



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:31 AM UTC

PDB ID : 8R09 / pdb_00008r09
EMDB ID : EMD-18787
Title : Cryo-EM structure of the cross-exon pre-B+5'ss+ATPgammaS complex
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on : 2023-10-31
Resolution : 4.30 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

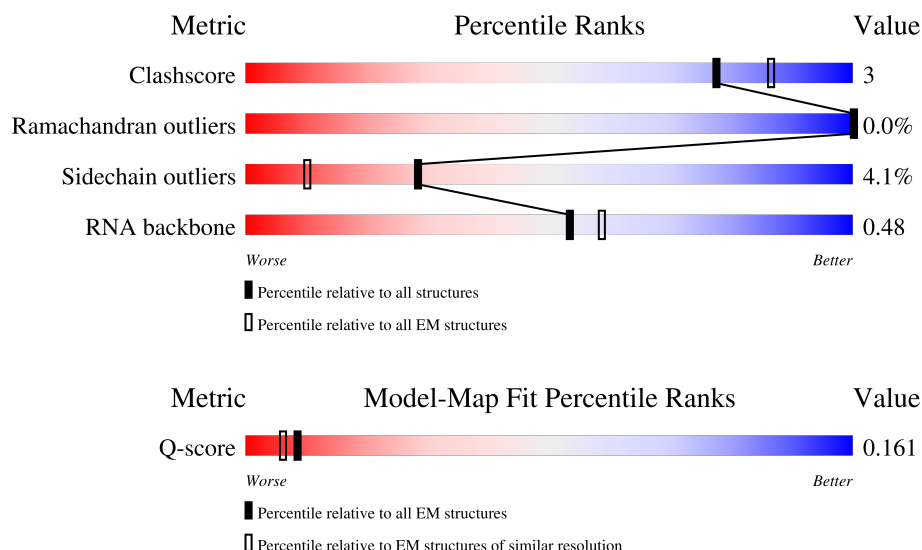
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



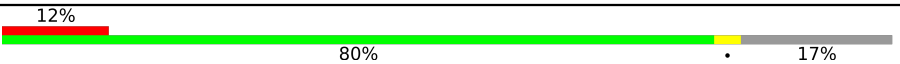
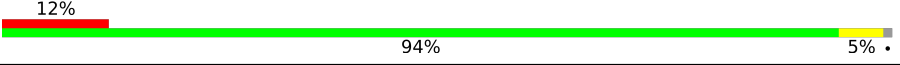
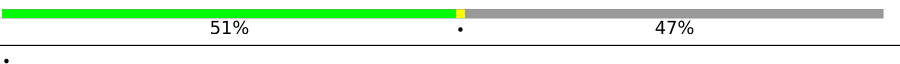
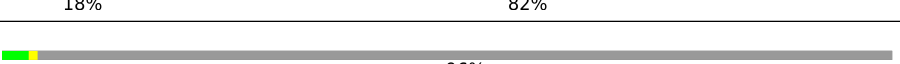
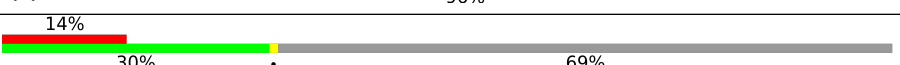
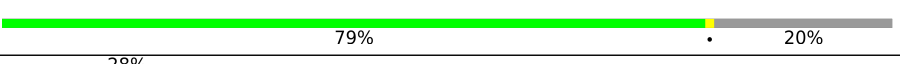
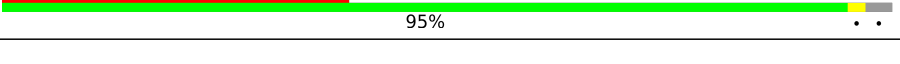
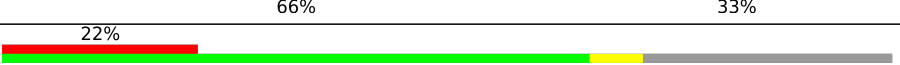
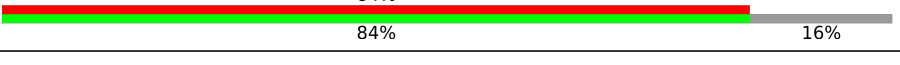
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	66	80	88% 10%
2	67	103	75% 25%
3	62	95	13% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	63	102	
5	68	96	
6	64	139	
7	65	91	
8	E	357	
9	B4	424	
10	Z	347	
11	8	464	
12	9	501	
13	B2	895	
14	B5	86	
15	2	188	
16	B3	1217	
17	BP	110	
18	B1	1304	
19	B6	125	
20	22	118	
20	42	118	
20	52	118	
21	2B	225	
22	2f	86	
22	4f	86	
22	5f	86	
23	2b	240	
23	4b	240	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
23	5b	240	
24	23	126	
24	43	126	
24	53	126	
25	2g	76	
25	4g	76	
25	5g	76	
26	2e	92	
26	4e	92	
26	5e	92	
27	21	119	
27	41	119	
27	51	119	
28	2A	255	
29	B	2136	
30	W	177	
31	G	820	
32	J	683	
33	L	499	
34	F	522	
35	N	941	
36	A	2335	
37	U	565	
38	S	800	
39	C	972	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	M	128	92% 5% .
41	D	142	99% ..
42	5	117	44% 40% 12% .
43	z	11	45% 36% 18%
44	7	793	13% 29% 71%
45	4	144	. 58% 31% 11%
46	6	106	44% 14% . 39%

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 82094 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 U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	66	72	Total	C	N	O	0	0
			357	213	72	72		

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	67	77	Total	C	N	O	0	0
			384	230	77	77		

- Molecule 3 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	62	95	Total	C	N	O	0	0
			478	288	95	95		

- Molecule 4 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	63	85	Total	C	N	O	0	0
			429	259	85	85		

- Molecule 5 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	68	95	Total	C	N	O	0	0
			469	279	95	95		

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	64	73	Total	C	N	O	0	0
			369	223	73	73		

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	65	76	Total	C	N	O	0	0
			378	226	76	76		

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	307	Total	C	N	O	0	0
			1531	917	307	307		

- Molecule 9 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	B4	78	Total	C	N	O	0	0
			391	235	78	78		

- Molecule 10 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	15	Total	C	N	O	P	0	0
			314	141	51	107	15		

- Molecule 11 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	8	144	Total	C	N	O	0	0
			729	441	144	144		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	9	383	Total	C	N	O	0	0
			1920	1154	383	383		

- Molecule 13 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B2	208	Total	C	N	O	0	0
			1072	656	208	208		

- Molecule 14 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	B5	69	Total	C	N	O	0	0
			347	209	69	69		

- Molecule 15 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	98	Total	C	N	O	P	0	0
			2072	926	349	699	98		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	B3	1186	Total	C	N	O	0	0
			5969	3597	1186	1186		

- Molecule 17 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	BP	100	Total	C	N	O	0	0
			498	298	100	100		

- Molecule 18 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	B1	870	Total	C	N	O	0	0
			4383	2643	870	870		

- Molecule 19 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	B6	90	Total	C	N	O	0	0
			455	275	90	90		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	22	95	Total	C	N	O		0	0
			482	292	95	95			
20	42	92	Total	C	N	O		0	0
			463	279	92	92			
20	52	98	Total	C	N	O	S	0	0
			796	498	144	148	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	2B	92	Total	C	N	O	0	0
			461	277	92	92		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2f	72	Total	C	N	O			
			359	215	72	72	0	0	
22	4f	72	Total	C	N	O			
			359	215	72	72	0	0	
22	5f	73	Total	C	N	O	S		
			567	367	94	101	5	0	

- Molecule 23 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2b	82	Total	C	N	O		0	0
			413	249	82	82			
23	4b	79	Total	C	N	O		0	0
			396	238	79	79			
23	5b	73	Total	C	N	O	S	0	0
			594	376	108	103	7		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	23	83	Total	C	N	O			
			415	249	83	83	0	0	
24	43	83	Total	C	N	O			
			415	249	83	83	0	0	
24	53	84	Total	C	N	O	S		
			657	412	116	123	6	0	

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	2g	73	Total	C	N	O	0	0
			364	218	73	73		
25	4g	74	Total	C	N	O	0	0
			369	221	74	74		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
25	5g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2e	81	Total	C	N	O		0	0
			403	241	81	81			
26	4e	76	Total	C	N	O		0	0
			378	226	76	76			
26	5e	77	Total	C	N	O	S	0	0
			638	405	113	115	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	21	80	Total	C	N	O		0	0
			402	242	80	80			
27	41	81	Total	C	N	O		0	0
			407	245	81	81			
27	51	81	Total	C	N	O	S	0	0
			641	408	112	118	3		

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2A	162	Total	C	N	O		0	0
			816	492	162	162			

- Molecule 29 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B	1714	Total	C	N	O		0	0
			8644	5216	1714	1714			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	169	Total	C	N	O		0	0
			844	506	169	169			

- Molecule 31 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	G	376	Total	C	N	O	6	0
			1930	1166	382	382		

- Molecule 32 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	J	224	Total	C	N	O	0	0
			1121	673	224	224		

- Molecule 33 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	L	376	Total	C	N	O	0	0
			1887	1135	376	376		

- Molecule 34 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	F	412	Total	C	N	O	0	0
			2060	1236	412	412		

- Molecule 35 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	N	834	Total	C	N	O	0	0
			4207	2539	834	834		

- Molecule 36 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	A	2218	Total	C	N	O	0	0
			10977	6541	2218	2218		

- Molecule 37 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	U	456	Total	C	N	O	0	0
			2308	1396	456	456		

- Molecule 38 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	S	154	Total	C	N	O	0	0
			778	470	154	154		

- Molecule 39 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	C	836	Total	C	N	O	0	0
			4223	2551	836	836		

- Molecule 40 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	M	124	Total	C	N	O	0	0
			627	379	124	124		

- Molecule 41 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	D	141	Total	C	N	O	0	0
			708	426	141	141		

- Molecule 42 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5	112	Total	C	N	O	P	0	0
			2356	1055	390	799	112		

- Molecule 43 is a RNA chain called 5'ss oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	z	11	Total	C	N	O	P	0	0
			239	107	46	75	11		

- Molecule 44 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	7	230	Total	C	N	O	0	0
			1158	698	230	230		

- Molecule 45 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4	128	Total	C	N	O	P	0	0
			2718	1216	477	898	127		

- Molecule 46 is a RNA chain called U6 snRNA.

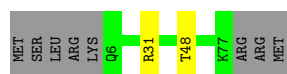
Mol	Chain	Residues	Atoms					AltConf	Trace
46	6	65	Total	C	N	O	P	0	0
			1392	622	253	452	65		

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.

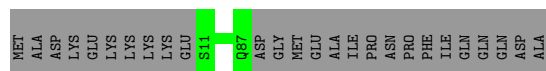
- Molecule 1: U6 snRNA-associated Sm-like protein LSm6

Chain 66:  88% 10%



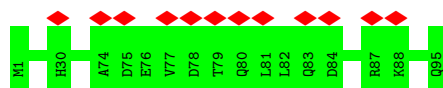
- Molecule 2: U6 snRNA-associated Sm-like protein LSm7

Chain 67:  75% 25%



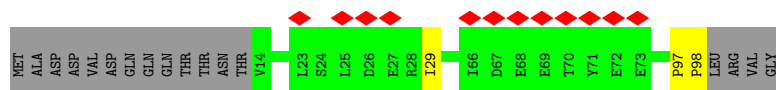
- Molecule 3: U6 snRNA-associated Sm-like protein LSm2

Chain 62:  13% 100%

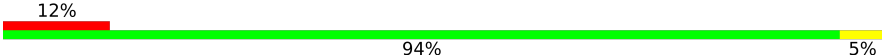


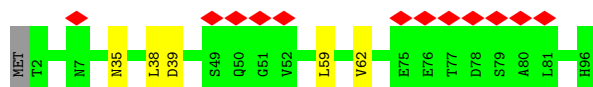
- Molecule 4: U6 snRNA-associated Sm-like protein LSm3

Chain 63:  12% 80% 17%

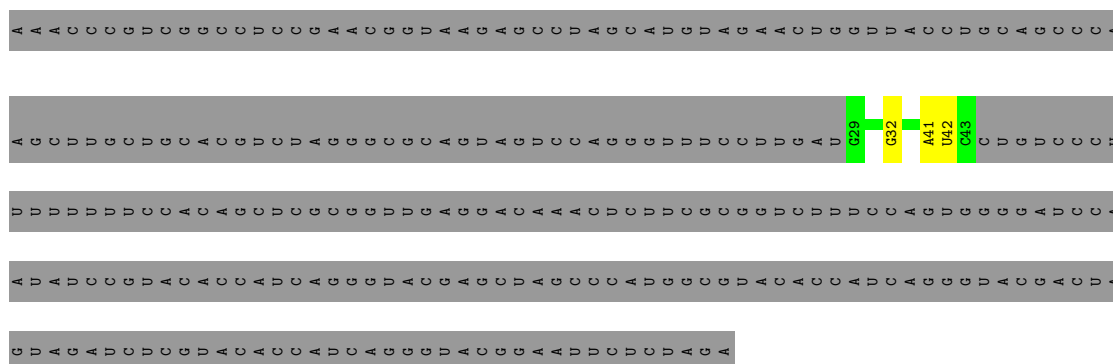


- Molecule 5: U6 snRNA-associated Sm-like protein LSm8

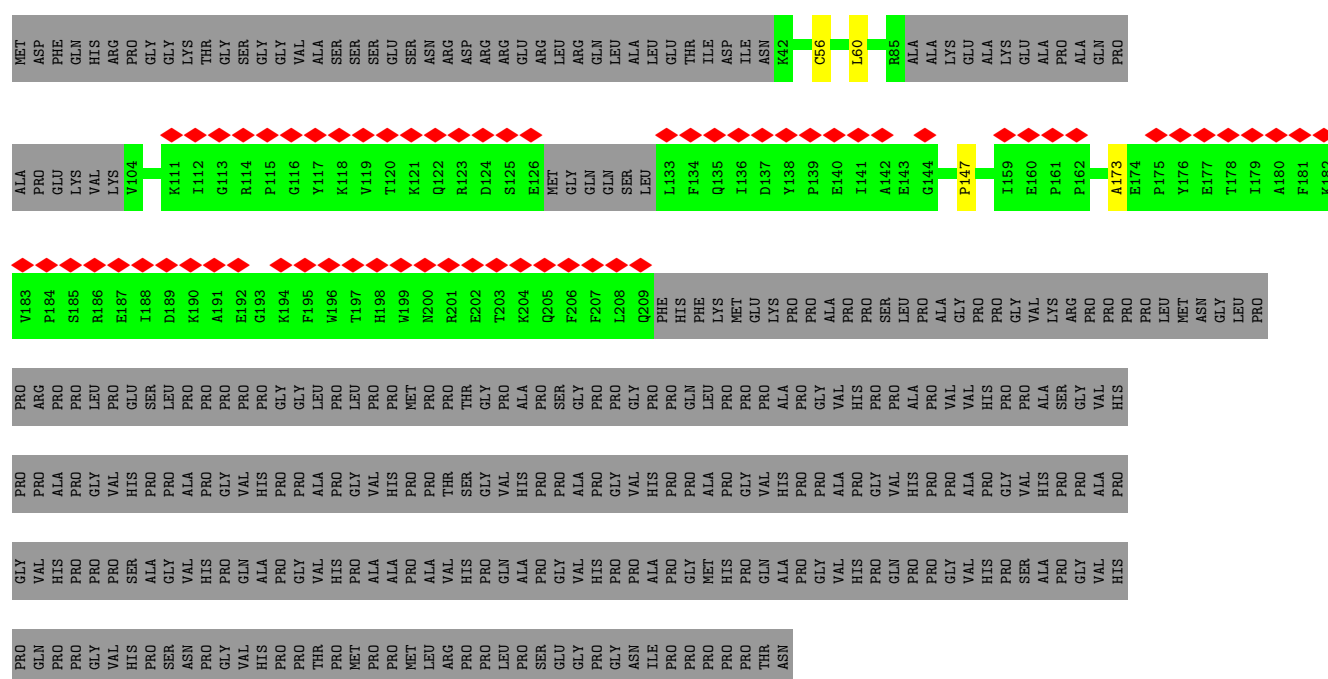
Chain 68:  12% 94% 5%



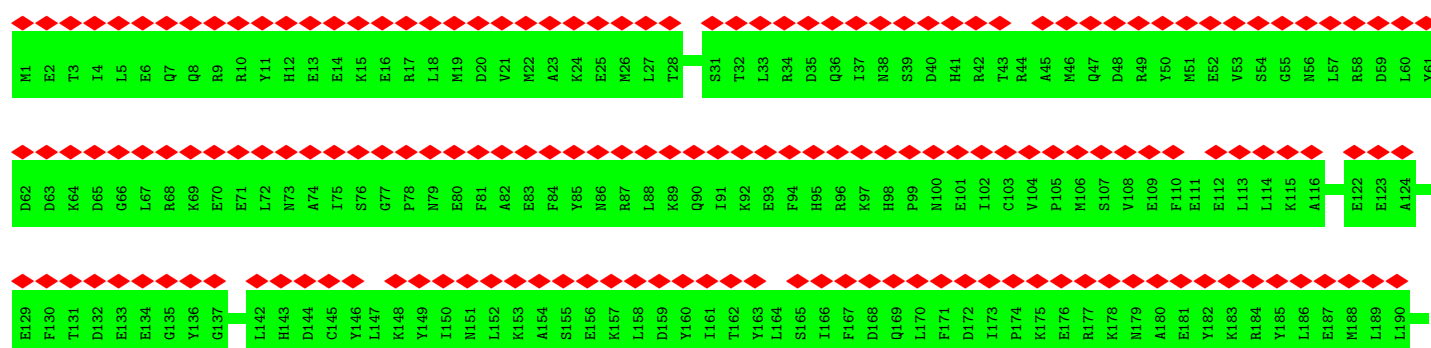
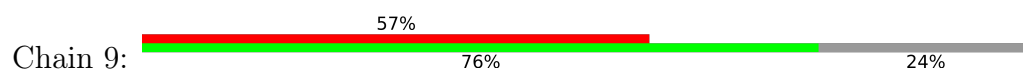
- Molecule 6: U6 snRNA-associated Sm-like protein LSm4

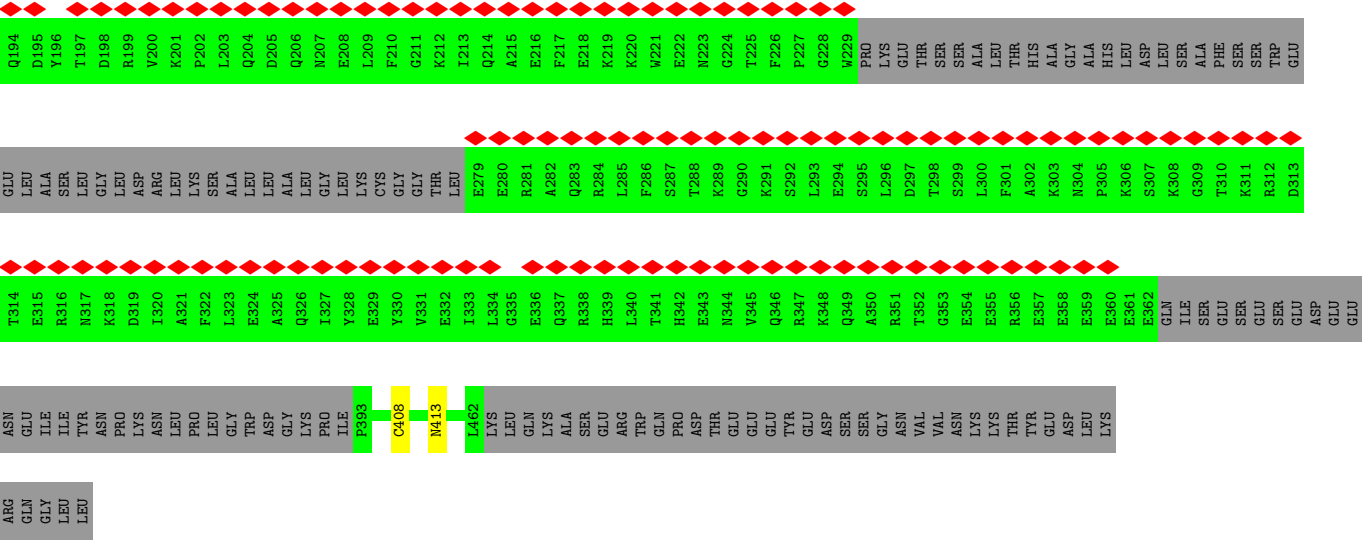


• Molecule 11: Splicing factor 3A subunit 2



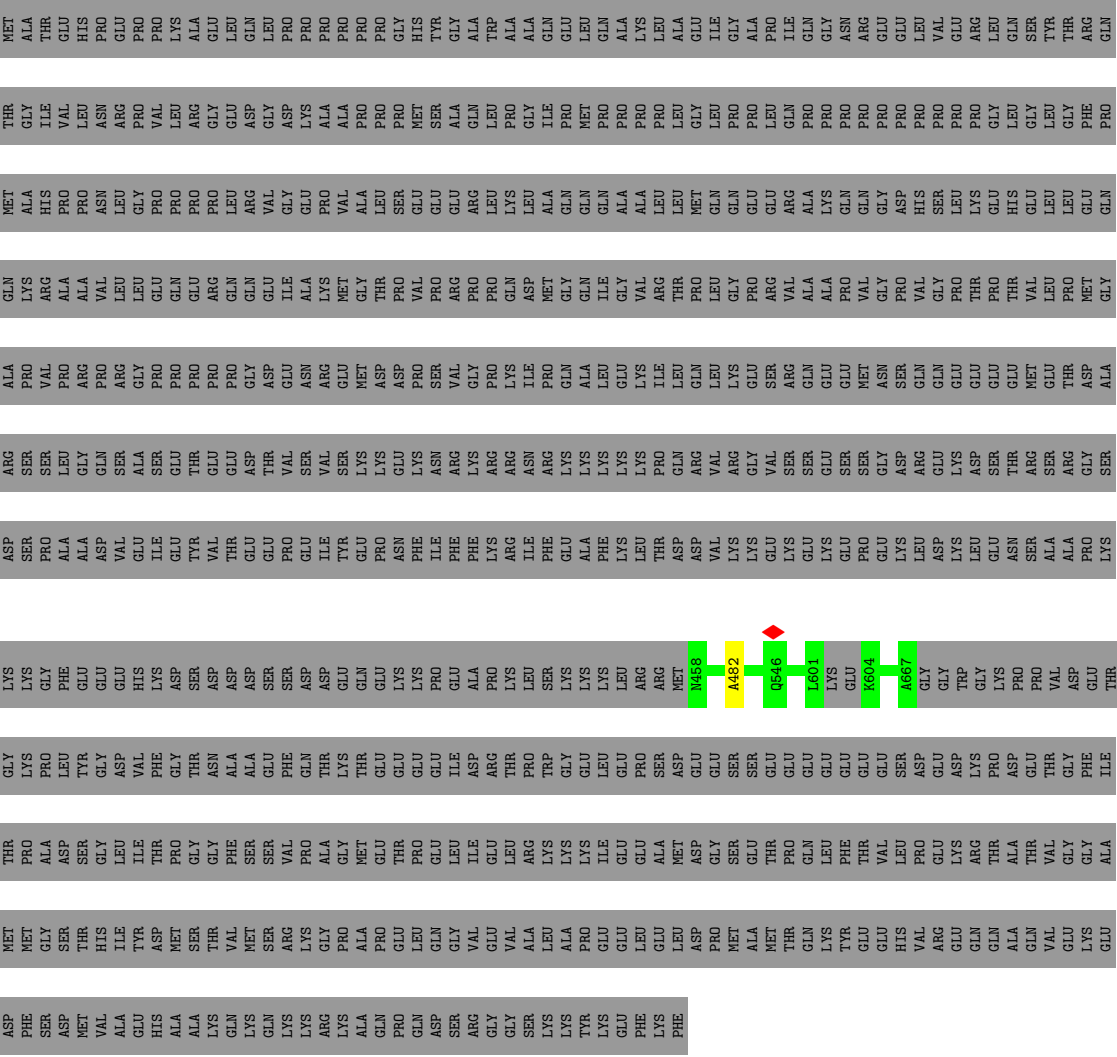
• Molecule 12: Splicing factor 3A subunit 3



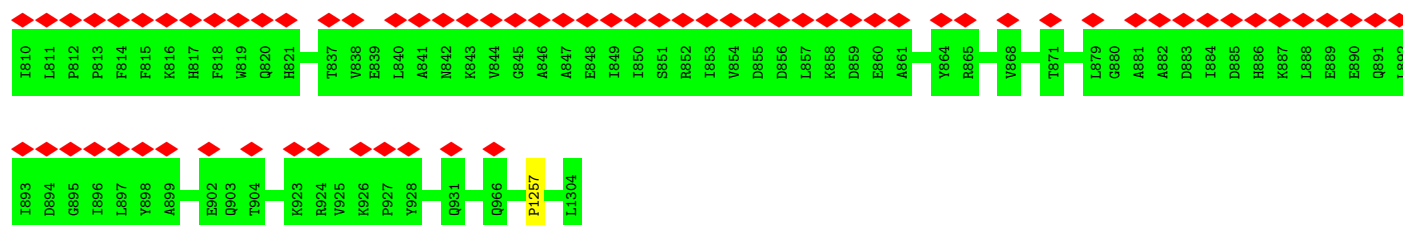


● Molecule 13: Splicing factor 3B subunit 2

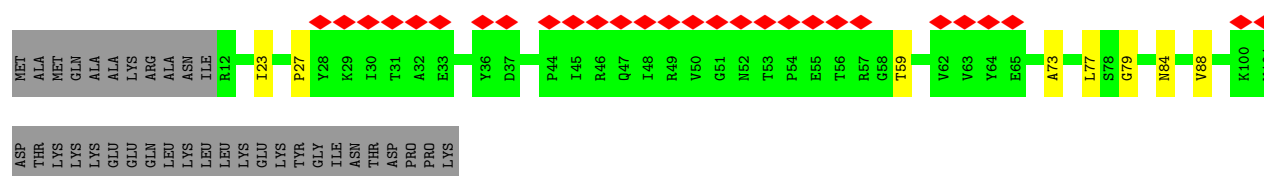
Chain B2: 23% 77%



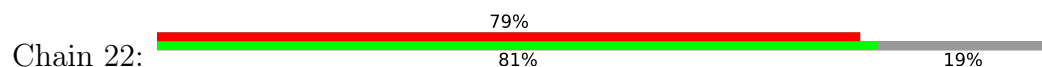




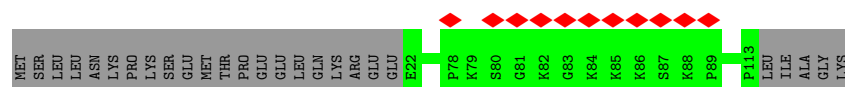
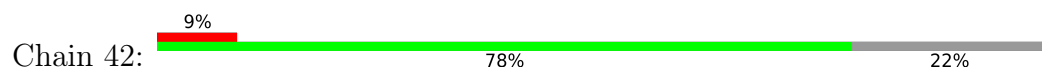
• Molecule 19: Splicing factor 3B subunit 6



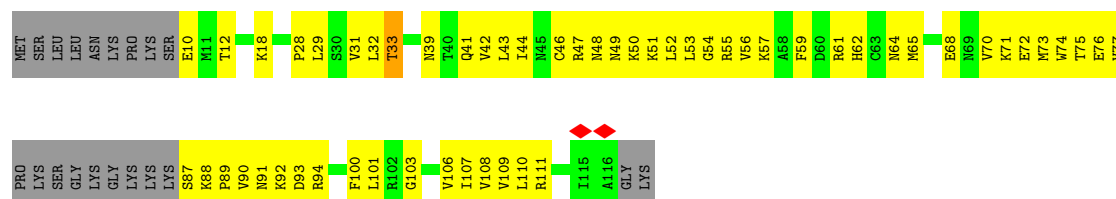
• Molecule 20: Small nuclear ribonucleoprotein Sm D2



• Molecule 20: Small nuclear ribonucleoprotein Sm D2

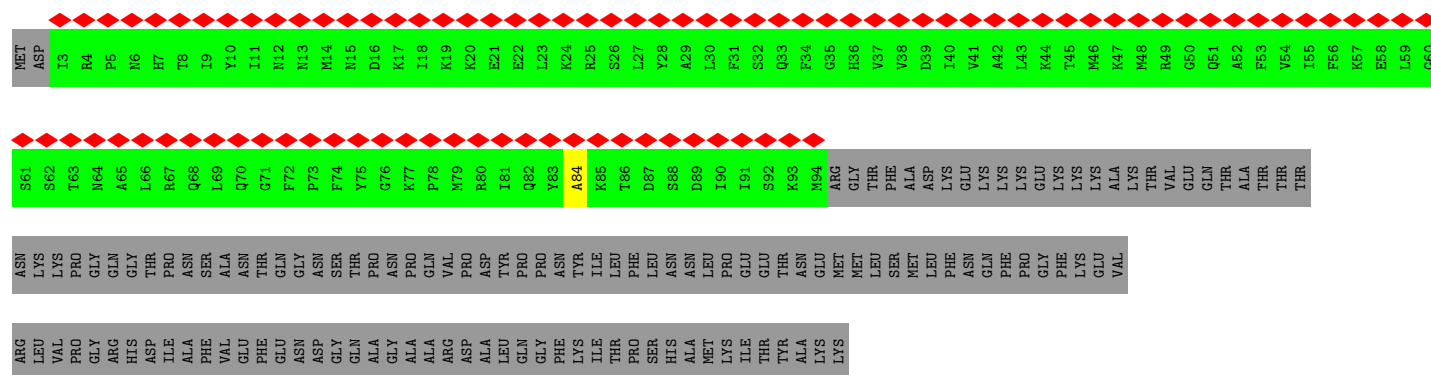


• Molecule 20: Small nuclear ribonucleoprotein Sm D2

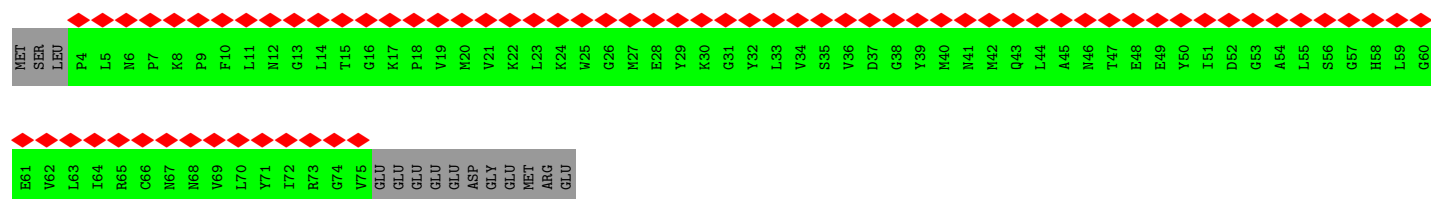
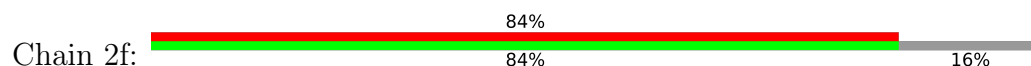


• Molecule 21: U2 small nuclear ribonucleoprotein B''

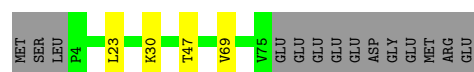
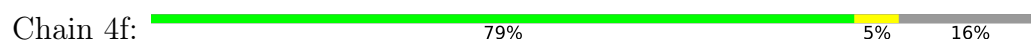




• Molecule 22: Small nuclear ribonucleoprotein F



• Molecule 22: Small nuclear ribonucleoprotein F

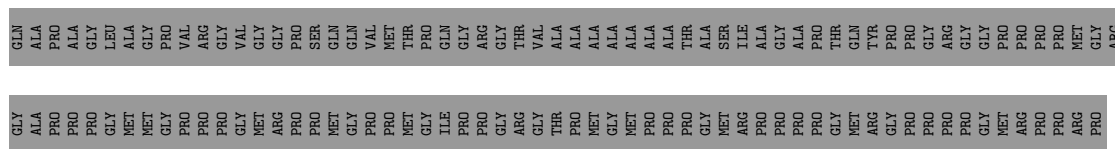


• Molecule 22: Small nuclear ribonucleoprotein F

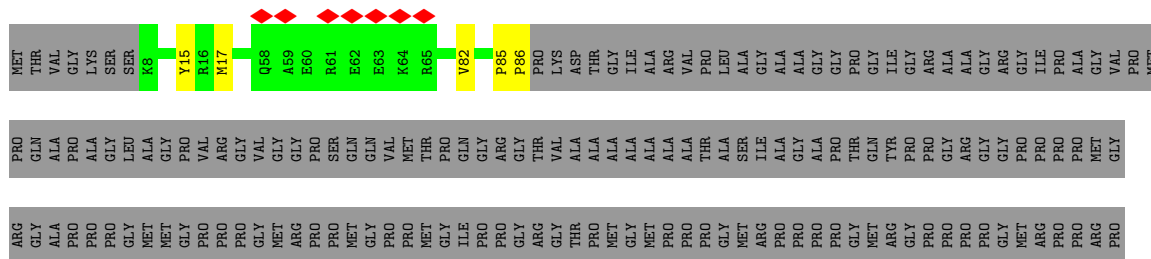


• Molecule 23: Small nuclear ribonucleoprotein-associated proteins B and B'

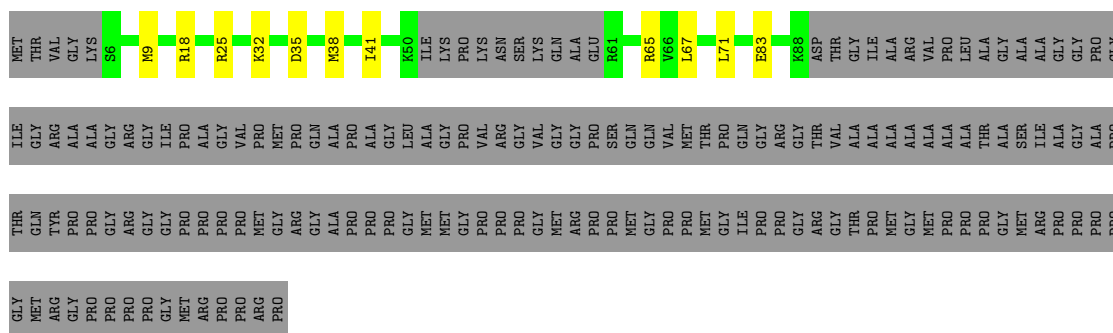




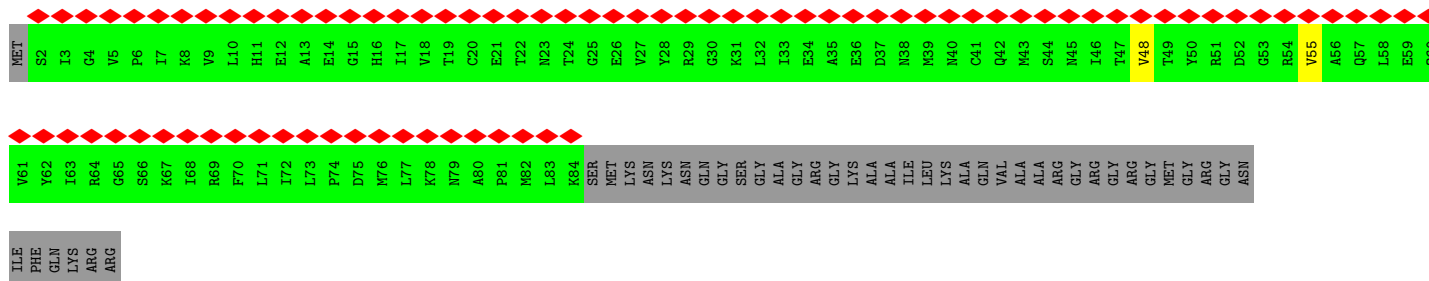
- Molecule 23: Small nuclear ribonucleoprotein-associated proteins B and B'



- Molecule 23: Small nuclear ribonucleoprotein-associated proteins B and B'

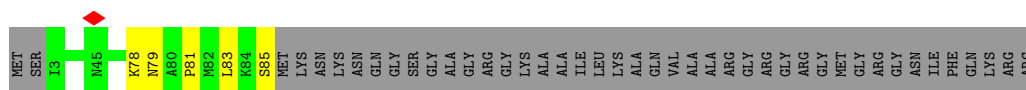


- Molecule 24: Small nuclear ribonucleoprotein Sm D3

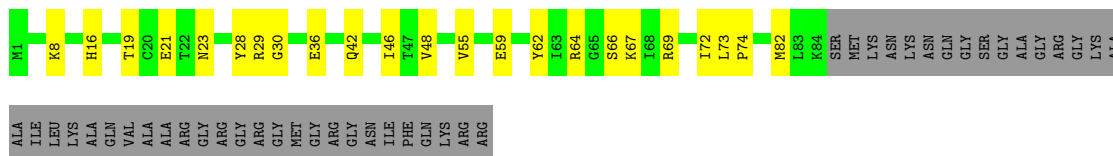


- Molecule 24: Small nuclear ribonucleoprotein Sm D3

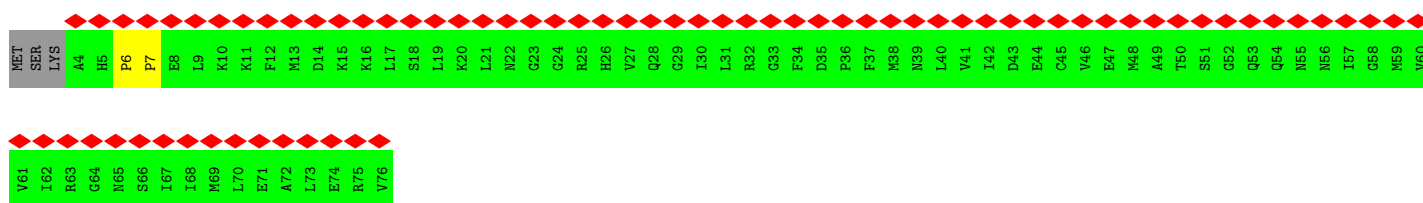




• Molecule 24: Small nuclear ribonucleoprotein Sm D3



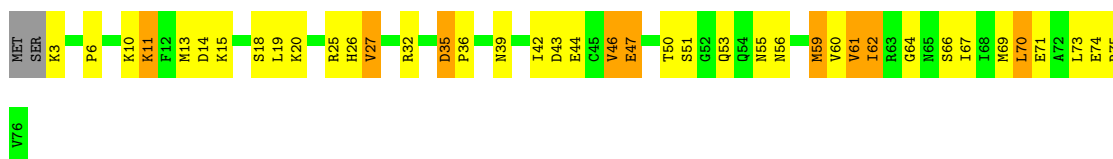
• Molecule 25: Small nuclear ribonucleoprotein G



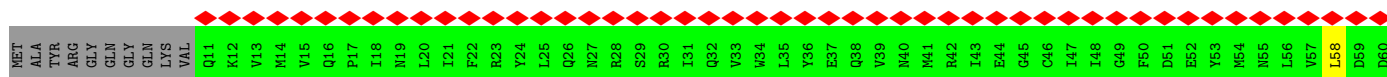
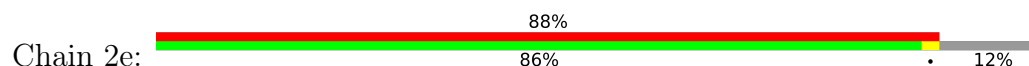
• Molecule 25: Small nuclear ribonucleoprotein G



• Molecule 25: Small nuclear ribonucleoprotein G



• Molecule 26: Small nuclear ribonucleoprotein E





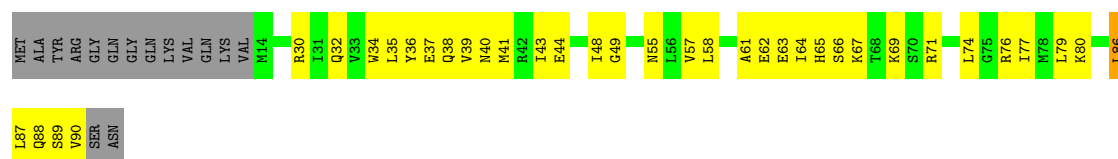
- Molecule 26: Small nuclear ribonucleoprotein E

Chain 4e: 78% 17%



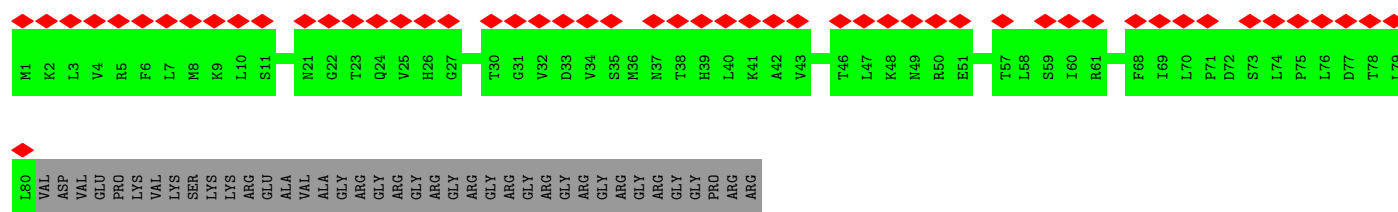
- Molecule 26: Small nuclear ribonucleoprotein E

Chain 5e: 45% 38% 16%



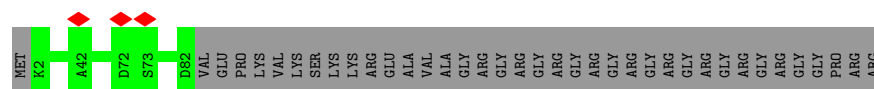
- Molecule 27: Small nuclear ribonucleoprotein Sm D1

Chain 21: 45% 67% 33%



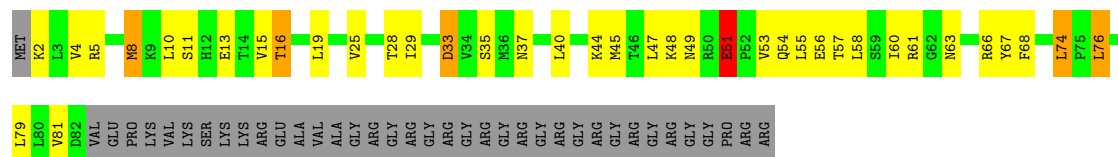
- Molecule 27: Small nuclear ribonucleoprotein Sm D1

Chain 41: 68% 32%

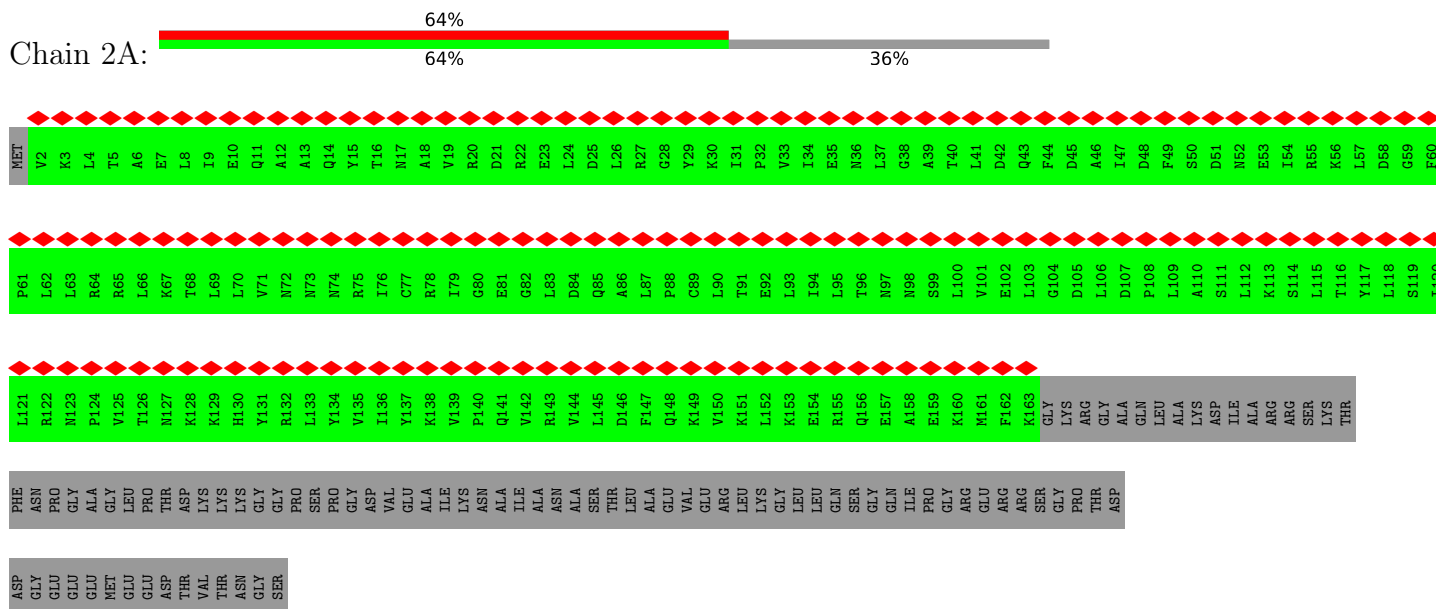


- Molecule 27: Small nuclear ribonucleoprotein Sm D1

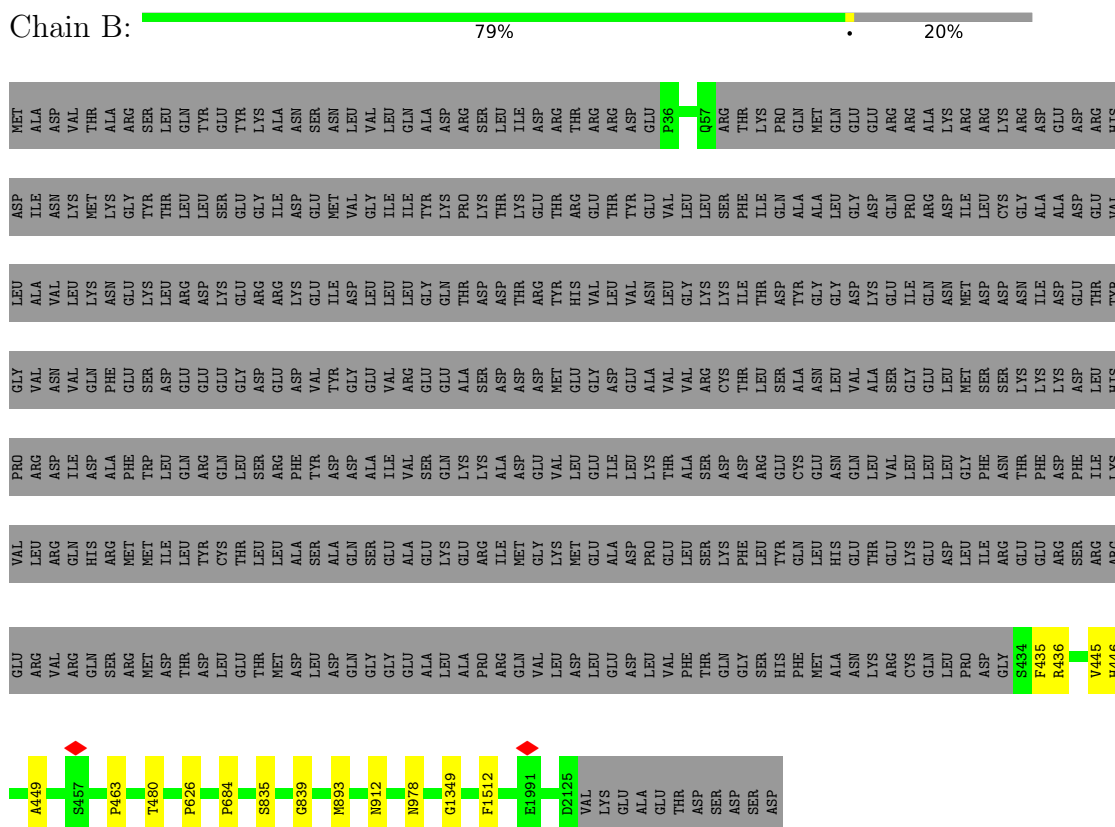
Chain 51: 35% 28% 32%



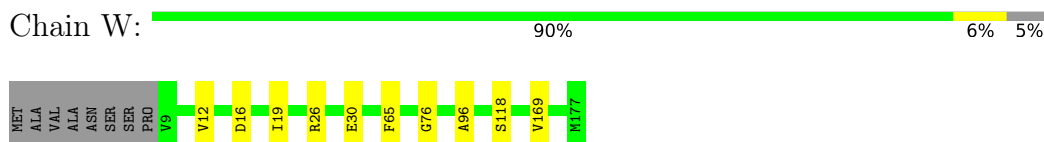
- Molecule 28: U2 small nuclear ribonucleoprotein A'



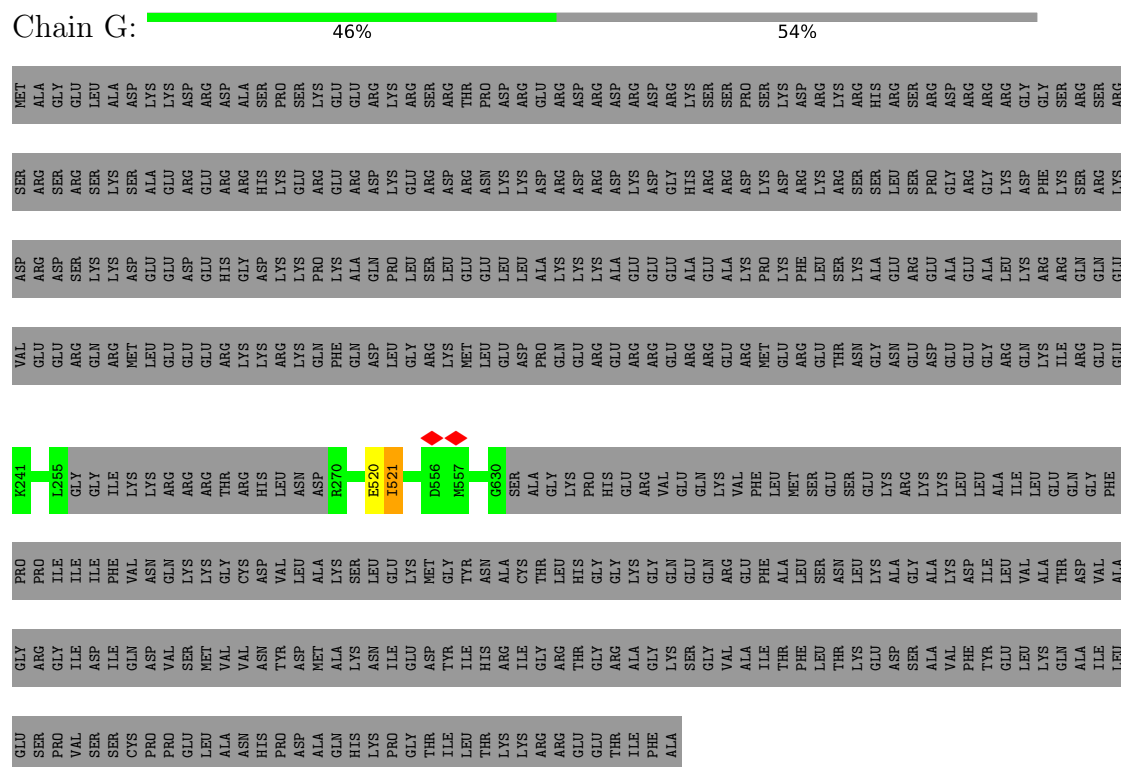
- Molecule 29: U5 small nuclear ribonucleoprotein 200 kDa helicase



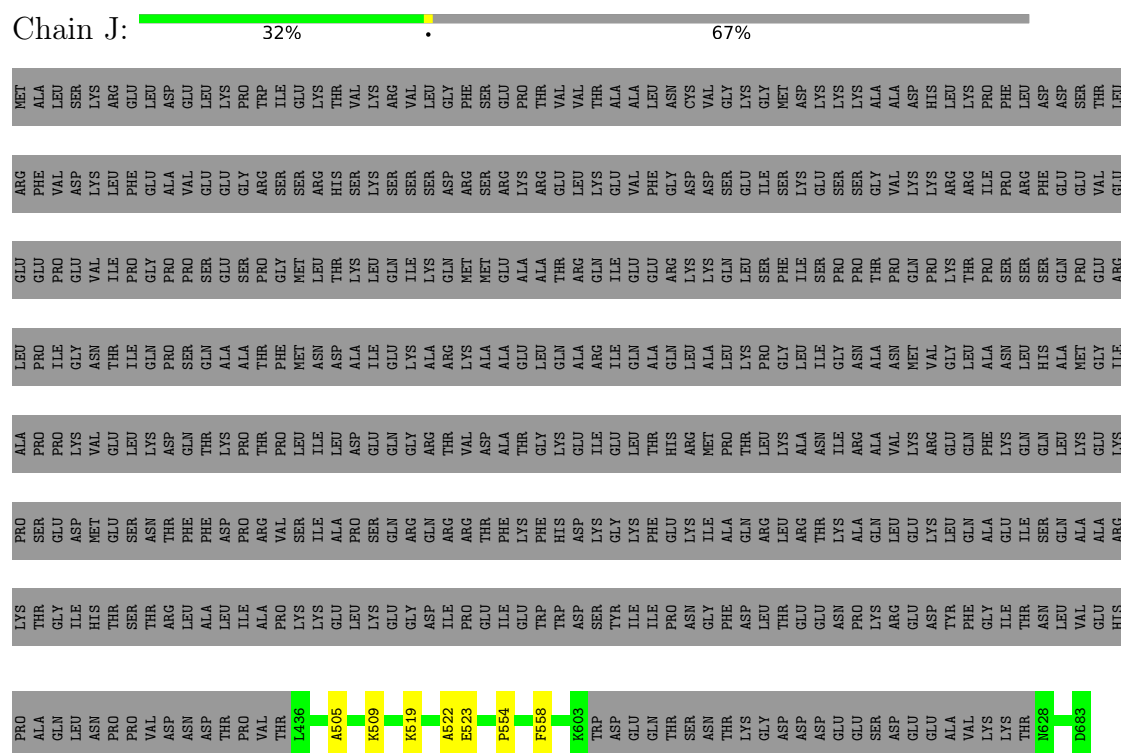
- Molecule 30: Peptidyl-prolyl cis-trans isomerase H



- Molecule 31: Probable ATP-dependent RNA helicase DDX23



- Molecule 32: U4/U6 small nuclear ribonucleoprotein Prp3

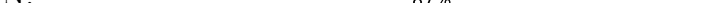


- Molecule 33: U4/U6 small nuclear ribonucleoprotein Prp31

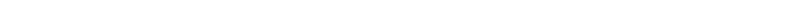
[illegible]

- Chain F: 75% • 21%

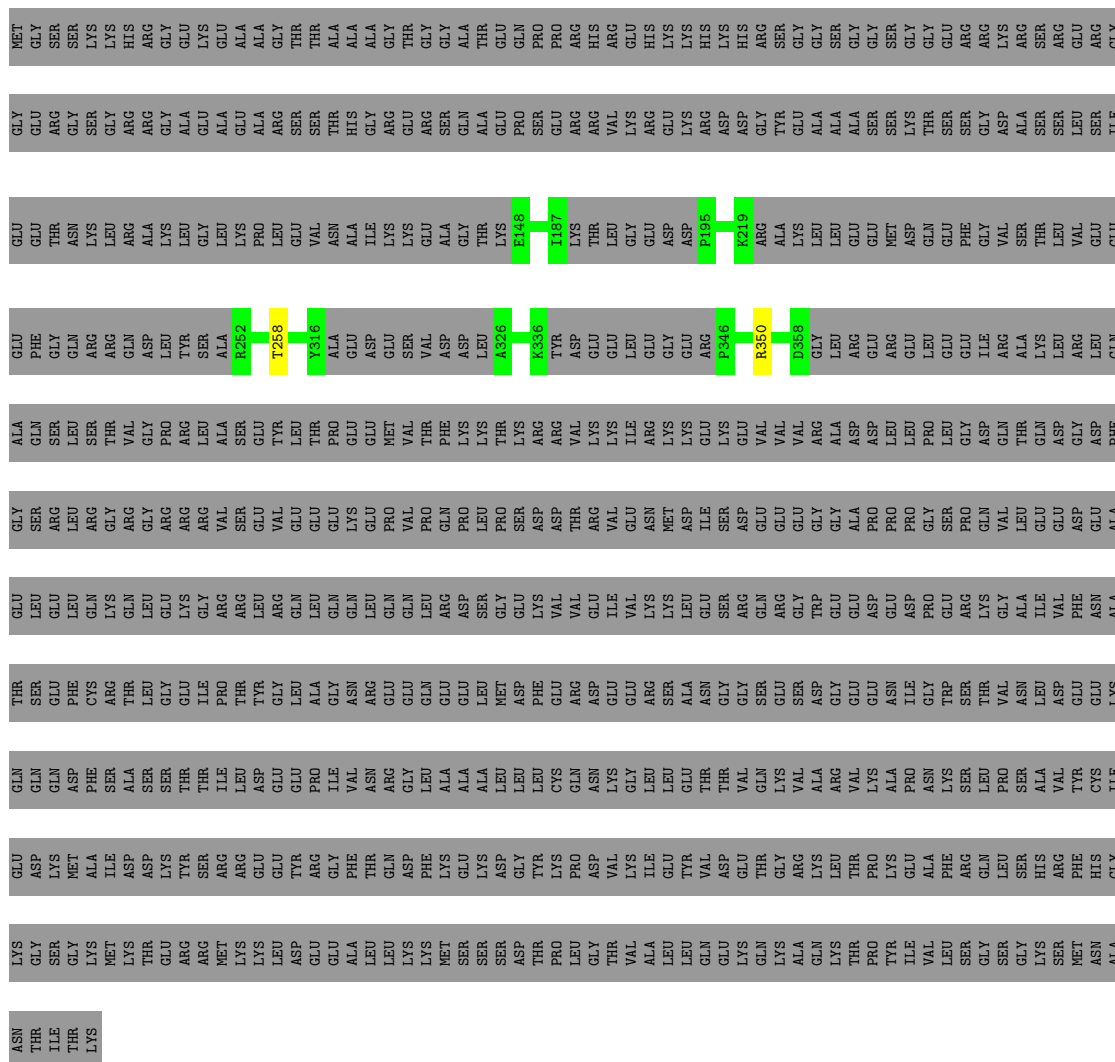
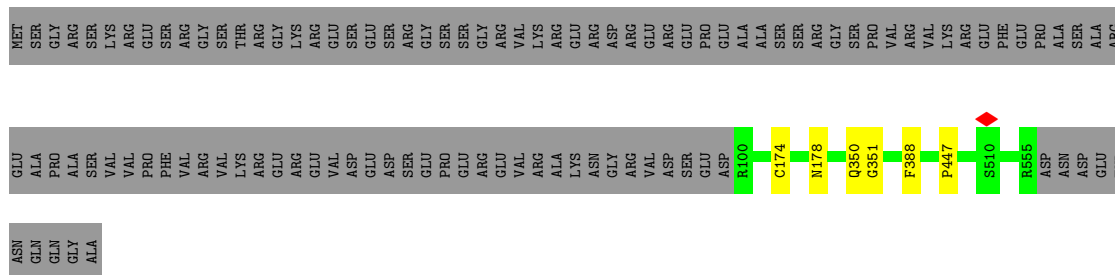
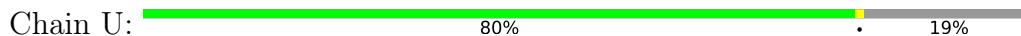
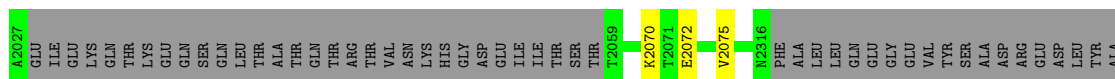
[illegible]

- Chain N:  87% • 11%

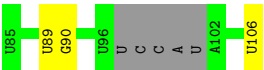
G395		C339	V411	E412	L413	E414	D686	S671	A672	R676	K680	S681	V682	A694	Q717	Y788	A796	K924	D928	V933	A934	F941																								
SER	GLY	PRO	TYR	GLU	X96	K178	G208	GLY	LEU	ASN	THR	TYR	PRO	PRO	GLY	GLY	GLY	THR	PRO	GLY	MET	ARG	LYS	ILE	GLN	ALA	R247	Q257	VAL	SER	ASP	SER	VAL	SER	SER	GLY	Q265									
MET	ASN	LYS	LYS	LYS	LYS	PRO	F8	A40	ASN	ASP	PRO	VAL	ASP	ASP	ARG	HIS	ALA	PRO	PRO	GLY	THR	ARG	THR	GLY	GLN	MET	LYS	ASN	GLN	ALA	ASP	ASP	ASP	ASP	GLU	LEU	ASN	THR	TYR	GLY	ALA	GLY	SER	LEU	PHE	SER

- Chain A:  94% . 5%

[illegible]



- | |
|-----|
| MET | PRO | ALA | PRO | GLY | VAL | GLN | ALA | VAL | PRO | PRO | PRO | PRO | PRO | VAL | THR | THR | GLU | GLU | LYS | GLN | PRO | THR | THR | GLU | GLU | GLU | ALA | ALA | SER | SER | LYS | GLU | ASP | SER | ALA | ALA | PRO | SER | LYS | VAL | VAL | VAL | GLY | ILE | ILE | TYR | PRO | PRO | PRO | PRO | GLU | GLU | VAL | ASP | LYS | THR | ALA | ALA | SER | SER | PHE | VAL |
|-----|



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	411185	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	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0068	Depositor
Map size ($\text{\AA}$)	556.8, 556.8, 556.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	66	0.17	0/358	0.49	0/497
2	67	0.14	0/386	0.39	0/537
3	62	0.23	0/480	0.55	0/671
4	63	0.17	0/432	0.52	0/604
5	68	0.18	0/469	0.54	0/651
6	64	0.24	0/372	0.50	0/520
7	65	0.16	0/380	0.42	0/528
8	E	0.16	0/1540	0.44	0/2148
9	B4	0.16	0/394	0.37	0/549
10	Z	0.14	0/349	0.26	0/540
11	8	0.19	0/734	0.53	0/1025
12	9	0.16	0/1928	0.44	0/2692
13	B2	0.21	0/1092	0.44	0/1536
14	B5	0.12	0/349	0.37	0/487
15	2	0.19	0/2308	0.40	3/3584 (0.1%)
16	B3	0.16	0/6024	0.43	0/8425
17	BP	0.14	0/501	0.46	0/697
18	B1	0.19	0/4421	0.50	0/6190
19	B6	0.18	0/459	0.44	0/642
20	22	0.15	0/485	0.37	0/677
20	42	0.17	0/466	0.46	0/651
20	52	0.32	0/805	0.77	0/1081
21	2B	0.14	0/463	0.33	0/646
22	2f	0.17	0/362	0.44	0/502
22	4f	0.20	0/362	0.44	0/502
22	5f	0.38	0/579	0.85	0/783
23	2b	0.15	0/416	0.45	0/581
23	4b	0.19	0/398	0.45	0/555
23	5b	0.33	0/602	0.55	0/801
24	23	0.18	0/417	0.49	0/581
24	43	0.20	0/417	0.53	1/581 (0.2%)
24	53	0.37	0/665	0.55	0/896
25	2g	0.17	0/366	0.41	0/509
25	4g	0.16	0/371	0.41	0/516

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	5g	0.38	0/584	0.78	0/779
26	2e	0.16	0/403	0.41	0/561
26	4e	0.17	0/378	0.48	0/526
26	5e	0.32	0/646	0.74	0/867
27	21	0.13	0/404	0.42	0/564
27	41	0.18	0/409	0.44	0/571
27	51	0.37	0/649	0.78	1/878 (0.1%)
28	2A	0.17	0/821	0.46	0/1149
29	B	0.13	0/8720	0.34	0/12217
30	W	0.15	0/853	0.40	0/1188
31	G	0.28	0/1949	0.46	0/2729
32	J	0.33	0/1127	0.53	0/1572
33	L	0.13	0/1899	0.28	0/2654
34	F	0.16	0/2074	0.41	0/2894
35	N	0.21	0/4239	0.43	0/5936
36	A	0.12	0/11081	0.32	0/15398
37	U	0.10	0/2330	0.31	0/3268
38	S	0.14	0/780	0.35	0/1084
39	C	0.16	0/4270	0.35	0/5983
40	M	0.16	0/632	0.45	0/885
41	D	0.12	0/712	0.31	0/995
42	5	0.16	0/2625	0.34	0/4079
43	z	0.11	0/268	0.17	0/416
44	7	0.14	0/1164	0.39	0/1625
45	4	0.11	0/3034	0.18	0/4718
46	6	0.10	0/1556	0.21	0/2419
All	All	0.18	0/83757	0.41	5/118340 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	106	G	P-O3'-C3'	5.34	128.22	120.20
24	43	79	ASN	CB-CA-C	-5.33	110.41	116.54
15	2	103	U	P-O3'-C3'	5.22	128.02	120.20
15	2	46	U	P-O3'-C3'	5.08	127.82	120.20
27	51	51	GLU	CB-CG-CD	5.02	121.13	112.60

There are no chirality outliers.

There are no planarity outliers.

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	66	357	0	169	1	0
2	67	384	0	178	0	0
3	62	478	0	222	0	0
4	63	429	0	199	2	0
5	68	469	0	220	3	0
6	64	369	0	172	1	0
7	65	378	0	174	2	0
8	E	1531	0	747	7	0
9	B4	391	0	197	0	0
10	Z	314	0	160	2	0
11	8	729	0	356	3	0
12	9	1920	0	902	1	0
13	B2	1072	0	563	1	0
14	B5	347	0	171	1	0
15	2	2072	0	1049	15	0
16	B3	5969	0	2985	15	0
17	BP	498	0	241	2	0
18	B1	4383	0	2195	2	0
19	B6	455	0	227	5	0
20	22	482	0	220	0	0
20	42	463	0	211	0	0
20	52	796	0	821	49	0
21	2B	461	0	218	1	0
22	2f	359	0	179	0	0
22	4f	359	0	179	2	0
22	5f	567	0	575	38	0
23	2b	413	0	194	1	0
23	4b	396	0	183	3	0
23	5b	594	0	615	8	0
24	23	415	0	198	1	0
24	43	415	0	198	2	0
24	53	657	0	675	17	0
25	2g	364	0	176	1	0
25	4g	369	0	178	1	0
25	5g	577	0	603	23	0
26	2e	403	0	173	1	0
26	4e	378	0	163	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	5e	638	0	657	42	0
27	21	402	0	184	0	0
27	41	407	0	183	0	0
27	51	641	0	681	16	0
28	2A	816	0	386	0	0
29	B	8644	0	4199	9	0
30	W	844	0	426	5	0
31	G	1930	0	946	1	0
32	J	1121	0	547	6	0
33	L	1887	0	934	3	0
34	F	2060	0	1021	12	0
35	N	4207	0	2161	12	0
36	A	10977	0	5122	17	0
37	U	2308	0	1104	5	0
38	S	778	0	382	1	0
39	C	4223	0	2099	11	0
40	M	627	0	315	5	0
41	D	708	0	328	1	0
42	5	2356	0	1194	28	0
43	z	239	0	119	2	0
44	7	1158	0	558	0	0
45	4	2718	0	1378	10	0
46	6	1392	0	702	9	0
All	All	82094	0	42512	347	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 3.

All (347) 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)
26:5e:58:LEU:O	26:5e:76:ARG:HA	1.63	0.96
32:J:558:PHE:CB	46:6:77:C:H3'	1.95	0.96
16:B3:886:GLU:HA	16:B3:910:ALA:O	1.74	0.88
8:E:56:GLN:H	8:E:96:TYR:HA	1.38	0.86
26:5e:44:GLU:O	26:5e:61:ALA:HA	1.75	0.85
29:B:436:ARG:H	29:B:445:VAL:HA	1.39	0.85
16:B3:699:VAL:HA	16:B3:715:MET:O	1.76	0.84
26:5e:63:GLU:O	26:5e:71:ARG:HA	1.78	0.83
25:5g:25:ARG:HH11	26:5e:39:VAL:HG12	1.43	0.82
26:5e:57:VAL:HA	26:5e:77:ILE:O	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:23:48:VAL:O	24:23:55:VAL:HA	1.78	0.81
39:C:737:PRO:HA	39:C:771:GLN:HA	1.62	0.81
19:B6:27:PRO:HG3	19:B6:84:ASN:H	1.42	0.81
29:B:435:PHE:H	29:B:446:HIS:H	1.27	0.80
22:5f:30:LYS:O	22:5f:47:THR:HA	1.82	0.79
16:B3:913:LEU:HA	16:B3:920:VAL:HA	1.63	0.78
16:B3:486:SER:O	16:B3:491:VAL:HA	1.85	0.74
1:66:31:ARG:O	1:66:48:THR:HA	1.86	0.74
20:52:75:THR:HA	20:52:91:ASN:HA	1.69	0.74
36:A:465:LYS:O	42:5:23:C:N4	2.21	0.73
22:5f:33:LEU:HD11	22:5f:42:MET:HB3	1.71	0.72
25:5g:42:ILE:O	25:5g:59:MET:HA	1.89	0.72
20:52:77:VAL:HG12	20:52:89:PRO:HG3	1.71	0.71
20:52:57:LYS:HE2	20:52:68:GLU:HB3	1.72	0.70
25:5g:47:GLU:HB3	25:5g:55:ASN:HB2	1.73	0.70
25:5g:60:VAL:HB	26:5e:86:LEU:HD11	1.73	0.70
37:U:174:CYS:O	37:U:178:ASN:HA	1.92	0.70
22:5f:43:GLN:HB2	20:52:28:PRO:HA	1.73	0.70
34:F:464:PHE:HA	34:F:478:THR:HA	1.73	0.70
41:D:139:LYS:H	42:5:41:U:H5'	1.57	0.70
37:U:174:CYS:O	37:U:178:ASN:N	2.25	0.70
24:53:48:VAL:O	24:53:55:VAL:HA	1.92	0.70
39:C:507:VAL:HA	39:C:568:PRO:HD3	1.74	0.70
8:E:56:GLN:N	8:E:96:TYR:HA	2.08	0.68
19:B6:79:GLY:H	19:B6:88:VAL:HA	1.57	0.68
22:4f:30:LYS:O	22:4f:47:THR:HA	1.94	0.68
42:5:8:G:H22	42:5:71:C:H5''	1.58	0.68
39:C:504:GLY:N	39:C:527:VAL:O	2.27	0.67
26:5e:44:GLU:HG2	26:5e:64:ILE:HD11	1.76	0.66
26:2e:58:LEU:O	26:2e:76:ARG:HA	1.95	0.66
22:5f:5:LEU:H	26:5e:48:ILE:HG22	1.62	0.65
29:B:435:PHE:H	29:B:446:HIS:N	1.95	0.65
42:5:93:U:O2'	22:5f:65:ARG:NH2	2.29	0.65
25:5g:35:ASP:OD1	25:5g:35:ASP:N	2.27	0.65
37:U:174:CYS:O	37:U:178:ASN:CA	2.44	0.64
22:5f:73:ARG:HB3	26:5e:77:ILE:HG22	1.79	0.63
42:5:46:U:O4	42:5:47:A:N6	2.31	0.63
20:52:42:VAL:O	20:52:53:LEU:HA	1.99	0.63
42:5:8:G:N2	42:5:70:A:O3'	2.31	0.62
20:52:10:GLU:HG2	20:52:12:THR:H	1.64	0.62
32:J:558:PHE:CB	46:6:77:C:C3'	2.75	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:J:554:PRO:HB2	46:6:78:A:OP2	2.00	0.62
22:5f:33:LEU:HD21	22:5f:42:MET:HG3	1.82	0.61
22:5f:20:MET:HE1	22:5f:73:ARG:HH11	1.65	0.61
40:M:11:TYR:N	40:M:12:PRO:HD2	2.15	0.61
29:B:449:ALA:HB1	29:B:684:PRO:HB2	1.82	0.61
40:M:11:TYR:N	40:M:12:PRO:CD	2.63	0.61
22:5f:69:VAL:HG23	26:5e:80:LYS:HG3	1.83	0.60
24:53:19:THR:HG23	24:53:72:ILE:HB	1.84	0.60
24:53:59:GLU:OE1	25:5g:75:ARG:NH1	2.35	0.60
26:5e:63:GLU:HG3	26:5e:74:LEU:HD11	1.84	0.60
40:M:12:PRO:HG2	40:M:82:PHE:CB	2.31	0.60
27:51:76:LEU:HA	27:51:79:LEU:HB2	1.84	0.59
25:5g:19:LEU:HB2	25:5g:27:VAL:HG12	1.85	0.59
36:A:1551:PHE:O	43:z:1:G:N1	2.34	0.59
31:G:520:GLU:O	31:G:521:ILE:C	2.46	0.58
26:5e:35:LEU:HB2	26:5e:38:GLN:HB3	1.86	0.58
20:52:53:LEU:HD11	20:52:71:LYS:HD3	1.86	0.58
35:N:335:GLY:O	35:N:339:CYS:N	2.37	0.58
20:52:39:ASN:O	20:52:55:ARG:NH1	2.36	0.58
25:5g:20:LYS:HD2	25:5g:69:MET:HE2	1.86	0.58
22:5f:50:TYR:HA	22:5f:54:ALA:O	2.04	0.57
20:52:46:CYS:SG	20:52:52:LEU:HD13	2.45	0.57
26:5e:74:LEU:HD23	26:5e:77:ILE:HG21	1.86	0.57
20:52:107:ILE:HG22	20:52:108:VAL:HG13	1.86	0.57
20:52:29:LEU:HB3	20:52:59:PHE:HE2	1.70	0.56
25:5g:60:VAL:HB	26:5e:86:LEU:CD1	2.35	0.56
34:F:484:PRO:O	34:F:485:LEU:C	2.48	0.56
27:51:25:VAL:HG22	27:51:45:MET:HG3	1.87	0.56
39:C:737:PRO:HA	39:C:771:GLN:CA	2.32	0.56
20:52:46:CYS:HB2	20:52:50:LYS:HB2	1.87	0.56
36:A:2070:LYS:HA	36:A:2075:VAL:CA	2.35	0.56
15:2:165:A:H61	21:2B:84:ALA:HB1	1.70	0.56
26:5e:43:ILE:HA	26:5e:62:GLU:O	2.06	0.56
40:M:12:PRO:HB2	40:M:81:VAL:HA	1.87	0.56
24:53:62:TYR:HB3	25:5g:70:LEU:HB2	1.88	0.56
35:N:788:TYR:CB	35:N:796:ALA:HB2	2.36	0.56
20:52:41:GLN:HE21	20:52:53:LEU:HD13	1.72	0.55
25:5g:25:ARG:HD3	26:5e:39:VAL:HG12	1.88	0.55
27:51:33:ASP:HB2	27:51:37:ASN:HB2	1.89	0.55
33:L:264:SER:O	33:L:269:PRO:HD3	2.06	0.55
26:5e:30:ARG:HB3	26:5e:90:VAL:HA	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:F:477:TRP:HA	34:F:483:SER:O	2.06	0.55
22:5f:64:ILE:HG22	20:52:108:VAL:HG12	1.87	0.55
8:E:52:CYS:O	8:E:340:PRO:HD2	2.08	0.54
20:52:75:THR:HA	20:52:90:VAL:O	2.08	0.54
26:5e:41:MET:HA	26:5e:64:ILE:O	2.07	0.54
16:B3:405:SER:N	16:B3:406:PRO:HD3	2.22	0.54
20:52:77:VAL:HA	20:52:89:PRO:HA	1.90	0.54
16:B3:336:ALA:HA	16:B3:351:SER:HA	1.90	0.54
35:N:682:VAL:HA	35:N:694:ALA:HA	1.88	0.54
25:5g:64:GLY:HA2	25:5g:67:ILE:HD12	1.90	0.54
20:52:44:ILE:HG23	20:52:106:VAL:HG23	1.90	0.53
39:C:504:GLY:CA	39:C:527:VAL:O	2.56	0.53
42:5:91:U:O2'	27:51:61:ARG:NH1	2.42	0.53
25:5g:35:ASP:OD2	25:5g:39:ASN:ND2	2.42	0.53
32:J:505:ALA:O	32:J:509:LYS:N	2.39	0.52
22:5f:21:VAL:HG22	22:5f:29:TYR:HB2	1.91	0.52
22:5f:11:LEU:O	22:5f:15:THR:OG1	2.23	0.52
24:53:42:GLN:HE22	25:5g:11:LYS:HD3	1.74	0.52
20:52:32:LEU:HD22	20:52:56:VAL:HG11	1.90	0.52
11:8:56:CYS:O	11:8:60:LEU:HA	2.09	0.52
36:A:1382:SER:HA	36:A:1415:GLY:HA2	1.91	0.52
30:W:65:PHE:HA	30:W:76:GLY:HA3	1.91	0.52
26:5e:89:SER:O	26:5e:90:VAL:C	2.53	0.52
20:52:76:GLU:OE1	20:52:92:LYS:HB2	2.10	0.51
20:52:54:GLY:HA3	20:52:70:VAL:HG12	1.92	0.51
38:S:258:THR:HA	38:S:350:ARG:HA	1.92	0.51
8:E:56:GLN:H	8:E:96:TYR:CA	2.16	0.51
26:5e:86:LEU:HD12	26:5e:87:LEU:N	2.26	0.51
22:5f:6:ASN:HA	26:5e:49:GLY:HA3	1.93	0.51
26:5e:44:GLU:HB2	26:5e:62:GLU:HG2	1.93	0.51
26:5e:66:SER:HB3	26:5e:67:LYS:HZ2	1.76	0.50
37:U:350:GLN:HA	37:U:388:PHE:O	2.10	0.50
24:43:83:LEU:C	24:43:85:SER:H	2.20	0.50
39:C:830:PRO:HG2	39:C:877:ALA:HB3	1.94	0.50
20:52:75:THR:CA	20:52:91:ASN:HA	2.40	0.50
29:B:835:SER:O	29:B:839:GLY:N	2.45	0.50
25:5g:42:ILE:HD13	25:5g:62:ILE:HG13	1.94	0.50
27:51:66:ARG:HH12	20:52:47:ARG:HB2	1.76	0.49
16:B3:427:CYS:O	16:B3:433:SER:HA	2.11	0.49
23:4b:15:TYR:HA	23:4b:86:PRO:HG3	1.94	0.49
33:L:378:MET:O	36:A:1503:TRP:N	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:53:73:LEU:HD11	23:5b:71:LEU:HB2	1.93	0.49
15:2:161:U:O2	15:2:163:G:N2	2.44	0.49
46:6:64:U:H2'	46:6:65:G:C8	2.47	0.49
29:B:626:PRO:HG3	29:B:893:MET:HA	1.94	0.49
34:F:234:ILE:HA	34:F:250:CYS:HA	1.95	0.49
27:51:29:ILE:HA	27:51:40:LEU:HD23	1.92	0.49
16:B3:1101:VAL:HA	16:B3:1121:THR:HA	1.93	0.49
46:6:89:U:H2'	46:6:90:G:H8	1.78	0.49
26:5e:34:TRP:CE2	26:5e:86:LEU:HD23	2.47	0.49
26:5e:38:GLN:NE2	26:5e:40:ASN:HB2	2.28	0.49
5:68:39:ASP:HA	5:68:59:LEU:H	1.78	0.49
36:A:1777:ILE:O	36:A:1812:PRO:HD2	2.12	0.49
42:5:4:C:O2	42:5:77:G:N2	2.46	0.49
29:B:463:PRO:HA	29:B:480:THR:HA	1.94	0.49
20:52:43:LEU:HB3	20:52:110:LEU:HD23	1.95	0.49
12:9:408:CYS:O	12:9:413:ASN:HA	2.13	0.48
35:N:680:LYS:CB	35:N:934:ALA:HB1	2.43	0.48
22:5f:33:LEU:HD11	22:5f:42:MET:CB	2.42	0.48
22:5f:36:VAL:HA	22:5f:41:ASN:O	2.13	0.48
16:B3:157:PRO:HD2	17:BP:16:GLY:HA2	1.94	0.48
24:53:23:ASN:O	24:53:69:ARG:NH2	2.46	0.48
22:4f:23:LEU:HA	22:4f:69:VAL:HA	1.95	0.48
16:B3:439:ARG:O	16:B3:774:PHE:HA	2.13	0.48
34:F:464:PHE:HA	34:F:479:HIS:H	1.78	0.48
35:N:928:ASP:HA	35:N:933:VAL:HA	1.95	0.48
39:C:683:ASN:HA	39:C:795:VAL:O	2.14	0.48
27:51:68:PHE:HB2	20:52:100:PHE:HB3	1.96	0.48
15:2:3:C:H2'	15:2:4:G:H8	1.78	0.48
40:M:52:GLU:O	40:M:79:PRO:HD2	2.13	0.48
7:65:53:ASP:HA	7:65:69:LEU:HA	1.96	0.48
22:5f:71:TYR:HB3	26:5e:79:LEU:CD1	2.44	0.48
45:4:75:C:O2	46:6:38:G:N2	2.39	0.47
34:F:410:ILE:HA	34:F:426:SER:HA	1.96	0.47
45:4:108:C:H2'	45:4:109:G:H8	1.80	0.47
20:52:32:LEU:HD11	20:52:109:VAL:HG11	1.95	0.47
5:68:38:LEU:O	5:68:59:LEU:HA	2.14	0.47
22:5f:73:ARG:HH21	26:5e:74:LEU:HA	1.80	0.47
16:B3:785:PRO:HA	16:B3:801:GLU:HA	1.96	0.47
42:5:67:A:C5	42:5:68:C:H2'	2.50	0.47
42:5:109:G:O3'	27:51:49:ASN:ND2	2.48	0.47
45:4:20:A:H2'	45:4:21:U:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:52:31:VAL:HG13	20:52:111:ARG:HE	1.79	0.47
46:6:44:G:O2'	46:6:46:G:OP1	2.27	0.47
22:5f:42:MET:HB2	22:5f:64:ILE:HD11	1.96	0.47
10:Z:42:U:H3	15:2:33:G:H1	1.62	0.47
15:2:32:U:H2'	15:2:33:G:H8	1.79	0.47
33:L:369:THR:O	33:L:373:LYS:N	2.47	0.47
20:52:53:LEU:HD23	20:52:73:MET:HE2	1.96	0.47
20:52:77:VAL:HA	20:52:88:LYS:C	2.40	0.47
34:F:276:VAL:HA	34:F:300:ALA:HA	1.96	0.47
30:W:96:ALA:HA	30:W:118:SER:HA	1.97	0.47
22:5f:37:ASP:OD1	22:5f:41:ASN:N	2.34	0.47
23:4b:17:MET:HA	23:4b:82:VAL:HA	1.96	0.47
34:F:477:TRP:HA	34:F:483:SER:C	2.39	0.47
36:A:2070:LYS:C	36:A:2072:GLU:N	2.72	0.47
39:C:769:GLY:HA3	39:C:812:ALA:HB3	1.97	0.47
20:52:29:LEU:HB3	20:52:59:PHE:CE2	2.50	0.47
25:5g:6:PRO:HA	25:5g:36:PRO:HA	1.96	0.46
8:E:295:PRO:HG2	8:E:337:PRO:HA	1.96	0.46
10:Z:32:G:N2	15:2:43:U:O2	2.48	0.46
42:5:89:U:O2'	24:53:64:ARG:NH2	2.48	0.46
30:W:19:ILE:HA	30:W:169:VAL:HA	1.96	0.46
24:53:16:HIS:HB3	24:53:74:PRO:HG2	1.98	0.46
11:8:147:PRO:HB3	11:8:173:ALA:HB2	1.98	0.46
15:2:166:G:N2	15:2:166:G:OP2	2.48	0.46
36:A:1821:ILE:O	36:A:1912:PRO:HA	2.16	0.46
36:A:2070:LYS:C	36:A:2072:GLU:H	2.23	0.46
22:5f:71:TYR:HB3	26:5e:79:LEU:HD12	1.97	0.46
20:52:77:VAL:HA	20:52:89:PRO:CA	2.45	0.46
22:5f:5:LEU:HB3	26:5e:48:ILE:HG21	1.96	0.46
27:51:19:LEU:HD21	27:51:60:ILE:HD13	1.98	0.46
35:N:411:VAL:C	35:N:413:LEU:N	2.73	0.46
22:5f:5:LEU:HB3	26:5e:48:ILE:CG2	2.46	0.46
22:5f:61:GLU:OE2	20:52:111:ARG:NE	2.48	0.46
15:2:63:G:H3'	15:2:64:A:H8	1.81	0.45
17:BP:42:LEU:HA	17:BP:70:TYR:HA	1.99	0.45
42:5:19:A:H4'	42:5:20:G:C8	2.52	0.45
42:5:75:G:H2'	42:5:76:A:C8	2.52	0.45
27:51:5:ARG:HD3	27:51:8:MET:HE2	1.99	0.45
20:52:62:HIS:O	20:52:103:GLY:HA3	2.17	0.45
24:53:64:ARG:NE	24:53:66:SER:OG	2.49	0.45
26:5e:65:HIS:HB2	26:5e:69:LYS:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:1198:PRO:HA	36:A:1226:ALA:HA	1.98	0.45
43:z:4:A:H61	46:6:43:A:H2	1.62	0.45
20:52:77:VAL:HA	20:52:89:PRO:N	2.32	0.45
42:5:88:A:N6	22:5f:38:GLY:O	2.50	0.45
34:F:483:SER:C	34:F:485:LEU:H	2.25	0.44
42:5:111:A:H2'	42:5:112:A:C8	2.53	0.44
20:52:65:MET:HE3	20:52:101:LEU:HD23	1.99	0.44
42:5:87:A:P	20:52:61:ARG:HE	2.39	0.44
27:51:67:TYR:HB3	20:52:101:LEU:HD12	1.98	0.44
24:43:78:LYS:O	24:43:81:PRO:HG3	2.16	0.44
35:N:676:ARG:O	35:N:680:LYS:N	2.50	0.44
23:5b:9:MET:HE3	23:5b:9:MET:HB2	1.90	0.44
25:5g:61:VAL:O	26:5e:86:LEU:HD12	2.17	0.44
45:4:111:C:H2'	45:4:112:A:C8	2.53	0.44
29:B:912:ASN:HA	29:B:978:ASN:HA	1.99	0.44
6:64:46:THR:HA	6:64:52:LYS:HA	2.00	0.44
15:2:180:G:H2'	15:2:181:G:H8	1.83	0.44
32:J:519:LYS:HA	46:6:66:C:O3'	2.18	0.44
34:F:373:PHE:HA	34:F:380:ALA:HA	1.99	0.44
22:5f:72:ILE:O	26:5e:77:ILE:HA	2.18	0.44
20:52:33:THR:HG23	20:52:59:PHE:CE1	2.52	0.44
20:52:48:ASN:O	20:52:49:ASN:C	2.60	0.44
19:B6:73:ALA:O	19:B6:77:LEU:CB	2.66	0.44
25:4g:46:VAL:HA	25:4g:56:ASN:HA	1.99	0.44
23:5b:65:ARG:HE	23:5b:67:LEU:HD21	1.83	0.44
45:4:108:C:H2'	45:4:109:G:C8	2.53	0.44
20:52:88:LYS:HA	20:52:88:LYS:HE2	1.99	0.44
18:B1:720:GLY:H	18:B1:756:LEU:CB	2.31	0.43
45:4:111:C:H2'	45:4:112:A:H8	1.82	0.43
20:52:18:LYS:HD3	20:52:18:LYS:HA	1.85	0.43
30:W:16:ASP:HA	30:W:26:ARG:HA	2.00	0.43
37:U:351:GLY:HA3	37:U:447:PRO:HD3	1.99	0.43
26:5e:30:ARG:HD2	26:5e:30:ARG:HA	1.77	0.43
34:F:478:THR:O	34:F:482:TRP:N	2.45	0.43
39:C:504:GLY:HA2	39:C:527:VAL:O	2.19	0.43
42:5:7:U:O2	42:5:75:G:N1	2.51	0.43
42:5:47:A:O2'	42:5:48:A:H5''	2.18	0.43
45:4:91:A:H2	45:4:110:G:H22	1.66	0.43
25:5g:13:MET:HE3	25:5g:13:MET:HB3	1.90	0.43
13:B2:482:ALA:HB2	18:B1:1257:PRO:HG3	2.01	0.43
22:5f:73:ARG:CB	26:5e:77:ILE:HG22	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:1404:THR:C	36:A:1406:GLU:H	2.25	0.43
22:5f:33:LEU:HD12	22:5f:44:LEU:HB3	2.00	0.43
20:52:74:TRP:HZ3	20:52:94:ARG:N	2.17	0.43
24:53:23:ASN:N	24:53:67:LYS:O	2.52	0.43
22:5f:20:MET:HA	22:5f:29:TYR:O	2.19	0.43
25:5g:14:ASP:OD1	25:5g:32:ARG:NH2	2.52	0.43
35:N:411:VAL:C	35:N:413:LEU:H	2.27	0.43
36:A:1706:ASP:O	36:A:1710:ASN:N	2.52	0.43
42:5:68:C:H1'	42:5:69:A:H2'	2.00	0.43
27:51:51:GLU:OE1	27:51:51:GLU:N	2.51	0.43
20:52:74:TRP:O	20:52:74:TRP:CG	2.71	0.43
20:52:77:VAL:O	20:52:87:SER:HB2	2.18	0.43
4:63:29:ILE:HA	4:63:98:PRO:HD3	2.00	0.43
35:N:717:GLN:CB	35:N:924:LYS:CB	2.97	0.43
36:A:1785:VAL:O	36:A:1805:GLY:HA3	2.18	0.43
45:4:92:C:H2'	45:4:93:G:H8	1.83	0.43
22:5f:5:LEU:O	26:5e:49:GLY:HA3	2.18	0.42
25:5g:46:VAL:HA	25:5g:56:ASN:HA	2.01	0.42
26:4e:58:LEU:O	26:4e:76:ARG:HA	2.19	0.42
36:A:425:PRO:HD3	42:5:26:A:H4'	2.00	0.42
42:5:92:U:OP1	27:51:63:ASN:ND2	2.52	0.42
24:53:19:THR:HB	24:53:29:ARG:HG3	2.01	0.42
24:53:30:GLY:HA3	24:53:46:ILE:HD13	2.00	0.42
19:B6:23:ILE:O	19:B6:59:THR:HA	2.19	0.42
15:2:37:U:H2'	15:2:38:A:C8	2.55	0.42
15:2:151:C:H2'	15:2:152:G:H8	1.85	0.42
39:C:836:VAL:O	39:C:870:THR:HA	2.20	0.42
7:65:48:ASN:HA	7:65:74:LEU:O	2.20	0.42
35:N:671:SER:O	35:N:672:ALA:C	2.63	0.42
5:68:35:ASN:HA	5:68:62:VAL:O	2.19	0.42
36:A:227:ARG:HA	36:A:416:GLY:O	2.19	0.42
22:5f:39:TYR:HB3	22:5f:66:CYS:SG	2.59	0.42
22:5f:63:LEU:HD21	20:52:29:LEU:HD23	2.01	0.42
20:52:74:TRP:CZ3	20:52:93:ASP:C	2.97	0.42
23:2b:19:CYS:HA	23:2b:80:MET:HA	2.02	0.42
42:5:61:A:H2'	42:5:62:G:C8	2.54	0.42
22:5f:73:ARG:HH21	26:5e:74:LEU:HG	1.85	0.42
8:E:53:SER:HA	8:E:339:GLU:CB	2.50	0.41
39:C:478:THR:HA	39:C:494:GLY:HA3	2.01	0.41
42:5:70:A:H4'	42:5:71:C:OP1	2.21	0.41
22:5f:41:ASN:ND2	22:5f:66:CYS:SG	2.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B6:27:PRO:HG3	19:B6:84:ASN:N	2.23	0.41
27:51:61:ARG:HG3	23:5b:38:MET:HG2	2.02	0.41
25:5g:59:MET:HE2	25:5g:59:MET:HB2	1.88	0.41
8:E:191:GLN:O	42:5:7:U:OP1	2.38	0.41
25:2g:6:PRO:HA	25:2g:7:PRO:HD3	1.97	0.41
26:4e:35:LEU:HA	26:4e:84:ILE:HA	2.00	0.41
42:5:93:U:H4'	42:5:94:U:H5''	2.00	0.41
27:51:13:GLU:HG2	27:51:74:LEU:HD11	2.02	0.41
15:2:64:A:C2	15:2:65:U:H1'	2.56	0.41
16:B3:84:SER:HA	16:B3:110:SER:HA	2.02	0.41
42:5:74:U:H2'	42:5:75:G:C8	2.56	0.41
22:5f:70:LEU:O	26:5e:79:LEU:HD12	2.20	0.41
22:5f:7:PRO:HG2	26:5e:55:ASN:O	2.20	0.41
34:F:244:LYS:O	34:F:261:PRO:HD2	2.20	0.41
24:53:28:TYR:OH	25:5g:69:MET:SD	2.59	0.41
23:5b:32:LYS:HB2	23:5b:41:ILE:HG22	2.02	0.41
20:52:59:PHE:HA	20:52:64:ASN:O	2.21	0.41
26:5e:36:TYR:O	26:5e:37:GLU:HB3	2.21	0.41
35:N:178:LYS:N	45:4:19:U:O4	2.52	0.41
24:53:8:LYS:HB3	24:53:82:MET:HE2	2.03	0.41
22:5f:29:TYR:HD2	22:5f:47:THR:HG21	1.84	0.41
27:51:16:THR:HA	27:51:25:VAL:O	2.20	0.41
20:52:47:ARG:C	20:52:49:ASN:H	2.28	0.41
14:B5:79:PRO:HD2	16:B3:196:PRO:HA	2.02	0.41
16:B3:515:ALA:HA	16:B3:528:ARG:HA	2.03	0.41
26:5e:32:GLN:O	26:5e:88:GLN:N	2.47	0.41
15:2:175:G:H2'	15:2:176:G:H8	1.86	0.40
42:5:47:A:O2'	42:5:48:A:H8	2.03	0.40
42:5:69:A:C2	42:5:70:A:C8	3.09	0.40
22:5f:70:LEU:HD21	26:5e:41:MET:HE1	2.03	0.40
23:5b:35:ASP:N	23:5b:35:ASP:OD1	2.54	0.40
25:5g:18:SER:HB2	25:5g:26:HIS:CE1	2.56	0.40
16:B3:405:SER:N	16:B3:406:PRO:CD	2.84	0.40
32:J:522:ALA:O	32:J:523:GLU:C	2.63	0.40
35:N:411:VAL:O	35:N:414:GLU:N	2.53	0.40
36:A:472:LEU:C	36:A:474:ARG:H	2.28	0.40
36:A:1792:LYS:HA	36:A:1798:LEU:HA	2.02	0.40
45:4:6:U:H2'	45:4:7:G:C8	2.56	0.40
24:53:21:GLU:OE1	23:5b:25:ARG:NH2	2.55	0.40
24:53:36:GLU:OE2	24:53:62:TYR:OH	2.39	0.40
20:52:51:LYS:O	20:52:72:GLU:HA	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:182:U:H2'	15:2:183:G:C8	2.56	0.40
30:W:12:VAL:HA	30:W:30:GLU:HA	2.03	0.40
23:5b:18:ARG:NE	23:5b:83:GLU:OE2	2.38	0.40
4:63:97:PRO:HA	4:63:98:PRO:HD3	1.91	0.40
11:8:56:CYS:O	11:8:60:LEU:CA	2.68	0.40
15:2:34:U:H2'	15:2:35:A:H8	1.86	0.40
23:4b:85:PRO:HA	23:4b:86:PRO:HD3	1.96	0.40
29:B:1349:GLY:N	29:B:1512:PHE:O	2.53	0.40
20:52:74:TRP:CZ2	20:52:92:LYS:HE3	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	66	70/80 (88%)	70 (100%)	0	0	100	100
2	67	75/103 (73%)	75 (100%)	0	0	100	100
3	62	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
4	63	83/102 (81%)	81 (98%)	2 (2%)	0	100	100
5	68	93/96 (97%)	93 (100%)	0	0	100	100
6	64	71/139 (51%)	70 (99%)	1 (1%)	0	100	100
7	65	74/91 (81%)	72 (97%)	2 (3%)	0	100	100
8	E	305/357 (85%)	300 (98%)	5 (2%)	0	100	100
9	B4	76/424 (18%)	76 (100%)	0	0	100	100
11	8	138/464 (30%)	136 (99%)	2 (1%)	0	100	100
12	9	377/501 (75%)	372 (99%)	5 (1%)	0	100	100
13	B2	204/895 (23%)	198 (97%)	6 (3%)	0	100	100
14	B5	67/86 (78%)	66 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	B3	1176/1217 (97%)	1131 (96%)	45 (4%)	0	100	100
17	BP	98/110 (89%)	96 (98%)	2 (2%)	0	100	100
18	B1	866/1304 (66%)	845 (98%)	21 (2%)	0	100	100
19	B6	88/125 (70%)	87 (99%)	1 (1%)	0	100	100
20	22	91/118 (77%)	90 (99%)	1 (1%)	0	100	100
20	42	90/118 (76%)	88 (98%)	2 (2%)	0	100	100
20	52	94/118 (80%)	85 (90%)	9 (10%)	0	100	100
21	2B	90/225 (40%)	89 (99%)	1 (1%)	0	100	100
22	2f	70/86 (81%)	68 (97%)	2 (3%)	0	100	100
22	4f	70/86 (81%)	67 (96%)	3 (4%)	0	100	100
22	5f	71/86 (83%)	63 (89%)	8 (11%)	0	100	100
23	2b	80/240 (33%)	80 (100%)	0	0	100	100
23	4b	77/240 (32%)	76 (99%)	1 (1%)	0	100	100
23	5b	69/240 (29%)	67 (97%)	2 (3%)	0	100	100
24	23	81/126 (64%)	80 (99%)	1 (1%)	0	100	100
24	43	81/126 (64%)	80 (99%)	1 (1%)	0	100	100
24	53	82/126 (65%)	77 (94%)	5 (6%)	0	100	100
25	2g	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
25	4g	72/76 (95%)	71 (99%)	1 (1%)	0	100	100
25	5g	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
26	2e	79/92 (86%)	79 (100%)	0	0	100	100
26	4e	74/92 (80%)	74 (100%)	0	0	100	100
26	5e	75/92 (82%)	71 (95%)	4 (5%)	0	100	100
27	21	78/119 (66%)	76 (97%)	2 (3%)	0	100	100
27	41	79/119 (66%)	77 (98%)	2 (2%)	0	100	100
27	51	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
28	2A	160/255 (63%)	157 (98%)	3 (2%)	0	100	100
29	B	1710/2136 (80%)	1683 (98%)	27 (2%)	0	100	100
30	W	167/177 (94%)	164 (98%)	3 (2%)	0	100	100
31	G	378/820 (46%)	373 (99%)	4 (1%)	1 (0%)	36	71
32	J	220/683 (32%)	217 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	L	372/499 (74%)	362 (97%)	10 (3%)	0	100	100
34	F	408/522 (78%)	399 (98%)	7 (2%)	2 (0%)	24	62
35	N	826/941 (88%)	797 (96%)	29 (4%)	0	100	100
36	A	2212/2335 (95%)	2120 (96%)	92 (4%)	0	100	100
37	U	454/565 (80%)	437 (96%)	17 (4%)	0	100	100
38	S	144/800 (18%)	141 (98%)	3 (2%)	0	100	100
39	C	834/972 (86%)	815 (98%)	19 (2%)	0	100	100
40	M	122/128 (95%)	120 (98%)	2 (2%)	0	100	100
41	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
44	7	224/793 (28%)	221 (99%)	3 (1%)	0	100	100
All	All	14049/20753 (68%)	13670 (97%)	376 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	G	521	ILE
34	F	480	PRO
34	F	485	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	66	2/70 (3%)	2 (100%)	0	100	100
2	67	3/91 (3%)	3 (100%)	0	100	100
3	62	3/88 (3%)	3 (100%)	0	100	100
4	63	4/94 (4%)	4 (100%)	0	100	100
5	68	1/82 (1%)	1 (100%)	0	100	100
6	64	4/111 (4%)	4 (100%)	0	100	100
7	65	3/80 (4%)	3 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	10/300 (3%)	10 (100%)	0	100	100
9	B4	4/336 (1%)	4 (100%)	0	100	100
11	8	8/382 (2%)	8 (100%)	0	100	100
12	9	11/446 (2%)	11 (100%)	0	100	100
13	B2	22/776 (3%)	22 (100%)	0	100	100
14	B5	3/77 (4%)	3 (100%)	0	100	100
16	B3	60/1051 (6%)	60 (100%)	0	100	100
17	BP	4/95 (4%)	4 (100%)	0	100	100
18	B1	40/1104 (4%)	40 (100%)	0	100	100
19	B6	5/109 (5%)	5 (100%)	0	100	100
20	22	5/110 (4%)	5 (100%)	0	100	100
20	42	4/110 (4%)	4 (100%)	0	100	100
20	52	93/110 (84%)	92 (99%)	1 (1%)	65	74
21	2B	3/195 (2%)	3 (100%)	0	100	100
22	2f	4/74 (5%)	4 (100%)	0	100	100
22	4f	4/74 (5%)	4 (100%)	0	100	100
22	5f	61/74 (82%)	60 (98%)	1 (2%)	55	69
23	2b	4/177 (2%)	4 (100%)	0	100	100
23	4b	3/177 (2%)	3 (100%)	0	100	100
23	5b	67/177 (38%)	67 (100%)	0	100	100
24	23	3/101 (3%)	3 (100%)	0	100	100
24	43	3/101 (3%)	3 (100%)	0	100	100
24	53	73/101 (72%)	73 (100%)	0	100	100
25	2g	3/66 (4%)	3 (100%)	0	100	100
25	4g	3/66 (4%)	3 (100%)	0	100	100
25	5g	64/66 (97%)	43 (67%)	21 (33%)	0	2
26	2e	1/84 (1%)	1 (100%)	0	100	100
26	4e	1/84 (1%)	1 (100%)	0	100	100
26	5e	72/84 (86%)	71 (99%)	1 (1%)	59	71
27	21	3/101 (3%)	3 (100%)	0	100	100
27	41	3/101 (3%)	3 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	51	76/101 (75%)	53 (70%)	23 (30%)	0	2
28	2A	6/218 (3%)	6 (100%)	0	100	100
29	B	78/1908 (4%)	78 (100%)	0	100	100
30	W	10/148 (7%)	10 (100%)	0	100	100
31	G	21/721 (3%)	21 (100%)	0	100	100
32	J	8/599 (1%)	8 (100%)	0	100	100
33	L	14/424 (3%)	14 (100%)	0	100	100
34	F	16/442 (4%)	16 (100%)	0	100	100
35	N	36/792 (4%)	36 (100%)	0	100	100
36	A	107/2108 (5%)	107 (100%)	0	100	100
37	U	23/511 (4%)	23 (100%)	0	100	100
38	S	7/681 (1%)	7 (100%)	0	100	100
39	C	48/866 (6%)	48 (100%)	0	100	100
40	M	6/111 (5%)	6 (100%)	0	100	100
41	D	5/130 (4%)	5 (100%)	0	100	100
44	7	9/709 (1%)	9 (100%)	0	100	100
All	All	1134/17994 (6%)	1087 (96%)	47 (4%)	28	49

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	5f	11	LEU
27	51	2	LYS
27	51	4	VAL
27	51	8	MET
27	51	10	LEU
27	51	11	SER
27	51	15	VAL
27	51	16	THR
27	51	28	THR
27	51	33	ASP
27	51	35	SER
27	51	44	LYS
27	51	47	LEU
27	51	48	LYS
27	51	51	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	51	53	VAL
27	51	54	GLN
27	51	55	LEU
27	51	56	GLU
27	51	57	THR
27	51	58	LEU
27	51	74	LEU
27	51	76	LEU
27	51	81	VAL
20	52	33	THR
25	5g	3	LYS
25	5g	10	LYS
25	5g	11	LYS
25	5g	15	LYS
25	5g	27	VAL
25	5g	35	ASP
25	5g	43	ASP
25	5g	44	GLU
25	5g	46	VAL
25	5g	47	GLU
25	5g	50	THR
25	5g	51	SER
25	5g	53	GLN
25	5g	59	MET
25	5g	61	VAL
25	5g	62	ILE
25	5g	66	SER
25	5g	70	LEU
25	5g	71	GLU
25	5g	73	LEU
25	5g	74	GLU
26	5e	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
24	53	42	GLN
24	53	57	GLN
24	53	79	ASN
22	5f	6	ASN
22	5f	12	ASN
22	5f	46	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	51	12	HIS
27	51	64	ASN
23	5b	22	GLN
20	52	34	GLN
20	52	38	ASN
20	52	41	GLN
25	5g	26	HIS
25	5g	28	GLN
25	5g	55	ASN
26	5e	26	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	Z	14/347 (4%)	1 (7%)	0
15	2	94/188 (50%)	21 (22%)	4 (4%)
42	5	110/117 (94%)	41 (37%)	5 (4%)
43	z	10/11 (90%)	6 (60%)	0
45	4	124/144 (86%)	30 (24%)	1 (0%)
46	6	62/106 (58%)	9 (14%)	2 (3%)
All	All	414/913 (45%)	108 (26%)	12 (2%)

All (108) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	Z	41	A
15	2	30	A
15	2	38	A
15	2	40	C
15	2	42	G
15	2	47	U
15	2	48	A
15	2	49	U
15	2	63	G
15	2	64	A
15	2	100	U
15	2	101	U
15	2	102	U
15	2	103	U
15	2	104	U
15	2	105	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	2	106	G
15	2	107	A
15	2	157	G
15	2	164	C
15	2	169	C
15	2	178	A
42	5	8	G
42	5	9	G
42	5	10	U
42	5	20	G
42	5	21	A
42	5	22	U
42	5	23	C
42	5	24	G
42	5	26	A
42	5	28	A
42	5	34	U
42	5	36	C
42	5	39	C
42	5	41	U
42	5	42	U
42	5	43	U
42	5	44	A
42	5	45	C
42	5	57	G
42	5	68	C
42	5	69	A
42	5	70	A
42	5	71	C
42	5	78	U
42	5	79	C
42	5	80	U
42	5	86	C
42	5	88	A
42	5	89	U
42	5	90	U
42	5	94	U
42	5	95	G
42	5	97	G
42	5	98	G
42	5	102	U
42	5	104	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	5	105	U
42	5	106	U
42	5	107	U
42	5	108	G
42	5	109	G
43	z	-2	A
43	z	1	G
43	z	3	A
43	z	4	A
43	z	6	U
43	z	8	U
45	4	9	G
45	4	11	A
45	4	18	G
45	4	25	A
45	4	26	G
45	4	31	U
45	4	36	U
45	4	39	A
45	4	40	U
45	4	41	C
45	4	44	A
45	4	45	G
45	4	53	U
45	4	55	U
45	4	58	C
45	4	66	A
45	4	68	A
45	4	69	C
45	4	70	U
45	4	71	U
45	4	72	U
45	4	73	U
45	4	74	C
45	4	114	U
45	4	115	G
45	4	121	U
45	4	122	U
45	4	123	U
45	4	125	G
45	4	126	A
46	6	35	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	6	37	C
46	6	40	U
46	6	46	G
46	6	50	A
46	6	52	U
46	6	77	C
46	6	78	A
46	6	106	U

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	2	37	U
15	2	46	U
15	2	103	U
15	2	106	G
42	5	70	A
42	5	77	G
42	5	78	U
42	5	96	A
42	5	105	U
45	4	114	U
46	6	51	U
46	6	77	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

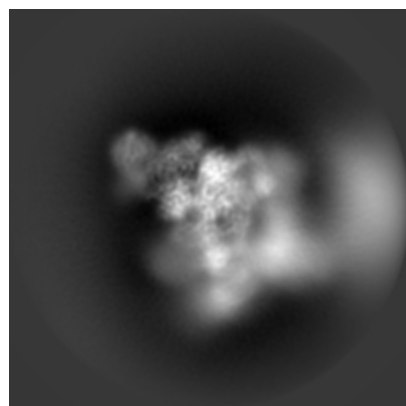
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18787. These allow visual inspection of the internal detail of the map and identification of artifacts.

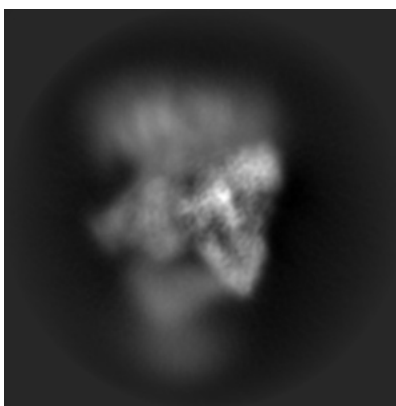
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

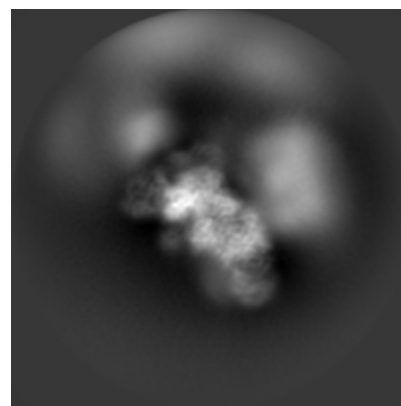
6.1.1 Primary map



X

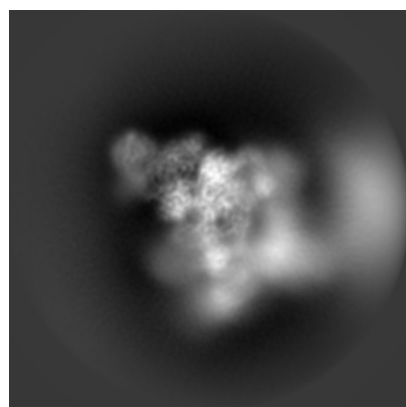


Y

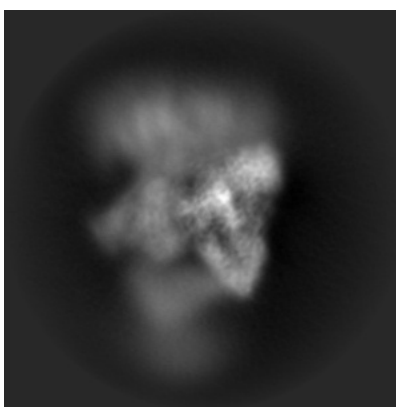


Z

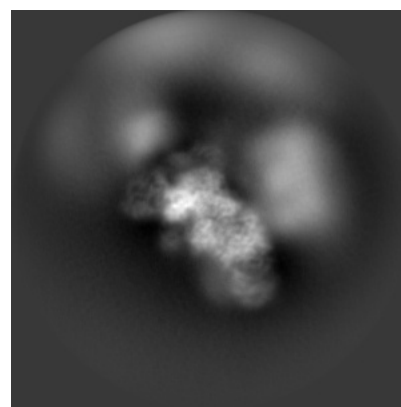
6.1.2 Raw map



X



Y

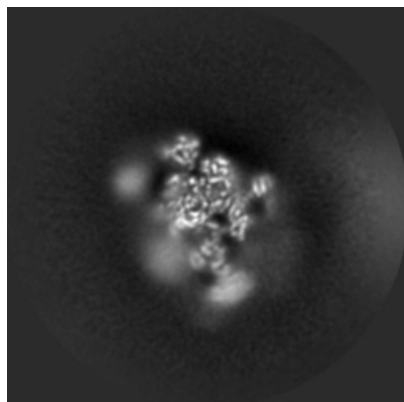


Z

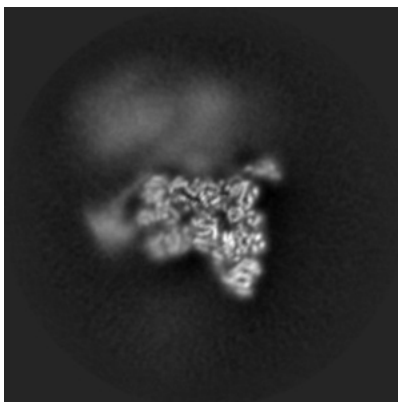
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

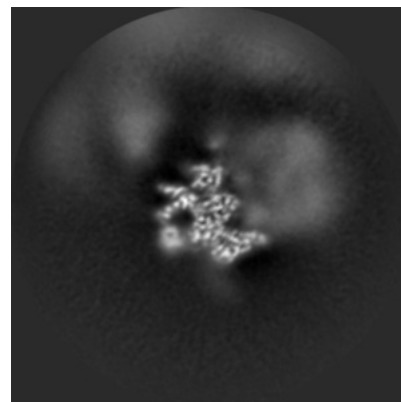
6.2.1 Primary map



X Index: 240

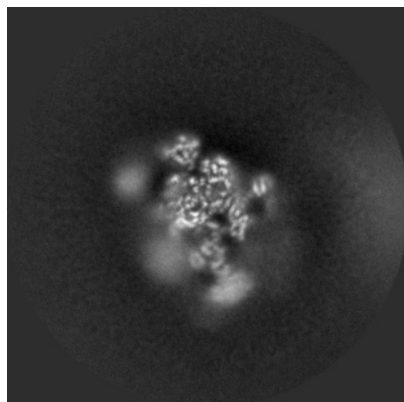


Y Index: 240

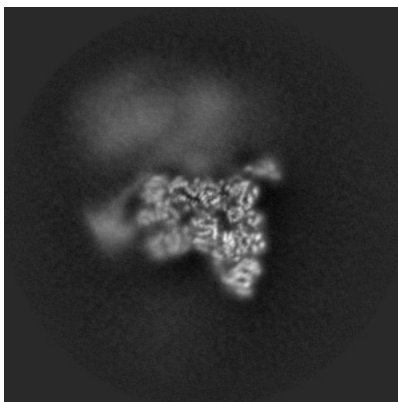


Z Index: 240

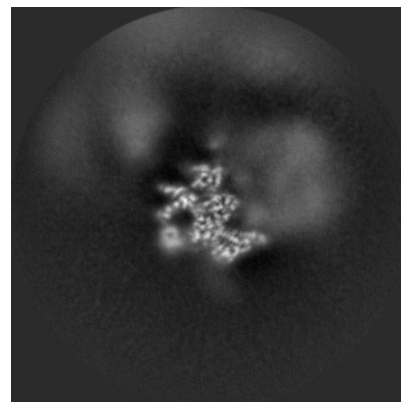
6.2.2 Raw map



X Index: 240



Y Index: 240

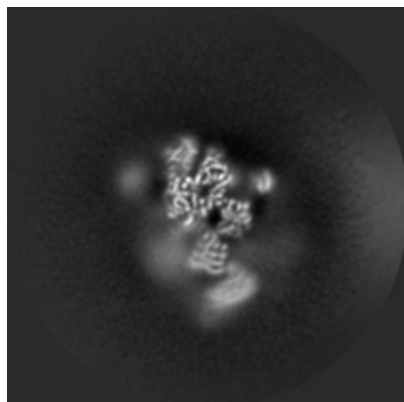


Z Index: 240

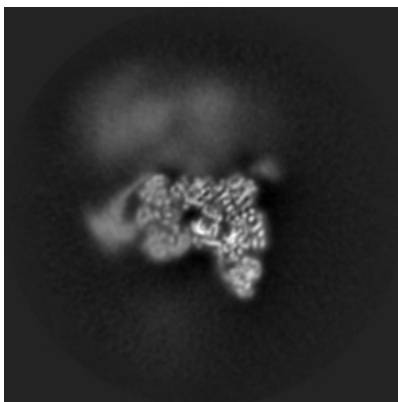
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

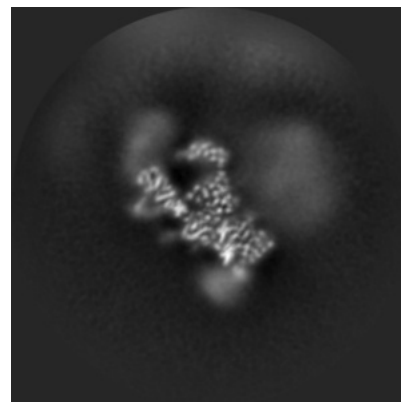
6.3.1 Primary map



X Index: 232

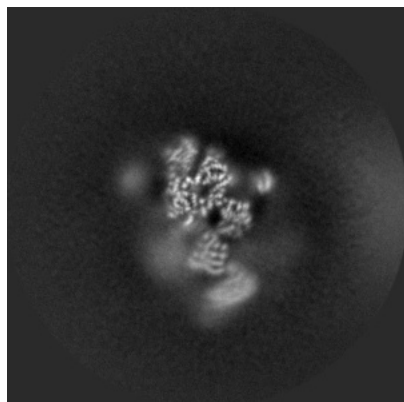


Y Index: 245

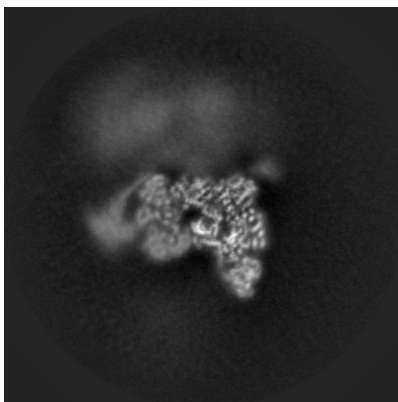


Z Index: 266

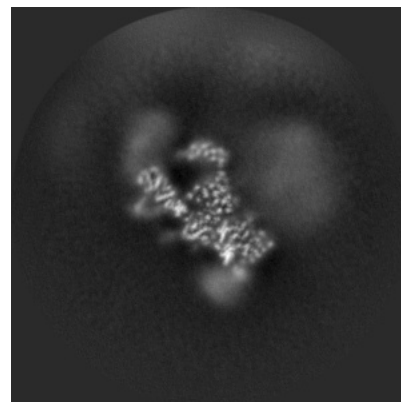
6.3.2 Raw map



X Index: 232



Y Index: 245

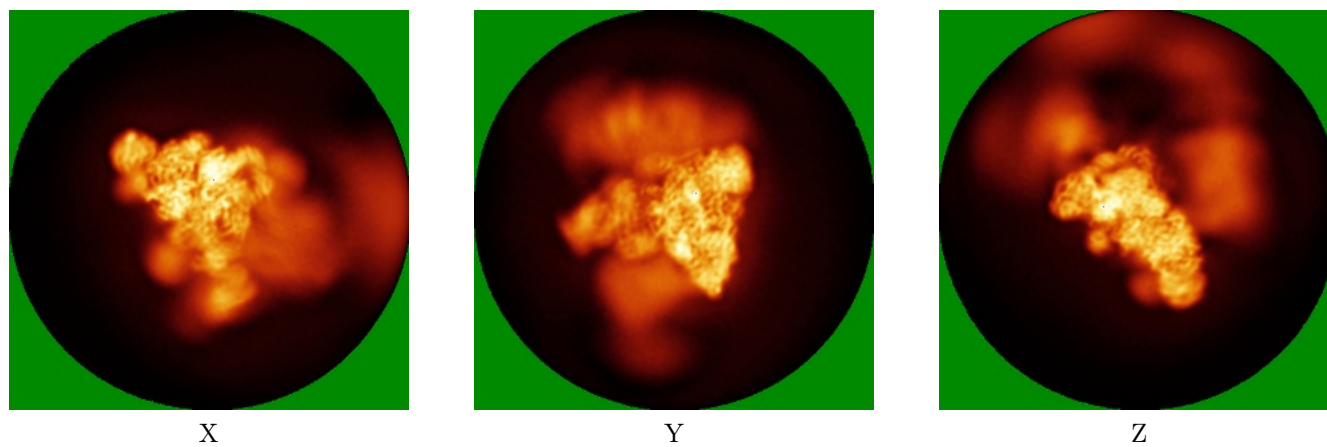


Z Index: 266

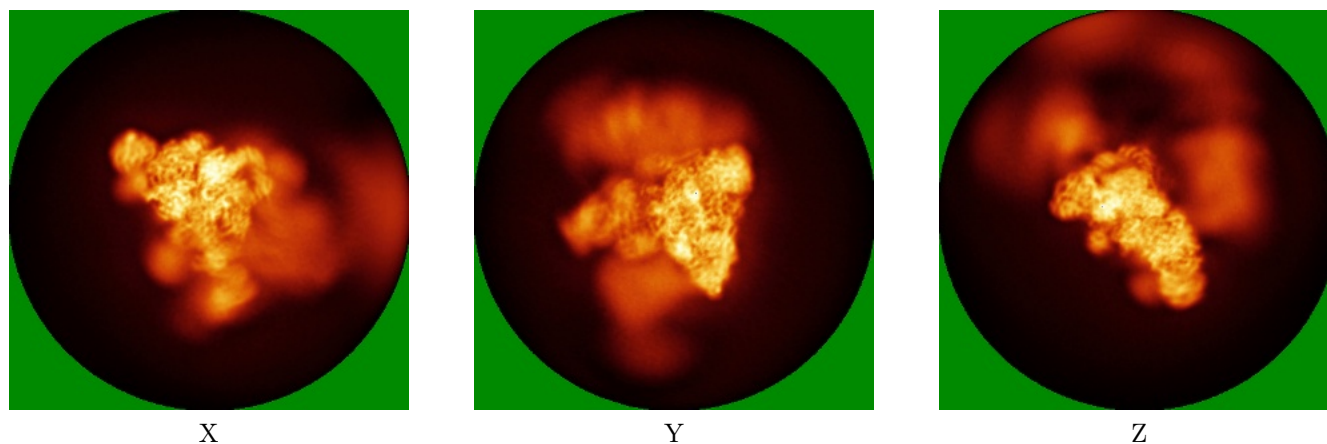
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

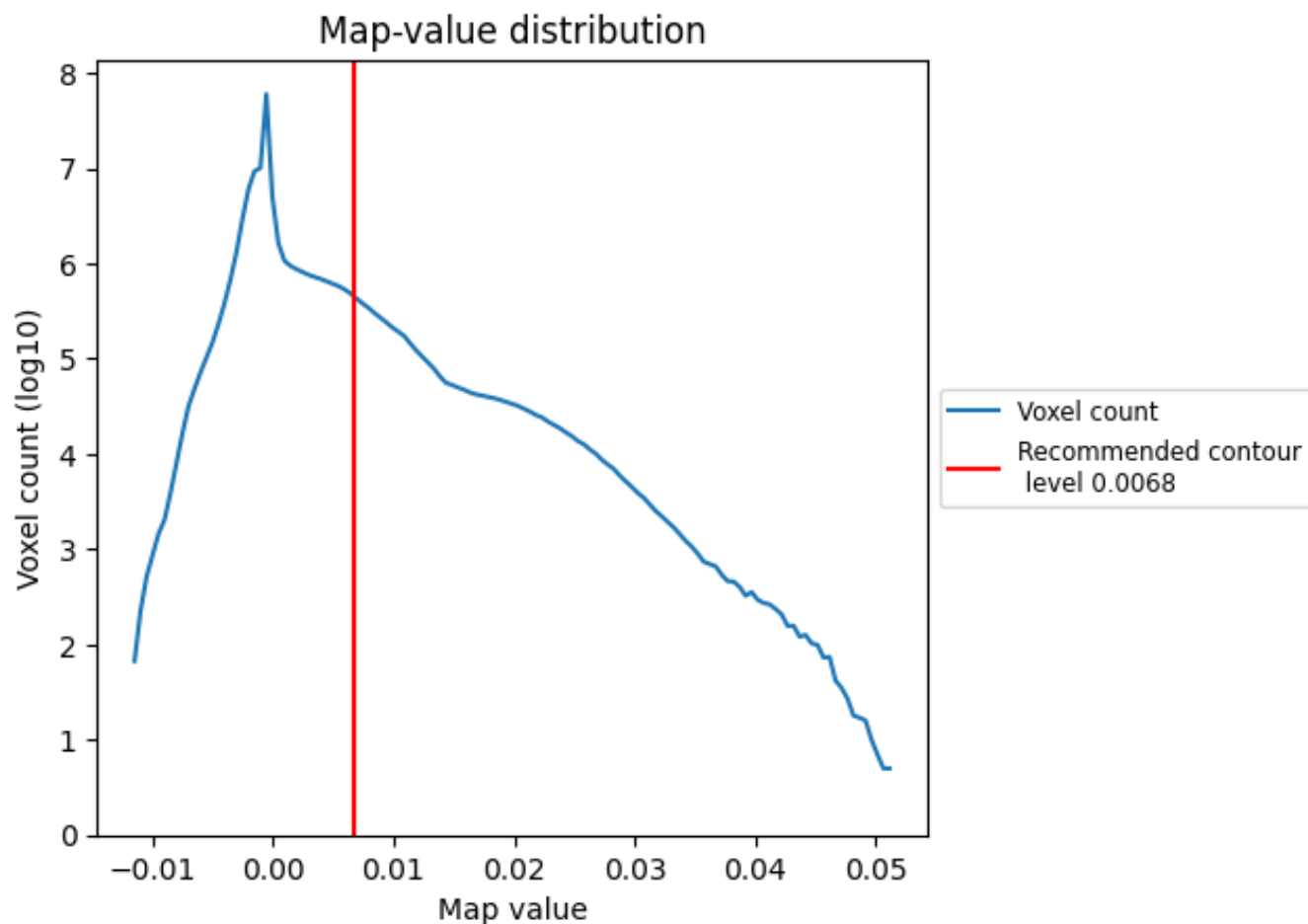
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

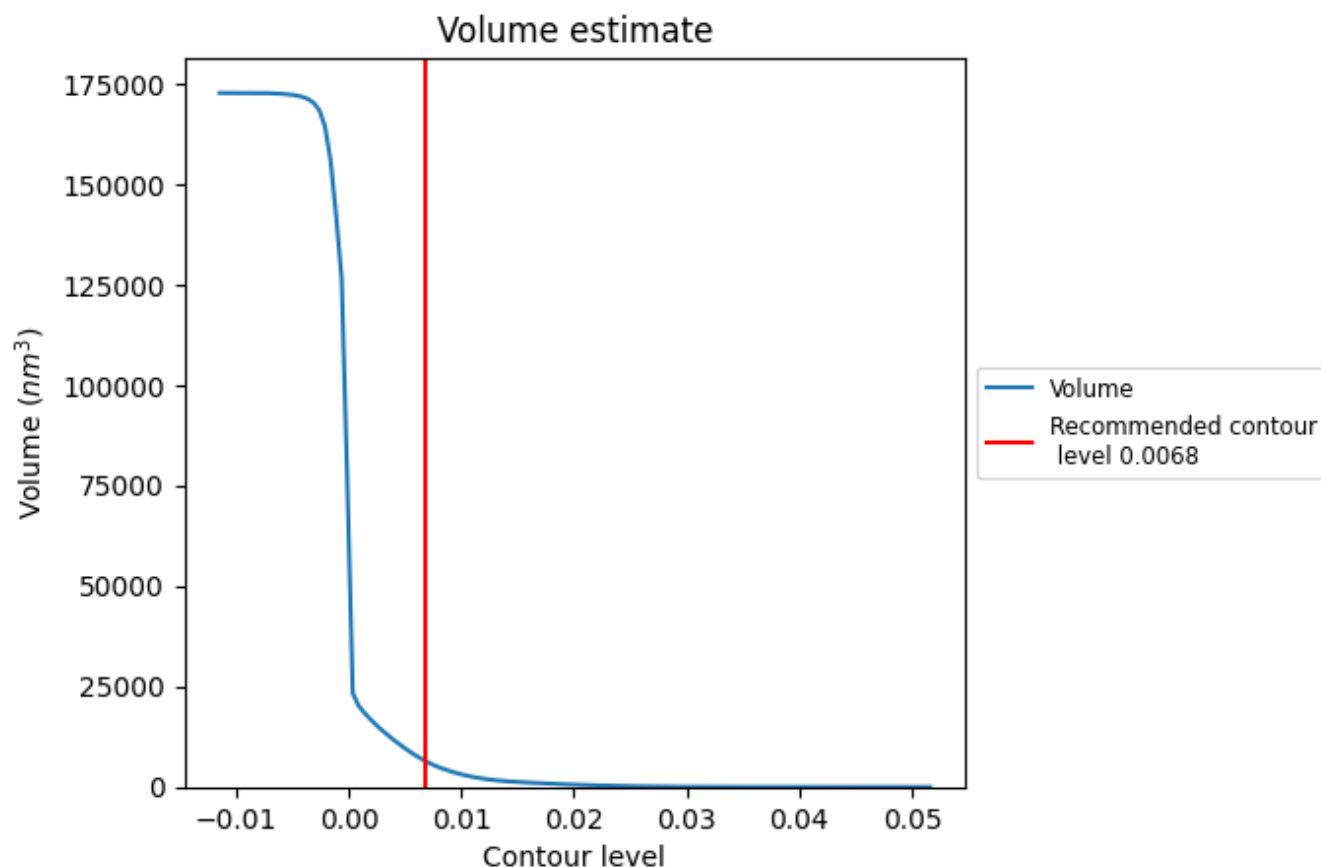
This section contains the results of statistical analysis of the map.

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.

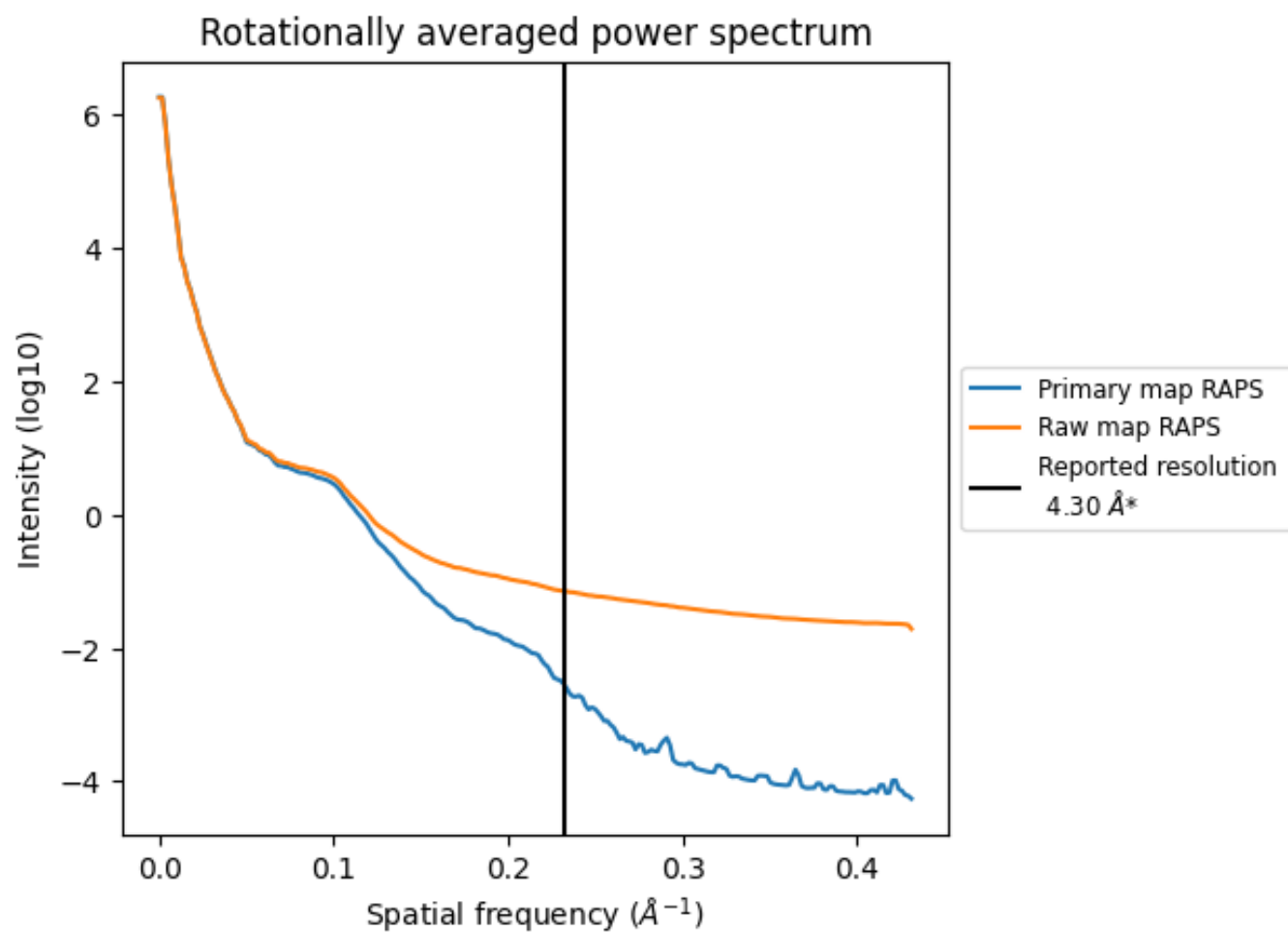
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6461 nm^3 ; this corresponds to an approximate mass of 5837 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

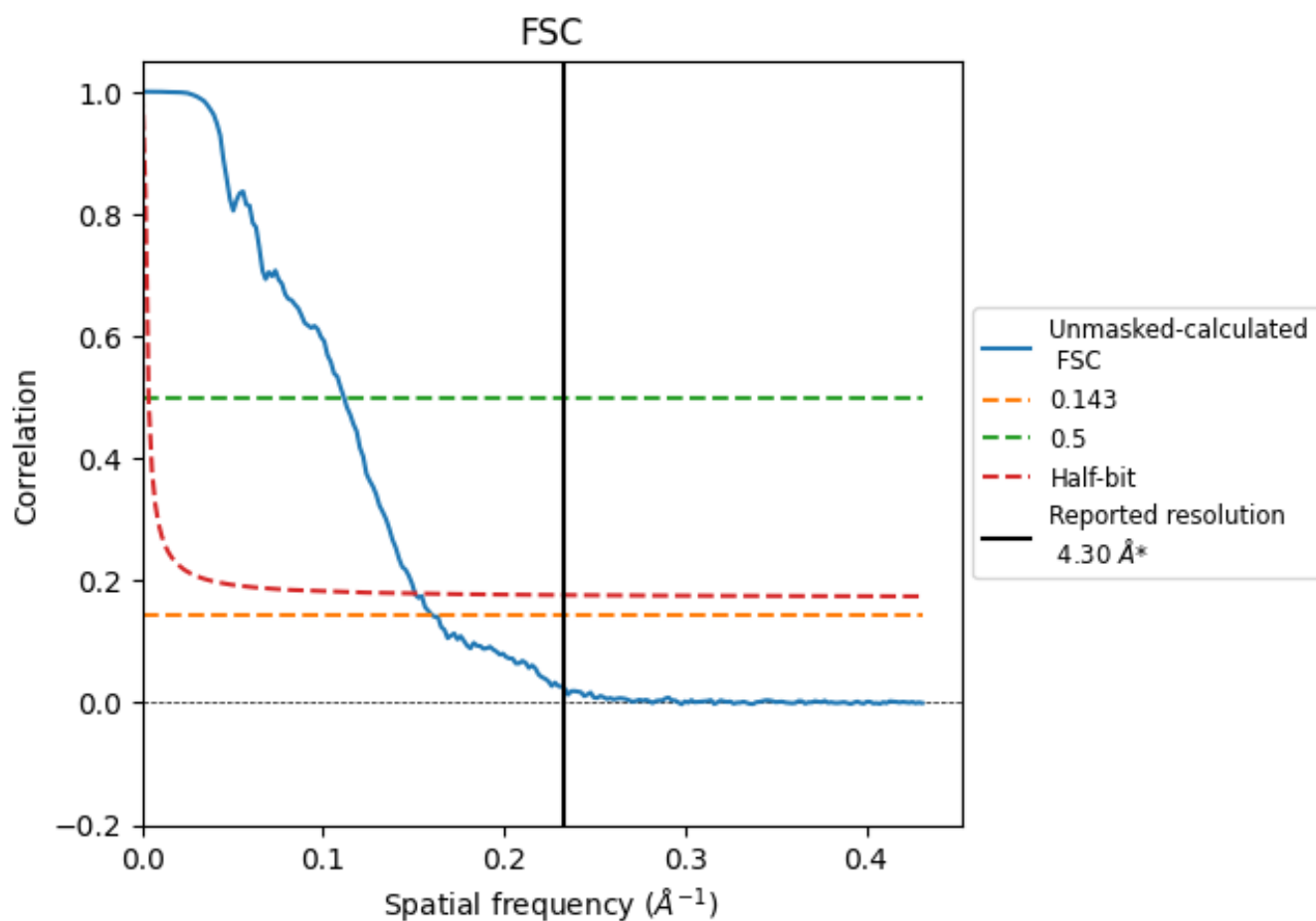


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.23	8.98	6.64

*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 6.23 differs from the reported value 4.3 by more than 10 %

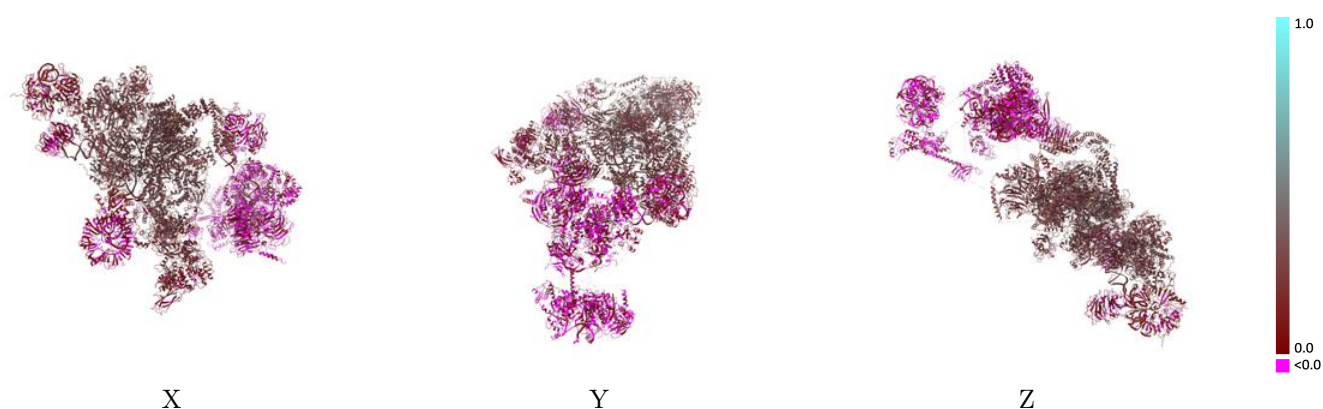
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18787 and PDB model 8R09. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

This section was not generated.

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

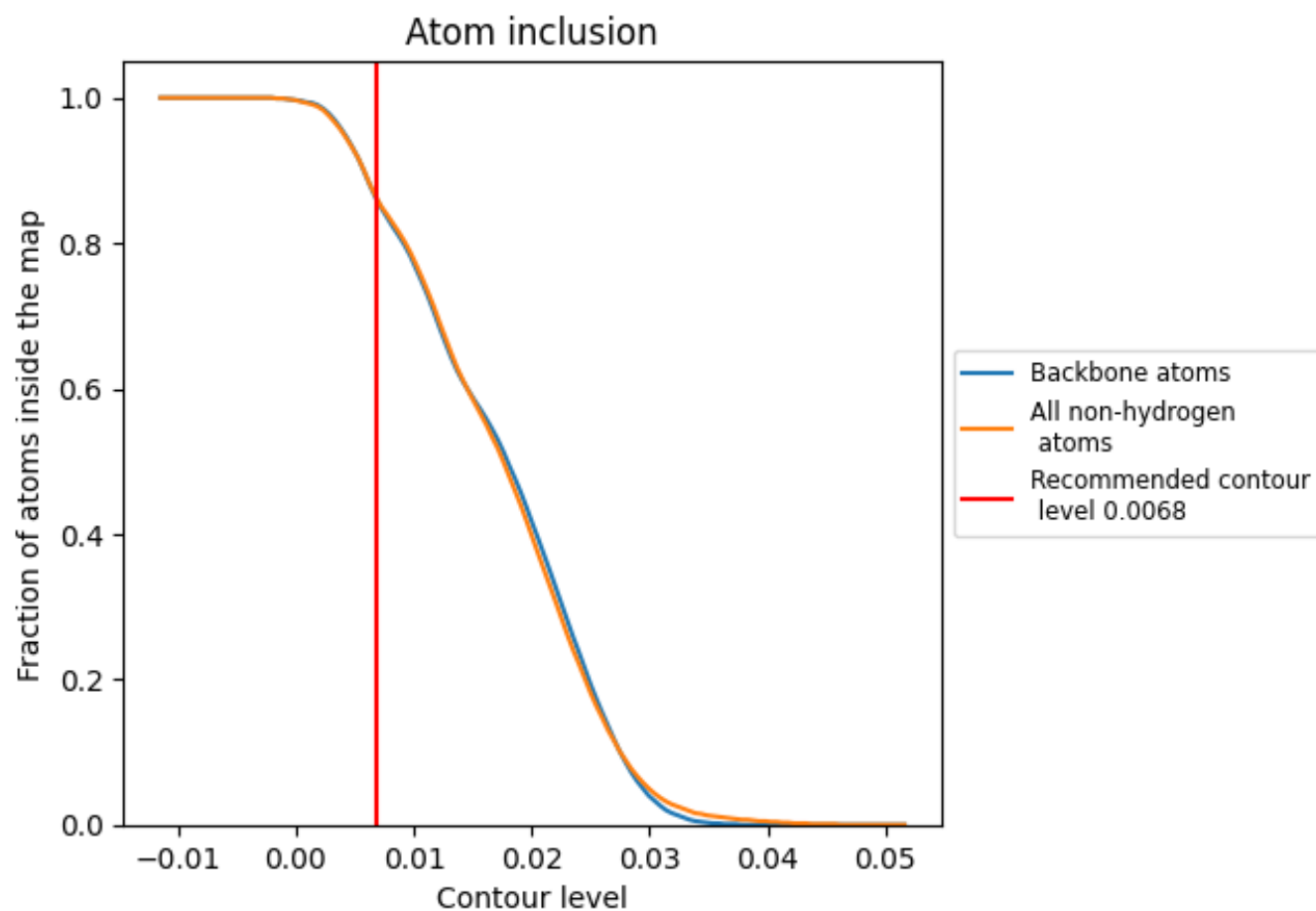


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.0068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.1610
2	 0.4510	 0.0180
21	 0.3560	 0.0010
22	 0.0460	 -0.0060
23	 0.0000	 0.0170
2A	 0.0010	 0.0020
2B	 0.0000	 0.0080
2b	 0.1140	 0.0270
2e	 0.0000	 0.0240
2f	 0.0000	 0.0530
2g	 0.0000	 0.0160
4	 0.9820	 0.1640
41	 0.9630	 0.0140
42	 0.8770	 0.0310
43	 0.9760	 -0.0000
4b	 0.8910	 0.0320
4e	 1.0000	 0.0570
4f	 1.0000	 0.0250
4g	 0.9890	 0.0300
5	 1.0000	 0.2090
51	 1.0000	 0.1180
52	 0.9830	 0.1070
53	 1.0000	 0.1770
5b	 1.0000	 0.1440
5e	 1.0000	 0.1120
5f	 1.0000	 0.1230
5g	 1.0000	 0.1310
6	 1.0000	 0.1960
62	 0.8890	 0.0150
63	 0.8630	 0.0180
64	 0.9950	 0.0580
65	 0.9760	 0.0310
66	 0.9920	 0.0560
67	 0.9920	 0.0460
68	 0.8700	 0.0430



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
7	 0.5570	 0.1470
8	 0.5390	 0.0100
9	 0.2570	 0.0070
A	 0.9990	 0.3030
B	 0.9980	 0.1860
B1	 0.8120	 0.0220
B2	 0.9940	 0.0540
B3	 0.5990	 0.0210
B4	 1.0000	 0.0430
B5	 1.0000	 0.0470
B6	 0.6810	 0.0420
BP	 1.0000	 0.0330
C	 1.0000	 0.2890
D	 1.0000	 0.3190
E	 0.9950	 0.0480
F	 1.0000	 0.2490
G	 0.9930	 0.1970
J	 1.0000	 0.2760
L	 0.9980	 0.3000
M	 1.0000	 0.3110
N	 0.9990	 0.2510
S	 0.9970	 0.2770
U	 0.9970	 0.2850
W	 1.0000	 0.1860
Z	 1.0000	 0.0440
z	 1.0000	 0.2830