



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 01:59 PM EST

PDB ID : 6BK8
EMDB ID : EMD-7109
Title : S. cerevisiae spliceosomal post-catalytic P complex
Authors : Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on : 2017-11-07
Resolution : 3.30 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

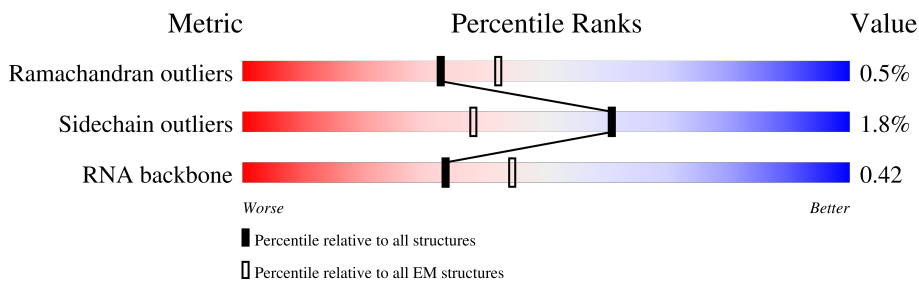
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.30 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1175	
2	5	214	
3	6	112	
4	e	34	
5	i	59	
6	A	2413	
7	B	1008	
8	D	451	

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Mol	Chain	Length	Quality of chain
9	E	379	7% 48% 51%
10	F	364	19% 54% 45%
11	G	339	7% 73% 25%
12	H	175	17% 37% 60%
13	I	157	99% 99%
14	K	135	36% 60% 39%
15	L	577	36% 71% 29%
16	M	455	24% 70% 28%
17	N	251	16% 66% 33%
18	O	382	24% 59% 40%
19	P	1145	51% 57% 43%
20	R	215	8% 46% 53%
21	S	590	40% 60%
22	T	687	33% 70% 30%
23	U	859	72% 73% 26%
24	X	219	60% 100%
25	Y	16	62% 100%
26	a	110	85% 85% 15%
26	q	110	82% 84% 15%
27	b	86	84% 84% 16%
27	m	86	81% 84% 16%
28	c	94	80% 78% 20%
28	l	94	80% 73% 6% 20%
29	d	77	90% 88% 10%
29	n	77	90% 88% 10%

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Mol	Chain	Length	Quality of chain
30	f	196	41% 41% 59%
30	k	196	40% 38% 60%
31	g	101	81% 81% 19%
31	o	101	77% 74% 23%
32	h	146	56% 55% 44%
32	p	146	54% 46% 8% 46%
33	r	111	76% 76% 24%
34	s	238	69% 66% 31%
35	u	503	86% 85% 14%
35	v	503	23% 22% 77%
35	w	503	87% 86% 13%
35	x	503	23% 23% 77%
36	y	175	63% 59% 37%

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 82745 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	135	2848	1272	472	969	135	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	103	2173	973	367	730	103	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	102	2170	972	386	710	102	0	0

- Molecule 4 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	e	34	707	319	107	247	34	0	0

- Molecule 5 is a RNA chain called RNA (59-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	i	59	1239	558	202	420	59	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor Prp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	1960	16159	10381	2786	2933	59	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	899	7179	4638	1191	1321	29	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	359	2826	1786	497	533	10	0	0

- Molecule 9 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	186	1494	939	276	273	6	0	0

- Molecule 10 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	199	1576	991	277	293	15	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	255	2048	1297	362	378	11	0	0

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	70	570	357	113	99	1	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	156	1283	803	239	231	10	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	82	550	332	106	111	1	0	0

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	L	412	3353	2160	556	620	17	0	0

- Molecule 16 is a protein called Pre-mRNA-processing factor Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	M	326	2607	1649	465	485	8	0	0

- Molecule 17 is a protein called Pre-mRNA-splicing factor Prp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	N	167	1326	856	233	233	4	0	0

- Molecule 18 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	229	1935	1211	347	368	9	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	653	3872	2393	736	740	3	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	R	101	813	499	150	163	1	0	0

- Molecule 21 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	238	Total	C	N	O	S	0	0
			1948	1218	355	368	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	483	Total	C	N	O	S	0	0
			3370	2113	624	625	8		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	637	Total	C	N	O	S	0	0
			3625	2226	689	703	7		

- Molecule 24 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	219	Total	C	N	O	0	0
			1095	657	219	219		

- Molecule 25 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
26	q	93	Total	C	N	O	S	0	0
			726	468	136	118	4		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
27	m	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
28	l	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
29	n	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	f	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
30	k	78	Total	C	N	O	S	0	0
			610	389	109	109	3		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	g	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
31	o	78	Total	C	N	O	S	0	0
			600	384	104	110	2		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
32	p	79	Total	C	N	O	S	0	0
			618	393	107	116	2		

- Molecule 33 is a protein called Lea1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	r	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 34 is a protein called Msl1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 35 is a protein called Pre-mRNA-processing factor Prp19.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	u	435	Total	C	N	O	0	0
			2156	1286	435	435		
35	v	118	Total	C	N	O	0	0
			588	352	118	118		
35	w	438	Total	C	N	O	0	0
			2171	1295	438	438		
35	x	116	Total	C	N	O	0	0
			578	346	116	116		

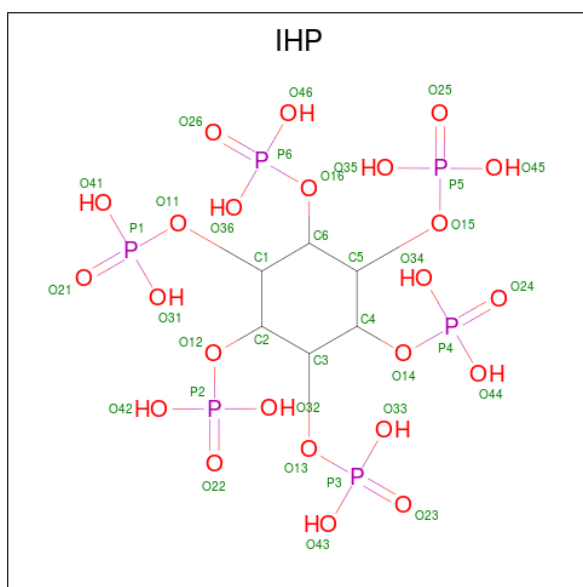
- Molecule 36 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	y	110	Total	C	N	O	0	0
			548	328	110	110		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

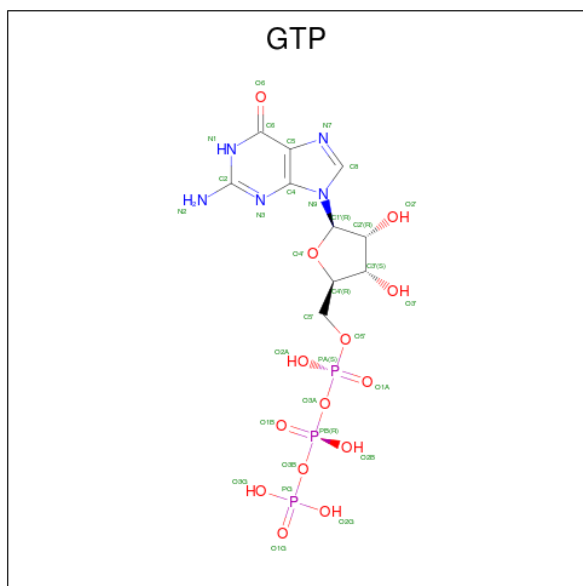
Mol	Chain	Residues	Atoms		AltConf
37	6	4	Total	Mg	0
			4	4	
37	B	1	Total	Mg	0
			1	1	

- Molecule 38 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
38	A	1	36	6	24	6	0

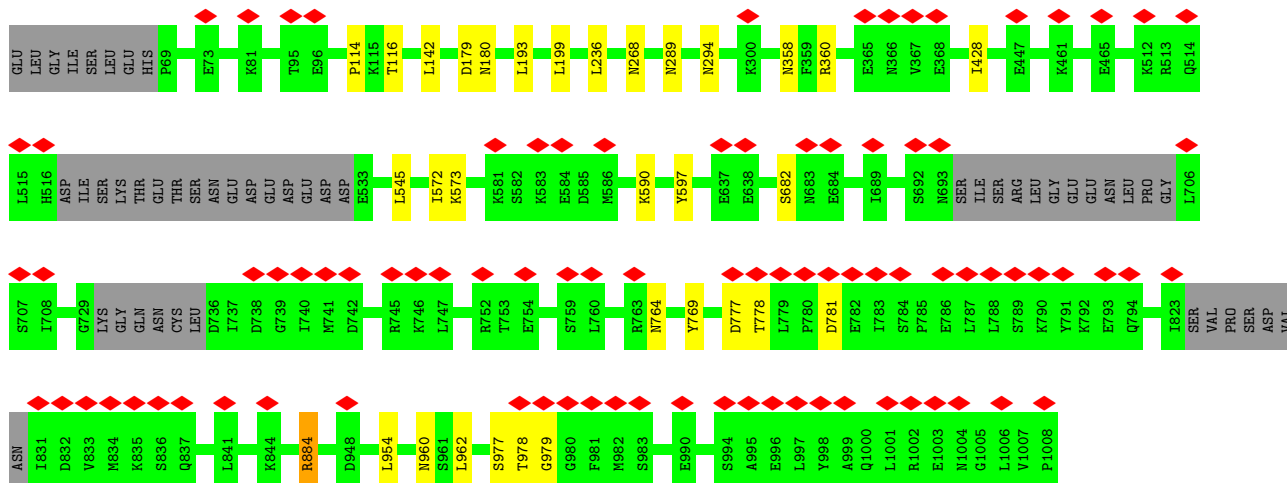
- Molecule 39 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



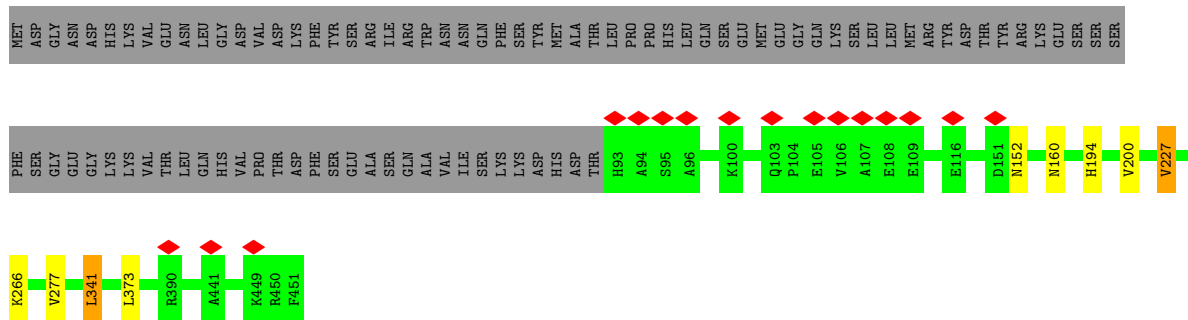
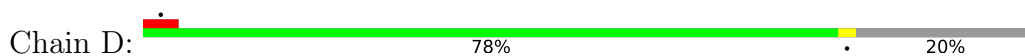
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	B	1	32	10	5	14	3	0

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

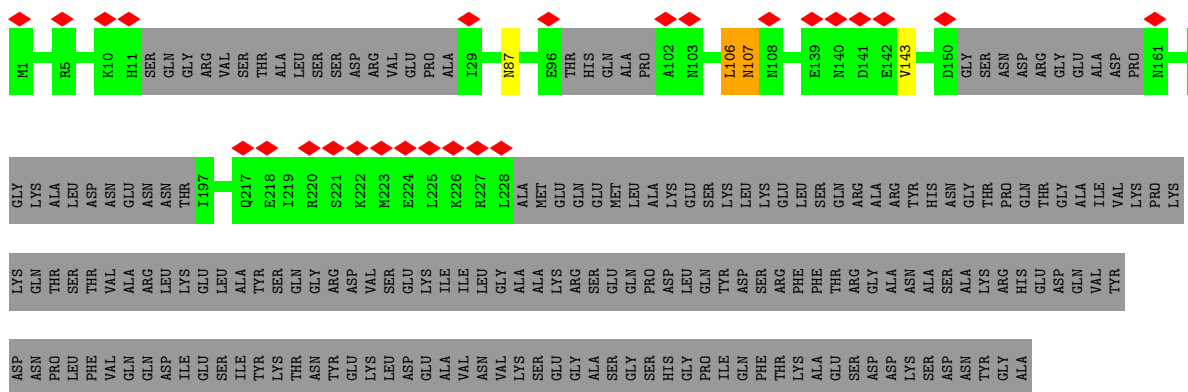
Mol	Chain	Residues	Atoms		AltConf
40	F	2	Total 2	Zn 2	0
40	G	1	Total 1	Zn 1	0
40	I	3	Total 3	Zn 3	0
40	O	1	Total 1	Zn 1	0



• Molecule 8: Pre-mRNA-splicing factor PRP46

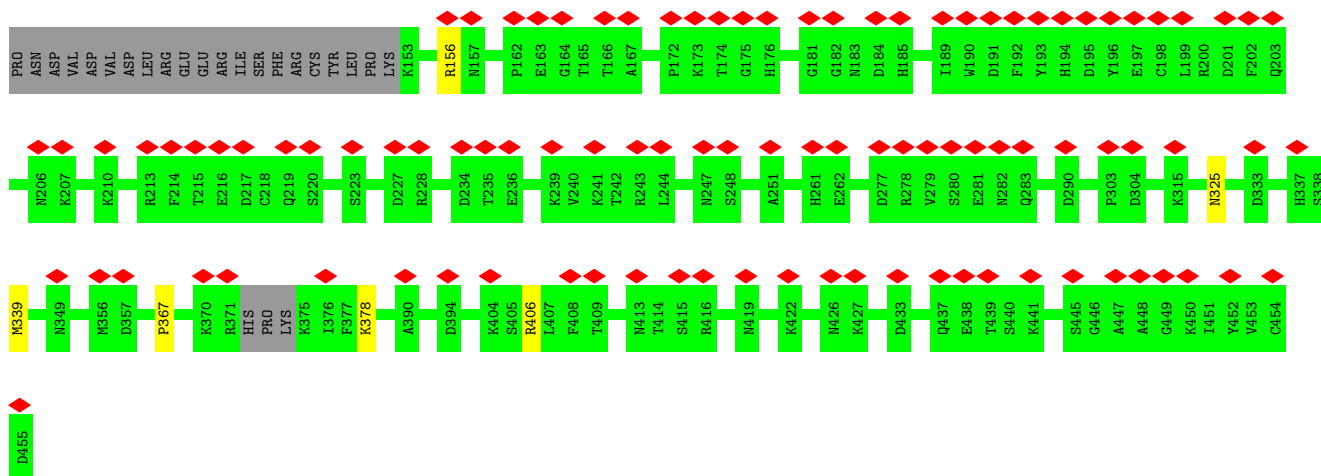


• Molecule 9: Pre-mRNA-processing protein 45

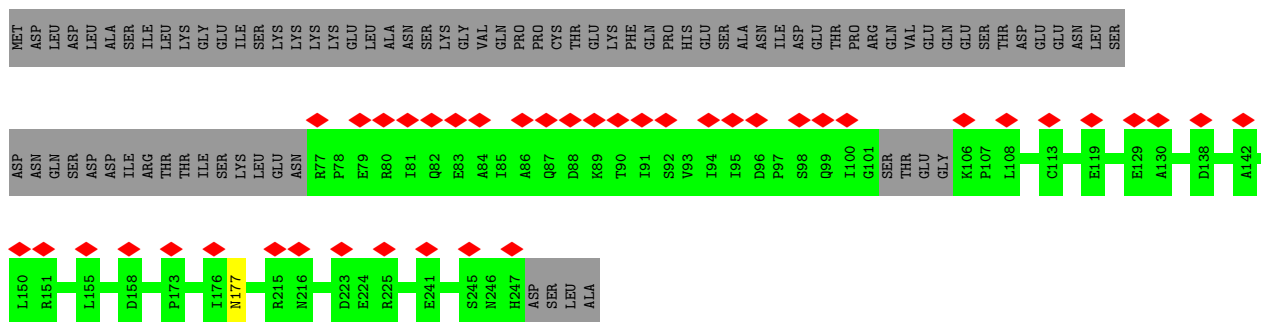


• Molecule 10: Pre-mRNA-splicing factor SLT11

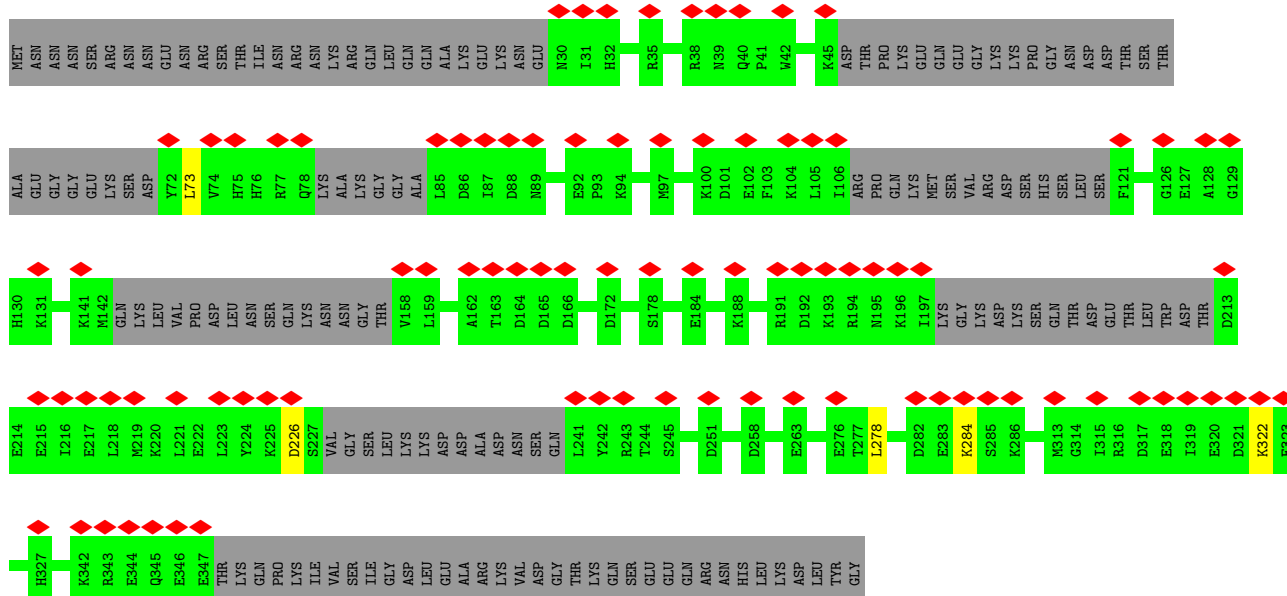


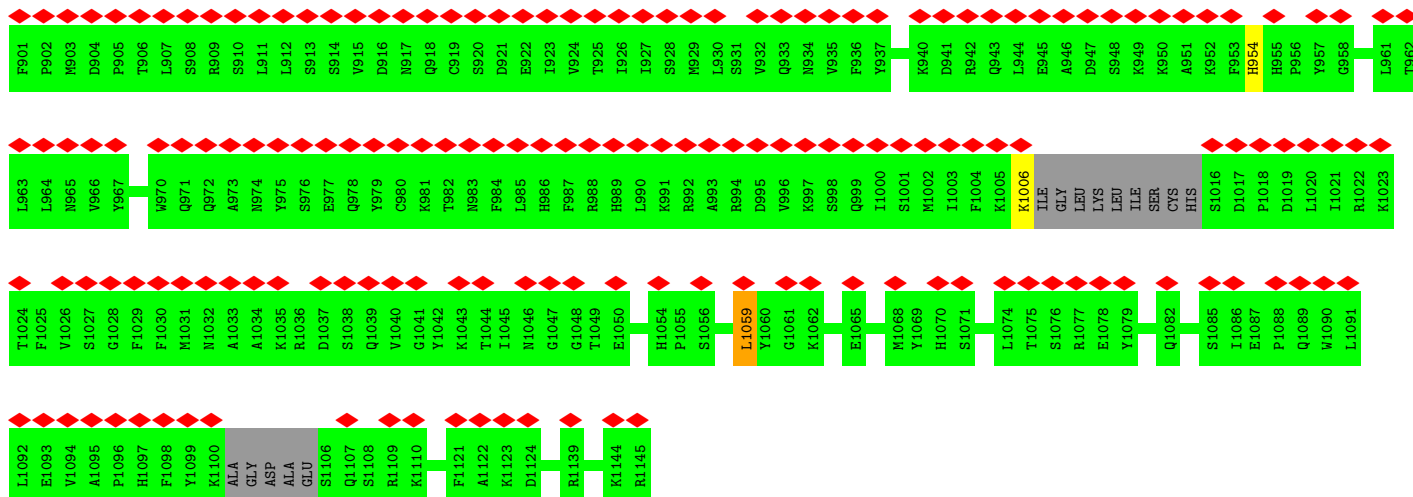


• Molecule 17: Pre-mRNA-splicing factor Prp18

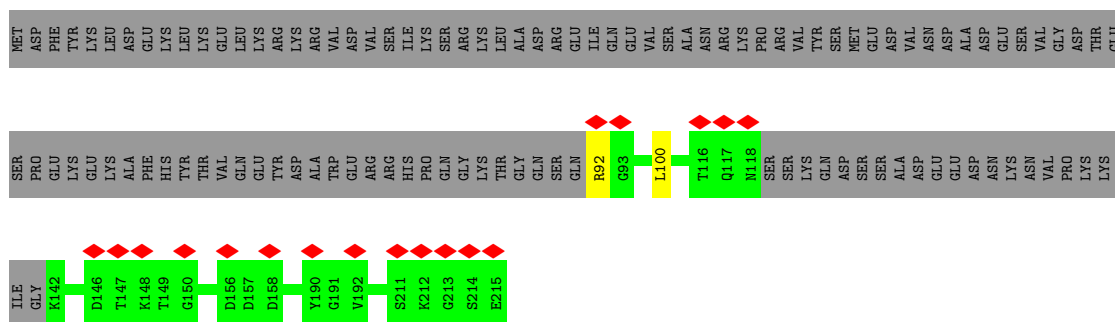


• Molecule 18: Pre-mRNA-splicing factor SLU7

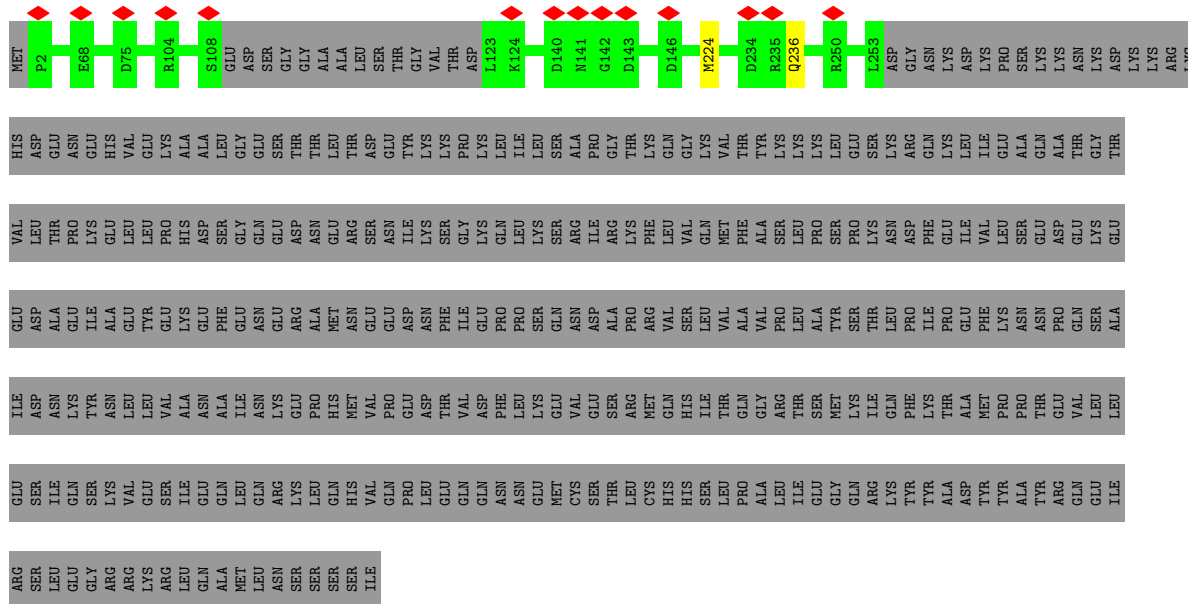


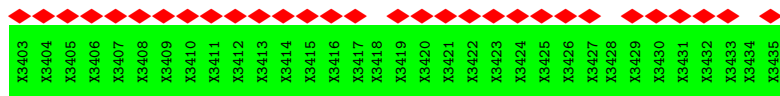


● Molecule 20: Pre-mRNA-splicing factor SYF2

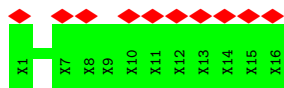


● Molecule 21: Pre-mRNA-splicing factor CEF1

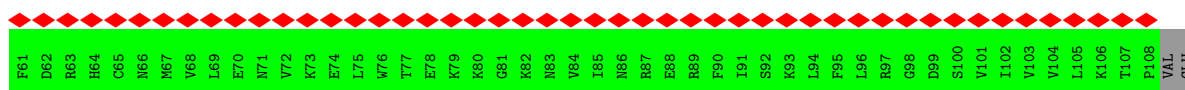
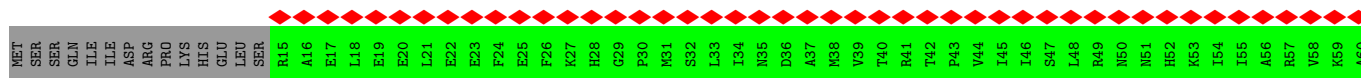
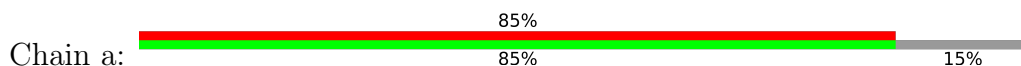




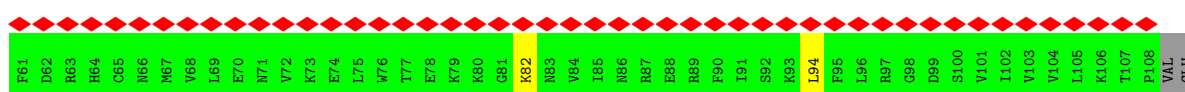
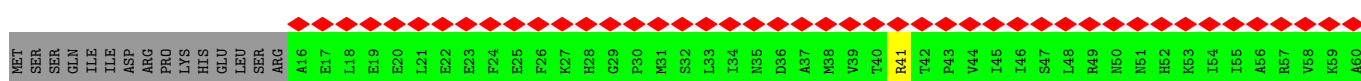
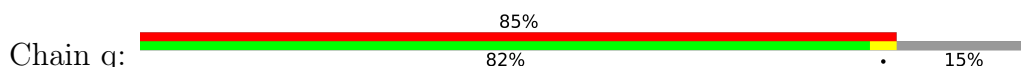
• Molecule 25: Unknown protein fragment



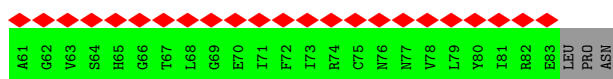
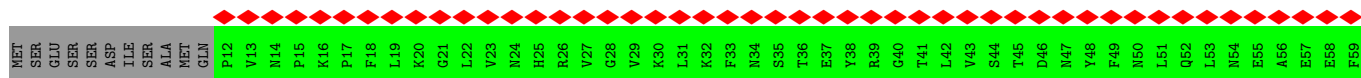
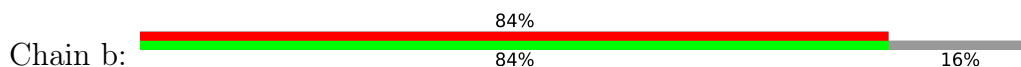
• Molecule 26: Small nuclear ribonucleoprotein Sm D2



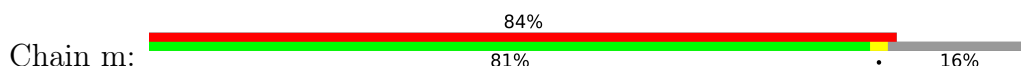
• Molecule 26: Small nuclear ribonucleoprotein Sm D2

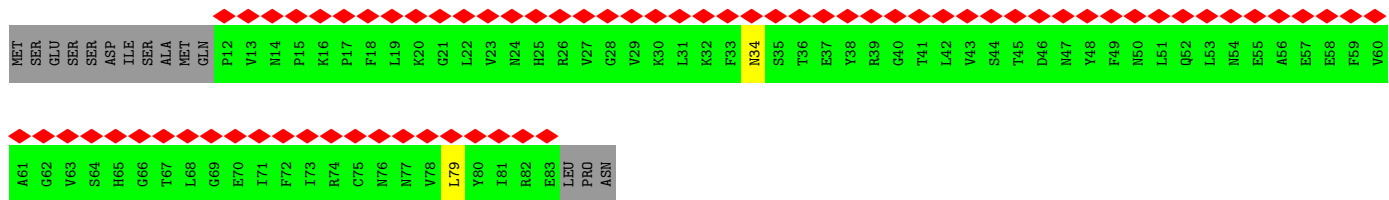


• Molecule 27: Small nuclear ribonucleoprotein F

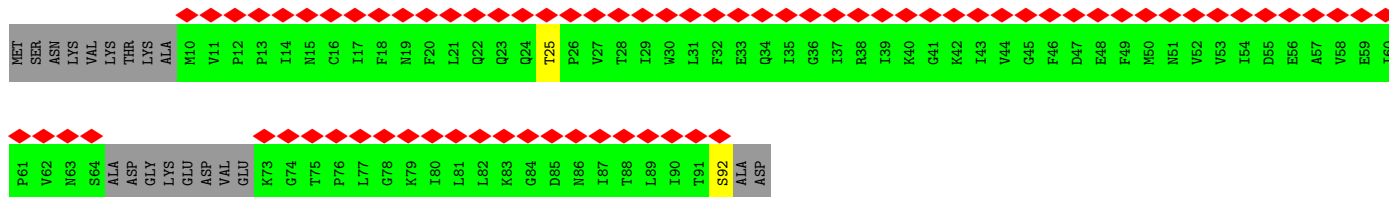
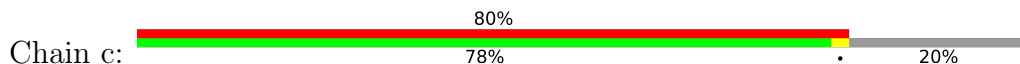


• Molecule 27: Small nuclear ribonucleoprotein F

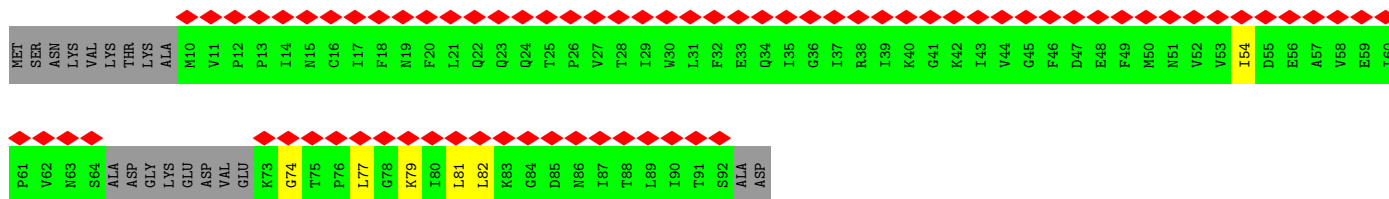
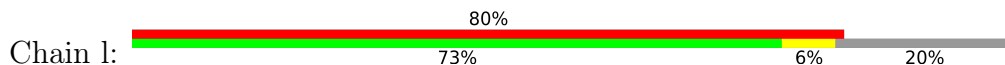




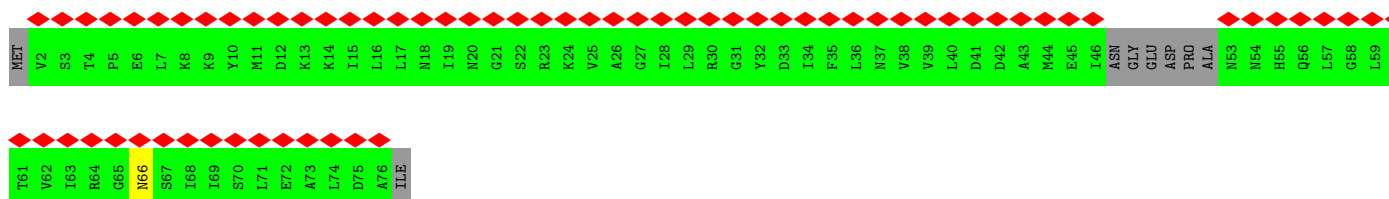
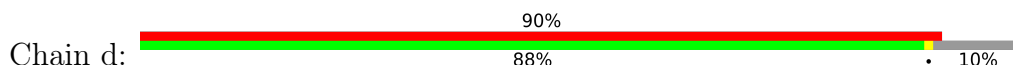
• Molecule 28: Small nuclear ribonucleoprotein E



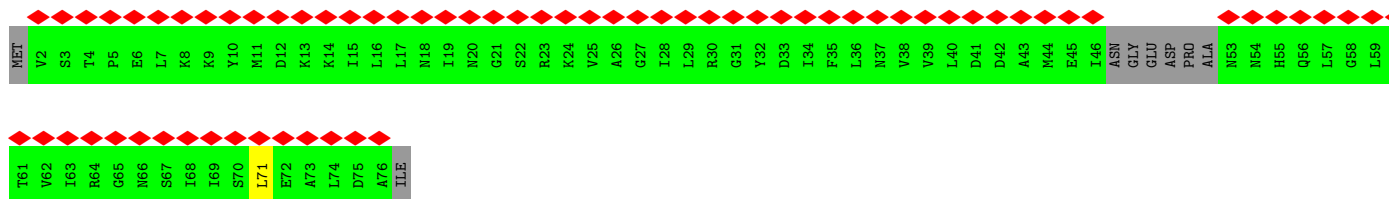
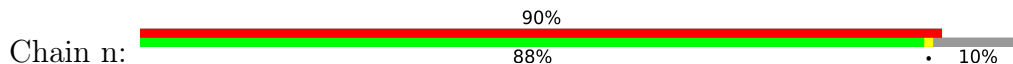
• Molecule 28: Small nuclear ribonucleoprotein E



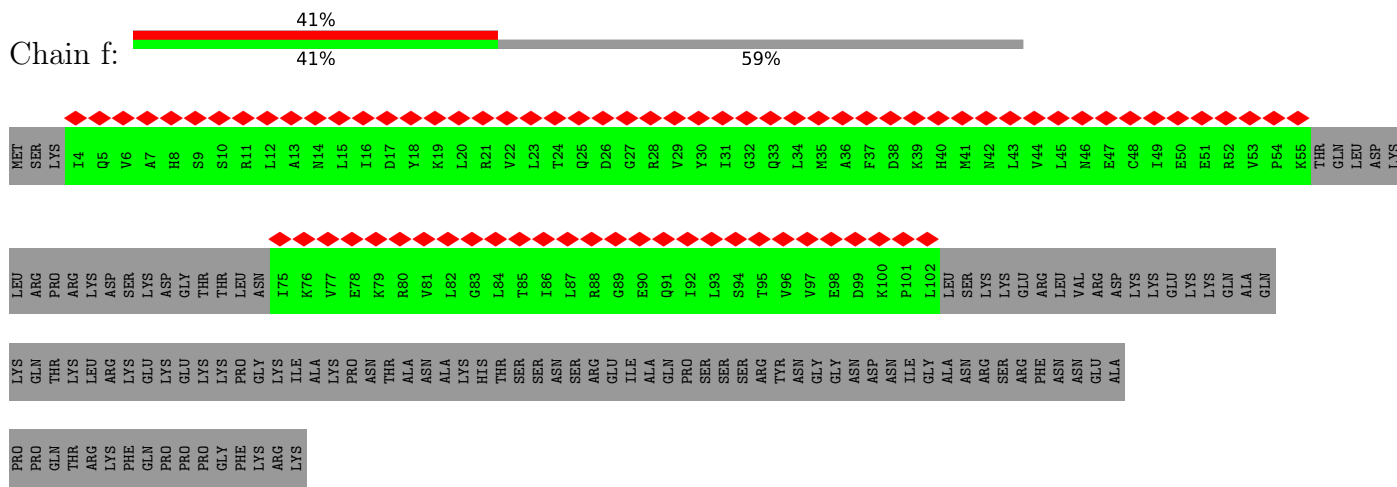
• Molecule 29: Small nuclear ribonucleoprotein G



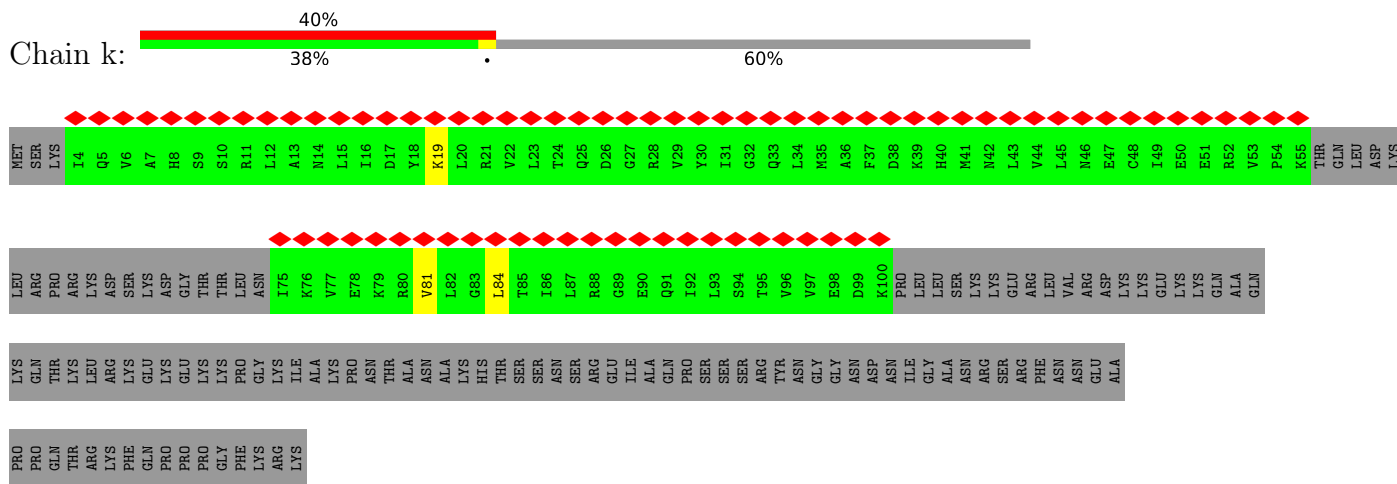
• Molecule 29: Small nuclear ribonucleoprotein G



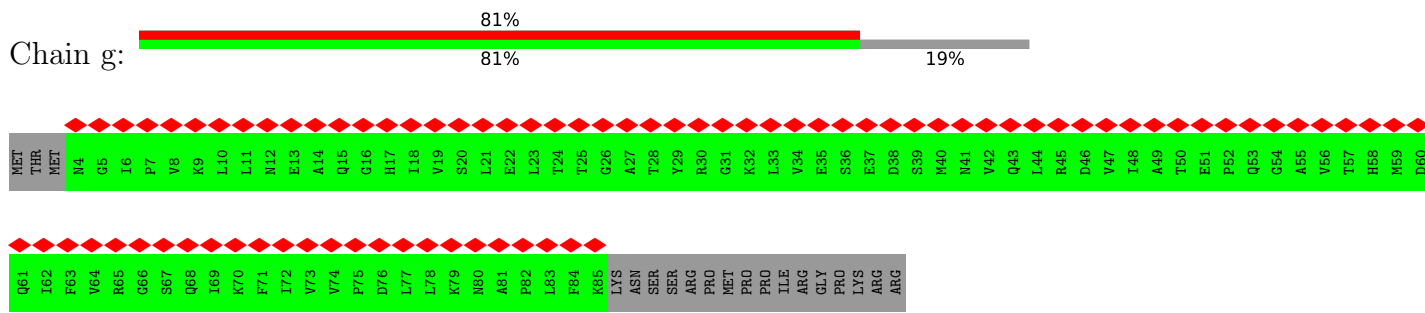
• Molecule 30: Small nuclear ribonucleoprotein-associated protein B



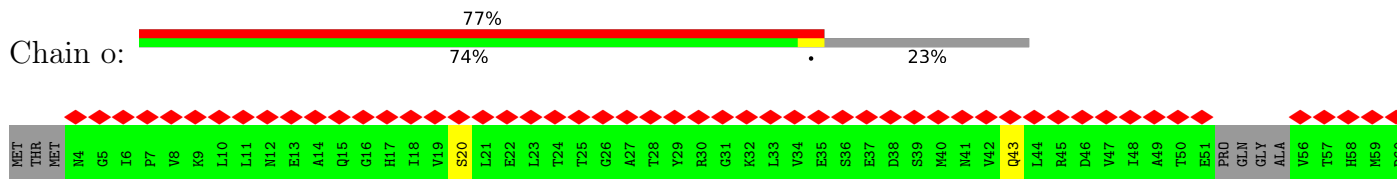
• Molecule 30: Small nuclear ribonucleoprotein-associated protein B

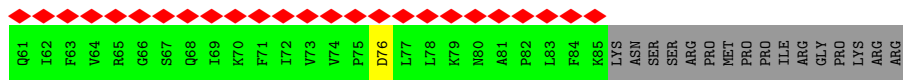


• Molecule 31: Small nuclear ribonucleoprotein Sm D3

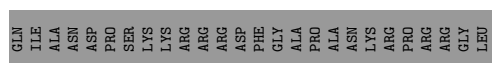
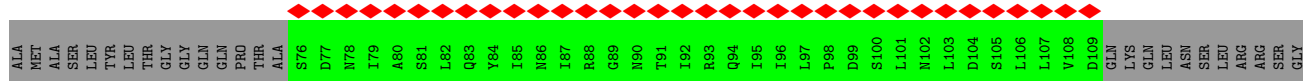
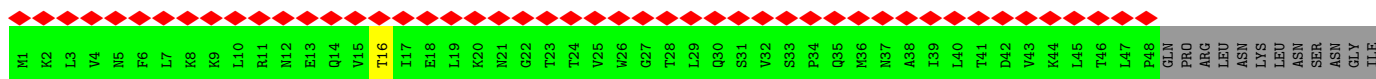


• Molecule 31: Small nuclear ribonucleoprotein Sm D3

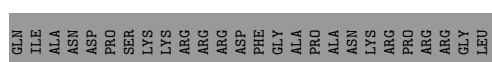
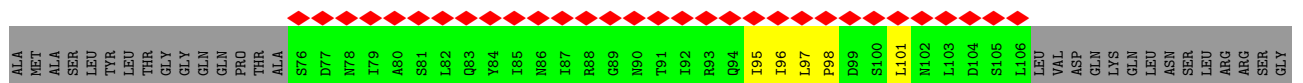
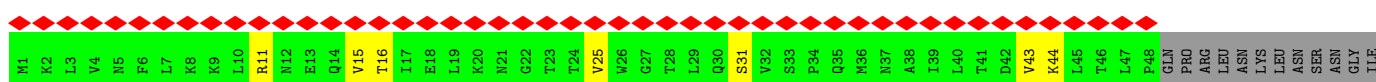




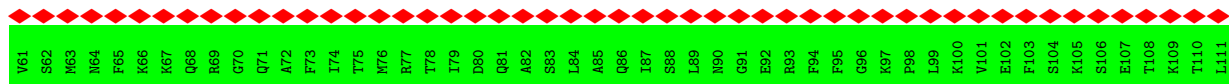
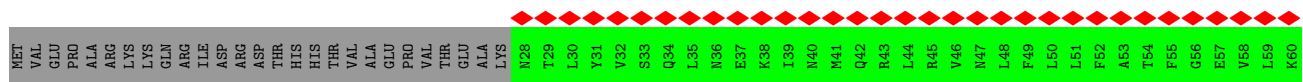
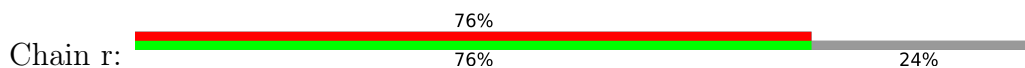
• Molecule 32: Small nuclear ribonucleoprotein Sm D1



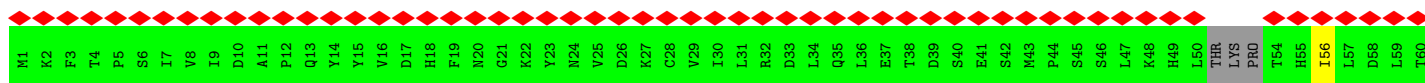
• Molecule 32: Small nuclear ribonucleoprotein Sm D1



• Molecule 33: Lea1

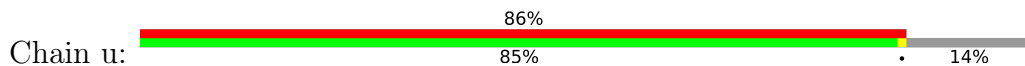


• Molecule 34: Msl1



N61	N62	D63	L64	I65	M66	I67	P68	D69	L70	S71	R72	R73	D74	D75	I76	H77	T78	L79	L80	L81	G82	R83	N84	N85	I86	V87	E88	V89	D90	G91	R92	L93	L94	P95	M96	N97	V98	Q99	N100	L101	T102	L103	S104	N105	S106	S107	I108	R109	R110	F111	E112	D113	L114	Q115	R116	L117	R118	R119	A120
P121	R122	T123	L124	K125	M126	L127	T128	L129	I130	G131	M132	Q133	V134	C135	H136	L137	A138	N139	Y140	R141	E142	H143	V144	L145	R146	L147	V148	P149	H150	L151	E152	T153	L154	D155	F156	Q157	N158	V159	T160	A161	E162	E163	R164	K165	S166	A167	MET	PHE	PRO	ARG	GLN	ALA	ASP	GLY	ASP	THR	LEU	GLY	
PRO	VAL	ASN	THR	ALA	ILE	ARG	ASP	ASN	GLY	SER	ARG	ASP	LYS	THR	MET	GLU	ILE	MET	ASN	LEU	VAL	VAL	SER	LYS	LYS	THR	THR	VAL	VAL	GLU	ARG	ARG	ASN	GLU	LEU	LEU	LEU	ILE	ALA	ARG	GLU	GLU	LYS	LEU	LEU	LEU	LEU	SER	GLY	GLY	VAL								

• Molecule 35: Pre-mRNA-processing factor Prp19



M1	L2	C3	A4	I5	S6	G7	K8	V9	P10	R11	R12	P13	V14	L15	S16	P17	K18	S19	R20	T21	I22	F23	E24	K25	S26	L27	L28	E29	Q30	Y31	V32	K33	D34	T35	G36	N37	D38	P39	I40	T41	M42	E43	P44	L45	S46	I47	E48	E49	I50	V51	ILE	VAL	PRO	SER	ALA	GLN	ALA					
SER	LEU	THR	GLU	SER	THR	ASN	SER	ALA	ALA	ASN	TYR	SER	I77	F78	N79	L80	L81	T82	S83	L84	Q85	N86	E87	W88	D89	A90	I91	N92	L93	E94	N95	F96	K97	L98	R99	S100	T101	L102	D103	S104	L105	T106	K107	K108	L109	S110	T111	V112	M113	Y114	E115	R116	D117	A118	A119	K120						
L121	V122	A123	A124	Q125	A126	L127	M128	E129	K130	M131	E132	D133	S134	K135	F136	L137	P138	K139	SER	GLN	GLN	S203	ALA	VAL	ALA	ILE	THR	GLU	GLU	PHE	W209	V210	C211	M212	C213	R214	C215	E216	D217	G218	A219	L220	H221	F222	T223	Q224	L225	K226	D227	S228	K229	T230	I231	T232	T233	I234	T235	T236	P237	N238	P239	R240
E181	L182	L183	Q184	H245	P246	M187	I248	I249	R190	M191	I192	K193	T194	F195	P196	Y197	K198	E199	L200	N201	K202	S203	M204	Y205	Y206	D207	K208	W209	V210	C211	M212	R214	C215	E216	D217	G218	A219	L220	H221	F222	T223	Q224	L225	K226	D227	S228	K229	T230	I231	T232	T233	I234	T235	T236	P237	N238	P239	R240				
T241	G242	G243	E244	H245	P246	A247	I248	I249	S250	R251	G252	P253	C254	N255	R256	L257	L258	L259	L260	Y261	P262	G263	N264	Q265	L266	T267	L268	L269	D270	S271	K272	T273	N274	K275	V276	L277	R278	E279	I280	E281	F282	D283	S284	A285	N286	E287	I288	L289	Y290	M291	Y292	G293	H294	N295	GLU	VAL	ASN	T299	E300			
Y301	F302	I303	W304	A305	D306	N307	R308	G309	T310	I311	G312	F313	Q314	S315	Y316	E317	D318	D319	S320	Q321	Y322	I323	V324	H325	S326	A327	K328	S329	D330	V331	E332	Y333	S334	S335	G336	V337	L338	H339	K340	D341	S342	L343	L344	L345	A346	L347	Y348	S349	P350	D351	G352	I353	L354	D355	V356	Y357	N358	L359	S360			
S361	P362	D363	Q364	A365	S366	S367	R368	F369	P370	V371	D372	E373	E374	A375	K376	I377	K378	E379	V380	K381	F382	A383	D384	N385	G386	Y387	W388	M389	V390	V391	C392	C393	D394	Q395	T396	V397	V398	C399	F400	D401	L402	R403	K404	D405	V406	G407	T408	L409	A410	Y411	P412	T413	Y414	T415	I416	PRO	GLU	PHE	LYS			
THR	G422	T423	V424	T425	Y426	D427	I428	D429	D430	S431	K432	K433	M434	M435	I436	A437	Y438	S439	M440	E441	S442	M443	S444	L445	T446	I447	Y448	K449	F450	D451	K452	K453	T454	K455	M456	W457	T458	K459	D460	E461	E462	S463	A464	L465	C466	L467	GLN	SER	ASP	THR	A472	D473	F474	T475	D476	M477	D478	V479	W480			
C481	G482	D483	G484	G485	I486	A487	A488	I489	L490	K491	T492	M493	D494	S495	F496	M497	I498	V499	A500	L501	T502	P503																																								

• Molecule 35: Pre-mRNA-processing factor Prp19



L121	K122	H123	Q124	E125	I126	V127	L128	D129	T130	L131	L132	P133	Q134	T135	V136	S137	N138	Q139	W140	R141	I142	N143	N144	D145	Y146	I147	R148	Q149	T150	C151	T152	I153	V154	E155	E156	M157	N158	I159	Q160	Q161	R162	K163	Q164	I165	N166	D167	L168	E169	I170	Y171	R172	K173	R174	LEU
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212219	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.197	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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: ZN, MG, GTP, IHP

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	0.50	1/3167 (0.0%)	0.92	8/4911 (0.2%)
2	5	0.88	0/2422	1.16	21/3762 (0.6%)
3	6	0.89	0/2427	1.13	15/3778 (0.4%)
4	e	0.82	4/787 (0.5%)	1.48	17/1219 (1.4%)
5	i	0.59	0/1379	1.10	3/2131 (0.1%)
6	A	0.52	0/16570	0.68	8/22456 (0.0%)
7	B	0.49	0/7331	0.70	8/9926 (0.1%)
8	D	0.56	1/2889 (0.0%)	0.71	2/3924 (0.1%)
9	E	0.44	0/1517	0.63	0/2043
10	F	0.43	0/1598	0.67	2/2151 (0.1%)
11	G	0.47	0/2094	0.62	2/2815 (0.1%)
12	H	0.41	0/584	0.76	1/781 (0.1%)
13	I	0.49	0/1307	0.59	0/1748
14	K	0.35	0/552	0.56	0/746
15	L	0.38	0/3406	0.63	1/4592 (0.0%)
16	M	0.37	0/2678	0.61	1/3619 (0.0%)
17	N	0.39	0/1354	0.59	0/1838
18	O	0.36	0/1967	0.62	2/2624 (0.1%)
19	P	0.29	0/3918	0.48	2/5386 (0.0%)
20	R	0.39	0/817	0.57	1/1083 (0.1%)
21	S	0.46	0/1978	0.63	1/2655 (0.0%)
22	T	0.45	0/3411	0.55	1/4632 (0.0%)
23	U	0.27	0/3625	0.45	0/4963
26	a	0.36	0/753	0.57	0/1013
26	q	0.38	0/738	0.61	0/995
27	b	0.41	0/585	0.57	0/791
27	m	0.40	0/585	0.61	0/791
28	c	0.42	0/585	0.61	0/795
28	l	0.40	0/585	0.56	0/795
29	d	0.50	0/532	0.61	0/715
29	n	0.36	0/529	0.50	0/711
30	f	0.36	0/636	0.63	0/856

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	k	0.35	0/614	0.57	0/826
31	g	0.35	0/634	0.56	0/859
31	o	0.37	0/607	0.53	0/820
32	h	0.38	0/649	0.54	0/880
32	p	0.40	0/623	0.65	0/844
33	r	0.33	0/415	0.55	0/577
34	s	0.31	0/814	0.53	0/1134
35	u	0.47	0/2150	0.68	2/2989 (0.1%)
35	v	0.59	0/586	0.89	3/816 (0.4%)
35	w	0.47	0/2165	0.71	3/3010 (0.1%)
35	x	0.58	0/576	0.79	0/802
36	y	0.58	0/546	0.80	0/760
All	All	0.49	6/83685 (0.0%)	0.72	104/115562 (0.1%)

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
6	A	0	6
7	B	0	9
8	D	0	2
9	E	0	3
10	F	0	1
11	G	0	2
15	L	0	1
18	O	0	1
30	k	0	1
35	u	0	1
35	v	0	1
35	w	0	2
36	y	0	2
All	All	0	32

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	9	U	C1'-N1	7.04	1.59	1.48
4	e	-13	U	C1'-N1	6.81	1.58	1.48
4	e	-11	U	C1'-N1	6.04	1.57	1.48
4	e	-2	A	N9-C4	-6.00	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	227	VAL	CB-CG1	-5.37	1.41	1.52
1	2	21	G	N7-C5	-5.24	1.36	1.39

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	954	LEU	CA-CB-CG	9.20	136.46	115.30
4	e	11	U	C2-N1-C1'	9.14	128.67	117.70
4	e	11	U	N1-C2-O2	8.22	128.55	122.80
35	w	134	SER	CA-C-O	-7.91	103.49	120.10
4	e	2	U	N1-C2-O2	7.86	128.30	122.80
7	B	193	LEU	CA-CB-CG	7.84	133.32	115.30
4	e	11	U	N3-C2-O2	-7.70	116.81	122.20
4	e	2	U	N3-C2-O2	-7.63	116.86	122.20
6	A	355	LEU	CA-CB-CG	7.48	132.50	115.30
18	O	73	LEU	CA-CB-CG	7.35	132.21	115.30
4	e	2	U	C2-N1-C1'	7.31	126.47	117.70
2	5	60	U	N1-C2-O2	7.30	127.91	122.80
8	D	341	LEU	CA-CB-CG	7.12	131.69	115.30
7	B	781	ASP	CB-CG-OD1	7.11	124.70	118.30
2	5	79	C	C2-N1-C1'	7.06	126.57	118.80
2	5	99	U	C5-C6-N1	7.04	126.22	122.70
4	e	-12	U	C2-N1-C1'	7.03	126.13	117.70
7	B	142	LEU	CA-CB-CG	6.99	131.37	115.30
21	S	224	MET	CA-CB-CG	6.97	125.15	113.30
11	G	151	LEU	CA-CB-CG	6.95	131.28	115.30
6	A	852	LEU	CB-CG-CD1	-6.84	99.38	111.00
2	5	60	U	N3-C2-O2	-6.83	117.42	122.20
2	5	60	U	C2-N1-C1'	6.76	125.81	117.70
4	e	17	U	P-O3'-C3'	6.75	127.80	119.70
4	e	4	U	C2-N1-C1'	6.66	125.69	117.70
3	6	67	C	C5-C6-N1	6.46	124.23	121.00
12	H	9	LEU	CA-CB-CG	6.46	130.16	115.30
2	5	97	U	C5-C6-N1	6.45	125.93	122.70
3	6	54	U	O4'-C1'-N1	6.45	113.36	108.20
7	B	236	LEU	CA-CB-CG	6.44	130.11	115.30
7	B	884	ARG	CA-CB-CG	6.43	127.55	113.40
7	B	199	LEU	CA-CB-CG	6.40	130.01	115.30
6	A	1634	LEU	CA-CB-CG	6.39	130.00	115.30
5	i	508	G	P-O3'-C3'	6.38	127.36	119.70
1	2	10	U	C2-N1-C1'	6.34	125.31	117.70
4	e	-12	U	N3-C2-O2	-6.29	117.80	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	11	U	N1-C2-O2	6.22	127.16	122.80
3	6	89	U	N3-C2-O2	-6.19	117.87	122.20
4	e	4	U	N3-C2-O2	-6.18	117.87	122.20
2	5	90	C	C6-N1-C2	-6.16	117.84	120.30
2	5	79	C	C6-N1-C2	-6.11	117.86	120.30
2	5	90	C	C5-C6-N1	6.09	124.04	121.00
2	5	125	C	C2-N1-C1'	6.06	125.47	118.80
4	e	-12	U	N1-C2-O2	6.05	127.03	122.80
4	e	11	U	C5-C6-N1	6.04	125.72	122.70
35	w	134	SER	O-C-N	6.00	132.30	122.70
6	A	593	LEU	CA-CB-CG	5.99	129.07	115.30
16	M	367	PRO	N-CA-CB	5.96	110.46	103.30
4	e	4	U	N1-C2-O2	5.94	126.96	122.80
3	6	80	U	C5-C6-N1	5.93	125.66	122.70
1	2	41	C	N1-C2-O2	5.92	122.45	118.90
15	L	303	LEU	CA-CB-CG	5.92	128.93	115.30
35	u	39	PRO	N-CA-CB	5.91	110.39	103.30
3	6	66	C	C6-N1-C2	-5.91	117.94	120.30
4	e	6	U	C2-N1-C1'	5.88	124.76	117.70
6	A	786	LEU	CA-CB-CG	5.80	128.64	115.30
3	6	14	C	P-O3'-C3'	5.79	126.64	119.70
2	5	90	C	C2-N1-C1'	5.77	125.14	118.80
3	6	64	U	C5-C6-N1	5.70	125.55	122.70
2	5	99	U	N1-C2-O2	5.69	126.78	122.80
7	B	962	LEU	CA-CB-CG	5.69	128.38	115.30
35	v	134	SER	CA-C-O	-5.69	108.16	120.10
1	2	41	C	P-O3'-C3'	5.67	126.50	119.70
4	e	17	U	OP1-P-O3'	5.66	117.66	105.20
10	F	94	VAL	C-N-CA	5.66	135.85	121.70
1	2	11	U	C5-C6-N1	5.66	125.53	122.70
4	e	11	U	C6-N1-C1'	-5.65	113.29	121.20
22	T	159	TRP	CA-CB-CG	5.63	124.40	113.70
2	5	112	C	C6-N1-C2	-5.63	118.05	120.30
3	6	43	C	N1-C2-O2	5.59	122.26	118.90
6	A	127	LEU	CA-CB-CG	5.59	128.15	115.30
3	6	48	C	C6-N1-C2	-5.57	118.07	120.30
2	5	78	A	OP1-P-O3'	5.52	117.35	105.20
2	5	125	C	C5-C6-N1	5.50	123.75	121.00
2	5	111	C	C6-N1-C2	-5.49	118.11	120.30
19	P	954	HIS	C-N-CA	5.48	135.40	121.70
10	F	37	CYS	CA-CB-SG	5.46	123.82	114.00
2	5	99	U	C2-N1-C1'	5.45	124.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	56	A	P-O3'-C3'	5.44	126.23	119.70
2	5	99	U	N3-C2-O2	-5.41	118.41	122.20
6	A	407	VAL	CG1-CB-CG2	-5.41	102.25	110.90
3	6	89	U	N1-C2-O2	5.38	126.57	122.80
5	i	1111	U	C2-N1-C1'	5.37	124.14	117.70
3	6	64	U	P-O3'-C3'	5.34	126.11	119.70
3	6	67	C	C6-N1-C2	-5.34	118.16	120.30
35	v	76	SER	N-CA-CB	5.33	118.49	110.50
18	O	226	ASP	CB-CG-OD1	5.30	123.07	118.30
1	2	41	C	C5-C6-N1	5.27	123.64	121.00
1	2	21	G	C8-N9-C1'	-5.22	120.21	127.00
6	A	582	LEU	CA-CB-CG	5.22	127.30	115.30
11	G	221	LEU	CA-CB-CG	5.20	127.25	115.30
19	P	1059	LEU	CA-CB-CG	5.17	127.19	115.30
35	v	134	SER	O-C-N	5.17	130.96	122.70
1	2	11	U	N3-C2-O2	-5.12	118.62	122.20
35	w	306	ASP	CB-CA-C	-5.12	100.17	110.40
3	6	89	U	C2-N1-C1'	5.09	123.81	117.70
35	u	306	ASP	CB-CA-C	-5.09	100.22	110.40
2	5	97	U	O5'-P-OP1	-5.07	101.14	105.70
5	i	1111	U	N3-C2-O2	-5.07	118.65	122.20
8	D	373	LEU	CA-CB-CG	5.06	126.94	115.30
2	5	101	C	N1-C2-O2	5.03	121.92	118.90
3	6	61	C	C6-N1-C2	-5.02	118.29	120.30
2	5	78	A	P-O3'-C3'	5.01	125.72	119.70
20	R	100	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	1474	ARG	Peptide
6	A	405	ASN	Peptide
6	A	542	HIS	Peptide
6	A	774	ILE	Peptide
6	A	775	ARG	Peptide
7	B	114	PRO	Peptide
7	B	179	ASP	Peptide
7	B	572	ILE	Peptide
7	B	597	TYR	Peptide
7	B	682	SER	Peptide

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Mol	Chain	Res	Type	Group
7	B	769	TYR	Peptide
7	B	777	ASP	Peptide
7	B	977	SER	Peptide
7	B	978	THR	Peptide
8	D	277	VAL	Peptide
8	D	341	LEU	Peptide
9	E	106	LEU	Peptide
9	E	107	ASN	Peptide
9	E	143	VAL	Peptide
10	F	120	LEU	Peptide
11	G	206	LEU	Peptide
11	G	23	PRO	Peptide
15	L	300	LYS	Peptide
18	O	322	LYS	Peptide
30	k	84	LEU	Peptide
35	u	134	SER	Mainchain
35	v	109	LEU	Mainchain
35	w	134	SER	Mainchain
35	w	3	CYS	Mainchain
36	y	111	VAL	Peptide
36	y	132	LEU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	1954/2413 (81%)	1813 (93%)	126 (6%)	15 (1%)	19	51
7	B	889/1008 (88%)	830 (93%)	55 (6%)	4 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	D	357/451 (79%)	329 (92%)	28 (8%)	0	100	100
9	E	176/379 (46%)	164 (93%)	11 (6%)	1 (1%)	25	57
10	F	193/364 (53%)	173 (90%)	19 (10%)	1 (0%)	29	61
11	G	253/339 (75%)	229 (90%)	23 (9%)	1 (0%)	34	66
12	H	64/175 (37%)	55 (86%)	8 (12%)	1 (2%)	9	36
13	I	154/157 (98%)	140 (91%)	14 (9%)	0	100	100
14	K	76/135 (56%)	72 (95%)	4 (5%)	0	100	100
15	L	406/577 (70%)	380 (94%)	26 (6%)	0	100	100
16	M	320/455 (70%)	302 (94%)	18 (6%)	0	100	100
17	N	163/251 (65%)	157 (96%)	6 (4%)	0	100	100
18	O	215/382 (56%)	196 (91%)	19 (9%)	0	100	100
19	P	645/1145 (56%)	610 (95%)	35 (5%)	0	100	100
20	R	97/215 (45%)	94 (97%)	3 (3%)	0	100	100
21	S	234/590 (40%)	223 (95%)	11 (5%)	0	100	100
22	T	451/687 (66%)	442 (98%)	9 (2%)	0	100	100
23	U	587/859 (68%)	555 (94%)	30 (5%)	2 (0%)	41	71
26	a	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
26	q	91/110 (83%)	84 (92%)	7 (8%)	0	100	100
27	b	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	m	70/86 (81%)	65 (93%)	5 (7%)	0	100	100
28	c	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
28	l	71/94 (76%)	66 (93%)	4 (6%)	1 (1%)	11	38
29	d	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
29	n	65/77 (84%)	57 (88%)	8 (12%)	0	100	100
30	f	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
30	k	74/196 (38%)	66 (89%)	7 (10%)	1 (1%)	11	38
31	g	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
31	o	74/101 (73%)	70 (95%)	4 (5%)	0	100	100
32	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
32	p	75/146 (51%)	65 (87%)	8 (11%)	2 (3%)	5	26
33	r	82/111 (74%)	76 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	s	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	2	14
35	u	423/503 (84%)	413 (98%)	8 (2%)	2 (0%)	29	61
35	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	5	27
35	w	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
35	x	112/503 (22%)	104 (93%)	8 (7%)	0	100	100
36	y	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	11
All	All	9709/14738 (66%)	9051 (93%)	610 (6%)	48 (0%)	32	61

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	1905	LEU
12	H	9	LEU
23	U	37	ILE
34	s	76	ILE
36	y	94	LYS
36	y	111	VAL
36	y	133	PRO
6	A	483	PRO
6	A	775	ARG
6	A	1675	VAL
7	B	778	THR
9	E	107	ASN
34	s	122	ARG
35	v	109	LEU
36	y	105	PRO
36	y	136	VAL
6	A	180	PRO
6	A	401	PRO
6	A	1475	LEU
6	A	1674	ASP
7	B	573	LYS
30	k	81	VAL
34	s	95	PRO
35	v	20	ARG
6	A	543	ASN
6	A	776	GLN
7	B	116	THR
10	F	120	LEU
11	G	120	TYR

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Mol	Chain	Res	Type
23	U	300	ASP
32	p	31	SER
34	s	68	PRO
34	s	94	LEU
34	s	129	LEU
35	u	20	ARG
36	y	119	SER
6	A	406	PRO
6	A	1328	PHE
6	A	1491	ILE
7	B	979	GLY
32	p	98	PRO
35	u	17	PRO
6	A	181	HIS
6	A	484	PHE
28	l	74	GLY
34	s	56	ILE
34	s	98	VAL
35	v	36	GLY

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	
6	A	1778/2182 (82%)	1741 (98%)	37 (2%)	53	75
7	B	809/910 (89%)	797 (98%)	12 (2%)	65	81
8	D	313/397 (79%)	307 (98%)	6 (2%)	57	77
9	E	168/328 (51%)	166 (99%)	2 (1%)	71	83
10	F	183/332 (55%)	183 (100%)	0	100	100
11	G	219/296 (74%)	216 (99%)	3 (1%)	67	82
12	H	58/151 (38%)	53 (91%)	5 (9%)	10	35
13	I	140/141 (99%)	139 (99%)	1 (1%)	84	90
14	K	44/121 (36%)	43 (98%)	1 (2%)	50	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	L	379/538 (70%)	377 (100%)	2 (0%)	88	93
16	M	288/413 (70%)	283 (98%)	5 (2%)	60	78
17	N	144/225 (64%)	143 (99%)	1 (1%)	84	90
18	O	210/346 (61%)	208 (99%)	2 (1%)	76	86
19	P	178/1029 (17%)	176 (99%)	2 (1%)	73	85
20	R	90/193 (47%)	89 (99%)	1 (1%)	73	85
21	S	208/525 (40%)	207 (100%)	1 (0%)	88	93
22	T	248/633 (39%)	244 (98%)	4 (2%)	62	79
23	U	131/786 (17%)	126 (96%)	5 (4%)	33	62
26	a	79/103 (77%)	79 (100%)	0	100	100
26	q	77/103 (75%)	74 (96%)	3 (4%)	32	62
27	b	63/77 (82%)	63 (100%)	0	100	100
27	m	63/77 (82%)	61 (97%)	2 (3%)	39	67
28	c	65/83 (78%)	63 (97%)	2 (3%)	40	67
28	l	65/83 (78%)	60 (92%)	5 (8%)	13	38
29	d	58/66 (88%)	57 (98%)	1 (2%)	60	78
29	n	57/66 (86%)	56 (98%)	1 (2%)	59	78
30	f	70/176 (40%)	70 (100%)	0	100	100
30	k	67/176 (38%)	66 (98%)	1 (2%)	65	81
31	g	69/89 (78%)	69 (100%)	0	100	100
31	o	67/89 (75%)	64 (96%)	3 (4%)	27	58
32	h	77/129 (60%)	76 (99%)	1 (1%)	69	82
32	p	73/129 (57%)	63 (86%)	10 (14%)	3	16
All	All	6538/10992 (60%)	6419 (98%)	119 (2%)	61	78

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	334	LYS
6	A	343	ASN
6	A	355	LEU
6	A	396	ARG
6	A	526	LEU
6	A	653	ILE

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Mol	Chain	Res	Type
6	A	705	GLN
6	A	716	ARG
6	A	760	ASN
6	A	848	ASN
6	A	906	LYS
6	A	944	TYR
6	A	1067	ASN
6	A	1105	ARG
6	A	1295	GLN
6	A	1346	PHE
6	A	1426	ARG
6	A	1456	ARG
6	A	1465	ARG
6	A	1466	GLN
6	A	1521	ARG
6	A	1529	ASN
6	A	1553	ILE
6	A	1561	LEU
6	A	1568	ASN
6	A	1695	ASN
6	A	1739	ARG
6	A	1753	ARG
6	A	1782	ASN
6	A	1803	ARG
6	A	1809	ASN
6	A	1903	LYS
6	A	1998	ARG
6	A	2018	ASN
6	A	2027	LEU
6	A	2086	GLN
6	A	2098	MET
7	B	180	ASN
7	B	268	ASN
7	B	289	ASN
7	B	294	ASN
7	B	358	ASN
7	B	360	ARG
7	B	428	ILE
7	B	545	LEU
7	B	590	LYS
7	B	764	ASN
7	B	884	ARG

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Mol	Chain	Res	Type
7	B	960	ASN
8	D	152	ASN
8	D	160	ASN
8	D	194	HIS
8	D	200	VAL
8	D	227	VAL
8	D	266	LYS
9	E	87	ASN
9	E	106	LEU
11	G	44	ASN
11	G	151	LEU
11	G	206	LEU
12	H	8	GLN
12	H	30	LEU
12	H	36	THR
12	H	135	ARG
12	H	157	ILE
13	I	128	GLN
14	K	71	ARG
15	L	84	ASN
15	L	201	ARG
16	M	156	ARG
16	M	325	ASN
16	M	339	MET
16	M	378	LYS
16	M	406	ARG
17	N	177	ASN
18	O	278	LEU
18	O	284	LYS
19	P	1006	LYS
19	P	1059	LEU
20	R	92	ARG
21	S	236	GLN
22	T	61	ASN
22	T	123	ASN
22	T	183	ASN
22	T	201	THR
23	U	663	LYS
23	U	726	ARG
23	U	760	ARG
23	U	777	ASN
23	U	801	LEU

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Mol	Chain	Res	Type
28	c	25	THR
28	c	92	SER
29	d	66	ASN
32	h	16	THR
30	k	19	LYS
28	l	54	ILE
28	l	77	LEU
28	l	79	LYS
28	l	81	LEU
28	l	82	LEU
27	m	34	ASN
27	m	79	LEU
29	n	71	LEU
31	o	20	SER
31	o	43	GLN
31	o	76	ASP
32	p	11	ARG
32	p	15	VAL
32	p	16	THR
32	p	25	VAL
32	p	43	VAL
32	p	44	LYS
32	p	95	ILE
32	p	96	ILE
32	p	97	LEU
32	p	101	LEU
26	q	41	ARG
26	q	82	LYS
26	q	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
6	A	310	ASN
6	A	343	ASN
6	A	481	HIS
6	A	648	GLN
6	A	676	GLN
6	A	748	GLN
6	A	974	ASN
6	A	1087	ASN
6	A	1156	HIS

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Mol	Chain	Res	Type
6	A	1368	GLN
6	A	1449	ASN
6	A	1455	GLN
6	A	1529	ASN
6	A	1548	GLN
6	A	1568	ASN
6	A	1687	HIS
6	A	1695	ASN
6	A	1782	ASN
6	A	1809	ASN
6	A	1824	GLN
6	A	1876	ASN
6	A	1895	HIS
7	B	101	GLN
7	B	103	HIS
7	B	180	ASN
7	B	255	GLN
7	B	268	ASN
7	B	289	ASN
7	B	294	ASN
7	B	358	ASN
7	B	511	GLN
7	B	514	GLN
7	B	647	ASN
7	B	764	ASN
7	B	869	HIS
7	B	960	ASN
7	B	1004	ASN
8	D	428	GLN
9	E	87	ASN
9	E	107	ASN
10	F	89	HIS
11	G	39	GLN
11	G	44	ASN
11	G	248	ASN
12	H	8	GLN
12	H	173	HIS
13	I	48	GLN
15	L	14	GLN
15	L	66	ASN
15	L	354	HIS
15	L	390	HIS

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Mol	Chain	Res	Type
15	L	441	ASN
15	L	457	HIS
16	M	219	GLN
16	M	261	HIS
16	M	325	ASN
16	M	380	HIS
17	N	177	ASN
17	N	208	HIS
18	O	39	ASN
18	O	327	HIS
19	P	960	HIS
19	P	986	HIS
19	P	989	HIS
19	P	1082	GLN
19	P	1107	GLN
20	R	184	GLN
20	R	200	ASN
20	R	204	ASN
22	T	61	ASN
22	T	183	ASN
22	T	210	ASN
22	T	277	ASN
23	U	777	ASN
32	h	94	GLN
29	n	53	ASN
32	p	14	GLN
32	p	21	ASN
32	p	86	ASN
32	p	94	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	127/1175 (10%)	44 (34%)	4 (3%)
2	5	100/214 (46%)	25 (25%)	2 (2%)
3	6	101/112 (90%)	28 (27%)	3 (2%)
4	e	33/34 (97%)	19 (57%)	0
5	i	54/59 (91%)	18 (33%)	0
All	All	415/1594 (26%)	134 (32%)	9 (2%)

All (134) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	A
1	2	11	U
1	2	16	U
1	2	17	U
1	2	18	U
1	2	19	U
1	2	20	G
1	2	21	G
1	2	23	U
1	2	24	U
1	2	25	A
1	2	30	A
1	2	31	A
1	2	32	G
1	2	40	U
1	2	41	C
1	2	42	U
1	2	63	U
1	2	64	G
1	2	141	A
1	2	1094	G
1	2	1096	C
1	2	1098	C
1	2	1099	G
1	2	1100	A
1	2	1101	C
1	2	1102	C
1	2	1103	C
1	2	1104	U
1	2	1106	G
1	2	1107	C
1	2	1108	A
1	2	1120	G
1	2	1123	C
1	2	1124	U
1	2	1125	U
1	2	1126	G
1	2	1139	G
1	2	1144	U
1	2	1145	U
1	2	1146	G
1	2	1149	G
1	2	1152	U

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Mol	Chain	Res	Type
1	2	1166	G
2	5	33	U
2	5	42	A
2	5	43	G
2	5	44	A
2	5	45	A
2	5	46	C
2	5	70	A
2	5	75	A
2	5	76	U
2	5	77	A
2	5	79	C
2	5	80	G
2	5	81	A
2	5	82	A
2	5	84	A
2	5	92	U
2	5	96	U
2	5	101	C
2	5	108	C
2	5	113	G
2	5	127	U
2	5	169	U
2	5	170	U
2	5	171	U
2	5	172	U
3	6	12	A
3	6	13	A
3	6	14	C
3	6	15	C
3	6	17	U
3	6	34	A
3	6	36	U
3	6	42	A
3	6	44	A
3	6	53	A
3	6	54	U
3	6	55	G
3	6	57	U
3	6	59	A
3	6	60	G
3	6	62	A

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Mol	Chain	Res	Type
3	6	64	U
3	6	65	U
3	6	66	C
3	6	67	C
3	6	73	A
3	6	74	U
3	6	80	U
3	6	81	G
3	6	85	C
3	6	86	G
3	6	88	U
3	6	99	A
4	e	-12	U
4	e	-11	U
4	e	-9	A
4	e	-4	A
4	e	3	A
4	e	4	U
4	e	5	A
4	e	6	U
4	e	8	U
4	e	9	U
4	e	10	U
4	e	11	U
4	e	13	U
4	e	15	U
4	e	17	U
4	e	18	U
4	e	19	U
4	e	20	A
4	e	21	U
5	i	2	U
5	i	9	U
5	i	505	C
5	i	508	G
5	i	509	U
5	i	511	A
5	i	514	A
5	i	515	A
5	i	516	C
5	i	518	U
5	i	1008	A

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Mol	Chain	Res	Type
5	i	1111	U
5	i	1112	U
5	i	1113	A
5	i	1114	U
5	i	1115	A
5	i	1117	A
5	i	1118	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	41	C
1	2	1123	C
1	2	1124	U
1	2	1145	U
2	5	78	A
2	5	81	A
3	6	14	C
3	6	56	A
3	6	64	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 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
38	IHP	A	3001	-	36,36,36	0.87	0	54,60,60	1.55	8 (14%)
39	GTP	B	2001	37	26,34,34	1.41	3 (11%)	32,54,54	1.84	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
38	IHP	A	3001	-	-	7/30/54/54	0/1/1/1
39	GTP	B	2001	37	-	5/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	2001	GTP	C5-C6	-4.67	1.37	1.47
39	B	2001	GTP	C5-C4	-2.39	1.37	1.43
39	B	2001	GTP	O4'-C4'	-2.13	1.40	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B	2001	GTP	PB-O3B-PG	-5.88	112.65	132.83
39	B	2001	GTP	C5-C6-N1	3.84	120.73	113.95
38	A	3001	IHP	C4-C3-C2	3.67	118.45	110.41
38	A	3001	IHP	C5-C6-C1	3.64	118.38	110.41
38	A	3001	IHP	C5-C4-C3	3.48	118.02	110.41
38	A	3001	IHP	O15-C5-C6	3.29	116.44	108.69
39	B	2001	GTP	PA-O3A-PB	-3.24	121.70	132.83
38	A	3001	IHP	C3-C2-C1	3.22	117.47	110.41
39	B	2001	GTP	C8-N7-C5	3.06	108.82	102.99
39	B	2001	GTP	C2-N1-C6	-2.90	119.75	125.10
38	A	3001	IHP	O11-C1-C2	2.42	114.38	108.69
38	A	3001	IHP	O11-C1-C6	2.32	114.15	108.69
38	A	3001	IHP	O15-C5-C4	2.30	114.11	108.69
39	B	2001	GTP	O6-C6-C5	-2.08	120.30	124.37
39	B	2001	GTP	N1-C2-N3	-2.03	119.52	123.32

There are no chirality outliers.

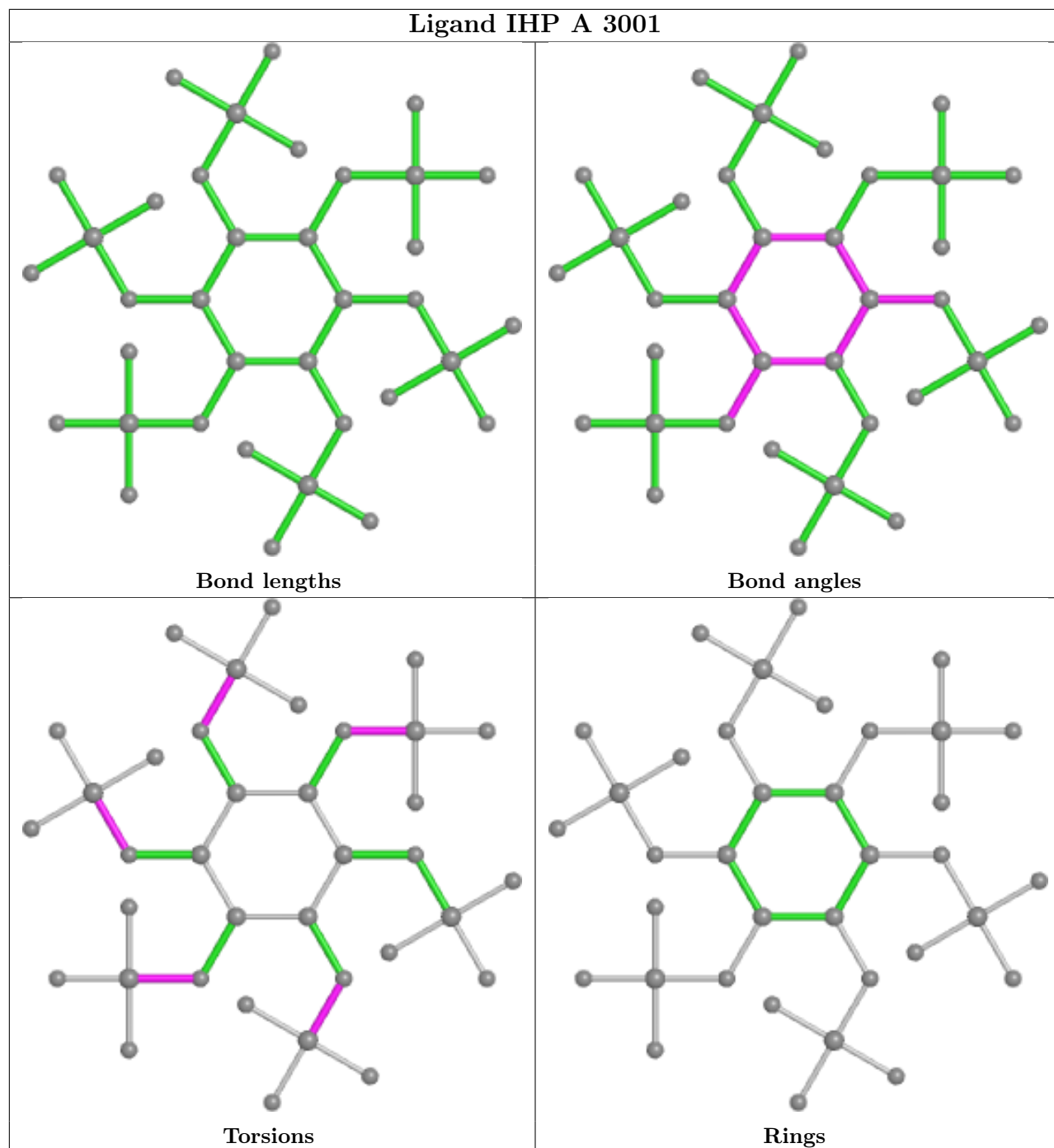
All (12) torsion outliers are listed below:

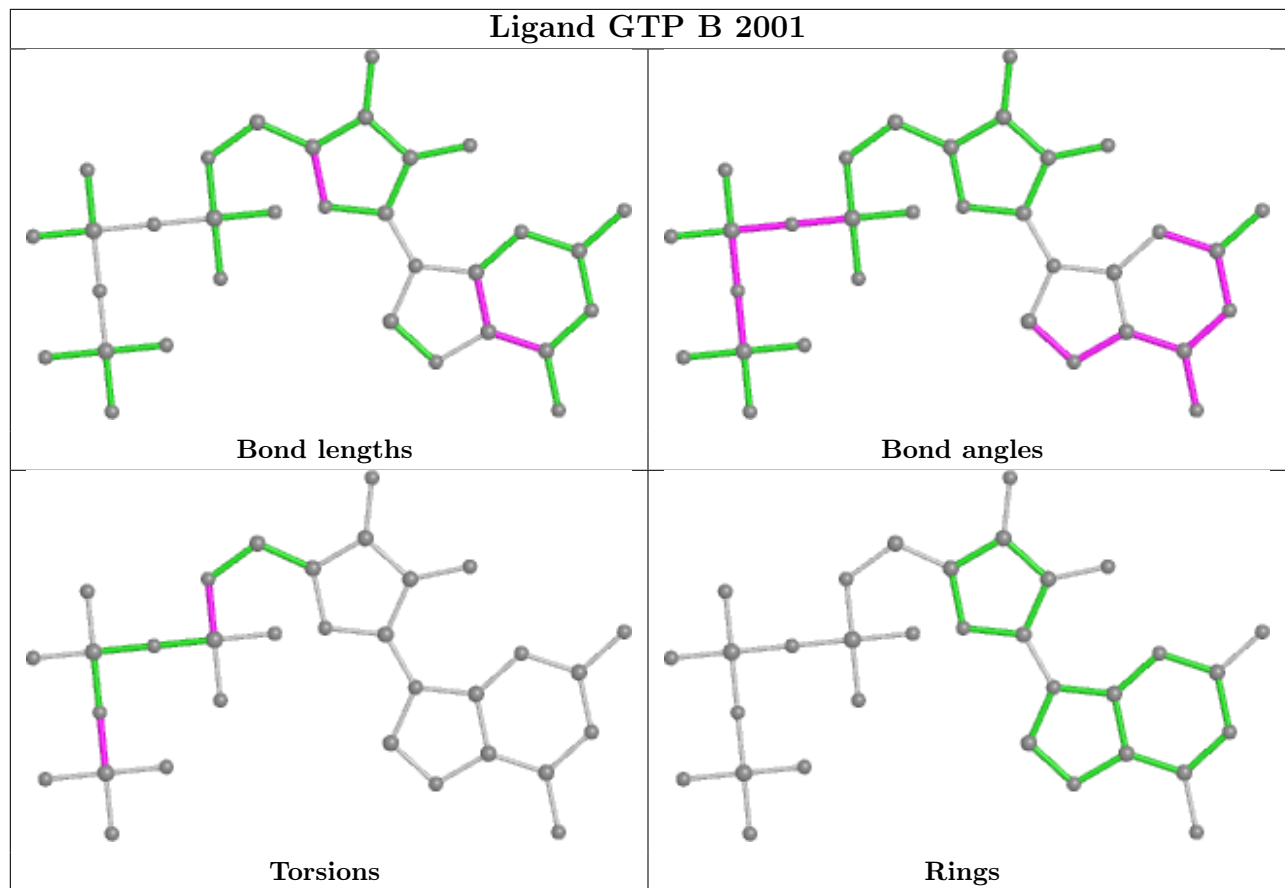
Mol	Chain	Res	Type	Atoms
38	A	3001	IHP	C1-O11-P1-O21
38	A	3001	IHP	C2-O12-P2-O22
38	A	3001	IHP	C3-O13-P3-O23
38	A	3001	IHP	C4-O14-P4-O34
38	A	3001	IHP	C6-O16-P6-O36
39	B	2001	GTP	PB-O3B-PG-O2G
39	B	2001	GTP	C5'-O5'-PA-O3A
39	B	2001	GTP	C5'-O5'-PA-O1A
39	B	2001	GTP	C5'-O5'-PA-O2A
39	B	2001	GTP	PB-O3B-PG-O3G
38	A	3001	IHP	C1-O11-P1-O41
38	A	3001	IHP	C3-O13-P3-O33

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	i	4
24	X	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	15:U	O3'	501:A	P	58.05
1	X	3370:UNK	C	3389:UNK	N	35.33
1	X	1031:UNK	C	2287:UNK	N	34.77
1	X	125:UNK	C	1001:UNK	N	25.13
1	X	2322:UNK	C	3364:UNK	N	19.85

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	628:U	O3'	1001:A	P	15.34
1	i	518:U	O3'	620:U	P	7.99
1	i	1008:A	O3'	1110:A	P	5.10

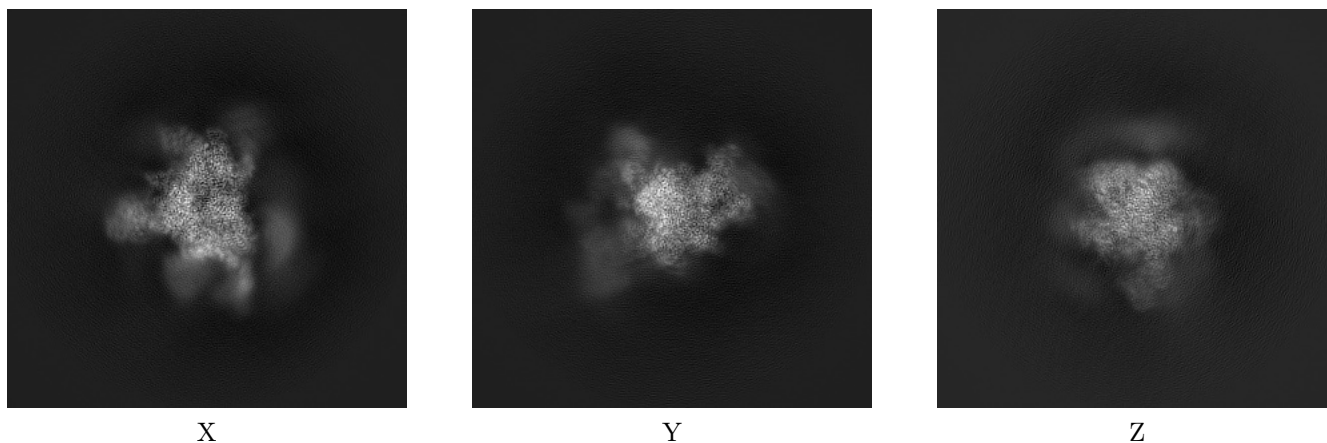
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7109. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

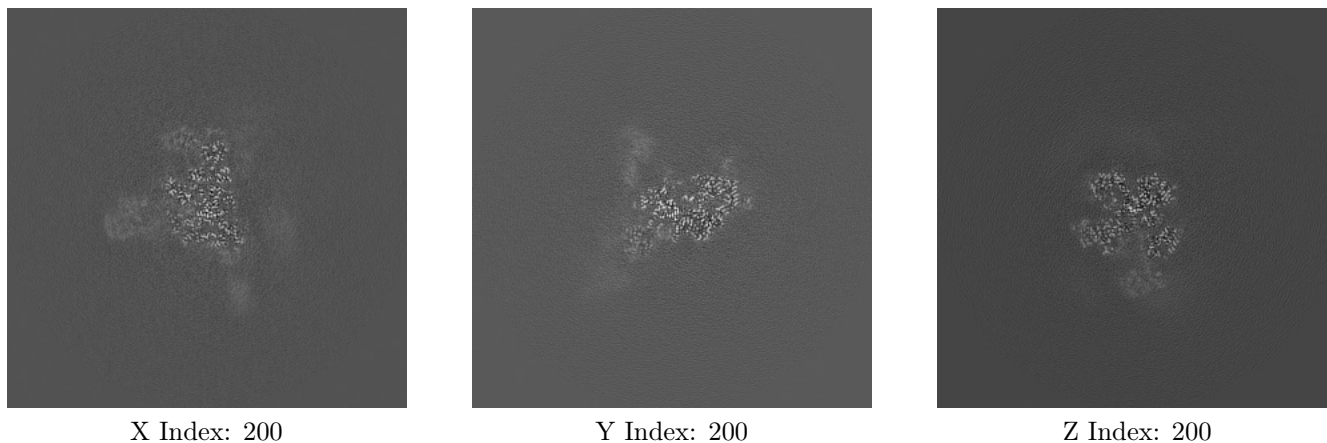
6.1.1 Primary map



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

6.2 Central slices [i](#)

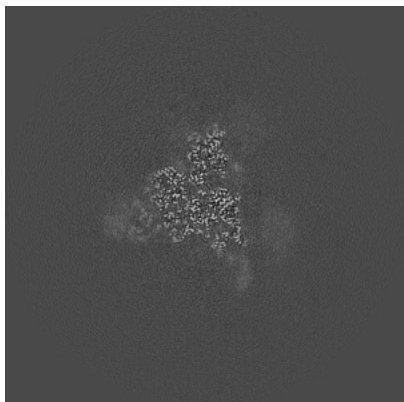
6.2.1 Primary map



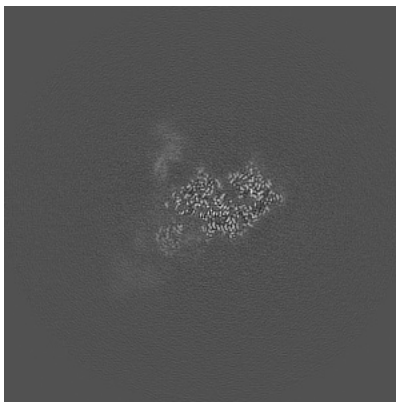
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

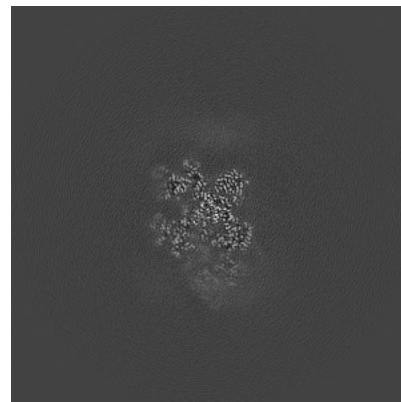
6.3.1 Primary map



X Index: 212



Y Index: 204

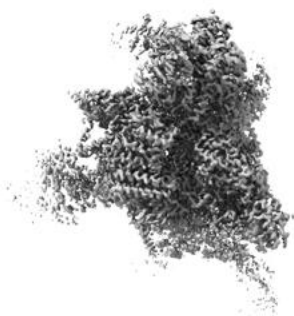


Z Index: 191

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

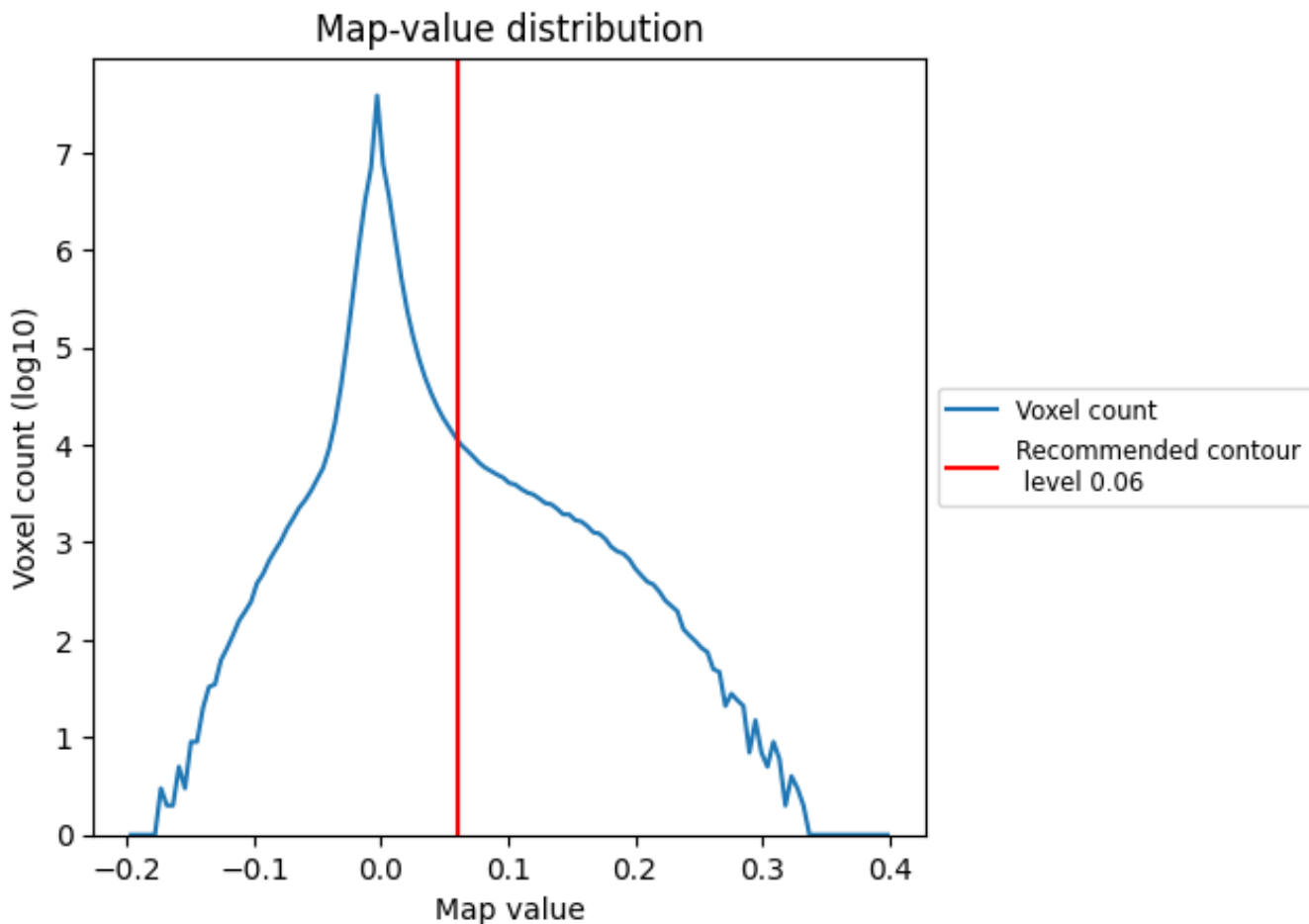
6.5 Mask visualisation

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

7 Map analysis [i](#)

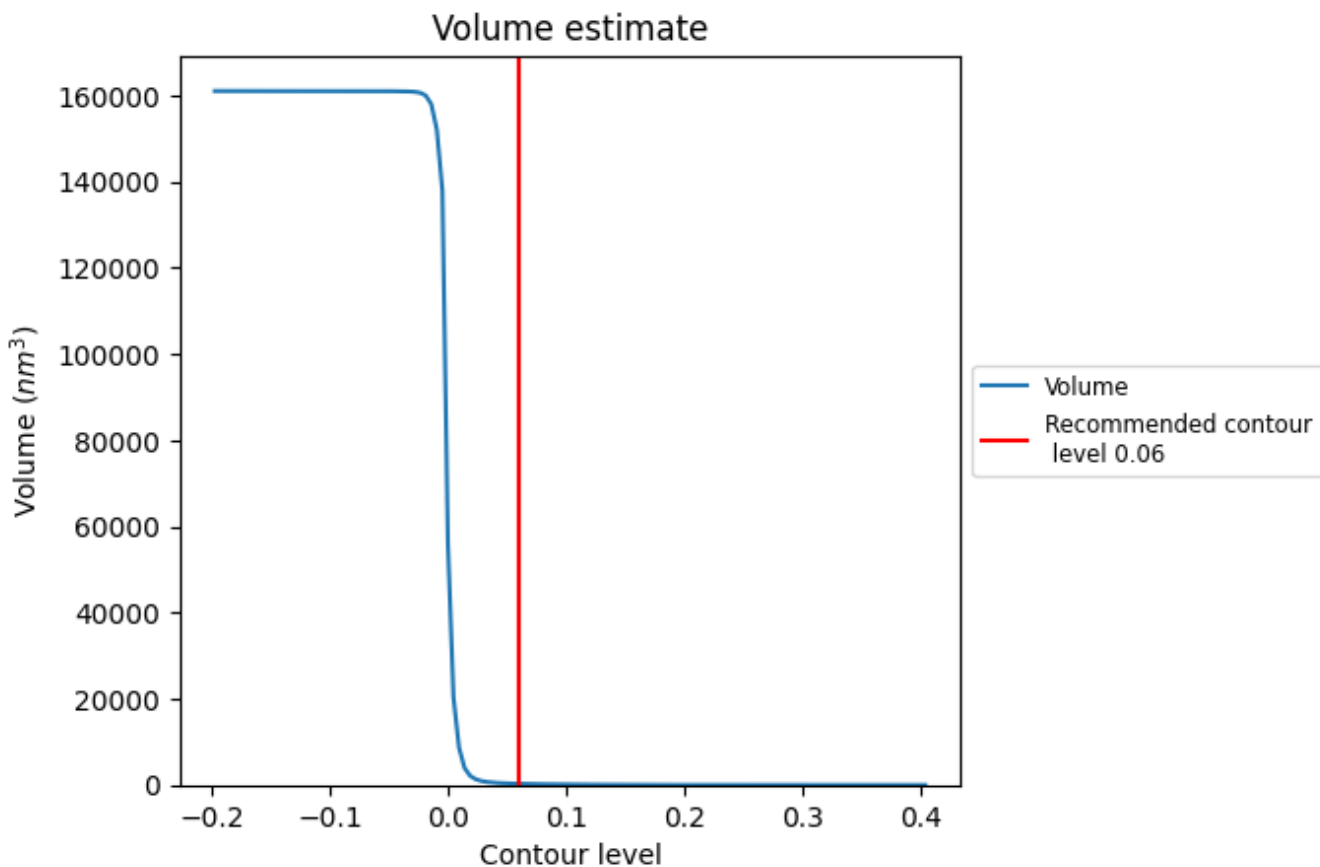
This section contains the results of statistical analysis of the map.

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.

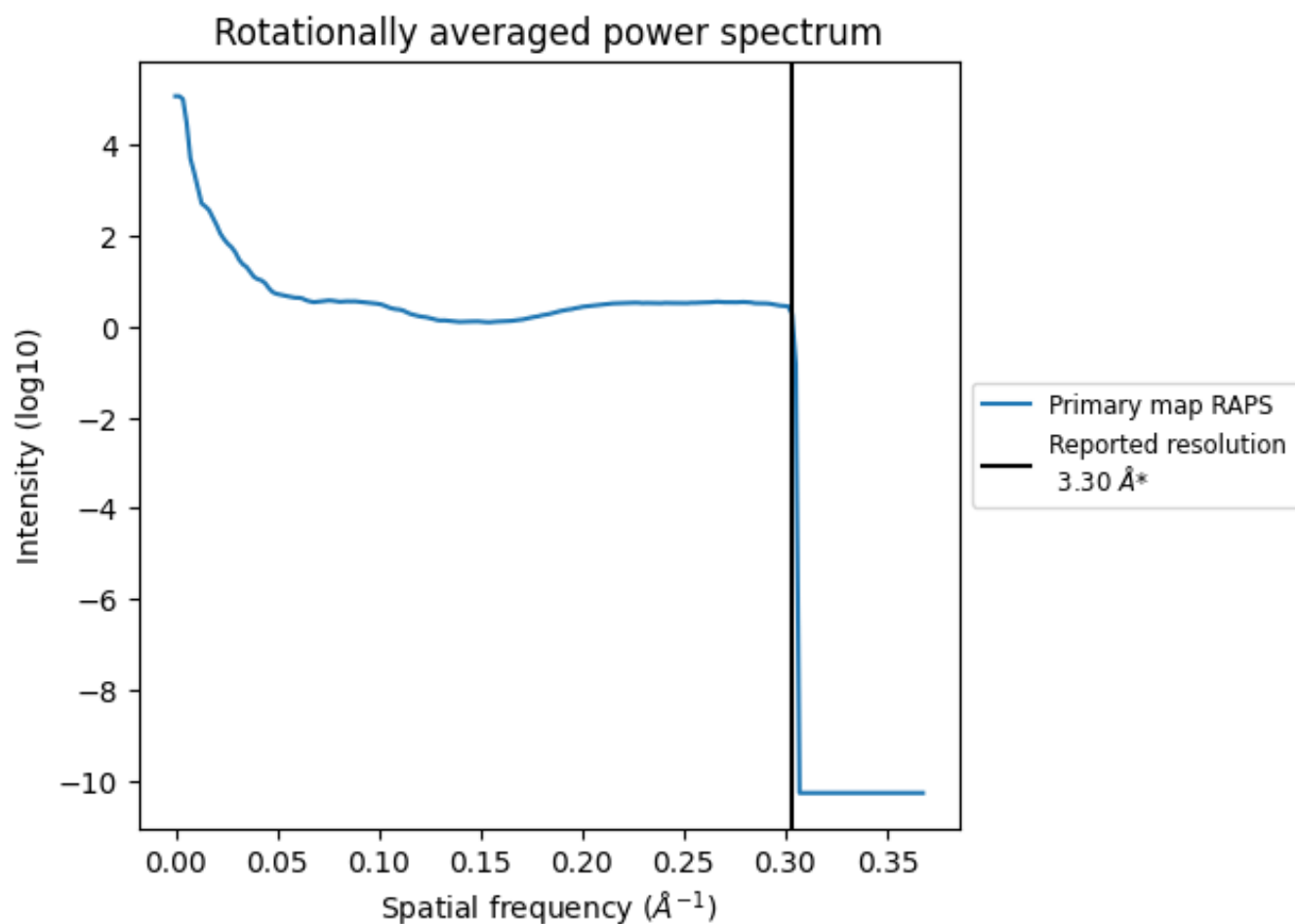
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 272 nm^3 ; this corresponds to an approximate mass of 246 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 0.303 Å⁻¹

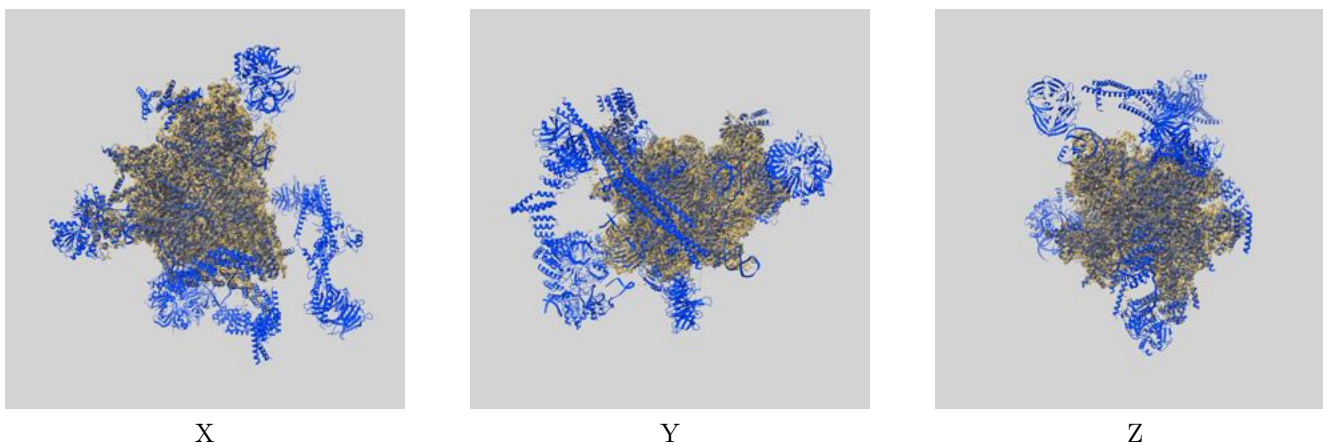
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

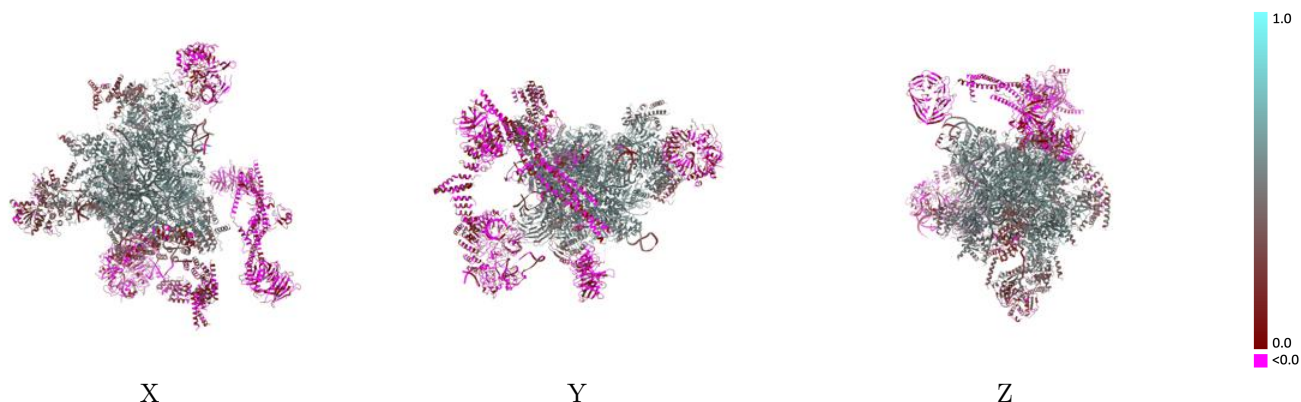
This section contains information regarding the fit between EMDB map EMD-7109 and PDB model 6BK8. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



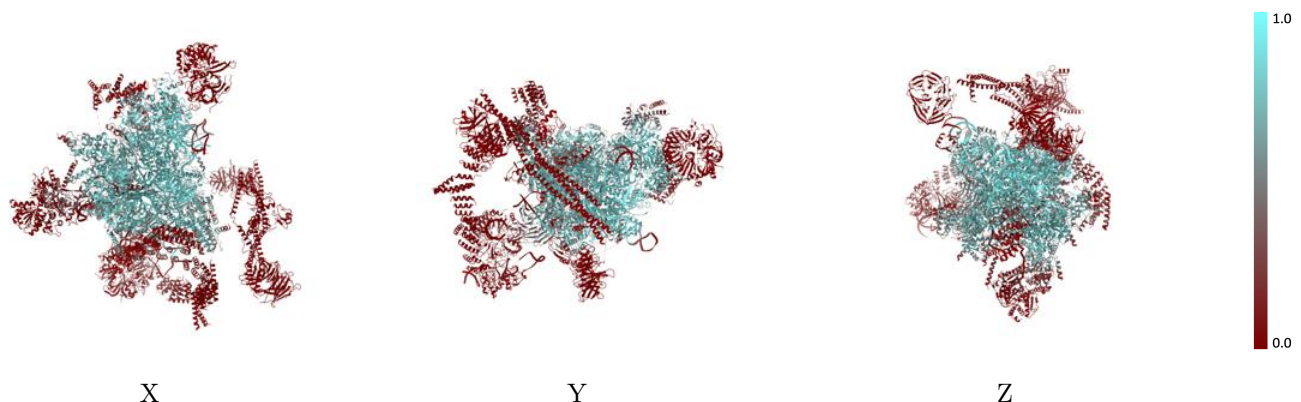
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



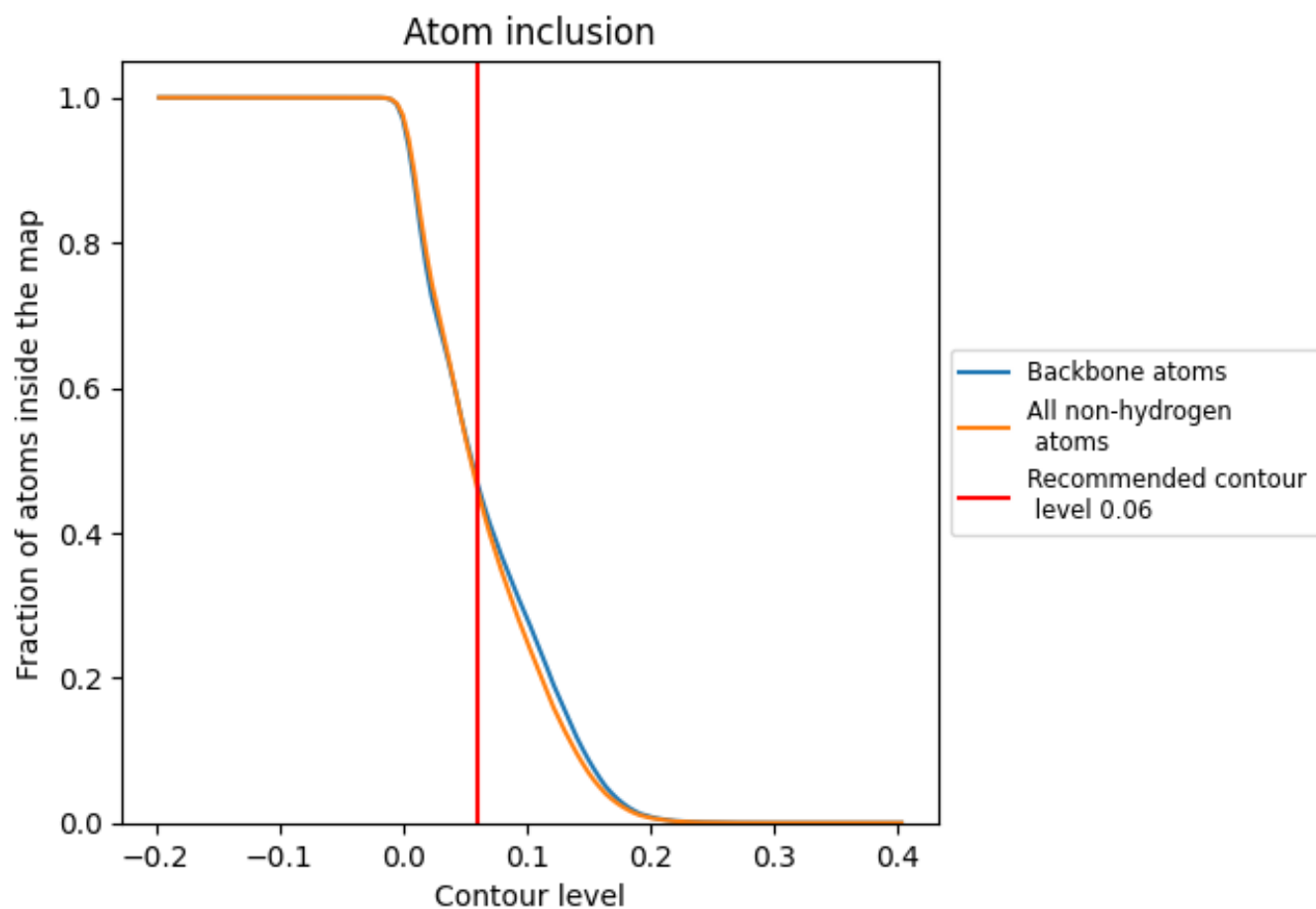
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 46% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4632	 0.3800
2	 0.2015	 0.1350
5	 0.7193	 0.4800
6	 0.7544	 0.5110
A	 0.7657	 0.5480
B	 0.7221	 0.5340
D	 0.7989	 0.5590
E	 0.6658	 0.5200
F	 0.5405	 0.4790
G	 0.6927	 0.5240
H	 0.5263	 0.5260
I	 0.7560	 0.5480
K	 0.3796	 0.4500
L	 0.4029	 0.3920
M	 0.5041	 0.5000
N	 0.5580	 0.4770
O	 0.4718	 0.4870
P	 0.1572	 0.3460
R	 0.5997	 0.5230
S	 0.7018	 0.5300
T	 0.5065	 0.4260
U	 0.0772	 0.2040
X	 0.4055	 0.4340
Y	 0.3375	 0.3790
a	 0.0000	 0.0440
b	 0.0000	 0.0190
c	 0.0000	 0.0250
d	 0.0000	 0.0920
e	 0.4158	 0.4330
f	 0.0000	 0.0780
g	 0.0000	 0.1650
h	 0.0000	 0.0050
i	 0.4262	 0.3650
k	 0.0000	 0.0040
l	 0.0000	 0.0130



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Chain	Atom inclusion	Q-score
m	0.0000	0.0240
n	0.0000	0.0090
o	0.0000	0.0240
p	0.0000	0.0100
q	0.0000	0.0120
r	0.0000	0.0330
s	0.0000	0.0040
u	0.0000	-0.0080
v	0.0000	-0.0290
w	0.0000	-0.0040
x	0.0000	-0.0220
y	0.0000	-0.0290