W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Oct 21, 2024 – 11:51 AM JST

PDB ID	:	6ID0
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)

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

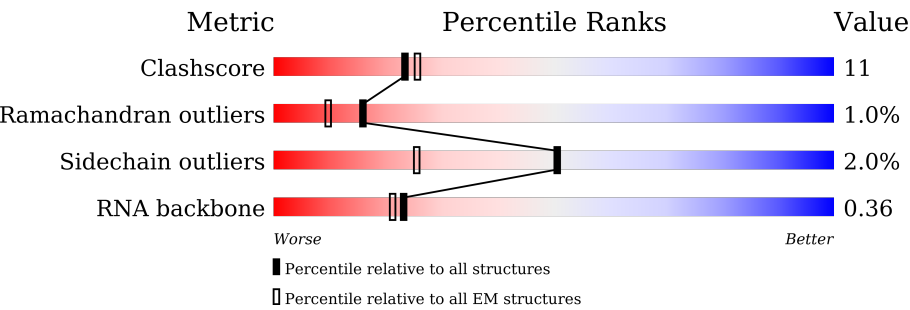|		
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1   Overall quality at a glance   ⓘ

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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		1.0%
Sidechain outliers		2.0%
RNA backbone		0.36

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2335	70% 14% • 15%
2	B	117	9% 32% 31% 19% • 16%
3	C	972	70% 19% • 9%
4	E	357	61% 23% • 15%
5	F	107	44% 25% 20% • 9%
6	J	848	21% 58% 7% • 34%
7	L	802	24% 52% 6% 41%

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Mol	Chain	Length	Quality of chain
8	M	243	45% 8% 47%
9	N	144	85% 11%
10	O	420	5% 54% 14% 31%
11	P	229	44% 7% 48%
12	R	536	40% 10% 49%
13	S	166	70% 25%
14	T	514	47% 13% 38%
15	W	579	6% 72% 15% 12%
16	G	272	7% 7% 10% 6% 74%
17	H	188	37% 12% 25% 33% 5% 26%
18	U	894	29% 8% 61%
19	I	855	30% 56% 10% 34%
20	a	126	13% 64% 36%
20	h	126	35% 64% 36%
21	b	231	19% 37% 63%
21	i	231	23% 37% 63%
22	c	119	17% 69% 31%
22	j	119	48% 69% 31%
23	d	118	22% 81% 18%
23	k	118	53% 71% 28%
24	f	86	40% 86% 14%
24	m	86	64% 86% 14%
25	e	92	43% 86% 14%
25	l	92	68% 86% 14%
26	g	76	49% 97%

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Mol	Chain	Length	Quality of chain
26	n	76	61% / 88% / 12%
27	q	504	25% / 25% / 74%
27	r	504	24% / 25% / 74%
27	s	504	12% / 13% / 87%
27	t	504	13% / 13% / 87%
28	K	225	56% / 57% / 9% / 32%
29	o	255	57% / 61% / 36%
30	p	225	30% / 42% / 58%
31	Q	1485	87% / 89% / 11%
32	y	301	17% / 26% / 74%

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 (i)

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 16477	C 10621	N 2883	O 2902	S 71	0	0

- Molecule 2 is a RNA chain called U5snRNA.

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

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

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

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

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

- Molecule 5 is a RNA chain called U6snRNA.

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

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

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

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

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

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

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

- Molecule 9 is a protein called Protein BUD31 homolog.

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called Pleiotropic regulator 1.

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

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

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

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

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

- Molecule 17 is a RNA chain called U2snRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 31 is a protein called RNA helicase aquarius.

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

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

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

- Molecule 33 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).
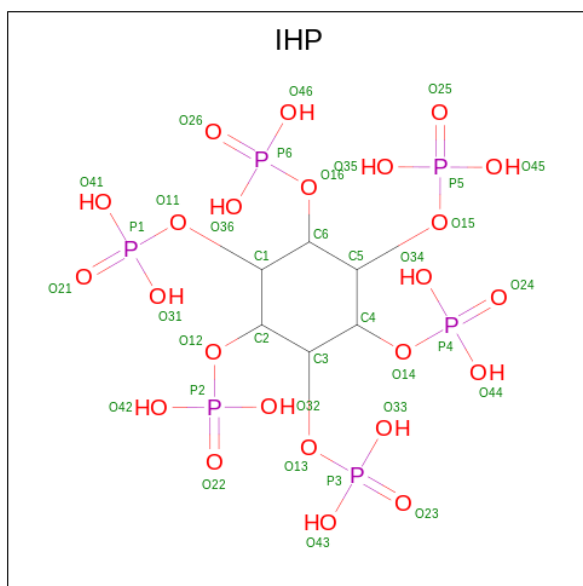
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total 36	C 6	O 24	P 6	0

- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).
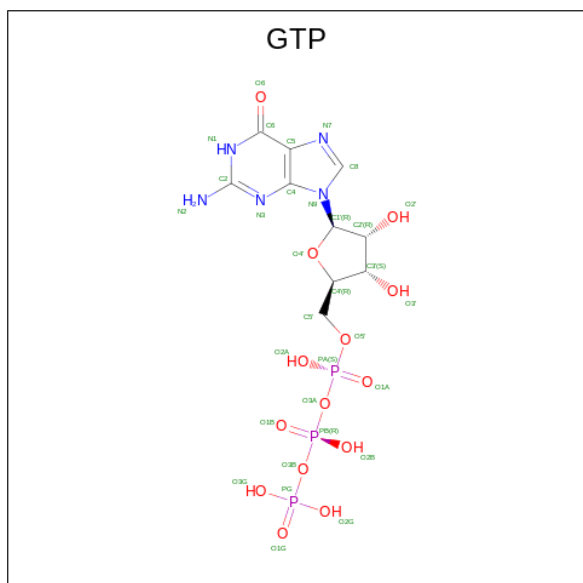
Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 35 is MAGNESIUM ION (three-letter code: 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 (three-letter code: 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

Chain B:

9%

32%   31%   19%   •   16%

• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:

70%   19%   •   9%

WORLDWIDE
wwPDB
PROTEIN DATA BANK
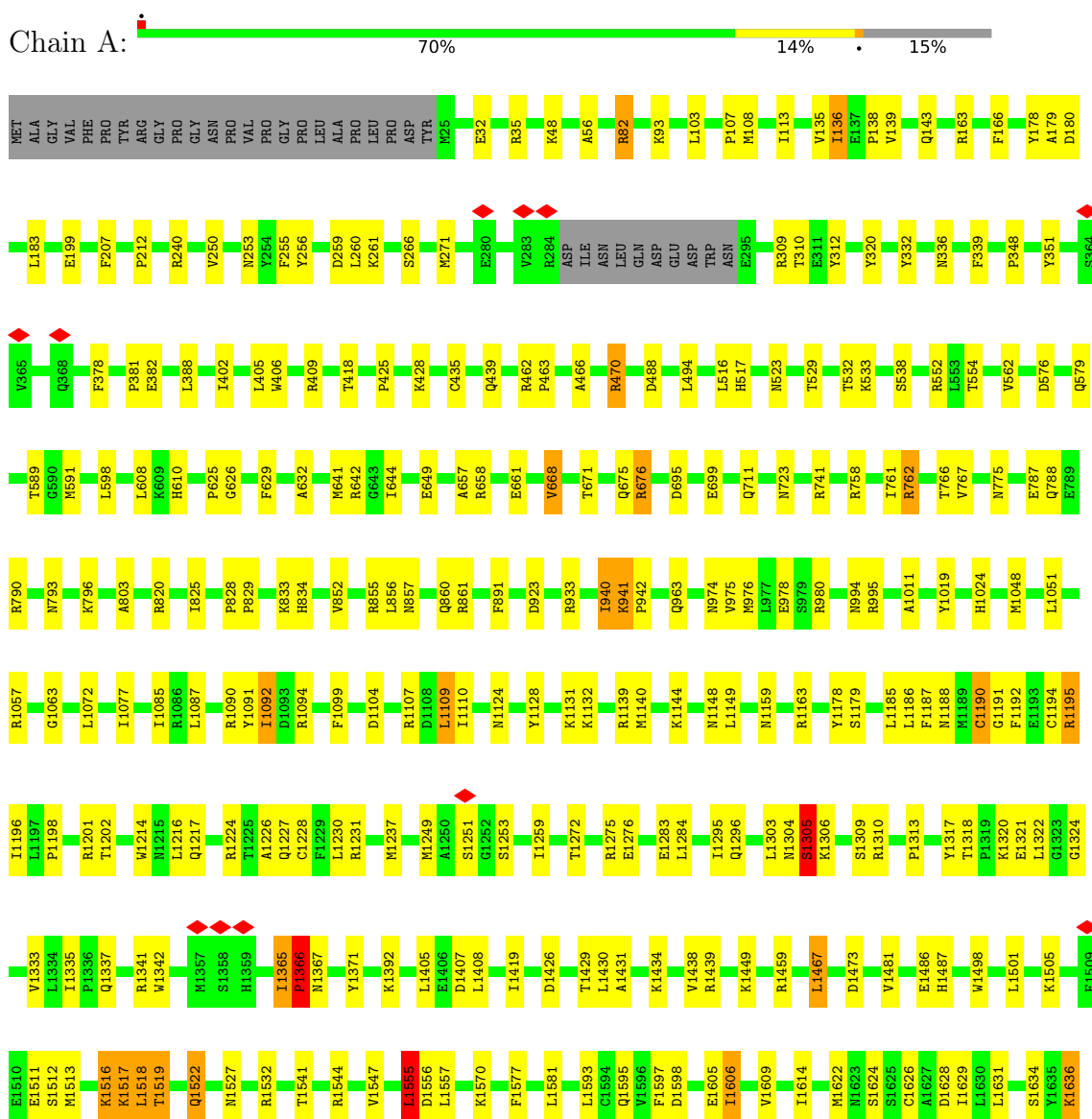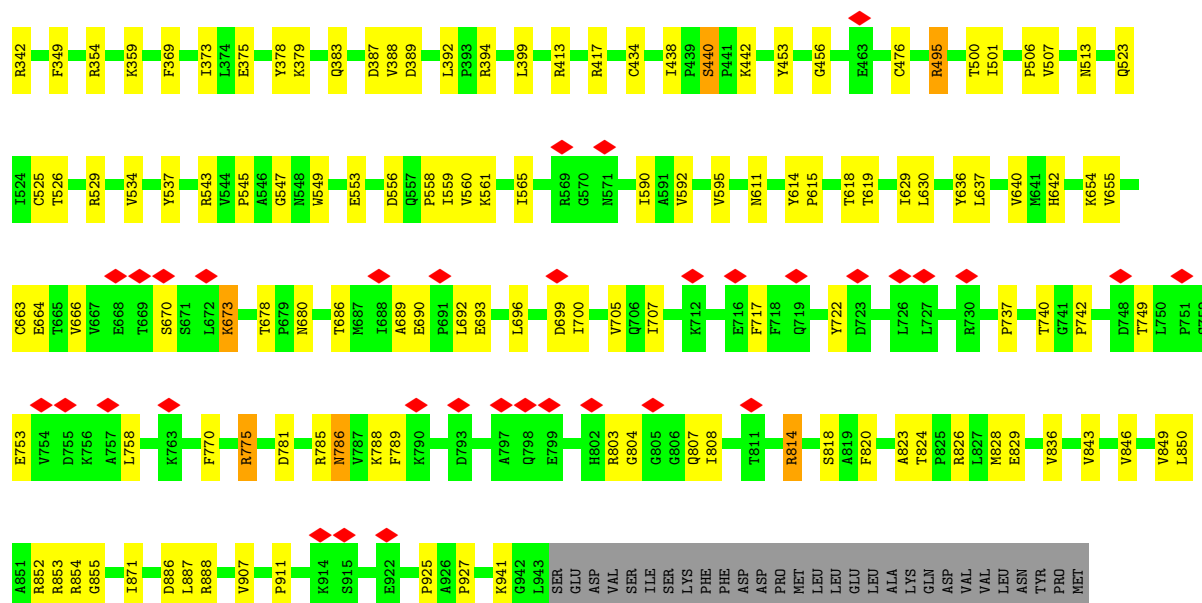
• Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E: 61%   23%   •   15%
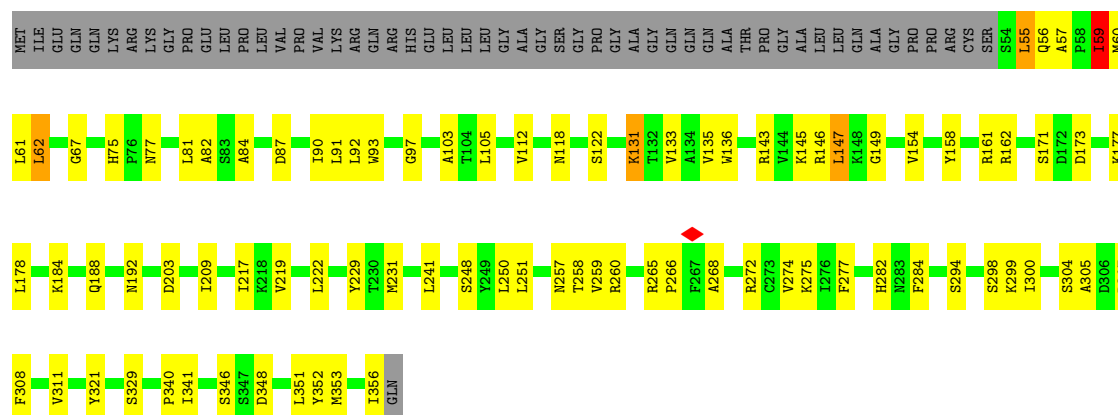
• Molecule 5: U6snRNA

Chain F: 44%   25%   20%   •   9%
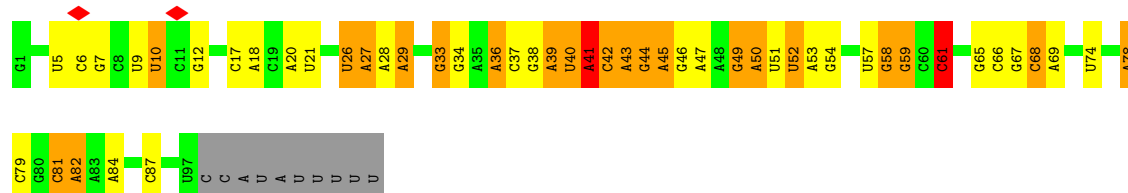
• Molecule 6: Crooked neck-like protein 1

Chain J: 21%   58%   7% •   34%
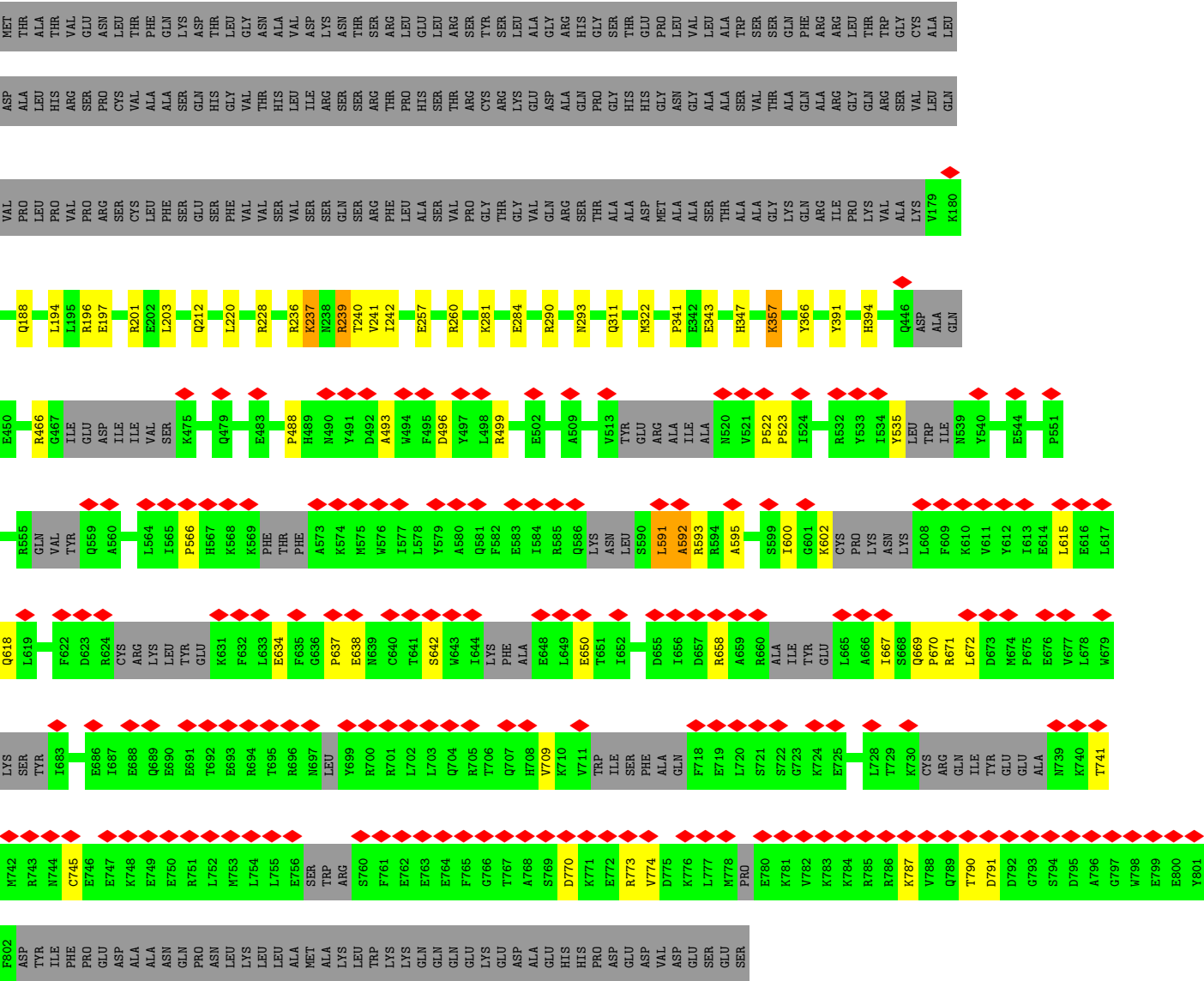
• Molecule 7: Cell division cycle 5-like protein

Chain L:

24%

52% 6% 41%
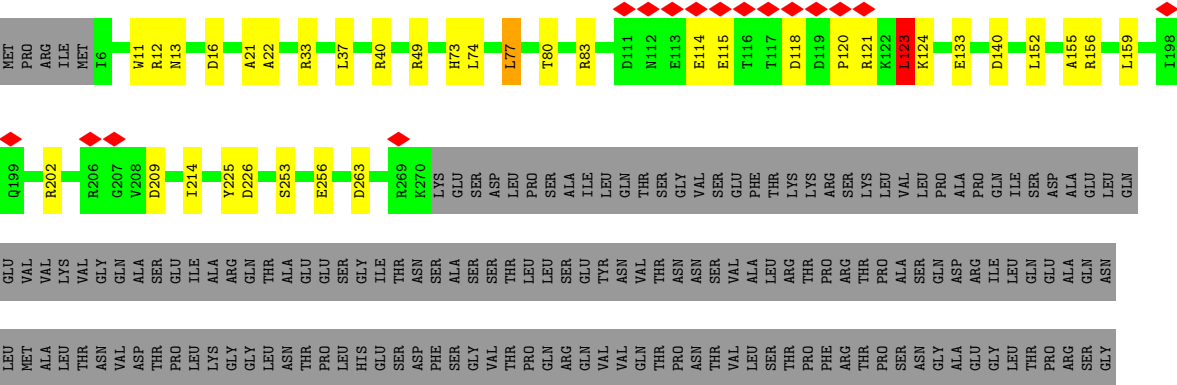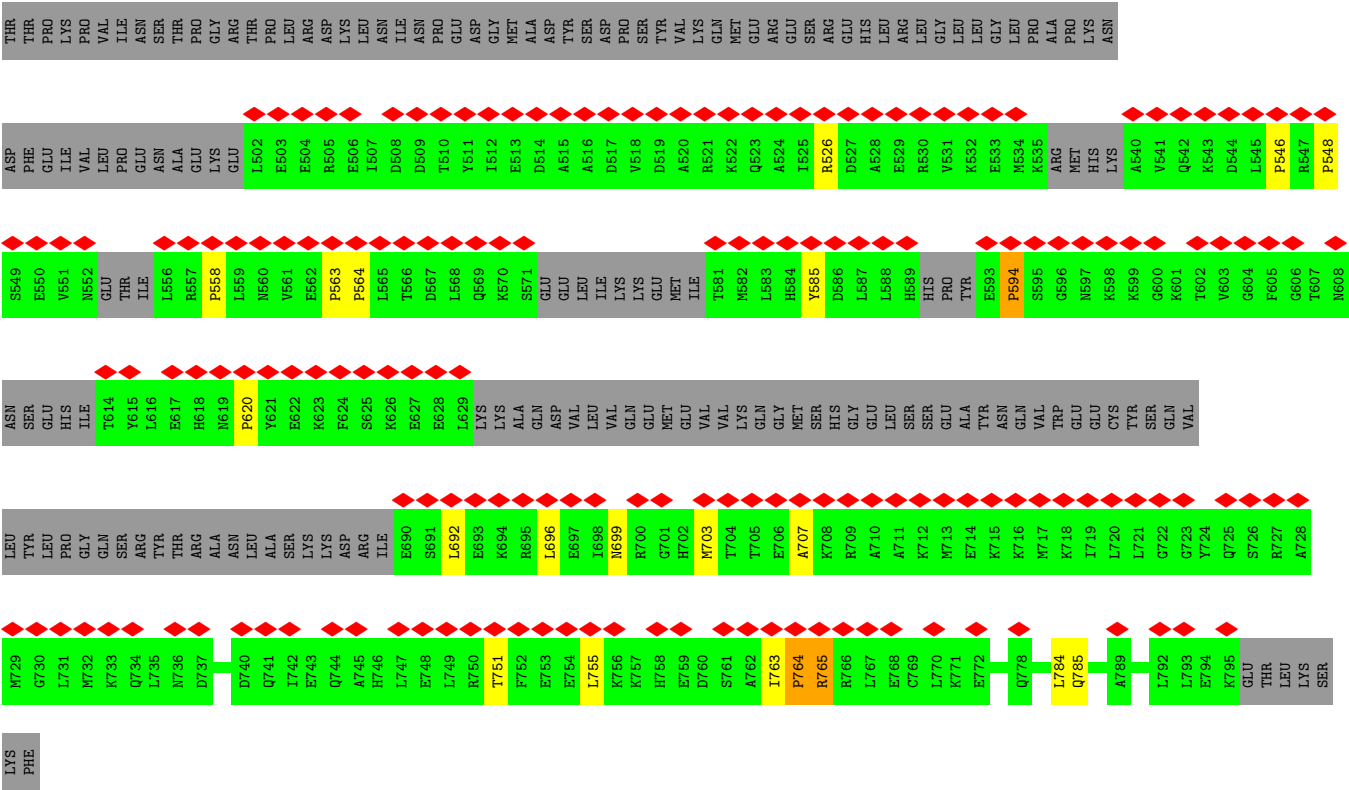
• Molecule 8: Pre-mRNA-splicing factor SYF2

Chain M:
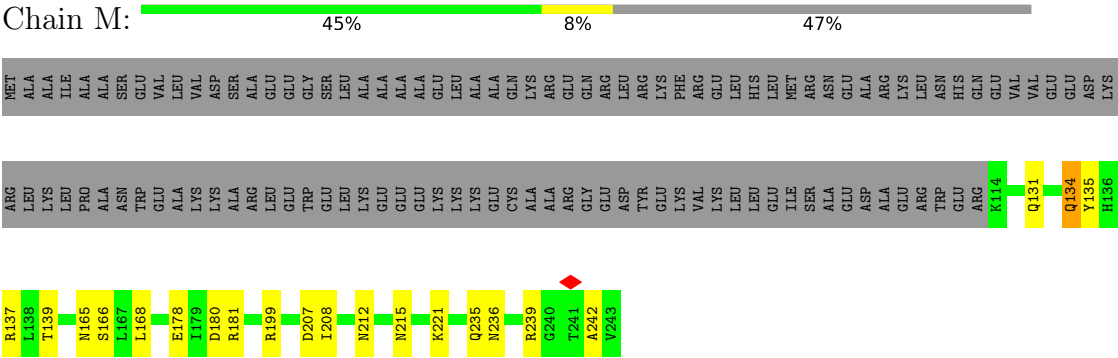
• Molecule 9: Protein BUD31 homolog

Chain N:

• Molecule 10: Pre-mRNA-splicing factor RBM22

Chain O:

MET ALA THR SER LEU GLY SER ASN THR TYR ASN ARG GLN N14 W15 E16 D17 A18 D19 F20 T26 C27 N31 P32 Y33 I34 P59 M63 R64 F65 K66 Q72 K78 N79 Q82 Y90 G91 L92 P93 I94 K104 S110 N113 T131 M136 L137

A140 M146 L150 A151 R152 R159 H63 V169 K174 R175 C179 R182 H183 E184 K185 L193 L213 R216 R222 L223 D224 P225 P226 E227 D228 K229 T233 L234 Y235 V236 G237 Q240 D241 T242 I243 T244 E245 L248 R249 Y253 Q254 F255 R259

T262 V263 C269 A270 F271 I272 A275 T276 R277 Q278 A279 A280 E281 E285 N289 K290 L291 I292 R296 N299 V300 K301 W302 G303 ARG SER GLN ALA ARG GLY LYS GLU LYS GLU LYS ASP GLY THR THR ASP SER GLY ILE LEU LYS GLU PRO VAL PRO GLY LEU PRO

GLY ALA LEU PRO PRO PRO ALA ALA GLU GLU GLU ALA SER ALA ASN TYR PHE ASN LEU PRO PRO SER GLY PRO ALA VAL ASN ILE ALA LEU PRO PRO GLY ILE ALA PRO PRO PRO PRO GLY PHE GLY PRO HIS PHE HIS PRO MET GLY PRO PRO PRO PRO

PHE MET ARG ALA PRO GLY ILE HIS HIS TYR PRO SER GLN ASP PRO GLN ARG MET GLY ALA HIS ALA GLY LYS HIS SER SER PRO

• Molecule 11: Spliceosome-associated protein CWC15 homolog

Chain P:

44%   7%   48%

MET THR T3 R6 R13 G17 K18 G19 E20 G21 D22 L23 L26 S32 L35 N75 R78 PRO THR ARG GLU HIS THR THR SER SER SER VAL SER LYS PRO ARG LEU ASP GLN ILE PRO ALA ALA ASN LEU ASP ALA ASP PRO LEU THR ASP GLU

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

GLY PRO SER GLN PRO GLN ALA ASN PHE LYS VAL LYS ARG ARG W188 N196 V201 D202 D203 Q204 K205 K206 D207 N212 K226 K229

• Molecule 12: SNW domain-containing protein 1

Chain R:

40%   10%   •   49%

MET ALA LEU THR SER PHE LEU PRO ALA PRO THR GLN LEU SER GLN ASP LEU GLU GLN ALA GLU GLU LYS ALA ARG SER GLN ARG SER ARG GLN THR SER LEU VAL SER SER ARG ARG GLU ARG PRO PRO PRO TYR GLY TYR R47 P52 R53 D60 G61 G62 A63 F64 I67 H68 V69

A70 Q71 D75 R78 K79 L86 K95 I96 K97 I101 Q104 G105 Q106 K110 Y113 L119 M125 L132 R148 L151 M163 P164 V165 R166 A167 A168 D169 K170 L171 A172 R178 Q184 G185 V186 N189 R195 V196 I197 S224 M230

H231 S232 P233 S234 R235 T238 E241 E244 P249 S252 K255 L268 R273 G274 L275 Q276 H279 I280 N281 E282 L291 R305 M312 E316 K317 E318 LYS HIS GLU GLU LYS LEU ARG GLU GLU MET ALA GLN LYS ALA ARG GLU ARG ARG ALA GLY ILE LYS

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

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

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

SER ARG PRO LYS GLU GLU HIS GLU HIS GLY LYS LYS ARG ARG LYS GLU

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

Chain S:

70%   25%

MET ALA ALA ILE PRO PRO ASP S8 P11 Y15 L25 E26 L27 Y28 W29 E41 R44 K52 R55 I56 I57 M61 I62 Q63 E83 D84 D89 L90 K91 F92 T93 G96 I97 L98 A99 N102 D106 T107 N108 W121 L122 D123 H126 T127 I128

F129 G130 R131 V132 C133 Q134 R141 E146 R152 D155 K158 I159 I160 K161 A162 Y163 G166

- Molecule 14: Pleiotropic regulator 1

Chain T:

47%   13% · 38%

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

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

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

LYS ALA PRO T184 W190 I200 E213 N216 Q217 W218 F219 V220 S223 A224 L238 T248 L261 V270 W273 N278 Y284 H287 L294 T299 L303 V304 T305 C306 S307 R308 A312 R313 I314 V323 H324 T325 L326 T330 V336

E342 P343 Q344 I345 S349 H350 D351 L356 L359 R365 H371 S374 V375 R376 L380 H381 P382 R383 G390 S391 P392 D393 W398 K399 F400 P401 D402 G403 S404 F405 I406 Q407 I415 I416 N417 T418 A431 N446 R449 V450 S463 A467 C468 D471

Q472 L478 I486 K487 V488 Y489 A495 T496 E497 T499 H500 PRO VAL SER TRP LYS PRO GLU ILE ILE LYS ARG LYS PHE

- Molecule 15: Pre-mRNA-processing factor 17

Chain W:

6%   72%   15% · 12%

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

ALA VAL LYS GLU ASP LEU GLU THR GLY V70 P74 A75 V76 K77 E78 N97 P98 F99 R100 Q103 R108 L111 I120 P141 S142 L143 D144 N145 V148 S149 I153 G154 S155 E158 N162 L165 Q172 L193 D204 V205 P208 L216

G227 K228 Q229 E230 E231 E232 K233 P234 G235 E236 I240 L241 H242 V243 M246 G251 Q259 D260 V261 G262 V263 N264 L265 R266 S267 T268 M269 P270 P271 E272 P277 K278 K279 Q280 G290 P298 L299 S300 G301 M309 V318 L325 G330 A334 F340 A343

• Molecule 16: pre-mRNA

• Molecule 17: U2snRNA

• Molecule 18: CWF19-like protein 2

• Molecule 19: Pre-mRNA-splicing factor SYF1

Chain I:

30%

56% 10% • 34%

• Molecule 20: Small nuclear ribonucleoprotein Sm D3

• Molecule 20: Small nuclear ribonucleoprotein Sm D3

• Molecule 21: Small nuclear ribonucleoprotein-associated protein

MET THR VAL G4 K5 S6 S7 L10 D14 C19 D23 G24 G29 T30 F31 K32 A33 F34 D35 K36 C45 D46 R49 K50 I51 K52 P53 K54 N55 S56 K57 Q58 A59 E60 R61 E62 E63 K64 R65 V66 L67 G68 L69 V70 L71 M80 G84 P85 P86 P87 K88

D89 THR GLY ILE ALA ARG VAL PRO LEU ALA GLY ALA ALA GLY GLY PRO GLY ILE GLY ARG ALA ALA GLY ARG GLY ILE PRO ALA GLY VAL PRO MET PRO GLN ALA PRO ALA GLY LEU ALA GLY PRO VAL ARG GLY VAL GLY GLY PRO SER GLN GLN VAL MET THR PRO GLN GLN ARG GLY GLY

THR VAL ALA ALA ALA ALA ALA THR ALA SER ILE ALA GLY ALA PRO THR GLN TYR PRO GLY ARG GLY GLY PRO PRO PRO MET GLY ARG GLY GLY ALA PRO PRO PRO GLY MET GLY PRO PRO GLY MET ARG PRO PRO MET GLY PRO PRO MET GLY ILE PRO PRO GLY

ARG GLY THR PRO MET GLY PRO PRO GLY MET ARG PRO PRO PRO GLY MET ARG GLY LEU LEU

• Molecule 21: Small nuclear ribonucleoprotein-associated protein

Chain i:

23%
37%
63%

MET THR VAL G4 K5 S6 S7 K8 M9 L10 Q11 H12 I13 D14 D23 G24 R25 F31 K32 A33 F34 D35 K36 H37 M38 I41 L42 C43 D44 C45 R49 K50 I51 K52 P53 K54 N55 S56 K57 Q58 A59 E60 R61 E62 E63 K64 R65 V66 L67 G68 L69 V70 V78 V82

E83 G84 P85 P86 P87 K88 D89 THR GLY ILE ALA ARG VAL PRO LEU ALA GLY ALA ALA GLY GLY PRO GLY ILE GLY ARG ALA ALA GLY ARG GLY ILE PRO ALA GLY VAL PRO MET PRO GLN ALA PRO ALA GLY LEU ALA GLY PRO VAL ARG GLY VAL GLY GLY PRO SER GLN GLN VAL MET

THR PRO GLN GLN ARG GLY THR VAL ALA ALA ALA ALA ALA THR ALA SER ILE ALA GLY ALA PRO THR GLN TYR PRO GLY ARG GLY GLY PRO PRO PRO MET GLY ARG GLY GLY ALA PRO PRO PRO GLY MET GLY PRO PRO GLY MET ARG PRO PRO MET GLY PRO PRO

MET GLY ILE PRO PRO GLY ARG GLY THR PRO MET GLY PRO PRO GLY MET ARG GLY LEU LEU

• Molecule 22: Small nuclear ribonucleoprotein Sm D1

Chain c:

17%
69%
31%

M1 H12 E13 T14 N21 T28 I29 T30 A42 V43 P52 V53 Q54 L55 N63 D72 S73 L74 L79 L80 V81 D82 VAL GLU PRO LYS VAL LYS SER LYS LYS ARG GLU ALA VAL ALA GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG

GLY ARG GLY GLY PRO ARG ARG

• Molecule 22: Small nuclear ribonucleoprotein Sm D1

Chain j:

48%
69%
31%

M1 K2 L3 F6 L7 M8 K9 L10 S11 H12 E13 T14 V15 E18 L19 K20 N21 Q24 V25 H26 G27 T28 I29 T30 G31 V32 D33 Y34 N37 T38 H39 L40 K41 A42 V43 K44 M45 T46 L47 K48 N49 R50 E51 P52 V53 Q54 L55 E56 S59 I65 R66 Y67 F68 I69

L70 P71 D72 S73 L74 P75 L76 D77 T78 L79 L80 V81 D82 VAL GLU PRO LYS VAL LYS SER LYS LYS ARG GLU VAL ALA GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY PRO ARG ARG

• Molecule 23: Small nuclear ribonucleoprotein Sm D2

Chain d:

22%

81%   18%

MET SER LEU LEU ASN LYS PRO LYS SER GLU MET THR PRO GLU GLU LEU GLN LYS ARG E20 E21 E22 E23 F24 N25 T26 R55 H62 L67 E76 V77 P78 K79 S80 G81 K82 G83 K84 K85 K86 S87 K88 P89 Y95 N112 P113 L114 I115 A116 GLY LYS

• Molecule 23: Small nuclear ribonucleoprotein Sm D2

Chain k:

53%

71%   28%

MET SER LEU LEU ASN LYS PRO LYS SER GLU MET THR PRO GLU GLU LEU GLN LYS ARG E20 E21 E22 E23 F24 N25 T26 G27 P28 L29 S30 V31 L32 T33 Q34 S35 V36 K37 N38 N39 T40 Q41 V42 L43 C46 R47 K50 K51 L52 L53 G54 R55 V56 K57 A58 F59 D60 R61 H62

C63 N64 M65 V66 L67 E68 N69 V70 K71 E72 M73 W74 T75 E76 VAL PRO LYS SER GLY LYS GLY LYS LYS SER LYS P89 V90 N91 K92 D93 R94 Y95 I96 S97 K98 M99 F100 R111 N112 P113 L114 I115 A116 GLY LYS

• Molecule 24: Small nuclear ribonucleoprotein F

Chain f:

40%

86%   14%

MET S2 L3 P4 L5 K8 P9 F10 L11 N12 G13 L14 T15 G16 K17 P18 W25 Y32 L33 V34 S35 V36 D37 G38 Y39 A45 N46 T47 E48 E49 D52 G53 A54 L55 S56 G57 H58 L59 G60 E61 V75 GLU GLU GLU GLU ASP GLY GLU MET ARG GLU

• Molecule 24: Small nuclear ribonucleoprotein F

Chain m:

64%

86%   14%

MET S2 L3 P4 L5 N6 P7 K8 P9 F10 L11 N12 G13 L14 T15 G16 K17 P18 V19 M20 W25 G26 M27 E28 Y29 K30 G31 Y32 L33 V34 S35 V36 D37 G38 Y39 M40 N41 M42 Q43 L44 A45 N46 T47 E48 E49 Y50 I51 D52 G53 A54 L55 S56 G57 H58 L59 G60 E61 V62 L63

I64 R65 C66 N67 Y71 G74 V75 GLU GLU GLU GLU GLU ASP GLY GLU MET ARG GLU

• Molecule 25: Small nuclear ribonucleoprotein E

Chain e:

43%

86%   14%

MET ALA TYR ARG GLY GLN GLY GLN LYS VAL GLN LYS VAL M14 I18 N19 L20 I21 F22 R23 Y24 L25 Q26 N27 R28 I31 V39 N40 M41 C46 I47 I48 G49 F50 D51 L56 V57 L58 D59 D60 A61 E62 E63 T68 K69 S70 R71 K72 Q73 R76 I77 M78 L79

K80 T85 L86 L87 Q88 S89 V90 S91 N92

• Molecule 25: Small nuclear ribonucleoprotein E

Chain l:

68%

86%   14%

MET ALA TYR ARG GLY GLN GLY GLN LYS VAL GLN LYS VAL M14 V15 Q16 P17 I18 N19 L20 I21 F22 R23 Y24 L25 Q26 N27 R28 S29 R30 I31 Q32 V33 W34 L35 Y36 E37 N40 M41 R42 I43 E44 G45 C46 I47 I48 G49 F50 D51 E52 Y53 M54 N55 L56 V57 L58 D59 D60 A61

E62 E63 I64 H65 S66 K67 T68 K69 S70 R71 K72 Q73 L74 G75 R76 I77 M78 L79 K80 G81 D82 N83 S89 V90 S91 N92

• Molecule 26: Small nuclear ribonucleoprotein G

Chain g:

MET SER K3 A4 H5 E8 L9 K10 K11 F12 M13 D14 K15 K16 G23 Q28 Q29 I30 L31 R32 G33 F34 L40 V41 I42 D43 E44 C45 V46 E47 M48 A49 T50 S51 G52 S53 Q54 N55 N56 I57 G58 M59 V60 I67 R75 V76

• Molecule 26: Small nuclear ribonucleoprotein G

Chain n:

MET SER LYS ALA H5 P6 L9 K10 K11 F12 M13 D14 K15 K16 L19 K20 G23 G24 R25 H26 V27 Q28 Q29 I30 L31 R32 G33 F34 D35 P36 F37 M38 N39 L40 D43 E44 C45 V46 E47 M48 ALA THR SER GLY GLN Q54 N55 N56 I57 G58 M59 V60 V61 I62 R63 G64

N65 A72 L73 E74 R75 V76

• Molecule 27: Pre-mRNA-processing factor 19

Chain q:

MET SER L3 I4 C5 S6 I7 S8 N9 E10 V11 P12 E13 H14 P15 C16 V17 S18 P19 V20 S21 N22 H23 V24 Y25 E26 R27 R28 L29 I30 E31 K32 Y33 I34 A35 E36 N37 G38 T39 D40 P41 I42 N43 N44 Q45 P46 L47 S48 E49 E50 Q51 L52 I53 D54 I55 K56 V57 A58 H59 P60

I61 R62 P63 K64 P65 P66 S67 A68 T69 S70 I71 P72 A73 I74 L75 K76 A77 L78 Q79 D80 E81 W82 D83 A84 V85 M86 L87 H88 S89 F90 T91 L92 R93 Q94 Q95 L96 Q97 T98 T99 R100 Q101 E102 L103 S104 H105 A106 L107 Y108 Q109 H110 D111 A112 A113 C114 R115 V116 I117 A118 R119 L120

T121 K122 E123 V124 T125 A126 A127 R128 E129 A130 L131 A132 T133 L134 LYS PRO GLN ALA GLY LEU ILE VAL PRO GLN ALA VAL PRO SER SER GLN PRO SER VAL VAL GLY ALA GLY GLU PRO MET ASP LEU GLY GLU LEU VAL GLY PRO ILE ILE GLN LYS LEU GLN ASP LYS ALA

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

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

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

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

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

VAL ALA PHE GLY HIS HIS ALA LYS PHE ILE ALA SER THR GLY MET ASP ARG SER LEU LYS PHE TYR SER LEU

• Molecule 27: Pre-mRNA-processing factor 19

Chain r:

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

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

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

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

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

ALA PHE GLY HIS HIS ALA LYS PHE ILE ALA SER THR GLY MET ASP ARG SER LEU LYS PHE TYR SER LEU

• Molecule 27: Pre-mRNA-processing factor 19

Chain s:

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

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

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

• Molecule 27: Pre-mRNA-processing factor 19

Chain t:

13%

13%   87%

• Molecule 28: Pre-mRNA-splicing factor SPF27

Chain K:

56%

57%   9%   32%

• Molecule 29: U2 small nuclear ribonucleoprotein A'

Chain o:

57%

61% • 36%

• Molecule 30: U2 small nuclear ribonucleoprotein B"

Chain p:

30%

42% 58%

• Molecule 31: RNA helicase aquarius

Chain Q:

87%

89% 11%

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

Chain y:

17%

26%   74%

R78 V79 N80 L81 A82 K83 PRO MET ARG ILE LYS GLU GLY SER SER ARG PRO VAL TRP SER ASP ASP ASP TRP LEU LYS LYS PHE SER GLY LYS THR LEU GLU GLU GLU ASN LYS GLU GLU GLU GLY SER GLU PRO PRO LYS ALA GLU THR GLN GLU GLY GLU PRO ILE ALA LYS LYS ALA

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

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

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

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 $(e^-/\text{Å}^2)$	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 (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MG, ZN, GTP, SEP, IHP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.41	0/16926	0.64	9/22947 (0.0%)
2	B	0.54	1/2296 (0.0%)	1.09	15/3569 (0.4%)
3	C	0.33	0/7181	0.65	3/9758 (0.0%)
4	E	0.32	0/2420	0.64	1/3281 (0.0%)
5	F	0.64	0/2323	1.14	11/3619 (0.3%)
6	J	0.43	0/3802	0.59	6/5162 (0.1%)
7	L	0.35	0/3267	0.61	9/4418 (0.2%)
8	M	0.33	0/1119	0.59	1/1497 (0.1%)
9	N	0.99	6/1210 (0.5%)	0.74	0/1622
10	O	0.39	0/2390	0.62	3/3227 (0.1%)
11	P	0.36	0/1000	0.58	0/1330
12	R	0.38	0/2186	0.71	4/2937 (0.1%)
13	S	0.33	0/1268	0.61	2/1714 (0.1%)
14	T	0.55	1/2562 (0.0%)	0.74	0/3492
15	W	0.47	0/3038	0.72	3/4171 (0.1%)
16	G	0.74	5/1378 (0.4%)	1.46	31/2133 (1.5%)
17	H	0.81	20/3308 (0.6%)	1.37	64/5135 (1.2%)
18	U	0.37	0/2928	0.71	4/3928 (0.1%)
19	I	0.34	0/2803	0.58	11/3870 (0.3%)
20	a	0.47	0/397	0.62	0/549
20	h	0.47	0/396	0.61	0/547
21	b	0.51	0/423	0.72	0/587
21	i	0.50	0/423	0.73	0/587
22	c	0.57	0/405	0.73	0/563
22	j	0.57	0/405	0.73	0/563
23	d	0.69	0/479	0.85	0/666
23	k	0.70	0/420	0.85	0/583
24	f	0.75	0/360	0.81	0/497
24	m	0.75	0/360	0.81	0/497
25	e	0.65	0/390	0.80	0/542
25	l	0.64	0/390	0.80	0/542
26	g	0.54	0/362	0.71	0/501

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
26	n	0.53	0/327	0.72	0/451
27	q	0.35	0/658	0.58	3/919 (0.3%)
27	r	0.33	0/653	0.56	2/912 (0.2%)
27	s	0.26	0/334	0.37	0/466
27	t	0.31	0/334	0.38	0/466
28	K	0.39	1/753 (0.1%)	0.53	3/1046 (0.3%)
29	o	0.64	0/803	1.49	5/1119 (0.4%)
30	p	0.62	0/463	1.27	0/643
31	Q	0.21	0/6565	0.42	0/9143
32	y	0.25	0/389	0.62	0/540
All	All	0.46	34/79894 (0.0%)	0.76	190/110739 (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 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	137	CYS	CB-SG	-11.04	1.63	1.82
9	N	119	CYS	CB-SG	-8.86	1.67	1.82
9	N	142	CYS	CB-SG	-8.41	1.68	1.82
9	N	101	CYS	CB-SG	-8.37	1.68	1.82
17	H	77	C	C1'-N1	7.34	1.59	1.48

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	147	C	O5'-P-OP1	-13.09	93.92	105.70
16	G	5	G	N3-C4-C5	-12.87	122.16	128.60
16	G	17	U	N1-C2-O2	9.52	129.47	122.80
16	G	2	U	N1-C1'-C2'	9.23	126.00	114.00
16	G	17	U	N3-C2-O2	-8.73	116.09	122.20

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	234	0
2	B	2060	0	1044	79	0
3	C	7022	0	7047	163	0
4	E	2366	0	2303	70	0
5	F	2075	0	1048	43	0
6	J	3758	0	2888	46	0
7	L	3237	0	2680	38	0
8	M	1098	0	1082	16	0
9	N	1184	0	1189	11	0
10	O	2340	0	2316	45	0
11	P	985	0	965	14	0
12	R	2165	0	2214	36	0
13	S	1236	0	1210	28	0
14	T	2496	0	2446	46	0
15	W	3008	0	1977	60	0
16	G	1246	0	631	212	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	H	2968	0	1504	256	0
18	U	2864	0	2814	80	0
19	I	2822	0	1319	64	0
20	a	399	0	173	0	0
20	h	398	0	172	0	0
21	b	424	0	179	0	0
21	i	424	0	179	0	0
22	c	406	0	170	0	0
22	j	406	0	170	0	0
23	d	480	0	200	0	0
23	k	422	0	175	0	0
24	f	361	0	158	0	0
24	m	361	0	158	0	0
25	e	391	0	163	0	0
25	l	391	0	163	0	0
26	g	363	0	160	0	0
26	n	329	0	138	0	0
27	q	659	0	296	0	0
27	r	654	0	294	0	0
27	s	335	0	168	0	0
27	t	335	0	168	0	0
28	K	757	0	338	18	0
29	o	804	0	350	0	0
30	p	464	0	205	0	0
31	Q	6562	0	2836	2	0
32	y	390	0	190	0	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	1359	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 1359 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 ⓘ

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	
1	A	1977/2335 (85%)	1793 (91%)	165 (8%)	19 (1%)	13	40
3	C	886/972 (91%)	788 (89%)	96 (11%)	2 (0%)	44	73
4	E	301/357 (84%)	280 (93%)	20 (7%)	1 (0%)	37	66
6	J	520/848 (61%)	473 (91%)	42 (8%)	5 (1%)	13	40
7	L	459/802 (57%)	423 (92%)	31 (7%)	5 (1%)	12	37
8	M	128/243 (53%)	116 (91%)	12 (9%)	0	100	100
9	N	141/144 (98%)	128 (91%)	12 (8%)	1 (1%)	19	49
10	O	288/420 (69%)	262 (91%)	25 (9%)	1 (0%)	37	66
11	P	114/229 (50%)	98 (86%)	15 (13%)	1 (1%)	14	43
12	R	268/536 (50%)	227 (85%)	38 (14%)	3 (1%)	12	37
13	S	157/166 (95%)	141 (90%)	16 (10%)	0	100	100
14	T	315/514 (61%)	292 (93%)	21 (7%)	2 (1%)	22	52
15	W	507/579 (88%)	433 (85%)	46 (9%)	28 (6%)	1	5
18	U	343/894 (38%)	277 (81%)	58 (17%)	8 (2%)	5	20
19	I	528/855 (62%)	491 (93%)	23 (4%)	14 (3%)	4	17
20	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100

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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%)	8	28
27	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8	29
27	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	29
28	K	144/225 (64%)	130 (90%)	8 (6%)	6 (4%)	2	9
29	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10	33
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%)	16	40

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%)	1767 (99%)	25 (1%)	62	86
3	C	787/866 (91%)	769 (98%)	18 (2%)	45	77
4	E	259/300 (86%)	254 (98%)	5 (2%)	52	81
6	J	242/751 (32%)	236 (98%)	6 (2%)	42	75
7	L	228/709 (32%)	225 (99%)	3 (1%)	65	88
8	M	117/209 (56%)	114 (97%)	3 (3%)	41	74
9	N	130/130 (100%)	129 (99%)	1 (1%)	79	93
10	O	259/361 (72%)	254 (98%)	5 (2%)	52	81
11	P	104/203 (51%)	101 (97%)	3 (3%)	37	72
12	R	227/457 (50%)	218 (96%)	9 (4%)	27	61
13	S	129/134 (96%)	127 (98%)	2 (2%)	58	84
14	T	273/441 (62%)	270 (99%)	3 (1%)	70	90
15	W	135/502 (27%)	133 (98%)	2 (2%)	60	85
18	U	313/806 (39%)	302 (96%)	11 (4%)	31	66
19	I	7/749 (1%)	2 (29%)	5 (71%)	0	0
All	All	5002/8726 (57%)	4901 (98%)	101 (2%)	50	79

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	M	134	GLN
12	R	165	VAL
19	I	526	MET
8	M	215	ASN
10	O	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
8	M	212	ASN
12	R	189	ASN
18	U	718	HIS
9	N	37	HIS
10	O	113	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%)	52 (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%)	192 (48%)	31 (7%)

5 of 192 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	0.85	0	8,12,14	2.02	1 (12%)
12	SEP	R	232	12	8,9,10	0.91	0	8,12,14	2.06	1 (12%)

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	-	1/5/8/10	-
12	SEP	R	232	12	-	3/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	R	232	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 (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	R	224	SEP	N-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	$\#|Z| > 2$
33	IHP	A	3000	-	36,36,36	0.70	0	54,60,60	0.97	0
34	GTP	C	1500	35	26,34,34	0.96	1 (3%)	32,54,54	1.46	4 (12%)

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
33	IHP	A	3000	-	-	8/30/54/54	0/1/1/1
34	GTP	C	1500	35	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1500	GTP	C6-N1	-2.74	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	1500	GTP	PA-O3A-PB	-3.98	119.17	132.83
34	C	1500	GTP	PB-O3B-PG	-3.53	120.71	132.83
34	C	1500	GTP	C5-C6-N1	2.44	118.26	113.95
34	C	1500	GTP	C8-N7-C5	2.43	107.61	102.99

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	A	3000	IHP	C6-C1-O11-P1
33	A	3000	IHP	C4-O14-P4-O44
33	A	3000	IHP	C6-O16-P6-O26
34	C	1500	GTP	C5'-O5'-PA-O3A
33	A	3000	IHP	C2-C1-O11-P1

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	3000	IHP	1	0
34	C	1500	GTP	22	0

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

Ligand IHP A 3000

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 1500

Bond lengths

Bond angles

Torsions

Rings
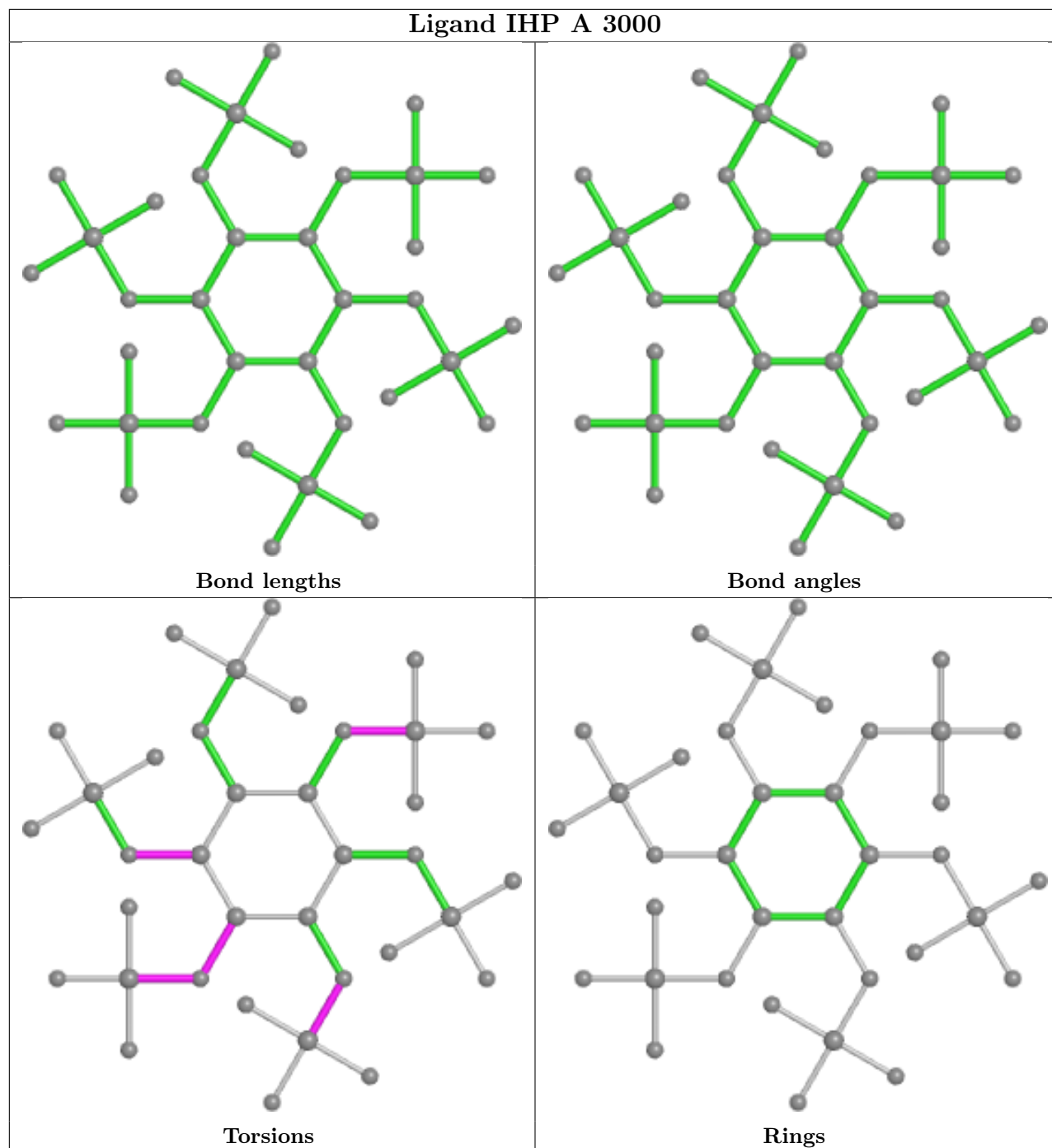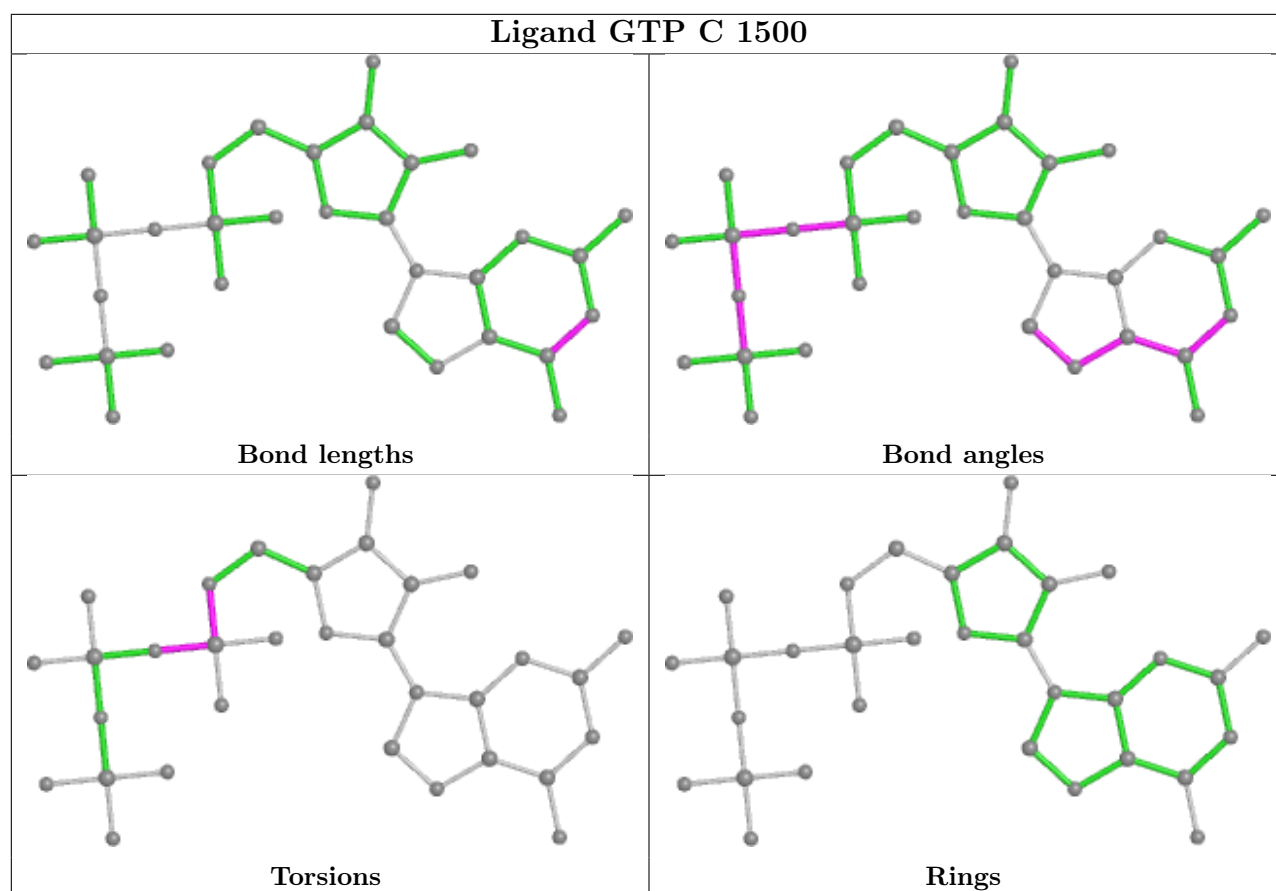
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-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 ⓘ

6.1.1 Primary map

| X | Y | Z |
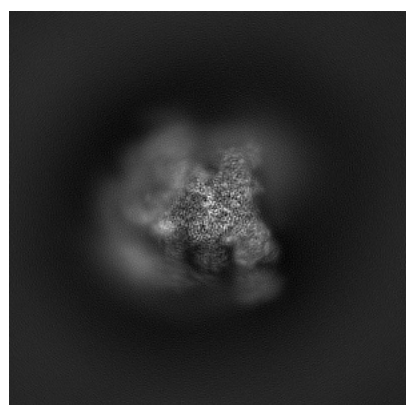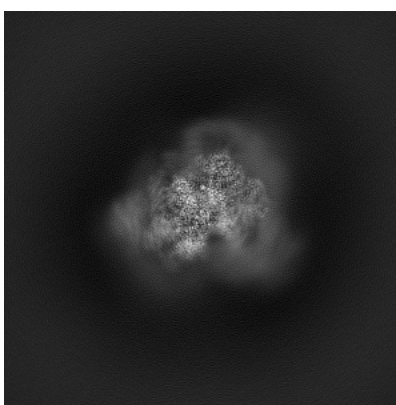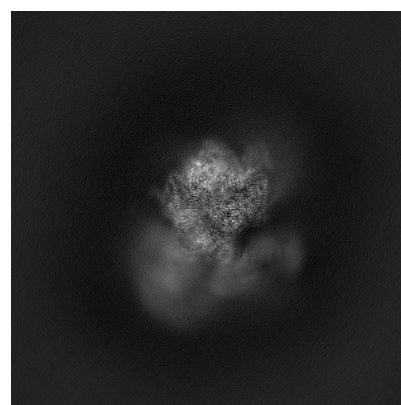
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
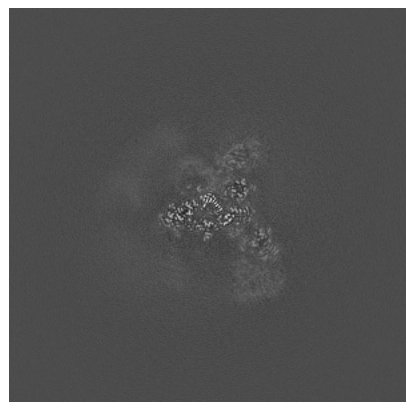
6.2.1 Primary map
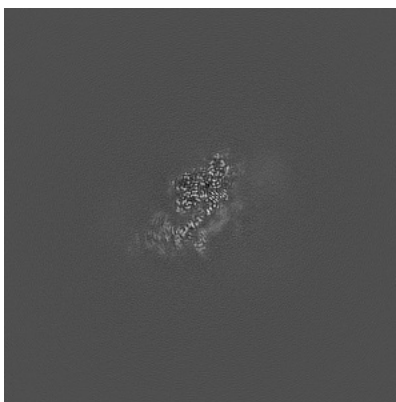
| X Index: 200 | Y Index: 200 | Z Index: 200 |
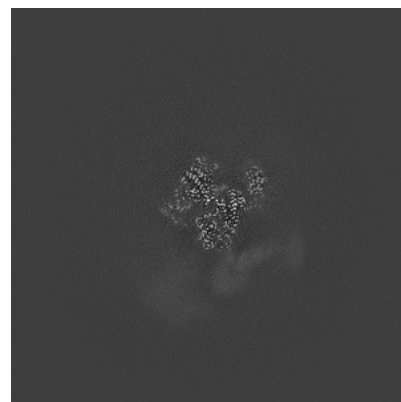
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
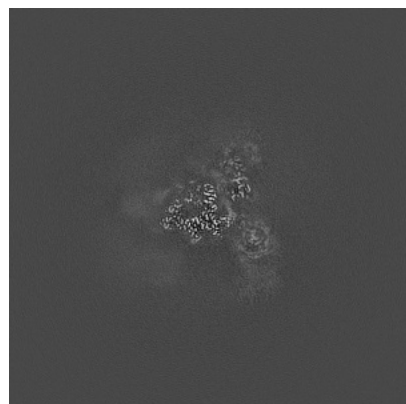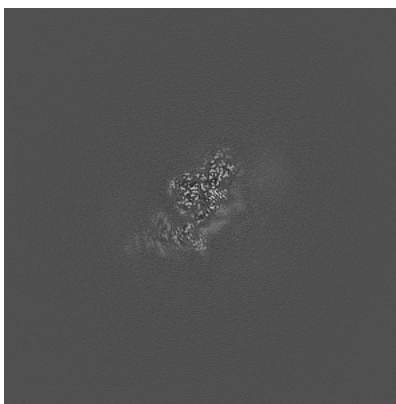
| X Index: 210 | Y Index: 201 | Z Index: 185 |
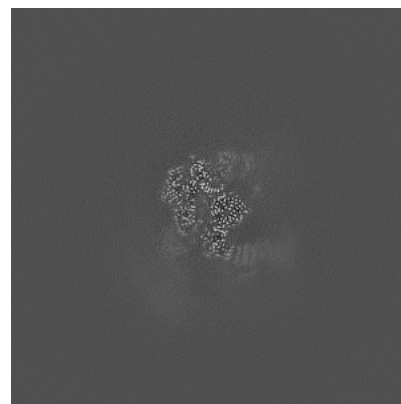
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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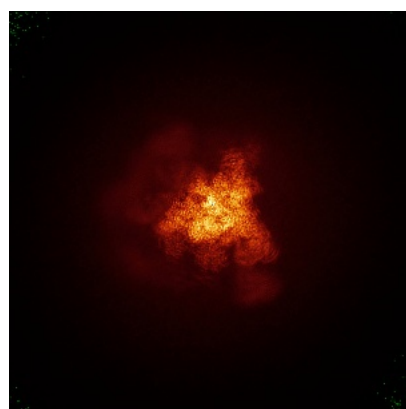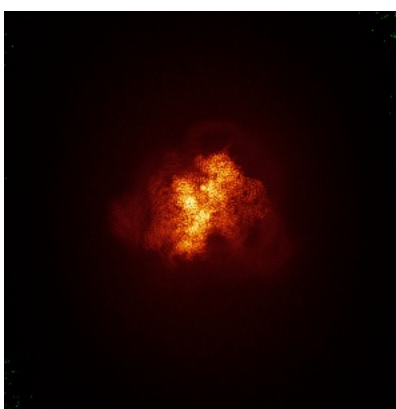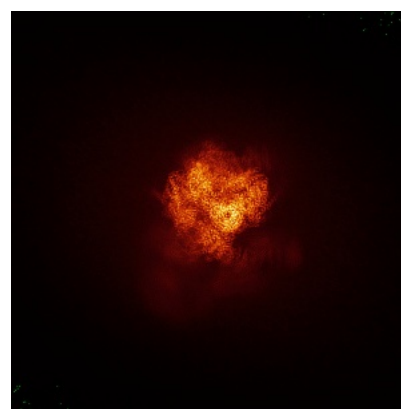
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 ⓘ

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

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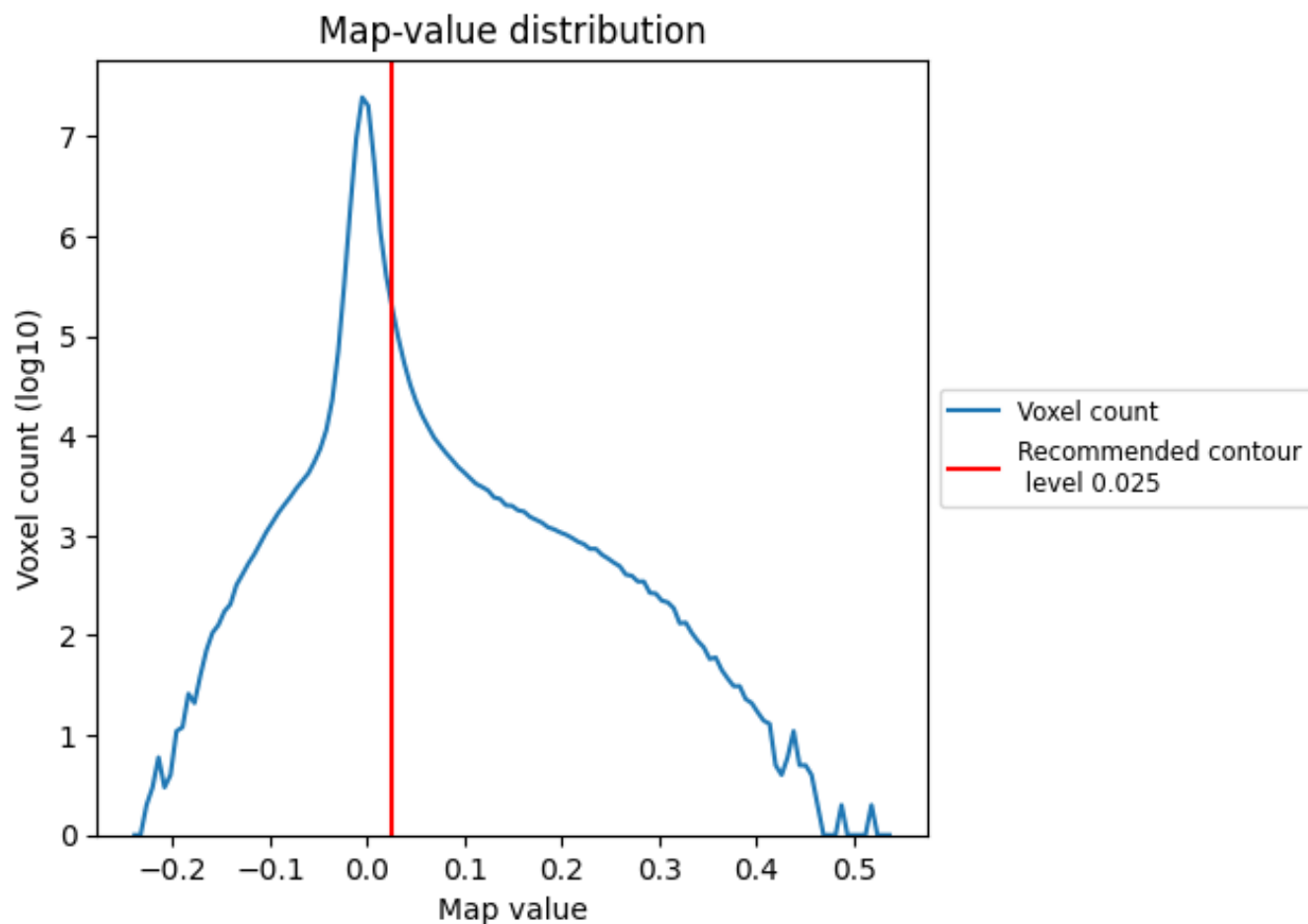
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

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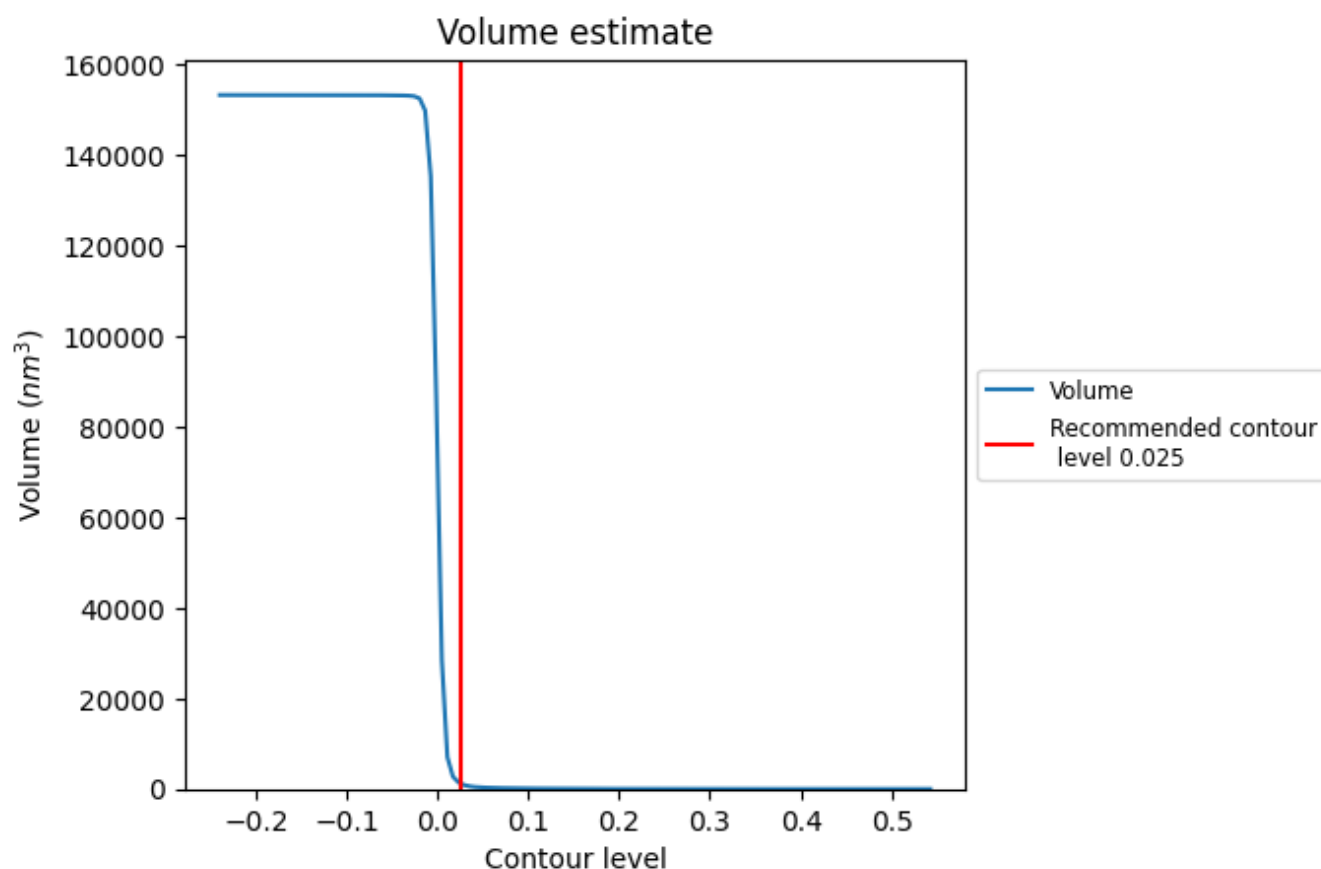
The volume at the recommended contour level is 1297 nm^3; this corresponds to an approximate mass of 1172 kDa.

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 (i)
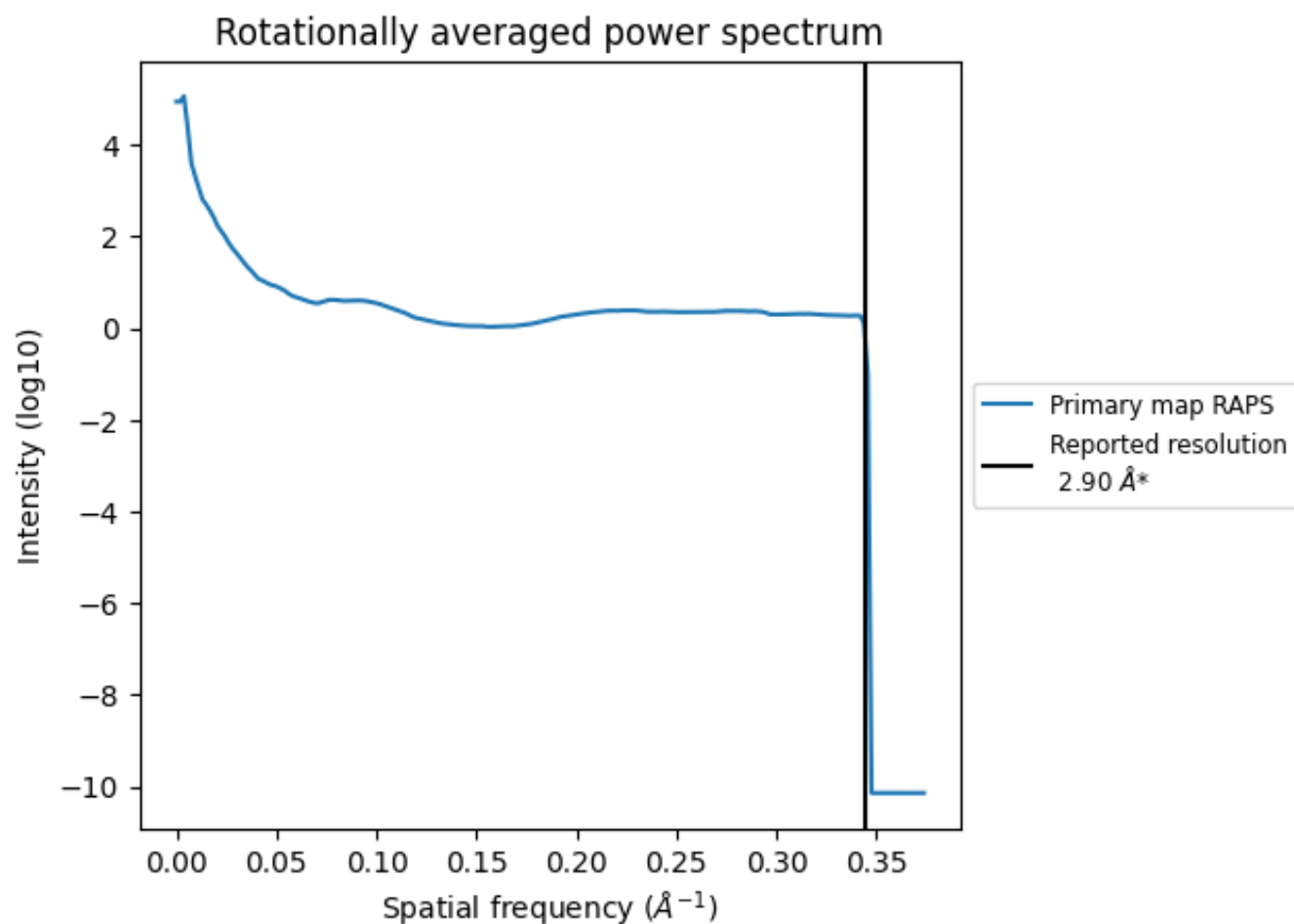
*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

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 ⓘ

<div align="center">X   Y   Z</div>
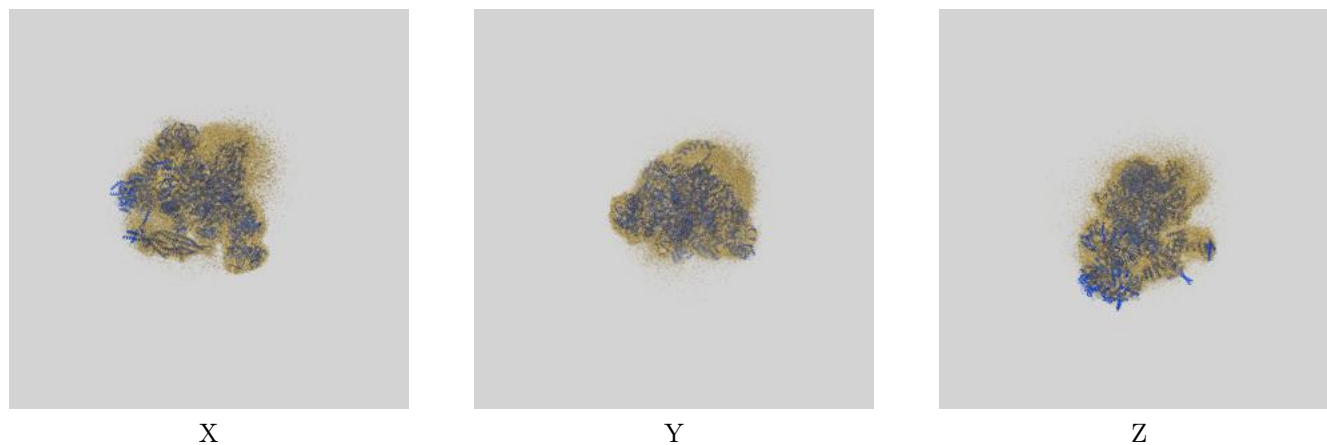
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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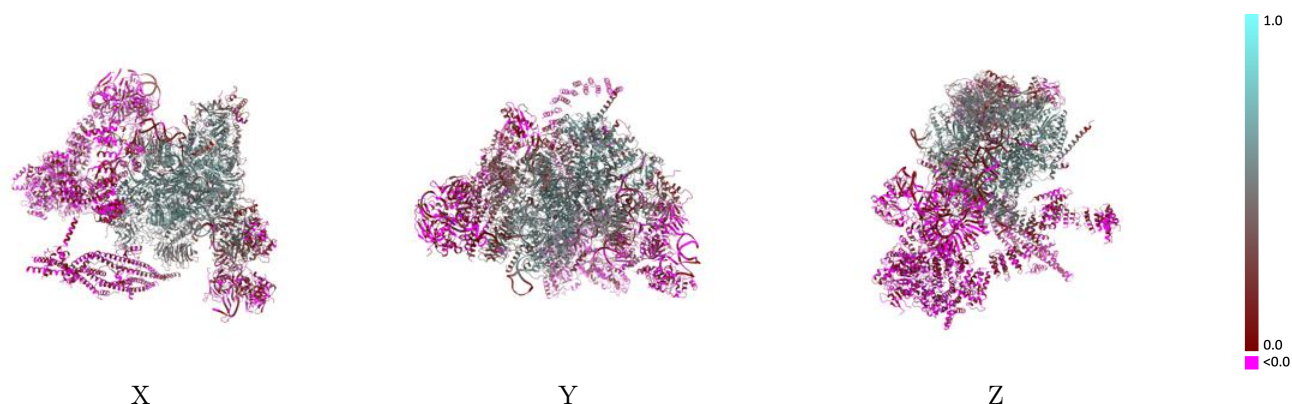
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

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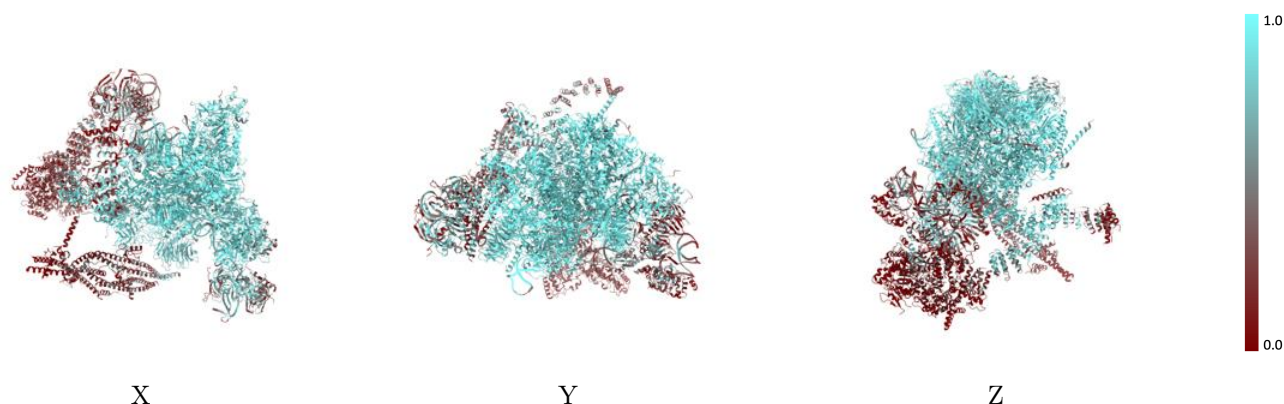
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4   Atom inclusion   ⓘ
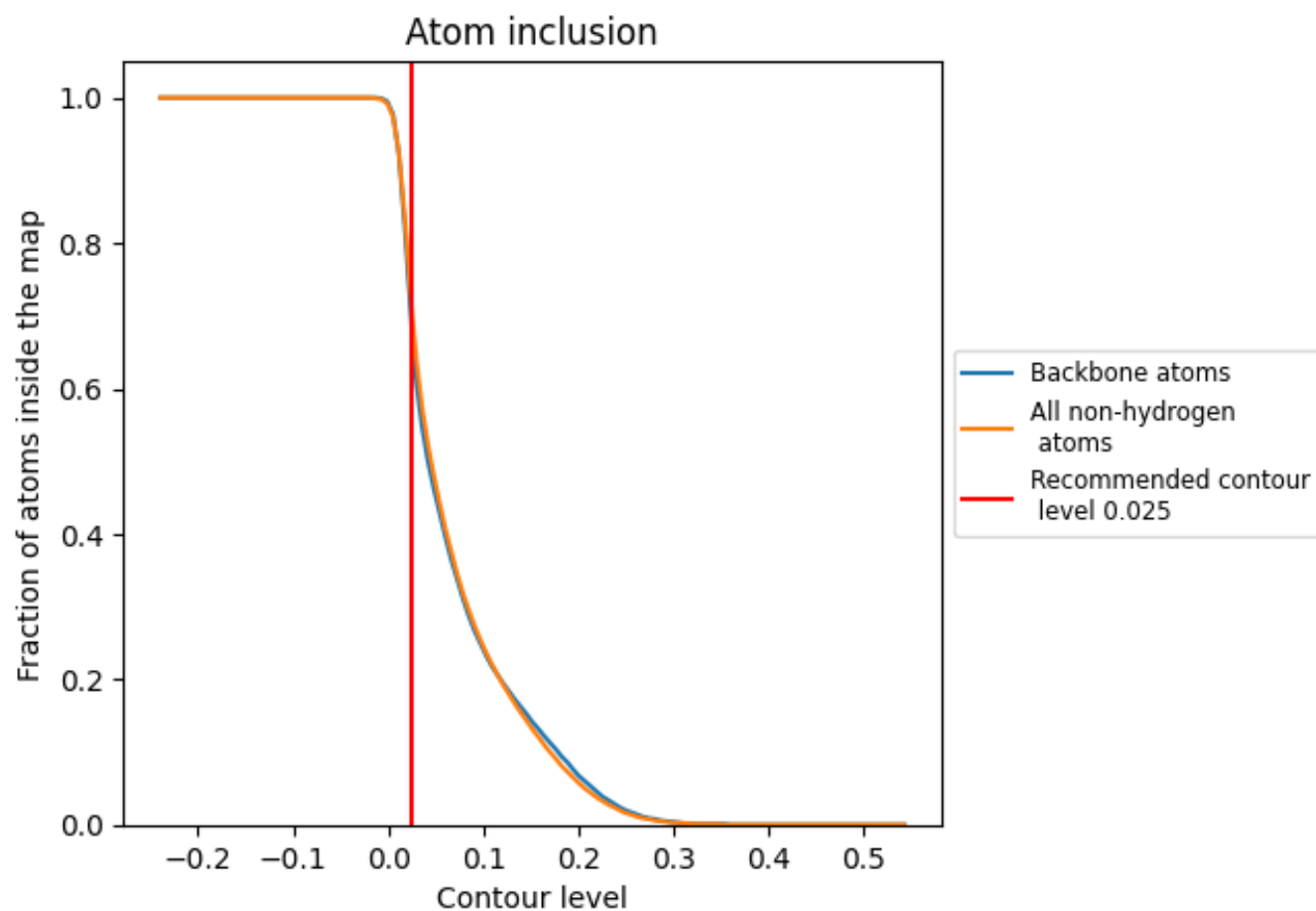
At the recommended contour level, 68% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

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

1.0

0.0
<0.0

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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