



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 10:51 PM UTC

PDB ID : 6ID0 / pdb_00006id0
EMDB ID : EMD-9646
Title : Cryo-EM structure of a human intron lariat spliceosome prior to Prp43 loaded (ILS1 complex) at 2.9 angstrom resolution
Authors : Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on : 2018-09-07
Resolution : 2.90 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 ⓘ 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:

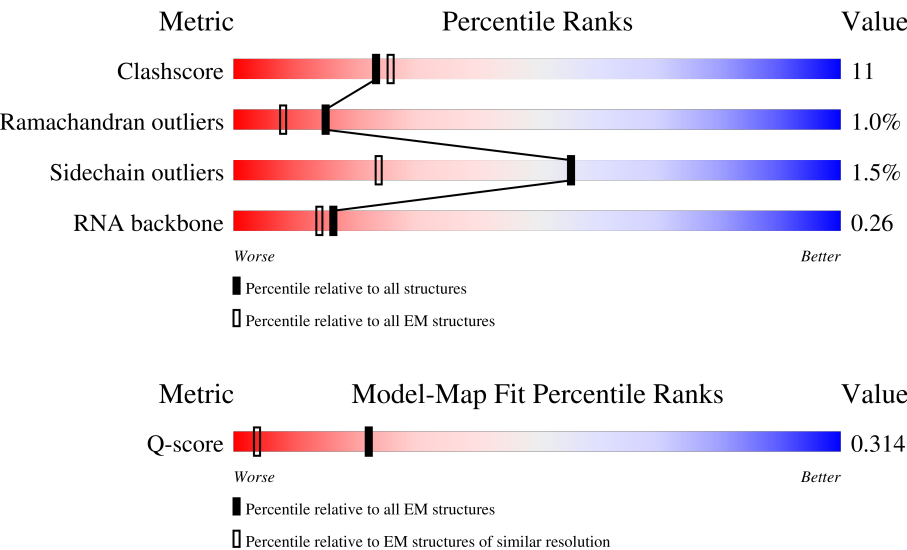
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 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	13054 (2.40 - 3.40)

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	A	2335	69%15%15%
2	B	117	9% 32%30%21%16%
3	C	972	70%20%9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	357	
5	F	107	
6	J	848	
7	L	802	
8	M	243	
9	N	144	
10	O	420	
11	P	229	
12	R	536	
13	S	166	
14	T	514	
15	W	579	
16	G	272	
17	H	188	
18	U	894	
19	I	855	
20	a	126	
20	h	126	
21	b	231	
21	i	231	
22	c	119	
22	j	119	
23	d	118	
23	k	118	
24	f	86	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
24	m	86	
25	e	92	
25	l	92	
26	g	76	
26	n	76	
27	q	504	
27	r	504	
27	s	504	
27	t	504	
28	K	225	
29	o	255	
30	p	225	
31	Q	1485	
32	y	301	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	GTP	C	1500	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 78004 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1981	Total	C	N	O	S	0	0
			16477	10621	2883	2902	71		

- Molecule 2 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	P	0	0
			2060	923	341	698	98		

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	888	Total	C	N	O	S	0	0
			7022	4494	1172	1322	34		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	303	Total	C	N	O	S	0	0
			2366	1487	415	451	13		

- Molecule 5 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 6 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	556	Total	C	N	O	S	0	0
			3758	2344	705	703	6		

- Molecule 7 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	475	Total	C	N	O	S	0	0
			3237	1985	627	619	6		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 9 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 10 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	290	Total	C	N	O	S	0	0
			2340	1469	415	436	20		

- Molecule 11 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	118	Total	C	N	O	S	0	0
			985	601	194	188	2		

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	272	Total	C	N	O	P	S	0	0
			2165	1357	393	401	2	12		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 14 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	317	Total	C	N	O	S	0	0
			2496	1574	453	461	8		

- Molecule 15 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	509	Total	C	N	O	S	0	0
			3008	1833	568	603	4		

- Molecule 16 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	70	Total	C	N	O	P	0	0
			1246	549	158	469	70		

- Molecule 17 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	140	Total	C	N	O	P	0	0
			2968	1327	511	990	140		

- Molecule 18 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	347	Total	C	N	O	S	0	0
			2864	1817	496	529	22		

- Molecule 19 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	568	Total	C	N	O	S	0	0
			2822	1683	569	569	1		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	a	81	Total	C	N	O	0	0
			399	237	81	81		
20	h	81	Total	C	N	O	0	0
			398	236	81	81		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	b	86	Total	C	N	O	0	0
			424	252	86	86		
21	i	86	Total	C	N	O	0	0
			424	252	86	86		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	c	82	Total	C	N	O	0	0
			406	242	82	82		
22	j	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	d	97	Total	C	N	O	0	0
			480	286	97	97		
23	k	85	Total	C	N	O	0	0
			422	252	85	85		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	f	74	Total	C	N	O	0	0
			361	213	74	74		
24	m	74	Total	C	N	O	0	0
			361	213	74	74		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	e	79	Total	C	N	O	0	0
			391	233	79	79		
25	l	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	g	74	Total	C	N	O	0	0
			363	215	74	74		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
26	n	67	Total	C	N	O	0	0
			329	195	67	67		

- Molecule 27 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	q	132	Total	C	N	O	0	0
			659	395	132	132		
27	r	131	Total	C	N	O	0	0
			654	392	131	131		
27	s	67	Total	C	N	O	0	0
			335	201	67	67		
27	t	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 28 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	K	152	Total	C	N	O	0	0
			757	453	152	152		

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	162	Total	C	N	O	0	0
			804	480	162	162		

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	p	94	Total	C	N	O	0	0
			464	276	94	94		

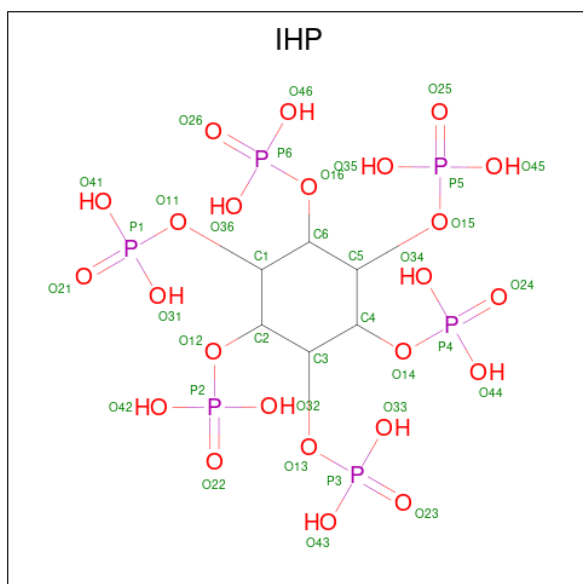
- Molecule 31 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Q	1322	Total	C	N	O	4	0
			6562	3918	1322	1322		

- Molecule 32 is a protein called Peptidyl-prolyl cis-trans isomerase E.

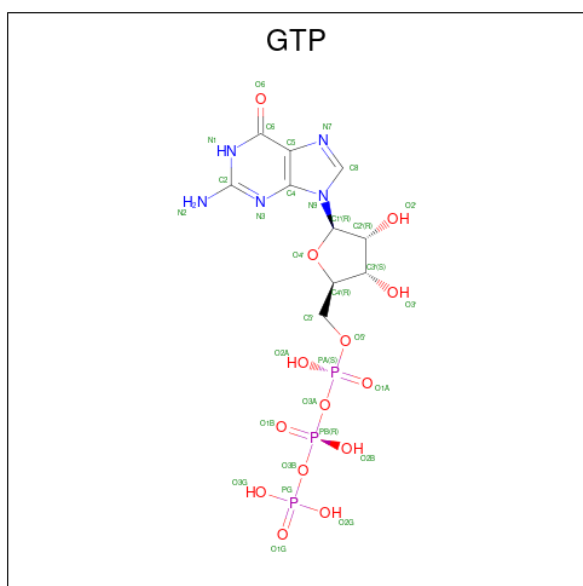
Mol	Chain	Residues	Atoms				AltConf	Trace
32	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 33 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$).



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

- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	C	1	Total	Mg	0
			1	1	
35	F	6	Total	Mg	0
			6	6	

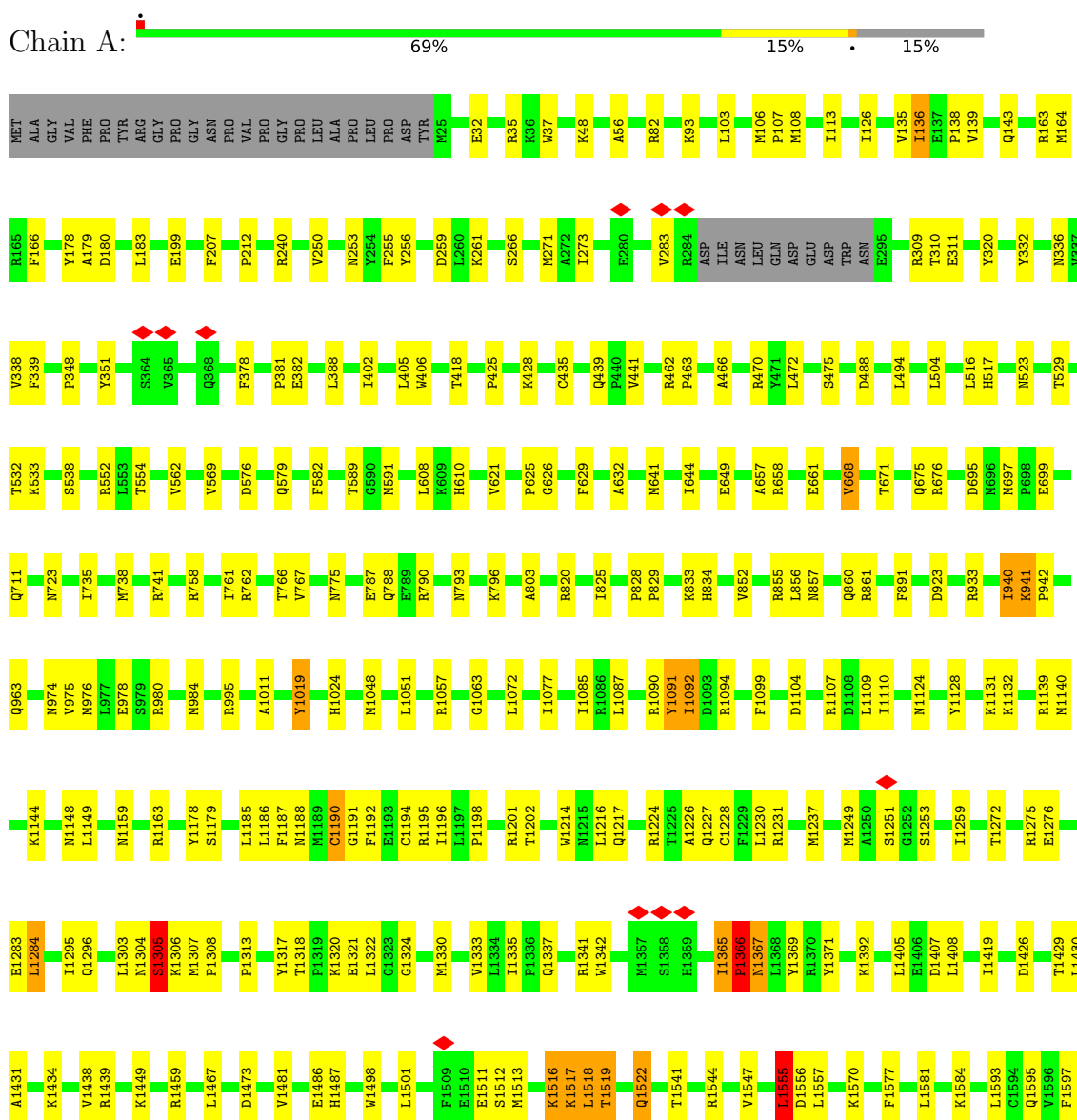
- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

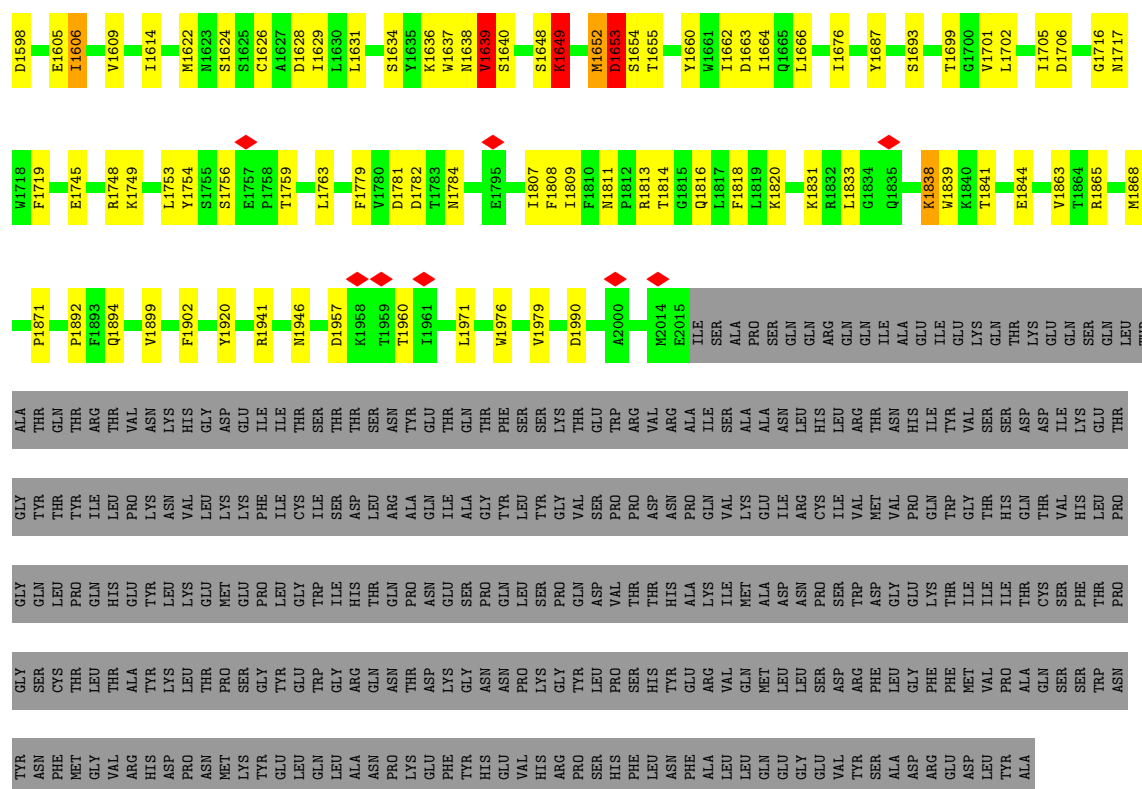
Mol	Chain	Residues	Atoms		AltConf
36	N	3	Total	Zn	0
			3	3	
36	O	3	Total	Zn	0
			3	3	
36	U	1	Total	Zn	0
			1	1	

3 Residue-property plots

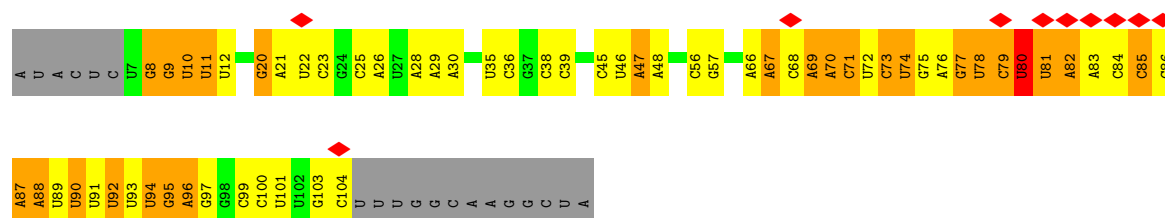
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Pre-mRNA-processing-splicing factor 8

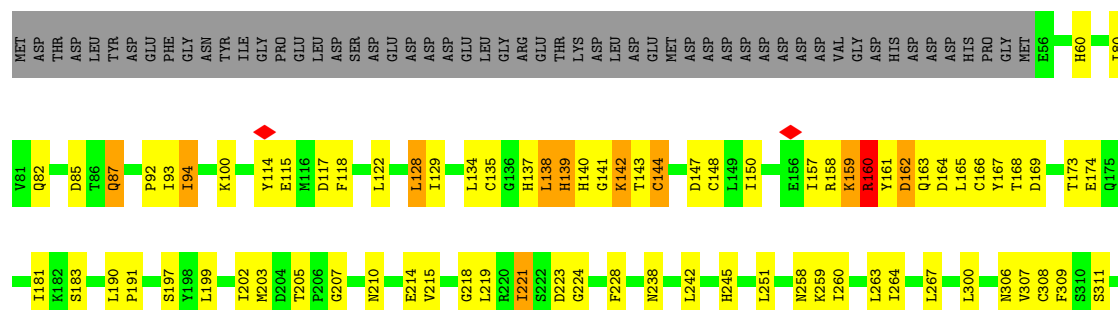


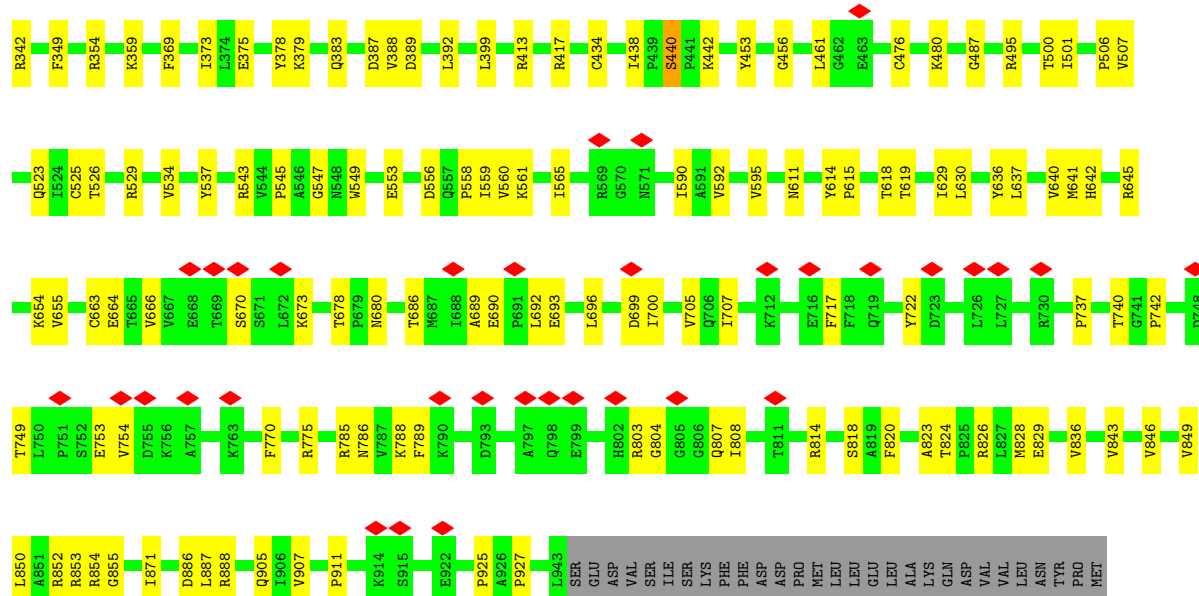


• Molecule 2: U5snRNA



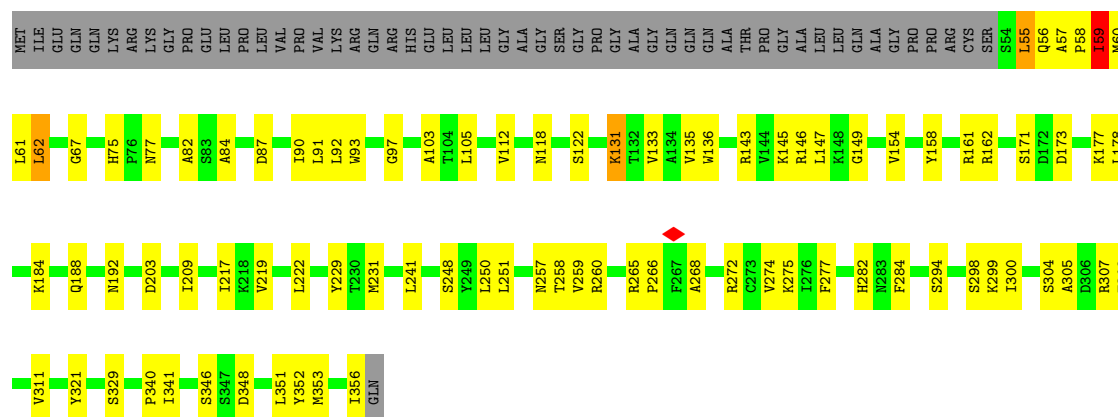
• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component





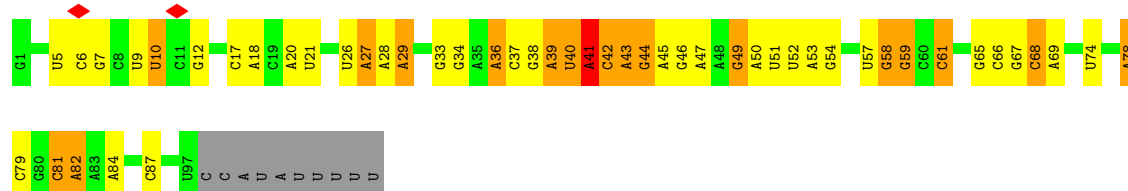
- Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E: 61% 23% 15%



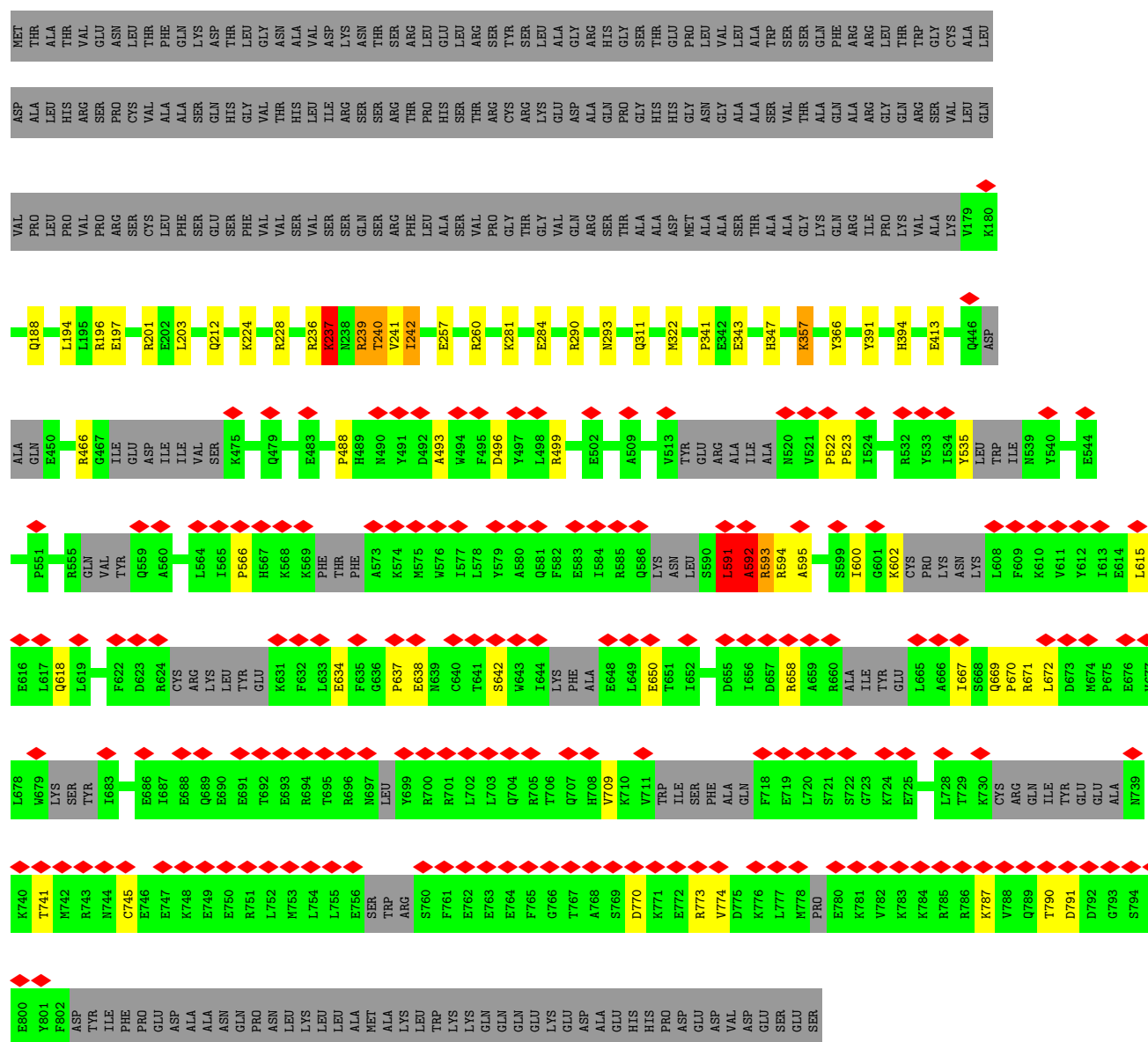
- Molecule 5: U6snRNA

Chain F: 44% 30% 16% 9%

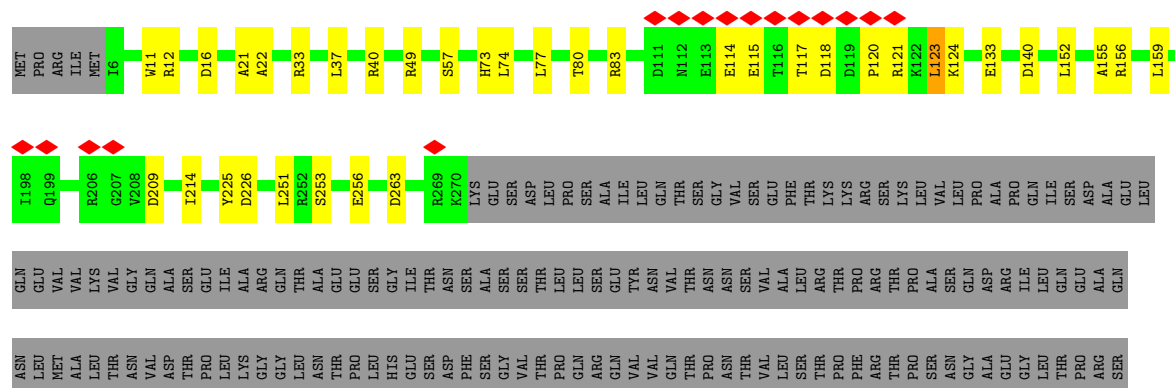


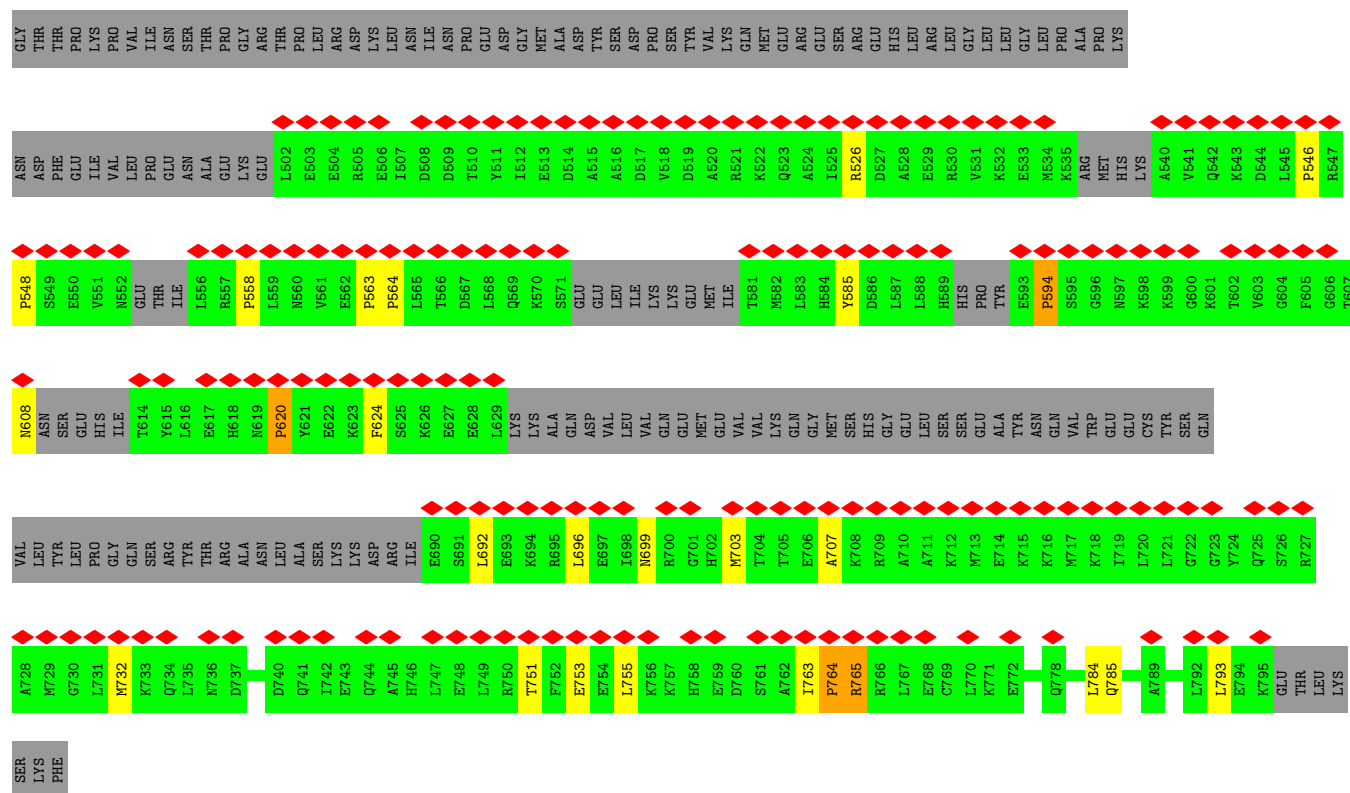
- Molecule 6: Crooked neck-like protein 1

Chain J: 21% 57% 7% 34%

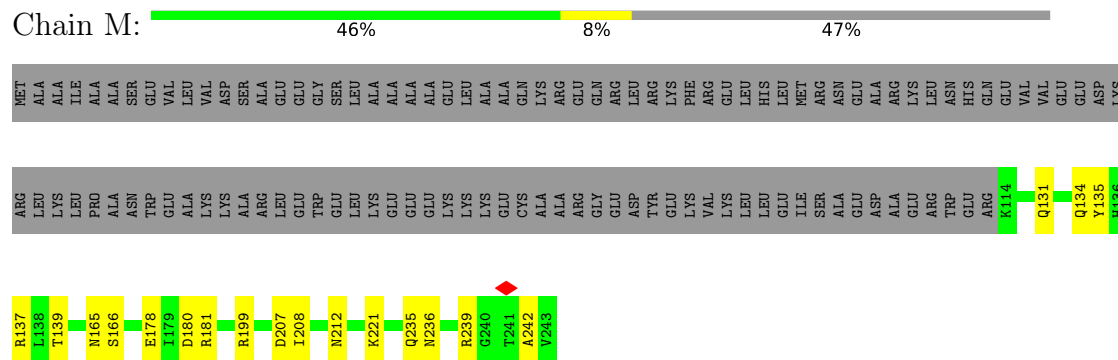


• Molecule 7: Cell division cycle 5-like protein

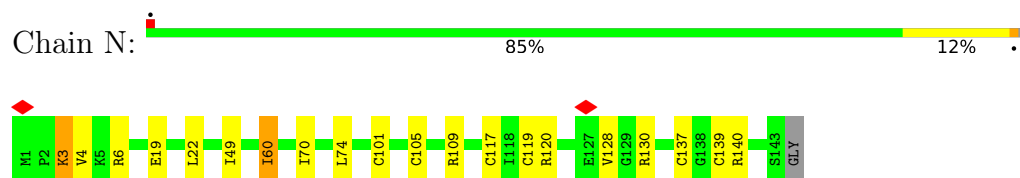




- Molecule 8: Pre-mRNA-splicing factor SYF2



- Molecule 9: Protein BUD31 homolog



- Molecule 10: Pre-mRNA-splicing factor RBM22



[illegible]

- Molecule 13: Peptidyl-prolyl cis-trans isomerase-like 1

[illegible]

- Molecule 14: Pleiotropic regulator 1

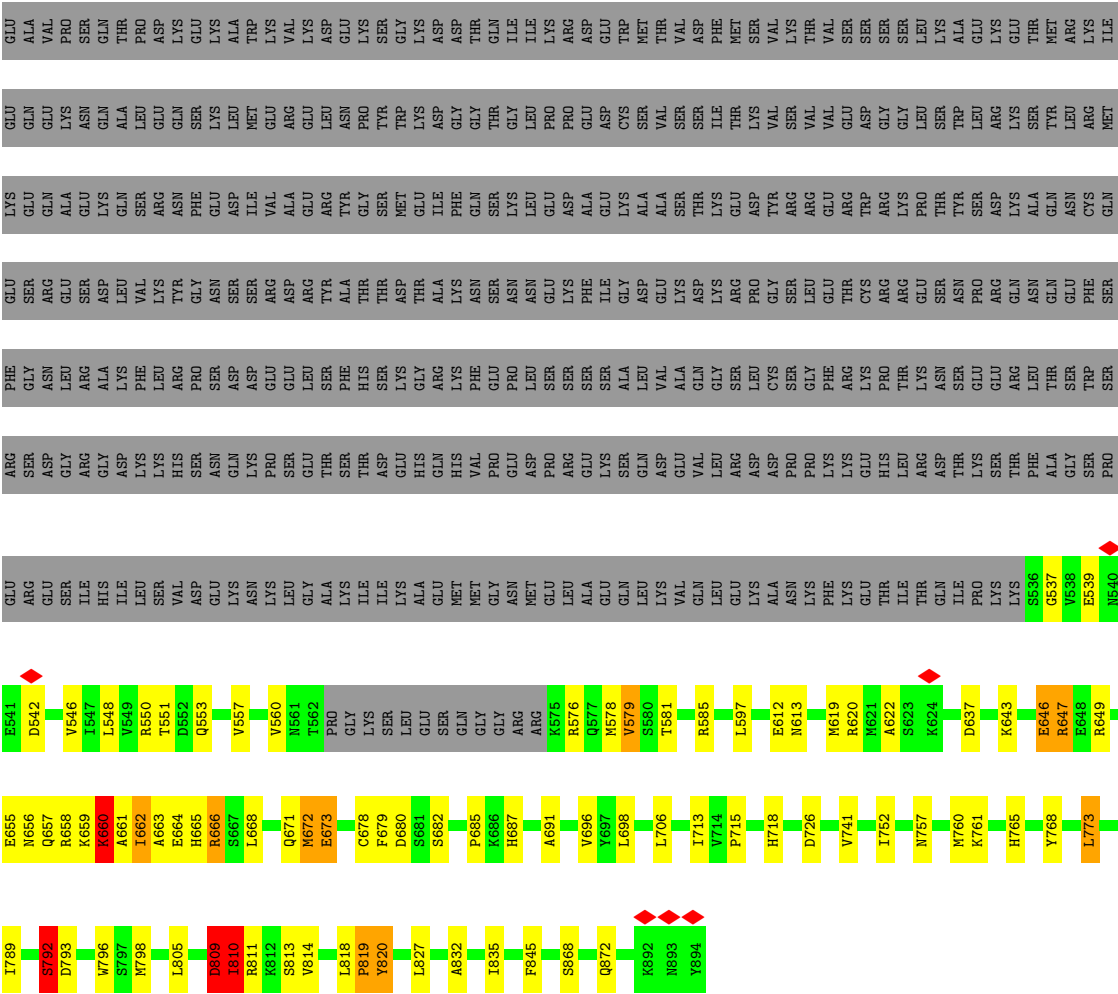


D471	P343	LYS	SER	SER	MET
Q472	Q344	ALA	ALA	LYS	VAL
L478	T345	PRO	ALA	GLU	GLU
I486	T346	T184	GLN	ASN	GLU
K487	T347	W190	SER	LEU	VAL
V488	G348		LEU	GLY	GLN
Y489	S349	I200	ALA	LYS	LYS
A495	H350	E213	VAL	GLY	HIS
T496	D351		ALA	PRO	VAL
E497	L356	E213	PRO	GLN	HIS
E498	L359	N216	LEU	ASN	THR
T499	R365	Q217	GLN	ALA	LEU
H500	R365	W218	THR	THR	VAL
PRO	H371	F219	LYS	ASP	PHE
VAL	K372	V220	ASP	SER	SER
SER	K373	S223	ALA	VAL	LEU
TRP	S374	A224	ASN	HIS	LYS
LYS	V375	L238	ARG	LYS	ARG
PRO	R376		THR	GLN	THR
GLU	L390	T248	ALA	TYR	HIS
ILE	H391		PRO	PRO	ASP
ILE	P392	L261	SER	ALA	MET
LYS	R393	V270	GLY	ASN	PHE
ARG			GLU	GLN	VAL
LYS	G390	W273	TYR	GLY	ALA
ARG	S391		ARG	VAL	GLY
PHE	P392	N278	HIS	GLU	LYS
	D393	Y284	PRO	TYR	PRO
			ALA	PHE	VAL
			SER	VAL	PRO
			ASP	ALA	LEU
			ARG	GLY	ASP
			PRO	THR	GLU
			GLN	HIS	GLU
			PRO	PRO	SER
			THR	TYR	HIS
			ALA	PRO	LYS
			MET	PRO	ARG
			ASN	GLY	LYS
			SER	PRO	MET
			ILE	GLY	ALA
			VAL	VAL	LYS
			MET	ALA	LYS
			GLU	LEU	LEU
			THR	THR	ARG
			GLY	ALA	ASN
			ASN	ASP	GLU
			THR	THR	TYR
			LYS	LYS	GLY
			ASN	ILE	PRO
			SER	GLN	VAL
			ALA	ARG	VAL
			LEU	MET	HIS
			MET	PRO	MET
			LYS	SER	THR
			ALA	LYS	PRO
			VAL	THR	THR
			YS	THR	THR

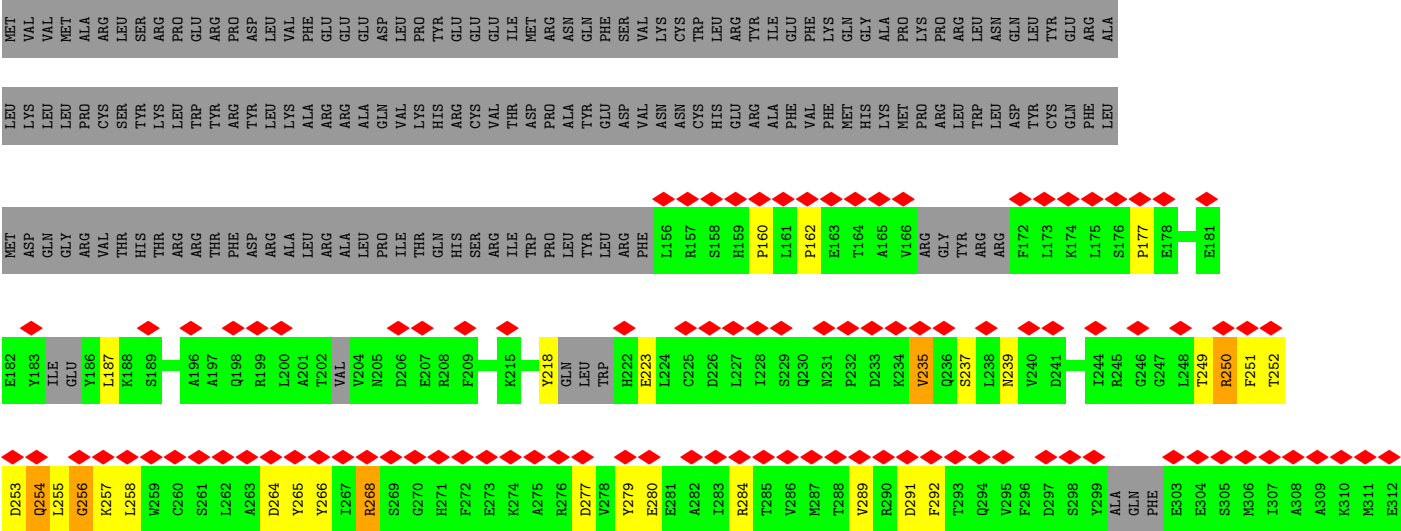
- Molecule 15: Pre-mRNA-processing factor 17

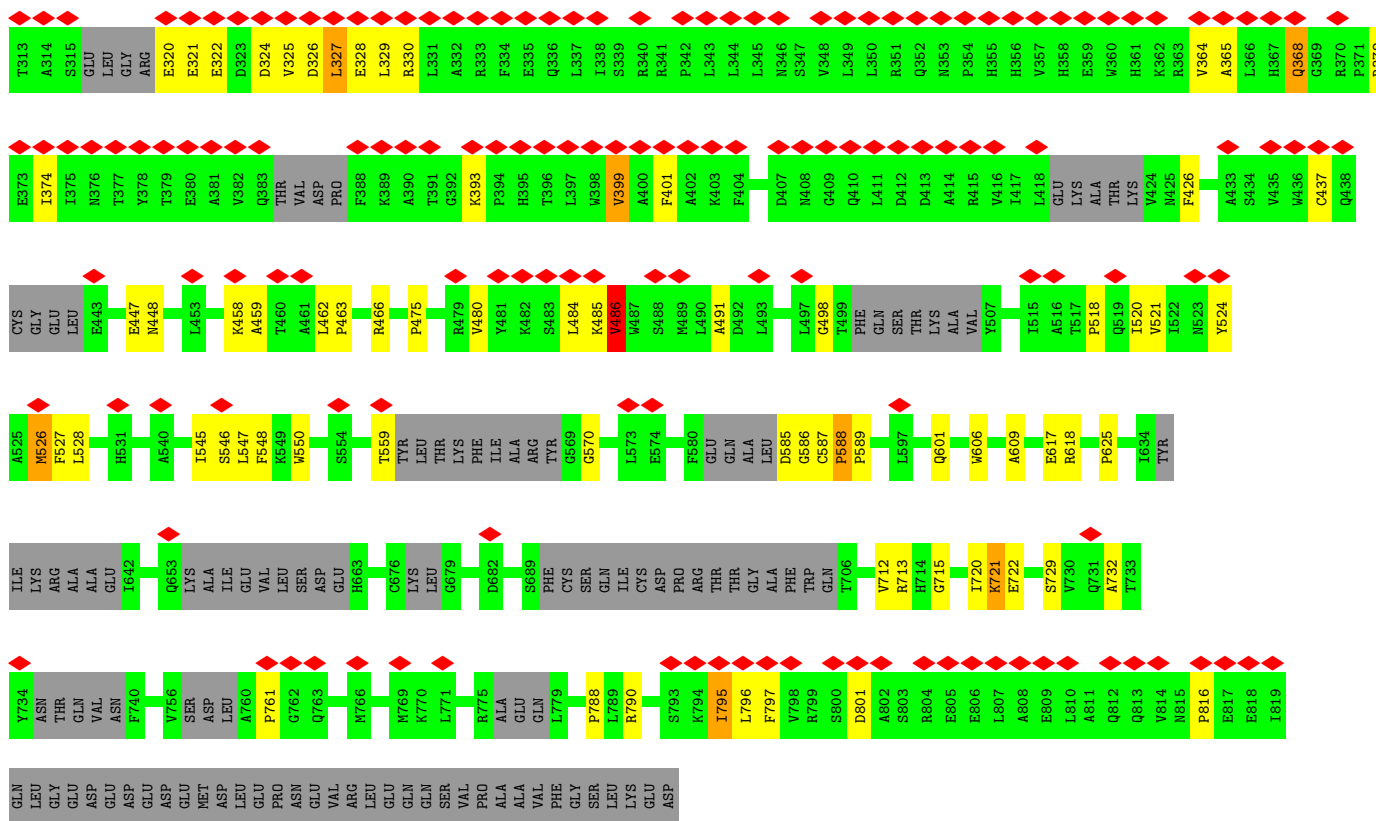


P208	P216	G227	K228	Q229	E230	E231	E232	K233	P234	G235	E236	I240	L241	H242	V243	M246	G251	I257	P258	Q259	D260	V261	G262	V263	M264	L265	R266	S267	T268	M269	P270	P271	E272	K273	C274	P277	K278	Q279	I281	S285	G290	F297												
ALA	VAL	LYS	GLU	ASP	LEU	GLU	THR	GLY	V70	P74	A75	R76	K77	E78	P83	M88	N97	P98	F99	R100	Q103	R108	L111	I120	P141	S142	L143	D144	N145	V148	S149	I153	G154	S155	E158	M162	L165	Q172	L193	D204														
MET	SER	ALA	ALA	ILE	ALA	LEU	ALA	ALA	SER	TVR	GLY	GLY	SER	GLY	SER	GLU	SER	ASP	ASP	SER	GLU	SER	SER	ARG	CYS	PRO	LEU	PRO	ALA	ALA	ASP	SER	LEU	MET	HIS	LEU	THR	LYS	SER	PRO	SER	SER	LYS	PRO	ALA	ALA	VAL	VAL	ASP	SER	PRO	ALA	GLU	VAL

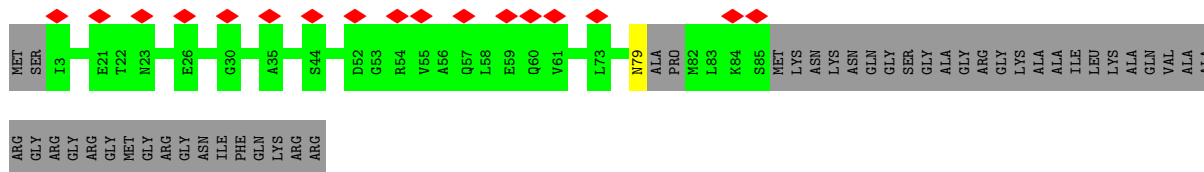


● Molecule 19: Pre-mRNA-splicing factor SYF1

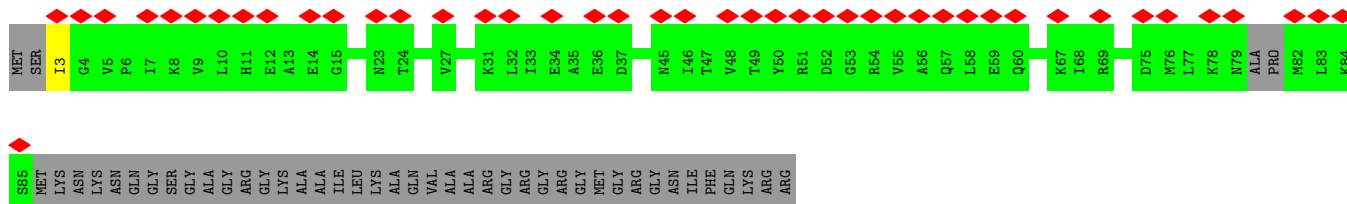




- Molecule 20: Small nuclear ribonucleoprotein Sm D3

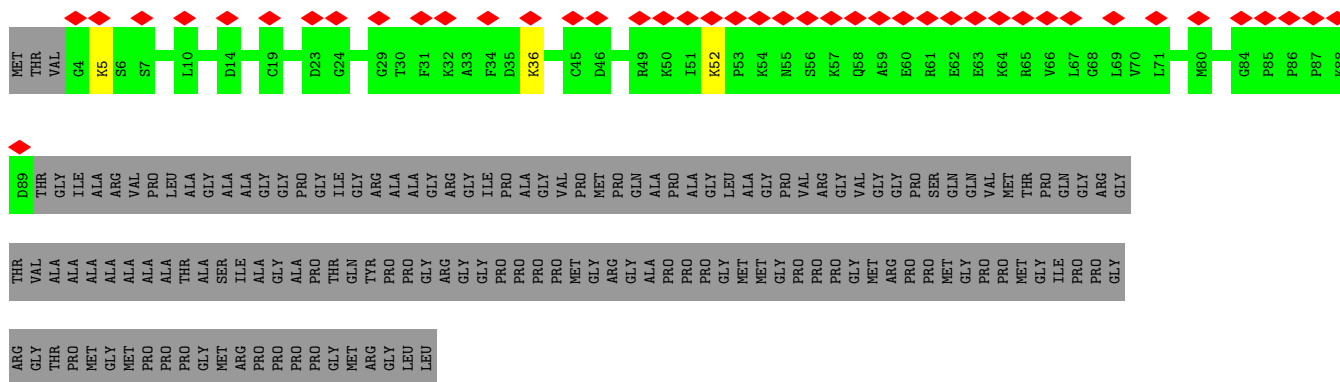


- Molecule 20: Small nuclear ribonucleoprotein Sm D3

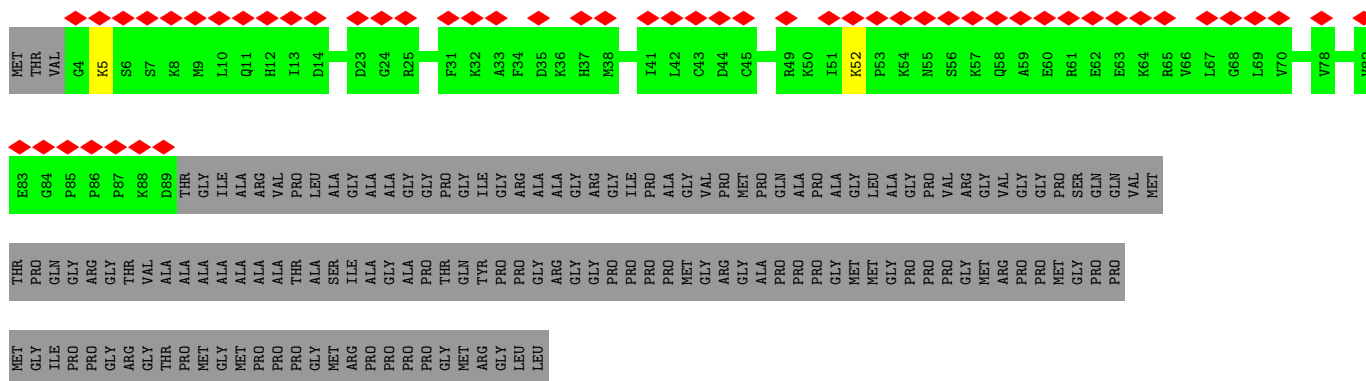


- Molecule 21: Small nuclear ribonucleoprotein-associated protein.

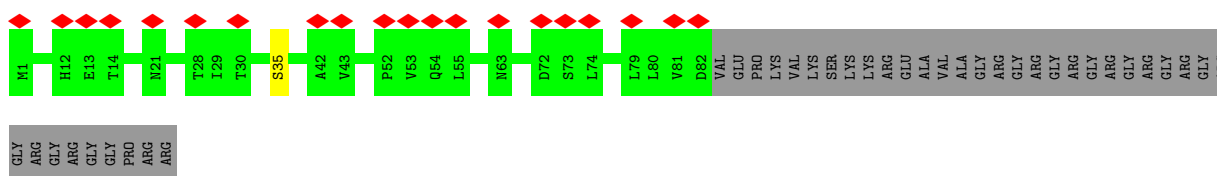




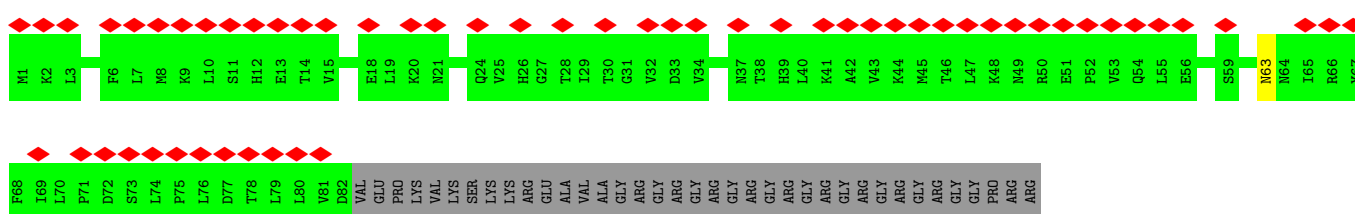
- Molecule 21: Small nuclear ribonucleoprotein-associated protein.



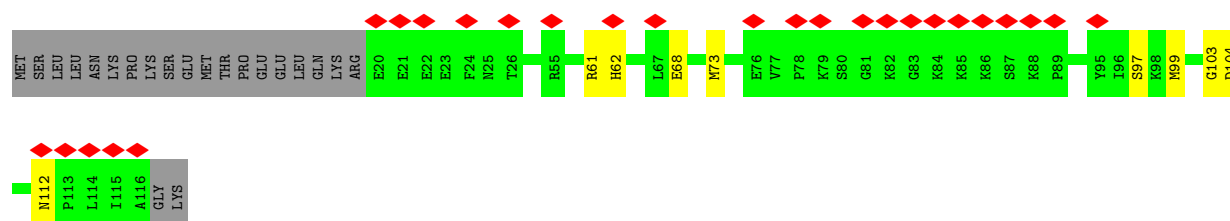
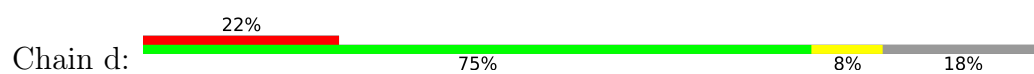
- Molecule 22: Small nuclear ribonucleoprotein Sm D1



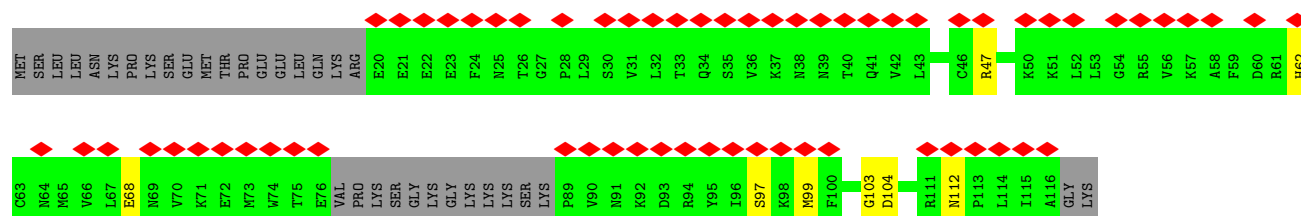
- Molecule 22: Small nuclear ribonucleoprotein Sm D1



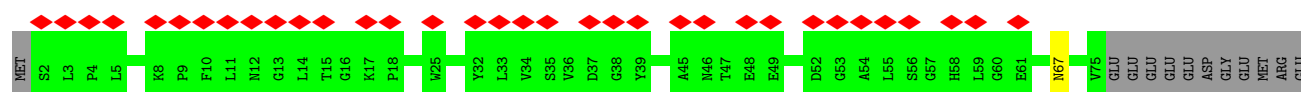
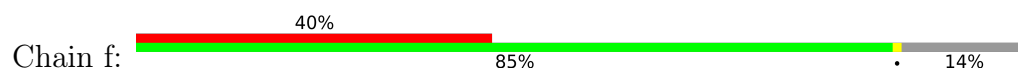
- Molecule 23: Small nuclear ribonucleoprotein Sm D2



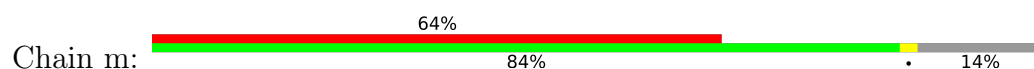
- Molecule 23: Small nuclear ribonucleoprotein Sm D2



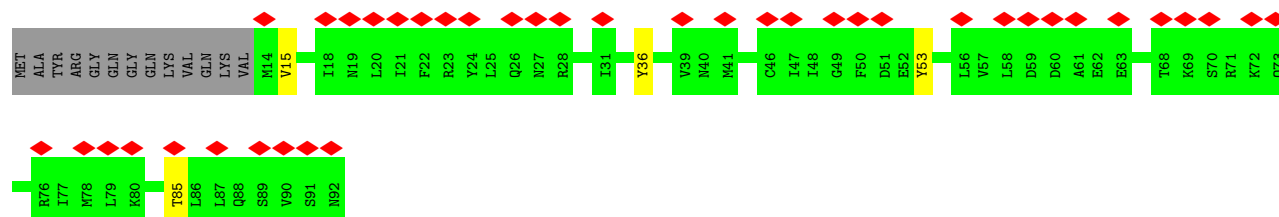
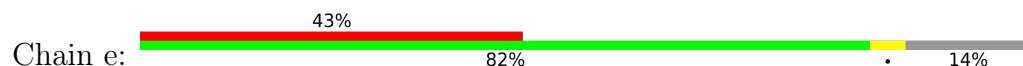
- Molecule 24: Small nuclear ribonucleoprotein F



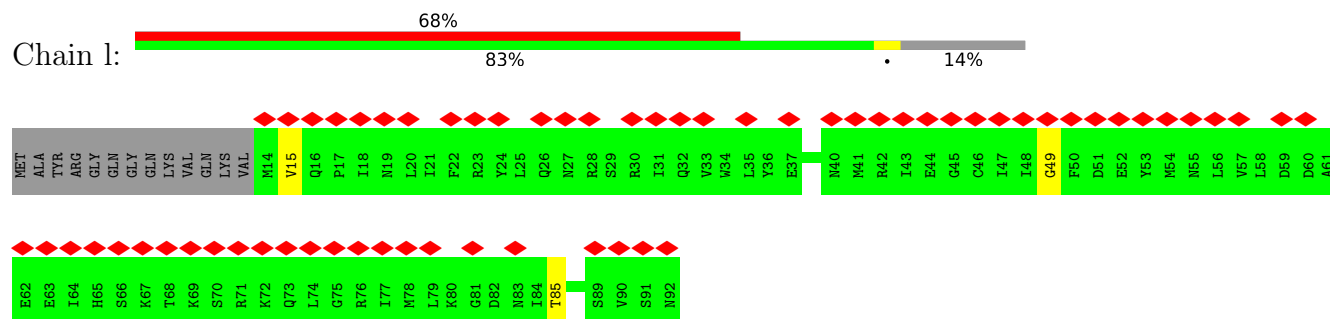
- Molecule 24: Small nuclear ribonucleoprotein F



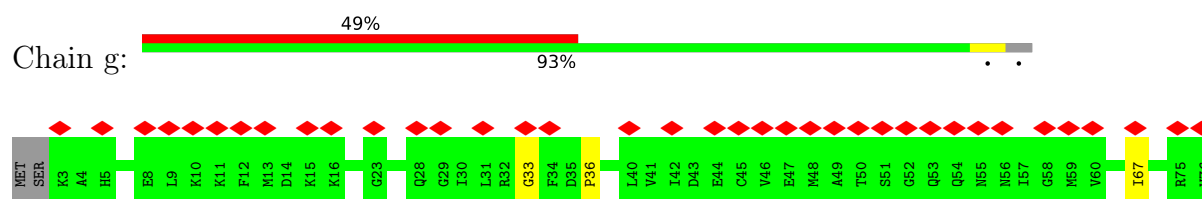
- Molecule 25: Small nuclear ribonucleoprotein E



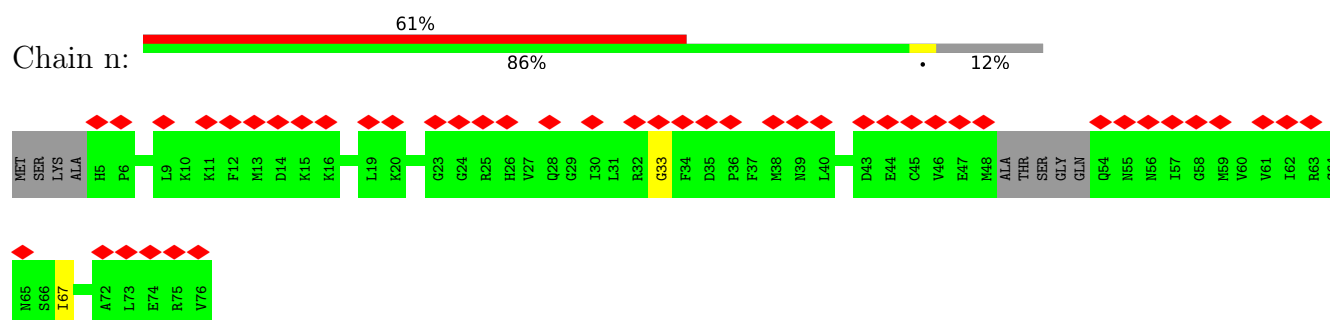
- Molecule 25: Small nuclear ribonucleoprotein E



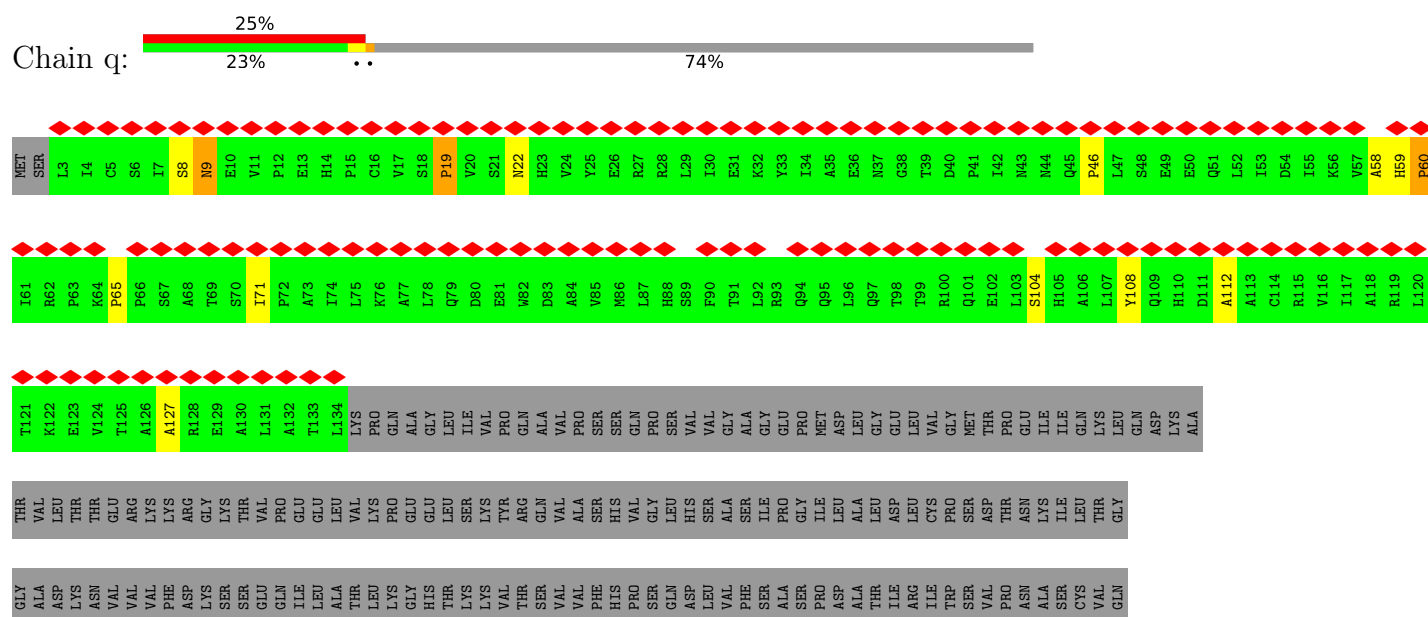
- Molecule 26: Small nuclear ribonucleoprotein G



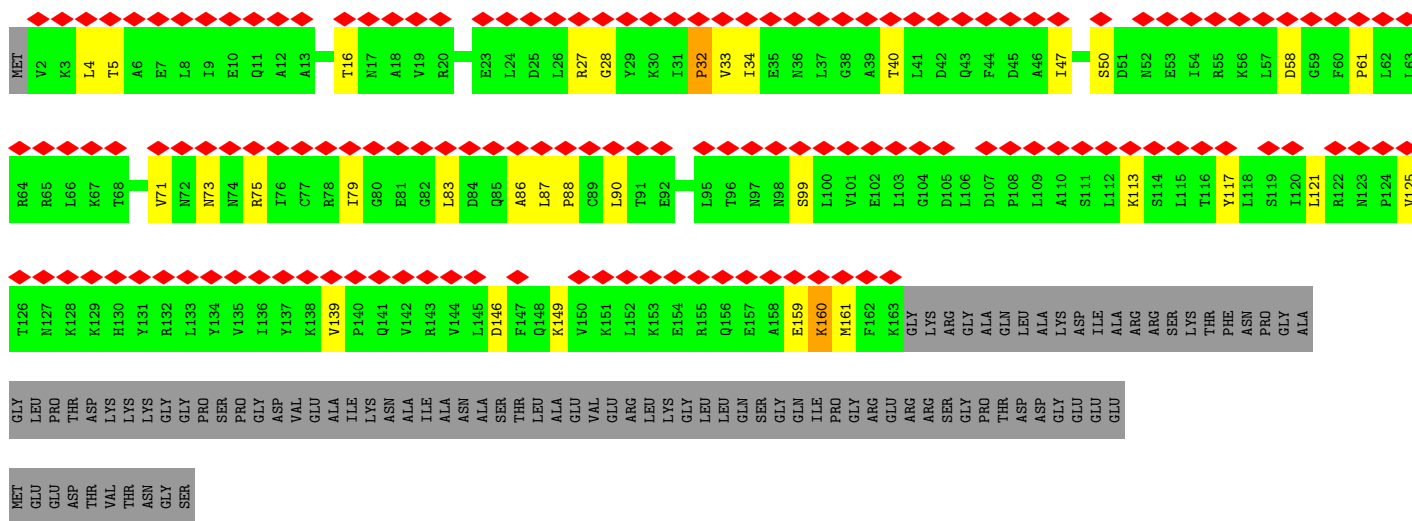
- Molecule 26: Small nuclear ribonucleoprotein G



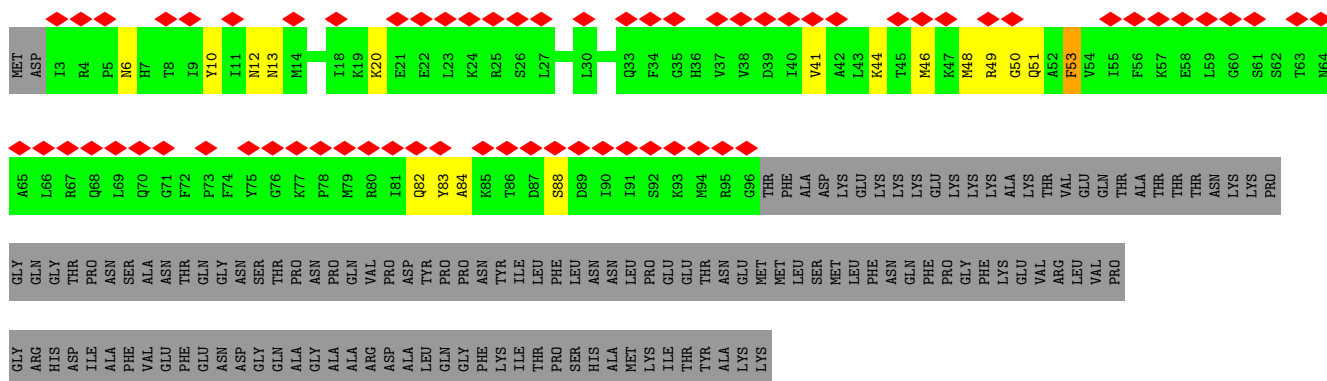
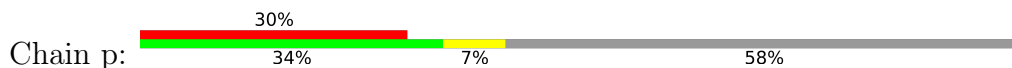
- Molecule 27: Pre-mRNA-processing factor 19



- Molecule 29: U2 small nuclear ribonucleoprotein A'

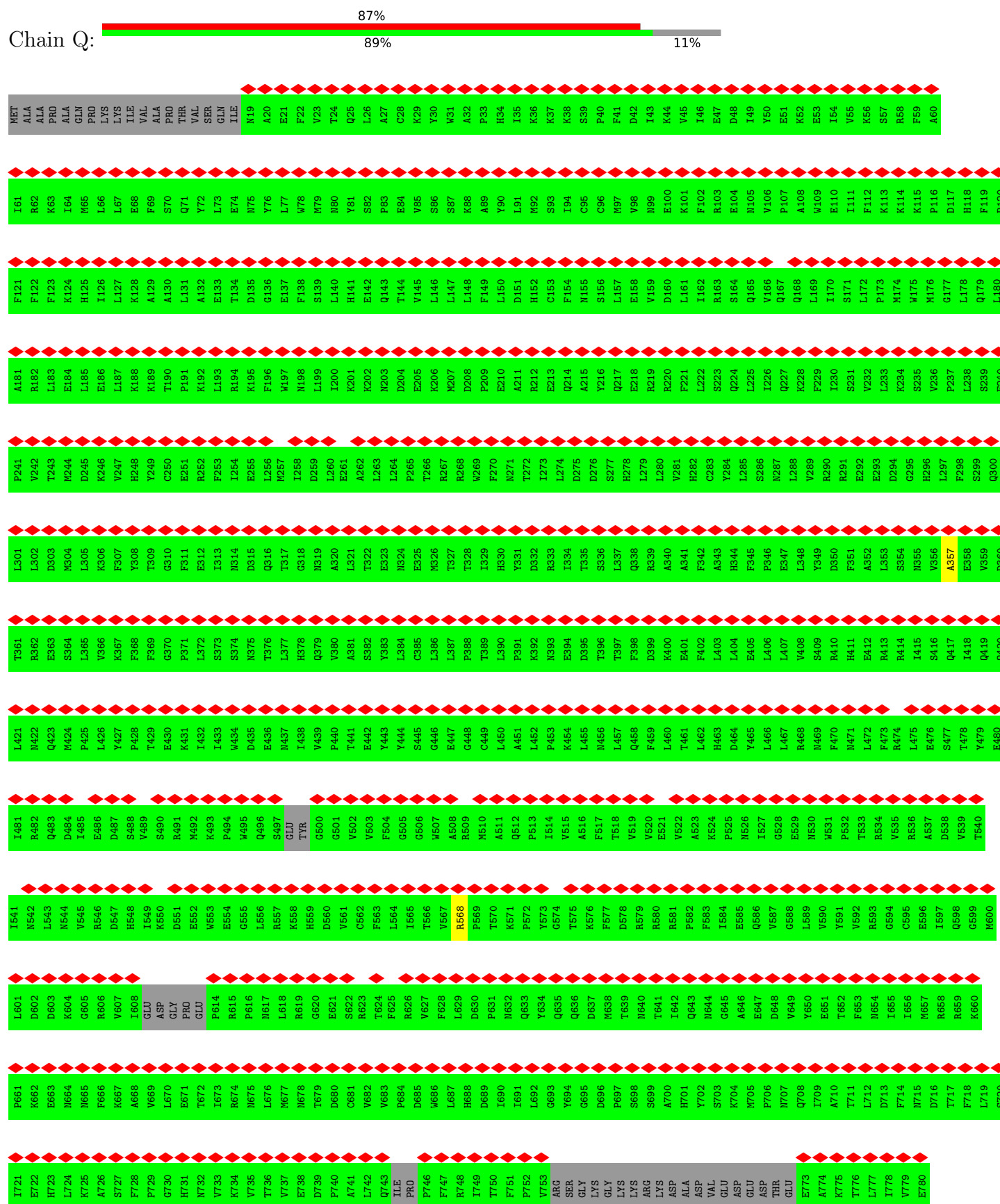


- Molecule 30: U2 small nuclear ribonucleoprotein B''



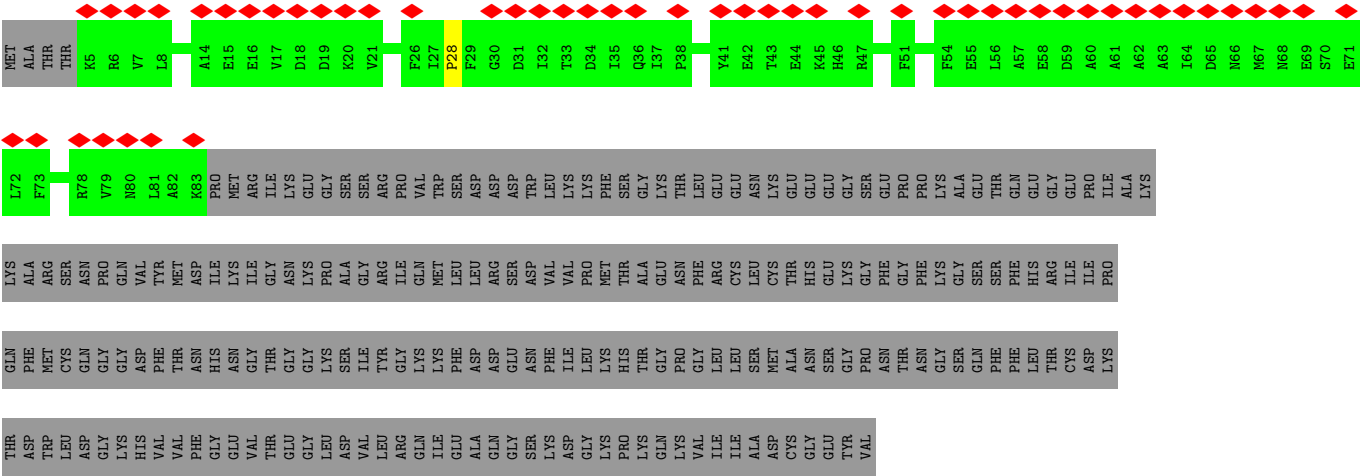
● Molecule 31: RNA helicase aquarius

Chain Q:



- Molecule 32: Peptidyl-prolyl cis-trans isomerase E





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	390072	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	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	0.543	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, IHP, GTP, MG, ZN

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	A	0.38	1/16926 (0.0%)	0.76	30/22947 (0.1%)
2	B	0.41	1/2296 (0.0%)	0.62	2/3569 (0.1%)
3	C	0.31	0/7181	0.81	7/9758 (0.1%)
4	E	0.27	0/2420	0.70	3/3281 (0.1%)
5	F	0.34	0/2323	0.54	0/3619
6	J	0.49	2/3802 (0.1%)	0.88	17/5162 (0.3%)
7	L	0.41	1/3267 (0.0%)	0.86	11/4418 (0.2%)
8	M	0.28	0/1119	0.66	0/1497
9	N	0.79	1/1210 (0.1%)	0.80	1/1622 (0.1%)
10	O	0.33	0/2390	0.72	3/3227 (0.1%)
11	P	0.33	0/1000	0.72	0/1330
12	R	0.36	0/2186	0.85	7/2937 (0.2%)
13	S	0.28	0/1268	0.70	0/1714
14	T	0.49	0/2562	0.83	1/3492 (0.0%)
15	W	0.70	1/3038 (0.0%)	1.16	30/4171 (0.7%)
16	G	0.65	5/1378 (0.4%)	1.12	13/2133 (0.6%)
17	H	0.72	22/3308 (0.7%)	1.17	34/5135 (0.7%)
18	U	0.37	0/2928	0.89	10/3928 (0.3%)
19	I	0.52	0/2803	1.09	28/3870 (0.7%)
20	a	0.78	0/397	0.99	0/549
20	h	0.78	0/396	0.99	0/547
21	b	0.85	0/423	1.14	3/587 (0.5%)
21	i	0.84	0/423	1.15	3/587 (0.5%)
22	c	0.88	0/405	1.12	0/563
22	j	0.87	0/405	1.11	0/563
23	d	1.12	1/479 (0.2%)	1.25	1/666 (0.2%)
23	k	1.14	0/420	1.24	1/583 (0.2%)
24	f	1.20	0/360	1.25	0/497
24	m	1.21	1/360 (0.3%)	1.24	0/497
25	e	1.04	0/390	1.24	1/542 (0.2%)
25	l	1.03	0/390	1.24	1/542 (0.2%)
26	g	0.86	0/362	1.09	1/501 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	n	0.83	0/327	1.08	1/451 (0.2%)
27	q	0.63	0/658	0.97	3/919 (0.3%)
27	r	0.57	0/653	1.06	6/912 (0.7%)
27	s	0.50	0/334	0.91	0/466
27	t	0.55	0/334	0.83	0/466
28	K	0.60	1/753 (0.1%)	1.01	4/1046 (0.4%)
29	o	0.97	0/803	2.25	43/1119 (3.8%)
30	p	0.95	0/463	1.88	7/643 (1.1%)
31	Q	0.38	0/6565	0.86	3/9143 (0.0%)
32	y	0.43	0/389	1.01	0/540
All	All	0.51	37/79894 (0.0%)	0.91	275/110739 (0.2%)

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
1	A	0	16
3	C	0	6
4	E	0	1
5	F	0	1
6	J	0	1
9	N	0	1
12	R	0	8
14	T	0	5
15	W	0	3
16	G	0	5
17	H	0	1
18	U	0	6
23	d	0	1
23	k	0	1
All	All	0	56

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	77	C	C1'-N1	7.54	1.59	1.48
15	W	278	LYS	CA-C	-7.39	1.44	1.53
28	K	186	VAL	CA-CB	-7.32	1.44	1.54
2	B	103	G	C1'-N9	-7.15	1.37	1.48
17	H	74	U	C1'-N1	7.12	1.59	1.48

The worst 5 of 275 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	32	U	C1'-C2'-O2'	11.22	128.62	111.80
2	B	104	C	C2'-C3'-O3'	-10.04	94.44	109.50
19	I	327	LEU	N-CA-C	-10.00	100.38	111.28
15	W	278	LYS	CB-CA-C	-9.99	95.78	111.17
16	G	142	U	C4'-C3'-O3'	9.97	124.35	109.40

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	TYR	Peptide
1	A	107	PRO	Peptide
1	A	135	VAL	Peptide
1	A	320	TYR	Peptide
1	A	940	ILE	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	A	16477	0	16462	244	0
2	B	2060	0	1044	93	0
3	C	7022	0	7047	167	0
4	E	2366	0	2303	70	0
5	F	2075	0	1048	43	0
6	J	3758	0	2888	47	0
7	L	3237	0	2680	49	0
8	M	1098	0	1082	16	0
9	N	1184	0	1189	11	0
10	O	2340	0	2316	46	0
11	P	985	0	965	14	0
12	R	2165	0	2214	40	0
13	S	1236	0	1210	27	0
14	T	2496	0	2446	48	0
15	W	3008	0	1977	66	0
16	G	1246	0	631	210	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	H	2968	0	1504	301	0
18	U	2864	0	2814	83	0
19	I	2822	0	1319	70	0
20	a	399	0	173	3	0
20	h	398	0	172	6	0
21	b	424	0	179	1	0
21	i	424	0	179	0	0
22	c	406	0	170	1	0
22	j	406	0	170	1	0
23	d	480	0	200	6	0
23	k	422	0	175	6	0
24	f	361	0	158	1	0
24	m	361	0	158	1	0
25	e	391	0	163	5	0
25	l	391	0	163	2	0
26	g	363	0	160	4	0
26	n	329	0	138	1	0
27	q	659	0	296	23	0
27	r	654	0	294	30	0
27	s	335	0	168	6	0
27	t	335	0	168	8	0
28	K	757	0	338	49	0
29	o	804	0	350	2	0
30	p	464	0	205	31	0
31	Q	6562	0	2836	2	0
32	y	390	0	190	2	0
33	A	36	0	6	1	0
34	C	32	0	12	22	0
35	C	1	0	0	0	0
35	F	6	0	0	0	0
36	N	3	0	0	0	0
36	O	3	0	0	0	0
36	U	1	0	0	0	0
All	All	78004	0	60360	1514	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 11.

The worst 5 of 1514 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)
19:I:437:CYS:CB	19:I:447:GLU:CB	1.98	1.42
5:F:44:G:N2	16:G:3:A:C2	1.84	1.38
18:U:546:VAL:HG21	18:U:665:HIS:CE1	1.56	1.38
5:F:44:G:N2	16:G:3:A:H2	1.14	1.36
5:F:41:A:N6	16:G:6:A:H61	1.17	1.34

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1977/2335 (85%)	1793 (91%)	165 (8%)	19 (1%)	12	39
3	C	886/972 (91%)	788 (89%)	96 (11%)	2 (0%)	43	72
4	E	301/357 (84%)	280 (93%)	20 (7%)	1 (0%)	36	65
6	J	520/848 (61%)	473 (91%)	42 (8%)	5 (1%)	12	39
7	L	459/802 (57%)	423 (92%)	31 (7%)	5 (1%)	11	36
8	M	128/243 (53%)	116 (91%)	12 (9%)	0	100	100
9	N	141/144 (98%)	128 (91%)	12 (8%)	1 (1%)	18	48
10	O	288/420 (69%)	262 (91%)	25 (9%)	1 (0%)	36	65
11	P	114/229 (50%)	98 (86%)	15 (13%)	1 (1%)	14	41
12	R	268/536 (50%)	227 (85%)	38 (14%)	3 (1%)	11	36
13	S	157/166 (95%)	141 (90%)	16 (10%)	0	100	100
14	T	315/514 (61%)	292 (93%)	21 (7%)	2 (1%)	21	51
15	W	507/579 (88%)	433 (85%)	46 (9%)	28 (6%)	1	4
18	U	343/894 (38%)	277 (81%)	58 (17%)	8 (2%)	5	19
19	I	528/855 (62%)	491 (93%)	23 (4%)	14 (3%)	4	16
20	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
21	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
21	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
22	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
22	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
23	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
23	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
24	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
24	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
25	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
25	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
26	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
26	n	63/76 (83%)	61 (97%)	2 (3%)	0	100	100
27	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3	14
27	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	7	27
27	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8	28
27	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	28
28	K	144/225 (64%)	130 (90%)	8 (6%)	6 (4%)	2	9
29	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	32
30	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
31	Q	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100	100
32	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
All	All	10193/16097 (63%)	9369 (92%)	718 (7%)	106 (1%)	15	39

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1306	LYS
1	A	1367	ASN
1	A	1639	VAL
1	A	1653	ASP
1	A	1654	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1792/2108 (85%)	1774 (99%)	18 (1%)	68	89
3	C	787/866 (91%)	773 (98%)	14 (2%)	51	80
4	E	259/300 (86%)	255 (98%)	4 (2%)	57	84
6	J	242/751 (32%)	236 (98%)	6 (2%)	42	74
7	L	228/709 (32%)	226 (99%)	2 (1%)	70	90
8	M	117/209 (56%)	116 (99%)	1 (1%)	70	90
9	N	130/130 (100%)	127 (98%)	3 (2%)	44	76
10	O	259/361 (72%)	258 (100%)	1 (0%)	84	94
11	P	104/203 (51%)	103 (99%)	1 (1%)	68	89
12	R	227/457 (50%)	221 (97%)	6 (3%)	40	73
13	S	129/134 (96%)	128 (99%)	1 (1%)	73	90
14	T	273/441 (62%)	271 (99%)	2 (1%)	76	92
15	W	135/502 (27%)	133 (98%)	2 (2%)	57	84
18	U	313/806 (39%)	306 (98%)	7 (2%)	45	77
19	I	7/749 (1%)	2 (29%)	5 (71%)	0	0
All	All	5002/8726 (57%)	4929 (98%)	73 (2%)	55	84

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	T	220	VAL
19	I	526	MET
15	W	76	VAL
18	U	673	GLU
3	C	159	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
12	R	281	ASN
18	U	717	GLN
13	S	102	ASN
15	W	102	GLN
3	C	238	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	G	69/272 (25%)	55 (79%)	12 (17%)
17	H	133/188 (70%)	53 (39%)	8 (6%)
2	B	97/117 (82%)	44 (45%)	5 (5%)
5	F	96/107 (89%)	41 (42%)	6 (6%)
All	All	395/684 (57%)	193 (48%)	31 (7%)

5 of 193 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	G
2	B	9	G
2	B	10	U
2	B	11	U
2	B	20	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	G	16	G
17	H	46	U
16	G	133	A
17	H	50	C
17	H	30	A

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

2 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	$\# Z > 2$
12	SEP	R	224	12	8,9,10	0.88	0	7,12,14	2.11	1 (14%)
12	SEP	R	232	12	8,9,10	0.94	0	7,12,14	2.19	1 (14%)

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
12	SEP	R	224	12	-	2/6/8/10	-
12	SEP	R	232	12	-	3/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	R	224	SEP	OG-CB-CA	5.17	113.17	108.14
12	R	224	SEP	OG-CB-CA	4.66	112.67	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	R	224	SEP	N-CA-CB-OG
12	R	224	SEP	C-CA-CB-OG
12	R	232	SEP	CB-OG-P-O1P
12	R	232	SEP	CB-OG-P-O2P
12	R	232	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	232	SEP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 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	$\# Z > 2$
34	GTP	C	1500	35	33,34,34	1.15	3 (9%)	50,54,54	1.72	6 (12%)
33	IHP	A	3000	-	36,36,36	0.71	0	60,60,60	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	GTP	C	1500	35	-	5/22/38/38	0/3/3/3
33	IHP	A	3000	-	-	8/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1500	GTP	C5-C4	2.85	1.46	1.38
34	C	1500	GTP	C6-N1	-2.70	1.33	1.38
34	C	1500	GTP	C5-N7	-2.37	1.34	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1500	GTP	C5-C4-N3	-6.20	118.52	128.39
34	C	1500	GTP	C2-N3-C4	5.07	121.04	112.30
34	C	1500	GTP	N9-C4-N3	4.58	135.11	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1500	GTP	C6-C5-N7	3.26	136.22	130.29
34	C	1500	GTP	C4-C5-N7	-2.59	106.56	110.67

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

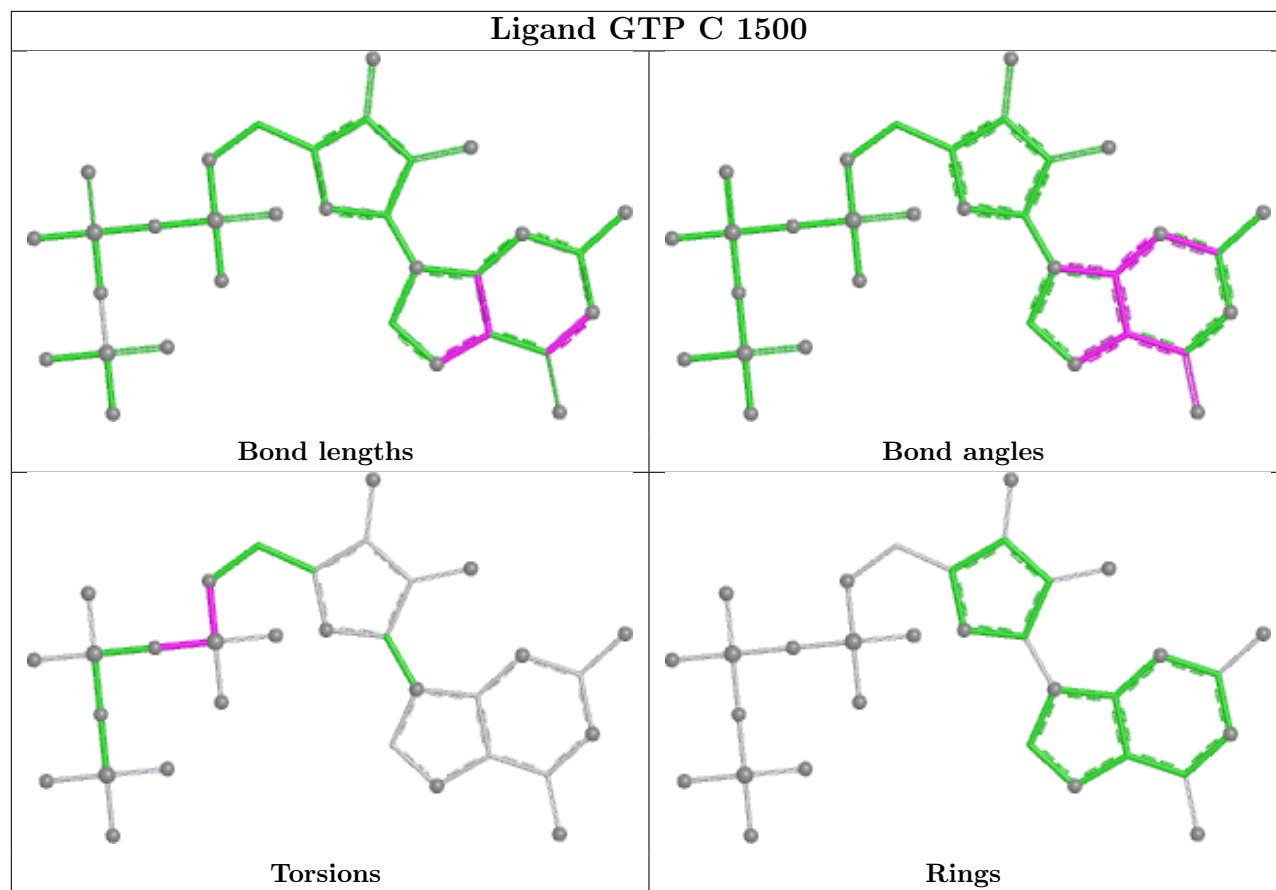
Mol	Chain	Res	Type	Atoms
33	A	3000	IHP	C6-C1-O11-P1
34	C	1500	GTP	C5'-O5'-PA-O2A
33	A	3000	IHP	C2-C1-O11-P1
33	A	3000	IHP	C1-C2-O12-P2
33	A	3000	IHP	C3-C2-O12-P2

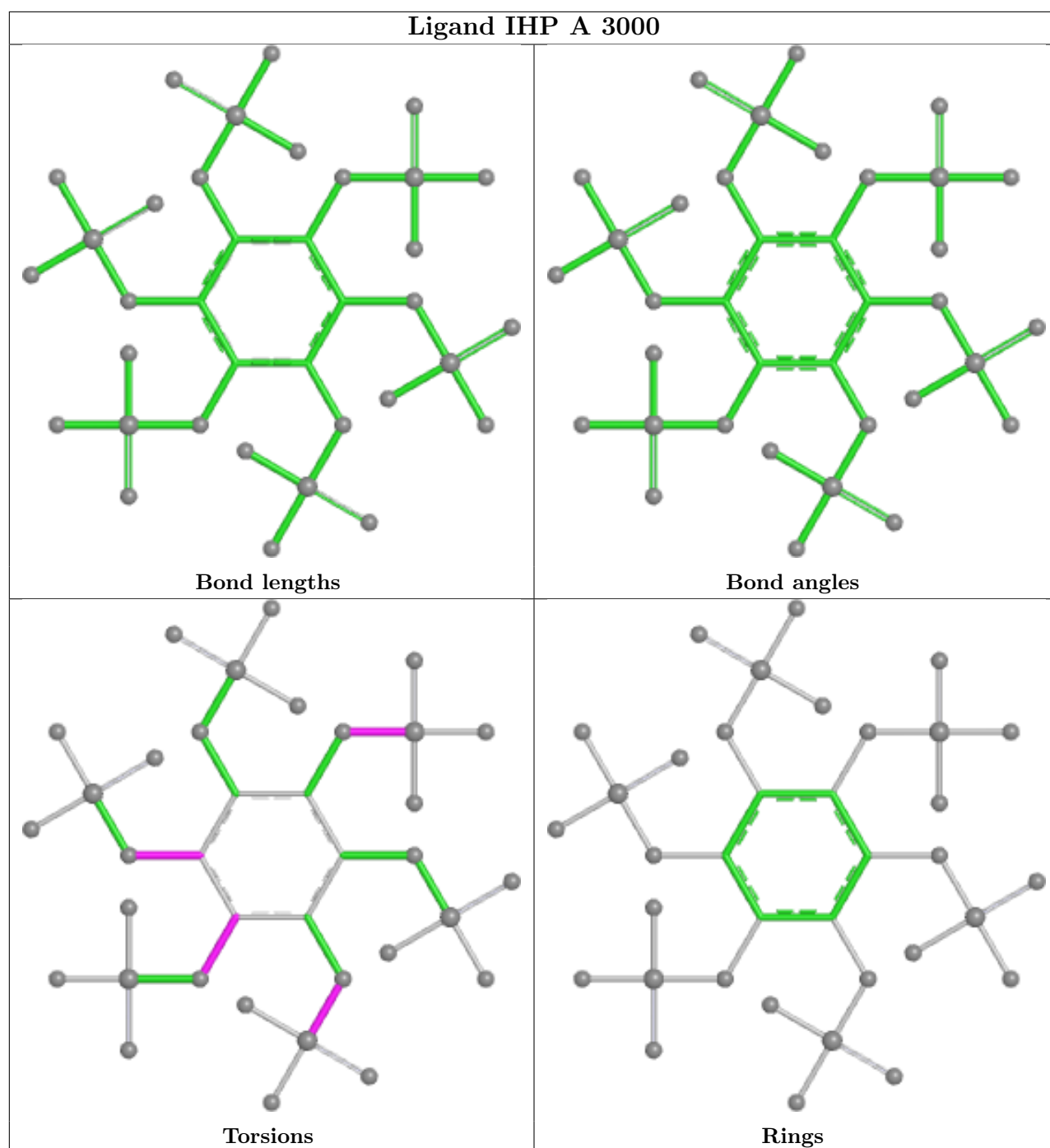
There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	1500	GTP	22	0
33	A	3000	IHP	1	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

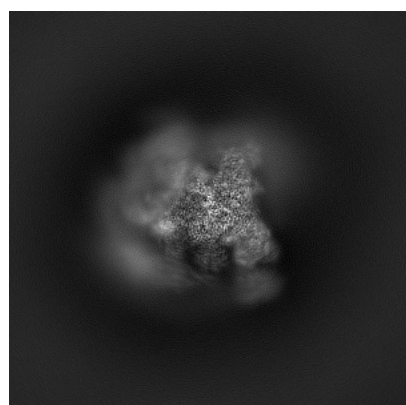
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9646. These allow visual inspection of the internal detail of the map and identification of artifacts.

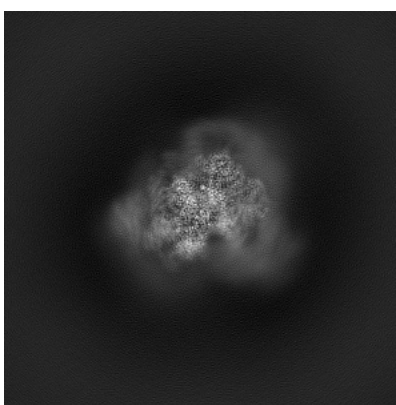
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

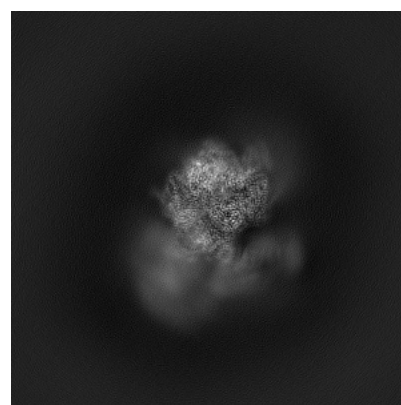
6.1.1 Primary map



X



Y

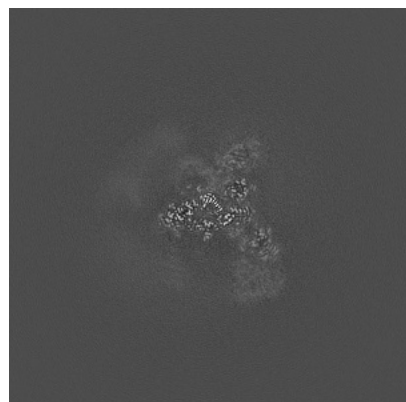


Z

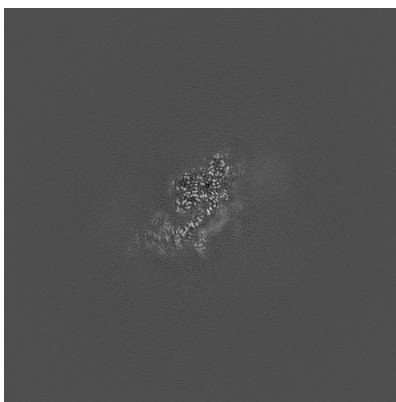
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

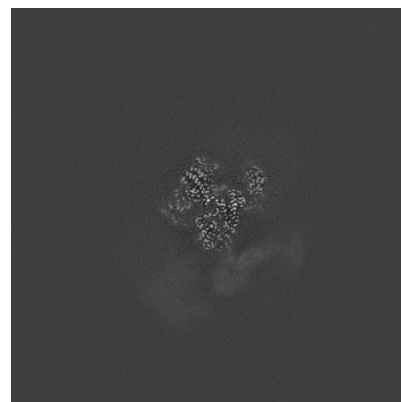
6.2.1 Primary map



X Index: 200



Y Index: 200

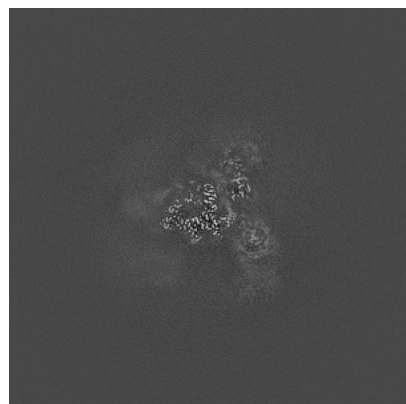


Z Index: 200

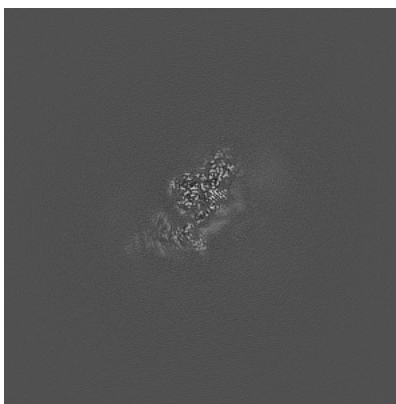
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

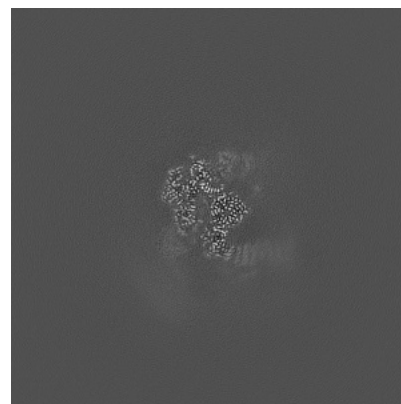
6.3.1 Primary map



X Index: 210



Y Index: 201

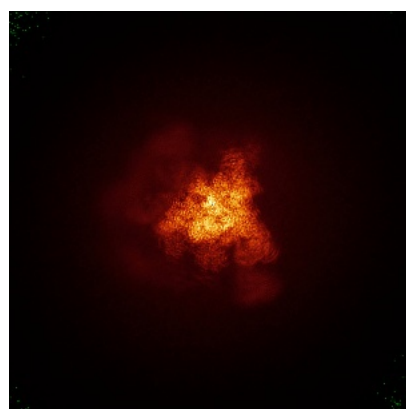


Z Index: 185

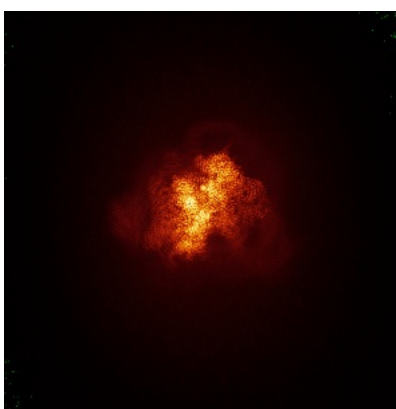
The images above show the largest variance slices of the map in three orthogonal directions.

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

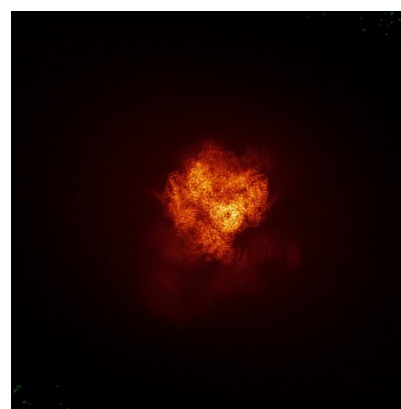
6.4.1 Primary map



X



Y



Z

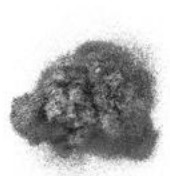
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

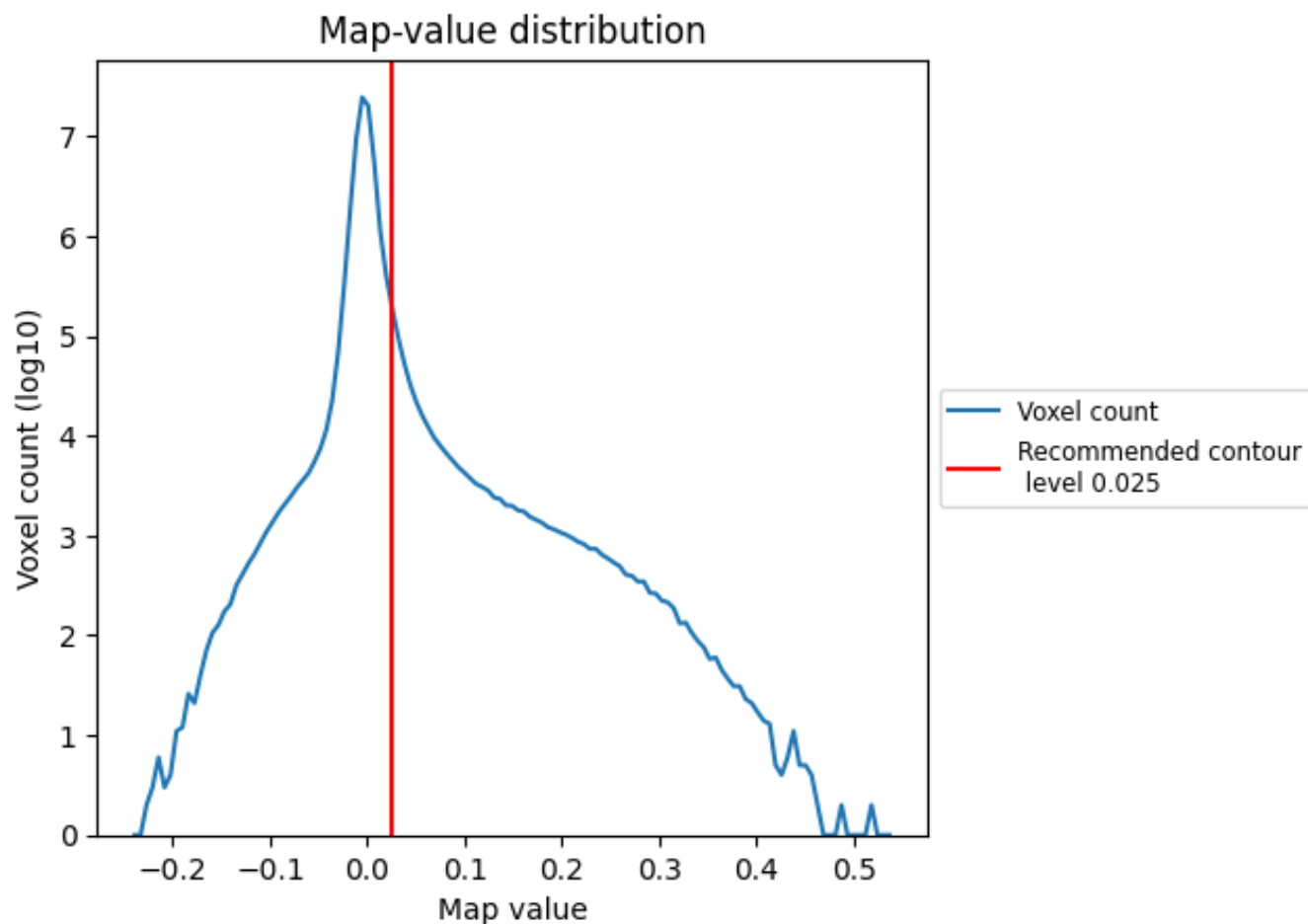
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

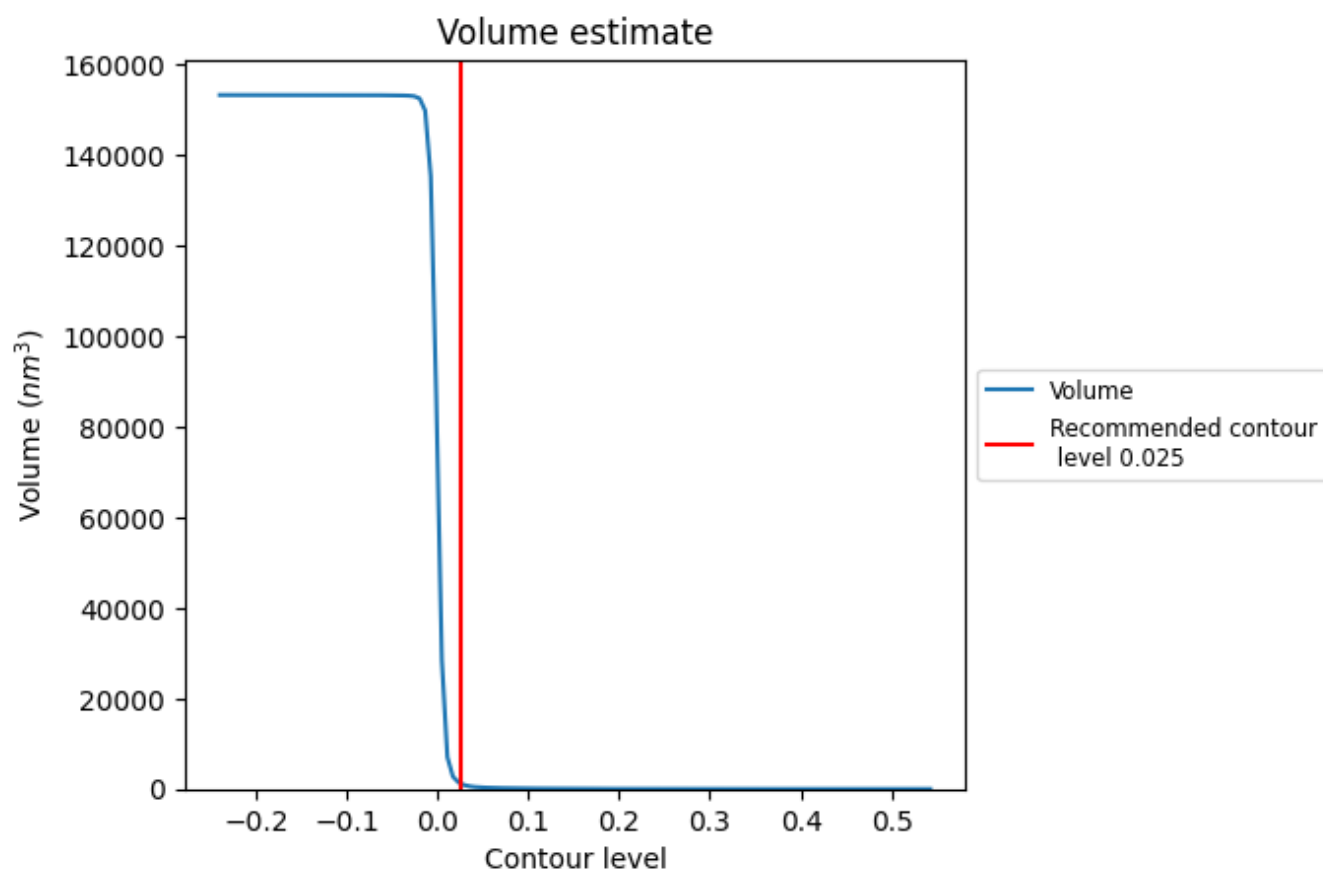
This section contains the results of statistical analysis of the map.

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.

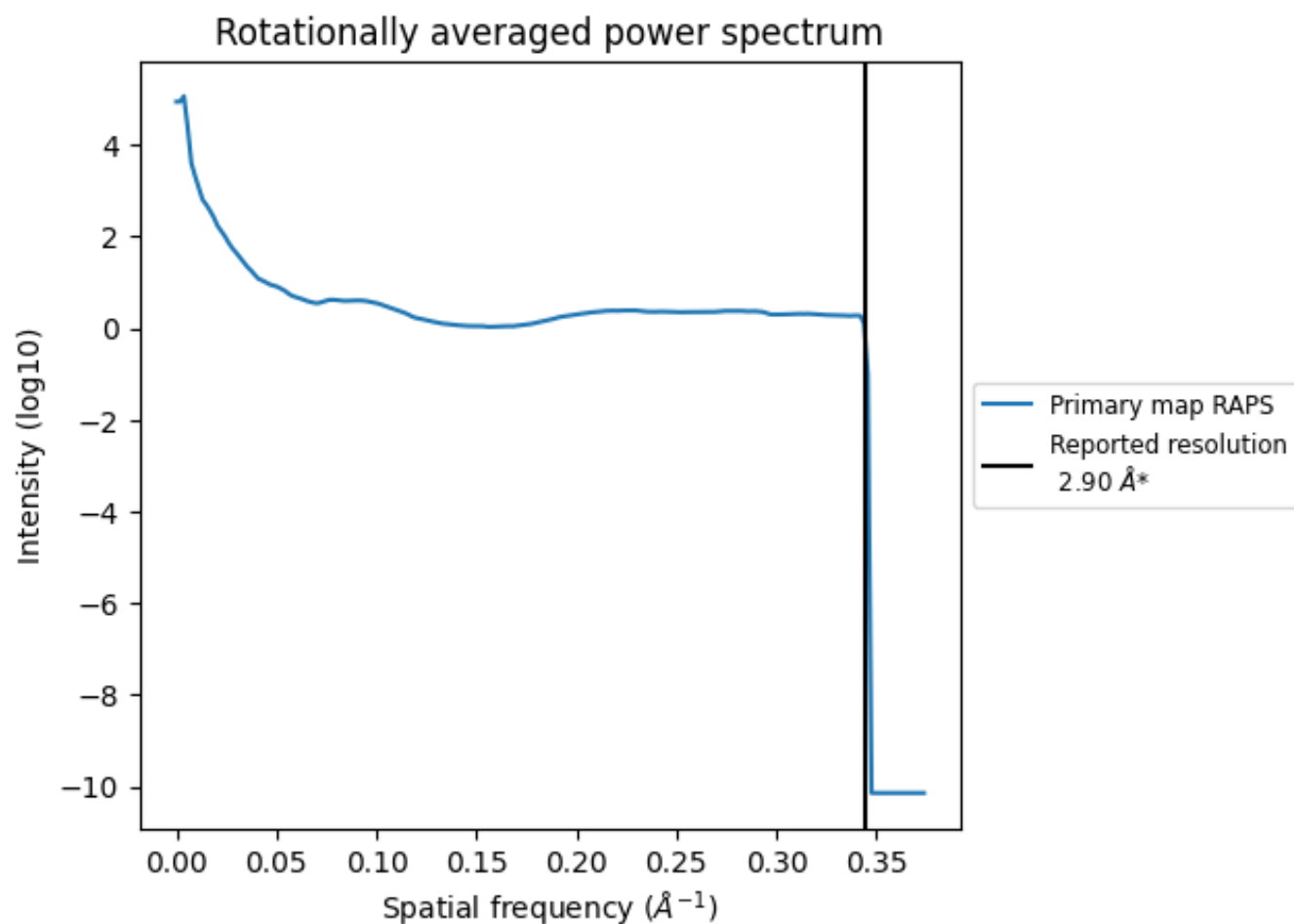
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1297 nm^3 ; this corresponds to an approximate mass of 1172 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

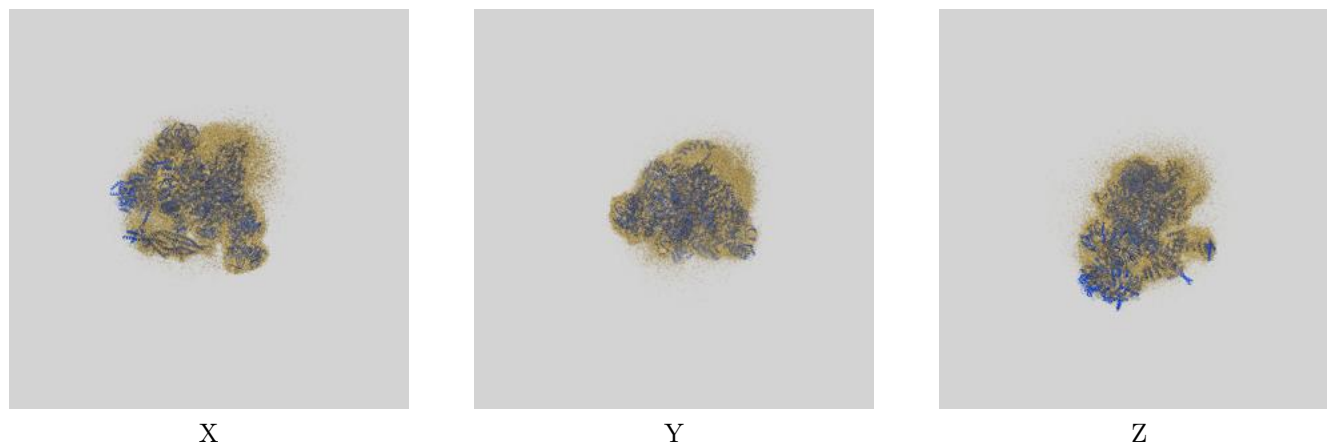
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

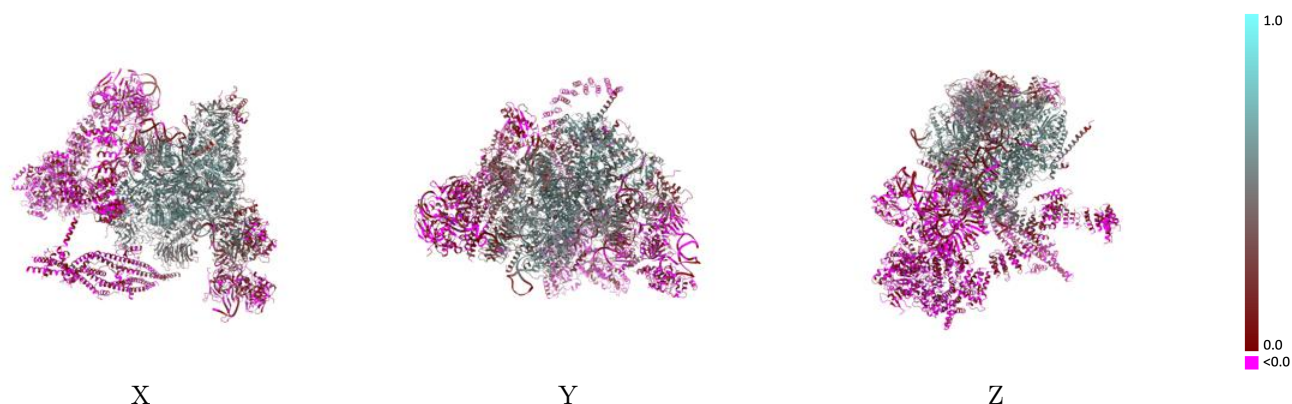
This section contains information regarding the fit between EMDB map EMD-9646 and PDB model 6ID0. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



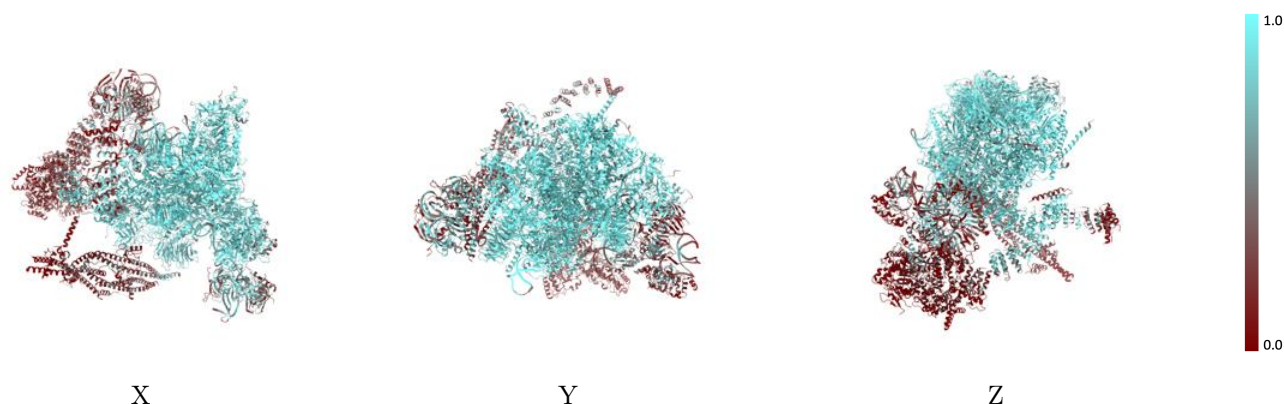
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



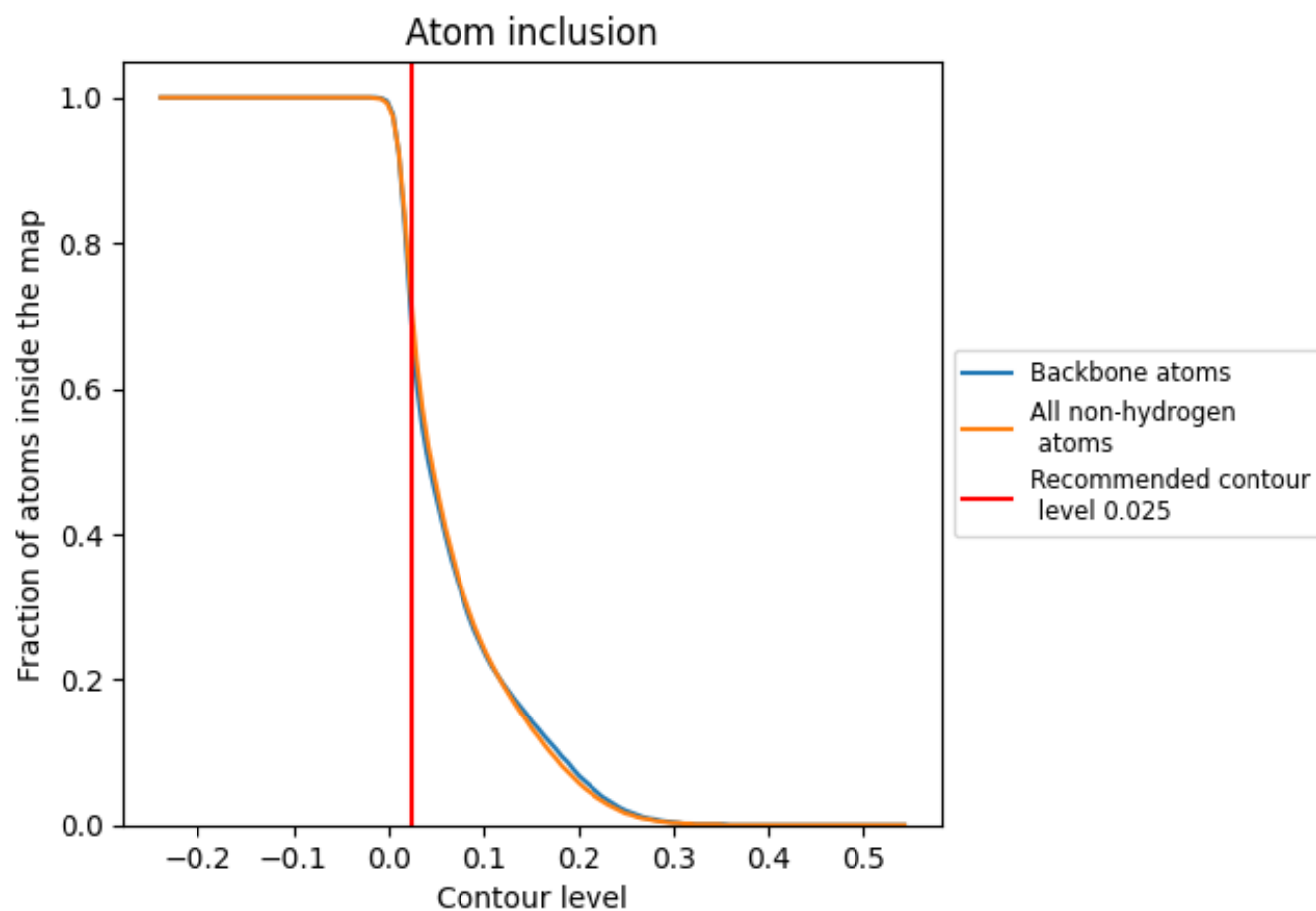
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7050	 0.3140
A	 0.9230	 0.5020
B	 0.8300	 0.3370
C	 0.8520	 0.3270
E	 0.8910	 0.4110
F	 0.9420	 0.4650
G	 0.6680	 0.1420
H	 0.5130	 0.1100
I	 0.5350	 0.0560
J	 0.7370	 0.3250
K	 0.2560	 0.0580
L	 0.6480	 0.3380
M	 0.8870	 0.4960
N	 0.9570	 0.5500
O	 0.8310	 0.3930
P	 0.8380	 0.4610
Q	 0.0690	 -0.0050
R	 0.8700	 0.4660
S	 0.9190	 0.4670
T	 0.9760	 0.5980
U	 0.8780	 0.4540
W	 0.8620	 0.3360
a	 0.6670	 0.1900
b	 0.4910	 0.0340
c	 0.6480	 0.0540
d	 0.6400	 0.0330
e	 0.4810	 0.0550
f	 0.4930	 -0.0020
g	 0.4850	 0.0500
h	 0.4700	 0.0160
i	 0.3660	 0.0240
j	 0.3520	 -0.0110
k	 0.3010	 -0.0100
l	 0.2530	 -0.0090
m	 0.3130	 0.0350



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n	 0.3830	 0.0330
o	 0.1870	 -0.0010
p	 0.3730	 0.0250
q	 0.1150	 0.0380
r	 0.1850	 0.0200
s	 0.2330	 0.0550
t	 0.1400	 0.0050
y	 0.3920	 0.0170