



# wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 11:01 PM EST

PDB ID : 8FL7  
EMDB ID : EMD-29269  
Title : Human nuclear pre-60S ribosomal subunit (State J2)  
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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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) : 2.40

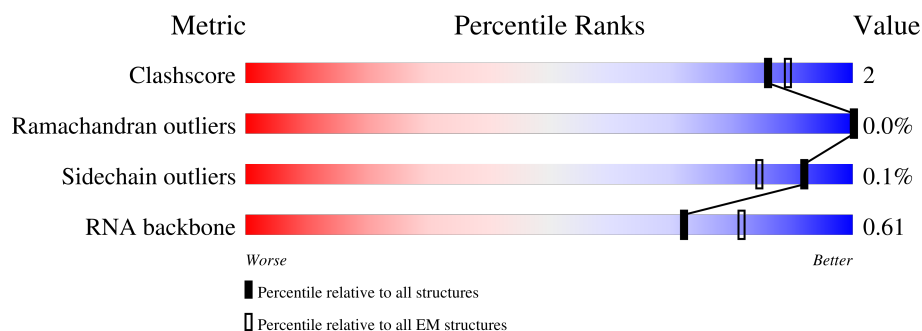
# 1 Overall quality at a glance

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.




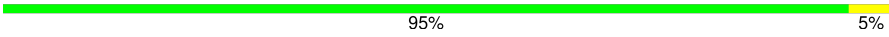

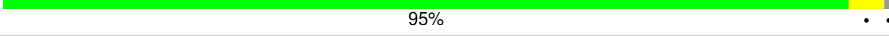
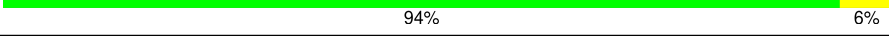

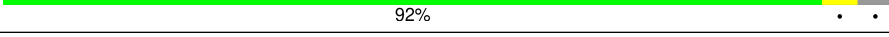

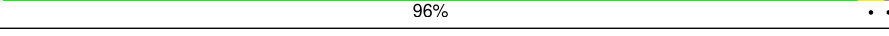

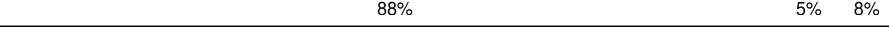
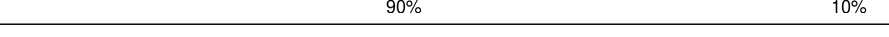
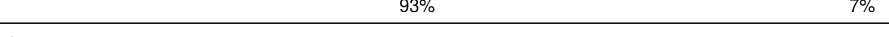
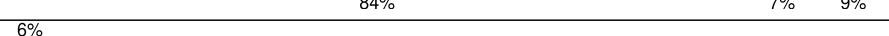

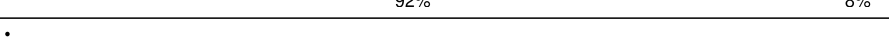
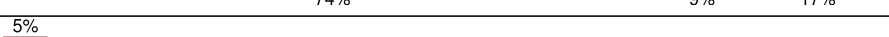

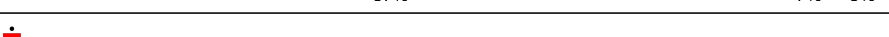






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	<div> <div>59%</div> <div>93%</div> </div>
2	L1	157	<div> <div>80%</div> <div>15%</div> </div>
3	L3	5070	<div> <div>53%</div> <div>12%</div> <div>33%</div> </div>
4	L4	121	<div> <div>83%</div> <div>14%</div> </div>
5	L5	178	<div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
6	L6	211	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>
7	L7	203	<div> <div>94%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
8	L8	215	
9	L9	204	
10	LA	184	
11	LB	188	
12	LC	176	
13	LD	196	
14	LE	160	
15	LF	128	
16	LG	140	
17	LH	156	
18	LI	145	
19	LJ	136	
20	LK	148	
21	LL	137	
22	LM	159	
23	LN	403	
24	LO	115	
25	LP	125	
26	LQ	135	
27	LR	117	
28	LS	123	
29	LT	110	
30	LU	105	
31	LV	106	
32	LW	97	

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Mol	Chain	Length	Quality of chain
33	LX	92	
34	LY	70	
35	LZ	51	
36	NC	731	
37	NF	260	
38	NK	129	
39	NL	478	
40	NP	134	
41	SA	427	
42	SB	297	
43	SC	288	
44	SD	248	
45	SE	266	
46	SF	257	
47	SG	192	
48	SH	293	
49	SI	255	
50	SK	245	
51	SM	588	
52	SQ	239	
53	SR	634	
54	SV	163	

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149506 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
1	BA	160	Total	C	N	O	S	0	0
			954	570	188	193	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	3409	Total	C	N	O	P	0	0
			73178	32611	13401	23757	3409		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
28	LS	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

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

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

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

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

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

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

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

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

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

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

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

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

- 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 Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NC	44	Total	C	N	O	S	0	0
			219	131	44	44			

- Molecule 37 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NF	71	Total	C	N	O	S	0	0
			626	392	129	102	3		

- Molecule 38 is a protein called Protein LLP homolog.

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

- Molecule 39 is a protein called Ribosome biogenesis protein NOP53.

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

- Molecule 40 is a protein called Zinc finger protein 593.

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

- Molecule 41 is a protein called 60S ribosomal protein L4.

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

- Molecule 42 is a protein called 60S ribosomal protein L5.

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

- Molecule 43 is a protein called 60S ribosomal protein L6.

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

- Molecule 44 is a protein called 60S ribosomal protein L7.

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

- Molecule 45 is a protein called 60S ribosomal protein L7a.

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

- Molecule 46 is a protein called 60S ribosomal protein L8.

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

- Molecule 47 is a protein called 60S ribosomal protein L9.

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

- Molecule 48 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

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

- Molecule 49 is a protein called 60S ribosomal protein L7-like 1.

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

- Molecule 50 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 51 is a protein called Pescadillo homolog.

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

- Molecule 52 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SQ	217	Total	C	N	O	S	0	0
			1771	1129	311	320	11		

- Molecule 53 is a protein called GTP-binding protein 4.

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

- Molecule 54 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	L1	4	Total	Mg	0
			4	4	
55	L3	73	Total	Mg	0
			73	73	
55	L4	3	Total	Mg	0
			3	3	

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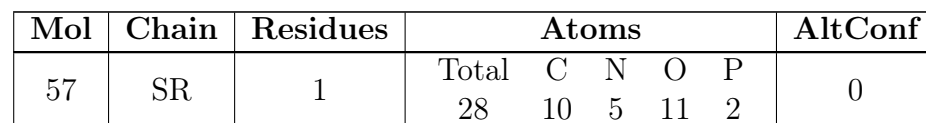
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Mol	Chain	Residues	Atoms		AltConf
55	LG	1	Total 1	Mg 1	0
55	LQ	1	Total 1	Mg 1	0
55	LR	1	Total 1	Mg 1	0
55	LT	1	Total 1	Mg 1	0
55	LW	1	Total 1	Mg 1	0
55	SA	1	Total 1	Mg 1	0
55	SF	1	Total 1	Mg 1	0
55	SR	1	Total 1	Mg 1	0

- Molecule 56 is ZINC ION (three-letter code: 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 (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

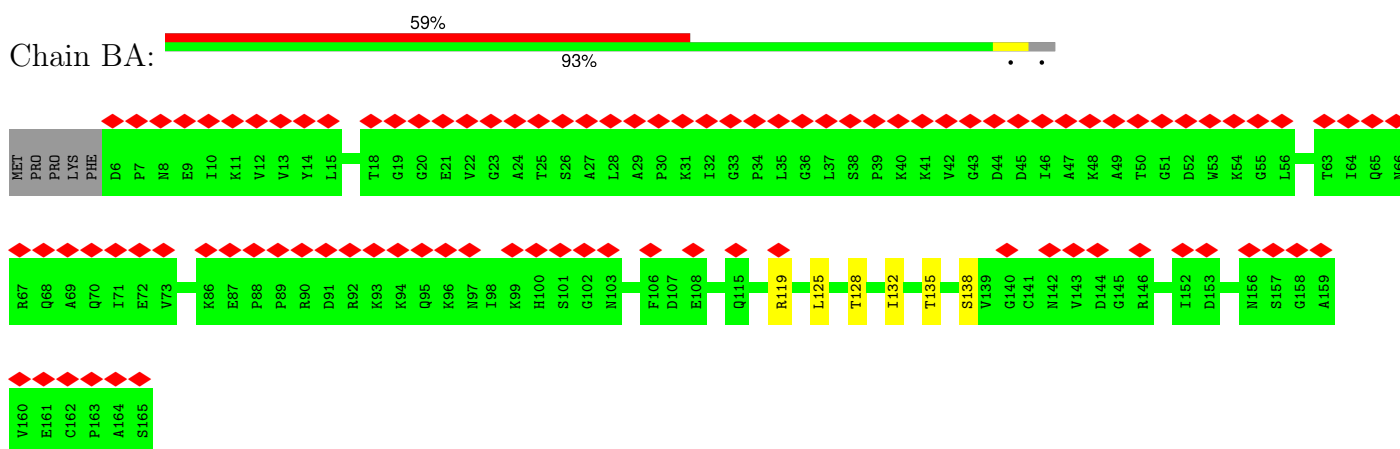


- | Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 58  | SR    | 1        | Total K<br>1 1 | 0       |

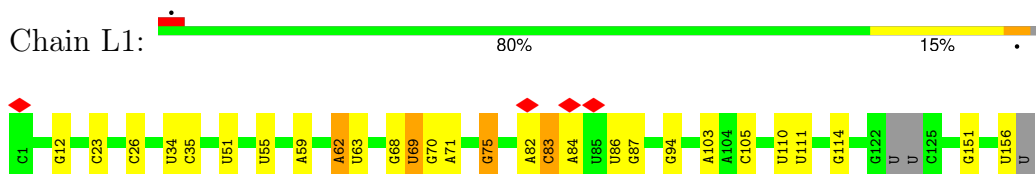
### 3 Residue-property plots

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.

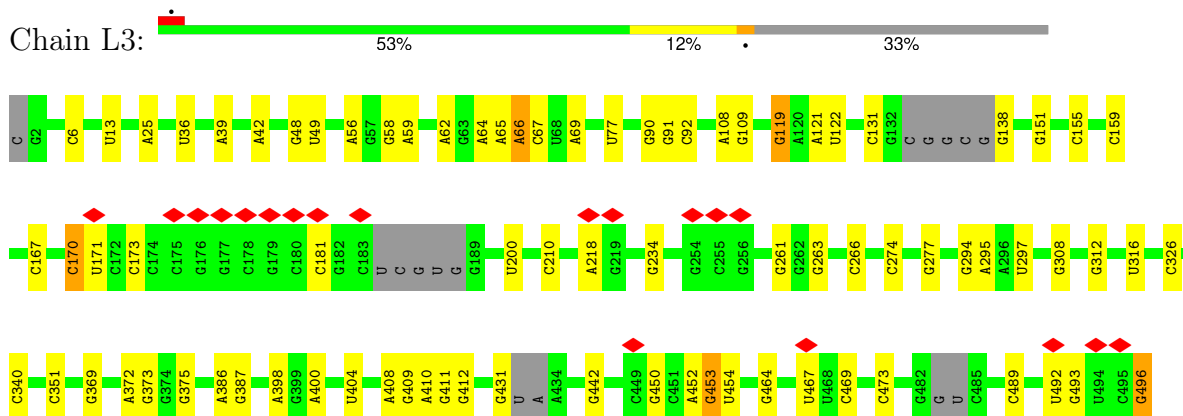
#### • Molecule 1: 60S ribosomal protein L12



#### • Molecule 2: 5.8S rRNA

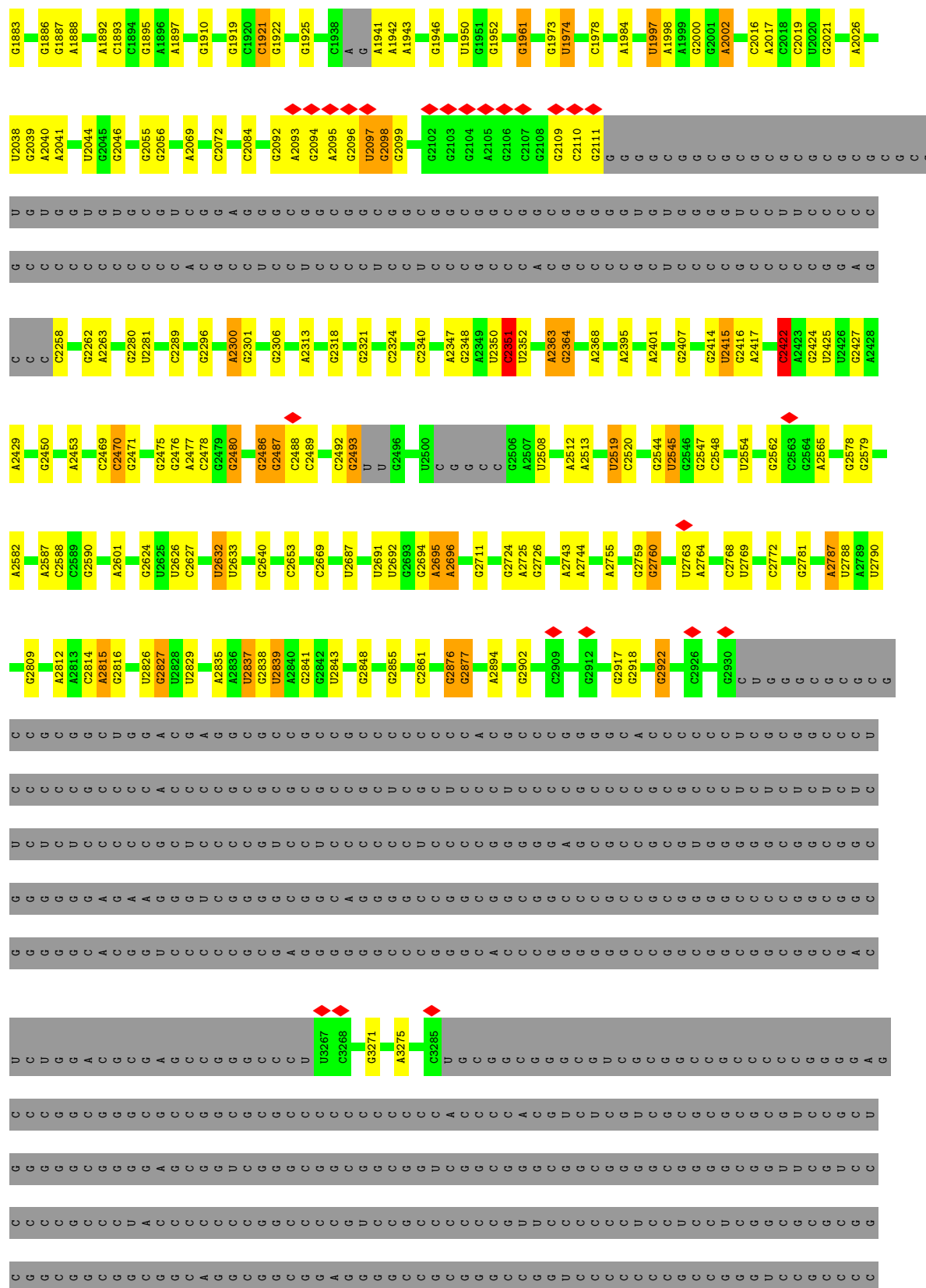


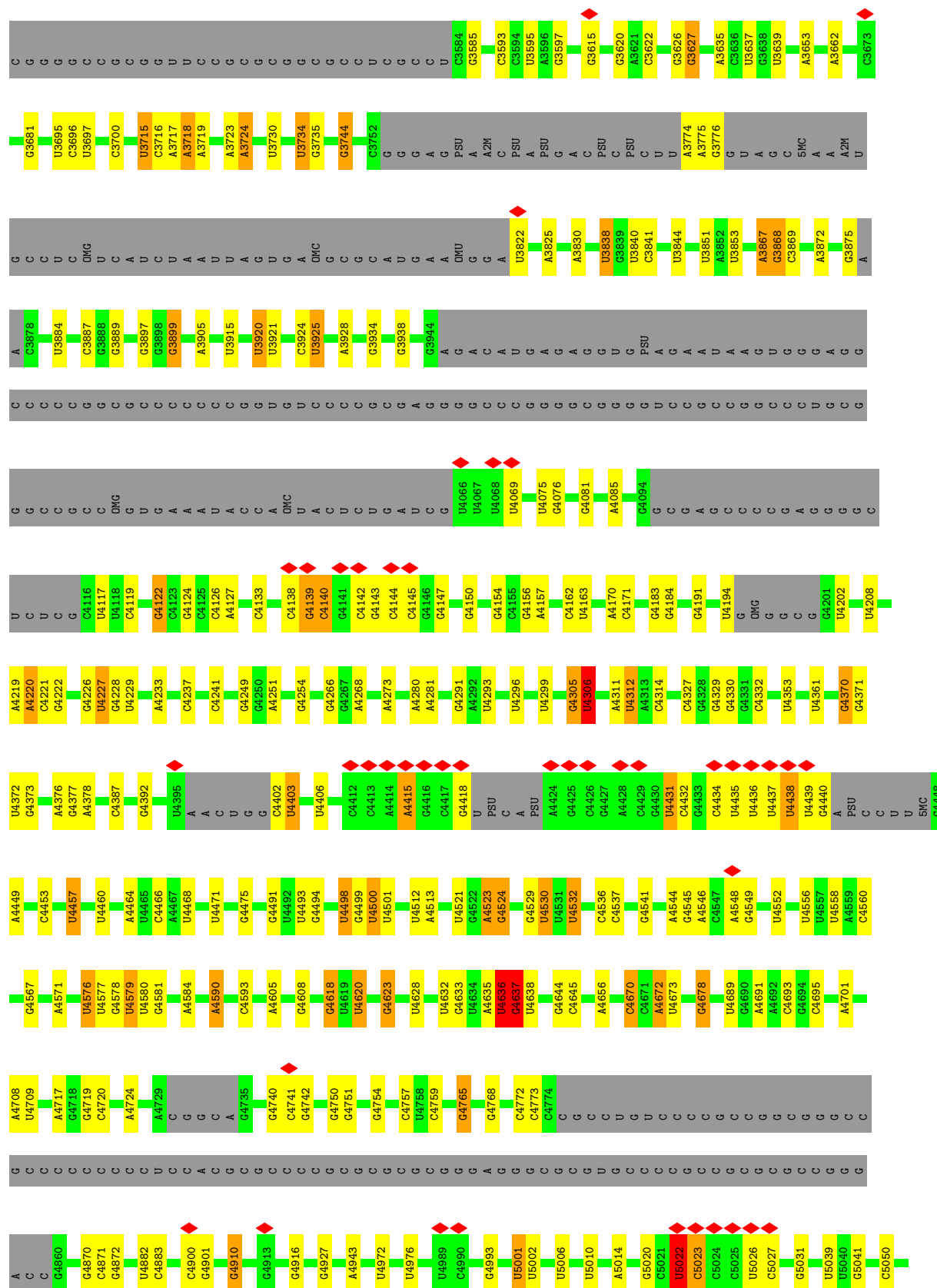
#### • Molecule 3: 28S rRNA





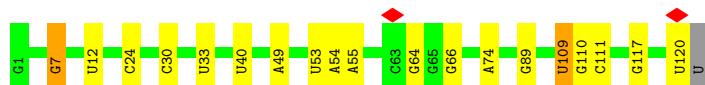
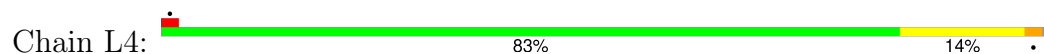




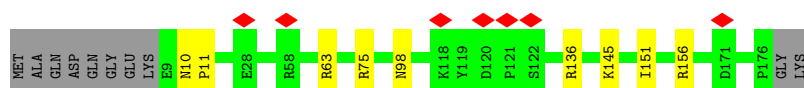




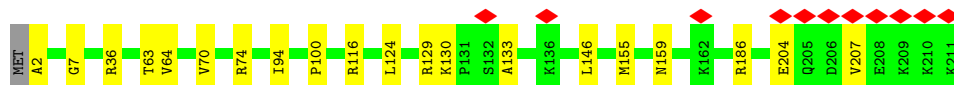
• Molecule 4: 5S rRNA



• Molecule 5: 60S ribosomal protein L11



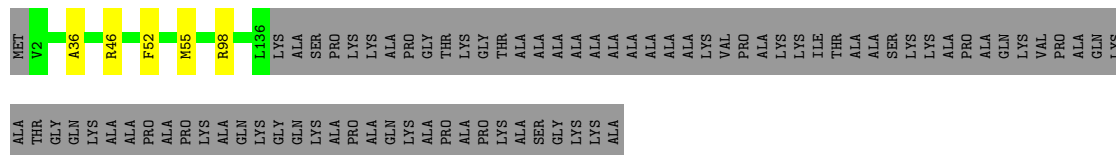
• Molecule 6: 60S ribosomal protein L13



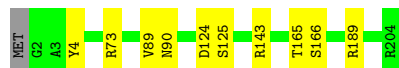
• Molecule 7: 60S ribosomal protein L13a



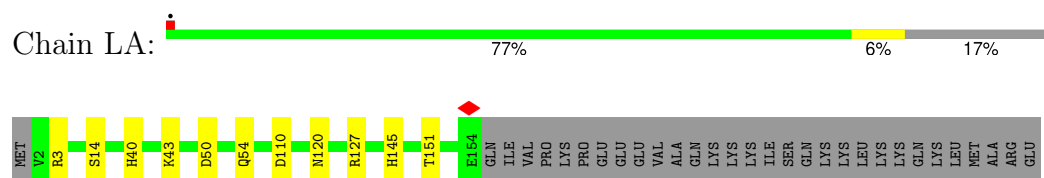
• Molecule 8: 60S ribosomal protein L14



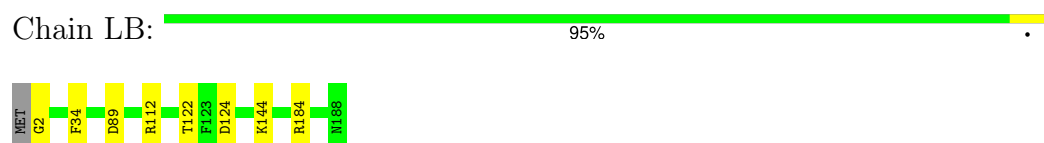
• Molecule 9: 60S ribosomal protein L15



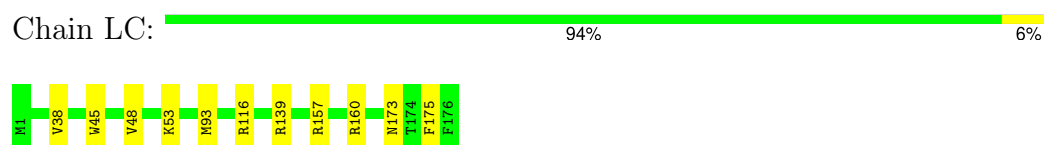
## • Molecule 10: 60S ribosomal protein L17



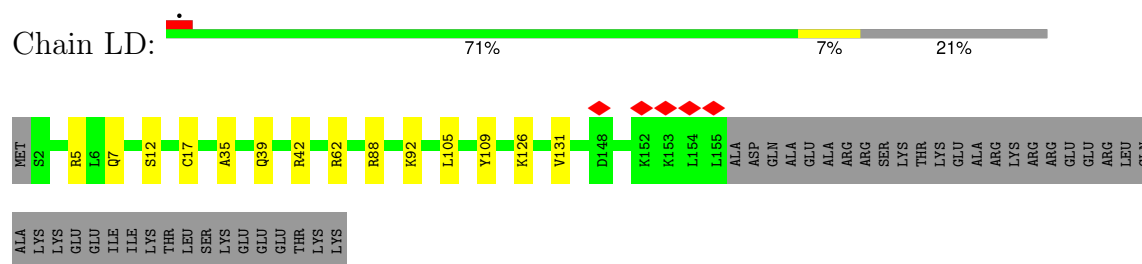
## • Molecule 11: 60S ribosomal protein L18



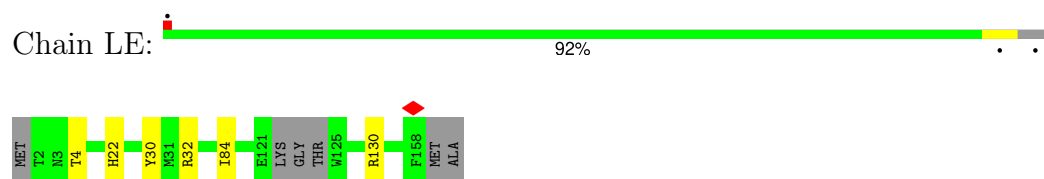
## • Molecule 12: 60S ribosomal protein L18a



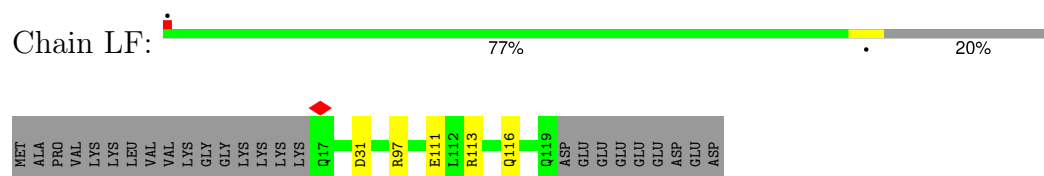
## • Molecule 13: 60S ribosomal protein L19



## • Molecule 14: 60S ribosomal protein L21



## • Molecule 15: 60S ribosomal protein L22

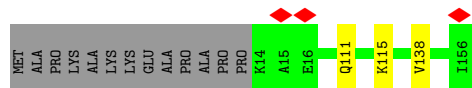


## • Molecule 16: 60S ribosomal protein L23

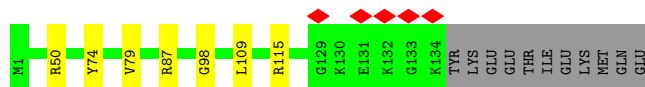




- Molecule 17: 60S ribosomal protein L23a



- Molecule 18: 60S ribosomal protein L26



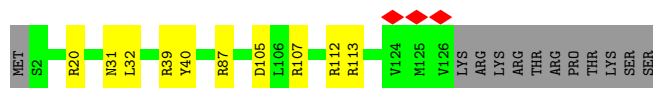
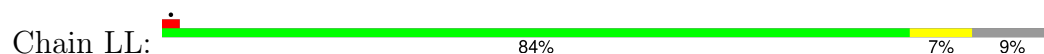
- Molecule 19: 60S ribosomal protein L27



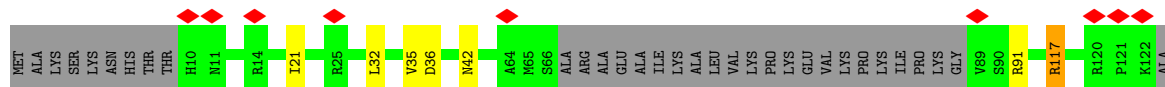
- Molecule 20: 60S ribosomal protein L27a



- Molecule 21: 60S ribosomal protein L28



- Molecule 22: 60S ribosomal protein L29




LYS  
ALA  
LYS  
LYS  
LYS  
LYS  
LYS  
ASP  
GLN  
THR  
LYS  
ALA  
GLN  
ALA  
ALA  
ALA  
PRO  
ALA  
SER  
VAL  
PRO  
GLN  
GLN  
ALA  
PRO  
LYS  
ARG  
THR  
GLN  
ALA  
PRO  
THR  
LYS  
ALA  
SER  
GLU

- Molecule 23: 60S ribosomal protein L3

Chain LN:  92% 8%


MET S2 R10 L14 V29 K30 V67 Y92 T95 G98 T104 A107 D141 E182 L201 I217 I220 G221 V222 T223 K224 Y228 H245 R246 A252 T278 E279 D295 G296 D306 Y307 D308 L333 V338 G339 T340 R343  
R348 T370 K385 E400 E401 G402 A403

- Molecule 24: 60S ribosomal protein L30

Chain LO:  74% 9% 17%


MET VAL ALA ALA LYS LYS THR LYS LYS SER SER LEU GLU S13 I14 N15 S16 R17 Y31 E59 N78 I79 S102 R106 S107 MET PRO GLU GLN THR GLY GLU LYS

- Molecule 25: 60S ribosomal protein L31

Chain LP:  5% 82% 15%

MET ALA PRO ALA LYS LYS GLY GLY GLU LYS LYS LYS GLY ARG SER ALA ILE N18 M57 R90 E94 D95 E96 D97 S98 D123 GLU ASN

- Molecule 26: 60S ribosomal protein L32

Chain LQ:  87% 7% 5%

MET A2 D26 R27 I31 L78 E84 V87 L88 L89 E98 L118 R128 L129 ARG SER GLU GLU ASN GLU

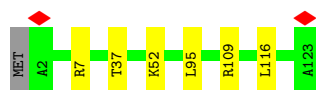
- Molecule 27: 60S ribosomal protein L34

Chain LR:  91% 5%

MET Y2 K40 S44 A45 C46 R93 I97 E98 Q112 S113 GLN LYS LYS ALA LYS

- Molecule 28: 60S ribosomal protein L35

Chain LS:  94% 5%



- Molecule 29: 60S ribosomal protein L35a

Chain LT: 95% 5% .



- Molecule 30: 60S ribosomal protein L36

Chain LU: 5% 90% 8% .



- Molecule 31: 60S ribosomal protein L36a

Chain LV: 5% 92% 7% .



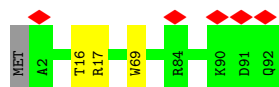
- Molecule 32: 60S ribosomal protein L37

Chain LW: 82% 6% 11%



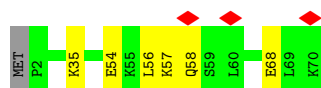
- Molecule 33: 60S ribosomal protein L37a

Chain LX: 5% 96% . .

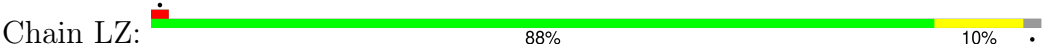


- Molecule 34: 60S ribosomal protein L38

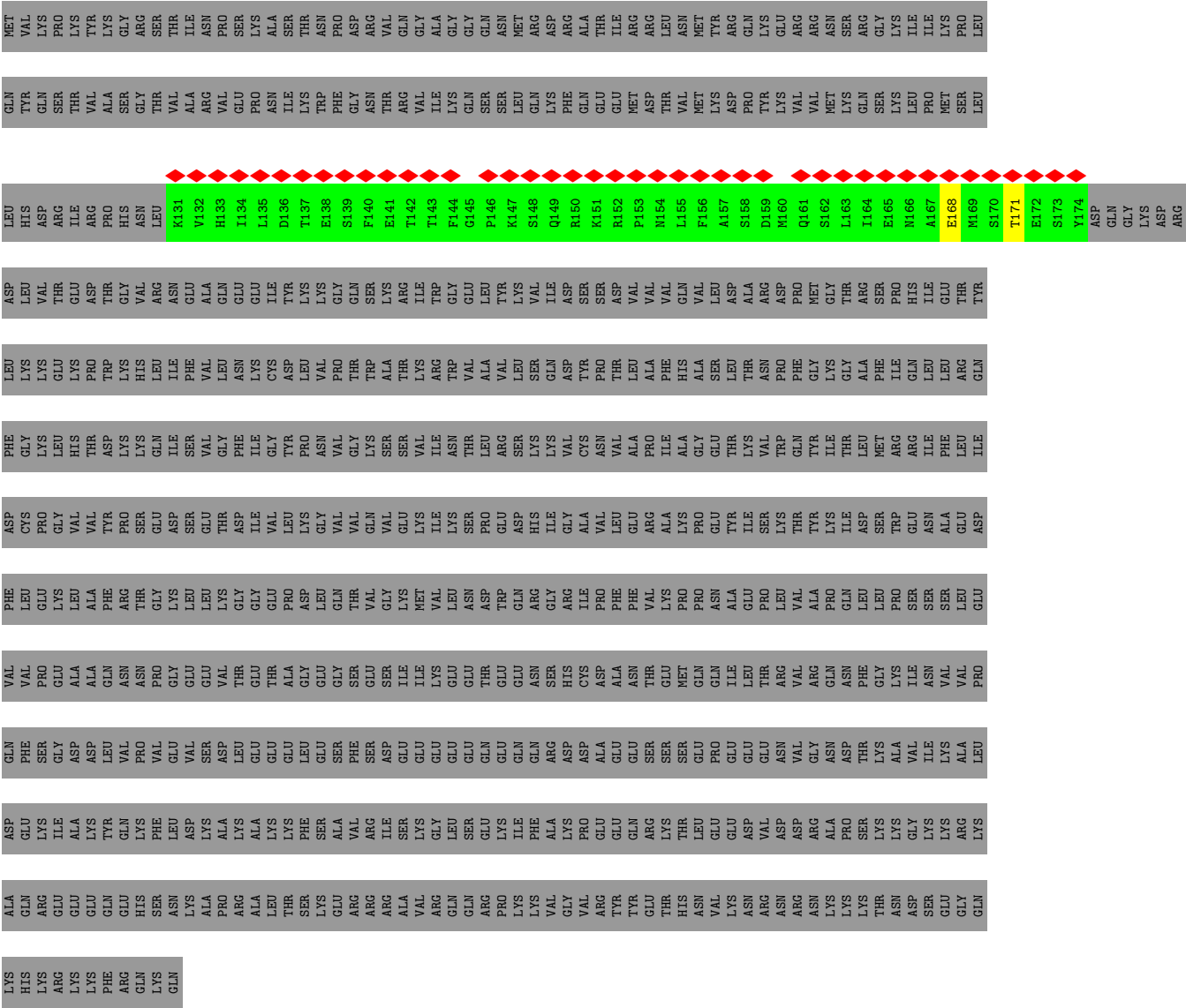
Chain LY: 5% 90% 9% .



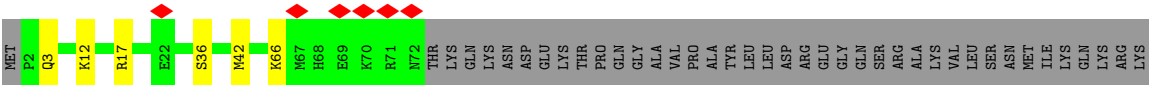
- Molecule 35: 60S ribosomal protein L39



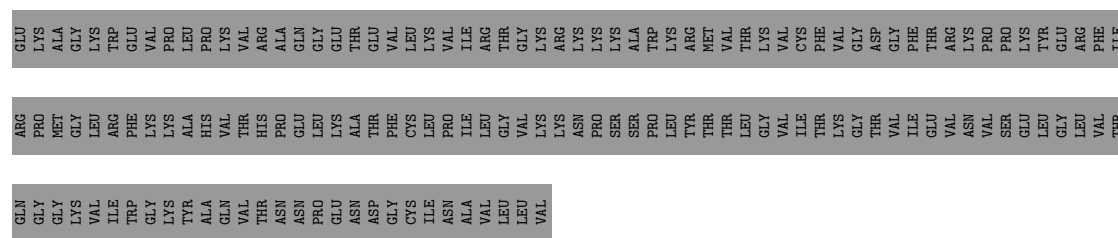
● Molecule 36: Nucleolar GTP-binding protein 2



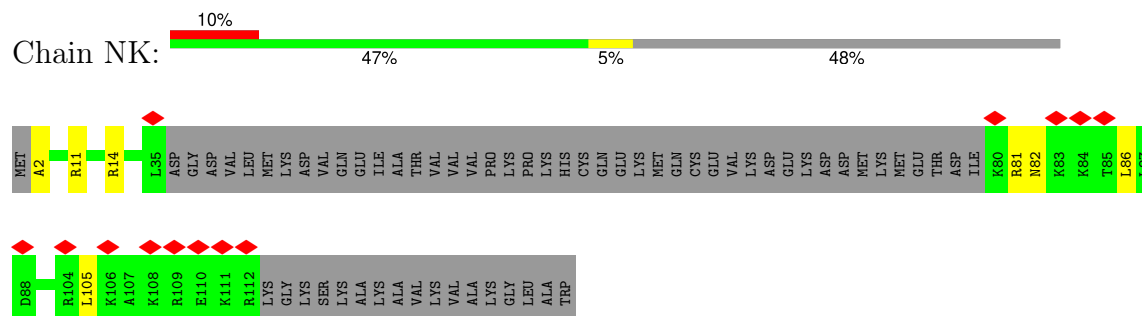
● Molecule 37: Ribosome biogenesis protein NSA2 homolog



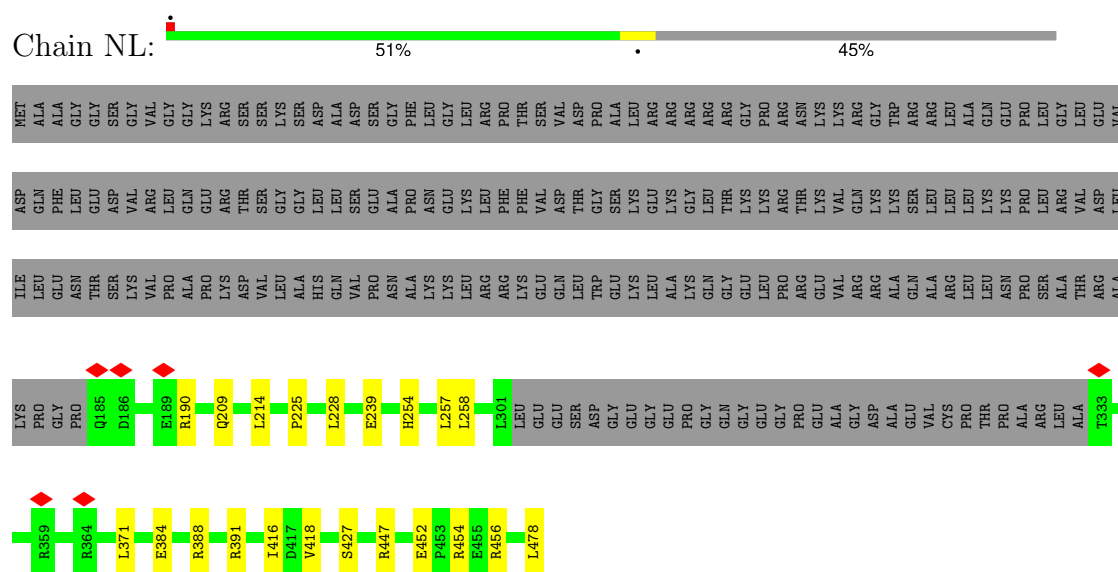




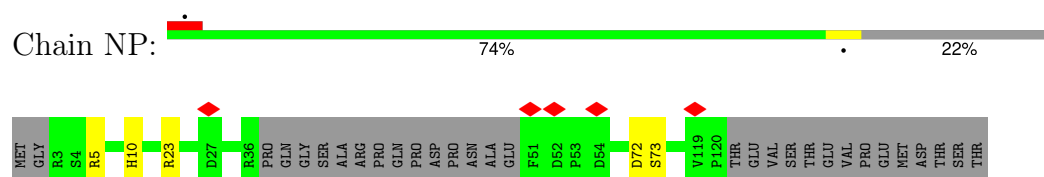
- Molecule 38: Protein LLP homolog



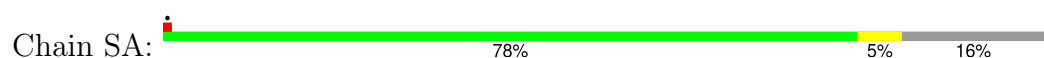
- Molecule 39: Ribosome biogenesis protein NOP53

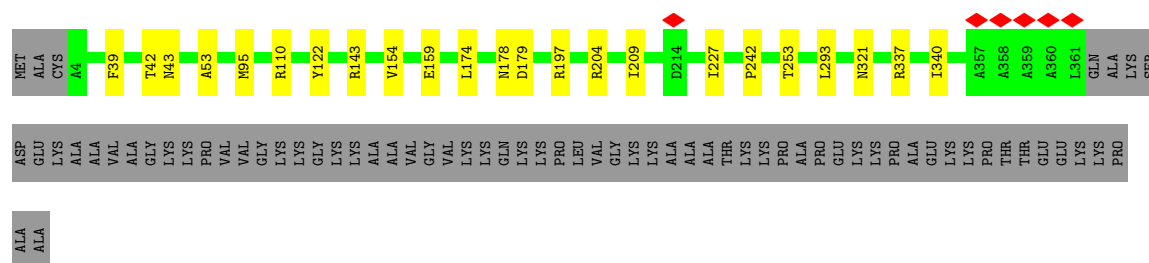


- Molecule 40: Zinc finger protein 593

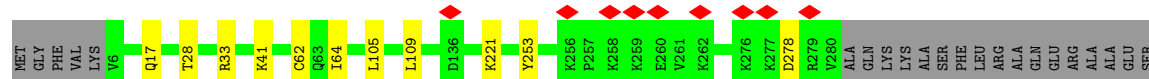
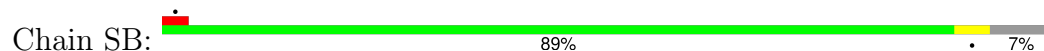


- Molecule 41: 60S ribosomal protein L4

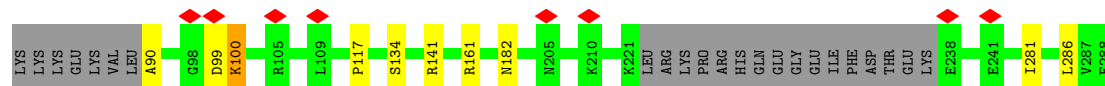
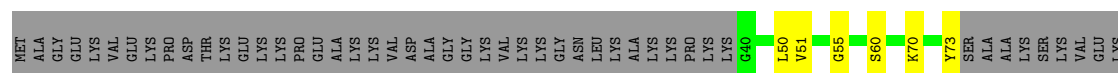




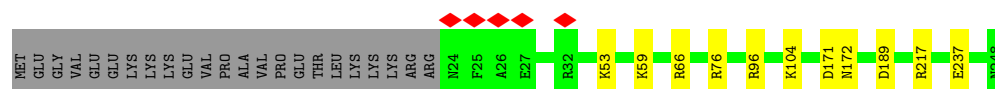
- Molecule 42: 60S ribosomal protein L5



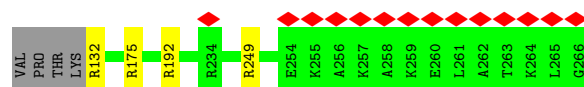
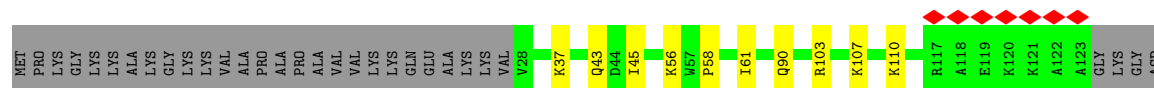
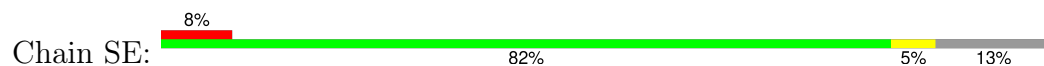
- Molecule 43: 60S ribosomal protein L6



- Molecule 44: 60S ribosomal protein L7



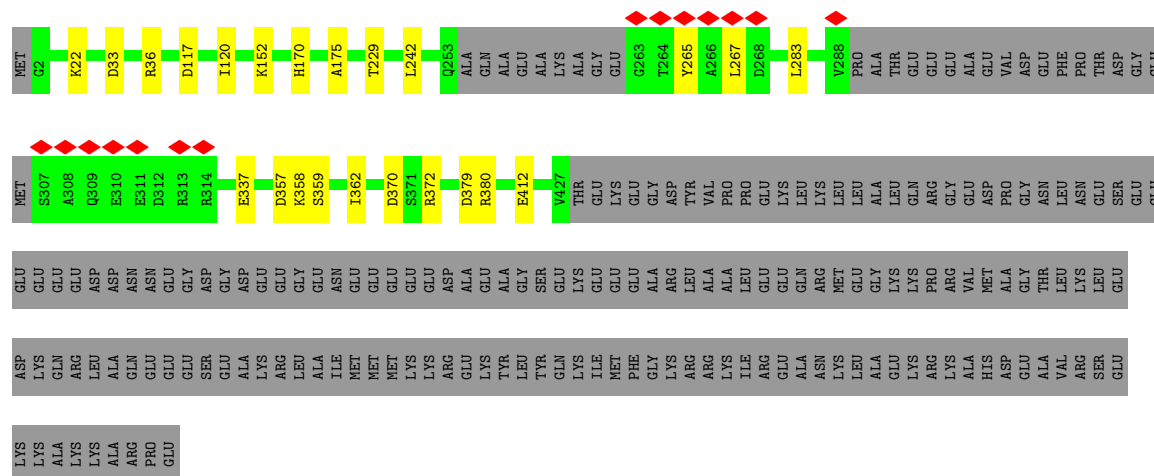
- Molecule 45: 60S ribosomal protein L7a



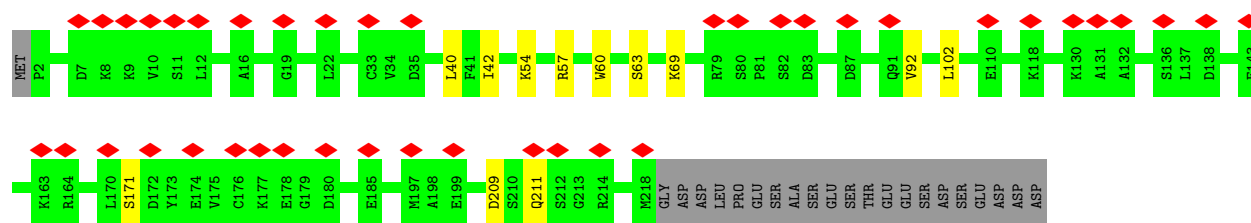
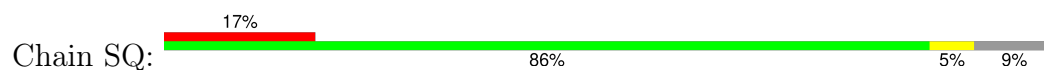
- Molecule 46: 60S ribosomal protein L8



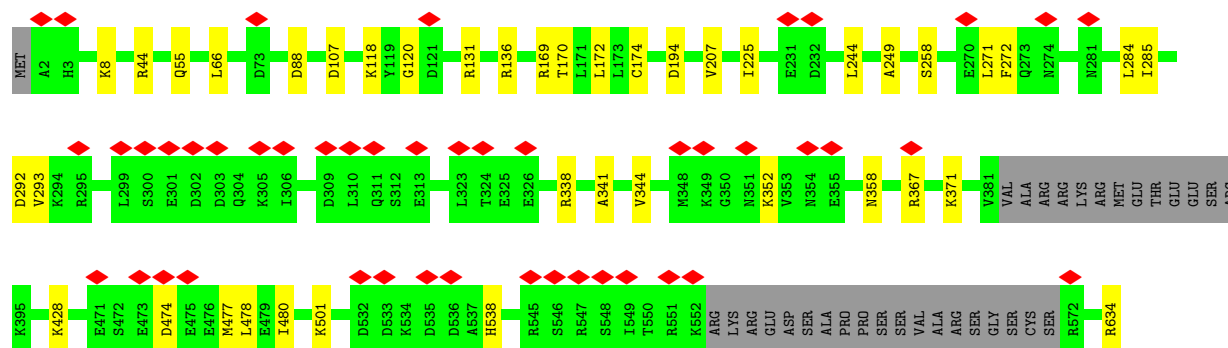
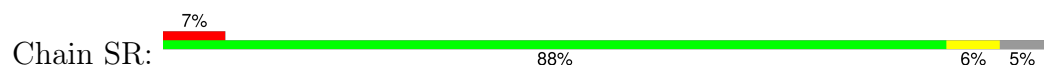




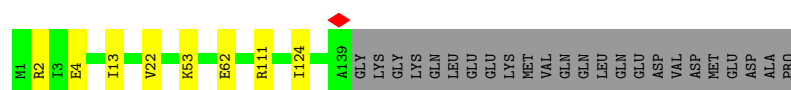
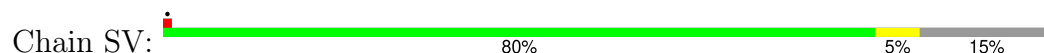
- Molecule 52: mRNA turnover protein 4 homolog



- Molecule 53: GTP-binding protein 4



- Molecule 54: Probable ribosome biogenesis protein RLP24



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74556	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	8.592	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.184	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: OMU, K, 6MZ, PSU, UR3, A2M, OMC, MG, OMG, HIC, ZN, GDP

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	0.24	0/959	0.47	0/1312
2	L1	0.35	0/3589	0.74	0/5589
3	L3	0.33	0/79388	0.77	9/123813 (0.0%)
4	L4	0.43	0/2861	0.79	0/4459
5	L5	0.26	0/1372	0.57	0/1836
6	L6	0.25	0/1732	0.59	0/2315
7	L7	0.26	0/1682	0.55	0/2250
8	L8	0.25	0/1133	0.51	0/1516
9	L9	0.27	0/1746	0.63	0/2338
10	LA	0.25	0/1268	0.53	0/1701
11	LB	0.26	0/1536	0.64	0/2052
12	LC	0.30	0/1501	0.58	0/2013
13	LD	0.23	0/1305	0.60	0/1727
14	LE	0.28	0/1291	0.56	0/1724
15	LF	0.26	0/856	0.51	0/1149
16	LG	0.26	0/1048	0.57	0/1402
17	LH	0.25	0/1175	0.52	0/1572
18	LI	0.27	0/1132	0.59	0/1504
19	LJ	0.29	0/1130	0.55	0/1507
20	LK	0.26	0/1191	0.54	0/1591
21	LL	0.24	0/1017	0.59	0/1364
22	LM	0.26	0/763	0.58	0/1005
23	LN	0.26	0/3294	0.54	0/4406
24	LO	0.26	0/748	0.48	0/1004
25	LP	0.25	0/894	0.58	0/1204
26	LQ	0.25	0/1071	0.56	0/1429
27	LR	0.26	0/898	0.61	0/1197
28	LS	0.24	0/1023	0.56	0/1351
29	LT	0.26	0/895	0.61	0/1198
30	LU	0.24	0/843	0.58	0/1115
31	LV	0.28	0/864	0.60	0/1140
32	LW	0.27	0/720	0.64	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	LX	0.25	0/718	0.55	0/953
34	LY	0.25	0/575	0.50	0/761
35	LZ	0.24	0/454	0.60	0/599
36	NC	0.21	0/218	0.36	0/303
37	NF	0.26	0/637	0.55	0/834
38	NK	0.23	0/587	0.59	0/767
39	NL	0.24	0/2207	0.58	0/2955
40	NP	0.24	0/864	0.61	0/1154
41	SA	0.25	0/2907	0.56	0/3905
42	SB	0.29	0/2287	0.54	0/3065
43	SC	0.25	0/1781	0.55	0/2388
44	SD	0.26	0/1905	0.56	0/2539
45	SE	0.26	0/1903	0.55	0/2559
46	SF	0.26	0/1914	0.60	0/2567
47	SG	0.25	0/1537	0.54	0/2066
48	SH	0.26	0/794	0.50	0/1071
49	SI	0.24	0/2003	0.52	0/2688
50	SK	0.25	0/1877	0.52	0/2554
51	SM	0.26	0/3357	0.51	0/4529
52	SQ	0.25	0/1806	0.51	0/2420
53	SR	0.24	0/5014	0.51	0/6727
54	SV	0.26	0/1207	0.52	0/1600
All	All	0.30	0/157477	0.69	9/229739 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	2469	C	C2-N1-C1'	6.66	126.12	118.80
3	L3	170	C	C6-N1-C2	-6.42	117.73	120.30
3	L3	2486	G	N1-C6-O6	-5.91	116.36	119.90
3	L3	5022	U	O4'-C1'-N1	5.79	112.83	108.20
3	L3	1961	G	O4'-C1'-N9	5.57	112.65	108.20

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	954	0	690	6	0
2	L1	3278	0	1665	11	0
3	L3	73178	0	37073	293	0
4	L4	2561	0	1295	7	0
5	L5	1349	0	1383	7	0
6	L6	1701	0	1818	15	0
7	L7	1650	0	1794	7	0
8	L8	1111	0	1174	4	0
9	L9	1701	0	1749	7	0
10	LA	1242	0	1269	7	0
11	LB	1512	0	1628	6	0
12	LC	1461	0	1502	9	0
13	LD	1289	0	1429	10	0
14	LE	1264	0	1328	7	0
15	LF	842	0	864	3	0
16	LG	1034	0	1097	3	0
17	LH	1156	0	1268	2	0
18	LI	1115	0	1205	7	0
19	LJ	1107	0	1182	7	0
20	LK	1162	0	1213	8	0
21	LL	1002	0	1068	7	0
22	LM	751	0	820	6	0
23	LN	3239	0	3377	26	0
24	LO	738	0	774	6	0
25	LP	879	0	924	2	0
26	LQ	1053	0	1147	7	0
27	LR	888	0	977	4	0
28	LS	1015	0	1148	6	0
29	LT	876	0	912	4	0
30	LU	832	0	917	7	0
31	LV	851	0	920	6	0
32	LW	705	0	737	5	0
33	LX	708	0	756	3	0
34	LY	569	0	637	5	0
35	LZ	444	0	483	4	0
36	NC	219	0	92	1	0
37	NF	626	0	665	7	0
38	NK	581	0	656	7	0
39	NL	2175	0	2235	15	0
40	NP	847	0	854	4	0
41	SA	2853	0	3028	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	SB	2243	0	2268	11	0
43	SC	1747	0	1897	16	0
44	SD	1870	0	1996	9	0
45	SE	1869	0	2014	13	0
46	SF	1876	0	1970	9	0
47	SG	1518	0	1601	7	0
48	SH	773	0	755	4	0
49	SI	1952	0	2086	7	0
50	SK	1852	0	1828	13	0
51	SM	3278	0	3332	16	0
52	SQ	1771	0	1810	8	0
53	SR	4932	0	5070	29	0
54	SV	1184	0	1248	6	0
55	L1	4	0	0	0	0
55	L3	73	0	0	0	0
55	L4	3	0	0	0	0
55	LG	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	LW	1	0	0	0	0
55	SA	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	149506	0	113640	523	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 523 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)
4:L4:40:U:O2	5:L5:75:ARG:NH1	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:4075:U:OP1	45:SE:249:ARG:NH1	2.11	0.84
2:L1:51:U:OP2	35:LZ:21:ARG:NH2	2.11	0.83
3:L3:2520:C:O2	3:L3:2640:G:N2	2.11	0.82
3:L3:4156:G:OP2	3:L3:4157:A:O2'	1.98	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	158/165 (96%)	157 (99%)	1 (1%)	0	100	100
5	L5	166/178 (93%)	164 (99%)	2 (1%)	0	100	100
6	L6	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
7	L7	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
8	L8	133/215 (62%)	131 (98%)	2 (2%)	0	100	100
9	L9	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
10	LA	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
11	LB	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
12	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
13	LD	152/196 (78%)	151 (99%)	1 (1%)	0	100	100
14	LE	150/160 (94%)	146 (97%)	4 (3%)	0	100	100
15	LF	101/128 (79%)	100 (99%)	1 (1%)	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%)	131 (99%)	1 (1%)	0	100	100
19	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	LK	145/148 (98%)	144 (99%)	1 (1%)	0	100	100
21	LL	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
22	LM	87/159 (55%)	86 (99%)	1 (1%)	0	100	100
23	LN	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
24	LO	93/115 (81%)	93 (100%)	0	0	100	100
25	LP	104/125 (83%)	104 (100%)	0	0	100	100
26	LQ	126/135 (93%)	126 (100%)	0	0	100	100
27	LR	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
28	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
29	LT	107/110 (97%)	107 (100%)	0	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%)	87 (98%)	2 (2%)	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	NC	42/731 (6%)	42 (100%)	0	0	100	100
37	NF	69/260 (26%)	68 (99%)	1 (1%)	0	100	100
38	NK	63/129 (49%)	63 (100%)	0	0	100	100
39	NL	259/478 (54%)	258 (100%)	1 (0%)	0	100	100
40	NP	100/134 (75%)	100 (100%)	0	0	100	100
41	SA	356/427 (83%)	351 (99%)	5 (1%)	0	100	100
42	SB	273/297 (92%)	270 (99%)	3 (1%)	0	100	100
43	SC	211/288 (73%)	206 (98%)	5 (2%)	0	100	100
44	SD	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
45	SE	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
46	SF	243/257 (95%)	236 (97%)	7 (3%)	0	100	100
47	SG	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
48	SH	91/293 (31%)	90 (99%)	1 (1%)	0	100	100
49	SI	233/255 (91%)	230 (99%)	3 (1%)	0	100	100
50	SK	242/245 (99%)	234 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	SM	393/588 (67%)	389 (99%)	4 (1%)	0	100	100
52	SQ	215/239 (90%)	214 (100%)	1 (0%)	0	100	100
53	SR	595/634 (94%)	589 (99%)	5 (1%)	1 (0%)	44	56
54	SV	137/163 (84%)	135 (98%)	2 (2%)	0	100	100
All	All	8586/11002 (78%)	8472 (99%)	113 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
53	SR	88	ASP

### 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	BA	53/137 (39%)	53 (100%)	0	100	100
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%)	92 (99%)	1 (1%)	70	82
16	LG	106/107 (99%)	106 (100%)	0	100	100
17	LH	124/133 (93%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	75 (97%)	2 (3%)	41	59
23	LN	347/348 (100%)	346 (100%)	1 (0%)	91	96
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
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
37	NF	65/228 (28%)	65 (100%)	0	100	100
38	NK	61/115 (53%)	61 (100%)	0	100	100
39	NL	227/402 (56%)	227 (100%)	0	100	100
40	NP	88/114 (77%)	88 (100%)	0	100	100
41	SA	298/348 (86%)	297 (100%)	1 (0%)	91	96
42	SB	234/250 (94%)	234 (100%)	0	100	100
43	SC	192/252 (76%)	191 (100%)	1 (0%)	86	93
44	SD	194/215 (90%)	194 (100%)	0	100	100
45	SE	198/223 (89%)	197 (100%)	1 (0%)	86	93
46	SF	188/199 (94%)	188 (100%)	0	100	100
47	SG	169/171 (99%)	169 (100%)	0	100	100
48	SH	85/274 (31%)	85 (100%)	0	100	100
49	SI	212/228 (93%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	SK	212/213 (100%)	211 (100%)	1 (0%)	86	93
51	SM	354/509 (70%)	354 (100%)	0	100	100
52	SQ	194/214 (91%)	194 (100%)	0	100	100
53	SR	545/574 (95%)	544 (100%)	1 (0%)	92	97
54	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	7440/8850 (84%)	7431 (100%)	9 (0%)	92	98

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	SK	57	ARG
53	SR	8	LYS
23	LN	246	ARG
41	SA	122	TYR
43	SC	100	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
49	SI	94	HIS
51	SM	211	HIS
53	SR	209	HIS
53	SR	157	HIS
42	SB	17	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	18 (11%)	0
3	L3	3376/5070 (66%)	413 (12%)	6 (0%)
4	L4	119/121 (98%)	12 (10%)	1 (0%)
All	All	3647/5348 (68%)	443 (12%)	7 (0%)

5 of 443 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	23	C
2	L1	34	U

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Mol	Chain	Res	Type
2	L1	35	C
2	L1	59	A
2	L1	62	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L3	1324	A
3	L3	1633	G
4	L4	109	U
3	L3	2095	A
3	L3	503	C

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

107 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	PSU	L3	3730	3	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
3	OMU	L3	4227	3	19,22,23	2.02	6 (31%)	25,31,34	1.80	4 (16%)
3	A2M	L3	1524	3	18,25,26	1.26	2 (11%)	20,36,39	1.51	3 (15%)
3	OMU	L3	4498	3	19,22,23	2.09	7 (36%)	25,31,34	1.81	5 (20%)
3	OMC	L3	3887	3	19,22,23	0.55	0	25,31,34	0.68	0
3	OMG	L3	4499	3	19,26,27	1.11	2 (10%)	21,38,41	0.81	1 (4%)
3	PSU	L3	3822	3	18,21,22	1.14	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L3	4689	3	18,21,22	1.06	1 (5%)	21,30,33	1.96	4 (19%)
3	PSU	L3	4403	3	18,21,22	1.08	1 (5%)	21,30,33	1.96	5 (23%)
3	PSU	L3	4361	3	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
3	UR3	L3	4530	3	19,22,23	1.12	3 (15%)	26,32,35	1.52	2 (7%)
3	PSU	L3	5010	3	18,21,22	1.06	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L3	4521	3	18,21,22	1.09	1 (5%)	21,30,33	1.92	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	A2M	L3	398	3	18,25,26	1.27	2 (11%)	20,36,39	1.35	2 (10%)
3	OMC	L3	2351	3,55	19,22,23	0.58	0	25,31,34	0.83	1 (4%)
3	PSU	L3	4552	3	18,21,22	1.07	1 (5%)	21,30,33	1.92	5 (23%)
3	OMG	L3	3899	3	19,26,27	1.18	2 (10%)	21,38,41	0.82	1 (4%)
3	A2M	L3	3825	3	18,25,26	1.26	2 (11%)	20,36,39	1.29	2 (10%)
3	PSU	L3	1536	3	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
3	OMC	L3	4536	3	19,22,23	0.54	0	25,31,34	0.65	0
3	OMG	L3	1625	3	19,26,27	1.20	2 (10%)	21,38,41	0.85	1 (4%)
3	OMG	L3	2876	3	19,26,27	1.15	2 (10%)	21,38,41	0.79	1 (4%)
3	PSU	L3	3844	3	18,21,22	1.12	1 (5%)	21,30,33	1.97	5 (23%)
3	PSU	L3	4636	3	18,21,22	1.10	1 (5%)	21,30,33	2.02	6 (28%)
3	PSU	L3	3639	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
3	OMG	L3	4494	3	19,26,27	1.19	2 (10%)	21,38,41	0.85	1 (4%)
3	PSU	L3	4431	3	18,21,22	1.13	1 (5%)	21,30,33	1.97	5 (23%)
3	OMG	L3	3627	3	19,26,27	1.17	2 (10%)	21,38,41	0.85	1 (4%)
3	OMU	L3	2837	3	19,22,23	2.05	7 (36%)	25,31,34	1.85	5 (20%)
3	A2M	L3	4571	3	18,25,26	1.27	2 (11%)	20,36,39	1.24	1 (5%)
3	PSU	L3	4579	3	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
2	OMG	L1	75	2	19,26,27	1.17	2 (10%)	21,38,41	0.81	1 (4%)
3	PSU	L3	2839	3	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
3	PSU	L3	1860	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
3	OMG	L3	4370	3	19,26,27	1.22	3 (15%)	21,38,41	0.88	1 (4%)
3	PSU	L3	5001	3	18,21,22	1.12	1 (5%)	21,30,33	1.93	4 (19%)
3	A2M	L3	3724	3	18,25,26	1.29	2 (11%)	20,36,39	1.29	1 (5%)
3	OMG	L3	4228	3	19,26,27	1.25	3 (15%)	21,38,41	0.90	1 (4%)
3	OMG	L3	4623	3	19,26,27	1.18	2 (10%)	21,38,41	0.88	1 (4%)
3	PSU	L3	4293	3	18,21,22	1.03	1 (5%)	21,30,33	1.77	4 (19%)
3	A2M	L3	2815	3	18,25,26	1.27	2 (11%)	20,36,39	1.29	2 (10%)
3	OMC	L3	2422	3,55	19,22,23	0.53	0	25,31,34	0.72	1 (4%)
3	OMU	L3	4620	3	19,22,23	1.98	6 (31%)	25,31,34	1.70	4 (16%)
3	PSU	L3	3695	3	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
3	OMU	L3	4306	3	19,22,23	2.01	6 (31%)	25,31,34	1.82	4 (16%)
2	PSU	L1	55	2	18,21,22	1.06	1 (5%)	21,30,33	1.93	5 (23%)
3	A2M	L3	1326	3	18,25,26	1.28	3 (16%)	20,36,39	1.30	2 (10%)
3	OMC	L3	3841	3	19,22,23	0.54	0	25,31,34	0.71	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	L3	4299	3	18,21,22	1.03	2 (11%)	21,30,33	2.02	5 (23%)
3	OMC	L3	3869	3	19,22,23	0.55	0	25,31,34	0.68	0
3	A2M	L3	4590	3	18,25,26	1.25	3 (16%)	20,36,39	1.46	3 (15%)
3	OMC	L3	4456	3	19,22,23	0.55	0	25,31,34	0.66	0
3	PSU	L3	3734	3	18,21,22	1.12	1 (5%)	21,30,33	1.96	6 (28%)
3	OMG	L3	4392	3	19,26,27	1.19	2 (10%)	21,38,41	0.83	1 (4%)
3	PSU	L3	2508	3	18,21,22	1.07	1 (5%)	21,30,33	1.96	4 (19%)
2	PSU	L1	69	2	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L3	3884	3	18,21,22	1.06	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L3	1677	3	18,21,22	1.06	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L3	4576	3	18,21,22	1.11	1 (5%)	21,30,33	1.97	6 (28%)
3	PSU	L3	2632	3	18,21,22	1.08	1 (5%)	21,30,33	1.88	5 (23%)
3	OMC	L3	2824	3	19,22,23	0.53	0	25,31,34	0.67	0
3	A2M	L3	2363	3,55	18,25,26	1.29	2 (11%)	20,36,39	1.29	1 (5%)
3	OMG	L3	4618	3	19,26,27	1.18	2 (10%)	21,38,41	0.90	1 (4%)
3	A2M	L3	2401	3	18,25,26	1.29	3 (16%)	20,36,39	1.41	2 (10%)
3	PSU	L3	4471	3	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
3	PSU	L3	3853	3	18,21,22	1.06	1 (5%)	21,30,33	1.81	4 (19%)
3	OMG	L3	2364	3	19,26,27	1.17	2 (10%)	21,38,41	0.85	1 (4%)
3	PSU	L3	1683	3	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
3	OMG	L3	1316	3	19,26,27	1.18	2 (10%)	21,38,41	0.84	1 (4%)
3	PSU	L3	4457	3	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
3	OMG	L3	2424	3	19,26,27	1.21	2 (10%)	21,38,41	0.77	1 (4%)
3	OMG	L3	1522	3	19,26,27	1.20	3 (15%)	21,38,41	0.83	1 (4%)
3	OMU	L3	2415	3	19,22,23	2.03	6 (31%)	25,31,34	1.82	5 (20%)
3	PSU	L3	4532	3	18,21,22	1.09	1 (5%)	21,30,33	2.00	5 (23%)
3	A2M	L3	3867	3	18,25,26	1.23	2 (11%)	20,36,39	1.36	1 (5%)
3	OMC	L3	1340	3	19,22,23	0.59	0	25,31,34	0.79	0
3	PSU	L3	3715	3	18,21,22	1.13	1 (5%)	21,30,33	1.94	6 (28%)
3	PSU	L3	4673	3	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
3	PSU	L3	4493	3	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
3	OMU	L3	3925	3	19,22,23	2.03	6 (31%)	25,31,34	1.82	5 (20%)
3	PSU	L3	1792	3	18,21,22	1.09	1 (5%)	21,30,33	1.93	6 (28%)
3	OMC	L3	2365	3	19,22,23	0.54	0	25,31,34	0.69	0
23	HIC	LN	245	23	8,11,12	1.64	2 (25%)	5,14,16	0.99	0
3	OMC	L3	2861	3	19,22,23	0.52	0	25,31,34	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMG	L3	4637	3	19,26,27	1.15	2 (10%)	21,38,41	0.85	1 (4%)
3	PSU	L3	4628	3	18,21,22	1.06	2 (11%)	21,30,33	1.97	6 (28%)
3	PSU	L3	4353	3	18,21,22	1.06	1 (5%)	21,30,33	1.99	6 (28%)
3	PSU	L3	1862	3	18,21,22	1.12	1 (5%)	21,30,33	1.92	5 (23%)
3	PSU	L3	4972	3	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L3	3920	3,55	18,21,22	1.11	2 (11%)	21,30,33	1.89	4 (19%)
3	PSU	L3	1582	3	18,21,22	1.04	1 (5%)	21,30,33	1.93	5 (23%)
3	OMC	L3	2804	3	19,22,23	0.54	0	25,31,34	0.69	0
3	A2M	L3	4523	3	18,25,26	1.25	2 (11%)	20,36,39	1.31	2 (10%)
3	OMG	L3	3744	3	19,26,27	1.14	2 (10%)	21,38,41	0.84	1 (4%)
3	A2M	L3	1534	3,55	18,25,26	1.27	3 (16%)	20,36,39	1.39	2 (10%)
3	A2M	L3	3718	3	18,25,26	1.28	3 (16%)	20,36,39	1.24	1 (5%)
3	6MZ	L3	4220	3	17,25,26	1.19	3 (17%)	15,36,39	2.17	4 (26%)
3	PSU	L3	4296	3	18,21,22	1.05	2 (11%)	21,30,33	2.02	5 (23%)
3	PSU	L3	3637	3	18,21,22	1.06	1 (5%)	21,30,33	2.01	5 (23%)
3	A2M	L3	3830	3	18,25,26	1.25	2 (11%)	20,36,39	1.32	2 (10%)
3	A2M	L3	400	3	18,25,26	1.26	2 (11%)	20,36,39	1.36	2 (10%)
3	A2M	L3	2787	3	18,25,26	1.25	2 (11%)	20,36,39	1.40	2 (10%)
3	PSU	L3	4312	3	18,21,22	1.04	1 (5%)	21,30,33	1.97	4 (19%)
3	A2M	L3	1871	3	18,25,26	1.27	2 (11%)	20,36,39	1.47	1 (5%)
3	PSU	L3	4500	3	18,21,22	1.09	1 (5%)	21,30,33	1.93	6 (28%)
3	OMC	L3	3701	3	19,22,23	0.49	0	25,31,34	0.63	0
3	PSU	L3	3851	3	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)

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	PSU	L3	3730	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	4227	3	-	1/9/27/28	0/2/2/2
3	A2M	L3	1524	3	-	1/5/27/28	0/3/3/3
3	OMU	L3	4498	3	-	0/9/27/28	0/2/2/2
3	OMC	L3	3887	3	-	2/9/27/28	0/2/2/2
3	OMG	L3	4499	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	3822	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4361	3	-	0/7/25/26	0/2/2/2
3	UR3	L3	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4521	3	-	2/7/25/26	0/2/2/2
3	A2M	L3	398	3	-	1/5/27/28	0/3/3/3
3	OMC	L3	2351	3,55	-	2/9/27/28	0/2/2/2
3	PSU	L3	4552	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	3899	3	-	1/5/27/28	0/3/3/3
3	A2M	L3	3825	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	1536	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	1625	3	-	2/5/27/28	0/3/3/3
3	OMG	L3	2876	3	-	3/5/27/28	0/3/3/3
3	PSU	L3	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L3	4636	3	-	3/7/25/26	0/2/2/2
3	PSU	L3	3639	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4494	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	4431	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	3627	3	-	1/5/27/28	0/3/3/3
3	OMU	L3	2837	3	-	1/9/27/28	0/2/2/2
3	A2M	L3	4571	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	4579	3	-	0/7/25/26	0/2/2/2
2	OMG	L1	75	2	-	1/5/27/28	0/3/3/3
3	PSU	L3	2839	3	-	2/7/25/26	0/2/2/2
3	PSU	L3	1860	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4370	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	5001	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3724	3	-	2/5/27/28	0/3/3/3
3	OMG	L3	4228	3	-	0/5/27/28	0/3/3/3
3	OMG	L3	4623	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2815	3	-	1/5/27/28	0/3/3/3
3	OMC	L3	2422	3,55	-	2/9/27/28	0/2/2/2
3	OMU	L3	4620	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	3695	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	4306	3	-	4/9/27/28	0/2/2/2
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
3	A2M	L3	1326	3	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L3	3841	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4299	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	3869	3	-	0/9/27/28	0/2/2/2
3	A2M	L3	4590	3	-	4/5/27/28	0/3/3/3
3	OMC	L3	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	3734	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4392	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	2508	3	-	0/7/25/26	0/2/2/2
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
3	PSU	L3	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1677	3	-	4/7/25/26	0/2/2/2
3	PSU	L3	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	2632	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2824	3	-	0/9/27/28	0/2/2/2
3	A2M	L3	2363	3,55	-	0/5/27/28	0/3/3/3
3	OMG	L3	4618	3	-	2/5/27/28	0/3/3/3
3	A2M	L3	2401	3	-	2/5/27/28	0/3/3/3
3	PSU	L3	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3853	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	2364	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	1683	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	1316	3	-	2/5/27/28	0/3/3/3
3	PSU	L3	4457	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	2424	3	-	0/5/27/28	0/3/3/3
3	OMG	L3	1522	3	-	0/5/27/28	0/3/3/3
3	OMU	L3	2415	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4532	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3867	3	-	1/5/27/28	0/3/3/3
3	OMC	L3	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4493	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	1792	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2365	3	-	0/9/27/28	0/2/2/2
23	HIC	LN	245	23	-	2/5/6/8	0/1/1/1
3	OMC	L3	2861	3	-	1/9/27/28	0/2/2/2
3	OMG	L3	4637	3	-	3/5/27/28	0/3/3/3
3	PSU	L3	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4353	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	1862	3	-	2/7/25/26	0/2/2/2
3	PSU	L3	4972	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3920	3,55	-	0/7/25/26	0/2/2/2
3	PSU	L3	1582	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2804	3	-	0/9/27/28	0/2/2/2
3	A2M	L3	4523	3	-	2/5/27/28	0/3/3/3
3	OMG	L3	3744	3	-	1/5/27/28	0/3/3/3
3	A2M	L3	1534	3,55	-	1/5/27/28	0/3/3/3
3	A2M	L3	3718	3	-	1/5/27/28	0/3/3/3
3	6MZ	L3	4220	3	-	3/5/27/28	0/3/3/3
3	PSU	L3	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3637	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3830	3	-	2/5/27/28	0/3/3/3
3	A2M	L3	400	3	-	0/5/27/28	0/3/3/3
3	A2M	L3	2787	3	-	2/5/27/28	0/3/3/3
3	PSU	L3	4312	3	-	1/7/25/26	0/2/2/2
3	A2M	L3	1871	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	4500	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	3701	3	-	6/9/27/28	0/2/2/2
3	PSU	L3	3851	3	-	0/7/25/26	0/2/2/2

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	4498	OMU	C6-N1	4.81	1.49	1.38
3	L3	2837	OMU	C6-N1	4.72	1.49	1.38
3	L3	4620	OMU	C6-N1	4.67	1.49	1.38
3	L3	2415	OMU	C6-N1	4.67	1.49	1.38
3	L3	4306	OMU	C6-N1	4.66	1.49	1.38

The worst 5 of 323 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4220	6MZ	C2-N1-C6	5.73	121.05	116.60
3	L3	2837	OMU	C4-N3-C2	-5.50	119.78	126.61
3	L3	4498	OMU	C4-N3-C2	-5.45	119.84	126.61
3	L3	3925	OMU	C4-N3-C2	-5.40	119.91	126.61
3	L3	4227	OMU	C4-N3-C2	-5.37	119.95	126.61

There are no chirality outliers.

5 of 86 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	C1'-C2'-O2'-CM'

There are no ring outliers.

51 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	4227	OMU	2	0
3	L3	1524	A2M	1	0
3	L3	4403	PSU	1	0
3	L3	4530	UR3	2	0
3	L3	2351	OMC	3	0
3	L3	3899	OMG	1	0
3	L3	4536	OMC	1	0
3	L3	2876	OMG	2	0
3	L3	4636	PSU	1	0
3	L3	4431	PSU	2	0
3	L3	3627	OMG	1	0
3	L3	2837	OMU	1	0
3	L3	4579	PSU	1	0
2	L1	75	OMG	2	0
3	L3	2839	PSU	1	0
3	L3	1860	PSU	1	0
3	L3	4370	OMG	1	0
3	L3	5001	PSU	1	0
3	L3	3724	A2M	1	0
3	L3	4623	OMG	1	0
3	L3	2815	A2M	2	0
3	L3	2422	OMC	2	0
3	L3	4620	OMU	2	0
3	L3	4306	OMU	3	0
3	L3	1326	A2M	3	0
3	L3	3841	OMC	1	0
3	L3	3869	OMC	1	0
3	L3	3734	PSU	1	0
2	L1	69	PSU	2	0
3	L3	1677	PSU	2	0
3	L3	4576	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	2632	PSU	1	0
3	L3	2363	A2M	1	0
3	L3	4618	OMG	1	0
3	L3	2364	OMG	2	0
3	L3	4457	PSU	2	0
3	L3	1522	OMG	1	0
3	L3	2415	OMU	5	0
3	L3	3867	A2M	1	0
3	L3	1340	OMC	1	0
3	L3	3715	PSU	1	0
3	L3	3925	OMU	2	0
3	L3	2861	OMC	1	0
3	L3	4637	OMG	2	0
3	L3	3920	PSU	1	0
3	L3	3744	OMG	1	0
3	L3	1534	A2M	2	0
3	L3	3718	A2M	5	0
3	L3	4220	6MZ	2	0
3	L3	4312	PSU	1	0
3	L3	4500	PSU	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	25,30,30	2.66	9 (36%)	30,47,47	1.55	7 (23%)

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	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	SR	1001	GDP	O6-C6	7.28	1.40	1.23
57	SR	1001	GDP	PA-O3A	5.24	1.65	1.59
57	SR	1001	GDP	O4'-C1'	4.97	1.47	1.40
57	SR	1001	GDP	C2-N2	4.85	1.45	1.34
57	SR	1001	GDP	C1'-N9	-2.48	1.43	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	SR	1001	GDP	C5-C6-N1	2.96	119.71	114.07
57	SR	1001	GDP	O2B-PB-O3A	2.93	114.47	104.64
57	SR	1001	GDP	C2-N1-C6	-2.90	119.80	125.11
57	SR	1001	GDP	C2'-C3'-C4'	2.73	107.89	102.61
57	SR	1001	GDP	O3B-PB-O3A	2.71	113.72	104.64

There are no chirality outliers.

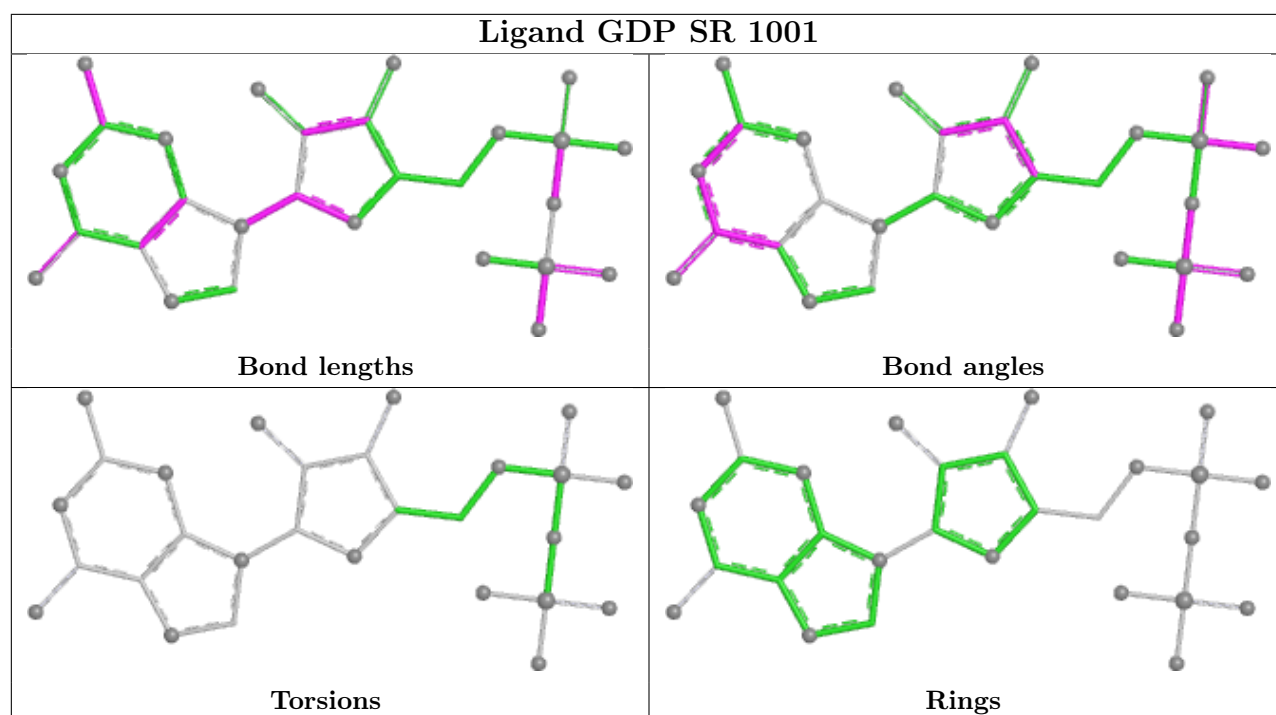
There are no torsion outliers.

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.

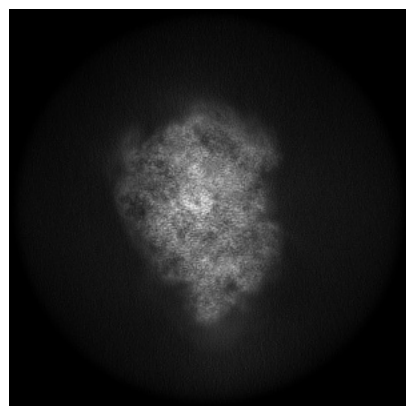
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29269. These allow visual inspection of the internal detail of the map and identification of artifacts.

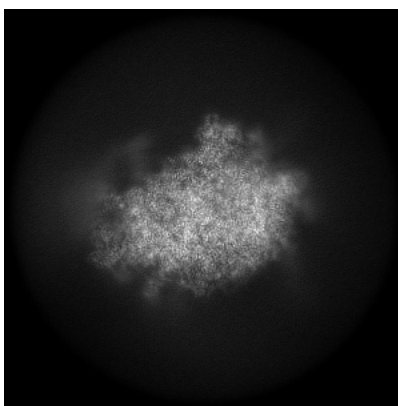
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

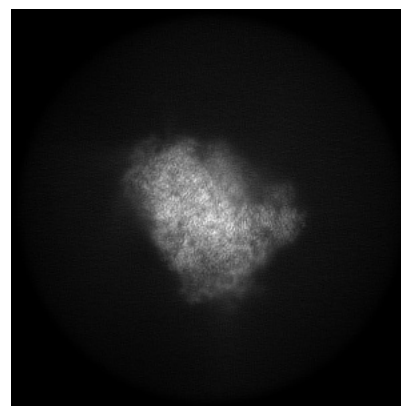
#### 6.1.1 Primary map



X

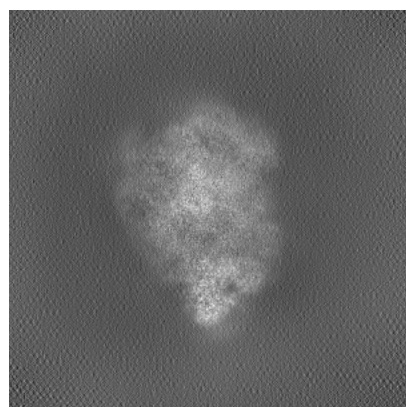


Y

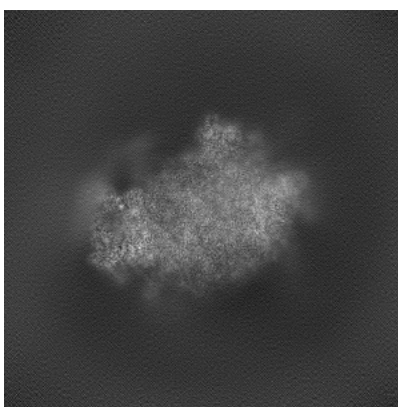


Z

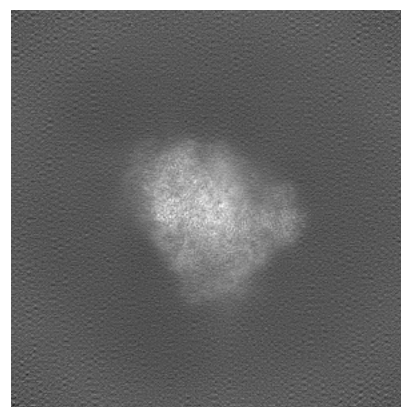
#### 6.1.2 Raw map



X



Y

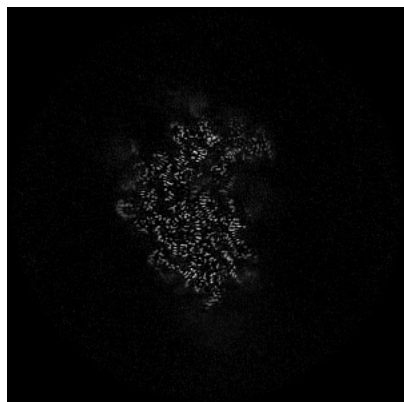


Z

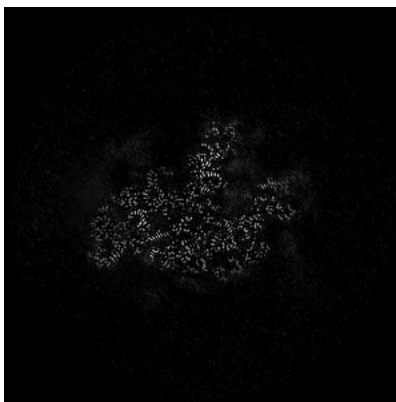
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

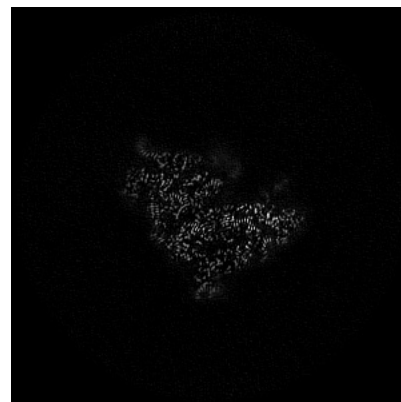
### 6.2.1 Primary map



X Index: 240

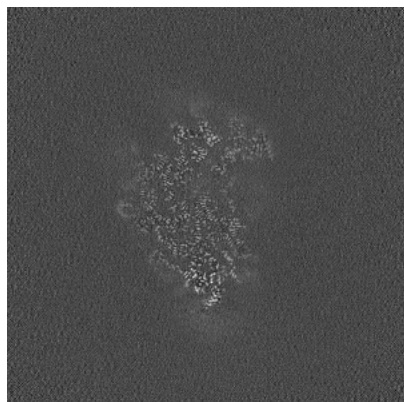


Y Index: 240

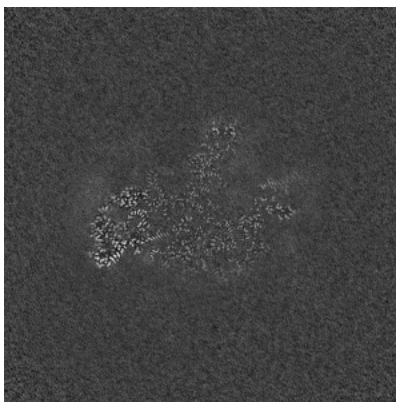


Z Index: 240

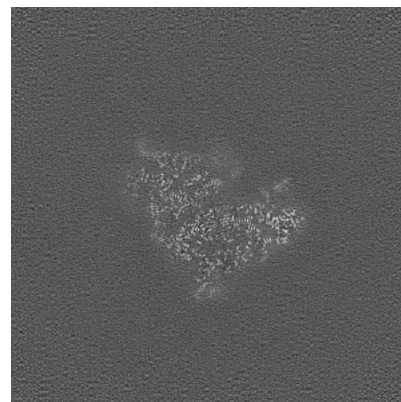
### 6.2.2 Raw map



X Index: 240



Y Index: 240

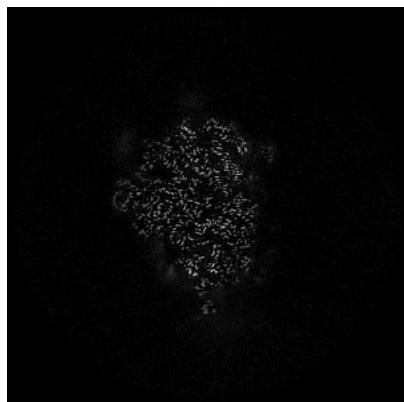


Z Index: 240

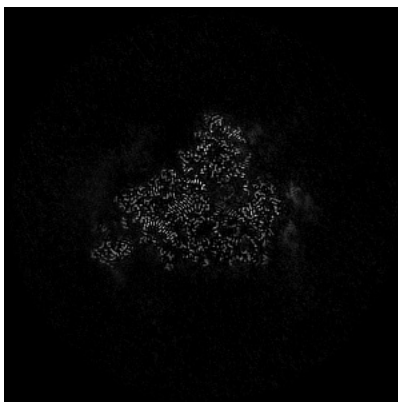
The images above show central slices of the map in three orthogonal directions.

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

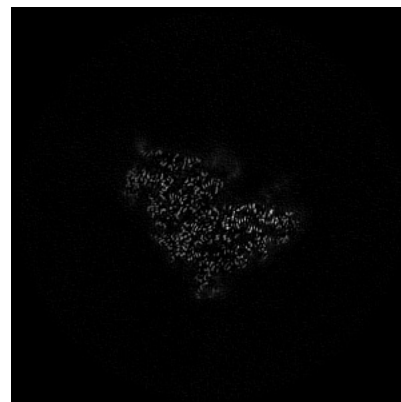
### 6.3.1 Primary map



X Index: 226

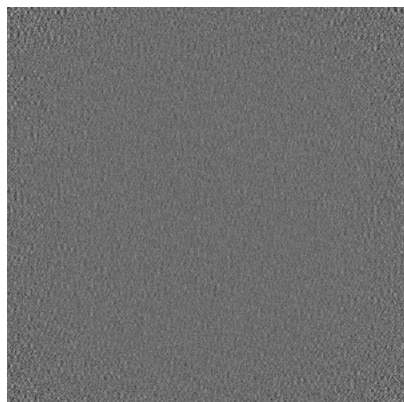


Y Index: 227

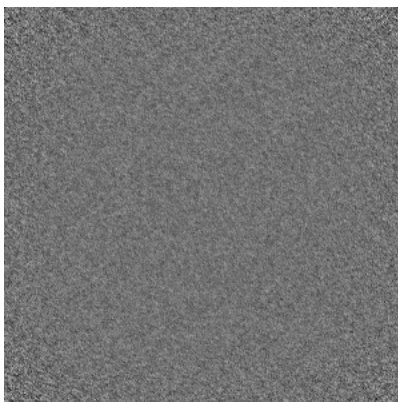


Z Index: 239

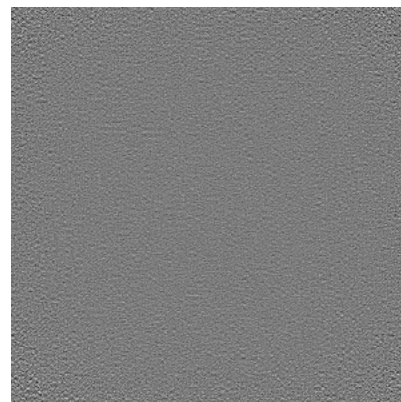
### 6.3.2 Raw map



X Index: 0



Y Index: 0



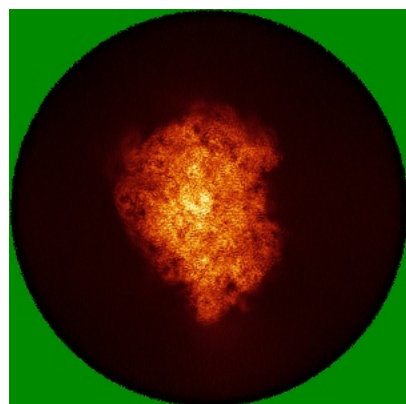
Z Index: 0

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

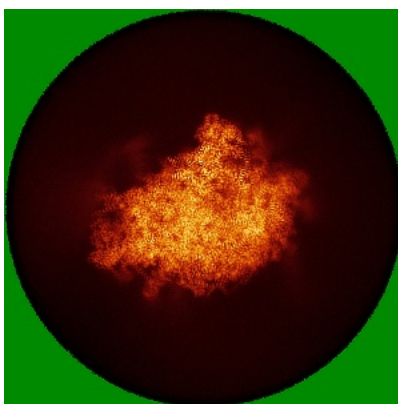


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

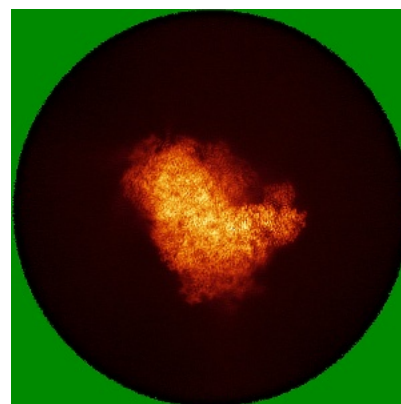
### 6.4.1 Primary map



X

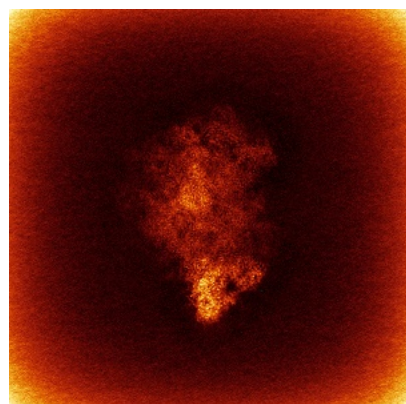


Y

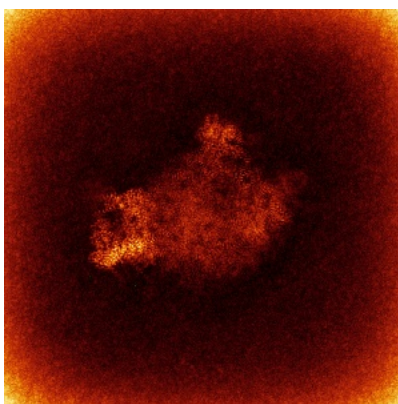


Z

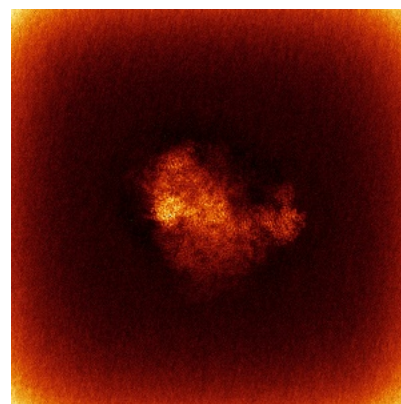
### 6.4.2 Raw map



X



Y

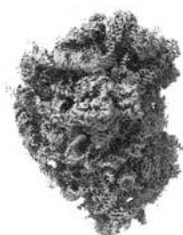


Z

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](#)

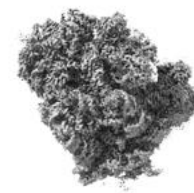
### 6.5.1 Primary map



X



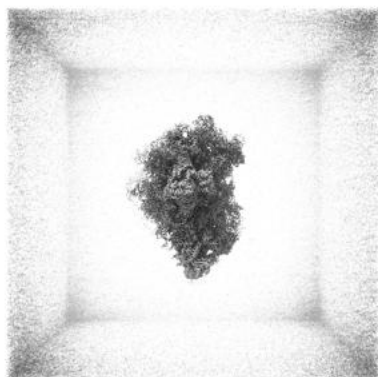
Y



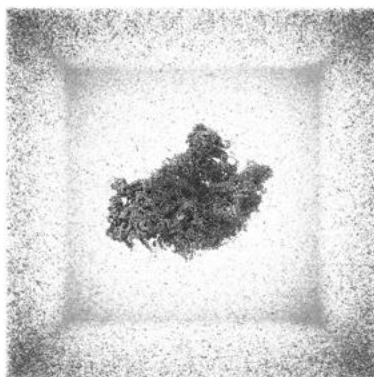
Z

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.

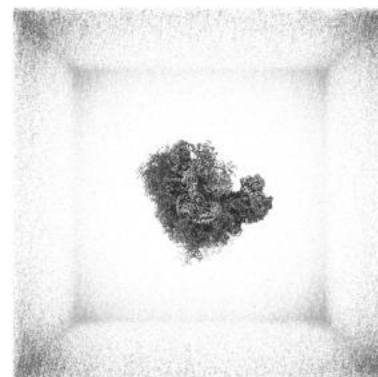
### 6.5.2 Raw map



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.

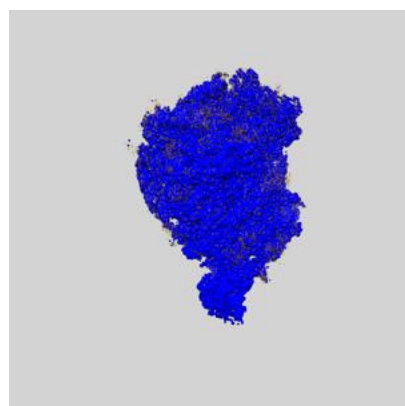
## 6.6 Mask visualisation [i](#)

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

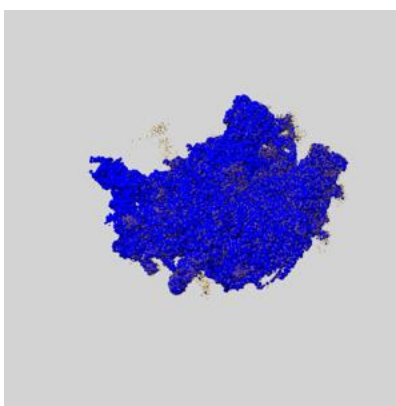
A mask typically either:

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

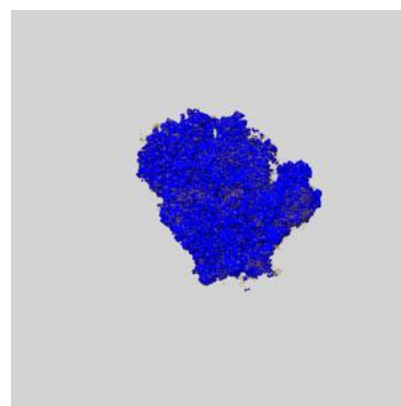
### 6.6.1 emd\_29269\_msk\_1.map [i](#)



X



Y

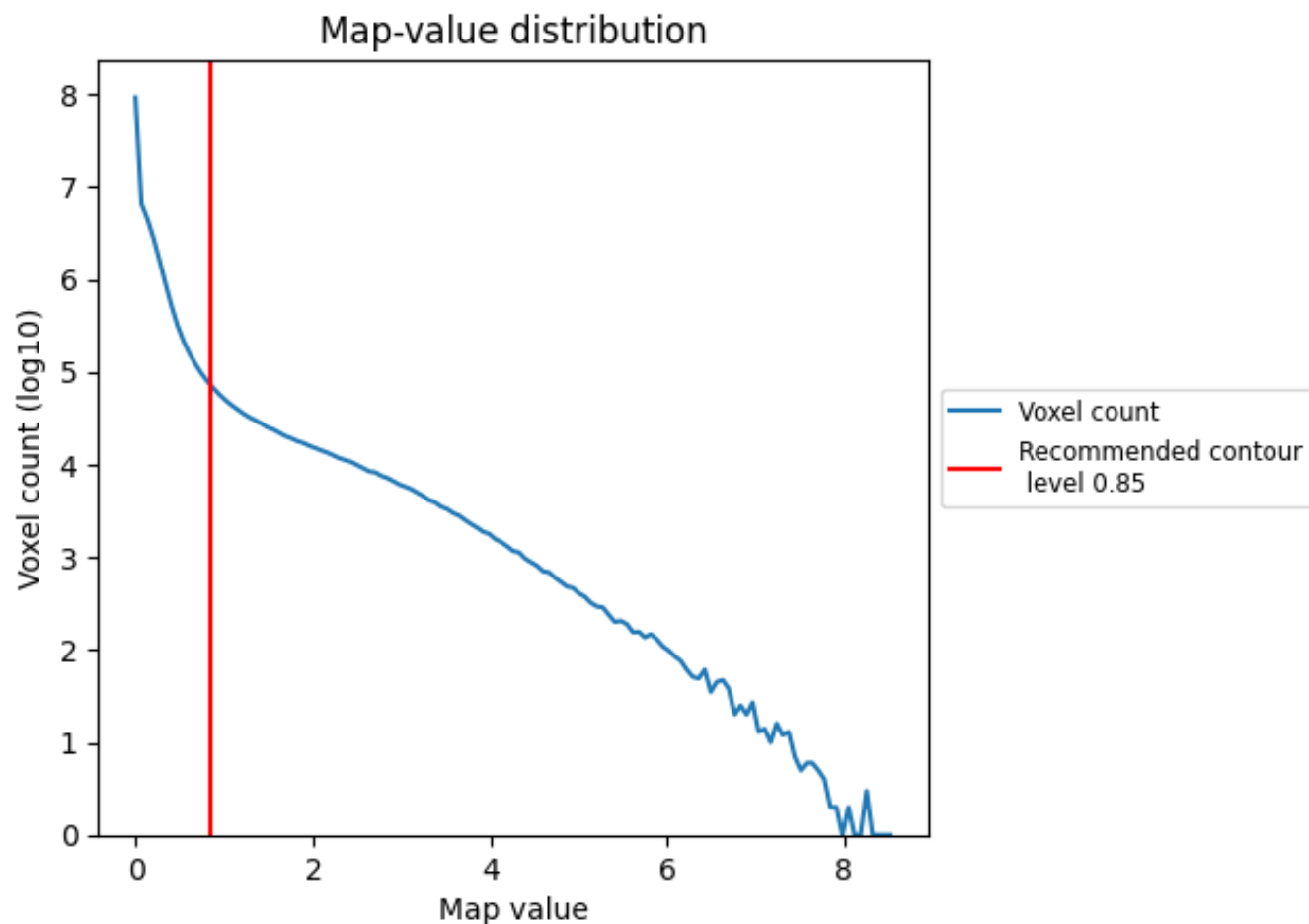


Z

## 7 Map analysis [i](#)

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

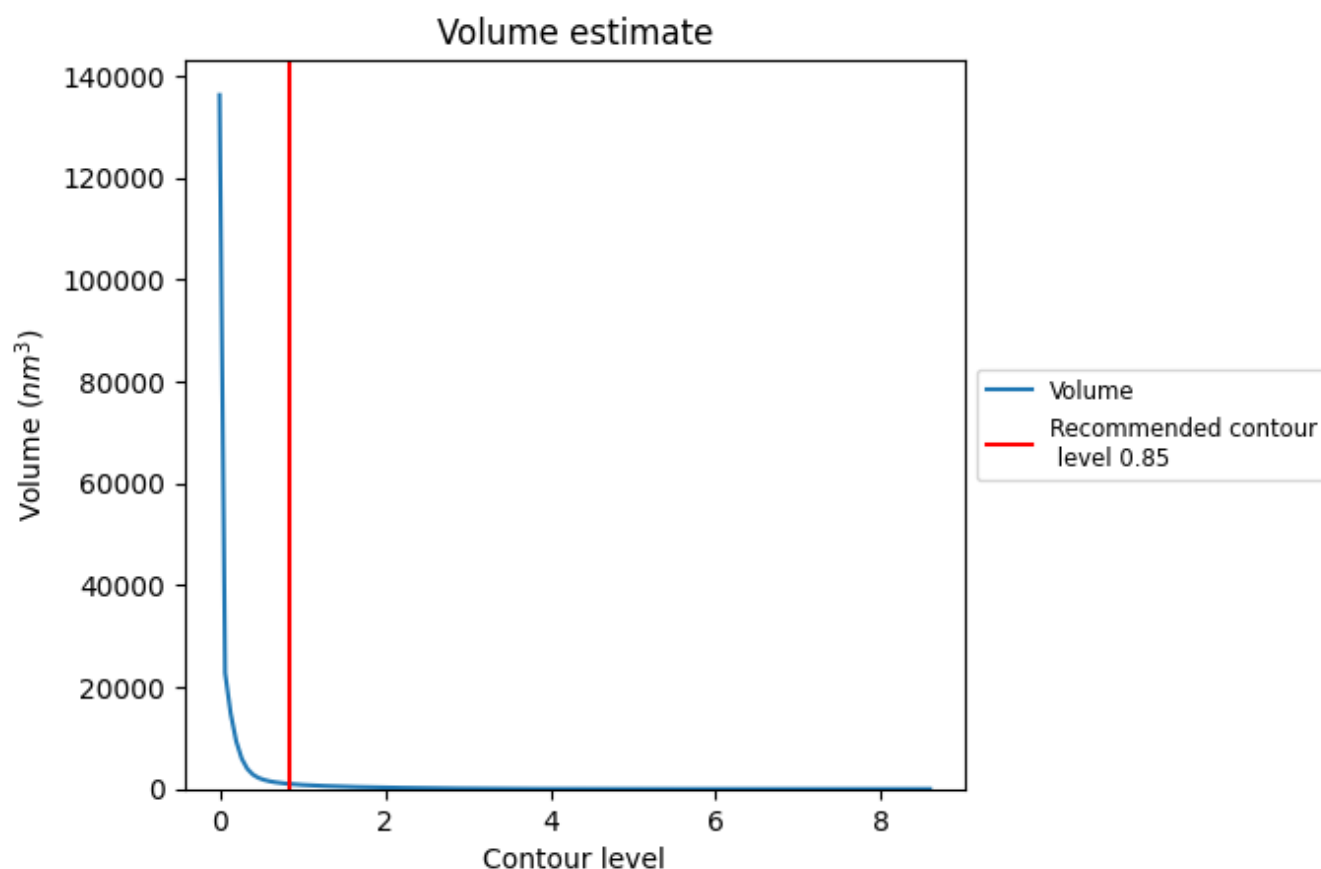
### 7.1 Map-value distribution [i](#)



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.



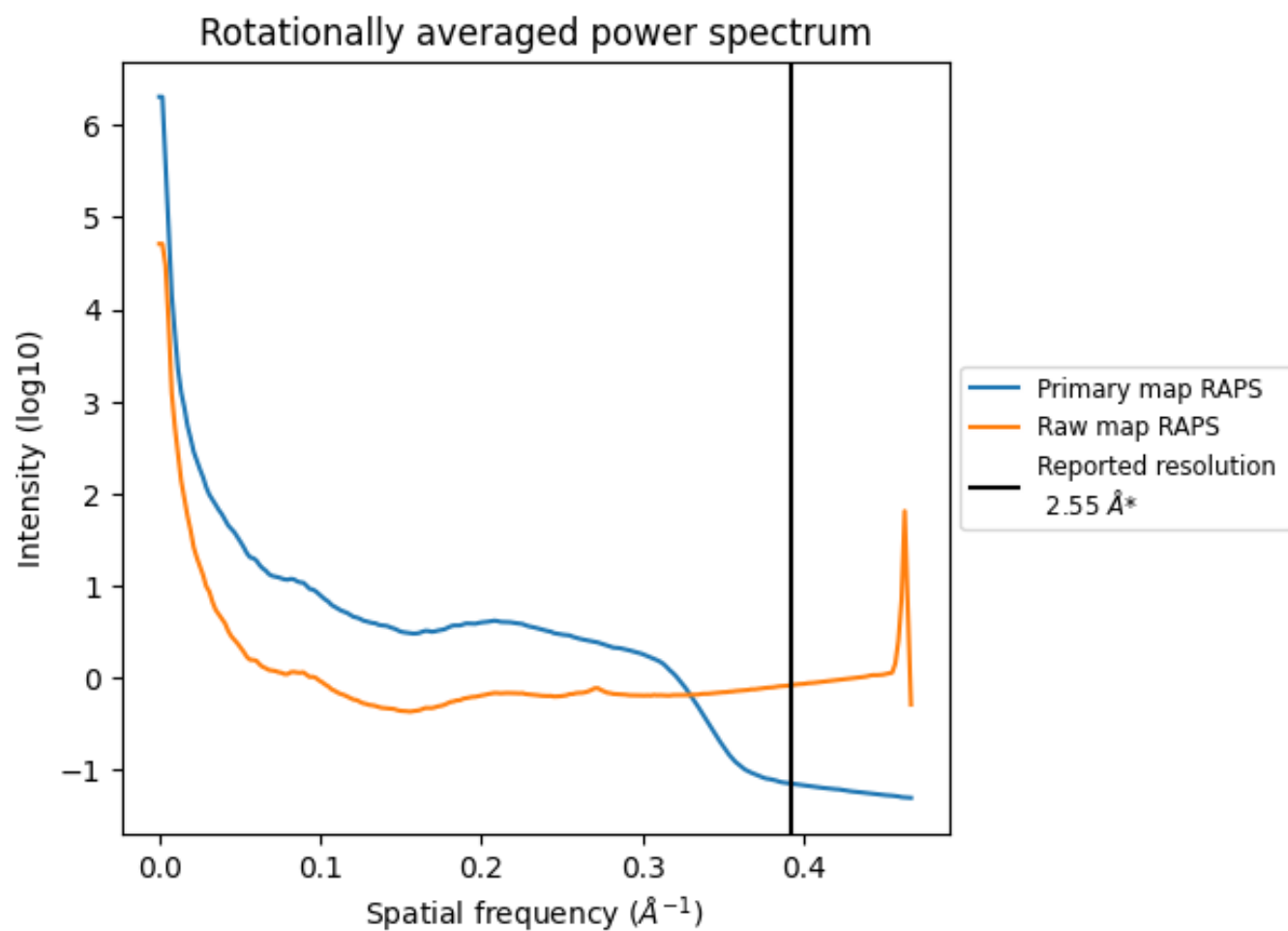
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $979 \text{ nm}^3$ ; this corresponds to an approximate mass of 884 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 ⓘ

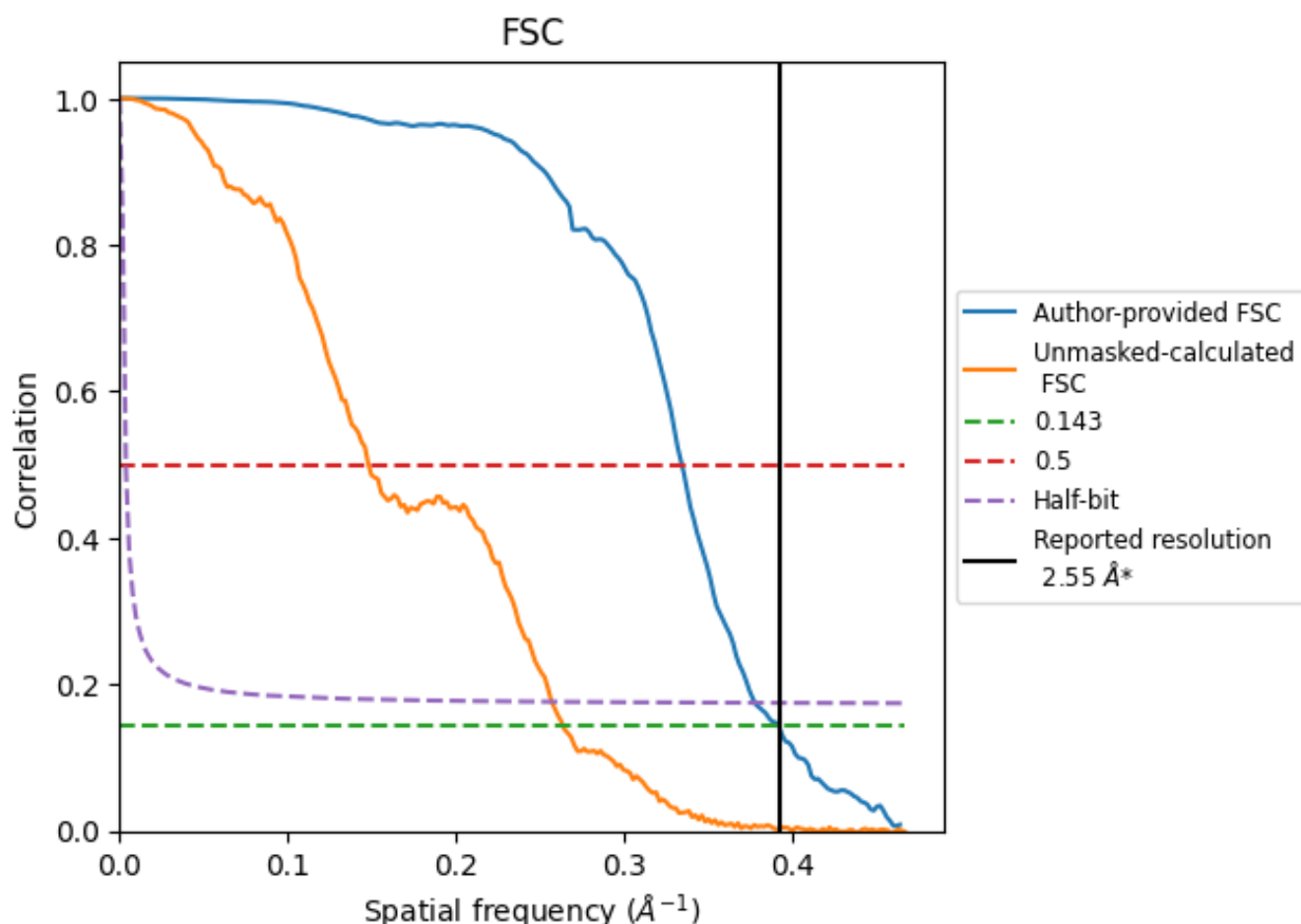


\*Reported resolution corresponds to spatial frequency of 0.392  $\text{\AA}^{-1}$

## 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  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

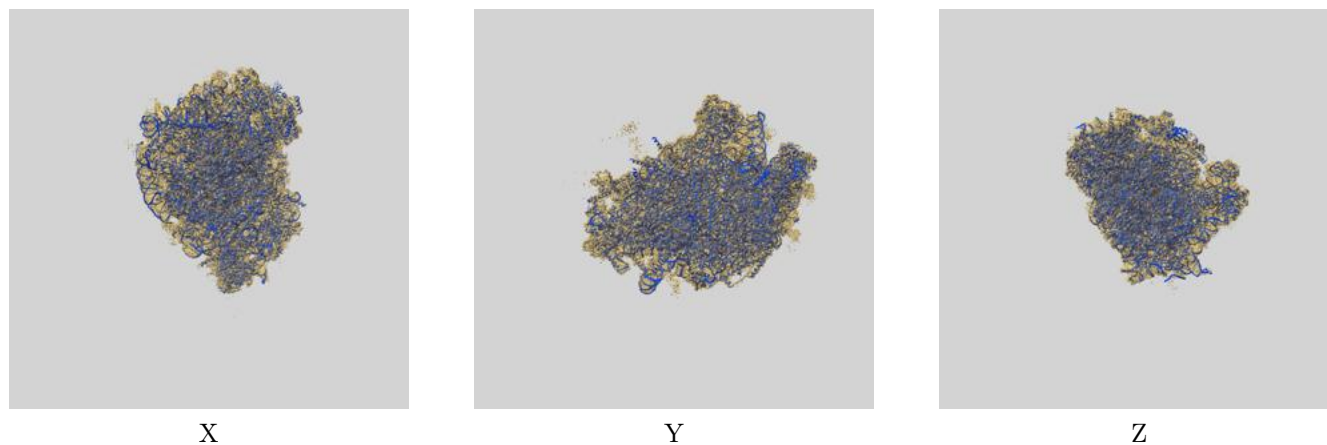
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.99	2.65
Unmasked-calculated*	3.80	6.76	3.90

\*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 3.80 differs from the reported value 2.55 by more than 10 %

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

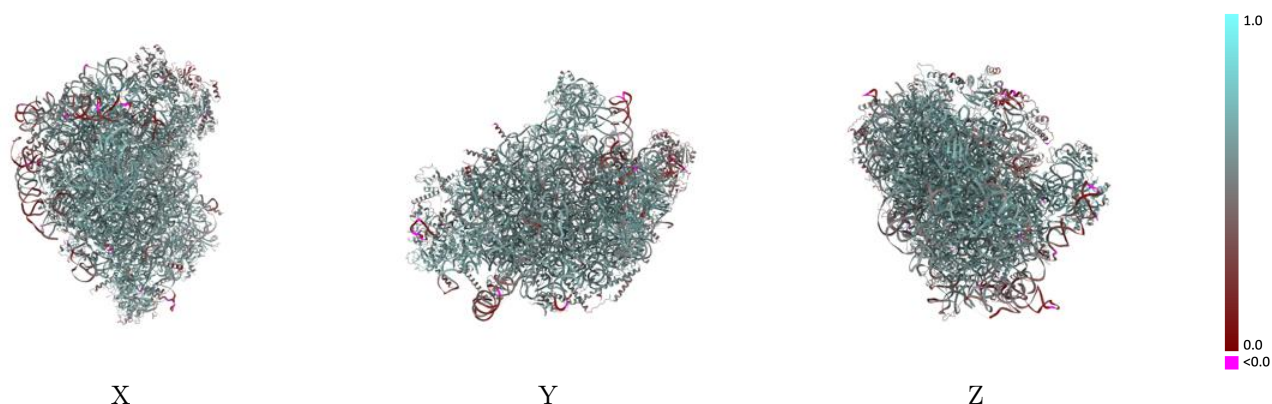
This section contains information regarding the fit between EMDB map EMD-29269 and PDB model 8FL7. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



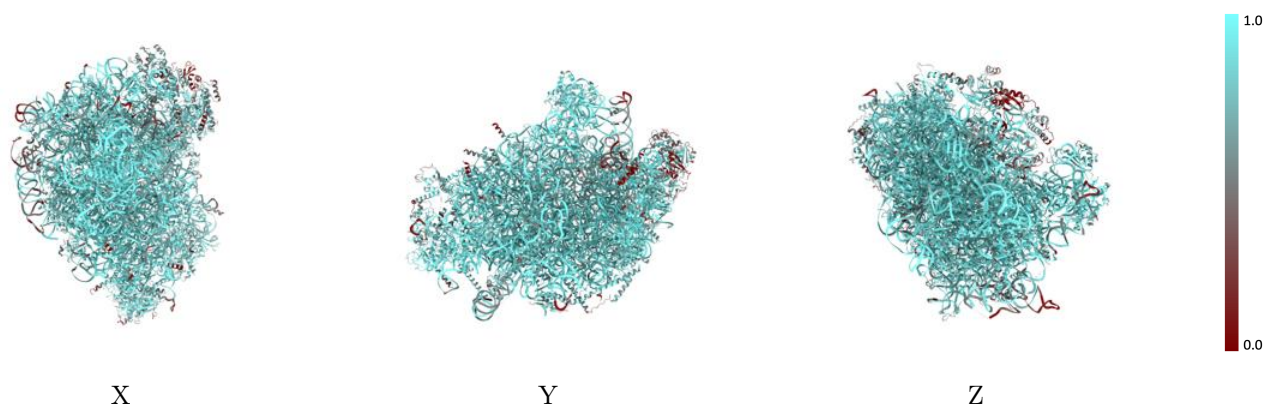
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



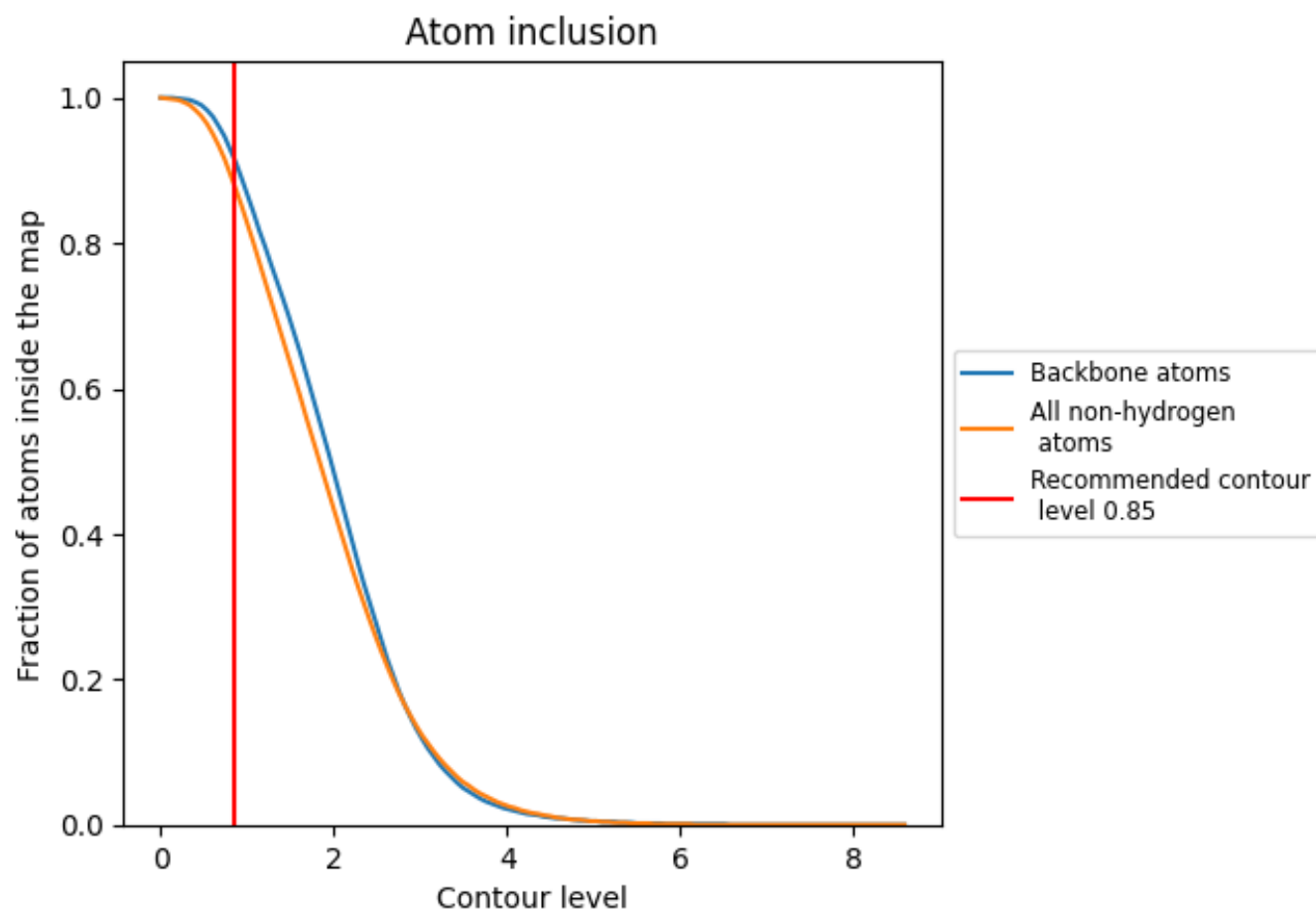
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 92% of all backbone atoms, 88% 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	 0.8800	 0.5700
BA	 0.3720	 0.3380
L1	 0.9540	 0.6100
L3	 0.9090	 0.5590
L4	 0.9810	 0.6210
L5	 0.8050	 0.5410
L6	 0.8220	 0.5660
L7	 0.9070	 0.6160
L8	 0.9180	 0.6070
L9	 0.9620	 0.6400
LA	 0.8860	 0.5960
LB	 0.9100	 0.6100
LC	 0.9560	 0.6440
LD	 0.8570	 0.5760
LE	 0.8910	 0.5810
LF	 0.8060	 0.5490
LG	 0.8890	 0.6090
LH	 0.8720	 0.6060
LI	 0.8430	 0.5710
LJ	 0.9300	 0.6210
LK	 0.9200	 0.6150
LL	 0.8750	 0.5820
LM	 0.7380	 0.5260
LN	 0.8990	 0.6020
LO	 0.8100	 0.5600
LP	 0.8460	 0.5760
LQ	 0.8880	 0.5960
LR	 0.9140	 0.6080
LS	 0.8650	 0.5890
LT	 0.9320	 0.6140
LU	 0.7990	 0.5570
LV	 0.8570	 0.5990
LW	 0.9360	 0.6150
LX	 0.8040	 0.5670
LY	 0.7590	 0.5590



*Continued on next page...*



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Chain	Atom inclusion	Q-score
LZ	 0.9240	 0.6130
NC	 0.0590	 0.3230
NF	 0.7120	 0.5510
NK	 0.6960	 0.5190
NL	 0.8240	 0.5680
NP	 0.8110	 0.5620
SA	 0.8930	 0.5970
SB	 0.8830	 0.5900
SC	 0.7820	 0.5360
SD	 0.8950	 0.5950
SE	 0.8650	 0.5910
SF	 0.9160	 0.6160
SG	 0.9130	 0.6140
SH	 0.6810	 0.5000
SI	 0.7460	 0.5260
SK	 0.8430	 0.5750
SM	 0.9050	 0.6150
SQ	 0.6070	 0.4720
SR	 0.7590	 0.5430
SV	 0.8390	 0.5720