



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:30 AM UTC

PDB ID : 6EXN / pdb_00006exn
EMDB ID : EMD-3979
Title : Post-catalytic P complex spliceosome with 3' splice site docked
Authors : Wilkinson, M.E.; Fica, S.M.; Galej, W.P.; Norman, C.M.; Newman, A.J.; Nagai, K.
Deposited on : 2017-11-08
Resolution : 3.70 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:

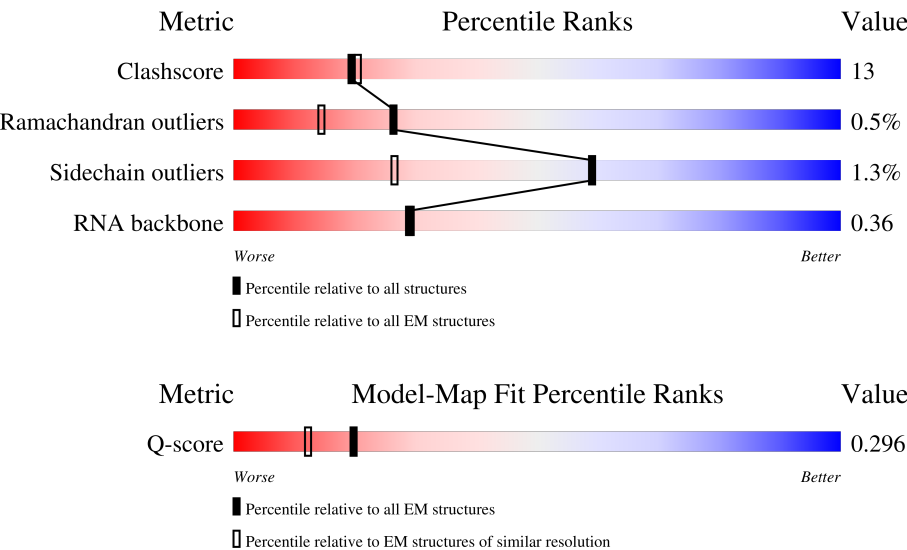
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.70 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	11569 (3.20 - 4.20)

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	179	
3	6	112	

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Mol	Chain	Length	Quality of chain
4	A	2413	
5	C	1008	
6	D	278	
7	E	39	
8	H	577	
9	I	95	
10	J	451	
11	K	379	
12	L	157	
13	M	339	
14	N	364	
15	O	590	
16	P	175	
17	R	135	
18	S	687	
19	T	859	
20	V	1145	
21	W	238	
22	X	95	
23	Y	111	
24	a	251	
25	b	196	
25	k	196	
26	c	382	
27	d	101	

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Mol	Chain	Length	Quality of chain
27	n	101	
28	e	94	
28	p	94	
29	f	86	
29	q	86	
30	g	77	
30	r	77	
31	h	146	
31	l	146	
32	j	110	
32	m	110	
33	o	455	
34	s	175	
35	t	503	
35	u	503	
35	v	503	
35	w	503	
36	y	215	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 80677 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
1	2	136	Total	C	N	O	P	0	0
			2868	1282	476	974	136		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	171	Total	C	N	O	P	0	0
			3626	1623	630	1203	170		

- Molecule 3 is a RNA chain called U6 snRNA.

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

- Molecule 4 is a protein called Pre-mRNA-splicing factor Prp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1945	Total	C	N	O	S	0	0
			16046	10308	2764	2915	59		

- Molecule 5 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	880	Total	C	N	O	S	0	0
			6999	4522	1169	1280	28		

- Molecule 6 is a protein called Pre-mRNA-splicing factor CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	97	Total	C	N	O	S	0	0
			579	347	108	123	1		

- Molecule 7 is a RNA chain called Ligated exons: UBC4 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	32	Total	C	N	O	P	0	0
			586	258	86	210	32		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	411	Total	C	N	O	S	0	0
			2689	1685	477	521	6		

- Molecule 9 is a RNA chain called Intron lariat: UBC4 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	39	Total	C	N	O	P	0	0
			804	360	136	269	39		

- Molecule 10 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	342	Total	C	N	O	S	0	0
			2691	1699	475	507	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	80	THR	ALA	conflict	UNP Q12417

- Molecule 11 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	170	Total	C	N	O	S	0	0
			1355	847	249	254	5		

- Molecule 12 is a protein called Pre-mRNA-splicing factor BUD31.

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

- Molecule 13 is a protein called Pre-mRNA-splicing factor CWC2.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	242	Total	C	N	O	S	0	0
			1917	1217	335	350	15		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2350	1457	437	449	7		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	125	VAL	ALA	conflict	UNP Q03654
O	285	PRO	SER	conflict	UNP Q03654
O	341	GLU	ASP	conflict	UNP Q03654
O	342	PRO	SER	conflict	UNP Q03654
O	417	SER	PRO	conflict	UNP Q03654
O	425	PRO	ARG	conflict	UNP Q03654

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	73	Total	C	N	O	S	0	0
			600	378	119	102	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	49	LYS	ARG	conflict	UNP Q03772
P	58	ASN	SER	conflict	UNP Q03772
P	66	VAL	ALA	conflict	UNP Q03772
P	68	VAL	MET	conflict	UNP Q03772

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	73	Total	C	N	O	0	0
			423	252	82	89		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	472	Total	C	N	O	S	0	0
			3189	1989	599	593	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	561	LYS	GLU	conflict	UNP Q12309
S	615	MET	LEU	conflict	UNP Q12309
S	649	ASP	ASN	conflict	UNP Q12309
S	659	VAL	ILE	conflict	UNP Q12309

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	T	594	Total	C	N	O	0	0
			2957	1769	594	594		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	695	ILE	THR	conflict	UNP Q04048

- Molecule 20 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	638	Total	C	N	O	S	0	0
			5059	3217	854	959	29		

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	149	Total	C	N	O	S	0	0
			1211	756	223	228	4		

- Molecule 22 is a protein called Unassigned structure.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	95	Total	C	N	O	0	0
			475	285	95	95		

- Molecule 23 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Y	87	Total	C	N	O	S	0
			704	451	123	127	3	0

- Molecule 24 is a protein called Pre-mRNA-splicing factor Prp18.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	a	171	Total	C	N	O	S	0
			1372	878	244	246	4	0

- Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	b	80	Total	C	N	O	S	0
			631	403	114	111	3	0
25	k	70	Total	C	N	O	S	0
			563	360	98	102	3	0

- Molecule 26 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	c	204	Total	C	N	O	S	0
			1709	1072	315	314	8	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	d	82	Total	C	N	O	S	0
			625	399	109	115	2	0
27	n	82	Total	C	N	O	S	0
			632	402	109	119	2	0

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
28	p	77	Total	C	N	O	S	0	0
			602	396	95	108	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
29	q	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
30	r	75	Total	C	N	O	S	0	0
			577	363	100	112	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
31	l	87	Total	C	N	O	S	0	0
			679	435	118	123	3		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
32	m	92	Total	C	N	O	S	0	0
			752	481	136	131	4		

- Molecule 33 is a protein called Pre-mRNA-processing factor Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	322	Total	C	N	O	S	0	0
			2599	1655	462	474	8		

- Molecule 34 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	110	Total	C	N	O	0	0
			548	328	110	110		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
35	t	117	Total	C	N	O	0	0
			583	349	117	117		
35	u	116	Total	C	N	O	0	0
			578	346	116	116		
35	v	118	Total	C	N	O	0	0
			588	352	118	118		
35	w	114	Total	C	N	O	0	0
			568	340	114	114		

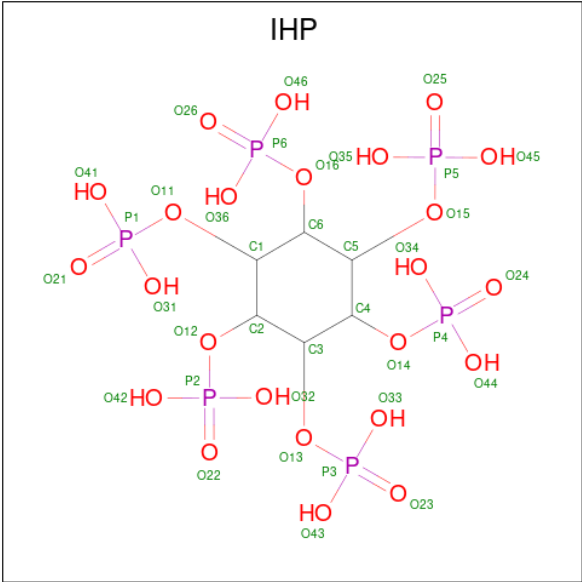
- Molecule 36 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	88	Total	C	N	O	S	0	0
			719	444	132	142	1		

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

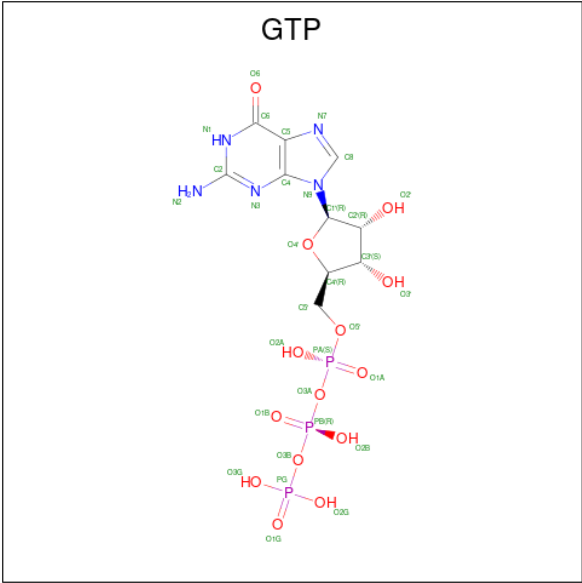
Mol	Chain	Residues	Atoms		AltConf
37	6	1	Total	Mg	0
			1	1	

- Molecule 38 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

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



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

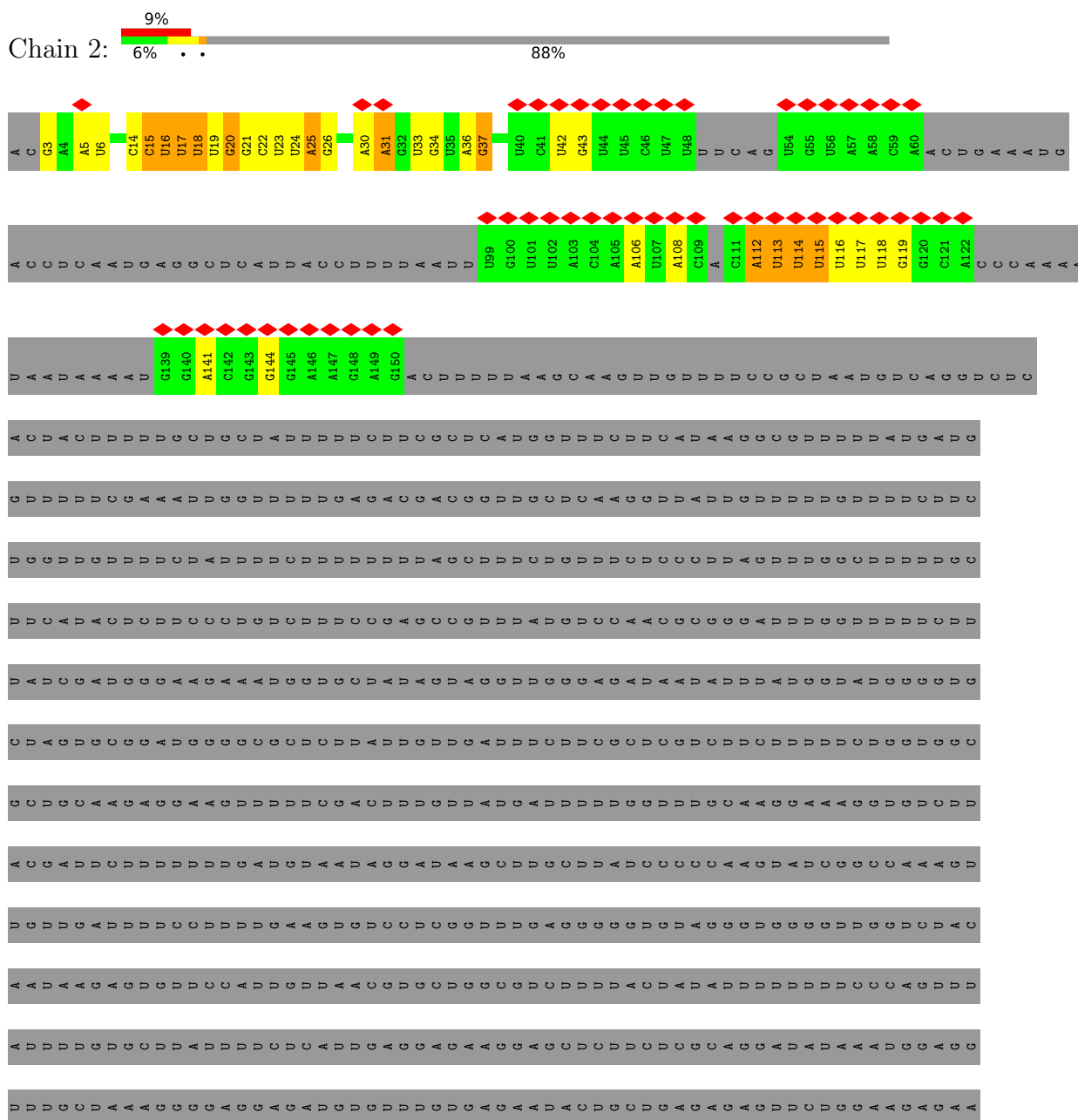
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

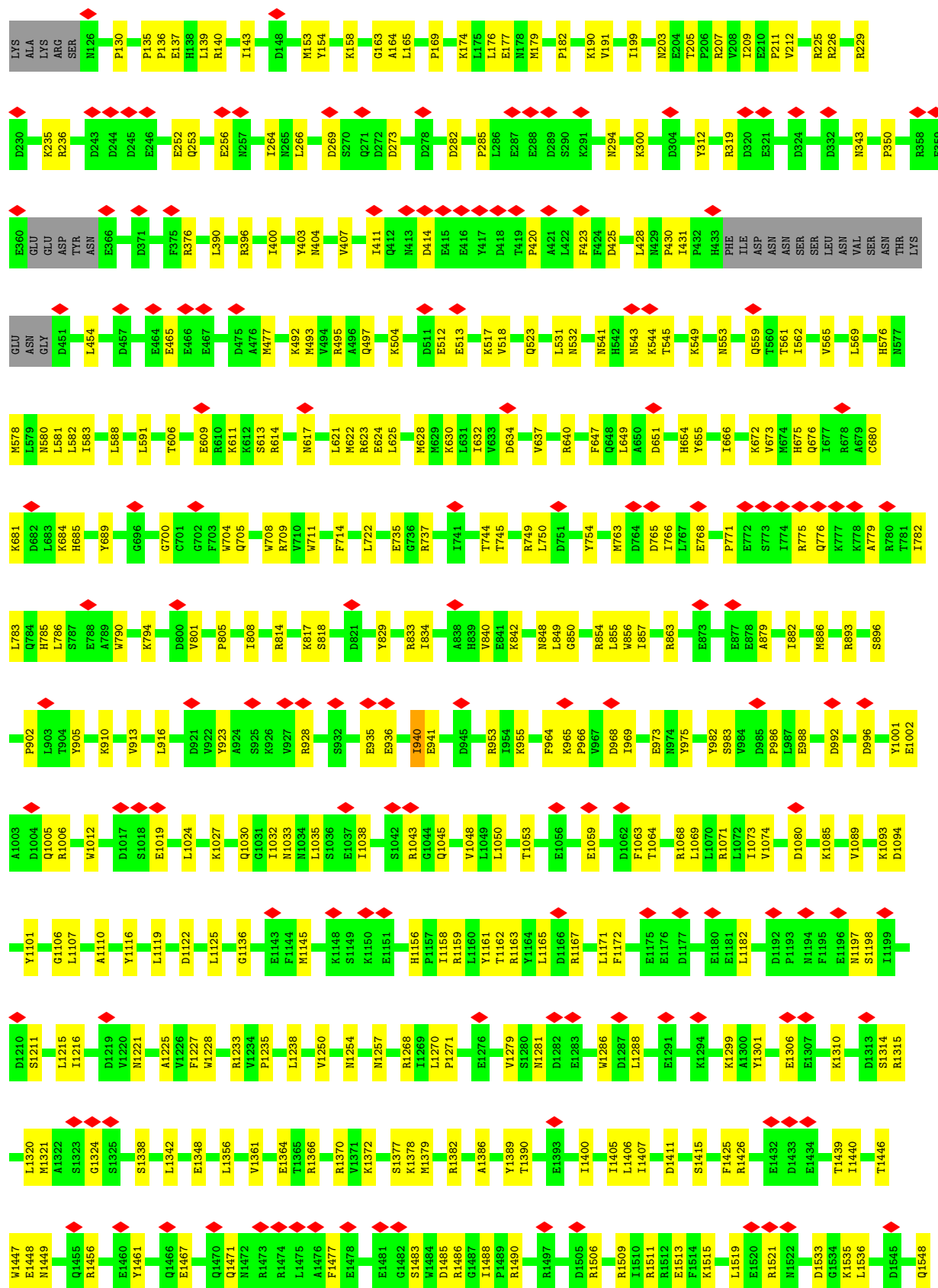
Mol	Chain	Residues	Atoms		AltConf
40	L	3	Total 3	Zn 3	0
40	M	1	Total 1	Zn 1	0
40	N	2	Total 2	Zn 2	0
40	c	1	Total 1	Zn 1	0

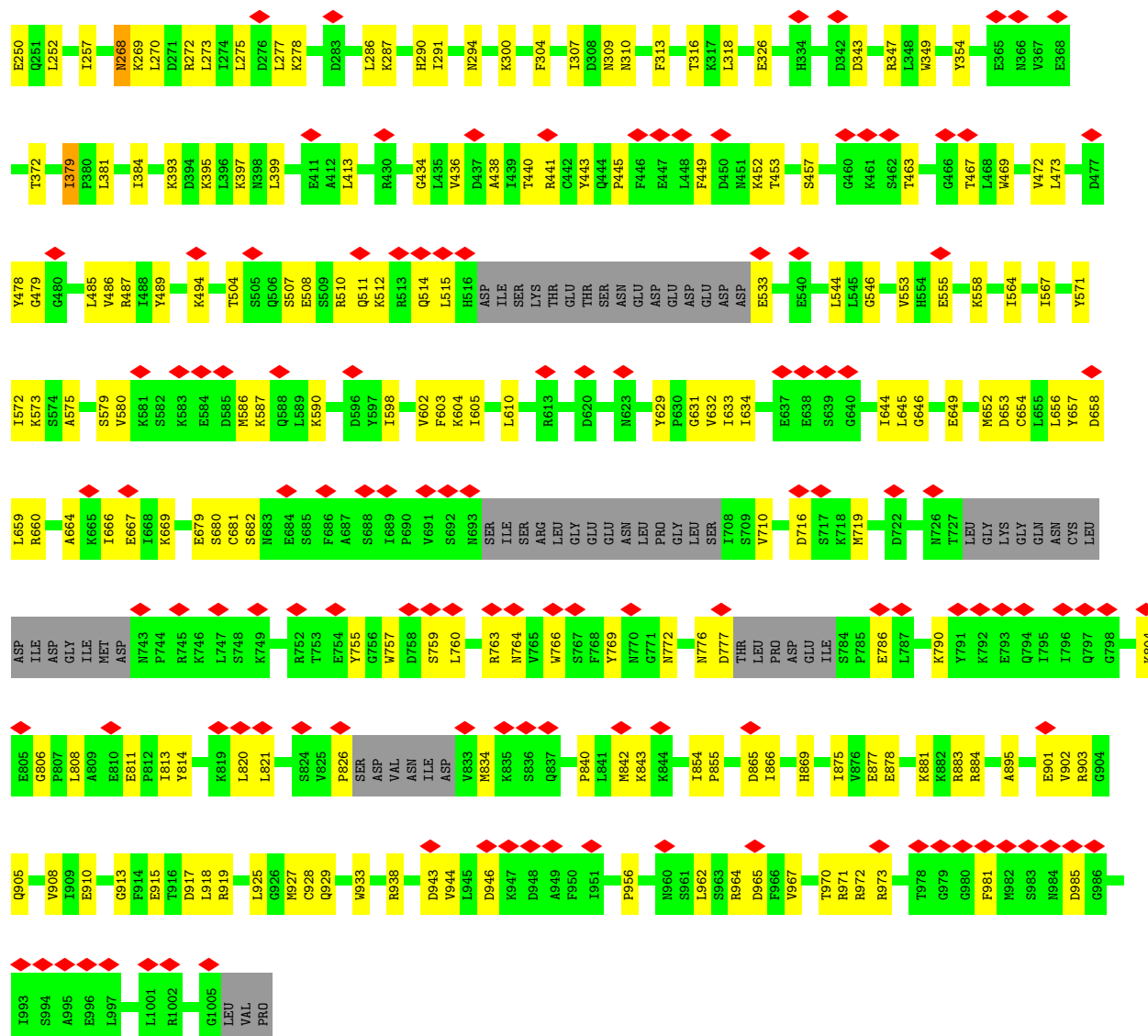
3 Residue-property plots [i](#)

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

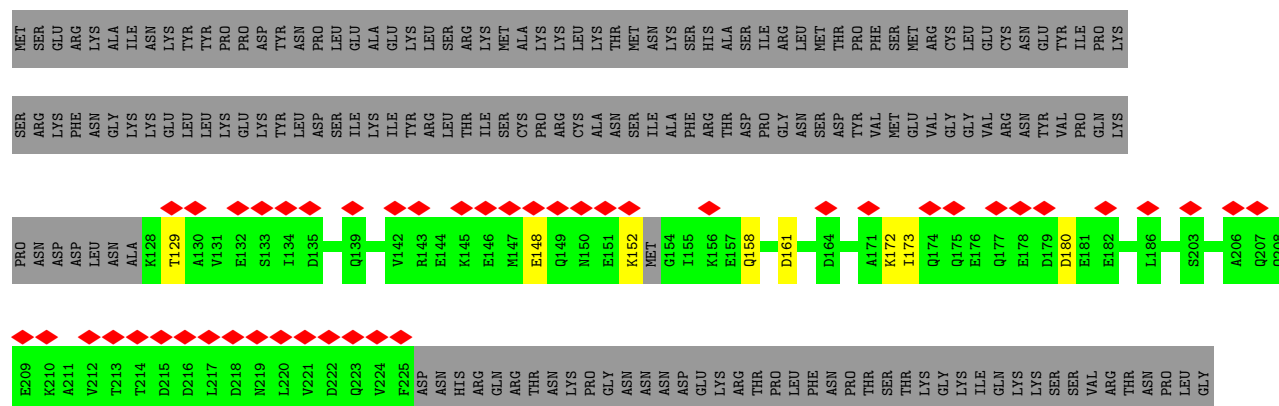
• Molecule 1: U2 snRNA





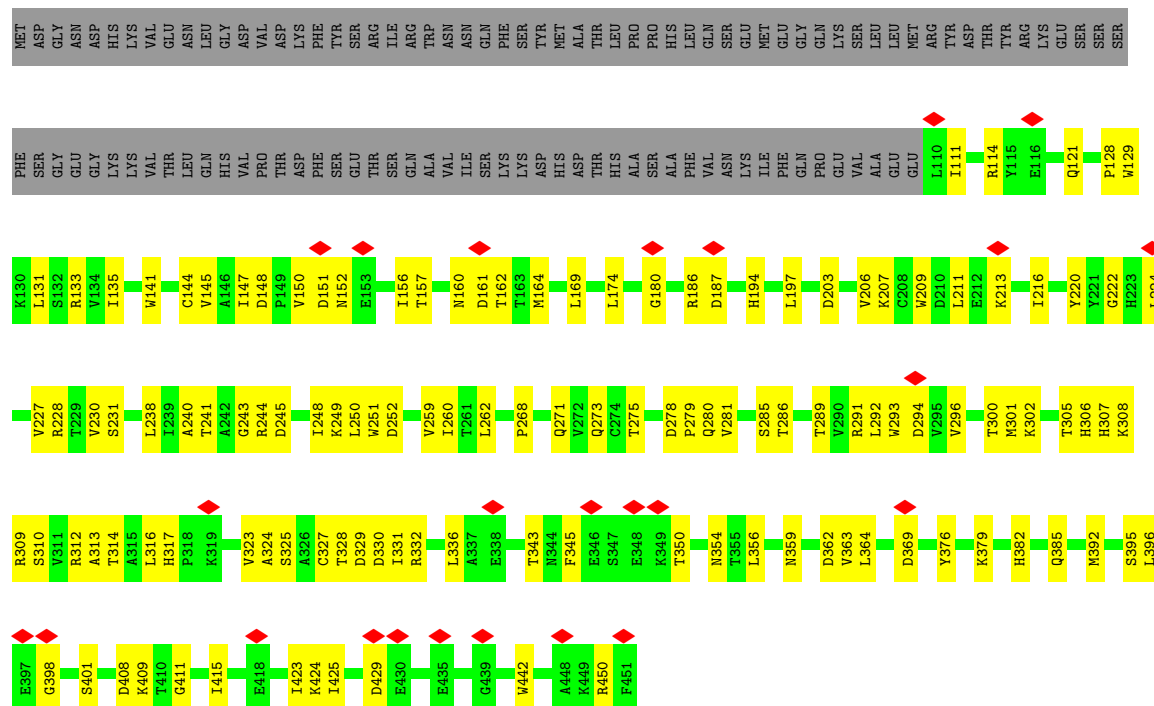


• Molecule 6: Pre-mRNA-splicing factor CWC16

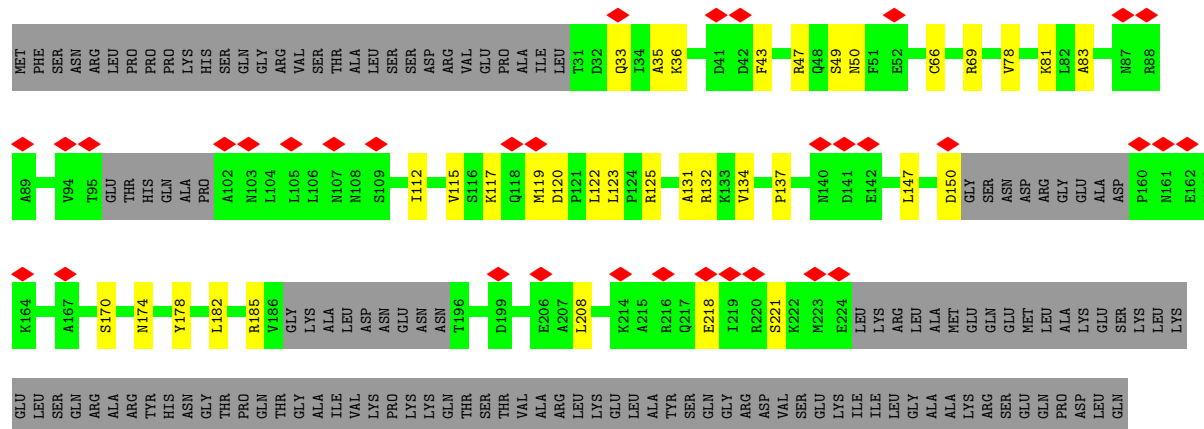
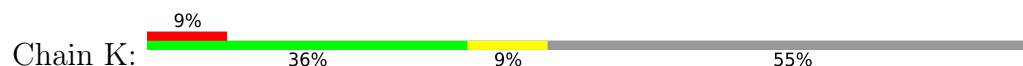




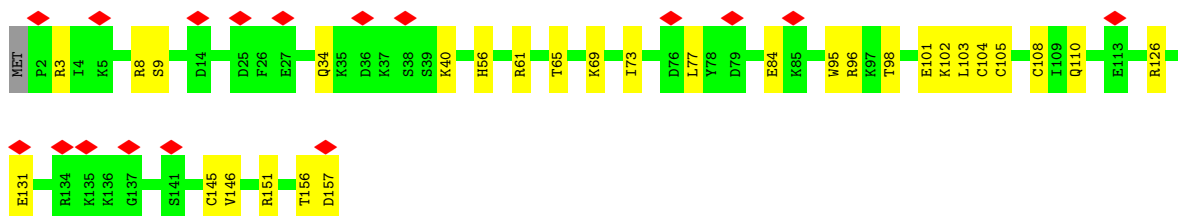
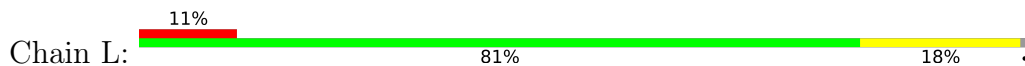
- Molecule 10: Pre-mRNA-splicing factor PRP46



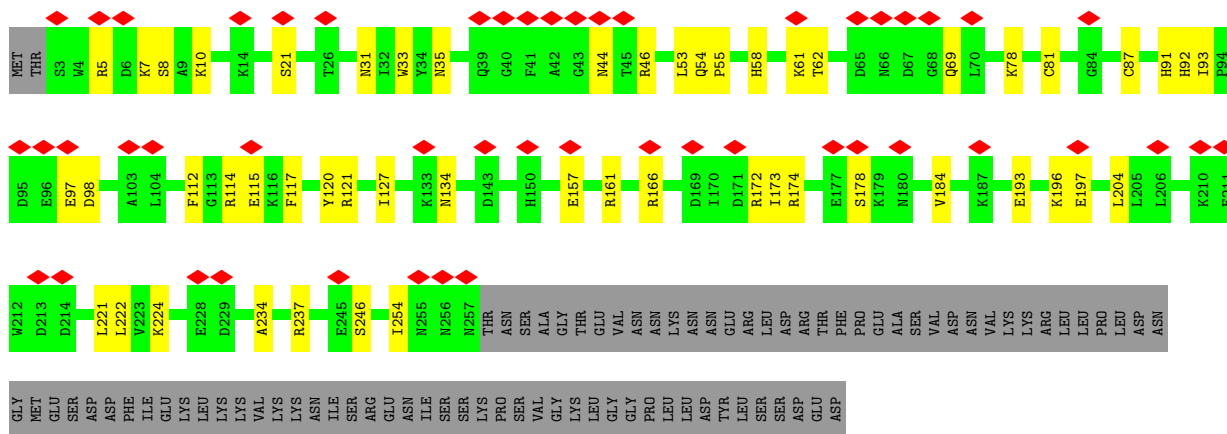
- Molecule 11: Pre-mRNA-processing protein 45



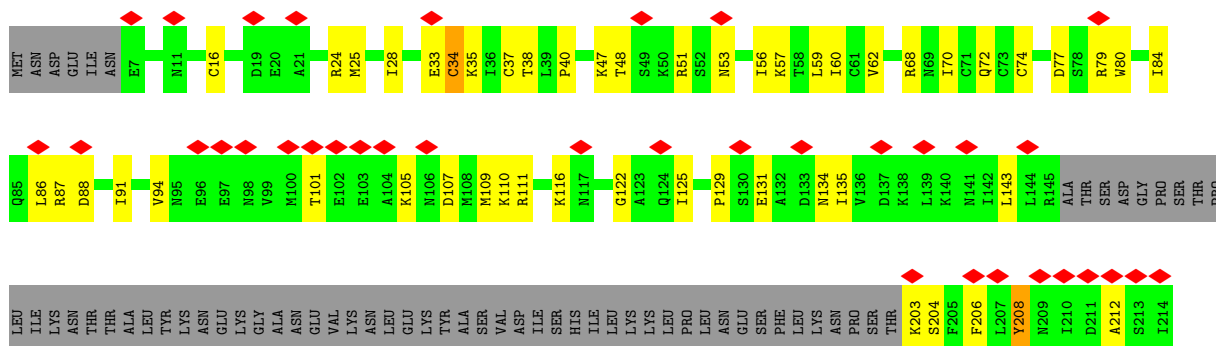
- Molecule 12: Pre-mRNA-splicing factor BUD31

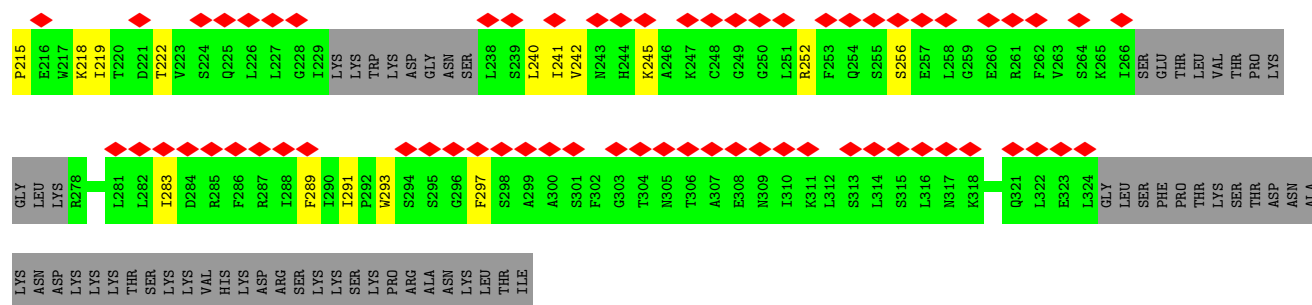


- Molecule 13: Pre-mRNA-splicing factor CWC2

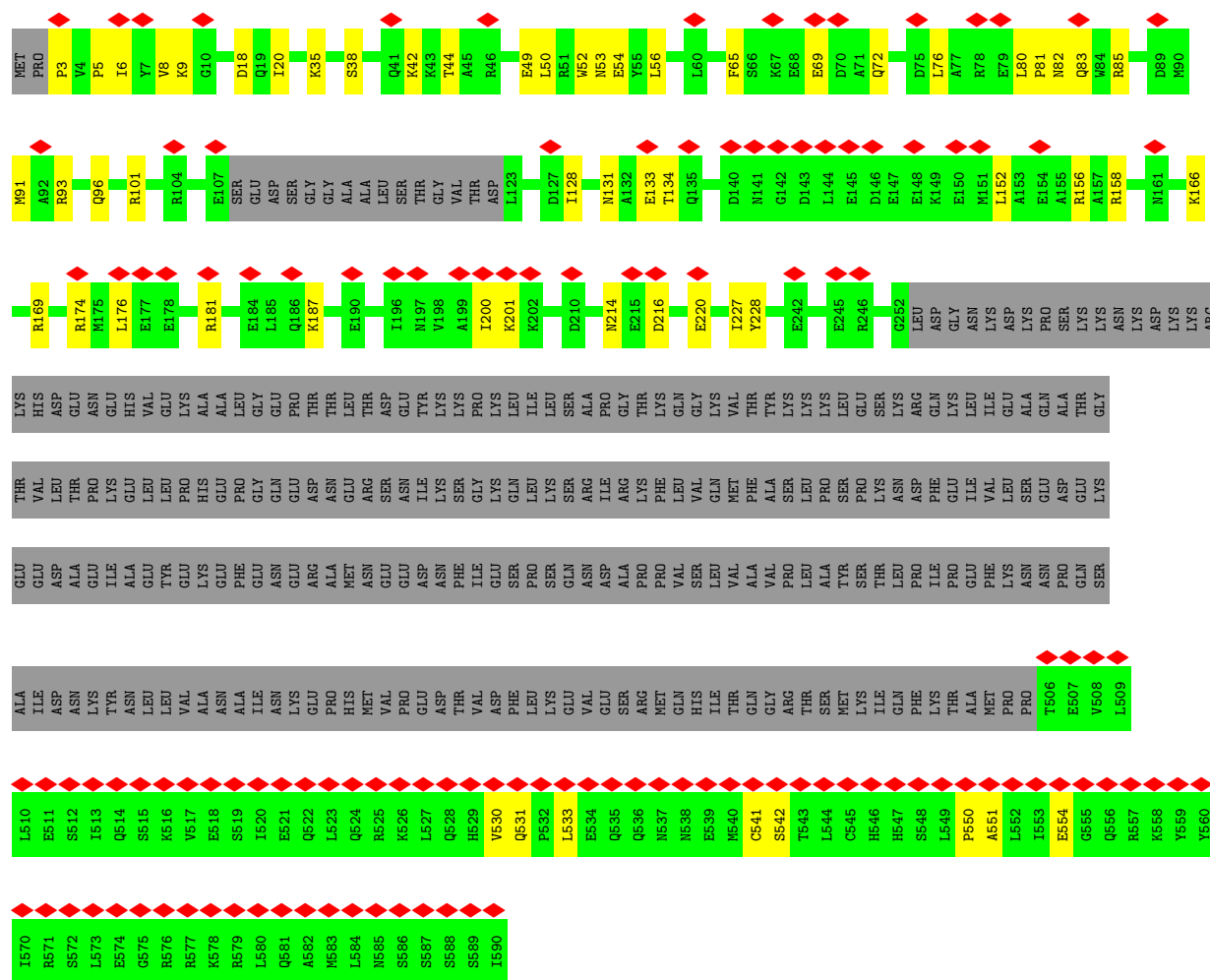
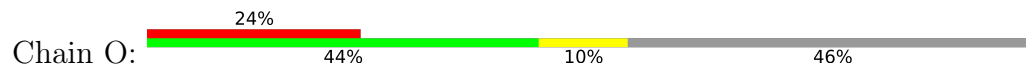


- Molecule 14: Pre-mRNA-splicing factor SLT11

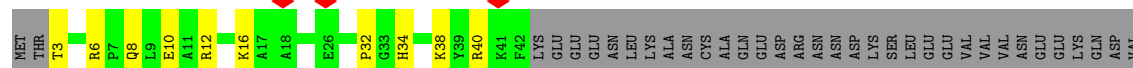
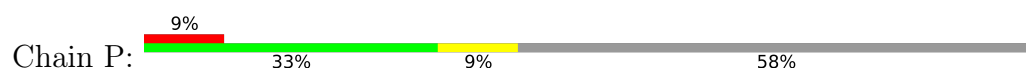




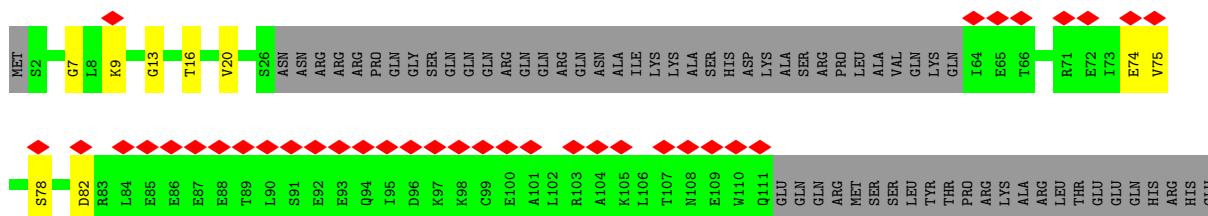
• Molecule 15: Pre-mRNA-splicing factor CEF1



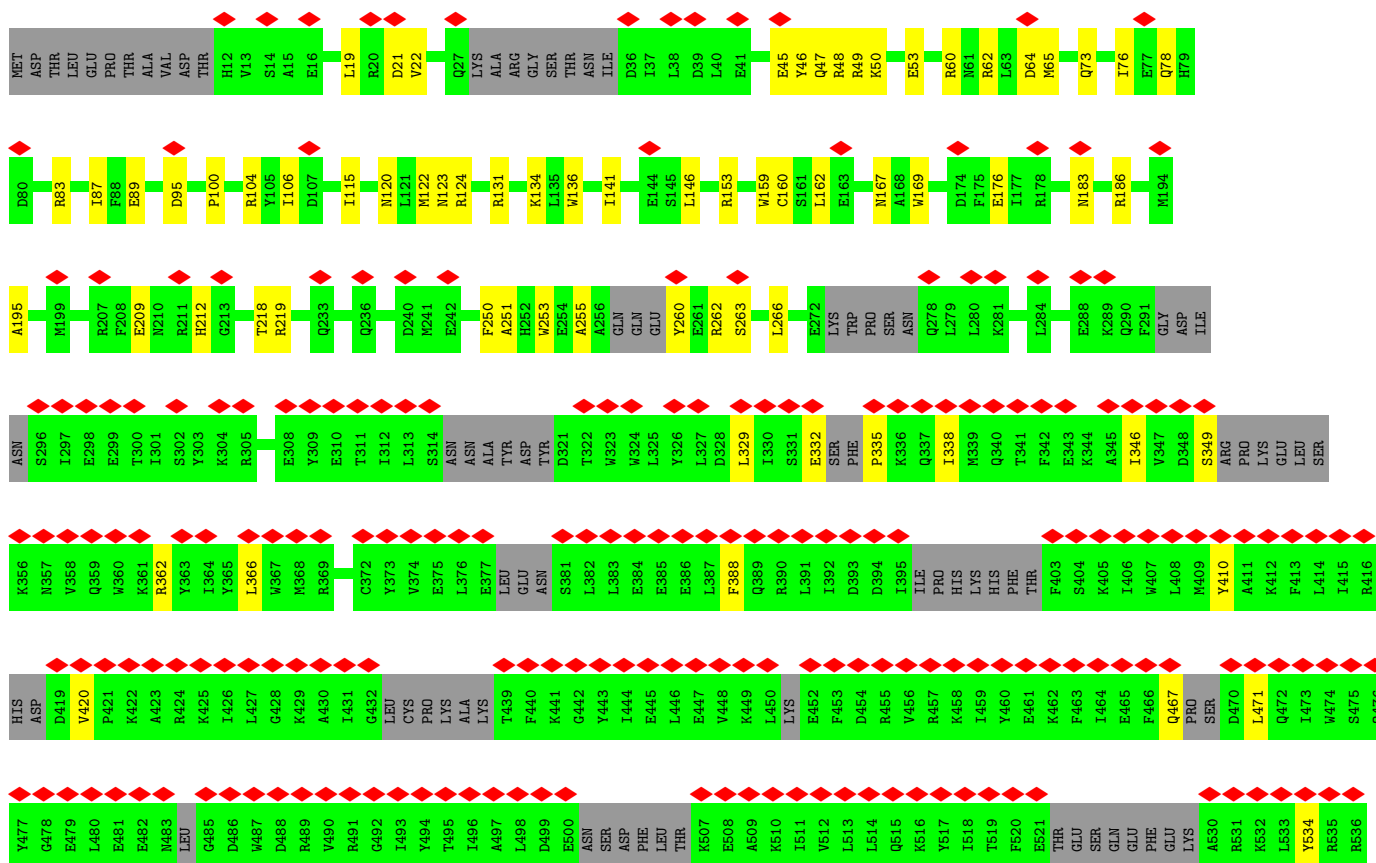
• Molecule 16: Pre-mRNA-splicing factor CWC15



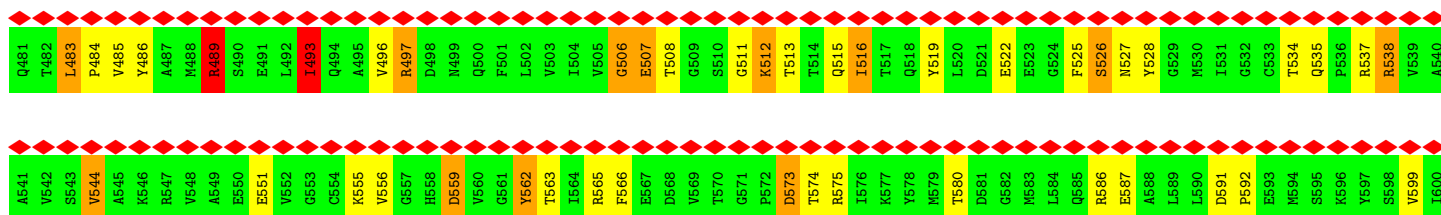
- Molecule 17: Pre-mRNA-splicing factor CWC21

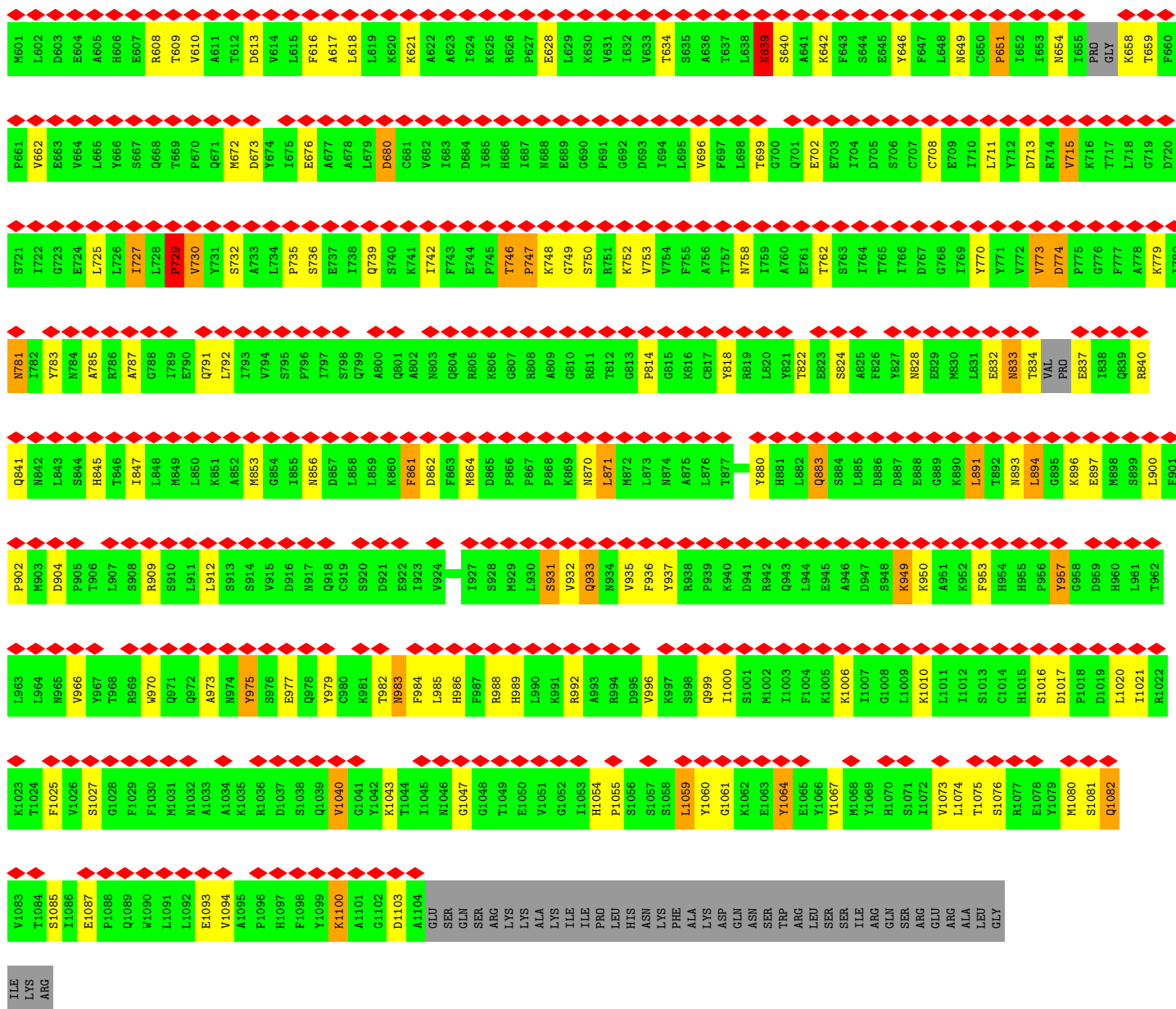


- Molecule 18: Pre-mRNA-splicing factor CLF1









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

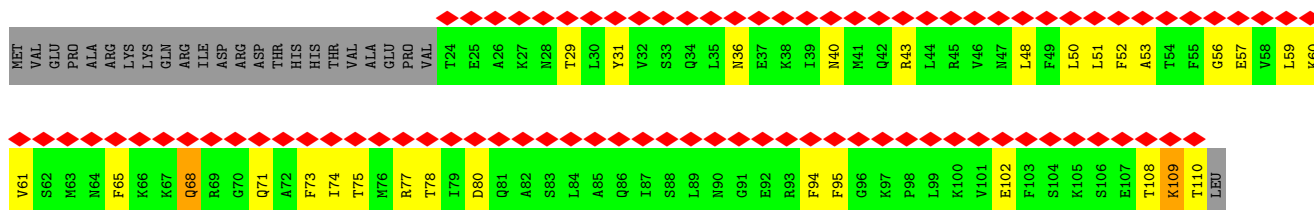
• Molecule 22: Unassigned structure

Chain X:



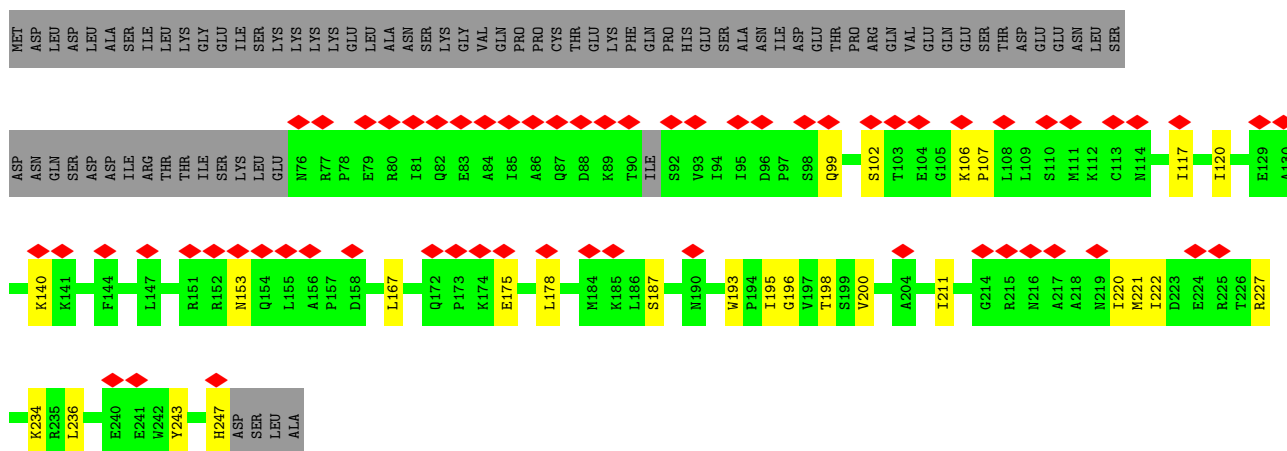
• Molecule 23: U2 small nuclear ribonucleoprotein B''

Chain Y:



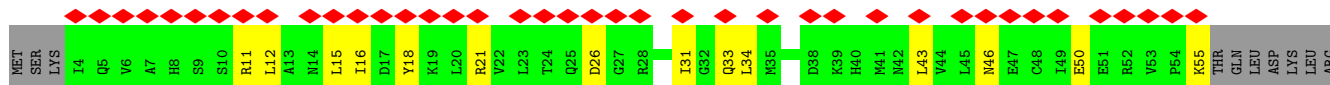
• Molecule 24: Pre-mRNA-splicing factor Prp18

Chain a:



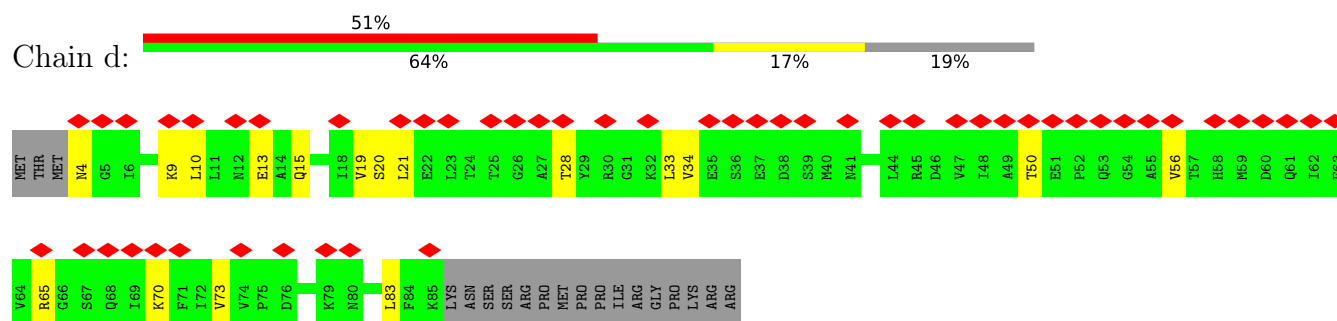
• Molecule 25: Small nuclear ribonucleoprotein-associated protein B

Chain b:

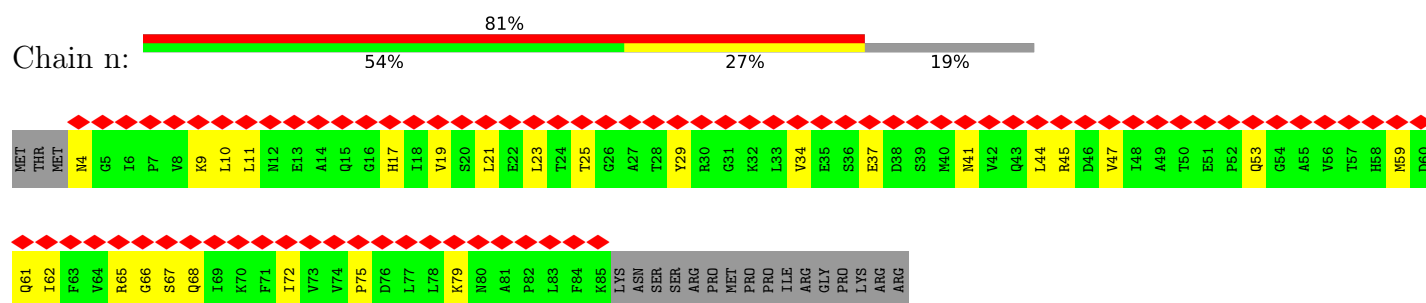




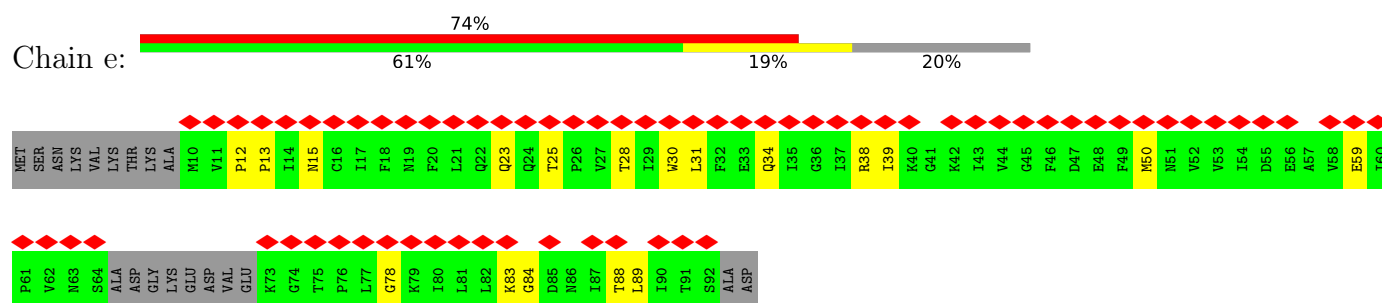
- Molecule 27: Small nuclear ribonucleoprotein Sm D3



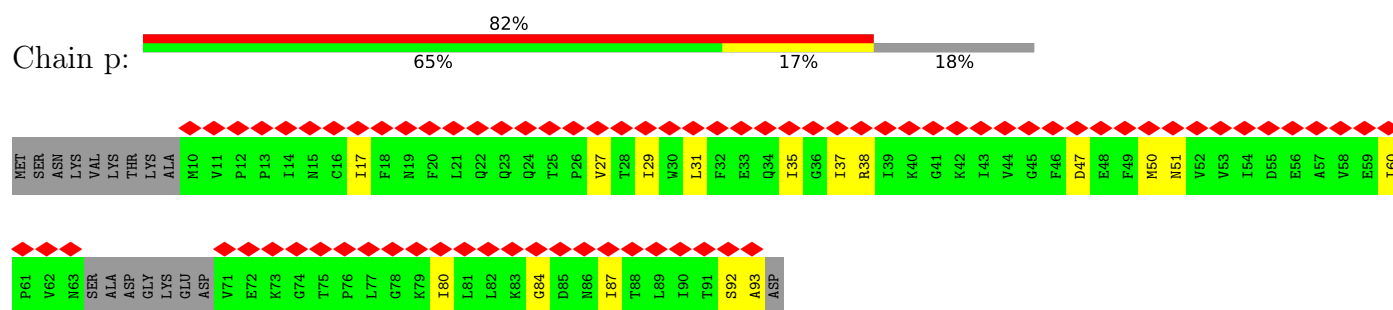
- Molecule 27: Small nuclear ribonucleoprotein Sm D3



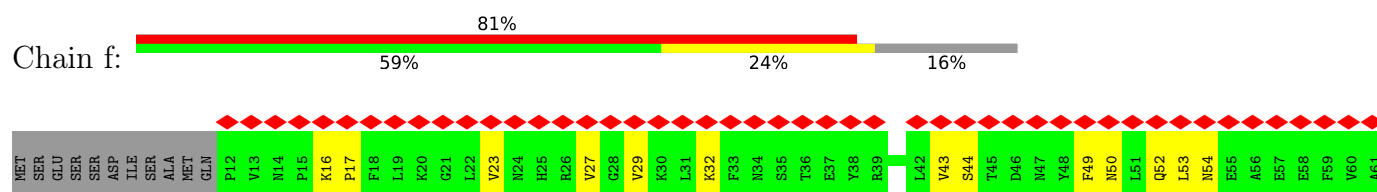
- Molecule 28: Small nuclear ribonucleoprotein E



- Molecule 28: Small nuclear ribonucleoprotein E

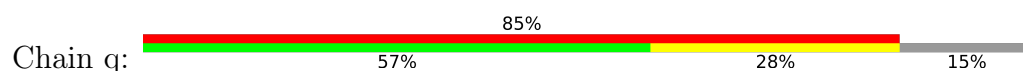


- Molecule 29: Small nuclear ribonucleoprotein F

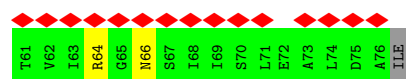
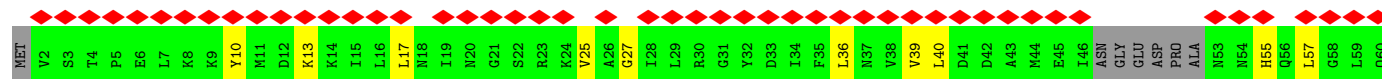
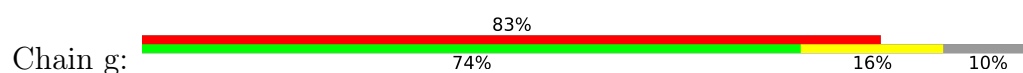




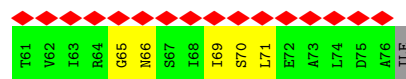
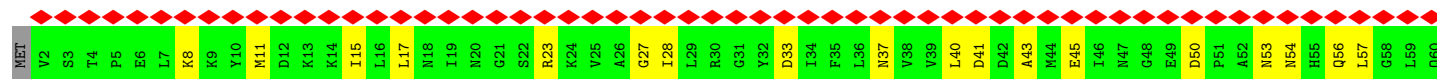
• Molecule 29: Small nuclear ribonucleoprotein F



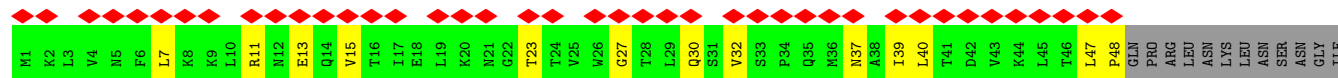
• Molecule 30: Small nuclear ribonucleoprotein G



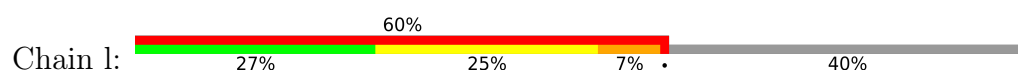
• Molecule 30: Small nuclear ribonucleoprotein G



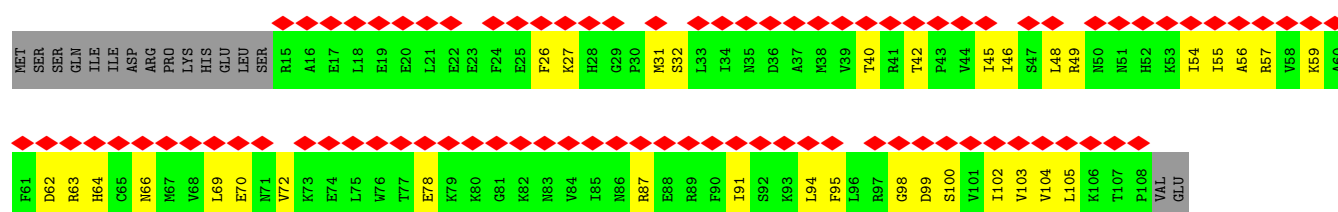
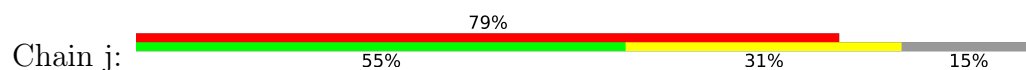
• Molecule 31: Small nuclear ribonucleoprotein Sm D1



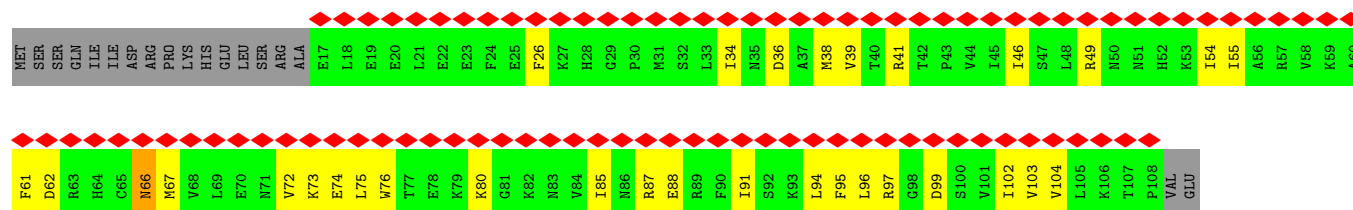
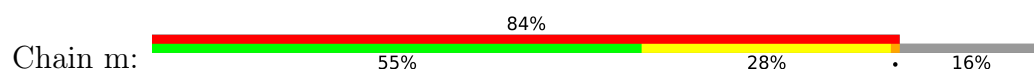
• Molecule 31: Small nuclear ribonucleoprotein Sm D1



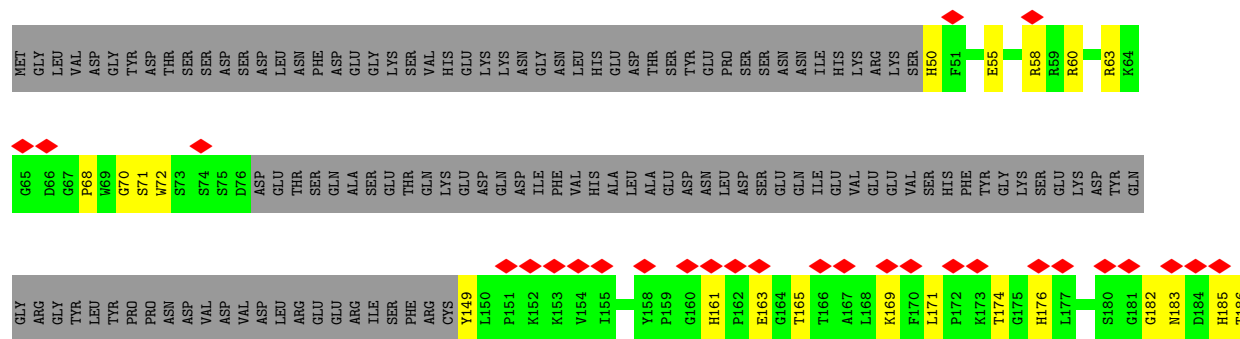
• Molecule 32: Small nuclear ribonucleoprotein Sm D2

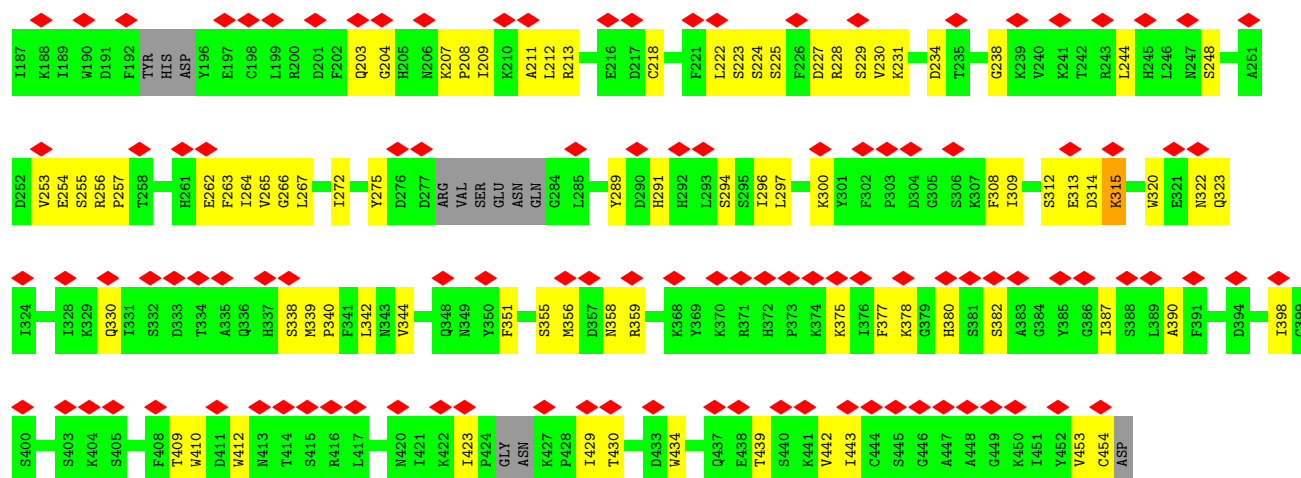


• Molecule 32: Small nuclear ribonucleoprotein Sm D2

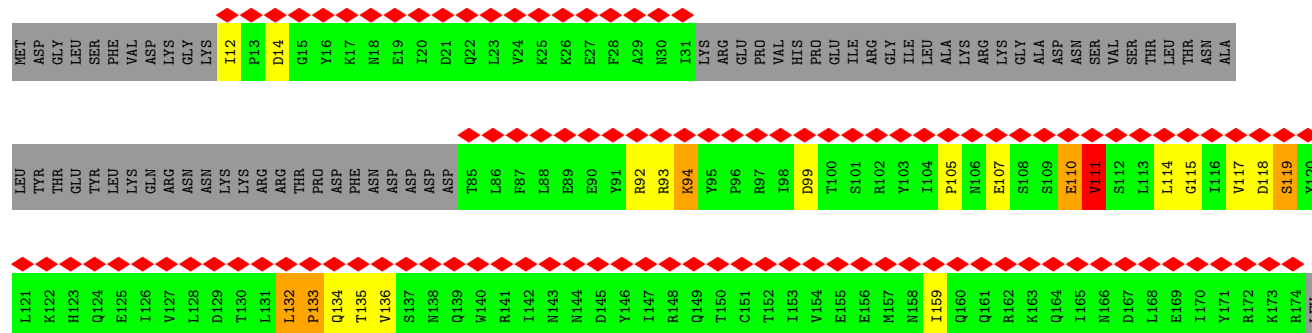


• Molecule 33: Pre-mRNA-processing factor Prp17

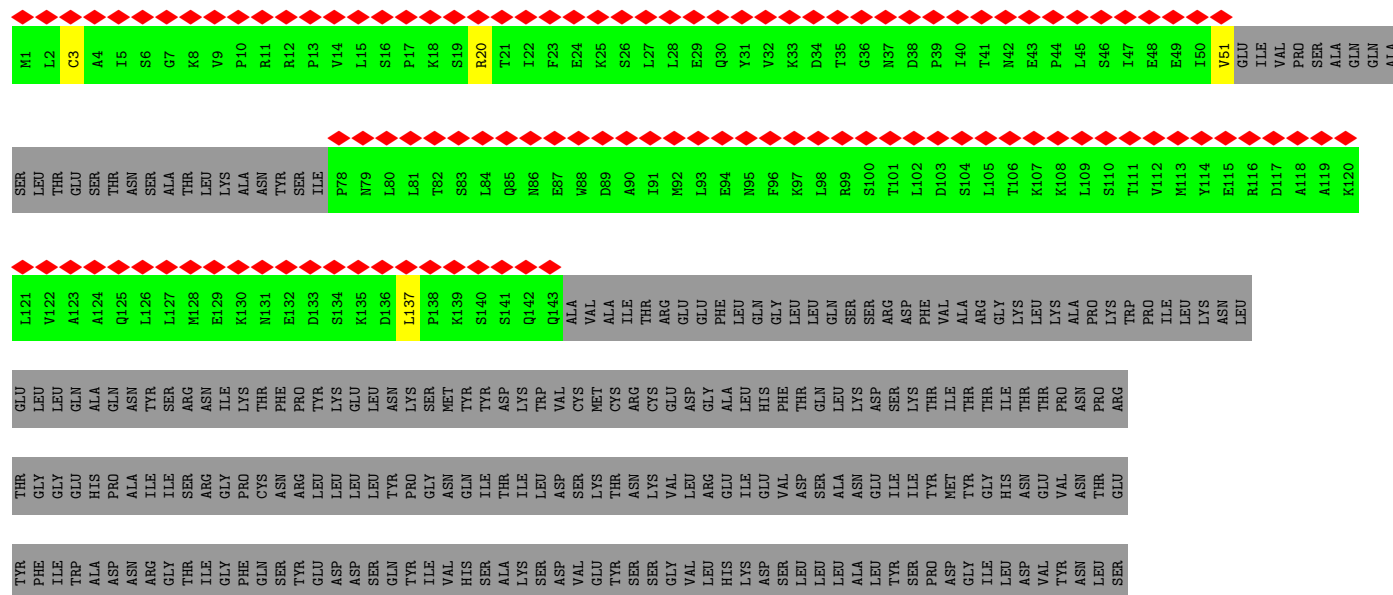




• Molecule 34: Pre-mRNA-splicing factor SNT309



• Molecule 35: Pre-mRNA-processing factor Prp19





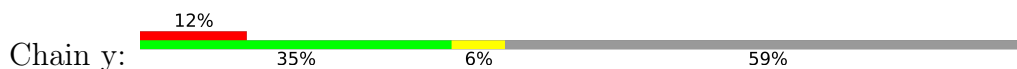
WORLD WIDE
PDB
PROTEIN DATA BANK

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

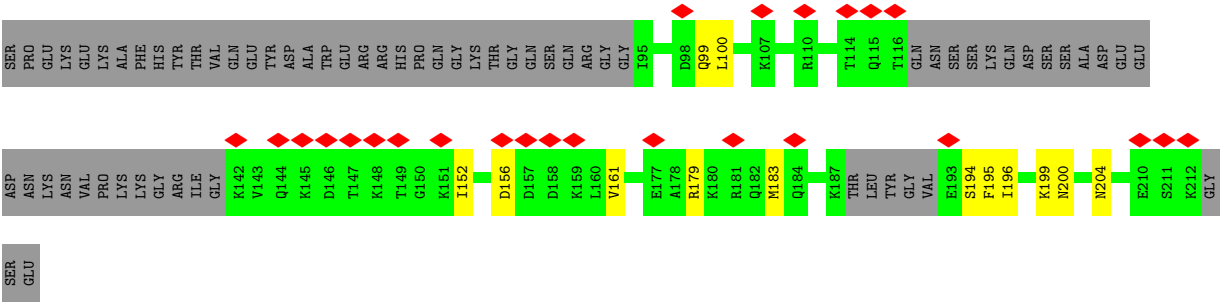
- Molecule 35: Pre-mRNA-processing factor Prp19

[illegible]

- Molecule 36: Pre-mRNA-splicing factor SYF2



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

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48617	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.174	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.35	0/3190	0.64	0/4946
2	5	0.25	0/4049	0.48	1/6300 (0.0%)
3	6	0.27	0/2427	0.47	0/3778
4	A	0.32	0/16452	0.57	0/22294
5	C	0.31	0/7147	0.57	0/9673
6	D	0.17	0/577	0.36	0/787
7	E	0.35	0/651	0.68	0/1008
8	H	0.39	0/2716	1.05	2/3702 (0.1%)
9	I	0.24	0/895	0.50	2/1384 (0.1%)
10	J	0.35	0/2750	0.57	2/3735 (0.1%)
11	K	0.26	0/1375	0.53	0/1854
12	L	0.27	0/1307	0.50	0/1748
13	M	0.26	0/2094	0.51	0/2815
14	N	0.25	0/1945	0.55	0/2617
15	O	0.47	0/2378	0.86	6/3212 (0.2%)
16	P	0.24	0/616	0.47	0/822
17	R	0.43	0/423	1.13	0/577
18	S	0.35	0/3221	0.97	1/4379 (0.0%)
19	T	0.48	1/2918 (0.0%)	1.32	6/4015 (0.1%)
20	V	0.83	2/5157 (0.0%)	1.62	49/6973 (0.7%)
21	W	0.36	0/1228	0.91	2/1663 (0.1%)
23	Y	0.27	0/713	0.71	1/952 (0.1%)
24	a	0.25	0/1400	0.57	0/1897
25	b	0.21	0/636	0.54	0/856
25	k	0.32	0/567	0.68	0/762
26	c	0.25	0/1737	0.60	0/2315
27	d	0.20	0/634	0.54	0/859
27	n	0.28	0/641	0.64	0/868
28	e	0.22	0/585	0.55	0/795
28	p	0.28	0/612	0.61	0/830
29	f	0.25	0/585	0.65	2/791 (0.3%)
29	q	0.32	0/597	0.73	0/807

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	g	0.19	0/532	0.56	0/715
30	r	0.30	0/582	0.71	0/785
31	h	0.19	0/649	0.51	0/880
31	l	0.32	0/685	0.96	8/926 (0.9%)
32	j	0.20	0/753	0.57	0/1013
32	m	0.31	0/764	0.78	2/1026 (0.2%)
33	o	0.25	0/2671	0.57	0/3605
34	s	0.98	1/546 (0.2%)	1.45	11/760 (1.4%)
35	t	0.79	0/581	1.30	2/809 (0.2%)
35	u	0.96	1/576 (0.2%)	1.34	3/802 (0.4%)
35	v	1.02	2/586 (0.3%)	1.56	7/816 (0.9%)
35	w	0.78	0/566	1.25	3/788 (0.4%)
36	y	0.24	0/721	0.49	0/954
All	All	0.40	7/82435 (0.0%)	0.80	110/113893 (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
14	N	0	1
18	S	0	1
20	V	0	23
21	W	0	3
22	X	0	3
26	c	0	2
30	r	0	1
34	s	0	2
35	t	0	1
35	v	0	1
35	w	0	1
All	All	0	39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	493	ILE	CA-CB	8.29	1.63	1.54
35	v	109	LEU	C-N	7.98	1.44	1.33
19	T	612	ILE	C-N	5.78	1.41	1.34
35	v	134	SER	C-O	-5.66	1.17	1.24
34	s	133	PRO	CA-C	5.64	1.60	1.52

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	V	493	ILE	N-CA-CB	19.36	131.72	110.62
20	V	493	ILE	CB-CA-C	-15.33	92.65	111.81
8	H	87	ILE	CA-C-N	14.34	134.48	118.85
8	H	87	ILE	C-N-CA	14.34	134.48	118.85
35	v	134	SER	CA-C-O	-11.55	108.17	120.42

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	208	TYR	Peptide
18	S	212	HIS	Peptide
20	V	489	ARG	Sidechain
20	V	493	ILE	Peptide
20	V	497	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2868	0	1455	90	0
2	5	3626	0	1834	56	0
3	6	2170	0	1095	41	0
4	A	16046	0	16046	391	0
5	C	6999	0	7168	187	0
6	D	579	0	376	8	0
7	E	586	0	294	73	0
8	H	2689	0	2087	26	0
9	I	804	0	404	14	0
10	J	2691	0	2690	92	0
11	K	1355	0	1383	30	0
12	L	1283	0	1301	23	0
13	M	2048	0	2011	44	0
14	N	1917	0	1974	49	0
15	O	2350	0	2134	52	0
16	P	600	0	589	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	R	423	0	286	24	0
18	S	3189	0	2485	85	0
19	T	2957	0	1259	26	0
20	V	5059	0	5064	226	0
21	W	1211	0	1230	189	0
22	X	475	0	106	20	0
23	Y	704	0	735	107	0
24	a	1372	0	1413	18	0
25	b	631	0	670	19	0
25	k	563	0	600	76	0
26	c	1709	0	1681	39	0
27	d	625	0	647	16	0
27	n	632	0	653	27	0
28	e	575	0	597	15	0
28	p	602	0	631	12	0
29	f	573	0	572	19	0
29	q	585	0	587	15	0
30	g	529	0	557	10	0
30	r	577	0	595	16	0
31	h	644	0	686	14	0
31	l	679	0	732	133	0
32	j	741	0	778	23	0
32	m	752	0	786	43	0
33	o	2599	0	2553	70	0
34	s	548	0	219	10	0
35	t	583	0	249	2	0
35	u	578	0	246	3	0
35	v	588	0	250	5	0
35	w	568	0	242	1	0
36	y	719	0	750	11	0
37	6	1	0	0	0	0
38	A	36	0	6	2	0
39	C	32	0	12	3	0
40	L	3	0	0	0	0
40	M	1	0	0	0	0
40	N	2	0	0	0	0
40	c	1	0	0	0	0
All	All	80677	0	70718	1898	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 13.

The worst 5 of 1898 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)
20:V:621:LYS:HE2	20:V:861:PHE:CE1	1.29	1.64
19:T:589:GLU:CB	22:X:216:UNK:CB	1.77	1.63
21:W:15:TYR:CZ	25:k:19:LYS:CE	1.81	1.57
21:W:50:LEU:HD12	21:W:73:ARG:CZ	1.31	1.56
21:W:35:GLN:HE22	23:Y:57:GLU:CG	1.11	1.55

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1935/2413 (80%)	1824 (94%)	111 (6%)	0	100	100
5	C	868/1008 (86%)	812 (94%)	56 (6%)	0	100	100
6	D	93/278 (34%)	91 (98%)	2 (2%)	0	100	100
8	H	403/577 (70%)	380 (94%)	23 (6%)	0	100	100
10	J	340/451 (75%)	318 (94%)	22 (6%)	0	100	100
11	K	162/379 (43%)	155 (96%)	7 (4%)	0	100	100
12	L	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
13	M	253/339 (75%)	238 (94%)	15 (6%)	0	100	100
14	N	234/364 (64%)	223 (95%)	11 (5%)	0	100	100
15	O	314/590 (53%)	293 (93%)	20 (6%)	1 (0%)	36	65
16	P	67/175 (38%)	64 (96%)	3 (4%)	0	100	100
17	R	69/135 (51%)	66 (96%)	3 (4%)	0	100	100
18	S	436/687 (64%)	427 (98%)	9 (2%)	0	100	100
19	T	516/859 (60%)	509 (99%)	6 (1%)	1 (0%)	43	72
20	V	630/1145 (55%)	549 (87%)	59 (9%)	22 (4%)	3	24
21	W	143/238 (60%)	122 (85%)	18 (13%)	3 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Y	85/111 (77%)	79 (93%)	6 (7%)	0	100	100
24	a	167/251 (66%)	148 (89%)	19 (11%)	0	100	100
25	b	76/196 (39%)	68 (90%)	8 (10%)	0	100	100
25	k	66/196 (34%)	59 (89%)	7 (11%)	0	100	100
26	c	186/382 (49%)	157 (84%)	29 (16%)	0	100	100
27	d	80/101 (79%)	74 (92%)	6 (8%)	0	100	100
27	n	80/101 (79%)	76 (95%)	4 (5%)	0	100	100
28	e	71/94 (76%)	66 (93%)	5 (7%)	0	100	100
28	p	73/94 (78%)	70 (96%)	3 (4%)	0	100	100
29	f	70/86 (81%)	57 (81%)	13 (19%)	0	100	100
29	q	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
30	g	65/77 (84%)	61 (94%)	4 (6%)	0	100	100
30	r	73/77 (95%)	62 (85%)	11 (15%)	0	100	100
31	h	78/146 (53%)	70 (90%)	8 (10%)	0	100	100
31	l	81/146 (56%)	74 (91%)	2 (2%)	5 (6%)	1	14
32	j	92/110 (84%)	86 (94%)	6 (6%)	0	100	100
32	m	90/110 (82%)	86 (96%)	4 (4%)	0	100	100
33	o	312/455 (69%)	274 (88%)	38 (12%)	0	100	100
34	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	15
35	t	113/503 (22%)	108 (96%)	5 (4%)	0	100	100
35	u	112/503 (22%)	104 (93%)	8 (7%)	0	100	100
35	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	4	28
35	w	110/503 (22%)	105 (96%)	3 (3%)	2 (2%)	6	34
36	y	82/215 (38%)	82 (100%)	0	0	100	100
All	All	9070/15016 (60%)	8455 (93%)	572 (6%)	43 (0%)	26	56

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	V	507	GLU
20	V	729	PRO
20	V	747	PRO
20	V	773	VAL
20	V	774	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1768/2182 (81%)	1762 (100%)	6 (0%)	86	83
5	C	783/910 (86%)	779 (100%)	4 (0%)	81	80
6	D	26/256 (10%)	26 (100%)	0	100	100
8	H	183/538 (34%)	181 (99%)	2 (1%)	65	73
10	J	299/398 (75%)	297 (99%)	2 (1%)	76	77
11	K	152/328 (46%)	152 (100%)	0	100	100
12	L	140/141 (99%)	140 (100%)	0	100	100
13	M	219/296 (74%)	219 (100%)	0	100	100
14	N	221/332 (67%)	220 (100%)	1 (0%)	81	80
15	O	205/526 (39%)	205 (100%)	0	100	100
16	P	60/152 (40%)	60 (100%)	0	100	100
17	R	22/121 (18%)	22 (100%)	0	100	100
18	S	216/633 (34%)	216 (100%)	0	100	100
20	V	562/1029 (55%)	495 (88%)	67 (12%)	5	23
21	W	142/219 (65%)	141 (99%)	1 (1%)	76	77
23	Y	78/100 (78%)	77 (99%)	1 (1%)	61	71
24	a	151/225 (67%)	151 (100%)	0	100	100
25	b	70/176 (40%)	70 (100%)	0	100	100
25	k	64/176 (36%)	63 (98%)	1 (2%)	55	68
26	c	184/346 (53%)	183 (100%)	1 (0%)	81	80
27	d	69/89 (78%)	69 (100%)	0	100	100
27	n	71/89 (80%)	71 (100%)	0	100	100
28	e	65/83 (78%)	65 (100%)	0	100	100
28	p	69/83 (83%)	69 (100%)	0	100	100
29	f	63/77 (82%)	63 (100%)	0	100	100
29	q	65/77 (84%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	g	58/66 (88%)	58 (100%)	0	100	100
30	r	64/66 (97%)	64 (100%)	0	100	100
31	h	77/129 (60%)	77 (100%)	0	100	100
31	l	78/129 (60%)	75 (96%)	3 (4%)	29	53
32	j	79/103 (77%)	79 (100%)	0	100	100
32	m	85/103 (82%)	85 (100%)	0	100	100
33	o	291/413 (70%)	290 (100%)	1 (0%)	86	83
36	y	81/193 (42%)	81 (100%)	0	100	100
All	All	6760/10784 (63%)	6670 (99%)	90 (1%)	59	71

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	V	871	LEU
20	V	1010	LYS
20	V	897	GLU
20	V	970	TRP
20	V	1059	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
20	V	978	GLN
27	n	4	ASN
21	W	105	ASN
26	c	300	ASN
33	o	336	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	128/1175 (10%)	44 (34%)	3 (2%)
2	5	169/179 (94%)	57 (33%)	6 (3%)
3	6	101/112 (90%)	26 (25%)	3 (2%)
7	E	32/39 (82%)	21 (65%)	4 (12%)
9	I	36/95 (37%)	10 (27%)	2 (5%)
All	All	466/1600 (29%)	158 (33%)	18 (3%)

5 of 158 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	A
1	2	6	U
1	2	14	C
1	2	16	U
1	2	17	U

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	E	2	G
9	I	91	A
9	I	66	A
2	5	174	G
7	E	1	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
39	GTP	C	2501	-	33,34,34	0.92	1 (3%)	50,54,54	1.60	10 (20%)
38	IHP	A	2500	-	36,36,36	0.70	0	60,60,60	0.69	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
39	GTP	C	2501	-	-	5/22/38/38	0/3/3/3
38	IHP	A	2500	-	-	2/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	2501	GTP	C5-N7	-2.12	1.34	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	C	2501	GTP	C5-C4-N3	-4.73	120.86	128.39
39	C	2501	GTP	C2-N3-C4	4.57	120.17	112.30
39	C	2501	GTP	N9-C4-N3	3.08	132.12	125.95
39	C	2501	GTP	C2-N1-C6	-2.93	119.80	125.11
39	C	2501	GTP	N9-C8-N7	-2.76	108.28	113.40

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	C	2501	GTP	C5'-O5'-PA-O3A
39	C	2501	GTP	C5'-O5'-PA-O1A
39	C	2501	GTP	C5'-O5'-PA-O2A
39	C	2501	GTP	PB-O3A-PA-O1A
38	A	2500	IHP	C2-O12-P2-O22

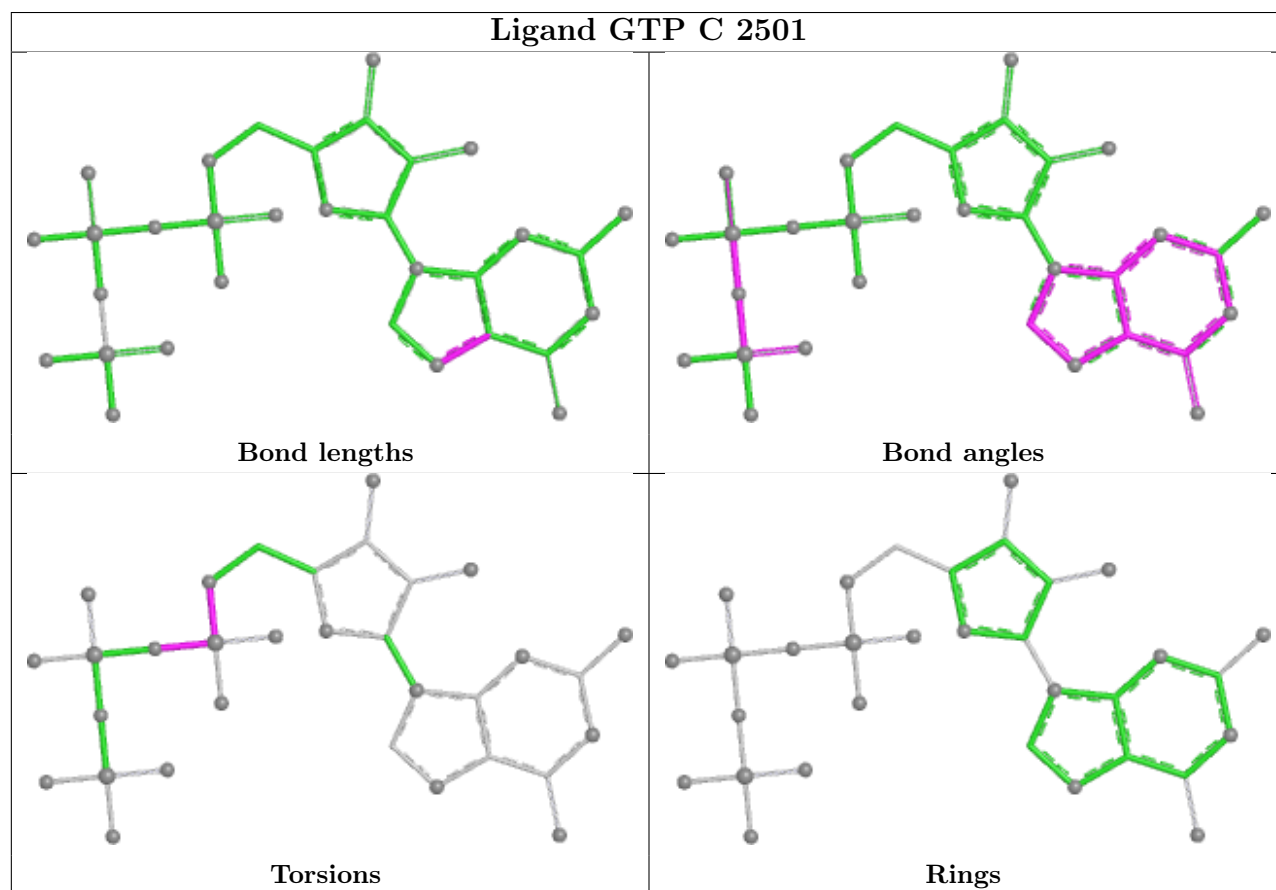
There are no ring outliers.

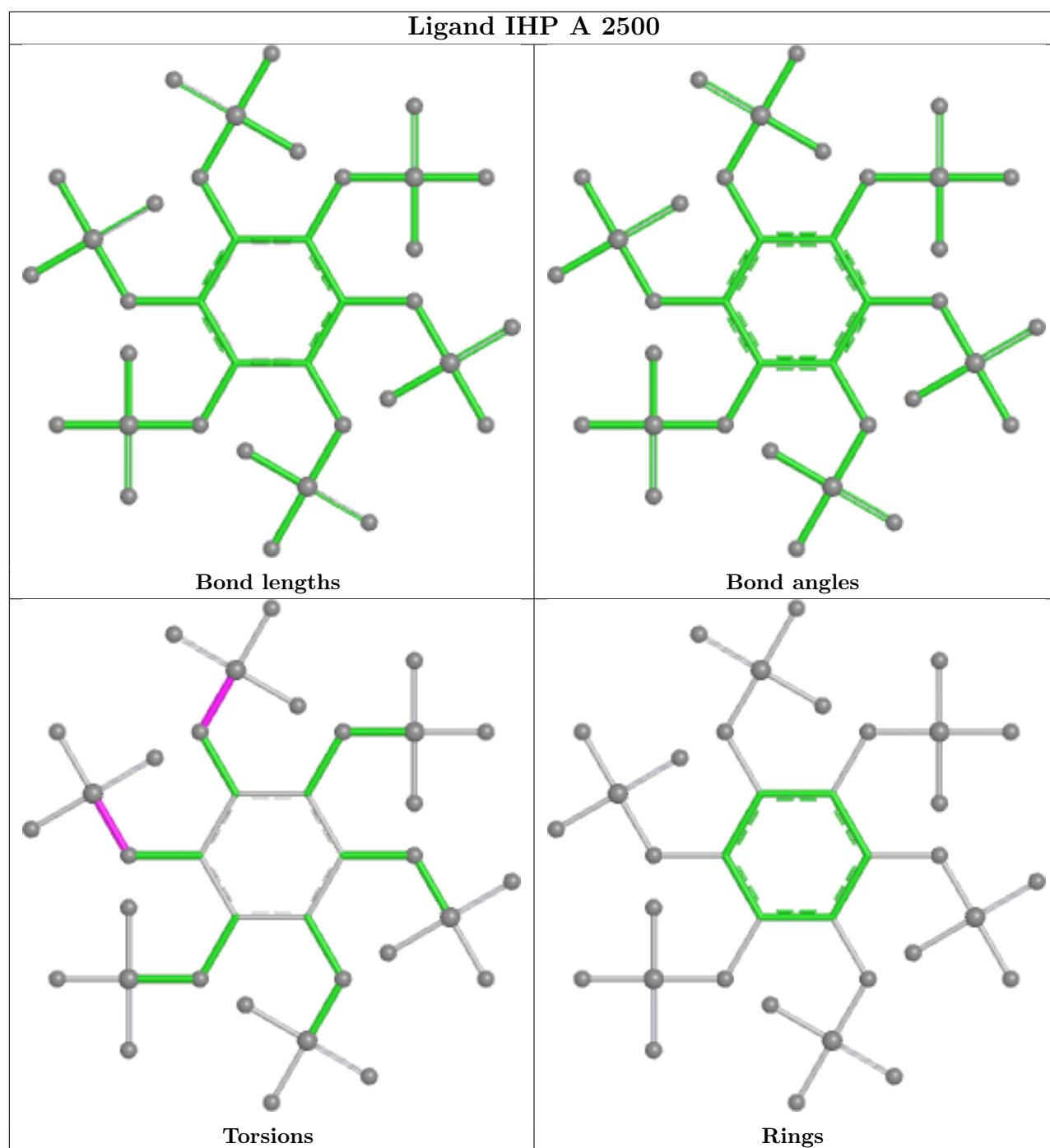
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	C	2501	GTP	3	0
38	A	2500	IHP	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	X	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	70:UNK	C	100:UNK	N	122.60
1	X	156:UNK	C	200:UNK	N	74.32
1	X	28:UNK	C	60:UNK	N	43.20
1	X	117:UNK	C	130:UNK	N	9.37
1	X	142:UNK	C	150:UNK	N	9.29

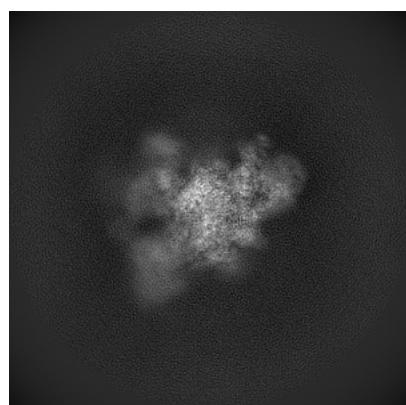
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3979. These allow visual inspection of the internal detail of the map and identification of artifacts.

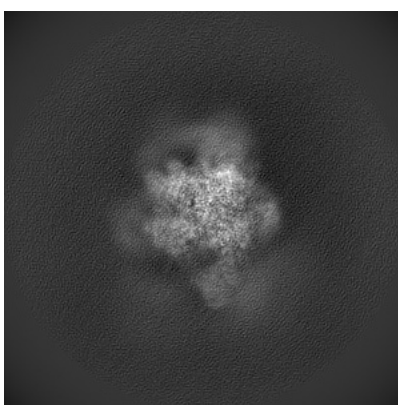
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

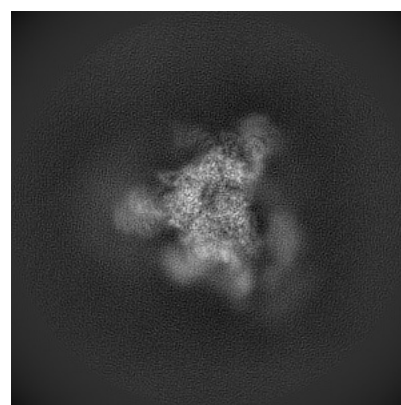
6.1.1 Primary map



X



Y

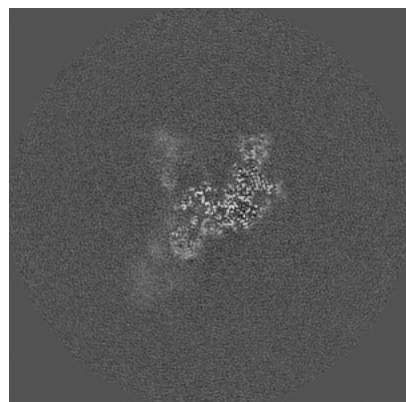


Z

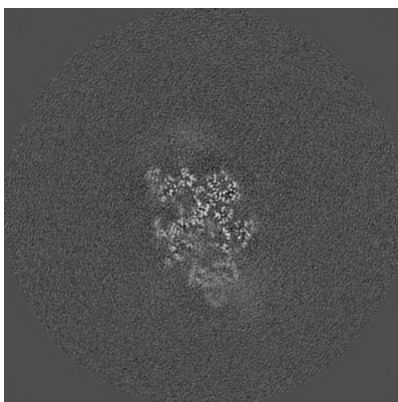
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

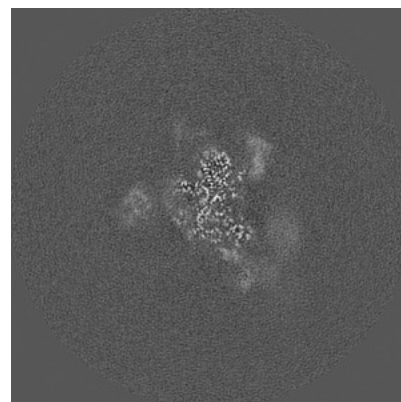
6.2.1 Primary map



X Index: 240



Y Index: 240

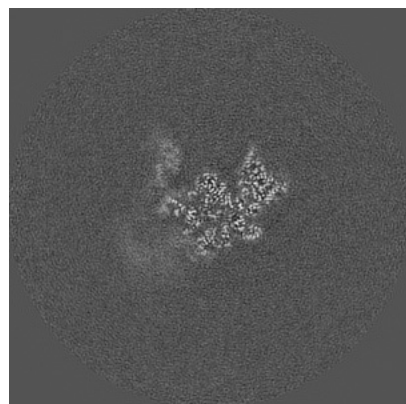


Z Index: 240

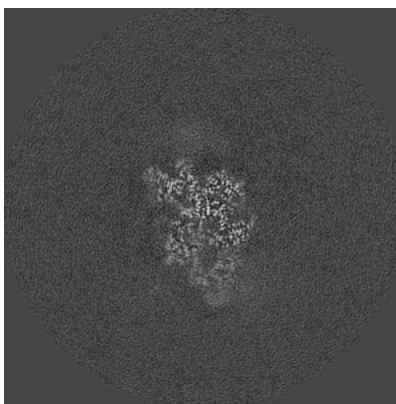
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

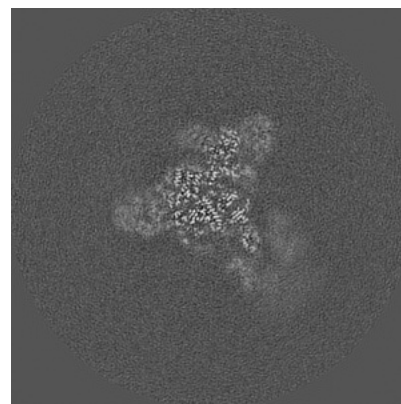
6.3.1 Primary map



X Index: 259



Y Index: 236

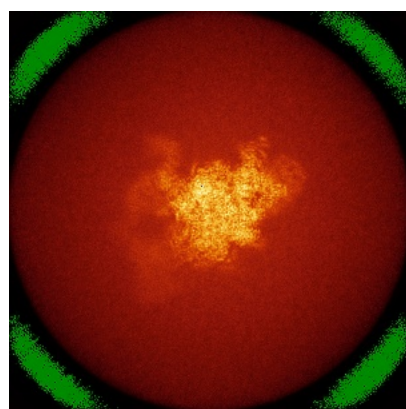


Z Index: 261

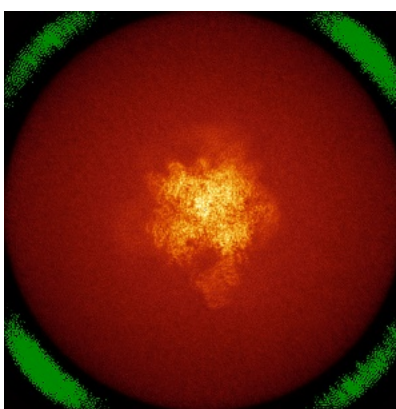
The images above show the largest variance slices of the map in three orthogonal directions.

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

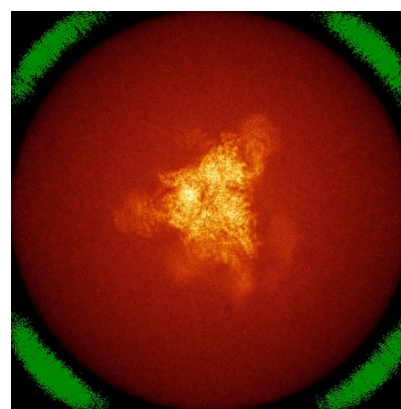
6.4.1 Primary map



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

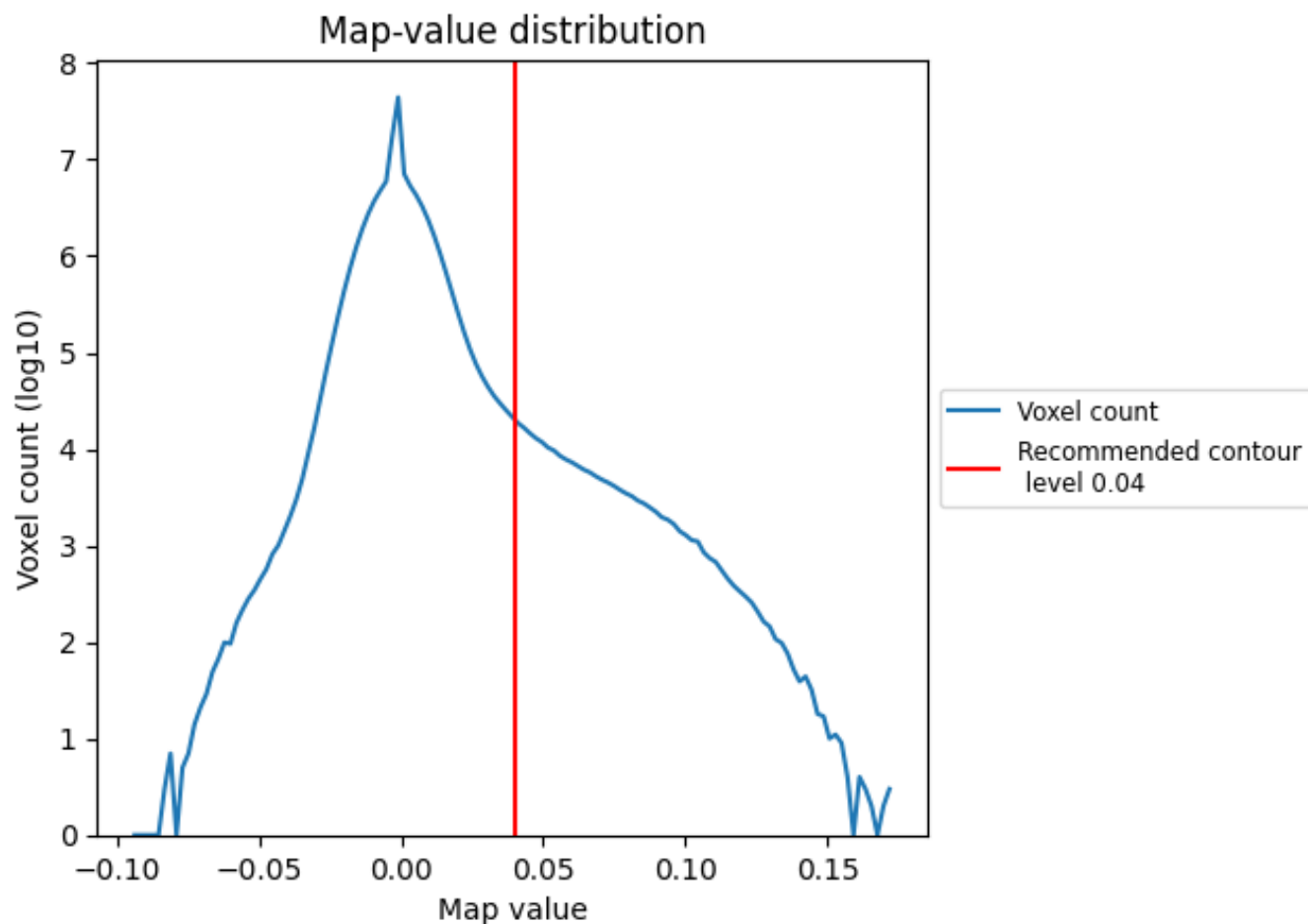
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

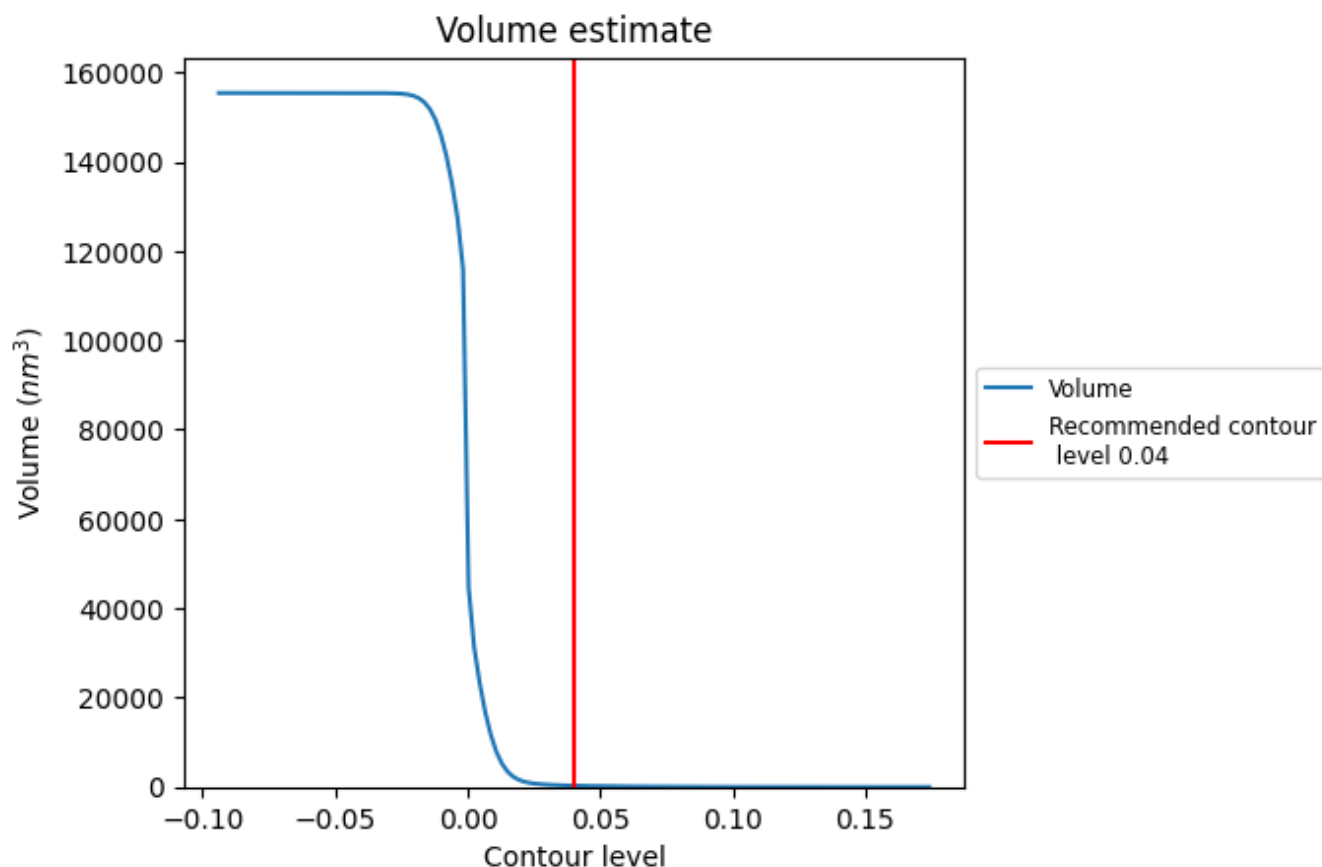
This section contains the results of statistical analysis of the map.

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.

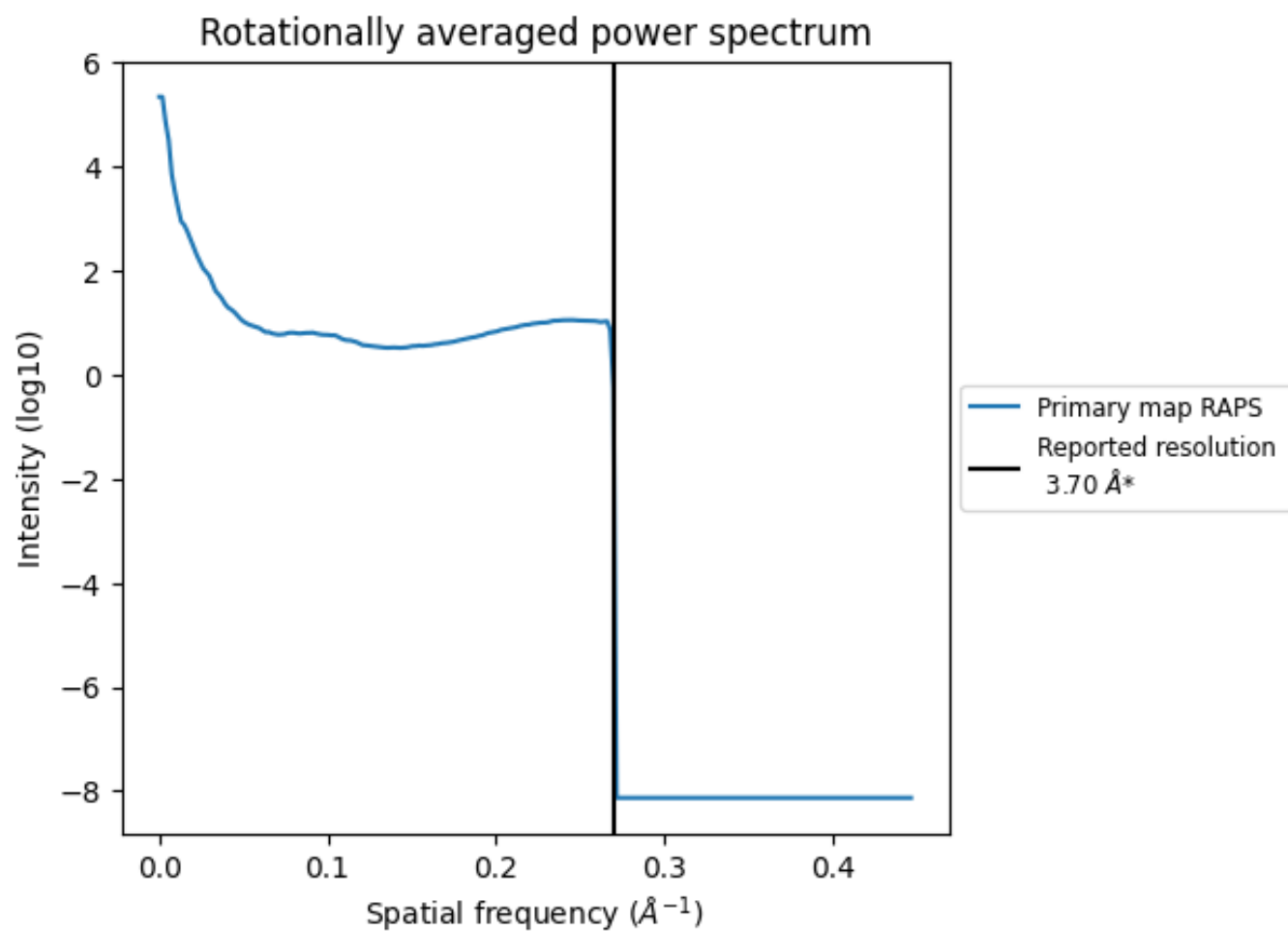
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287 nm³; this corresponds to an approximate mass of 259 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 ⓘ

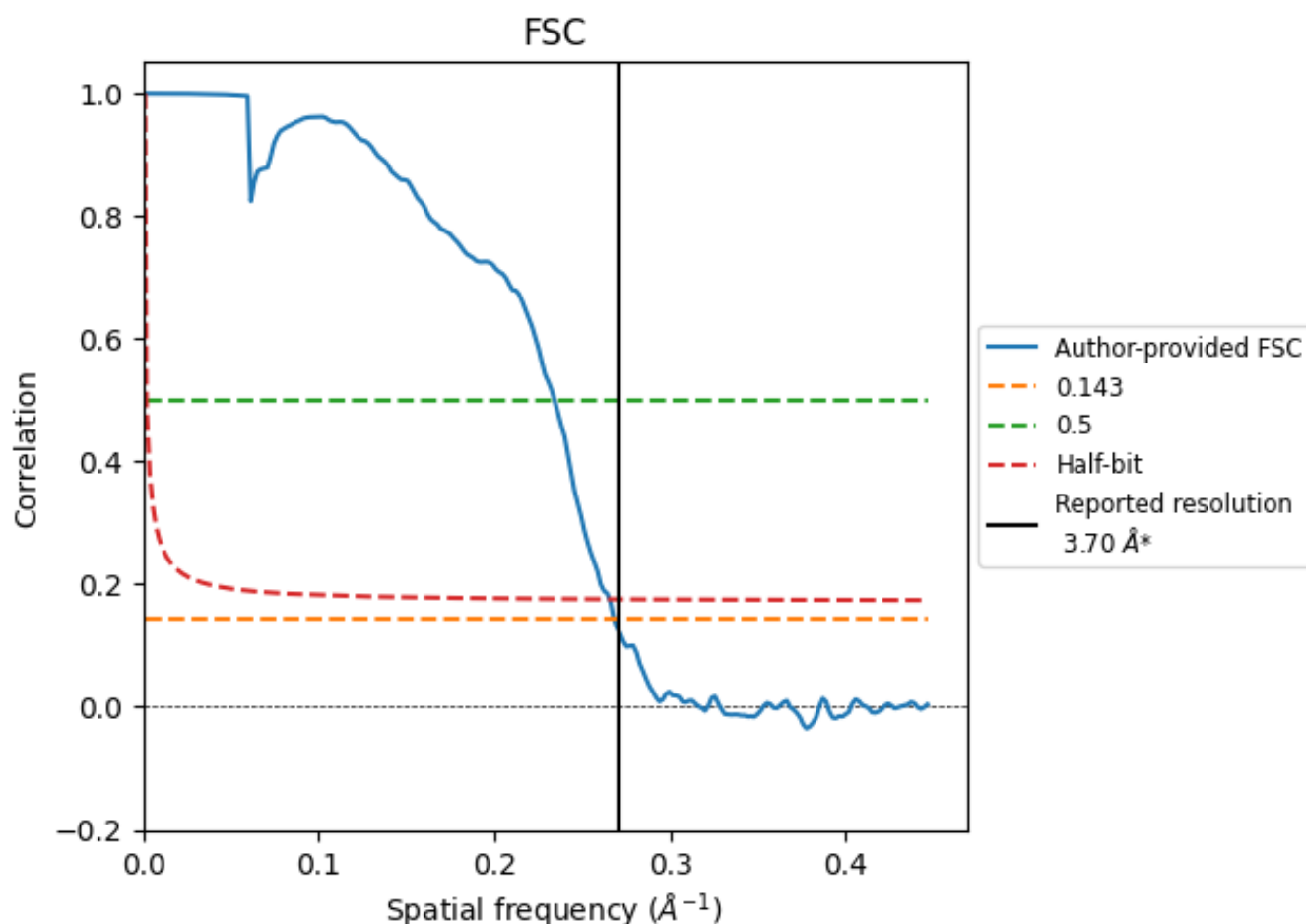


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

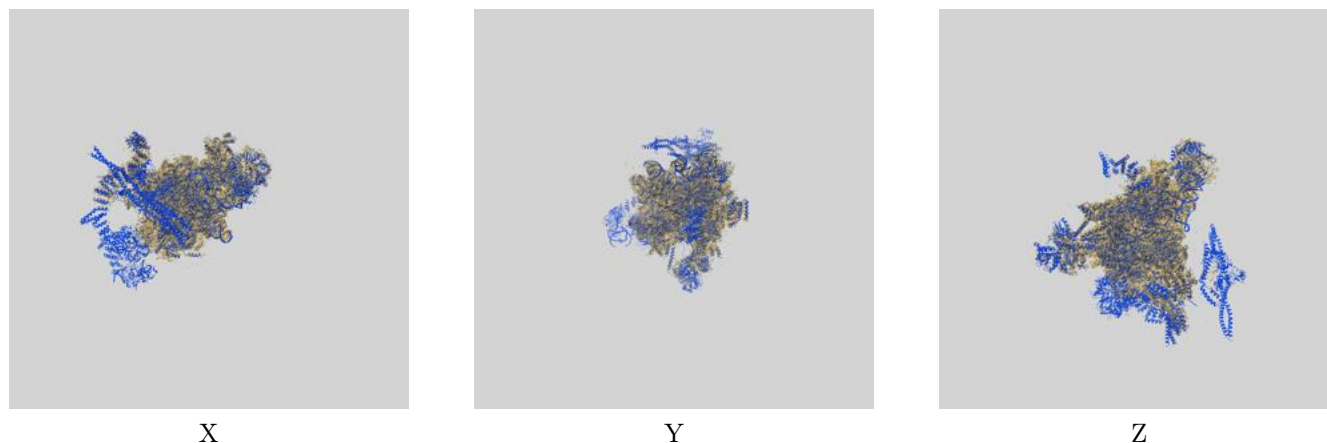
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.27	3.77
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

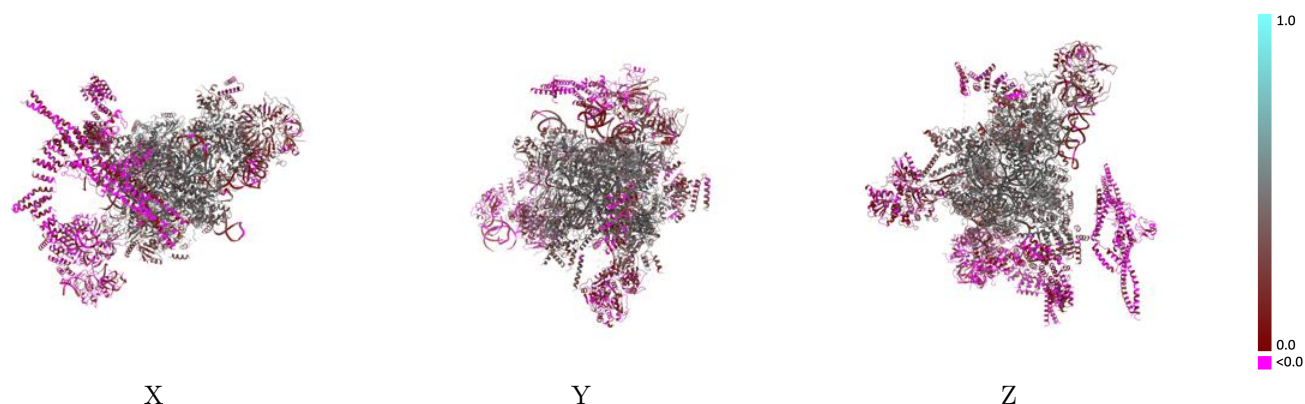
This section contains information regarding the fit between EMDB map EMD-3979 and PDB model 6EXN. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



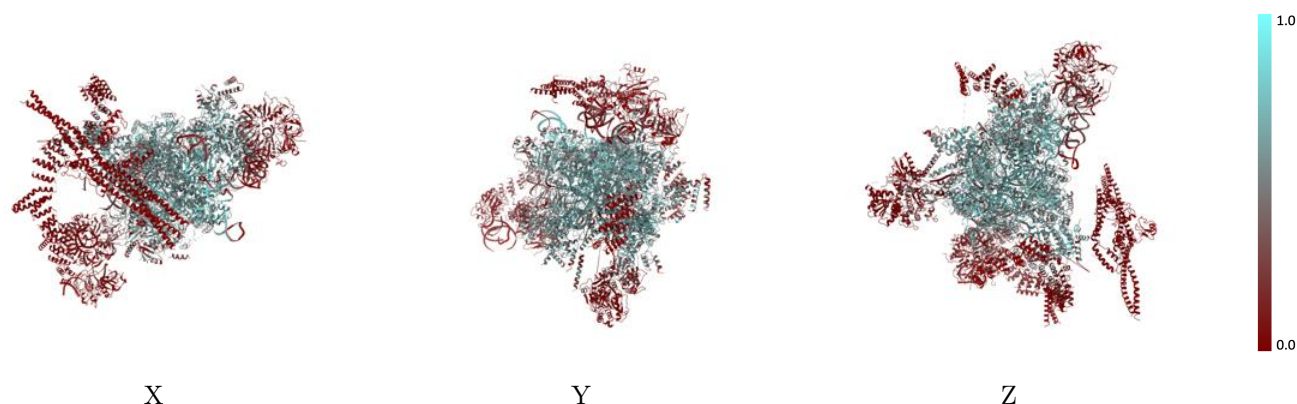
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



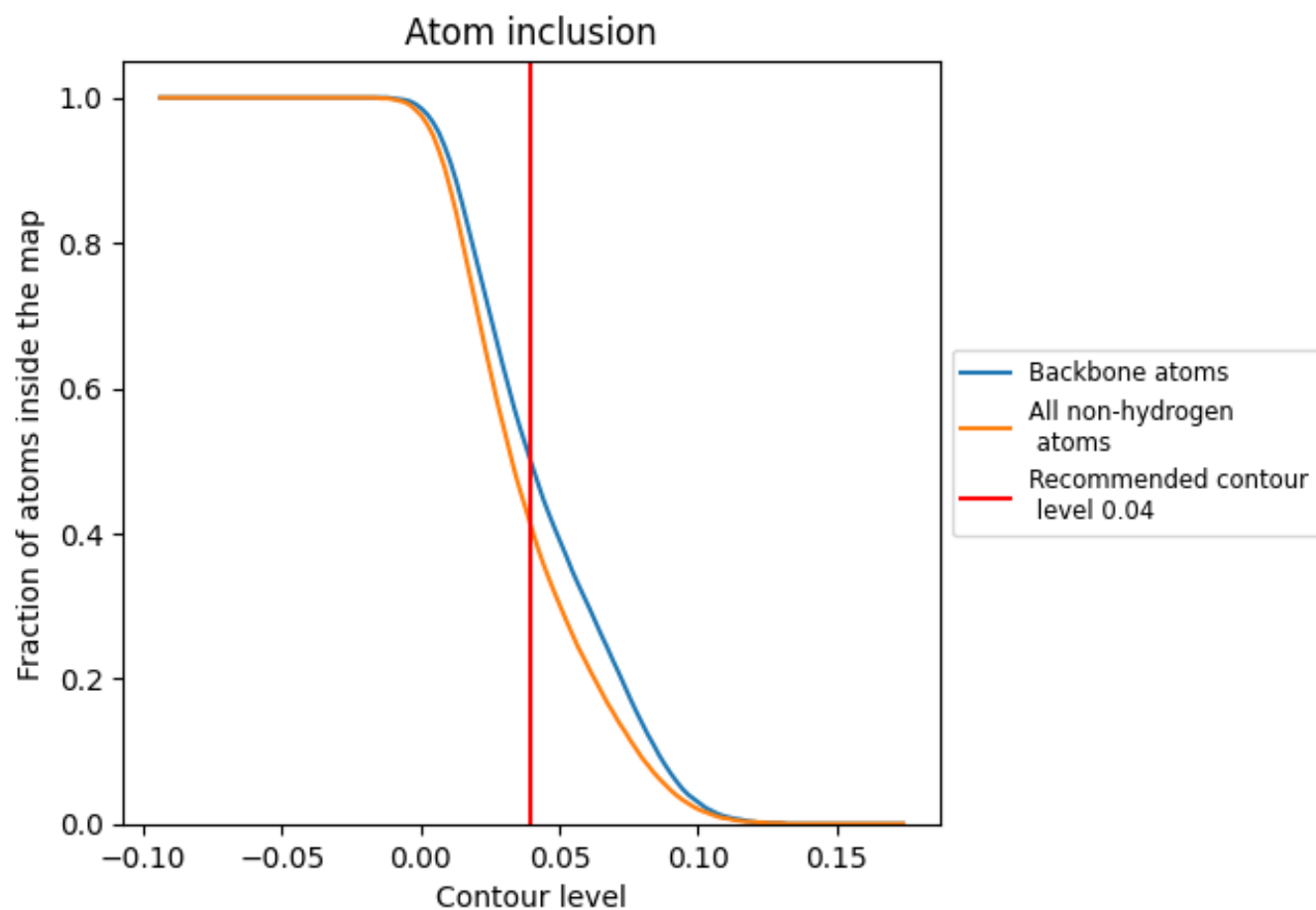
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 41% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4080	 0.2960
2	 0.1910	 0.1300
5	 0.4610	 0.2840
6	 0.6910	 0.3820
A	 0.6210	 0.4310
C	 0.5850	 0.4150
D	 0.4390	 0.3080
E	 0.4490	 0.3090
H	 0.3720	 0.2960
I	 0.5630	 0.3590
J	 0.6440	 0.4540
K	 0.5550	 0.4100
L	 0.6340	 0.4270
M	 0.5750	 0.3970
N	 0.4620	 0.3610
O	 0.4480	 0.3180
P	 0.5840	 0.4480
R	 0.4380	 0.2970
S	 0.4410	 0.2850
T	 0.1180	 0.0880
V	 0.1130	 0.1090
W	 0.0000	 0.0040
X	 0.3700	 0.2460
Y	 0.0000	 0.0310
a	 0.4740	 0.3540
b	 0.2660	 0.3200
c	 0.4590	 0.3660
d	 0.3300	 0.3480
e	 0.1080	 0.2290
f	 0.0980	 0.2000
g	 0.1460	 0.2540
h	 0.1670	 0.2620
j	 0.1050	 0.1980
k	 0.0020	 0.0530
l	 0.0000	 -0.0180



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Chain	Atom inclusion	Q-score
m	 0.0000	 0.0040
n	 0.0030	 0.0520
o	 0.4440	 0.3500
p	 0.0000	 -0.0040
q	 0.0020	 0.0330
r	 0.0000	 0.0440
s	 0.0070	 0.0320
t	 0.0000	 -0.0120
u	 0.0000	 0.0350
v	 0.0000	 -0.0410
w	 0.0020	 0.0170
y	 0.5370	 0.3950