wwPDB EM Validation Summary Report (i)

Mar 8, 2026 – 08:07 AM UTC

PDB ID	:	9L5R / pdb_00009l5r
EMDB ID	:	EMD-62841
Title	:	Cryo-EM structure of the thermophile spliceosome (state ILS)
Authors	:	Li, Y.; Fischer, P.; Wang, M.; Yuan, R.; Meng, W.; Luehrmann, R.; Lau, B.; Hurt, E.; Cheng, J.
Deposited on	:	2024-12-23
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

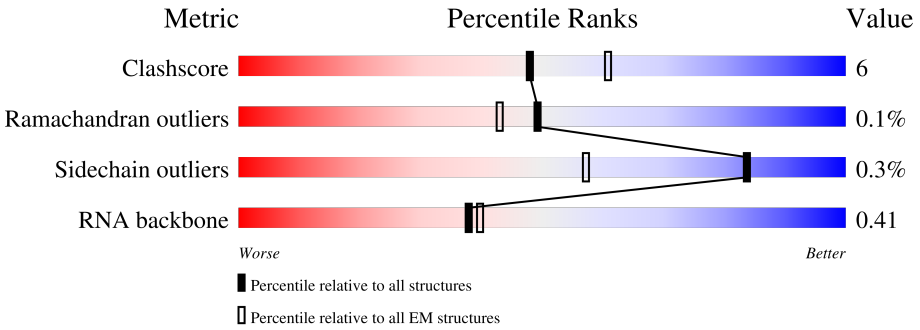
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

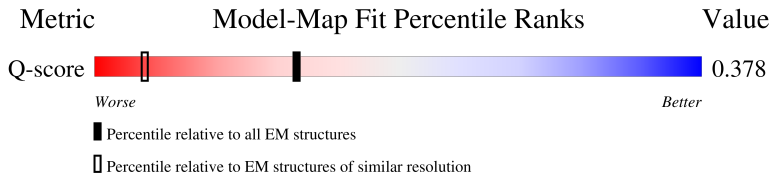
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	2	193	• 41% 12% • 45%
2	5	116	15% 70% 19% 7% •
3	6	101	55% 31% 11% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	A	2463	68% 13% 19%
5	B	326	70% 9% 21%
6	C	1011	77% 14% 9%
7	D	325	24% 6% 71%
8	E	352	68% 20% 12%
9	F	233	39% 8% 53%
10	I	839	69% 19% 12%
11	J	687	6% 77% 11% 11%
12	L	768	6% 72% 11% 17%
13	K	231	7% 84% 16%
14	q	480	22% 7% 71%
14	r	480	23% 7% 70%
14	s	480	25% 71%
14	t	480	22% 7% 71%
15	N	148	85% 14%
16	S	167	71% 23% 6%
17	T	496	55% 11% 34%
18	U	757	36% 10% 54%
19	M	395	49% 13% 37%
20	0	408	56% 10% 32%
21	R	578	50% 8% 41%
22	W	547	68% 27%
23	P	260	38% 6% 56%
24	Y	1416	15% 79% 16% 5%
25	a	98	9% 86% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
25	j	98	69% 20% 10%
26	b	94	71% 24%
26	l	94	67% 19% 14%
27	c	592	14% 86%
27	m	592	11% 85%
28	d	118	14% 69% 31%
28	o	118	51% 23% 26%
29	e	211	5% 36% 63%
29	p	211	5% 38% 11% 51%
30	f	114	68% 5% 26%
30	u	114	55% 24% 21%
31	g	82	16% 88% 12%
31	k	82	65% 24% 11%
32	h	242	6% 50% 50%
33	i	201	19% 51% 49%
34	CY	510	5% 18% 82%
35	Cb	975	14% 52% 48%
36	Cc	764	13% 93% 7%
37	7	101	7% 15% 74%
38	Ci	153	50% 5% 45%
39	H	22	9% 100%

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 104144 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 U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	106	2224	994	357	767	106	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	111	2343	1048	398	786	111	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	98	2090	935	379	678	98	0	0

- Molecule 4 is a protein called PRP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	2006	16540	10628	2874	2976	62	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	258	2071	1273	388	405	5	0	0

- Molecule 6 is a protein called SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	922	7301	4668	1229	1368	36	0	0

- Molecule 7 is a protein called SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	95	786	477	150	154	5	0	0

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4-like WD40 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	310	2379	1493	414	462	10	0	0

- Molecule 9 is a protein called CCDC12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	110	879	544	166	167	2	0	0

- Molecule 10 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	738	6135	3924	1071	1112	28	0	0

- Molecule 11 is a protein called Suppressor of forked domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	608	5176	3297	937	929	13	0	0

- Molecule 12 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	637	5052	3111	952	974	15	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	K	231	1797	1122	317	354	4	0	0

- Molecule 14 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	139	Total	C	N	O	S	0	0
			1110	699	195	214	2		
14	t	141	Total	C	N	O	S	0	0
			1122	707	197	216	2		
14	r	143	Total	C	N	O	S	0	0
			1132	713	199	218	2		
14	s	140	Total	C	N	O	S	0	0
			1115	702	196	215	2		

- Molecule 15 is a protein called Putative bud site selection protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	148	Total	C	N	O	S	0	0
			1200	755	213	220	12		

- Molecule 16 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	157	Total	C	N	O	S	0	0
			1209	763	217	223	6		

- Molecule 17 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	328	Total	C	N	O	S	0	0
			2565	1621	461	469	14		

- Molecule 18 is a protein called Cell cycle control protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	348	Total	C	N	O	S	0	0
			2821	1770	516	524	11		

- Molecule 19 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	248	Total	C	N	O	S	0	0
			1964	1238	355	354	17		

- Molecule 20 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	0	276	2224	1381	424	412	7	0	0

- Molecule 21 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
21	R	340	2686	1664	509	503	2	8	0	0

- Molecule 22 is a protein called PRP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	397	2224	1336	444	440	4	0	0

- Molecule 23 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	114	925	577	182	165	1	0	0

- Molecule 24 is a protein called Pre-mRNA-splicing factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	1344	10819	6892	1900	2002	25	0	0

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
25	a	86	426	253	86	87		0	0
			Total	C	N	O	S		
25	j	88	704	456	121	126	1	0	0

- Molecule 26 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
26	b	71	351	209	71	71		0	0
			Total	C	N	O	S		
26	l	81	649	412	114	120	3	0	0

- Molecule 27 is a protein called Delta(14)-sterol reductase.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	c	84	Total C N O 416 247 84 85	0	0
27	m	86	Total C N O S 678 427 129 118 4	0	0

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	AltConf	Trace
28	d	81	Total C N O 401 239 81 81	0	0
28	o	87	Total C N O S 679 433 114 128 4	0	0

- Molecule 29 is a protein called Sm protein B.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	e	79	Total C N O 388 230 79 79	0	0
29	p	103	Total C N O S 788 490 148 145 5	0	0

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms	AltConf	Trace
30	f	84	Total C N O 414 246 84 84	0	0
30	u	90	Total C N O S 716 449 132 131 4	0	0

- Molecule 31 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	g	72	Total C N O 354 210 72 72	0	0
31	k	73	Total C N O S 577 369 101 105 2	0	0

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	h	122	605	361	122	122	0	0

- Molecule 33 is a protein called U2 small nuclear ribonucleoprotein B'-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	i	102	504	300	102	102	0	0

- Molecule 34 is a protein called Nineteen complex-related protein 2-domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	CY	91	444	262	91	91	0	0

- Molecule 35 is a protein called G-patch domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Cb	505	2496	1486	505	505	0	0

- Molecule 36 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	Cc	714	3541	2112	714	715	0	0

- Molecule 37 is a RNA chain called Unknown mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	7	26	494	241	68	159	26	0	0

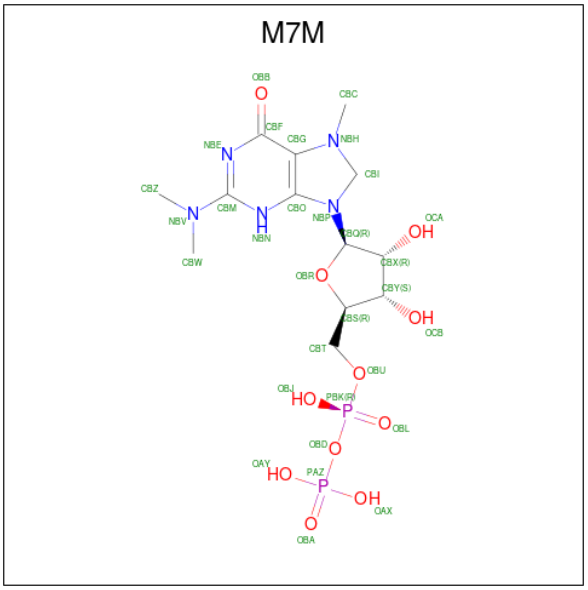
- Molecule 38 is a protein called Putative cyclophilin protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	Ci	84	415	247	84	84	0	0

- Molecule 39 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	H	22	110	66	22	22	0	0

- Molecule 40 is N,N,7-trimethylguanosine 5'-(trihydrogen diphosphate) (CCD ID: M7M) (formula: $C_{13}H_{23}N_5O_{11}P_2$).

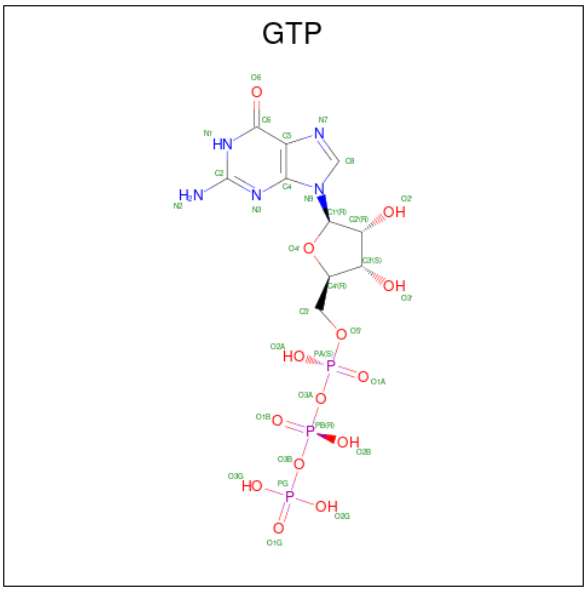


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
40	B	1	30	13	5	10	2	0

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

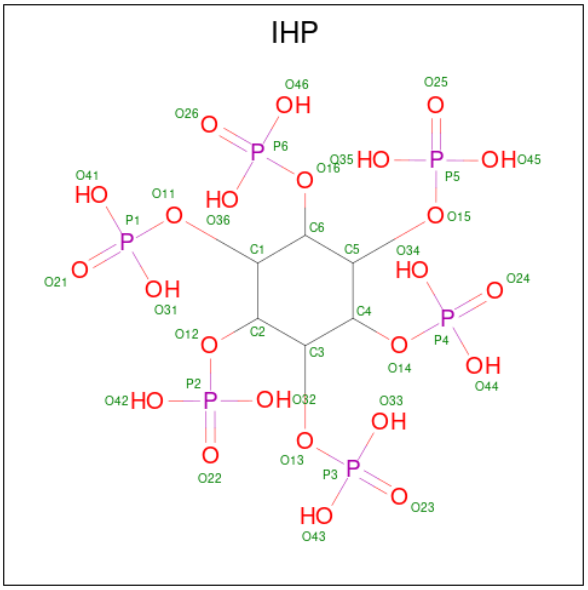
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
41	C	1	1	1	0

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 43 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
43	J	1	36	6	24	6	0

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

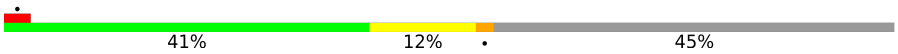
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
44	N	3	3	3	0
			Total	Zn	
44	U	1	1	1	0
			Total	Zn	
44	M	2	2	2	0

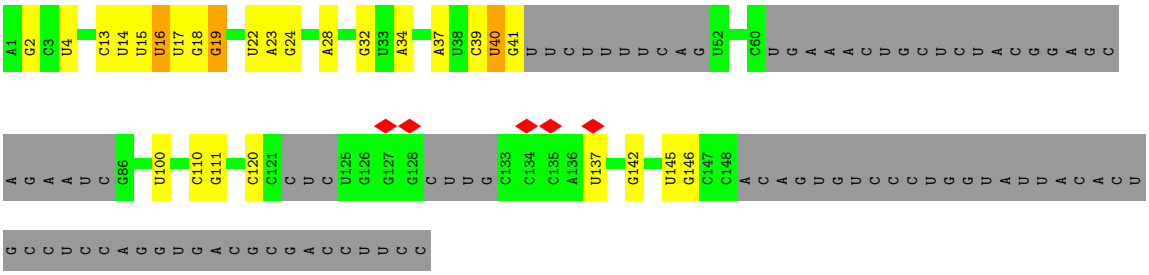
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: U2 snRNA

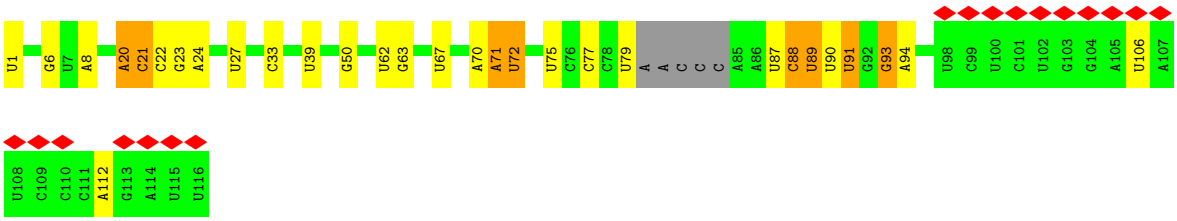
Chain 2:





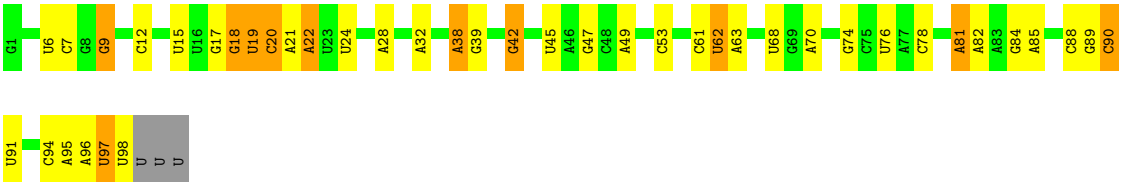
- Molecule 2: U5 snRNA

Chain 5:



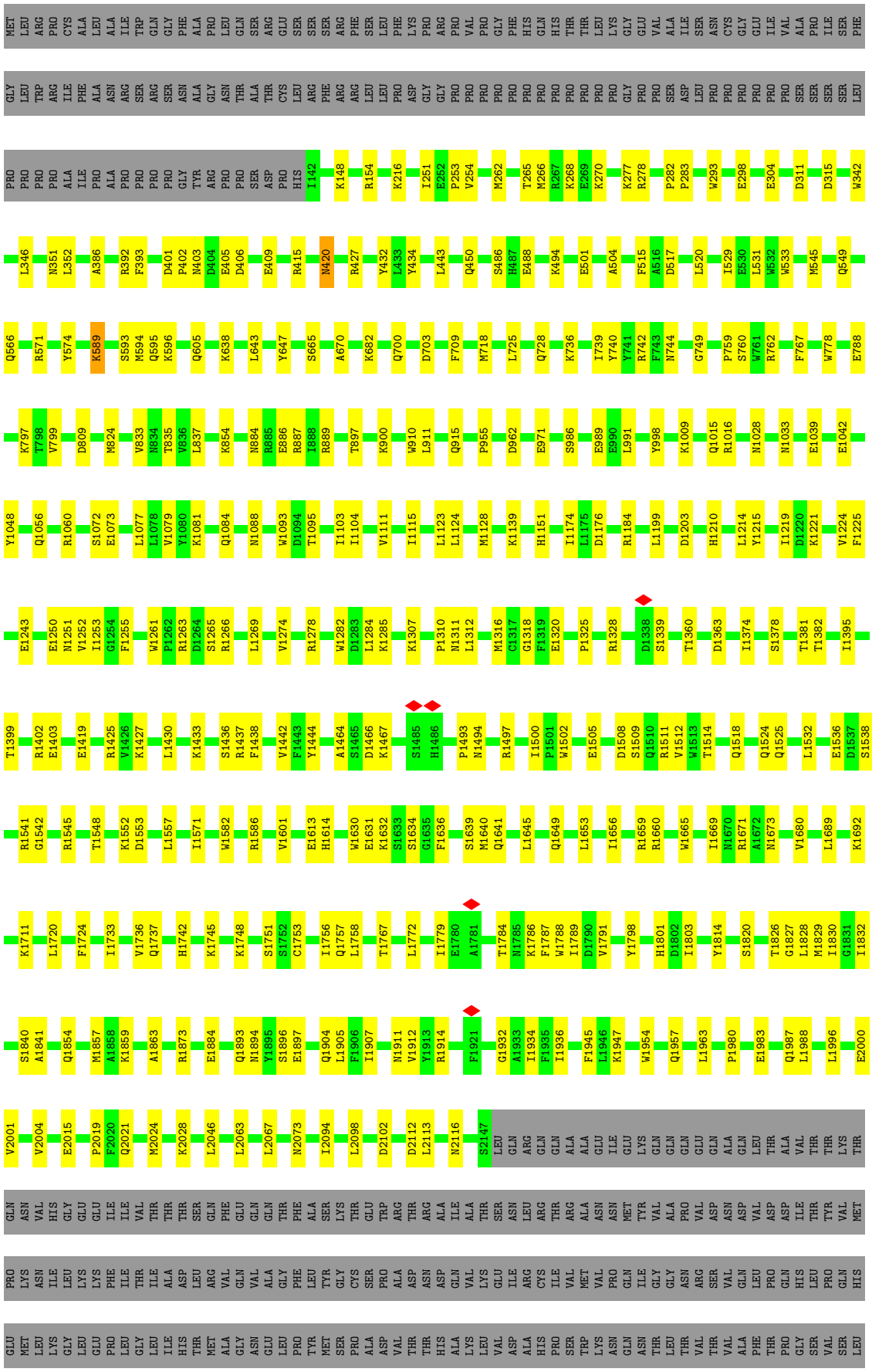
- Molecule 3: U6 snRNA

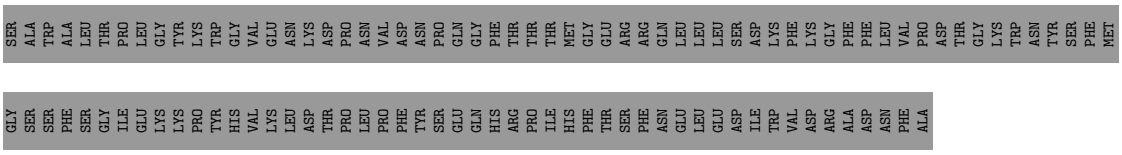
Chain 6:



- Molecule 4: PRP8

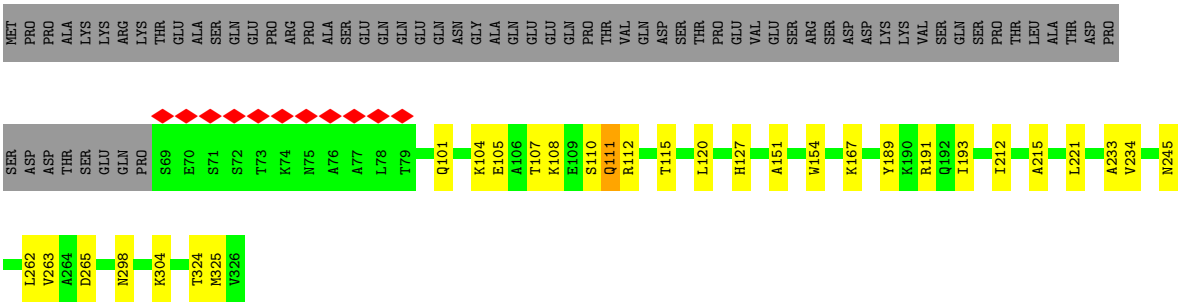
Chain A:


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



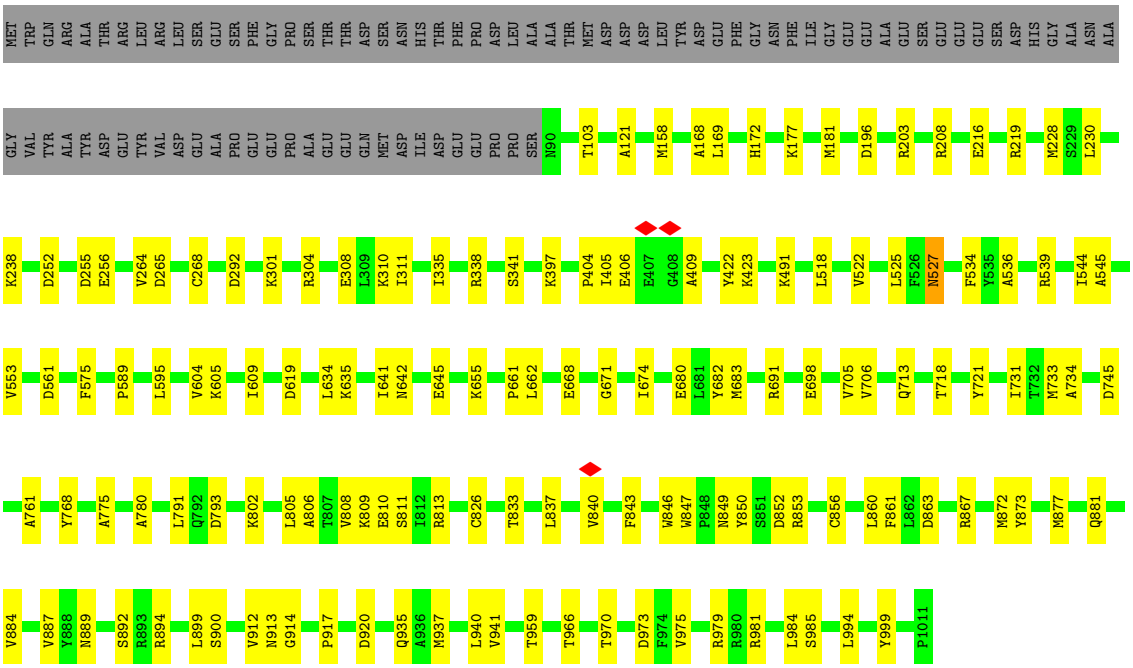
- Molecule 5: Pre-mRNA-splicing factor SYF2

Chain B:



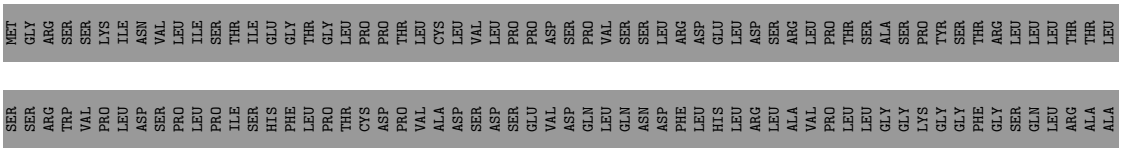
- Molecule 6: SNU114

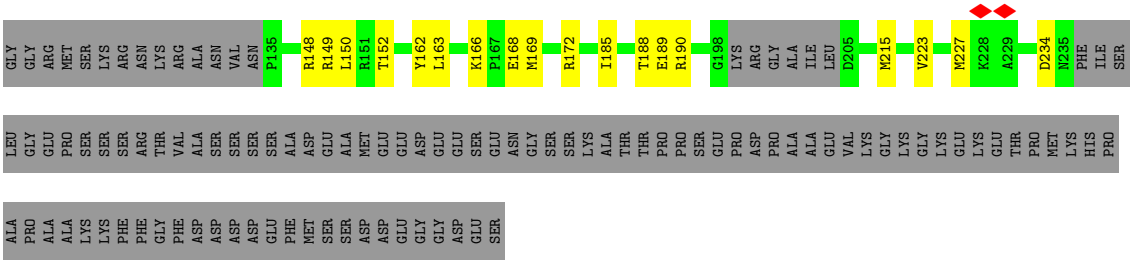
Chain C:



- Molecule 7: SDE2

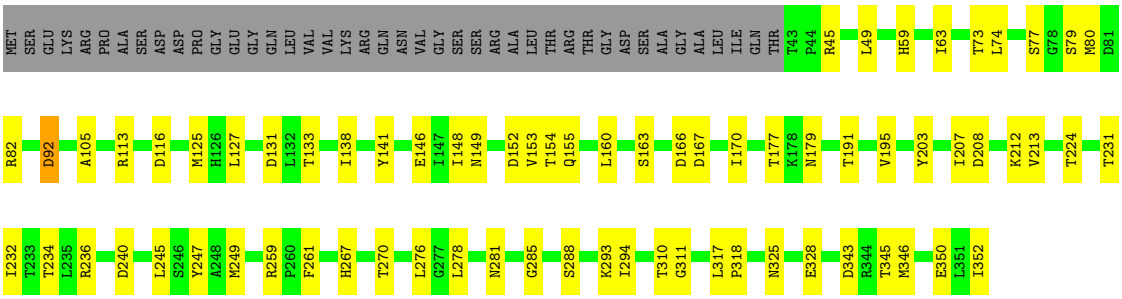
Chain D:





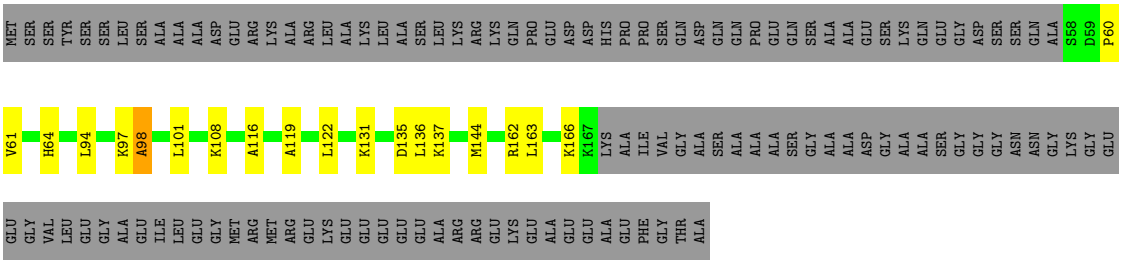
• Molecule 8: Anaphase-promoting complex subunit 4-like WD40 domain-containing protein

Chain E:



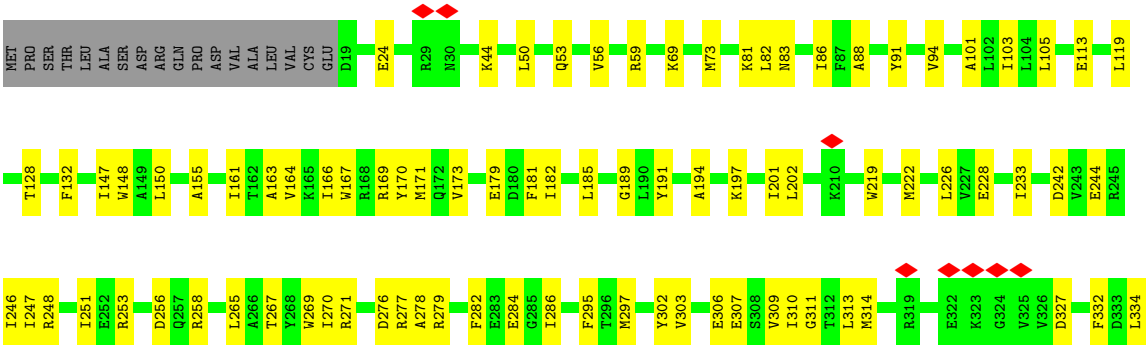
• Molecule 9: CCDC12

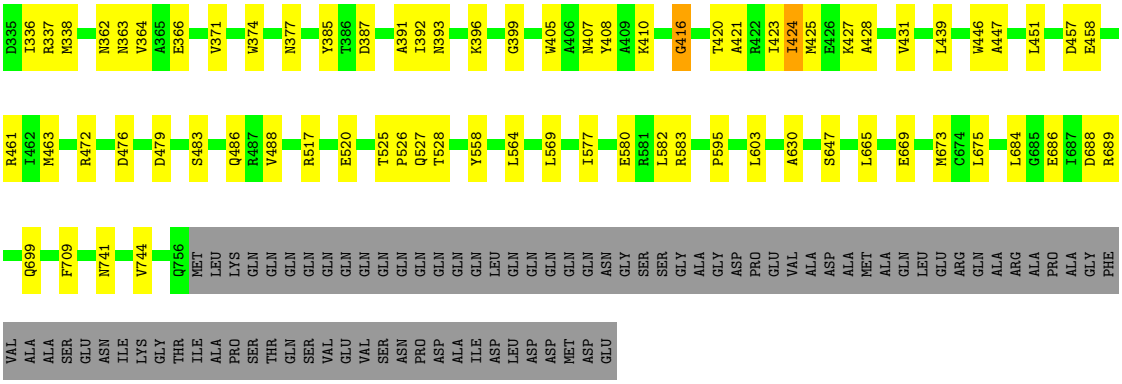
Chain F:



• Molecule 10: Putative pre-mRNA splicing protein

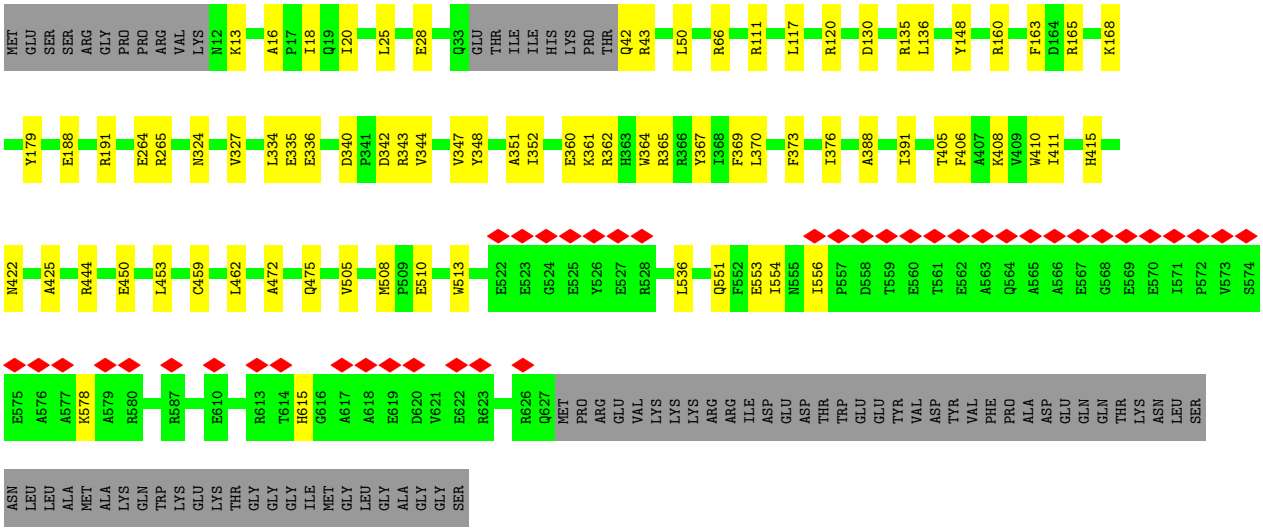
Chain I:





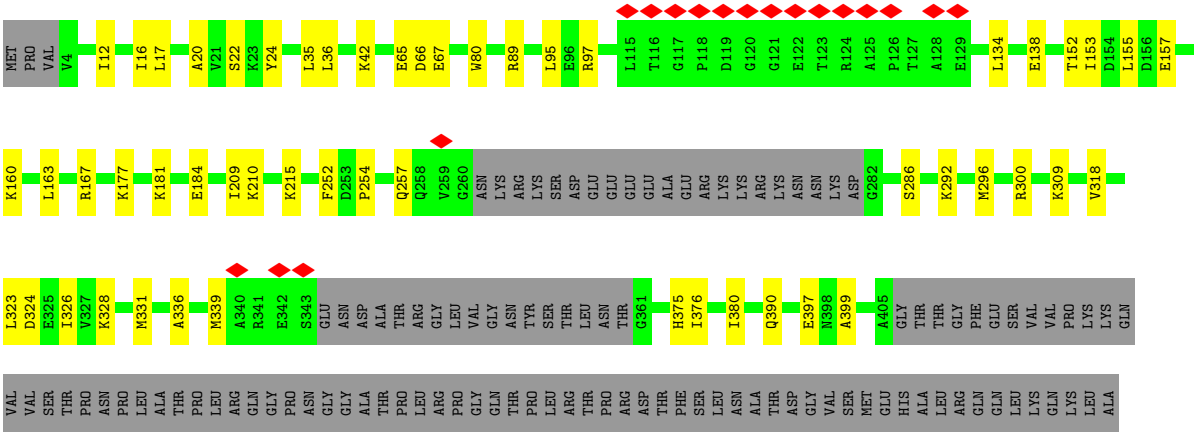
- Molecule 11: Suppressor of forked domain-containing protein

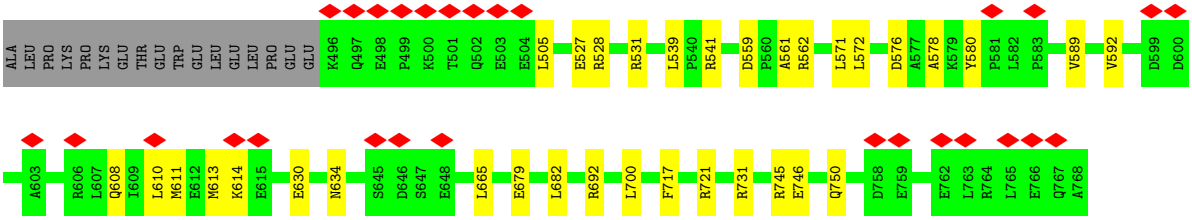
Chain J:



- Molecule 12: Putative pre-mRNA splicing protein

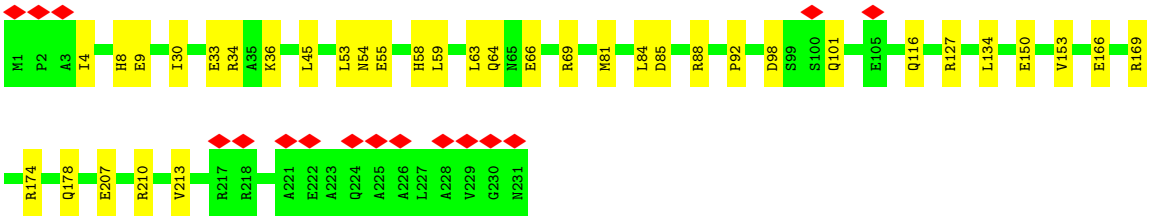
Chain L:





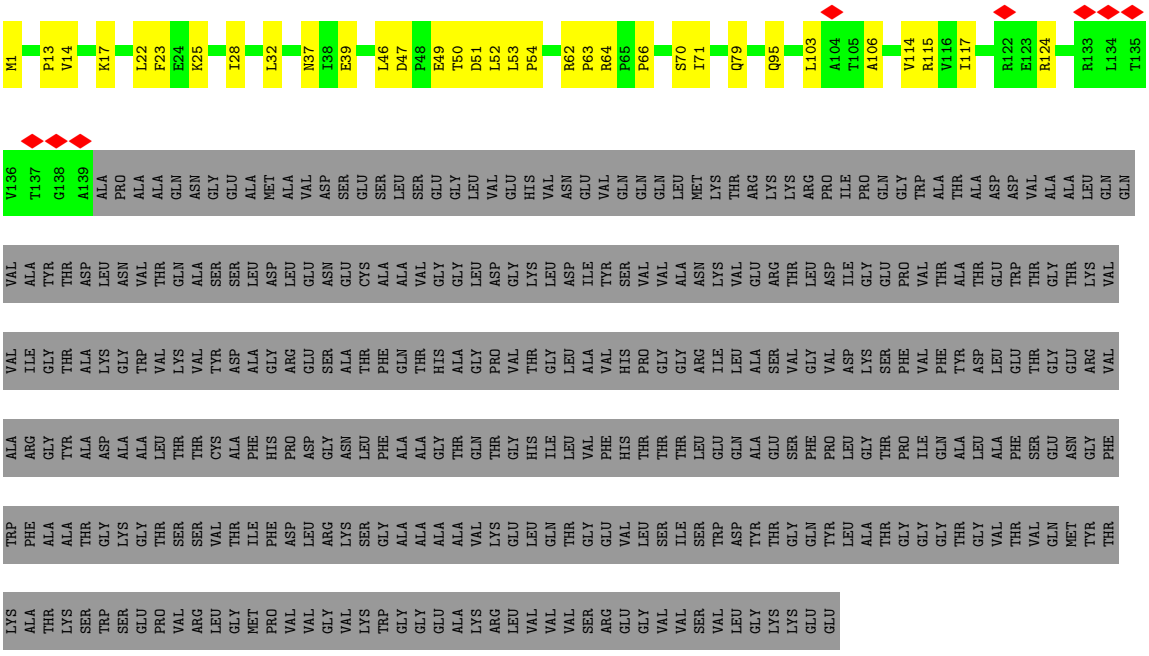
• Molecule 13: Pre-mRNA-splicing factor SPF27

Chain K:



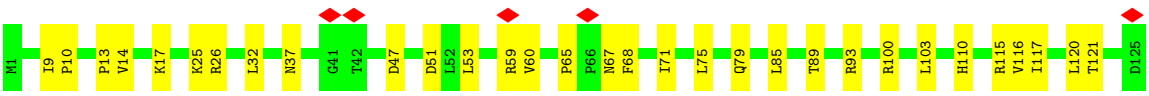
• Molecule 14: Pre-mRNA-processing factor 19

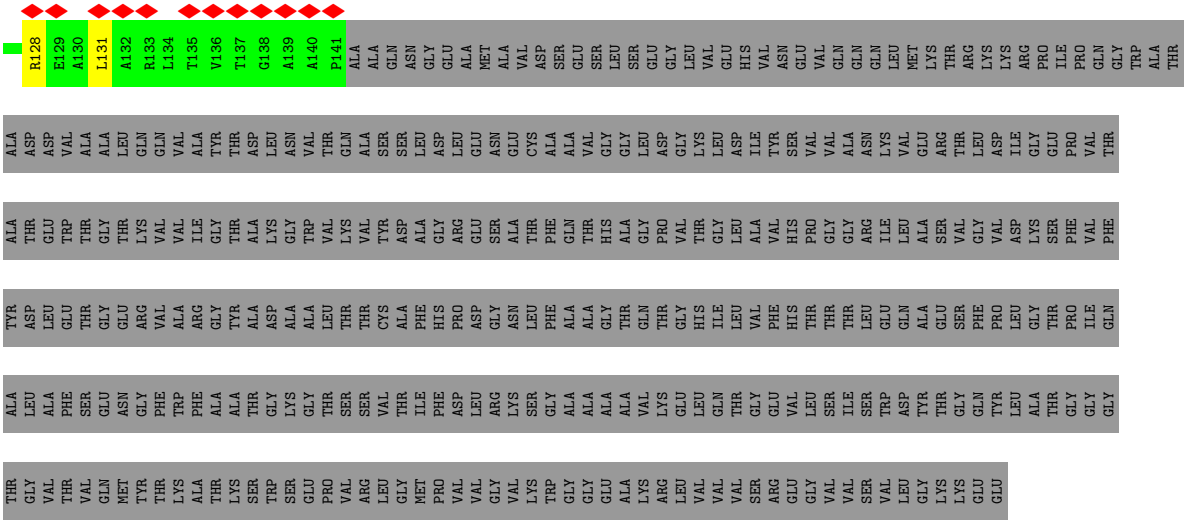
Chain q:



• Molecule 14: Pre-mRNA-processing factor 19

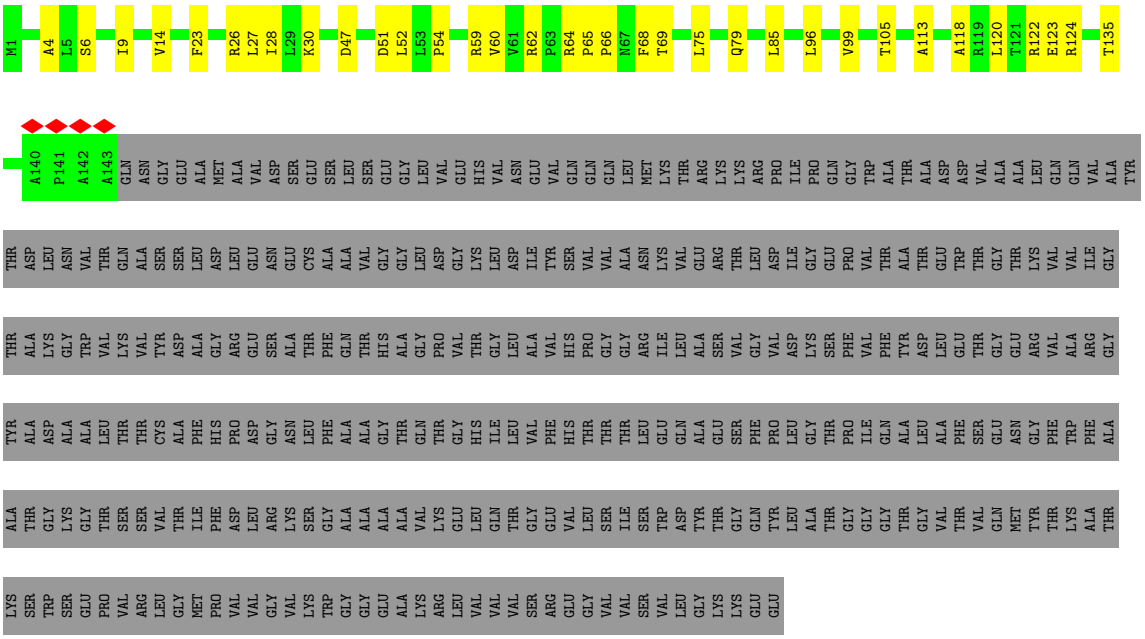
Chain t:





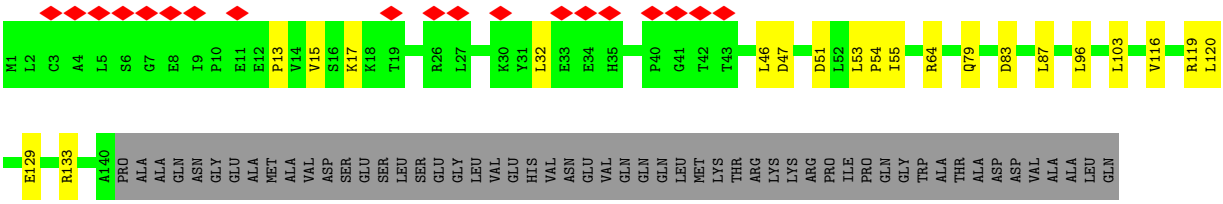
- Molecule 14: Pre-mRNA-processing factor 19

Chain r:



- Molecule 14: Pre-mRNA-processing factor 19

Chain s:



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

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

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

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

THR LYS ALA THR LYS SER TRP SER GLU PRO VAL ARG LEU GLY MET PRO VAL VAL GLY VAL LYS TRP GLY GLY GLU ALA LYS ARG LEU VAL VAL VAL SER ARG GLU GLY VAL VAL SER VAL LEU GLY LYS LYS GLU GLU

- Molecule 15: Putative bud site selection protein

Chain N: 85% 14% ••

M1 R5 P6 A7 S8 K9 H45 Q48 Y66 I72 K95 K101 L102 C103 I108 N116 C121 R122 R125 L128 K129 Q132 C144 A145 S146 T147 D148

- Molecule 16: Peptidyl-prolyl cis-trans isomerase

Chain S: 71% 23% 6%

M1 A2 T3 D4 E17 L18 Y19 N20 Q21 T26 C27 E28 K31 T32 L33 Y38 I43 R46 F51 M52 D57 G60 F73 E74 D75 F76 I77 T84 G85 A86 G87 S90 N99 F104 L105 T106 P109 T110 P111 G115 R132 V136

R143 I148 K149 V156 G157 GLU GLY GLU GLU ASP ASP LYS GLN LEU VAL

- Molecule 17: Pre-mRNA-splicing factor PRP46

Chain T: 55% 11% 34%

MET ALA THR ASP VAL ALA VAL ASN GLY PRO ASP VAL SER LYS LEU GLU ALA LEU LEU ARG ASP ASN GLU ARG THR THR ARG SER LEU TYR ALA SER THR THR PRO ASP SER GLY ARG LYS ARG ILE LYS LEU ASP PRO GLY LEU ALA SER GLU ASP PRO ASP ILE THR LYS SER ALA LEU

SER LEU ARG LEU HIS ALA GLU TYR GLY ASP VAL GLN THR LEU PRO GLU ALA ILE ALA LYS LYS LEU SER ALA ALA GLY PRO ARG LYS LYS LYS PRO PRO GLY VAL ALA GLU ASP GLU ALA PRO SER LYS SER GLU GLU HIS THR ARG LYS LEU ILE GLU GLY ILE PRO GLN ALA LYS

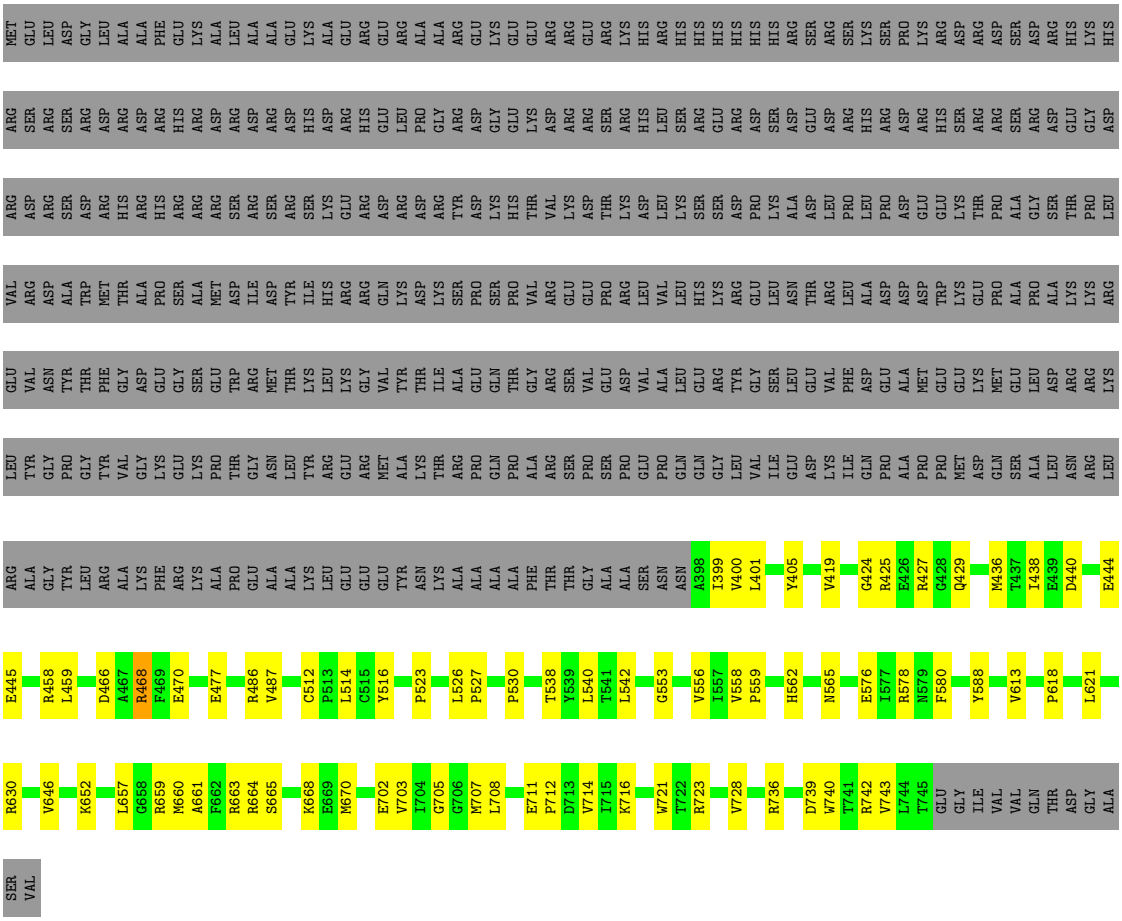
PRO SER ALA GLY ALA ALA SER SER ASN ALA LEU VAL LEU ALA HIS GLY LYS PRO SER ALA ALA GLY ALA GLY ALA ALA ARG PRO GLN ARG ASN GLU PRO GLN GLN LEU SER LEU VAL ARG ARG SER GLU SER LEU LEU ALA GLN P169 R170 P171 M180 S184 E196 P197 W201

R209 D215 S218 G219 Q220 I229 R233 P239 R240 E249 C255 R265 H270 P281 V287 A295 R296 V297 W298 S304 L309 L319 D325 P326 Q327 G331 A343 K356 A360 L361 T372 A373 I378 F392 N405

D406 Q407 F411 M419 Q438 R459 L460 W472 K473 I485 K488 P489 S490 L491 V492 R493 R494 K495 Y496

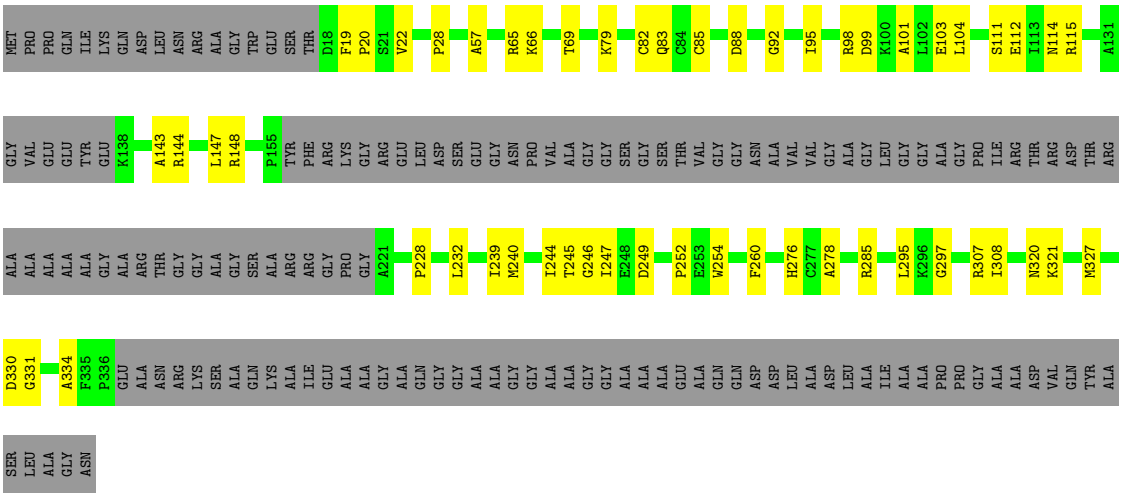
- Molecule 18: Cell cycle control protein

Chain U: 36% 10% 54%



- Molecule 19: Putative pre-mRNA splicing protein

Chain M: 49% 13% 37%



- Molecule 20: Putative pre-mRNA splicing protein

Chain 0: 56% 10% • 32%

MET ALA GLU LEU GLU THR ASN PRO ASP VAL ALA VAL ALA VAL ALA GLU ASP SER ASN GLU GLN LYS GLN GLU ASN GLN LEU VAL ALA VAL ASN ASN GLU VAL ALA ALA PRO ILE GLU LYS LYS VAL LYS LYS ILE ILE ARG LYS LYS ARG R51 R54 P59 V62 T72

S82 D85 R86 E87 D88 K89 Y90 L91 K97 G98 R99 C100 N101 I102 D105 T109 R110 A111 C120 F123 K130 L137 L140 P141 T142 I143 I193 W201 I204 I207 R208 V209 L210 N211 N212 R213 M233 S237 L238 E242 R260 A269

I273 I285 L304 Y307 A312 V313 A316 G326 ARG GLU GLU GLY PHE GLU LEU GLU ARG GLU GLN GLN LEU MET LEU GLU ALA PRO PRO GLU THR SER GLN PRO ALA GLN ILE GLU ALA PRO PRO GLN ALA GLN GLU LYS LYS LEU ALA GLY GLY ILE LEU SER SER ARG

THR LEU ALA ALA LEU GLN GLY ALA LYS VAL ALA VAL ALA THR LYS ASP SER LYS PRO GLU LYS PRO SER GLY PRO LEU VAL ALA TYR GLY SER ASP ASP GLU GLU ASP GLU

• Molecule 21: Pre-mRNA-processing protein 45

Chain R: • 50% 8% 41%

M1 P13 K16 R25 I33 V34 S35 I39 T42 GLN ILE VAL ILE ARG ARG THR GLY PRO P52 R57 P65 F68 P83 K92 D101 K105 I111 R120 L132 R157 T158 P175 K176 N177 V178 T182 K190 Y191 S194

A195 Q196 M197 G198 N199 R206 I207 P217 K224 S234 S242 P243 P244 P258 P259 P260 I272 E299 M303 R306 E310 R313 Q314 Q329 K330 E331 E332 H333 L334 R335 Q336 L337 A338 Q339 Q340 A341 R342 A343 E344 R345 A346 A347 A348 A349 ALA SER GLY

ARG ARG ARG SER THR ARG SER ARG SER GLY SER TYR SER GLY SER GLU SER GLY SER GLU THR ASP GLU SER GLU ARG GLU ARG ARG ARG ALA ARG ARG GLU LYS LEU LYS GLU GLU GLU ARG LYS LEU ARG GLN SER ARG MET GLY ALA GLU ARG ARG ALA GLN VAL LEU ALA ARG GLU

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

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

PRO PHE ASN VAL ASP LYS PHE LEU SER GLU VAL GLN LYS GLY SER ASN SER GLY GLY GLY LYS ARG GLY TYR GLY LEU GLN ASP GLU ASP SER ARG GLN ALA LYS ARG SER ARG VAL ASP ASP ASP GLU ASN ASP ASP

• Molecule 22: PRP17

Chain W: 68% • 27%

MET PRO ASP PHE GLY GLU TYR PRO PRO ASN LEU PRO VAL ARG ASP ALA LEU ILE LEU ARG GLU SER GLN ALA GLN ALA PRO THR ALA ASN HIS ALA VAL V34 P35 Y36 N40 P51 F52 ARG ASP THR SER SER SER ALA SER ALA SER GLY SER LEU LYS ARG K69 N70 N71

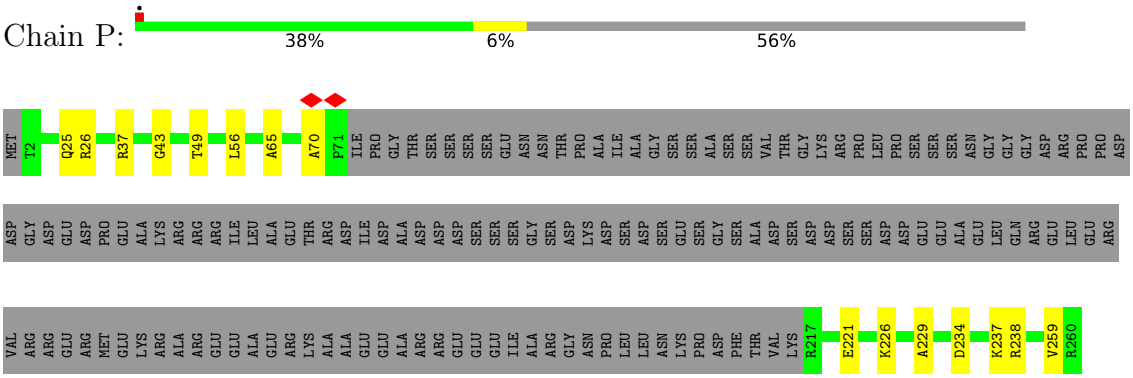
V72 L73 T74 M80 Y81 I82 K90 V101 N105 R106 E107 M108 A125 Y134 R143 ARG GLU GLU TYR GLU VAL VAL ASP LYS LYS GLY GLU GLU GLU ASP GLY ASP GLU TYR GLU GLU VAL GLU VAL THR ASP GLU GLU GLU GLU VAL ILE GLU SER GLY THR VAL LEU

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

K242 P254 I255 S272 A273 V282 R286 V409 I418 K544 LEU TRP ASP

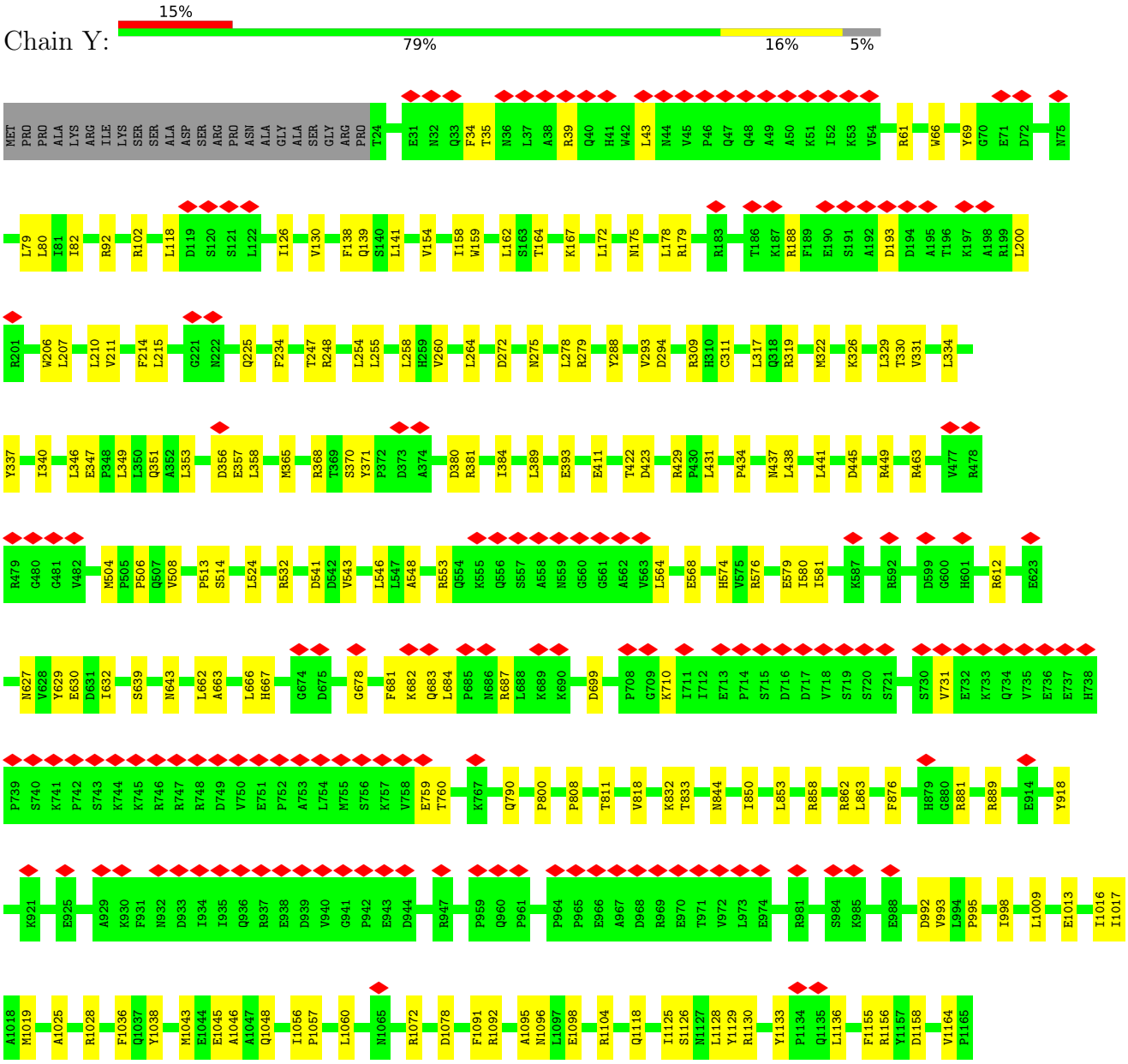
- Molecule 23: Putative pre-mRNA splicing protein

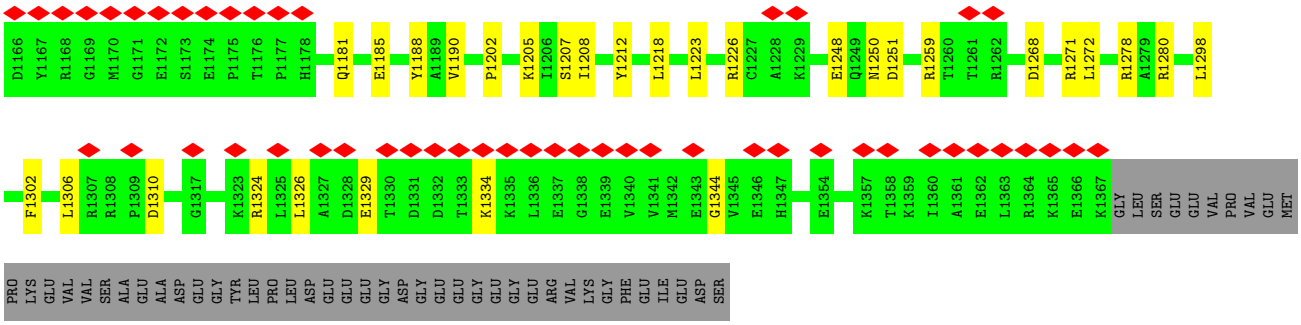
Chain P:



- Molecule 24: Pre-mRNA-splicing factor

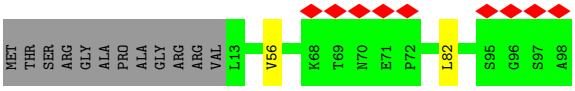
Chain Y:





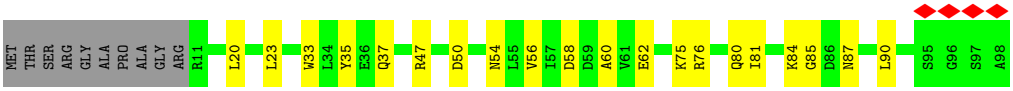
• Molecule 25: Small nuclear ribonucleoprotein E

Chain a:



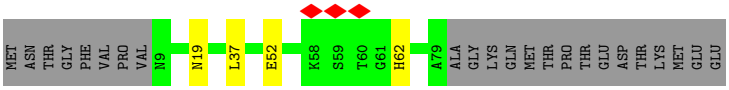
• Molecule 25: Small nuclear ribonucleoprotein E

Chain j:



• Molecule 26: Sm protein F

Chain b:

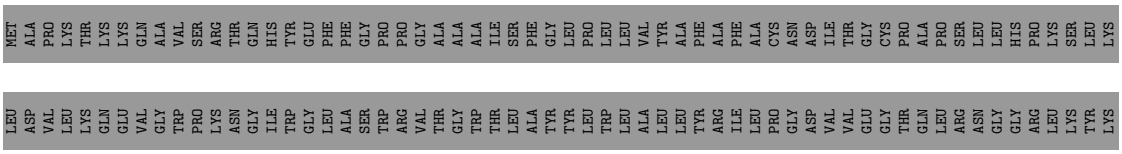


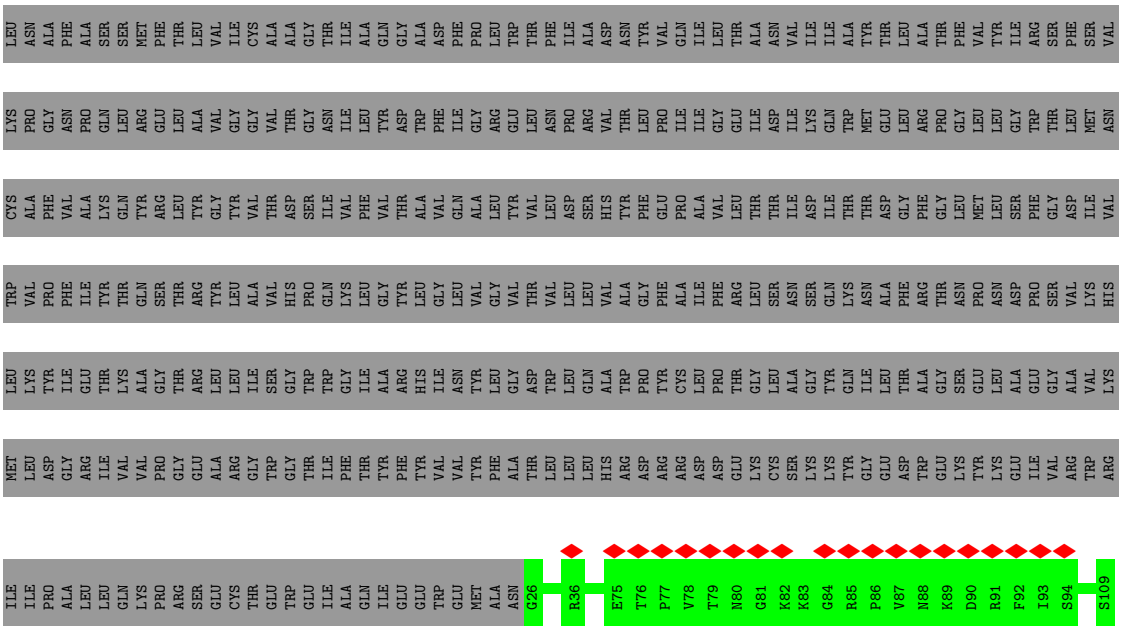
• Molecule 26: Sm protein F

Chain l:

• Molecule 27: Delta(14)-sterol reductase

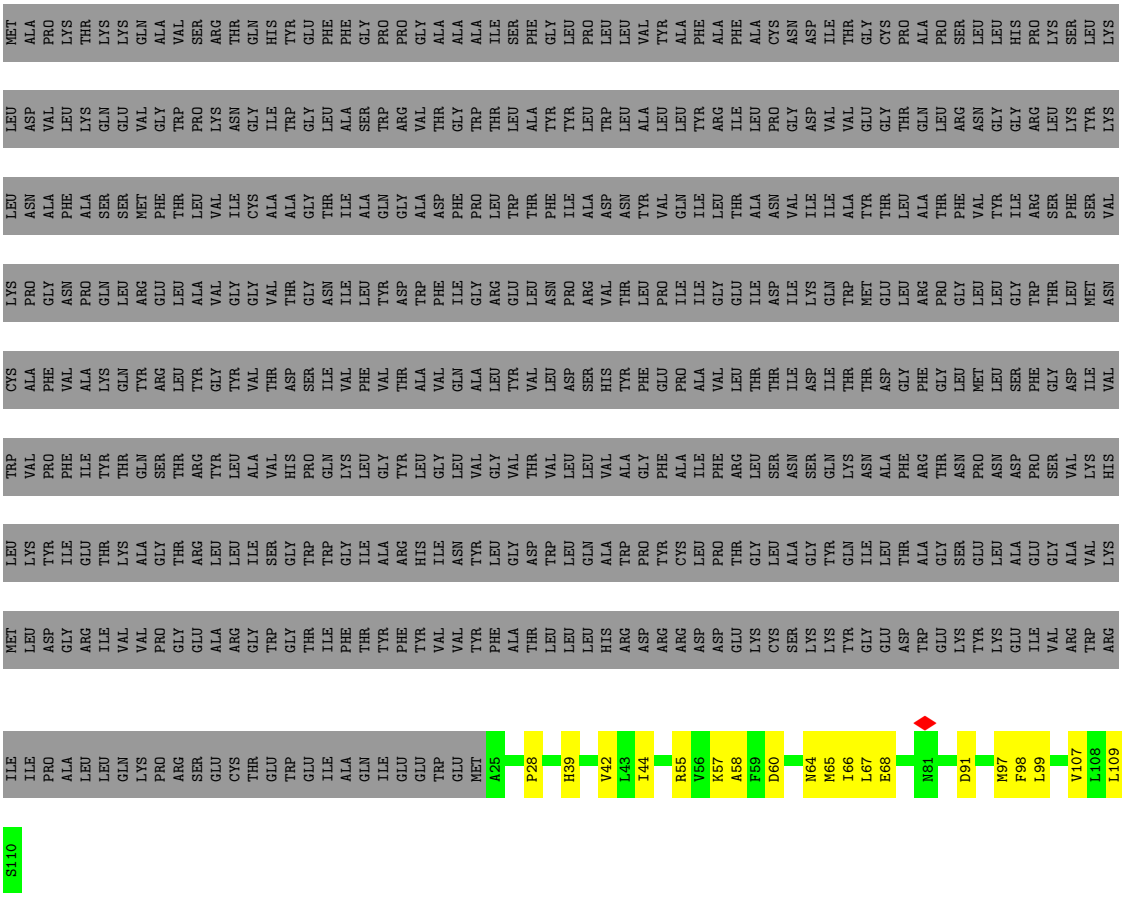
Chain c:





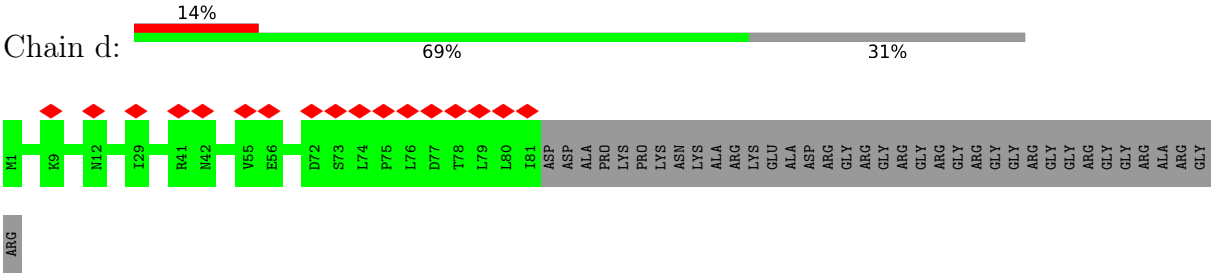
• Molecule 27: Delta(14)-sterol reductase

Chain m: 11% • 85%



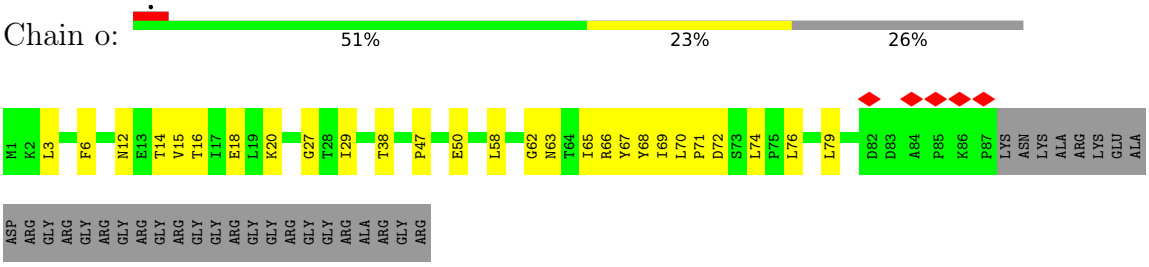
• Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain d:



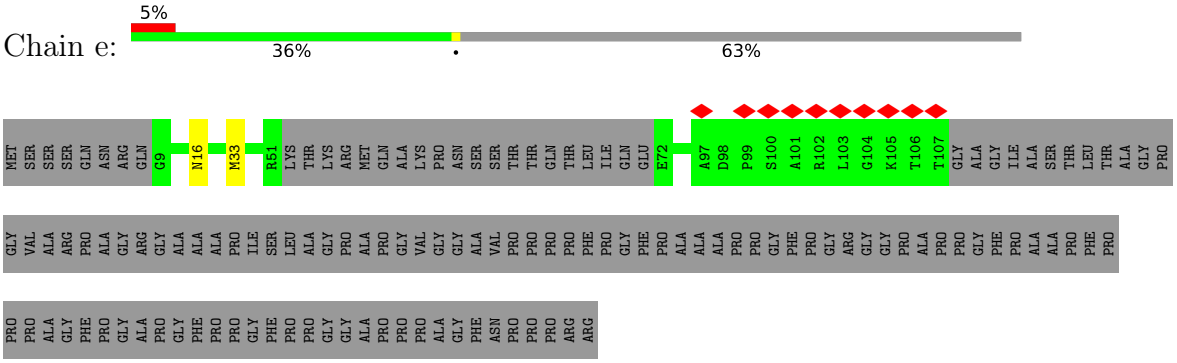
• Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain o:



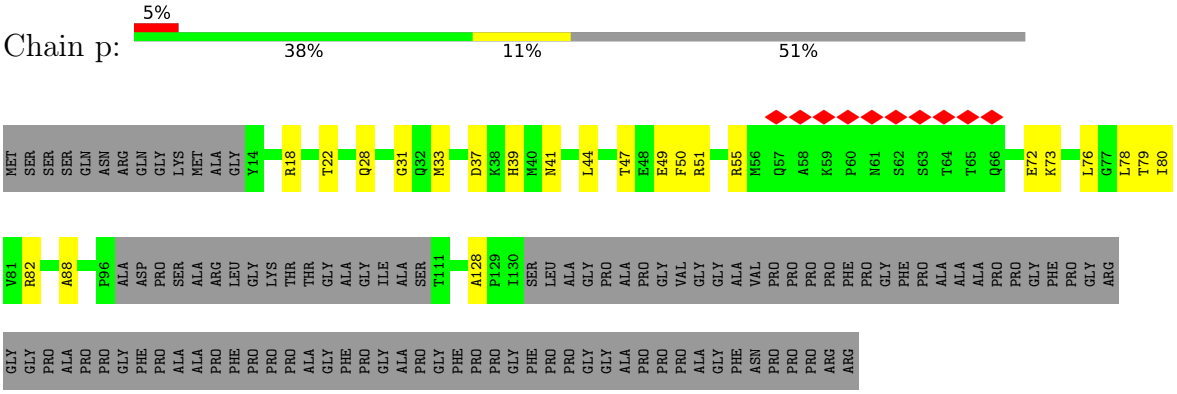
• Molecule 29: Sm protein B

Chain e:



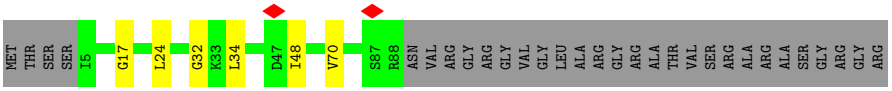
• Molecule 29: Sm protein B

Chain p:



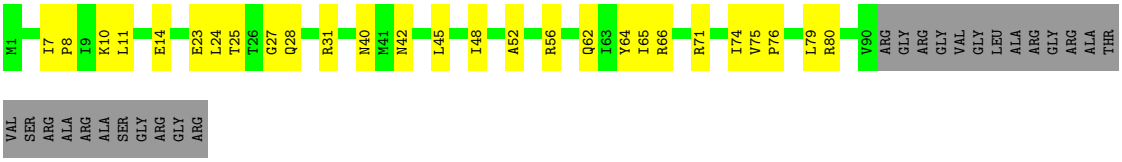
• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain f:



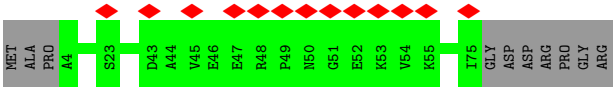
• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain u:



• Molecule 31: Small nuclear ribonucleoprotein G

Chain g:

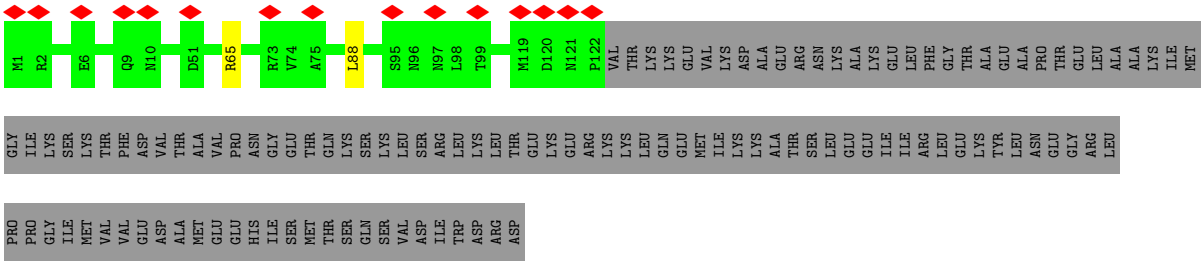


• Molecule 31: Small nuclear ribonucleoprotein G

Chain k:

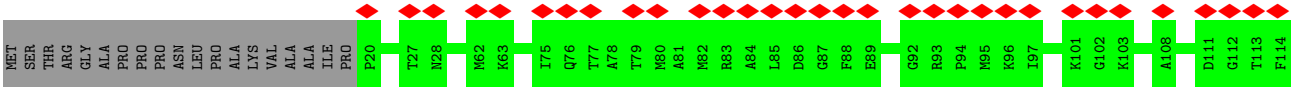
• Molecule 32: U2 small nuclear ribonucleoprotein A'

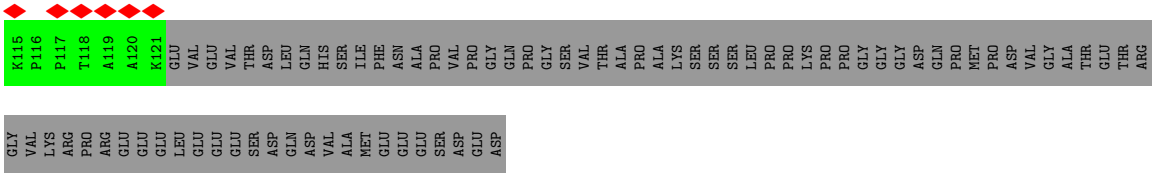
Chain h:



• Molecule 33: U2 small nuclear ribonucleoprotein B'-like protein

Chain i:



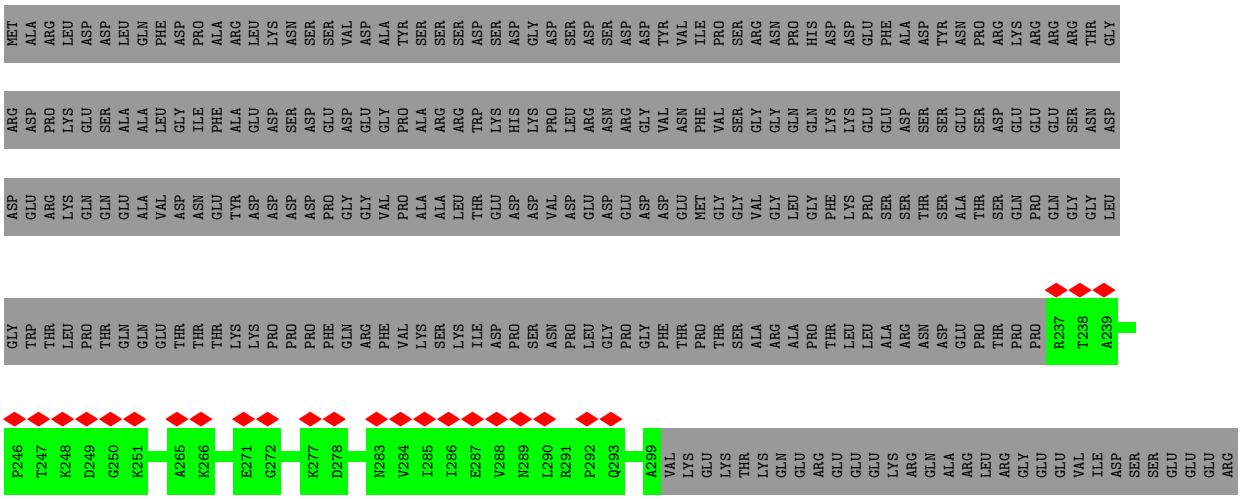


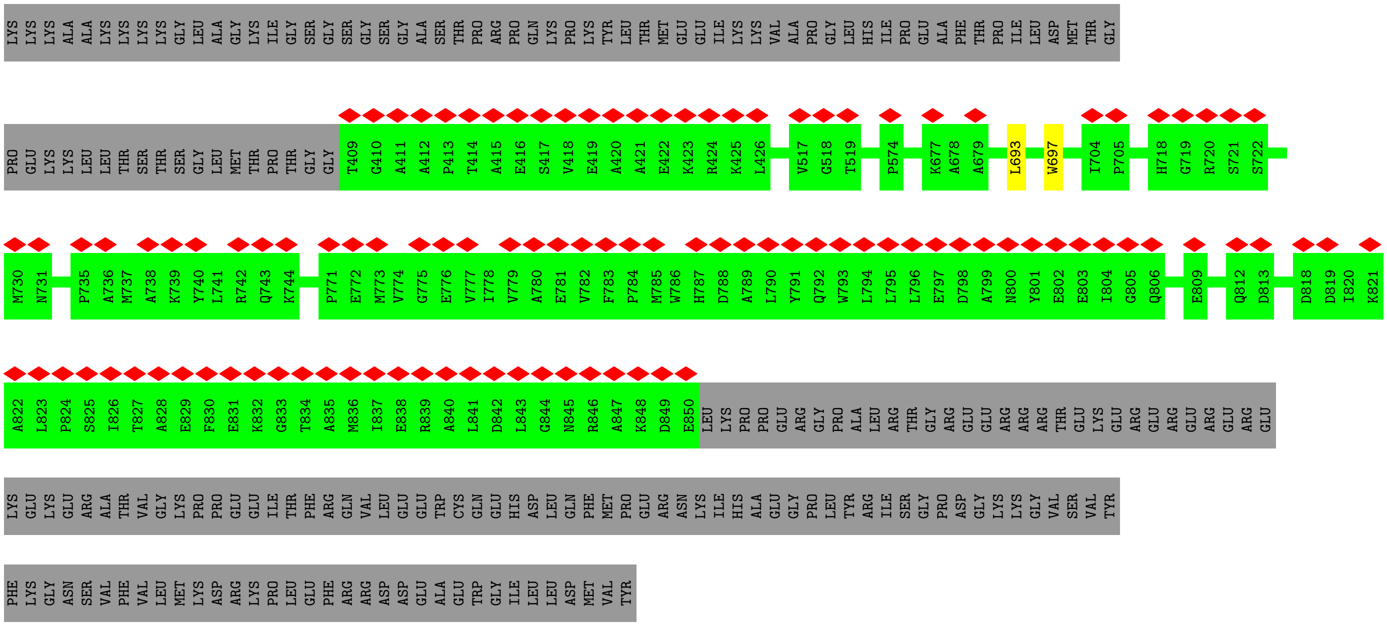
• Molecule 34: Nineteen complex-related protein 2-domain-containing protein

Chain CY:

• Molecule 35: G-patch domain-containing protein

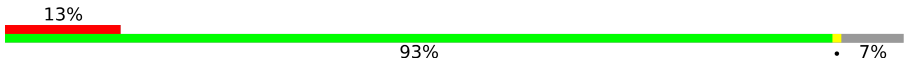
Chain Cb:

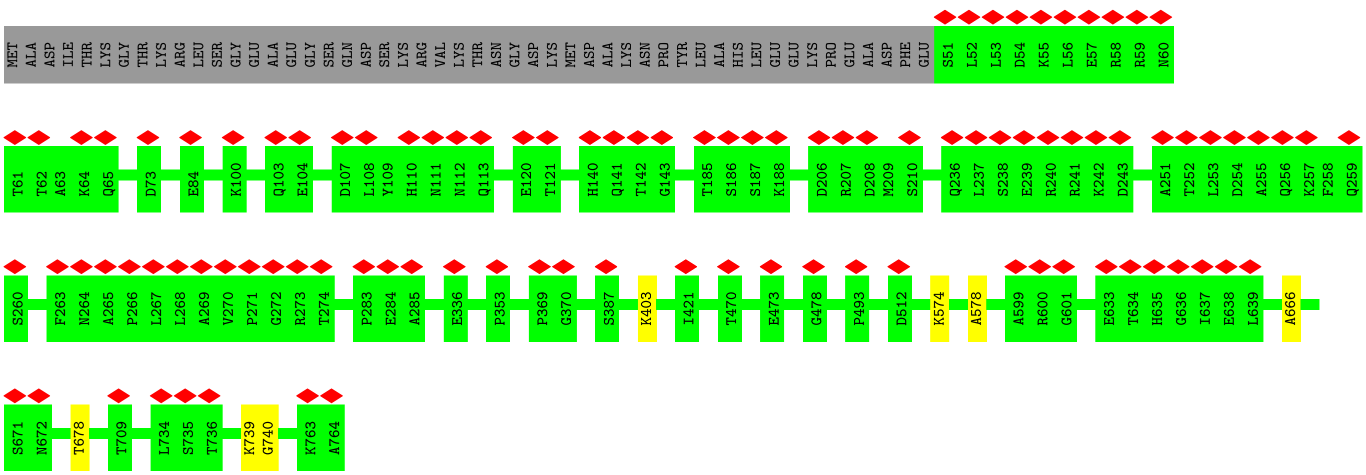




• Molecule 36: RNA helicase

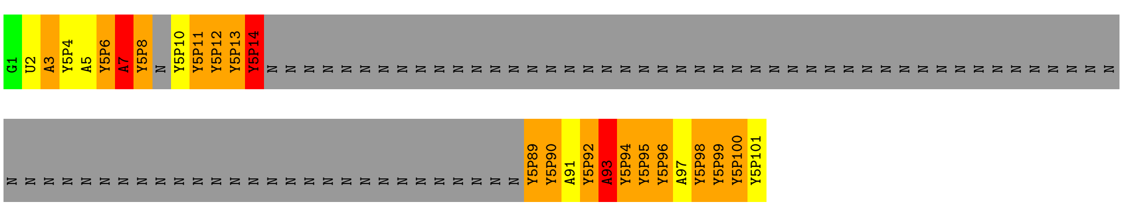
Chain Cc:





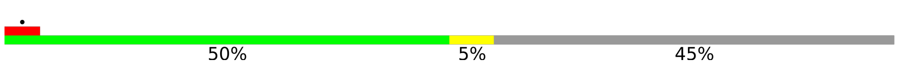
• Molecule 37: Unknown mRNA

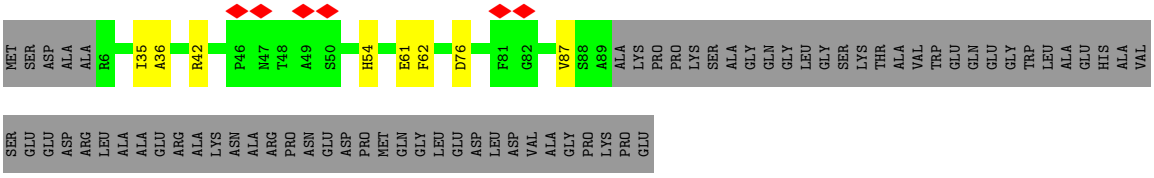
Chain 7:



• Molecule 38: Putative cyclophilin protein

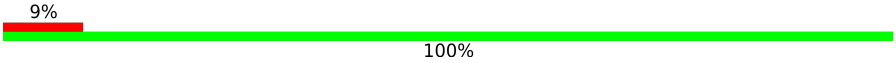
Chain Ci:

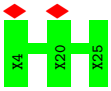




- Molecule 39: Unknown protein

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77668	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.259	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	447.36, 447.36, 447.36	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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: IHP, P5P, ZN, MG, GTP, M7M, Y5P, SEP

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	2	0.26	0/2471	0.36	0/3832
2	5	0.39	0/2612	0.44	0/4059
3	6	0.48	0/2338	0.54	0/3639
4	A	0.39	0/16969	0.57	3/23006 (0.0%)
5	B	0.35	0/2099	0.53	0/2806
6	C	0.32	0/7464	0.50	0/10117
7	D	0.25	0/793	0.62	0/1051
8	E	0.31	0/2428	0.61	2/3295 (0.1%)
9	F	0.27	0/891	0.61	0/1201
10	I	0.24	0/6282	0.51	1/8491 (0.0%)
11	J	0.34	0/5301	0.50	0/7149
12	L	0.30	0/5120	0.53	0/6882
13	K	0.20	0/1833	0.46	0/2493
14	q	0.19	0/1128	0.49	0/1533
14	r	0.18	0/1151	0.42	0/1566
14	s	0.16	0/1133	0.37	0/1540
14	t	0.16	0/1141	0.41	0/1552
15	N	0.55	0/1227	0.79	3/1655 (0.2%)
16	S	0.28	0/1235	0.53	0/1671
17	T	0.54	0/2635	0.79	0/3582
18	U	0.27	0/2883	0.51	0/3895
19	M	0.31	0/2006	0.60	1/2703 (0.0%)
20	0	0.36	0/2278	0.57	0/3081
21	R	0.41	0/2724	0.60	2/3675 (0.1%)
22	W	0.24	0/2237	0.50	1/3068 (0.0%)
23	P	0.38	0/945	0.58	0/1264
24	Y	0.13	0/11057	0.33	0/14995
25	a	0.11	0/425	0.31	0/589
25	j	0.16	0/716	0.47	0/969
26	b	0.12	0/350	0.35	0/486
26	l	0.20	0/661	0.53	0/898
27	c	0.10	0/415	0.31	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	m	0.18	0/687	0.50	0/922
28	d	0.12	0/400	0.31	0/556
28	o	0.25	0/691	0.56	0/940
29	e	0.12	0/386	0.34	0/533
29	p	0.23	0/799	0.62	0/1079
30	f	0.10	0/413	0.30	0/573
30	u	0.25	0/726	0.65	0/979
31	g	0.12	0/353	0.37	0/489
31	k	0.21	0/584	0.66	0/787
32	h	0.11	0/604	0.34	0/841
33	i	0.08	0/503	0.24	0/699
34	CY	0.11	0/443	0.30	0/612
35	Cb	0.10	0/2494	0.27	0/3471
36	Cc	0.10	0/3540	0.28	0/4935
37	7	0.55	0/71	0.95	0/106
38	Ci	0.09	0/414	0.26	0/575
All	All	0.31	0/106056	0.51	13/145415 (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
4	A	0	1
8	E	0	1
10	I	0	1
12	L	0	2
16	S	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	N	144	CYS	CB-CA-C	-8.33	95.08	109.07
4	A	833	VAL	N-CA-C	-7.05	107.01	113.71
22	W	108	MET	CA-CB-CG	6.49	127.08	114.10
15	N	108	ILE	N-CA-C	-6.46	106.69	112.90
8	E	92	ASP	CA-C-N	5.99	132.99	121.54

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1437	ARG	Peptide
8	E	92	ASP	Peptide
10	I	416	GLY	Peptide
12	L	505	LEU	Peptide
12	L	539	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2224	0	1130	15	0
2	5	2343	0	1190	14	0
3	6	2090	0	1058	18	0
4	A	16540	0	16528	217	0
5	B	2071	0	2054	23	0
6	C	7301	0	7338	94	0
7	D	786	0	782	15	0
8	E	2379	0	2343	46	0
9	F	879	0	899	15	0
10	I	6135	0	6049	106	0
11	J	5176	0	5069	56	0
12	L	5052	0	5108	62	0
13	K	1797	0	1783	28	0
14	q	1110	0	1136	27	0
14	r	1132	0	1158	30	0
14	s	1115	0	1141	18	0
14	t	1122	0	1148	26	0
15	N	1200	0	1184	11	0
16	S	1209	0	1207	23	0
17	T	2565	0	2516	33	0
18	U	2821	0	2773	51	0
19	M	1964	0	1969	37	0
20	0	2224	0	2131	38	0
21	R	2686	0	2686	39	0
22	W	2224	0	1400	18	0
23	P	925	0	918	12	0
24	Y	10819	0	10842	137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	a	426	0	182	1	0
25	j	704	0	743	13	0
26	b	351	0	152	3	0
26	l	649	0	652	12	0
27	c	416	0	178	0	0
27	m	678	0	723	14	0
28	d	401	0	175	0	0
28	o	679	0	711	20	0
29	e	388	0	180	2	0
29	p	788	0	816	20	0
30	f	414	0	182	4	0
30	u	716	0	738	22	0
31	g	354	0	152	0	0
31	k	577	0	611	12	0
32	h	605	0	265	1	0
33	i	504	0	238	0	0
34	CY	444	0	199	0	0
35	Cb	2496	0	1148	1	0
36	Cc	3541	0	1590	4	0
37	7	494	0	301	23	0
38	Ci	415	0	199	4	0
39	H	110	0	24	0	0
40	B	30	0	19	0	0
41	C	1	0	0	0	0
42	C	32	0	12	0	0
43	J	36	0	6	4	0
44	M	2	0	0	0	0
44	N	3	0	0	0	0
44	U	1	0	0	0	0
All	All	104144	0	93736	1161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1161 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:o:14:THR:HA	28:o:27:GLY:O	1.23	1.29
19:M:297:GLY:HA2	19:M:308:ILE:O	1.37	1.18
19:M:99:ASP:O	19:M:103:GLU:HA	1.64	0.97
4:A:1532:LEU:O	4:A:1536:GLU:HB2	1.67	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:o:14:THR:CA	28:o:27:GLY:O	2.19	0.85

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	2004/2463 (81%)	1911 (95%)	90 (4%)	3 (0%)	48	77
5	B	256/326 (78%)	249 (97%)	6 (2%)	1 (0%)	30	60
6	C	920/1011 (91%)	889 (97%)	29 (3%)	2 (0%)	43	72
7	D	91/325 (28%)	90 (99%)	1 (1%)	0	100	100
8	E	308/352 (88%)	285 (92%)	23 (8%)	0	100	100
9	F	108/233 (46%)	104 (96%)	3 (3%)	1 (1%)	14	41
10	I	736/839 (88%)	705 (96%)	29 (4%)	2 (0%)	36	66
11	J	604/687 (88%)	592 (98%)	12 (2%)	0	100	100
12	L	629/768 (82%)	602 (96%)	26 (4%)	1 (0%)	43	72
13	K	229/231 (99%)	224 (98%)	5 (2%)	0	100	100
14	q	137/480 (28%)	135 (98%)	2 (2%)	0	100	100
14	r	141/480 (29%)	140 (99%)	1 (1%)	0	100	100
14	s	138/480 (29%)	137 (99%)	1 (1%)	0	100	100
14	t	139/480 (29%)	136 (98%)	3 (2%)	0	100	100
15	N	146/148 (99%)	136 (93%)	8 (6%)	2 (1%)	9	30
16	S	155/167 (93%)	148 (96%)	7 (4%)	0	100	100
17	T	326/496 (66%)	311 (95%)	14 (4%)	1 (0%)	36	66
18	U	346/757 (46%)	321 (93%)	23 (7%)	2 (1%)	21	51
19	M	242/395 (61%)	225 (93%)	17 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	0	274/408 (67%)	261 (95%)	13 (5%)	0	100	100
21	R	334/578 (58%)	312 (93%)	21 (6%)	1 (0%)	36	66
22	W	391/547 (72%)	376 (96%)	14 (4%)	1 (0%)	36	66
23	P	110/260 (42%)	102 (93%)	8 (7%)	0	100	100
24	Y	1342/1416 (95%)	1315 (98%)	27 (2%)	0	100	100
25	a	84/98 (86%)	83 (99%)	1 (1%)	0	100	100
25	j	86/98 (88%)	84 (98%)	2 (2%)	0	100	100
26	b	69/94 (73%)	69 (100%)	0	0	100	100
26	l	79/94 (84%)	77 (98%)	2 (2%)	0	100	100
27	c	82/592 (14%)	80 (98%)	2 (2%)	0	100	100
27	m	84/592 (14%)	80 (95%)	4 (5%)	0	100	100
28	d	79/118 (67%)	76 (96%)	3 (4%)	0	100	100
28	o	85/118 (72%)	78 (92%)	7 (8%)	0	100	100
29	e	75/211 (36%)	73 (97%)	2 (3%)	0	100	100
29	p	99/211 (47%)	92 (93%)	7 (7%)	0	100	100
30	f	82/114 (72%)	79 (96%)	3 (4%)	0	100	100
30	u	88/114 (77%)	83 (94%)	5 (6%)	0	100	100
31	g	70/82 (85%)	69 (99%)	1 (1%)	0	100	100
31	k	71/82 (87%)	68 (96%)	3 (4%)	0	100	100
32	h	120/242 (50%)	117 (98%)	3 (2%)	0	100	100
33	i	100/201 (50%)	100 (100%)	0	0	100	100
34	CY	89/510 (18%)	88 (99%)	1 (1%)	0	100	100
35	Cb	501/975 (51%)	495 (99%)	6 (1%)	0	100	100
36	Cc	712/764 (93%)	694 (98%)	18 (2%)	0	100	100
38	Ci	82/153 (54%)	82 (100%)	0	0	100	100
All	All	12843/19790 (65%)	12373 (96%)	453 (4%)	17 (0%)	49	77

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	494	LYS
4	A	1219	ILE
5	B	111	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	C	840	VAL
9	F	98	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1813/2212 (82%)	1809 (100%)	4 (0%)	87	96
5	B	208/270 (77%)	208 (100%)	0	100	100
6	C	809/884 (92%)	808 (100%)	1 (0%)	88	97
7	D	80/276 (29%)	80 (100%)	0	100	100
8	E	254/287 (88%)	254 (100%)	0	100	100
9	F	92/179 (51%)	92 (100%)	0	100	100
10	I	646/729 (89%)	646 (100%)	0	100	100
11	J	525/592 (89%)	525 (100%)	0	100	100
12	L	520/635 (82%)	518 (100%)	2 (0%)	84	94
13	K	186/186 (100%)	186 (100%)	0	100	100
14	q	122/385 (32%)	122 (100%)	0	100	100
14	r	123/385 (32%)	123 (100%)	0	100	100
14	s	122/385 (32%)	122 (100%)	0	100	100
14	t	123/385 (32%)	123 (100%)	0	100	100
15	N	131/131 (100%)	129 (98%)	2 (2%)	57	84
16	S	126/135 (93%)	126 (100%)	0	100	100
17	T	276/408 (68%)	271 (98%)	5 (2%)	51	82
18	U	294/649 (45%)	293 (100%)	1 (0%)	86	95
19	M	210/293 (72%)	210 (100%)	0	100	100
20	0	227/335 (68%)	219 (96%)	8 (4%)	32	67
21	R	278/476 (58%)	277 (100%)	1 (0%)	84	94
22	W	73/459 (16%)	73 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	P	91/213 (43%)	91 (100%)	0	100	100
24	Y	1173/1231 (95%)	1173 (100%)	0	100	100
25	j	79/85 (93%)	79 (100%)	0	100	100
26	l	72/84 (86%)	72 (100%)	0	100	100
27	m	77/497 (16%)	77 (100%)	0	100	100
28	o	78/95 (82%)	78 (100%)	0	100	100
29	p	84/152 (55%)	84 (100%)	0	100	100
30	u	80/94 (85%)	80 (100%)	0	100	100
31	k	64/71 (90%)	64 (100%)	0	100	100
All	All	9036/13198 (68%)	9012 (100%)	24 (0%)	84	95

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	U	468	ARG
20	0	89	LYS
20	0	88	ASP
20	0	91	LEU
12	L	210	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	127	GLN
24	Y	653	GLN
17	T	220	GLN
20	0	258	GLN
26	l	50	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	101/193 (52%)	18 (17%)	2 (1%)
2	5	109/116 (93%)	21 (19%)	1 (0%)
3	6	97/101 (96%)	36 (37%)	2 (2%)
37	7	23/101 (22%)	7 (30%)	0
All	All	330/511 (64%)	82 (24%)	5 (1%)

5 of 82 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	U
1	2	14	U
1	2	16	U
1	2	17	U
1	2	18	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	13	C
1	2	23	A
2	5	70	A
3	6	15	U
3	6	38	A

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

25 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	$\#\|Z\| > 2$
37	Y5P	7	90	37	14,19,20	4.58	2 (14%)	18,26,29	1.34	2 (11%)
21	SEP	R	242	21	8,9,10	0.70	0	7,12,14	1.24	1 (14%)
37	Y5P	7	12	37	14,19,20	4.20	2 (14%)	18,26,29	1.05	1 (5%)
37	Y5P	7	10	37	14,19,20	4.22	2 (14%)	18,26,29	1.03	1 (5%)
37	P5P	7	5	37	20,23,24	1.00	2 (10%)	27,33,36	1.87	3 (11%)
37	P5P	7	3	3,37	20,23,24	0.43	0	27,33,36	0.70	1 (3%)
37	Y5P	7	98	37	14,19,20	4.15	2 (14%)	18,26,29	1.00	1 (5%)
21	SEP	R	234	21	8,9,10	1.42	1 (12%)	7,12,14	0.84	0
37	Y5P	7	100	37	14,19,20	4.59	2 (14%)	18,26,29	1.37	2 (11%)
37	Y5P	7	89	37	14,19,20	4.26	2 (14%)	18,26,29	0.99	1 (5%)
37	Y5P	7	14	37	14,19,20	4.18	2 (14%)	18,26,29	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	Y5P	7	96	37	14,19,20	4.17	2 (14%)	18,26,29	1.05	1 (5%)
37	Y5P	7	101	37	14,19,20	4.23	2 (14%)	18,26,29	1.05	1 (5%)
37	Y5P	7	4	37	14,19,20	4.24	2 (14%)	18,26,29	1.15	1 (5%)
37	Y5P	7	95	37	14,19,20	4.19	2 (14%)	18,26,29	1.02	1 (5%)
37	Y5P	7	99	37	14,19,20	4.61	2 (14%)	18,26,29	1.38	2 (11%)
37	P5P	7	91	1,37	20,23,24	0.46	0	27,33,36	0.68	1 (3%)
37	P5P	7	7	3,37	20,23,24	0.90	1 (5%)	27,33,36	1.89	4 (14%)
37	P5P	7	93	1,37	20,23,24	0.48	0	27,33,36	0.70	1 (3%)
37	Y5P	7	94	37	14,19,20	4.58	2 (14%)	18,26,29	1.38	2 (11%)
37	Y5P	7	13	37	14,19,20	4.19	2 (14%)	18,26,29	1.03	1 (5%)
37	Y5P	7	6	37	14,19,20	4.16	2 (14%)	18,26,29	0.97	1 (5%)
37	Y5P	7	8	37	14,19,20	4.55	2 (14%)	18,26,29	1.37	2 (11%)
37	Y5P	7	92	37	14,19,20	4.25	2 (14%)	18,26,29	0.98	1 (5%)
37	Y5P	7	11	37	14,19,20	4.23	2 (14%)	18,26,29	1.02	1 (5%)

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
37	Y5P	7	90	37	-	2/7/33/34	0/2/2/2
21	SEP	R	242	21	-	3/6/8/10	-
37	Y5P	7	12	37	-	4/7/33/34	0/2/2/2
37	Y5P	7	10	37	-	3/7/33/34	0/2/2/2
37	P5P	7	5	37	-	0/7/25/26	0/3/3/3
37	P5P	7	3	3,37	-	2/7/25/26	0/3/3/3
37	Y5P	7	98	37	-	1/7/33/34	0/2/2/2
21	SEP	R	234	21	-	2/6/8/10	-
37	Y5P	7	100	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	89	37	-	3/7/33/34	0/2/2/2
37	Y5P	7	14	37	-	2/7/33/34	0/2/2/2
37	Y5P	7	96	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	101	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	4	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	95	37	-	4/7/33/34	0/2/2/2
37	Y5P	7	99	37	-	1/7/33/34	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	P5P	7	91	1,37	-	1/7/25/26	0/3/3/3
37	P5P	7	7	3,37	-	2/7/25/26	0/3/3/3
37	P5P	7	93	1,37	-	1/7/25/26	0/3/3/3
37	Y5P	7	94	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	13	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	6	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	8	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	92	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	11	37	-	4/7/33/34	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	7	99	Y5P	C4-N3	-13.78	1.33	1.46
37	7	94	Y5P	C4-N3	-13.56	1.33	1.46
37	7	92	Y5P	C2-N3	13.47	1.37	1.27
37	7	89	Y5P	C2-N3	13.45	1.37	1.27
37	7	101	Y5P	C2-N3	13.45	1.37	1.27

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	7	P5P	C6-N1-C2	7.84	125.06	115.80
37	7	5	P5P	C6-N1-C2	7.75	124.94	115.80
37	7	94	Y5P	C5-C4-N3	4.92	122.08	114.15
37	7	99	Y5P	C5-C4-N3	4.91	122.06	114.15
37	7	100	Y5P	C5-C4-N3	4.88	122.02	114.15

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	R	234	SEP	N-CA-CB-OG
21	R	234	SEP	C-CA-CB-OG
21	R	242	SEP	C-CA-CB-OG
37	7	6	Y5P	O4'-C1'-N1-C2
37	7	11	Y5P	O4'-C1'-N1-C2

There are no ring outliers.

17 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	7	90	Y5P	1	0
37	7	12	Y5P	2	0
37	7	98	Y5P	1	0
21	R	234	SEP	1	0
37	7	100	Y5P	1	0
37	7	89	Y5P	2	0
37	7	14	Y5P	2	0
37	7	96	Y5P	1	0
37	7	95	Y5P	5	0
37	7	99	Y5P	1	0
37	7	7	P5P	2	0
37	7	93	P5P	1	0
37	7	94	Y5P	1	0
37	7	13	Y5P	3	0
37	7	6	Y5P	1	0
37	7	8	Y5P	2	0
37	7	92	Y5P	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
42	GTP	C	1102	41	33,34,34	0.99	2 (6%)	50,54,54	1.63	10 (20%)
40	M7M	B	401	-	28,32,33	3.94	16 (57%)	31,49,52	1.19	3 (9%)
43	IHP	J	1001	-	36,36,36	1.53	6 (16%)	60,60,60	1.13	6 (10%)

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
42	GTP	C	1102	41	-	6/22/38/38	0/3/3/3
40	M7M	B	401	-	-	2/17/47/48	0/3/3/3
43	IHP	J	1001	-	-	10/30/54/54	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B	401	M7M	CBY-CBS	-7.16	1.34	1.53
40	B	401	M7M	CBG-NBH	7.09	1.44	1.35
40	B	401	M7M	CBI-NBP	7.05	1.50	1.45
40	B	401	M7M	OBR-CBS	6.95	1.60	1.45
40	B	401	M7M	CBO-NBP	5.73	1.44	1.35

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	C	1102	GTP	C5-C4-N3	-4.87	120.64	128.39
42	C	1102	GTP	C2-N3-C4	4.44	119.94	112.30
43	J	1001	IHP	C5-C4-C3	-3.73	102.25	110.43
43	J	1001	IHP	O15-C5-C4	3.36	115.91	108.76
40	B	401	M7M	CBO-CBG-NBH	3.31	109.30	106.86

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	C	1102	GTP	C5'-O5'-PA-O3A
42	C	1102	GTP	C5'-O5'-PA-O1A
42	C	1102	GTP	C5'-O5'-PA-O2A
43	J	1001	IHP	C4-C5-O15-P5
42	C	1102	GTP	PA-O3A-PB-O1B

There are no ring outliers.

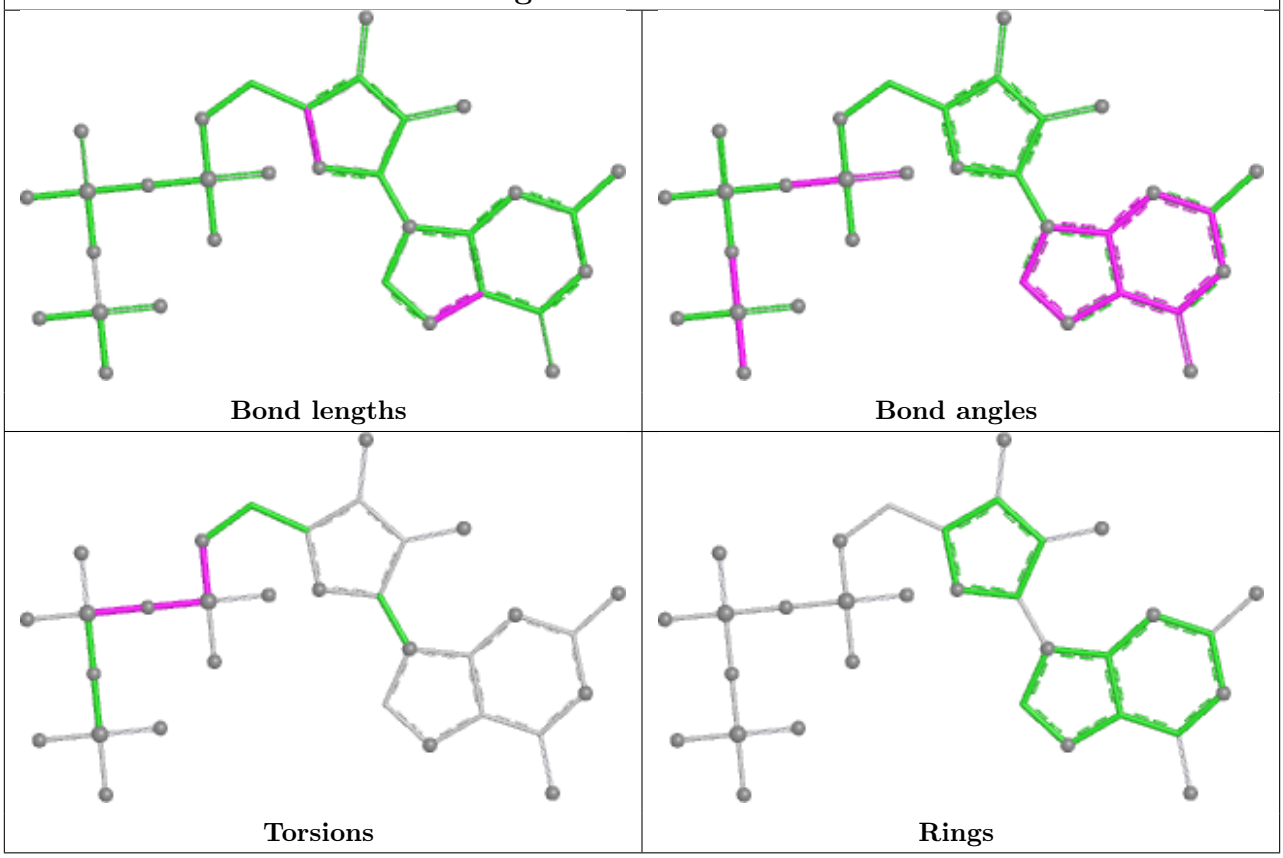
1 monomer is involved in 4 short contacts:

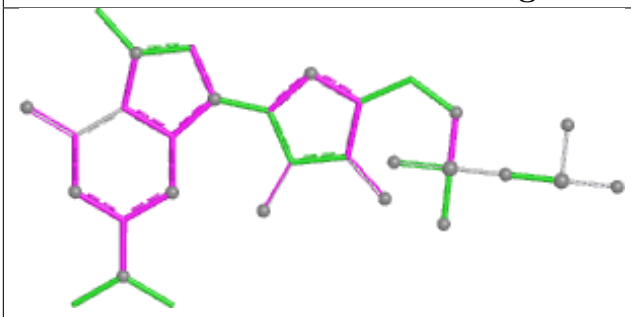
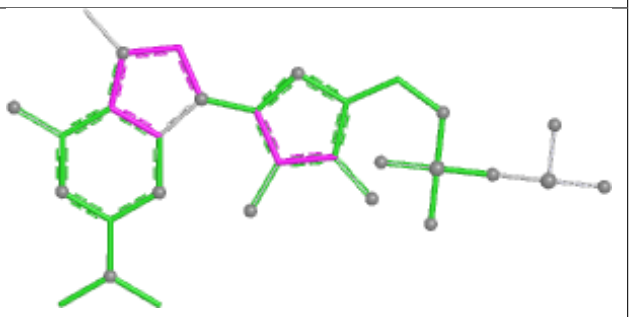
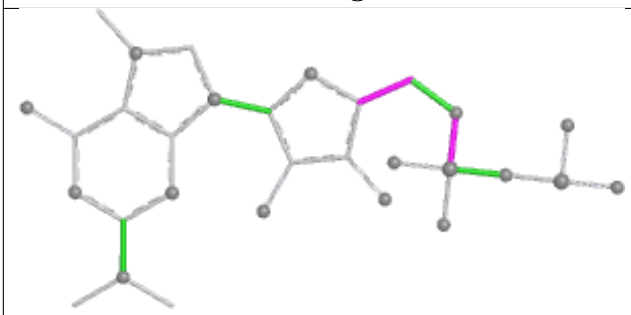
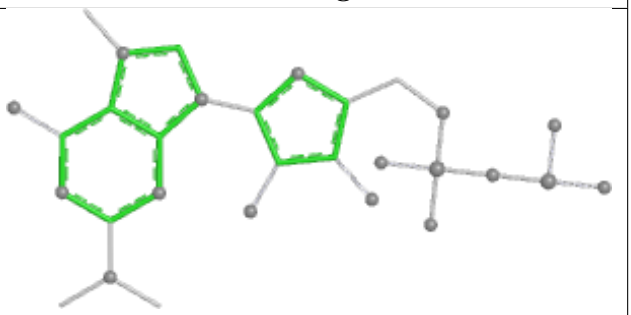
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	J	1001	IHP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

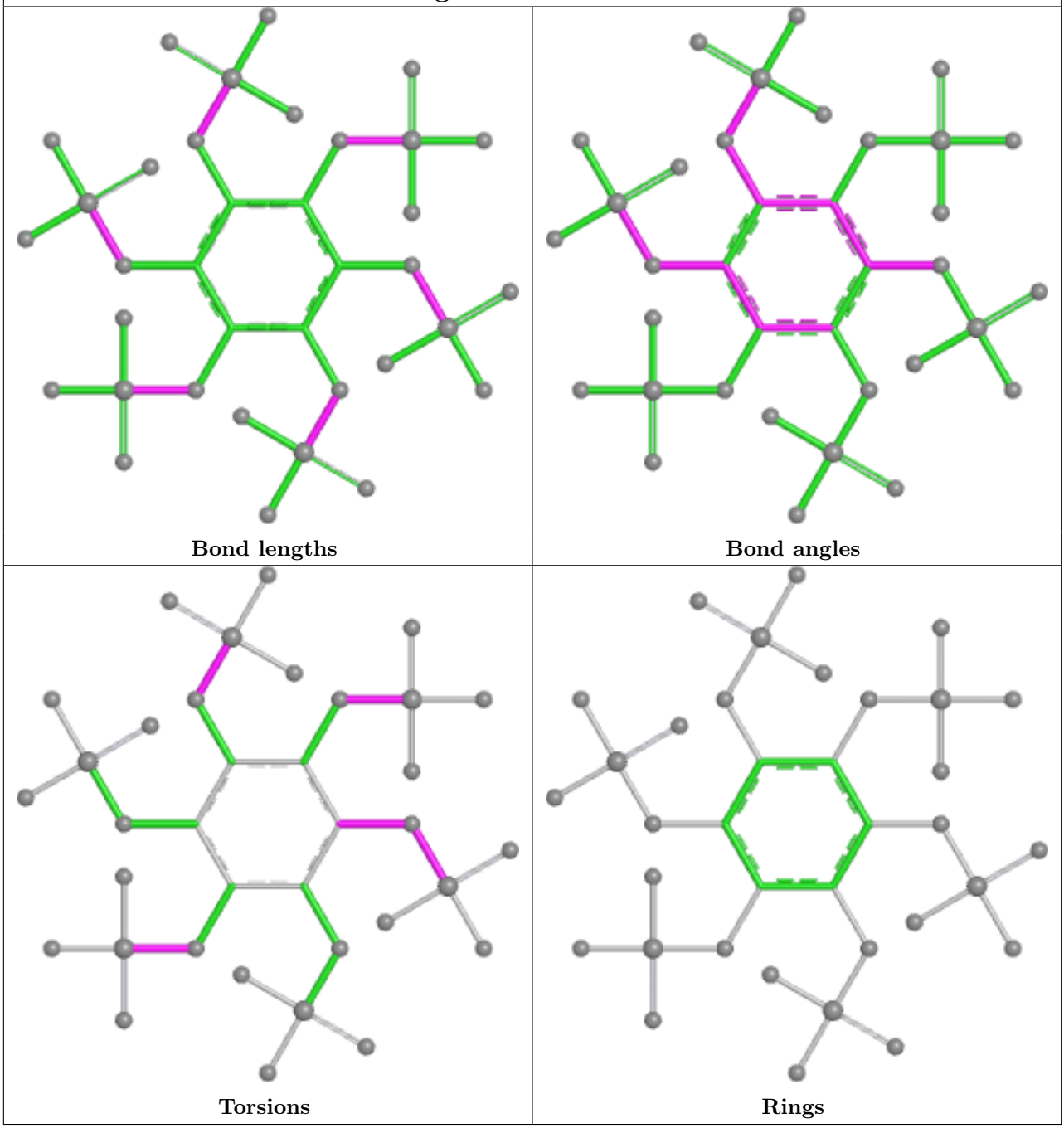
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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 C 1102



Ligand M7M B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IHP J 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

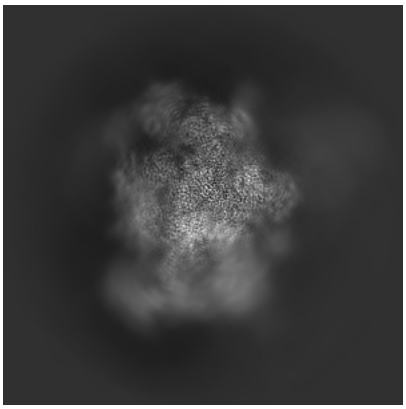
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-62841. These allow visual inspection of the internal detail of the map and identification of artifacts.

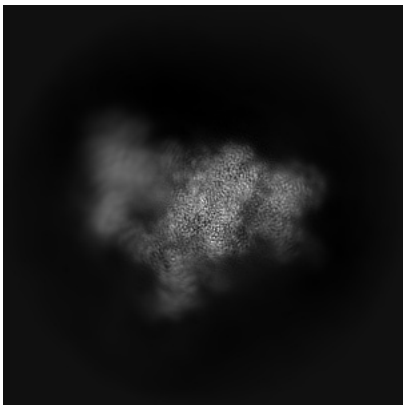
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

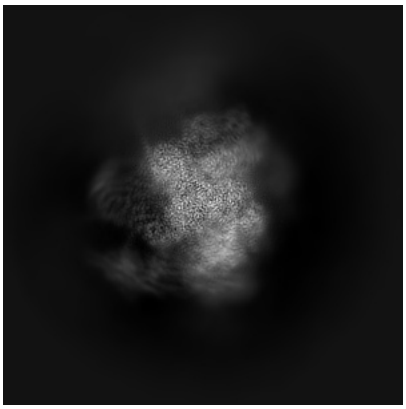
6.1.1 Primary map



X

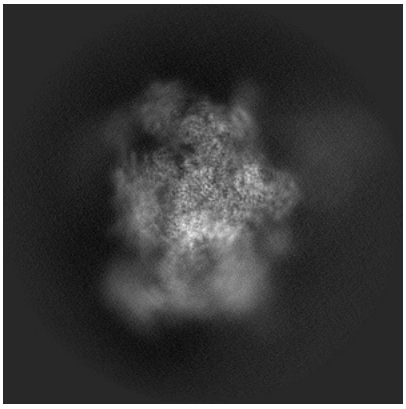


Y

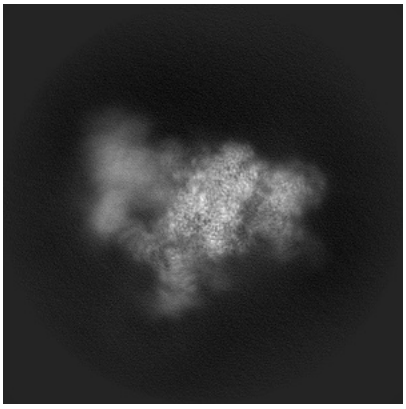


Z

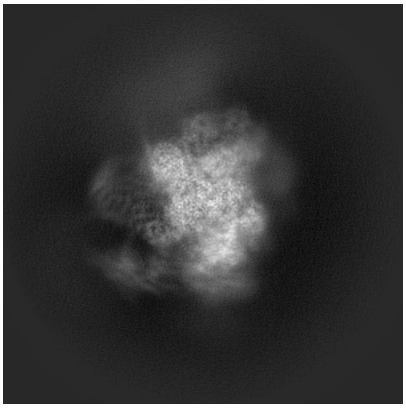
6.1.2 Raw map



X



Y

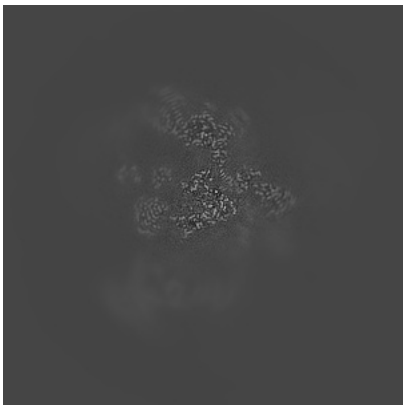


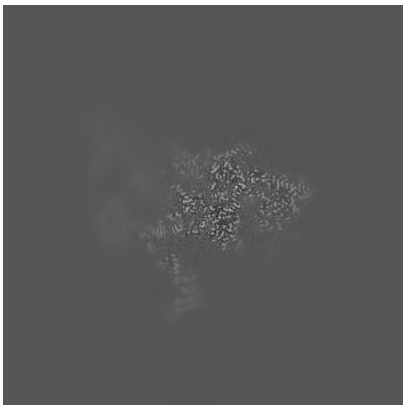
Z

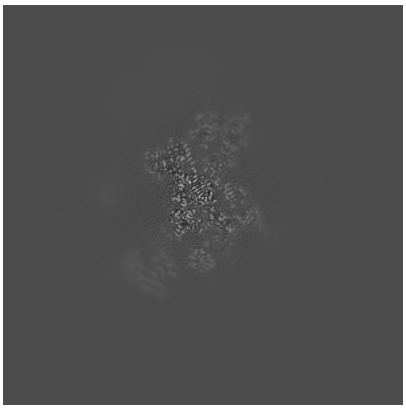
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

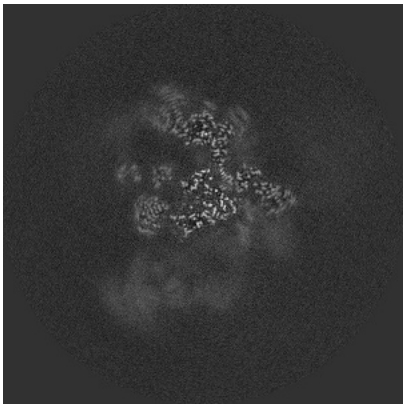
6.2.1 Primary map

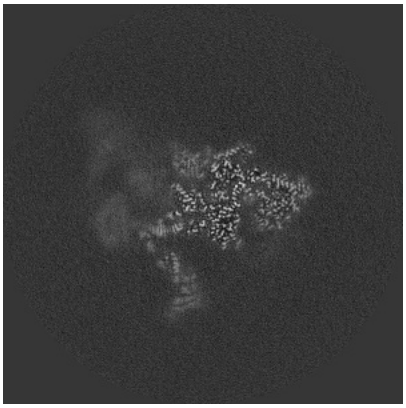

X Index: 240

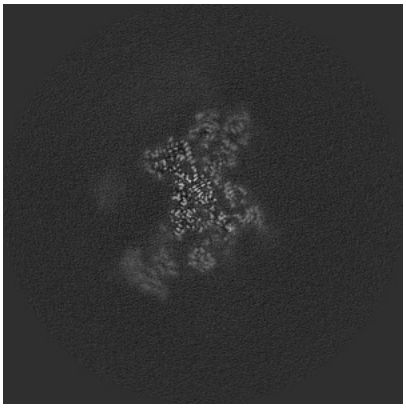

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

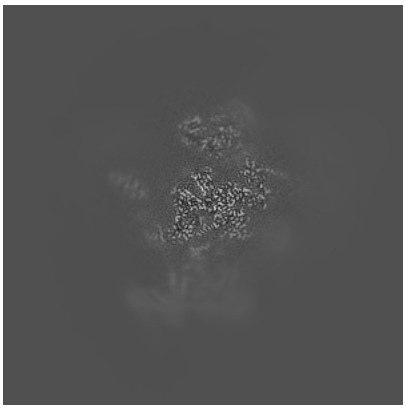

Y Index: 240


Z Index: 240

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

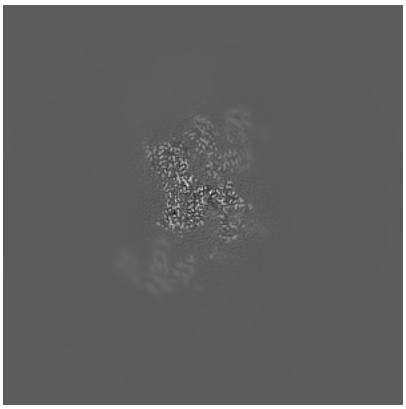
6.3 Largest variance slices (i)

6.3.1 Primary map



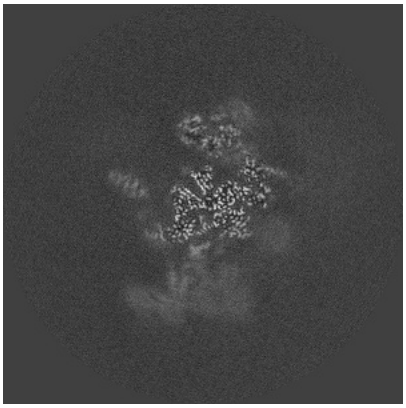
X Index: 215

Y Index: 249

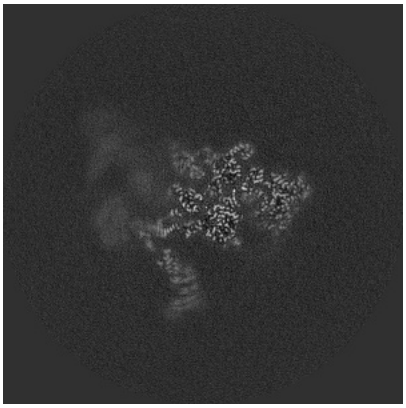


Z Index: 253

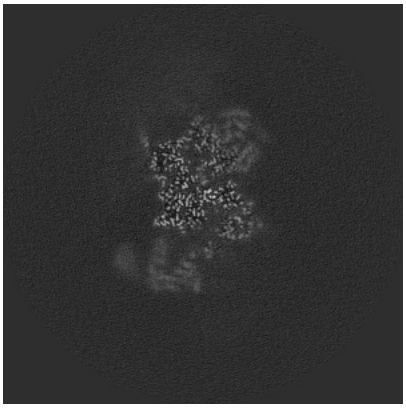
6.3.2 Raw map



X Index: 215



Y Index: 238

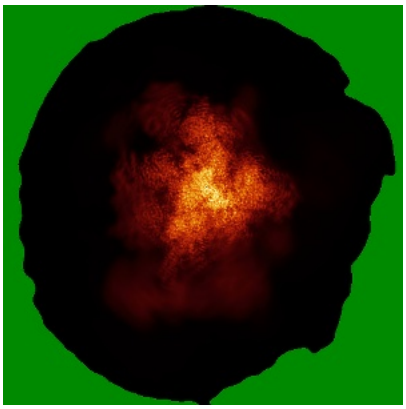


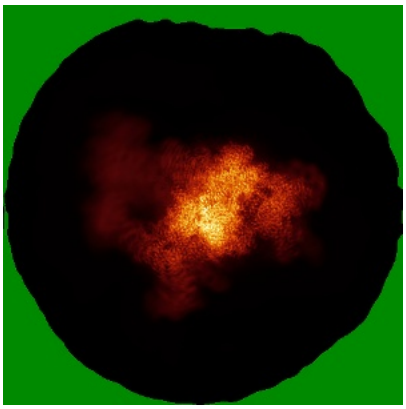
Z Index: 258

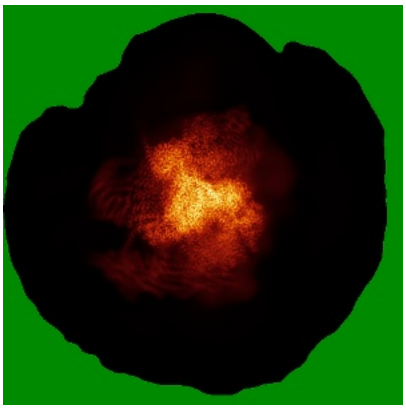
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

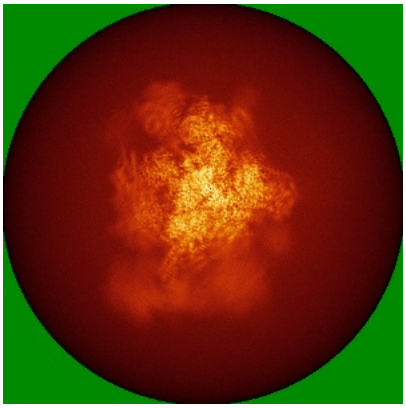
6.4.1 Primary map

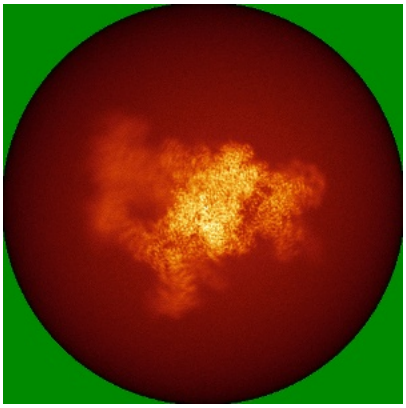

X

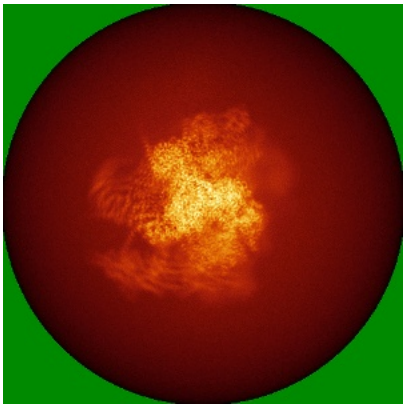

Y


Z

6.4.2 Raw map


X

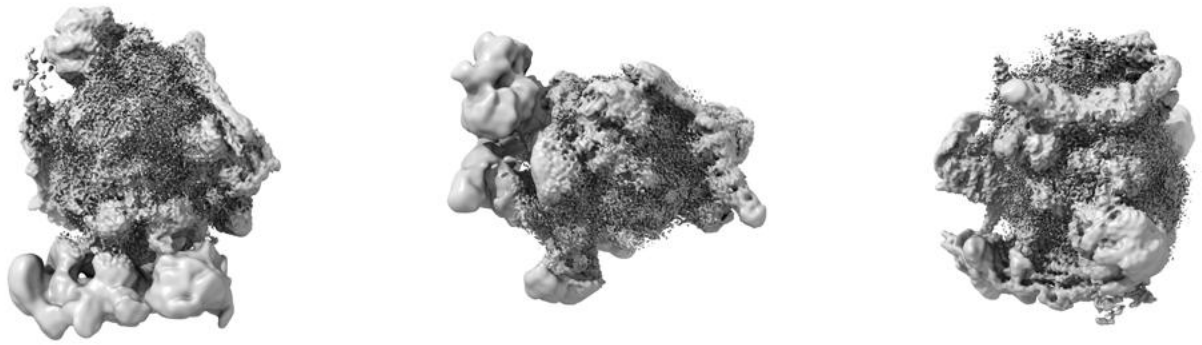

Y


Z

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

6.5 Orthogonal surface views (i)

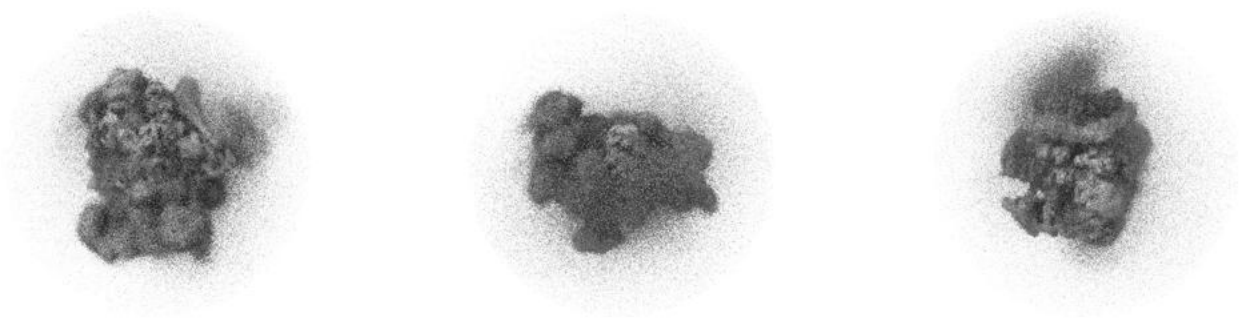
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

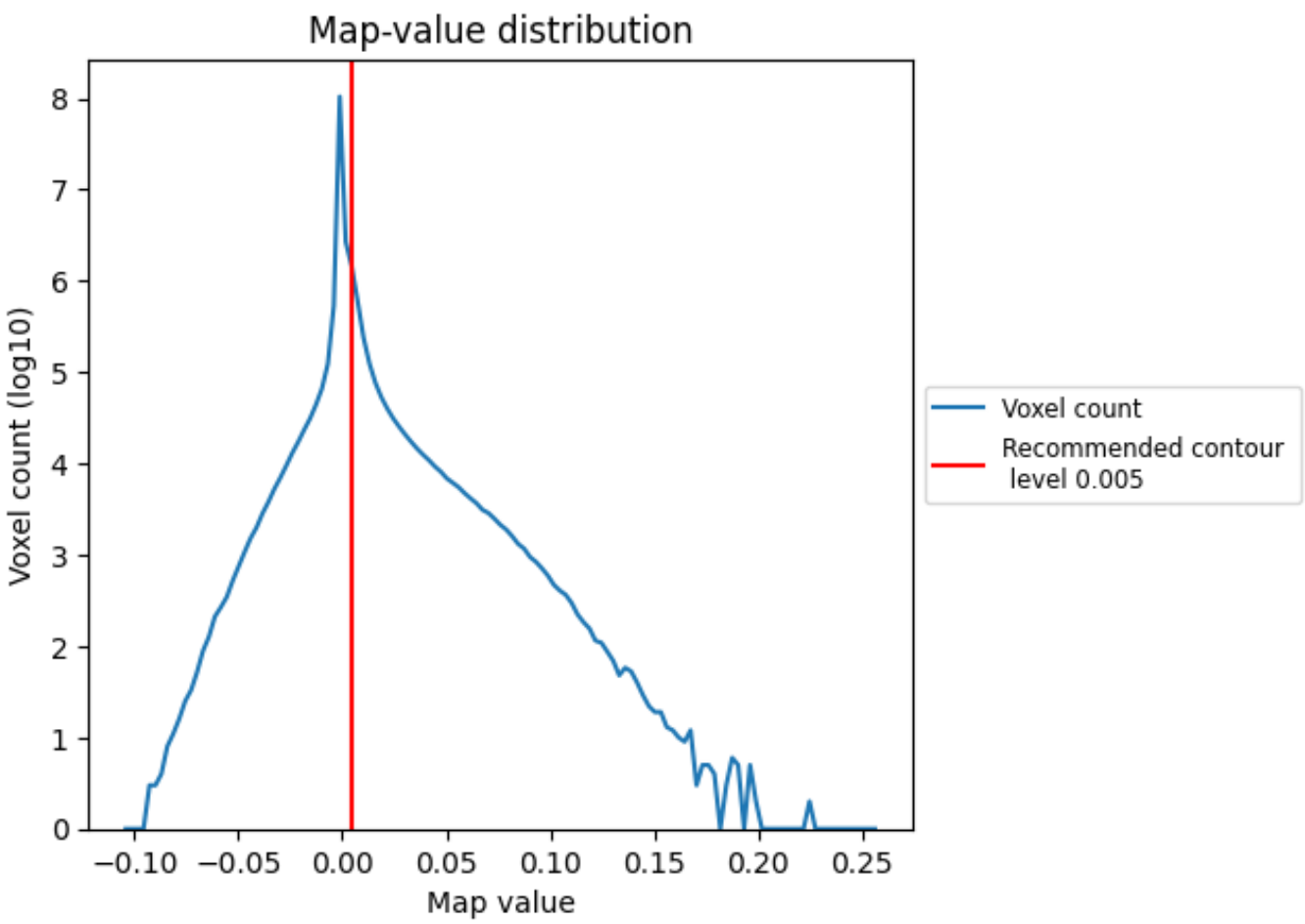
6.6 Mask visualisation (i)

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

7 Map analysis (i)

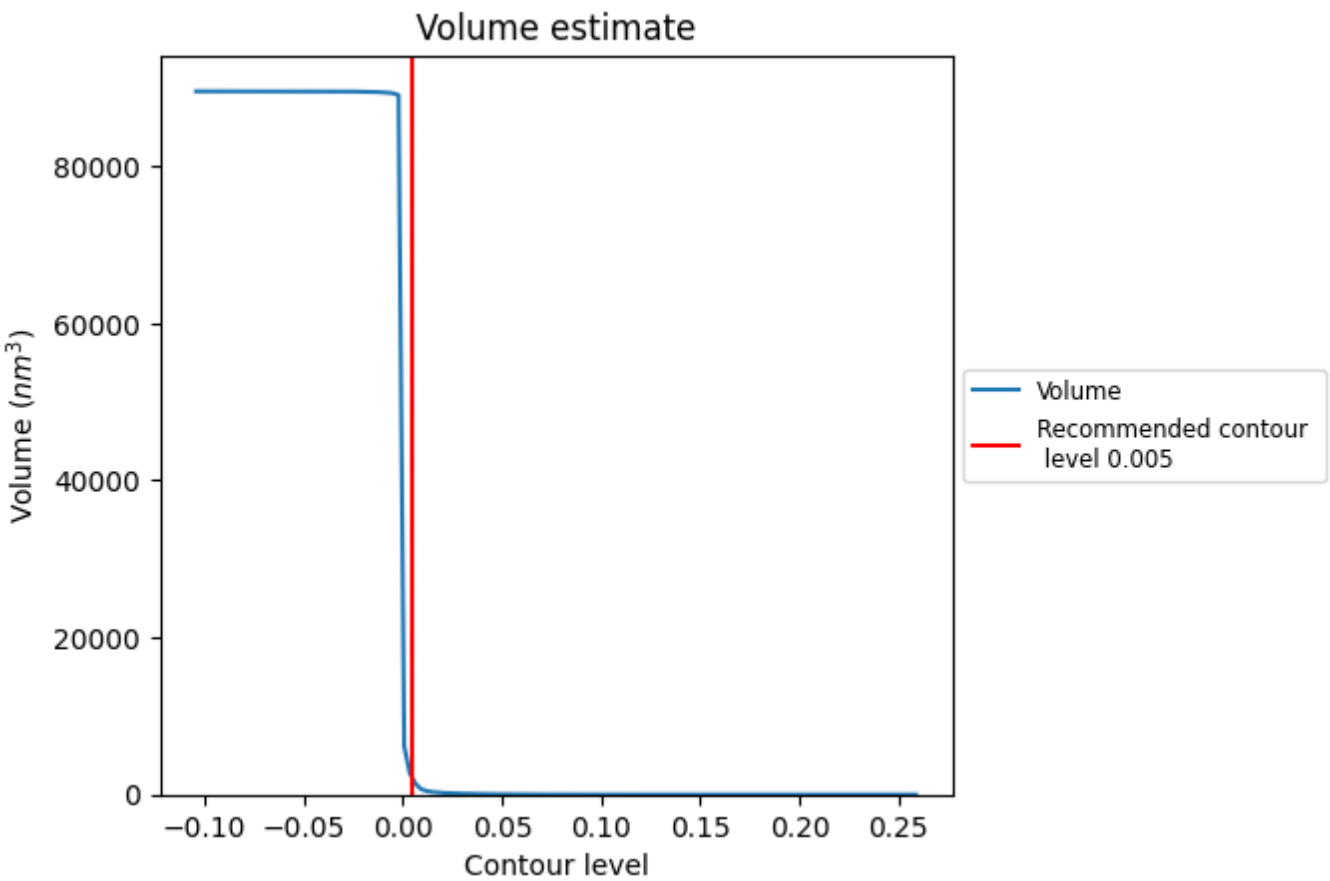
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

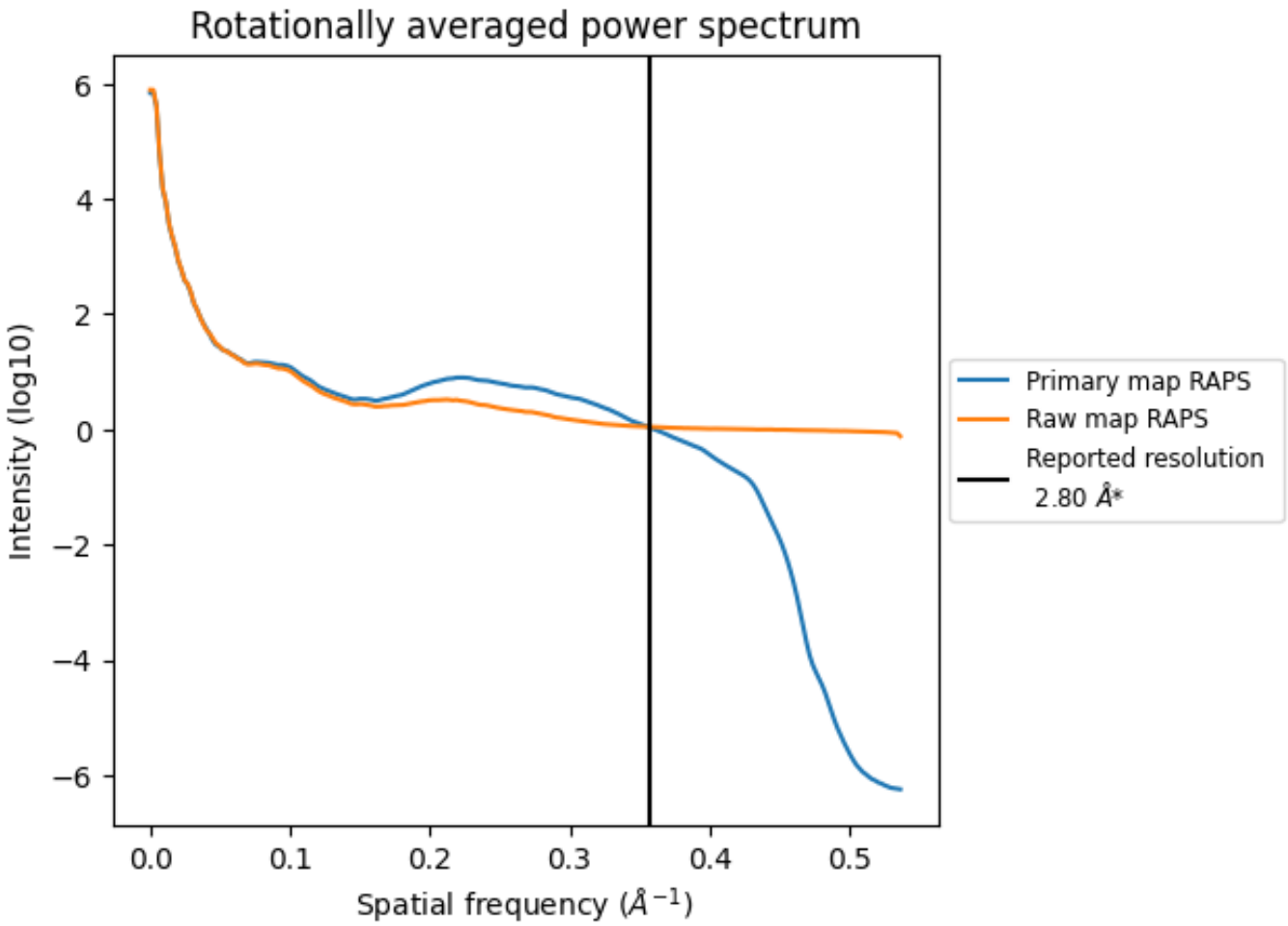
7.2 Volume estimate (i)



The volume at the recommended contour level is 2080 nm^3; this corresponds to an approximate mass of 1879 kDa.

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

7.3 Rotationally averaged power spectrum (i)

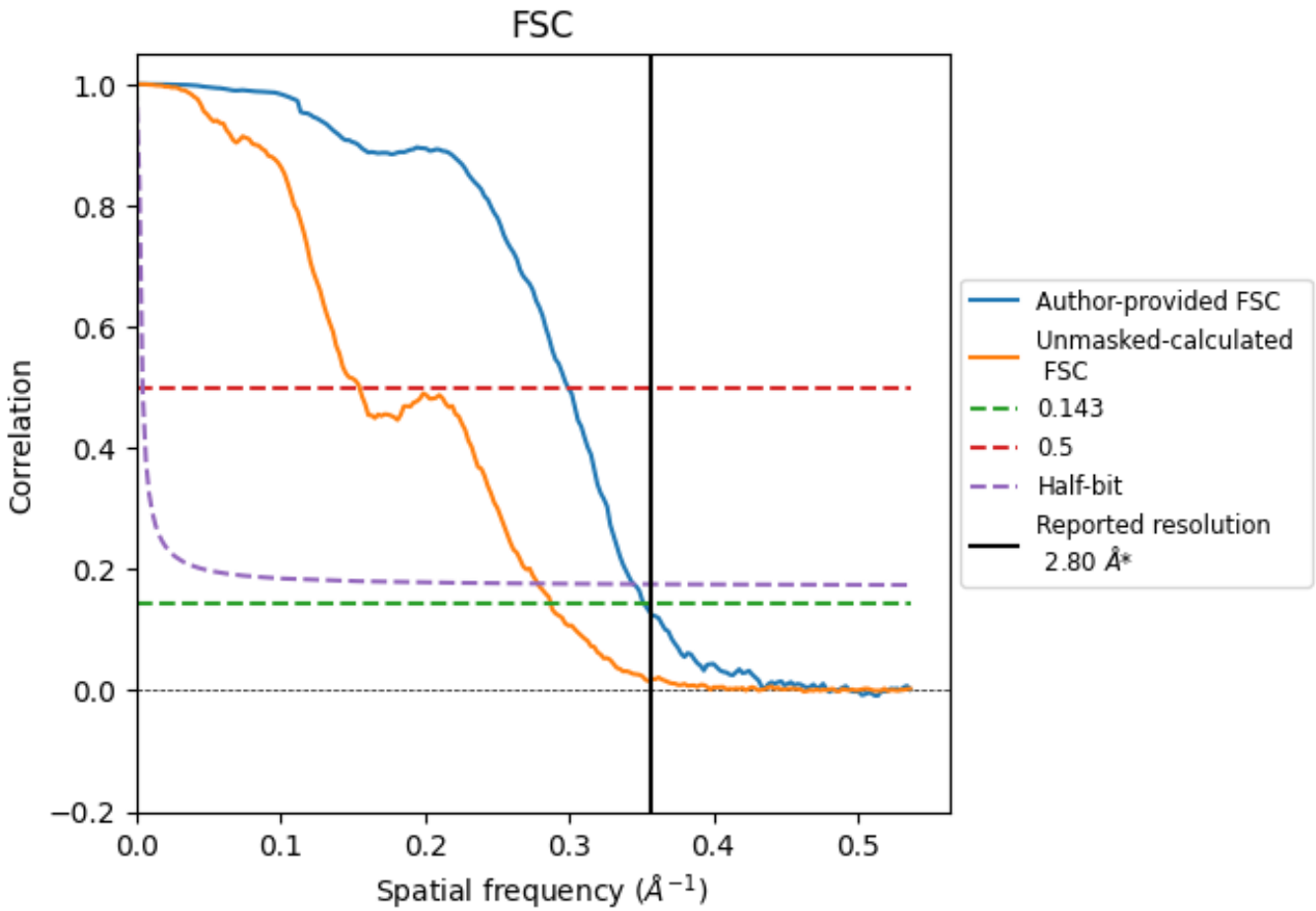


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

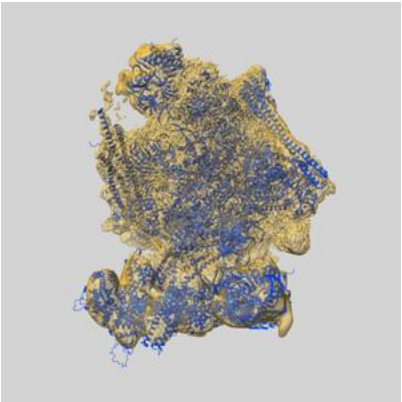
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.34	2.90
Unmasked-calculated*	3.48	6.46	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 2.8 by more than 10 %

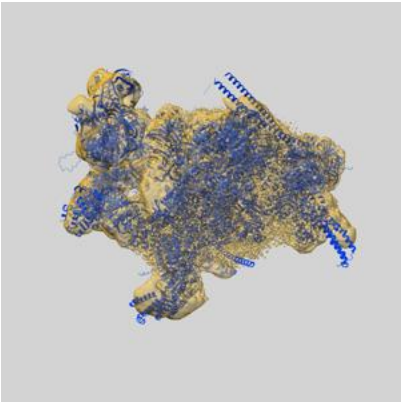
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-62841 and PDB model 9L5R. Per-residue inclusion information can be found in section 3 on page 14.

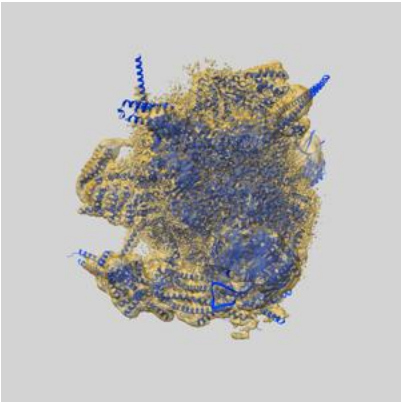
9.1 Map-model overlay (i)



X



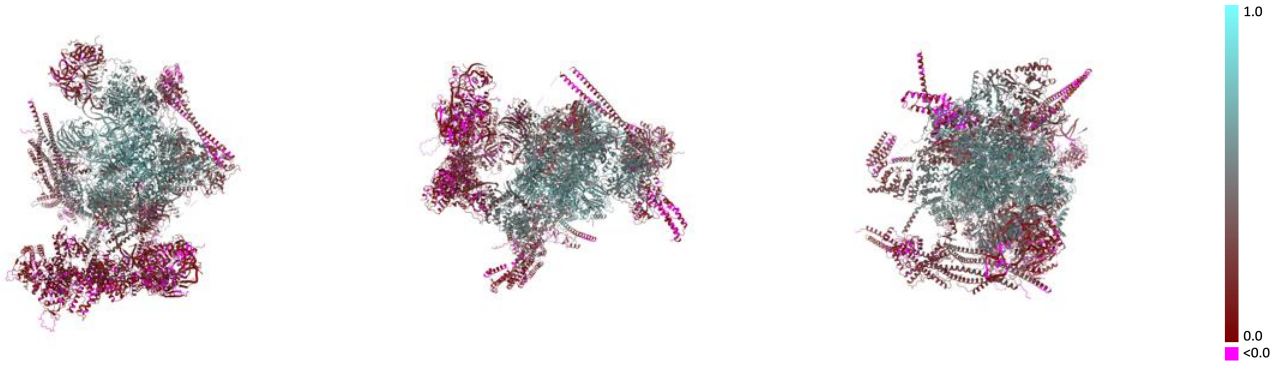
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

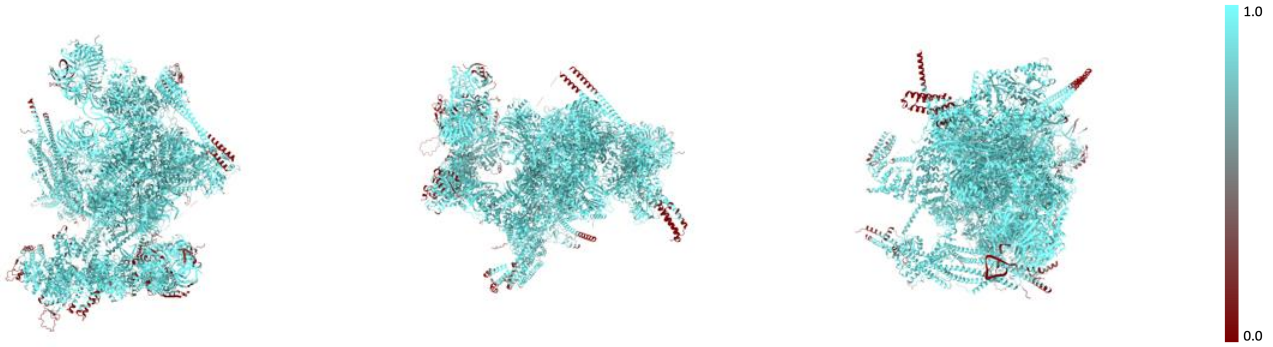
9.2 Q-score mapped to coordinate model (i)



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.

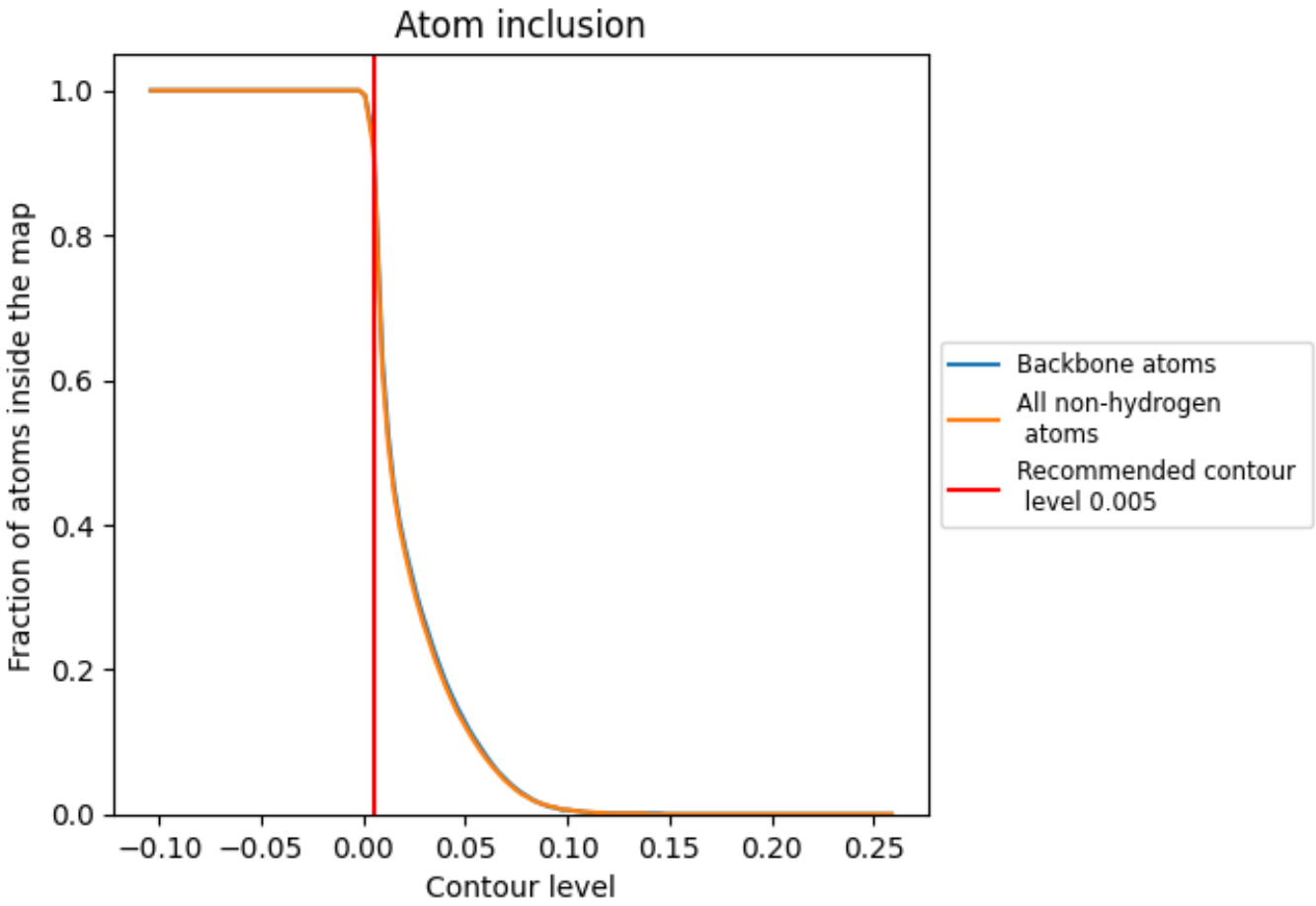
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9190	0.3780
0	0.9860	0.5070
2	0.9400	0.2700
5	0.8500	0.4260
6	0.9960	0.5910
7	0.9980	0.4500
A	0.9730	0.5640
B	0.9430	0.5100
C	0.9770	0.5260
CY	0.6760	0.1490
Cb	0.7170	0.1570
Cc	0.8480	0.1140
Ci	0.9370	0.1060
D	0.9220	0.3380
E	0.9940	0.5630
F	0.9450	0.3960
H	0.8640	0.3100
I	0.9620	0.3230
J	0.9060	0.4120
K	0.8850	0.2530
L	0.8810	0.3730
M	0.9720	0.4620
N	0.9960	0.6200
P	0.9700	0.6030
R	0.9170	0.5450
S	0.9870	0.5530
T	0.9990	0.7070
U	0.9690	0.4820
W	0.9940	0.3670
Y	0.8110	0.0880
a	0.8830	0.0680
b	0.9520	0.0560
c	0.7570	0.0630
d	0.7950	0.1020
e	0.8790	0.0950

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.9640	0.1220
g	0.7910	0.0450
h	0.8690	0.0980
i	0.6390	0.1040
j	0.9100	0.1980
k	0.9610	0.2850
l	0.9120	0.1370
m	0.9440	0.1390
o	0.9220	0.1580
p	0.8590	0.3260
q	0.9110	0.2090
r	0.9060	0.2140
s	0.8240	0.1680
t	0.8410	0.1250
u	0.9640	0.4050