Full wwPDB EM Validation Report ⓘ

Nov 11, 2023 – 09:03 pm GMT

PDB ID	:	8PV6
EMDB ID	:	EMD-17955
Title	:	Chaetomium thermophilum pre-60S State 3 - post-5S rotation with Rix1 complex with Foot - composite structure
Authors	:	Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2023-07-17
Resolution	:	2.94 Å(reported)

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

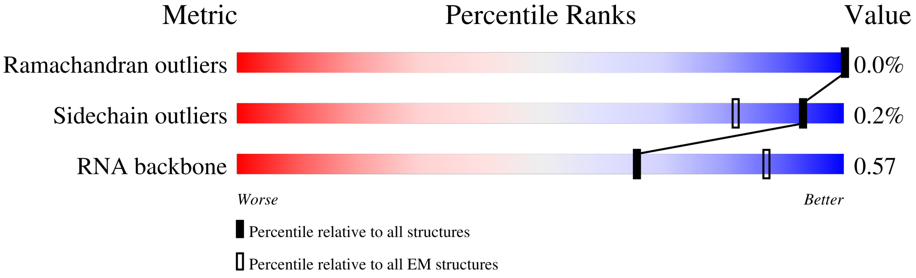
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

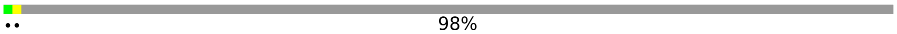
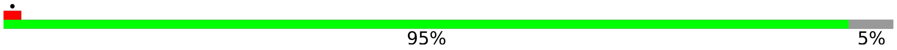
The reported resolution of this entry is 2.94 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	C1	3342	 • 75% 17% • 7%
2	C2	156	 • 85% 15%
3	C3	162	 • • 98%
4	C4	119	 76% 20% • •
5	CF	270	 • 91% 9%
6	CH	661	 • 95% 5%
7	CI	414	 • 22% 78%
8	CJ	679	 • 56% 44%

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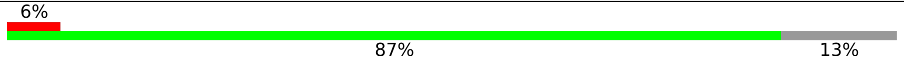
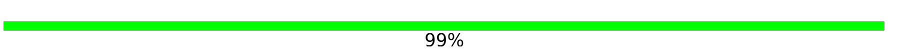
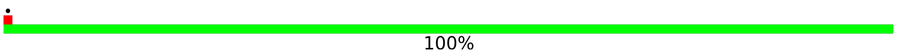
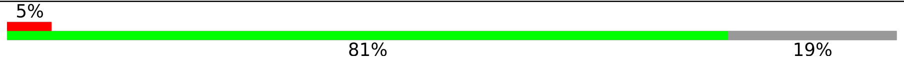
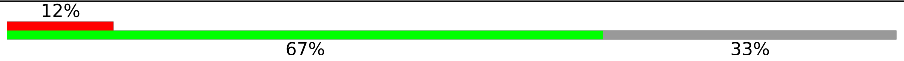
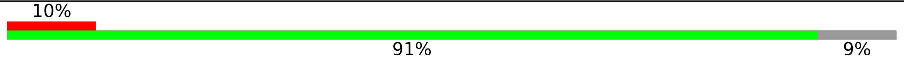
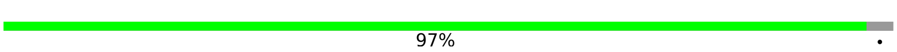
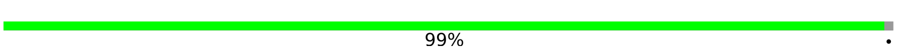
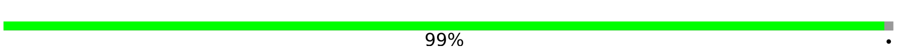
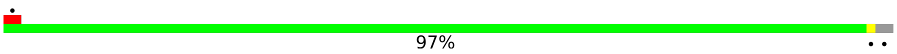
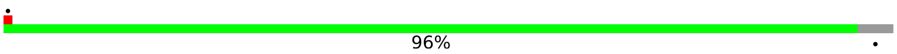
Mol	Chain	Length	Quality of chain
9	CK	261	 89% 11%
10	CL	558	 14% 86%
11	CM	249	 6% 87% 13%
11	LF	249	 99%
12	CN	246	 100%
13	CO	120	 52% 48%
14	CQ	225	 5% 81% 19%
15	CR	767	 12% 67% 33%
16	CS	338	 10% 91% 9%
17	CT	437	 90% 10%
17	CU	437	 90% 10%
18	CV	781	 70% 30%
18	CW	781	 70% 30%
19	Cb	117	 86% 14%
20	Cd	627	 72% 28%
21	Ce	443	 68% 32%
22	Ch	517	 75% 25%
23	Cz	123	 84% 16%
24	LA	254	 97%
25	LB	392	 99%
26	LC	365	 99%
27	LD	304	 97%
28	LE	200	 96%
29	LG	262	 90% 10%
30	LH	229	 83% 17%

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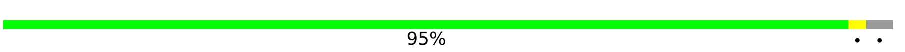
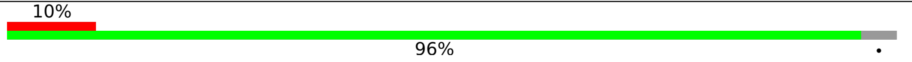
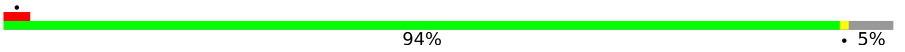
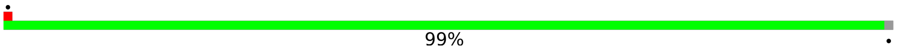
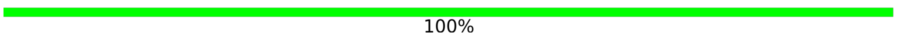
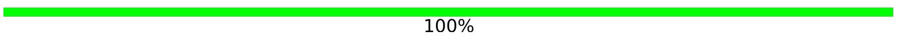
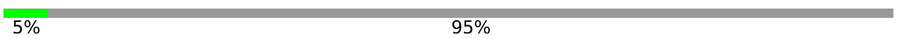
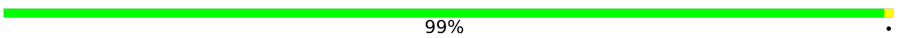
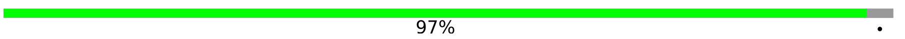
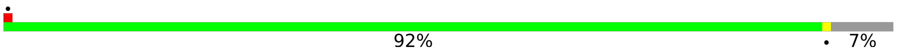
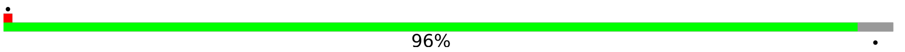
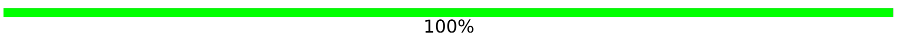
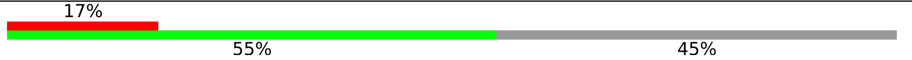
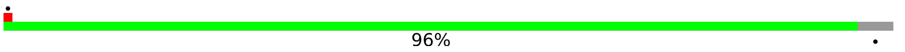
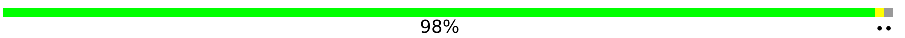
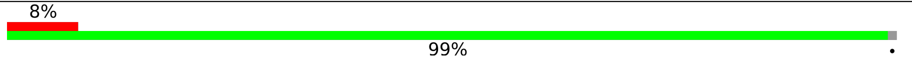
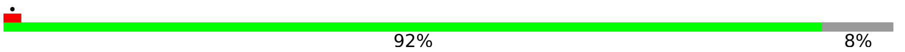
Mol	Chain	Length	Quality of chain
31	LJ	173	
32	LK	165	
33	LL	213	
34	LM	142	
35	LN	203	
36	LO	204	
37	LP	187	
38	LQ	213	
39	LR	2898	
40	LS	174	
41	LT	160	
42	LU	127	
43	LV	139	
44	LX	156	
45	LY	138	
46	LZ	135	
47	La	149	
48	Lb	65	
49	Lc	108	
50	Ld	120	
51	Le	131	
52	Lf	109	
53	Lg	119	
54	Lh	935	
55	Li	110	

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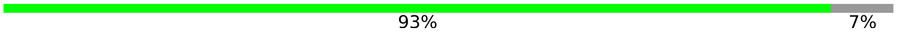
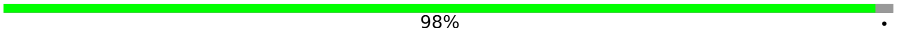
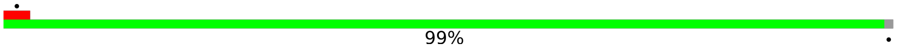
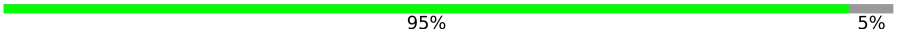
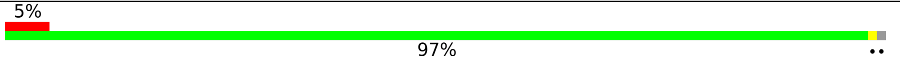
Mol	Chain	Length	Quality of chain
56	Lj	95	
57	Lk	94	
58	Ll	51	
59	Lp	92	
60	Lq	147	
61	Lr	217	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 172014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	3100	66359	29636	12012	21611	3100	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	156	3319	1484	589	1090	156	0	0

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C3	3	60	27	7	23	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	C4	115	2451	1093	438	805	115	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CF	245	1934	1215	350	360	9	0	0

- Molecule 6 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CH	627	5061	3180	924	938	19	0	0

- Molecule 7 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CI	93	Total 729	C 472	N 132	O 122	S 3	0	0

- Molecule 8 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CJ	382	Total 3116	C 2008	N 548	O 550	S 10	0	0

- Molecule 9 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CK	233	Total 1878	C 1183	N 363	O 328	S 4	0	0

- Molecule 10 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	CL	79	Total 618	C 386	N 124	O 108	0	0

- Molecule 11 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CM	217	Total 1773	C 1144	N 329	O 297	S 3	0	0
11	LF	248	Total 2023	C 1297	N 377	O 346	S 3	0	0

- Molecule 12 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CN	246	Total 1850	C 1154	N 322	O 368	S 6	0	0

- Molecule 13 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CO	62	Total 468	C 290	N 94	O 82	S 2	0	0

- Molecule 14 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CQ	183	Total 1476	C 923	N 304	O 239	S 10	0	0

- Molecule 15 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CR	516	Total 3844	C 2445	N 683	O 703	S 13	0	0

- Molecule 16 is a protein called Pre-rRNA-processing protein IPI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CS	307	Total 2391	C 1520	N 418	O 446	S 7	0	0

- Molecule 17 is a protein called Pre-rRNA-processing protein IPI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CT	393	Total 2941	C 1865	N 492	O 566	S 18	0	0
17	CU	393	Total 2953	C 1873	N 494	O 568	S 18	0	0

- Molecule 18 is a protein called Pre-rRNA-processing protein RIX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CV	550	Total 4217	C 2691	N 735	O 777	S 14	0	0
18	CW	550	Total 4204	C 2685	N 729	O 776	S 14	0	0

- Molecule 19 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Cb	101	Total 830	C 517	N 161	O 148	S 4	0	0

- Molecule 20 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Cd	451	3614	2301	660	642	11	0	0

- Molecule 21 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Ce	302	2476	1541	471	460	4	0	0

- Molecule 22 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Ch	389	3050	1916	568	557	9	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	117	ASP	GLU	engineered mutation	UNP G0SC29

- Molecule 23 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Cz	103	884	548	183	149	4	0	0

- Molecule 24 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LA	247	1878	1175	374	326	3	0	0

- Molecule 25 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LB	388	3097	1969	578	537	13	0	0

- Molecule 26 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LC	363	2745	1734	524	478	9	0	0

- Molecule 27 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LD	298	2366	1496	424	443	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LE	191	1470	941	267	259	3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LG	235	1880	1204	348	323	5	0	0

- Molecule 30 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LH	190	1495	949	268	272	6	0	0

- Molecule 31 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LJ	168	1367	854	266	241	6	0	0

- Molecule 32 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	LK	158	1184	743	215	224	2	0	0

- Molecule 33 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LL	203	Total	C	N	O	S	0	0
			1587	989	325	271	2		

- Molecule 34 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LM	141	Total	C	N	O	S	0	0
			1126	714	216	195	1		

- Molecule 35 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LN	202	Total	C	N	O	S	0	0
			1704	1062	360	278	4		

- Molecule 36 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LO	203	Total	C	N	O	S	0	0
			1611	1034	305	267	5		

- Molecule 37 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LP	171	Total	C	N	O	S	0	0
			1343	834	274	232	3		

- Molecule 38 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LQ	146	Total	C	N	O	S	0	0
			1156	730	228	196	2		

- Molecule 39 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LR	155	Total	C	N	O	S	0	0
			1241	772	262	203	4		

- Molecule 40 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LS	174	Total 1430	C 920	N 267	O 238	S 5	0	0

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LT	141	Total 1124	C 712	N 215	O 195	S 2	0	0

- Molecule 42 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LU	105	Total 838	C 542	N 144	O 151	S 1	0	0

- Molecule 43 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LV	135	Total 991	C 630	N 184	O 170	S 7	0	0

- Molecule 44 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	LX	145	Total 1113	C 709	N 206	O 198	0	0

- Molecule 45 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LY	133	Total 1056	C 658	N 213	O 183	S 2	0	0

- Molecule 46 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LZ	135	Total 1102	C 707	N 203	O 188	S 4	0	0

- Molecule 47 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	La	108	Total	C	N	O	S	0	0
			872	556	168	147	1		

- Molecule 48 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Lb	36	Total	C	N	O	0	0
			286	178	61	47		

- Molecule 49 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lc	95	Total	C	N	O	S	0	0
			705	449	122	129	5		

- Molecule 50 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ld	110	Total	C	N	O	S	0	0
			875	555	171	148	1		

- Molecule 51 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Le	126	Total	C	N	O	S	0	0
			1017	640	208	163	6		

- Molecule 52 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 53 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lg	118	Total	C	N	O	S	0	0
			901	561	184	152	4		

- Molecule 54 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	Lh	122	Total 1003	C 637	N 198	O 168	0	0

- Molecule 55 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Li	101	Total 821	C 506	N 178	O 136	S 1	0	0

- Molecule 56 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lj	88	Total 698	C 427	N 154	O 112	S 5	0	0

- Molecule 57 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lk	76	Total 624	C 394	N 119	O 109	S 2	0	0

- Molecule 58 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Ll	50	Total 436	C 275	N 97	O 64	0	0

- Molecule 59 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Lp	91	Total 694	C 428	N 138	O 122	S 6	0	0

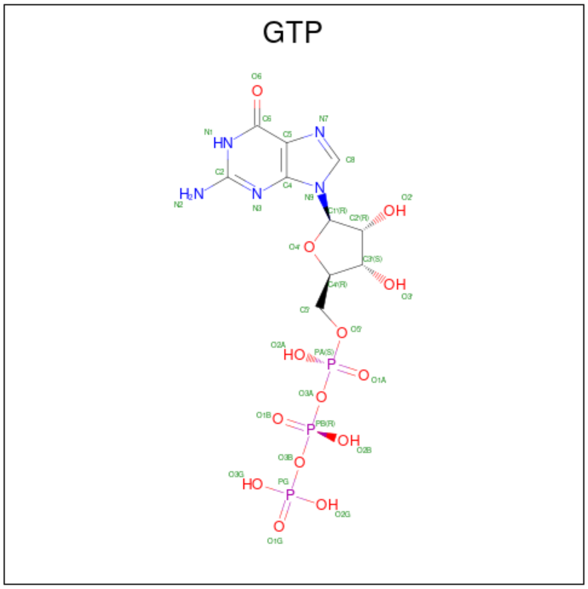
- Molecule 60 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	Lq	139	Total 1061	C 666	N 207	O 188	0	0

- Molecule 61 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	Lr	214	1660	1056	296	300	8	0	0

- Molecule 62 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
62	CH	1	32	10	5	14	3	0
62	Cd	1	32	10	5	14	3	0

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
63	CH	1	1	1	0
63	Cd	2	2	2	0

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	CQ	1	1	1	0
64	Cb	1	1	1	0

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Mol	Chain	Residues	Atoms	AltConf
64	Lg	1	Total Zn 1 1	0
64	Lj	1	Total Zn 1 1	0
64	Lp	1	Total Zn 1 1	0

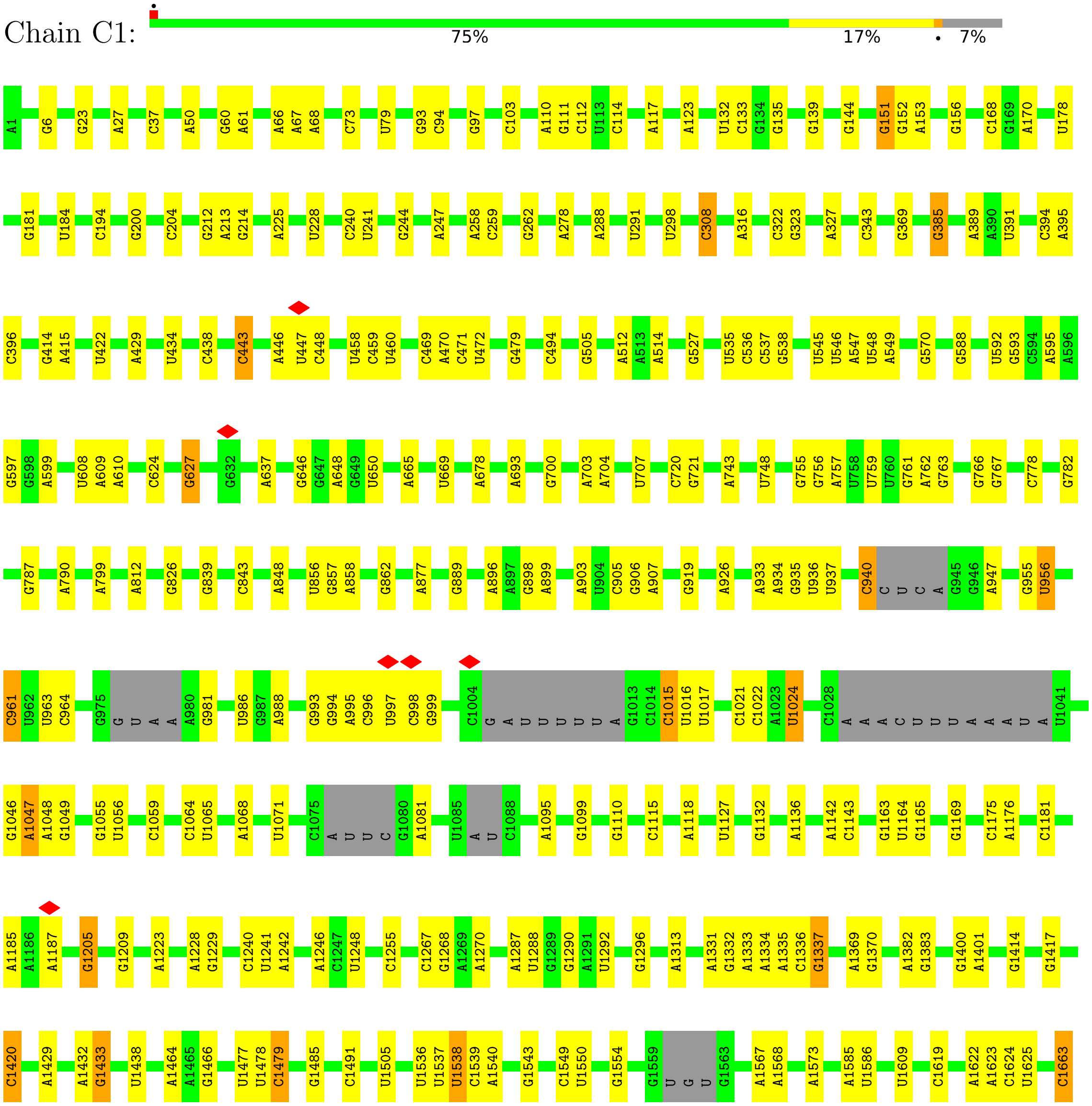
- Molecule 65 is water.

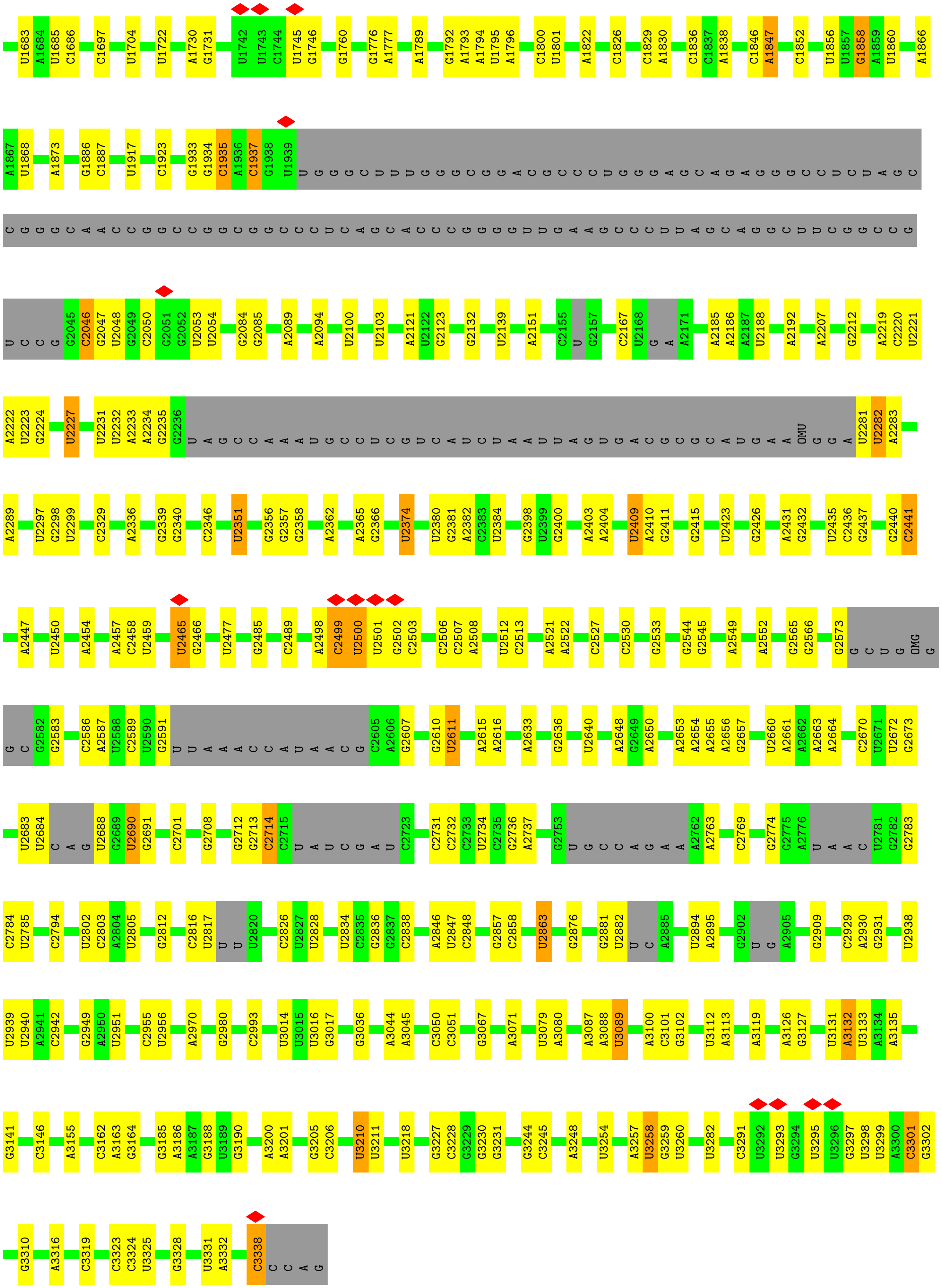
Mol	Chain	Residues	Atoms	AltConf
65	C1	1	Total O 1 1	0
65	CH	1	Total O 1 1	0
65	Cd	2	Total O 2 2	0

3 Residue-property plots ⓘ

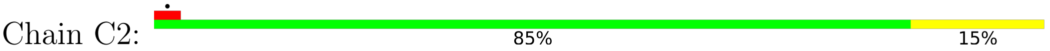
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

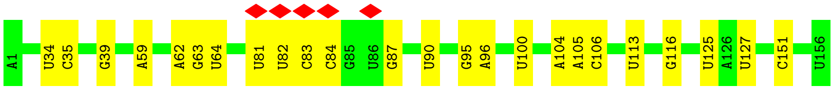
- Molecule 1: 26S rRNA





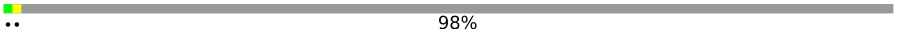
- Molecule 2: 5.8S rRNA

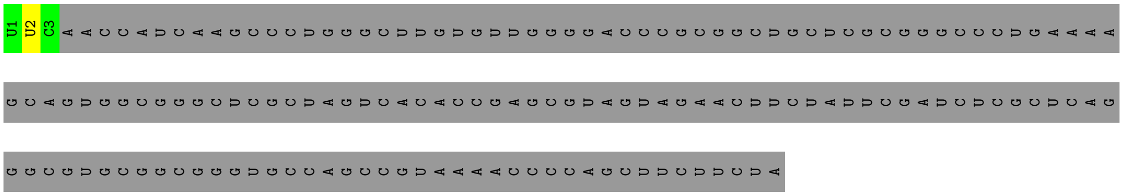




- Molecule 3: ITS2

Chain C3:



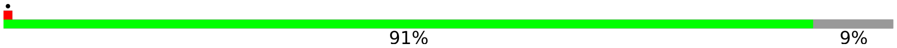


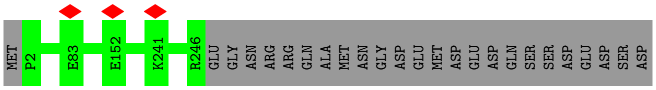
- Molecule 4: 5S rRNA

Chain C4:

- Molecule 5: Large ribosomal subunit protein uL10

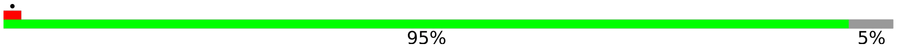
Chain CF:

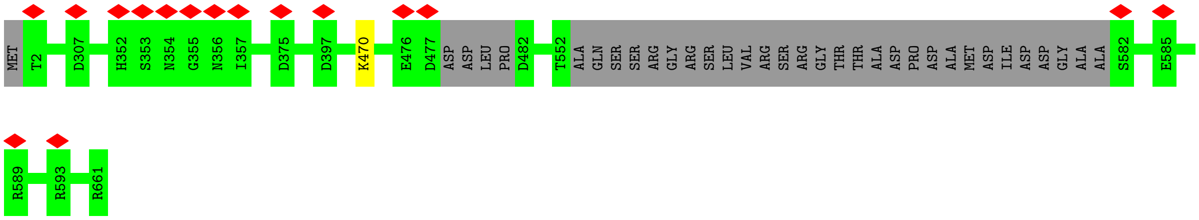




- Molecule 6: Nucleolar GTP-binding protein 1

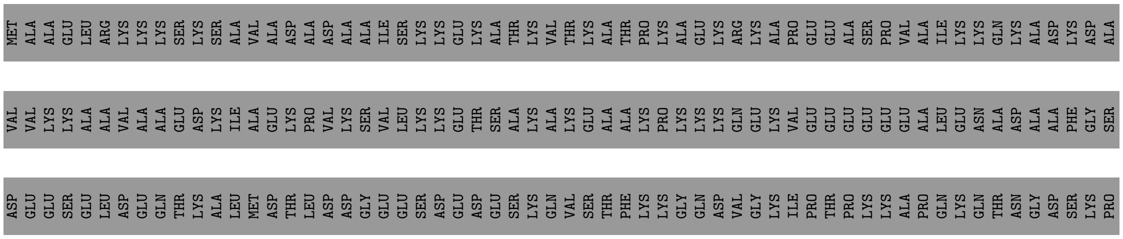
Chain CH:

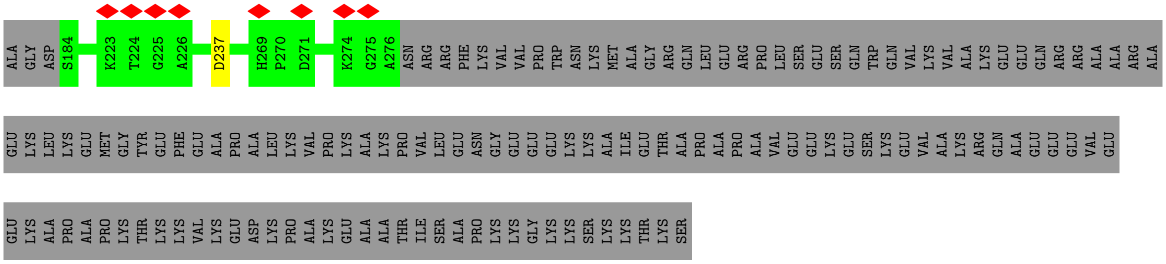




- Molecule 7: Putative RNA-binding protein

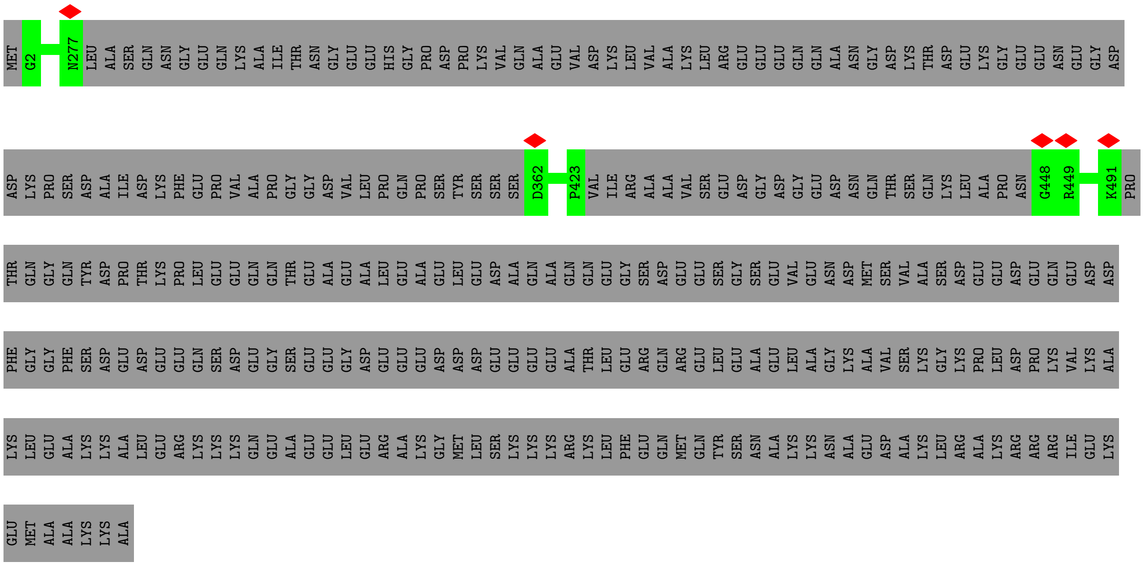
Chain CI:





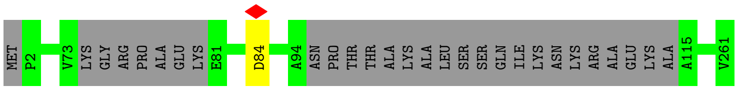
- Molecule 8: Pescadillo homolog

Chain CJ:



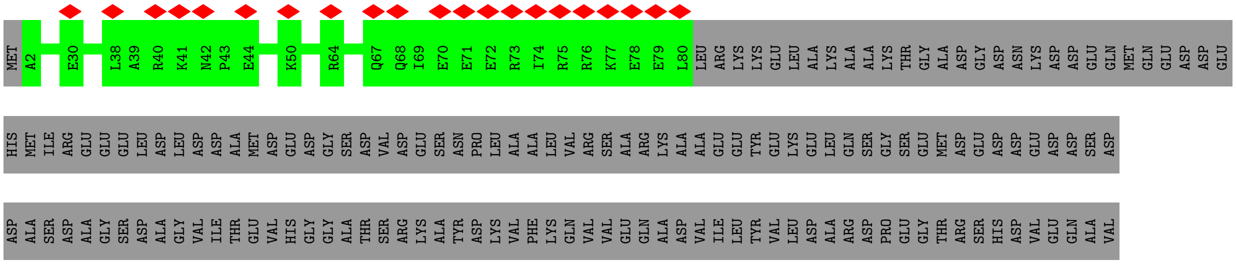
- Molecule 9: Ribosome biogenesis protein NSA2 homolog

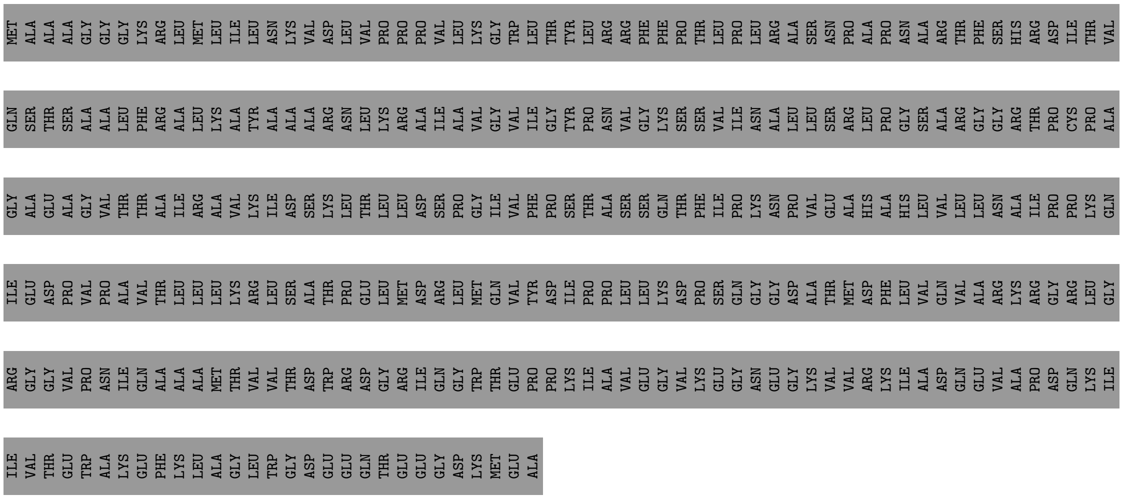
Chain CK:



- Molecule 10: Putative GTP binding protein

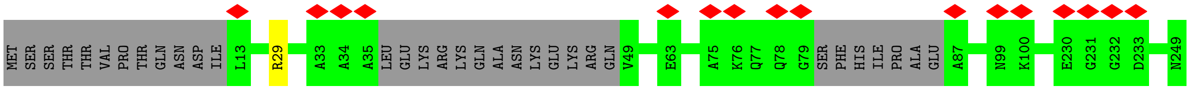
Chain CL:





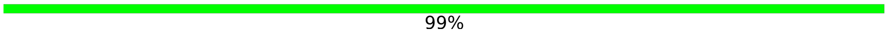
- Molecule 11: 60S ribosomal protein l7-like protein

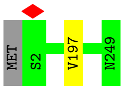
Chain CM:



- Molecule 11: 60S ribosomal protein l7-like protein

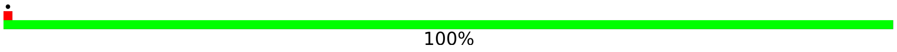
Chain LF:

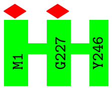




- Molecule 12: Eukaryotic translation initiation factor 6

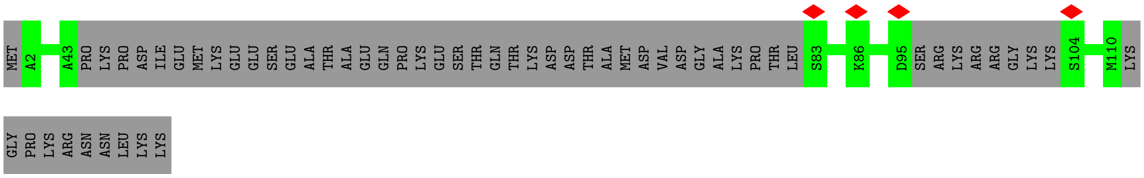
Chain CN:





- Molecule 13: DUF2423 domain-containing protein

Chain CO:

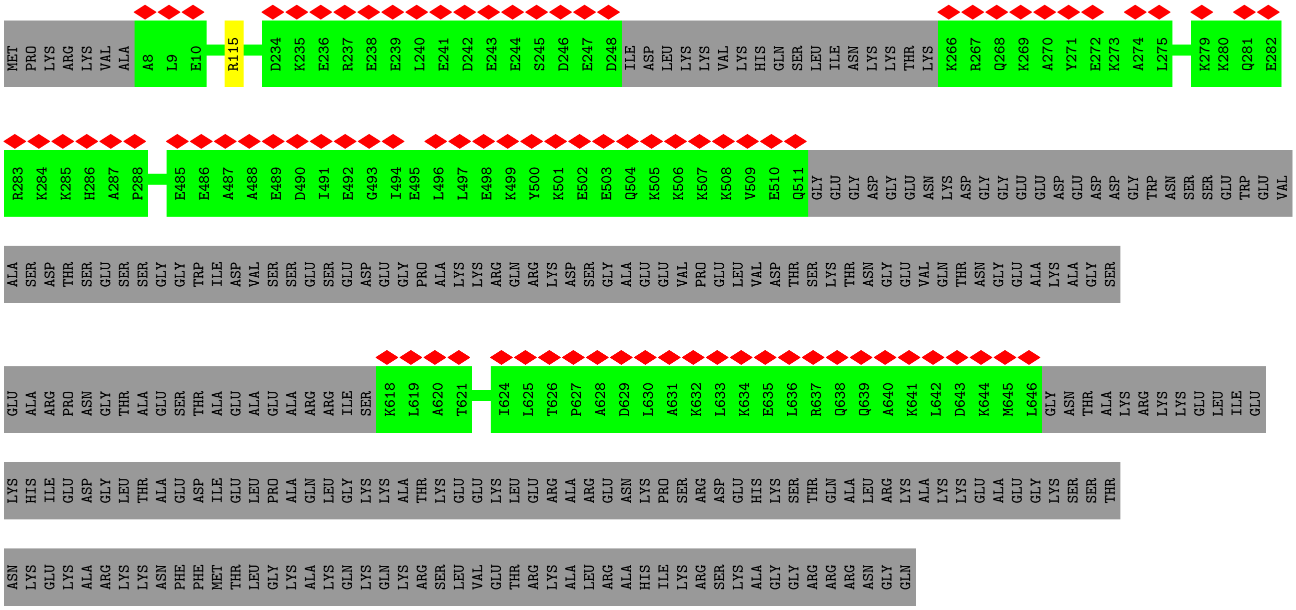


- Molecule 14: Ribosome biogenesis protein RLP24

Chain CQ:

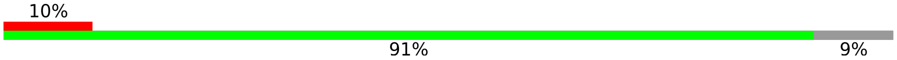
- Molecule 15: Protein SDA1

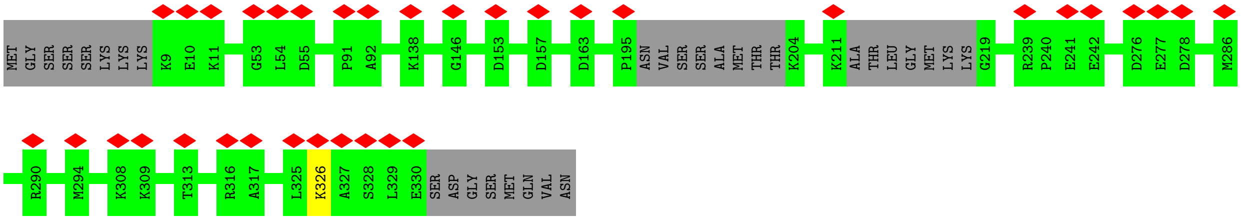
Chain CR:



- Molecule 16: Pre-rRNA-processing protein IPI1

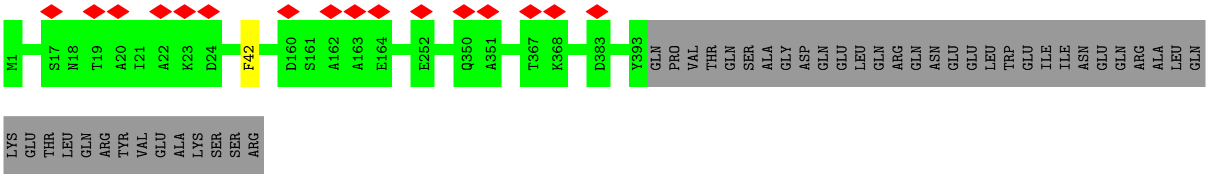
Chain CS:





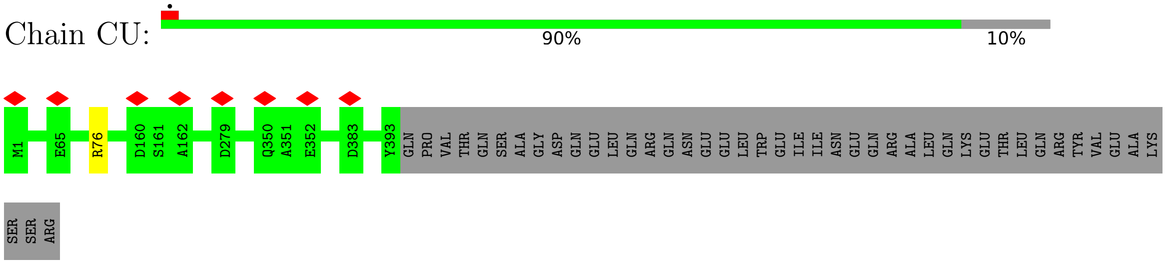
- Molecule 17: Pre-rRNA-processing protein IPI3

Chain CT:



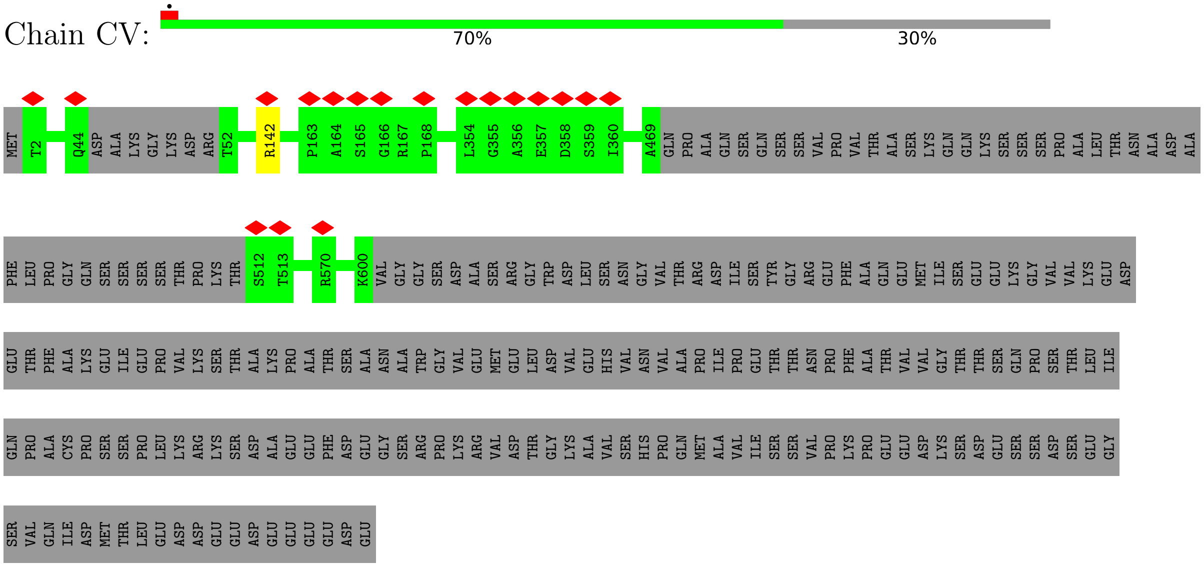
- Molecule 17: Pre-rRNA-processing protein IPI3

Chain CU:



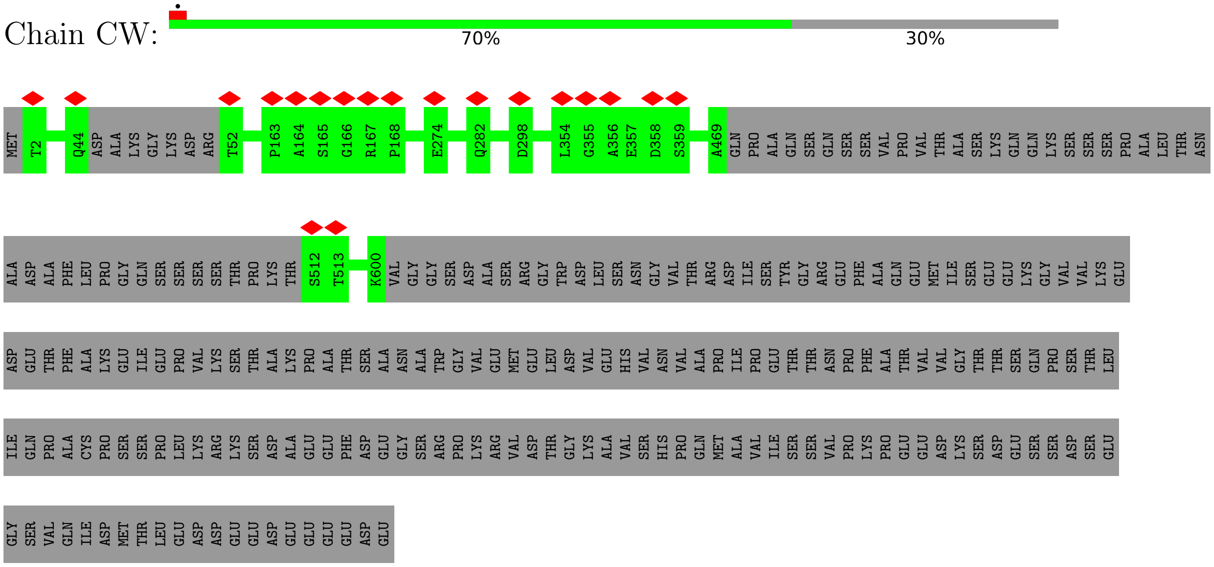
- Molecule 18: Pre-rRNA-processing protein RIX1

Chain CV:



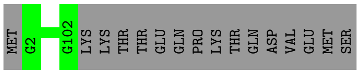
- Molecule 18: Pre-rRNA-processing protein RIX1

Chain CW:



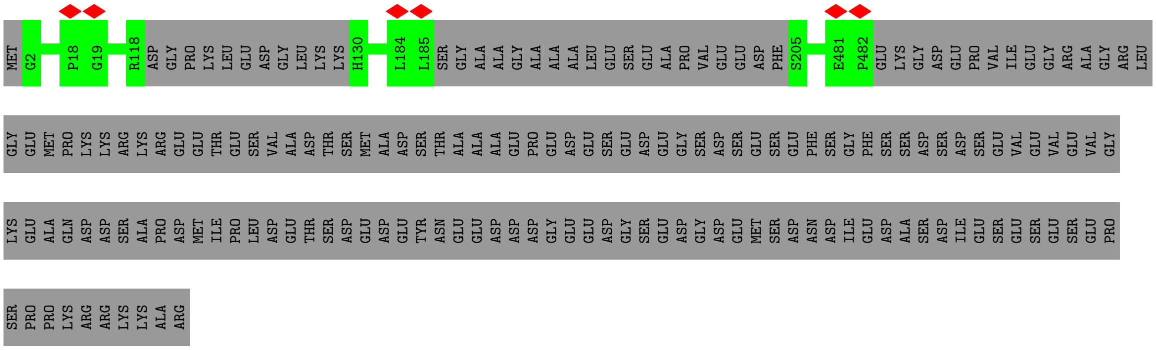
- Molecule 19: Zinc finger domain-containing protein

Chain Cb:



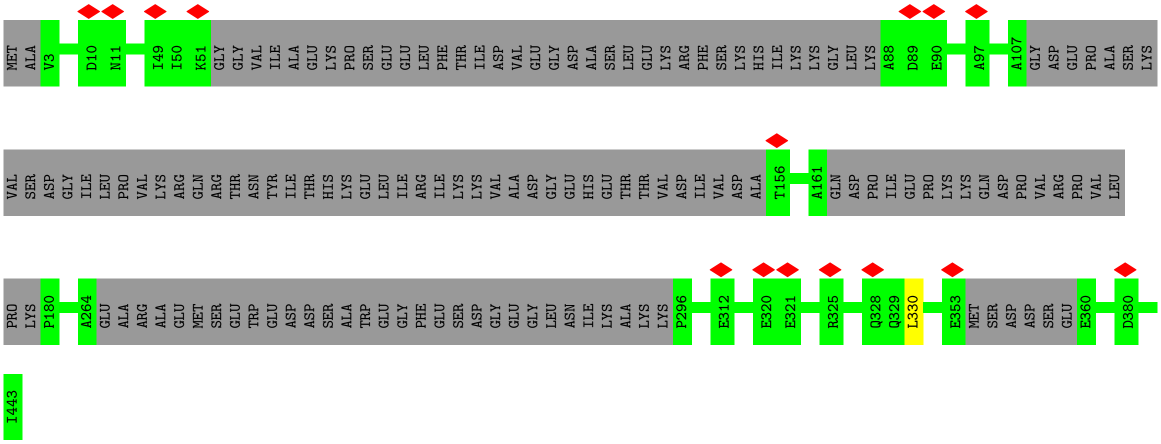
- Molecule 20: Nucleolar GTP-binding protein 2

Chain Cd:



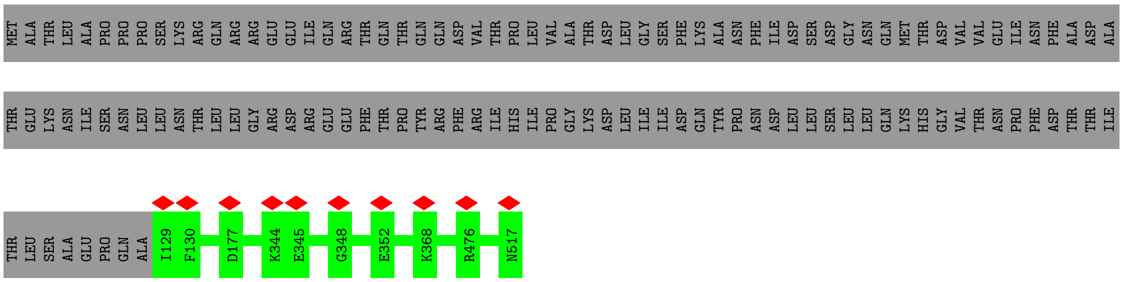
- Molecule 21: Ribosome biogenesis protein NOP53

Chain Ce:



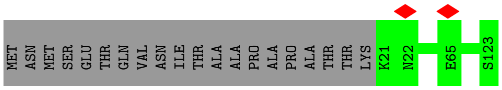
- Molecule 22: Ribosome assembly protein 4

Chain Ch:



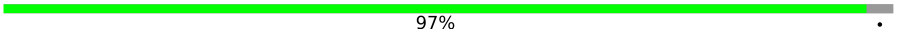
- Molecule 23: rRNA-processing protein

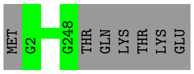
Chain Cz:



- Molecule 24: 60S ribosomal protein L2-like protein

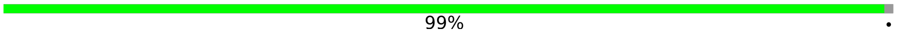
Chain LA:

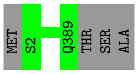




- Molecule 25: 60S ribosomal protein L3-like protein

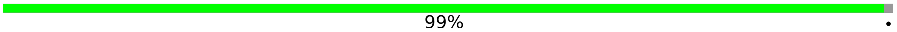
Chain LB:

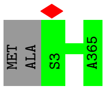




- Molecule 26: 60S ribosomal protein L4-like protein

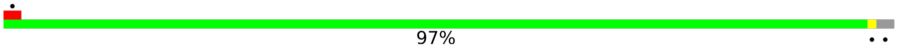
Chain LC:

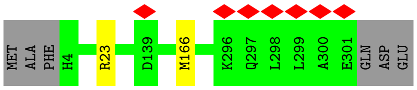




- Molecule 27: 60S ribosomal protein l5-like protein

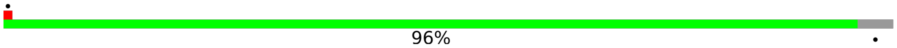
Chain LD:

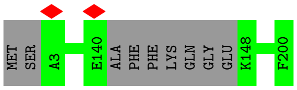




- Molecule 28: 60S ribosomal protein L6

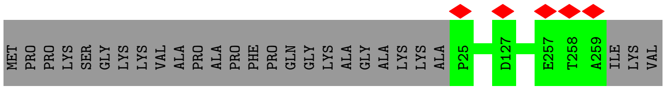
Chain LE:



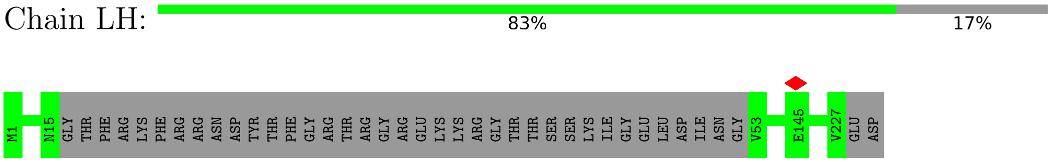


- Molecule 29: 60S ribosomal protein L8

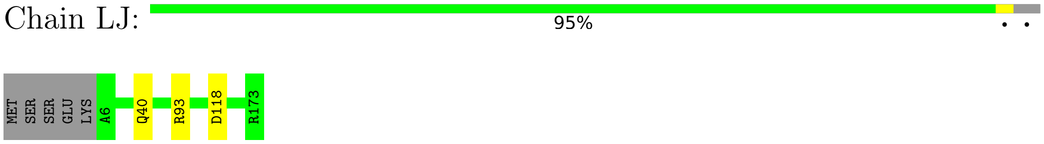
Chain LG:



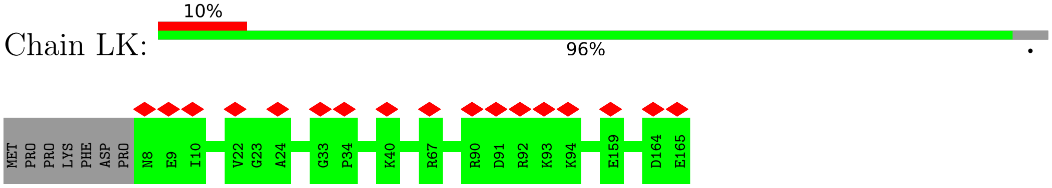
- Molecule 30: 60S ribosomal protein l9-like protein



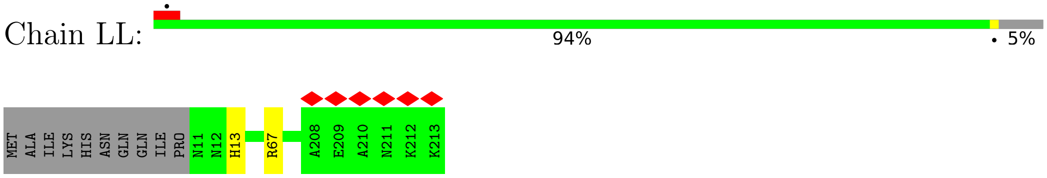
- Molecule 31: Putative ribosomal protein



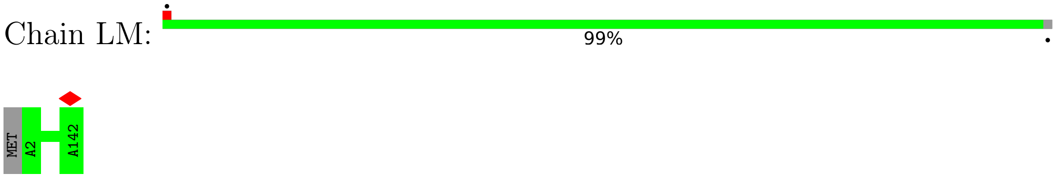
- Molecule 32: 60S ribosomal protein L12-like protein



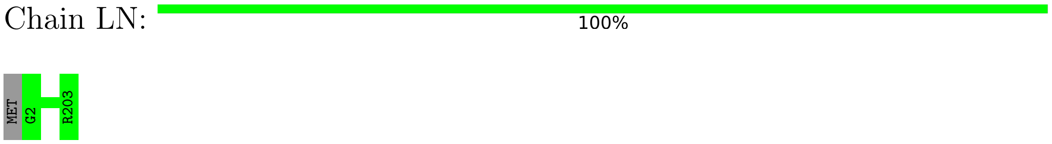
- Molecule 33: 60S ribosomal protein L13



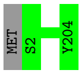
- Molecule 34: 60S ribosomal protein L14-like protein



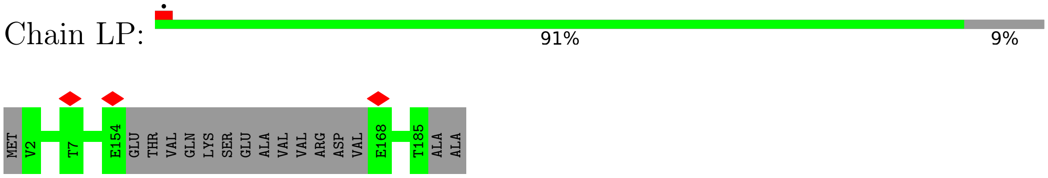
- Molecule 35: Ribosomal protein L15



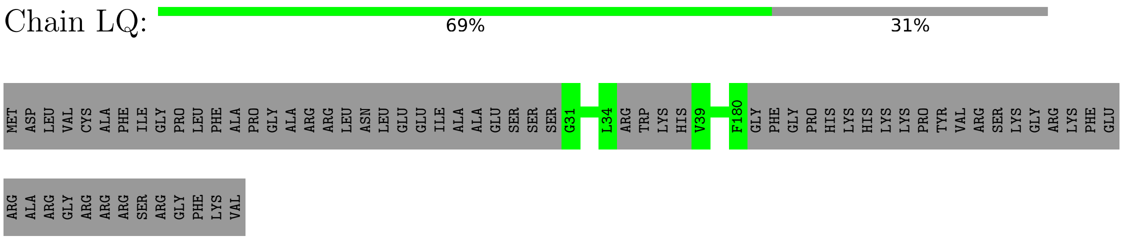
- Molecule 36: 60S ribosomal protein L16-like protein



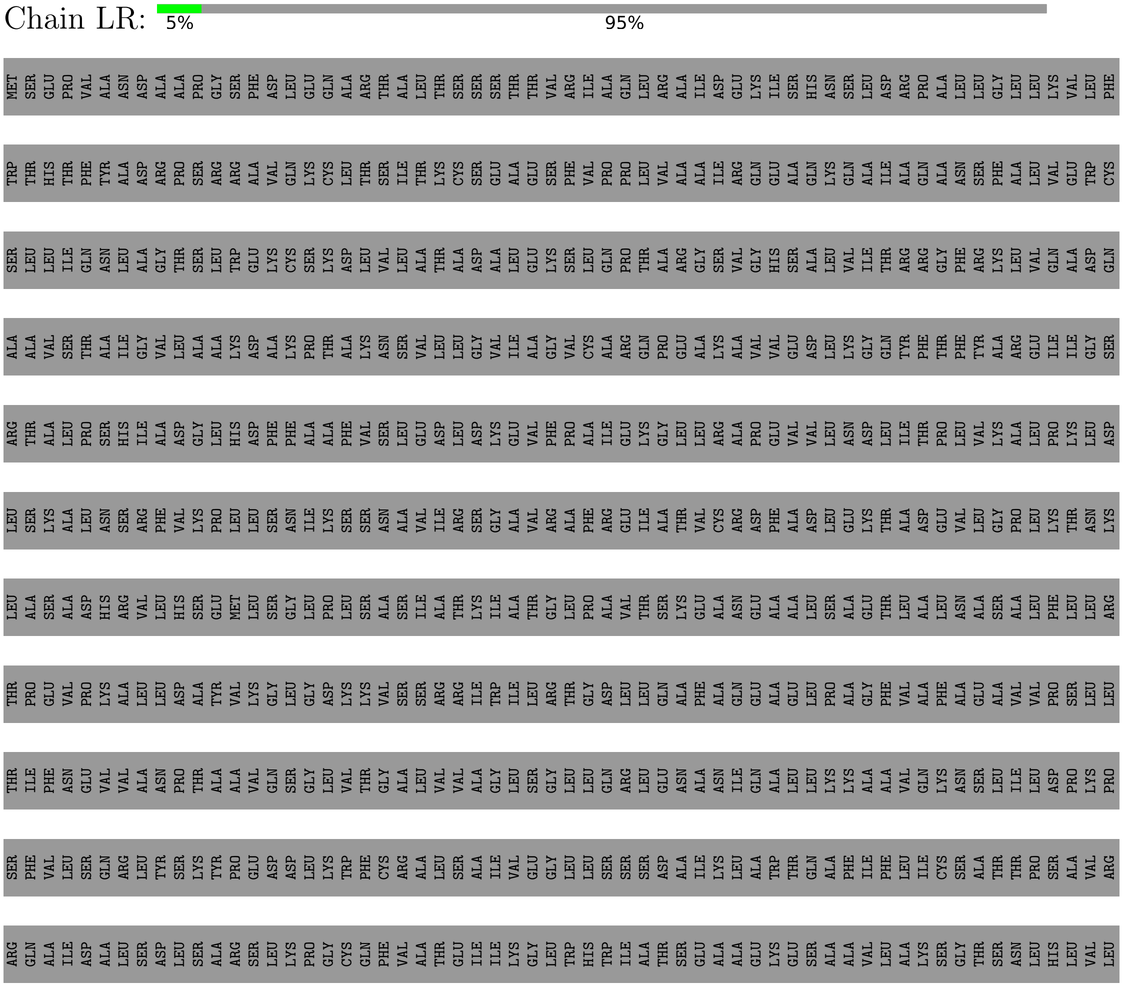
- Molecule 37: 60S ribosomal protein l17-like protein

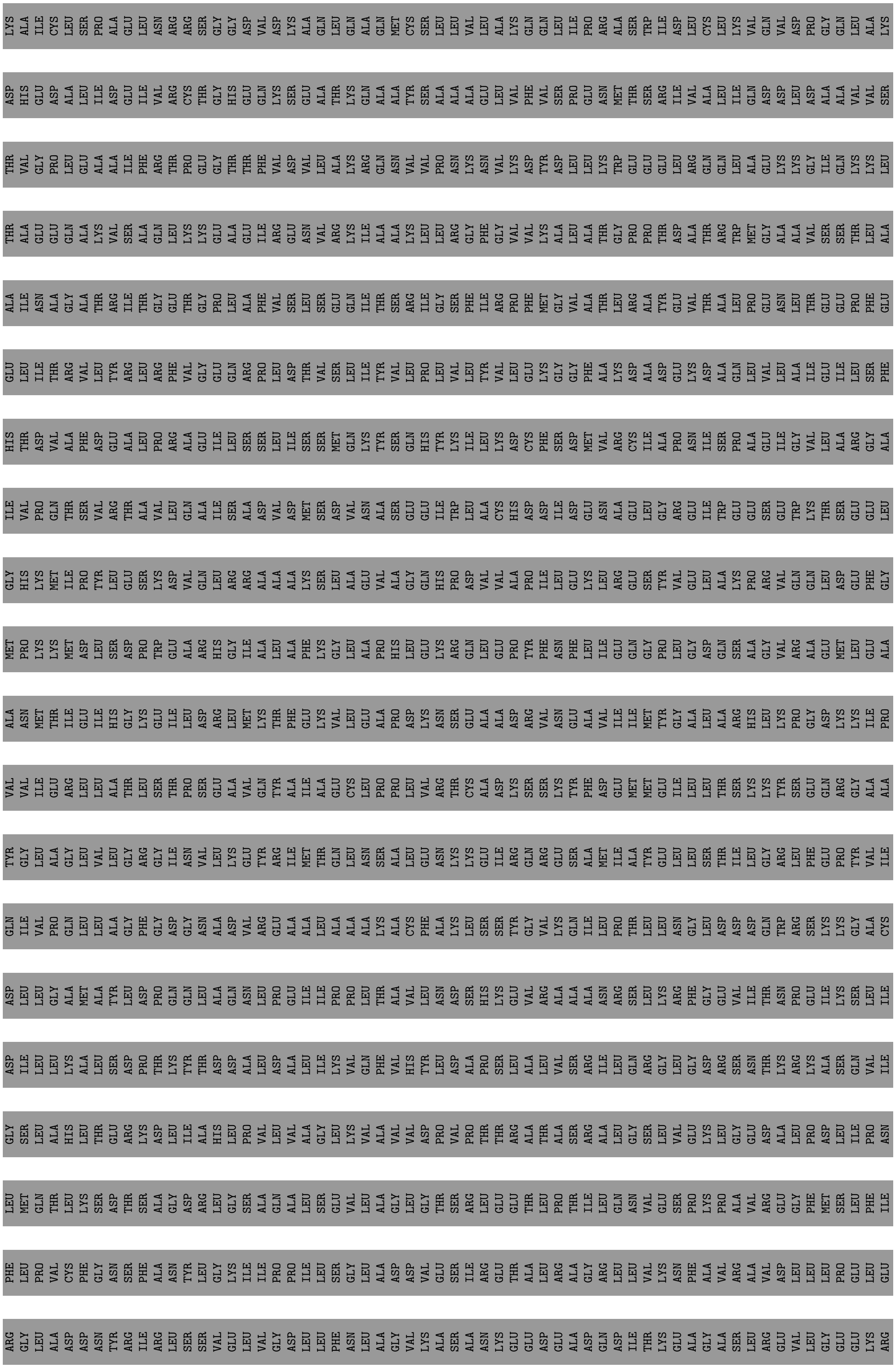


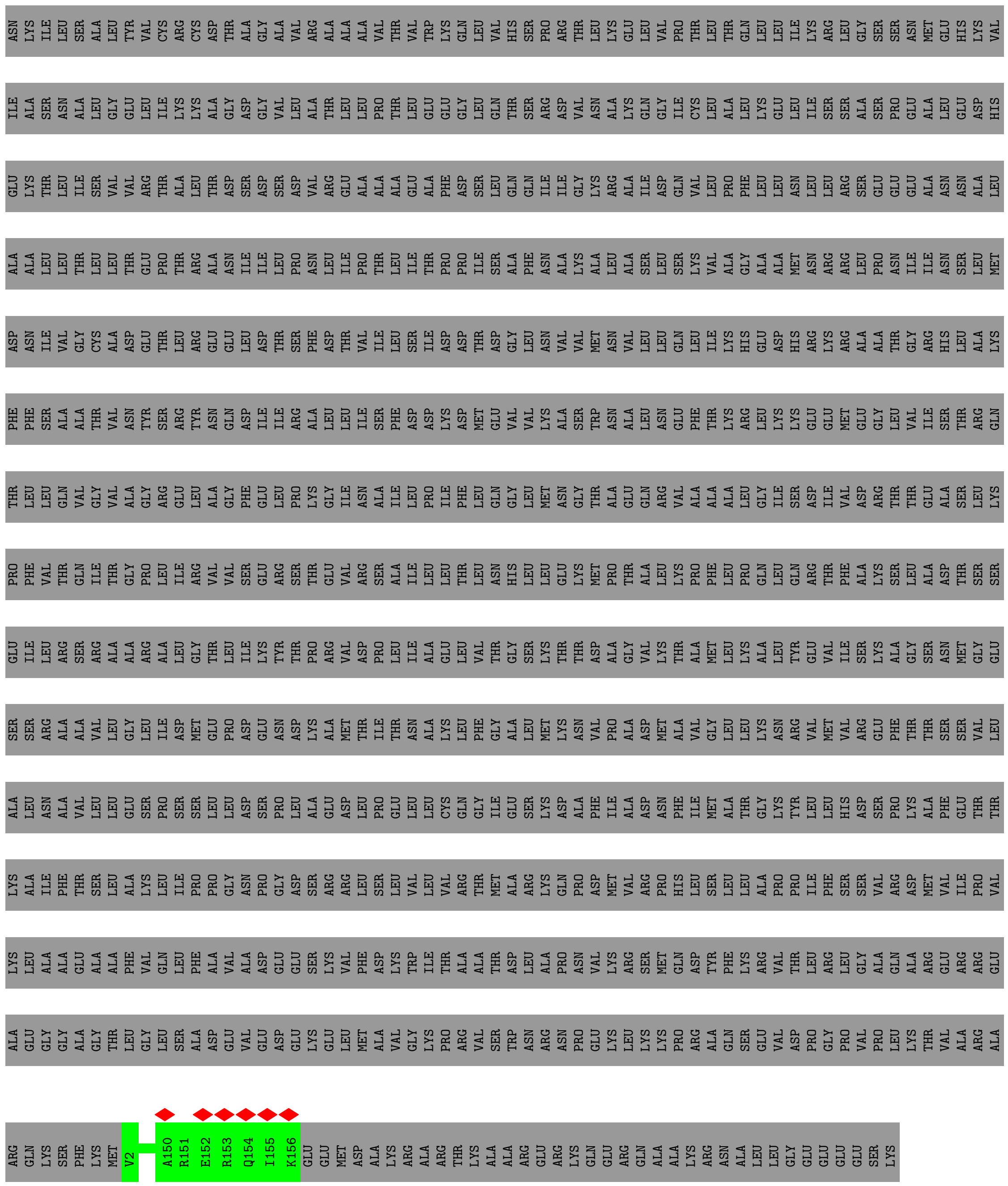
- Molecule 38: Ribosomal protein L18-like protein



- Molecule 39: Ribosomal protein L19

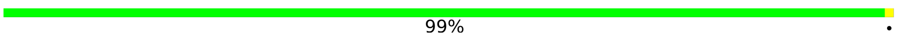


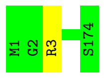

LYS ALA ILE CYS LEU SER PRO ALA GLU LEU ASN ARG ARG SER GLY GLY ASP VAL ASP LYS ALA GLN LEU GLN ALA GLN MET CYS SER LEU LEU VAL LEU ALA LYS GLN GLN LEU ILE PRO ARG ALA SER TRP ILE ASP LEU CYS LEU LYS VAL GLN VAL ASP PRO GLY GLN LEU ALA LYS
ASP HIS GLU ASP ALA LEU ILE ASP GLU ILE VAL ARG CYS THR GLY HIS GLU GLN LYS SER GLU ALA THR LYS GLN ALA ALA TYR SER ALA ALA ALA GLU LEU VAL PHE VAL SER PRO GLU ASN MET THR SER ARG ILE VAL ALA LEU ILE GLN ASP ASP LEU ASP ALA ALA VAL VAL SER
THR VAL GLY PRO LEU GLU ALA ALA ILE PHE ARG THR PRO GLU GLY THR THR PHE VAL ASP VAL LEU ALA LYS ARG GLN ASN VAL VAL PRO ASN LYS ASN VAL LYS ASP TYR ASP LEU LEU LYS TRP GLU GLU GLU LEU ARG GLN GLN LEU ALA GLU LYS LYS GLY ILE GLN LYS LYS LEU
THR ALA GLU GLU GLN ALA LYS VAL SER ALA GLN LEU LYS LYS GLU ALA GLU ILE ARG GLU ASN VAL ARG LYS ILE ALA ALA LYS LEU LEU ARG GLY PHE GLY VAL VAL LYS ALA LEU ALA THR GLY PRO PRO THR ASP ALA THR ARG TRP MET GLY ALA ALA VAL SER SER THR LEU ALA
ALA ILE ASN ALA GLY ALA THR ARG ILE THR GLY GLU THR GLY PRO LEU ALA PHE VAL SER LEU SER GLU GLN ILE THR SER ARG ILE GLY SER PHE ILE ARG PRO PHE MET GLY VAL ALA THR LEU ARG ALA TYR GLU VAL THR ALA LEU PRO GLU ASN LEU THR GLU GLU PRO PHE GLU
GLU LEU ILE THR ARG VAL LEU TYR ARG LEU ARG PHE VAL GLY GLU GLN ARG PRO LEU ASP THR VAL SER LEU ILE TYR VAL LEU PRO LEU VAL LEU TYR VAL LEU GLU LYS GLY GLY PHE ALA LYS ASP ALA ASP GLU LYS ASP ALA GLN LEU VAL LEU ALA ILE GLU ILE LEU SER PHE
HIS THR ASP VAL ALA PHE ASP GLU ALA LEU PRO ARG ALA GLU ILE LEU SER SER LEU ILE SER SER MET GLN LYS TYR SER GLN HIS TYR LYS ILE LEU LYS ASP CYS PHE SER ASP MET VAL ARG CYS ILE ALA PRO ASN ILE SER PRO ALA GLU ILE GLY VAL LEU ALA ARG GLY ALA
ILE VAL PRO GLN THR SER VAL ARG THR ALA VAL LEU GLN ALA ILE SER ALA ASP VAL ASP MET SER ASP VAL ASN ALA SER GLU GLU ILE TRP LEU ALA CYS HIS ASP ASP ILE ASP GLU ASN ALA GLU LEU GLY ARG GLU ILE TRP GLU GLU SER GLU TRP LYS THR SER GLU GLU LEU
GLY HIS LYS MET ILE PRO TYR LEU GLU SER LYS ASP VAL GLN LEU ARG ALA ALA ALA LYS SER LEU ALA GLU VAL ALA GLY GLN HIS PRO ASP VAL VAL ALA PRO ILE LEU GLU LYS LEU ARG GLU SER TYR VAL GLU LEU ALA LYS PRO ARG VAL GLN GLN LEU ASP GLU PHE GLY
MET PRO LYS LYS MET ASP LEU SER ASP PRO TRP GLU ALA ARG HIS GLY ILE ALA LEU ALA PHE LYS GLY LEU ALA PRO HIS LEU GLU LYS ARG GLN LEU GLU PRO TYR PHE ASN PHE LEU ILE GLU GLN GLY PRO LEU GLY ASP GLN SER ALA GLY VAL ARG ALA GLU MET LEU GLU ALA
ALA ASN MET THR ILE GLU ILE HIS GLY LYS GLU ILE LEU ASP ARG LEU MET LYS THR PHE GLU LYS VAL LEU GLU ALA PRO ASP LYS ASN SER GLU ALA ALA ASP ARG VAL ASN GLU ALA VAL ILE ILE MET TYR GLY ALA LEU ALA ARG HIS LEU LYS PRO GLY ASP LYS LYS ILE PRO
VAL VAL ILE GLU ARG LEU LEU ALA THR LEU SER THR PRO SER GLU ALA VAL GLN TYR ALA ILE ALA GLU CYS LEU PRO PRO LEU VAL ARG THR CYS ALA ASP LYS SER SER LYS TYR PHE ASP GLU MET MET GLU ILE LEU LEU THR SER LYS LYS TYR SER GLU GLN ARG GLY ALA ALA
TYR GLY LEU ALA GLY LEU VAL LEU GLY ARG GLY ILE ASN VAL LEU LYS GLU TYR ARG ILE MET THR GLN LEU ASN SER ALA LEU GLU ASN LYS LYS GLU ILE ARG GLN ARG GLU SER ALA MET ILE ALA TYR GLU LEU LEU SER THR ILE LEU GLY ARG LEU PHE GLU PRO TYR VAL ILE
GLN ILE VAL PRO GLN LEU LEU ALA GLY PHE GLY ASP GLY ASN ALA ASP VAL ARG GLU ALA ALA LEU ALA ALA LYS ALA CYS PHE ALA LYS LEU SER SER TYR GLY VAL LYS GLN ILE LEU PRO THR LEU LEU ASN GLY LEU ASP ASP ASP GLN TRP ARG SER LYS LYS GLY ALA CYS
ASP LEU LEU GLY ALA MET ALA TYR LEU ASP PRO GLN GLN LEU ALA GLN ASN LEU PRO GLU ILE ILE PRO PRO LEU THR ALA VAL LEU ASN ASP SER HIS LYS GLU VAL ARG ALA ALA ALA ASN ARG SER LEU LYS ARG PHE GLY GLU VAL ILE THR ASN PRO GLU ILE LYS SER LEU ILE
ASP ILE LEU LEU LYS ALA LEU SER ASP PRO THR LYS TYR THR ASP ASP ALA LEU ASP ALA LEU ILE LYS VAL GLN PHE VAL HIS TYR LEU ASP ALA PRO SER LEU ALA LEU VAL SER ARG ILE LEU GLN ARG GLY LEU GLY ASP ARG SER ASN THR LYS ARG LYS ALA SER GLN VAL ILE
GLY SER LEU ALA HIS LEU THR GLU ARG LYS ASP LEU ILE ALA HIS LEU PRO VAL LEU VAL ALA GLY LEU LYS VAL ALA VAL VAL ASP PRO VAL PRO THR THR ARG ALA THR ALA SER ARG ALA LEU GLY SER LEU VAL GLU LYS LEU GLY GLU ASP ALA LEU PRO ASP LEU ILE PRO ASN
LEU MET GLN THR LEU LYS SER ASP THR SER ALA GLY ASP ARG LEU GLY SER ALA GLN ALA LEU SER GLU VAL LEU ALA GLY LEU GLY THR SER ARG LEU GLU GLU THR LEU PRO THR ILE LEU GLN ASN VAL GLU SER PRO LYS PRO ALA VAL ARG GLU GLY PHE MET SER LEU PHE ILE
PHE LEU PRO VAL CYS PHE GLY ASN SER PHE ALA ASN TYR LEU GLY LYS ILE ILE PRO PRO ILE LEU SER GLY LEU ALA ASP ASP VAL GLU SER ILE ARG GLU THR ALA LEU ARG ALA GLY ARG LEU LEU VAL LYS ASN PHE ALA VAL ARG ALA VAL ASP LEU LEU LEU PRO GLU LEU GLU
ARG GLY LEU ALA ASP ASP ASN TYR ARG ILE ARG LEU SER SER VAL GLU LEU VAL GLY ASP LEU LEU PHE ASN LEU ALA GLY VAL LYS ALA SER ALA ASN LYS GLU GLU ASP GLU ALA ASP GLN ASP ILE THR LYS GLU ALA GLY ALA SER LEU ARG GLU VAL LEU GLY GLU GLU LYS ARG



- Molecule 40: 60S ribosomal protein L20

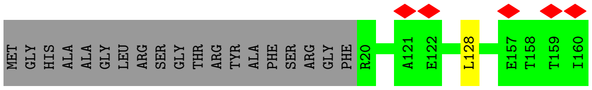
Chain LS:





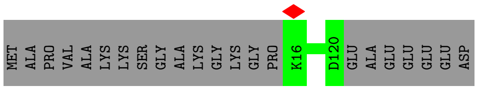
- Molecule 41: 60S ribosomal protein l21-like protein

Chain LT:



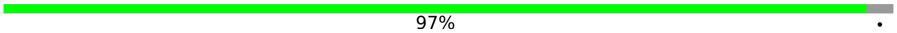
- Molecule 42: 60S ribosomal protein L22-like protein

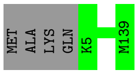
Chain LU:



- Molecule 43: 60S ribosomal protein l23-like protein

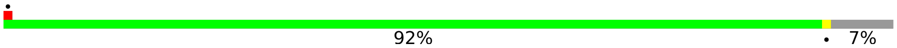
Chain LV:

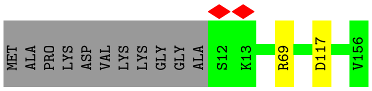




- Molecule 44: 60S ribosomal protein L25-like protein

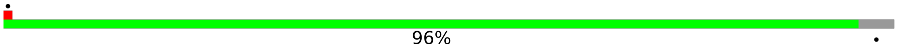
Chain LX:

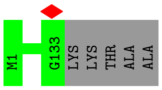




- Molecule 45: 60S ribosomal protein L26-like protein

Chain LY:





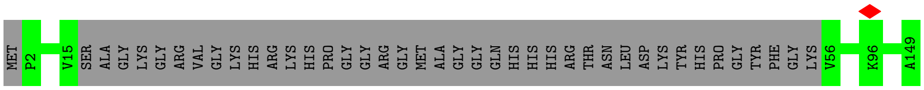
- Molecule 46: 60S ribosomal protein L27

Chain LZ:

There are no outlier residues recorded for this chain.

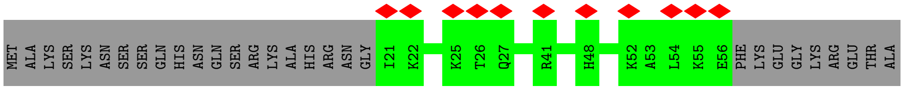
- Molecule 47: 60S ribosomal protein L28-like protein

Chain La:



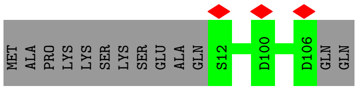
- Molecule 48: 60S ribosomal protein L29

Chain Lb:



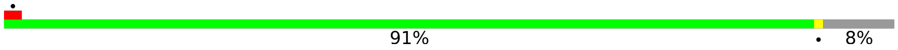
- Molecule 49: 60S ribosomal protein l30-like protein

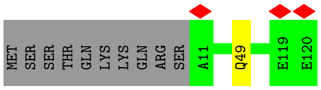
Chain Lc:



- Molecule 50: Putative 60S ribosomal protein

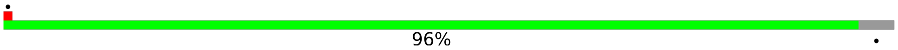
Chain Ld:

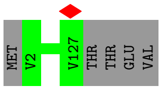




- Molecule 51: 60S ribosomal protein L32-like protein

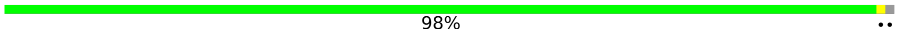
Chain Le:

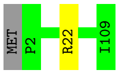




- Molecule 52: 60S ribosomal protein l33-like protein

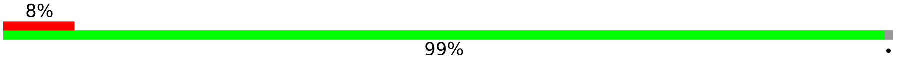
Chain Lf:

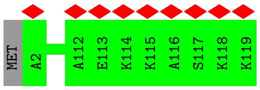




- Molecule 53: Ribosomal protein l34-like protein

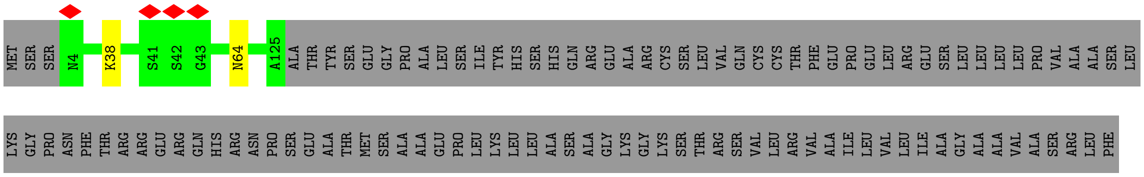
Chain Lg:

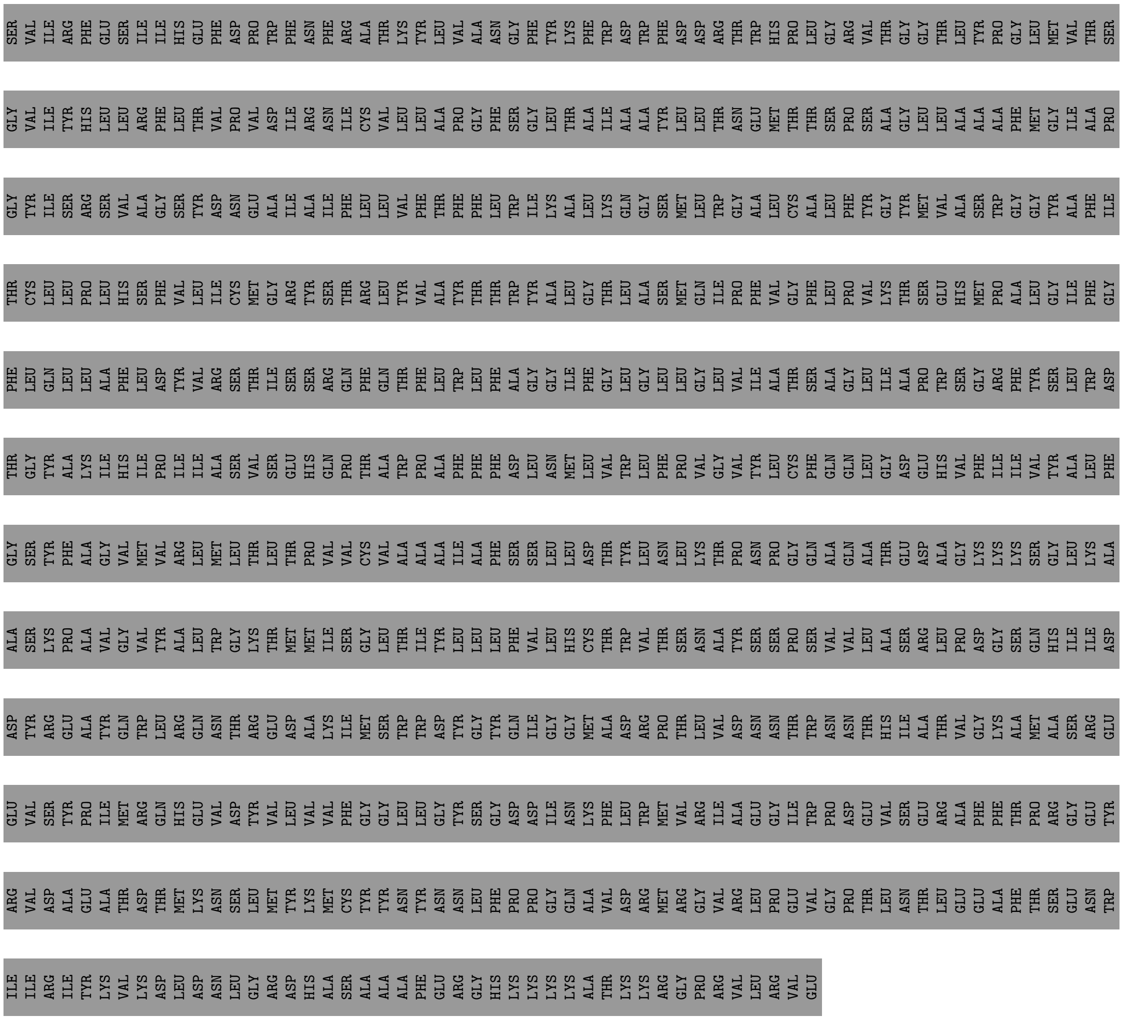




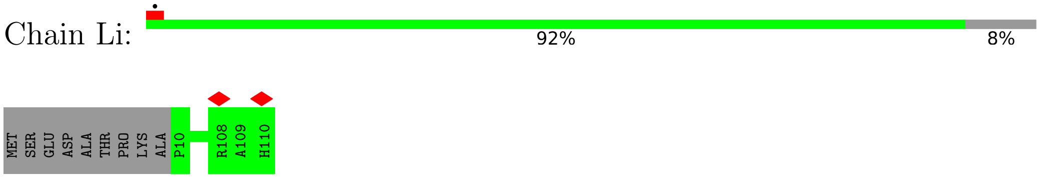
- Molecule 54: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:

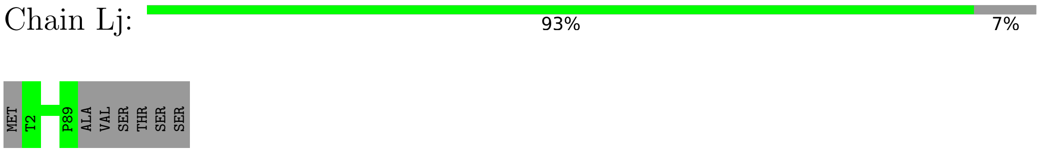




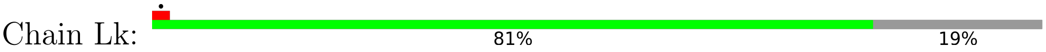
- Molecule 55: 60S ribosomal protein L36

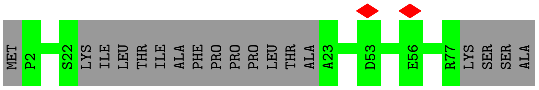


- Molecule 56: Ribosomal protein L37



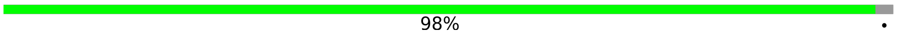
- Molecule 57: 60S ribosomal protein L38-like protein

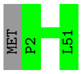




- Molecule 58: Ribosomal protein eL39

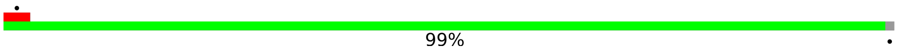
Chain Ll:

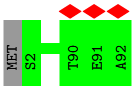




- Molecule 59: 60S ribosomal protein L43-like protein

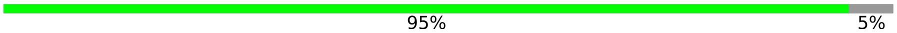
Chain Lp:

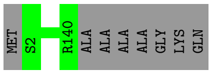




- Molecule 60: Putative 60S ribosomal protein

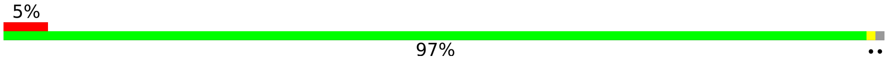
Chain Lq:

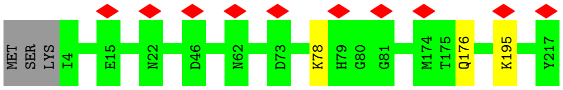




- Molecule 61: Ribosomal protein

Chain Lr:





4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25753	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 ($e^-/\text{Å}^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.708	Depositor
Minimum map value	0.000	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, OMU, ZN, OMC, A2M, OMG

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	C1	0.31	0/73447	0.90	93/114487 (0.1%)
2	C2	0.30	0/3710	0.86	4/5778 (0.1%)
3	C3	0.19	0/65	0.79	0/98
4	C4	0.32	0/2737	1.01	11/4262 (0.3%)
5	CF	0.25	0/1972	0.53	0/2660
6	CH	0.26	0/5145	0.53	0/6923
7	CI	0.28	0/749	0.64	1/1013 (0.1%)
8	CJ	0.26	0/3196	0.50	0/4319
9	CK	0.26	0/1913	0.56	1/2571 (0.0%)
10	CL	0.30	0/627	0.65	0/839
11	CM	0.26	0/1805	0.51	0/2417
11	LF	0.27	0/2061	0.54	0/2765
12	CN	0.27	0/1875	0.55	0/2552
13	CO	0.30	0/470	0.59	0/619
14	CQ	0.28	0/1500	0.62	0/1995
15	CR	0.26	0/3912	0.48	0/5320
16	CS	0.26	0/2442	0.49	0/3315
17	CT	0.27	0/3009	0.56	0/4113
17	CU	0.27	0/3021	0.54	0/4128
18	CV	0.27	0/4312	0.54	0/5897
18	CW	0.28	0/4299	0.53	0/5882
19	Cb	0.28	0/845	0.60	0/1128
20	Cd	0.26	0/3691	0.51	0/4975
21	Ce	0.26	0/2506	0.57	1/3338 (0.0%)
22	Ch	0.25	0/3137	0.55	0/4262
23	Cz	0.27	0/892	0.60	0/1167
24	LA	0.28	0/1917	0.58	0/2580
25	LB	0.26	0/3165	0.54	0/4250
26	LC	0.27	0/2802	0.52	0/3778
27	LD	0.26	0/2412	0.52	1/3247 (0.0%)
28	LE	0.27	0/1497	0.54	0/2018
29	LG	0.27	0/1909	0.53	0/2556

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	LH	0.26	0/1515	0.53	0/2037
31	LJ	0.28	0/1389	0.63	1/1856 (0.1%)
32	LK	0.26	0/1198	0.54	0/1611
33	LL	0.26	0/1614	0.58	0/2168
34	LM	0.26	0/1145	0.55	0/1539
35	LN	0.29	0/1741	0.61	0/2332
36	LO	0.27	0/1645	0.53	0/2205
37	LP	0.26	0/1364	0.57	0/1835
38	LQ	0.26	0/1170	0.57	0/1573
39	LR	0.26	0/1260	0.53	0/1683
40	LS	0.27	0/1465	0.55	0/1970
41	LT	0.27	0/1146	0.58	1/1546 (0.1%)
42	LU	0.28	0/851	0.53	0/1143
43	LV	0.28	0/1009	0.55	0/1357
44	LX	0.27	0/1131	0.58	1/1526 (0.1%)
45	LY	0.29	0/1070	0.61	0/1432
46	LZ	0.30	0/1125	0.59	0/1508
47	La	0.26	0/892	0.53	0/1200
48	Lb	0.24	0/293	0.55	0/392
49	Lc	0.27	0/714	0.52	0/960
50	Ld	0.27	0/889	0.58	1/1192 (0.1%)
51	Le	0.29	0/1035	0.62	0/1379
52	Lf	0.29	0/883	0.58	0/1187
53	Lg	0.29	0/914	0.62	0/1228
54	Lh	0.26	0/1014	0.55	0/1349
55	Li	0.26	0/828	0.60	0/1092
56	Lj	0.27	0/712	0.62	0/944
57	Lk	0.30	0/632	0.58	0/842
58	Ll	0.25	0/446	0.56	0/593
59	Lp	0.29	0/702	0.63	0/935
60	Lq	0.27	0/1079	0.55	0/1454
61	Lr	0.30	0/1684	0.56	0/2266
All	All	0.29	0/181595	0.74	116/261586 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	CT	0	1

There are no bond length outliers.

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1538	U	N3-C2-O2	-9.75	115.38	122.20
1	C1	1538	U	N1-C2-O2	9.52	129.47	122.80
1	C1	1478	U	C2-N1-C1’	9.25	128.80	117.70
1	C1	1538	U	C2-N1-C1’	8.87	128.34	117.70
1	C1	1478	U	N1-C2-O2	7.95	128.36	122.80
44	LX	117	ASP	CB-CG-OD1	7.90	125.41	118.30
1	C1	2441	C	N1-C2-O2	7.88	123.63	118.90
1	C1	1478	U	N3-C2-O2	-7.63	116.86	122.20
1	C1	1935	C	C2-N1-C1’	7.54	127.10	118.80
1	C1	3089	U	C2-N1-C1’	7.37	126.55	117.70
1	C1	1937	C	C2-N1-C1’	7.14	126.66	118.80
4	C4	50	U	N1-C2-O2	7.10	127.77	122.80
4	C4	103	U	C2-N1-C1’	7.00	126.10	117.70
1	C1	2046	C	N1-C2-O2	6.85	123.01	118.90
4	C4	50	U	N3-C2-O2	-6.83	117.42	122.20
31	LJ	118	ASP	CB-CG-OD1	6.74	124.37	118.30
4	C4	103	U	N1-C2-O2	6.64	127.45	122.80
1	C1	103	C	N1-C2-O2	6.46	122.78	118.90
1	C1	2586	C	C2-N1-C1’	6.42	125.86	118.80
1	C1	961	C	C2-N1-C1’	6.41	125.85	118.80
1	C1	3016	U	C2-N1-C1’	6.35	125.32	117.70
2	C2	64	U	N3-C2-O2	-6.32	117.78	122.20
1	C1	2441	C	C2-N1-C1’	6.31	125.74	118.80
1	C1	308	C	C2-N1-C1’	6.31	125.74	118.80
4	C4	42	C	N1-C2-O2	6.31	122.69	118.90
1	C1	2282	U	P-O3’-C3’	6.31	127.27	119.70
1	C1	3258	U	P-O3’-C3’	6.25	127.20	119.70
1	C1	1478	U	C6-N1-C1’	-6.21	112.51	121.20
1	C1	2499	C	N1-C2-O2	6.19	122.62	118.90
1	C1	1935	C	N1-C2-O2	6.12	122.57	118.90
1	C1	1937	C	C5-C6-N1	6.11	124.06	121.00
1	C1	2281	U	C2-N1-C1’	6.09	125.01	117.70
1	C1	2441	C	N3-C2-O2	-6.04	117.67	121.90
1	C1	2499	C	C2-N1-C1’	6.01	125.41	118.80
1	C1	1337	G	C4-N9-C1’	6.01	134.31	126.50
1	C1	2351	U	N3-C2-O2	-6.01	117.99	122.20
7	CI	237	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C1	2046	C	C2-N1-C1’	5.97	125.37	118.80
9	CK	84	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C1	2500	U	C2-N1-C1’	5.96	124.85	117.70
1	C1	1479	C	C2-N1-C1’	5.92	125.31	118.80
4	C4	50	U	C2-N1-C1’	5.91	124.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	956	U	C2-N1-C1'	5.91	124.79	117.70
4	C4	103	U	N3-C2-O2	-5.90	118.07	122.20
1	C1	438	C	C2-N1-C1'	5.87	125.26	118.80
1	C1	2794	C	C2-N1-C1'	5.87	125.25	118.80
1	C1	103	C	N3-C2-O2	-5.86	117.80	121.90
1	C1	2500	U	N1-C2-O2	5.79	126.86	122.80
1	C1	114	C	C2-N1-C1'	5.78	125.16	118.80
1	C1	3338	C	C2-N1-C1'	5.78	125.16	118.80
1	C1	443	C	C2-N1-C1'	5.77	125.14	118.80
1	C1	1937	C	N1-C2-O2	5.74	122.34	118.90
1	C1	1937	C	C6-N1-C2	-5.73	118.01	120.30
1	C1	79	U	N3-C2-O2	-5.73	118.19	122.20
1	C1	2611	U	N3-C2-O2	-5.73	118.19	122.20
1	C1	2046	C	C5-C6-N1	5.70	123.85	121.00
1	C1	2611	U	C2-N1-C1'	5.68	124.52	117.70
2	C2	100	U	C2-N1-C1'	5.66	124.49	117.70
1	C1	3338	C	N1-C2-O2	5.64	122.29	118.90
1	C1	2611	U	N1-C2-O2	5.62	126.73	122.80
1	C1	2227	U	C2-N1-C1'	5.60	124.42	117.70
1	C1	3016	U	N1-C2-O2	5.60	126.72	122.80
1	C1	1663	C	N1-C2-O2	5.58	122.25	118.90
1	C1	2465	U	C2-N1-C1'	5.56	124.37	117.70
1	C1	1015	C	C2-N1-C1'	5.52	124.87	118.80
1	C1	3089	U	N1-C2-O2	5.50	126.65	122.80
1	C1	37	C	N1-C2-O2	5.45	122.17	118.90
1	C1	2282	U	N3-C2-O2	-5.43	118.40	122.20
1	C1	1852	C	N1-C2-O2	5.42	122.15	118.90
1	C1	2220	C	C2-N1-C1'	5.40	124.74	118.80
1	C1	2100	U	C2-N1-C1'	5.40	124.18	117.70
1	C1	3301	C	P-O3'-C3'	5.39	126.17	119.70
1	C1	1538	U	C6-N1-C2	-5.39	117.77	121.00
1	C1	1205	G	O4'-C1'-N9	5.39	112.51	108.20
1	C1	151	G	P-O3'-C3'	5.38	126.16	119.70
1	C1	1047	A	P-O3'-C3'	5.38	126.16	119.70
1	C1	2374	U	N3-C2-O2	-5.36	118.45	122.20
1	C1	2500	U	N3-C2-O2	-5.35	118.45	122.20
1	C1	2351	U	N1-C2-O2	5.34	126.54	122.80
1	C1	2046	C	N3-C2-O2	-5.33	118.17	121.90
1	C1	2863	U	C2-N1-C1'	5.33	124.09	117.70
4	C4	105	C	C2-N1-C1'	5.33	124.66	118.80
27	LD	166	MET	CA-CB-CG	5.31	122.33	113.30
2	C2	113	U	C2-N1-C1'	5.30	124.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1337	G	C8-N9-C1'	-5.30	120.11	127.00
1	C1	103	C	C6-N1-C2	-5.29	118.18	120.30
1	C1	1538	U	C6-N1-C1'	-5.27	113.82	121.20
1	C1	3210	U	P-O3'-C3'	5.26	126.01	119.70
50	Ld	49	GLN	CA-CB-CG	5.25	124.95	113.40
1	C1	1935	C	C6-N1-C1'	-5.23	114.52	120.80
1	C1	2441	C	C6-N1-C2	-5.22	118.21	120.30
4	C4	109	G	C4-N9-C1'	5.22	133.28	126.50
1	C1	1858	G	C4-N9-C1'	5.20	133.26	126.50
1	C1	2282	U	N1-C2-O2	5.18	126.42	122.80
1	C1	2465	U	N1-C2-O2	5.17	126.42	122.80
1	C1	1686	C	N1-C2-O2	5.16	122.00	118.90
1	C1	2499	C	C5-C6-N1	5.16	123.58	121.00
1	C1	961	C	N1-C2-O2	5.15	121.99	118.90
21	Ce	330	LEU	CA-CB-CG	5.15	127.15	115.30
1	C1	940	C	C2-N1-C1'	5.13	124.44	118.80
1	C1	2220	C	N1-C2-O2	5.11	121.96	118.90
1	C1	2993	C	N1-C2-O2	5.10	121.96	118.90
1	C1	2282	U	C2-N1-C1'	5.08	123.80	117.70
1	C1	2714	C	C2-N1-C1'	5.08	124.39	118.80
1	C1	1024	U	C2-N1-C1'	5.07	123.78	117.70
1	C1	2046	C	C6-N1-C2	-5.06	118.28	120.30
1	C1	1015	C	N1-C2-O2	5.06	121.94	118.90
1	C1	3132	A	P-O3'-C3'	5.06	125.77	119.70
2	C2	64	U	N1-C2-O2	5.05	126.33	122.80
4	C4	109	G	N3-C4-N9	5.04	129.03	126.00
41	LT	128	LEU	CA-CB-CG	5.03	126.87	115.30
1	C1	168	C	C2-N1-C1'	5.02	124.32	118.80
1	C1	2409	U	P-O3'-C3'	5.01	125.72	119.70
4	C4	42	C	N3-C2-O2	-5.01	118.39	121.90
1	C1	103	C	C2-N1-C1'	5.01	124.31	118.80
1	C1	2329	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	CT	42	PHE	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
5	CF	243/270 (90%)	241 (99%)	2 (1%)	0	100	100
6	CH	621/661 (94%)	616 (99%)	5 (1%)	0	100	100
7	CI	91/414 (22%)	90 (99%)	1 (1%)	0	100	100
8	CJ	376/679 (55%)	374 (100%)	2 (0%)	0	100	100
9	CK	227/261 (87%)	223 (98%)	4 (2%)	0	100	100
10	CL	77/558 (14%)	76 (99%)	1 (1%)	0	100	100
11	CM	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
11	LF	246/249 (99%)	241 (98%)	4 (2%)	1 (0%)	34	64
12	CN	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
13	CO	56/120 (47%)	54 (96%)	2 (4%)	0	100	100
14	CQ	181/225 (80%)	178 (98%)	3 (2%)	0	100	100
15	CR	510/767 (66%)	504 (99%)	6 (1%)	0	100	100
16	CS	301/338 (89%)	298 (99%)	3 (1%)	0	100	100
17	CT	391/437 (90%)	384 (98%)	7 (2%)	0	100	100
17	CU	391/437 (90%)	380 (97%)	11 (3%)	0	100	100
18	CV	544/781 (70%)	535 (98%)	9 (2%)	0	100	100
18	CW	544/781 (70%)	536 (98%)	8 (2%)	0	100	100
19	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
20	Cd	445/627 (71%)	437 (98%)	8 (2%)	0	100	100
21	Ce	290/443 (66%)	285 (98%)	5 (2%)	0	100	100
22	Ch	388/517 (75%)	375 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Cz	101/123 (82%)	100 (99%)	1 (1%)	0	100	100
24	LA	245/254 (96%)	238 (97%)	7 (3%)	0	100	100
25	LB	386/392 (98%)	380 (98%)	6 (2%)	0	100	100
26	LC	361/365 (99%)	356 (99%)	5 (1%)	0	100	100
27	LD	296/304 (97%)	289 (98%)	7 (2%)	0	100	100
28	LE	187/200 (94%)	182 (97%)	5 (3%)	0	100	100
29	LG	233/262 (89%)	230 (99%)	3 (1%)	0	100	100
30	LH	188/229 (82%)	184 (98%)	4 (2%)	0	100	100
31	LJ	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
32	LK	156/165 (94%)	156 (100%)	0	0	100	100
33	LL	201/213 (94%)	199 (99%)	2 (1%)	0	100	100
34	LM	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
35	LN	200/203 (98%)	196 (98%)	4 (2%)	0	100	100
36	LO	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
37	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
38	LQ	142/213 (67%)	140 (99%)	2 (1%)	0	100	100
39	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
40	LS	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
41	LT	139/160 (87%)	136 (98%)	3 (2%)	0	100	100
42	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
43	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
44	LX	143/156 (92%)	139 (97%)	4 (3%)	0	100	100
45	LY	131/138 (95%)	126 (96%)	5 (4%)	0	100	100
46	LZ	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
47	La	104/149 (70%)	101 (97%)	3 (3%)	0	100	100
48	Lb	34/65 (52%)	34 (100%)	0	0	100	100
49	Lc	93/108 (86%)	92 (99%)	1 (1%)	0	100	100
50	Ld	108/120 (90%)	108 (100%)	0	0	100	100
51	Le	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
52	Lf	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
53	Lg	116/119 (98%)	114 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Lh	120/935 (13%)	116 (97%)	4 (3%)	0	100	100
55	Li	99/110 (90%)	99 (100%)	0	0	100	100
56	Lj	86/95 (90%)	86 (100%)	0	0	100	100
57	Lk	74/94 (79%)	74 (100%)	0	0	100	100
58	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
59	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
60	Lq	137/147 (93%)	134 (98%)	3 (2%)	0	100	100
61	Lr	212/217 (98%)	209 (99%)	3 (1%)	0	100	100
All	All	12502/19275 (65%)	12289 (98%)	212 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	LF	197	VAL

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	
5	CF	212/236 (90%)	212 (100%)	0	100	100
6	CH	548/575 (95%)	547 (100%)	1 (0%)	93	98
7	CI	70/336 (21%)	70 (100%)	0	100	100
8	CJ	331/579 (57%)	331 (100%)	0	100	100
9	CK	203/225 (90%)	203 (100%)	0	100	100
10	CL	60/458 (13%)	60 (100%)	0	100	100
11	CM	185/215 (86%)	184 (100%)	1 (0%)	88	96
11	LF	213/215 (99%)	213 (100%)	0	100	100
12	CN	204/206 (99%)	204 (100%)	0	100	100
13	CO	48/99 (48%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	143/192 (74%)	143 (100%)	0	100	100
15	CR	374/663 (56%)	373 (100%)	1 (0%)	92	97
16	CS	260/291 (89%)	259 (100%)	1 (0%)	91	97
17	CT	323/376 (86%)	323 (100%)	0	100	100
17	CU	327/376 (87%)	326 (100%)	1 (0%)	92	97
18	CV	472/675 (70%)	471 (100%)	1 (0%)	93	98
18	CW	469/675 (70%)	469 (100%)	0	100	100
19	Cb	85/101 (84%)	85 (100%)	0	100	100
20	Cd	395/541 (73%)	395 (100%)	0	100	100
21	Ce	262/383 (68%)	262 (100%)	0	100	100
22	Ch	322/436 (74%)	322 (100%)	0	100	100
23	Cz	91/107 (85%)	91 (100%)	0	100	100
24	LA	190/198 (96%)	190 (100%)	0	100	100
25	LB	328/331 (99%)	328 (100%)	0	100	100
26	LC	281/285 (99%)	281 (100%)	0	100	100
27	LD	233/253 (92%)	232 (100%)	1 (0%)	91	97
28	LE	155/166 (93%)	155 (100%)	0	100	100
29	LG	197/222 (89%)	197 (100%)	0	100	100
30	LH	167/200 (84%)	167 (100%)	0	100	100
31	LJ	144/150 (96%)	142 (99%)	2 (1%)	67	86
32	LK	127/136 (93%)	127 (100%)	0	100	100
33	LL	158/176 (90%)	156 (99%)	2 (1%)	69	88
34	LM	116/117 (99%)	116 (100%)	0	100	100
35	LN	179/180 (99%)	179 (100%)	0	100	100
36	LO	162/163 (99%)	162 (100%)	0	100	100
37	LP	133/152 (88%)	133 (100%)	0	100	100
38	LQ	124/178 (70%)	124 (100%)	0	100	100
39	LR	125/2396 (5%)	125 (100%)	0	100	100
40	LS	153/154 (99%)	152 (99%)	1 (1%)	84	94
41	LT	120/135 (89%)	120 (100%)	0	100	100
42	LU	90/108 (83%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	LV	98/102 (96%)	98 (100%)	0	100	100
44	LX	117/129 (91%)	116 (99%)	1 (1%)	78	92
45	LY	116/119 (98%)	116 (100%)	0	100	100
46	LZ	119/121 (98%)	119 (100%)	0	100	100
47	La	93/122 (76%)	93 (100%)	0	100	100
48	Lb	28/55 (51%)	28 (100%)	0	100	100
49	Lc	76/88 (86%)	76 (100%)	0	100	100
50	Ld	90/105 (86%)	90 (100%)	0	100	100
51	Le	109/114 (96%)	109 (100%)	0	100	100
52	Lf	89/90 (99%)	88 (99%)	1 (1%)	73	90
53	Lg	91/102 (89%)	91 (100%)	0	100	100
54	Lh	109/781 (14%)	107 (98%)	2 (2%)	59	82
55	Li	84/93 (90%)	84 (100%)	0	100	100
56	Lj	72/78 (92%)	72 (100%)	0	100	100
57	Lk	71/88 (81%)	71 (100%)	0	100	100
58	Ll	45/46 (98%)	45 (100%)	0	100	100
59	Lp	72/74 (97%)	72 (100%)	0	100	100
60	Lq	107/112 (96%)	107 (100%)	0	100	100
61	Lr	186/189 (98%)	183 (98%)	3 (2%)	62	84
All	All	10551/16268 (65%)	10532 (100%)	19 (0%)	93	98

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CH	470	LYS
11	CM	29	ARG
15	CR	115	ARG
16	CS	326	LYS
17	CU	76	ARG
18	CV	142	ARG
27	LD	23	ARG
31	LJ	40	GLN
31	LJ	93	ARG
33	LL	13	HIS
33	LL	67	ARG

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Mol	Chain	Res	Type
40	LS	3	ARG
44	LX	69	ARG
52	Lf	22	ARG
54	Lh	38	LYS
54	Lh	64	ASN
61	Lr	78	LYS
61	Lr	176	GLN
61	Lr	195	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
6	CH	53	GLN
16	CS	45	ASN
18	CV	383	HIS
18	CW	382	HIS
20	Cd	326	GLN
30	LH	5	HIS
30	LH	95	HIS
61	Lr	11	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3079/3342 (92%)	557 (18%)	17 (0%)
2	C2	155/156 (99%)	21 (13%)	0
3	C3	2/162 (1%)	1 (50%)	0
4	C4	113/119 (94%)	21 (18%)	0
All	All	3349/3779 (88%)	600 (17%)	17 (0%)

All (600) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	G
1	C1	23	G
1	C1	27	A
1	C1	50	A
1	C1	60	G
1	C1	61	A
1	C1	66	A

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Mol	Chain	Res	Type
1	C1	67	A
1	C1	68	A
1	C1	73	C
1	C1	93	G
1	C1	94	C
1	C1	97	G
1	C1	110	A
1	C1	111	G
1	C1	112	C
1	C1	117	A
1	C1	123	A
1	C1	132	U
1	C1	133	C
1	C1	135	G
1	C1	139	G
1	C1	144	G
1	C1	151	G
1	C1	152	G
1	C1	153	A
1	C1	156	G
1	C1	170	A
1	C1	178	U
1	C1	181	G
1	C1	184	U
1	C1	194	C
1	C1	200	G
1	C1	204	C
1	C1	212	G
1	C1	213	A
1	C1	214	G
1	C1	225	A
1	C1	228	U
1	C1	240	C
1	C1	241	U
1	C1	244	G
1	C1	247	A
1	C1	258	A
1	C1	259	C
1	C1	262	G
1	C1	278	A
1	C1	288	A
1	C1	291	U

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Mol	Chain	Res	Type
1	C1	298	U
1	C1	308	C
1	C1	316	A
1	C1	322	C
1	C1	323	G
1	C1	327	A
1	C1	343	C
1	C1	369	G
1	C1	385	OMG
1	C1	391	U
1	C1	394	C
1	C1	395	A
1	C1	396	C
1	C1	414	G
1	C1	415	A
1	C1	422	U
1	C1	429	A
1	C1	434	U
1	C1	443	C
1	C1	446	A
1	C1	447	U
1	C1	448	C
1	C1	458	U
1	C1	459	C
1	C1	460	U
1	C1	469	C
1	C1	470	A
1	C1	471	C
1	C1	472	U
1	C1	479	G
1	C1	494	C
1	C1	505	G
1	C1	512	A
1	C1	514	A
1	C1	527	G
1	C1	535	U
1	C1	536	C
1	C1	537	C
1	C1	538	G
1	C1	545	U
1	C1	546	U
1	C1	547	A

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Mol	Chain	Res	Type
1	C1	548	U
1	C1	549	A
1	C1	570	G
1	C1	588	G
1	C1	592	U
1	C1	593	G
1	C1	595	A
1	C1	597	G
1	C1	599	A
1	C1	608	U
1	C1	609	A
1	C1	610	A
1	C1	624	C
1	C1	627	OMG
1	C1	648	A
1	C1	650	U
1	C1	665	A
1	C1	669	U
1	C1	678	A
1	C1	693	A
1	C1	700	G
1	C1	703	A
1	C1	704	A
1	C1	707	U
1	C1	720	C
1	C1	721	G
1	C1	743	A
1	C1	748	U
1	C1	755	G
1	C1	756	G
1	C1	757	A
1	C1	759	U
1	C1	761	G
1	C1	762	A
1	C1	763	G
1	C1	766	G
1	C1	767	G
1	C1	782	G
1	C1	790	A
1	C1	799	A
1	C1	812	A
1	C1	826	G

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Mol	Chain	Res	Type
1	C1	839	G
1	C1	843	C
1	C1	856	U
1	C1	857	G
1	C1	862	G
1	C1	877	A
1	C1	889	G
1	C1	896	A
1	C1	898	G
1	C1	899	A
1	C1	903	A
1	C1	905	C
1	C1	906	G
1	C1	907	A
1	C1	919	G
1	C1	926	A
1	C1	933	A
1	C1	934	A
1	C1	935	G
1	C1	936	U
1	C1	937	U
1	C1	940	C
1	C1	947	A
1	C1	955	G
1	C1	956	U
1	C1	961	C
1	C1	963	U
1	C1	964	C
1	C1	981	G
1	C1	986	U
1	C1	988	A
1	C1	993	G
1	C1	994	G
1	C1	995	A
1	C1	996	C
1	C1	997	U
1	C1	998	C
1	C1	999	G
1	C1	1015	C
1	C1	1016	U
1	C1	1017	U
1	C1	1021	C

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Mol	Chain	Res	Type
1	C1	1022	C
1	C1	1024	U
1	C1	1046	G
1	C1	1047	A
1	C1	1048	A
1	C1	1049	G
1	C1	1055	G
1	C1	1056	U
1	C1	1059	C
1	C1	1064	C
1	C1	1065	U
1	C1	1068	A
1	C1	1071	U
1	C1	1081	A
1	C1	1095	A
1	C1	1099	G
1	C1	1110	G
1	C1	1115	C
1	C1	1118	A
1	C1	1127	U
1	C1	1132	G
1	C1	1136	A
1	C1	1142	A
1	C1	1143	C
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1169	G
1	C1	1175	C
1	C1	1176	A
1	C1	1181	C
1	C1	1185	A
1	C1	1187	A
1	C1	1205	G
1	C1	1209	G
1	C1	1228	A
1	C1	1229	G
1	C1	1240	C
1	C1	1241	U
1	C1	1242	A
1	C1	1246	A
1	C1	1248	U

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Mol	Chain	Res	Type
1	C1	1255	C
1	C1	1268	G
1	C1	1270	A
1	C1	1287	A
1	C1	1288	U
1	C1	1290	G
1	C1	1292	U
1	C1	1296	G
1	C1	1313	A
1	C1	1331	A
1	C1	1332	G
1	C1	1333	A
1	C1	1334	A
1	C1	1335	A
1	C1	1336	C
1	C1	1337	G
1	C1	1369	A
1	C1	1370	G
1	C1	1382	A
1	C1	1383	G
1	C1	1400	G
1	C1	1401	A
1	C1	1414	G
1	C1	1417	G
1	C1	1420	OMC
1	C1	1429	A
1	C1	1433	OMG
1	C1	1438	U
1	C1	1464	A
1	C1	1466	G
1	C1	1477	U
1	C1	1479	C
1	C1	1485	G
1	C1	1491	OMC
1	C1	1505	U
1	C1	1536	U
1	C1	1538	U
1	C1	1539	C
1	C1	1540	A
1	C1	1543	G
1	C1	1549	C
1	C1	1550	U

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Mol	Chain	Res	Type
1	C1	1554	G
1	C1	1567	A
1	C1	1568	A
1	C1	1573	A
1	C1	1585	A
1	C1	1586	U
1	C1	1609	U
1	C1	1619	C
1	C1	1622	A
1	C1	1623	A
1	C1	1624	C
1	C1	1625	U
1	C1	1663	C
1	C1	1683	U
1	C1	1685	U
1	C1	1697	C
1	C1	1704	U
1	C1	1722	U
1	C1	1730	A
1	C1	1731	G
1	C1	1745	U
1	C1	1746	G
1	C1	1760	G
1	C1	1776	G
1	C1	1777	A
1	C1	1789	A
1	C1	1792	G
1	C1	1793	A
1	C1	1794	A
1	C1	1795	U
1	C1	1796	A
1	C1	1800	C
1	C1	1801	U
1	C1	1822	A
1	C1	1826	C
1	C1	1829	C
1	C1	1830	A
1	C1	1838	A
1	C1	1846	C
1	C1	1847	A2M
1	C1	1856	U
1	C1	1858	G

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Mol	Chain	Res	Type
1	C1	1860	U
1	C1	1866	A
1	C1	1873	A
1	C1	1886	G
1	C1	1887	C
1	C1	1923	C
1	C1	1933	G
1	C1	1934	G
1	C1	1935	C
1	C1	1937	C
1	C1	2046	C
1	C1	2047	G
1	C1	2048	U
1	C1	2050	C
1	C1	2053	U
1	C1	2054	U
1	C1	2084	G
1	C1	2085	G
1	C1	2089	A
1	C1	2094	A
1	C1	2103	U
1	C1	2121	A
1	C1	2123	G
1	C1	2132	G
1	C1	2139	U
1	C1	2151	A
1	C1	2167	C
1	C1	2185	A
1	C1	2186	A
1	C1	2188	U
1	C1	2192	A
1	C1	2207	A
1	C1	2212	G
1	C1	2219	A
1	C1	2221	U
1	C1	2222	A
1	C1	2223	U
1	C1	2224	G
1	C1	2227	U
1	C1	2231	U
1	C1	2232	U
1	C1	2233	A

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Mol	Chain	Res	Type
1	C1	2235	G
1	C1	2283	A
1	C1	2297	U
1	C1	2298	G
1	C1	2299	U
1	C1	2336	A
1	C1	2339	G
1	C1	2340	G
1	C1	2346	C
1	C1	2351	U
1	C1	2356	G
1	C1	2357	G
1	C1	2362	A
1	C1	2365	A
1	C1	2366	G
1	C1	2374	U
1	C1	2381	G
1	C1	2382	A
1	C1	2398	G
1	C1	2400	G
1	C1	2403	A
1	C1	2404	A
1	C1	2409	U
1	C1	2410	A
1	C1	2411	G
1	C1	2415	G
1	C1	2423	U
1	C1	2426	G
1	C1	2431	A
1	C1	2432	G
1	C1	2435	U
1	C1	2436	C
1	C1	2437	G
1	C1	2440	G
1	C1	2441	C
1	C1	2447	A
1	C1	2450	U
1	C1	2454	A
1	C1	2457	A
1	C1	2458	C
1	C1	2459	U
1	C1	2465	U

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Mol	Chain	Res	Type
1	C1	2466	G
1	C1	2477	U
1	C1	2485	G
1	C1	2489	C
1	C1	2498	A
1	C1	2499	C
1	C1	2500	U
1	C1	2501	U
1	C1	2502	G
1	C1	2503	C
1	C1	2506	C
1	C1	2507	C
1	C1	2508	A
1	C1	2512	U
1	C1	2513	C
1	C1	2521	A
1	C1	2522	A
1	C1	2527	C
1	C1	2530	C
1	C1	2533	G
1	C1	2544	G
1	C1	2545	G
1	C1	2549	A
1	C1	2552	A
1	C1	2565	G
1	C1	2566	G
1	C1	2573	G
1	C1	2583	G
1	C1	2587	A
1	C1	2589	C
1	C1	2591	G
1	C1	2607	G
1	C1	2610	G
1	C1	2611	U
1	C1	2615	A
1	C1	2616	A
1	C1	2633	A
1	C1	2636	G
1	C1	2640	U
1	C1	2648	A
1	C1	2650	A
1	C1	2653	A

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Mol	Chain	Res	Type
1	C1	2654	A
1	C1	2655	A
1	C1	2656	A
1	C1	2657	G
1	C1	2660	U
1	C1	2661	A
1	C1	2663	A
1	C1	2664	A
1	C1	2670	C
1	C1	2672	U
1	C1	2673	G
1	C1	2684	U
1	C1	2690	OMU
1	C1	2691	G
1	C1	2701	C
1	C1	2708	G
1	C1	2712	G
1	C1	2713	G
1	C1	2714	C
1	C1	2731	C
1	C1	2732	C
1	C1	2734	U
1	C1	2736	G
1	C1	2737	A
1	C1	2763	A
1	C1	2769	C
1	C1	2783	G
1	C1	2784	C
1	C1	2785	U
1	C1	2802	U
1	C1	2803	C
1	C1	2805	U
1	C1	2812	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	U
1	C1	2834	U
1	C1	2836	G
1	C1	2846	A
1	C1	2847	U
1	C1	2848	C

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Mol	Chain	Res	Type
1	C1	2857	G
1	C1	2858	C
1	C1	2863	U
1	C1	2882	U
1	C1	2894	U
1	C1	2895	A
1	C1	2909	G
1	C1	2929	C
1	C1	2930	A
1	C1	2931	G
1	C1	2938	U
1	C1	2939	U
1	C1	2940	U
1	C1	2942	C
1	C1	2949	G
1	C1	2951	U
1	C1	2955	C
1	C1	2956	U
1	C1	2970	A
1	C1	2980	G
1	C1	3014	U
1	C1	3017	G
1	C1	3036	G
1	C1	3044	A
1	C1	3045	A
1	C1	3050	C
1	C1	3051	C
1	C1	3067	G
1	C1	3071	A
1	C1	3080	A
1	C1	3087	A
1	C1	3088	A
1	C1	3089	U
1	C1	3100	A
1	C1	3101	C
1	C1	3102	G
1	C1	3112	U
1	C1	3113	A
1	C1	3119	A
1	C1	3126	A
1	C1	3127	G
1	C1	3131	U

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Mol	Chain	Res	Type
1	C1	3133	U
1	C1	3135	A
1	C1	3141	G
1	C1	3146	C
1	C1	3155	A
1	C1	3162	C
1	C1	3163	A
1	C1	3164	G
1	C1	3185	G
1	C1	3186	A
1	C1	3188	G
1	C1	3190	G
1	C1	3200	A
1	C1	3201	A
1	C1	3206	C
1	C1	3210	U
1	C1	3211	U
1	C1	3218	U
1	C1	3227	G
1	C1	3228	C
1	C1	3231	G
1	C1	3244	G
1	C1	3245	C
1	C1	3248	A
1	C1	3254	U
1	C1	3257	A
1	C1	3258	U
1	C1	3259	G
1	C1	3260	U
1	C1	3282	U
1	C1	3291	C
1	C1	3293	U
1	C1	3295	U
1	C1	3297	G
1	C1	3299	U
1	C1	3302	G
1	C1	3310	G
1	C1	3316	A
1	C1	3319	C
1	C1	3323	C
1	C1	3324	C
1	C1	3325	U

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Mol	Chain	Res	Type
1	C1	3328	G
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	39	G
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	83	C
2	C2	84	C
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	96	A
2	C2	104	A
2	C2	105	A
2	C2	106	C
2	C2	116	G
2	C2	125	U
2	C2	127	U
2	C2	151	C
3	C3	2	U
4	C4	7	G
4	C4	8	A
4	C4	9	C
4	C4	18	G
4	C4	26	C
4	C4	29	G
4	C4	54	U
4	C4	55	A
4	C4	64	A
4	C4	65	G
4	C4	72	G
4	C4	73	U
4	C4	75	A
4	C4	76	G
4	C4	87	G
4	C4	88	G

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Mol	Chain	Res	Type
4	C4	98	G
4	C4	101	A
4	C4	109	G
4	C4	110	U
4	C4	111	G

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	151	G
1	C1	1021	C
1	C1	1047	A
1	C1	1267	C
1	C1	1537	U
1	C1	2234	A
1	C1	2282	U
1	C1	2409	U
1	C1	2712	G
1	C1	3079	U
1	C1	3132	A
1	C1	3205	G
1	C1	3210	U
1	C1	3230	G
1	C1	3258	U
1	C1	3298	U
1	C1	3301	C

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

32 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	C1	787	1	18,26,27	1.15	2 (11%)	19,38,41	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	OMU	C1	2384	1	19,22,23	3.04	6 (31%)	26,31,34	1.67	4 (15%)
1	OMG	C1	646	1	18,26,27	1.16	2 (11%)	19,38,41	0.87	1 (5%)
1	OMC	C1	2300	1	19,22,23	0.53	0	26,31,34	0.70	0
1	OMU	C1	2380	1	19,22,23	3.00	6 (31%)	26,31,34	1.70	5 (19%)
1	OMC	C1	2838	1	19,22,23	0.61	0	26,31,34	0.95	1 (3%)
1	OMG	C1	2358	1	18,26,27	1.14	2 (11%)	19,38,41	0.89	1 (5%)
1	OMU	C1	1917	1	19,22,23	3.09	6 (31%)	26,31,34	1.80	5 (19%)
1	OMG	C1	2881	1	18,26,27	1.12	2 (11%)	19,38,41	0.82	1 (5%)
1	A2M	C1	848	1	18,25,26	4.35	9 (50%)	18,36,39	3.83	4 (22%)
1	OMC	C1	1420	1	19,22,23	0.58	0	26,31,34	1.02	1 (3%)
1	OMU	C1	1868	1	19,22,23	3.04	6 (31%)	26,31,34	1.76	5 (19%)
1	OMG	C1	2774	1	18,26,27	1.13	2 (11%)	19,38,41	0.85	1 (5%)
1	A2M	C1	1432	1	18,25,26	4.36	9 (50%)	18,36,39	3.88	4 (22%)
1	OMC	C1	1812	1	19,22,23	0.57	0	26,31,34	0.75	0
1	A2M	C1	2289	1	18,25,26	4.37	8 (44%)	18,36,39	3.74	4 (22%)
1	A2M	C1	637	1	18,25,26	4.34	9 (50%)	18,36,39	3.85	4 (22%)
1	OMC	C1	1836	1	19,22,23	0.61	0	26,31,34	0.94	1 (3%)
1	OMU	C1	2690	1	19,22,23	3.19	6 (31%)	26,31,34	1.77	6 (23%)
1	OMC	C1	778	1	19,22,23	0.58	0	26,31,34	0.88	1 (3%)
1	OMG	C1	1433	1	18,26,27	1.14	2 (11%)	19,38,41	0.83	1 (5%)
1	OMG	C1	627	1	18,26,27	1.19	2 (11%)	19,38,41	0.84	1 (5%)
1	A2M	C1	858	1	18,25,26	4.37	9 (50%)	18,36,39	3.95	4 (22%)
1	A2M	C1	1847	1	18,25,26	4.33	9 (50%)	18,36,39	3.94	4 (22%)
1	OMC	C1	2918	1	19,22,23	0.57	0	26,31,34	0.77	0
1	A2M	C1	389	1	18,25,26	4.31	9 (50%)	18,36,39	3.88	4 (22%)
1	OMG	C1	2876	1	18,26,27	1.15	2 (11%)	19,38,41	0.85	1 (5%)
1	A2M	C1	1223	1	18,25,26	4.34	9 (50%)	18,36,39	3.80	4 (22%)
1	OMU	C1	2688	1	19,22,23	3.11	6 (31%)	26,31,34	1.66	4 (15%)
1	OMG	C1	385	1	18,26,27	1.12	2 (11%)	19,38,41	0.84	1 (5%)
1	OMC	C1	1491	1	19,22,23	0.56	0	26,31,34	0.76	0
1	OMU	C1	2683	1	19,22,23	3.05	6 (31%)	26,31,34	1.74	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	C1	787	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	2384	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	646	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	2300	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2838	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2358	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	1917	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	2881	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	848	1	-	1/5/27/28	0/3/3/3
1	OMC	C1	1420	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2774	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	1432	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	1812	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	2289	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	637	1	-	1/5/27/28	0/3/3/3
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2690	1	-	3/9/27/28	0/2/2/2
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	1433	1	-	2/5/27/28	0/3/3/3
1	OMG	C1	627	1	-	2/5/27/28	0/3/3/3
1	A2M	C1	858	1	-	1/5/27/28	0/3/3/3
1	A2M	C1	1847	1	-	3/5/27/28	0/3/3/3
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	389	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	2876	1	-	2/5/27/28	0/3/3/3
1	A2M	C1	1223	1	-	3/5/27/28	0/3/3/3
1	OMU	C1	2688	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	385	1	-	2/5/27/28	0/3/3/3
1	OMC	C1	1491	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	2683	1	-	2/9/27/28	0/2/2/2

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C3'-C2'	-12.82	1.24	1.52
1	C1	848	A2M	C3'-C2'	-12.77	1.24	1.52
1	C1	858	A2M	C3'-C2'	-12.76	1.24	1.52
1	C1	1223	A2M	C3'-C2'	-12.71	1.24	1.52
1	C1	637	A2M	C3'-C2'	-12.70	1.24	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1432	A2M	C3'-C2'	-12.70	1.24	1.52
1	C1	1847	A2M	C3'-C2'	-12.60	1.24	1.52
1	C1	389	A2M	C3'-C2'	-12.42	1.25	1.52
1	C1	2289	A2M	O4'-C1'	8.09	1.52	1.41
1	C1	858	A2M	O4'-C1'	8.06	1.52	1.41
1	C1	1432	A2M	O4'-C1'	8.03	1.52	1.41
1	C1	2690	OMU	C2-N1	8.00	1.51	1.38
1	C1	1847	A2M	O4'-C1'	7.98	1.52	1.41
1	C1	848	A2M	O4'-C1'	7.98	1.52	1.41
1	C1	1223	A2M	O4'-C1'	7.94	1.52	1.41
1	C1	637	A2M	O4'-C1'	7.86	1.52	1.41
1	C1	389	A2M	O4'-C1'	7.74	1.51	1.41
1	C1	1917	OMU	C2-N1	7.58	1.50	1.38
1	C1	2688	OMU	C2-N1	7.48	1.50	1.38
1	C1	2690	OMU	C2-N3	7.26	1.50	1.38
1	C1	2683	OMU	C2-N1	7.19	1.50	1.38
1	C1	1868	OMU	C2-N1	7.18	1.50	1.38
1	C1	2384	OMU	C2-N1	7.18	1.50	1.38
1	C1	2688	OMU	C2-N3	7.17	1.50	1.38
1	C1	2683	OMU	C2-N3	7.11	1.50	1.38
1	C1	2384	OMU	C2-N3	7.07	1.50	1.38
1	C1	1917	OMU	C2-N3	7.05	1.50	1.38
1	C1	1868	OMU	C2-N3	7.04	1.50	1.38
1	C1	2380	OMU	C2-N3	7.04	1.50	1.38
1	C1	2380	OMU	C2-N1	6.92	1.49	1.38
1	C1	389	A2M	O4'-C4'	-6.87	1.29	1.45
1	C1	1847	A2M	O4'-C4'	-6.57	1.30	1.45
1	C1	637	A2M	O4'-C4'	-6.53	1.30	1.45
1	C1	858	A2M	O4'-C4'	-6.52	1.30	1.45
1	C1	1432	A2M	O4'-C4'	-6.50	1.30	1.45
1	C1	848	A2M	O4'-C4'	-6.47	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.42	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.42	1.30	1.45
1	C1	2688	OMU	C6-C5	6.26	1.49	1.35
1	C1	2683	OMU	C6-C5	6.24	1.49	1.35
1	C1	2690	OMU	C6-C5	6.24	1.49	1.35
1	C1	1868	OMU	C6-C5	6.23	1.49	1.35
1	C1	2384	OMU	C6-C5	6.16	1.49	1.35
1	C1	1917	OMU	C6-C5	6.14	1.49	1.35
1	C1	2380	OMU	C6-C5	6.09	1.49	1.35
1	C1	2289	A2M	C3'-C4'	5.27	1.66	1.53
1	C1	1432	A2M	C3'-C4'	5.26	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1223	A2M	C3'-C4'	5.23	1.66	1.53
1	C1	858	A2M	C3'-C4'	5.20	1.66	1.53
1	C1	848	A2M	C3'-C4'	5.17	1.66	1.53
1	C1	637	A2M	C3'-C4'	5.12	1.66	1.53
1	C1	389	A2M	C3'-C4'	5.09	1.66	1.53
1	C1	1847	A2M	C3'-C4'	5.06	1.65	1.53
1	C1	2688	OMU	C4-N3	4.31	1.46	1.38
1	C1	2690	OMU	C4-N3	4.27	1.46	1.38
1	C1	2683	OMU	C4-N3	4.20	1.46	1.38
1	C1	2380	OMU	C4-N3	4.18	1.46	1.38
1	C1	2384	OMU	C4-N3	4.17	1.46	1.38
1	C1	1868	OMU	C4-N3	4.16	1.46	1.38
1	C1	1917	OMU	C4-N3	4.13	1.46	1.38
1	C1	389	A2M	O2'-C2'	3.72	1.52	1.42
1	C1	637	A2M	O2'-C2'	3.54	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.46	1.51	1.42
1	C1	858	A2M	O2'-C2'	3.44	1.51	1.42
1	C1	1432	A2M	O2'-C2'	3.44	1.51	1.42
1	C1	848	A2M	O2'-C2'	3.42	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.37	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.35	1.51	1.42
1	C1	1223	A2M	C6-N6	3.15	1.45	1.34
1	C1	858	A2M	C6-N6	3.14	1.45	1.34
1	C1	389	A2M	C6-N6	3.14	1.45	1.34
1	C1	637	A2M	C6-N6	3.13	1.45	1.34
1	C1	1432	A2M	C6-N6	3.13	1.45	1.34
1	C1	2289	A2M	C6-N6	3.11	1.45	1.34
1	C1	848	A2M	C6-N6	3.10	1.45	1.34
1	C1	1847	A2M	C6-N6	3.09	1.45	1.34
1	C1	646	OMG	C8-N7	-2.97	1.30	1.35
1	C1	627	OMG	C8-N7	-2.96	1.30	1.35
1	C1	1433	OMG	C8-N7	-2.95	1.30	1.35
1	C1	385	OMG	C8-N7	-2.91	1.30	1.35
1	C1	2876	OMG	C8-N7	-2.84	1.30	1.35
1	C1	2881	OMG	C8-N7	-2.82	1.30	1.35
1	C1	2690	OMU	C6-N1	2.82	1.44	1.38
1	C1	2688	OMU	C6-N1	2.81	1.44	1.38
1	C1	2358	OMG	C8-N7	-2.77	1.30	1.35
1	C1	2774	OMG	C8-N7	-2.76	1.30	1.35
1	C1	1847	A2M	C5-C4	-2.73	1.33	1.40
1	C1	637	A2M	C5-C4	-2.73	1.33	1.40
1	C1	389	A2M	C5-C4	-2.73	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C5-C4	-2.73	1.33	1.40
1	C1	1432	A2M	C5-C4	-2.71	1.33	1.40
1	C1	2683	OMU	C6-N1	2.71	1.44	1.38
1	C1	848	A2M	C5-C4	-2.70	1.33	1.40
1	C1	858	A2M	C5-C4	-2.70	1.33	1.40
1	C1	787	OMG	C8-N7	-2.67	1.30	1.35
1	C1	1917	OMU	C6-N1	2.66	1.44	1.38
1	C1	2380	OMU	C6-N1	2.64	1.44	1.38
1	C1	1223	A2M	C5-C4	-2.64	1.33	1.40
1	C1	2384	OMU	C6-N1	2.63	1.44	1.38
1	C1	1868	OMU	C6-N1	2.63	1.44	1.38
1	C1	627	OMG	C5-C6	-2.51	1.42	1.47
1	C1	646	OMG	C5-C6	-2.47	1.42	1.47
1	C1	2876	OMG	C5-C6	-2.39	1.42	1.47
1	C1	1433	OMG	C5-C6	-2.35	1.42	1.47
1	C1	787	OMG	C5-C6	-2.35	1.42	1.47
1	C1	2688	OMU	C5-C4	2.35	1.48	1.43
1	C1	2774	OMG	C5-C6	-2.34	1.42	1.47
1	C1	385	OMG	C5-C6	-2.31	1.42	1.47
1	C1	2881	OMG	C5-C6	-2.31	1.42	1.47
1	C1	2683	OMU	C5-C4	2.31	1.48	1.43
1	C1	2358	OMG	C5-C6	-2.28	1.42	1.47
1	C1	1868	OMU	C5-C4	2.27	1.48	1.43
1	C1	2380	OMU	C5-C4	2.25	1.48	1.43
1	C1	1847	A2M	O3'-C3'	2.23	1.48	1.43
1	C1	637	A2M	C2-N3	2.22	1.35	1.32
1	C1	2384	OMU	C5-C4	2.21	1.48	1.43
1	C1	1432	A2M	C2-N3	2.21	1.35	1.32
1	C1	2690	OMU	C5-C4	2.21	1.48	1.43
1	C1	848	A2M	O3'-C3'	2.18	1.48	1.43
1	C1	1223	A2M	O3'-C3'	2.17	1.48	1.43
1	C1	1223	A2M	C2-N3	2.16	1.35	1.32
1	C1	1432	A2M	O3'-C3'	2.13	1.48	1.43
1	C1	1917	OMU	C5-C4	2.13	1.48	1.43
1	C1	389	A2M	C2-N3	2.12	1.35	1.32
1	C1	848	A2M	C2-N3	2.12	1.35	1.32
1	C1	1847	A2M	C2-N3	2.11	1.35	1.32
1	C1	2289	A2M	O3'-C3'	2.10	1.47	1.43
1	C1	858	A2M	C2-N3	2.08	1.35	1.32
1	C1	858	A2M	O3'-C3'	2.07	1.47	1.43
1	C1	637	A2M	O3'-C3'	2.04	1.47	1.43
1	C1	389	A2M	O3'-C3'	2.00	1.47	1.43

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C4	10.91	145.81	126.64
1	C1	858	A2M	C1'-N9-C4	10.77	145.56	126.64
1	C1	1432	A2M	C1'-N9-C4	10.75	145.53	126.64
1	C1	389	A2M	C1'-N9-C4	10.56	145.20	126.64
1	C1	637	A2M	C1'-N9-C4	10.52	145.12	126.64
1	C1	1223	A2M	C1'-N9-C4	10.30	144.74	126.64
1	C1	848	A2M	C1'-N9-C4	10.12	144.42	126.64
1	C1	2289	A2M	C1'-N9-C4	9.79	143.84	126.64
1	C1	858	A2M	C5-C6-N6	9.22	134.37	120.35
1	C1	848	A2M	C5-C6-N6	9.03	134.08	120.35
1	C1	1847	A2M	C5-C6-N6	8.97	133.98	120.35
1	C1	2289	A2M	C5-C6-N6	8.95	133.95	120.35
1	C1	1223	A2M	C5-C6-N6	8.90	133.87	120.35
1	C1	1432	A2M	C5-C6-N6	8.89	133.86	120.35
1	C1	389	A2M	C5-C6-N6	8.89	133.86	120.35
1	C1	637	A2M	C5-C6-N6	8.88	133.85	120.35
1	C1	848	A2M	N6-C6-N1	-6.15	105.81	118.57
1	C1	858	A2M	N6-C6-N1	-6.15	105.81	118.57
1	C1	1847	A2M	N6-C6-N1	-6.10	105.92	118.57
1	C1	637	A2M	N6-C6-N1	-6.04	106.04	118.57
1	C1	1432	A2M	N6-C6-N1	-6.00	106.12	118.57
1	C1	2289	A2M	N6-C6-N1	-5.98	106.15	118.57
1	C1	389	A2M	N6-C6-N1	-5.97	106.19	118.57
1	C1	1223	A2M	N6-C6-N1	-5.91	106.31	118.57
1	C1	858	A2M	N3-C2-N1	-5.78	119.65	128.68
1	C1	1847	A2M	N3-C2-N1	-5.76	119.68	128.68
1	C1	848	A2M	N3-C2-N1	-5.72	119.74	128.68
1	C1	389	A2M	N3-C2-N1	-5.60	119.92	128.68
1	C1	2289	A2M	N3-C2-N1	-5.59	119.94	128.68
1	C1	1432	A2M	N3-C2-N1	-5.58	119.96	128.68
1	C1	637	A2M	N3-C2-N1	-5.57	119.98	128.68
1	C1	1223	A2M	N3-C2-N1	-5.55	120.00	128.68
1	C1	1868	OMU	C4-N3-C2	-5.42	119.43	126.58
1	C1	2380	OMU	C4-N3-C2	-5.31	119.58	126.58
1	C1	2683	OMU	C4-N3-C2	-5.27	119.63	126.58
1	C1	2688	OMU	C4-N3-C2	-5.09	119.86	126.58
1	C1	2384	OMU	C4-N3-C2	-5.05	119.92	126.58
1	C1	1917	OMU	C4-N3-C2	-4.89	120.12	126.58
1	C1	2690	OMU	C4-N3-C2	-4.68	120.41	126.58
1	C1	2683	OMU	N3-C2-N1	4.04	120.25	114.89
1	C1	1917	OMU	N3-C2-N1	3.94	120.12	114.89
1	C1	2380	OMU	N3-C2-N1	3.84	119.99	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1868	OMU	N3-C2-N1	3.84	119.99	114.89
1	C1	2384	OMU	N3-C2-N1	3.83	119.98	114.89
1	C1	2690	OMU	N3-C2-N1	3.79	119.92	114.89
1	C1	2688	OMU	N3-C2-N1	3.71	119.81	114.89
1	C1	1917	OMU	C1'-N1-C2	3.61	124.10	117.57
1	C1	1868	OMU	C5-C4-N3	3.47	120.03	114.84
1	C1	2380	OMU	C5-C4-N3	3.40	119.93	114.84
1	C1	2688	OMU	C5-C4-N3	3.27	119.74	114.84
1	C1	2683	OMU	C5-C4-N3	3.22	119.66	114.84
1	C1	2384	OMU	C5-C4-N3	3.20	119.63	114.84
1	C1	1917	OMU	C5-C4-N3	3.08	119.45	114.84
1	C1	2690	OMU	C1'-N1-C2	3.07	123.13	117.57
1	C1	2690	OMU	C5-C4-N3	3.03	119.38	114.84
1	C1	1420	OMC	C1'-N1-C2	2.93	124.97	118.42
1	C1	1868	OMU	O4-C4-C5	-2.85	120.15	125.16
1	C1	2380	OMU	O4-C4-C5	-2.83	120.19	125.16
1	C1	2683	OMU	O4-C4-C5	-2.82	120.20	125.16
1	C1	2688	OMU	O4-C4-C5	-2.79	120.25	125.16
1	C1	2690	OMU	O4-C4-C5	-2.79	120.25	125.16
1	C1	2384	OMU	O4-C4-C5	-2.77	120.28	125.16
1	C1	2838	OMC	C1'-N1-C2	2.77	124.61	118.42
1	C1	1917	OMU	O4-C4-C5	-2.74	120.34	125.16
1	C1	1836	OMC	C1'-N1-C2	2.72	124.50	118.42
1	C1	778	OMC	C1'-N1-C2	2.48	123.96	118.42
1	C1	646	OMG	O6-C6-C5	2.43	129.12	124.37
1	C1	2358	OMG	O6-C6-C5	2.37	129.00	124.37
1	C1	2881	OMG	O6-C6-C5	2.37	129.00	124.37
1	C1	385	OMG	O6-C6-C5	2.37	129.00	124.37
1	C1	2774	OMG	O6-C6-C5	2.36	128.98	124.37
1	C1	2876	OMG	O6-C6-C5	2.34	128.94	124.37
1	C1	2683	OMU	O2-C2-N1	-2.33	119.69	122.79
1	C1	1433	OMG	O6-C6-C5	2.32	128.91	124.37
1	C1	627	OMG	O6-C6-C5	2.29	128.85	124.37
1	C1	787	OMG	O6-C6-C5	2.28	128.83	124.37
1	C1	1868	OMU	O2-C2-N1	-2.28	119.76	122.79
1	C1	2380	OMU	O2-C2-N1	-2.24	119.81	122.79
1	C1	2690	OMU	C6-N1-C2	-2.05	118.37	120.99

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	385	OMG	C3'-C4'-C5'-O5'
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	627	OMG	C3'-C4'-C5'-O5'
1	C1	637	A2M	C1'-C2'-O2'-CM'
1	C1	1223	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'
1	C1	1433	OMG	C3'-C4'-C5'-O5'
1	C1	1847	A2M	C3'-C4'-C5'-O5'
1	C1	2384	OMU	C1'-C2'-O2'-CM2
1	C1	2683	OMU	C1'-C2'-O2'-CM2
1	C1	2688	OMU	C3'-C4'-C5'-O5'
1	C1	2688	OMU	O4'-C4'-C5'-O5'
1	C1	1223	A2M	O4'-C4'-C5'-O5'
1	C1	2690	OMU	C4'-C5'-O5'-P
1	C1	389	A2M	O4'-C4'-C5'-O5'
1	C1	627	OMG	O4'-C4'-C5'-O5'
1	C1	1847	A2M	O4'-C4'-C5'-O5'
1	C1	385	OMG	O4'-C4'-C5'-O5'
1	C1	1223	A2M	C3'-C4'-C5'-O5'
1	C1	1847	A2M	C4'-C5'-O5'-P
1	C1	2683	OMU	C3'-C2'-O2'-CM2
1	C1	848	A2M	O4'-C4'-C5'-O5'
1	C1	2690	OMU	C2'-C1'-N1-C6
1	C1	2876	OMG	C3'-C2'-O2'-CM2
1	C1	2690	OMU	C2'-C1'-N1-C2
1	C1	858	A2M	O4'-C4'-C5'-O5'
1	C1	2876	OMG	C1'-C2'-O2'-CM2
1	C1	1491	OMC	O4'-C4'-C5'-O5'
1	C1	1917	OMU	C2'-C1'-N1-C2
1	C1	389	A2M	C3'-C4'-C5'-O5'
1	C1	1420	OMC	O4'-C4'-C5'-O5'
1	C1	1917	OMU	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	GTP	CH	701	63	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
62	GTP	Cd	1000	63	26,34,34	1.17	2 (7%)	32,54,54	1.55	7 (21%)

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
62	GTP	CH	701	63	-	4/18/38/38	0/3/3/3
62	GTP	Cd	1000	63	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	Cd	1000	GTP	C5-C6	-4.12	1.39	1.47
62	CH	701	GTP	C5-C6	-4.04	1.39	1.47
62	Cd	1000	GTP	C2-N3	2.20	1.38	1.33
62	CH	701	GTP	C2-N3	2.08	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	CH	701	GTP	PA-O3A-PB	-3.91	119.40	132.83
62	CH	701	GTP	PB-O3B-PG	-3.75	119.96	132.83
62	Cd	1000	GTP	PB-O3B-PG	-3.51	120.78	132.83
62	Cd	1000	GTP	C5-C6-N1	3.32	119.81	113.95
62	CH	701	GTP	C5-C6-N1	3.24	119.68	113.95
62	CH	701	GTP	C8-N7-C5	3.03	108.77	102.99
62	Cd	1000	GTP	C3'-C2'-C1'	3.00	105.50	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	Cd	1000	GTP	C8-N7-C5	2.96	108.64	102.99
62	Cd	1000	GTP	C2-N1-C6	-2.93	119.70	125.10
62	CH	701	GTP	C3'-C2'-C1'	2.88	105.32	100.98
62	CH	701	GTP	C2-N1-C6	-2.87	119.81	125.10
62	Cd	1000	GTP	O6-C6-C5	-2.22	120.03	124.37
62	Cd	1000	GTP	PA-O3A-PB	-2.12	125.54	132.83
62	CH	701	GTP	O6-C6-C5	-2.10	120.26	124.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

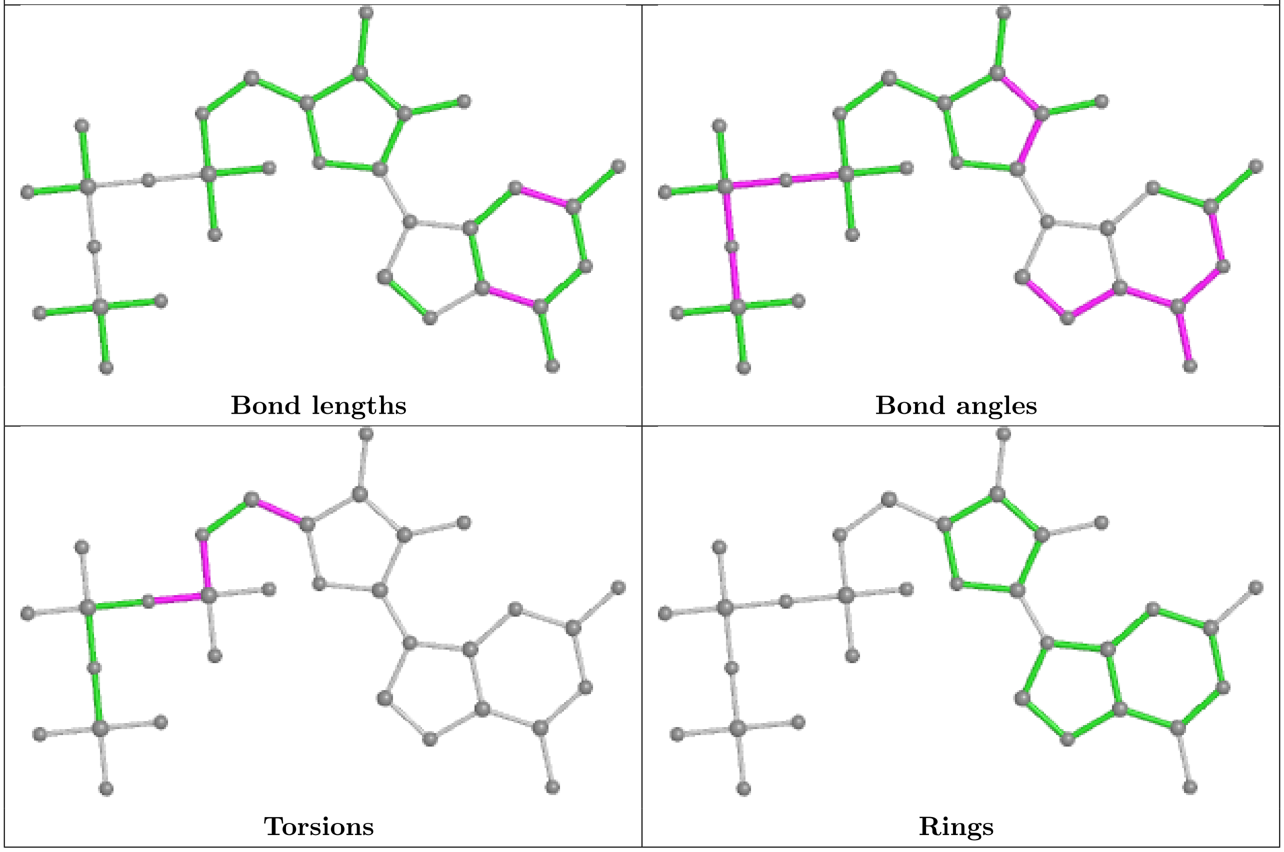
Mol	Chain	Res	Type	Atoms
62	CH	701	GTP	C5'-O5'-PA-O1A
62	CH	701	GTP	O4'-C4'-C5'-O5'
62	Cd	1000	GTP	C3'-C4'-C5'-O5'
62	Cd	1000	GTP	O4'-C4'-C5'-O5'
62	CH	701	GTP	PB-O3A-PA-O1A
62	CH	701	GTP	PB-O3A-PA-O2A
62	Cd	1000	GTP	C5'-O5'-PA-O1A

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 then 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.

Ligand GTP CH 701



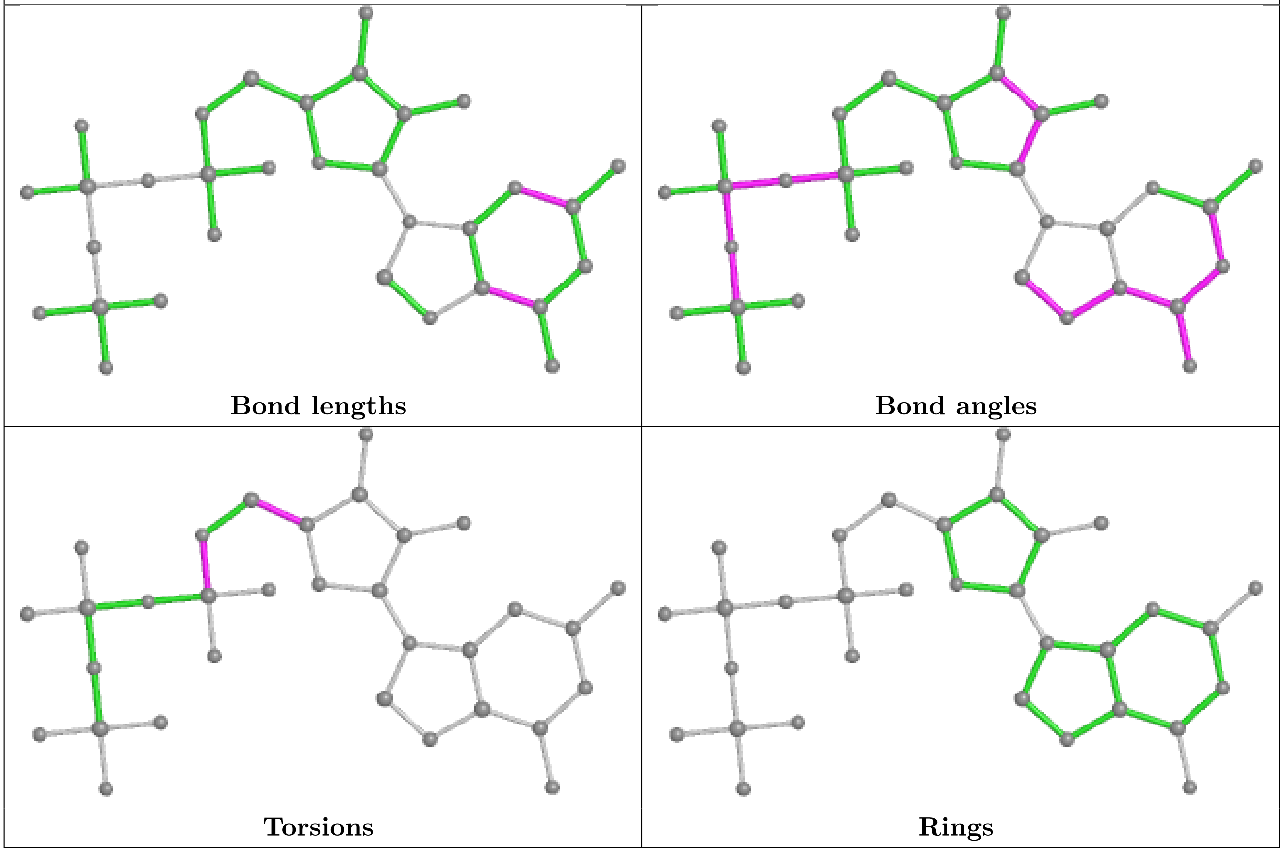
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP Cd 1000



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

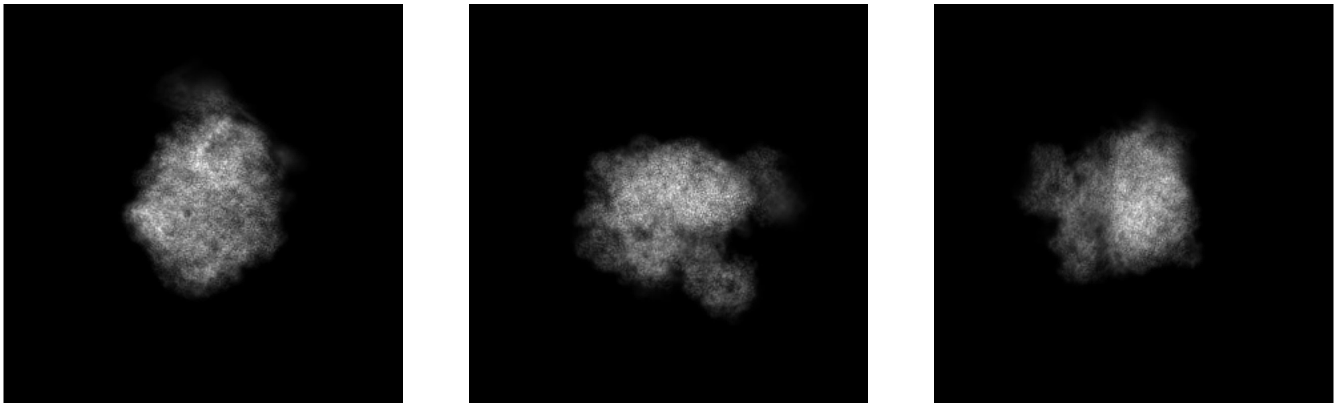
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-17955. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

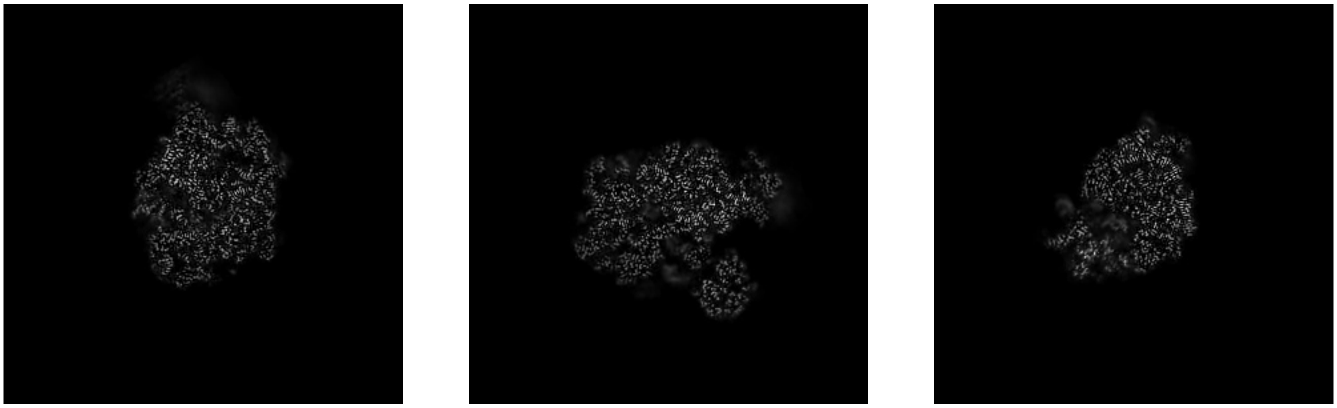


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

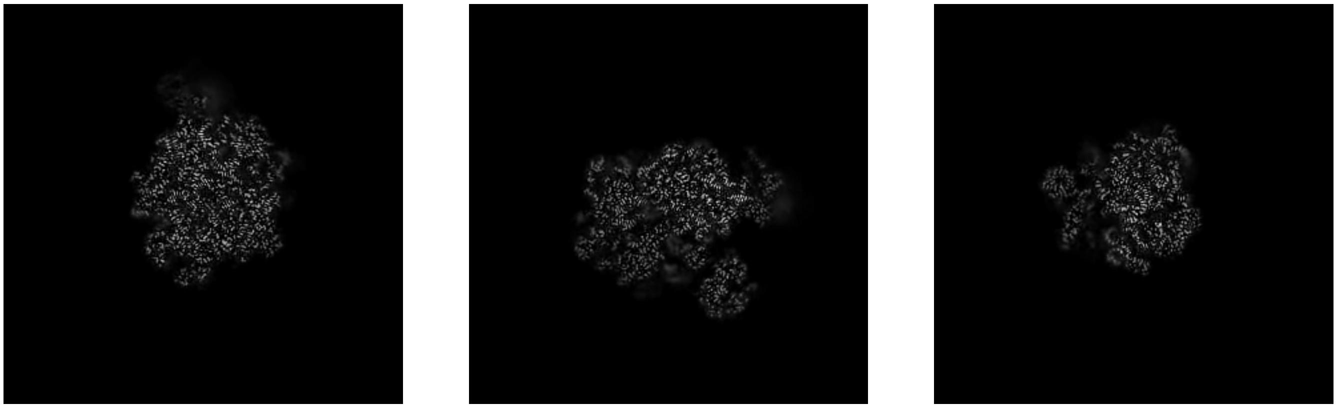


X Index: 250 Y Index: 250 Z Index: 250

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

6.3 Largest variance slices

6.3.1 Primary map

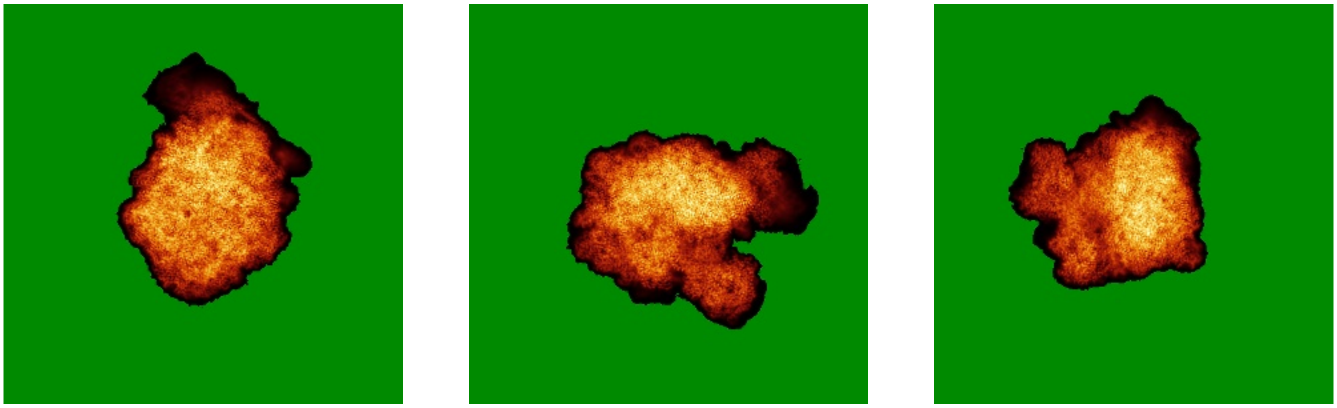


X Index: 259 Y Index: 248 Z Index: 274

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

6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

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

6.5 Orthogonal surface views

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

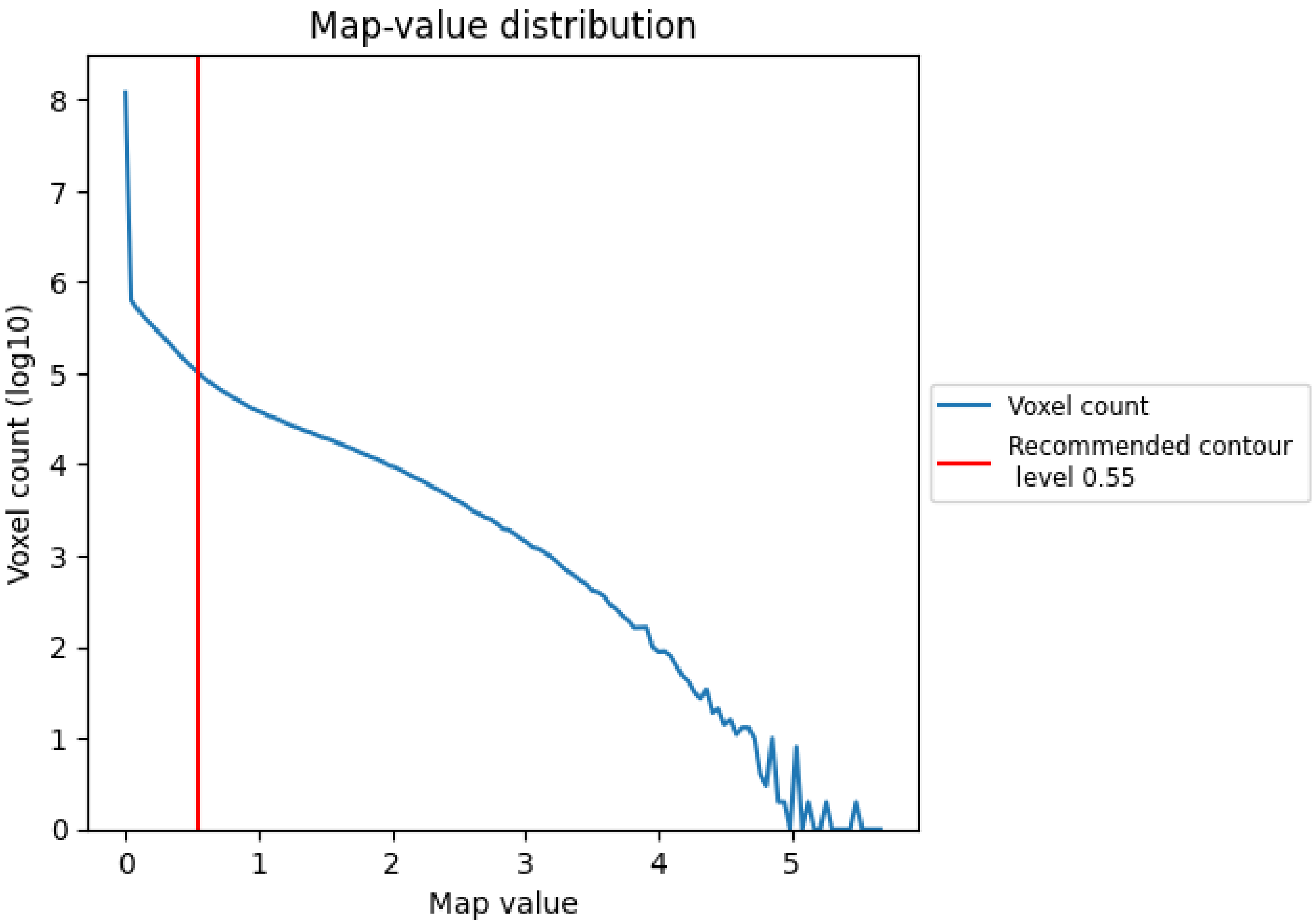
6.6 Mask visualisation

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

7 Map analysis ⓘ

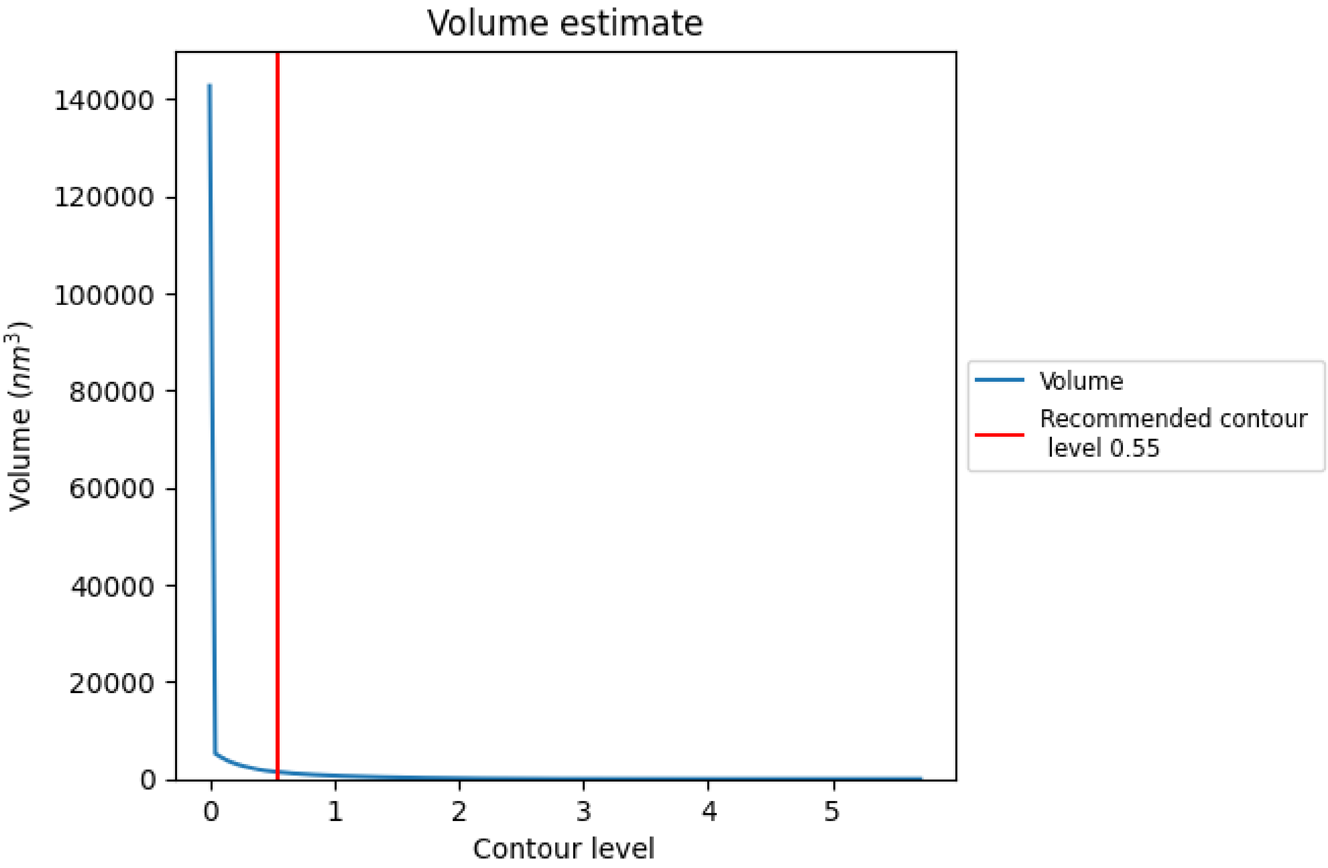
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

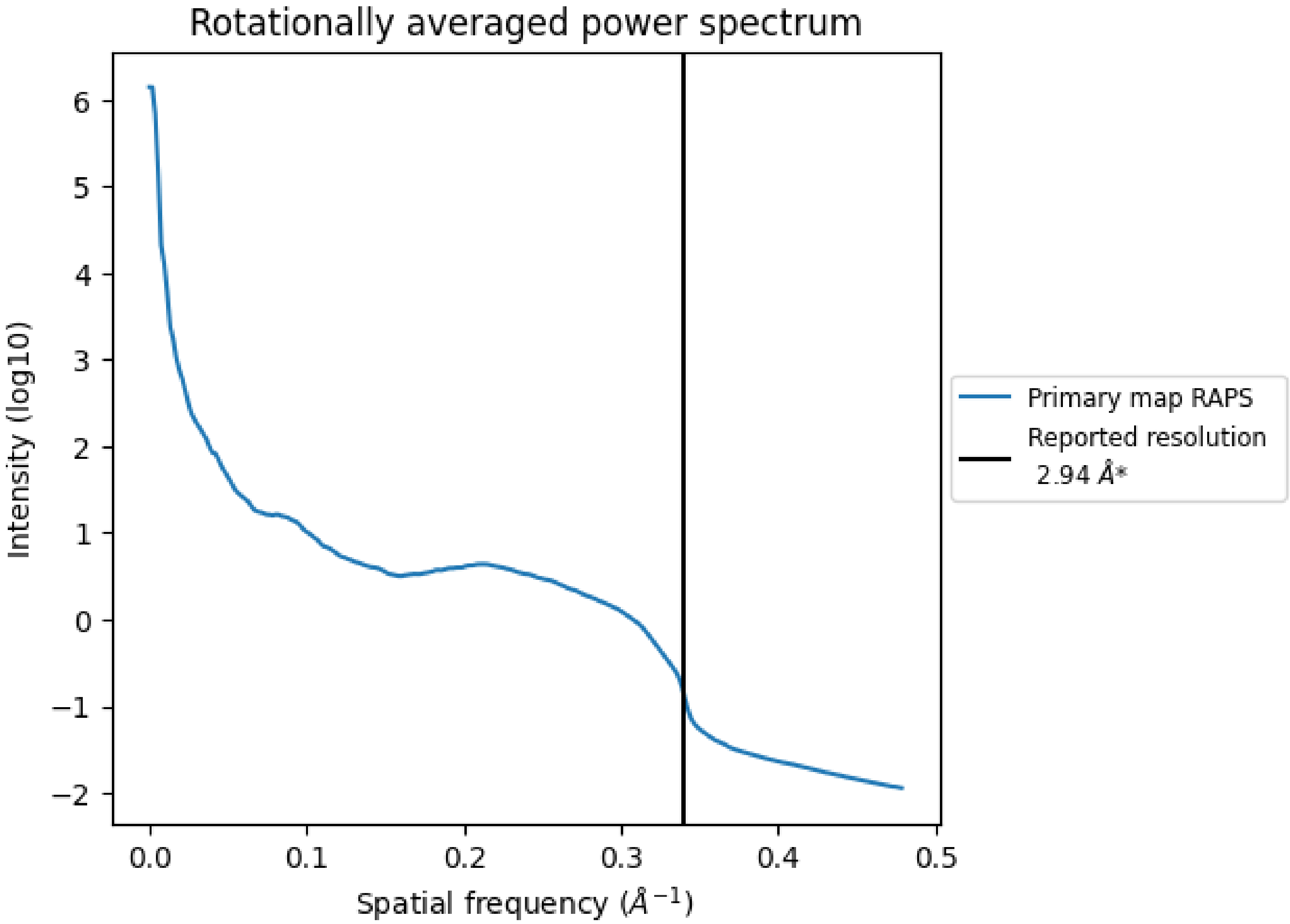
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1418 nm^3; this corresponds to an approximate mass of 1281 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 0.340 Å^{-1}

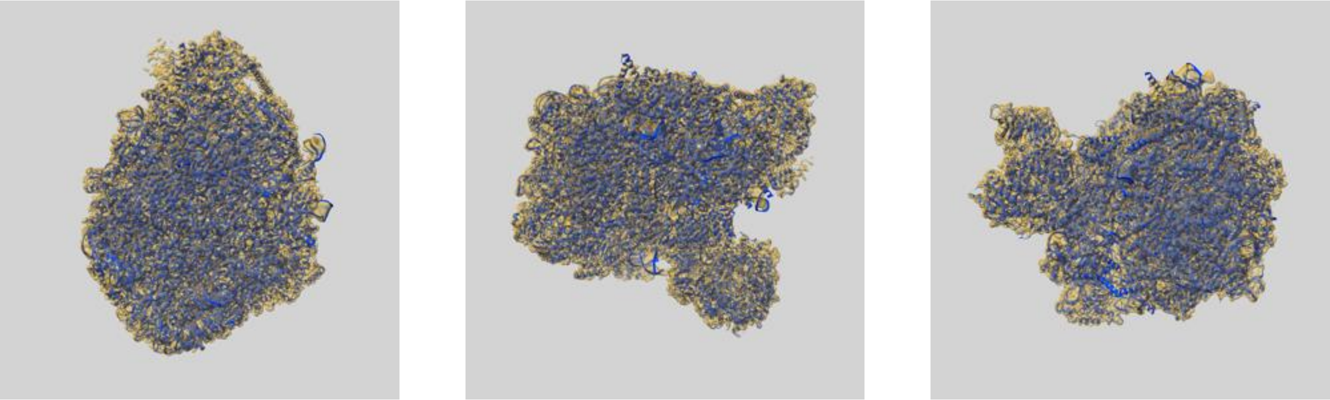
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-17955 and PDB model 8PV6. Per-residue inclusion information can be found in section 3 on page 17.

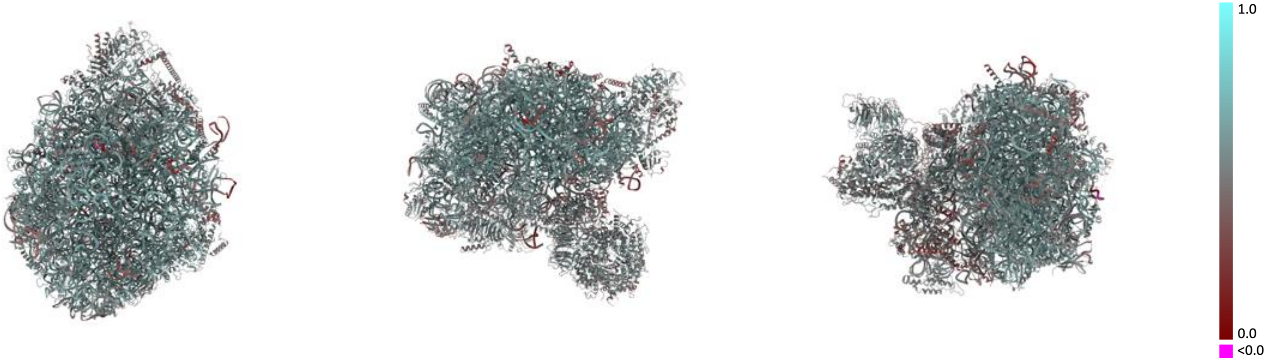
9.1 Map-model overlay (i)



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

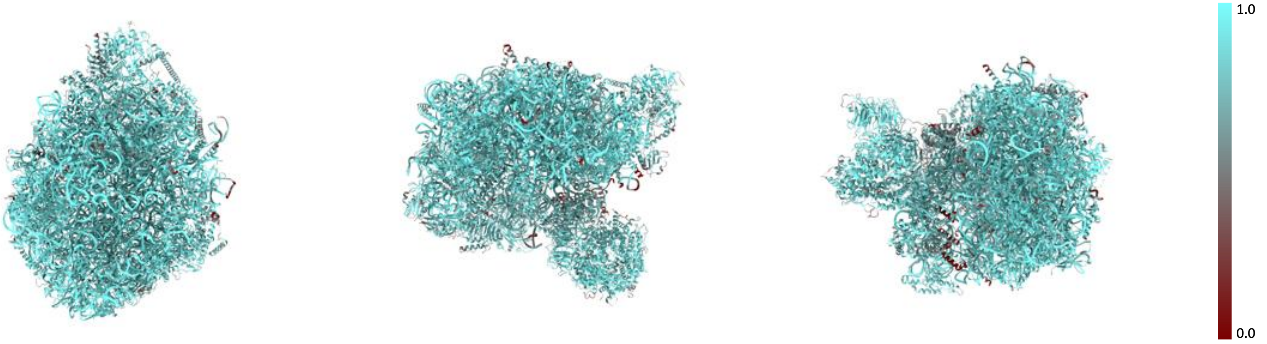
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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.

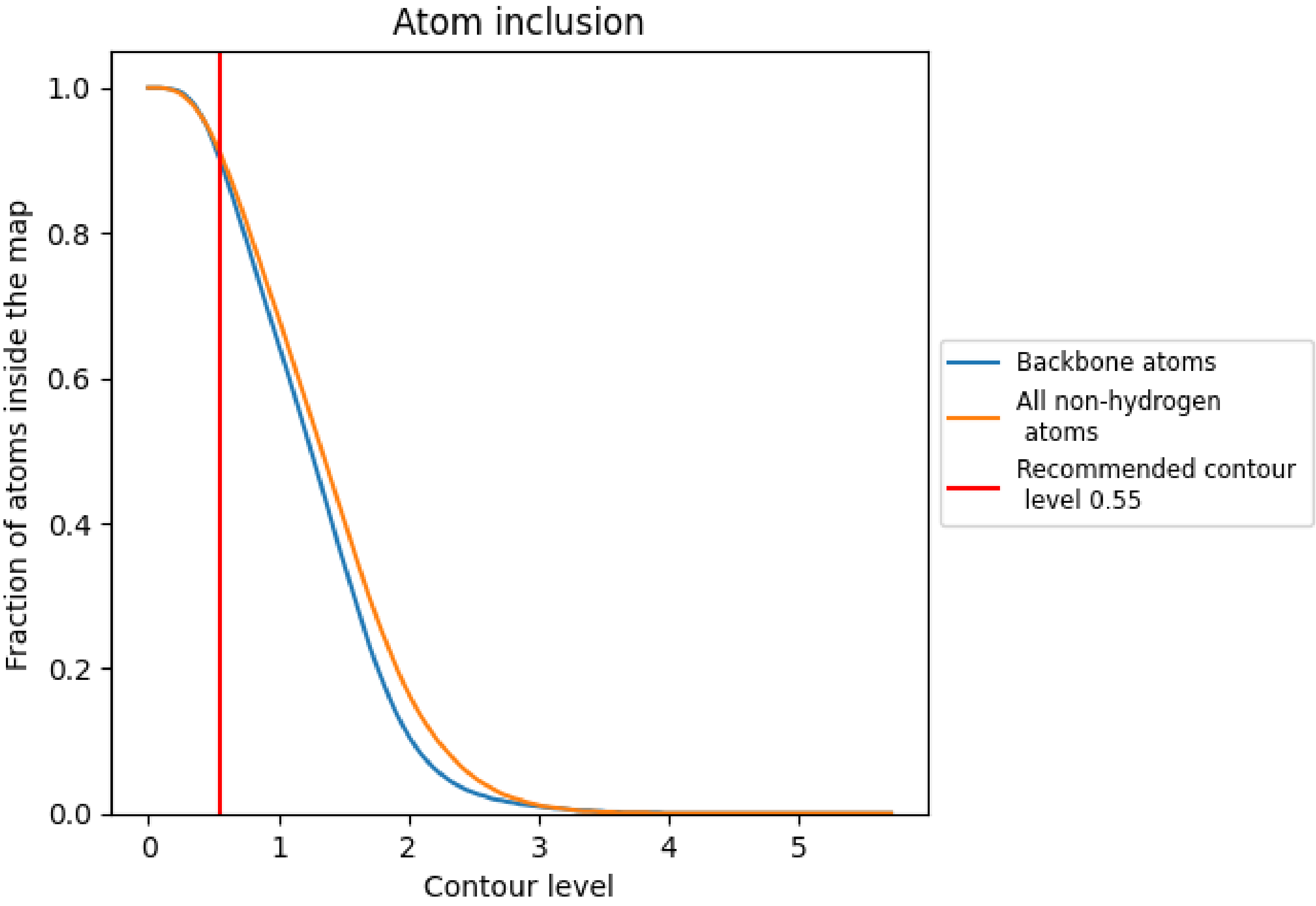
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 (0.55).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.5470
C1	0.9730	0.5650
C2	0.9650	0.5840
C3	0.7830	0.4850
C4	0.9910	0.5130
CF	0.8150	0.5010
CH	0.8540	0.5350
CI	0.7360	0.4770
CJ	0.8890	0.5370
CK	0.9190	0.5800
CL	0.5890	0.4240
CM	0.7900	0.4600
CN	0.9200	0.5660
CO	0.8470	0.5430
CQ	0.8550	0.5330
CR	0.7820	0.4910
CS	0.6840	0.4670
CT	0.8430	0.4930
CU	0.8490	0.5120
CV	0.8310	0.4910
CW	0.8550	0.4970
Cb	0.9090	0.5610
Cd	0.8710	0.5560
Ce	0.7550	0.4740
Ch	0.8490	0.5090
Cz	0.7980	0.4710
LA	0.9700	0.6120
LB	0.9610	0.6020
LC	0.9410	0.5920
LD	0.8980	0.4940
LE	0.8840	0.5500
LF	0.9210	0.5670
LG	0.9160	0.5630
LH	0.8920	0.5670
LJ	0.9350	0.5140

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Chain	Atom inclusion	Q-score
LK	0.7190	0.4370
LL	0.9070	0.5690
LM	0.9040	0.5690
LN	0.9900	0.6170
LO	0.9480	0.5970
LP	0.9550	0.5920
LQ	0.9470	0.5870
LR	0.9320	0.5800
LS	0.9300	0.5750
LT	0.8690	0.4840
LU	0.8710	0.5320
LV	0.9550	0.5910
LX	0.9200	0.5650
LY	0.9140	0.5690
LZ	0.9310	0.5550
La	0.9280	0.5810
Lb	0.5310	0.3630
Lc	0.8850	0.5530
Ld	0.9190	0.5820
Le	0.9420	0.5920
Lf	0.9760	0.6190
Lg	0.9080	0.5770
Lh	0.8800	0.5300
Li	0.9350	0.5590
Lj	0.9780	0.6190
Lk	0.8410	0.5310
Ll	0.9810	0.6210
Lp	0.8880	0.5630
Lq	0.9410	0.5790
Lr	0.6770	0.3720