



## Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 09:03 pm BST

PDB ID : 8CH6  
EMDB ID : EMD-16658  
Title : Structure of a late-stage activated spliceosome (BAqr) arrested with a dominant-negative Aquarius mutant (state B complex).  
Authors : Cretu, C.; Schmitzova, J.; Pena, V.  
Deposited on : 2023-02-07  
Resolution : 5.90 Å (reported)  
Based on initial models : 5Z57, 6FF4, 6FF7

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

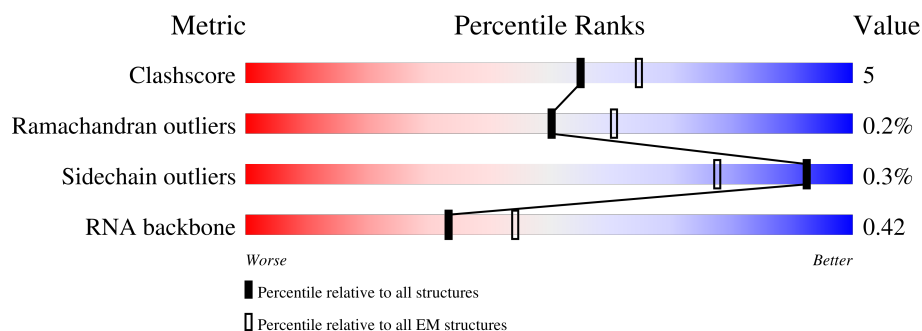
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


The reported resolution of this entry is 5.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	92	
1	i	92	
2	2	86	
2	h	86	
3	3	126	
3	j	126	
4	4	118	

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Mol	Chain	Length	Quality of chain
4	l	118	
5	5	119	
5	k	119	
6	8	240	
6	n	240	
7	9	76	
7	m	76	
8	A	1217	
9	B	86	
10	C	1304	
11	D	110	
12	E	895	
13	F	424	
14	G	476	
15	H	793	
16	I	464	
17	J	501	
18	K	504	
18	M	504	
18	R	504	
18	v	504	
19	L	619	
20	N	1041	
21	O	514	
22	P	802	

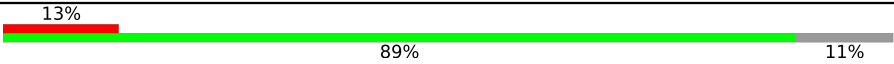

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Mol	Chain	Length	Quality of chain
23	Q	229	
24	S	225	
25	T	144	
26	U	420	
27	V	492	
28	W	908	
29	X	848	
30	Y	536	
31	Z	343	
32	a	2335	
33	b	972	
34	c	2136	
35	d	106	
36	e	117	
37	f	188	
38	g	319	
39	o	357	
40	p	166	
41	q	2752	
42	r	255	
43	s	225	
44	t	285	
45	u	520	
46	w	301	
47	x	579	

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Mol	Chain	Length	Quality of chain
48	y	1485	 13% 89% 11%
49	z	855	 19% 80% 19%

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 119058 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 Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	79	Total	C	N	O	0	0
			391	233	79	79		
1	i	70	Total	C	N	O	0	0
			346	206	70	70		

- Molecule 2 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	74	Total	C	N	O	0	0
			361	213	74	74		
2	h	66	Total	C	N	O	0	0
			322	190	66	66		

- Molecule 3 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	76	Total	C	N	O	0	0
			373	221	76	76		
3	j	68	Total	C	N	O	0	0
			335	199	68	68		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	85	Total	C	N	O	0	0
			422	252	85	85		
4	l	68	Total	C	N	O	0	0
			337	201	68	68		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	82	Total	C	N	O	0	0
			406	242	82	82		
5	k	78	Total	C	N	O	0	0
			388	232	78	78		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	8	86	Total	C	N	O	0	0
			422	250	86	86		
6	n	64	Total	C	N	O	0	0
			315	187	64	64		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	9	68	Total	C	N	O	0	0
			334	198	68	68		
7	m	63	Total	C	N	O	0	0
			309	183	63	63		

- Molecule 8 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	A	1158	Total	C	N	O	0	0
			5714	3398	1158	1158		

- Molecule 9 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	B	70	Total	C	N	O	0	0
			350	210	70	70		

- Molecule 10 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	815	Total	C	N	O	S	0	0
			5115	3242	928	930	15		

- Molecule 11 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	89	Total	C	N	O	S	0	0
			649	399	117	120	13		

- Molecule 12 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	198	Total	C	N	O	S	0	0
			1350	855	249	241	5		

- Molecule 13 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	F	78	Total	C	N	O	0	0
			383	227	78	78		

- Molecule 14 is a protein called G-patch domain and KOW motifs-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	G	67	Total	C	N	O	0	0
			364	228	68	68		

- Molecule 15 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	H	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 16 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	185	Total	C	N	O	S	0	0
			1034	620	215	197	2		

- Molecule 17 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	410	Total	C	N	O	S	0	0
			2187	1326	431	426	4		

- Molecule 18 is a protein called Pre-mRNA-processing factor 19.



Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	118	Total	C	N	O	S	0	0
			938	586	167	181	4		
18	M	125	Total	C	N	O	S	0	0
			988	618	176	190	4		
18	R	118	Total	C	N	O	S	0	0
			938	586	167	181	4		
18	v	125	Total	C	N	O	S	0	0
			988	618	176	190	4		

- Molecule 19 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	28	Total	C	N	O	S	0	0
			177	111	32	32	2		

- Molecule 20 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	791	Total	C	N	O	S	0	0
			6147	3893	1089	1137	28		

- Molecule 21 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	320	Total	C	N	O	S	0	0
			2517	1592	457	460	8		

- Molecule 22 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	330	Total	C	N	O	S	0	0
			2432	1522	446	454	10		

- Molecule 23 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	100	Total	C	N	O	S	0	0
			823	509	161	151	2		

- Molecule 24 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	159	Total	C	N	O	S	0	0
			1323	820	246	248	9		

- Molecule 25 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	142	Total	C	N	O	S	0	0
			1176	741	216	208	11		

- Molecule 26 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	295	Total	C	N	O	S	0	0
			2080	1290	380	392	18		

- Molecule 27 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	285	Total	C	N	O	S	0	0
			1996	1252	338	396	10		

- Molecule 28 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	459	Total	C	N	O	S	0	0
			2921	1817	533	559	12		

- Molecule 29 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	241	Total	C	N	O	S	0	0
			1587	1017	298	270	2		

- Molecule 30 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	306	Total	C	N	O	S	0	0
			2250	1412	411	417	10		

- Molecule 31 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	95	Total	C	N	O	S	0	0
			607	378	109	117	3		

- Molecule 32 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	2183	Total	C	N	O	S	0	0
			16415	10472	2956	2922	65		

- Molecule 33 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	898	Total	C	N	O	S	0	0
			7046	4513	1172	1327	34		

- Molecule 34 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	1722	Total	C	N	O		0	0
			8530	5086	1722	1722			

- Molecule 35 is a RNA chain called RNU6-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	93	Total	C	N	O	P	0	0
			1989	889	364	643	93		

- Molecule 36 is a RNA chain called RNU5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	98	Total	C	N	O	P	0	0
			2070	926	347	699	98		

- Molecule 37 is a RNA chain called RNU2-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	137	Total	C	N	O	P	0	0
			2906	1298	501	970	137		

- Molecule 38 is a RNA chain called MINX-M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	76	Total	C	N	O	P	0	0
			1559	697	250	536	76		

- Molecule 39 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 40 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	p	159	Total	C	N	O	0	0
			776	457	159	160		

- Molecule 41 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	q	74	Total	C	N	O	S	0	0
			461	285	89	85	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	162	Total	C	N	O	0	0
			804	480	162	162		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
43	s	165	Total	C	N	O	0	0
			813	483	165	165		

- Molecule 44 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	48	Total	C	N	O	S	0	0
			407	261	64	81	1		

- Molecule 45 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	367	Total	C	N	O	S	0	0
			1963	1181	382	399	1		

- Molecule 46 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	w	224	Total	C	N	O		0	0
			1093	645	224	224			

- Molecule 47 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	362	Total	C	N	O		0	0
			1787	1063	362	362			

- Molecule 48 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	1327	Total	C	N	O	S	0	0
			10878	6988	1871	1965	54		

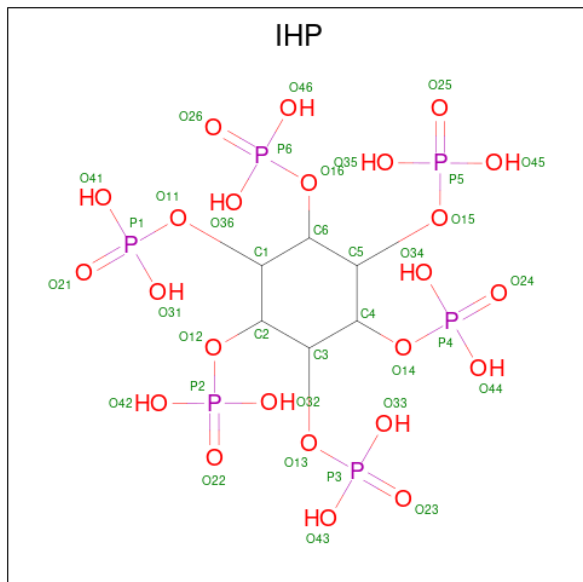
- Molecule 49 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	692	Total	C	N	O	S	0	0
			4511	2853	837	807	14		

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

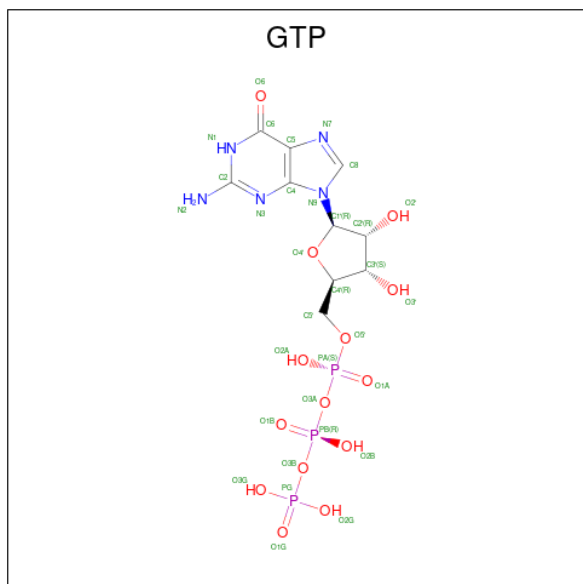
Mol	Chain	Residues	Atoms		AltConf
50	D	3	Total	Zn	0
			3	3	
50	I	1	Total	Zn	0
			1	1	
50	J	1	Total	Zn	0
			1	1	
50	T	3	Total	Zn	0
			3	3	
50	U	3	Total	Zn	0
			3	3	
50	Z	1	Total	Zn	0
			1	1	

- Molecule 51 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
51	a	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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


- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

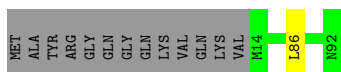
Mol	Chain	Residues	Atoms		AltConf
53	b	1	Total 1	Mg 1	0
53	d	6	Total 6	Mg 6	0

### 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: Small nuclear ribonucleoprotein E

Chain 1:  85% 14%



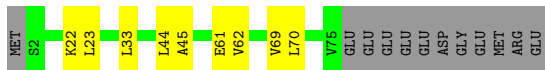
- Molecule 1: Small nuclear ribonucleoprotein E

Chain i:  76% 24%




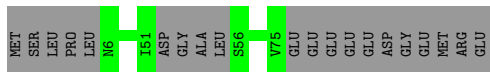
- Molecule 2: Small nuclear ribonucleoprotein F

Chain 2:  76% 10% 14%



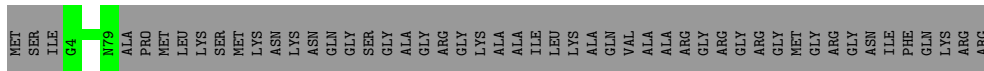
- Molecule 2: Small nuclear ribonucleoprotein F

Chain h:  77% 23%



- Molecule 3: Small nuclear ribonucleoprotein Sm D3

Chain 3:  60% 40%



- Molecule 3: Small nuclear ribonucleoprotein Sm D3



ARG	MET	SER	ILE	GLY	V5	I72	LEU	PRO	ASP	MET	LEU	LYS	ASN	ALA	PRO	MET	LEU	LYS	SER	MET	LYS	ASN	LYS	ASN	GLN	GLY	SER	GLY	ALA	GLY	ARG	GLY	LYS	ALA	ALA	ILE	LEU	LYS	ALA	GLN	VAL	ALA	ALA	ARG	GLY	ARG	GLY	ARG	GLY	GLY	MET	GLY	ARG	GLY	ASN	ILE	PHE	GLN	LYS	ASP
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- Chain 4:  69% 28%

MET	SEU	LEU	ASN	LYS	PRO	LYS	SER	GLU	MET	THR	PRO	GLU	GLU	LEU	GLN	LYS	ARG	E20	V66	S76	VAL	PRO	LYS	SER	GLY	LYS	GLY	LYS	LYS	SER	LYS	P89	M99	F100	L110	A116	GLY
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- Chain I:  58% 42%

[illegible]

- Chain 5:  65% 1% 31%

[illegible]

- Chain k:  66% 34%

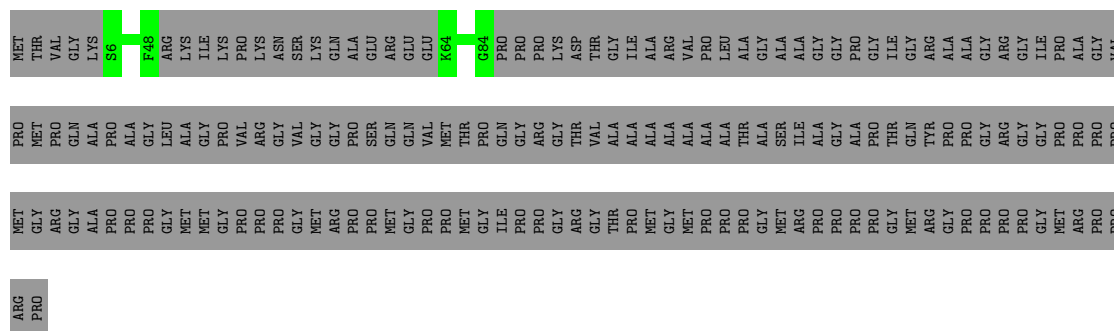
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- Chain 8:  35% . 64%


[illegible]

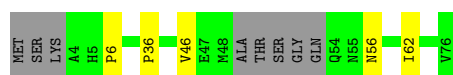
- Molecule 6: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain n:  27% 73%




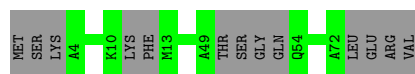
- Molecule 7: Small nuclear ribonucleoprotein G

Chain 9:  83% 7% 11%



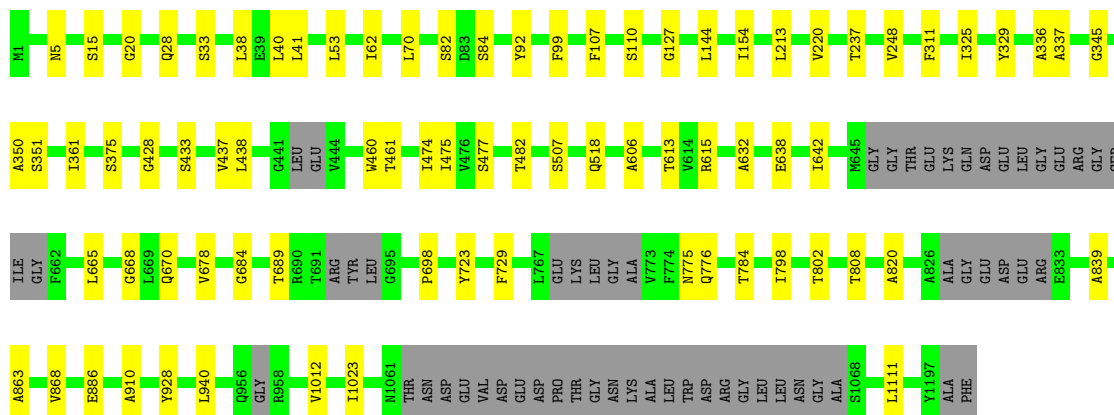
- Molecule 7: Small nuclear ribonucleoprotein G

Chain m:  83% 17%




- Molecule 8: Splicing factor 3B subunit 3

Chain A:  89% 6% 5%

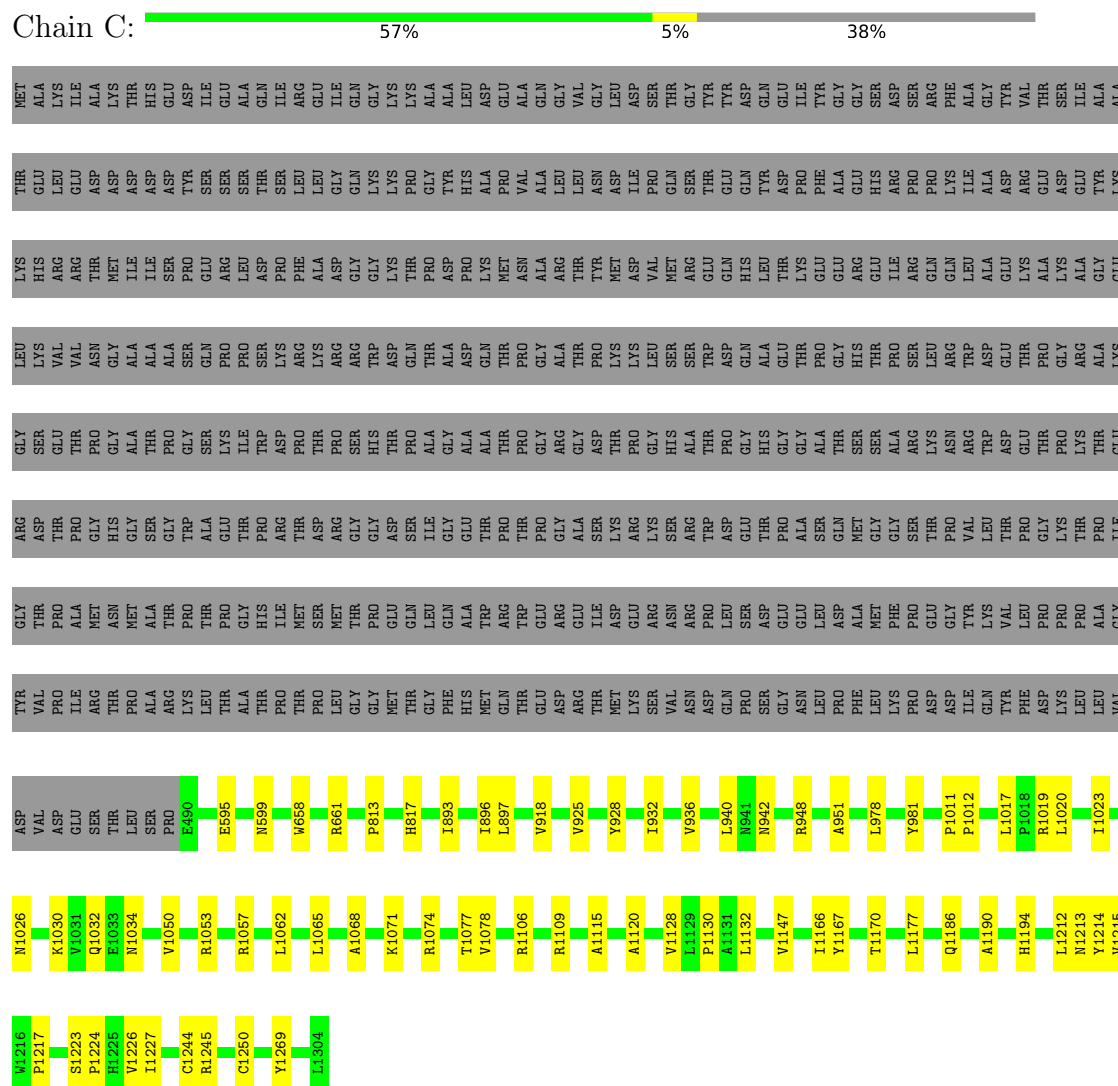


- Molecule 9: Splicing factor 3B subunit 5

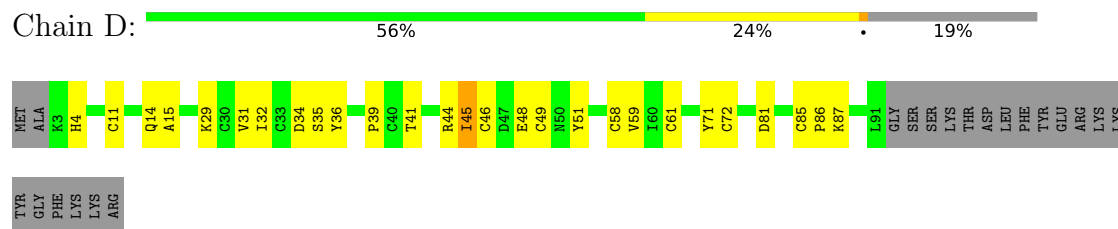
Chain B:  80% 19%



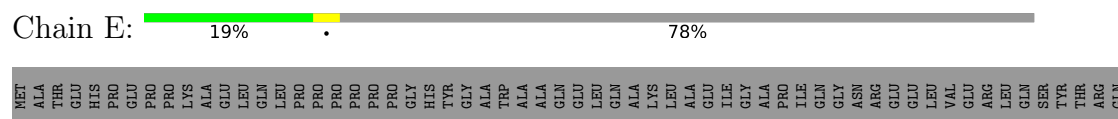
- Molecule 10: Splicing factor 3B subunit 1



- Molecule 11: PHD finger-like domain-containing protein 5A

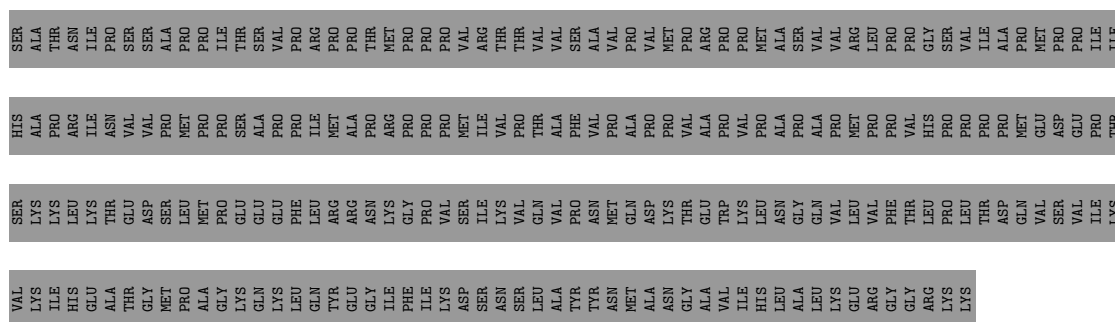


- Molecule 12: Splicing factor 3B subunit 2

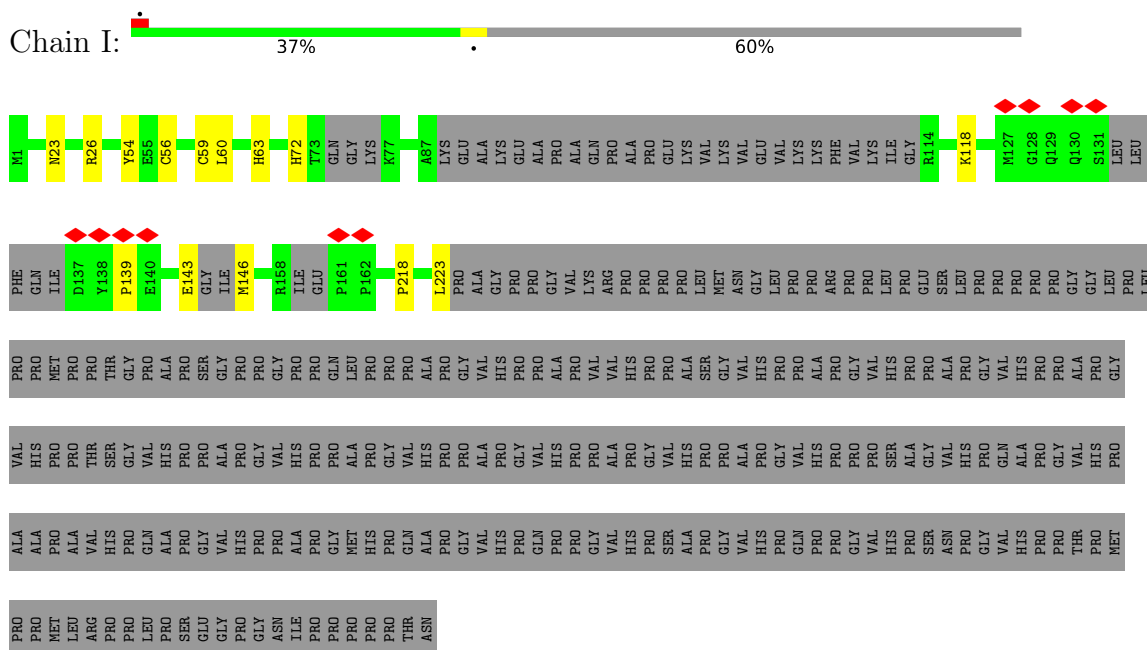




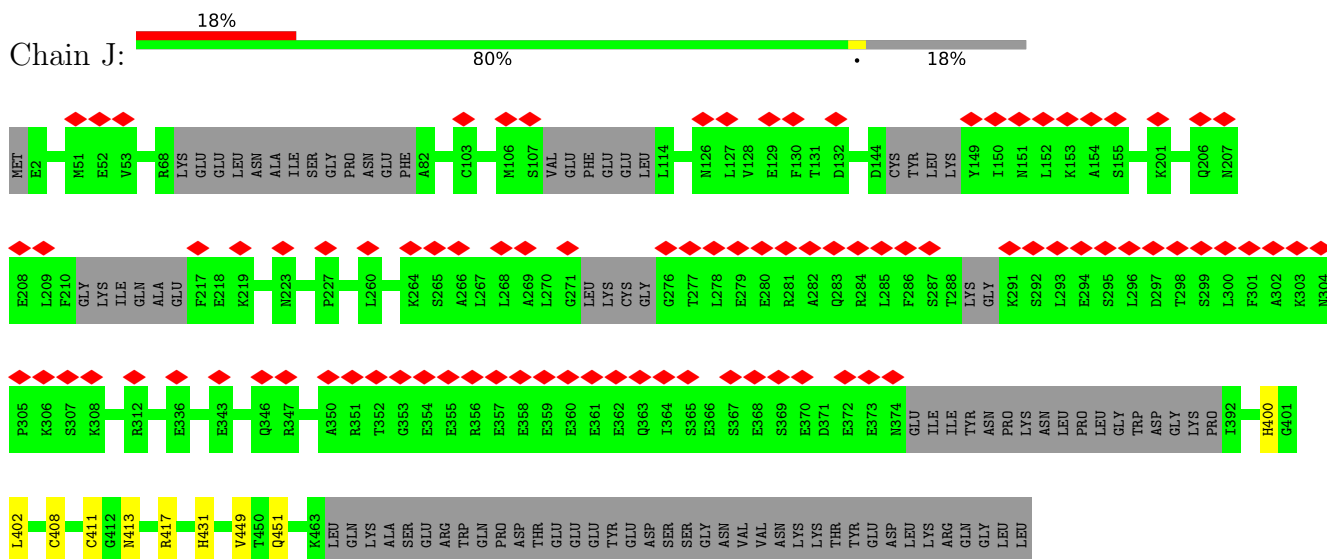




- Molecule 16: Splicing factor 3A subunit 2



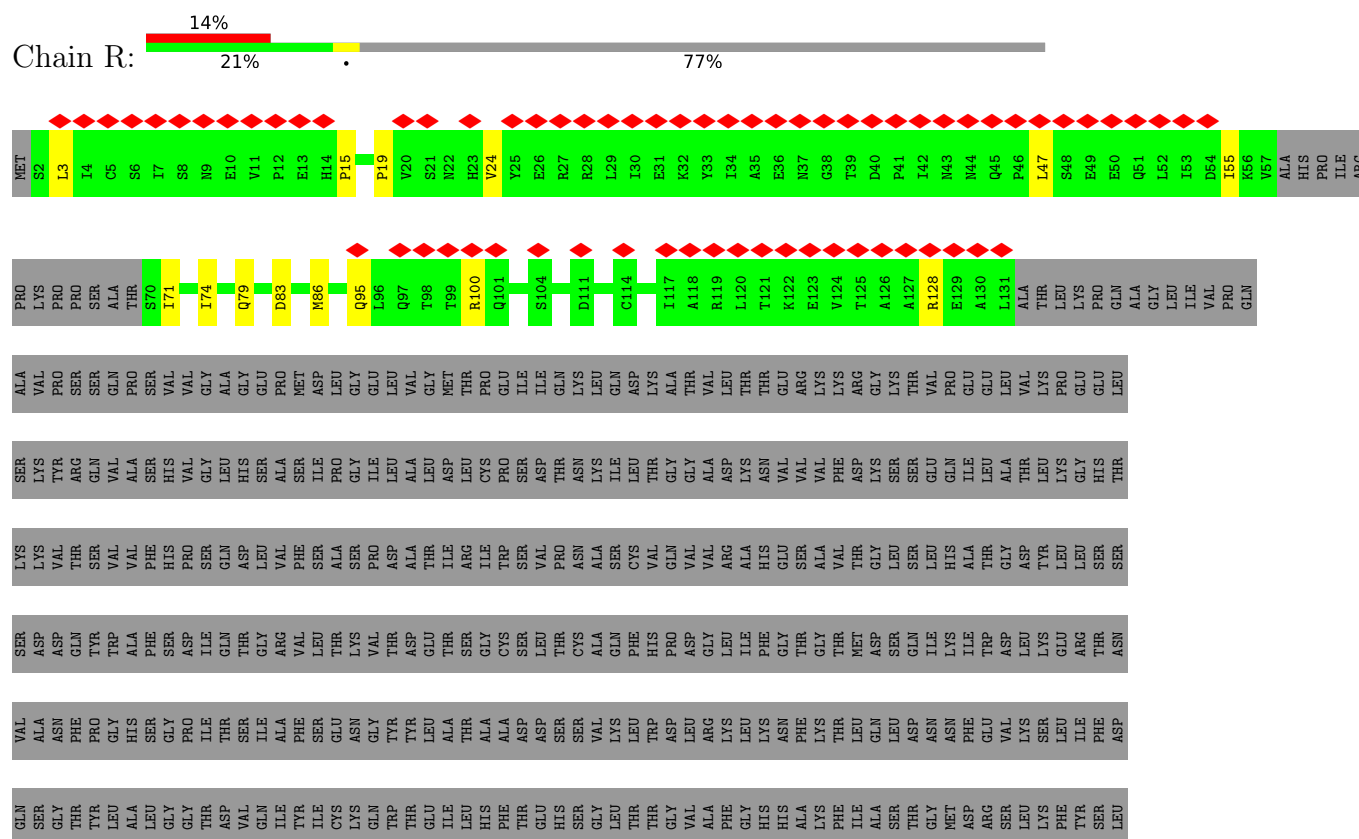
- Molecule 17: Splicing factor 3A subunit 3



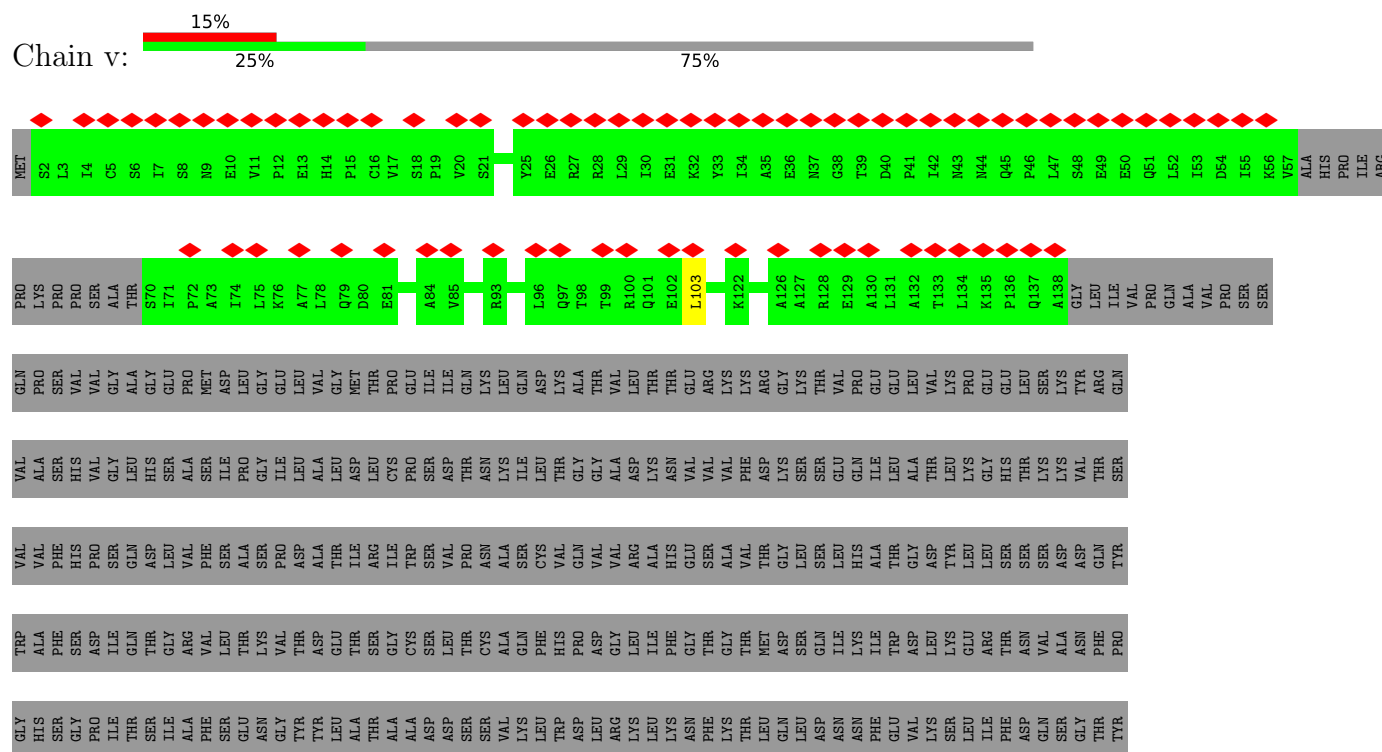
- Molecule 18: Pre-mRNA-processing factor 19



## ● Molecule 18: Pre-mRNA-processing factor 19



## ● Molecule 18: Pre-mRNA-processing factor 19



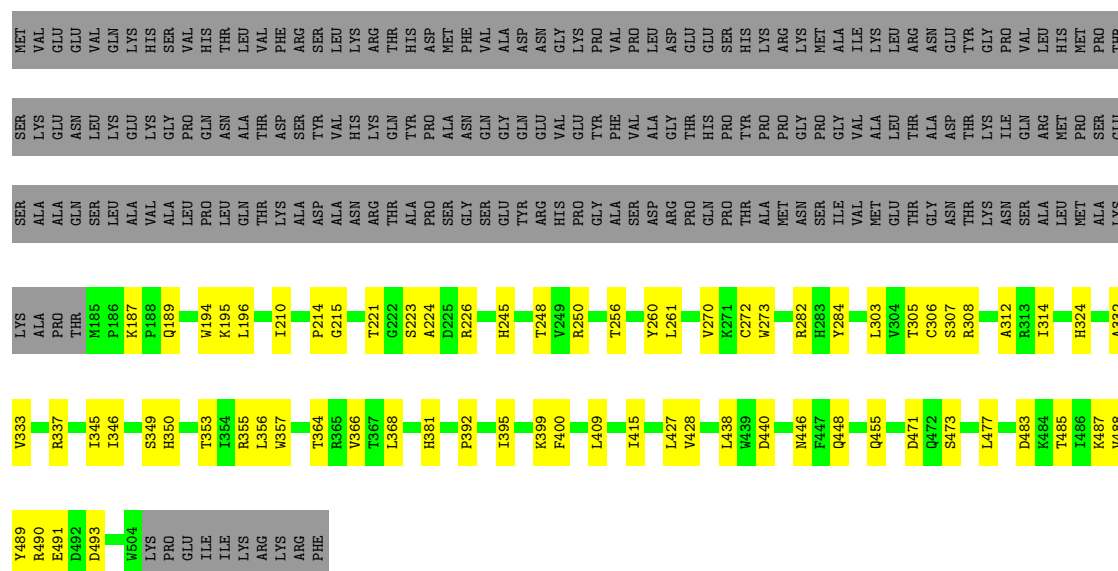






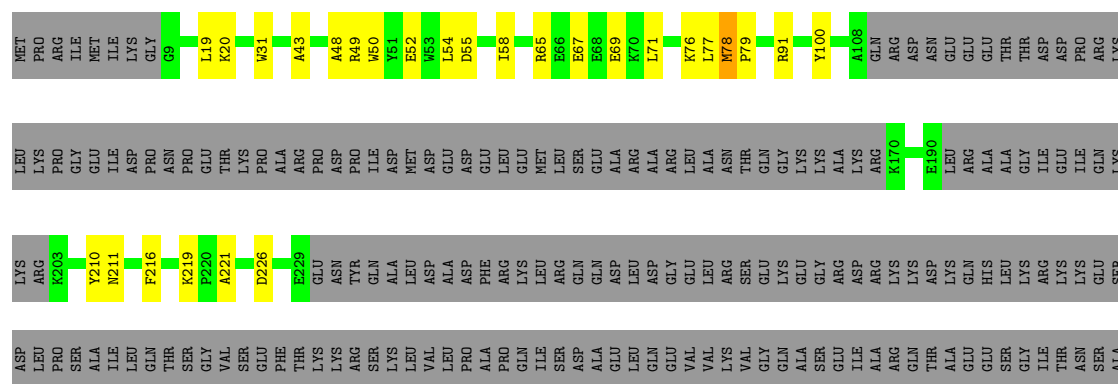
• Molecule 21: Pleiotropic regulator 1

Chain O: 49% 14% 38%

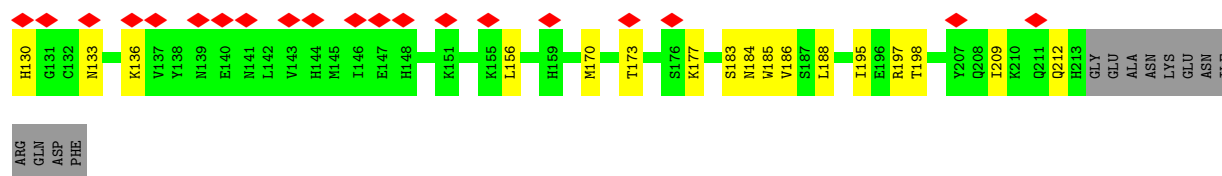


• Molecule 22: Cell division cycle 5-like protein

Chain P: 11% 36% 5% 50%







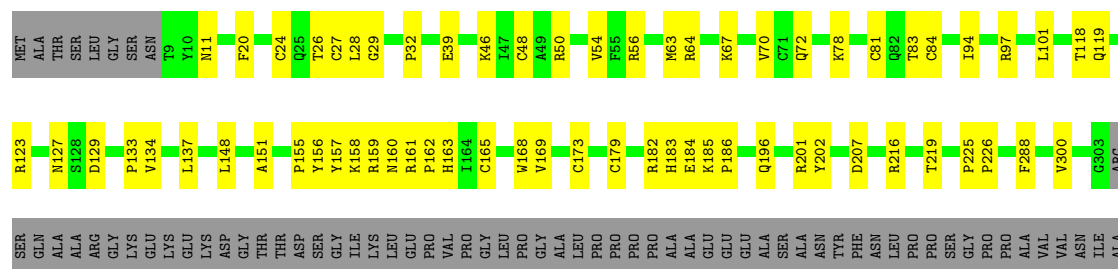
- Molecule 25: Protein BUD31 homolog

Chain T: 84% 15%



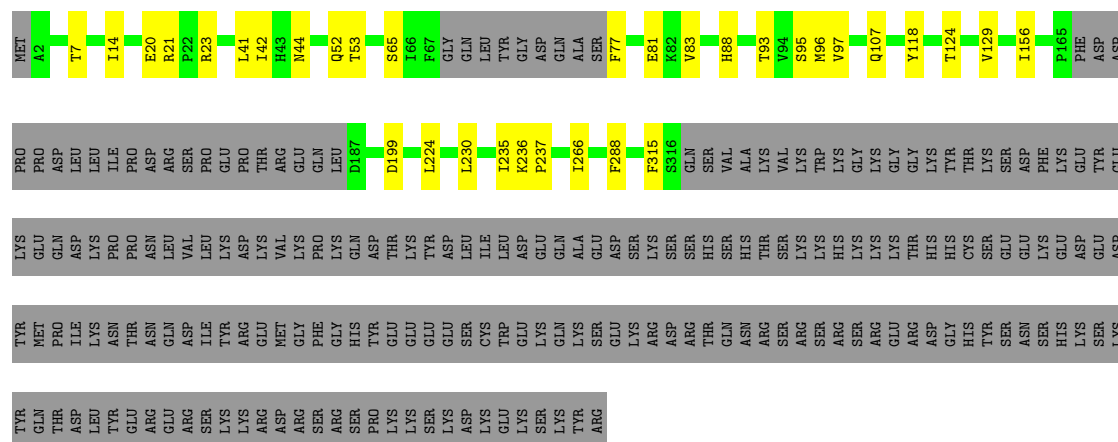
- Molecule 26: Pre-mRNA-splicing factor RBM22

Chain U: 55% 15% 30%



- Molecule 27: Peptidyl-prolyl cis-trans isomerase-like 4

Chain V: 51% 7% 42%



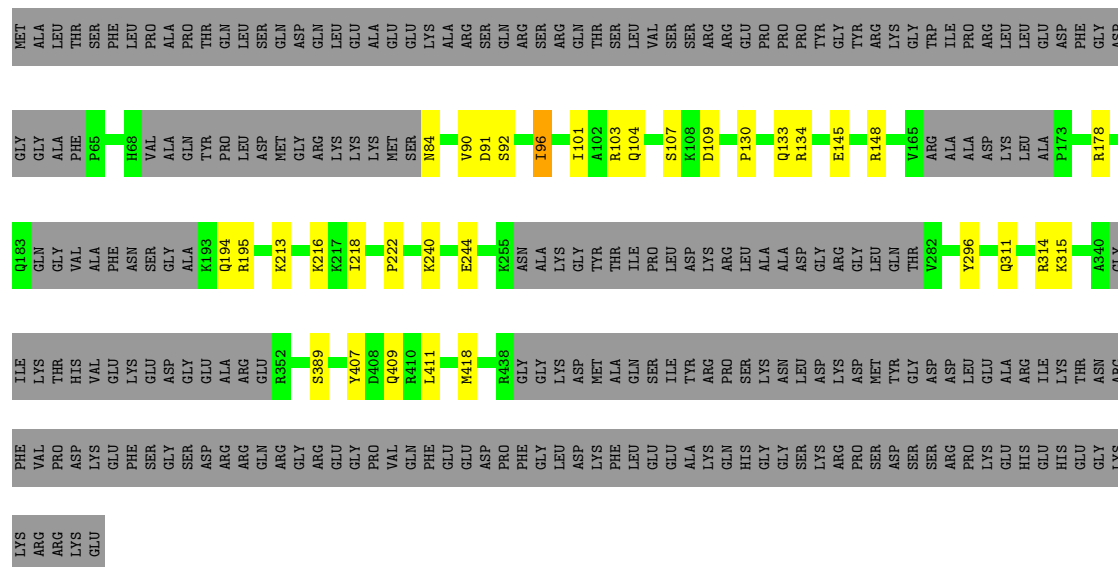
- Molecule 28: Pre-mRNA-splicing factor CWC22 homolog

Chain W: 48% 49%

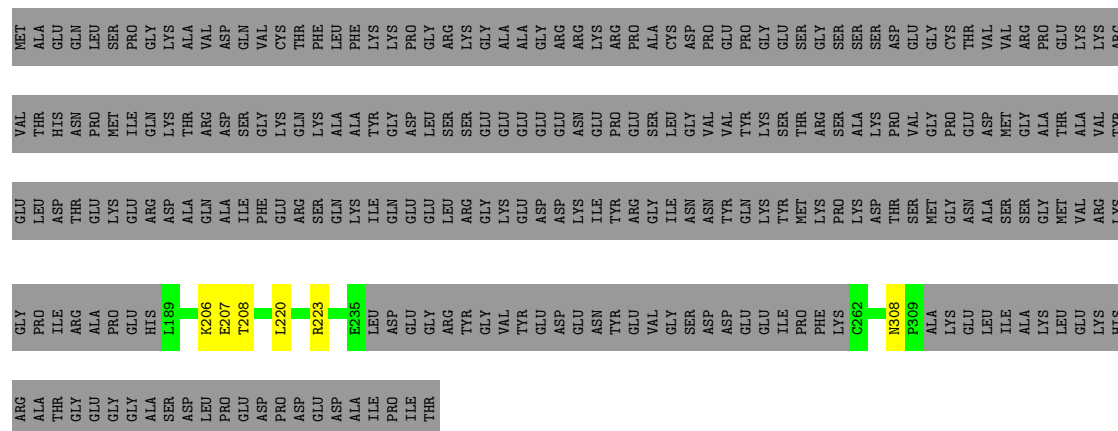


ASP	ALA	ALA	ASN	GLN	PRO	ASN	LEU	LYS	LEU	LEU	ALA	MET	ALA	LYS	LEU	TRP	LYS	LYS	GLN	GLN	GLN	GLU	LYS	GLU	GLU	ASP	ALA	GLU	HIS	HIS	PRO	ASP	ASP	GLU	GLU	ASP	VAL	ASP	GLU	SER	GLU	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 30: SNW domain-containing protein 1

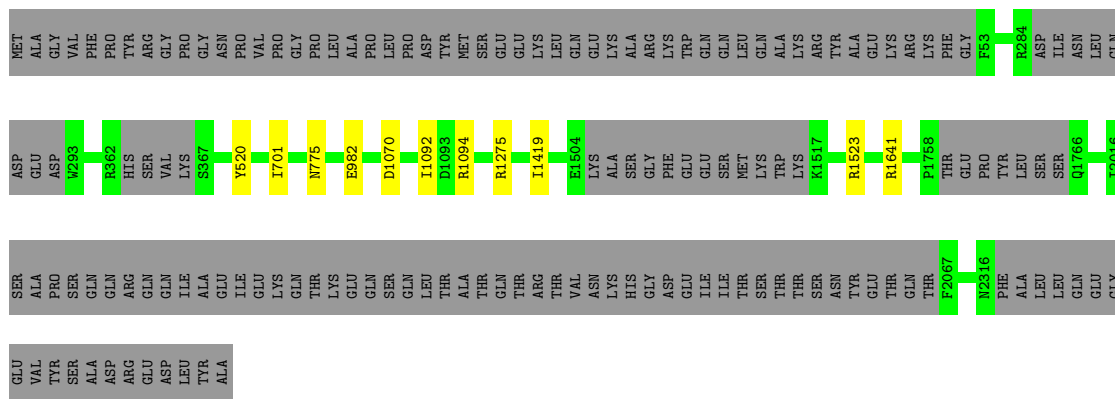


- Molecule 31: RING finger protein 113A



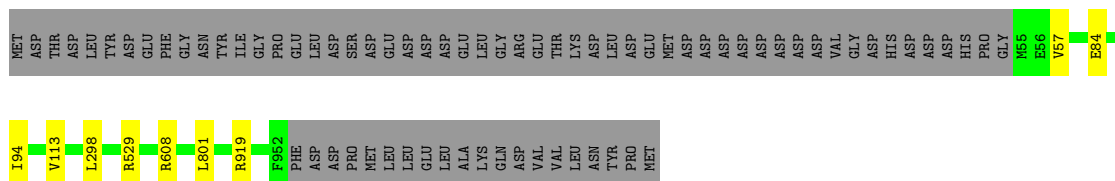
- Molecule 32: Pre-mRNA-processing-splicing factor 8






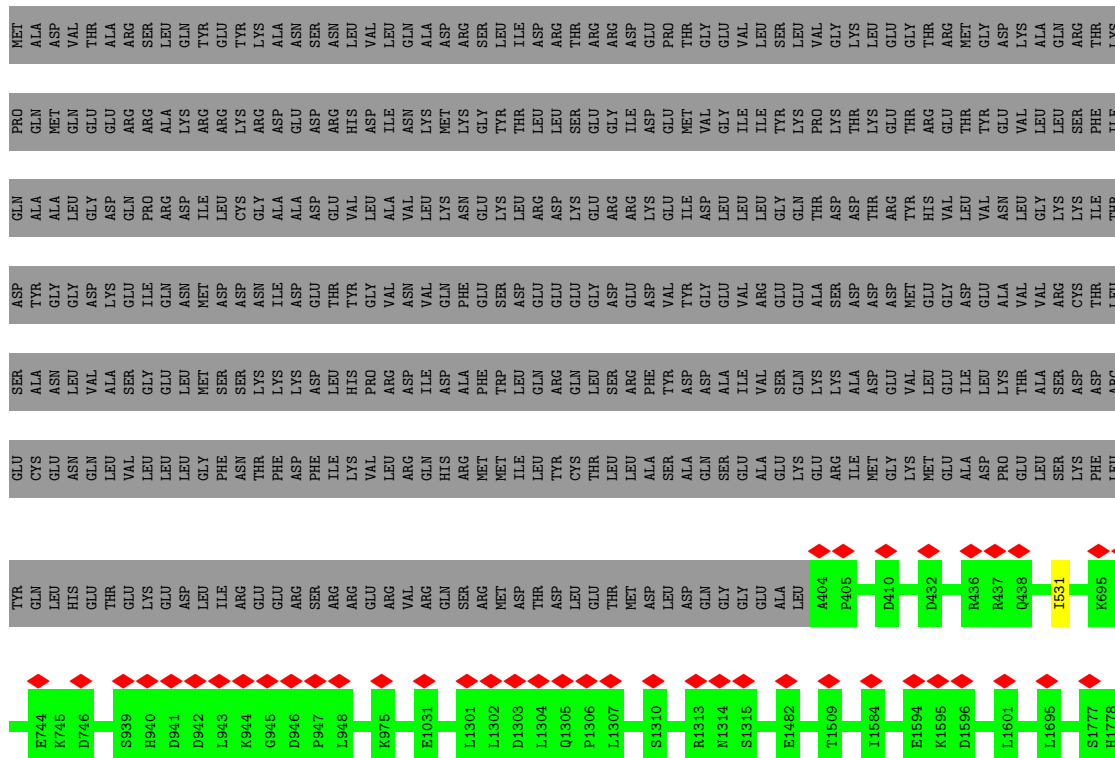
- Molecule 33: 116 kDa U5 small nuclear ribonucleoprotein component

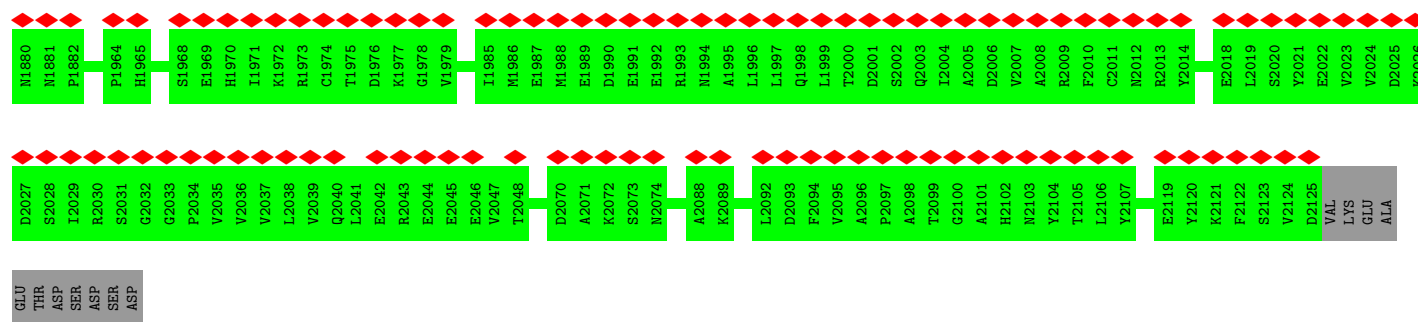
Chain b:  91% • 8%



- Molecule 34: U5 small nuclear ribonucleoprotein 200 kDa helicase

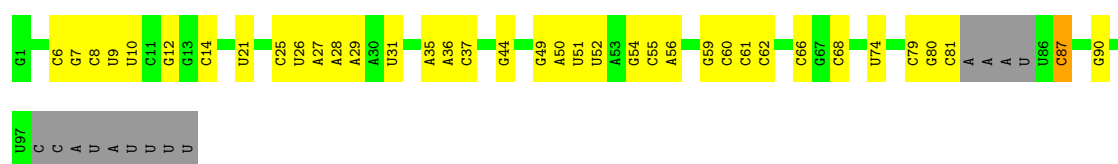
Chain c:  7% 81% 19%





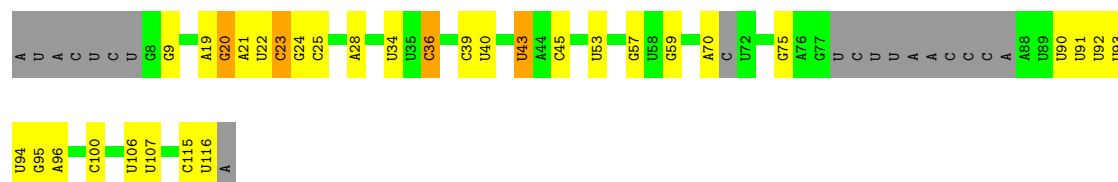
• Molecule 35: RNU6-1

Chain d: 53% 34% 12%



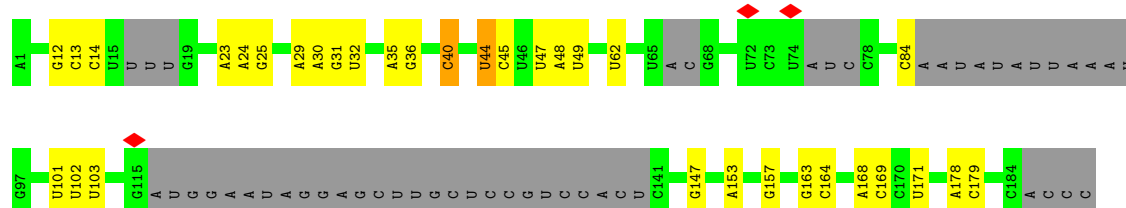
• Molecule 36: RNU5A-1

Chain e: 56% 24% 16%



• Molecule 37: RNU2-1

Chain f: 55% 16% 27%

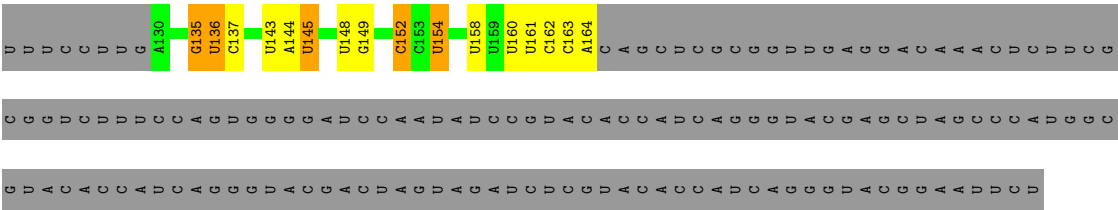


• Molecule 38: MINX-M3

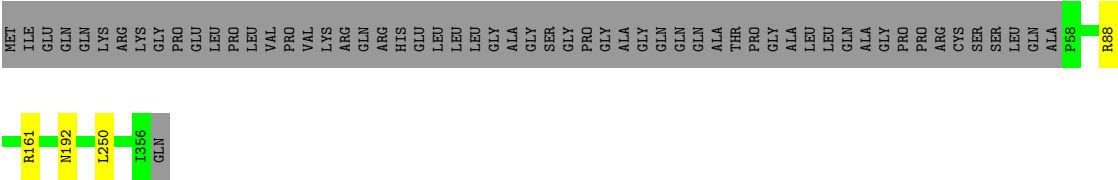
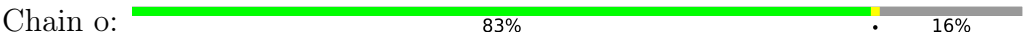
Chain g: 13% 9% 76%



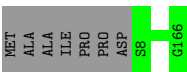




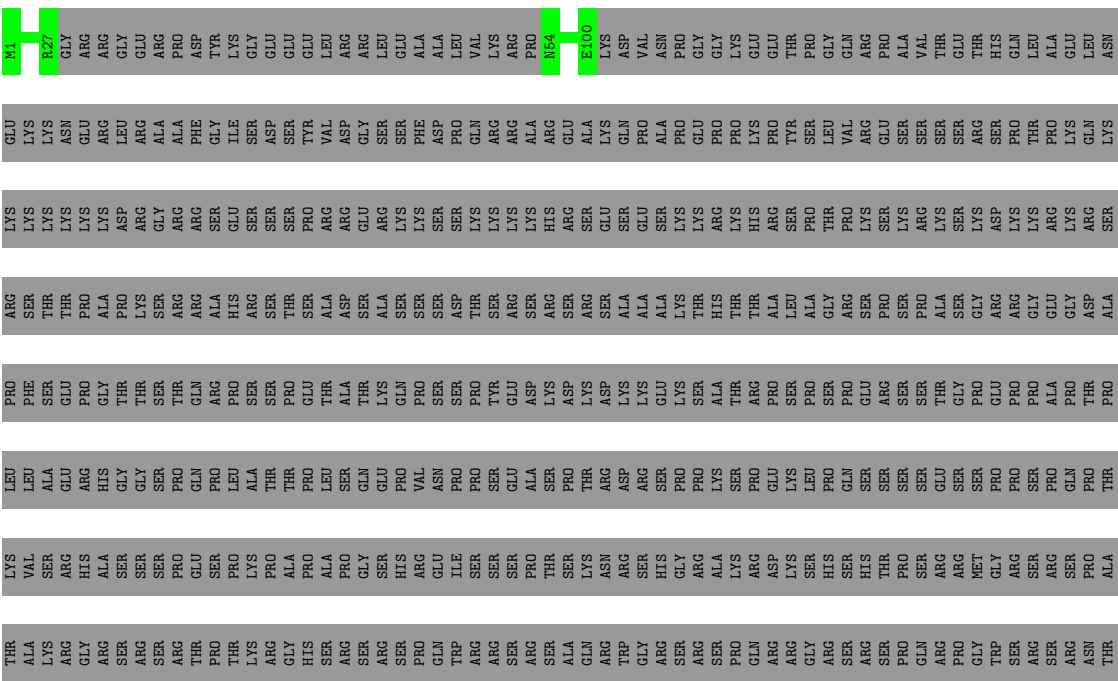
• Molecule 39: U5 small nuclear ribonucleoprotein 40 kDa protein



• Molecule 40: Peptidyl-prolyl cis-trans isomerase-like 1



• Molecule 41: Serine/arginine repetitive matrix protein 2

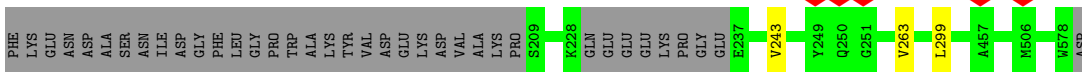
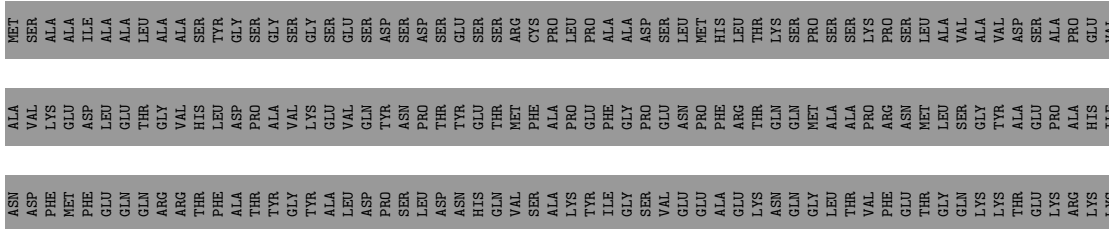


WORLDWIDE  
PDB  
PROTEIN DATA BANK

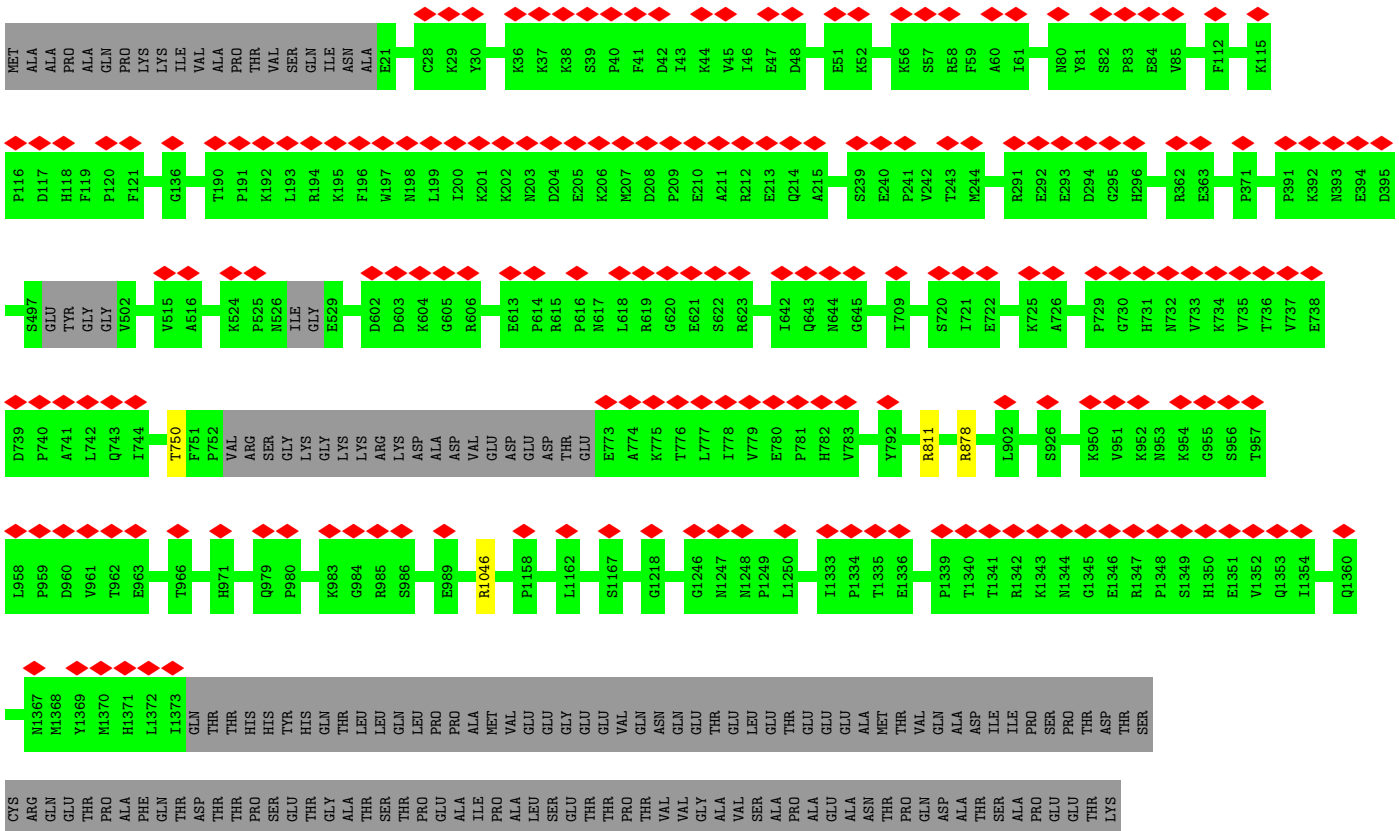
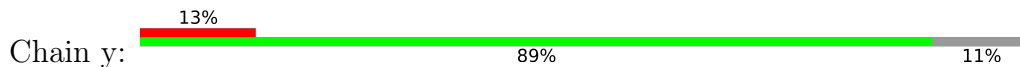




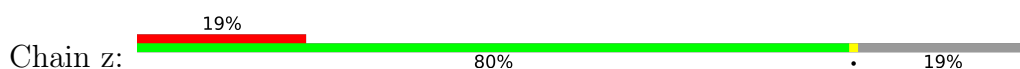
- Molecule 47: Pre-mRNA-processing factor 17

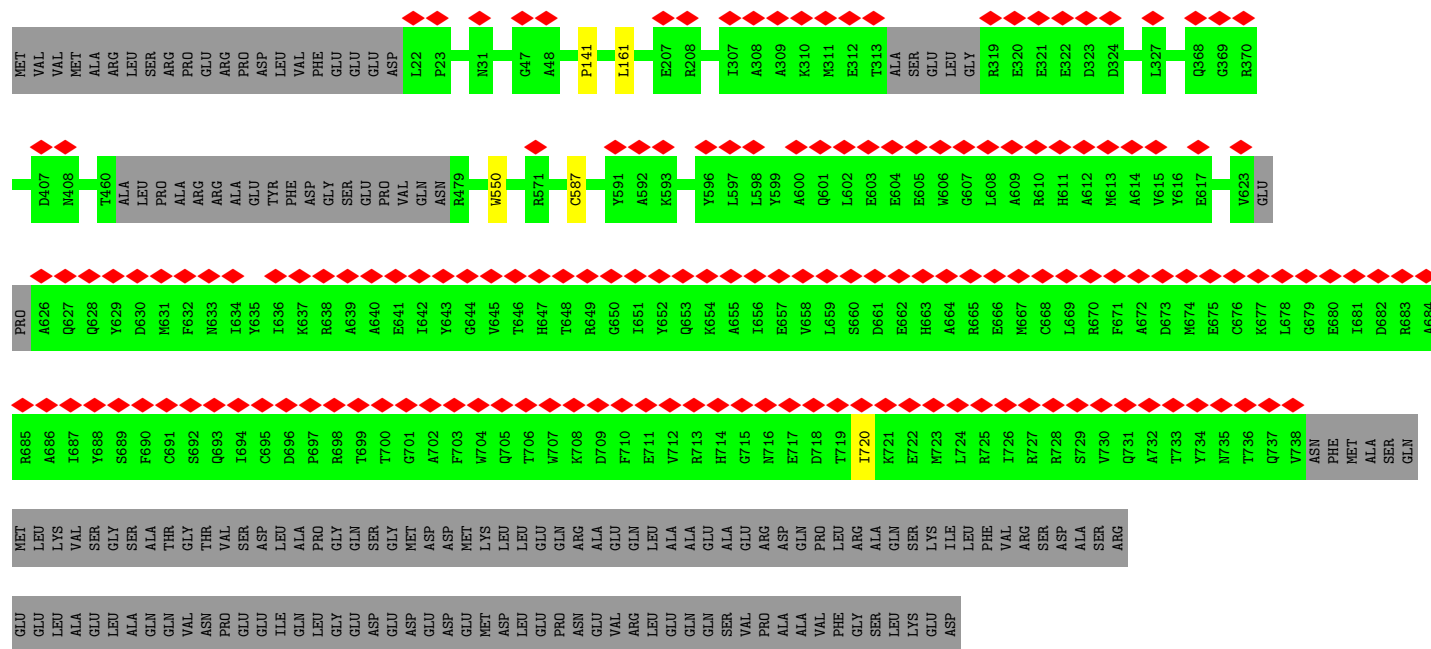


- Molecule 48: Intron-binding protein aquarium



- Molecule 49: Pre-mRNA-splicing factor SYF1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12395	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45.47	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.24	0/390	0.46	0/542
1	i	0.25	0/344	0.48	0/476
2	2	0.25	0/360	0.48	0/497
2	h	0.25	0/320	0.48	0/440
3	3	0.25	0/372	0.47	0/515
3	j	0.25	0/334	0.50	0/463
4	4	0.25	0/420	0.47	0/583
4	l	0.24	0/335	0.46	0/464
5	5	0.27	0/405	0.45	0/563
5	k	0.25	0/387	0.46	0/537
6	8	0.26	0/421	0.50	0/583
6	n	0.24	0/313	0.47	0/432
7	9	0.25	0/332	0.47	0/458
7	m	0.25	0/306	0.50	0/420
8	A	0.26	0/5706	0.48	0/7930
9	B	0.24	0/351	0.37	0/489
10	C	0.28	0/5209	0.52	0/7211
11	D	0.30	0/660	0.65	0/893
12	E	0.27	0/1383	0.53	0/1887
13	F	0.25	0/382	0.46	0/529
14	G	0.28	0/370	0.54	0/513
15	H	0.22	0/524	0.34	0/724
16	I	0.28	0/1037	0.50	0/1420
17	J	0.24	0/2195	0.42	0/3036
18	K	0.26	0/953	0.57	0/1295
18	M	0.27	0/1004	0.60	1/1365 (0.1%)
18	R	0.24	0/953	0.55	0/1295
18	v	0.26	0/1004	0.54	1/1365 (0.1%)
19	L	0.27	0/178	0.53	0/240
20	N	0.31	0/6267	0.67	4/8491 (0.0%)
21	O	0.29	0/2586	0.61	0/3527
22	P	0.26	0/2463	0.55	2/3317 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
23	Q	0.32	0/836	0.68	0/1117
24	S	0.26	0/1342	0.66	1/1804 (0.1%)
25	T	0.32	0/1202	0.66	0/1611
26	U	0.30	0/2118	0.62	1/2881 (0.0%)
27	V	0.28	0/2026	0.57	0/2760
28	W	0.28	0/2954	0.51	0/4033
29	X	0.26	0/1623	0.47	0/2240
30	Y	0.27	0/2290	0.56	1/3103 (0.0%)
31	Z	0.27	0/618	0.52	1/845 (0.1%)
32	a	0.28	0/16807	0.56	1/22895 (0.0%)
33	b	0.30	0/7206	0.60	1/9800 (0.0%)
34	c	0.25	0/8529	0.43	0/11891
35	d	0.33	0/2225	1.02	6/3464 (0.2%)
36	e	0.34	0/2307	1.12	13/3584 (0.4%)
37	f	0.29	1/3239 (0.0%)	0.96	8/5031 (0.2%)
38	g	0.31	0/1734	1.09	16/2691 (0.6%)
39	o	0.29	0/2392	0.62	1/3242 (0.0%)
40	p	0.26	0/775	0.46	0/1070
41	q	0.28	0/466	0.57	0/639
42	r	0.25	0/803	0.48	0/1119
43	s	0.24	0/810	0.44	0/1122
44	t	0.31	0/414	0.63	0/555
45	u	0.27	0/1969	0.52	0/2722
46	w	0.25	0/1087	0.47	0/1497
47	x	0.25	0/1785	0.51	0/2482
48	y	0.28	0/11144	0.57	1/15101 (0.0%)
49	z	0.29	0/4593	0.57	1/6317 (0.0%)
All	All	0.28	1/121558 (0.0%)	0.61	60/168116 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	D	0	1
20	N	0	1
24	S	0	2
39	o	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	f	168	A	N9-C4	5.57	1.41	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	82	LEU	CA-CB-CG	8.59	135.04	115.30
38	g	-6	C	N1-C2-O2	7.54	123.42	118.90
22	P	773	ASP	CB-CG-OD1	7.15	124.73	118.30
36	e	20	G	C4-N9-C1'	7.09	135.72	126.50
38	g	152	C	N1-C2-O2	7.05	123.13	118.90
36	e	20	G	N3-C4-N9	6.97	130.18	126.00
36	e	20	G	N3-C4-C5	-6.84	125.18	128.60
37	f	168	A	C2-N3-C4	6.72	113.96	110.60
36	e	23	C	N1-C2-O2	6.71	122.93	118.90
33	b	298	LEU	CA-CB-CG	6.65	130.59	115.30
38	g	154	U	N1-C2-O2	6.49	127.34	122.80
38	g	154	U	C2-N1-C1'	6.39	125.37	117.70
35	d	50	A	P-O3'-C3'	6.30	127.26	119.70
38	g	136	U	P-O3'-C3'	6.28	127.24	119.70
20	N	799	LEU	CA-CB-CG	6.17	129.50	115.30
36	e	23	C	C2-N1-C1'	6.16	125.58	118.80
38	g	135	G	N3-C4-N9	6.13	129.68	126.00
38	g	-6	C	N3-C2-O2	-6.11	117.62	121.90
48	y	750	THR	C-N-CA	6.05	136.82	121.70
37	f	168	A	C4-N9-C1'	6.02	137.14	126.30
38	g	22	C	N1-C2-O2	6.02	122.51	118.90
36	e	20	G	C8-N9-C1'	-5.98	119.23	127.00
36	e	36	C	N1-C2-O2	5.94	122.47	118.90
18	M	54	ASP	CB-CG-OD1	5.88	123.59	118.30
38	g	154	U	N3-C2-O2	-5.87	118.09	122.20
36	e	43	U	N3-C2-O2	-5.82	118.13	122.20
36	e	36	C	C6-N1-C2	-5.80	117.98	120.30
35	d	14	C	C6-N1-C2	-5.78	117.99	120.30
36	e	43	U	N1-C2-O2	5.76	126.83	122.80
31	Z	220	LEU	CA-CB-CG	5.73	128.48	115.30
35	d	87	C	N1-C2-O2	5.71	122.33	118.90
36	e	39	C	P-O3'-C3'	5.67	126.50	119.70
38	g	145	U	C5-C6-N1	5.65	125.53	122.70
32	a	1070	ASP	CB-CG-OD1	5.58	123.32	118.30
38	g	152	C	N3-C2-O2	-5.48	118.06	121.90
37	f	168	A	N3-C4-N9	5.48	131.78	127.40
37	f	40	C	N1-C2-O2	5.45	122.17	118.90
39	o	250	LEU	CA-CB-CG	5.43	127.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	643	LEU	CA-CB-CG	5.39	127.70	115.30
37	f	40	C	C6-N1-C2	-5.39	118.14	120.30
38	g	-6	C	C6-N1-C2	-5.37	118.15	120.30
36	e	23	C	N3-C2-O2	-5.36	118.15	121.90
35	d	31	U	N1-C2-O2	5.33	126.53	122.80
35	d	87	C	C6-N1-C2	-5.31	118.18	120.30
22	P	78	MET	CA-CB-CG	5.28	122.27	113.30
26	U	63	MET	CB-CG-SD	5.26	128.19	112.40
35	d	31	U	N3-C2-O2	-5.24	118.54	122.20
30	Y	418	MET	CA-CB-CG	5.22	122.17	113.30
38	g	135	G	C4-N9-C1'	5.19	133.25	126.50
38	g	145	U	N1-C2-O2	5.18	126.43	122.80
37	f	44	U	N3-C2-O2	-5.12	118.62	122.20
38	g	22	C	C2-N1-C1'	5.12	124.43	118.80
20	N	506	LEU	CA-CB-CG	5.10	127.03	115.30
38	g	-6	C	C2-N1-C1'	5.10	124.41	118.80
36	e	36	C	N3-C2-O2	-5.09	118.34	121.90
18	v	103	LEU	CA-CB-CG	5.04	126.90	115.30
37	f	168	A	N3-C4-C5	-5.02	123.28	126.80
20	N	546	LEU	CA-CB-CG	5.01	126.83	115.30
49	z	161	LEU	CA-CB-CG	5.01	126.82	115.30
37	f	168	A	C8-N9-C1'	-5.00	118.69	127.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	D	45	ILE	Peptide
20	N	504	GLU	Peptide
24	S	77	GLN	Peptide
24	S	89	LEU	Peptide
39	o	192	ASN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	391	0	163	1	0
1	i	346	0	144	0	0
2	2	361	0	158	5	0
2	h	322	0	138	0	0
3	3	373	0	163	0	0
3	j	335	0	148	0	0
4	4	422	0	175	3	0
4	l	337	0	139	0	0
5	5	406	0	170	3	0
5	k	388	0	164	0	0
6	8	422	0	177	1	0
6	n	315	0	134	0	0
7	9	334	0	143	3	0
7	m	309	0	135	0	0
8	A	5714	0	2549	42	0
9	B	350	0	167	0	0
10	C	5115	0	4128	42	0
11	D	649	0	597	16	0
12	E	1350	0	1111	18	0
13	F	383	0	173	4	0
14	G	364	0	226	2	0
15	H	530	0	218	1	0
16	I	1034	0	621	6	0
17	J	2187	0	1161	8	0
18	K	938	0	938	5	0
18	M	988	0	994	11	0
18	R	938	0	938	10	0
18	v	988	0	994	0	0
19	L	177	0	140	0	0
20	N	6147	0	5981	87	0
21	O	2517	0	2466	46	0
22	P	2432	0	2205	35	0
23	Q	823	0	779	14	0
24	S	1323	0	1311	13	0
25	T	1176	0	1178	15	0
26	U	2080	0	1803	40	0
27	V	1996	0	1727	21	0
28	W	2921	0	2168	12	0
29	X	1587	0	1176	12	0
30	Y	2250	0	2095	23	0
31	Z	607	0	402	3	0
32	a	16415	0	14878	0	0
33	b	7046	0	7030	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	c	8530	0	3747	0	0
35	d	1989	0	1006	0	0
36	e	2070	0	1046	0	0
37	f	2906	0	1473	0	0
38	g	1559	0	794	0	0
39	o	2338	0	2275	0	0
40	p	776	0	358	0	0
41	q	461	0	354	0	0
42	r	804	0	350	0	0
43	s	813	0	366	0	0
44	t	407	0	393	0	0
45	u	1963	0	1065	0	0
46	w	1093	0	497	0	0
47	x	1787	0	780	0	0
48	y	10878	0	10826	0	0
49	z	4511	0	3545	0	0
50	D	3	0	0	0	0
50	I	1	0	0	0	0
50	J	1	0	0	0	0
50	T	3	0	0	0	0
50	U	3	0	0	0	0
50	Z	1	0	0	0	0
51	a	36	0	6	0	0
52	b	32	0	12	0	0
53	b	1	0	0	0	0
53	d	6	0	0	0	0
All	All	119058	0	91198	453	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (453) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:139:CYS:SG	25:T:142:CYS:HB3	1.98	1.02
26:U:24:CYS:SG	26:U:81:CYS:HB2	2.12	0.90
27:V:65:SER:HG	27:V:77:PHE:N	1.74	0.86
26:U:27:CYS:HB3	26:U:84:CYS:SG	2.26	0.75
11:D:46:CYS:SG	11:D:85:CYS:HB2	2.26	0.75
22:P:48:ALA:O	22:P:52:GLU:HB2	1.87	0.73
20:N:504:GLU:O	20:N:508:GLU:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:179:CYS:HB3	26:U:183:HIS:NE2	2.06	0.70
27:V:95:SER:HA	27:V:124:THR:O	1.94	0.67
16:I:54:TYR:HB2	16:I:63:HIS:HB2	1.77	0.66
17:J:411:CYS:HB3	17:J:431:HIS:ND1	2.10	0.66
17:J:411:CYS:CB	17:J:431:HIS:HD1	2.10	0.64
25:T:117:CYS:SG	25:T:118:ILE:N	2.70	0.63
17:J:408:CYS:O	17:J:413:ASN:HA	1.99	0.62
20:N:644:VAL:HA	20:N:670:VAL:O	1.99	0.62
30:Y:240:LYS:O	30:Y:244:GLU:HB2	2.00	0.62
20:N:988:GLU:HB3	20:N:998:ARG:HB2	1.81	0.62
24:S:133:ASN:HA	24:S:136:LYS:HB2	1.81	0.62
26:U:39:GLU:HB2	26:U:54:VAL:HB	1.83	0.61
25:T:105:CYS:SG	25:T:117:CYS:HB3	2.41	0.60
22:P:216:PHE:O	29:X:267:ARG:NH1	2.35	0.60
21:O:272:CYS:HB3	21:O:282:ARG:HB2	1.84	0.60
17:J:411:CYS:HB3	17:J:431:HIS:HD1	1.63	0.59
13:F:39:VAL:HA	13:F:61:PHE:HA	1.85	0.59
23:Q:187:ARG:HE	27:V:118:TYR:HB2	1.67	0.59
20:N:615:LEU:HD12	20:N:621:ILE:HG13	1.84	0.59
21:O:270:VAL:HB	21:O:284:TYR:HB2	1.85	0.59
21:O:477:LEU:O	21:O:488:VAL:HA	2.03	0.59
8:A:336:ALA:HA	8:A:351:SER:HA	1.85	0.58
20:N:873:LEU:H	20:N:880:VAL:HG22	1.69	0.58
22:P:226:ASP:HB2	29:X:297:ASN:HD21	1.68	0.57
30:Y:178:ARG:HH11	30:Y:194:GLN:HB3	1.70	0.57
25:T:12:PRO:HB2	25:T:74:LEU:HD22	1.86	0.57
18:R:19:PRO:HD2	18:R:47:LEU:HD11	1.87	0.56
20:N:765:LEU:HD22	20:N:822:PRO:HG3	1.86	0.56
21:O:195:LYS:HE2	21:O:490:ARG:HH21	1.68	0.56
10:C:1244:CYS:SG	10:C:1245:ARG:NH1	2.79	0.56
20:N:251:LEU:HD11	20:N:273:LYS:HB3	1.87	0.56
20:N:752:VAL:O	20:N:757:ARG:NH1	2.39	0.56
18:M:81:GLU:HB3	18:R:71:ILE:HG12	1.88	0.56
21:O:210:ILE:HG12	21:O:221:THR:HG22	1.87	0.56
8:A:461:THR:HA	8:A:474:ILE:HA	1.88	0.56
20:N:232:ARG:HD2	27:V:237:PRO:HG3	1.88	0.56
20:N:700:TYR:HB2	20:N:707:GLU:HG3	1.86	0.56
22:P:221:ALA:O	29:X:301:ARG:NH1	2.38	0.56
26:U:24:CYS:O	26:U:28:LEU:HB2	2.06	0.56
11:D:29:LYS:HE2	11:D:34:ASP:HB3	1.87	0.55
26:U:84:CYS:O	26:U:201:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:133:PRO:HD2	26:U:137:LEU:HD22	1.88	0.55
8:A:437:VAL:O	8:A:776:GLN:HA	2.06	0.55
20:N:656:GLN:HA	20:N:659:ILE:HD12	1.87	0.55
18:K:26:GLU:HB3	18:K:29:LEU:HB2	1.88	0.55
20:N:511:LEU:HB3	20:N:514:TYR:HB2	1.88	0.55
20:N:649:ALA:O	20:N:906:ARG:NH2	2.40	0.55
21:O:314:ILE:HB	21:O:324:HIS:HB2	1.88	0.55
27:V:14:ILE:HG12	27:V:129:VAL:HG22	1.87	0.55
25:T:120:ARG:NH1	25:T:142:CYS:SG	2.78	0.55
8:A:820:ALA:HA	8:A:839:ALA:HB1	1.89	0.55
11:D:4:HIS:NE2	11:D:32:ILE:O	2.40	0.55
18:M:116:VAL:HG13	18:M:119:ARG:HH21	1.71	0.55
20:N:416:GLN:HG3	20:N:417:VAL:HG13	1.88	0.55
20:N:497:THR:H	20:N:500:MET:HE2	1.72	0.54
21:O:195:LYS:NZ	21:O:491:GLU:O	2.41	0.54
20:N:612:LEU:HB3	20:N:689:VAL:HG22	1.89	0.54
20:N:612:LEU:O	20:N:689:VAL:HA	2.06	0.54
12:E:508:ARG:HH11	12:E:513:GLY:H	1.56	0.54
20:N:453:PRO:HG3	20:N:524:GLU:HG3	1.89	0.54
26:U:168:TRP:O	26:U:185:LYS:NZ	2.41	0.54
21:O:381:HIS:O	30:Y:134:ARG:NH2	2.41	0.54
26:U:78:LYS:NZ	26:U:202:TYR:O	2.41	0.54
12:E:530:ARG:HH22	12:E:578:TRP:HB3	1.73	0.54
26:U:162:PRO:O	26:U:182:ARG:NE	2.38	0.54
21:O:307:SER:OG	21:O:308:ARG:N	2.41	0.53
21:O:485:THR:OG1	21:O:487:LYS:NZ	2.41	0.53
26:U:288:PHE:HA	26:U:300:VAL:H	1.73	0.53
7:9:46:VAL:HA	7:9:56:ASN:HA	1.90	0.53
8:A:15:SER:N	8:A:33:SER:O	2.42	0.53
10:C:1068:ALA:O	10:C:1074:ARG:NH1	2.41	0.53
10:C:1190:ALA:O	10:C:1194:HIS:ND1	2.41	0.53
20:N:559:ARG:HH22	20:N:782:ASP:HB3	1.72	0.53
21:O:356:LEU:HB2	21:O:366:VAL:HB	1.91	0.53
10:C:940:LEU:HD23	10:C:948:ARG:HB3	1.89	0.53
20:N:460:SER:OG	20:N:464:ARG:NH1	2.41	0.53
20:N:648:TYR:HB2	20:N:651:LEU:HB2	1.91	0.53
27:V:7:THR:HG22	27:V:156:ILE:HG12	1.89	0.53
11:D:41:THR:HB	11:D:71:TYR:HB2	1.91	0.53
20:N:945:ALA:HA	20:N:1011:VAL:HG21	1.91	0.52
21:O:189:GLN:NE2	21:O:440:ASP:OD1	2.42	0.52
22:P:779:GLU:HA	22:P:782:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:V:96:MET:HB3	27:V:124:THR:HB	1.90	0.52
27:V:7:THR:HA	27:V:156:ILE:HA	1.91	0.52
10:C:942:ASN:O	10:C:948:ARG:NH1	2.42	0.52
10:C:1062:LEU:HD22	10:C:1077:THR:HG23	1.91	0.52
20:N:752:VAL:HG13	20:N:757:ARG:HH11	1.75	0.52
26:U:26:THR:HG22	26:U:155:PRO:HA	1.91	0.52
10:C:1062:LEU:HA	10:C:1065:LEU:HB2	1.92	0.52
10:C:1106:ARG:O	10:C:1109:ARG:NH1	2.43	0.52
20:N:960:ARG:NH1	20:N:961:THR:O	2.43	0.52
22:P:211:ASN:OD1	29:X:228:ARG:NH1	2.40	0.52
30:Y:103:ARG:NH1	30:Y:107:SER:O	2.43	0.52
30:Y:145:GLU:OE2	30:Y:148:ARG:NH1	2.43	0.52
10:C:1019:ARG:O	10:C:1019:ARG:NH1	2.43	0.52
24:S:73:LEU:HD23	24:S:76:ARG:HH22	1.74	0.52
14:G:120:GLU:O	20:N:184:ARG:NH2	2.43	0.52
21:O:282:ARG:NH1	23:Q:38:HIS:O	2.42	0.52
20:N:479:TYR:HE2	20:N:484:GLU:HB3	1.75	0.51
21:O:306:CYS:HB2	21:O:333:VAL:HB	1.93	0.51
27:V:42:ILE:HG23	27:V:53:THR:HB	1.92	0.51
27:V:266:ILE:HA	27:V:288:PHE:HA	1.92	0.51
17:J:402:LEU:HD13	17:J:417:ARG:HH21	1.75	0.51
22:P:777:GLN:OE1	24:S:185:TRP:NE1	2.44	0.51
23:Q:52:GLU:O	23:Q:56:ASN:ND2	2.43	0.51
8:A:606:ALA:HA	8:A:615:ARG:O	2.10	0.51
18:R:15:PRO:HG2	18:R:55:ILE:HB	1.91	0.51
2:2:22:LYS:O	2:2:70:LEU:N	2.44	0.51
8:A:107:PHE:O	11:D:14:GLN:NE2	2.43	0.51
20:N:754:GLU:OE1	20:N:757:ARG:NH2	2.44	0.51
22:P:226:ASP:O	30:Y:84:ASN:N	2.44	0.51
21:O:345:ILE:HB	21:O:357:TRP:HB2	1.92	0.51
21:O:349:SER:OG	21:O:350:HIS:N	2.43	0.51
26:U:32:PRO:HA	30:Y:195:ARG:HG2	1.93	0.51
28:W:562:TRP:HA	28:W:565:LEU:HD13	1.92	0.51
20:N:835:SER:OG	20:N:836:CYS:N	2.43	0.51
26:U:26:THR:O	26:U:160:ASN:ND2	2.44	0.51
30:Y:311:GLN:HG2	30:Y:314:ARG:HH12	1.75	0.51
8:A:70:LEU:HA	8:A:127:GLY:HA3	1.92	0.51
10:C:1017:LEU:HD13	10:C:1050:VAL:HG21	1.92	0.51
26:U:50:ARG:HH22	26:U:118:THR:HG22	1.75	0.51
8:A:798:ILE:HA	8:A:868:VAL:HA	1.93	0.51
10:C:925:VAL:HA	10:C:928:TYR:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:48:GLU:HA	11:D:51:TYR:HB3	1.93	0.51
22:P:71:LEU:HD11	22:P:100:TYR:HB2	1.93	0.51
10:C:1078:VAL:HG22	10:C:1115:ALA:HB2	1.93	0.51
10:C:813:PRO:O	10:C:817:HIS:ND1	2.44	0.51
21:O:261:LEU:HB3	21:O:273:TRP:HB2	1.93	0.51
27:V:21:ARG:NH1	27:V:81:GLU:O	2.43	0.51
8:A:928:TYR:HA	8:A:940:LEU:H	1.76	0.50
20:N:331:GLU:HA	20:N:334:LEU:HB2	1.93	0.50
22:P:19:LEU:HD23	22:P:54:LEU:HD22	1.93	0.50
28:W:487:LYS:O	28:W:491:ASN:ND2	2.40	0.50
8:A:62:ILE:HA	8:A:82:SER:HA	1.92	0.50
30:Y:130:PRO:HA	30:Y:133:GLN:HB2	1.93	0.50
20:N:948:PHE:O	20:N:1016:TYR:OH	2.27	0.50
22:P:221:ALA:HB3	29:X:301:ARG:HD3	1.93	0.50
20:N:232:ARG:NH2	27:V:315:PHE:O	2.44	0.50
28:W:498:ALA:HB1	28:W:543:LYS:HG2	1.93	0.50
20:N:937:ILE:HD12	20:N:940:ARG:HE	1.77	0.50
18:R:79:GLN:NE2	18:R:83:ASP:OD2	2.45	0.50
24:S:195:ILE:O	24:S:198:THR:OG1	2.29	0.50
30:Y:213:LYS:O	30:Y:216:LYS:NZ	2.43	0.50
11:D:45:ILE:HG22	11:D:86:PRO:HD2	1.93	0.50
10:C:893:ILE:HD13	10:C:896:ILE:HD11	1.93	0.50
21:O:427:LEU:O	21:O:438:LEU:HA	2.11	0.50
8:A:40:LEU:O	8:A:53:LEU:N	2.44	0.49
10:C:658:TRP:HA	10:C:661:ARG:HE	1.77	0.49
11:D:35:SER:OG	11:D:36:TYR:N	2.44	0.49
28:W:542:ASN:OD1	28:W:545:ARG:NH1	2.44	0.49
26:U:64:ARG:NH1	26:U:161:ARG:O	2.44	0.49
27:V:97:VAL:HB	27:V:107:GLN:HG3	1.93	0.49
20:N:520:ASP:N	20:N:520:ASP:OD1	2.45	0.49
5:5:19:LEU:HA	5:5:65:ILE:HA	1.95	0.49
10:C:1030:LYS:O	10:C:1034:ASN:ND2	2.45	0.49
20:N:653:SER:HG	30:Y:389:SER:HG	1.58	0.49
21:O:215:GLY:O	23:Q:57:ARG:NH2	2.44	0.49
2:2:23:LEU:HA	2:2:69:VAL:HA	1.94	0.49
8:A:507:SER:O	8:A:518:GLN:HA	2.13	0.49
20:N:629:GLN:NE2	30:Y:409:GLN:OE1	2.46	0.49
7:9:6:PRO:HA	7:9:36:PRO:HA	1.94	0.49
12:E:574:ALA:HA	12:E:578:TRP:HB2	1.95	0.49
21:O:392:PRO:HG3	21:O:415:ILE:HA	1.94	0.49
25:T:134:CYS:SG	25:T:135:THR:N	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:29:GLY:O	30:Y:195:ARG:NH2	2.45	0.49
26:U:158:LYS:O	26:U:161:ARG:NH1	2.46	0.49
10:C:918:VAL:HG13	10:C:925:VAL:HG21	1.94	0.49
20:N:602:ILE:O	20:N:668:ARG:NH1	2.45	0.49
20:N:782:ASP:N	20:N:782:ASP:OD1	2.46	0.49
22:P:67:GLU:OE1	22:P:91:ARG:NH2	2.46	0.49
26:U:26:THR:OG1	26:U:159:ARG:NH2	2.45	0.49
11:D:58:CYS:O	11:D:87:LYS:NZ	2.40	0.49
26:U:56:ARG:HD2	26:U:67:LYS:HD3	1.94	0.49
8:A:92:TYR:HA	8:A:99:PHE:HA	1.93	0.49
10:C:1020:LEU:HD23	10:C:1023:ILE:HD12	1.94	0.49
20:N:580:ASP:OD1	20:N:580:ASP:N	2.45	0.49
21:O:438:LEU:HB2	21:O:448:GLN:HB3	1.94	0.49
18:K:29:LEU:HD11	18:R:86:MET:HE1	1.94	0.49
25:T:120:ARG:NH1	25:T:142:CYS:O	2.46	0.49
17:J:400:HIS:HB3	17:J:402:LEU:HG	1.94	0.48
26:U:196:GLN:NE2	26:U:207:ASP:OD1	2.45	0.48
8:A:237:THR:HA	8:A:248:VAL:HA	1.94	0.48
13:F:40:VAL:N	13:F:60:GLU:O	2.46	0.48
18:K:95:GLN:HB3	18:R:100:ARG:HH22	1.78	0.48
30:Y:407:TYR:HB3	30:Y:411:LEU:HD11	1.95	0.48
20:N:835:SER:OG	20:N:932:CYS:SG	2.69	0.48
10:C:1026:ASN:O	10:C:1032:GLN:NE2	2.46	0.48
20:N:455:ARG:NH2	20:N:482:ARG:O	2.43	0.48
20:N:577:PHE:HB3	20:N:731:ALA:HA	1.94	0.48
29:X:295:ALA:HA	29:X:298:ILE:HD12	1.94	0.48
10:C:1167:TYR:HB3	12:E:582:PRO:HD3	1.95	0.48
12:E:558:ARG:NH1	31:Z:207:GLU:O	2.46	0.48
17:J:411:CYS:CB	17:J:431:HIS:ND1	2.71	0.48
18:R:15:PRO:HB2	18:R:55:ILE:HD12	1.94	0.48
26:U:123:ARG:O	26:U:127:ASN:ND2	2.44	0.48
27:V:44:ASN:HB3	27:V:52:GLN:HB3	1.94	0.48
18:M:15:PRO:HG2	18:M:55:ILE:HB	1.95	0.48
21:O:224:ALA:HA	21:O:248:THR:HG23	1.96	0.48
23:Q:54:VAL:HG13	23:Q:59:PHE:HZ	1.77	0.48
26:U:78:LYS:HE2	26:U:94:ILE:HG12	1.94	0.48
28:W:609:GLN:HA	28:W:612:PHE:HB2	1.96	0.48
10:C:897:LEU:HD11	10:C:932:ILE:HG12	1.96	0.48
11:D:31:VAL:HG23	11:D:32:ILE:HG12	1.96	0.48
20:N:897:TRP:O	20:N:901:ASN:ND2	2.40	0.48
20:N:951:THR:HA	20:N:985:LEU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S:173:THR:O	24:S:177:LYS:NZ	2.45	0.48
10:C:1223:SER:HB3	10:C:1226:VAL:HG12	1.95	0.47
20:N:500:MET:SD	20:N:500:MET:N	2.87	0.47
15:H:221:PRO:O	15:H:227:SER:N	2.47	0.47
11:D:11:CYS:HB2	11:D:85:CYS:HB3	1.95	0.47
16:I:23:ASN:OD1	16:I:26:ARG:NH2	2.46	0.47
18:K:100:ARG:NH2	18:R:95:GLN:OE1	2.46	0.47
20:N:325:GLU:HA	20:N:328:ARG:HB3	1.96	0.47
20:N:430:THR:HG21	20:N:464:ARG:HE	1.79	0.47
21:O:471:ASP:N	21:O:471:ASP:OD1	2.44	0.47
21:O:493:ASP:OD1	21:O:493:ASP:N	2.43	0.47
22:P:49:ARG:HG3	22:P:54:LEU:HD13	1.97	0.47
12:E:531:THR:HG22	12:E:570:LYS:HG2	1.97	0.47
20:N:273:LYS:HD3	20:N:273:LYS:HA	1.77	0.47
25:T:13:ASP:N	25:T:13:ASP:OD1	2.47	0.47
12:E:569:GLN:HA	12:E:572:HIS:HB3	1.96	0.47
22:P:50:TRP:HA	22:P:54:LEU:HB2	1.95	0.47
20:N:423:GLU:HB3	20:N:574:GLY:HA3	1.96	0.47
21:O:305:THR:O	21:O:312:ALA:HA	2.15	0.47
8:A:802:THR:HA	8:A:863:ALA:O	2.15	0.47
20:N:525:ARG:HD2	20:N:525:ARG:HA	1.77	0.47
30:Y:90:VAL:HG22	30:Y:96:ILE:H	1.80	0.47
6:8:41:ILE:HA	6:8:71:LEU:HA	1.97	0.47
16:I:143:GLU:O	16:I:146:MET:N	2.48	0.46
8:A:20:GLY:O	8:A:28:GLN:HA	2.16	0.46
18:M:19:PRO:HG3	18:M:51:GLN:HB3	1.97	0.46
20:N:654:ASP:N	20:N:654:ASP:OD1	2.47	0.46
24:S:170:MET:HA	24:S:173:THR:HG22	1.97	0.46
28:W:526:GLU:HG3	28:W:560:LEU:HD22	1.95	0.46
1:1:86:LEU:HA	7:9:62:ILE:HA	1.98	0.46
10:C:1120:ALA:HA	10:C:1128:VAL:HG21	1.97	0.46
22:P:773:ASP:HA	22:P:776:ARG:HE	1.79	0.46
26:U:148:LEU:HD13	26:U:151:ALA:HB3	1.98	0.46
27:V:199:ASP:HA	30:Y:315:LYS:HE3	1.95	0.46
20:N:716:LYS:N	20:N:748:GLU:O	2.48	0.46
21:O:226:ARG:NH1	21:O:245:HIS:O	2.45	0.46
22:P:20:LYS:HG3	22:P:54:LEU:HD23	1.98	0.46
26:U:182:ARG:NH1	26:U:184:GLU:OE2	2.47	0.46
23:Q:51:PRO:HA	23:Q:54:VAL:HB	1.98	0.46
21:O:353:THR:HA	21:O:368:LEU:O	2.15	0.46
21:O:332:ALA:O	21:O:350:HIS:ND1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:211:ASN:ND2	29:X:221:ASN:O	2.49	0.46
30:Y:101:ILE:O	30:Y:104:GLN:NE2	2.49	0.46
20:N:408:LEU:HD21	20:N:432:ILE:HG12	1.98	0.46
10:C:1224:PRO:HA	10:C:1227:ILE:HG22	1.98	0.46
8:A:325:ILE:H	8:A:375:SER:H	1.63	0.45
23:Q:213:ASP:OD2	23:Q:216:ARG:NH1	2.48	0.45
25:T:58:ARG:NH2	25:T:98:GLU:O	2.39	0.45
12:E:682:LEU:HA	12:E:687:PHE:HA	1.96	0.45
22:P:31:TRP:HB3	22:P:43:ALA:HB1	1.99	0.45
8:A:670:GLN:HA	8:A:698:PRO:HA	1.97	0.45
20:N:273:LYS:HA	20:N:276:VAL:HG12	1.98	0.45
20:N:981:PRO:HG2	20:N:984:LEU:HB3	1.98	0.45
21:O:303:LEU:O	21:O:314:ILE:HA	2.17	0.45
26:U:97:ARG:HH11	26:U:101:LEU:HD12	1.81	0.45
27:V:224:LEU:HD13	27:V:230:LEU:HD12	1.97	0.45
10:C:1212:LEU:HA	10:C:1215:VAL:HB	1.98	0.45
26:U:46:LYS:HB2	26:U:70:VAL:HG12	1.98	0.45
26:U:48:CYS:SG	26:U:50:ARG:NH1	2.89	0.45
29:X:365:ILE:HG12	29:X:368:ARG:HH21	1.81	0.45
21:O:194:TRP:NE1	21:O:491:GLU:OE2	2.49	0.45
22:P:756:LYS:HG3	24:S:170:MET:HE1	1.99	0.45
8:A:144:LEU:HA	8:A:154:ILE:HA	1.98	0.45
20:N:796:LEU:HB3	20:N:802:LEU:HG	1.98	0.45
24:S:126:LEU:O	24:S:130:HIS:ND1	2.50	0.45
30:Y:91:ASP:OD1	30:Y:91:ASP:N	2.46	0.45
4:4:99:MET:HA	5:5:69:ILE:HA	1.99	0.45
8:A:345:GLY:HA2	8:A:361:ILE:H	1.81	0.45
8:A:613:THR:HA	8:A:632:ALA:HA	1.98	0.45
10:C:978:LEU:HA	10:C:981:TYR:HB2	1.97	0.45
20:N:606:GLN:HA	20:N:607:PRO:HD3	1.83	0.45
31:Z:206:LYS:HG2	31:Z:223:ARG:HA	1.98	0.45
8:A:41:LEU:HA	8:A:53:LEU:H	1.80	0.45
10:C:1130:PRO:HG3	12:E:528:ILE:HG12	1.99	0.45
11:D:39:PRO:HA	11:D:72:CYS:HA	1.98	0.45
21:O:214:PRO:HG2	21:O:256:THR:HA	1.99	0.45
2:2:62:VAL:HA	4:4:110:LEU:HA	1.99	0.44
8:A:84:SER:HA	8:A:110:SER:HA	1.99	0.44
22:P:781:GLU:HA	22:P:784:LEU:HB2	1.99	0.44
27:V:20:GLU:HB3	27:V:83:VAL:HG21	1.98	0.44
22:P:749:LEU:HD11	24:S:156:LEU:HD22	2.00	0.44
26:U:20:PHE:O	26:U:72:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:428:GLY:HA3	8:A:433:SER:HA	1.99	0.44
8:A:642:ILE:HA	8:A:665:LEU:HA	1.99	0.44
8:A:808:THR:HA	8:A:863:ALA:HB2	1.99	0.44
16:I:59:CYS:SG	16:I:72:HIS:HE1	2.32	0.44
20:N:561:SER:HA	20:N:567:ALA:HB3	1.98	0.44
21:O:428:VAL:HG11	21:O:477:LEU:HD21	2.00	0.44
26:U:169:VAL:HG22	26:U:186:PRO:HD3	1.98	0.44
28:W:554:LEU:HD22	28:W:560:LEU:HG	1.99	0.44
13:F:14:THR:HA	13:F:60:GLU:HA	1.99	0.44
20:N:1005:SER:HA	20:N:1008:LEU:HB3	2.00	0.44
28:W:621:PRO:HB2	28:W:625:ARG:HH21	1.82	0.44
20:N:480:SER:HA	20:N:485:ASP:HA	1.98	0.44
20:N:691:ASP:OD2	20:N:736:ARG:NH1	2.49	0.44
20:N:826:LYS:HA	20:N:829:LEU:HB2	1.98	0.44
25:T:80:LYS:HA	25:T:80:LYS:HD3	1.79	0.44
26:U:11:ASN:HB3	30:Y:218:ILE:HG13	2.00	0.44
29:X:263:SER:OG	29:X:267:ARG:NH1	2.51	0.44
8:A:337:ALA:N	8:A:350:ALA:O	2.50	0.44
22:P:65:ARG:HE	22:P:69:GLU:HG3	1.83	0.44
28:W:616:LEU:HG	28:W:643:LEU:HD11	2.00	0.44
8:A:784:THR:O	8:A:802:THR:N	2.51	0.44
10:C:595:GLU:O	10:C:599:ASN:ND2	2.47	0.44
10:C:1166:ILE:O	10:C:1170:THR:OG1	2.29	0.44
20:N:725:ARG:HH11	20:N:728:ARG:HH22	1.64	0.44
26:U:11:ASN:OD1	26:U:119:GLN:NE2	2.48	0.44
18:M:99:THR:HA	18:M:102:GLU:HB2	1.99	0.44
21:O:455:GLN:N	21:O:483:ASP:OD2	2.51	0.44
22:P:65:ARG:HH21	22:P:69:GLU:HG3	1.82	0.44
26:U:156:TYR:CZ	26:U:158:LYS:HB2	2.53	0.44
20:N:519:VAL:HB	20:N:550:VAL:HA	1.99	0.43
22:P:50:TRP:O	22:P:55:ASP:N	2.51	0.43
11:D:15:ALA:HB1	11:D:44:ARG:HB2	2.00	0.43
20:N:611:ILE:HA	20:N:688:TYR:O	2.18	0.43
27:V:199:ASP:OD1	27:V:199:ASP:N	2.50	0.43
20:N:396:ARG:NH2	20:N:468:GLU:O	2.51	0.43
20:N:541:ARG:HA	20:N:541:ARG:HD3	1.79	0.43
23:Q:218:GLU:OE2	23:Q:221:LYS:NZ	2.46	0.43
8:A:213:LEU:HA	8:A:220:VAL:HA	2.00	0.43
20:N:613:VAL:HG22	20:N:690:LEU:HB2	2.01	0.43
21:O:187:LYS:HA	21:O:187:LYS:HD3	1.86	0.43
22:P:700:ARG:NH2	24:S:89:LEU:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:275:ASN:OD1	29:X:278:LEU:N	2.51	0.43
8:A:886:GLU:HA	8:A:910:ALA:O	2.18	0.43
11:D:59:VAL:HG12	11:D:87:LYS:HD2	2.00	0.43
12:E:461:THR:HG23	12:E:464:GLU:H	1.83	0.43
12:E:567:ASP:OD1	12:E:567:ASP:N	2.52	0.43
26:U:123:ARG:HH22	30:Y:222:PRO:HD2	1.84	0.43
2:2:45:ALA:HA	2:2:61:GLU:HA	1.99	0.43
20:N:839:GLU:O	20:N:842:THR:OG1	2.31	0.43
21:O:223:SER:OG	21:O:224:ALA:N	2.50	0.43
22:P:78:MET:HA	22:P:79:PRO:HD3	1.83	0.43
16:I:56:CYS:O	16:I:60:LEU:N	2.52	0.43
21:O:337:ARG:HA	21:O:337:ARG:HD3	1.80	0.43
18:M:100:ARG:HD2	18:M:100:ARG:HA	1.90	0.43
20:N:708:SER:HB2	20:N:991:LEU:HD23	2.00	0.43
21:O:337:ARG:HB2	21:O:346:ILE:HB	2.01	0.43
28:W:494:LEU:HD12	28:W:547:VAL:HG22	2.01	0.43
5:5:29:ILE:HA	5:5:40:LEU:HA	2.01	0.42
10:C:1071:LYS:HA	10:C:1074:ARG:HE	1.84	0.42
14:G:180:GLY:O	20:N:756:GLN:NE2	2.46	0.42
18:K:121:THR:HA	18:K:124:VAL:HB	2.02	0.42
18:M:17:VAL:HG23	18:M:55:ILE:HD11	2.01	0.42
20:N:451:THR:O	20:N:452:GLN:NE2	2.52	0.42
21:O:395:ILE:HB	21:O:409:LEU:HB2	2.01	0.42
25:T:15:TRP:NE1	25:T:19:GLU:OE1	2.52	0.42
8:A:723:TYR:O	8:A:729:PHE:HA	2.19	0.42
10:C:1227:ILE:HD12	10:C:1227:ILE:HA	1.95	0.42
20:N:940:ARG:HG2	20:N:1001:LEU:HD11	2.01	0.42
23:Q:182:PHE:HB3	23:Q:183:LYS:H	1.69	0.42
23:Q:218:GLU:HA	23:Q:221:LYS:HD2	2.01	0.42
28:W:606:GLU:HA	28:W:609:GLN:HG2	2.00	0.42
20:N:688:TYR:HA	20:N:733:LYS:HB2	2.02	0.42
20:N:784:PRO:HG2	20:N:789:LEU:HD11	2.01	0.42
22:P:752:PHE:HA	22:P:755:LEU:HB2	2.02	0.42
22:P:764:PRO:HA	22:P:767:LEU:HB2	2.01	0.42
23:Q:224:MET:O	23:Q:228:ILE:HB	2.19	0.42
27:V:88:HIS:HA	27:V:93:THR:HG21	2.00	0.42
27:V:236:LYS:HA	27:V:236:LYS:HD3	1.80	0.42
4:4:66:VAL:HA	4:4:100:PHE:HA	2.01	0.42
8:A:678:VAL:H	8:A:684:GLY:HA3	1.85	0.42
18:M:121:THR:HA	18:M:124:VAL:HG22	2.00	0.42
20:N:539:VAL:HG13	20:N:543:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:270:VAL:HG21	21:O:305:THR:HG21	2.02	0.42
24:S:209:ILE:HA	24:S:212:GLN:HB2	2.00	0.42
2:2:33:LEU:HA	2:2:44:LEU:HA	2.01	0.42
8:A:638:GLU:N	8:A:668:GLY:O	2.45	0.42
10:C:1020:LEU:HA	10:C:1023:ILE:HD12	2.01	0.42
17:J:449:VAL:HG22	17:J:451:GLN:H	1.84	0.42
21:O:399:LYS:NZ	21:O:400:PHE:O	2.48	0.42
21:O:473:SER:HB2	23:Q:60:ARG:HG2	2.01	0.42
12:E:510:TYR:HE1	12:E:592:TYR:HA	1.85	0.42
20:N:808:LEU:O	20:N:813:ARG:NH1	2.53	0.42
22:P:76:LYS:O	30:Y:296:TYR:OH	2.36	0.42
25:T:134:CYS:SG	25:T:136:HIS:N	2.86	0.42
8:A:438:LEU:HA	8:A:775:ASN:O	2.19	0.41
11:D:49:CYS:HB3	11:D:87:LYS:HD3	2.02	0.41
12:E:524:LEU:O	12:E:529:LYS:NZ	2.45	0.41
13:F:16:TYR:HA	13:F:58:PHE:HA	2.02	0.41
21:O:355:ARG:HH11	21:O:364:THR:HG21	1.85	0.41
26:U:165:CYS:SG	26:U:173:CYS:HB2	2.60	0.41
21:O:260:TYR:HE2	23:Q:41:ILE:HG23	1.85	0.41
10:C:1250:CYS:HB3	10:C:1269:TYR:HB2	2.03	0.41
20:N:419:ILE:HB	20:N:569:VAL:HG22	2.02	0.41
20:N:601:GLN:HA	20:N:604:VAL:HG22	2.02	0.41
18:R:3:LEU:HD12	18:R:24:VAL:HG21	2.02	0.41
24:S:184:ASN:O	24:S:188:LEU:HB2	2.19	0.41
10:C:1186:GLN:HB2	10:C:1226:VAL:HG23	2.01	0.41
20:N:611:ILE:O	20:N:670:VAL:HA	2.20	0.41
8:A:1012:VAL:HA	8:A:1023:ILE:HA	2.02	0.41
20:N:415:HIS:CG	20:N:568:PRO:HG3	2.56	0.41
20:N:476:GLU:HA	20:N:491:THR:HA	2.03	0.41
22:P:55:ASP:HB3	22:P:58:ILE:HG13	2.02	0.41
22:P:226:ASP:H	29:X:293:ASN:HB3	1.85	0.41
22:P:796:GLU:HA	22:P:799:LYS:HD2	2.01	0.41
8:A:5:ASN:HA	8:A:1111:LEU:HA	2.03	0.41
10:C:1053:ARG:HD3	12:E:559:PRO:HG2	2.01	0.41
20:N:293:GLU:HA	20:N:296:ASN:HB2	2.03	0.41
21:O:196:LEU:HB2	21:O:489:TYR:CZ	2.56	0.41
8:A:689:THR:HA	31:Z:308:ASN:HA	2.03	0.41
22:P:210:TYR:O	29:X:260:ARG:NH1	2.44	0.41
26:U:83:THR:OG1	26:U:84:CYS:N	2.53	0.41
10:C:1057:ARG:NH1	12:E:557:VAL:O	2.47	0.41
10:C:1132:LEU:HG	10:C:1147:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:74:ILE:HG23	18:R:74:ILE:HG23	2.03	0.41
22:P:219:LYS:HD3	22:P:219:LYS:HA	1.90	0.41
28:W:477:LEU:HD11	28:W:517:LEU:HD13	2.02	0.41
10:C:936:VAL:HG13	10:C:951:ALA:HB1	2.01	0.41
10:C:1011:PRO:HA	10:C:1012:PRO:HD3	1.97	0.41
10:C:1177:LEU:HD13	10:C:1214:TYR:HB2	2.02	0.41
12:E:537:ARG:HH21	12:E:564:ILE:HD11	1.85	0.41
16:I:118:LYS:HA	16:I:223:LEU:HA	2.03	0.41
18:M:40:ASP:N	18:M:45:GLN:O	2.53	0.41
20:N:708:SER:HA	20:N:991:LEU:HB3	2.02	0.41
8:A:460:TRP:O	8:A:475:ILE:N	2.48	0.41
20:N:596:VAL:HA	20:N:599:VAL:HG12	2.03	0.41
21:O:471:ASP:OD2	21:O:473:SER:OG	2.37	0.41
23:Q:53:GLU:O	23:Q:57:ARG:HB2	2.20	0.41
25:T:58:ARG:HA	25:T:58:ARG:HD3	1.84	0.41
26:U:157:TYR:HA	26:U:160:ASN:HD22	1.86	0.41
18:M:96:LEU:HD23	18:M:96:LEU:HA	1.93	0.40
20:N:502:LEU:HD21	20:N:766:LEU:HD13	2.03	0.40
22:P:77:LEU:O	30:Y:296:TYR:OH	2.39	0.40
10:C:1213:ASN:OD1	12:E:586:ILE:O	2.40	0.40
20:N:511:LEU:O	20:N:543:ARG:NH1	2.53	0.40
26:U:129:ASP:OD1	26:U:129:ASP:N	2.43	0.40
27:V:41:LEU:HD23	27:V:41:LEU:HA	1.93	0.40
8:A:33:SER:HA	8:A:38:LEU:HA	2.03	0.40
8:A:311:PHE:HA	8:A:329:TYR:HA	2.03	0.40
8:A:477:SER:HA	8:A:482:THR:HA	2.02	0.40
11:D:81:ASP:OD1	11:D:81:ASP:N	2.55	0.40
24:S:183:SER:HA	24:S:186:VAL:HG22	2.03	0.40
26:U:64:ARG:HD2	26:U:163:HIS:CD2	2.56	0.40
10:C:1217:PRO:HG2	12:E:591:TYR:H	1.87	0.40
20:N:877:ASP:OD1	20:N:877:ASP:N	2.49	0.40
25:T:111:THR:OG1	25:T:115:THR:N	2.49	0.40
26:U:216:ARG:O	26:U:219:THR:OG1	2.30	0.40
30:Y:109:ASP:OD1	30:Y:109:ASP:N	2.55	0.40
21:O:250:ARG:HA	21:O:250:ARG:HD2	1.88	0.40
25:T:25:LEU:HD23	25:T:28:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	77/92 (84%)	77 (100%)	0	0	100	100
1	i	66/92 (72%)	64 (97%)	2 (3%)	0	100	100
2	2	72/86 (84%)	72 (100%)	0	0	100	100
2	h	62/86 (72%)	58 (94%)	4 (6%)	0	100	100
3	3	74/126 (59%)	72 (97%)	2 (3%)	0	100	100
3	j	66/126 (52%)	63 (96%)	3 (4%)	0	100	100
4	4	81/118 (69%)	79 (98%)	2 (2%)	0	100	100
4	l	64/118 (54%)	61 (95%)	3 (5%)	0	100	100
5	5	80/119 (67%)	78 (98%)	2 (2%)	0	100	100
5	k	74/119 (62%)	68 (92%)	6 (8%)	0	100	100
6	8	84/240 (35%)	81 (96%)	3 (4%)	0	100	100
6	n	60/240 (25%)	60 (100%)	0	0	100	100
7	9	64/76 (84%)	64 (100%)	0	0	100	100
7	m	57/76 (75%)	55 (96%)	2 (4%)	0	100	100
8	A	1142/1217 (94%)	1069 (94%)	73 (6%)	0	100	100
9	B	68/86 (79%)	65 (96%)	2 (3%)	1 (2%)	10	45
10	C	813/1304 (62%)	779 (96%)	34 (4%)	0	100	100
11	D	87/110 (79%)	75 (86%)	11 (13%)	1 (1%)	14	51
12	E	190/895 (21%)	177 (93%)	13 (7%)	0	100	100
13	F	76/424 (18%)	68 (90%)	8 (10%)	0	100	100
14	G	63/476 (13%)	60 (95%)	3 (5%)	0	100	100
15	H	94/793 (12%)	94 (100%)	0	0	100	100
16	I	173/464 (37%)	161 (93%)	10 (6%)	2 (1%)	13	50
17	J	394/501 (79%)	369 (94%)	25 (6%)	0	100	100
18	K	114/504 (23%)	113 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	M	121/504 (24%)	120 (99%)	1 (1%)	0	100	100
18	R	114/504 (23%)	111 (97%)	3 (3%)	0	100	100
18	v	121/504 (24%)	121 (100%)	0	0	100	100
19	L	26/619 (4%)	24 (92%)	2 (8%)	0	100	100
20	N	779/1041 (75%)	723 (93%)	53 (7%)	3 (0%)	34	72
21	O	318/514 (62%)	304 (96%)	14 (4%)	0	100	100
22	P	316/802 (39%)	308 (98%)	8 (2%)	0	100	100
23	Q	96/229 (42%)	89 (93%)	7 (7%)	0	100	100
24	S	153/225 (68%)	142 (93%)	11 (7%)	0	100	100
25	T	140/144 (97%)	130 (93%)	10 (7%)	0	100	100
26	U	293/420 (70%)	270 (92%)	20 (7%)	3 (1%)	15	54
27	V	279/492 (57%)	257 (92%)	21 (8%)	1 (0%)	34	72
28	W	455/908 (50%)	439 (96%)	16 (4%)	0	100	100
29	X	237/848 (28%)	232 (98%)	5 (2%)	0	100	100
30	Y	294/536 (55%)	270 (92%)	22 (8%)	2 (1%)	22	62
31	Z	91/343 (26%)	83 (91%)	7 (8%)	1 (1%)	14	51
32	a	2171/2335 (93%)	2070 (95%)	95 (4%)	6 (0%)	41	76
33	b	896/972 (92%)	849 (95%)	42 (5%)	5 (1%)	25	65
34	c	1720/2136 (80%)	1668 (97%)	51 (3%)	1 (0%)	51	85
39	o	297/357 (83%)	278 (94%)	19 (6%)	0	100	100
40	p	157/166 (95%)	145 (92%)	12 (8%)	0	100	100
41	q	70/2752 (2%)	65 (93%)	5 (7%)	0	100	100
42	r	160/255 (63%)	154 (96%)	6 (4%)	0	100	100
43	s	159/225 (71%)	153 (96%)	6 (4%)	0	100	100
44	t	46/285 (16%)	45 (98%)	1 (2%)	0	100	100
45	u	359/520 (69%)	339 (94%)	19 (5%)	1 (0%)	41	76
46	w	213/301 (71%)	207 (97%)	6 (3%)	0	100	100
47	x	358/579 (62%)	332 (93%)	23 (6%)	3 (1%)	19	60
48	y	1319/1485 (89%)	1272 (96%)	47 (4%)	0	100	100
49	z	684/855 (80%)	636 (93%)	44 (6%)	4 (1%)	25	65
All	All	16637/30344 (55%)	15818 (95%)	785 (5%)	34 (0%)	50	81

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	I	139	PRO
16	I	218	PRO
26	U	225	PRO
26	U	226	PRO
33	b	57	VAL
47	x	243	VAL
49	z	720	ILE
20	N	860	LYS
26	U	134	VAL
31	Z	208	THR
32	a	520	TYR
32	a	1092	ILE
47	x	263	VAL
49	z	550	TRP
11	D	61	CYS
32	a	1275	ARG
33	b	801	LEU
45	u	235	LYS
30	Y	96	ILE
32	a	982	GLU
33	b	94	ILE
20	N	639	ILE
20	N	854	PHE
32	a	701	ILE
27	V	235	ILE
30	Y	92	SER
33	b	84	GLU
47	x	299	LEU
33	b	113	VAL
49	z	141	PRO
9	B	78	PRO
49	z	587	CYS
34	c	531	ILE
32	a	1419	ILE

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	k	1/101 (1%)	1 (100%)	0	100	100
9	B	2/77 (3%)	2 (100%)	0	100	100
10	C	342/1104 (31%)	342 (100%)	0	100	100
11	D	69/95 (73%)	69 (100%)	0	100	100
12	E	102/776 (13%)	102 (100%)	0	100	100
14	G	10/397 (2%)	10 (100%)	0	100	100
16	I	33/382 (9%)	33 (100%)	0	100	100
17	J	42/446 (9%)	42 (100%)	0	100	100
18	K	106/435 (24%)	106 (100%)	0	100	100
18	M	111/435 (26%)	111 (100%)	0	100	100
18	R	106/435 (24%)	105 (99%)	1 (1%)	78	87
18	v	111/435 (26%)	111 (100%)	0	100	100
19	L	11/545 (2%)	11 (100%)	0	100	100
20	N	624/897 (70%)	620 (99%)	4 (1%)	86	92
21	O	274/441 (62%)	273 (100%)	1 (0%)	91	94
22	P	208/709 (29%)	208 (100%)	0	100	100
23	Q	83/203 (41%)	82 (99%)	1 (1%)	71	84
24	S	144/196 (74%)	143 (99%)	1 (1%)	84	90
25	T	129/130 (99%)	129 (100%)	0	100	100
26	U	181/361 (50%)	181 (100%)	0	100	100
27	V	180/451 (40%)	179 (99%)	1 (1%)	86	92
28	W	180/838 (22%)	176 (98%)	4 (2%)	52	71
29	X	85/751 (11%)	85 (100%)	0	100	100
30	Y	209/459 (46%)	209 (100%)	0	100	100
31	Z	35/294 (12%)	35 (100%)	0	100	100
32	a	1496/2108 (71%)	1492 (100%)	4 (0%)	92	94
33	b	784/866 (90%)	781 (100%)	3 (0%)	91	94
39	o	256/300 (85%)	254 (99%)	2 (1%)	81	89
41	q	30/2432 (1%)	30 (100%)	0	100	100
44	t	41/240 (17%)	40 (98%)	1 (2%)	49	69
45	u	45/456 (10%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	y	1200/1336 (90%)	1197 (100%)	3 (0%)	92	94
49	z	290/749 (39%)	290 (100%)	0	100	100
All	All	7520/19880 (38%)	7494 (100%)	26 (0%)	92	94

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	N	472	LYS
20	N	640	ARG
20	N	703	ARG
20	N	938	ARG
21	O	446	ASN
23	Q	61	ARG
18	R	128	ARG
24	S	197	ARG
27	V	23	ARG
28	W	458	THR
28	W	557	THR
28	W	575	THR
28	W	580	ARG
32	a	775	ASN
32	a	1094	ARG
32	a	1523	ARG
32	a	1641	ARG
33	b	529	ARG
33	b	608	ARG
33	b	919	ARG
39	o	88	ARG
39	o	161	ARG
44	t	148	ARG
48	y	811	ARG
48	y	878	ARG
48	y	1046	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
17	J	431	HIS
20	N	629	GLN
20	N	773	HIS

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Mol	Chain	Res	Type
23	Q	56	ASN
18	R	79	GLN
26	U	183	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	d	91/106 (85%)	34 (37%)	0
36	e	95/117 (81%)	31 (32%)	0
37	f	131/188 (69%)	32 (24%)	0
38	g	74/319 (23%)	35 (47%)	0
All	All	391/730 (53%)	132 (33%)	0

All (132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	d	6	C
35	d	7	G
35	d	8	C
35	d	9	U
35	d	10	U
35	d	12	G
35	d	21	U
35	d	25	C
35	d	26	U
35	d	27	A
35	d	28	A
35	d	29	A
35	d	35	A
35	d	36	A
35	d	37	C
35	d	44	G
35	d	49	G
35	d	51	U
35	d	52	U
35	d	54	G
35	d	55	C
35	d	56	A
35	d	59	G
35	d	60	C
35	d	61	C

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Mol	Chain	Res	Type
35	d	62	C
35	d	66	C
35	d	68	C
35	d	74	U
35	d	79	C
35	d	80	G
35	d	81	C
35	d	87	C
35	d	90	G
36	e	9	G
36	e	19	A
36	e	20	G
36	e	21	A
36	e	22	U
36	e	23	C
36	e	24	G
36	e	25	C
36	e	28	A
36	e	34	U
36	e	36	C
36	e	40	U
36	e	43	U
36	e	45	C
36	e	53	U
36	e	57	G
36	e	59	G
36	e	70	A
36	e	75	G
36	e	90	U
36	e	91	U
36	e	92	U
36	e	93	U
36	e	94	U
36	e	95	G
36	e	96	A
36	e	100	C
36	e	106	U
36	e	107	U
36	e	115	C
36	e	116	U
37	f	12	G
37	f	13	C

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Mol	Chain	Res	Type
37	f	14	C
37	f	23	A
37	f	24	A
37	f	25	G
37	f	29	A
37	f	30	A
37	f	31	G
37	f	32	U
37	f	35	A
37	f	36	G
37	f	40	C
37	f	44	U
37	f	45	C
37	f	47	U
37	f	48	A
37	f	49	U
37	f	62	U
37	f	84	C
37	f	101	U
37	f	102	U
37	f	103	U
37	f	147	G
37	f	153	A
37	f	157	G
37	f	163	G
37	f	164	C
37	f	169	C
37	f	171	U
37	f	178	A
37	f	179	C
38	g	-13	C
38	g	-12	G
38	g	-11	G
38	g	-9	C
38	g	-6	C
38	g	1	G
38	g	2	U
38	g	3	A
38	g	9	C
38	g	14	A
38	g	16	G
38	g	17	U

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Mol	Chain	Res	Type
38	g	18	A
38	g	20	A
38	g	21	A
38	g	22	C
38	g	23	U
38	g	25	G
38	g	27	U
38	g	135	G
38	g	136	U
38	g	137	C
38	g	143	U
38	g	144	A
38	g	145	U
38	g	148	U
38	g	149	G
38	g	152	C
38	g	154	U
38	g	158	U
38	g	160	U
38	g	161	U
38	g	162	C
38	g	163	C
38	g	164	A

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 19 are monoatomic - leaving 2 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	IHP	a	3001	-	36,36,36	1.54	6 (16%)	54,60,60	1.23	6 (11%)
52	GTP	b	1500	53	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)

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
51	IHP	a	3001	-	-	6/30/54/54	0/1/1/1
52	GTP	b	1500	53	-	3/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	b	1500	GTP	C5-C6	-4.12	1.39	1.47
51	a	3001	IHP	P3-O13	3.66	1.66	1.59
51	a	3001	IHP	P4-O14	3.55	1.66	1.59
51	a	3001	IHP	P2-O12	3.13	1.65	1.59
51	a	3001	IHP	P6-O16	3.07	1.65	1.59
51	a	3001	IHP	P5-O15	3.04	1.65	1.59
51	a	3001	IHP	P1-O11	2.93	1.64	1.59
52	b	1500	GTP	C2-N3	2.01	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	b	1500	GTP	PB-O3B-PG	-4.52	117.32	132.83
51	a	3001	IHP	C6-C5-C4	3.86	118.86	110.41
51	a	3001	IHP	C5-C6-C1	3.77	118.66	110.41
51	a	3001	IHP	O13-C3-C2	3.43	116.77	108.69
52	b	1500	GTP	C5-C6-N1	3.16	119.54	113.95
52	b	1500	GTP	C8-N7-C5	3.02	108.73	102.99
51	a	3001	IHP	O14-C4-C5	2.72	115.10	108.69
52	b	1500	GTP	C2-N1-C6	-2.70	120.12	125.10
51	a	3001	IHP	C6-C1-C2	2.70	116.32	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	b	1500	GTP	C3'-C2'-C1'	2.61	104.91	100.98
52	b	1500	GTP	PA-O3A-PB	-2.40	124.59	132.83
52	b	1500	GTP	O6-C6-C5	-2.15	120.17	124.37
51	a	3001	IHP	C5-C4-C3	2.11	115.03	110.41

There are no chirality outliers.

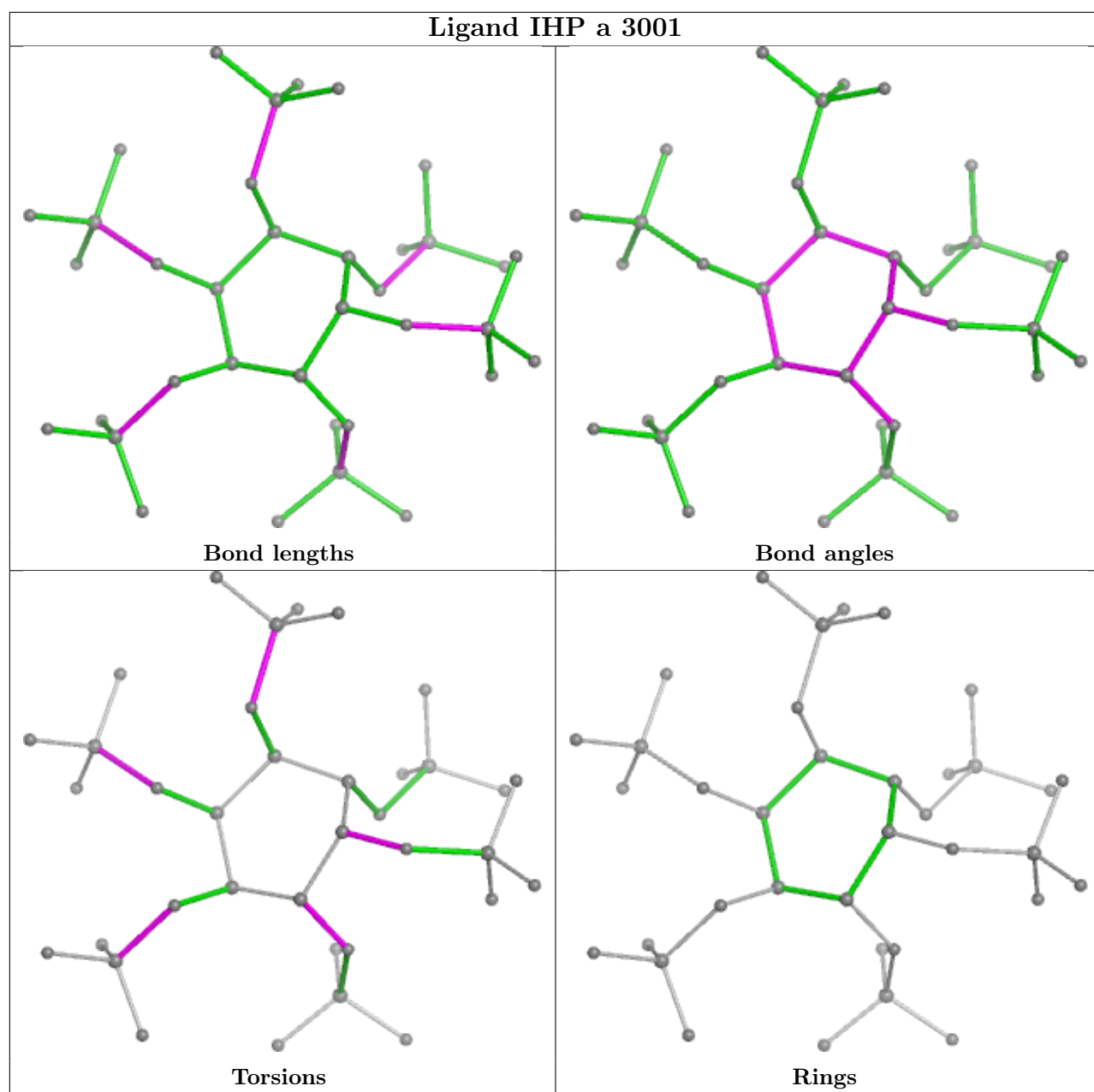
All (9) torsion outliers are listed below:

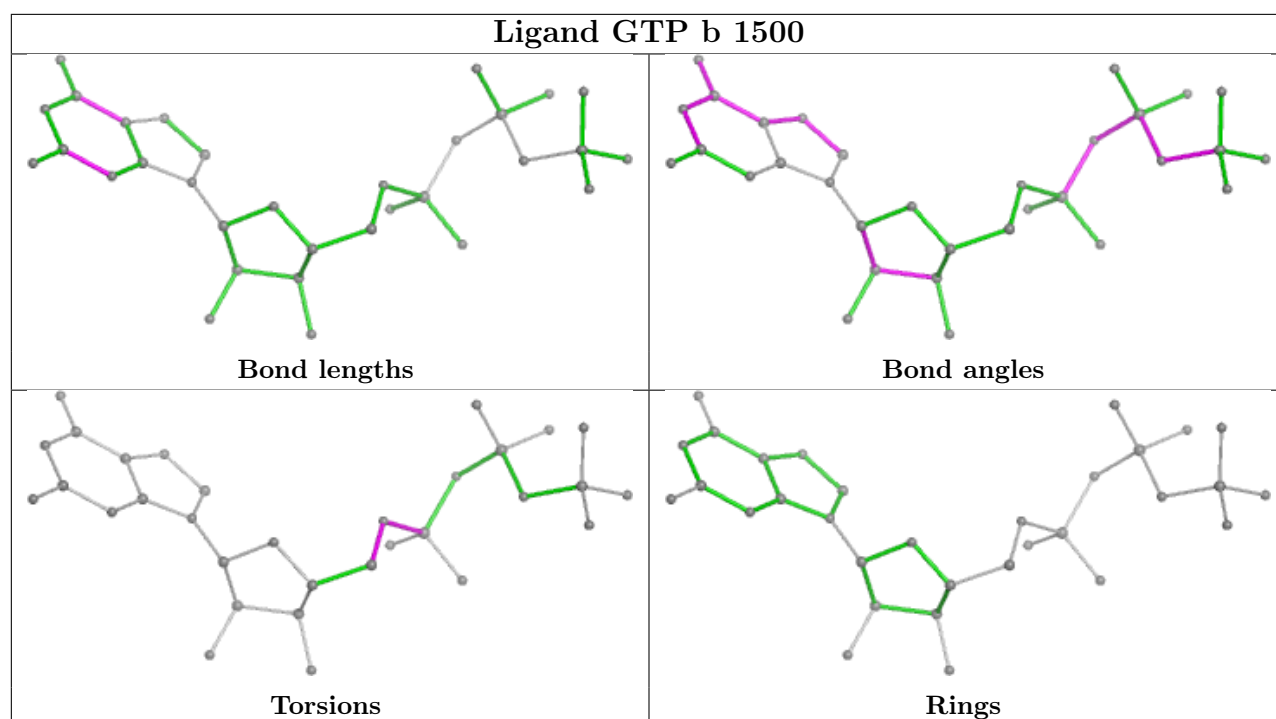
Mol	Chain	Res	Type	Atoms
51	a	3001	IHP	C2-C3-O13-P3
51	a	3001	IHP	C5-C4-O14-P4
51	a	3001	IHP	C5-O15-P5-O45
52	b	1500	GTP	C5'-O5'-PA-O3A
51	a	3001	IHP	C1-O11-P1-O21
52	b	1500	GTP	C5'-O5'-PA-O1A
52	b	1500	GTP	C4'-C5'-O5'-PA
51	a	3001	IHP	C5-O15-P5-O35
51	a	3001	IHP	C6-O16-P6-O36

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

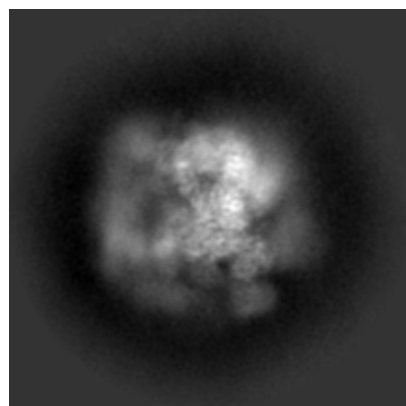
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16658. These allow visual inspection of the internal detail of the map and identification of artifacts.

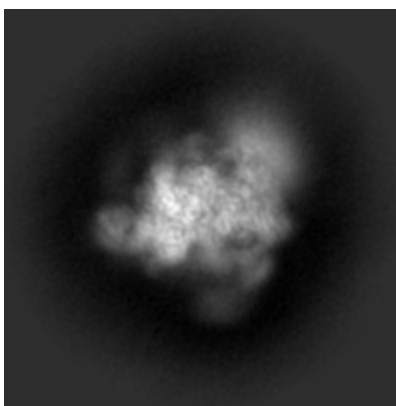
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

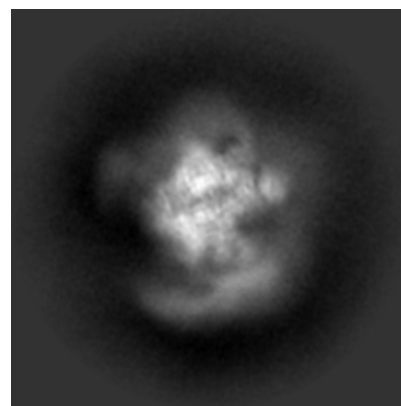
#### 6.1.1 Primary map



X

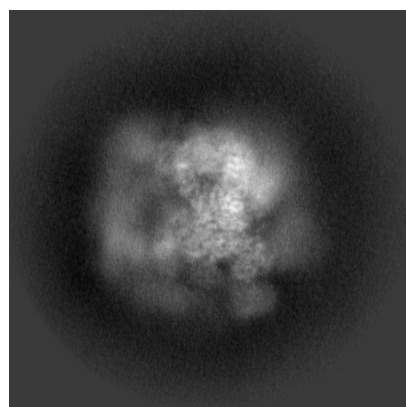


Y

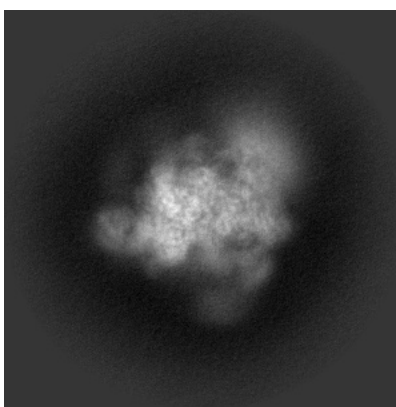


Z

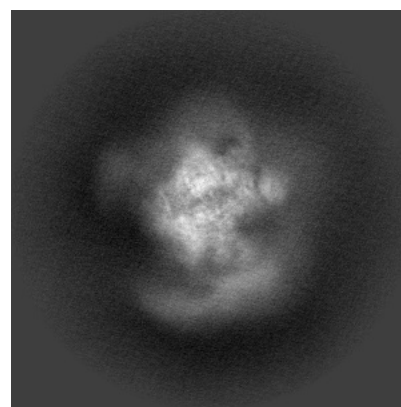
#### 6.1.2 Raw map



X



Y

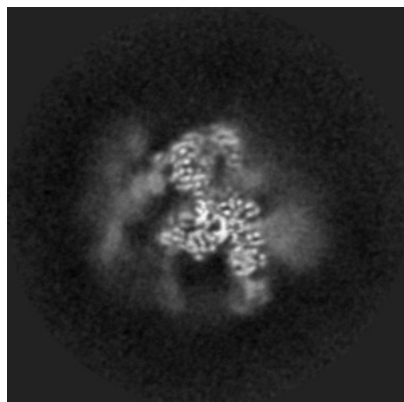


Z

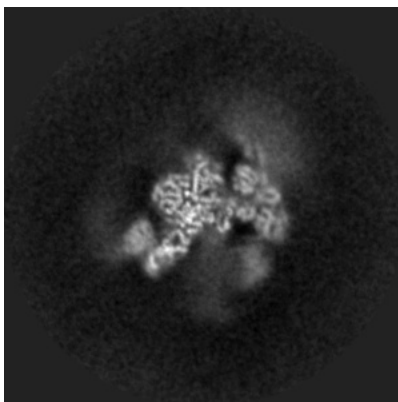
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

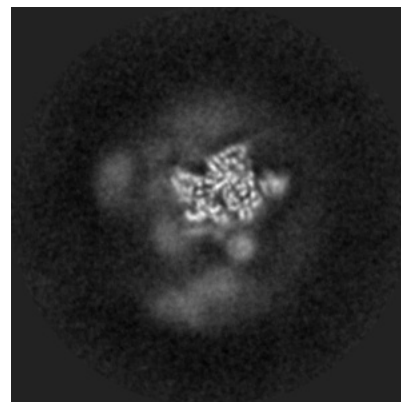
### 6.2.1 Primary map



X Index: 260

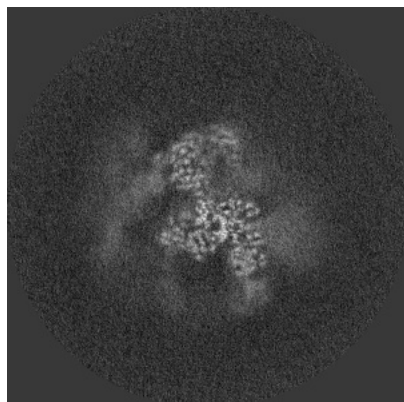


Y Index: 260

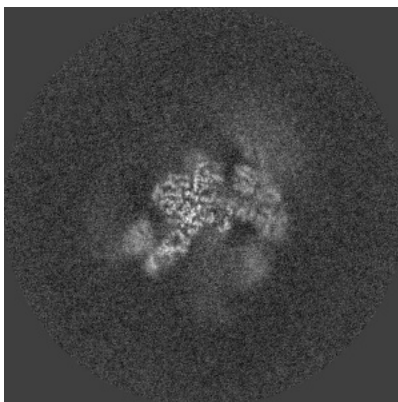


Z Index: 260

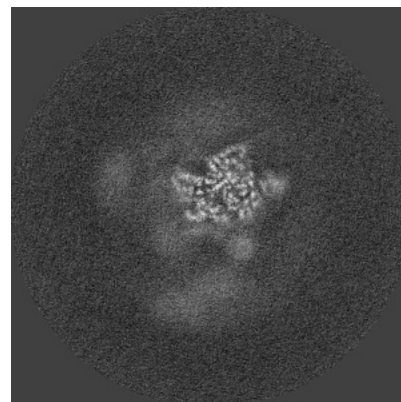
### 6.2.2 Raw map



X Index: 260



Y Index: 260



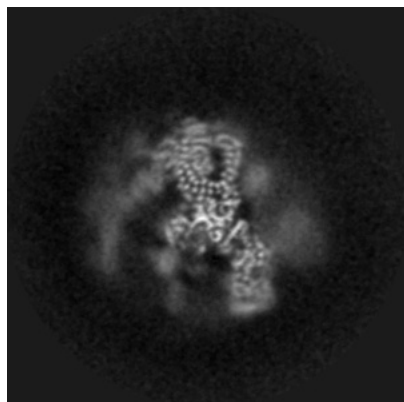
Z Index: 260

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

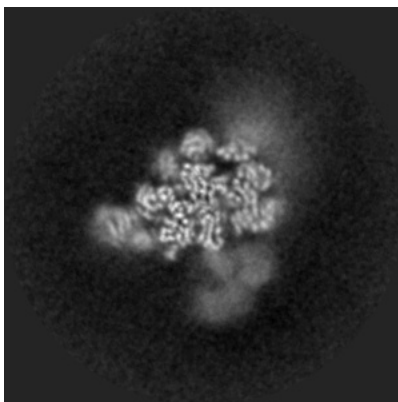


## 6.3 Largest variance slices [i](#)

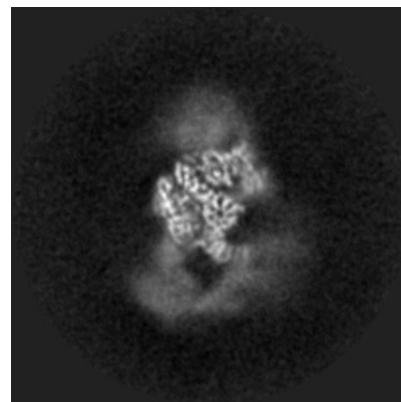
### 6.3.1 Primary map



X Index: 248

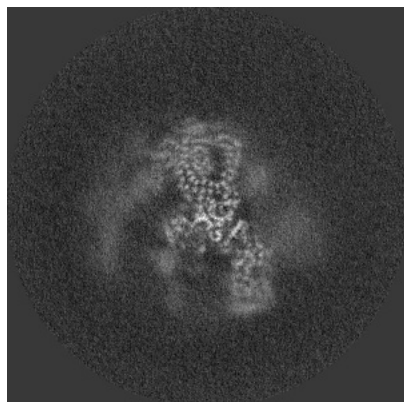


Y Index: 295

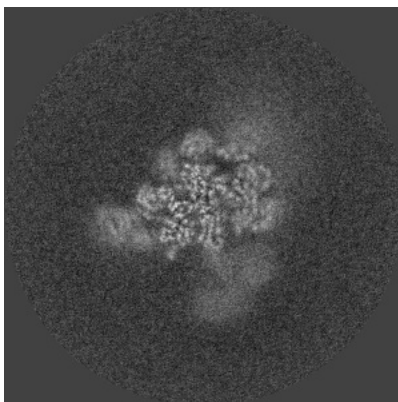


Z Index: 216

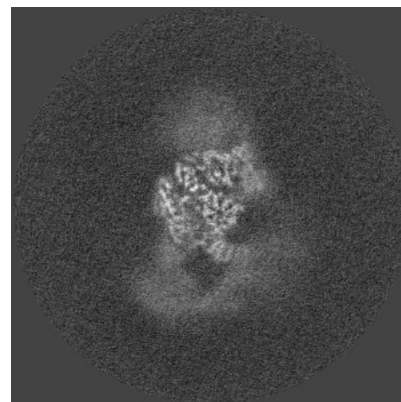
### 6.3.2 Raw map



X Index: 248



Y Index: 295



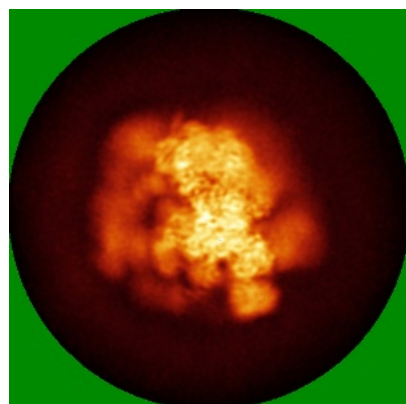
Z Index: 215

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

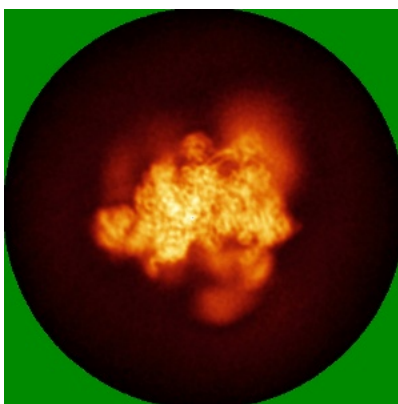


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

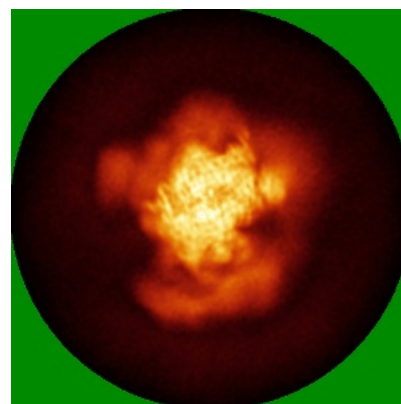
### 6.4.1 Primary map



X

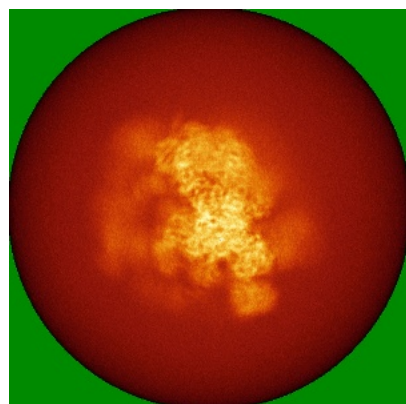


Y

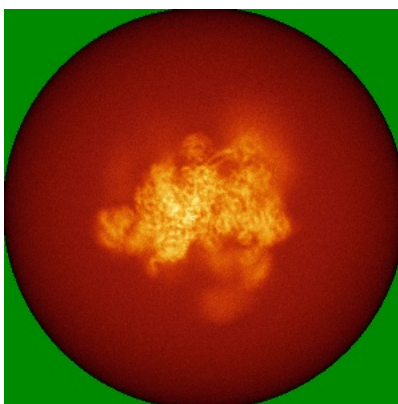


Z

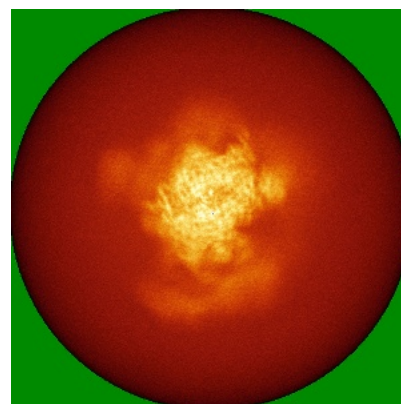
### 6.4.2 Raw map



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](#)

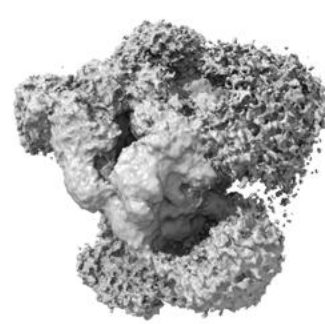
### 6.5.1 Primary map



X



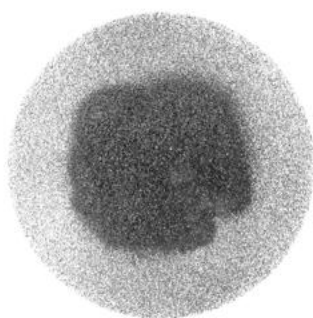
Y



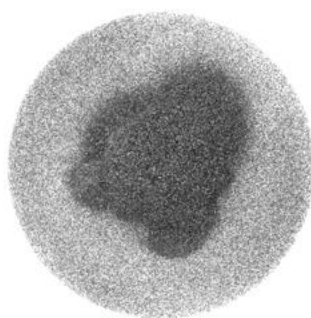
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

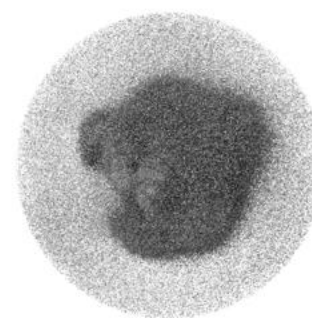
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

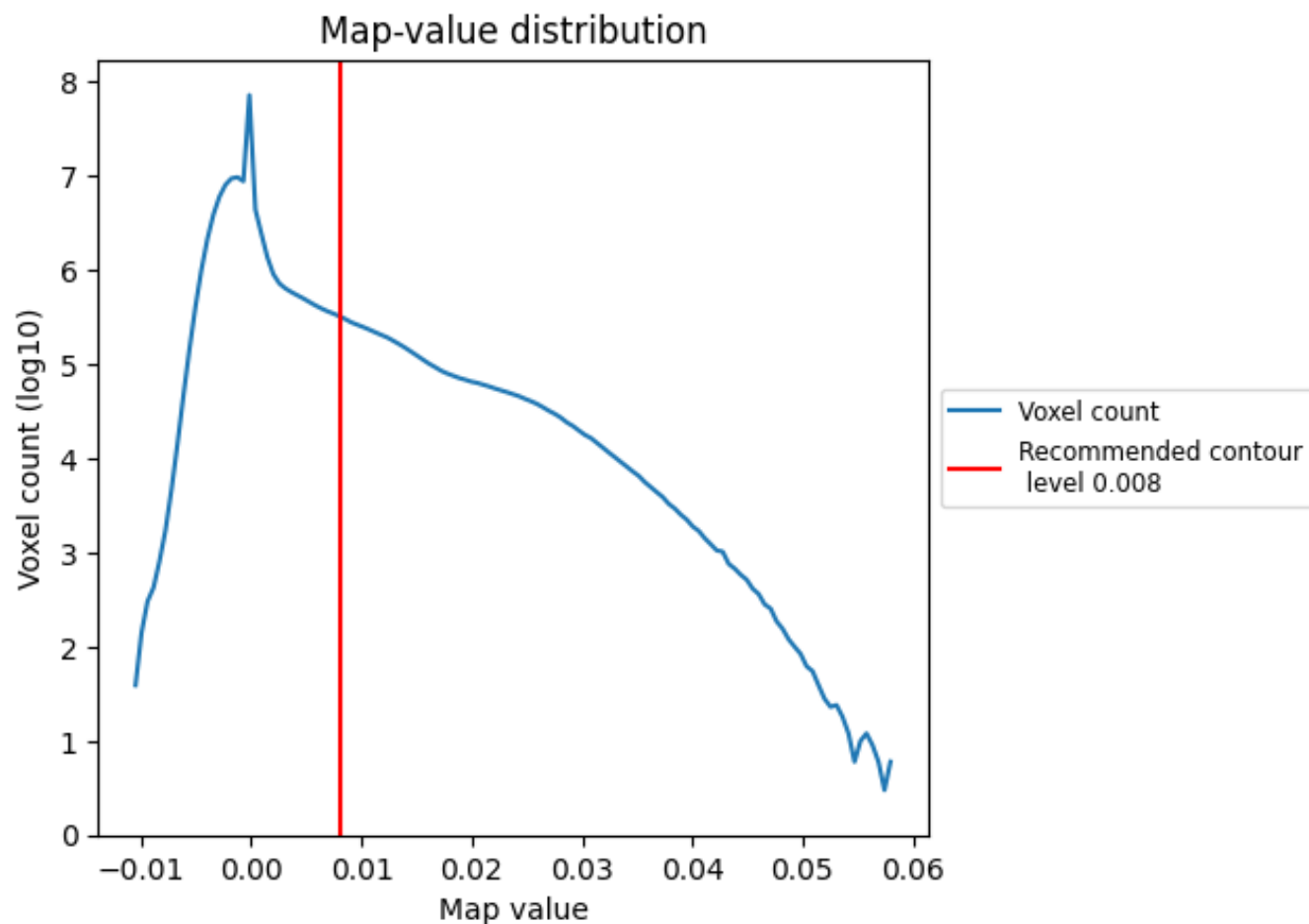
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

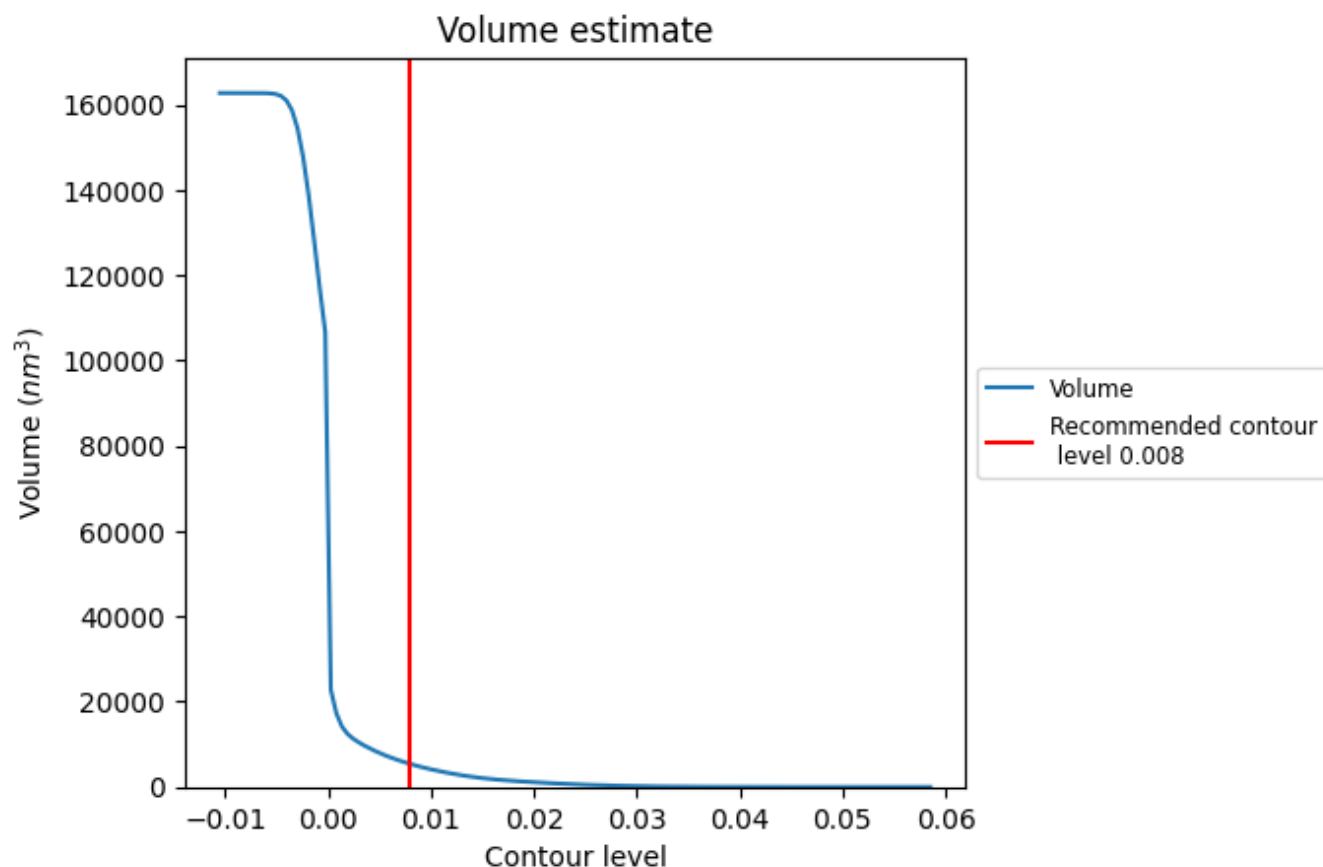
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

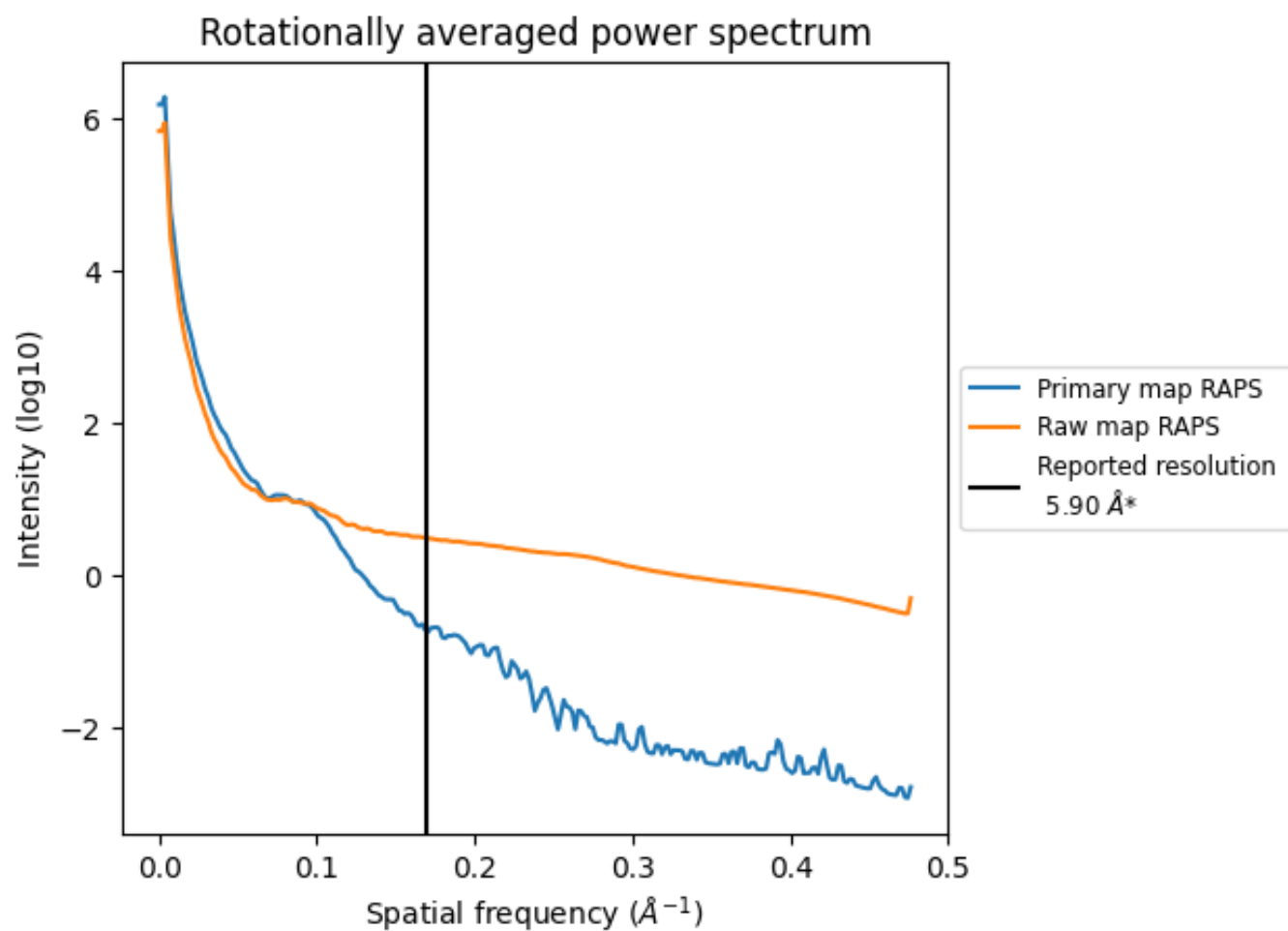
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5401  $\text{nm}^3$ ; this corresponds to an approximate mass of 4879 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](#)

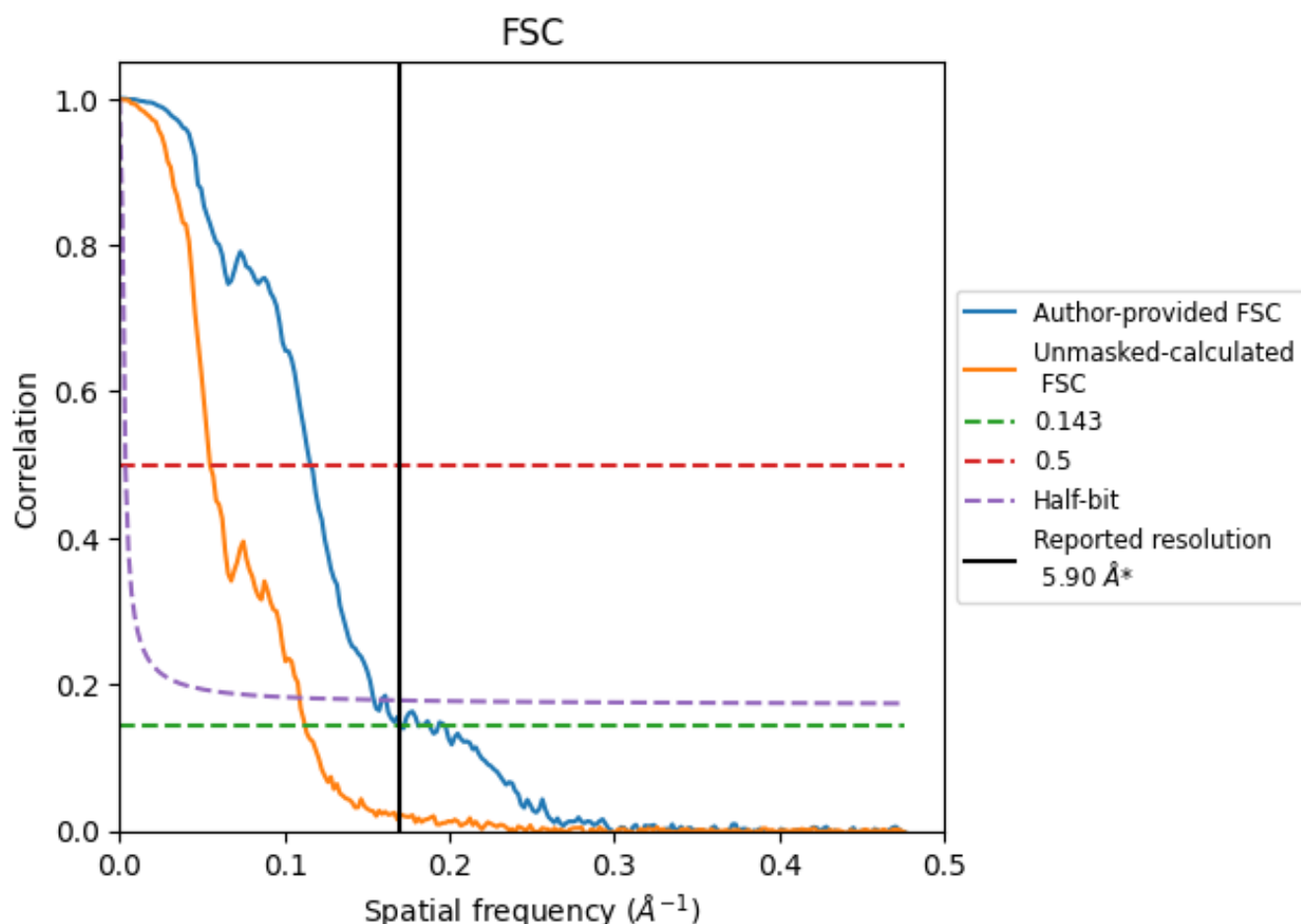


\*Reported resolution corresponds to spatial frequency of 0.169 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.169 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

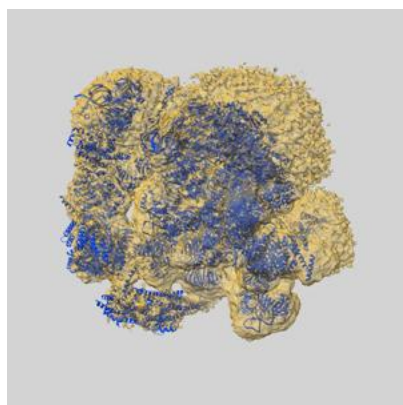
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	5.85	8.63	6.48
Unmasked-calculated*	8.88	18.21	9.17

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.88 differs from the reported value 5.9 by more than 10 %

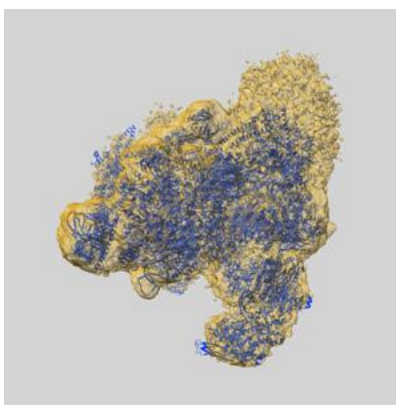
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16658 and PDB model 8CH6. Per-residue inclusion information can be found in section 3 on page 16.

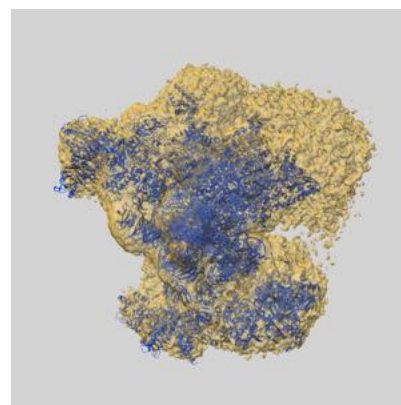
### 9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

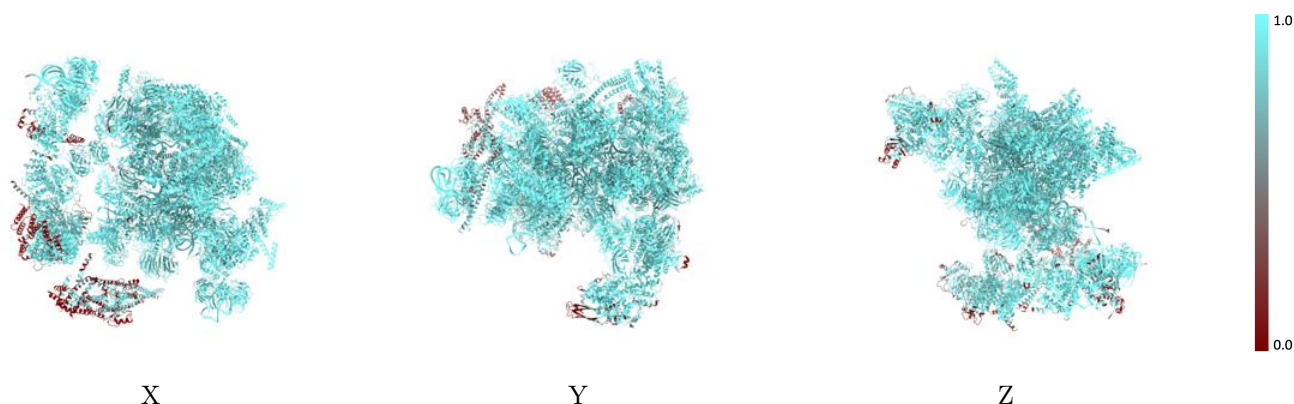


## 9.2 Q-score mapped to coordinate model [i](#)



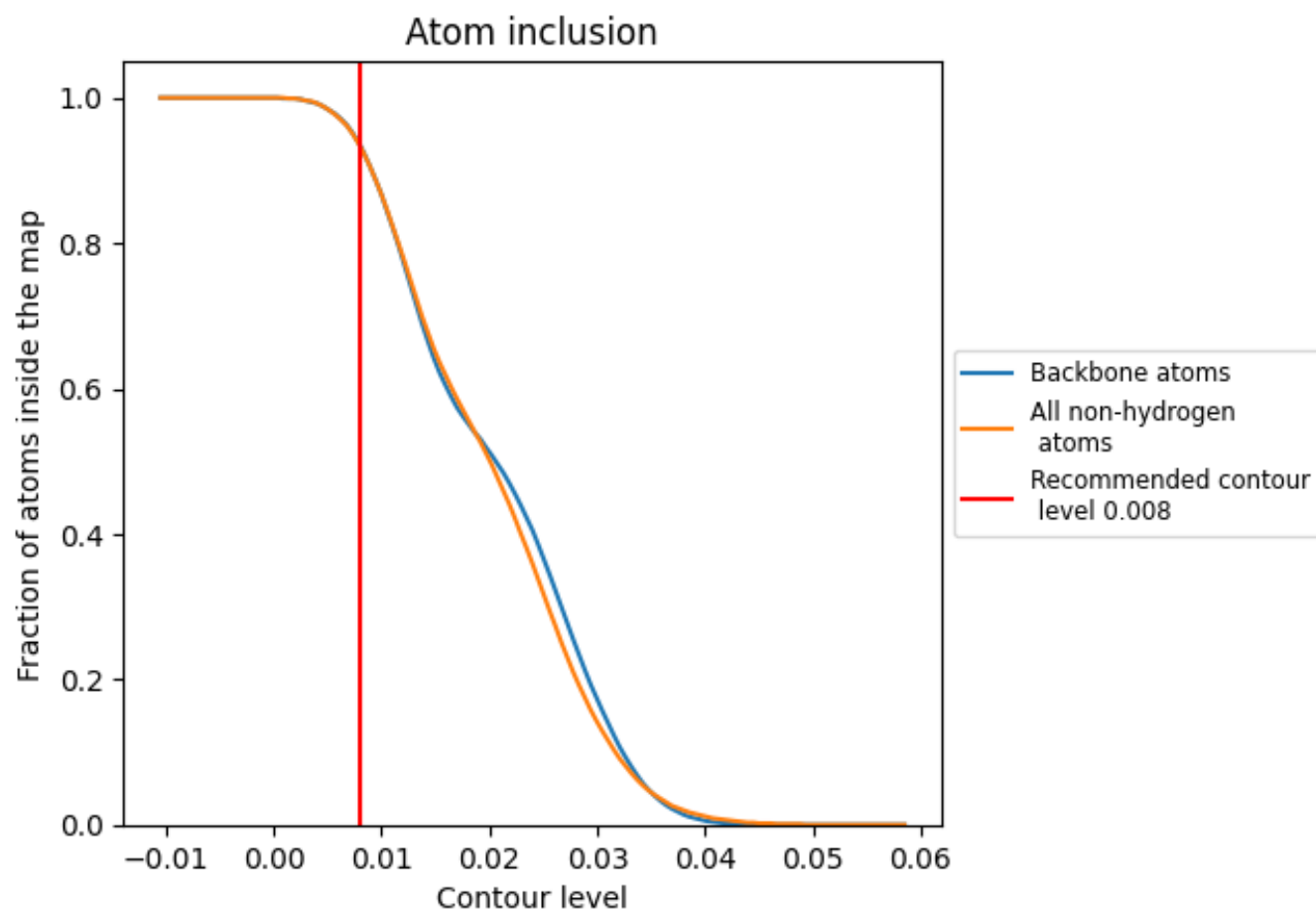
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.1540
1	 1.0000	 0.0660
2	 0.9970	 0.0750
3	 1.0000	 0.0880
4	 0.9760	 0.0500
5	 1.0000	 0.0540
8	 1.0000	 0.0560
9	 1.0000	 0.1280
A	 1.0000	 0.2080
B	 1.0000	 0.2630
C	 1.0000	 0.2250
D	 1.0000	 0.1730
E	 1.0000	 0.2060
F	 0.9240	 0.1030
G	 1.0000	 0.2420
H	 0.9060	 0.0660
I	 0.9500	 0.1610
J	 0.7820	 0.0980
K	 0.4960	 0.0470
L	 1.0000	 0.2100
M	 0.5760	 0.0740
N	 1.0000	 0.1800
O	 1.0000	 0.2300
P	 0.7290	 0.1480
Q	 1.0000	 0.2160
R	 0.4040	 0.0800
S	 0.4540	 0.0980
T	 1.0000	 0.1910
U	 1.0000	 0.1740
V	 1.0000	 0.1690
W	 1.0000	 0.1580
X	 1.0000	 0.2050
Y	 1.0000	 0.2280
Z	 0.9970	 0.1790
a	 1.0000	 0.2030



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
b	 1.0000	 0.2060
c	 0.9060	 0.0830
d	 1.0000	 0.2540
e	 1.0000	 0.2500
f	 0.9650	 0.1380
g	 1.0000	 0.2490
h	 1.0000	 0.2580
i	 1.0000	 0.1840
j	 1.0000	 0.1550
k	 1.0000	 0.2230
l	 1.0000	 0.2280
m	 1.0000	 0.1410
n	 1.0000	 0.1570
o	 0.9970	 0.1020
p	 1.0000	 0.1470
q	 1.0000	 0.2510
r	 0.9690	 0.0720
s	 0.9130	 0.0600
t	 0.7880	 0.0750
u	 0.9840	 0.1530
v	 0.3870	 0.0640
w	 0.9930	 0.0850
x	 0.9730	 0.0850
y	 0.8370	 0.0520
z	 0.8100	 0.0550