Full wwPDB EM Validation Report

Nov 4, 2024 – 07:21 AM JST

PDB ID	:	7W5A
EMDB ID	:	EMD-32319
Title	:	The cryo-EM structure of human pre-C*-II complex
Authors	:	Zhan, X.; Lu, Y.; Shi, Y.
Deposited on	:	2021-11-29
Resolution	:	3.60 Å(reported)

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

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

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

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

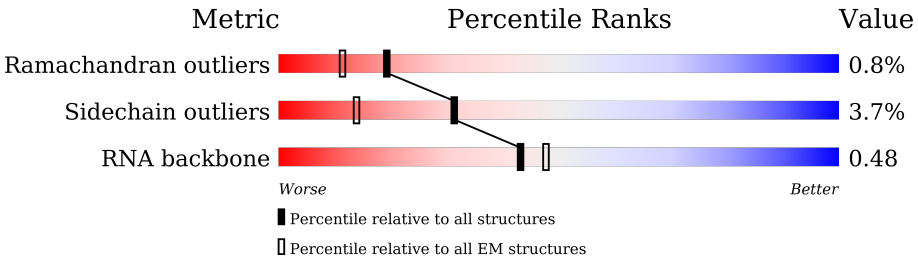
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	A	2335	77% 7% 15%
2	B	117	54% 16% 28%
3	C	972	86% 11%
4	E	357	83% 16%
5	F	107	46% 43% 9%
6	4	46	9% 15% 72%
7	G	174	7% 9% 30% 9% 53%
8	H	188	28% 43% 26%

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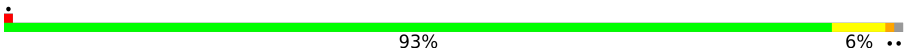
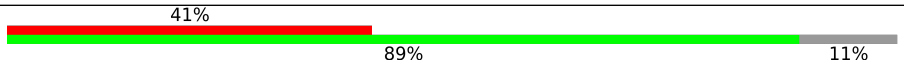
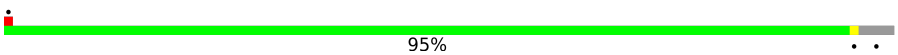
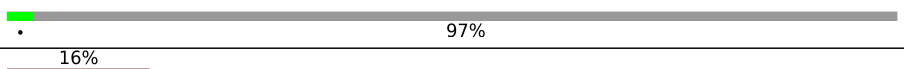
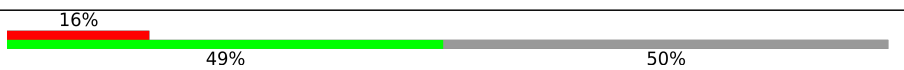
Mol	Chain	Length	Quality of chain
9	I	855	
10	J	848	
11	K	225	
12	L	802	
13	M	243	
14	N	144	
15	O	420	
16	P	229	
17	Q	1485	
18	R	536	
19	S	166	
20	T	514	
21	U	2752	
22	V	908	
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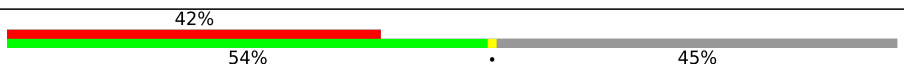
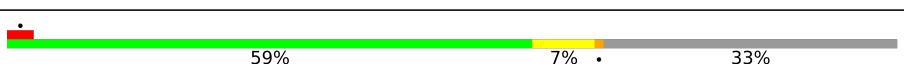
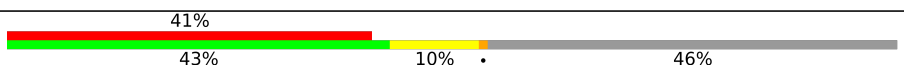
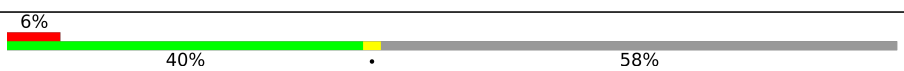
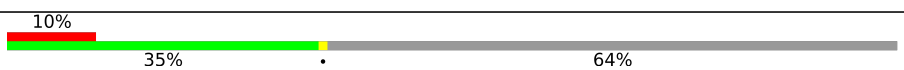
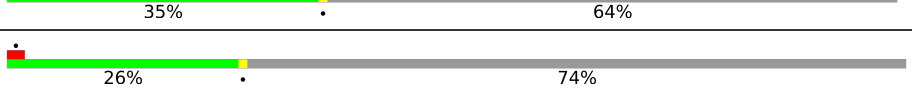
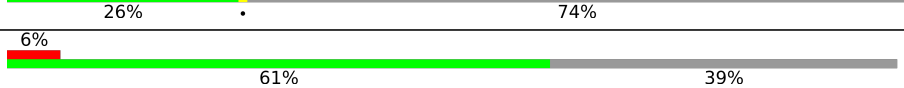
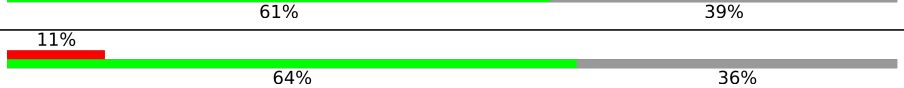
24	X	254	
25	Y	1220	
26	Z	758	
27	2	184	
28	z	112	
29	b	240	
29	i	240	
30	y	301	
31	a	126	
31	h	126	

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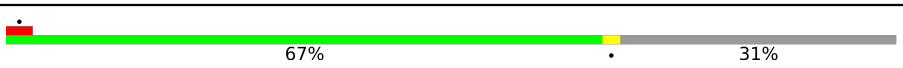
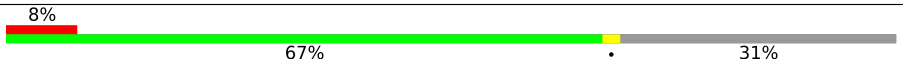
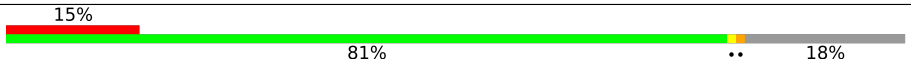
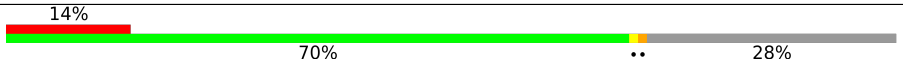
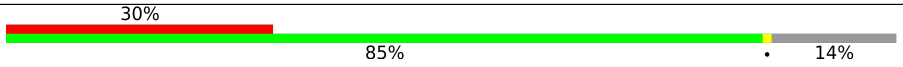
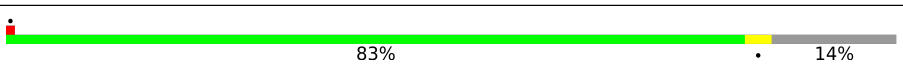
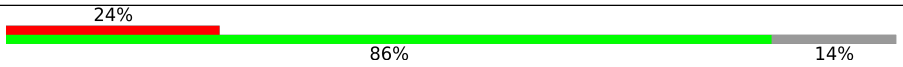
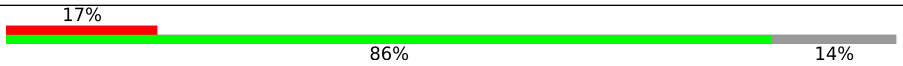
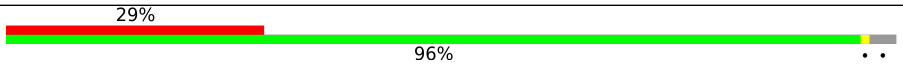
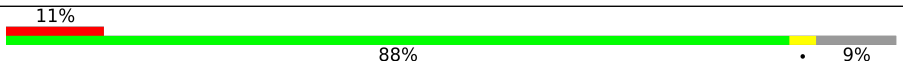
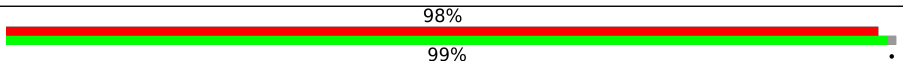
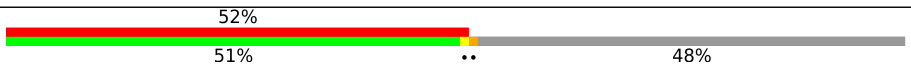
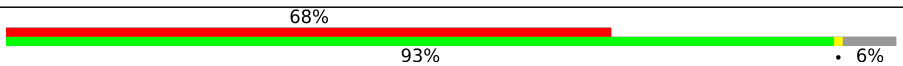
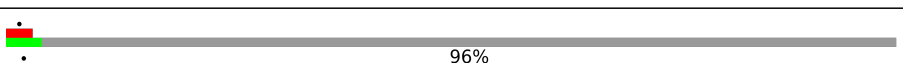
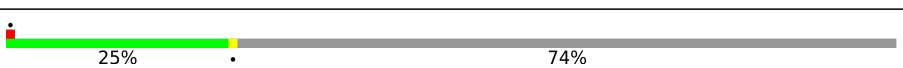
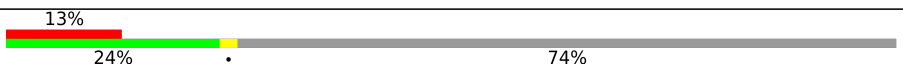
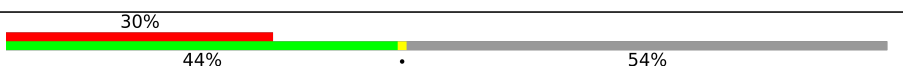
Mol	Chain	Length	Quality of chain
32	c	119	
32	j	119	
33	d	118	
33	k	118	
34	f	86	
34	m	86	
35	e	92	
35	l	92	
36	g	76	
36	n	76	
37	v	146	
38	w	174	
39	u	411	
40	x	703	
41	q	504	
41	r	504	
41	s	504	
41	t	504	
42	o	255	
43	p	225	
44	1	586	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 96822 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
			Total	C	N	O	S		
1	A	1984	16449	10601	2879	2899	70	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	84	1768	792	295	597	84	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	862	6791	4341	1138	1280	32	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	299	2338	1470	410	445	13	0	0

- Molecule 5 is a RNA chain called U6 snRNA.

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

- Molecule 6 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	4	13	276	123	50	90	13	0	0

- Molecule 7 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	82	Total	C	N	O	P	0	0
			1510	666	210	552	82		

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	P	0	0
			2966	1326	510	990	140		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	618	Total	C	N	O	S	0	0
			3857	2389	722	735	11		

- Molecule 10 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	567	Total	C	N	O	S	0	0
			3809	2373	716	714	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	155	Total	C	N	O	0	0
			772	462	155	155		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	437	Total	C	N	O	S	0	0
			3015	1859	584	565	7		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SYF2.

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

- Molecule 14 is a protein called Protein BUD31 homolog.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	285	Total	C	N	O	S	0	0
			2296	1442	408	426	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	113	Total	C	N	O	S	0	0
			953	583	189	179	2		

- Molecule 17 is a protein called RNA helicase aquarius.

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

- Molecule 18 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	261	Total	C	N	O	P	S	0	0
			2073	1300	373	386	2	12		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 20 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	312	Total	C	N	O	S	0	0
			2454	1550	446	450	8		

- Molecule 21 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	452	Total	C	N	O	S	0	0
			2632	1639	492	495	6		

- Molecule 23 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	509	Total	C	N	O	S	0	0
			4129	2628	715	762	24		

- Molecule 24 is a protein called PSME3-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	87	Total	C	N	O	S	0	0
			702	431	128	142	1		

- Molecule 25 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	667	Total	C	N	O	S	4	0
			3431	2057	680	693	1		

- Molecule 26 is a protein called Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	101	Total	C	N	O	S	0	0
			902	592	167	141	2		

- Molecule 27 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	123	Total	C	N	O	S	0	0
			1013	635	193	180	5		

- Molecule 28 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	z	60	Total	C	N	O	S	0	0
			504	314	96	92	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	102	Total	C	N	O	S	0	0
			786	492	148	139	7		
29	i	86	Total	C	N	O	S	0	0
			690	434	126	123	7		

- Molecule 30 is a protein called Peptidyl-prolyl cis-trans isomerase E.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	77	Total	C	N	O	S	0	0
			609	381	108	115	5		
31	h	81	Total	C	N	O	S	0	0
			633	397	112	118	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	82	Total	C	N	O	S	0	0
			649	413	113	119	4		
32	j	82	Total	C	N	O	S	0	0
			649	413	113	119	4		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	97	Total	C	N	O	S	0	0
			776	488	143	140	5		
33	k	85	Total	C	N	O	S	0	0
			688	432	125	126	5		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	74	Total	C	N	O	S	0	0
			576	373	95	103	5		
34	m	74	Total	C	N	O	S	0	0
			572	370	94	103	5		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	79	Total	C	N	O	S	0	0
			652	412	116	119	5		
35	l	79	Total	C	N	O	S	0	0
			652	412	116	119	5		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		
36	n	69	Total	C	N	O	S	0	0
			542	345	97	94	6		

- Molecule 37 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	v	144	Total	C	N	O	0	0
			711	423	144	144		

- Molecule 38 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	w	91	Total	C	N	O	0	0
			445	263	91	91		

- Molecule 39 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	u	386	Total	C	N	O	0	0
			1907	1135	386	386		

- Molecule 40 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	x	25	Total	C	N	O	0	0
			124	74	25	25		

- Molecule 41 is a protein called Pre-mRNA-processing factor 19.

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

- Molecule 42 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	162	Total	C	N	O	S	0	0
			1282	820	219	240	3		

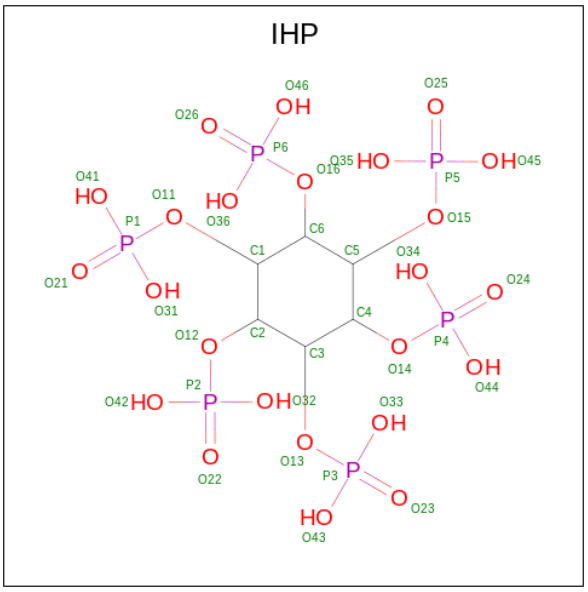
- Molecule 43 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	94	Total	C	N	O	S	0	0
			760	488	135	132	5		

- Molecule 44 is a protein called Pre-mRNA-splicing factor SLU7.

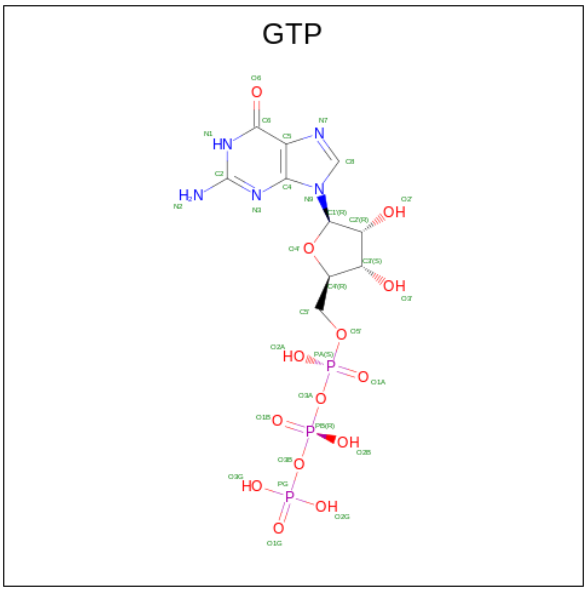
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	267	Total	C	N	O	S	0	0
			2194	1378	392	416	8		

- Molecule 45 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 46 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

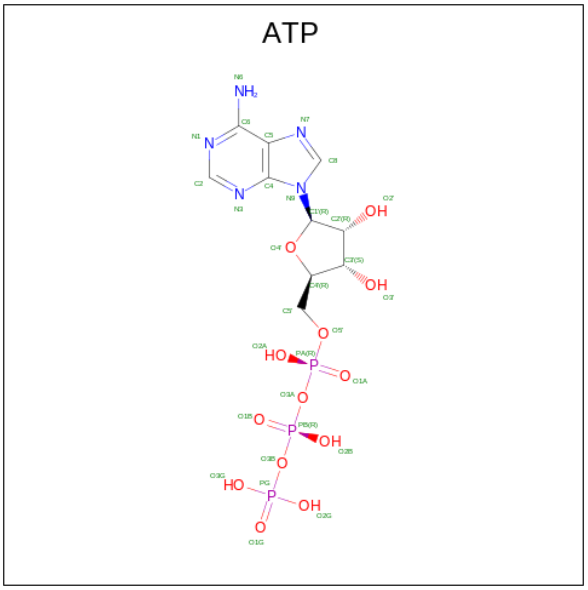
- Molecule 47 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
47	C	1	Total Mg 1 1	0
47	F	6	Total Mg 6 6	0
47	Q	2	Total Mg 2 2	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
48	N	3	Total Zn 3 3	0
48	O	3	Total Zn 3 3	0
48	1	1	Total Zn 1 1	0

- Molecule 49 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



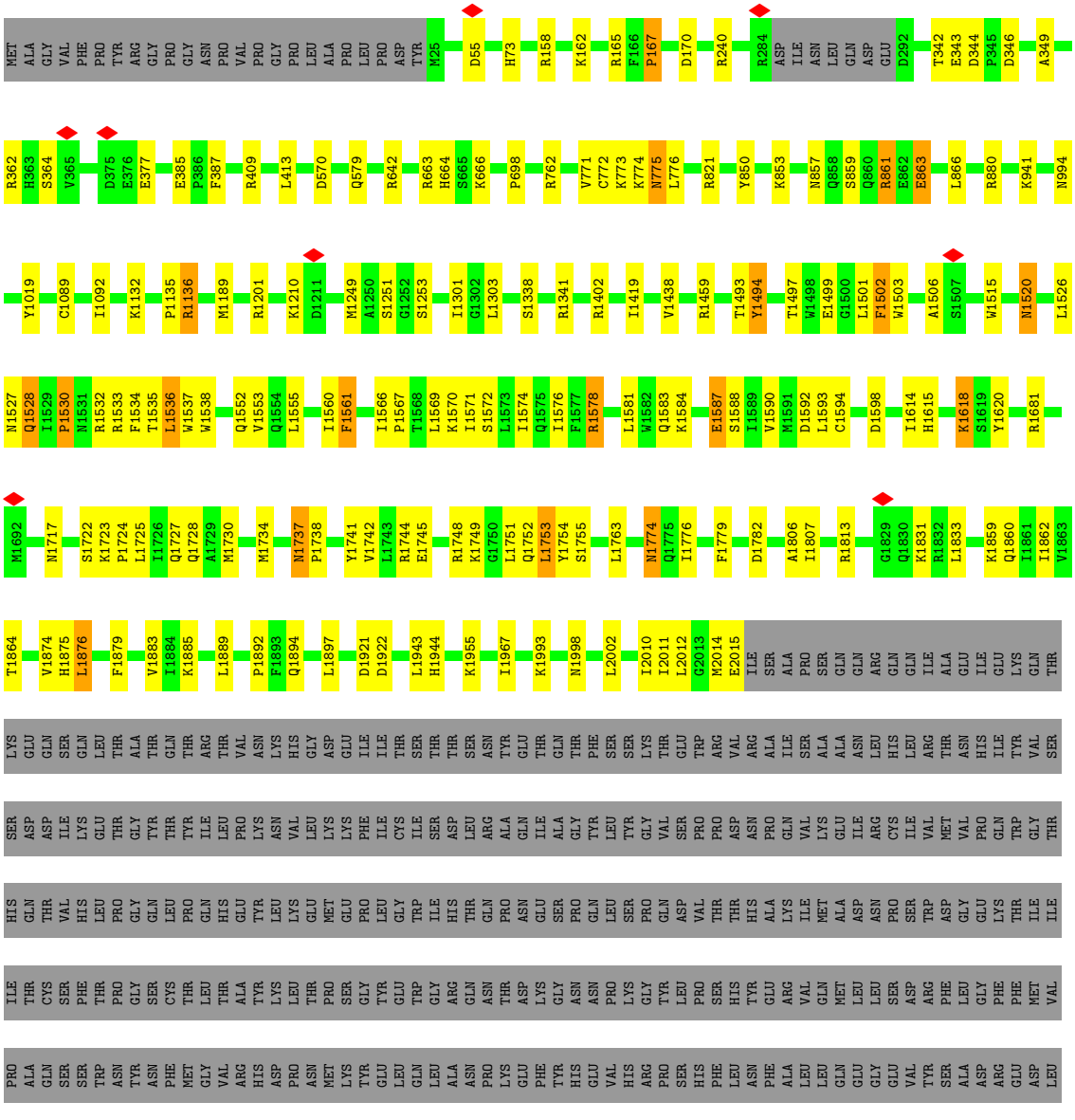
Mol	Chain	Residues	Atoms	AltConf
49	Q	1	Total C N O P 31 10 5 13 3	0

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.

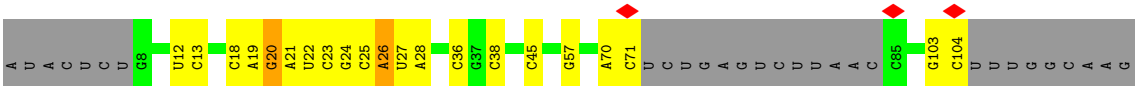
• Molecule 1: Pre-mRNA-processing-splicing factor 8

Chain A:



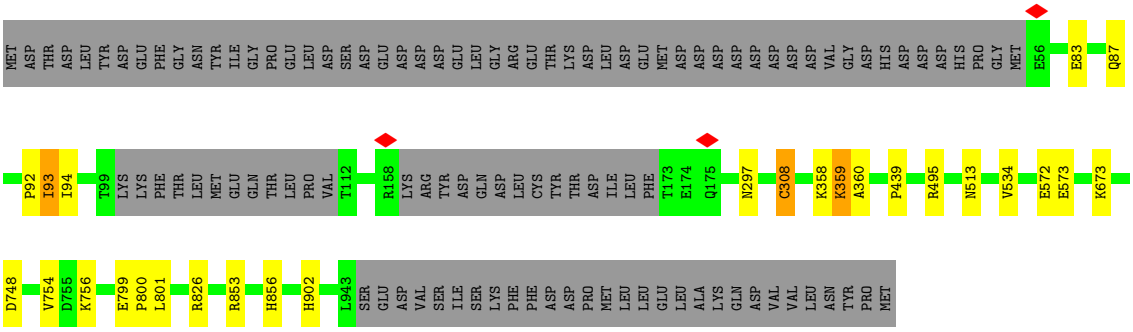
• Molecule 2: U5 snRNA

Chain B:



• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:



• Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:

• Molecule 5: U6 snRNA

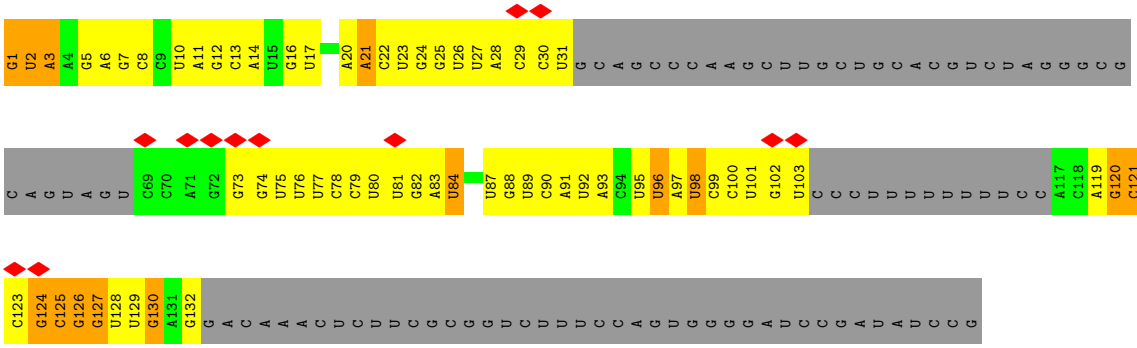
Chain F:

• Molecule 6: Pre-mRNA

Chain 4:

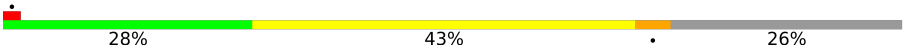
• Molecule 7: Pre-mRNA

Chain G:



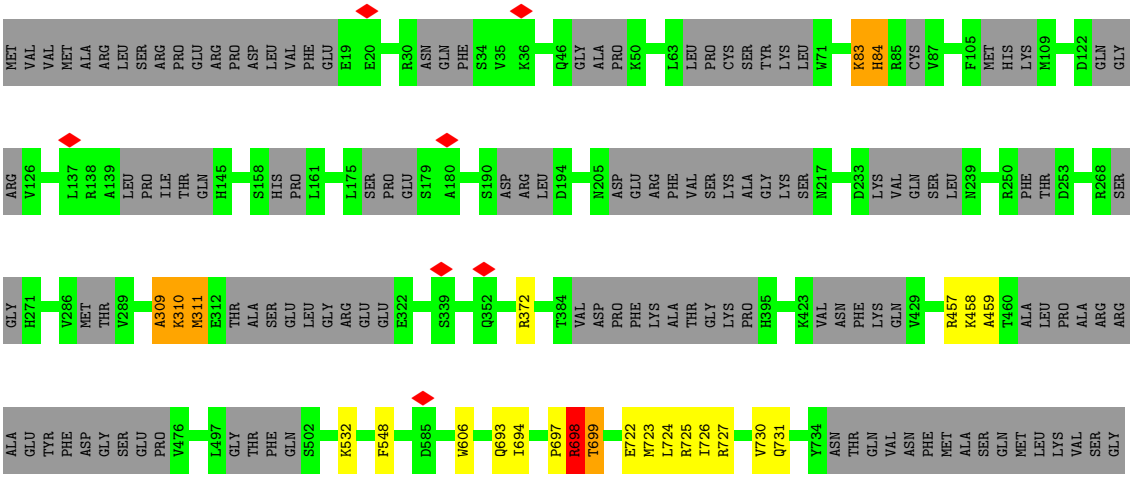
• Molecule 8: U2 snRNA

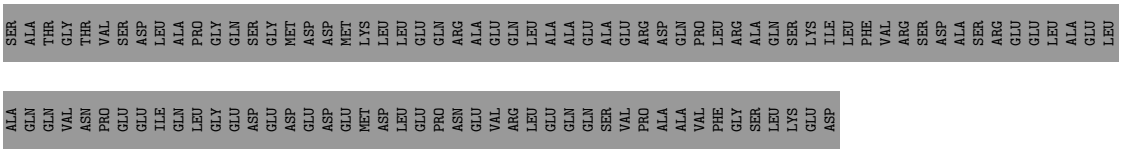
Chain H:



• Molecule 9: Pre-mRNA-splicing factor SYF1

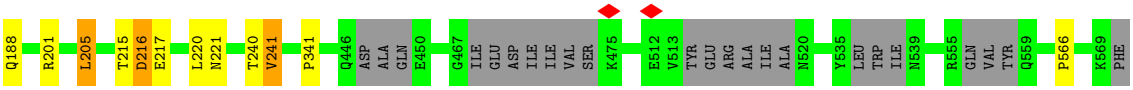
Chain I:

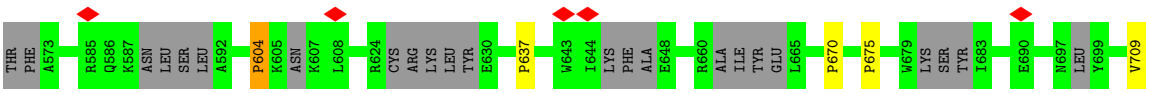


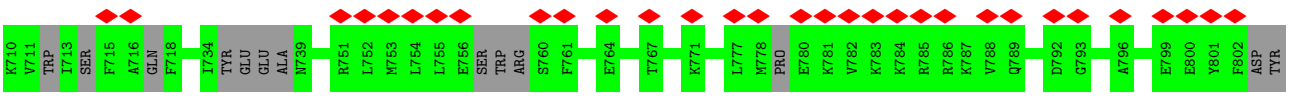


• Molecule 10: Crooked neck-like protein 1

Chain J:

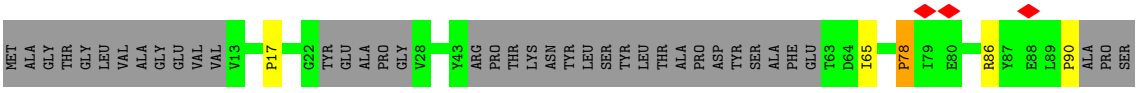


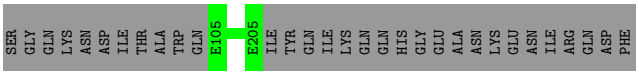




• Molecule 11: Pre-mRNA-splicing factor SPF27

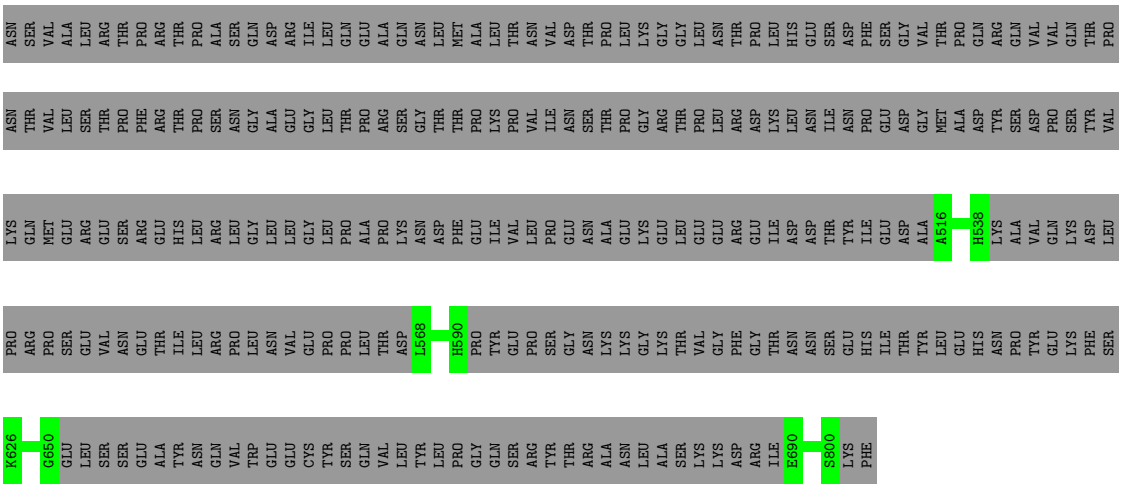
Chain K:





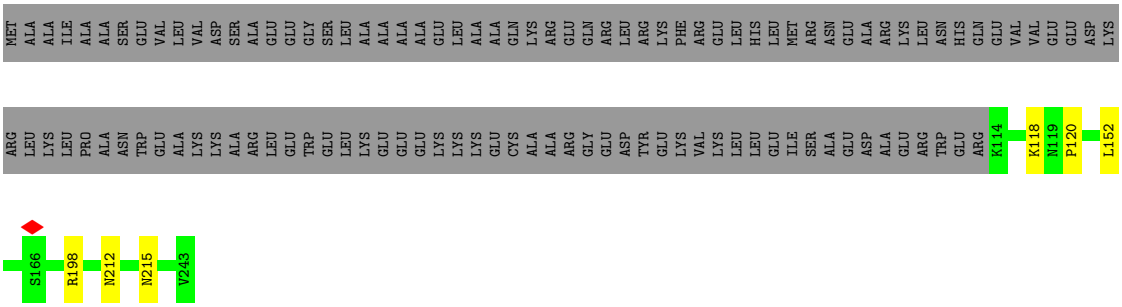
• Molecule 12: Cell division cycle 5-like protein

Chain L:



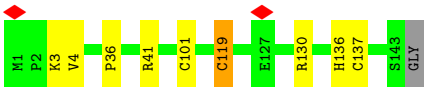
• Molecule 13: Pre-mRNA-splicing factor SYF2

Chain M:



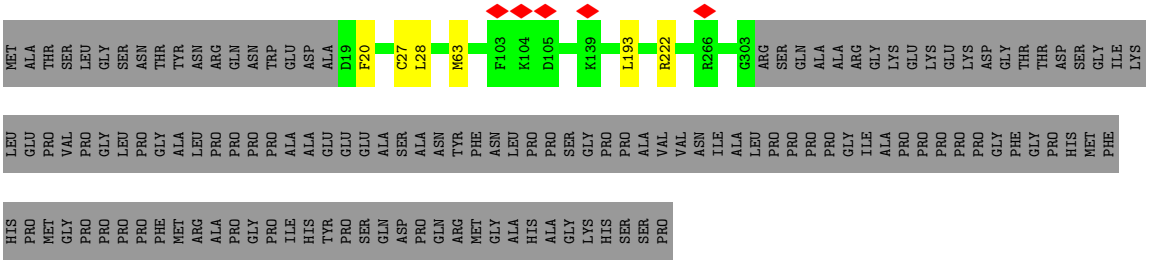
• Molecule 14: Protein BUD31 homolog

Chain N:



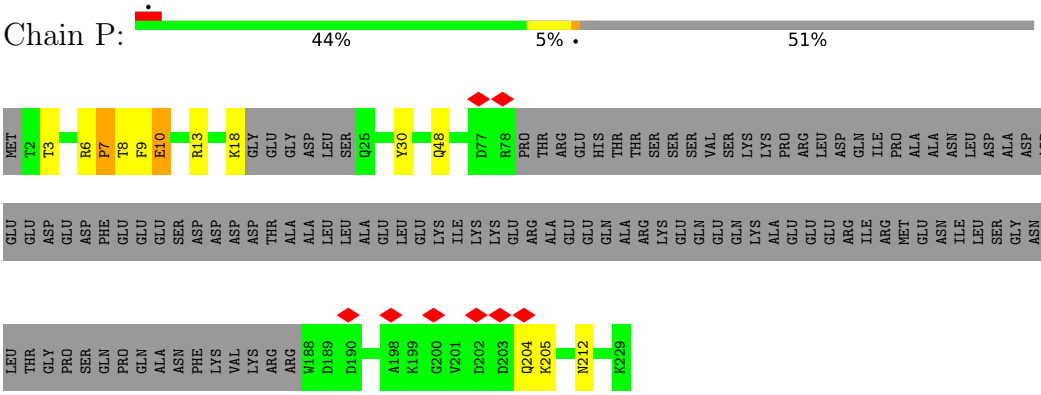
• Molecule 15: Pre-mRNA-splicing factor RBM22

Chain O:



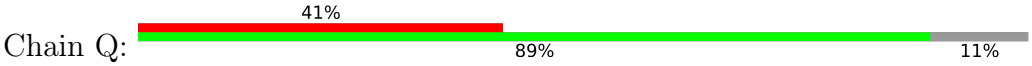
• Molecule 16: Spliceosome-associated protein CWC15 homolog

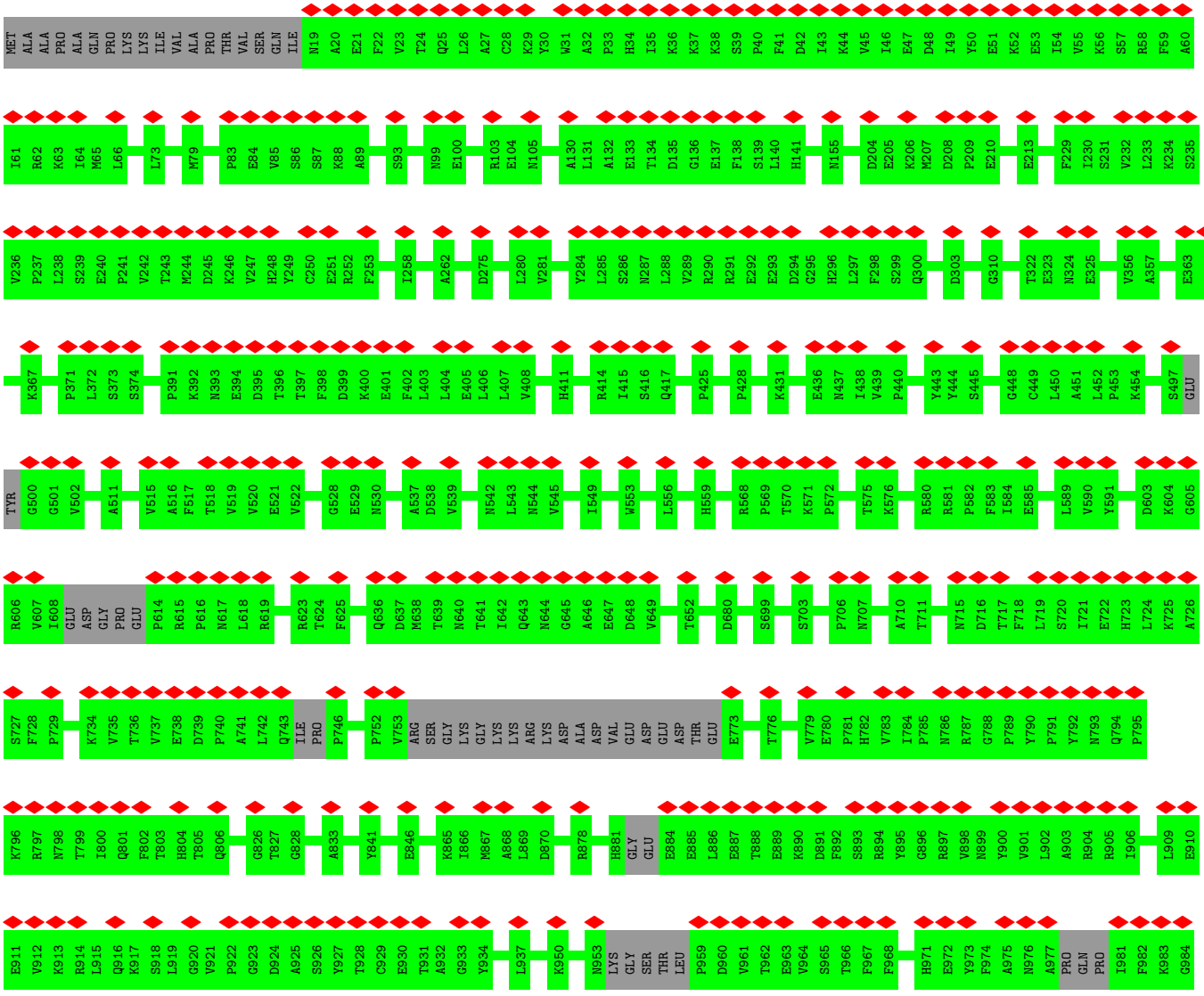
Chain P:

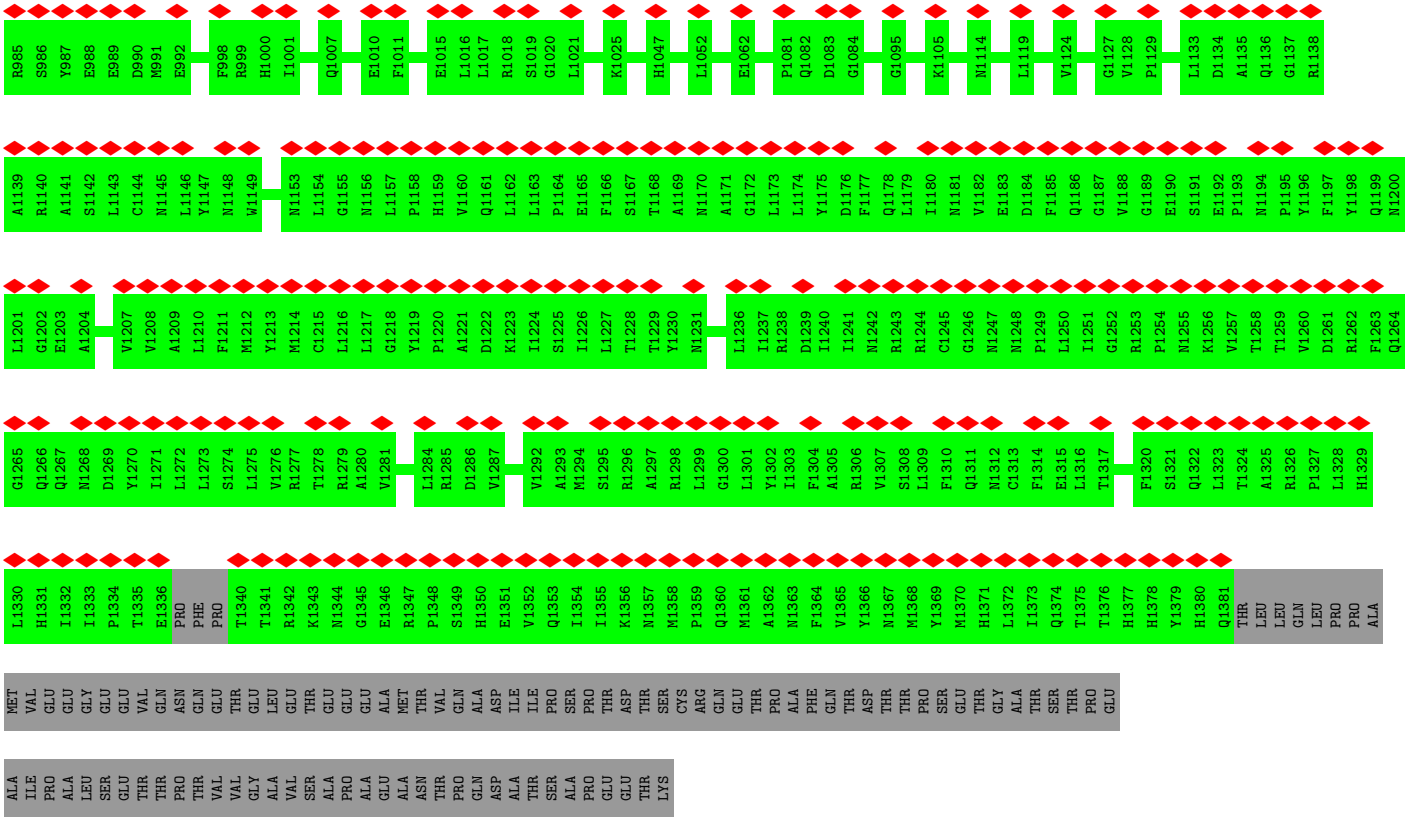


• Molecule 17: RNA helicase aquarius

Chain Q:

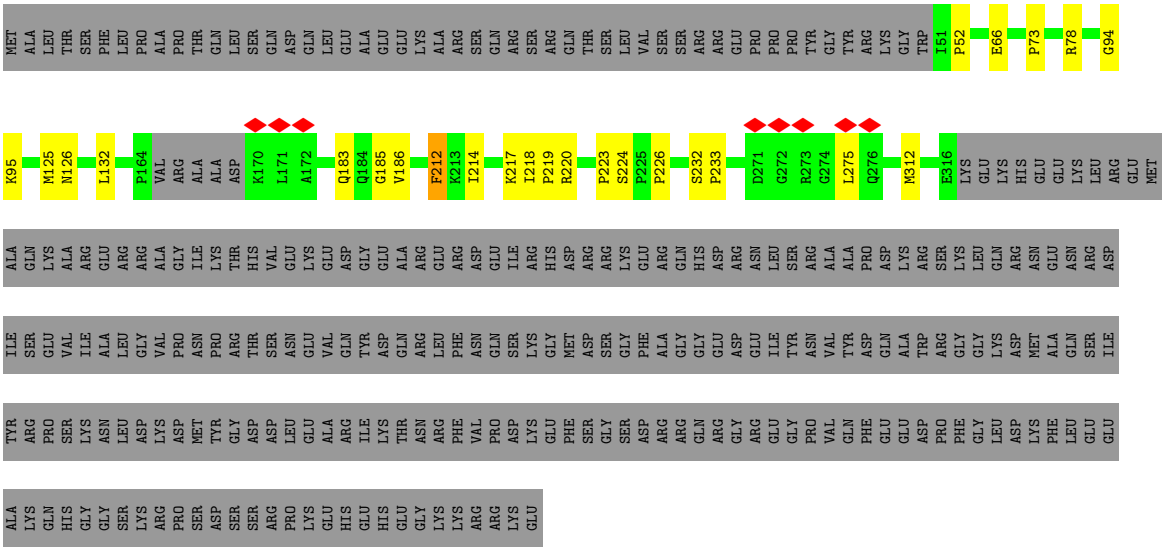






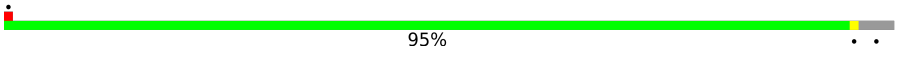
• Molecule 18: SNW domain-containing protein 1

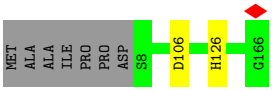
Chain R:



• Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1

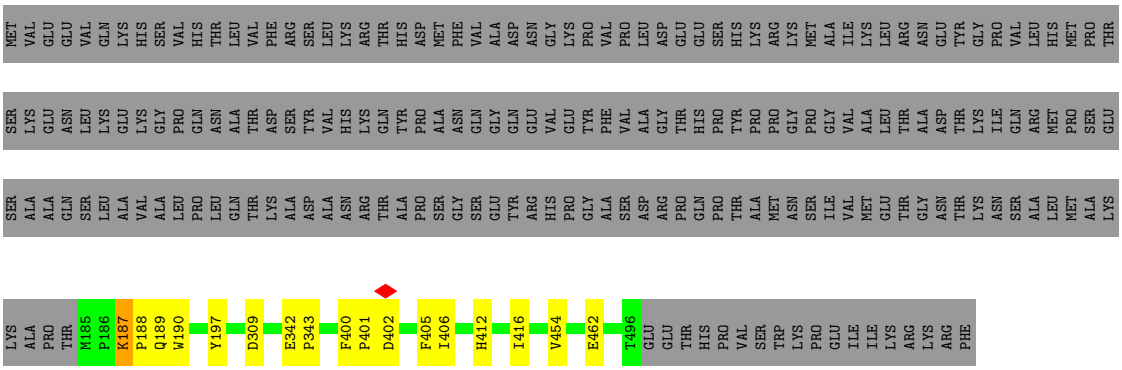
Chain S:





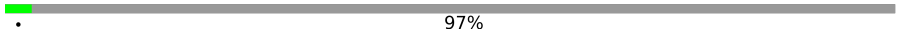
• Molecule 20: Pleiotropic regulator 1

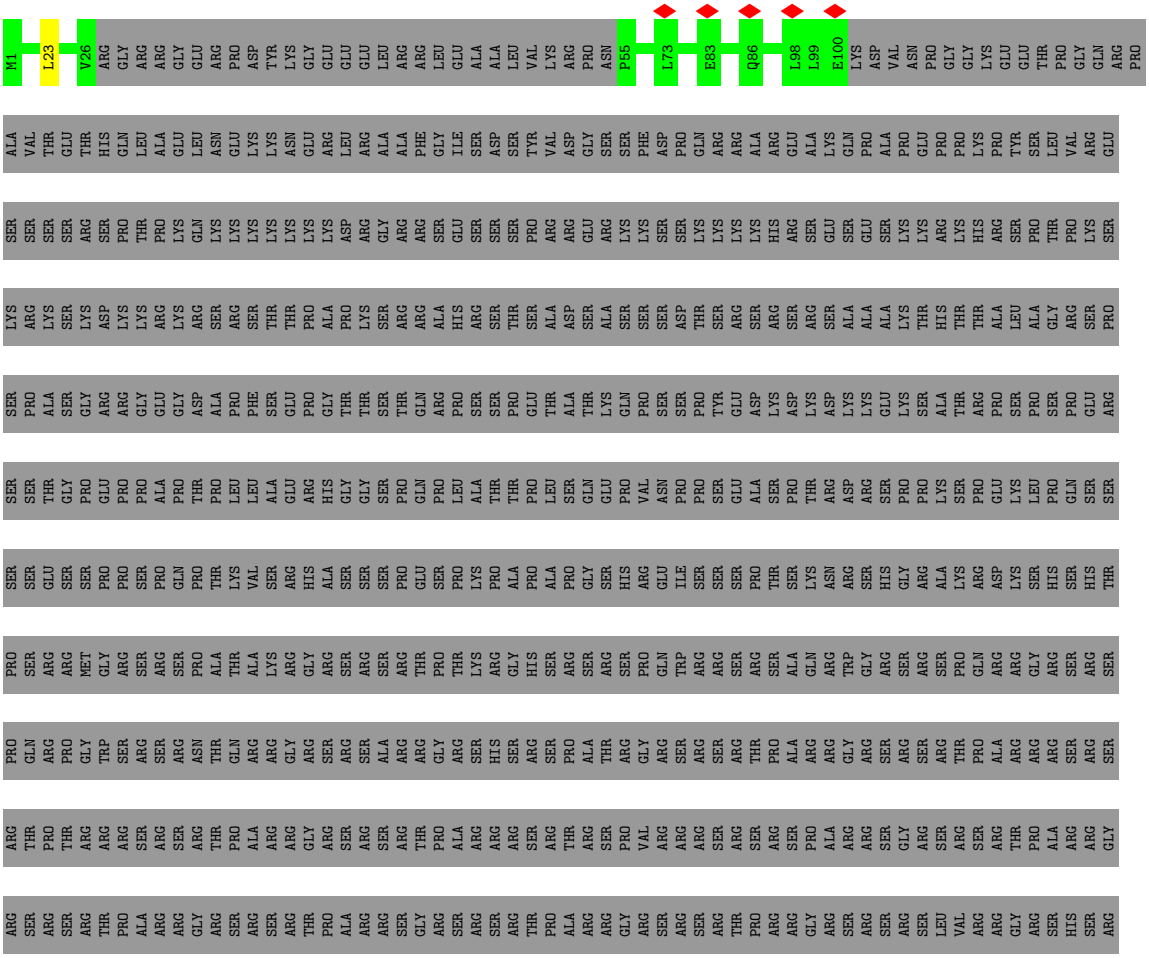
Chain T:

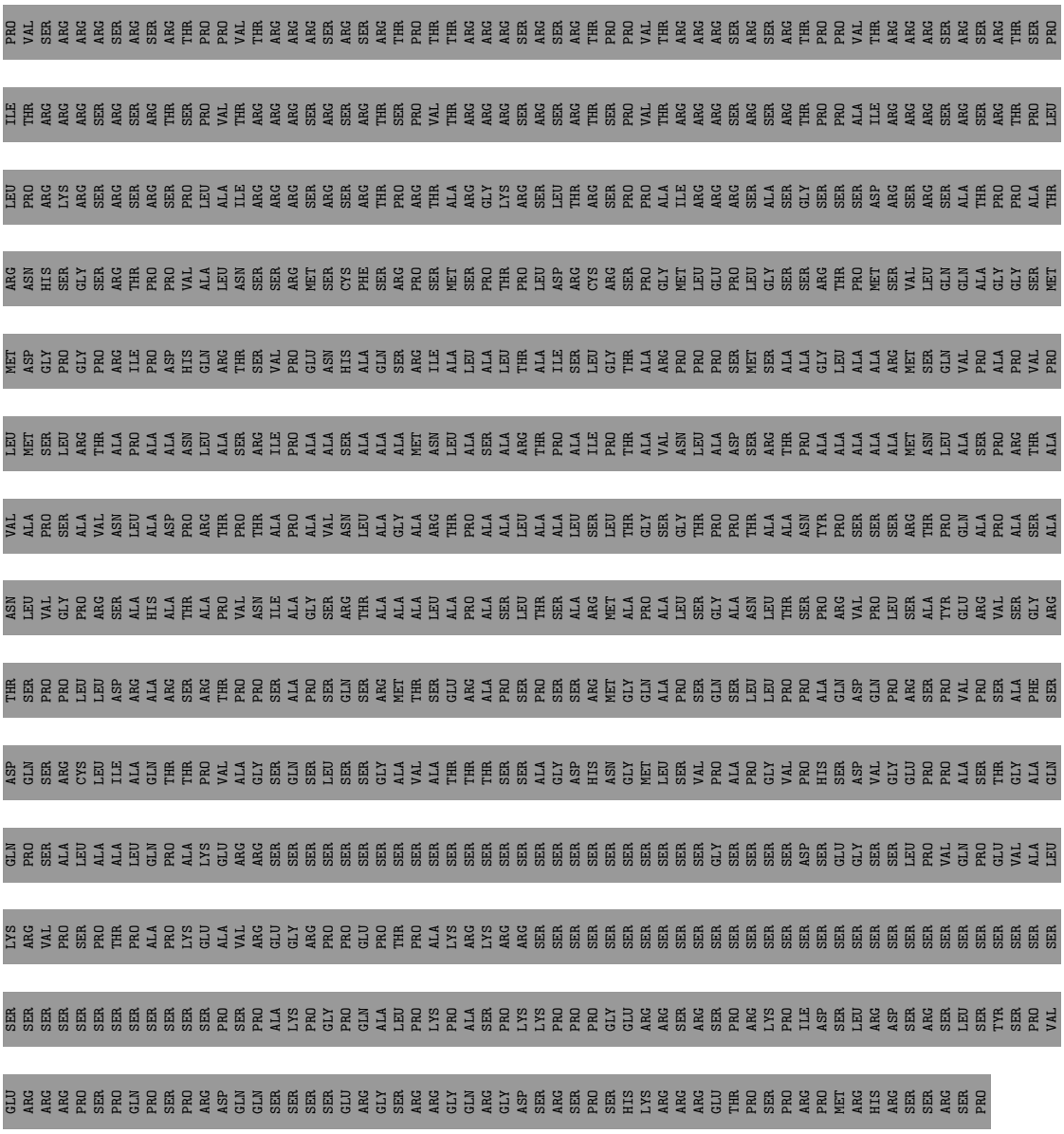


• Molecule 21: Serine/arginine repetitive matrix protein 2

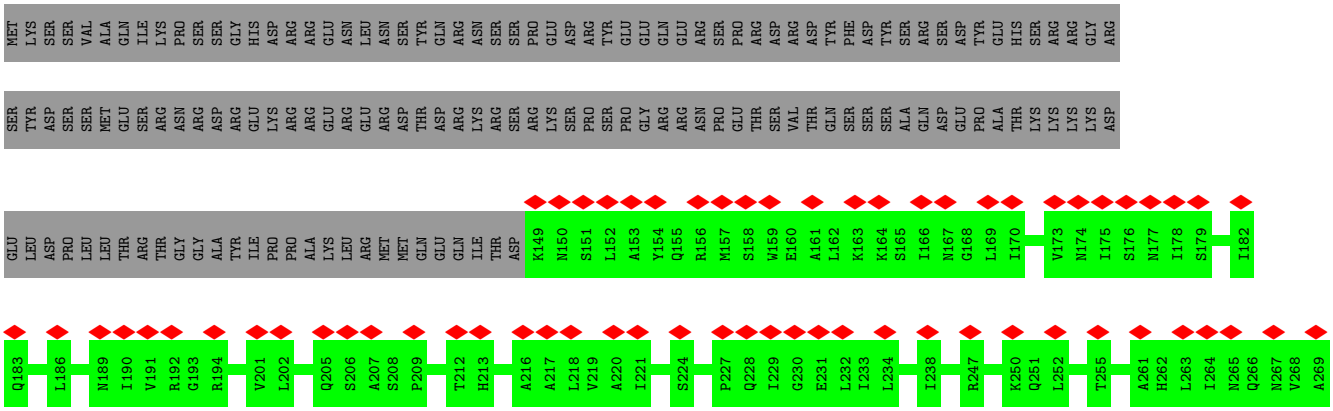
Chain U:

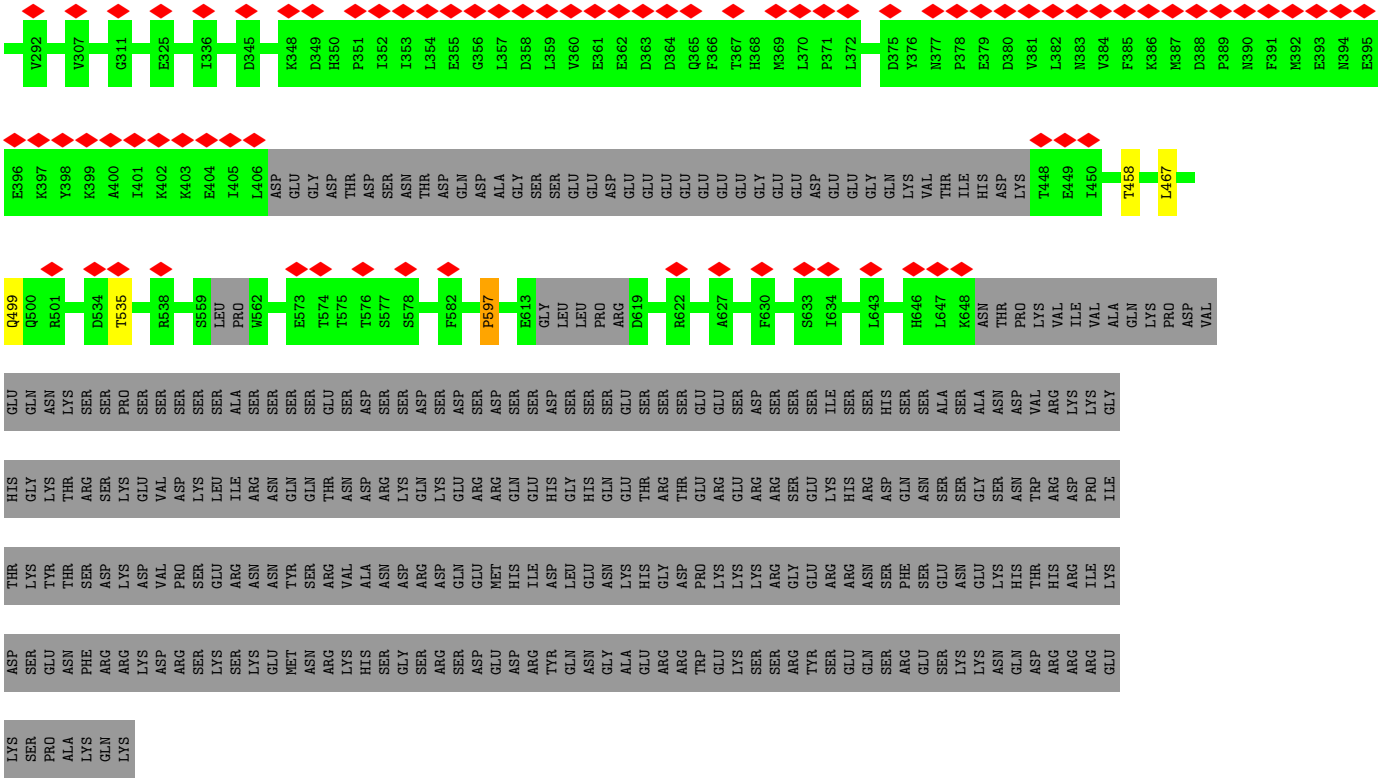






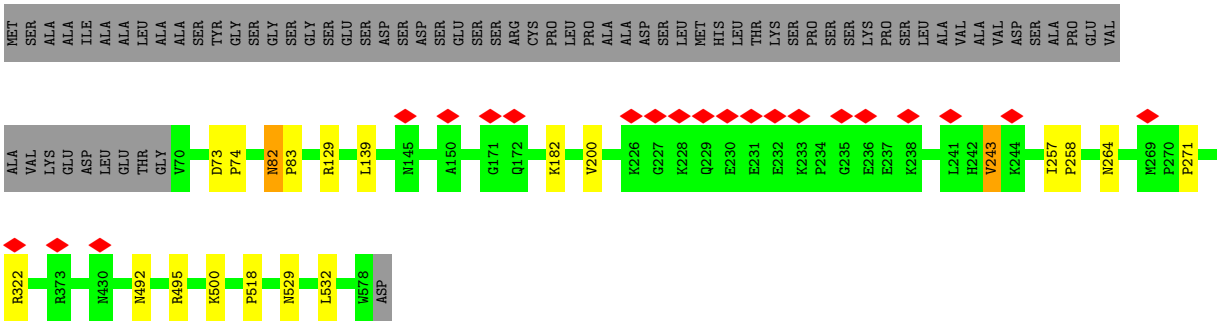
• Molecule 22: Pre-mRNA-splicing factor CWC22 homolog





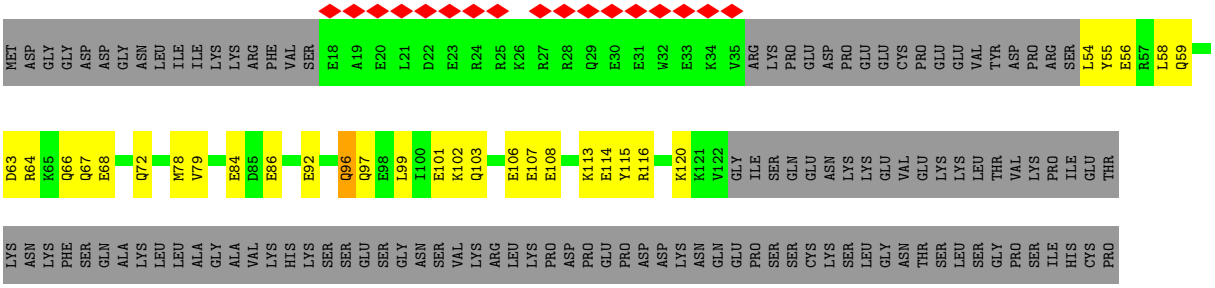
• Molecule 23: Pre-mRNA-processing factor 17

Chain W:

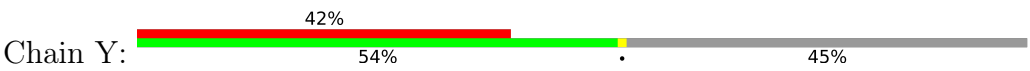


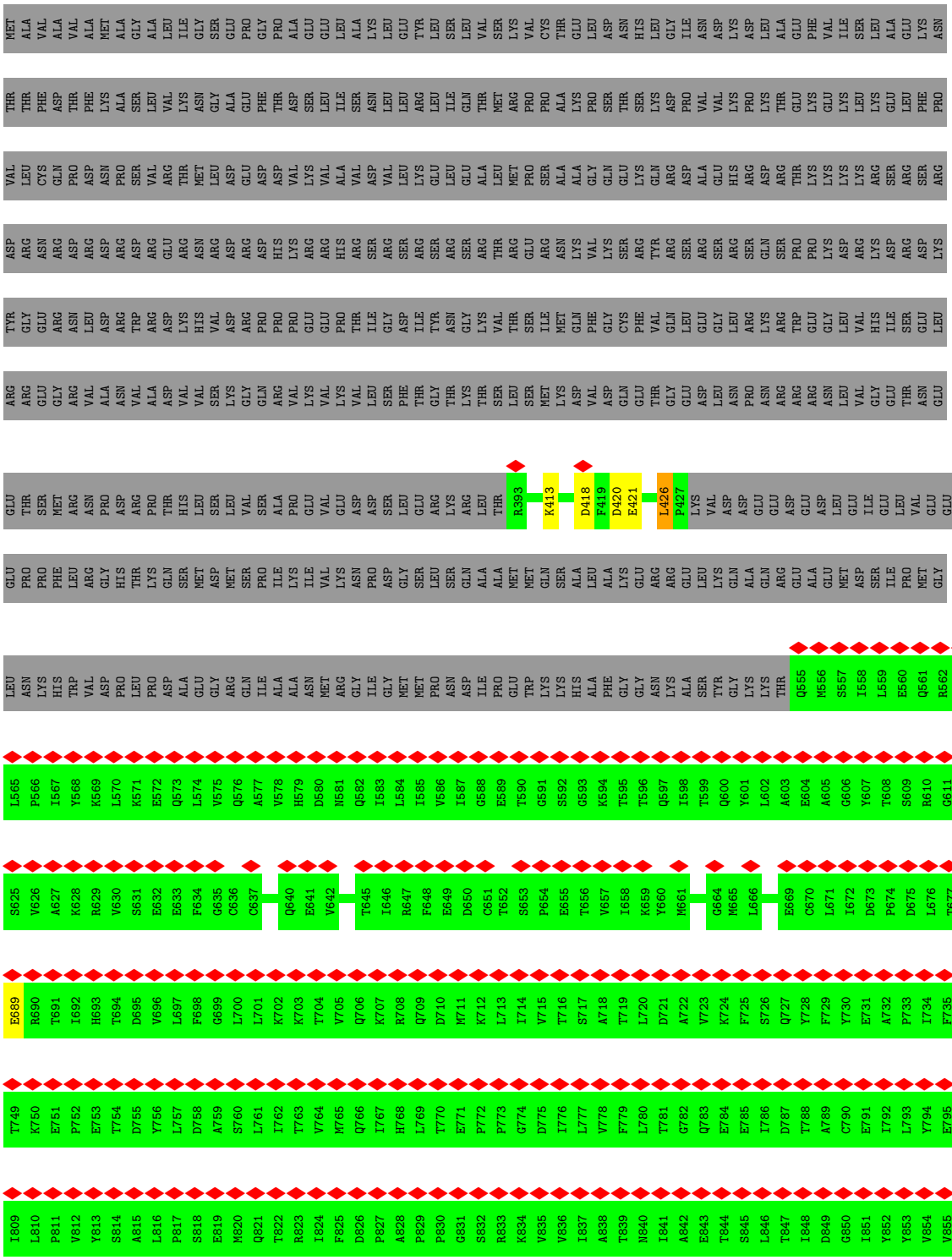
• Molecule 24: PSME3-interacting protein

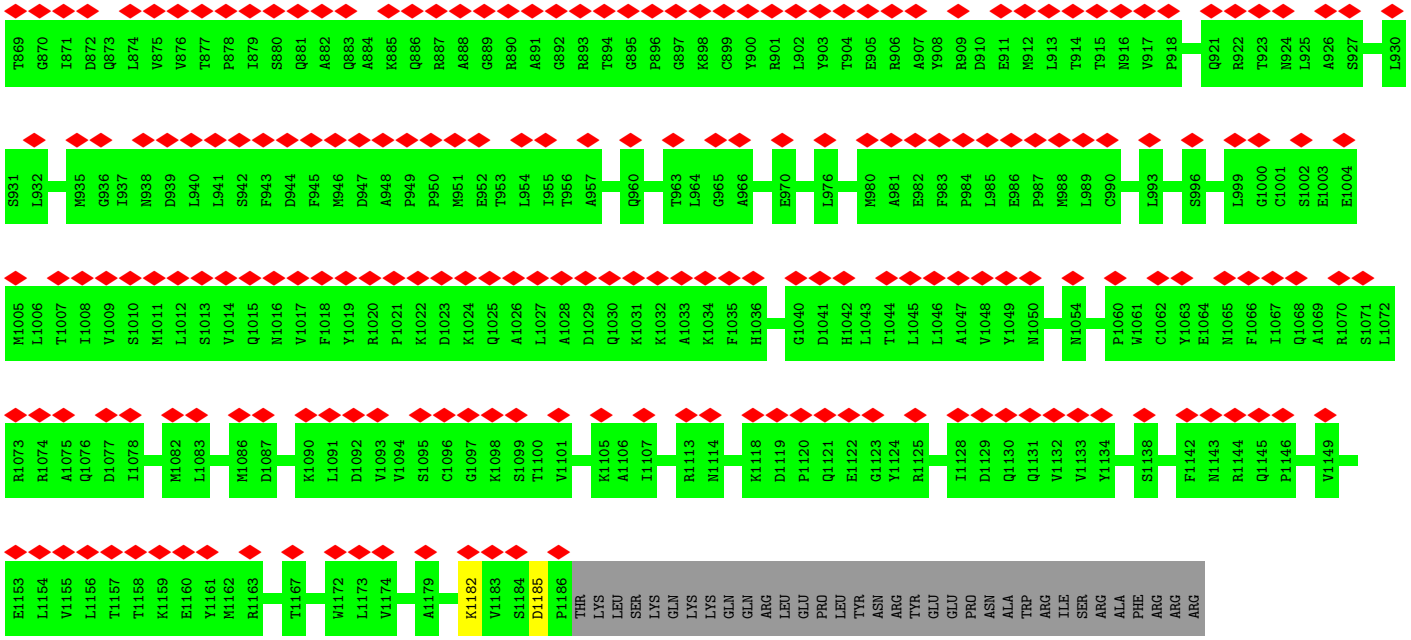
Chain X:



• Molecule 25: ATP-dependent RNA helicase DHX8

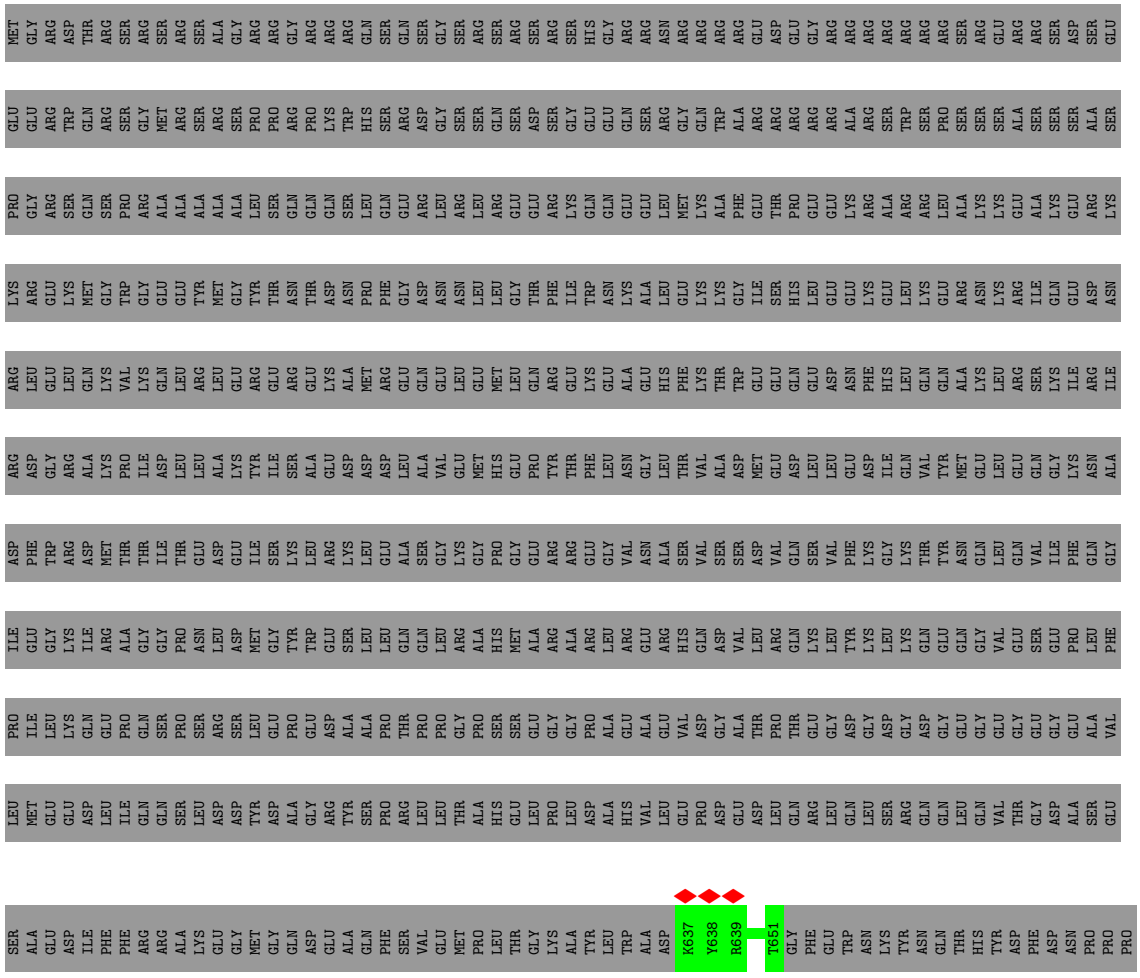


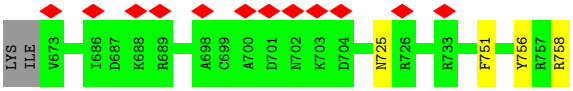




- Molecule 26: Cactin

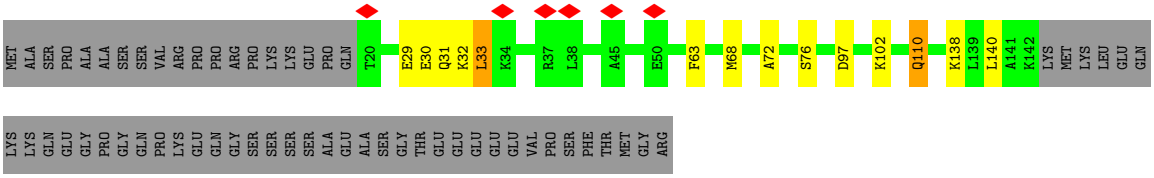
Chain Z:





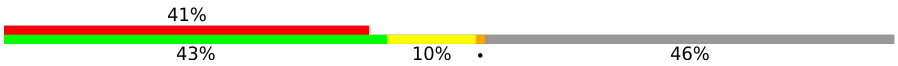
• Molecule 27: PRKR-interacting protein 1

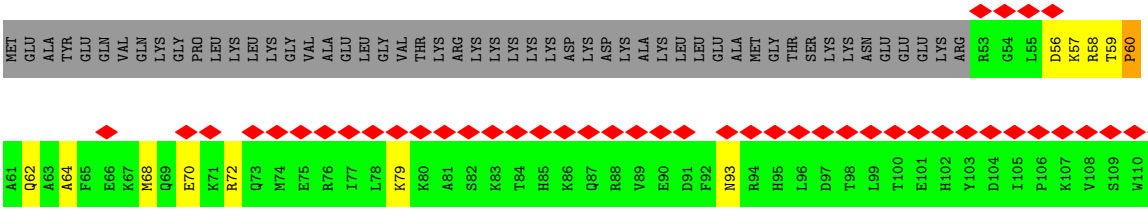
Chain 2:



• Molecule 28: Protein FAM32A

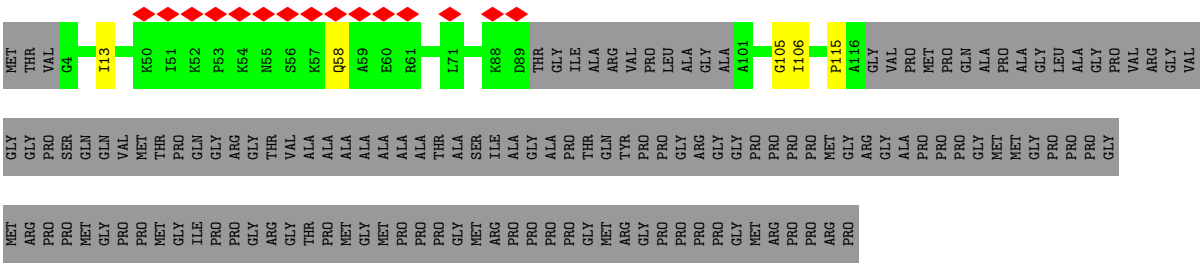
Chain z:





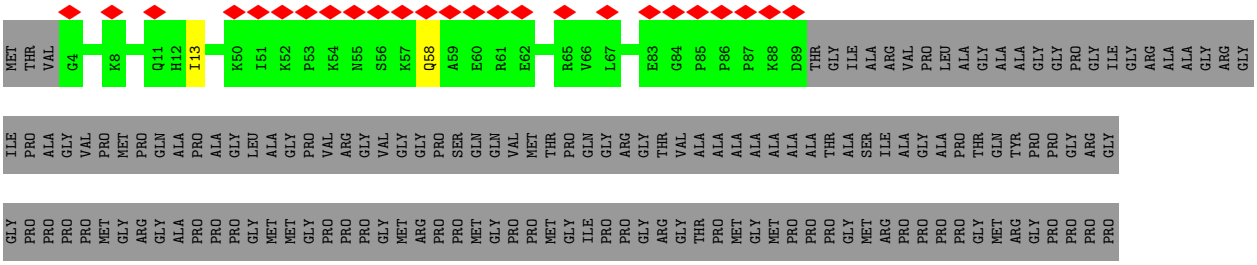
• Molecule 29: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain b:

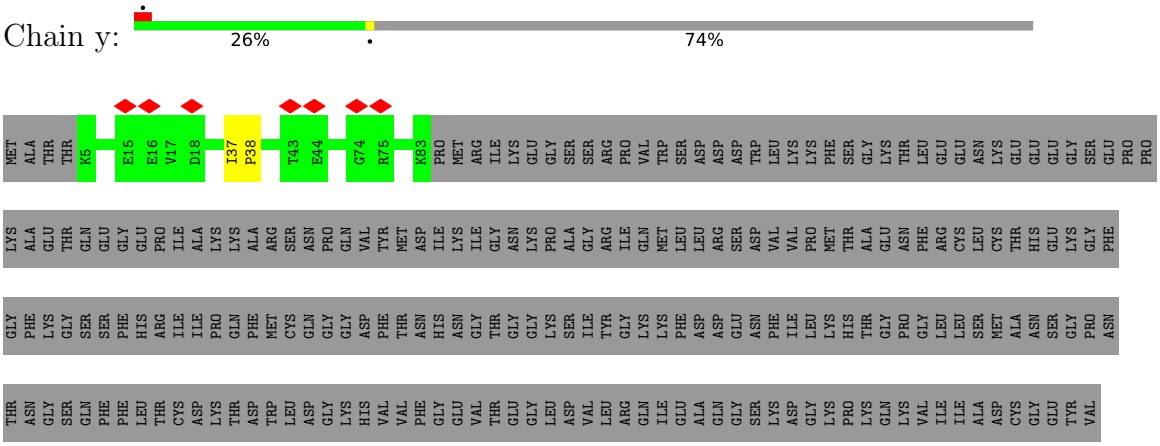


• Molecule 29: Small nuclear ribonucleoprotein-associated proteins B and B'

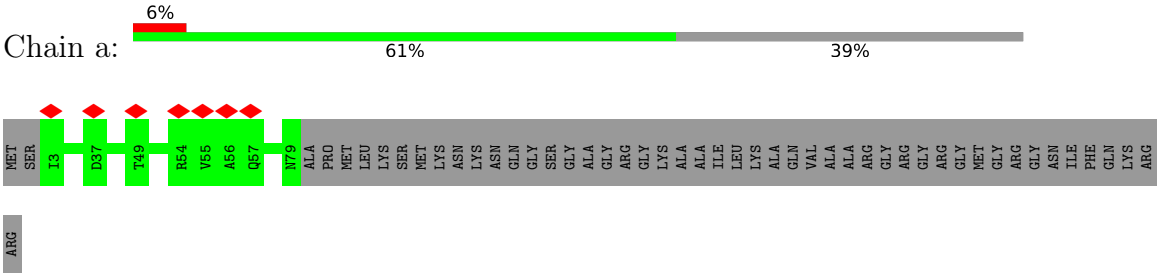
Chain i:



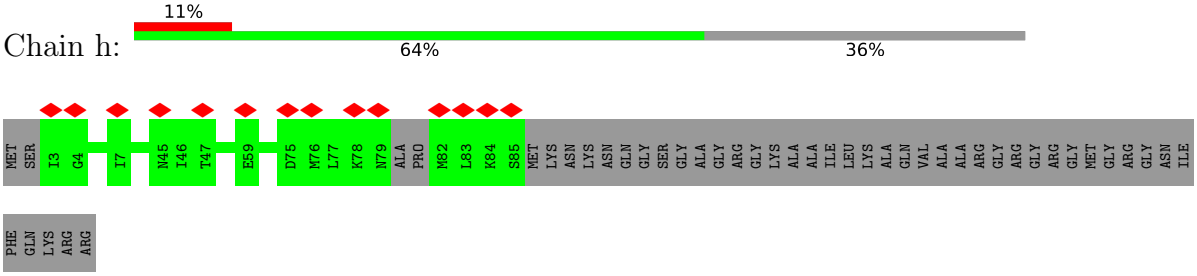
• Molecule 30: Peptidyl-prolyl cis-trans isomerase E



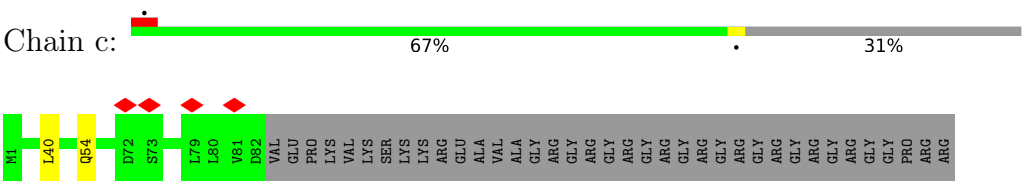
• Molecule 31: Small nuclear ribonucleoprotein Sm D3



• Molecule 31: Small nuclear ribonucleoprotein Sm D3

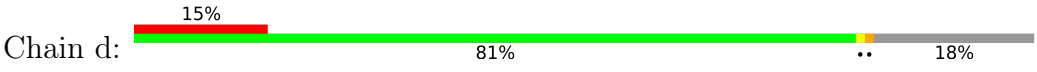


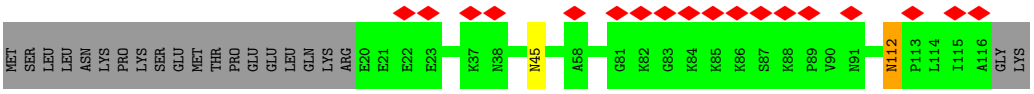
• Molecule 32: Small nuclear ribonucleoprotein Sm D1



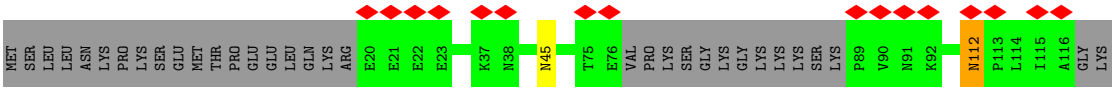
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

• Molecule 33: Small nuclear ribonucleoprotein Sm D2

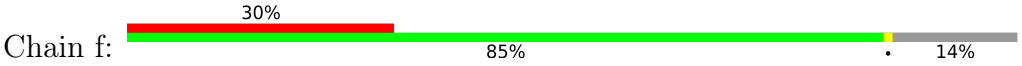


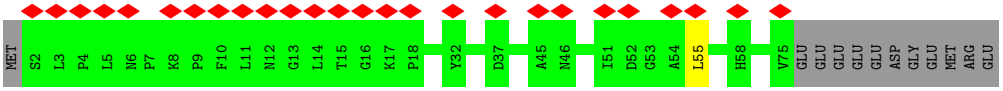


• Molecule 33: Small nuclear ribonucleoprotein Sm D2

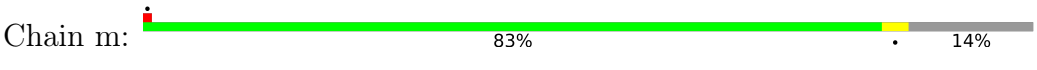


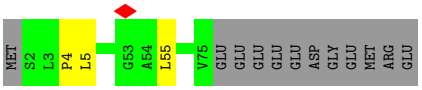
• Molecule 34: Small nuclear ribonucleoprotein F



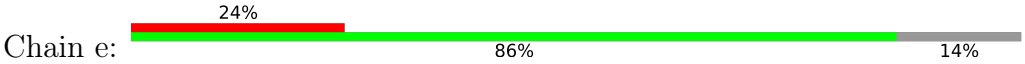


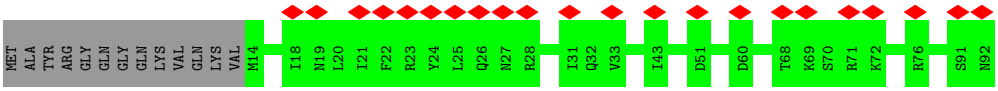
• Molecule 34: Small nuclear ribonucleoprotein F



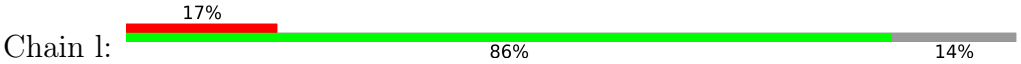


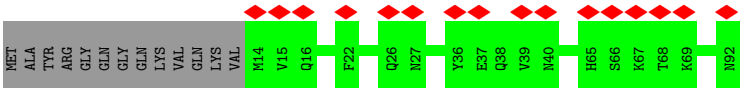
• Molecule 35: Small nuclear ribonucleoprotein E





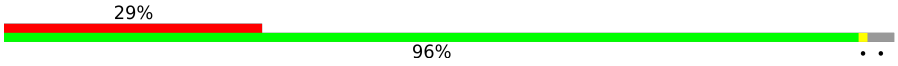
• Molecule 35: Small nuclear ribonucleoprotein E

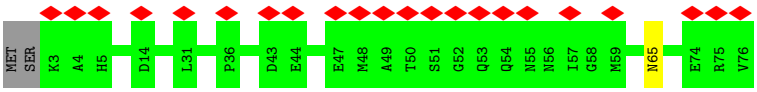




• Molecule 36: Small nuclear ribonucleoprotein G

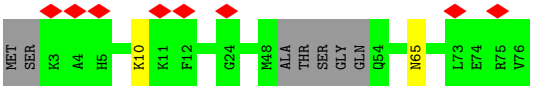
Chain g:





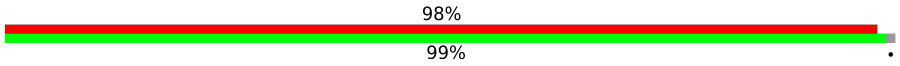
• Molecule 36: Small nuclear ribonucleoprotein G

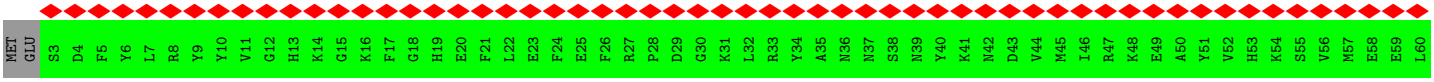
Chain n:

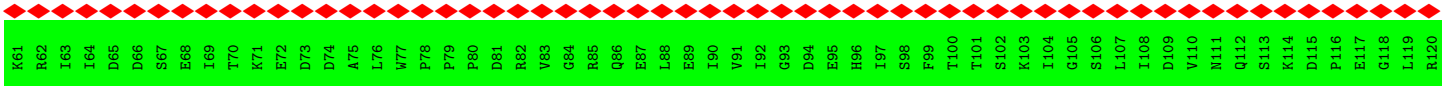


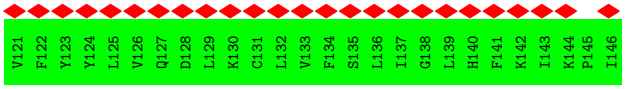
• Molecule 37: Protein mago nashi homolog

Chain v:



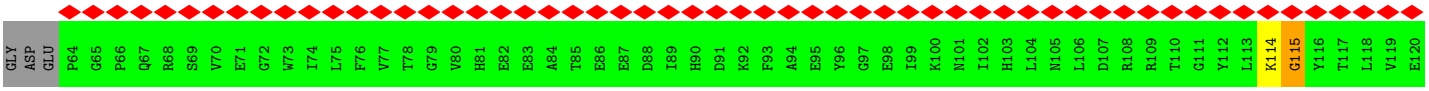


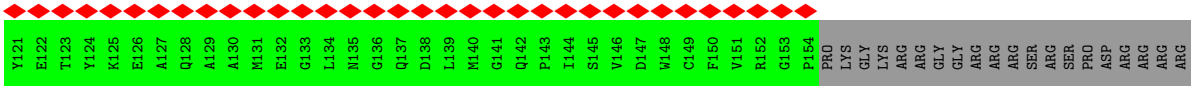




• Molecule 38: RNA-binding protein 8A

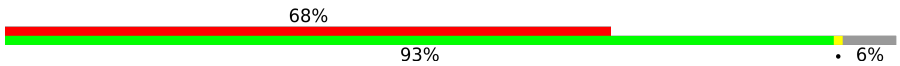
Chain w:

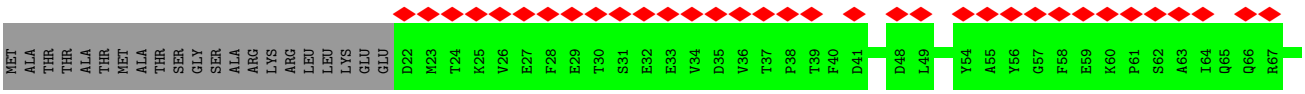


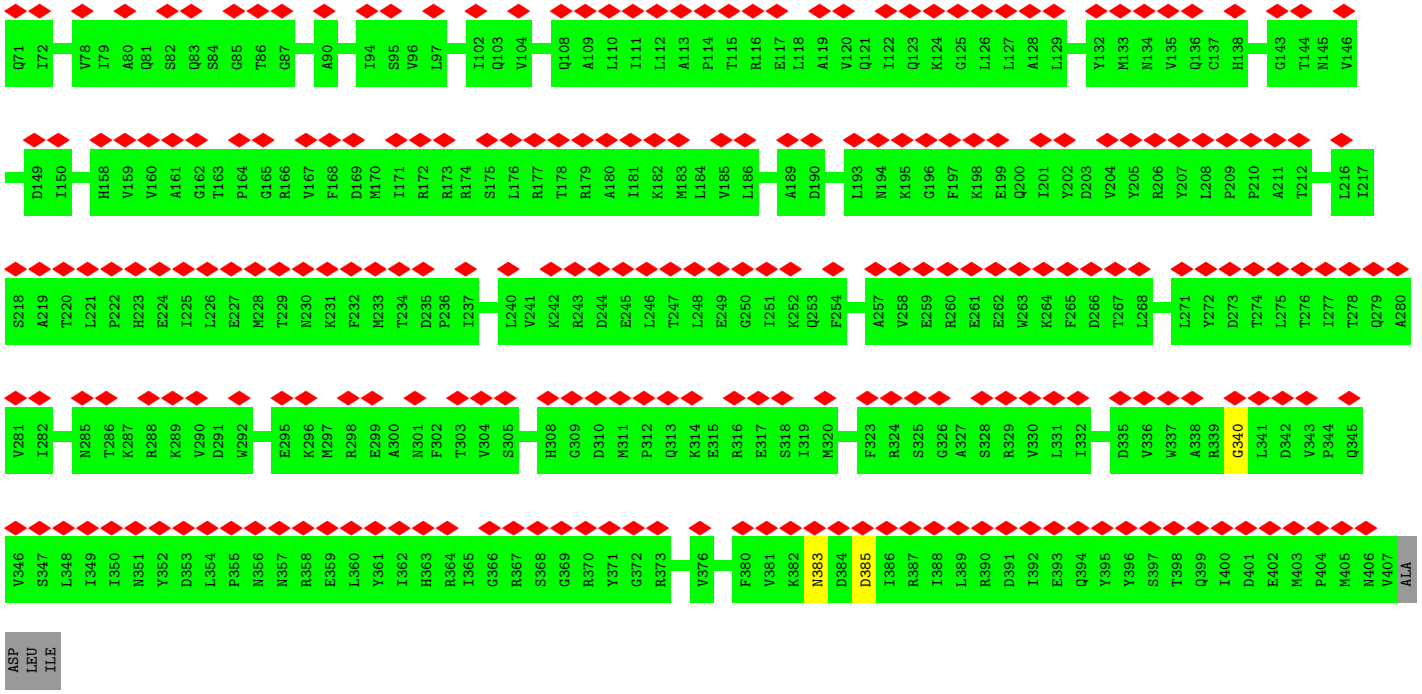


• Molecule 39: Eukaryotic initiation factor 4A-III

Chain u:

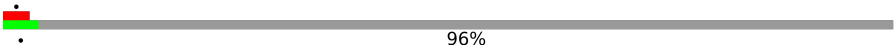


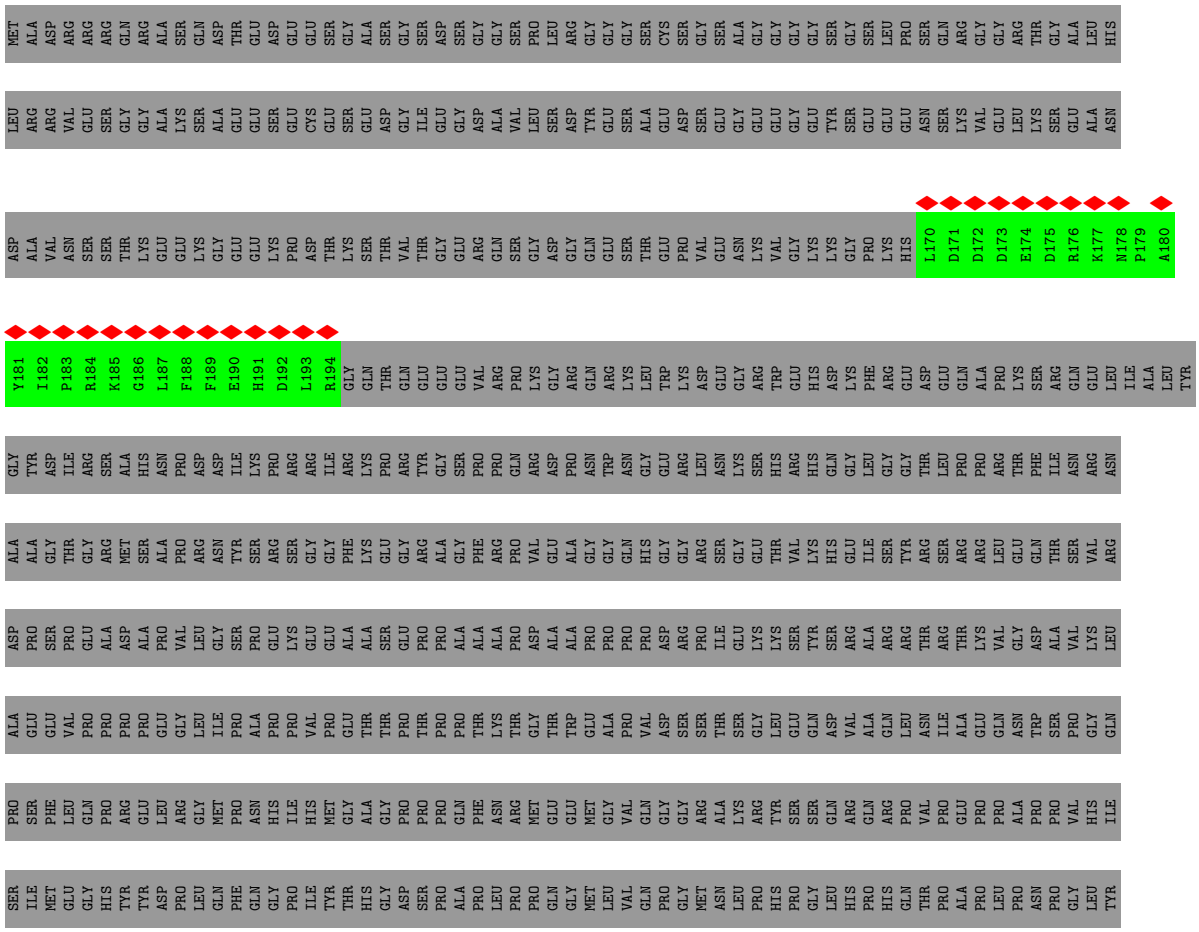


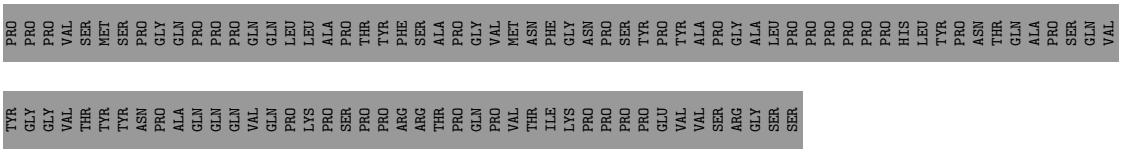


- Molecule 40: Protein CASC3

Chain x:

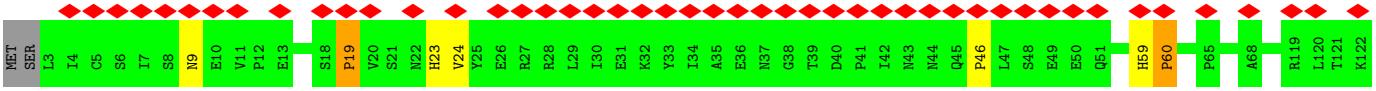


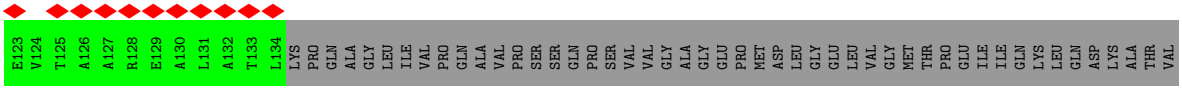


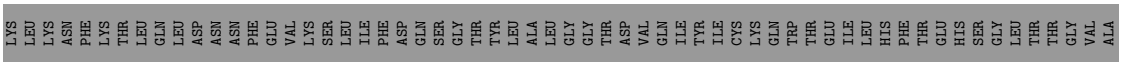


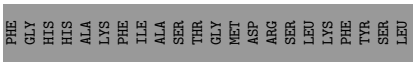
• Molecule 41: Pre-mRNA-processing factor 19

Chain q:



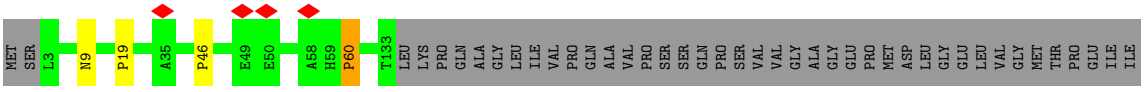






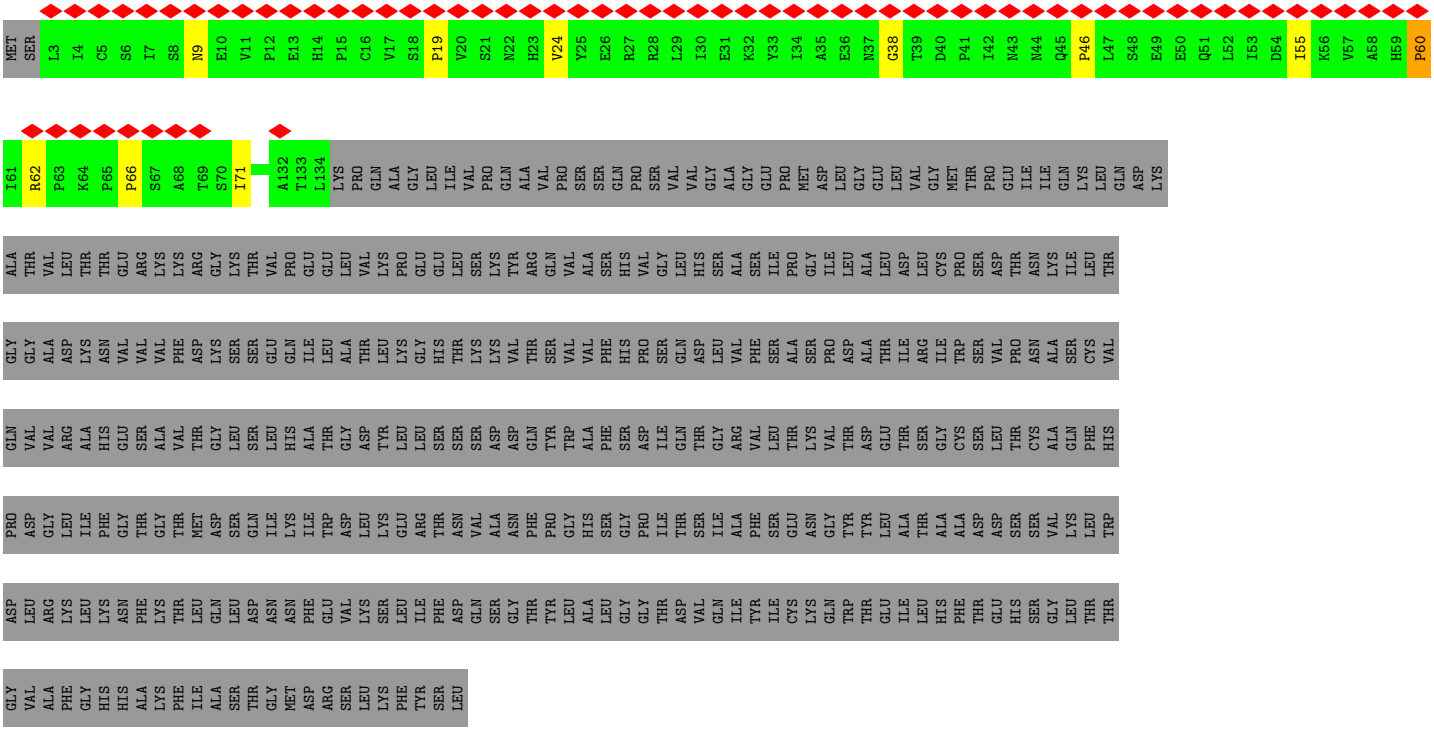
• Molecule 41: Pre-mRNA-processing factor 19

Chain r:



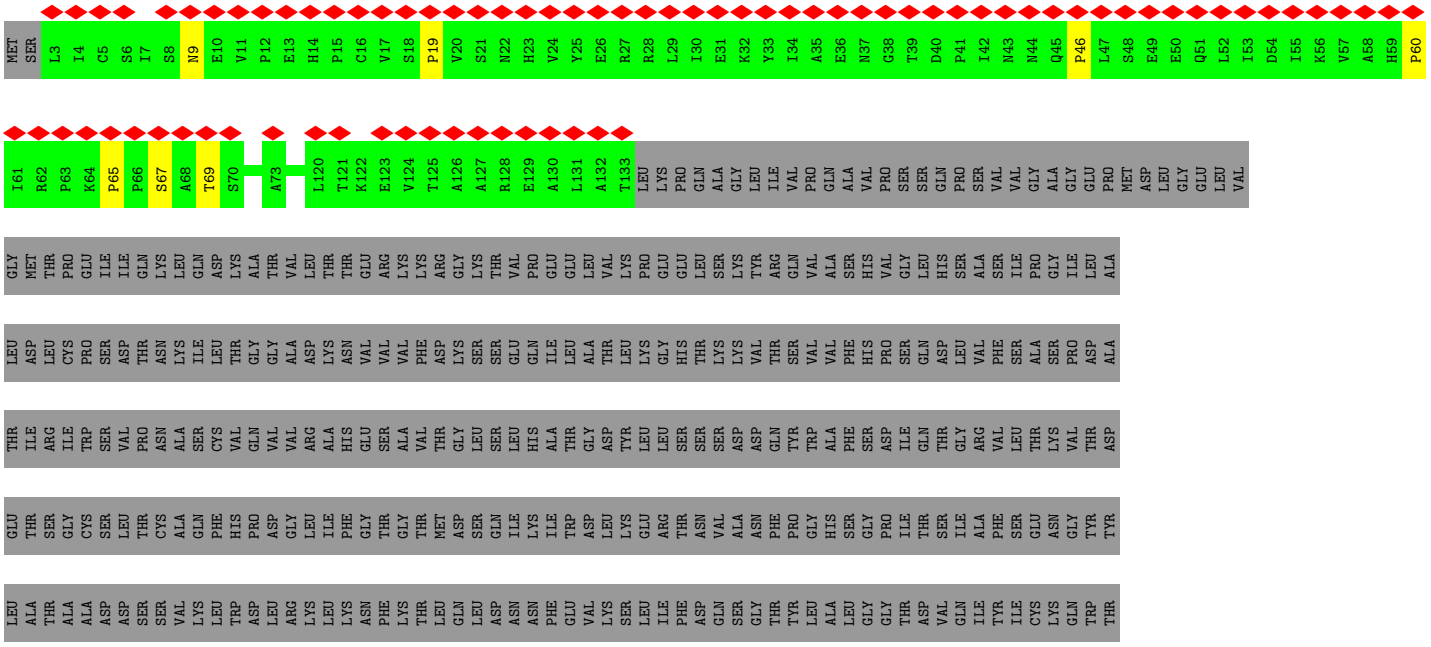
• Molecule 41: Pre-mRNA-processing factor 19

Chain s:

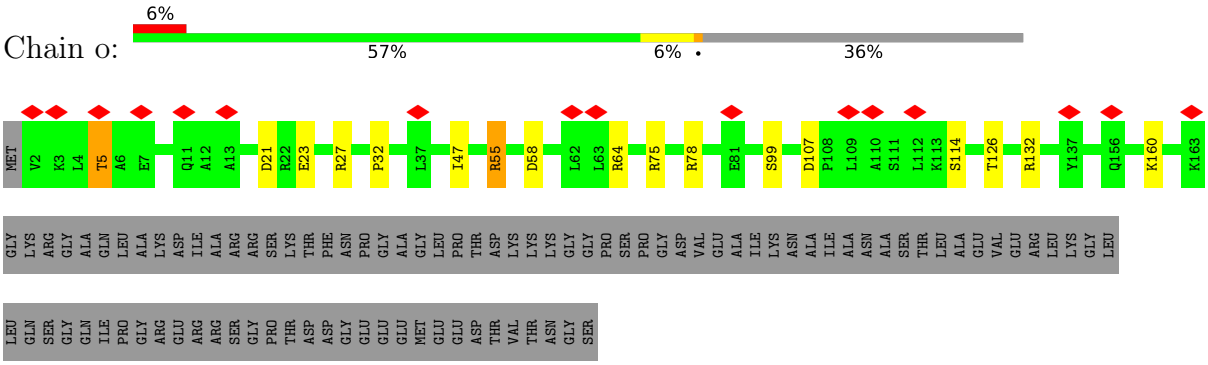


• Molecule 41: Pre-mRNA-processing factor 19

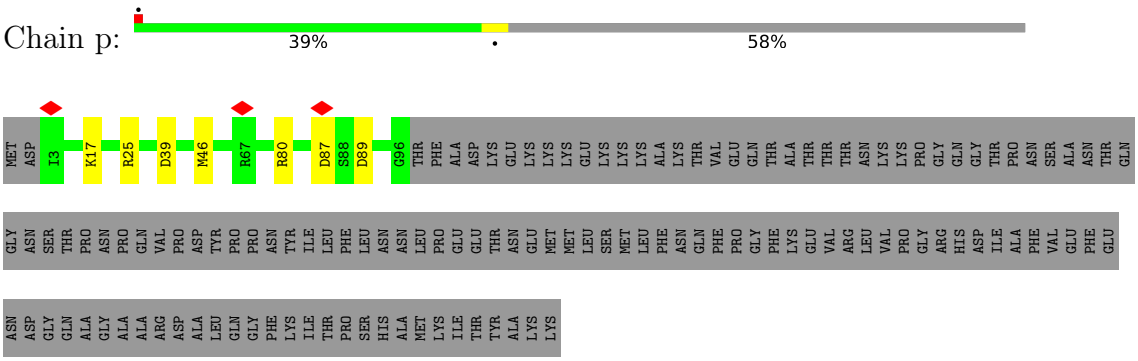
Chain t:



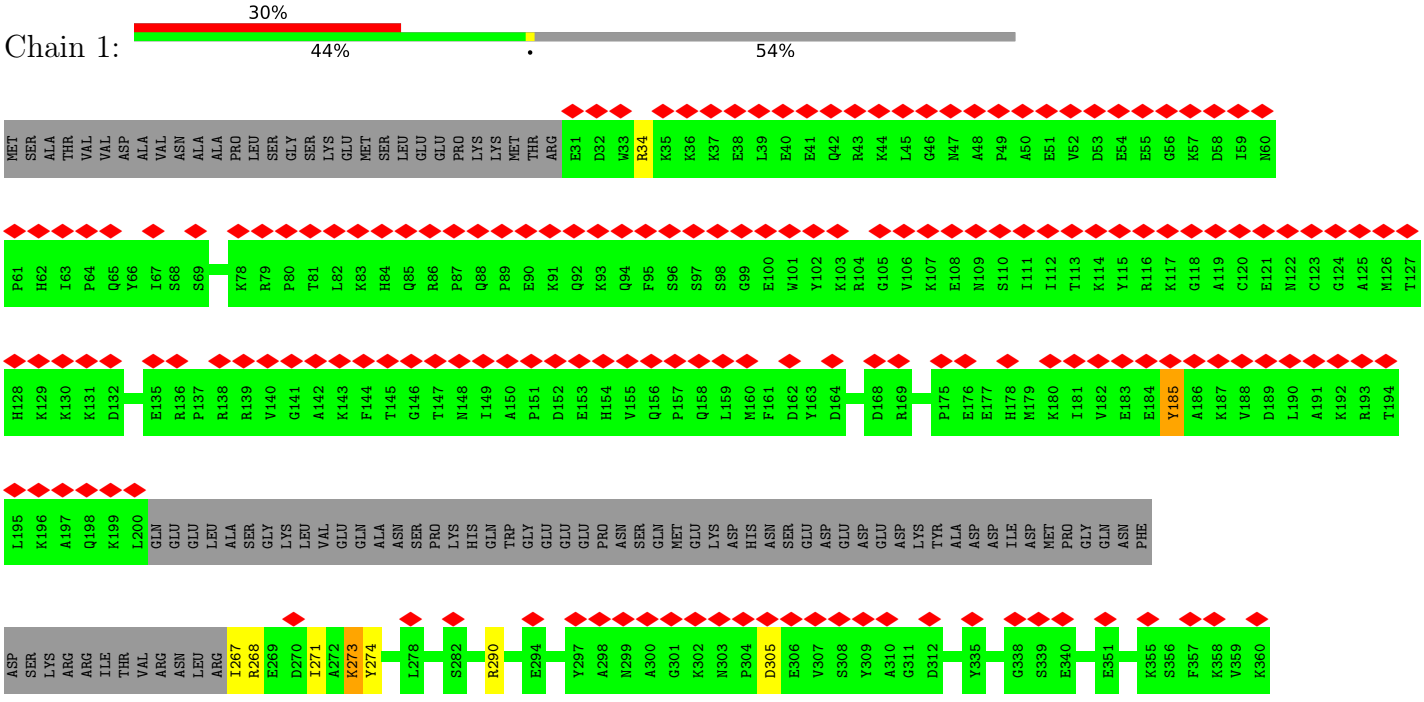
• Molecule 42: U2 small nuclear ribonucleoprotein A'

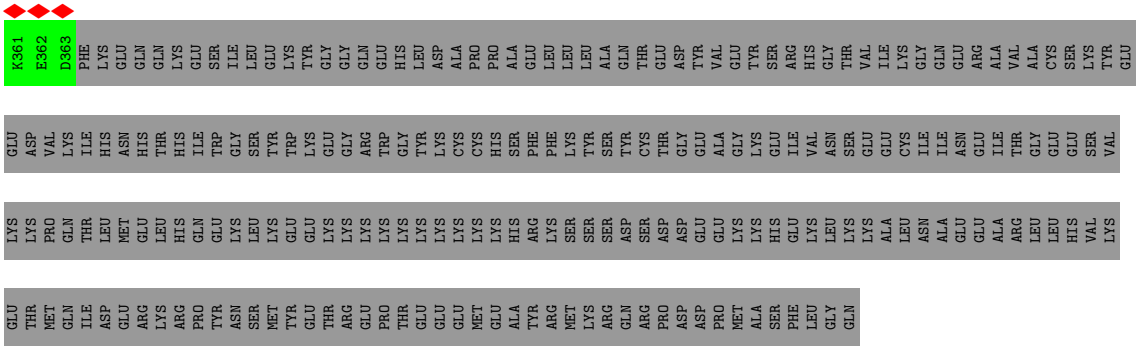


• Molecule 43: U2 small nuclear ribonucleoprotein B"



• Molecule 44: Pre-mRNA-splicing factor SLU7




K361 E362 D363 PHE LYS GLU GLN GLN LYS GLU SER ILE LEU GLU LYS TYR GLY GLY GLN GLU HIS LEU ASP ALA PRO PRO ALA GLU LEU LEU LEU ALA GLN THR GLU ASP TYR VAL GLU TYR SER ARG HIS GLY THR VAL ILE LYS GLY GLN GLU ARG ALA VAL ALA CYS SER LYS TYR GLU
GLU ASP VAL LYS ILE HIS ASN HIS THR HIS ILE TRP GLY SER TYR TRP LYS GLU GLY ARG TRP GLY TYR LYS CYS CYS HIS SER PHE PHE LYS TYR SER TYR CYS THR GLY GLU ALA GLY LYS GLU ILE VAL ASN SER GLU GLU CYS ILE ILE ASN GLU ILE THR GLY GLU GLU SER VAL
LYS LYS PRO GLN THR LEU MET GLU LEU HIS GLN GLU LYS LEU LYS GLU GLU LYS LYS LYS LYS LYS LYS LYS LYS LYS HIS ARG LYS SER SER SER ASP SER ASP ASP GLU GLU LYS LYS HIS GLU LYS LEU LYS LYS ALA LEU ASN ALA GLU GLU ALA ARG LEU LEU HIS VAL LYS
GLU THR MET GLN ILE ASP GLU ARG LYS ARG PRO TYR ASN SER MET TYR GLU THR ARG GLU PRO THR GLU GLU GLU MET GLU ALA TYR ARG MET LYS ARG GLN ARG PRO ASP ASP PRO MET ALA SER PHE LEU GLY GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212224	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.505	Depositor
Minimum map value	-1.600	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.39	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, SEP, 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	A	0.82	16/16897 (0.1%)	0.90	55/22917 (0.2%)
2	B	0.61	1/1970 (0.1%)	0.84	4/3060 (0.1%)
3	C	0.58	0/6942	0.73	3/9432 (0.0%)
4	E	0.56	0/2392	0.66	0/3242
5	F	0.49	0/2323	0.78	2/3619 (0.1%)
6	4	1.34	0/307	1.53	7/476 (1.5%)
7	G	0.63	4/1674 (0.2%)	1.24	19/2594 (0.7%)
8	H	0.95	26/3305 (0.8%)	1.63	112/5130 (2.2%)
9	I	0.46	0/3884	0.86	10/5301 (0.2%)
10	J	0.57	0/3851	0.61	6/5227 (0.1%)
11	K	0.39	0/768	0.51	2/1067 (0.2%)
12	L	0.49	0/3046	0.64	2/4115 (0.0%)
13	M	0.54	0/1119	0.70	1/1497 (0.1%)
14	N	0.77	3/1210 (0.2%)	0.69	0/1622
15	O	0.60	1/2344 (0.0%)	0.69	3/3163 (0.1%)
16	P	0.66	0/967	0.87	2/1285 (0.2%)
17	Q	0.23	0/6565	0.43	0/9143
18	R	0.72	2/2091 (0.1%)	0.83	7/2809 (0.2%)
19	S	0.51	0/1268	0.64	1/1714 (0.1%)
20	T	0.81	0/2519	0.82	5/3433 (0.1%)
21	U	0.49	0/424	0.59	0/582
22	V	0.34	0/2642	0.56	1/3602 (0.0%)
23	W	0.46	0/4237	0.72	4/5723 (0.1%)
24	X	0.78	0/706	1.35	6/941 (0.6%)
25	Y	0.55	1/3436 (0.0%)	0.78	4/4774 (0.1%)
26	Z	0.36	0/936	0.65	0/1258
27	2	0.45	0/1030	0.85	4/1371 (0.3%)
28	z	0.73	2/513 (0.4%)	0.96	3/683 (0.4%)
29	b	0.55	0/797	0.81	0/1062
29	i	0.53	0/700	0.82	0/933
30	y	0.86	2/389 (0.5%)	0.75	0/540
31	a	0.46	0/616	0.66	0/830

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	h	0.47	0/639	0.68	0/857
32	c	0.56	0/657	0.77	0/888
32	j	0.56	0/657	0.77	0/888
33	d	0.69	0/786	0.86	0/1053
33	k	0.69	0/696	0.86	0/935
34	f	0.82	0/588	0.84	0/795
34	m	0.82	0/584	0.86	0/791
35	e	0.62	0/660	0.83	0/886
35	l	0.62	0/660	0.84	0/886
36	g	0.53	0/584	0.78	0/779
36	n	0.53	0/548	0.86	1/729 (0.1%)
37	v	0.31	0/710	0.65	0/987
38	w	0.31	0/444	0.78	2/614 (0.3%)
39	u	0.32	0/1906	0.69	0/2653
40	x	0.34	0/123	0.70	0/170
41	q	0.35	0/658	0.63	3/919 (0.3%)
41	r	0.32	0/653	0.59	3/912 (0.3%)
41	s	0.34	0/658	0.66	3/919 (0.3%)
41	t	0.35	0/653	0.59	3/912 (0.3%)
42	o	0.59	0/1299	1.63	17/1761 (1.0%)
43	p	0.56	0/774	1.35	6/1035 (0.6%)
44	1	0.40	0/2247	0.65	2/3024 (0.1%)
All	All	0.61	58/99052 (0.1%)	0.84	303/136538 (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	21
3	C	0	9
4	E	0	1
9	I	0	7
10	J	0	5
14	N	0	4
15	O	0	1
16	P	0	3
18	R	0	7
20	T	0	3
23	W	0	2
27	2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	d	0	1
33	k	0	1
All	All	0	66

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	y	38	PRO	N-CA	14.01	1.71	1.47
1	A	1724	PRO	N-CA	12.47	1.68	1.47
28	z	60	PRO	N-CA	12.15	1.68	1.47
18	R	223	PRO	N-CA	11.88	1.67	1.47
25	Y	426	LEU	C-N	9.37	1.52	1.34
1	A	1955	LYS	C-N	9.33	1.51	1.34
7	G	21	A	O3'-P	-8.42	1.51	1.61
1	A	1572	SER	CA-CB	-8.06	1.40	1.52
8	H	142	C	C1'-N1	7.46	1.59	1.48
8	H	77	C	C1'-N1	7.45	1.59	1.48
7	G	98	U	O3'-P	-7.28	1.52	1.61
8	H	55	U	C1'-N1	7.00	1.59	1.48
8	H	72	U	C1'-N1	7.00	1.59	1.48
2	B	103	G	C1'-N9	-6.98	1.37	1.46
8	H	54	U	C1'-N1	6.97	1.59	1.48
8	H	92	U	C1'-N1	6.96	1.59	1.48
8	H	74	U	C1'-N1	6.93	1.59	1.48
14	N	101	CYS	CB-SG	-6.92	1.70	1.82
8	H	60	U	C1'-N1	6.90	1.59	1.48
8	H	89	U	C1'-N1	6.89	1.59	1.48
8	H	69	U	C1'-N1	6.89	1.59	1.48
8	H	58	U	C1'-N1	6.88	1.59	1.48
8	H	91	U	C1'-N1	6.86	1.59	1.48
8	H	150	U	C1'-N1	6.78	1.58	1.48
8	H	182	U	C1'-N1	6.78	1.58	1.48
8	H	151	C	C1'-N1	6.49	1.58	1.48
8	H	73	C	C1'-N1	6.47	1.58	1.48
8	H	141	C	C1'-N1	6.43	1.58	1.48
8	H	184	C	C1'-N1	6.39	1.58	1.48
8	H	67	C	C1'-N1	6.37	1.58	1.48
8	H	97	G	C1'-N9	-6.37	1.38	1.46
8	H	71	C	C1'-N1	6.34	1.58	1.48
8	H	148	C	C1'-N1	6.33	1.58	1.48
30	y	37	ILE	C-N	6.29	1.46	1.34
8	H	70	C	C1'-N1	6.28	1.58	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	78	C	C1'-N1	6.27	1.58	1.48
8	H	84	C	C1'-N1	6.27	1.58	1.48
1	A	1534	PHE	C-O	-6.24	1.11	1.23
7	G	121	C	O3'-P	6.12	1.68	1.61
1	A	1535	THR	C-O	-6.07	1.11	1.23
1	A	167	PRO	N-CD	-6.03	1.39	1.47
1	A	863	GLU	CD-OE1	-6.03	1.19	1.25
1	A	776	LEU	C-O	-5.95	1.12	1.23
7	G	3	A	O3'-P	-5.86	1.54	1.61
1	A	863	GLU	CD-OE2	-5.85	1.19	1.25
18	R	219	PRO	C-O	-5.82	1.11	1.23
28	z	59	THR	C-N	5.80	1.45	1.34
15	O	27	CYS	CB-SG	-5.62	1.72	1.81
1	A	771	VAL	C-O	-5.43	1.13	1.23
1	A	1536	LEU	C-O	-5.41	1.13	1.23
14	N	137	CYS	CB-SG	-5.40	1.73	1.81
14	N	119	CYS	CB-SG	-5.31	1.73	1.81
1	A	1883	VAL	C-N	5.25	1.46	1.34
1	A	1537	TRP	C-O	-5.24	1.13	1.23
1	A	859	SER	CA-CB	-5.24	1.45	1.52
1	A	1552	GLN	C-O	-5.13	1.13	1.23
8	H	110	A	C1'-N9	-5.11	1.39	1.46
1	A	1438	VAL	CB-CG1	-5.09	1.42	1.52

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	o	55	ARG	NE-CZ-NH1	15.10	127.85	120.30
1	A	772	CYS	CA-CB-SG	-13.85	89.08	114.00
42	o	55	ARG	CD-NE-CZ	13.73	142.82	123.60
7	G	120	G	O4'-C1'-N9	-12.98	97.81	108.20
1	A	1741	TYR	CB-CA-C	-12.20	86.00	110.40
8	H	167	U	C5-C4-O4	11.85	133.01	125.90
42	o	55	ARG	NE-CZ-NH2	-11.44	114.58	120.30
7	G	130	G	N9-C1'-C2'	-11.44	99.13	114.00
1	A	167	PRO	CA-N-CD	-11.26	95.73	111.50
42	o	75	ARG	NE-CZ-NH1	-11.26	114.67	120.30
27	2	29	GLU	CB-CA-C	11.13	132.66	110.40
1	A	1534	PHE	CB-CA-C	-11.09	88.22	110.40
6	4	-12	G	N9-C1'-C2'	-11.03	99.66	114.00
1	A	1561	PHE	CB-CA-C	-10.28	89.84	110.40
1	A	1530	PRO	CA-N-CD	-10.23	97.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	164	C	N1-C2-O2	-10.08	112.85	118.90
24	X	115	TYR	CB-CA-C	9.93	130.26	110.40
8	H	31	G	N9-C1'-C2'	-9.83	101.18	112.00
25	Y	420	ASP	CB-CA-C	-9.74	90.92	110.40
1	A	1584	LYS	CB-CA-C	-9.68	91.04	110.40
1	A	1744	ARG	CB-CG-CD	-9.45	87.02	111.60
7	G	130	G	C4'-C3'-O3'	9.45	131.89	113.00
1	A	1883	VAL	C-N-CA	-9.42	98.16	121.70
1	A	1587	GLU	CB-CA-C	-9.25	91.90	110.40
7	G	1	G	N9-C1'-C2'	-9.24	101.84	112.00
24	X	96	GLN	CB-CA-C	-9.21	91.98	110.40
43	p	25	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	A	1744	ARG	CB-CA-C	-8.98	92.44	110.40
5	F	56	A	O5'-P-OP1	-8.94	97.66	105.70
8	H	162	U	N3-C2-O2	-8.91	115.96	122.20
24	X	107	GLU	CB-CA-C	-8.87	92.67	110.40
43	p	80	ARG	CD-NE-CZ	8.85	135.99	123.60
2	B	20	G	N9-C1'-C2'	8.51	125.06	114.00
6	4	-6	C	C2-N1-C1'	8.49	128.13	118.80
1	A	1754	TYR	CB-CA-C	-8.40	93.61	110.40
28	z	60	PRO	CA-N-CD	-8.36	99.80	111.50
8	H	164	C	C5'-C4'-O4'	-8.35	99.08	109.10
7	G	3	A	N9-C1'-C2'	-8.31	102.86	112.00
8	H	169	C	P-O3'-C3'	8.21	129.55	119.70
1	A	861	ARG	CG-CD-NE	-8.20	94.59	111.80
9	I	84	HIS	O-C-N	-8.14	109.67	122.70
9	I	83	LYS	O-C-N	-8.14	109.68	122.70
9	I	311	MET	O-C-N	-8.13	109.69	122.70
9	I	310	LYS	O-C-N	-8.12	109.71	122.70
8	H	166	G	O4'-C1'-N9	8.07	114.65	108.20
1	A	1571	ILE	CB-CA-C	-8.06	95.47	111.60
9	I	309	ALA	O-C-N	-8.05	109.83	122.70
8	H	167	U	N3-C4-O4	-8.04	113.77	119.40
15	O	193	LEU	CA-CB-CG	7.88	133.42	115.30
7	G	1	G	C1'-C2'-O2'	-7.87	86.99	110.60
36	n	10	LYS	CB-CA-C	7.85	126.10	110.40
7	G	125	C	P-O3'-C3'	7.80	129.06	119.70
20	T	402	ASP	CB-CG-OD1	7.68	125.21	118.30
42	o	107	ASP	CB-CG-OD1	7.62	125.15	118.30
8	H	167	U	N1-C2-O2	7.59	128.11	122.80
8	H	164	C	P-O3'-C3'	7.49	128.69	119.70
1	A	1530	PRO	N-CA-CB	7.42	112.20	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	164	C	N3-C2-O2	7.41	127.09	121.90
1	A	663	ARG	CG-CD-NE	-7.40	96.26	111.80
42	o	27	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	1724	PRO	N-CA-C	-7.36	92.97	112.10
8	H	69	U	OP2-P-O3'	7.28	121.21	105.20
7	G	122	U	N1-C1'-C2'	-7.28	103.99	112.00
8	H	114	A	OP2-P-O3'	7.27	121.19	105.20
8	H	73	C	OP2-P-O3'	7.25	121.16	105.20
8	H	148	C	OP2-P-O3'	7.25	121.14	105.20
8	H	183	G	OP2-P-O3'	7.23	121.11	105.20
8	H	59	A	OP2-P-O3'	7.22	121.09	105.20
8	H	88	A	OP2-P-O3'	7.22	121.10	105.20
8	H	70	C	OP2-P-O3'	7.22	121.09	105.20
8	H	82	G	OP2-P-O3'	7.22	121.08	105.20
8	H	55	U	OP2-P-O3'	7.22	121.08	105.20
18	R	223	PRO	CA-N-CD	-7.22	101.40	111.50
8	H	71	C	OP2-P-O3'	7.21	121.07	105.20
8	H	149	A	OP2-P-O3'	7.21	121.07	105.20
8	H	113	G	OP2-P-O3'	7.21	121.07	105.20
8	H	72	U	OP2-P-O3'	7.21	121.06	105.20
8	H	77	C	OP2-P-O3'	7.21	121.05	105.20
8	H	141	C	OP2-P-O3'	7.21	121.06	105.20
8	H	180	G	OP2-P-O3'	7.20	121.04	105.20
8	H	182	U	OP2-P-O3'	7.20	121.04	105.20
8	H	81	G	OP2-P-O3'	7.20	121.03	105.20
8	H	92	U	OP2-P-O3'	7.20	121.04	105.20
8	H	91	U	OP2-P-O3'	7.20	121.03	105.20
8	H	54	U	OP2-P-O3'	7.20	121.03	105.20
8	H	78	C	OP2-P-O3'	7.19	121.03	105.20
8	H	79	G	OP2-P-O3'	7.19	121.02	105.20
8	H	57	A	OP2-P-O3'	7.19	121.02	105.20
8	H	68	G	OP2-P-O3'	7.19	121.02	105.20
8	H	90	A	OP2-P-O3'	7.19	121.01	105.20
8	H	93	A	OP2-P-O3'	7.18	121.01	105.20
8	H	74	U	OP2-P-O3'	7.18	121.00	105.20
8	H	181	G	OP2-P-O3'	7.18	121.00	105.20
8	H	67	C	OP2-P-O3'	7.18	120.99	105.20
8	H	58	U	OP2-P-O3'	7.17	120.98	105.20
8	H	89	U	OP2-P-O3'	7.17	120.98	105.20
8	H	84	C	OP2-P-O3'	7.17	120.97	105.20
8	H	150	U	OP2-P-O3'	7.16	120.96	105.20
8	H	56	A	OP2-P-O3'	7.16	120.95	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	80	A	OP2-P-O3'	7.15	120.94	105.20
8	H	83	A	OP2-P-O3'	7.14	120.90	105.20
8	H	168	A	P-O5'-C5'	-7.12	109.52	120.90
41	s	60	PRO	N-CA-CB	7.10	111.83	103.30
8	H	167	U	N3-C2-O2	-7.10	117.23	122.20
20	T	187	LYS	C-N-CD	-7.01	105.19	120.60
7	G	127	G	C4'-C3'-O3'	6.96	126.91	113.00
1	A	775	ASN	CA-CB-CG	-6.90	98.22	113.40
1	A	1583	GLN	CB-CA-C	-6.88	96.64	110.40
1	A	1533	ARG	CB-CG-CD	6.87	129.45	111.60
8	H	82	G	O3'-P-O5'	-6.86	90.96	104.00
8	H	183	G	O3'-P-O5'	-6.84	91.00	104.00
8	H	77	C	O3'-P-O5'	-6.82	91.05	104.00
8	H	59	A	O3'-P-O5'	-6.82	91.05	104.00
8	H	141	C	O3'-P-O5'	-6.82	91.05	104.00
8	H	68	G	O3'-P-O5'	-6.81	91.05	104.00
8	H	113	G	O3'-P-O5'	-6.81	91.06	104.00
8	H	56	A	O3'-P-O5'	-6.81	91.07	104.00
8	H	91	U	O3'-P-O5'	-6.81	91.07	104.00
1	A	1497	THR	CA-CB-OG1	-6.81	94.71	109.00
27	2	63	PHE	CB-CA-C	-6.80	96.79	110.40
1	A	1874	VAL	O-C-N	6.80	133.58	122.70
8	H	78	C	O3'-P-O5'	-6.80	91.07	104.00
8	H	148	C	O3'-P-O5'	-6.80	91.09	104.00
8	H	150	U	O3'-P-O5'	-6.80	91.09	104.00
8	H	54	U	O3'-P-O5'	-6.79	91.10	104.00
8	H	73	C	O3'-P-O5'	-6.79	91.10	104.00
8	H	182	U	O3'-P-O5'	-6.79	91.10	104.00
18	R	132	LEU	CA-CB-CG	6.79	130.92	115.30
8	H	74	U	O3'-P-O5'	-6.79	91.10	104.00
8	H	180	G	O3'-P-O5'	-6.79	91.10	104.00
2	B	104	C	C2'-C3'-O3'	-6.79	94.57	109.50
8	H	57	A	O3'-P-O5'	-6.78	91.12	104.00
8	H	90	A	O3'-P-O5'	-6.78	91.12	104.00
8	H	181	G	O3'-P-O5'	-6.78	91.12	104.00
8	H	93	A	O3'-P-O5'	-6.78	91.12	104.00
8	H	81	G	O3'-P-O5'	-6.77	91.13	104.00
8	H	72	U	O3'-P-O5'	-6.77	91.14	104.00
8	H	89	U	O3'-P-O5'	-6.77	91.14	104.00
8	H	69	U	O3'-P-O5'	-6.77	91.14	104.00
8	H	55	U	O3'-P-O5'	-6.76	91.15	104.00
8	H	79	G	O3'-P-O5'	-6.76	91.15	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	80	A	O3'-P-O5'	-6.76	91.16	104.00
8	H	149	A	O3'-P-O5'	-6.76	91.16	104.00
8	H	84	C	O3'-P-O5'	-6.75	91.17	104.00
8	H	155	C	P-O3'-C3'	6.75	127.80	119.70
8	H	58	U	O3'-P-O5'	-6.75	91.17	104.00
8	H	67	C	O3'-P-O5'	-6.75	91.17	104.00
8	H	92	U	O3'-P-O5'	-6.75	91.17	104.00
8	H	71	C	O3'-P-O5'	-6.75	91.18	104.00
8	H	114	A	O3'-P-O5'	-6.74	91.20	104.00
8	H	83	A	O3'-P-O5'	-6.74	91.20	104.00
8	H	88	A	O3'-P-O5'	-6.74	91.20	104.00
1	A	775	ASN	CB-CA-C	-6.74	96.93	110.40
1	A	1860	GLN	CB-CA-C	-6.73	96.94	110.40
8	H	166	G	C8-N9-C4	-6.72	103.71	106.40
42	o	23	GLU	OE1-CD-OE2	-6.72	115.23	123.30
8	H	70	C	O3'-P-O5'	-6.71	91.25	104.00
41	t	60	PRO	N-CA-CB	6.69	111.33	103.30
1	A	1535	THR	CB-CA-C	-6.66	93.62	111.60
22	V	467	LEU	CA-CB-CG	6.65	130.59	115.30
43	p	89	ASP	CB-CG-OD1	6.62	124.26	118.30
41	q	46	PRO	N-CA-CB	6.61	111.24	103.30
1	A	343	GLU	CB-CA-C	6.61	123.62	110.40
7	G	127	G	N9-C1'-C2'	-6.60	104.74	112.00
1	A	1620	TYR	C-N-CA	-6.58	105.26	121.70
41	s	46	PRO	N-CA-CB	6.57	111.19	103.30
41	r	46	PRO	N-CA-CB	6.51	111.11	103.30
11	K	90	PRO	N-CA-CB	6.48	111.07	103.30
41	q	60	PRO	N-CA-CB	6.48	111.07	103.30
38	w	114	LYS	N-CA-C	-6.40	93.71	111.00
12	L	159	LEU	CA-CB-CG	6.40	130.02	115.30
1	A	1535	THR	CA-CB-OG1	-6.36	95.65	109.00
7	G	84	U	C2'-C3'-O3'	-6.36	95.52	109.50
1	A	1502	PHE	C-N-CA	6.35	137.58	121.70
1	A	1618	LYS	CB-CA-C	-6.34	97.71	110.40
42	o	5	THR	N-CA-CB	-6.34	98.26	110.30
1	A	1537	TRP	CB-CA-C	6.33	123.07	110.40
7	G	124	G	C2'-C3'-O3'	6.33	123.83	113.70
8	H	165	A	O4'-C1'-N9	-6.32	103.15	108.20
11	K	78	PRO	N-CA-CB	6.30	110.87	103.30
27	2	110	GLN	CB-CA-C	-6.30	97.80	110.40
1	A	162	LYS	CB-CA-C	-6.27	97.86	110.40
3	C	308	CYS	CA-CB-SG	6.27	125.29	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	108	GLU	CB-CA-C	-6.25	97.91	110.40
12	L	9	GLY	C-N-CA	6.25	137.31	121.70
44	1	273	LYS	CB-CA-C	-6.21	97.99	110.40
1	A	342	THR	CB-CA-C	-6.17	94.94	111.60
8	H	166	G	N9-C4-C5	6.17	107.87	105.40
7	G	21	A	O3'-P-O5'	6.16	115.71	104.00
6	4	-6	C	C6-N1-C1'	-6.12	113.46	120.80
8	H	162	U	N1-C2-O2	6.10	127.07	122.80
18	R	226	PRO	N-CD-CG	-6.06	94.11	103.20
28	z	64	ALA	C-N-CA	-6.05	106.57	121.70
42	o	78	ARG	NE-CZ-NH2	-6.05	117.28	120.30
42	o	132	ARG	CD-NE-CZ	6.03	132.04	123.60
15	O	193	LEU	CB-CG-CD2	-6.00	100.80	111.00
10	J	220	LEU	CA-CB-CG	5.98	129.05	115.30
24	X	66	GLN	CB-CA-C	-5.98	98.45	110.40
24	X	103	GLN	CB-CA-C	-5.97	98.45	110.40
20	T	401	PRO	C-N-CA	5.97	136.62	121.70
18	R	226	PRO	CB-CA-C	-5.97	97.08	112.00
42	o	21	ASP	CB-CG-OD1	5.95	123.66	118.30
10	J	670	PRO	N-CA-CB	5.95	110.44	103.30
16	P	7	PRO	C-N-CA	5.94	136.55	121.70
1	A	663	ARG	CB-CA-C	-5.94	98.52	110.40
41	t	46	PRO	N-CA-CB	5.93	110.41	103.30
1	A	1499	GLU	N-CA-CB	-5.93	99.93	110.60
8	H	166	G	N3-C4-C5	-5.92	125.64	128.60
1	A	1528	GLN	CB-CA-C	5.91	122.23	110.40
10	J	637	PRO	N-CA-CB	5.91	110.39	103.30
9	I	458	LYS	O-C-N	5.90	132.14	122.70
43	p	25	ARG	CD-NE-CZ	5.90	131.86	123.60
42	o	64	ARG	NE-CZ-NH1	5.90	123.25	120.30
10	J	675	PRO	N-CA-CB	5.89	110.37	103.30
8	H	172	C	P-O3'-C3'	5.89	126.76	119.70
8	H	168	A	C5'-C4'-C3'	-5.87	106.61	116.00
42	o	27	ARG	CB-CA-C	-5.86	98.67	110.40
10	J	604	PRO	N-CA-CB	5.86	110.33	103.30
7	G	21	A	P-O3'-C3'	-5.86	112.67	119.70
2	B	26	A	P-O5'-C5'	-5.84	111.55	120.90
8	H	164	C	C5-C4-N4	-5.84	116.11	120.20
9	I	459	ALA	O-C-N	5.82	132.02	122.70
44	1	185	TYR	CB-CA-C	5.81	122.02	110.40
41	q	19	PRO	N-CA-CB	5.81	110.27	103.30
1	A	158	ARG	CB-CA-C	-5.81	98.79	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	r	19	PRO	N-CA-CB	5.78	110.24	103.30
10	J	566	PRO	N-CA-CB	5.78	110.24	103.30
9	I	457	ARG	O-C-N	5.76	131.92	122.70
8	H	167	U	O3'-P-O5'	-5.73	93.12	104.00
23	W	139	LEU	CA-CB-CG	5.69	128.39	115.30
18	R	214	ILE	CG1-CB-CG2	-5.69	98.89	111.40
1	A	158	ARG	CG-CD-NE	-5.67	99.89	111.80
8	H	156	U	P-O3'-C3'	-5.66	112.90	119.70
41	t	19	PRO	N-CA-CB	5.64	110.07	103.30
6	4	-12	G	C4'-C3'-O3'	5.64	124.28	113.00
42	o	75	ARG	NH1-CZ-NH2	5.64	125.60	119.40
16	P	10	GLU	CB-CA-C	5.62	121.65	110.40
8	H	166	G	C6-N1-C2	-5.61	121.73	125.10
1	A	1737	ASN	CB-CA-C	5.59	121.58	110.40
42	o	58	ASP	N-CA-CB	-5.55	100.60	110.60
7	G	2	U	N1-C1'-C2'	-5.55	105.89	112.00
41	s	19	PRO	N-CA-CB	5.54	109.95	103.30
23	W	532	LEU	CB-CG-CD1	-5.48	101.69	111.00
7	G	121	C	O5'-P-OP2	-5.47	100.78	105.70
41	r	60	PRO	N-CA-CB	5.46	109.86	103.30
5	F	73	A	P-O3'-C3'	5.46	126.25	119.70
2	B	20	G	O4'-C1'-N9	5.45	112.56	108.20
1	A	1779	PHE	CB-CA-C	-5.40	99.61	110.40
8	H	106	G	O5'-P-OP1	5.40	117.18	110.70
8	H	157	G	O4'-C1'-N9	-5.36	103.91	108.20
1	A	1874	VAL	CA-C-N	-5.36	105.41	117.20
8	H	156	U	OP2-P-O3'	5.34	116.95	105.20
19	S	106	ASP	CB-CG-OD1	5.33	123.09	118.30
42	o	47	ILE	N-CA-CB	5.32	123.04	110.80
1	A	1459	ARG	NE-CZ-NH1	-5.32	117.64	120.30
18	R	275	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	1532	ARG	CB-CG-CD	-5.29	97.85	111.60
20	T	309	ASP	CB-CG-OD1	5.29	123.06	118.30
20	T	309	ASP	O-C-N	5.28	131.15	122.70
23	W	82	ASN	C-N-CD	-5.28	108.99	120.60
43	p	39	ASP	CB-CG-OD2	-5.27	113.55	118.30
18	R	217	LYS	CB-CA-C	-5.27	99.87	110.40
6	4	-6	C	N1-C2-O2	5.26	122.06	118.90
1	A	1753	LEU	N-CA-CB	-5.25	99.90	110.40
1	A	1301	ILE	CG1-CB-CG2	-5.25	99.85	111.40
8	H	162	U	C2-N3-C4	-5.25	123.85	127.00
25	Y	685	ASP	C-N-CA	5.23	134.78	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1530	PRO	CA-CB-CG	-5.23	94.07	104.00
8	H	157	G	P-O5'-C5'	-5.23	112.54	120.90
1	A	863	GLU	CB-CG-CD	-5.22	100.10	114.20
8	H	156	U	C4'-C3'-C2'	5.22	107.82	102.60
6	4	-6	C	O4'-C1'-N1	5.21	112.37	108.20
15	O	28	LEU	CB-CG-CD2	-5.20	102.16	111.00
28	z	56	ASP	CB-CG-OD2	5.19	122.97	118.30
38	w	115	GLY	N-CA-C	5.19	126.07	113.10
1	A	1745	GLU	CB-CA-C	-5.18	100.04	110.40
8	H	170	C	N3-C4-C5	-5.18	119.83	121.90
7	G	2	U	C3'-C2'-C1'	5.18	105.64	101.50
43	p	39	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	344	ASP	CB-CA-C	-5.17	100.06	110.40
23	W	243	VAL	CG1-CB-CG2	-5.16	102.64	110.90
7	G	96	U	N1-C1'-C2'	-5.14	106.35	112.00
1	A	1303	LEU	CA-CB-CG	-5.14	103.49	115.30
8	H	160	A	P-O5'-C5'	-5.13	112.69	120.90
27	2	97	ASP	CB-CA-C	-5.13	100.15	110.40
1	A	1578	ARG	CG-CD-NE	5.12	122.56	111.80
8	H	176	G	OP1-P-OP2	-5.12	111.92	119.60
1	A	1520	ASN	O-C-N	-5.11	114.53	122.70
25	Y	686	GLU	C-N-CA	5.10	134.46	121.70
9	I	697	PRO	C-N-CA	5.09	134.44	121.70
3	C	93	ILE	CG1-CB-CG2	-5.09	100.20	111.40
25	Y	689	GLU	N-CA-C	-5.08	97.28	111.00
1	A	1515	TRP	N-CA-C	-5.07	97.30	111.00
7	G	126	G	O5'-P-OP2	-5.06	101.15	105.70
8	H	160	A	C4'-C3'-C2'	-5.06	97.54	102.60
9	I	698	ARG	N-CA-CB	5.06	119.70	110.60
1	A	1748	ARG	NE-CZ-NH1	-5.04	117.78	120.30
42	o	99	SER	N-CA-CB	-5.04	102.94	110.50
1	A	1744	ARG	NE-CZ-NH1	-5.03	117.78	120.30
6	4	-6	C	N3-C2-O2	-5.03	118.38	121.90
8	H	170	C	O4'-C1'-C2'	-5.03	100.77	105.80
13	M	120	PRO	CB-CA-C	-5.03	99.43	112.00
3	C	359	LYS	CA-CB-CG	5.03	124.46	113.40

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	2	31	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	1019	TYR	Peptide
1	A	1201	ARG	Peptide
1	A	1210	LYS	Peptide
1	A	1338	SER	Peptide
1	A	1493	THR	Mainchain
1	A	1506	ALA	Mainchain
1	A	1520	ASN	Mainchain
1	A	1576	ILE	Mainchain
1	A	170	ASP	Mainchain
1	A	1717	ASN	Mainchain
1	A	1749	LYS	Mainchain
1	A	1806	ALA	Mainchain
1	A	1876	LEU	Mainchain
1	A	2010	ILE	Mainchain
1	A	377	GLU	Peptide
1	A	385	GLU	Peptide
1	A	55	ASP	Peptide
1	A	698	PRO	Peptide
1	A	73	HIS	Peptide
1	A	775	ASN	Sidechain
1	A	941	LYS	Peptide
3	C	308	CYS	Peptide
3	C	358	LYS	Peptide
3	C	360	ALA	Peptide
3	C	534	VAL	Peptide
3	C	799	GLU	Peptide
3	C	800	PRO	Peptide
3	C	902	HIS	Peptide
3	C	92	PRO	Peptide
3	C	93	ILE	Peptide
4	E	192	ASN	Peptide
9	I	309	ALA	Mainchain
9	I	310	LYS	Mainchain
9	I	311	MET	Mainchain
9	I	693	GLN	Mainchain
9	I	722	GLU	Mainchain
9	I	83	LYS	Mainchain
9	I	84	HIS	Mainchain
10	J	205	LEU	Peptide
10	J	215	THR	Peptide
10	J	216	ASP	Peptide
10	J	240	THR	Peptide

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Mol	Chain	Res	Type	Group
10	J	241	VAL	Peptide
14	N	136	HIS	Peptide
14	N	3	LYS	Peptide
14	N	36	PRO	Peptide
14	N	4	VAL	Peptide
15	O	63	MET	Peptide
16	P	204	GLN	Peptide
16	P	30	TYR	Peptide
16	P	48	GLN	Peptide
18	R	125	MET	Peptide
18	R	126	ASN	Peptide
18	R	183	GLN	Peptide
18	R	185	GLY	Peptide
18	R	212	PHE	Peptide
18	R	66	GLU	Peptide
18	R	94	GLY	Peptide
20	T	342	GLU	Peptide
20	T	400	PHE	Peptide
20	T	405	PHE	Peptide
23	W	257	ILE	Peptide
23	W	518	PRO	Peptide
33	d	112	ASN	Peptide
33	k	112	ASN	Peptide

5.2 Too-close contacts

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

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	1980/2335 (85%)	1782 (90%)	181 (9%)	17 (1%)	14 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	856/972 (88%)	781 (91%)	71 (8%)	4 (0%)	25 59
4	E	297/357 (83%)	275 (93%)	22 (7%)	0	100 100
9	I	576/855 (67%)	557 (97%)	15 (3%)	4 (1%)	19 53
10	J	528/848 (62%)	487 (92%)	33 (6%)	8 (2%)	8 39
11	K	147/225 (65%)	137 (93%)	6 (4%)	4 (3%)	4 28
12	L	425/802 (53%)	408 (96%)	15 (4%)	2 (0%)	25 59
13	M	128/243 (53%)	117 (91%)	11 (9%)	0	100 100
14	N	141/144 (98%)	124 (88%)	16 (11%)	1 (1%)	19 53
15	O	283/420 (67%)	259 (92%)	23 (8%)	1 (0%)	30 63
16	P	107/229 (47%)	89 (83%)	15 (14%)	3 (3%)	4 27
17	Q	1308/1485 (88%)	1282 (98%)	26 (2%)	0	100 100
18	R	255/536 (48%)	228 (89%)	23 (9%)	4 (2%)	8 38
19	S	157/166 (95%)	147 (94%)	10 (6%)	0	100 100
20	T	310/514 (60%)	275 (89%)	29 (9%)	6 (2%)	6 35
21	U	68/2752 (2%)	60 (88%)	8 (12%)	0	100 100
22	V	444/908 (49%)	431 (97%)	12 (3%)	1 (0%)	44 73
23	W	507/579 (88%)	432 (85%)	69 (14%)	6 (1%)	11 43
24	X	83/254 (33%)	81 (98%)	2 (2%)	0	100 100
25	Y	667/1220 (55%)	642 (96%)	23 (3%)	2 (0%)	37 67
26	Z	97/758 (13%)	87 (90%)	10 (10%)	0	100 100
27	2	121/184 (66%)	113 (93%)	5 (4%)	3 (2%)	4 29
28	z	58/112 (52%)	55 (95%)	3 (5%)	0	100 100
29	b	98/240 (41%)	93 (95%)	2 (2%)	3 (3%)	3 26
29	i	84/240 (35%)	82 (98%)	2 (2%)	0	100 100
30	y	77/301 (26%)	75 (97%)	2 (3%)	0	100 100
31	a	75/126 (60%)	74 (99%)	1 (1%)	0	100 100
31	h	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
32	c	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
32	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
33	d	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
33	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	f	72/86 (84%)	68 (94%)	4 (6%)	0	100 100
34	m	72/86 (84%)	69 (96%)	2 (3%)	1 (1%)	9 40
35	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
35	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
36	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
36	n	65/76 (86%)	63 (97%)	2 (3%)	0	100 100
37	v	142/146 (97%)	138 (97%)	4 (3%)	0	100 100
38	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	12 45
39	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	16 51
40	x	23/703 (3%)	22 (96%)	1 (4%)	0	100 100
41	q	130/504 (26%)	117 (90%)	7 (5%)	6 (5%)	2 18
41	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	8 38
41	s	130/504 (26%)	115 (88%)	7 (5%)	8 (6%)	1 13
41	t	129/504 (26%)	116 (90%)	9 (7%)	4 (3%)	3 26
42	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10 41
43	p	92/225 (41%)	90 (98%)	2 (2%)	0	100 100
44	1	263/586 (45%)	244 (93%)	19 (7%)	0	100 100
All	All	12396/23429 (53%)	11559 (93%)	741 (6%)	96 (1%)	19 51

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	A	1092	ILE
1	A	1136	ARG
1	A	1494	TYR
1	A	1503	TRP
1	A	1831	LYS
3	C	801	LEU
9	I	698	ARG
10	J	217	GLU
10	J	241	VAL
11	K	78	PRO
12	L	10	VAL
12	L	125	PRO
16	P	8	THR

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Mol	Chain	Res	Type
18	R	233	PRO
20	T	187	LYS
20	T	188	PRO
20	T	190	TRP
23	W	73	ASP
23	W	74	PRO
23	W	82	ASN
23	W	83	PRO
27	2	76	SER
39	u	383	ASN
41	q	24	VAL
41	q	59	HIS
41	q	60	PRO
41	s	9	ASN
41	s	55	ILE
41	s	60	PRO
41	s	66	PRO
41	s	71	ILE
41	t	9	ASN
41	t	69	THR
34	m	4	PRO
1	A	349	ALA
3	C	94	ILE
3	C	439	PRO
9	I	532	LYS
10	J	709	VAL
20	T	406	ILE
25	Y	1185	ASP
27	2	33	LEU
38	w	115	GLY
39	u	340	GLY
39	u	385	ASP
41	q	9	ASN
41	q	19	PRO
41	s	24	VAL
42	o	160	LYS
1	A	1538	TRP
1	A	1774	ASN
1	A	1782	ASP
9	I	699	THR
10	J	188	GLN
10	J	205	LEU

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Mol	Chain	Res	Type
11	K	86	ARG
16	P	6	ARG
18	R	52	PRO
18	R	186	VAL
22	V	597	PRO
23	W	258	PRO
27	2	72	ALA
41	q	23	HIS
41	r	9	ASN
41	t	67	SER
1	A	570	ASP
1	A	1567	PRO
1	A	1598	ASP
3	C	83	GLU
10	J	341	PRO
10	J	604	PRO
11	K	65	ILE
14	N	41	ARG
16	P	205	LYS
18	R	73	PRO
25	Y	1182	LYS
41	t	65	PRO
42	o	32	PRO
1	A	364	SER
20	T	343	PRO
20	T	462	GLU
29	b	105	GLY
29	b	106	ILE
41	s	62	ARG
9	I	372	ARG
10	J	216	ASP
15	O	20	PHE
29	b	115	PRO
1	A	1135	PRO
1	A	1419	ILE
11	K	17	PRO
23	W	271	PRO
1	A	1892	PRO
41	s	38	GLY
41	r	60	PRO

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
1	A	1780/2108 (84%)	1678 (94%)	102 (6%)	17 46
3	C	760/866 (88%)	746 (98%)	14 (2%)	54 74
4	E	256/300 (85%)	256 (100%)	0	100 100
9	I	199/749 (27%)	187 (94%)	12 (6%)	16 45
10	J	241/751 (32%)	239 (99%)	2 (1%)	79 88
12	L	218/709 (31%)	209 (96%)	9 (4%)	26 55
13	M	117/209 (56%)	112 (96%)	5 (4%)	25 54
14	N	130/130 (100%)	128 (98%)	2 (2%)	60 78
15	O	255/361 (71%)	254 (100%)	1 (0%)	89 95
16	P	101/203 (50%)	94 (93%)	7 (7%)	13 40
18	R	219/457 (48%)	213 (97%)	6 (3%)	40 65
19	S	129/134 (96%)	128 (99%)	1 (1%)	79 88
20	T	268/441 (61%)	263 (98%)	5 (2%)	52 73
21	U	21/2432 (1%)	20 (95%)	1 (5%)	21 51
22	V	98/838 (12%)	94 (96%)	4 (4%)	26 55
23	W	448/502 (89%)	438 (98%)	10 (2%)	47 69
24	X	67/230 (29%)	42 (63%)	25 (37%)	0 1
25	Y	32/1085 (3%)	28 (88%)	4 (12%)	3 20
26	Z	91/655 (14%)	87 (96%)	4 (4%)	24 53
27	2	106/157 (68%)	98 (92%)	8 (8%)	11 37
28	z	54/99 (54%)	45 (83%)	9 (17%)	2 11
29	b	83/177 (47%)	81 (98%)	2 (2%)	44 67
29	i	77/177 (44%)	75 (97%)	2 (3%)	41 65
31	a	68/101 (67%)	68 (100%)	0	100 100
31	h	70/101 (69%)	70 (100%)	0	100 100
32	c	77/101 (76%)	75 (97%)	2 (3%)	41 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	j	77/101 (76%)	75 (97%)	2 (3%)	41	65
33	d	90/110 (82%)	88 (98%)	2 (2%)	47	69
33	k	80/110 (73%)	78 (98%)	2 (2%)	42	66
34	f	63/74 (85%)	62 (98%)	1 (2%)	58	76
34	m	62/74 (84%)	60 (97%)	2 (3%)	34	61
35	e	74/84 (88%)	74 (100%)	0	100	100
35	l	74/84 (88%)	74 (100%)	0	100	100
36	g	64/66 (97%)	63 (98%)	1 (2%)	58	76
36	n	60/66 (91%)	59 (98%)	1 (2%)	56	75
42	o	139/218 (64%)	135 (97%)	4 (3%)	37	63
43	p	82/195 (42%)	79 (96%)	3 (4%)	29	58
44	1	233/520 (45%)	224 (96%)	9 (4%)	27	57
All	All	7063/15775 (45%)	6799 (96%)	264 (4%)	31	58

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ARG
1	A	240	ARG
1	A	346	ASP
1	A	362	ARG
1	A	387	PHE
1	A	409	ARG
1	A	413	LEU
1	A	579	GLN
1	A	642	ARG
1	A	664	HIS
1	A	666	LYS
1	A	762	ARG
1	A	773	LYS
1	A	774	LYS
1	A	821	ARG
1	A	850	TYR
1	A	853	LYS
1	A	857	ASN
1	A	861	ARG
1	A	863	GLU
1	A	866	LEU

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Mol	Chain	Res	Type
1	A	880	ARG
1	A	994	ASN
1	A	1089	CYS
1	A	1132	LYS
1	A	1136	ARG
1	A	1189	MET
1	A	1249	MET
1	A	1251	SER
1	A	1253	SER
1	A	1341	ARG
1	A	1402	ARG
1	A	1494	TYR
1	A	1501	LEU
1	A	1502	PHE
1	A	1526	LEU
1	A	1527	ASN
1	A	1528	GLN
1	A	1530	PRO
1	A	1536	LEU
1	A	1553	VAL
1	A	1555	LEU
1	A	1560	ILE
1	A	1561	PHE
1	A	1566	ILE
1	A	1569	LEU
1	A	1570	LYS
1	A	1574	ILE
1	A	1578	ARG
1	A	1581	LEU
1	A	1587	GLU
1	A	1588	SER
1	A	1590	VAL
1	A	1592	ASP
1	A	1593	LEU
1	A	1594	CYS
1	A	1614	ILE
1	A	1615	HIS
1	A	1618	LYS
1	A	1681	ARG
1	A	1722	SER
1	A	1723	LYS
1	A	1725	LEU

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Mol	Chain	Res	Type
1	A	1727	GLN
1	A	1728	GLN
1	A	1730	MET
1	A	1734	MET
1	A	1737	ASN
1	A	1738	PRO
1	A	1742	VAL
1	A	1751	LEU
1	A	1752	GLN
1	A	1753	LEU
1	A	1755	SER
1	A	1763	LEU
1	A	1774	ASN
1	A	1776	ILE
1	A	1807	ILE
1	A	1813	ARG
1	A	1833	LEU
1	A	1859	LYS
1	A	1862	ILE
1	A	1864	THR
1	A	1875	HIS
1	A	1876	LEU
1	A	1879	PHE
1	A	1885	LYS
1	A	1889	LEU
1	A	1894	GLN
1	A	1897	LEU
1	A	1921	ASP
1	A	1922	ASP
1	A	1943	LEU
1	A	1944	HIS
1	A	1967	ILE
1	A	1993	LYS
1	A	1998	ASN
1	A	2002	LEU
1	A	2011	ILE
1	A	2012	LEU
1	A	2014	MET
1	A	2015	GLU
3	C	87	GLN
3	C	297	ASN
3	C	359	LYS

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Mol	Chain	Res	Type
3	C	495	ARG
3	C	513	ASN
3	C	572	GLU
3	C	573	GLU
3	C	673	LYS
3	C	748	ASP
3	C	754	VAL
3	C	756	LYS
3	C	826	ARG
3	C	853	ARG
3	C	856	HIS
9	I	548	PHE
9	I	606	TRP
9	I	694	ILE
9	I	698	ARG
9	I	699	THR
9	I	723	MET
9	I	724	LEU
9	I	725	ARG
9	I	726	ILE
9	I	727	ARG
9	I	730	VAL
9	I	731	GLN
10	J	201	ARG
10	J	221	ASN
12	L	4	ILE
12	L	5	MET
12	L	6	ILE
12	L	7	LYS
12	L	10	VAL
12	L	123	LEU
12	L	133	GLU
12	L	181	ARG
12	L	240	ARG
13	M	118	LYS
13	M	152	LEU
13	M	198	ARG
13	M	212	ASN
13	M	215	ASN
14	N	119	CYS
14	N	130	ARG
15	O	222	ARG

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Mol	Chain	Res	Type
16	P	3	THR
16	P	7	PRO
16	P	9	PHE
16	P	10	GLU
16	P	13	ARG
16	P	18	LYS
16	P	212	ASN
18	R	78	ARG
18	R	95	LYS
18	R	212	PHE
18	R	218	ILE
18	R	220	ARG
18	R	312	MET
19	S	126	HIS
20	T	189	GLN
20	T	197	TYR
20	T	412	HIS
20	T	416	ILE
20	T	454	VAL
21	U	23	LEU
22	V	458	THR
22	V	499	GLN
22	V	535	THR
22	V	597	PRO
23	W	129	ARG
23	W	182	LYS
23	W	200	VAL
23	W	243	VAL
23	W	264	ASN
23	W	322	ARG
23	W	492	ASN
23	W	495	ARG
23	W	500	LYS
23	W	529	ASN
24	X	54	LEU
24	X	55	TYR
24	X	56	GLU
24	X	58	LEU
24	X	59	GLN
24	X	63	ASP
24	X	64	ARG
24	X	67	GLN

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Mol	Chain	Res	Type
24	X	68	GLU
24	X	72	GLN
24	X	78	MET
24	X	79	VAL
24	X	84	GLU
24	X	86	GLU
24	X	92	GLU
24	X	96	GLN
24	X	97	GLN
24	X	99	LEU
24	X	101	GLU
24	X	102	LYS
24	X	106	GLU
24	X	113	LYS
24	X	114	GLU
24	X	116	ARG
24	X	120	LYS
25	Y	413	LYS
25	Y	418	ASP
25	Y	421	GLU
25	Y	426	LEU
26	Z	725	ASN
26	Z	751	PHE
26	Z	756	TYR
26	Z	758	ARG
27	2	30	GLU
27	2	32	LYS
27	2	33	LEU
27	2	68	MET
27	2	102	LYS
27	2	110	GLN
27	2	138	LYS
27	2	140	LEU
28	z	57	LYS
28	z	58	ARG
28	z	60	PRO
28	z	62	GLN
28	z	68	MET
28	z	70	GLU
28	z	72	ARG
28	z	79	LYS
28	z	93	ASN

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Mol	Chain	Res	Type
29	b	13	ILE
29	b	58	GLN
32	c	40	LEU
32	c	54	GLN
33	d	45	ASN
33	d	112	ASN
34	f	55	LEU
36	g	65	ASN
29	i	13	ILE
29	i	58	GLN
32	j	40	LEU
32	j	54	GLN
33	k	45	ASN
33	k	112	ASN
34	m	5	LEU
34	m	55	LEU
36	n	65	ASN
42	o	5	THR
42	o	55	ARG
42	o	114	SER
42	o	126	THR
43	p	17	LYS
43	p	46	MET
43	p	87	ASP
44	1	34	ARG
44	1	185	TYR
44	1	267	ILE
44	1	268	ARG
44	1	271	ILE
44	1	273	LYS
44	1	274	TYR
44	1	290	ARG
44	1	305	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	78	ASN
1	A	105	ASN
1	A	181	ASN
1	A	244	GLN

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Mol	Chain	Res	Type
1	A	361	HIS
1	A	457	ASN
1	A	467	GLN
1	A	495	GLN
1	A	573	GLN
1	A	584	HIS
1	A	703	GLN
1	A	704	ASN
1	A	711	GLN
1	A	792	HIS
1	A	793	ASN
1	A	994	ASN
1	A	1014	ASN
1	A	1124	ASN
1	A	1148	ASN
1	A	1359	HIS
1	A	1460	HIS
1	A	1476	GLN
1	A	1487	HIS
1	A	1527	ASN
1	A	1528	GLN
1	A	1554	GLN
1	A	1599	GLN
1	A	1717	ASN
1	A	1727	GLN
1	A	1766	GLN
1	A	1775	GLN
1	A	1784	ASN
1	A	1875	HIS
1	A	1890	GLN
1	A	1965	HIS
1	A	1998	ASN
1	A	2004	GLN
3	C	60	HIS
3	C	137	HIS
3	C	208	HIS
3	C	210	ASN
3	C	245	HIS
3	C	297	ASN
3	C	451	HIS
3	C	513	ASN
3	C	856	HIS

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Mol	Chain	Res	Type
4	E	101	ASN
4	E	253	ASN
9	I	601	GLN
10	J	212	GLN
10	J	221	ASN
10	J	331	GLN
10	J	347	HIS
12	L	186	GLN
12	L	266	HIS
13	M	212	ASN
14	N	37	HIS
14	N	54	HIS
15	O	113	ASN
15	O	196	GLN
15	O	294	ASN
18	R	106	GLN
18	R	189	ASN
18	R	279	HIS
19	S	87	HIS
19	S	111	GLN
19	S	126	HIS
20	T	189	GLN
20	T	278	ASN
20	T	437	HIS
20	T	455	GLN
22	V	474	HIS
23	W	71	HIS
23	W	82	ASN
23	W	242	HIS
23	W	472	ASN
23	W	492	ASN
23	W	529	ASN
23	W	549	HIS
24	X	61	GLN
24	X	72	GLN
24	X	96	GLN
26	Z	725	ASN
27	2	31	GLN
27	2	110	GLN
28	z	69	GLN
28	z	93	ASN
29	b	22	GLN

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Mol	Chain	Res	Type
29	b	76	ASN
31	a	60	GLN
32	c	64	ASN
33	d	69	ASN
34	f	58	HIS
36	g	65	ASN
31	h	60	GLN
29	i	22	GLN
29	i	76	ASN
32	j	64	ASN
33	k	69	ASN
34	m	12	ASN
34	m	58	HIS
36	n	65	ASN
42	o	130	HIS
43	p	7	HIS
44	1	85	GLN
44	1	154	HIS
44	1	156	GLN
44	1	344	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	82/117 (70%)	17 (20%)	4 (4%)
5	F	96/107 (89%)	45 (46%)	16 (16%)
6	4	13/46 (28%)	8 (61%)	3 (23%)
7	G	80/174 (45%)	63 (78%)	20 (25%)
8	H	133/188 (70%)	34 (25%)	10 (7%)
All	All	404/632 (63%)	167 (41%)	53 (13%)

All (167) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C

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Mol	Chain	Res	Type
2	B	24	G
2	B	25	C
2	B	26	A
2	B	28	A
2	B	36	C
2	B	38	C
2	B	45	C
2	B	57	G
2	B	70	A
2	B	71	C
5	F	6	C
5	F	7	G
5	F	8	C
5	F	9	U
5	F	10	U
5	F	12	G
5	F	25	C
5	F	26	U
5	F	27	A
5	F	28	A
5	F	29	A
5	F	31	U
5	F	33	G
5	F	34	G
5	F	35	A
5	F	36	A
5	F	37	C
5	F	38	G
5	F	40	U
5	F	43	A
5	F	45	A
5	F	46	G
5	F	47	A
5	F	48	A
5	F	49	G
5	F	51	U
5	F	54	G
5	F	56	A
5	F	59	G
5	F	60	C
5	F	61	C
5	F	62	C

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Mol	Chain	Res	Type
5	F	68	C
5	F	73	A
5	F	74	U
5	F	78	A
5	F	79	C
5	F	80	G
5	F	81	C
5	F	82	A
5	F	83	A
5	F	84	A
5	F	85	U
5	F	86	U
5	F	87	C
6	4	-12	G
6	4	-11	G
6	4	-10	C
6	4	-9	C
6	4	-7	C
6	4	-6	C
6	4	-4	A
6	4	-1	G
7	G	2	U
7	G	3	A
7	G	5	G
7	G	6	A
7	G	7	G
7	G	8	C
7	G	10	U
7	G	11	A
7	G	12	G
7	G	13	C
7	G	14	A
7	G	17	U
7	G	21	A
7	G	22	C
7	G	23	U
7	G	24	G
7	G	25	G
7	G	26	U
7	G	27	U
7	G	28	A
7	G	29	C

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Mol	Chain	Res	Type
7	G	30	C
7	G	31	U
7	G	73	G
7	G	74	G
7	G	75	U
7	G	76	U
7	G	77	U
7	G	78	C
7	G	79	C
7	G	80	U
7	G	81	U
7	G	82	G
7	G	83	A
7	G	84	U
7	G	87	U
7	G	88	G
7	G	89	U
7	G	90	C
7	G	91	A
7	G	92	U
7	G	93	A
7	G	96	U
7	G	97	A
7	G	98	U
7	G	99	C
7	G	100	C
7	G	101	U
7	G	102	G
7	G	103	U
7	G	119	A
7	G	120	G
7	G	121	C
7	G	122	U
7	G	123	C
7	G	124	G
7	G	125	C
7	G	126	G
7	G	127	G
7	G	128	U
7	G	129	U
7	G	130	G
7	G	132	G

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Mol	Chain	Res	Type
8	H	13	C
8	H	14	C
8	H	15	U
8	H	16	U
8	H	17	U
8	H	19	G
8	H	24	A
8	H	25	G
8	H	28	C
8	H	29	A
8	H	30	A
8	H	31	G
8	H	33	G
8	H	37	U
8	H	39	U
8	H	40	C
8	H	41	U
8	H	42	G
8	H	43	U
8	H	112	G
8	H	143	A
8	H	147	G
8	H	152	G
8	H	153	A
8	H	154	C
8	H	156	U
8	H	157	G
8	H	164	C
8	H	165	A
8	H	168	A
8	H	169	C
8	H	177	A
8	H	178	A
8	H	179	C

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	18	C
2	B	19	A
2	B	20	G
2	B	27	U

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Mol	Chain	Res	Type
5	F	5	U
5	F	7	G
5	F	25	C
5	F	26	U
5	F	33	G
5	F	34	G
5	F	35	A
5	F	36	A
5	F	45	A
5	F	50	A
5	F	58	G
5	F	59	G
5	F	73	A
5	F	81	C
5	F	84	A
5	F	86	U
6	4	-13	C
6	4	-12	G
6	4	-11	G
7	G	1	G
7	G	16	G
7	G	20	A
7	G	21	A
7	G	22	C
7	G	23	U
7	G	90	C
7	G	95	U
7	G	96	U
7	G	97	A
7	G	98	U
7	G	100	C
7	G	119	A
7	G	120	G
7	G	121	C
7	G	124	G
7	G	125	C
7	G	126	G
7	G	128	U
7	G	129	U
8	H	15	U
8	H	28	C
8	H	29	A

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Mol	Chain	Res	Type
8	H	30	A
8	H	38	A
8	H	39	U
8	H	40	C
8	H	156	U
8	H	164	C
8	H	168	A

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

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	$\#\|Z\| > 2$
18	SEP	R	232	18	8,9,10	1.55	1 (12%)	8,12,14	1.71	2 (25%)
18	SEP	R	224	18	8,9,10	1.42	2 (25%)	8,12,14	1.60	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
18	SEP	R	232	18	-	1/5/8/10	-
18	SEP	R	224	18	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	232	SEP	P-O1P	3.40	1.61	1.50
18	R	224	SEP	P-O2P	-2.41	1.45	1.54
18	R	224	SEP	P-O3P	-2.21	1.46	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	232	SEP	P-OG-CB	-4.05	107.13	118.30
18	R	224	SEP	OG-CB-CA	-3.55	104.69	108.14
18	R	232	SEP	OG-CB-CA	2.37	110.46	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	232	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 16 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	$\#\|Z\| > 2$
46	GTP	C	1500	47	26,34,34	1.51	3 (11%)	32,54,54	1.95	7 (21%)
49	ATP	Q	1501	47	26,33,33	1.72	8 (30%)	31,52,52	1.85	10 (32%)
45	IHP	A	3000	-	36,36,36	0.71	0	54,60,60	1.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GTP	C	1500	47	-	1/18/38/38	0/3/3/3
49	ATP	Q	1501	47	-	4/18/38/38	0/3/3/3
45	IHP	A	3000	-	-	3/30/54/54	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	C	1500	GTP	C5-C6	-4.83	1.37	1.47
49	Q	1501	ATP	C2'-C1'	-3.61	1.48	1.53
49	Q	1501	ATP	C4-N3	3.43	1.40	1.35
49	Q	1501	ATP	C6-N6	3.34	1.46	1.34
49	Q	1501	ATP	C2'-C3'	-2.74	1.45	1.53
46	C	1500	GTP	C5-C4	-2.42	1.36	1.43
46	C	1500	GTP	O4'-C4'	-2.27	1.39	1.45
49	Q	1501	ATP	O2'-C2'	-2.25	1.37	1.43
49	Q	1501	ATP	C2-N3	2.20	1.35	1.32
49	Q	1501	ATP	O3'-C3'	-2.17	1.37	1.43
49	Q	1501	ATP	C3'-C4'	-2.16	1.47	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	C	1500	GTP	PA-O3A-PB	-5.64	113.48	132.83
49	Q	1501	ATP	PB-O3B-PG	-5.46	114.08	132.83
46	C	1500	GTP	PB-O3B-PG	-4.36	117.85	132.83
49	Q	1501	ATP	N3-C2-N1	-4.17	122.16	128.68
46	C	1500	GTP	C5-C6-N1	3.72	120.52	113.95
46	C	1500	GTP	C2-N1-C6	-3.47	118.71	125.10
46	C	1500	GTP	C3'-C2'-C1'	3.22	105.83	100.98
46	C	1500	GTP	C8-N7-C5	2.82	108.37	102.99
49	Q	1501	ATP	PA-O3A-PB	-2.61	123.86	132.83
49	Q	1501	ATP	C1'-N9-C4	-2.51	122.22	126.64
49	Q	1501	ATP	O2G-PG-O1G	-2.41	101.23	110.68
49	Q	1501	ATP	O2A-PA-O1A	-2.35	100.64	112.24
49	Q	1501	ATP	O2G-PG-O3B	2.26	112.20	104.64
46	C	1500	GTP	O6-C6-C5	-2.22	120.04	124.37
49	Q	1501	ATP	O2B-PB-O1B	-2.08	101.96	112.24
49	Q	1501	ATP	O5'-C5'-C4'	2.07	116.11	108.99
49	Q	1501	ATP	O3G-PG-O3B	2.05	111.50	104.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

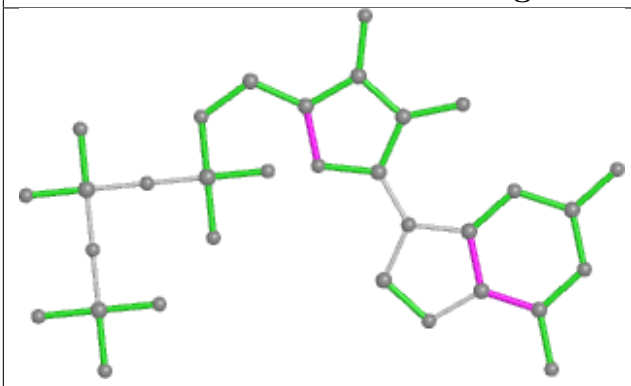
Mol	Chain	Res	Type	Atoms
45	A	3000	IHP	C3-O13-P3-O43
46	C	1500	GTP	O4'-C4'-C5'-O5'
49	Q	1501	ATP	C5'-O5'-PA-O1A
49	Q	1501	ATP	C5'-O5'-PA-O2A
45	A	3000	IHP	C3-C4-O14-P4
49	Q	1501	ATP	PB-O3A-PA-O2A
45	A	3000	IHP	C4-O14-P4-O44
49	Q	1501	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

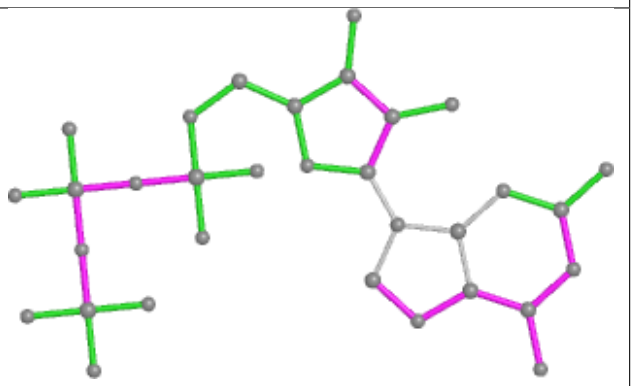
No monomer is involved in short contacts.

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.

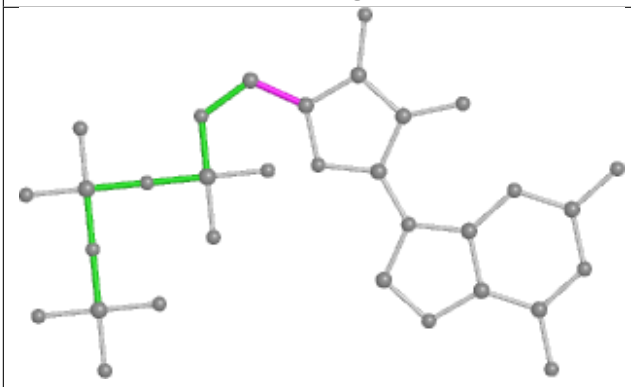
Ligand GTP C 1500



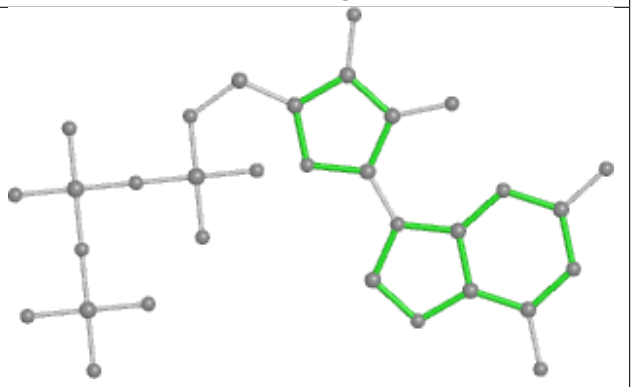
Bond lengths



Bond angles

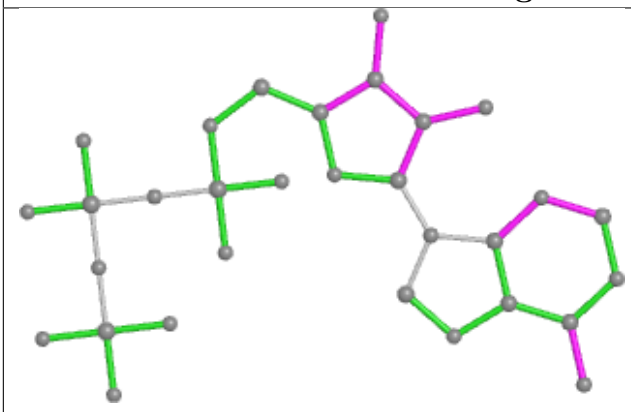


Torsions

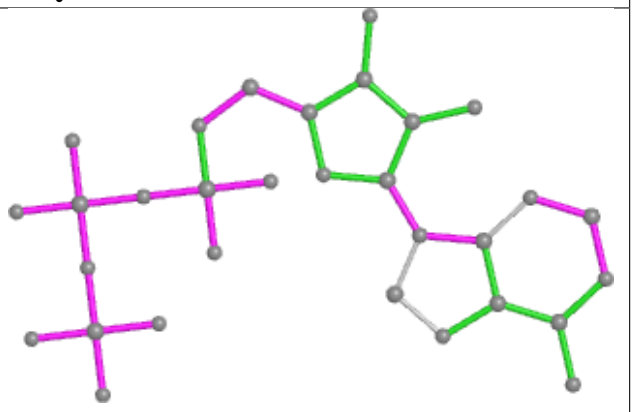


Rings

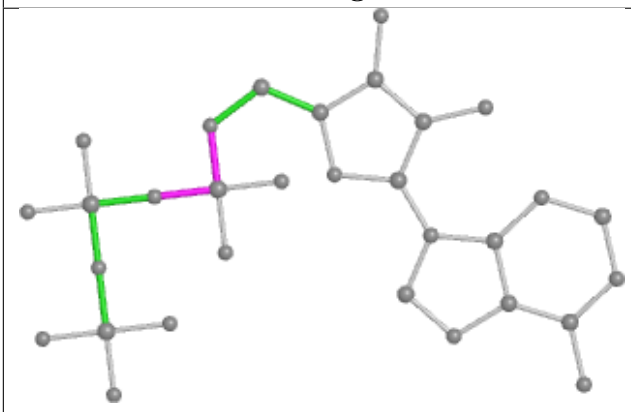
Ligand ATP Q 1501



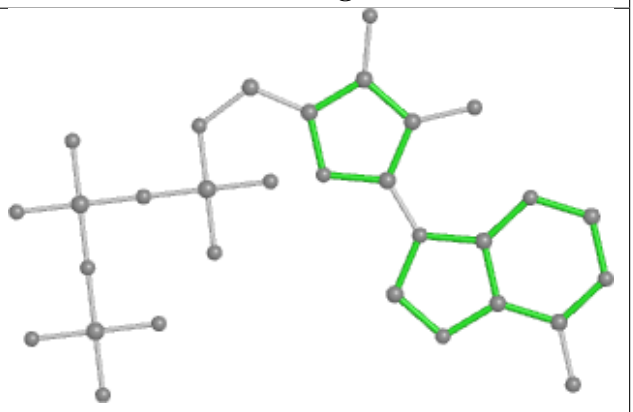
Bond lengths



Bond angles

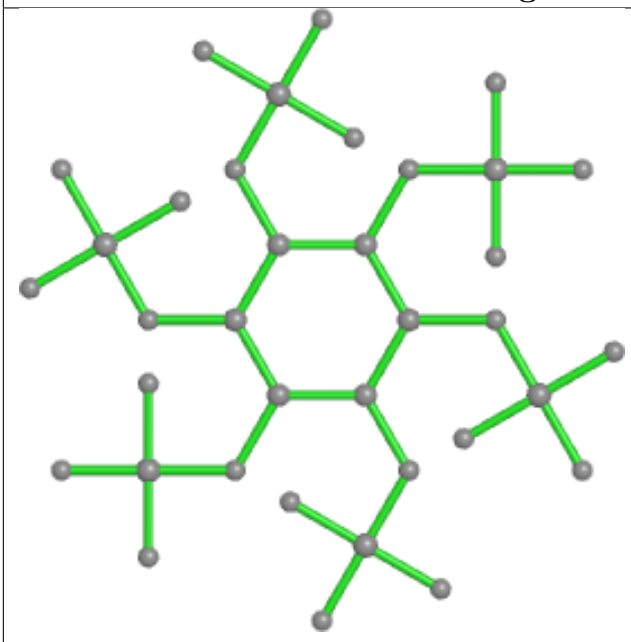


Torsions

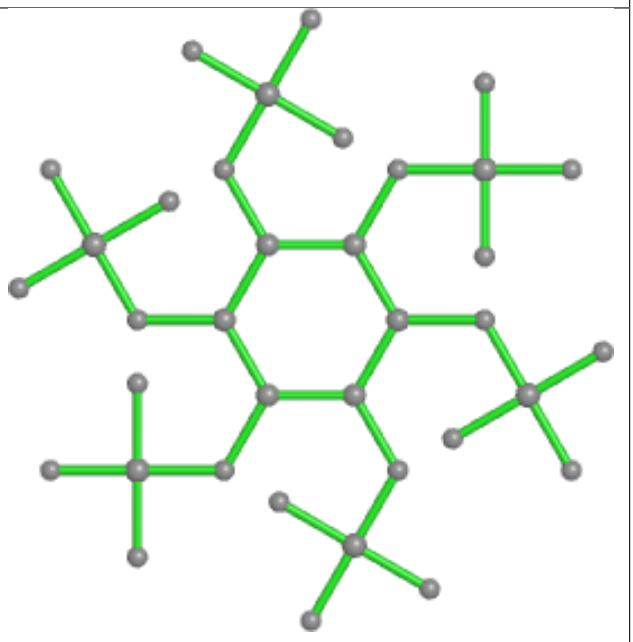


Rings

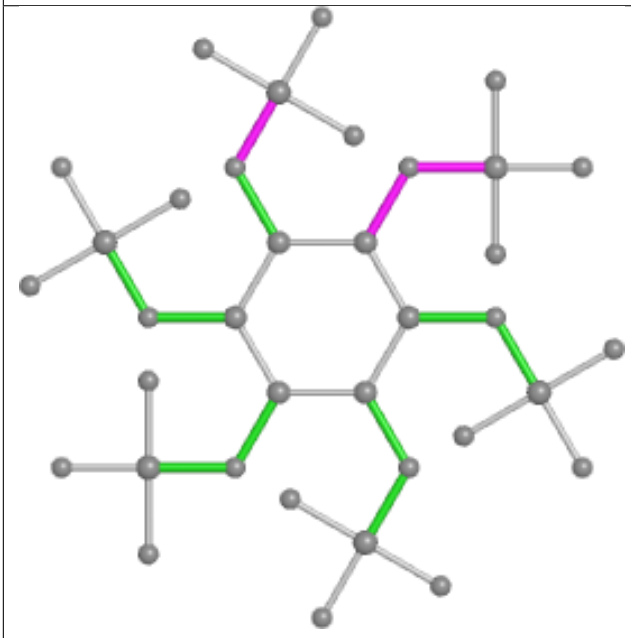
Ligand IHP A 3000



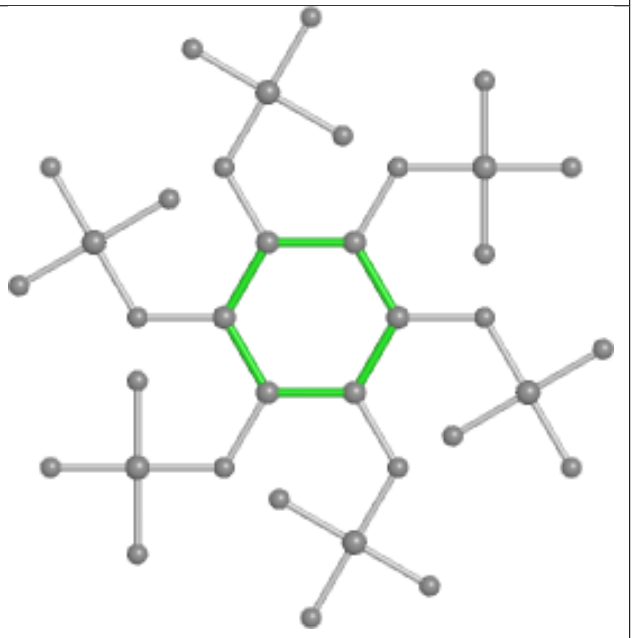
Bond lengths



Bond angles



Torsions



Rings

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.

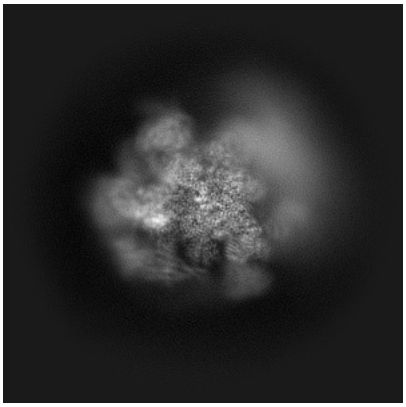
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32319. These allow visual inspection of the internal detail of the map and identification of artifacts.

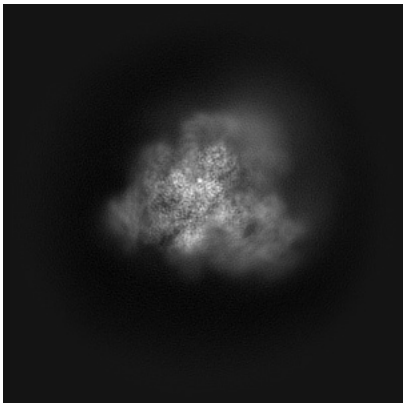
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

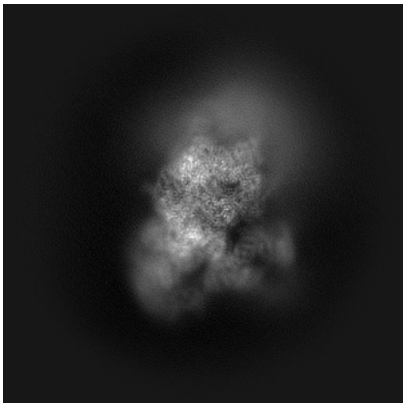
6.1.1 Primary map



X



Y

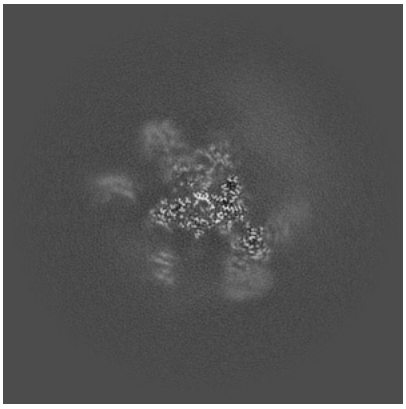


Z

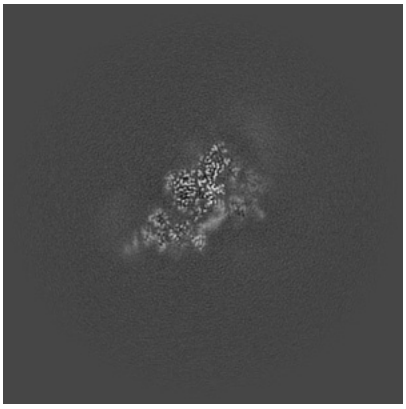
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 200



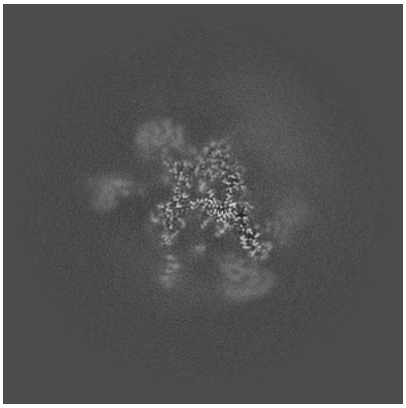
Y Index: 200

Z Index: 200

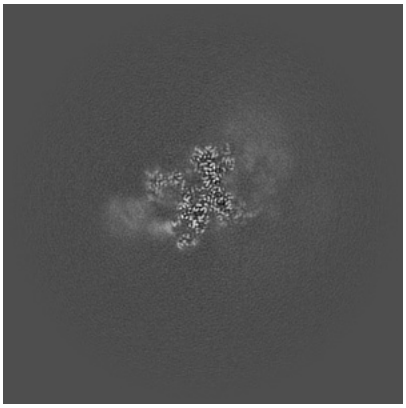
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

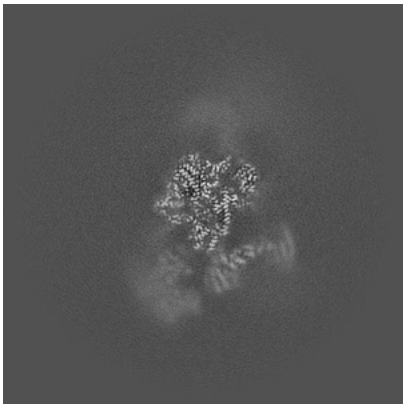
6.3.1 Primary map



X Index: 194



Y Index: 227

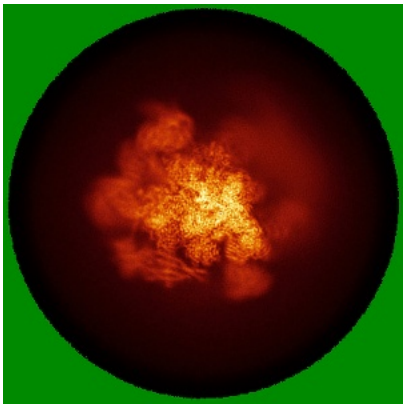


Z Index: 197

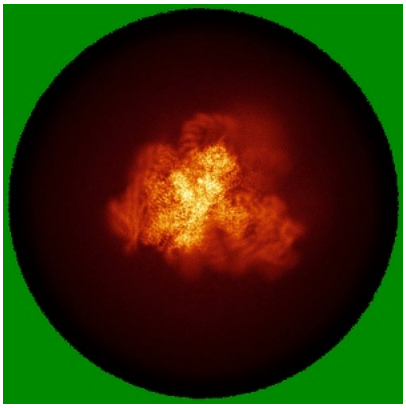
The images above show the largest variance slices of the map in three orthogonal directions.

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

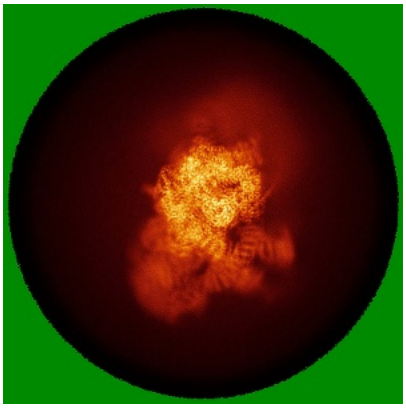
6.4.1 Primary map



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

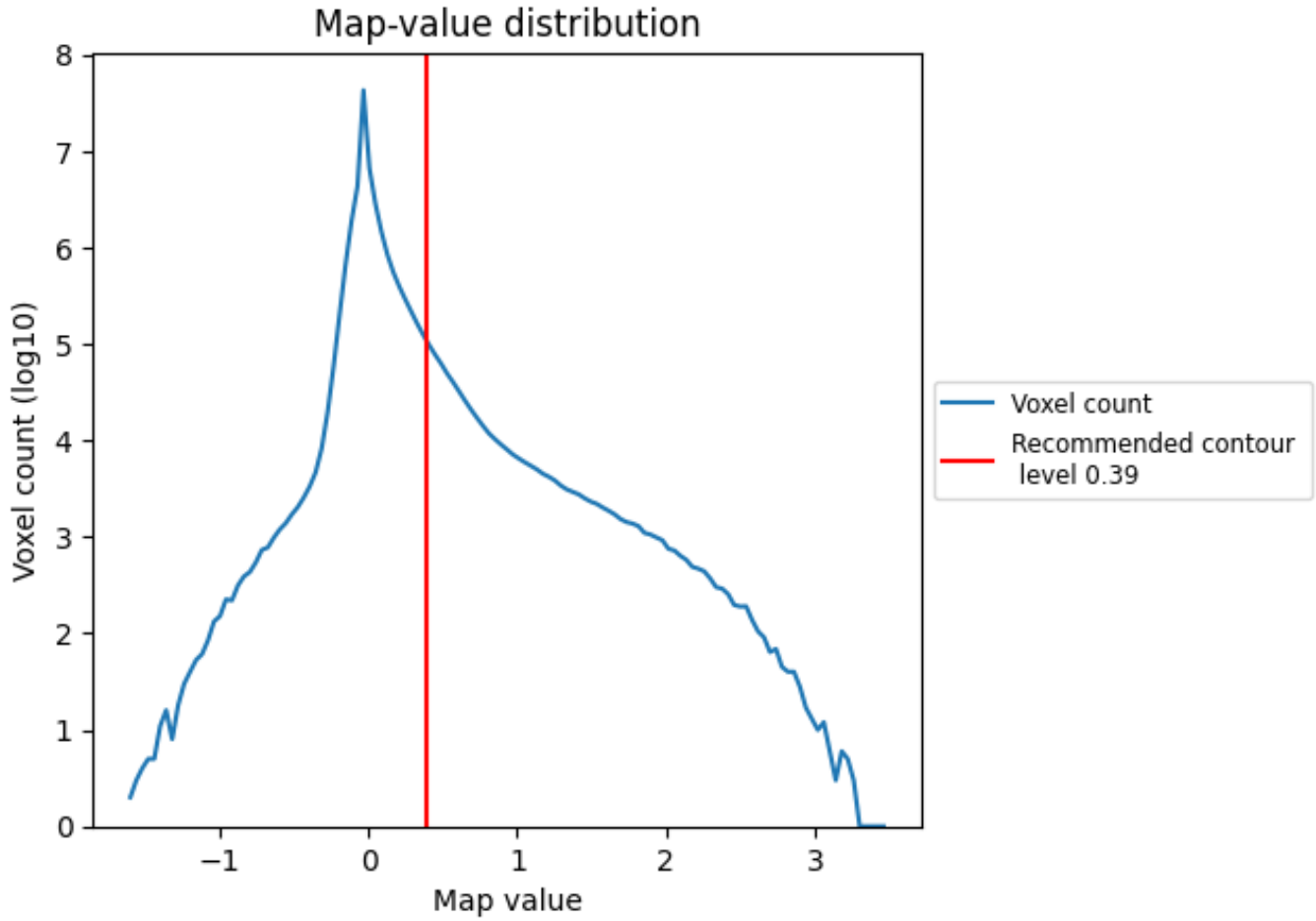
6.6 Mask visualisation (i)

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

7 Map analysis

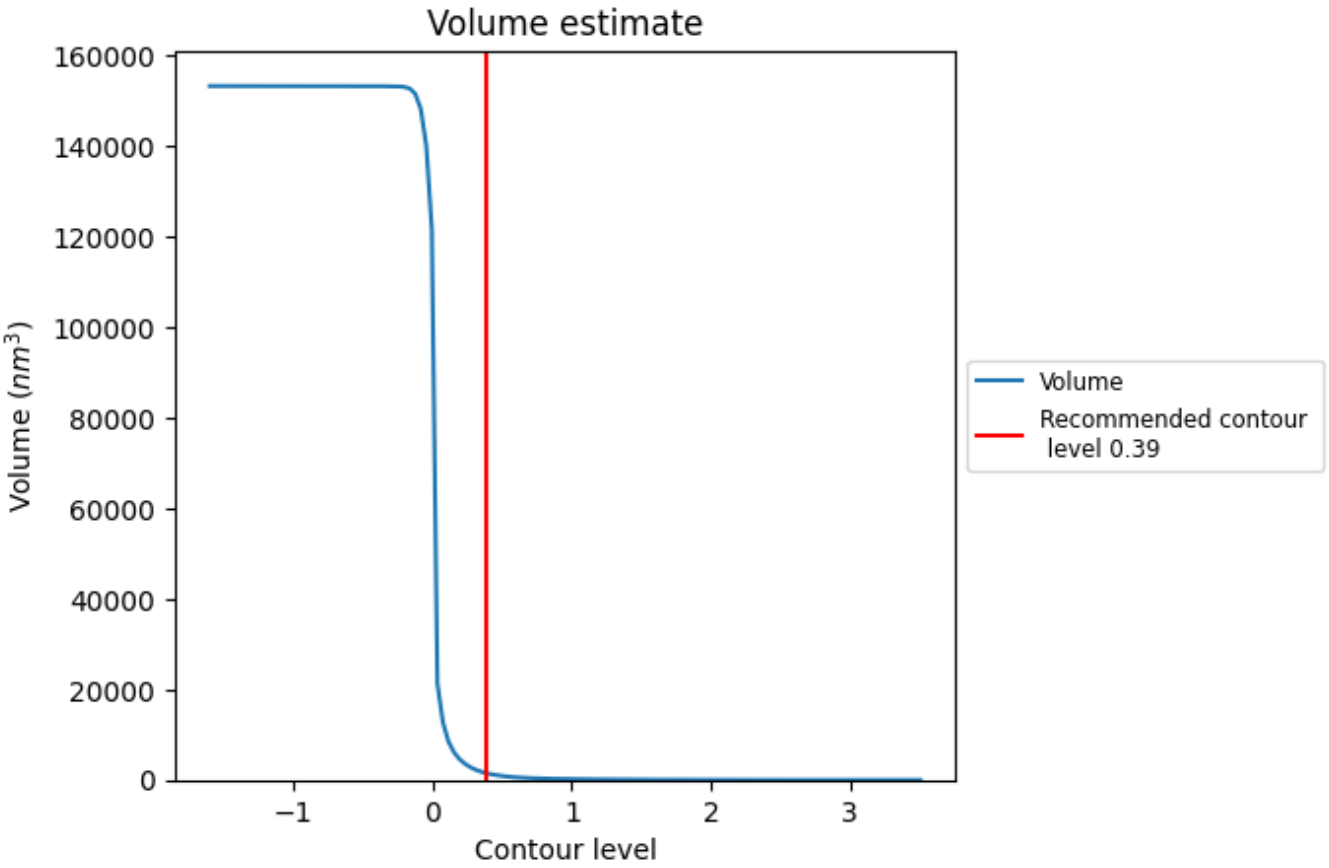
This section contains the results of statistical analysis of the map.

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.

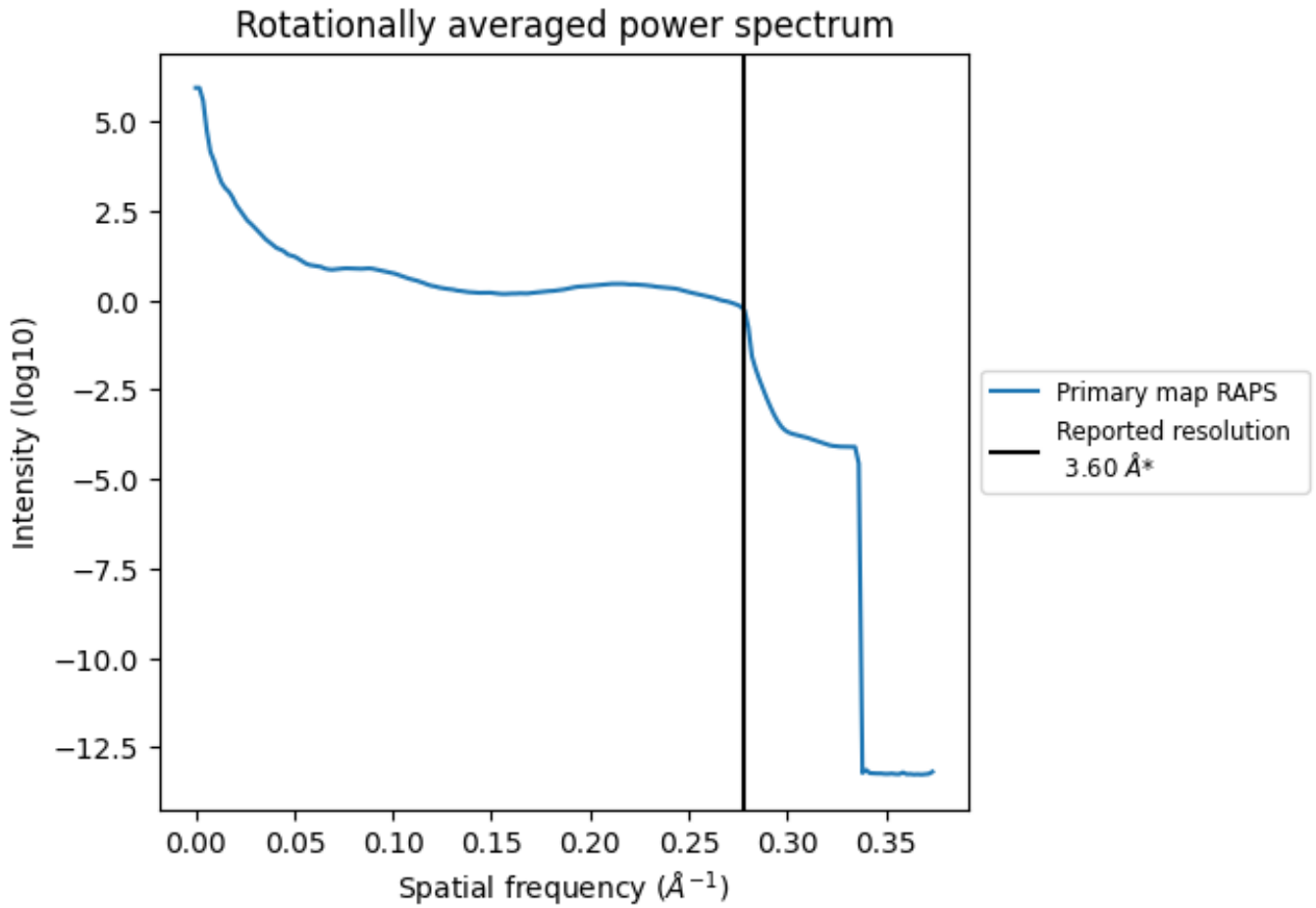
7.2 Volume estimate



The volume at the recommended contour level is 1478 nm^3; this corresponds to an approximate mass of 1335 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 0.278 $Å^{-1}$

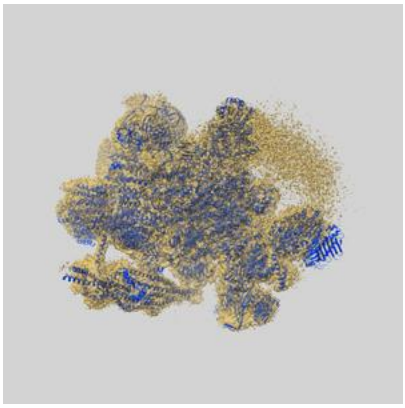
8 Fourier-Shell correlation (i)

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

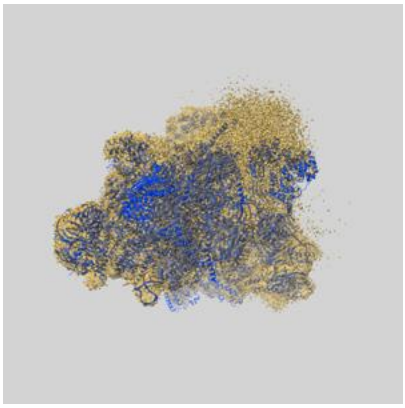
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32319 and PDB model 7W5A. Per-residue inclusion information can be found in section 3 on page 14.

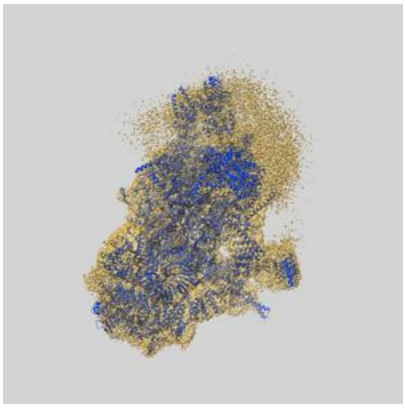
9.1 Map-model overlay



X



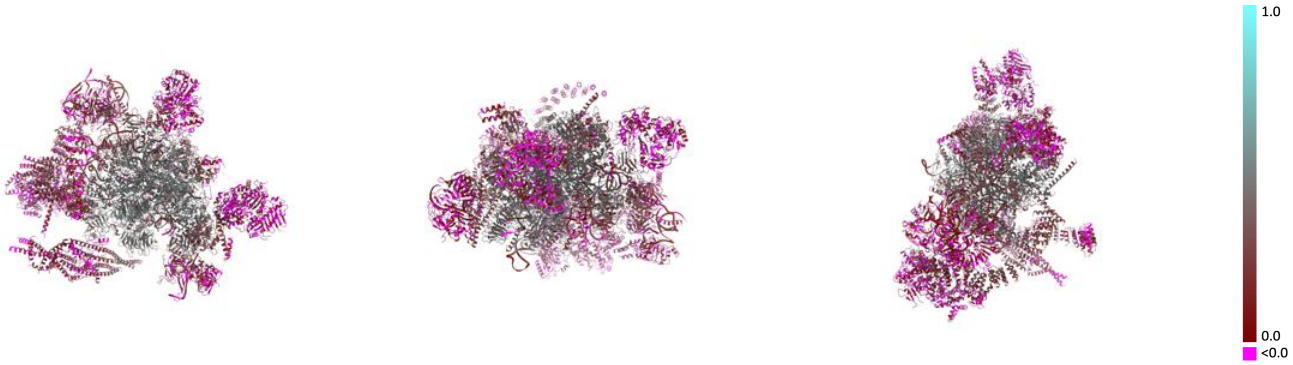
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.39 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.

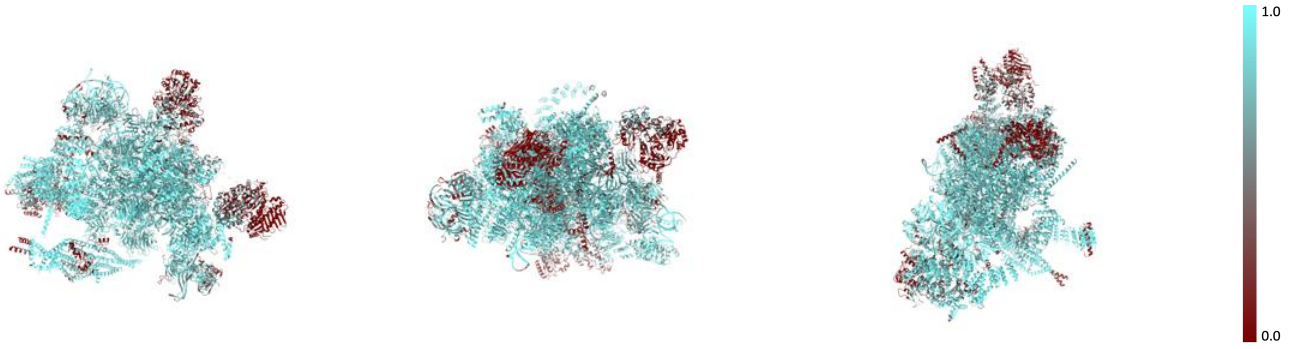
9.2 Q-score mapped to coordinate model (i)



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.

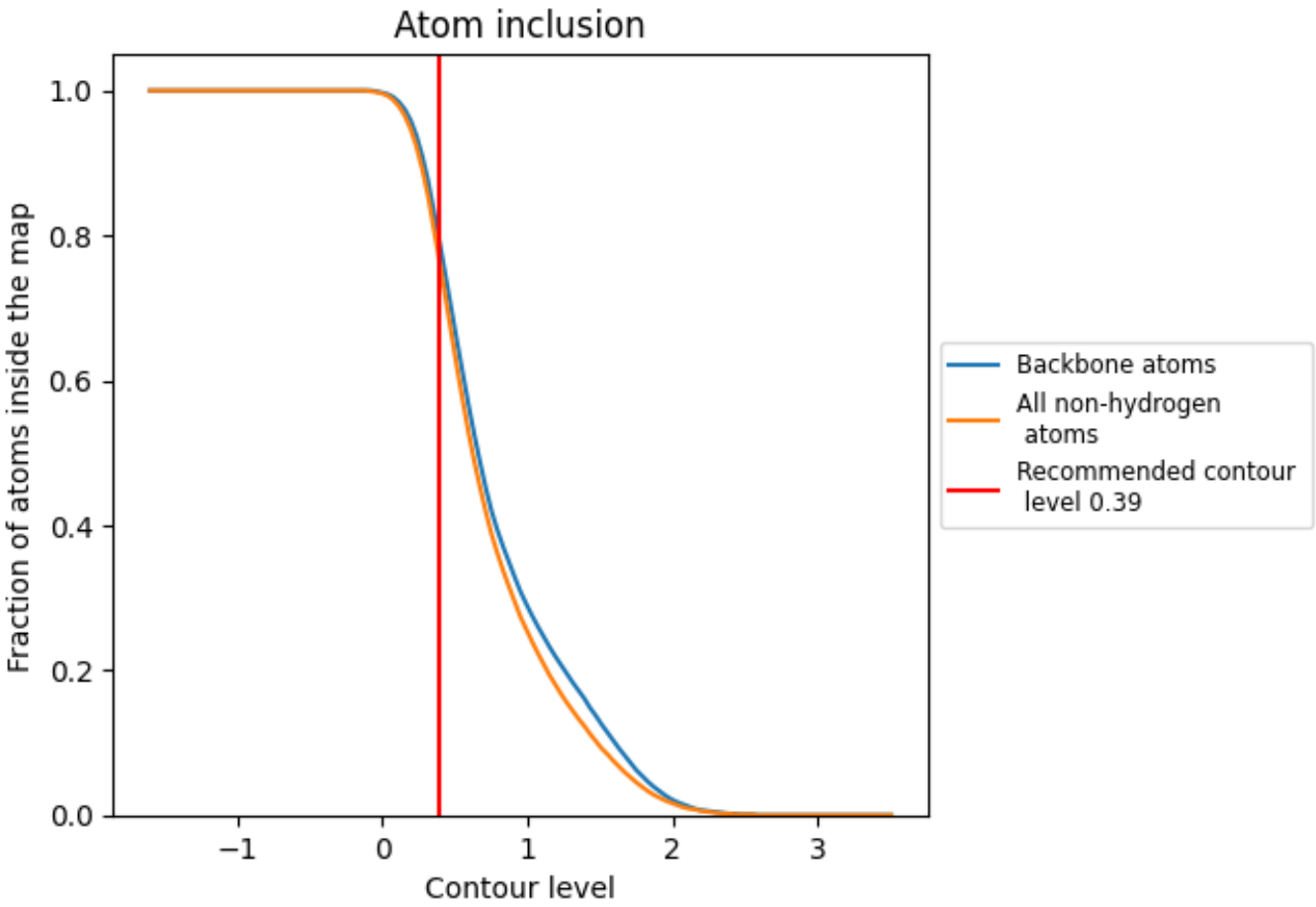
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.39).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.2690
1	0.2940	0.2090
2	0.7600	0.2290
4	0.9860	0.4820
A	0.9110	0.4460
B	0.9280	0.3030
C	0.8950	0.3900
E	0.9280	0.4200
F	0.9520	0.3700
G	0.7950	0.2110
H	0.9090	0.1640
I	0.9080	0.2300
J	0.8770	0.3030
K	0.9640	0.2140
L	0.8930	0.3370
M	0.8520	0.3870
N	0.9250	0.4370
O	0.8840	0.3700
P	0.8070	0.3930
Q	0.5250	0.0520
R	0.8550	0.4010
S	0.9260	0.4110
T	0.9550	0.4950
U	0.8850	0.2950
V	0.6440	0.1890
W	0.8190	0.2890
X	0.7270	0.3180
Y	0.2740	0.0650
Z	0.6840	0.3220
a	0.7370	0.1700
b	0.7180	0.1150
c	0.8310	0.0590
d	0.7320	0.0270
e	0.6020	0.0550
f	0.6110	0.0080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	0.5610	0.0960
h	0.6810	0.0850
i	0.6090	0.0580
j	0.7920	0.0500
k	0.7260	0.0950
l	0.6630	0.0860
m	0.9060	0.1440
n	0.7140	0.1320
o	0.7790	0.0570
p	0.8830	0.0900
q	0.5660	0.0450
r	0.9270	0.1650
s	0.4870	0.1010
t	0.3980	0.0490
u	0.3010	0.0250
v	0.0110	0.0060
w	0.0130	-0.0000
x	0.0970	0.0270
y	0.8590	0.1390
z	0.1890	0.1200