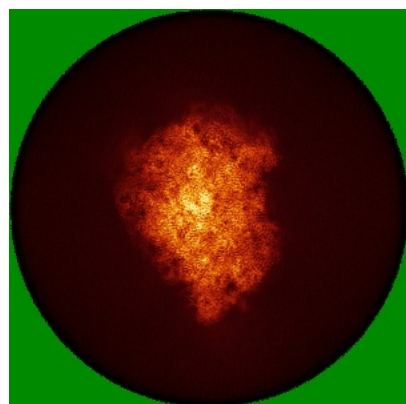


Z Index: 0

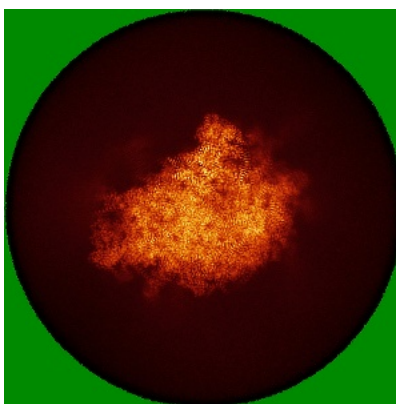
The images above show the largest variance slices of the map in three orthogonal directions.

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

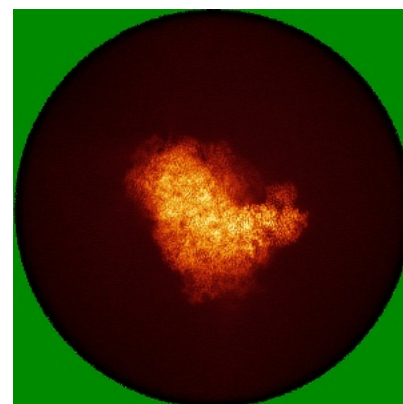
### 6.4.1 Primary map



X

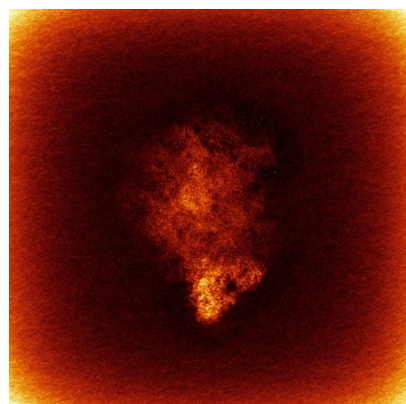


Y

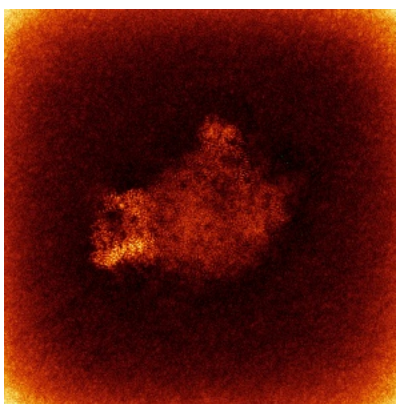


Z

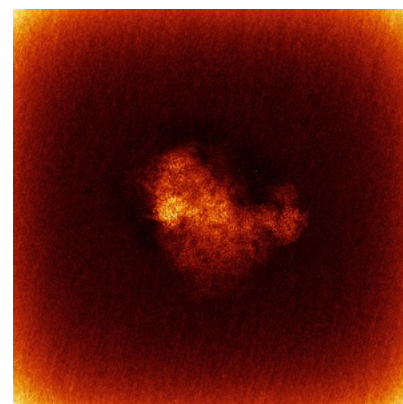
### 6.4.2 Raw map



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



X



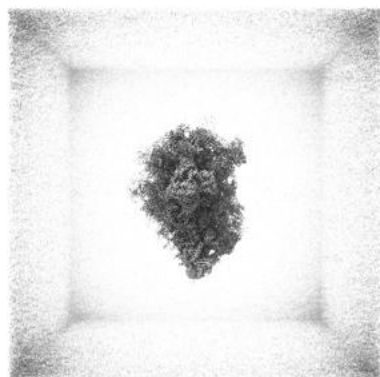
Y



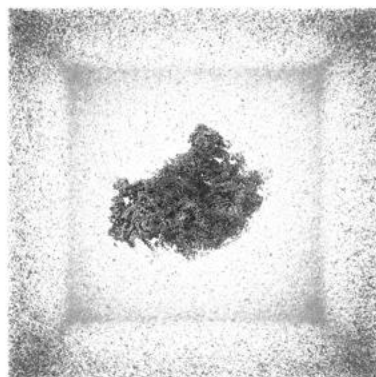
Z

The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

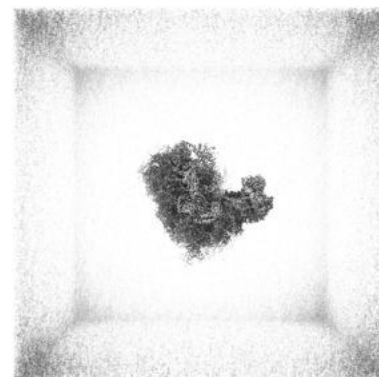
### 6.5.2 Raw map



X



Y



Z

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.

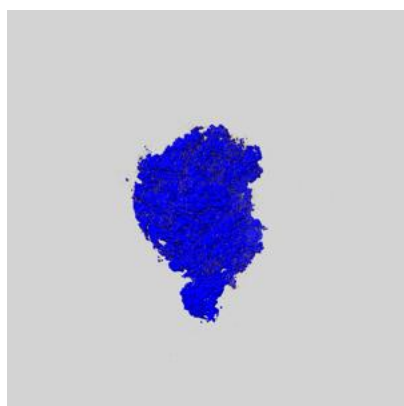
## 6.6 Mask visualisation [i](#)

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

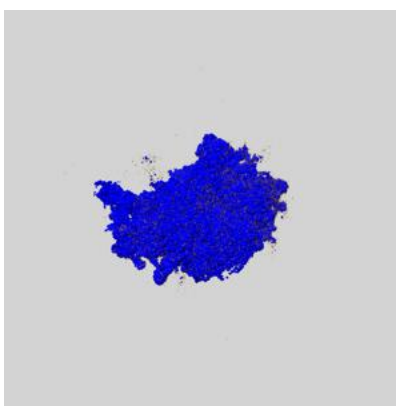
A mask typically either:

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

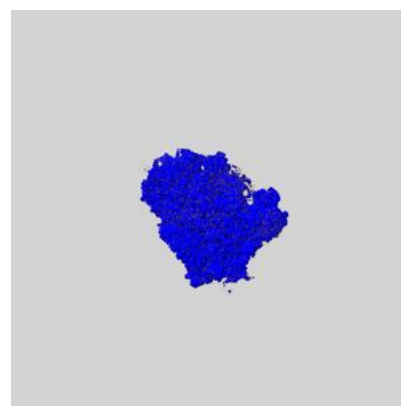
### 6.6.1 emd\_29273\_msk\_1.map [i](#)



X



Y

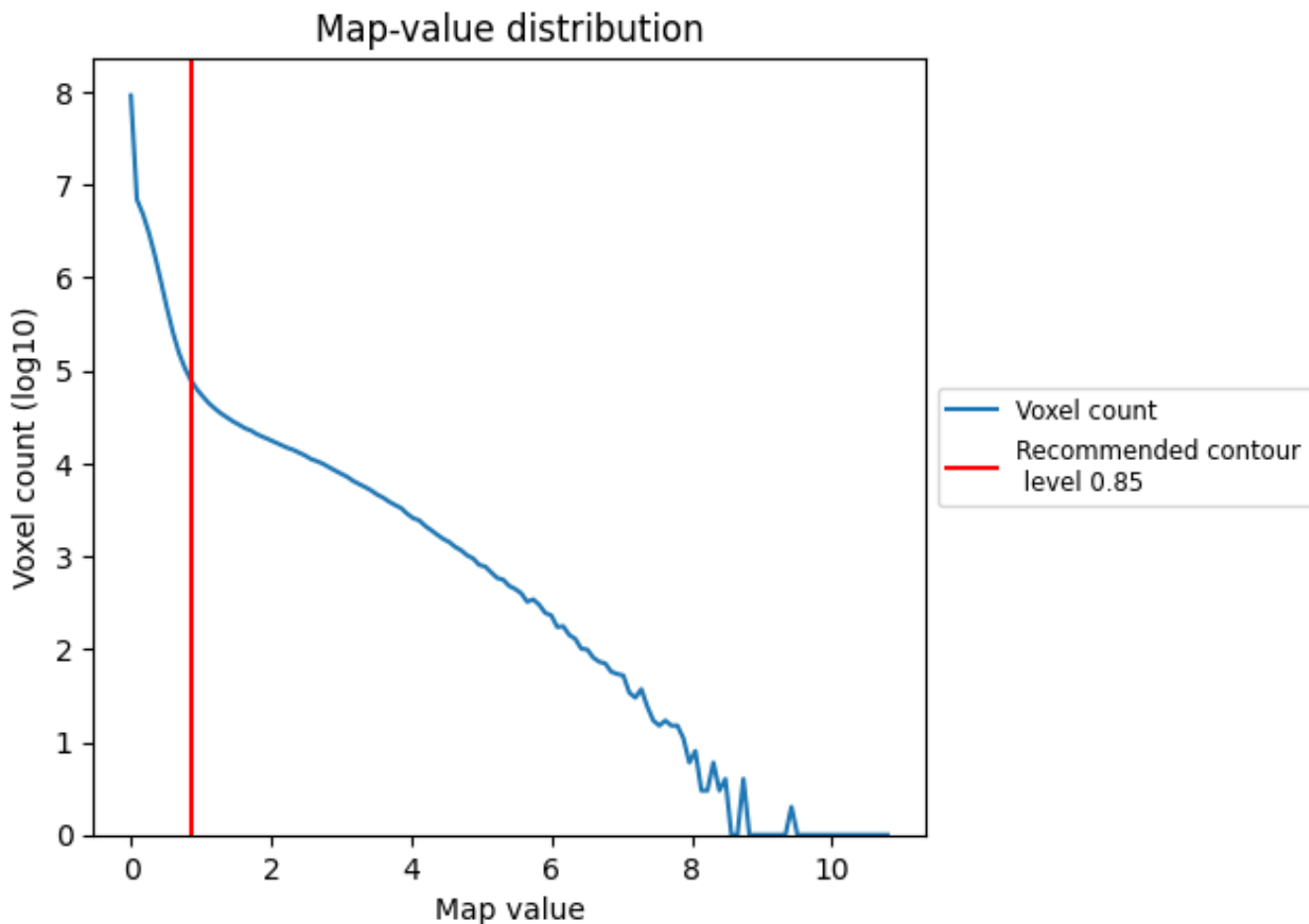


Z

## 7 Map analysis [i](#)

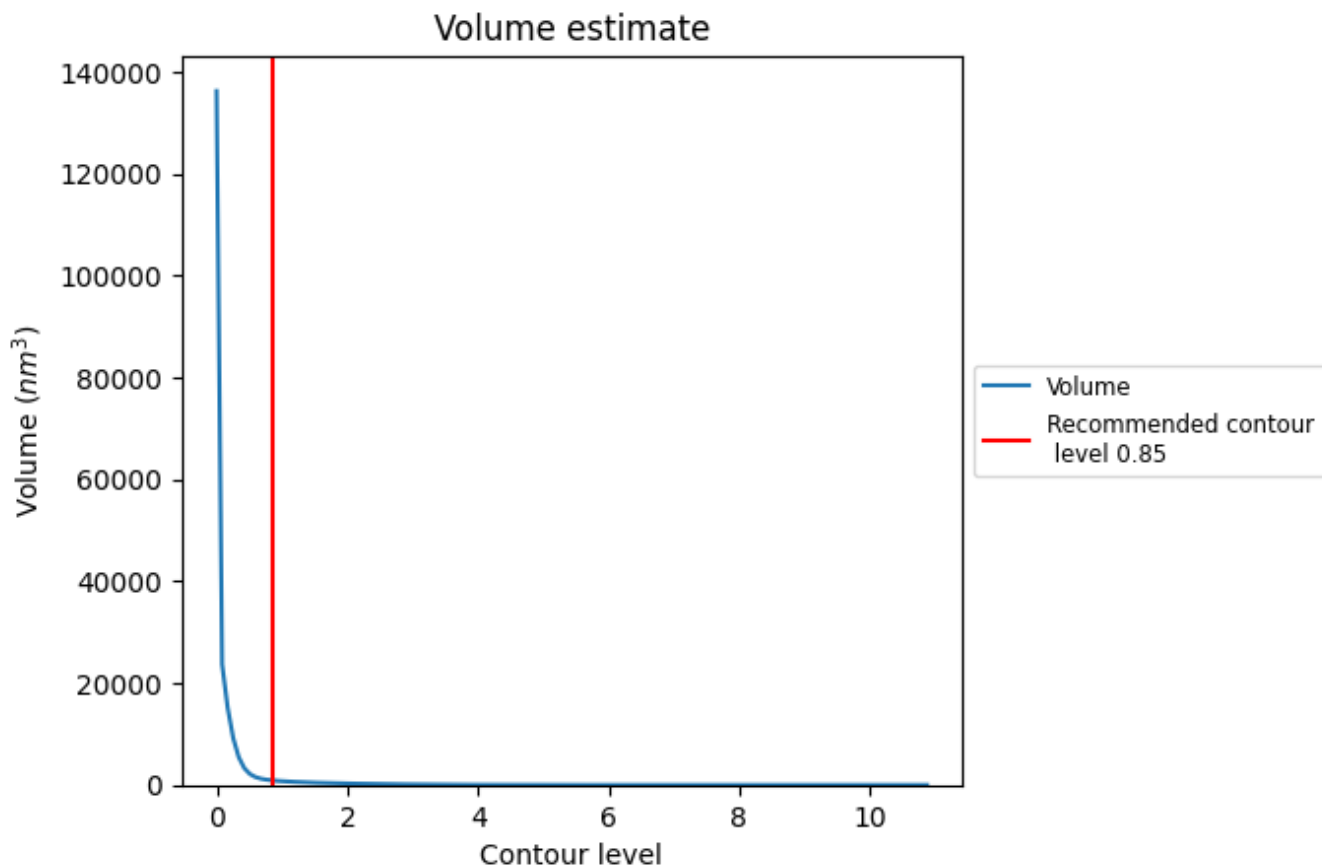
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

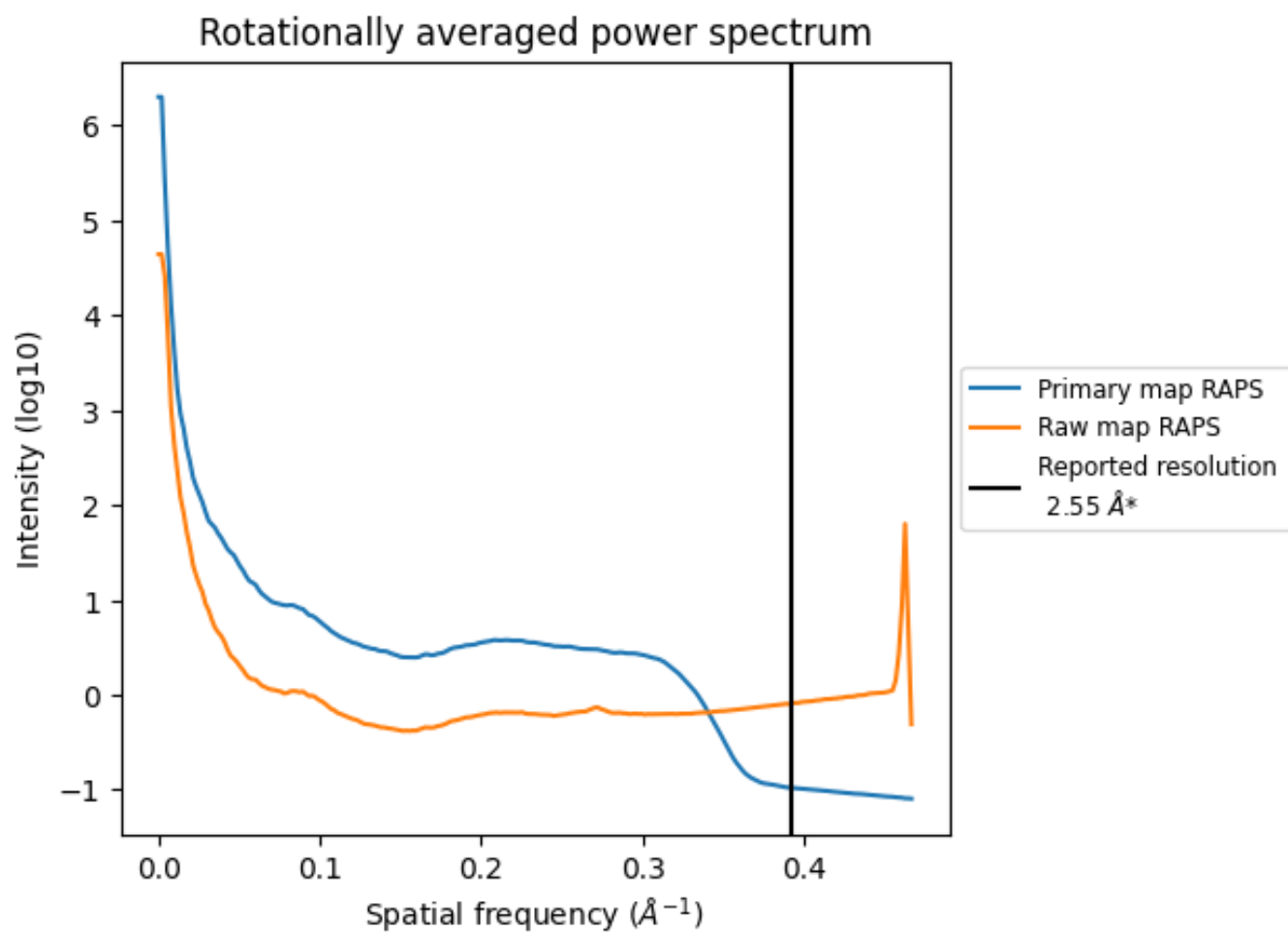
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 895  $\text{nm}^3$ ; this corresponds to an approximate mass of 809 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

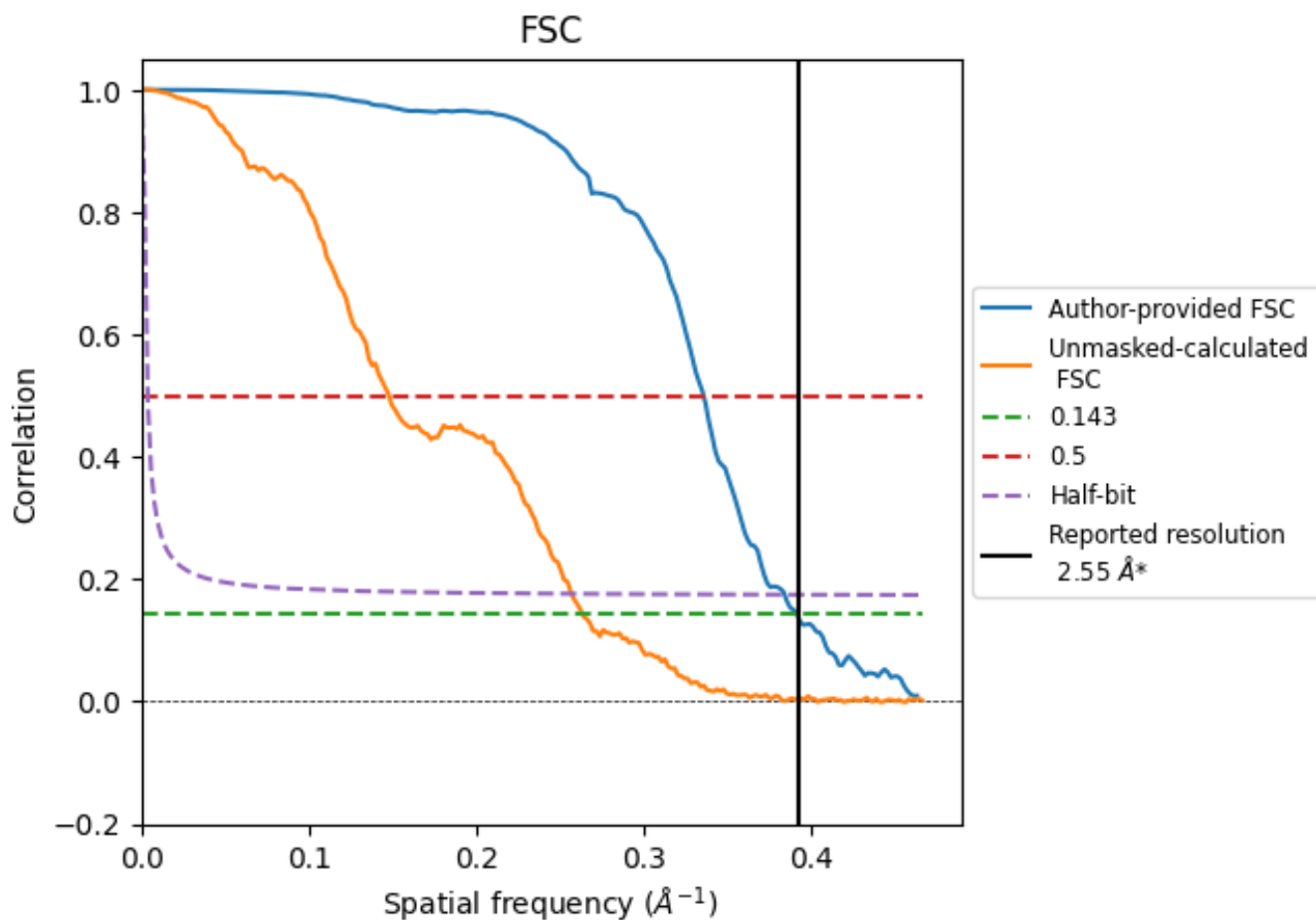


\*Reported resolution corresponds to spatial frequency of  $0.392 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.392 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

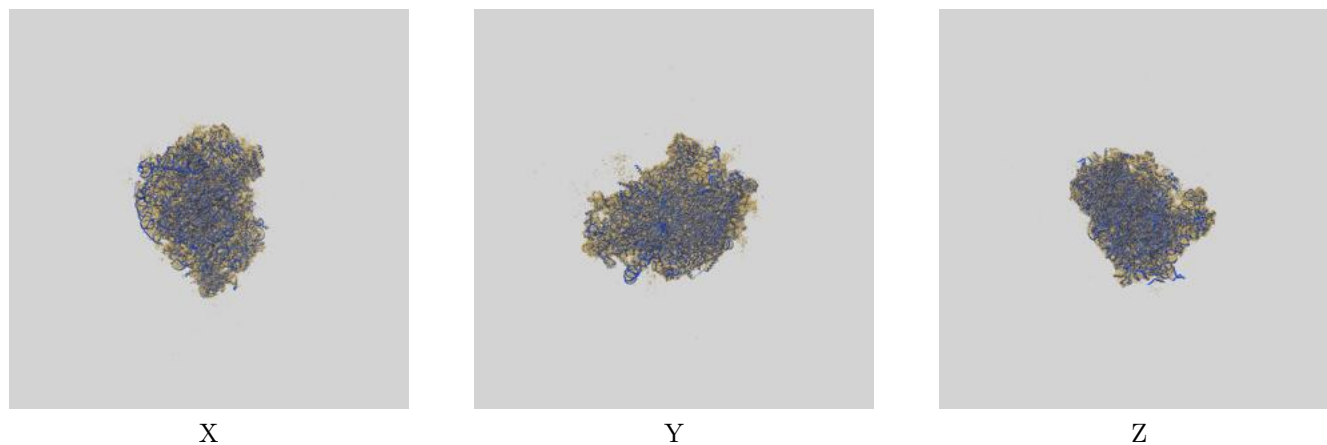
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.98	2.60
Unmasked-calculated*	3.79	6.76	3.89

\*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 3.79 differs from the reported value 2.55 by more than 10 %

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

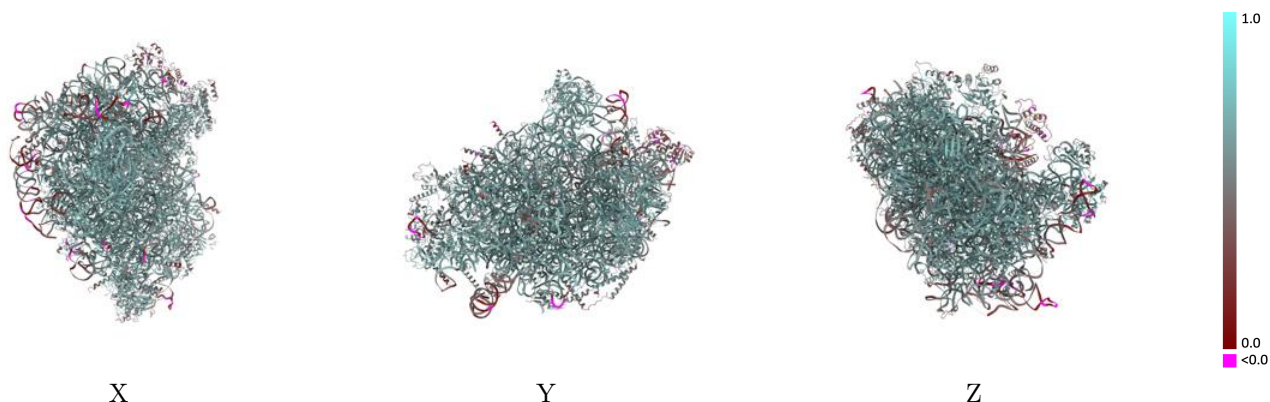
This section contains information regarding the fit between EMDB map EMD-29273 and PDB model 8FLB. Per-residue inclusion information can be found in section 3 on page 16.

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



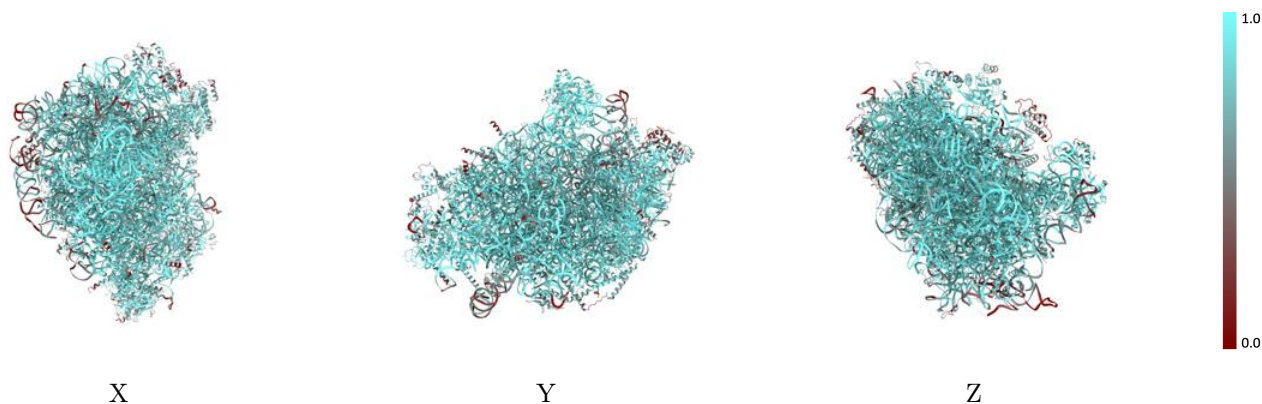
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



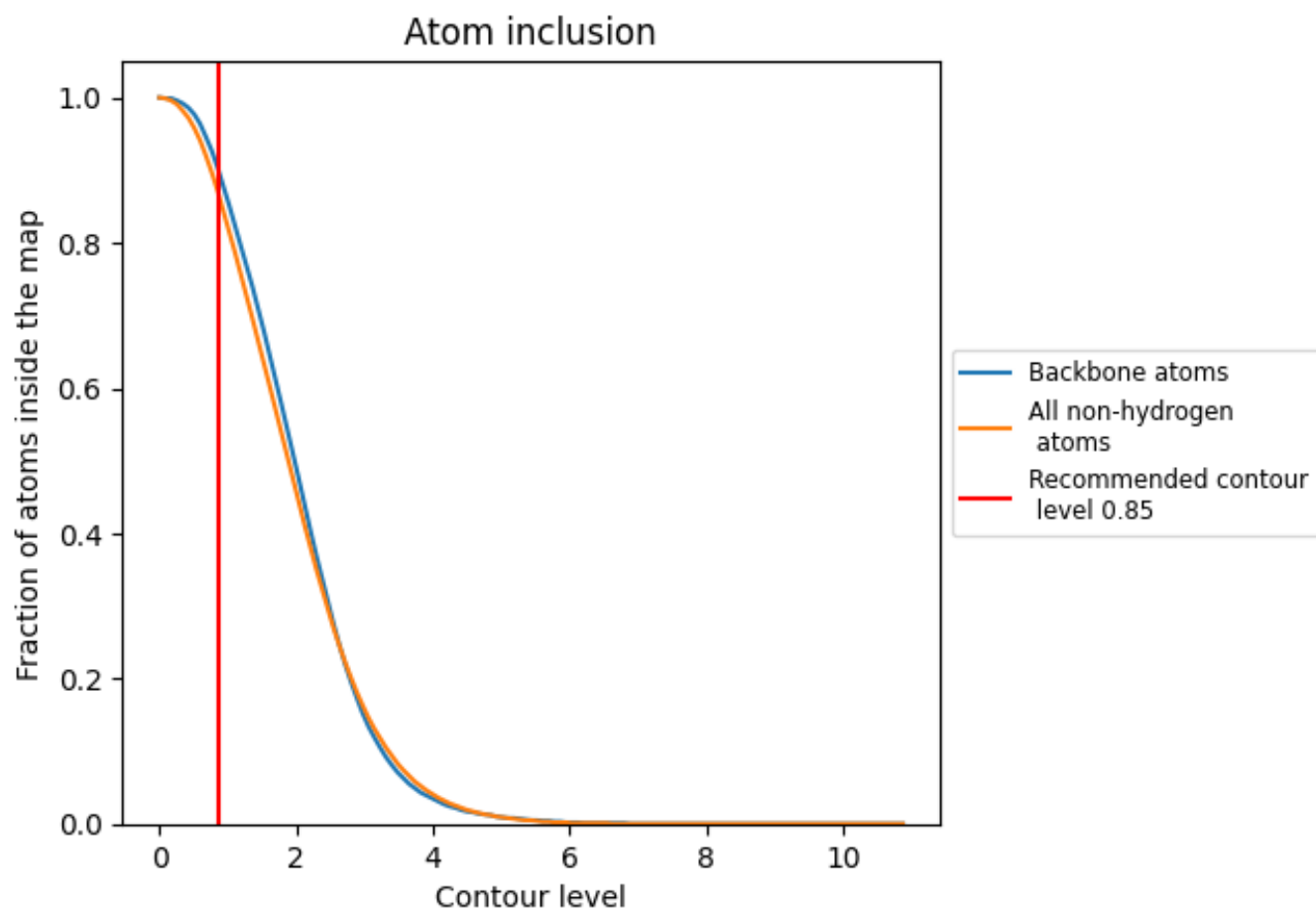
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.5870
BA	 0.3030	 0.2780
L1	 0.9500	 0.6260
L3	 0.8850	 0.5750
L4	 0.9790	 0.6330
L5	 0.8200	 0.5590
L6	 0.8020	 0.5790
L7	 0.9030	 0.6290
L8	 0.8980	 0.6220
L9	 0.9670	 0.6580
LA	 0.8850	 0.6160
LB	 0.9200	 0.6320
LC	 0.9630	 0.6630
LD	 0.8400	 0.6000
LE	 0.8890	 0.6040
LF	 0.7830	 0.5740
LG	 0.9050	 0.6230
LH	 0.8680	 0.6240
LI	 0.8510	 0.5950
LJ	 0.9210	 0.6290
LK	 0.9230	 0.6380
LL	 0.8790	 0.6050
LM	 0.7290	 0.5260
LN	 0.8920	 0.6210
LO	 0.8040	 0.5850
LP	 0.8400	 0.6000
LQ	 0.8940	 0.6210
LR	 0.9180	 0.6230
LS	 0.8590	 0.6110
LT	 0.9410	 0.6420
LU	 0.7890	 0.5700
LV	 0.8900	 0.6120
LW	 0.9420	 0.6400
LX	 0.8070	 0.5880
LY	 0.7380	 0.5760



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Chain	Atom inclusion	Q-score
LZ	 0.9410	 0.6340
NK	 0.6580	 0.5260
NL	 0.8070	 0.5740
NP	 0.8310	 0.5860
NR	 0.7370	 0.5440
SA	 0.8940	 0.6190
SB	 0.8880	 0.6060
SC	 0.7640	 0.5620
SD	 0.8830	 0.6170
SE	 0.8610	 0.5990
SF	 0.9230	 0.6360
SG	 0.9000	 0.6130
SH	 0.6820	 0.5050
SI	 0.7270	 0.5360
SK	 0.8420	 0.5870
SM	 0.9010	 0.6190
SQ	 0.6030	 0.3730
SR	 0.7780	 0.5580
SV	 0.8330	 0.5850
VB	 0.6450	 0.5280