Full wwPDB EM Validation Report (i)

Nov 10, 2024 – 07:25 am GMT

PDB ID	:	8RO0
EMDB ID	:	EMD-19397
Title	:	Structure of the C. elegans Intron Lariat Spliceosome primed for disassembly (ILS')
Authors	:	Vorlaender, M.K.; Rothe, P.; Plaschka, C.
Deposited on	:	2024-01-11
Resolution	:	2.90 Å(reported)
Based on initial model	:	.

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

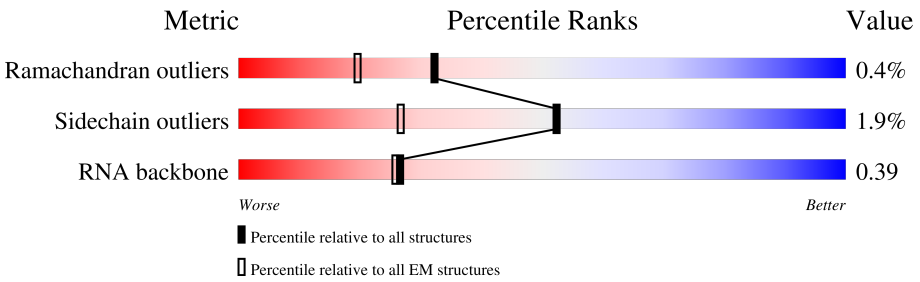
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	2	191	5%, 28%, •, 68%
2	5	121	•, 54%, 31%, 7%, •, 8%
3	6	101	31%, 48%, 36%, 6%, 11%
4	A	2329	12%, 93%, •, •
5	B	2145	•, 83%, •, 16%
6	C	974	•, 90%, •, 8%
7	D	267	13%, 32%, •, 67%
8	E	331	•, 93%, •, 6%

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Mol	Chain	Length	Quality of chain
9	I	855	82% 15%
10	J	744	9% 75% 23%
11	K	238	12% 85% 15%
12	L	755	23% 79% 19%
13	M	234	16% 82% 16%
14	N	147	95%
15	O	408	8% 82% 16%
16	P	230	38% 62% 35%
17	PX	809	24% 58% 42%
18	Q	1467	7% 93% 6%
19	R	535	6% 49% 47%
20	S	169	9% 98%
21	T	494	76% 22%
22	TF	830	59% 40%
23	W	567	26% 84% 13%
24	Z	169	15% 39% 59%
25	a	136	58% 40%
25	h	136	10% 57% 40%
26	b	160	59% 39%
26	i	160	22% 48% 51%
27	c	127	61% 37%
27	j	127	26% 63% 37%
28	d	118	10% 77% 20%
28	k	118	29% 66% 33%
29	e	90	88% 11%

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Mol	Chain	Length	Quality of chain
29	l	90	28% 86% 11%
30	f	85	84% 15%
30	m	85	16% 81% 15%
31	g	77	8% 97%
31	n	77	17% 96%
32	o	253	26% 63% 36%
33	p	217	11% 35% 65%
34	q	492	24% 75%
34	r	492	11% 26% 73%
34	s	492	55% 93% 5%
34	t	492	10% 26% 74%
35	y	331	12% 23% 76%
36	In	19	21% 100%

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 121370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	61	947	410	82	394	61	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	111	2349	1052	405	781	111	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	90	1927	863	358	616	90	0	0

- Molecule 4 is a protein called Pre-mRNA-splicing factor 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	2231	18444	11870	3216	3272	86	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	1806	14404	9175	2476	2669	84	0	0

- Molecule 6 is a protein called Tr-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	898	7152	4558	1211	1337	46	0	0

- Molecule 7 is a protein called Protein isy-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	88	726	458	122	143	3	0	0

- Molecule 8 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	312	2443	1528	429	466	20	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	724	5995	3813	1047	1092	43	0	0

- Molecule 10 is a protein called TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	574	4893	3122	855	896	20	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	203	1665	1041	298	309	17	0	0

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	609	4898	3039	902	934	23	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor syf-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	196	1652	1021	308	317	6	0	0

- Molecule 14 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	142	1163	731	212	208	12	0	0

- Molecule 15 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	342	2717	1703	493	502	19	0	0

- Molecule 16 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	150	1204	729	232	237	6	0	0

- Molecule 17 is a protein called GCF C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	PX	472	3838	2396	695	720	27	0	0

- Molecule 18 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	1378	11292	7218	1964	2063	47	0	0

- Molecule 19 is a protein called Uncharacterized protein T27F2.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	282	2207	1379	404	414	10	0	0

- Molecule 20 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	169	1301	818	233	243	7	0	0

- Molecule 21 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	387	3066	1937	555	555	19	0	0

- Molecule 22 is a protein called Septin and tuftelin-interacting protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	TF	497	4094	2637	685	750	22	0	0

- Molecule 23 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	496	4071	2584	726	746	15	0	0

- Molecule 24 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	69	567	356	104	105	2	0	0

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a	81	634	396	113	119	6	0	0
25	h	81	634	396	113	119	6	0	0

- Molecule 26 is a protein called Probable small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	b	98	754	475	141	130	8	0	0
26	i	79	638	405	117	110	6	0	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	c	80	621	396	109	112	4	0	0
27	j	80	621	396	109	112	4	0	0

- Molecule 28 is a protein called Probable small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	d	94	747	469	135	138	5	0	0
28	k	79	630	398	118	109	5	0	0

- Molecule 29 is a protein called Probable small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	e	80	663	424	118	119	2	0	0
29	l	80	663	424	118	119	2	0	0

- Molecule 30 is a protein called Probable small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	f	72	557	359	93	101	4	0	0
30	m	72	557	359	93	101	4	0	0

- Molecule 31 is a protein called Probable small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	g	77	606	379	107	113	7	0	0
31	n	77	606	379	107	113	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	o	162	1335	849	236	243	7	0	0

- Molecule 33 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	p	76	626	402	114	106	4	0	0

- Molecule 34 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	q	121	939	585	165	184	5	0	0
34	r	131	1003	621	179	198	5	0	0
34	s	469	3570	2239	620	702	9	0	0
34	t	128	991	620	173	193	5	0	0

- Molecule 35 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	y	79	618	396	100	117	5	0	0

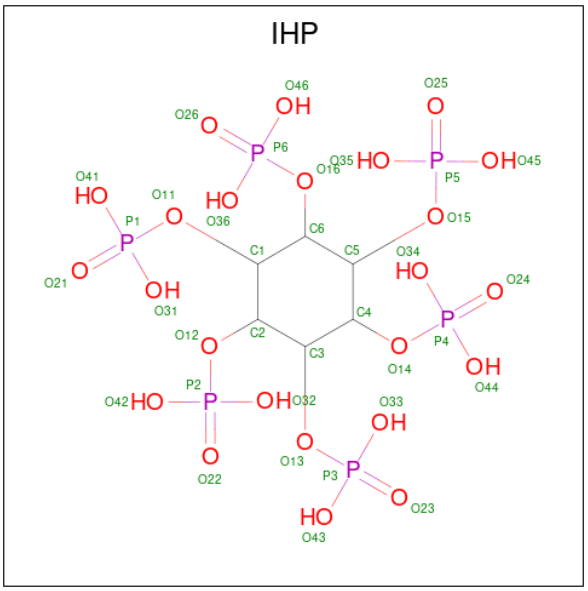
- Molecule 36 is a DNA chain called Intron lariat RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	O	P		
36	In	19	225	95	112	18	0	0

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

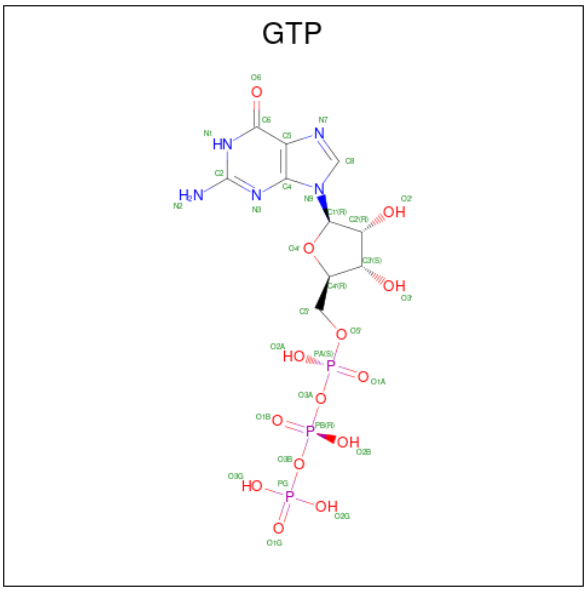
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	6	6	6	6	0
37	C	1	1	1	0

- Molecule 38 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

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



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

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

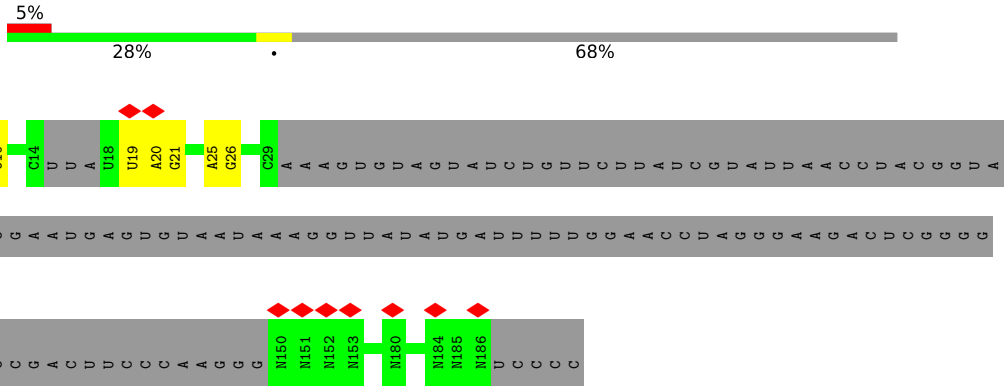
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
40	N	3	3	3	0
40	O	3	3	3	0

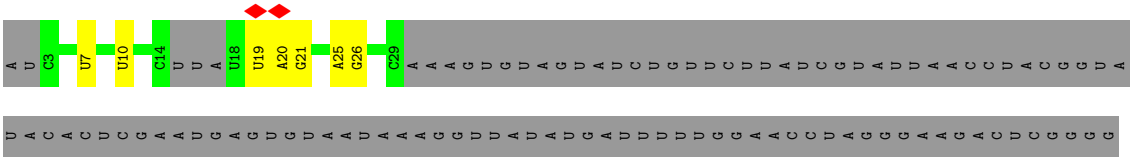
3 Residue-property plots (i)

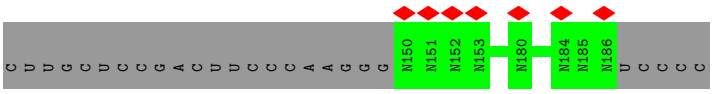
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: U2 snRNA

Chain 2:

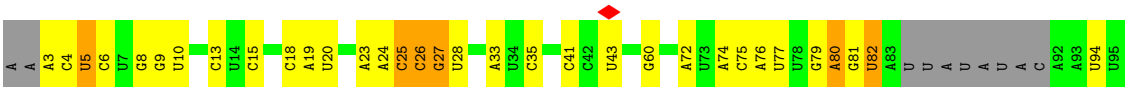






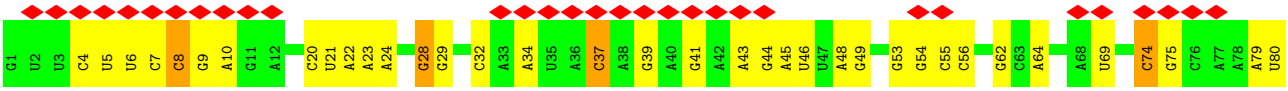
- Molecule 2: U5 snRNA

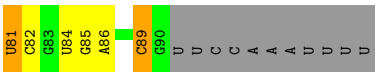
Chain 5:



- Molecule 3: U6 snRNA

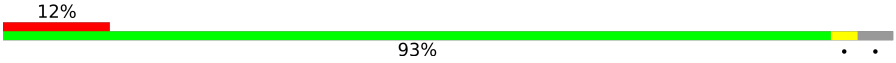
Chain 6:

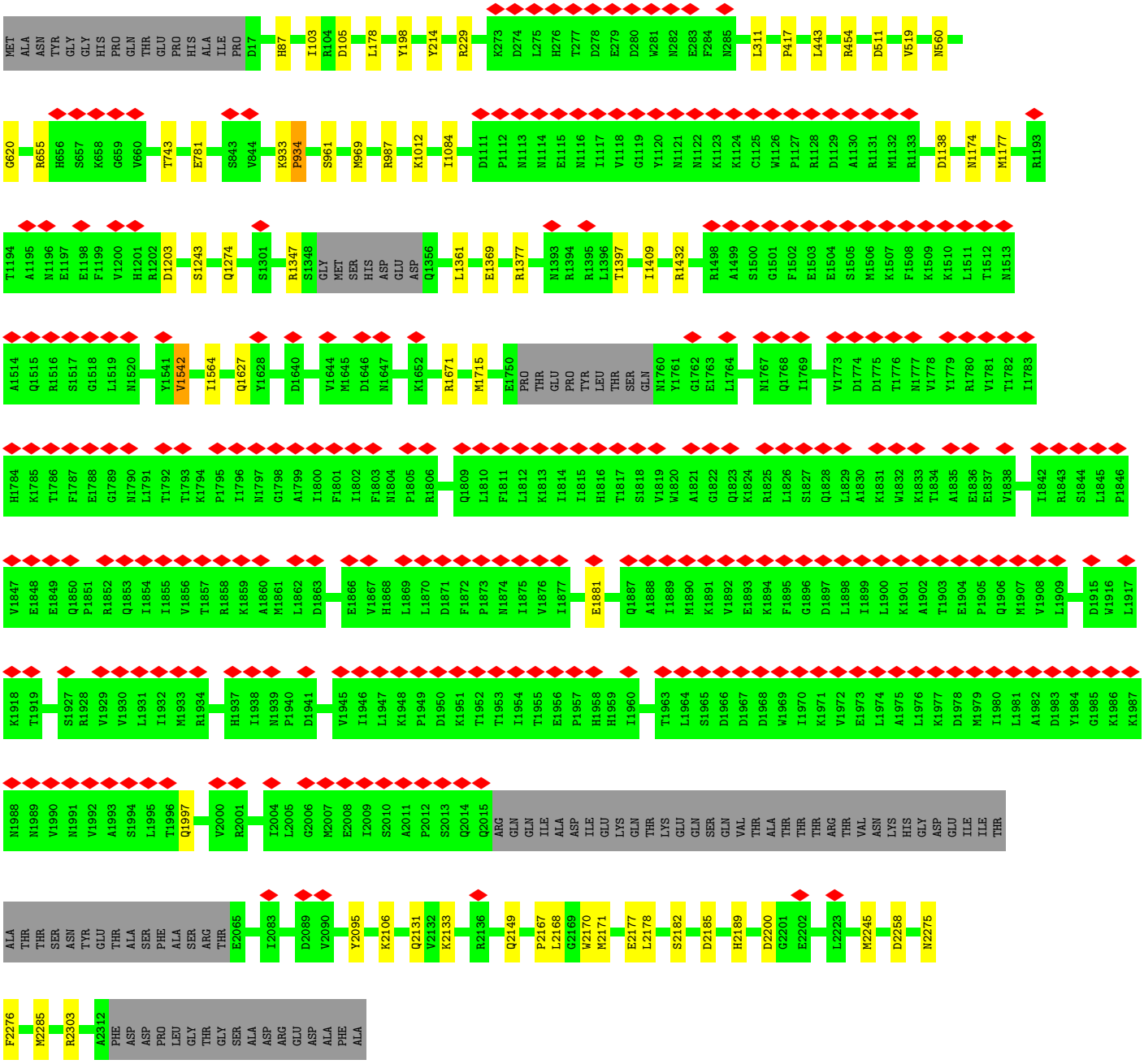




- Molecule 4: Pre-mRNA-splicing factor 8 homolog

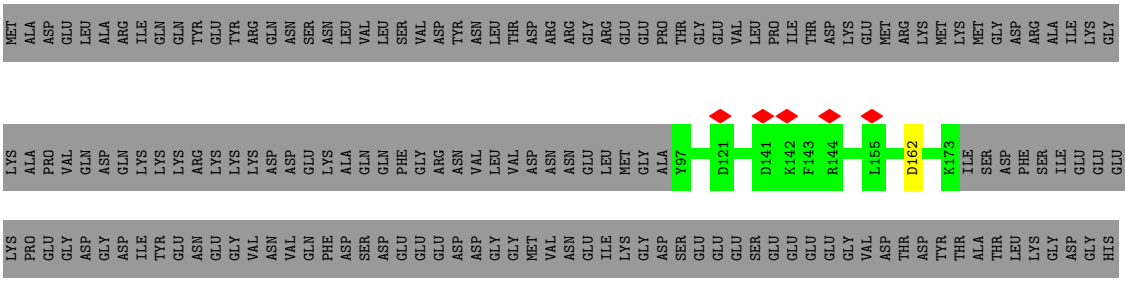
Chain A:

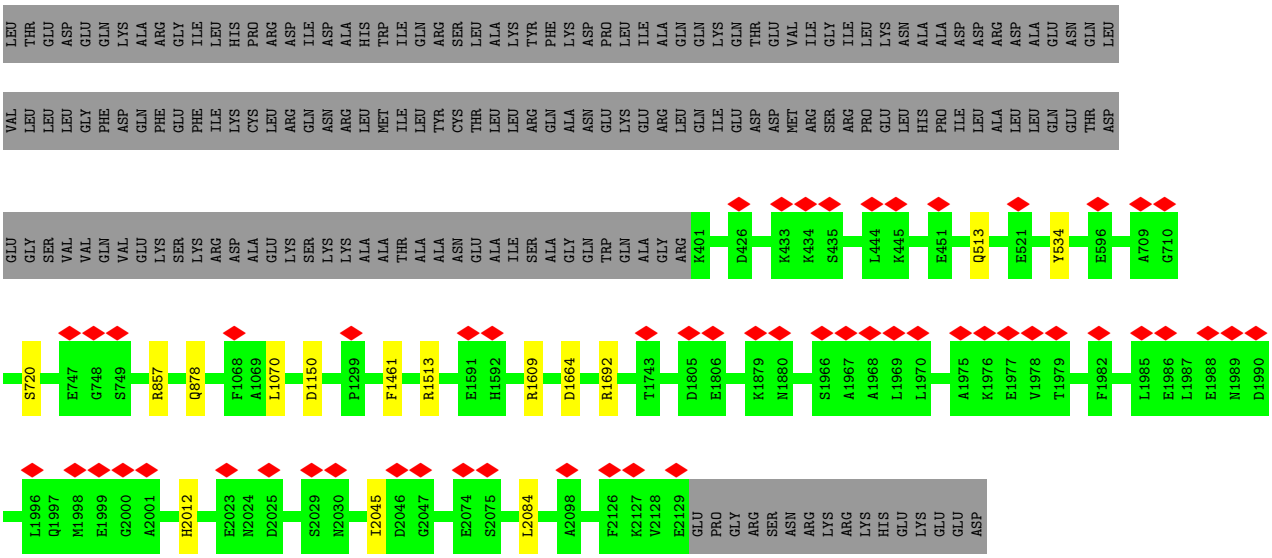




- Molecule 5: U5 small nuclear ribonucleoprotein 200 kDa helicase

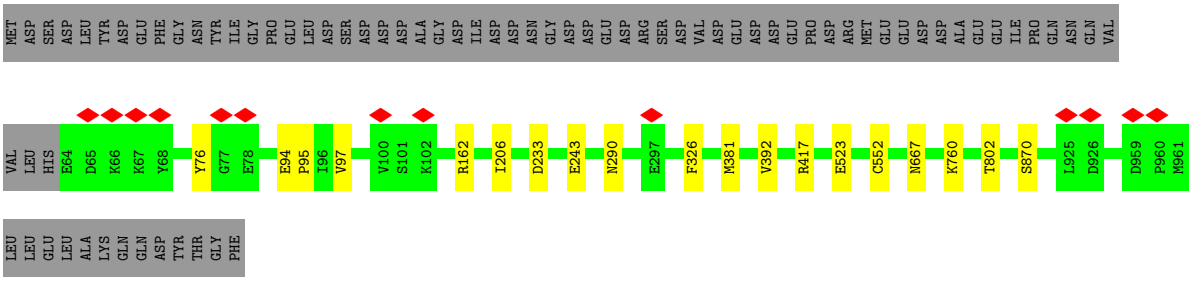
Chain B:





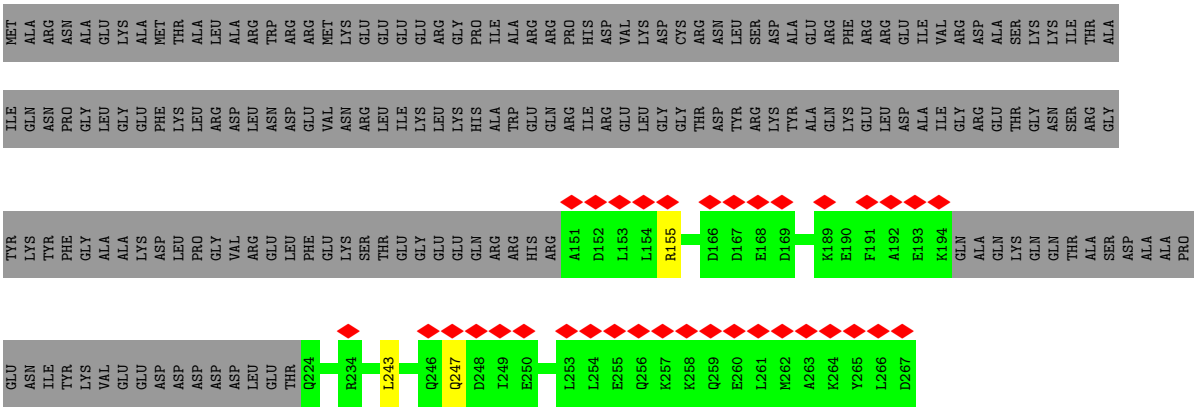
- Molecule 6: Tr-type G domain-containing protein

Chain C:



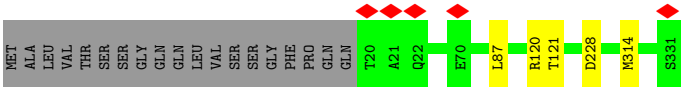
- Molecule 7: Protein isy-1

Chain D:



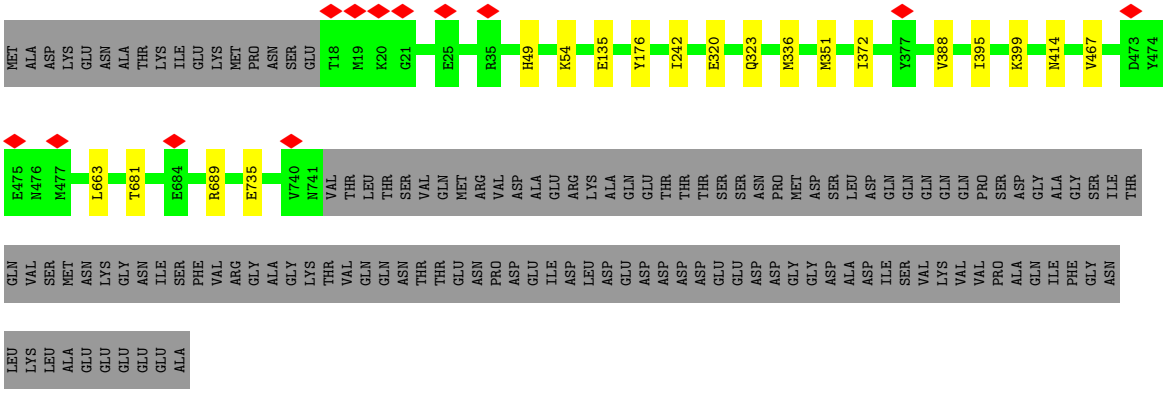
- Molecule 8: WD_REPEATS_REGION domain-containing protein

Chain E:



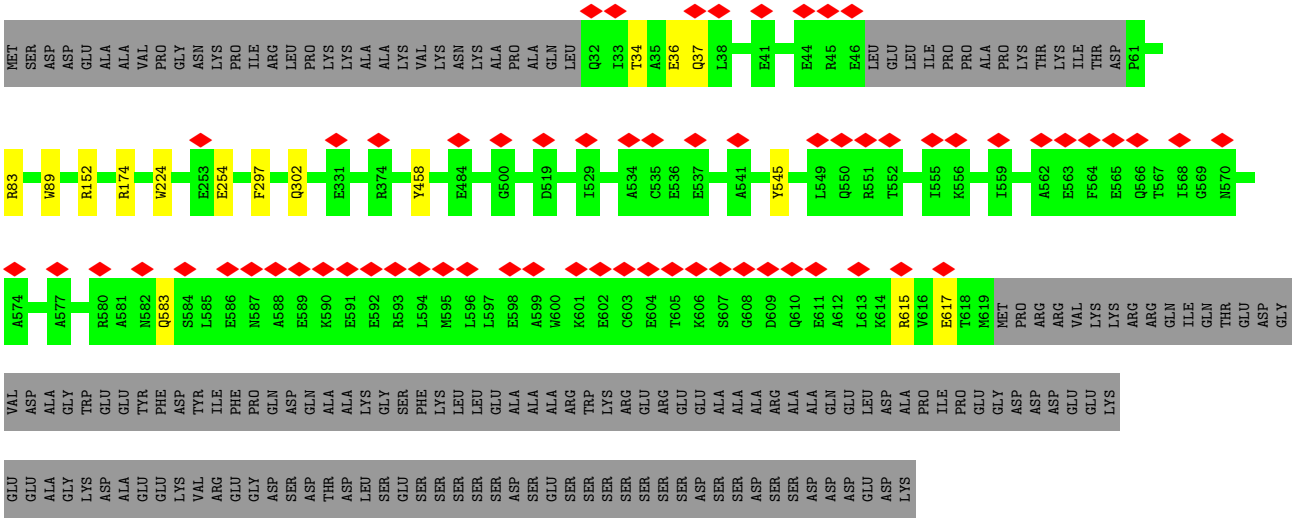
• Molecule 9: Pre-mRNA-splicing factor SYF1

Chain I:



• Molecule 10: TPR_REGION domain-containing protein

Chain J:

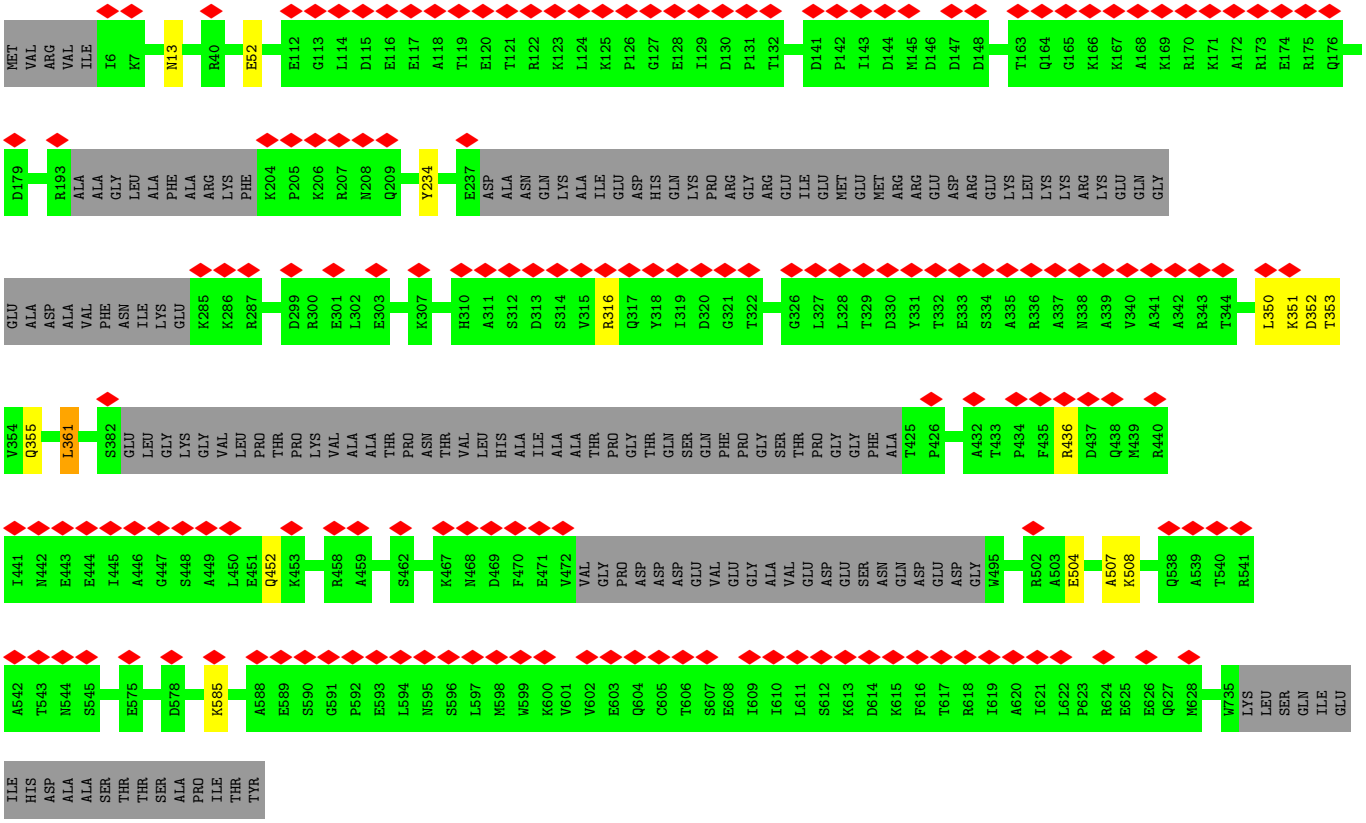


• Molecule 11: Pre-mRNA-splicing factor SPF27

Chain K:

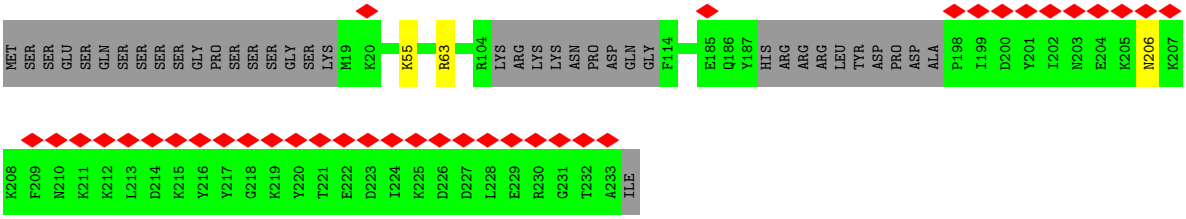
• Molecule 12: Cell division cycle 5-like protein

Chain L: 23% 79% 19%



• Molecule 13: Pre-mRNA-splicing factor syf-2

Chain M: 16% 82% 16%

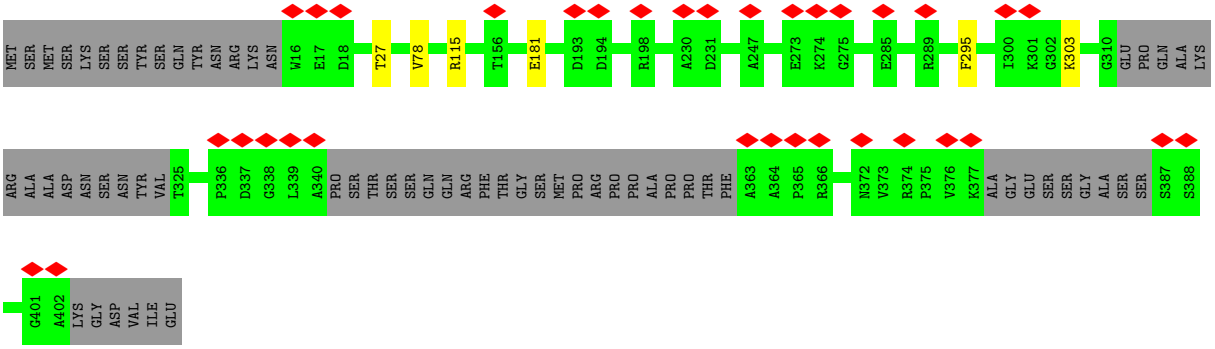


• Molecule 14: Protein BUD31 homolog

Chain N: 95%

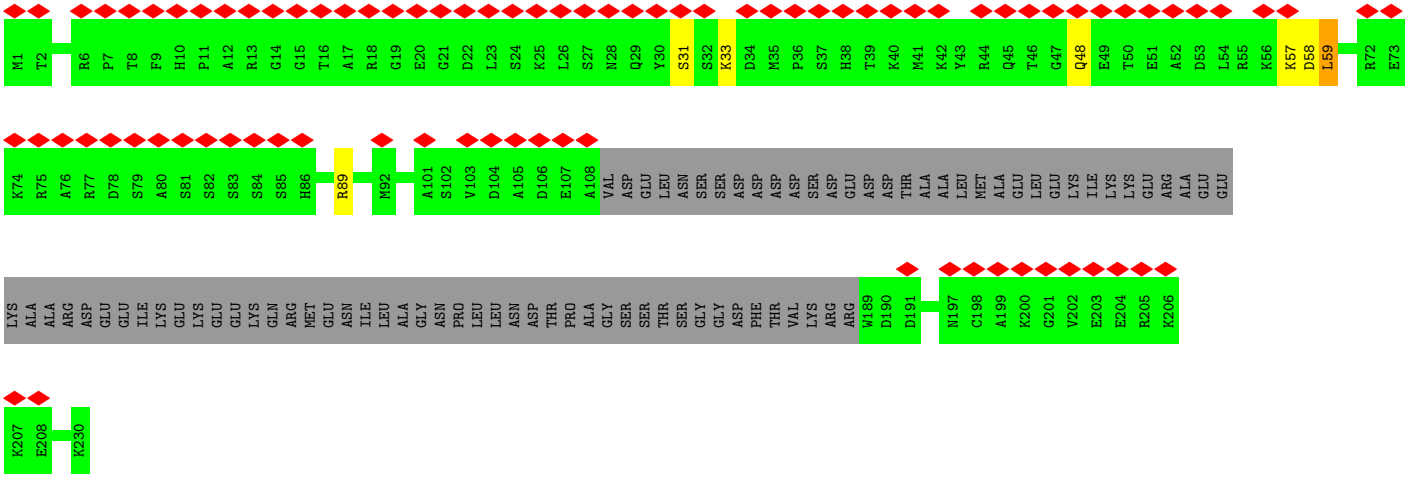
• Molecule 15: Pre-mRNA-splicing factor RBM22

Chain O: 8% 82% 16%



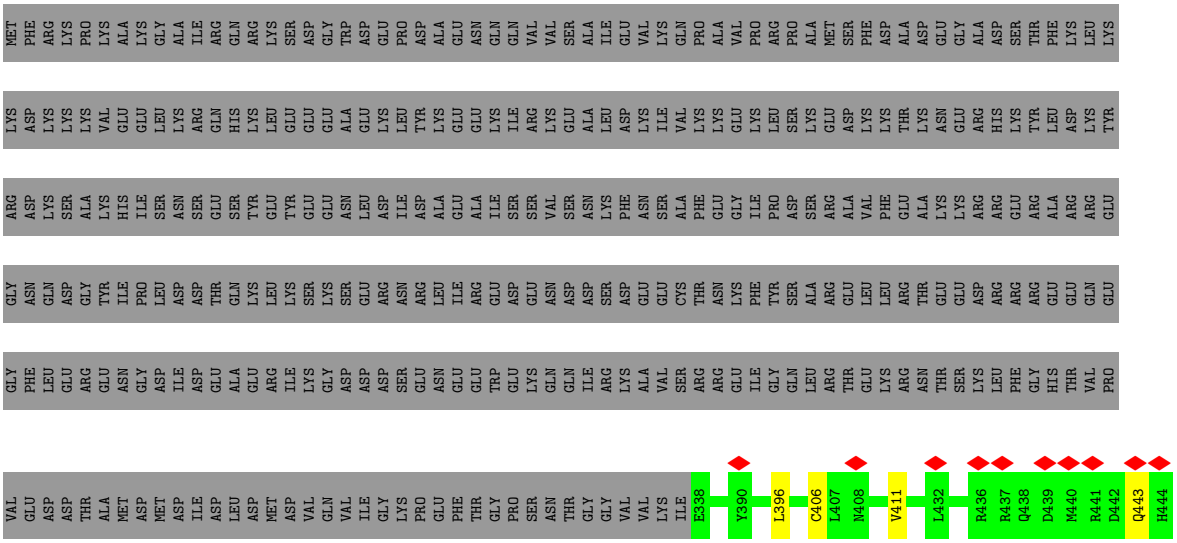
• Molecule 16: Spliceosome-associated protein CWC15 homolog

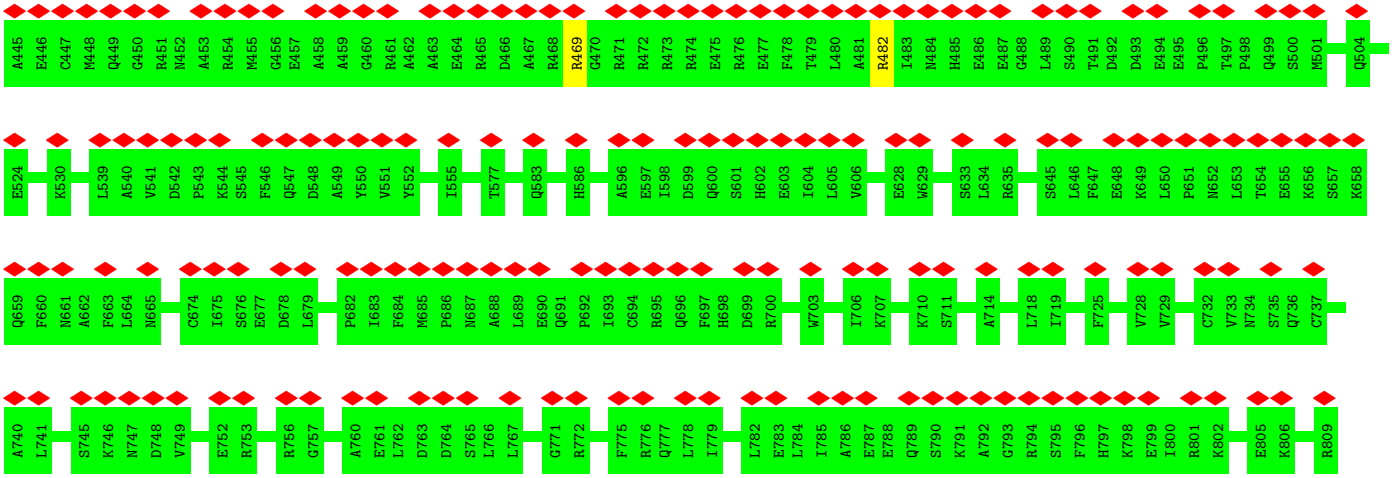
Chain P:



• Molecule 17: GCF C-terminal domain-containing protein

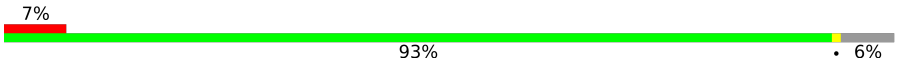
Chain PX:

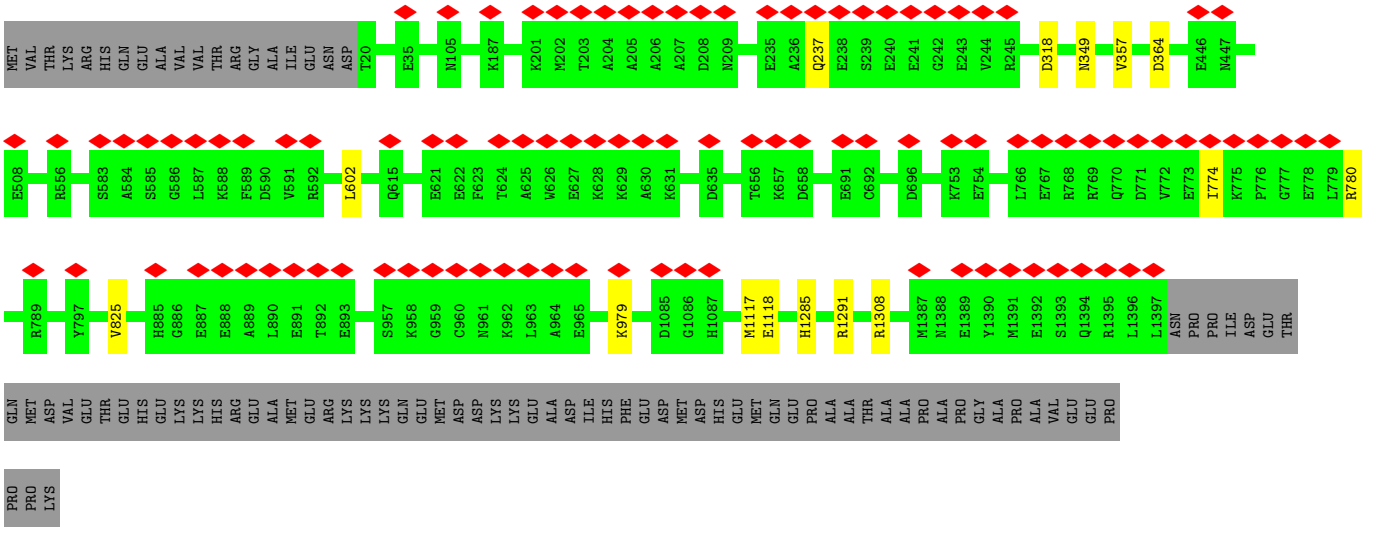




- Molecule 18: Intron-binding protein aquarius

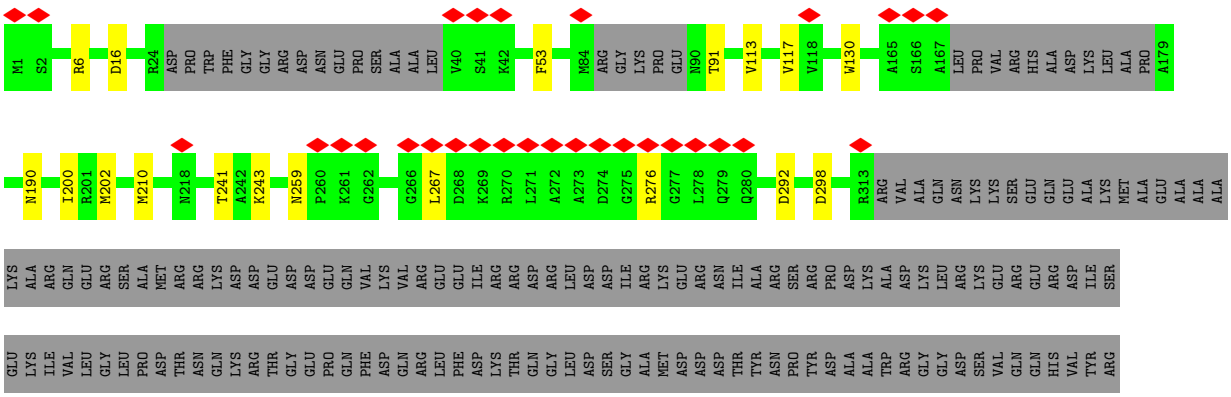
Chain Q:

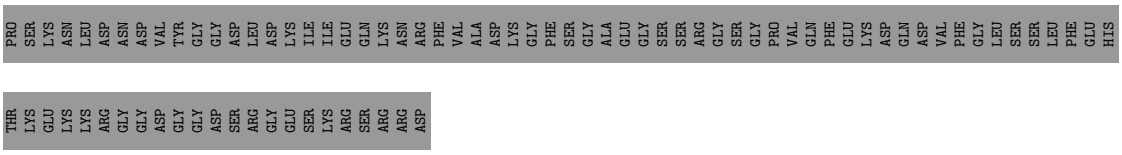




- Molecule 19: Uncharacterized protein T27F2.1

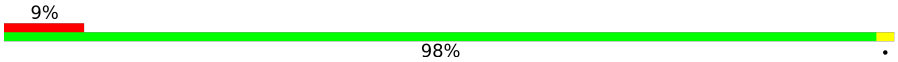
Chain R:

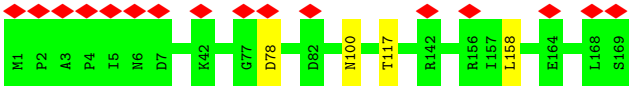




• Molecule 20: Peptidyl-prolyl cis-trans isomerase

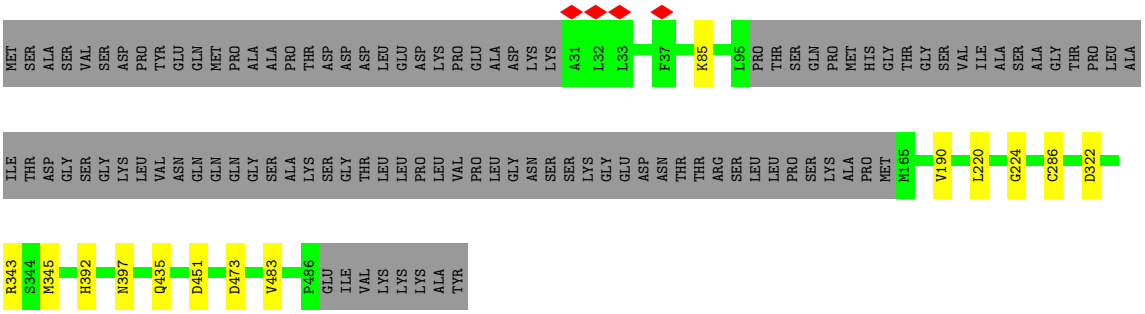
Chain S:





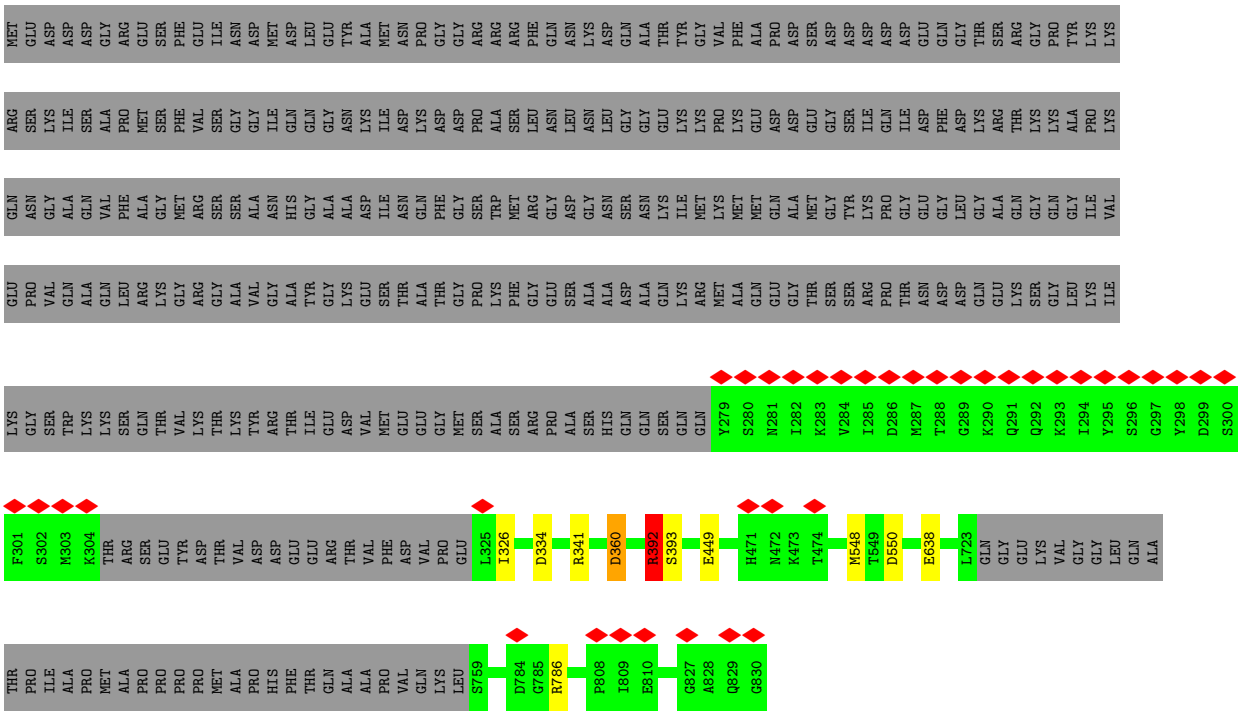
• Molecule 21: WD_REPEATS_REGION domain-containing protein

Chain T:



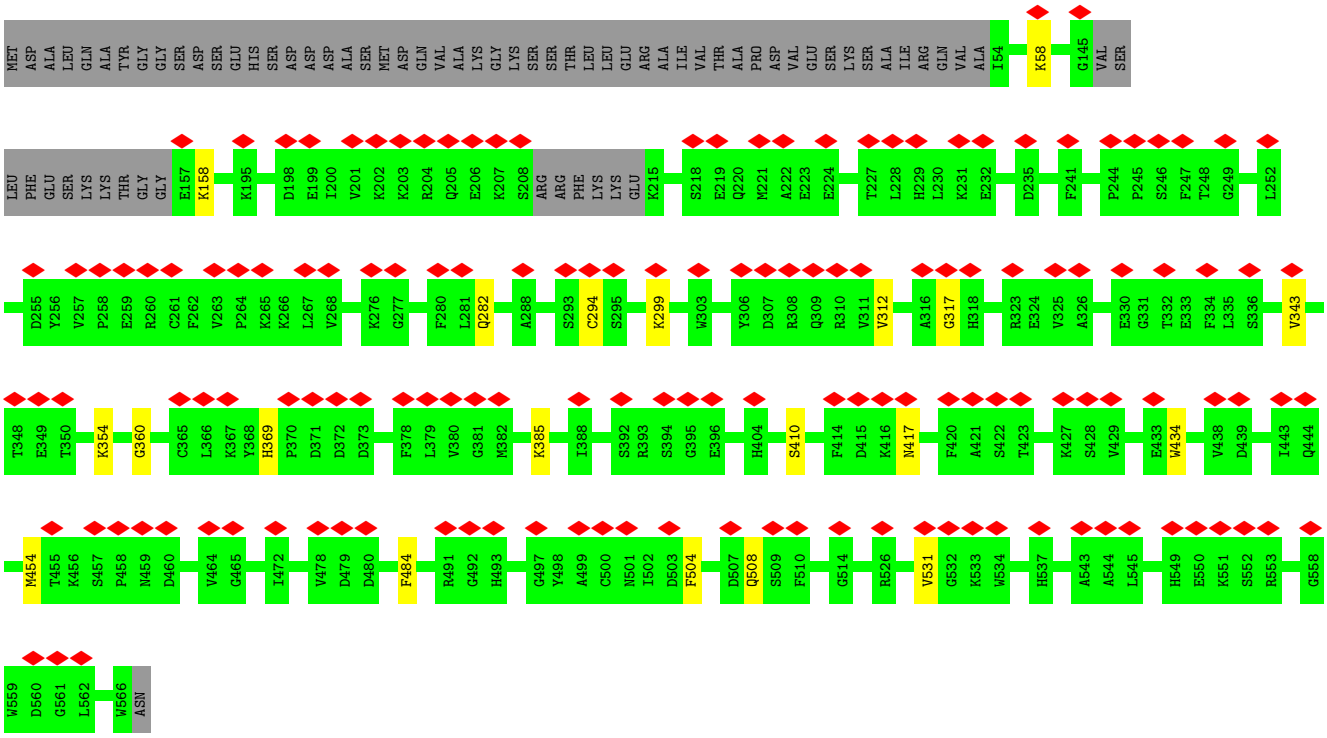
• Molecule 22: Septin and tuftelin-interacting protein 1 homolog

Chain TF:



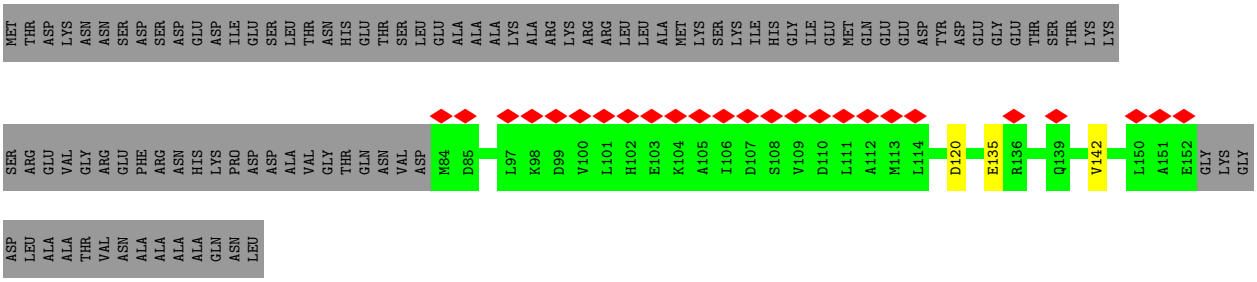
- Molecule 23: WD_REPEATS_REGION domain-containing protein

Chain W:



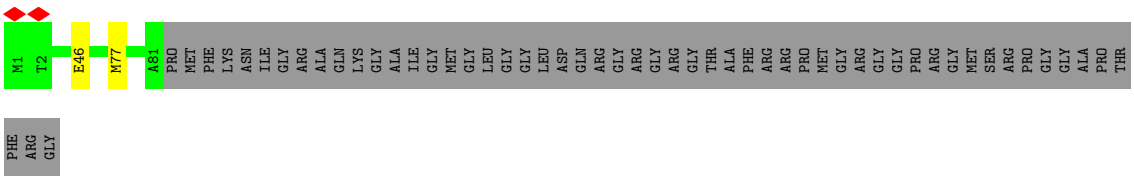
- Molecule 24: Coiled-coil domain-containing protein 12

Chain Z:



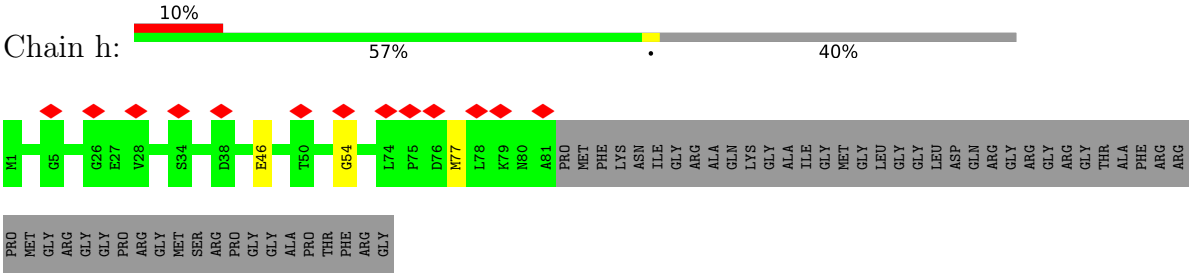
- Molecule 25: Small nuclear ribonucleoprotein Sm D3

Chain a:



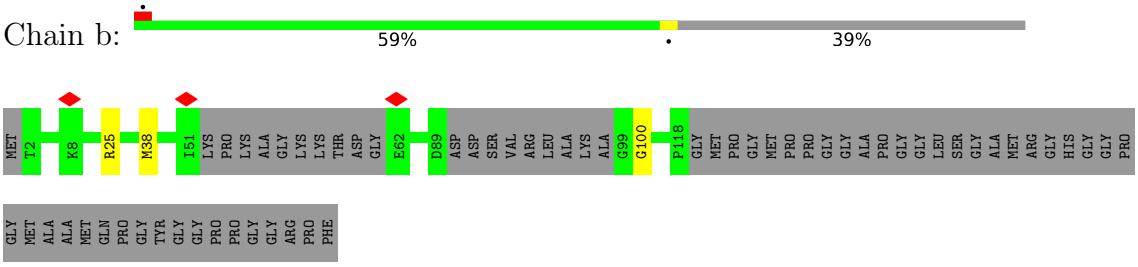
- Molecule 25: Small nuclear ribonucleoprotein Sm D3

Chain h:



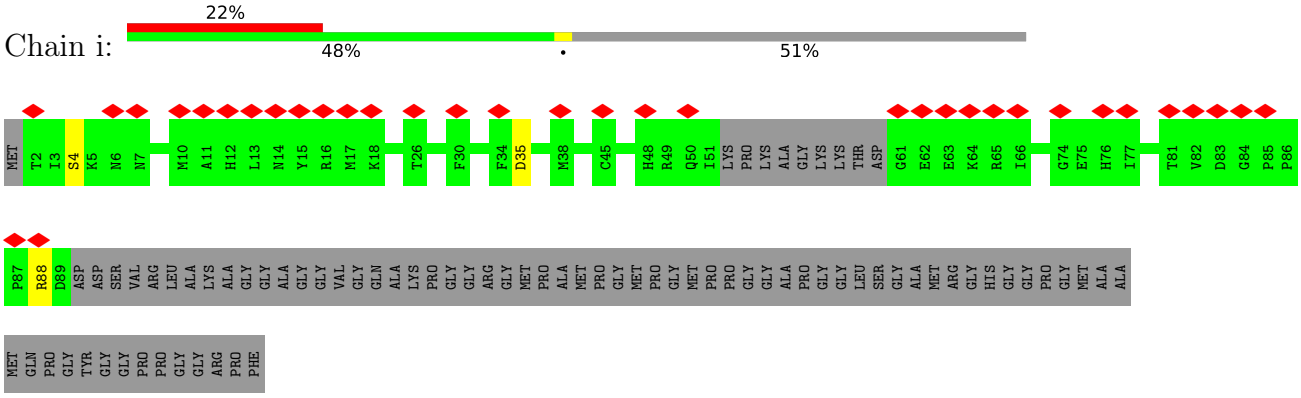
- Molecule 26: Probable small nuclear ribonucleoprotein-associated protein B

Chain b:



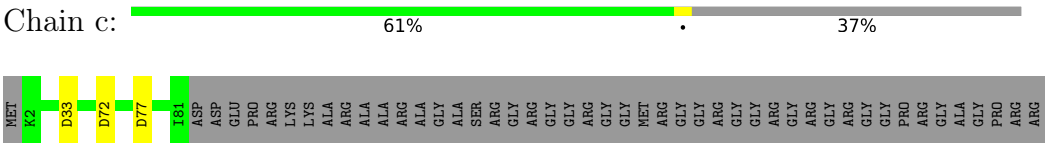
- Molecule 26: Probable small nuclear ribonucleoprotein-associated protein B

Chain i:



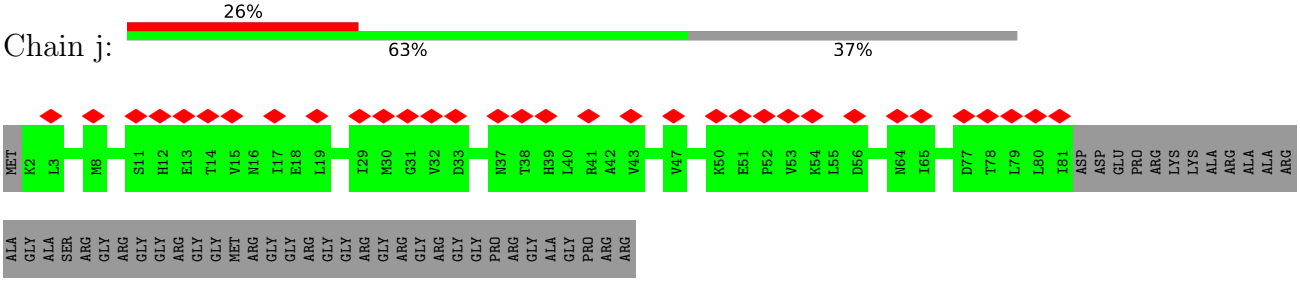
- Molecule 27: Small nuclear ribonucleoprotein Sm D1

Chain c:



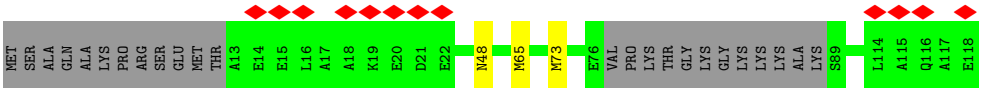
- Molecule 27: Small nuclear ribonucleoprotein Sm D1

Chain j:



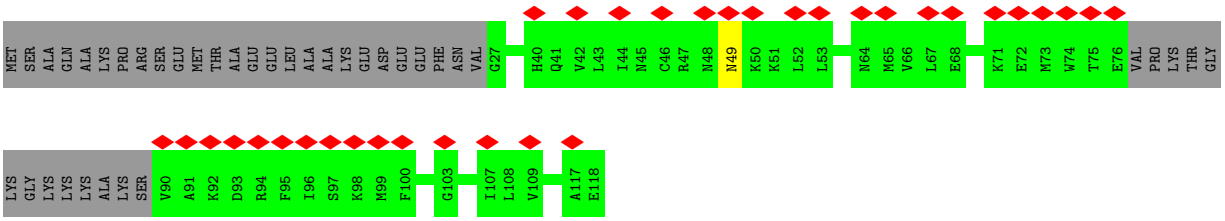
- Molecule 28: Probable small nuclear ribonucleoprotein Sm D2

Chain d:



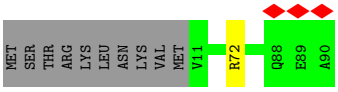
• Molecule 28: Probable small nuclear ribonucleoprotein Sm D2

Chain k:



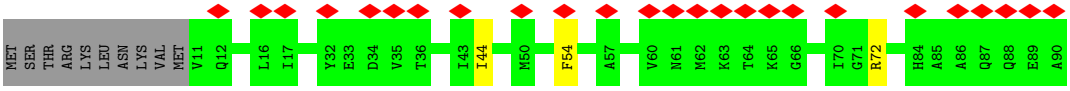
• Molecule 29: Probable small nuclear ribonucleoprotein E

Chain e:



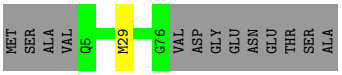
• Molecule 29: Probable small nuclear ribonucleoprotein E

Chain l:



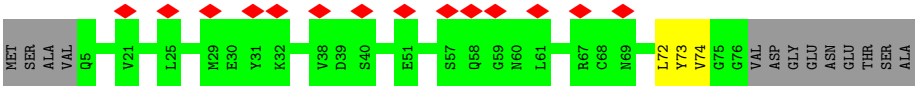
• Molecule 30: Probable small nuclear ribonucleoprotein F

Chain f:



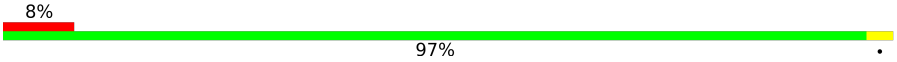
• Molecule 30: Probable small nuclear ribonucleoprotein F

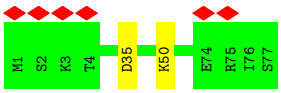
Chain m:



• Molecule 31: Probable small nuclear ribonucleoprotein G

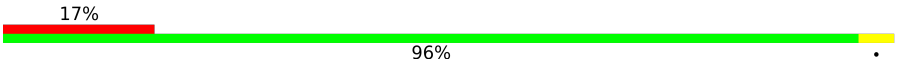
Chain g:

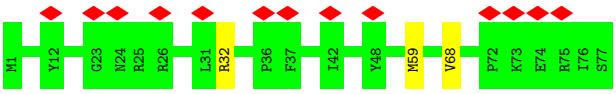




• Molecule 31: Probable small nuclear ribonucleoprotein G

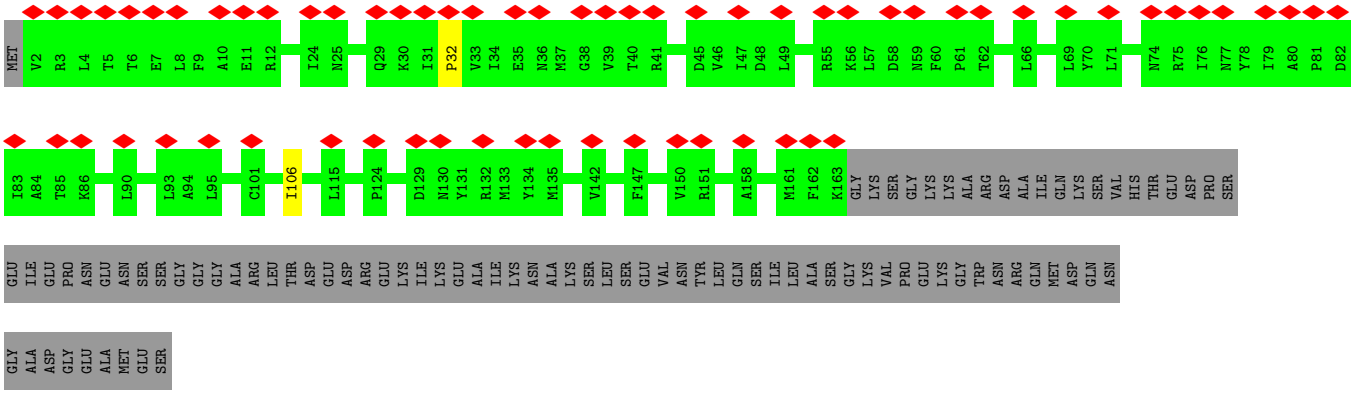
Chain n:





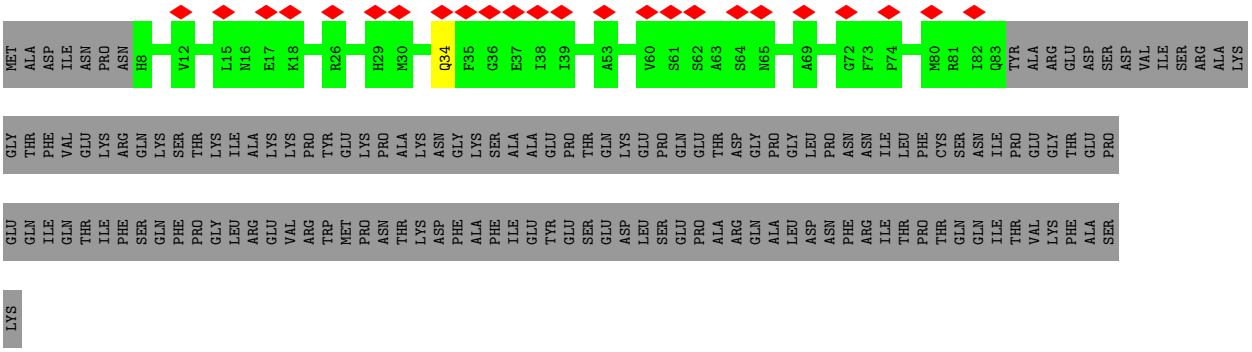
• Molecule 32: Probable U2 small nuclear ribonucleoprotein A'

Chain o:



• Molecule 33: RRM domain-containing protein

Chain p:



• Molecule 34: Pre-mRNA-processing factor 19

Chain q:

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

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

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

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

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

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

- Molecule 34: Pre-mRNA-processing factor 19

Chain r:

M1 S2 F3 V4 C5 G6 I7 S8 G9 E10 L11 T12 E13 D14 V20 S21 G22 F25 D26 R27 R28 L29 I30 V31 K32 F33 I34 A35 E36 N37 G38 T39 I42 S43 H44 G45 E46 L47 S48 E49 D50 Q51 L52 L55 K56 S57 G58 G59 T60 H111 C115 R120 L121

S122 K123 E124 L125 T126 A127 A128 R129 E130 A131 LEU SER THR LEU LYS PRO HIS THR SER ALA LYS VAL ASP ASP ASP VAL SER ILE ASP GLU SER GLU ASP GLN GLN GLY LEU SER GLU ALA ILE LEU ALA LYS LEU GLU GLU LYS SER LYS SER LEU THR ALA GLU ARG LYS GLN ARG GLY

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

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

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

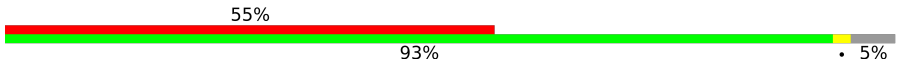
VAL LYS ILE TRP ASP LEU LYS ASN GLN THR VAL ALA ALA ALA PHE PRO GLY HIS THR ALA ALA VAL ARG SER ILE ALA PHE SER GLU GLU ASN GLY TYR TYR LEU ALA THR GLY SER GLU VAL LYS LEU TRP ASP LEU ARG LYS LEU LYS ASN LEU LYS THR PHE ALA ASN GLU

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

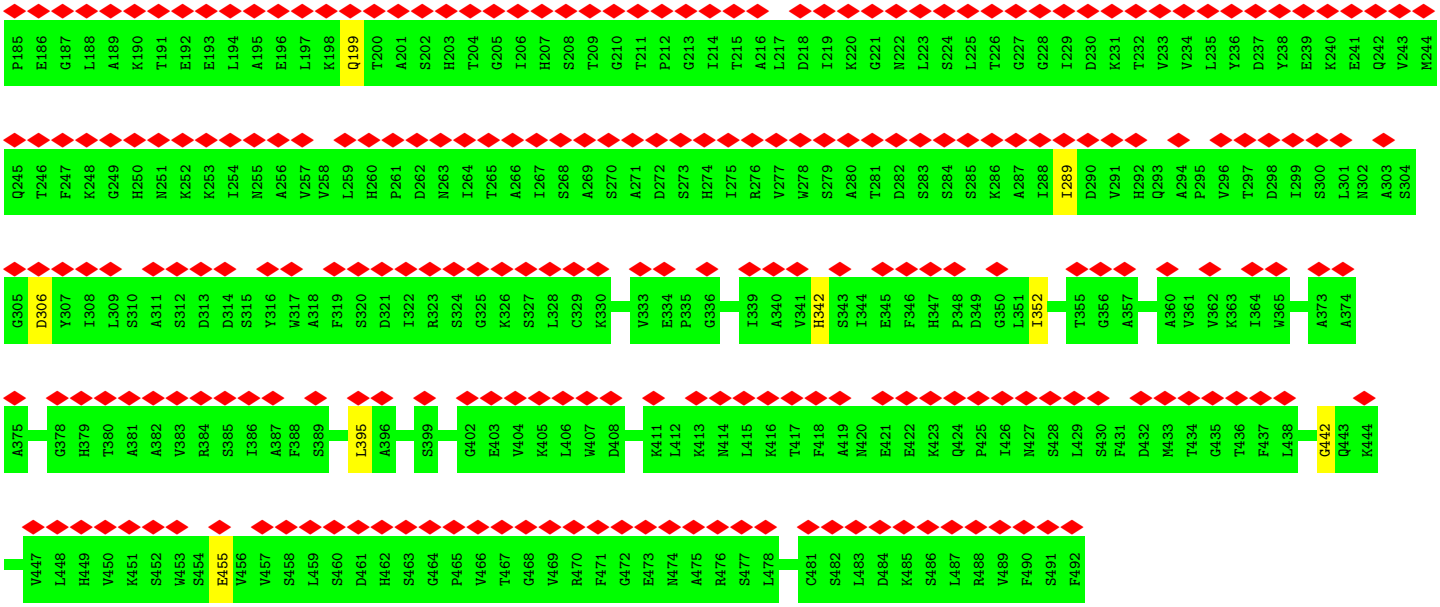
SER LEU ASP LYS SER LEU ARG VAL PHE SER PHE

- Molecule 34: Pre-mRNA-processing factor 19

Chain s:

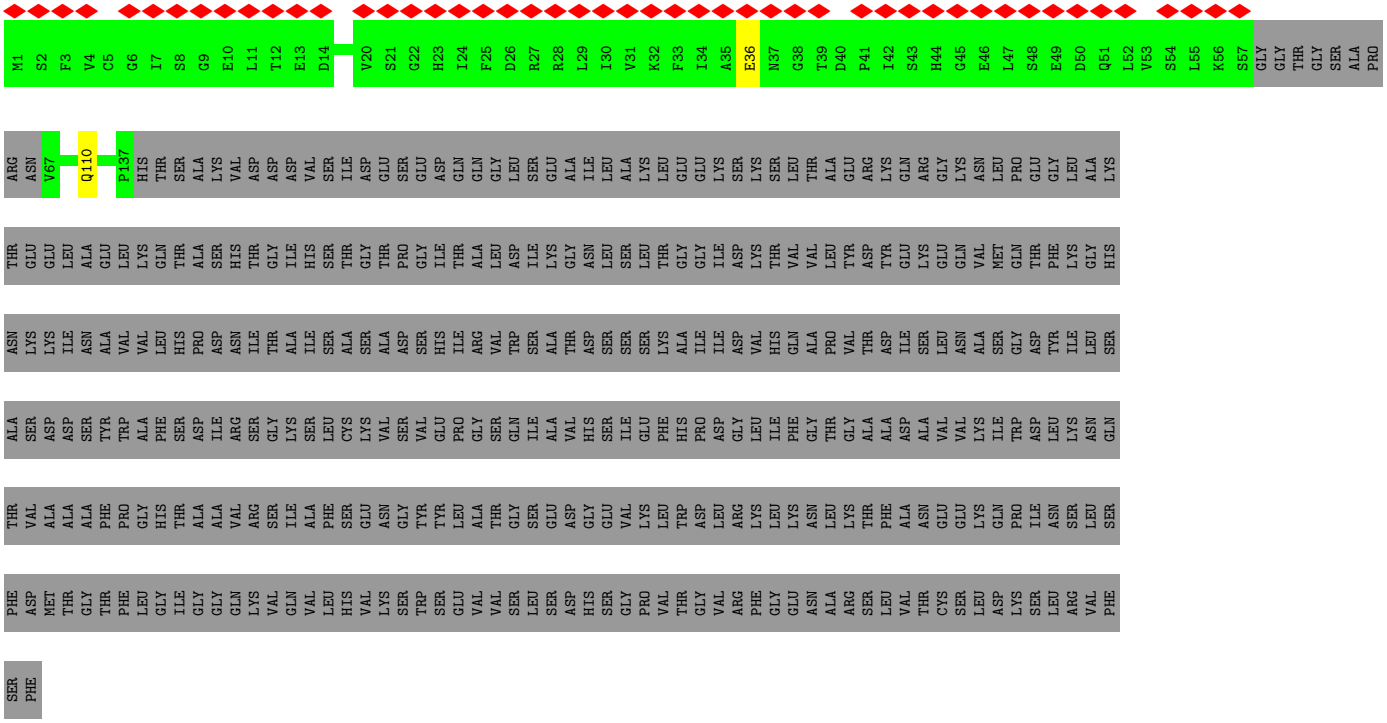


M1 S2 E13 Q19 E46 E49 K56 S57 G58 G59 T60 G61 S62 P137 HIS THR SER ALA LYS VAL ASP ASP ASP VAL SER ILE ASP GLU SER GLU ASP GLN GLN GLY LEU SER GLU A161 A164 S170 K171 S172 E176 R177 K178 Q179 R180 G181 K182 N183 L184



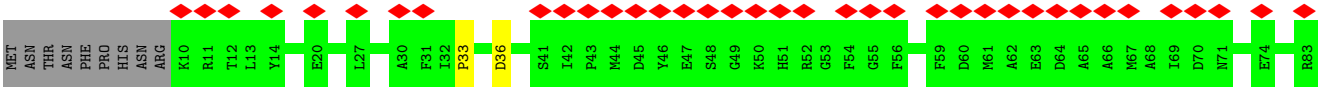
- Molecule 34: Pre-mRNA-processing factor 19

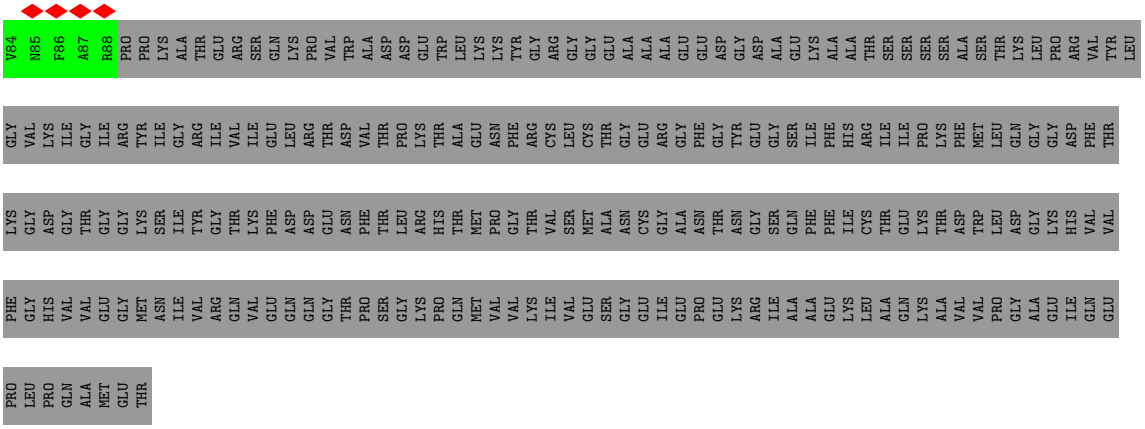
Chain t:



- Molecule 35: Peptidyl-prolyl cis-trans isomerase E

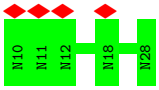
Chain y:





• Molecule 36: Intron lariat RNA

Chain In: 21% 100%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	879523	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.985	Depositor
Minimum map value	0.000	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	582.9824, 582.9824, 582.9824	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3013, 1.3013, 1.3013	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, IHP, ZN, 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	0.56	0/558	1.16	1/863 (0.1%)
2	5	1.19	5/2622 (0.2%)	1.47	28/4077 (0.7%)
3	6	0.54	0/2159	1.21	7/3363 (0.2%)
4	A	0.50	2/18943 (0.0%)	0.70	1/25695 (0.0%)
5	B	0.31	0/14697	0.61	1/19895 (0.0%)
6	C	0.60	1/7309 (0.0%)	0.72	1/9906 (0.0%)
7	D	0.37	0/734	0.70	0/984
8	E	0.44	0/2500	0.71	2/3384 (0.1%)
9	I	0.45	0/6133	0.68	0/8286
10	J	0.45	0/5006	0.68	0/6735
11	K	0.33	0/1688	0.62	0/2260
12	L	0.32	0/4970	0.68	1/6673 (0.0%)
13	M	0.35	0/1678	0.67	0/2238
14	N	0.57	1/1190 (0.1%)	0.70	0/1597
15	O	0.49	0/2779	0.71	0/3764
16	P	0.33	0/1220	0.74	0/1624
17	PX	0.34	0/3893	0.71	0/5223
18	Q	0.41	0/11554	0.65	1/15626 (0.0%)
19	R	0.40	0/2252	0.74	1/3040 (0.0%)
20	S	0.33	0/1330	0.70	0/1800
21	T	0.51	1/3144 (0.0%)	0.75	0/4259
22	TF	0.53	0/4202	0.72	4/5711 (0.1%)
23	W	0.41	0/4179	0.77	0/5638
24	Z	0.27	0/571	0.66	0/765
25	a	0.44	0/642	0.76	0/864
25	h	0.37	0/642	0.76	0/864
26	b	0.42	0/766	0.76	0/1021
26	i	0.34	0/648	0.75	0/865
27	c	0.36	0/627	0.77	1/848 (0.1%)
27	j	0.34	0/627	0.69	0/848
28	d	0.36	0/755	0.69	0/1013
28	k	0.37	0/637	0.79	0/854

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	e	0.39	0/674	0.70	0/909
29	l	0.36	0/674	0.77	0/909
30	f	0.41	0/568	0.67	0/769
30	m	0.42	0/568	0.79	0/769
31	g	0.39	0/614	0.76	1/820 (0.1%)
31	n	0.36	0/614	0.73	0/820
32	o	0.33	0/1358	0.70	0/1837
33	p	0.37	0/638	0.72	0/850
34	q	0.32	0/951	0.65	0/1282
34	r	0.30	0/1017	0.67	0/1373
34	s	0.32	0/3632	0.67	0/4913
34	t	0.30	0/1004	0.62	0/1355
35	y	0.42	0/630	0.76	0/846
All	All	0.46	10/123597 (0.0%)	0.73	50/168035 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	5	0	1
4	A	0	5
5	B	0	3
6	C	0	1
9	I	0	1
10	J	0	2
17	PX	0	1
19	R	0	1
22	TF	0	1
26	b	0	1
34	q	0	1
All	All	0	18

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	26	C	N1-C6	-7.06	1.32	1.37
21	T	286	CYS	CB-SG	-6.26	1.71	1.82
14	N	142	CYS	CB-SG	-5.94	1.72	1.81
6	C	552	CYS	CB-SG	-5.92	1.72	1.81
2	5	60	G	C6-N1	-5.78	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	15	C	N1-C6	-5.27	1.33	1.37
4	A	198	TYR	CD1-CE1	-5.15	1.31	1.39
2	5	26	C	C5-C6	-5.14	1.30	1.34
4	A	214	TYR	CE1-CZ	-5.09	1.31	1.38
2	5	13	C	C4-C5	-5.01	1.39	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	109	C	C6-N1-C2	-11.45	115.72	120.30
2	5	5	U	C5-C4-O4	-11.34	119.10	125.90
2	5	5	U	N3-C4-O4	11.19	127.23	119.40
2	5	27	G	O4'-C1'-N9	-10.79	99.57	108.20
2	5	25	C	C6-N1-C2	-10.04	116.28	120.30
3	6	89	C	C6-N1-C2	-7.98	117.11	120.30
2	5	115	A	O4'-C1'-N9	7.56	114.25	108.20
2	5	26	C	C4-C5-C6	7.44	121.12	117.40
2	5	13	C	C6-N1-C2	-7.37	117.35	120.30
19	R	292	ASP	CB-CG-OD1	7.21	124.79	118.30
22	TF	392	ARG	C-N-CA	6.92	139.00	121.70
2	5	5	U	C6-N1-C2	-6.81	116.91	121.00
2	5	41	C	C6-N1-C2	-6.80	117.58	120.30
3	6	37	C	C6-N1-C2	-6.70	117.62	120.30
3	6	89	C	C2-N1-C1'	6.70	126.16	118.80
2	5	109	C	O4'-C1'-N1	6.69	113.55	108.20
4	A	511	ASP	CB-CG-OD1	6.68	124.32	118.30
27	c	33	ASP	CB-CG-OD1	6.64	124.27	118.30
2	5	18	C	C6-N1-C2	-6.21	117.82	120.30
12	L	361	LEU	CA-CB-CG	6.18	129.51	115.30
22	TF	360	ASP	CB-CG-OD1	6.18	123.86	118.30
2	5	25	C	C2'-C3'-O3'	6.08	123.42	113.70
2	5	82	U	C6-N1-C2	-6.04	117.38	121.00
2	5	35	C	C6-N1-C2	-5.94	117.93	120.30
31	g	35	ASP	CB-CG-OD1	5.91	123.62	118.30
1	2	7	U	C5-C6-N1	5.89	125.64	122.70
2	5	114	G	O4'-C1'-N9	5.86	112.89	108.20
5	B	1150	ASP	CB-CG-OD1	5.85	123.57	118.30
22	TF	334	ASP	CB-CG-OD1	5.82	123.54	118.30
2	5	33	A	C8-N9-C4	-5.78	103.49	105.80
2	5	116	G	O4'-C1'-N9	5.69	112.75	108.20
3	6	8	C	C6-N1-C2	-5.69	118.03	120.30
18	Q	364	ASP	CB-CG-OD1	5.67	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	109	C	C5-C6-N1	5.57	123.78	121.00
2	5	80	A	O4'-C1'-N9	5.56	112.65	108.20
3	6	81	U	P-O3'-C3'	5.53	126.33	119.70
2	5	100	G	C1'-O4'-C4'	-5.50	105.50	109.90
2	5	5	U	O4'-C1'-N1	5.47	112.57	108.20
2	5	13	C	C5-C6-N1	5.41	123.70	121.00
8	E	87	LEU	CA-CB-CG	5.41	127.73	115.30
3	6	74	C	C6-N1-C2	-5.24	118.20	120.30
2	5	15	C	C5-C6-N1	5.24	123.62	121.00
2	5	25	C	C5-C6-N1	5.24	123.62	121.00
8	E	228	ASP	CB-CG-OD1	5.22	123.00	118.30
3	6	28	G	P-O3'-C3'	5.16	125.89	119.70
2	5	33	A	N7-C8-N9	5.15	116.38	113.80
2	5	94	U	O4'-C1'-N1	5.14	112.31	108.20
6	C	233	ASP	CB-CG-OD1	5.05	122.84	118.30
2	5	9	G	C8-N9-C1'	-5.03	120.46	127.00
22	TF	786	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	5	109	C	Sidechain
4	A	1409	ILE	Peptide
4	A	1432	ARG	Sidechain
4	A	229	ARG	Sidechain
4	A	655	ARG	Sidechain
4	A	933	LYS	Peptide
5	B	1513	ARG	Sidechain
5	B	1692	ARG	Sidechain
5	B	857	ARG	Sidechain
6	C	162	ARG	Sidechain
9	I	689	ARG	Sidechain
10	J	152	ARG	Sidechain
10	J	174	ARG	Sidechain
17	PX	469	ARG	Sidechain
19	R	190	ASN	Peptide
22	TF	392	ARG	Peptide
26	b	25	ARG	Sidechain
34	q	28	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	2223/2329 (95%)	2118 (95%)	91 (4%)	14 (1%)	22	52
5	B	1802/2145 (84%)	1780 (99%)	20 (1%)	2 (0%)	48	77
6	C	896/974 (92%)	857 (96%)	36 (4%)	3 (0%)	37	66
7	D	84/267 (32%)	82 (98%)	2 (2%)	0	100	100
8	E	310/331 (94%)	294 (95%)	15 (5%)	1 (0%)	37	66
9	I	722/855 (84%)	702 (97%)	19 (3%)	1 (0%)	48	77
10	J	570/744 (77%)	547 (96%)	23 (4%)	0	100	100
11	K	201/238 (84%)	195 (97%)	5 (2%)	1 (0%)	25	56
12	L	599/755 (79%)	562 (94%)	33 (6%)	4 (1%)	19	49
13	M	190/234 (81%)	185 (97%)	5 (3%)	0	100	100
14	N	140/147 (95%)	130 (93%)	10 (7%)	0	100	100
15	O	334/408 (82%)	317 (95%)	15 (4%)	2 (1%)	22	52
16	P	146/230 (64%)	137 (94%)	5 (3%)	4 (3%)	4	17
17	PX	470/809 (58%)	464 (99%)	4 (1%)	2 (0%)	30	60
18	Q	1376/1467 (94%)	1330 (97%)	44 (3%)	2 (0%)	48	77
19	R	274/535 (51%)	249 (91%)	23 (8%)	2 (1%)	19	49
20	S	167/169 (99%)	156 (93%)	10 (6%)	1 (1%)	22	52
21	T	383/494 (78%)	361 (94%)	20 (5%)	2 (0%)	25	56
22	TF	491/830 (59%)	473 (96%)	16 (3%)	2 (0%)	30	60
23	W	490/567 (86%)	445 (91%)	40 (8%)	5 (1%)	13	40
24	Z	67/169 (40%)	62 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	a	79/136 (58%)	78 (99%)	1 (1%)	0	100	100
25	h	79/136 (58%)	68 (86%)	9 (11%)	2 (2%)	4	18
26	b	92/160 (58%)	83 (90%)	8 (9%)	1 (1%)	12	37
26	i	75/160 (47%)	69 (92%)	5 (7%)	1 (1%)	10	33
27	c	78/127 (61%)	76 (97%)	2 (3%)	0	100	100
27	j	78/127 (61%)	72 (92%)	6 (8%)	0	100	100
28	d	90/118 (76%)	84 (93%)	6 (7%)	0	100	100
28	k	75/118 (64%)	72 (96%)	3 (4%)	0	100	100
29	e	78/90 (87%)	75 (96%)	2 (3%)	1 (1%)	10	33
29	l	78/90 (87%)	73 (94%)	3 (4%)	2 (3%)	4	17
30	f	70/85 (82%)	68 (97%)	2 (3%)	0	100	100
30	m	70/85 (82%)	66 (94%)	3 (4%)	1 (1%)	9	31
31	g	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
31	n	75/77 (97%)	68 (91%)	5 (7%)	2 (3%)	4	17
32	o	160/253 (63%)	154 (96%)	5 (3%)	1 (1%)	22	52
33	p	74/217 (34%)	70 (95%)	4 (5%)	0	100	100
34	q	117/492 (24%)	112 (96%)	5 (4%)	0	100	100
34	r	129/492 (26%)	125 (97%)	4 (3%)	0	100	100
34	s	465/492 (94%)	443 (95%)	20 (4%)	2 (0%)	30	60
34	t	124/492 (25%)	119 (96%)	5 (4%)	0	100	100
35	y	77/331 (23%)	73 (95%)	4 (5%)	0	100	100
All	All	14173/19052 (74%)	13565 (96%)	547 (4%)	61 (0%)	32	60

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	934	PRO
6	C	97	VAL
12	L	350	LEU
12	L	507	ALA
16	P	57	LYS
16	P	58	ASP
18	Q	349	ASN
22	TF	392	ARG
22	TF	393	SER

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Mol	Chain	Res	Type
23	W	508	GLN
4	A	1084	ILE
4	A	1542	VAL
4	A	2095	TYR
4	A	2275	ASN
17	PX	411	VAL
29	l	72	ARG
4	A	1243	SER
4	A	2200	ASP
4	A	2285	MET
12	L	353	THR
15	O	295	PHE
16	P	59	LEU
19	R	113	VAL
25	h	46	GLU
31	n	59	MET
4	A	1881	GLU
6	C	95	PRO
6	C	523	GLU
8	E	120	ARG
9	I	242	ILE
11	K	71	PHE
15	O	303	LYS
21	T	483	VAL
23	W	317	GLY
29	e	72	ARG
25	h	54	GLY
26	i	4	SER
4	A	454	ARG
5	B	2045	ILE
12	L	352	ASP
17	PX	482	ARG
18	Q	774	ILE
20	S	78	ASP
23	W	360	GLY
23	W	484	PHE
31	n	68	VAL
34	s	171	LYS
5	B	1664	ASP
16	P	48	GLN
34	s	442	GLY
4	A	2303	ARG

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Mol	Chain	Res	Type
23	W	531	VAL
4	A	2167	PRO
30	m	74	VAL
4	A	620	GLY
19	R	117	VAL
21	T	224	GLY
29	l	44	ILE
32	o	32	PRO
4	A	417	PRO
26	b	100	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	2018/2100 (96%)	1972 (98%)	46 (2%)	45	77
5	B	1593/1886 (84%)	1583 (99%)	10 (1%)	84	95
6	C	793/861 (92%)	780 (98%)	13 (2%)	58	84
7	D	80/230 (35%)	77 (96%)	3 (4%)	28	63
8	E	275/291 (94%)	273 (99%)	2 (1%)	81	94
9	I	641/754 (85%)	624 (97%)	17 (3%)	40	73
10	J	508/650 (78%)	494 (97%)	14 (3%)	38	73
11	K	183/214 (86%)	183 (100%)	0	100	100
12	L	529/645 (82%)	517 (98%)	12 (2%)	45	77
13	M	178/212 (84%)	175 (98%)	3 (2%)	56	83
14	N	125/129 (97%)	122 (98%)	3 (2%)	44	76
15	O	295/351 (84%)	291 (99%)	4 (1%)	62	86
16	P	129/197 (66%)	125 (97%)	4 (3%)	35	70
17	PX	423/724 (58%)	420 (99%)	3 (1%)	81	94
18	Q	1235/1311 (94%)	1223 (99%)	12 (1%)	73	91
19	R	235/447 (53%)	221 (94%)	14 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	S	137/137 (100%)	134 (98%)	3 (2%)	47	78
21	T	333/421 (79%)	322 (97%)	11 (3%)	33	68
22	TF	451/718 (63%)	444 (98%)	7 (2%)	58	84
23	W	444/502 (88%)	429 (97%)	15 (3%)	32	67
24	Z	63/145 (43%)	60 (95%)	3 (5%)	21	54
25	a	71/106 (67%)	69 (97%)	2 (3%)	38	73
25	h	71/106 (67%)	70 (99%)	1 (1%)	62	86
26	b	79/116 (68%)	78 (99%)	1 (1%)	65	88
26	i	70/116 (60%)	68 (97%)	2 (3%)	37	72
27	c	73/98 (74%)	71 (97%)	2 (3%)	40	73
27	j	73/98 (74%)	73 (100%)	0	100	100
28	d	84/103 (82%)	81 (96%)	3 (4%)	30	65
28	k	72/103 (70%)	71 (99%)	1 (1%)	62	86
29	e	71/81 (88%)	71 (100%)	0	100	100
29	l	71/81 (88%)	70 (99%)	1 (1%)	62	86
30	f	61/71 (86%)	60 (98%)	1 (2%)	58	84
30	m	61/71 (86%)	59 (97%)	2 (3%)	33	68
31	g	69/69 (100%)	68 (99%)	1 (1%)	62	86
31	n	69/69 (100%)	68 (99%)	1 (1%)	62	86
32	o	151/225 (67%)	150 (99%)	1 (1%)	81	94
33	p	68/192 (35%)	67 (98%)	1 (2%)	60	85
34	q	108/417 (26%)	107 (99%)	1 (1%)	75	92
34	r	114/417 (27%)	109 (96%)	5 (4%)	24	57
34	s	396/417 (95%)	389 (98%)	7 (2%)	54	82
34	t	115/417 (28%)	113 (98%)	2 (2%)	56	83
35	y	64/270 (24%)	62 (97%)	2 (3%)	35	70
All	All	12679/16568 (76%)	12443 (98%)	236 (2%)	52	81

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	87	HIS
4	A	103	ILE

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Mol	Chain	Res	Type
4	A	105	ASP
4	A	178	LEU
4	A	311	LEU
4	A	443	LEU
4	A	519	VAL
4	A	560	ASN
4	A	743	THR
4	A	781	GLU
4	A	934	PRO
4	A	961	SER
4	A	969	MET
4	A	987	ARG
4	A	1012	LYS
4	A	1138	ASP
4	A	1174	ASN
4	A	1177	MET
4	A	1203	ASP
4	A	1274	GLN
4	A	1347	ARG
4	A	1361	LEU
4	A	1369	GLU
4	A	1377	ARG
4	A	1397	THR
4	A	1542	VAL
4	A	1564	ILE
4	A	1627	GLN
4	A	1671	ARG
4	A	1715	MET
4	A	1997	GLN
4	A	2106	LYS
4	A	2131	GLN
4	A	2133	LYS
4	A	2149	GLN
4	A	2168	LEU
4	A	2170	TRP
4	A	2171	MET
4	A	2177	GLU
4	A	2178	LEU
4	A	2182	SER
4	A	2185	ASP
4	A	2189	HIS
4	A	2245	MET

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Mol	Chain	Res	Type
4	A	2258	ASP
4	A	2276	PHE
5	B	162	ASP
5	B	513	GLN
5	B	534	TYR
5	B	720	SER
5	B	878	GLN
5	B	1070	LEU
5	B	1461	PHE
5	B	1609	ARG
5	B	2012	HIS
5	B	2084	LEU
6	C	76	TYR
6	C	94	GLU
6	C	206	ILE
6	C	243	GLU
6	C	290	ASN
6	C	326	PHE
6	C	381	MET
6	C	392	VAL
6	C	417	ARG
6	C	667	ASN
6	C	760	LYS
6	C	802	THR
6	C	870	SER
7	D	155	ARG
7	D	243	LEU
7	D	247	GLN
8	E	121	THR
8	E	314	MET
9	I	49	HIS
9	I	54	LYS
9	I	135	GLU
9	I	176	TYR
9	I	320	GLU
9	I	323	GLN
9	I	336	MET
9	I	351	MET
9	I	372	ILE
9	I	388	VAL
9	I	395	ILE
9	I	399	LYS

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Mol	Chain	Res	Type
9	I	414	ASN
9	I	467	VAL
9	I	663	LEU
9	I	681	THR
9	I	735	GLU
10	J	34	THR
10	J	36	GLU
10	J	37	GLN
10	J	83	ARG
10	J	89	TRP
10	J	224	TRP
10	J	254	GLU
10	J	297	PHE
10	J	302	GLN
10	J	458	TYR
10	J	545	TYR
10	J	583	GLN
10	J	615	ARG
10	J	617	GLU
12	L	13	ASN
12	L	52	GLU
12	L	234	TYR
12	L	316	ARG
12	L	351	LYS
12	L	355	GLN
12	L	361	LEU
12	L	436	ARG
12	L	452	GLN
12	L	504	GLU
12	L	508	LYS
12	L	585	LYS
13	M	55	LYS
13	M	63	ARG
13	M	206	ASN
14	N	19	ASP
14	N	48	ILE
14	N	142	CYS
15	O	27	THR
15	O	78	VAL
15	O	115	ARG
15	O	181	GLU
16	P	31	SER

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Mol	Chain	Res	Type
16	P	33	LYS
16	P	59	LEU
16	P	89	ARG
17	PX	396	LEU
17	PX	406	CYS
17	PX	443	GLN
18	Q	237	GLN
18	Q	318	ASP
18	Q	357	VAL
18	Q	602	LEU
18	Q	780	ARG
18	Q	825	VAL
18	Q	979	LYS
18	Q	1117	MET
18	Q	1118	GLU
18	Q	1285	HIS
18	Q	1291	ARG
18	Q	1308	ARG
19	R	6	ARG
19	R	16	ASP
19	R	53	PHE
19	R	91	THR
19	R	130	TRP
19	R	200	ILE
19	R	202	MET
19	R	210	MET
19	R	241	THR
19	R	243	LYS
19	R	259	ASN
19	R	267	LEU
19	R	276	ARG
19	R	298	ASP
20	S	100	ASN
20	S	117	THR
20	S	158	LEU
21	T	85	LYS
21	T	190	VAL
21	T	220	LEU
21	T	322	ASP
21	T	343	ARG
21	T	345	MET
21	T	392	HIS

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Mol	Chain	Res	Type
21	T	397	ASN
21	T	435	GLN
21	T	451	ASP
21	T	473	ASP
22	TF	326	ILE
22	TF	341	ARG
22	TF	360	ASP
22	TF	449	GLU
22	TF	548	MET
22	TF	550	ASP
22	TF	638	GLU
23	W	58	LYS
23	W	158	LYS
23	W	282	GLN
23	W	294	CYS
23	W	299	LYS
23	W	312	VAL
23	W	343	VAL
23	W	354	LYS
23	W	369	HIS
23	W	385	LYS
23	W	410	SER
23	W	417	ASN
23	W	434	TRP
23	W	454	MET
23	W	504	PHE
24	Z	120	ASP
24	Z	135	GLU
24	Z	142	VAL
25	a	46	GLU
25	a	77	MET
26	b	38	MET
27	c	72	ASP
27	c	77	ASP
28	d	48	ASN
28	d	65	MET
28	d	73	MET
30	f	29	MET
31	g	50	LYS
25	h	77	MET
26	i	35	ASP
26	i	88	ARG

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Mol	Chain	Res	Type
28	k	49	ASN
29	l	54	PHE
30	m	72	LEU
30	m	73	TYR
31	n	32	ARG
32	o	106	ILE
33	p	34	GLN
34	q	129	ARG
34	r	28	ARG
34	r	32	LYS
34	r	46	GLU
34	r	115	CYS
34	r	121	LEU
34	s	199	GLN
34	s	289	ILE
34	s	306	ASP
34	s	342	HIS
34	s	352	ILE
34	s	395	LEU
34	s	455	GLU
34	t	36	GLU
34	t	110	GLN
35	y	33	PRO
35	y	36	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	1997	GLN
5	B	681	GLN
17	PX	394	GLN
22	TF	346	GLN
22	TF	532	GLN
22	TF	819	ASN
30	f	70	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	22/191 (11%)	6 (27%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	5	110/121 (90%)	28 (25%)	13 (11%)
3	6	89/101 (88%)	39 (43%)	10 (11%)
All	All	221/413 (53%)	73 (33%)	23 (10%)

All (73) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	10	U
1	2	19	U
1	2	20	A
1	2	21	G
1	2	25	A
1	2	26	G
2	5	4	C
2	5	6	C
2	5	8	G
2	5	10	U
2	5	20	U
2	5	23	A
2	5	24	A
2	5	26	C
2	5	27	G
2	5	28	U
2	5	43	U
2	5	72	A
2	5	74	A
2	5	76	A
2	5	77	U
2	5	79	G
2	5	80	A
2	5	81	G
2	5	82	U
2	5	96	U
2	5	99	G
2	5	100	G
2	5	101	A
2	5	110	G
2	5	112	A
2	5	113	A
2	5	114	G
2	5	117	C
3	6	4	C

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Mol	Chain	Res	Type
3	6	5	U
3	6	6	U
3	6	7	C
3	6	8	C
3	6	9	G
3	6	10	A
3	6	20	C
3	6	21	U
3	6	22	A
3	6	23	A
3	6	24	A
3	6	29	G
3	6	32	C
3	6	34	A
3	6	37	C
3	6	39	G
3	6	41	G
3	6	43	A
3	6	44	G
3	6	46	U
3	6	48	A
3	6	49	G
3	6	54	G
3	6	55	C
3	6	56	C
3	6	62	G
3	6	64	A
3	6	69	U
3	6	74	C
3	6	75	G
3	6	79	A
3	6	80	U
3	6	81	U
3	6	82	C
3	6	84	U
3	6	85	G
3	6	86	A
3	6	89	C

All (23) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type

Mol	Chain	Res	Type
2	5	3	A
2	5	5	U
2	5	19	A
2	5	23	A
2	5	25	C
2	5	75	C
2	5	79	G
2	5	81	G
2	5	100	G
2	5	109	C
2	5	111	A
2	5	112	A
2	5	113	A
3	6	23	A
3	6	28	G
3	6	37	C
3	6	41	G
3	6	45	A
3	6	48	A
3	6	53	G
3	6	79	A
3	6	81	U
3	6	85	G

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 16 ligands modelled in this entry, 13 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	IHP	J	3000	-	36,36,36	2.23	10 (27%)	54,60,60	0.89	1 (1%)
39	GTP	C	1101	37	26,34,34	1.89	5 (19%)	32,54,54	1.82	6 (18%)
38	IHP	A	3000	-	36,36,36	2.22	10 (27%)	54,60,60	1.44	7 (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
38	IHP	J	3000	-	-	0/30/54/54	0/1/1/1
39	GTP	C	1101	37	-	0/18/38/38	0/3/3/3
38	IHP	A	3000	-	-	4/30/54/54	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	1101	GTP	C5-C6	-6.23	1.34	1.47
38	J	3000	IHP	C3-C2	-5.31	1.41	1.52
38	J	3000	IHP	P3-O13	4.91	1.68	1.59
38	A	3000	IHP	P5-O15	4.83	1.68	1.59
38	A	3000	IHP	P2-O12	4.64	1.68	1.59
38	A	3000	IHP	P6-O16	4.48	1.67	1.59
38	J	3000	IHP	P6-O16	4.37	1.67	1.59
38	A	3000	IHP	P3-O13	4.31	1.67	1.59
38	J	3000	IHP	P2-O12	4.30	1.67	1.59
38	A	3000	IHP	C3-C2	-4.24	1.43	1.52
38	J	3000	IHP	P5-O15	4.14	1.67	1.59
38	A	3000	IHP	P4-O14	4.13	1.67	1.59
38	A	3000	IHP	P1-O11	4.06	1.67	1.59
38	J	3000	IHP	P1-O11	4.01	1.66	1.59
38	J	3000	IHP	P4-O14	3.98	1.66	1.59
38	A	3000	IHP	C5-C4	3.25	1.59	1.52
39	C	1101	GTP	C5-C4	-3.04	1.35	1.43
38	J	3000	IHP	O12-C2	-2.85	1.33	1.44
38	J	3000	IHP	O13-C3	-2.82	1.33	1.44
38	A	3000	IHP	O12-C2	-2.71	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A	3000	IHP	O13-C3	-2.58	1.34	1.44
38	J	3000	IHP	C2-C1	-2.53	1.47	1.52
39	C	1101	GTP	C6-N1	-2.34	1.34	1.37
39	C	1101	GTP	PG-O3G	-2.08	1.46	1.54
39	C	1101	GTP	O4'-C4'	-2.01	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	C	1101	GTP	PB-O3B-PG	-5.24	114.86	132.83
38	A	3000	IHP	O15-C5-C4	5.13	120.78	108.69
39	C	1101	GTP	C5-C6-N1	4.51	121.91	113.95
38	A	3000	IHP	O15-C5-C6	4.13	118.42	108.69
39	C	1101	GTP	C2-N1-C6	-3.55	118.56	125.10
39	C	1101	GTP	O6-C6-C5	-3.19	118.15	124.37
39	C	1101	GTP	PA-O3A-PB	-2.86	123.00	132.83
38	A	3000	IHP	C6-C5-C4	-2.76	104.37	110.41
39	C	1101	GTP	C8-N7-C5	2.35	107.48	102.99
38	A	3000	IHP	O11-C1-C2	2.34	114.21	108.69
38	J	3000	IHP	C5-C4-C3	2.32	115.48	110.41
38	A	3000	IHP	O13-C3-C2	2.25	114.00	108.69
38	A	3000	IHP	C5-C6-C1	-2.13	105.74	110.41
38	A	3000	IHP	C3-C2-C1	2.11	115.04	110.41

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	A	3000	IHP	C4-C3-O13-P3
38	A	3000	IHP	C2-C3-O13-P3
38	A	3000	IHP	C3-O13-P3-O23
38	A	3000	IHP	C2-O12-P2-O32

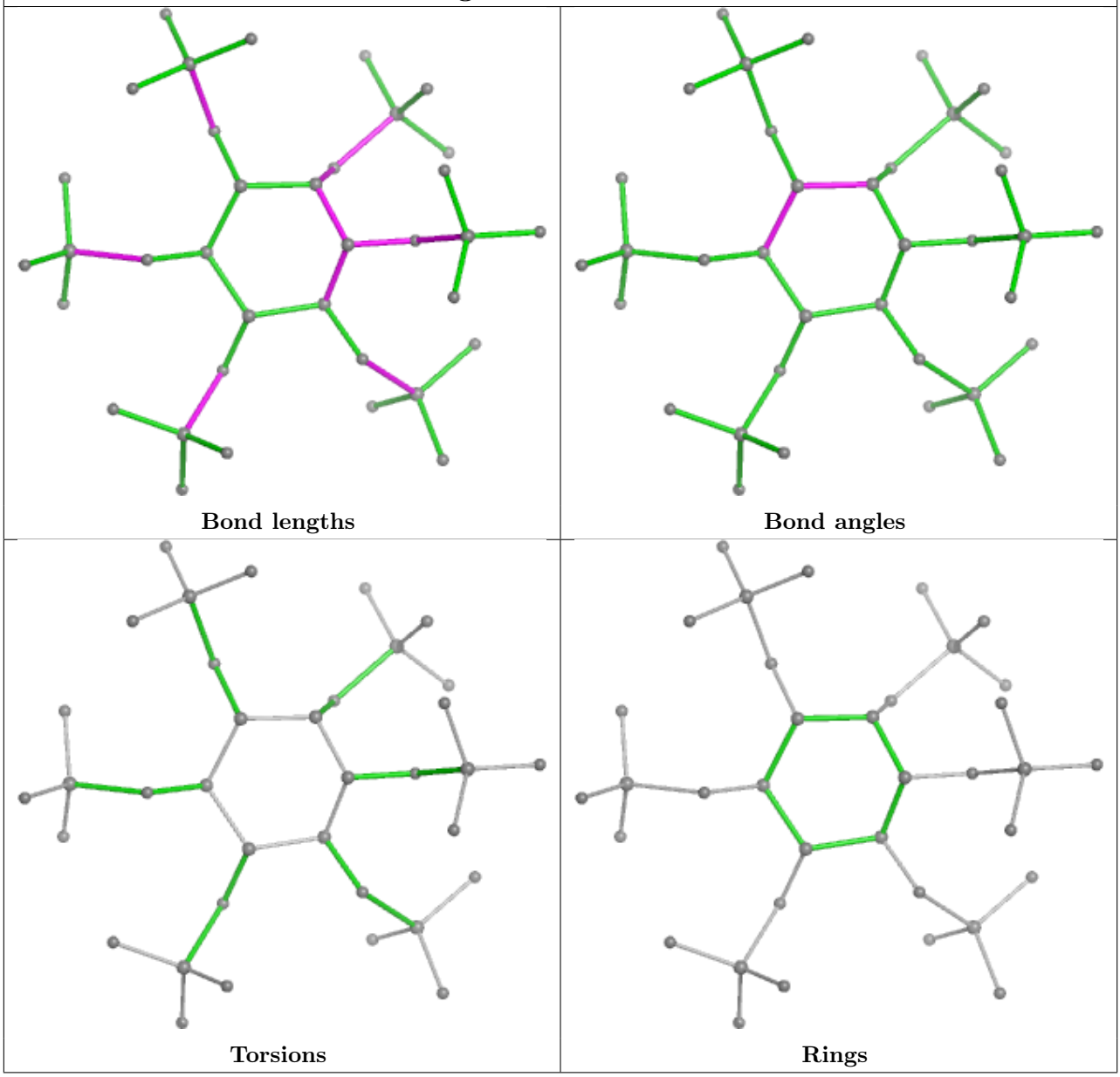
There are no ring outliers.

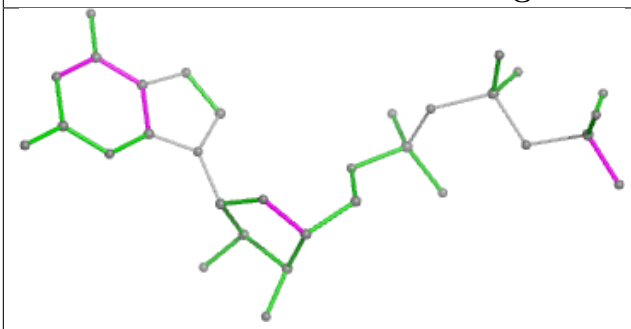
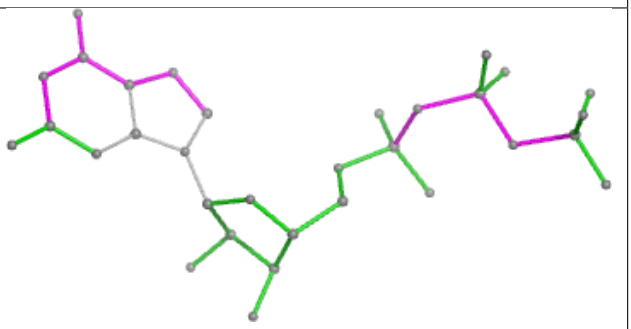
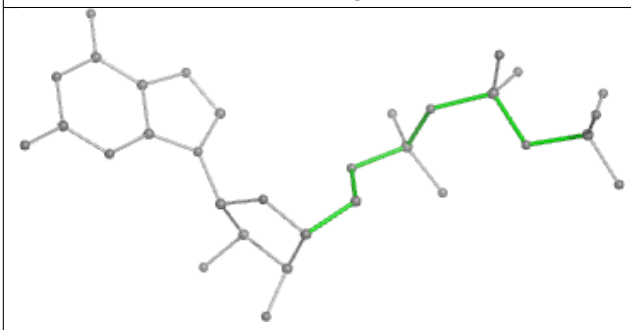
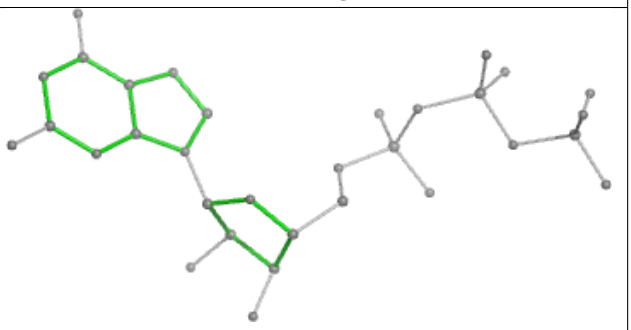
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

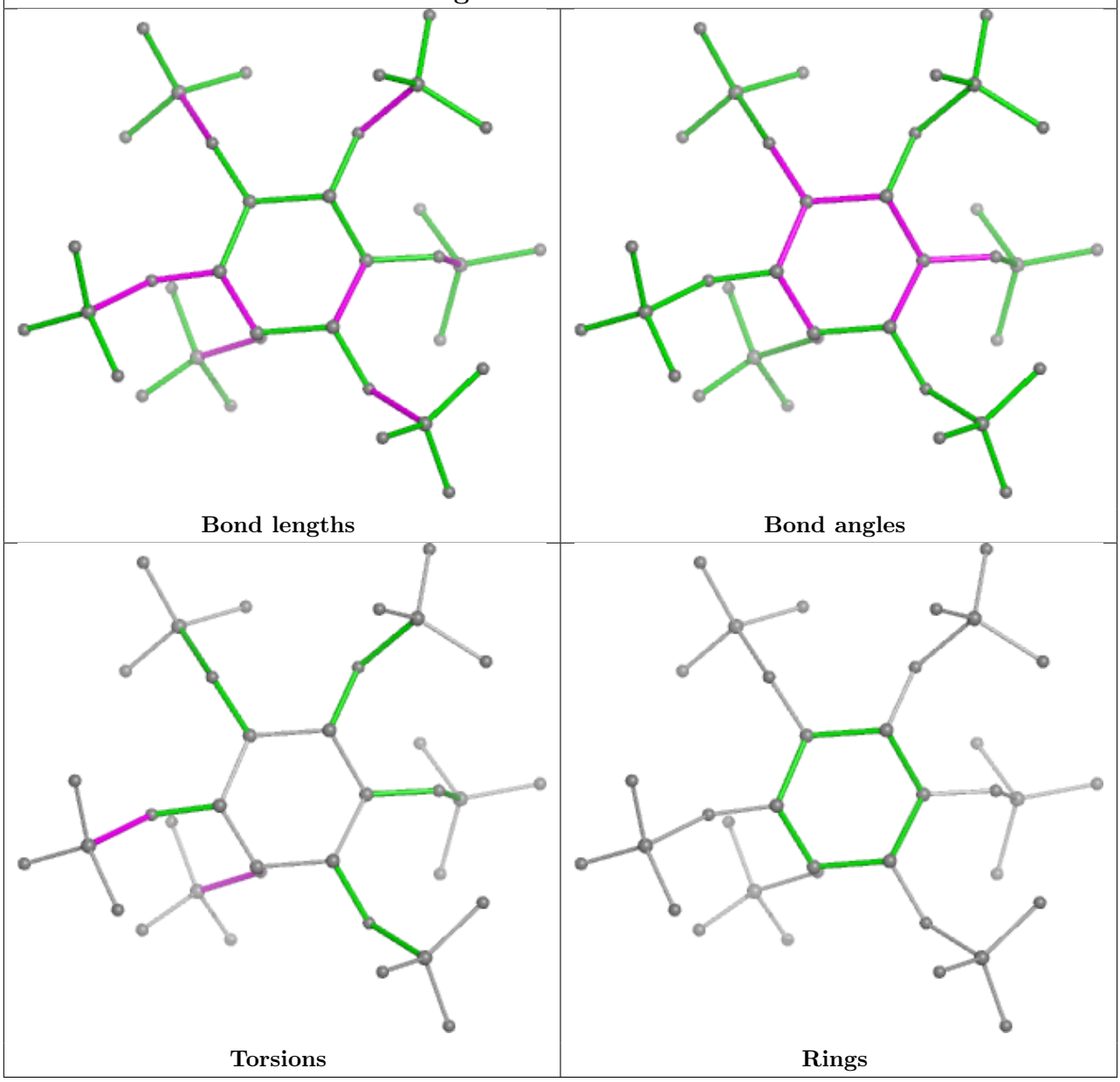
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 J 3000



Ligand GTP C 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IHP A 3000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

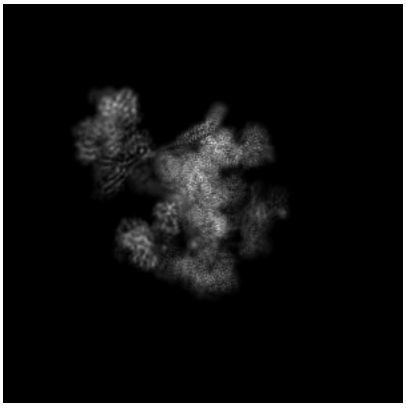
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19397. These allow visual inspection of the internal detail of the map and identification of artifacts.

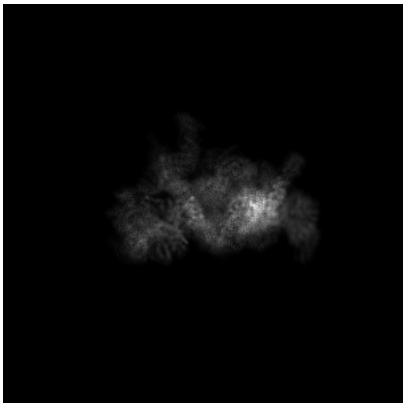
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

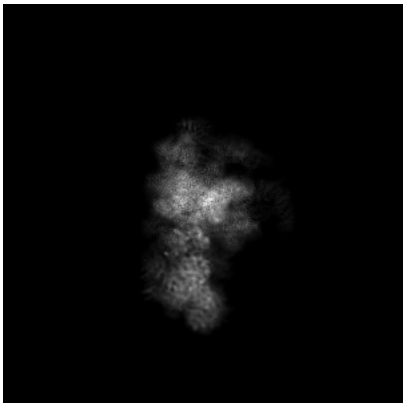
6.1.1 Primary map



X



Y



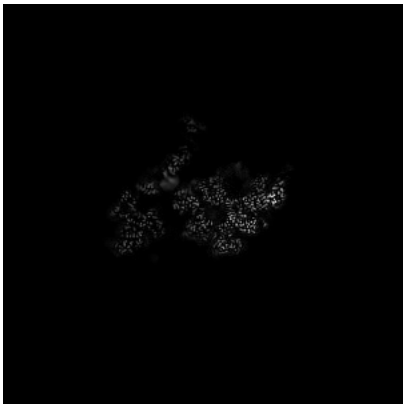
Z

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

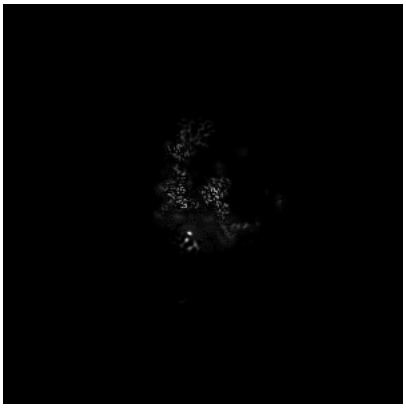
6.2 Central slices (i)

6.2.1 Primary map

X Index: 224



Y Index: 224



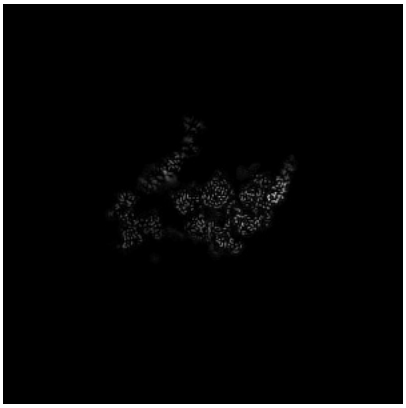
Z Index: 224

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: 221



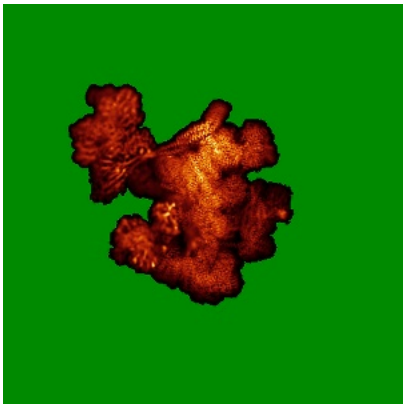
Y Index: 228

Z Index: 282

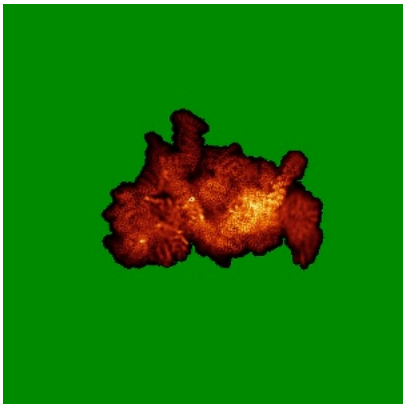
The images above show the largest variance slices of the map in three orthogonal directions.

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

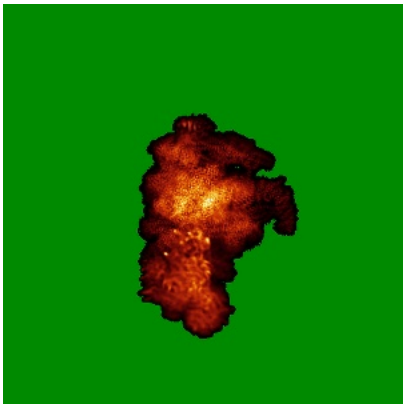
6.4.1 Primary map



X



Y

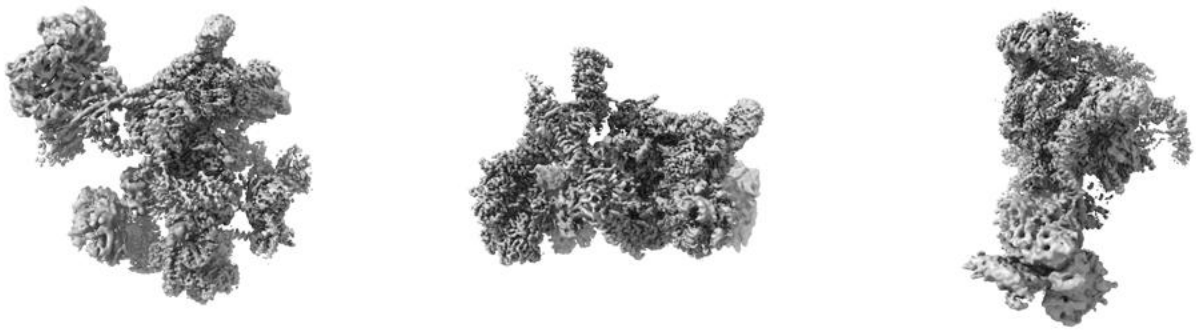


Z

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

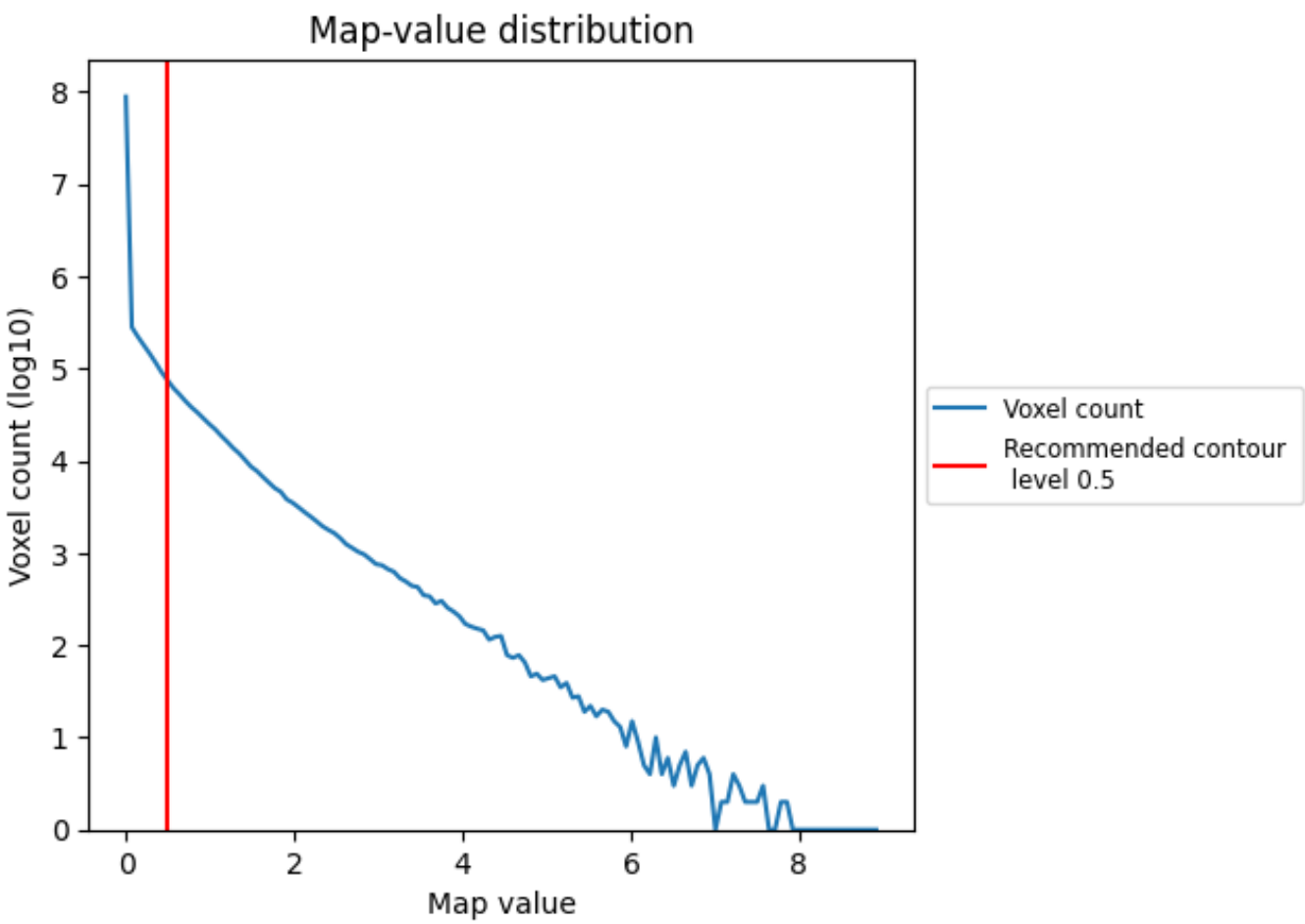
6.6 Mask visualisation (i)

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

7 Map analysis (i)

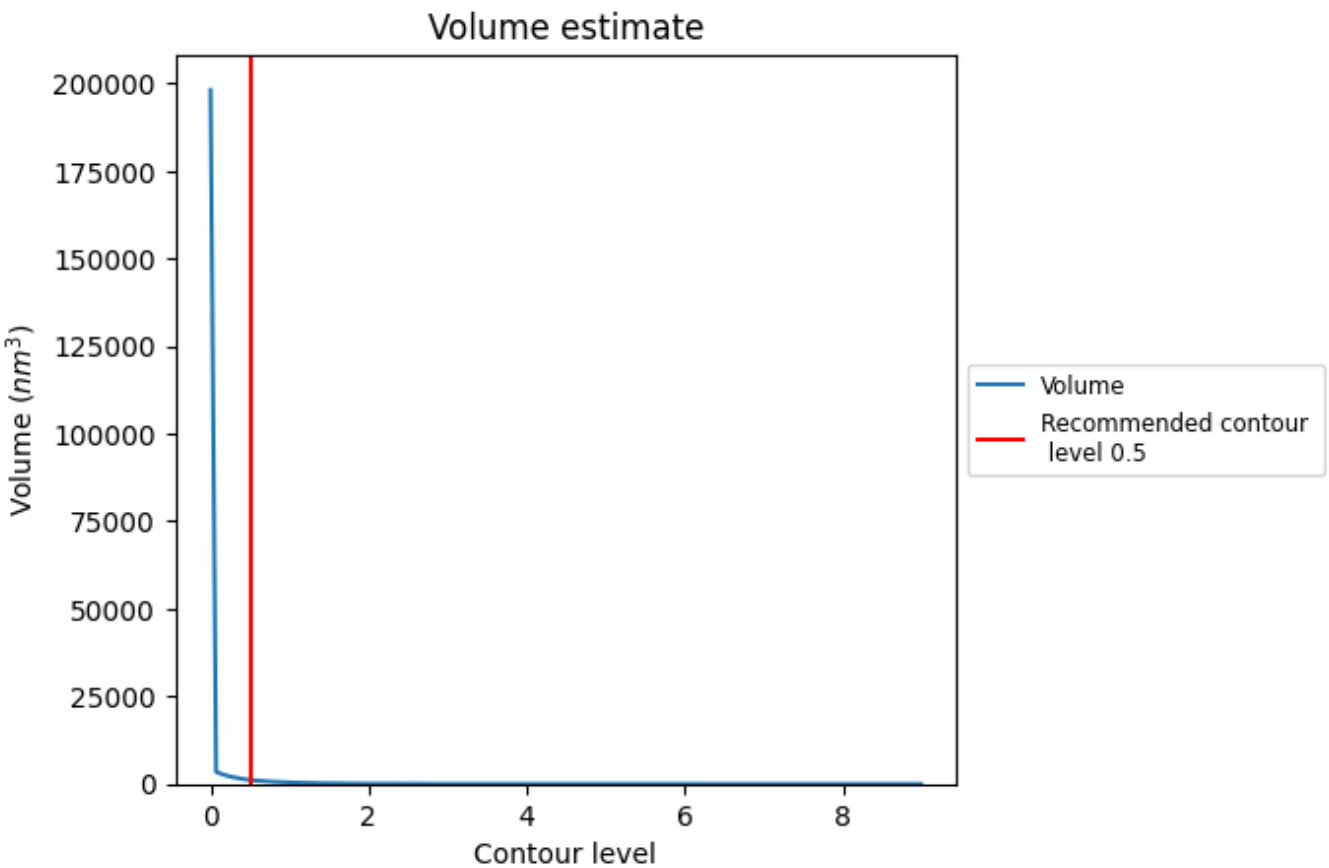
This section contains the results of statistical analysis of the map.

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.

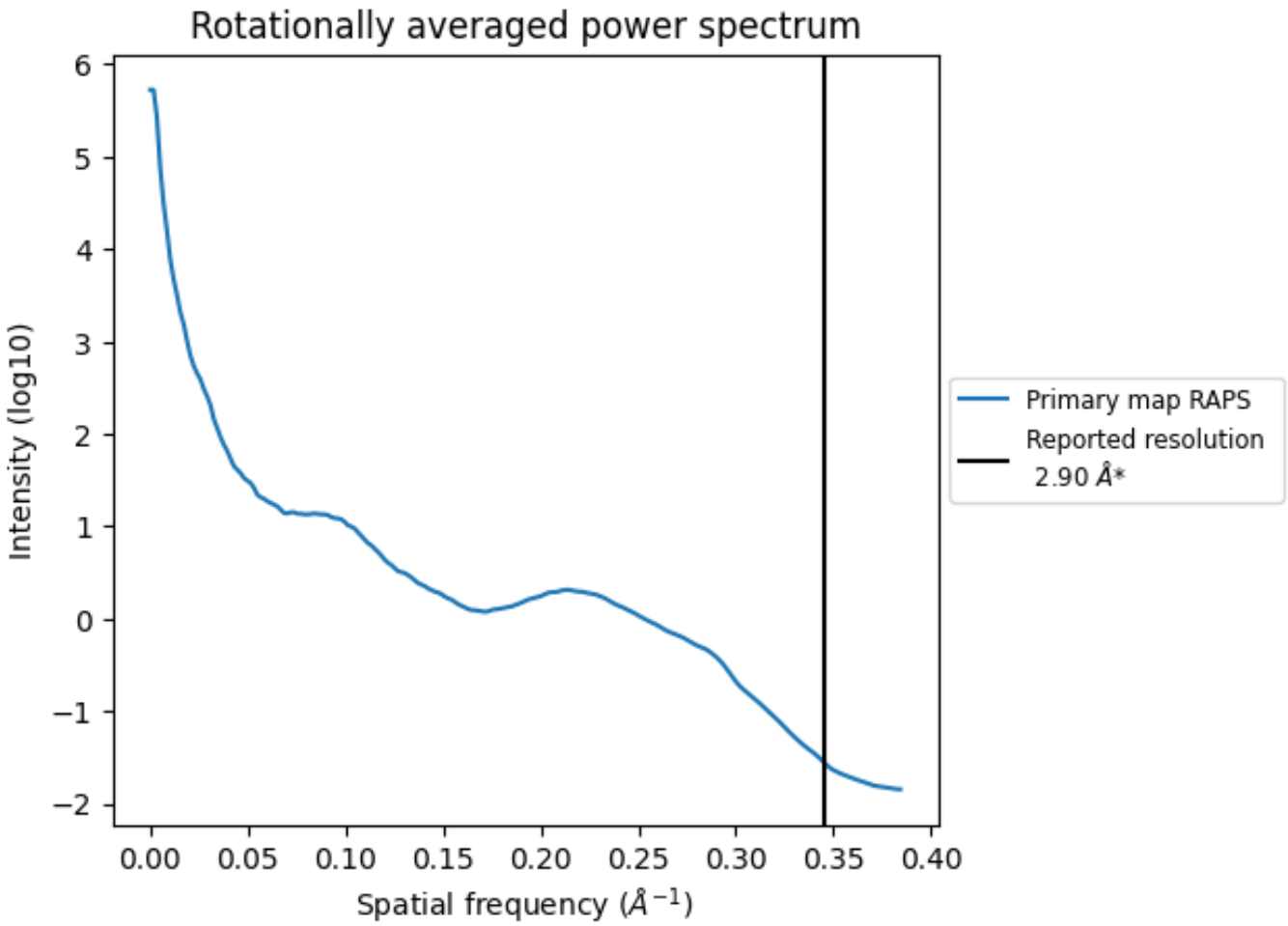
7.2 Volume estimate (i)



The volume at the recommended contour level is 1151 nm^3; this corresponds to an approximate mass of 1040 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}

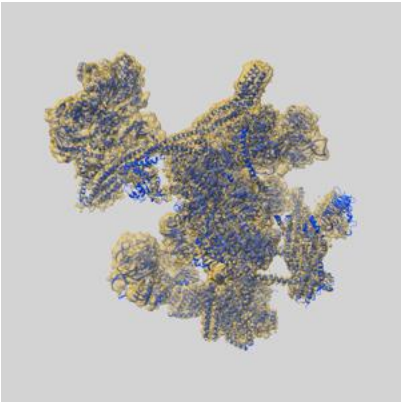
8 Fourier-Shell correlation (i)

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

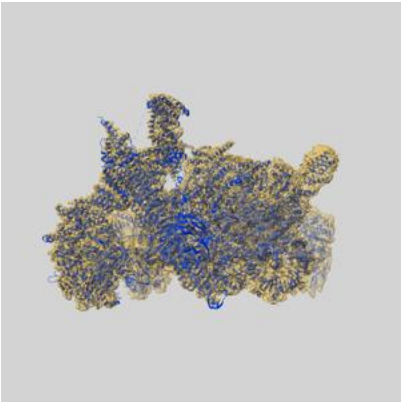
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19397 and PDB model 8RO0. Per-residue inclusion information can be found in section 3 on page 13.

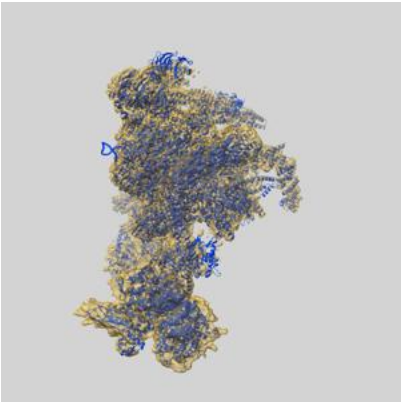
9.1 Map-model overlay (i)



X



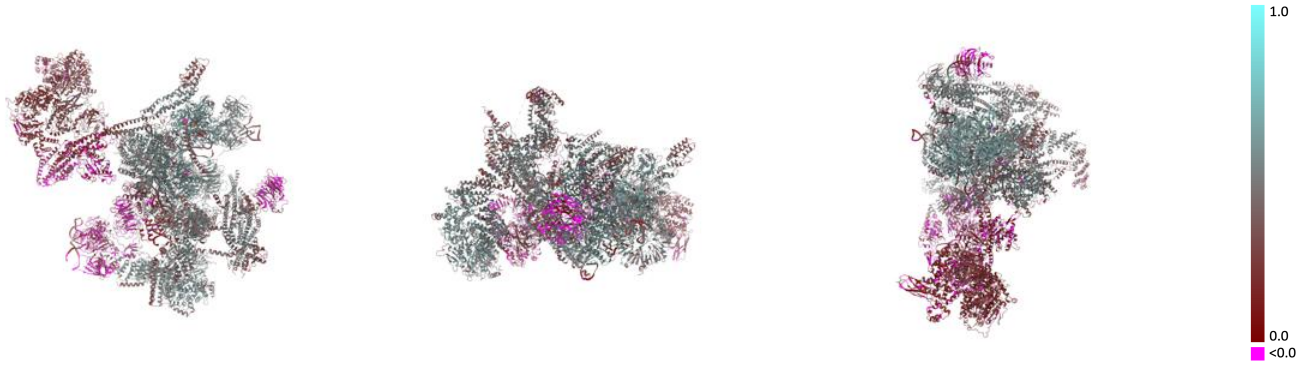
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

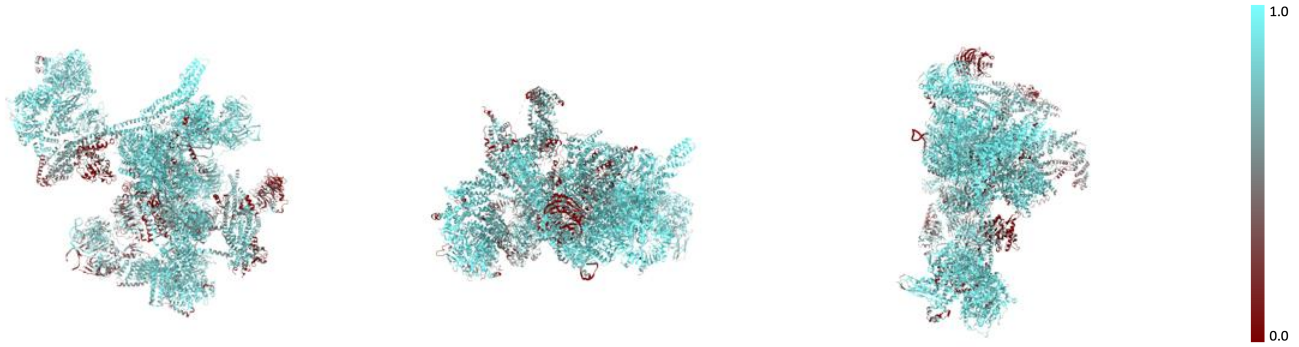
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

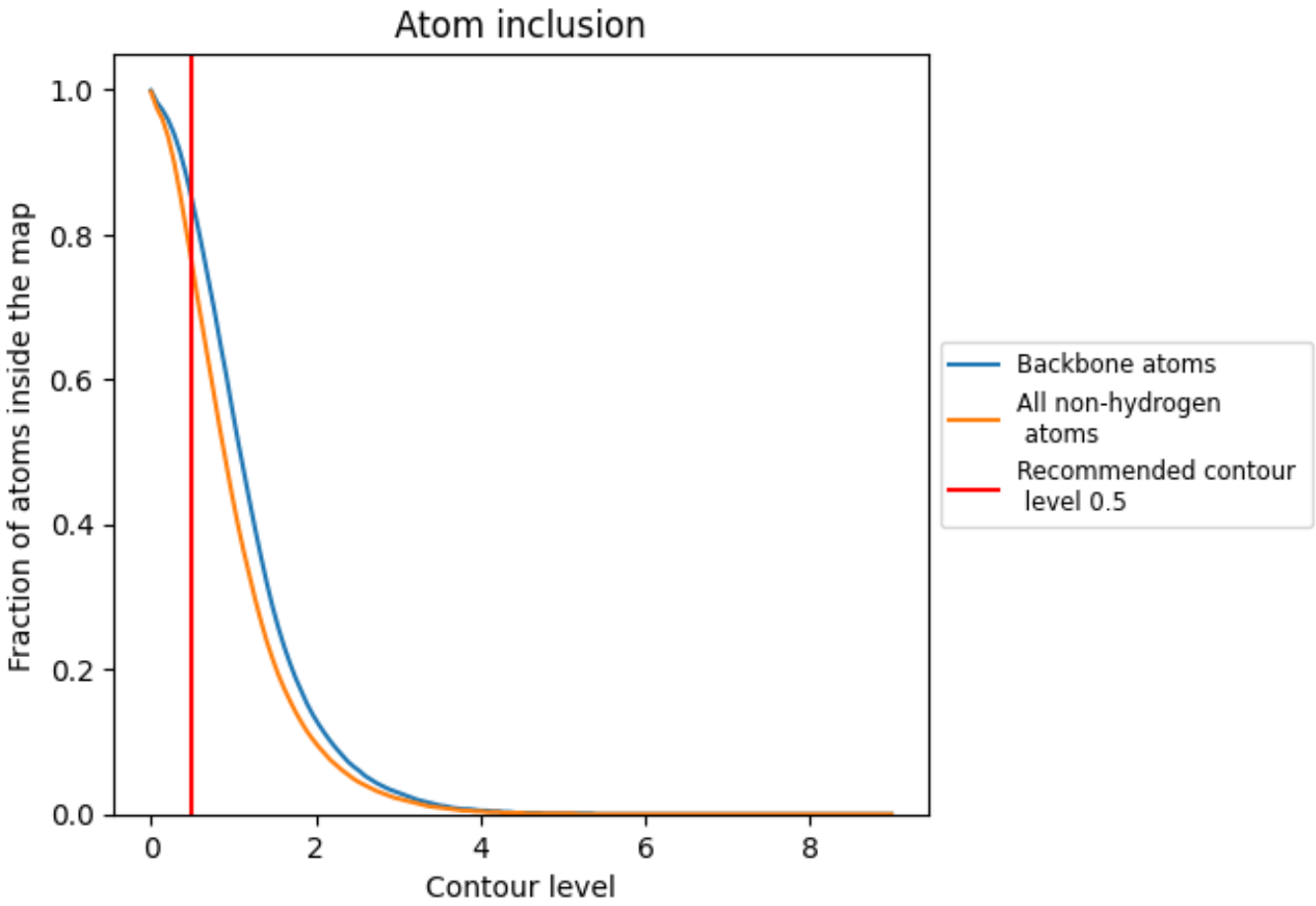
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.3720
2	0.7730	0.1980
5	0.9440	0.4570
6	0.6260	0.3220
A	0.8000	0.4350
B	0.8460	0.2000
C	0.9420	0.5700
D	0.4670	0.3640
E	0.8940	0.5330
I	0.8460	0.4750
In	0.6220	0.2310
J	0.7620	0.4580
K	0.6820	0.4230
L	0.5830	0.3790
M	0.7150	0.3100
N	0.9410	0.5520
O	0.8020	0.4680
P	0.3610	0.2980
PX	0.4710	0.0840
Q	0.8220	0.5150
R	0.7750	0.4450
S	0.7380	0.4350
T	0.9210	0.5490
TF	0.8490	0.3840
W	0.6190	0.1620
Z	0.4980	0.4050
a	0.9130	0.5030
b	0.8860	0.4550
c	0.9100	0.4790
d	0.7980	0.3850
e	0.8640	0.4680
f	0.8600	0.4670
g	0.8250	0.4430
h	0.7500	0.0960
i	0.4880	0.0510

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Chain	Atom inclusion	Q-score
j	0.5000	0.0490
k	0.4860	0.0630
l	0.6030	0.0520
m	0.6560	0.0740
n	0.6890	0.0690
o	0.5080	0.0310
p	0.5550	0.0610
q	0.7370	0.4590
r	0.4870	0.3880
s	0.3600	0.1630
t	0.5380	0.3930
y	0.4010	0.1490