



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 12:52 AM UTC

PDB ID : 9ZE3 / pdb_00009ze3
EMDB ID : EMD-74090
Title : Cryo-EM structure of the endogenous U2/branchpoint spliceosomal complex (Distal DHX15 state)
Authors : Liu, S.; Su, T.; Zhou, Z.H.
Deposited on : 2025-11-27
Resolution : 3.93 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:

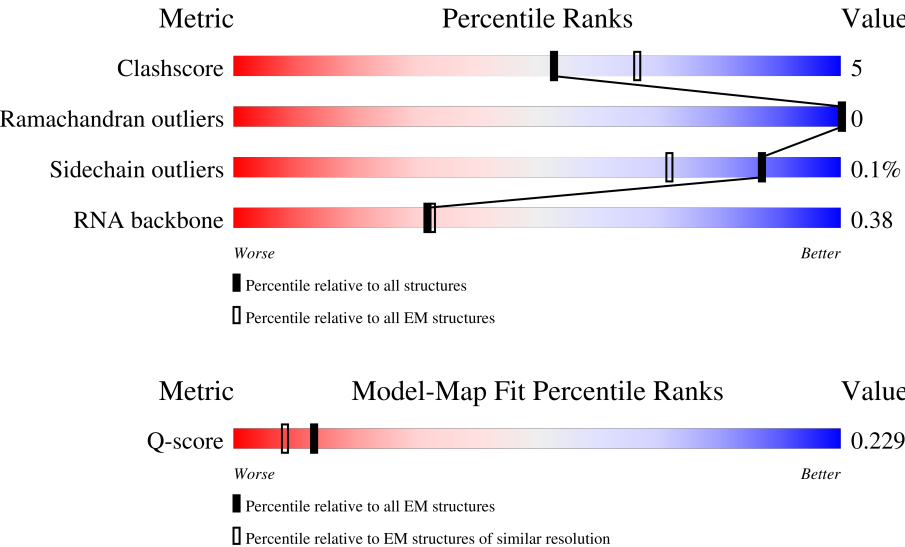
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.93 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	7811 (3.43 - 4.43)

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	A	824	<div> <div>16%</div> <div>14%</div> <div>83%</div> </div>
2	B	795	<div> <div>85%</div> <div>72%</div> <div>13%</div> <div>15%</div> </div>
3	C	1029	<div> <div>15%</div> <div>12%</div> <div>85%</div> </div>

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Mol	Chain	Length	Quality of chain
4	2	37	
5	H	110	
6	R	44	
7	B1	1304	
8	B2	895	
9	B3	1217	
10	B4	424	
11	B5	86	
12	B6	125	
13	A1	793	
14	A2	464	
15	A3	501	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 37987 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 RNA-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	137	Total	C	N	O	S	0	0
			1113	687	219	197	10		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	816	MET	-	expression tag	UNP P52756
A	817	ASP	-	expression tag	UNP P52756
A	818	TYR	-	expression tag	UNP P52756
A	819	LYS	-	expression tag	UNP P52756
A	820	ASP	-	expression tag	UNP P52756
A	821	ASP	-	expression tag	UNP P52756
A	822	ASP	-	expression tag	UNP P52756
A	823	ASP	-	expression tag	UNP P52756
A	824	LYS	-	expression tag	UNP P52756

- Molecule 2 is a protein called ATP-dependent RNA helicase DHX15.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	672	Total	C	N	O	S	0	0
			5409	3433	933	1008	35		

- Molecule 3 is a protein called U2 snRNP-associated SURP motif-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	152	Total	C	N	O	S	0	0
			1234	794	208	226	6		

- Molecule 4 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	37	Total	C	N	O	P	0	0
			781	352	127	265	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	103	Total	C	N	O	S	0	0
			794	490	142	148	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	44	Total	C	N	O	P	0	0
			882	397	93	348	44		

- Molecule 7 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B1	895	Total	C	N	O	S	0	0
			7142	4581	1225	1295	41		

- Molecule 8 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B2	250	Total	C	N	O	S	0	0
			1960	1260	348	345	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B3	1198	Total	C	N	O	S	0	0
			9396	5959	1598	1794	45		

- Molecule 10 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B4	205	Total	C	N	O	S	0	0
			1593	1011	270	305	7		

- Molecule 11 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B5	75	Total	C	N	O	S	0	0
			616	390	108	113	5		

- Molecule 12 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B6	98	Total	C	N	O	S	0	0
			805	515	144	142	4		

- Molecule 13 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	159	Total	C	N	O	S	0	0
			1344	864	229	249	2		

- Molecule 14 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A2	197	Total	C	N	O	S	0	0
			1645	1042	300	295	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A3	388	Total	C	N	O	S	0	0
			3270	2068	570	618	14		

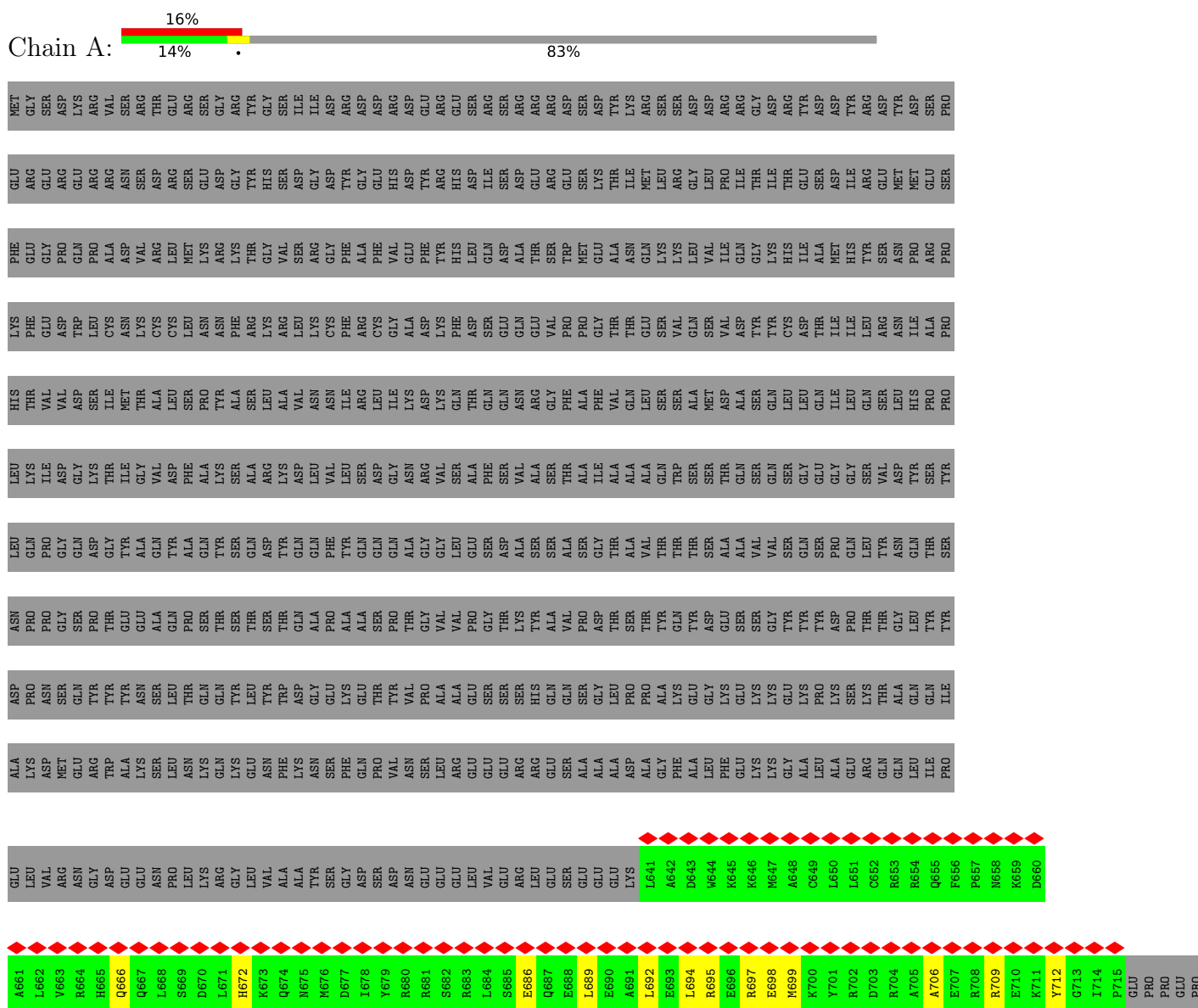
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

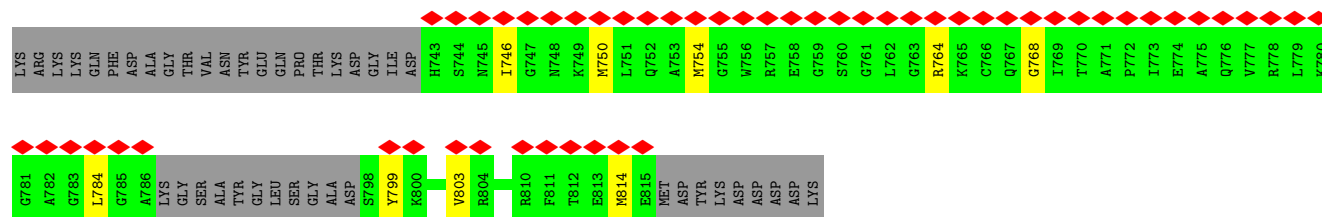
Mol	Chain	Residues	Atoms		AltConf
16	H	3	Total	Zn	0
			3	3	

3 Residue-property plots

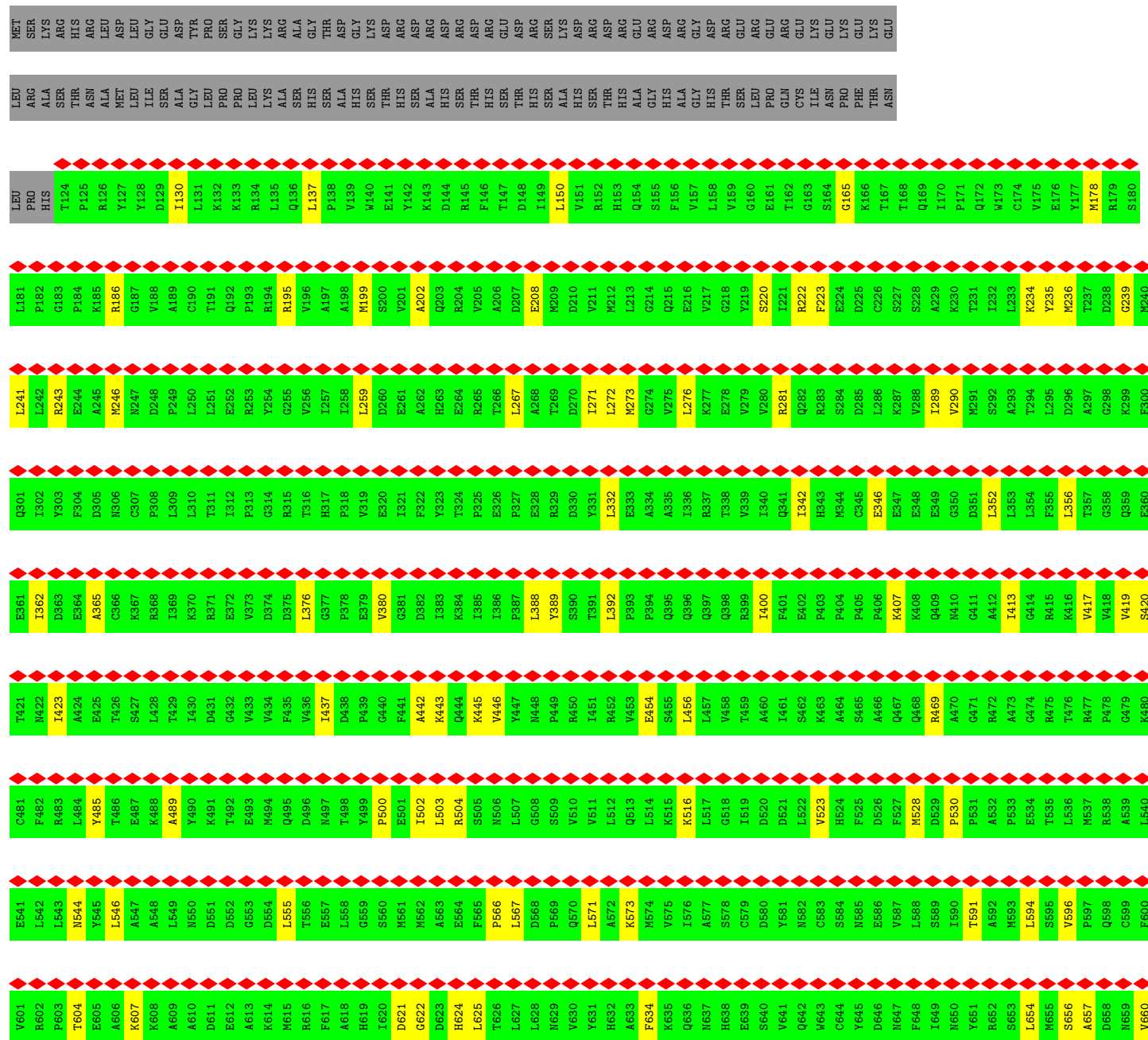
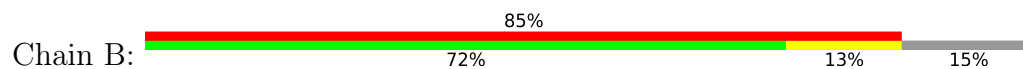
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: RNA-binding protein 5





• Molecule 2: ATP-dependent RNA helicase DHX15



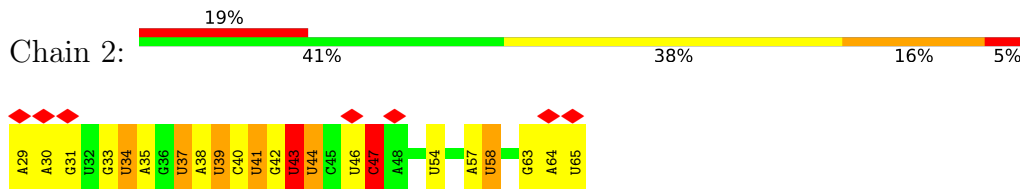
- Molecule 3: U2 snRNP-associated SURP motif-containing protein



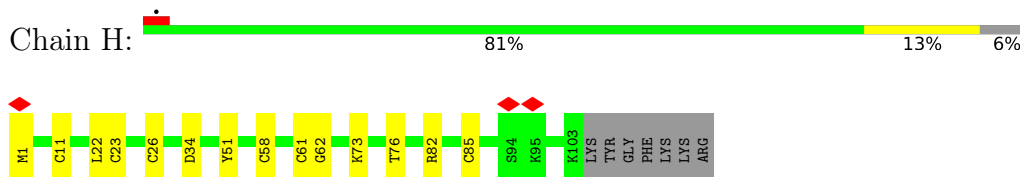
A661	V601	K541	LEU	TLE	HIS	ALA	GLN	SER	LEU	LEU	ARG	MET
I662	L602	L542	GLY	THR	ILE	VAL	LEU	LEU	SER	LEU	ARG	ALA
Y663	Y603	E543	ASP	GLU	TYR	LYS	VAL	VAL	LYS	PHE	ALA	ALA
P664	N604	E544	SER	ASN	TYR	ILE	MET	GLU	GLY	GLY	ASP	THR
E665	S605	I645	PRO	ASN	PRO	MET	TRP	THR	THR	THR	ASP	GLY
P666	S606	L546	THR	LEU	PRO	TRP	PRO	PRO	LYS	ASP	SER	GLY
F667	A607	L546	LYS	LEU	MET	ARG	PRO	PRO	PRO	GLY	HIS	SER
L668	K608	G548	ARG	ALA	THR	THR	ARG	THR	PRO	ASN	GLN	GLN
I669	V609	L549	THR	ILE	GLU	ASP	ARG	PRO	LYS	ASN	LYS	ALA
K670	A610	T550	ASP	ARG	HIS	GLU	ASN	LEU	VAL	VAL	ALA	ALA
L671	N611	P551	PHE	MET	THR	GLU	ARG	LYS	LYS	SER	SER	SER
K672	A612	R552	ARG	ILE	LEU	ARG	SER	LYS	THR	ARG	ARG	LYS
N673	S613	K553	MET	GLU	PRO	ALA	SER	GLY	PHE	PRO	PRO	THR
I674	Y614	L554	PHE	PHE	PRO	ARG	VAL	VAL	ARG	VAL	VAL	THR
F675	Y615	D555	LYS	VAL	PRO	ARG	LEU	LYS	GLY	GLY	GLY	SER
L676	R616	I556	ASN	ARG	SER	ASN	ASP	LYS	GLY	ASN	ASN	SER
G677	K617	G557	GLY	VAL	GLY	CYS	ASP	LYS	VAL	VAL	VAL	ASP
L678	F618	D558	SER	GLU	LEU	TYR	TYR	LYS	VAL	VAL	VAL	LYS
F619	V679	A559	PHE	GLY	PRO	PHE	ALA	SER	ASN	ASN	ALA	HIS
E620	E620	M560	ARG	MET	ASN	VAL	GLY	ALA	PRO	ALA	ALA	SER
N680	E620	F561	PRO	PHE	ALA	PHE	SER	GLU	GLY	ALA	ALA	SER
I681	T621	F562	PRO	ILE	PRO	ARG	ASP	GLY	GLY	GLY	GLY	GLY
GLU	K622	C563	ASN	MET	GLU	ASP	ASP	GLU	GLY	GLY	GLY	GLY
GLY	L623	L564	TYR	ASN	LEU	ALA	ALA	GLU	GLY	GLY	GLY	GLY
LYS	C624	M565	LEU	ARG	ASN	LEU	LYS	LYS	GLY	GLY	GLY	GLY
GLU	Q625	N566	LEU	ILE	PRO	ALA	THR	ILE	GLN	GLY	GLY	GLY
THR	I626	A567	GLY	ILE	PRO	ALA	THR	ILE	GLN	GLY	GLY	GLY
ASP	F627	E568	MET	ASN	ASN	LEU	LEU	GLY	GLY	GLY	GLY	GLY
VAL	S628	A569	SER	ASN	PRO	LYS	LEU	GLU	GLY	GLY	GLY	GLY
PRO	D629	A570	GLU	PRO	ALA	ASN	TYR	GLU	GLY	GLY	GLY	GLY
ASP	L630	E571	GLU	MET	MET	LEU	TYR	ARG	ARG	GLY	GLY	GLY
LEU	N631	E572	GLN	PHE	LEU	ASN	GLY	ASP	GLY	GLY	GLY	GLY
ASP	A632	E573	GLU	ARG	PRO	GLY	ASN	ARG	GLY	GLY	GLY	GLY
GLY	T633	I573	THR	PHE	PRO	LYS	ILE	ARG	GLY	GLY	GLY	GLY
ALA	Y634	V574	GLU	LEU	PRO	MET	ASN	HIS	SER	SER	GLY	GLY
PRO	R635	D575	PHE	PHE	LYS	ILE	PRO	LYS	THR	THR	GLY	GLY
ILE	L636	C576	VAL	GLN	GLU	PHE	GLY	GLY	GLY	GLY	GLY	GLY
GLU	T636	I577	GLU	THR	ASP	GLY	GLY	ARG	GLY	GLY	GLY	GLY
GLU	I637	T578	PRO	PRO	PHE	MET	GLY	GLY	GLY	GLY	GLY	GLY
GLU	Q638	E579	SER	ALA	GLU	LYS	MET	SER	GLY	GLY	GLY	GLY
LEU	K639	S580	K530	HIS	LYS	LEU	LEU	LEU	GLY	GLY	GLY	GLY
ASP	G639	L581	K531	TYR	LEU	TRP	GLY	PHE	GLY	GLY	GLY	GLY
ALA	H640	A533	A533	ARG	GLN	LYS	PHE	PRO	PRO	PRO	GLY	GLY
PRO	L641	S582	F535	THR	SER	GLY	GLY	PRO	GLN	GLN	GLY	GLY
LEU	Q642	I583	L534	TRP	ALA	VAL	GLY	GLM	SER	SER	ALA	ALA
GLU	S643	L584	F535	LYS	ILE	VAL	ARG	GLY	GLY	GLY	ALA	ALA
ASP	E644	K585	E536	THR	VAL	PRO	PHE	ASP	ASN	ASN	ALA	ALA
VAL	N645	F536	K585	TYR	LYS	ILE	GLY	GLY	GLY	GLY	ALA	ALA
ASP	F646	T586	E537	THR	VAL	PRO	THR	GLY	GLY	GLY	ALA	ALA
GLY												

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

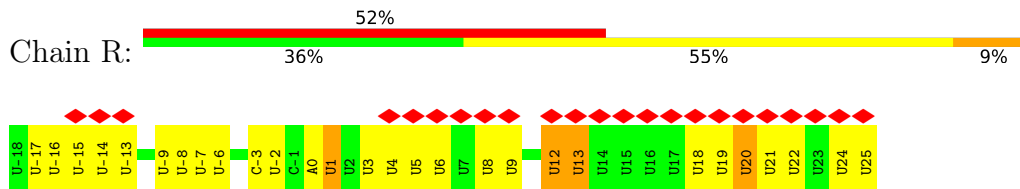
- Molecule 4: U2 snRNA



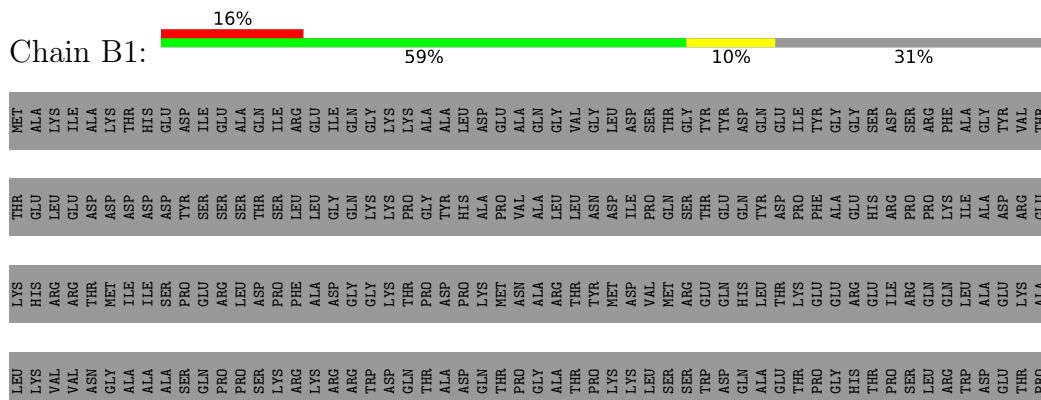
- Molecule 5: PHD finger-like domain-containing protein 5A

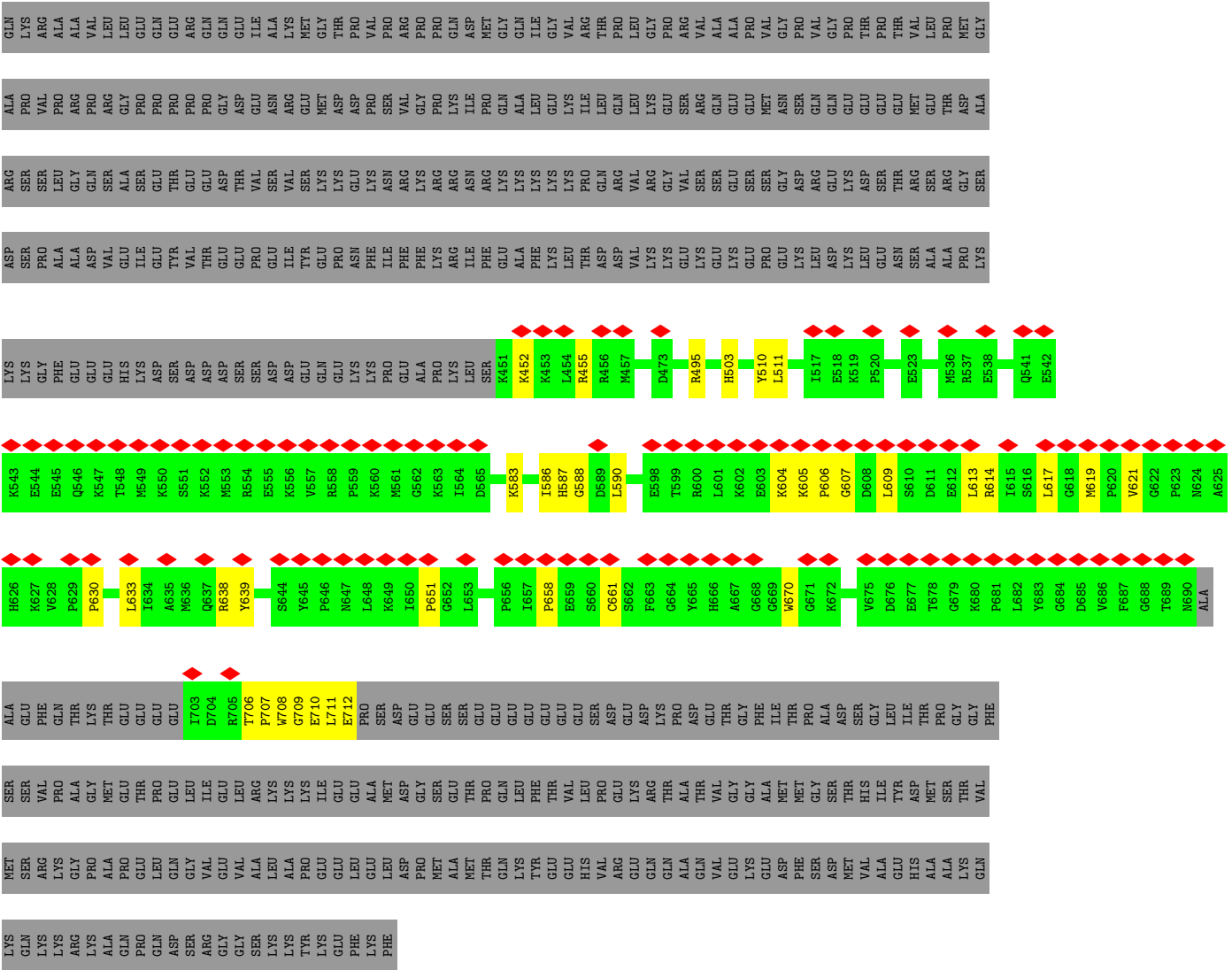


- Molecule 6: Pre-mRNA

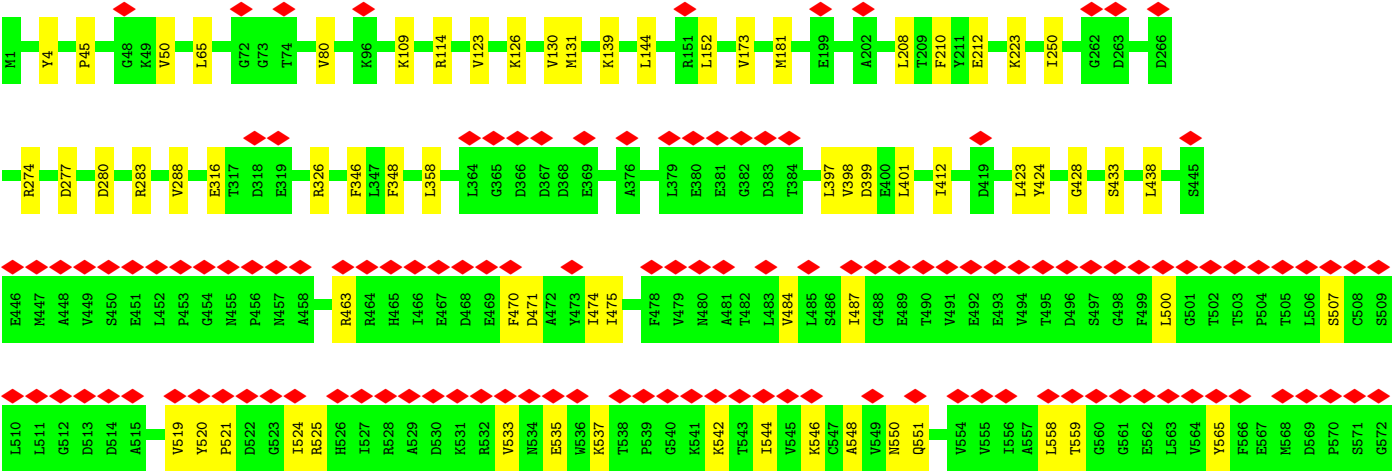
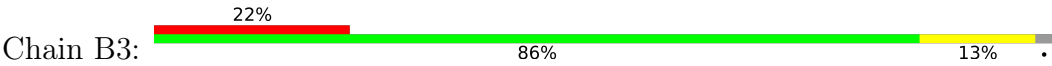


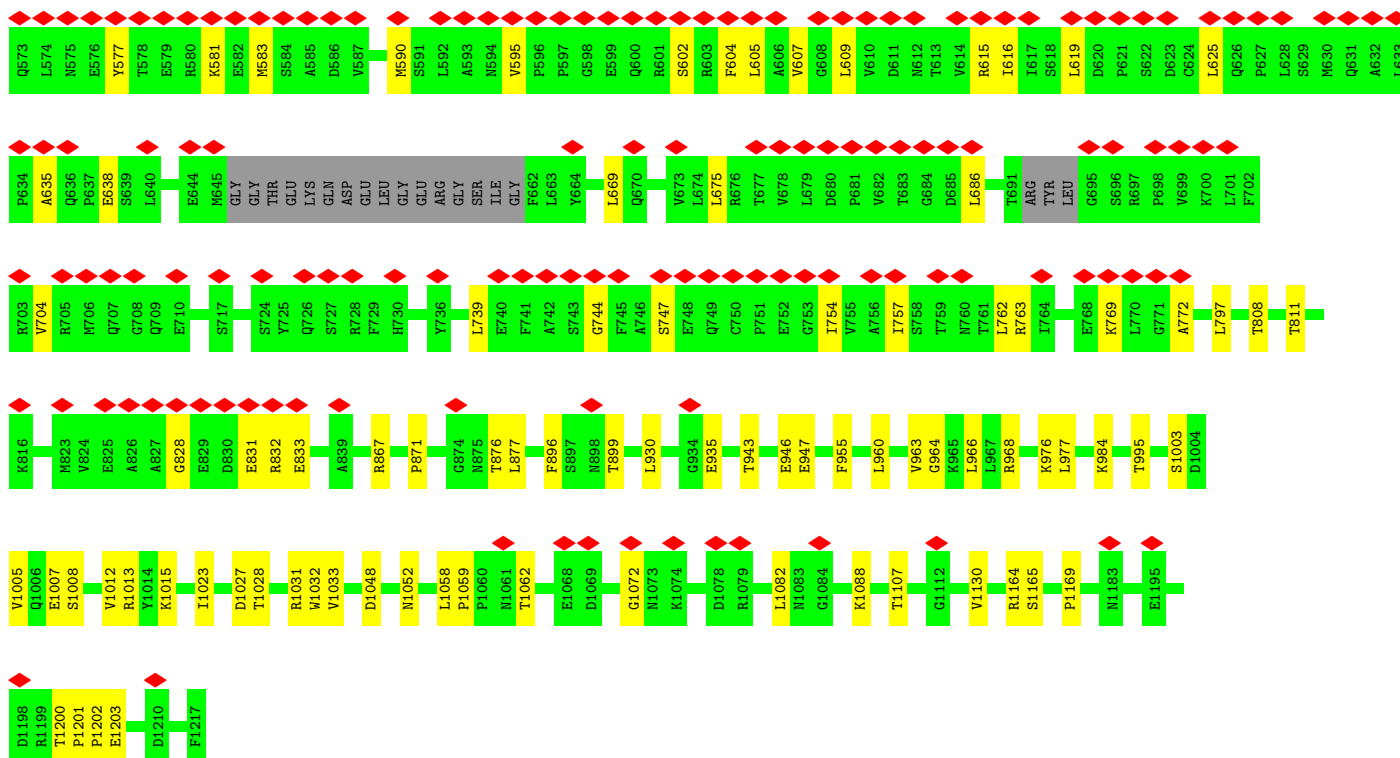
- Molecule 7: Splicing factor 3B subunit 1



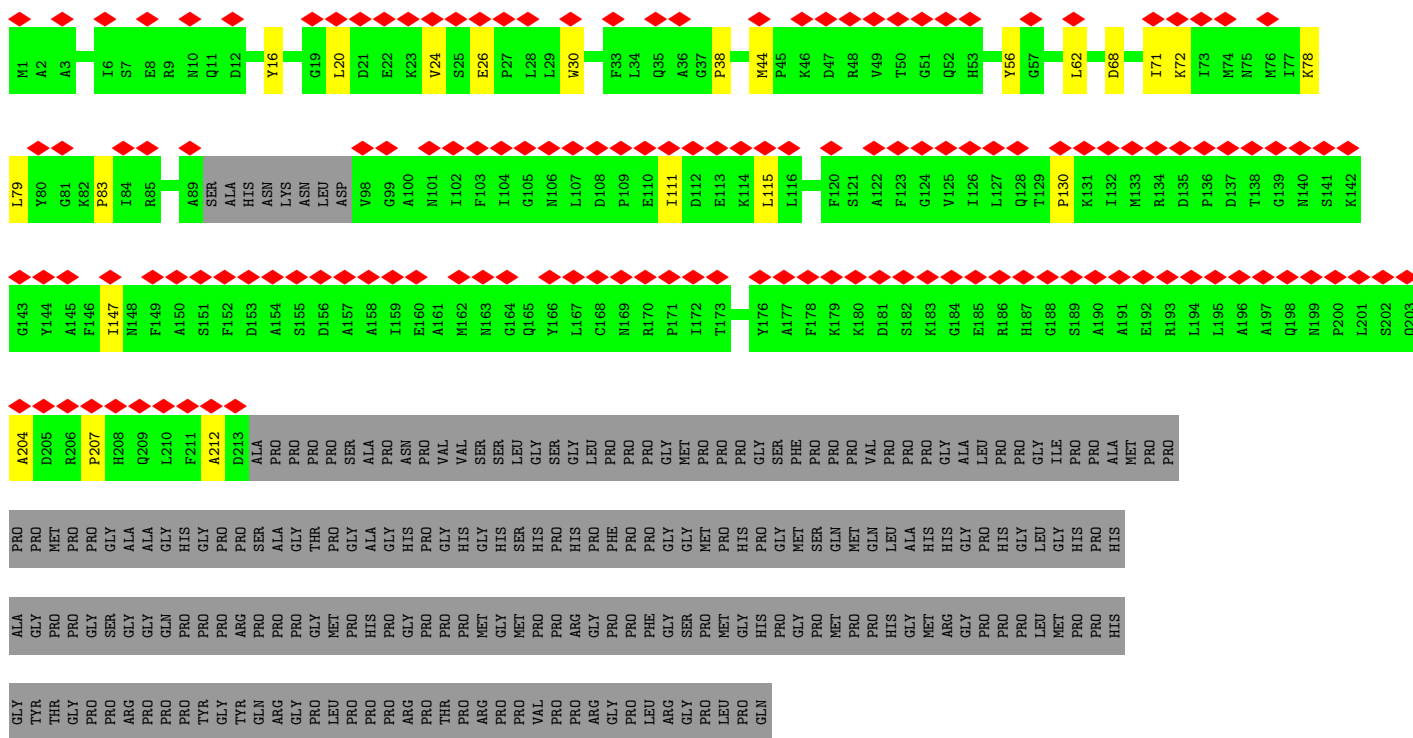
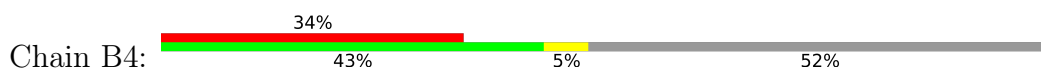


● Molecule 9: Splicing factor 3B subunit 3





• Molecule 10: Splicing factor 3B subunit 4



• Molecule 11: Splicing factor 3B subunit 5

Chain B5:

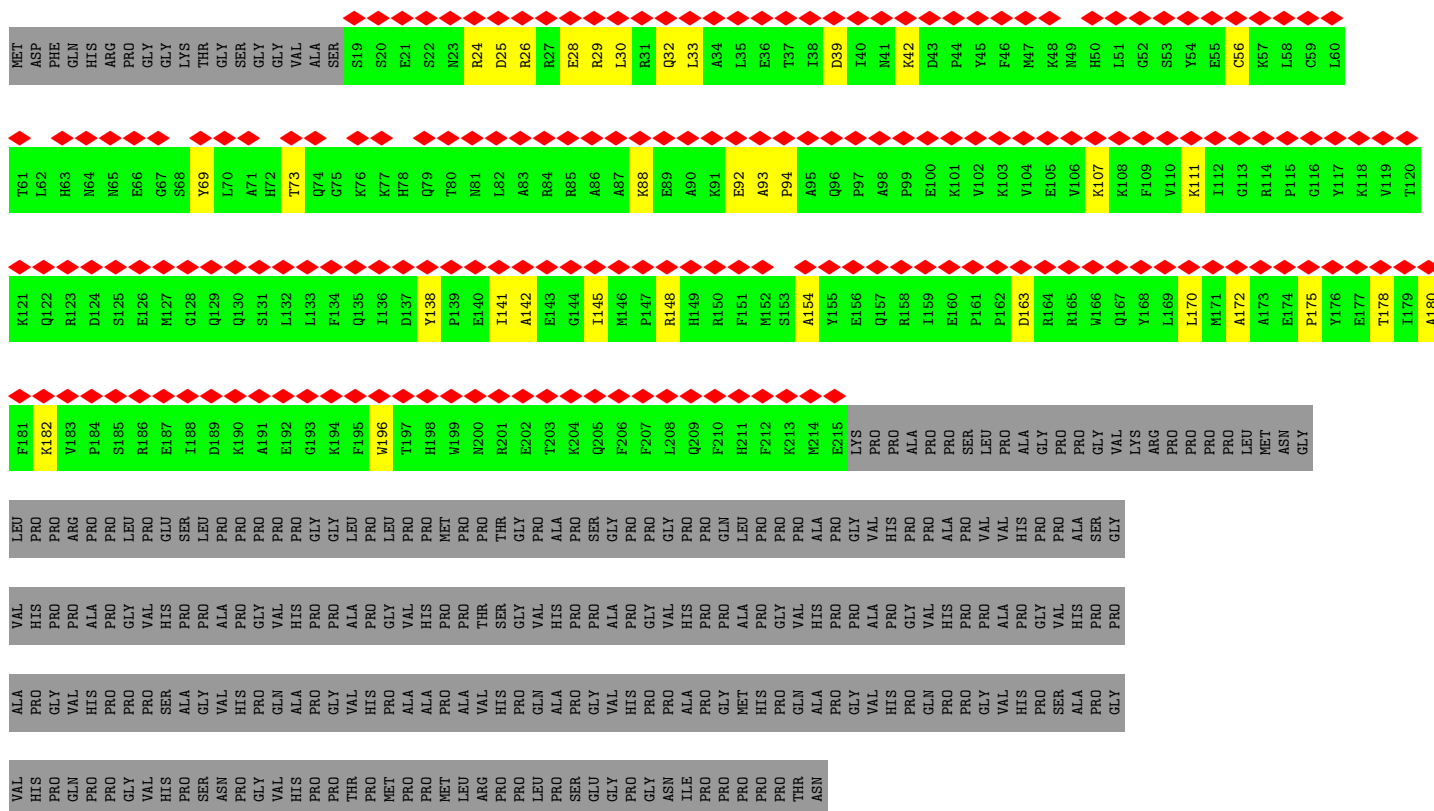
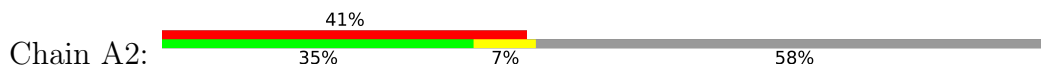
Chain B6:

Chain A1:

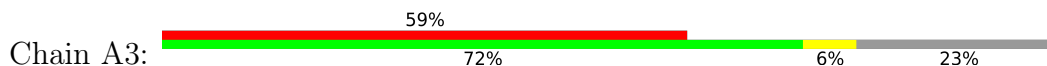


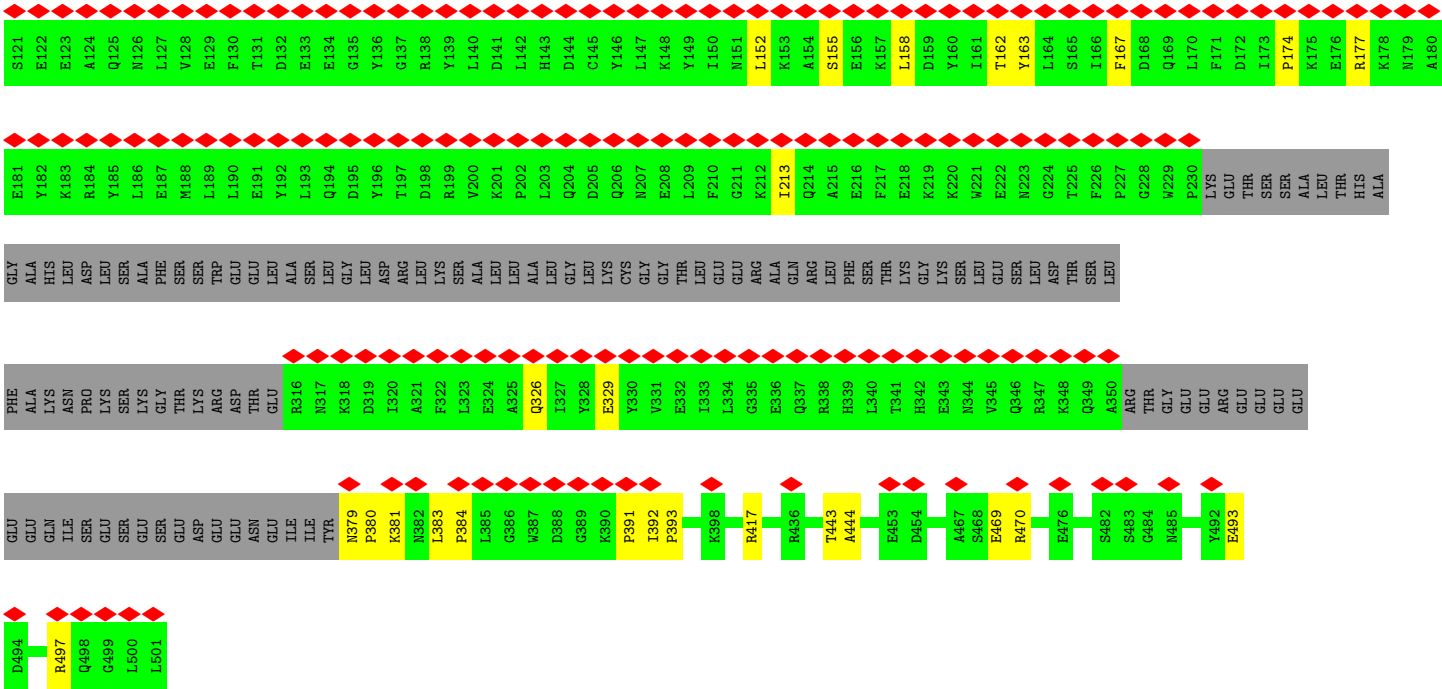
[illegible]

- Molecule 14: Splicing factor 3A subunit 2



- Molecule 15: Splicing factor 3A subunit 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49971	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.340	Depositor
Minimum map value	-1.398	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, ZN, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/1127	0.23	0/1496
2	B	0.08	0/5521	0.23	0/7479
3	C	0.08	0/1257	0.20	0/1696
4	2	0.09	0/625	0.21	0/972
5	H	0.15	0/807	0.36	0/1082
6	R	0.09	0/970	0.24	0/1497
7	B1	0.13	0/7284	0.33	0/9868
8	B2	0.18	0/2017	0.40	0/2735
9	B3	0.14	0/9590	0.33	0/13015
10	B4	0.09	0/1627	0.24	0/2200
11	B5	0.13	0/634	0.27	0/857
12	B6	0.09	0/823	0.25	0/1114
13	A1	0.08	0/1377	0.20	0/1857
14	A2	0.09	0/1686	0.23	0/2264
15	A3	0.08	0/3345	0.21	0/4503
All	All	0.12	0/38690	0.29	0/52635

There are no bond length outliers.

There are no bond angle outliers.

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	A	1113	0	1128	20	0
2	B	5409	0	5433	66	0
3	C	1234	0	1257	20	0
4	2	781	0	398	17	0
5	H	794	0	775	9	0
6	R	882	0	444	10	0
7	B1	7142	0	7319	92	0
8	B2	1960	0	1911	28	0
9	B3	9396	0	9309	96	0
10	B4	1593	0	1556	15	0
11	B5	616	0	579	9	0
12	B6	805	0	802	10	0
13	A1	1344	0	1309	14	0
14	A2	1645	0	1629	21	0
15	A3	3270	0	3163	21	0
16	H	3	0	0	0	0
All	All	37987	0	37012	399	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 (399) 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)
2:B:243:ARG:HA	2:B:246:MET:HG3	1.59	0.83
9:B3:704:VAL:HG11	9:B3:754:ILE:HG22	1.65	0.78
5:H:58:CYS:HB3	5:H:62:GLY:H	1.47	0.78
2:B:443:LYS:HB3	2:B:456:LEU:HD11	1.67	0.77
5:H:1:MET:HA	5:H:34:ASP:OD2	1.87	0.74
8:B2:605:LYS:HG3	8:B2:607:GLY:H	1.52	0.73
13:A1:273:GLN:HA	14:A2:107:LYS:HG2	1.71	0.73
7:B1:968:GLU:HG3	7:B1:1004:ILE:HD11	1.72	0.72
7:B1:460:PRO:HD3	7:B1:467:LEU:HD11	1.73	0.71
13:A1:271:TYR:HB2	14:A2:148:ARG:HD2	1.74	0.70
1:A:803:VAL:HG22	7:B1:623:TYR:HB3	1.72	0.69
2:B:407:LYS:HE2	2:B:413:ILE:HG12	1.73	0.69
9:B3:423:LEU:HB2	9:B3:438:LEU:HB2	1.75	0.69
8:B2:630:PRO:HD2	8:B2:633:LEU:HD22	1.74	0.69
4:2:42:G:H1	6:R:-9:U:H3	1.39	0.68
15:A3:213:ILE:HG12	15:A3:329:GLU:HG3	1.75	0.67
2:B:332:LEU:HD11	2:B:365:ALA:HB2	1.77	0.67
1:A:754:MET:HE2	2:B:523:VAL:HG23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:445:LYS:HE2	2:B:454:GLU:HB3	1.78	0.66
1:A:746:ILE:HG13	1:A:750:MET:HE3	1.78	0.65
9:B3:507:SER:HB3	9:B3:519:VAL:HB	1.77	0.65
9:B3:542:LYS:HD2	9:B3:559:THR:HB	1.79	0.65
15:A3:152:LEU:HB2	15:A3:155:SER:HB3	1.78	0.65
7:B1:918:VAL:HG12	7:B1:961:VAL:HG21	1.79	0.64
8:B2:710:GLU:HG3	8:B2:711:LEU:N	2.13	0.63
7:B1:477:LYS:HZ3	7:B1:494:GLU:HG3	1.65	0.62
9:B3:604:PHE:HB3	9:B3:616:ILE:HD11	1.82	0.62
13:A1:268:ARG:HA	13:A1:271:TYR:HB3	1.82	0.62
8:B2:605:LYS:HD2	8:B2:606:PRO:HD2	1.82	0.62
3:C:611:ASN:H	7:B1:902:GLU:HG3	1.65	0.62
7:B1:1017:LEU:HD21	7:B1:1042:ILE:HG21	1.81	0.61
9:B3:1058:LEU:HG	9:B3:1062:THR:HG21	1.81	0.61
9:B3:635:ALA:HB3	9:B3:669:LEU:HD23	1.82	0.61
7:B1:1193:GLN:HB2	7:B1:1233:ALA:HA	1.81	0.61
5:H:11:CYS:HB3	5:H:85:CYS:HB3	1.82	0.61
9:B3:877:LEU:HD13	9:B3:935:GLU:HG3	1.82	0.60
2:B:423:ILE:HD12	6:R:21:U:H5'	1.83	0.60
3:C:560:MET:HE2	3:C:597:LEU:HD13	1.82	0.60
13:A1:246:ARG:HH21	13:A1:249:TRP:HE1	1.48	0.60
9:B3:65:LEU:HD12	9:B3:80:VAL:HG12	1.83	0.60
2:B:376:LEU:HB3	2:B:380:VAL:HG21	1.84	0.60
14:A2:26:ARG:HG2	14:A2:29:ARG:HH21	1.66	0.59
4:2:33:G:H1	6:R:1:U:H3	1.49	0.59
8:B2:588:GLY:HA3	9:B3:1082:LEU:HD11	1.84	0.59
9:B3:1028:THR:HG22	9:B3:1088:LYS:HE3	1.83	0.59
7:B1:424:ILE:H	12:B6:44:PRO:HB3	1.68	0.59
15:A3:383:LEU:HD21	15:A3:392:ILE:HG22	1.85	0.59
2:B:259:LEU:HD11	2:B:276:LEU:HD12	1.85	0.58
7:B1:619:ASN:HD22	7:B1:624:VAL:HG11	1.68	0.58
12:B6:24:ARG:HG3	12:B6:88:VAL:HB	1.85	0.58
3:C:534:LEU:HD21	3:C:566:ASN:HB3	1.85	0.58
10:B4:26:GLU:HG3	10:B4:44:MET:HG3	1.86	0.57
8:B2:605:LYS:HG2	8:B2:609:LEU:HD23	1.84	0.57
7:B1:387:ARG:HH22	7:B1:469:PRO:HG2	1.69	0.57
9:B3:828:GLY:HA2	9:B3:832:ARG:HD3	1.87	0.57
2:B:445:LYS:HB2	6:R:20:U:O4	2.04	0.57
2:B:342:ILE:HG23	2:B:346:GLU:HG3	1.86	0.57
7:B1:953:ASP:O	7:B1:957:ARG:HG2	2.04	0.57
2:B:735:LEU:HB2	2:B:753:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B3:114:ARG:HG3	11:B5:41:CYS:SG	2.45	0.56
9:B3:797:LEU:HG	9:B3:871:PRO:HG3	1.87	0.56
15:A3:384:PRO:HG3	15:A3:417:ARG:HH12	1.71	0.56
7:B1:556:ILE:HA	7:B1:559:ILE:HG22	1.88	0.55
9:B3:544:ILE:HA	9:B3:558:LEU:HA	1.88	0.55
9:B3:1165:SER:HB2	9:B3:1169:PRO:HA	1.87	0.55
5:H:23:CYS:HB3	5:H:58:CYS:HB2	1.89	0.55
8:B2:638:ARG:NE	10:B4:212:ALA:HA	2.21	0.55
9:B3:131:MET:HE2	9:B3:139:LYS:HB3	1.89	0.55
9:B3:173:VAL:HG21	9:B3:210:PHE:HE1	1.72	0.55
2:B:621:ASP:HB2	2:B:625:LEU:HD12	1.87	0.55
10:B4:111:ILE:HG23	10:B4:115:LEU:HD23	1.89	0.55
7:B1:1281:ILE:HD11	11:B5:39:SER:HA	1.89	0.55
9:B3:565:TYR:HD2	9:B3:577:TYR:HB2	1.72	0.55
15:A3:392:ILE:HG13	15:A3:393:PRO:HD2	1.88	0.55
1:A:712:TYR:HB3	7:B1:943:LYS:HD3	1.90	0.55
2:B:220:SER:HB3	2:B:236:MET:HB3	1.89	0.54
2:B:773:GLN:HA	2:B:777:LYS:HD3	1.89	0.54
9:B3:316:GLU:HG3	9:B3:326:ARG:HE	1.72	0.54
9:B3:963:VAL:HG21	9:B3:968:ARG:HE	1.72	0.54
9:B3:548:ALA:HB2	9:B3:590:MET:HB3	1.89	0.54
1:A:686:GLU:HA	1:A:689:LEU:HD12	1.90	0.54
7:B1:806:ILE:HG12	7:B1:810:ILE:HD12	1.90	0.54
2:B:202:ALA:HB2	2:B:235:TYR:HB2	1.89	0.54
2:B:220:SER:HB2	2:B:234:LYS:HE2	1.90	0.54
3:C:600:ASP:HA	3:C:603:TYR:HB3	1.90	0.54
2:B:691:LYS:O	2:B:695:THR:HG23	2.08	0.53
9:B3:428:GLY:HA3	9:B3:433:SER:HA	1.90	0.53
7:B1:622:GLU:HG3	7:B1:625:ARG:NH2	2.23	0.53
7:B1:1152:SER:HB2	7:B1:1191:VAL:HG22	1.91	0.53
2:B:223:PHE:CD2	2:B:660:VAL:HG22	2.44	0.53
9:B3:463:ARG:HG2	9:B3:471:ASP:HA	1.90	0.53
9:B3:474:ILE:HG13	9:B3:487:ILE:HD11	1.90	0.53
7:B1:1103:VAL:HG13	7:B1:1105:GLU:H	1.73	0.53
15:A3:383:LEU:HD13	15:A3:391:PRO:HB2	1.90	0.53
7:B1:1140:GLU:HB2	7:B1:1143:VAL:HG22	1.89	0.53
2:B:388:LEU:HB2	2:B:400:ILE:HD11	1.89	0.53
7:B1:471:ASP:HB2	7:B1:475:PHE:CD2	2.44	0.53
14:A2:30:LEU:HA	14:A2:33:LEU:HD12	1.90	0.53
14:A2:111:LYS:HD2	14:A2:175:PRO:HA	1.91	0.53
9:B3:1008:SER:OG	9:B3:1031:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B3:208:LEU:HD22	9:B3:250:ILE:HD11	1.90	0.52
3:C:534:LEU:HG	3:C:569:ALA:HB3	1.91	0.52
3:C:660:TRP:HB3	7:B1:938:TRP:HZ3	1.74	0.52
7:B1:1041:ARG:HH12	7:B1:1045:ARG:HH21	1.57	0.52
4:2:33:G:H2'	4:2:34:PSU:H6	1.73	0.52
7:B1:397:ARG:HH21	7:B1:399:LEU:HD13	1.74	0.52
7:B1:471:ASP:HB2	7:B1:475:PHE:HD2	1.74	0.52
9:B3:520:TYR:HE1	9:B3:525:ARG:HG3	1.74	0.52
7:B1:1006:MET:HG2	7:B1:1046:GLY:HA3	1.90	0.52
7:B1:388:TRP:O	7:B1:391:GLU:HG2	2.09	0.52
9:B3:500:LEU:HB2	9:B3:525:ARG:HH12	1.74	0.52
4:2:37:PSU:H2'	4:2:38:A:H8	1.75	0.52
14:A2:138:TYR:HB3	14:A2:141:ILE:HB	1.91	0.52
9:B3:412:ILE:HG21	9:B3:1107:THR:HG21	1.92	0.52
9:B3:470:PHE:HB3	9:B3:747:SER:HA	1.92	0.52
7:B1:621:ASP:HB2	7:B1:624:VAL:HG23	1.91	0.51
9:B3:274:ARG:HB2	9:B3:277:ASP:HB3	1.92	0.51
9:B3:769:LYS:HZ2	9:B3:772:ALA:H	1.58	0.51
2:B:222:ARG:HG2	2:B:223:PHE:CD2	2.45	0.51
2:B:362:ILE:HG12	2:B:419:VAL:HG12	1.91	0.51
8:B2:651:PRO:HB3	8:B2:658:PRO:HD3	1.93	0.51
9:B3:1072:GLY:HA3	15:A3:470:ARG:HH22	1.76	0.51
1:A:694:LEU:HA	1:A:697:ARG:HD3	1.92	0.51
4:2:34:PSU:H2'	4:2:35:A:C8	2.46	0.51
2:B:571:LEU:HD22	2:B:591:THR:HG23	1.93	0.51
2:B:656:SER:O	2:B:660:VAL:HG23	2.11	0.51
7:B1:644:LEU:HD23	7:B1:644:LEU:H	1.76	0.51
1:A:692:LEU:O	1:A:695:ARG:HG2	2.11	0.50
7:B1:869:MET:HE1	7:B1:896:ILE:HG22	1.94	0.50
2:B:407:LYS:HG2	2:B:413:ILE:HA	1.93	0.50
3:C:549:LEU:HD21	3:C:597:LEU:HD23	1.92	0.50
9:B3:123:VAL:HG23	9:B3:130:VAL:HG23	1.92	0.50
15:A3:158:LEU:HD11	15:A3:162:THR:HB	1.94	0.50
15:A3:213:ILE:HG21	15:A3:326:GLN:HG2	1.94	0.50
7:B1:523:ALA:HB1	7:B1:559:ILE:HD13	1.92	0.50
7:B1:811:LEU:HG	7:B1:812:PRO:HD3	1.93	0.50
7:B1:380:PRO:HA	7:B1:383:LEU:HD12	1.94	0.50
2:B:352:LEU:HB2	2:B:417:VAL:HG22	1.93	0.50
7:B1:873:GLU:HG3	7:B1:913:GLY:HA2	1.94	0.50
7:B1:793:LYS:HG3	7:B1:839:GLU:HG2	1.92	0.50
13:A1:301:PRO:HG3	14:A2:196:TRP:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B1:856:ASP:HB3	7:B1:864:TYR:HE2	1.77	0.49
9:B3:963:VAL:HG21	9:B3:968:ARG:HH21	1.76	0.49
9:B3:1003:SER:HB2	9:B3:1033:VAL:HG21	1.94	0.49
10:B4:78:LYS:HA	10:B4:83:PRO:HA	1.93	0.49
13:A1:176:ARG:HG2	15:A3:75:ILE:HG13	1.93	0.49
1:A:706:ALA:HA	1:A:709:ARG:HE	1.76	0.49
12:B6:22:TYR:HE1	12:B6:59:THR:HB	1.76	0.49
1:A:698:GLU:HG3	1:A:699:MET:HE2	1.95	0.49
9:B3:520:TYR:CE1	9:B3:525:ARG:HG3	2.47	0.49
9:B3:739:LEU:HD22	9:B3:763:ARG:HH22	1.78	0.49
8:B2:638:ARG:HG3	8:B2:639:TYR:CD1	2.47	0.49
9:B3:704:VAL:HG13	9:B3:744:GLY:HA2	1.94	0.49
9:B3:946:GLU:CD	9:B3:947:GLU:HG3	2.38	0.49
12:B6:98:PHE:HA	12:B6:101:MET:HE3	1.95	0.49
14:A2:172:ALA:HB2	14:A2:178:THR:HA	1.94	0.49
7:B1:884:ILE:HG23	7:B1:888:LEU:HD23	1.94	0.49
7:B1:1094:LEU:HD22	7:B1:1128:VAL:HG23	1.94	0.49
7:B1:665:ILE:HG23	7:B1:690:ILE:HD12	1.93	0.49
1:A:764:ARG:HH12	2:B:281:ARG:HH22	1.61	0.49
2:B:195:ARG:O	2:B:199:MET:HG3	2.13	0.48
5:H:82:ARG:HG3	9:B3:109:LYS:HA	1.94	0.48
15:A3:383:LEU:HD23	15:A3:384:PRO:HD2	1.95	0.48
9:B3:808:THR:HG22	9:B3:811:THR:HG22	1.94	0.48
3:C:645:ASN:O	3:C:648:GLN:HG3	2.14	0.48
1:A:750:MET:HE1	2:B:544:ASN:HB2	1.94	0.48
5:H:73:LYS:O	5:H:76:THR:HG22	2.14	0.48
7:B1:386:TRP:O	7:B1:389:GLU:HG3	2.13	0.48
2:B:546:LEU:HD22	2:B:573:LYS:HG2	1.96	0.48
15:A3:443:THR:HG22	15:A3:444:ALA:H	1.79	0.48
7:B1:477:LYS:NZ	7:B1:494:GLU:HG3	2.29	0.48
7:B1:1185:ARG:HD2	7:B1:1218:ASN:HD21	1.79	0.48
9:B3:581:LYS:HE3	9:B3:625:LEU:HG	1.94	0.48
7:B1:625:ARG:HD3	7:B1:659:GLN:HG3	1.95	0.48
13:A1:240:LEU:HD23	15:A3:47:GLN:HG3	1.96	0.48
14:A2:142:ALA:HB3	14:A2:145:ILE:HD12	1.96	0.47
3:C:660:TRP:HE3	3:C:662:ILE:HD11	1.78	0.47
7:B1:553:VAL:O	7:B1:556:ILE:HG22	2.15	0.47
7:B1:856:ASP:HB3	7:B1:864:TYR:CE2	2.49	0.47
9:B3:358:LEU:HD21	9:B3:399:ASP:HB3	1.96	0.47
7:B1:1245:ARG:HD2	8:B2:587:HIS:ND1	2.29	0.47
1:A:784:LEU:HB3	2:B:485:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2:40:OMC:H2'	4:2:41:PSU:H6	1.80	0.47
8:B2:503:HIS:CG	8:B2:510:TYR:HB2	2.50	0.47
8:B2:604:LYS:HZ1	10:B4:30:TRP:CG	2.32	0.47
10:B4:20:LEU:HD11	10:B4:24:VAL:HG11	1.96	0.47
2:B:259:LEU:HD13	2:B:273:MET:HG2	1.97	0.47
14:A2:39:ASP:HB2	14:A2:42:LYS:HG3	1.97	0.47
7:B1:1244:CYS:HB2	7:B1:1283:HIS:CE1	2.50	0.47
9:B3:152:LEU:HD23	9:B3:152:LEU:HA	1.81	0.47
4:2:33:G:N2	6:R:1:U:O2	2.35	0.46
2:B:389:TYR:CE2	2:B:392:LEU:HG	2.51	0.46
2:B:694:VAL:HG13	2:B:758:LEU:HD23	1.97	0.46
9:B3:867:ARG:HH11	9:B3:876:THR:HG21	1.80	0.46
1:A:784:LEU:HG	2:B:489:ALA:HB1	1.98	0.46
6:R:-3:C:H2'	6:R:-2:U:H6	1.81	0.46
8:B2:614:ARG:HB2	8:B2:621:VAL:HG12	1.97	0.46
2:B:150:LEU:HD13	2:B:289:ILE:HD11	1.98	0.46
7:B1:1272:ILE:HG22	7:B1:1280:LEU:HD11	1.97	0.46
10:B4:16:TYR:HE1	10:B4:56:TYR:HB2	1.81	0.46
4:2:39:PSU:H2'	4:2:40:OMC:H6	1.80	0.46
4:2:47:OMC:C6	15:A3:381:LYS:HB2	2.51	0.46
9:B3:475:ILE:HD13	9:B3:484:VAL:HG13	1.98	0.46
12:B6:35:MET:SD	12:B6:48:ILE:HG21	2.56	0.46
7:B1:806:ILE:HA	7:B1:810:ILE:HB	1.98	0.46
9:B3:955:PHE:HB2	9:B3:995:THR:HG21	1.97	0.46
3:C:559:ALA:HB3	3:C:597:LEU:HD11	1.98	0.46
3:C:586:THR:HB	3:C:591:LYS:HE2	1.98	0.46
5:H:51:TYR:CE2	7:B1:676:GLY:HA3	2.51	0.45
5:H:58:CYS:SG	5:H:61:CYS:HB2	2.55	0.45
9:B3:602:SER:HB3	9:B3:619:LEU:HD13	1.98	0.45
2:B:634:PHE:CG	2:B:654:LEU:HD13	2.52	0.45
9:B3:424:TYR:HE2	9:B3:871:PRO:HB3	1.81	0.45
7:B1:490:GLU:HG2	7:B1:491:GLU:N	2.32	0.45
9:B3:533:VAL:HG12	9:B3:535:GLU:HB2	1.97	0.45
2:B:664:LEU:O	2:B:668:MET:HG3	2.16	0.45
7:B1:735:ILE:HD11	7:B1:747:LEU:HD12	1.99	0.45
8:B2:452:LYS:HG3	8:B2:455:ARG:HH21	1.82	0.45
9:B3:519:VAL:HG22	9:B3:524:ILE:HD12	1.99	0.45
9:B3:546:LYS:HA	9:B3:546:LYS:HD3	1.77	0.45
7:B1:1290:ASP:OD1	7:B1:1291:ASP:N	2.50	0.45
13:A1:273:GLN:HB2	14:A2:107:LYS:HA	1.98	0.45
2:B:500:PRO:HD2	2:B:503:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:VAL:HG21	2:B:657:ALA:HB2	1.98	0.45
4:2:63:G:H2'	4:2:64:A:C8	2.52	0.45
9:B3:583:MET:HB3	9:B3:609:LEU:HD21	1.98	0.45
1:A:814:MET:SD	7:B1:576:VAL:HG11	2.57	0.45
2:B:604:THR:HA	2:B:607:LYS:HE3	1.99	0.45
2:B:130:ILE:HG21	2:B:208:GLU:HG2	1.98	0.44
6:R:12:U:H5''	6:R:13:U:C6	2.51	0.44
7:B1:921:LEU:HD23	7:B1:921:LEU:HA	1.80	0.44
14:A2:25:ASP:O	14:A2:29:ARG:HG3	2.17	0.44
7:B1:494:GLU:HA	7:B1:497:ILE:HG12	1.99	0.44
9:B3:769:LYS:NZ	9:B3:772:ALA:H	2.16	0.44
12:B6:35:MET:HA	12:B6:38:ILE:HG12	1.99	0.44
2:B:594:LEU:HD11	2:B:624:HIS:CD2	2.52	0.44
7:B1:1041:ARG:NH2	7:B1:1045:ARG:HE	2.16	0.44
8:B2:590:LEU:HD23	8:B2:590:LEU:HA	1.81	0.44
10:B4:38:PRO:HB2	10:B4:62:LEU:HB2	1.99	0.44
8:B2:706:THR:O	8:B2:707:PRO:C	2.60	0.44
9:B3:412:ILE:HD13	9:B3:1107:THR:HG21	1.98	0.44
9:B3:976:LYS:HG2	9:B3:977:LEU:O	2.17	0.44
9:B3:1048:ASP:OD1	9:B3:1052:ASN:HB2	2.18	0.44
14:A2:24:ARG:O	14:A2:28:GLU:HG2	2.17	0.44
2:B:178:MET:HE2	2:B:186:ARG:HB2	2.00	0.44
9:B3:943:THR:HG21	9:B3:977:LEU:H	1.83	0.44
14:A2:32:GLN:OE1	14:A2:32:GLN:HA	2.17	0.44
9:B3:4:TYR:HB3	9:B3:1130:VAL:HG23	2.00	0.44
2:B:239:GLY:HA3	6:R:24:U:H5'	2.00	0.44
7:B1:1281:ILE:HD12	11:B5:42:SER:HB3	1.98	0.44
8:B2:708:TRP:CG	8:B2:709:GLY:N	2.85	0.44
9:B3:946:GLU:OE1	9:B3:947:GLU:HG3	2.17	0.44
12:B6:69:ASP:HA	12:B6:72:ASN:HD21	1.83	0.44
14:A2:56:CYS:HB2	14:A2:69:TYR:HE1	1.83	0.44
2:B:259:LEU:HD12	2:B:290:VAL:HG22	2.00	0.43
7:B1:1009:MET:HG3	7:B1:1011:PRO:HD2	2.00	0.43
7:B1:1154:LEU:O	7:B1:1158:ILE:HG12	2.18	0.43
7:B1:653:LYS:HB2	7:B1:653:LYS:HE2	1.73	0.43
9:B3:590:MET:SD	9:B3:607:VAL:HG22	2.58	0.43
13:A1:264:LYS:HA	13:A1:267:GLU:HG2	2.00	0.43
9:B3:50:VAL:HG21	9:B3:401:LEU:HD11	2.00	0.43
9:B3:348:PHE:HD1	9:B3:358:LEU:HB3	1.83	0.43
11:B5:49:LEU:HD23	11:B5:49:LEU:HA	1.77	0.43
9:B3:638:GLU:HG2	9:B3:669:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B3:1008:SER:HB2	9:B3:1027:ASP:HB3	2.00	0.43
4:2:42:G:H2'	4:2:43:PSU:O4	2.18	0.43
7:B1:488:SER:HB2	7:B1:491:GLU:HG2	1.99	0.43
7:B1:1025:LYS:HA	7:B1:1025:LYS:HD2	1.86	0.43
9:B3:288:VAL:HG12	11:B5:62:ALA:HB3	1.99	0.43
3:C:613:SER:N	7:B1:901:GLN:HG2	2.33	0.43
9:B3:520:TYR:HB2	9:B3:521:PRO:HD2	2.00	0.43
9:B3:757:ILE:HG22	9:B3:762:LEU:HD22	2.01	0.43
13:A1:270:ALA:O	13:A1:273:GLN:HG2	2.18	0.43
2:B:442:ALA:HB2	2:B:469:ARG:HH22	1.84	0.43
4:2:33:G:H2'	4:2:34:PSU:C6	2.53	0.43
7:B1:789:LEU:HD13	7:B1:818:PHE:CE2	2.54	0.43
8:B2:710:GLU:CG	8:B2:711:LEU:N	2.80	0.43
2:B:267:LEU:HD13	2:B:502:ILE:HA	2.01	0.43
4:2:29:A:H61	12:B6:61:TYR:HE1	1.66	0.43
4:2:40:OMC:H2'	4:2:41:PSU:C6	2.54	0.43
4:2:57:A:H2'	4:2:58:PSU:O4'	2.19	0.43
8:B2:613:LEU:H	8:B2:613:LEU:HD23	1.83	0.43
9:B3:1164:ARG:HD3	9:B3:1164:ARG:HA	1.76	0.43
3:C:556:ILE:HD13	3:C:596:TYR:CD2	2.53	0.43
7:B1:787:ILE:O	7:B1:791:VAL:HG23	2.19	0.43
2:B:744:LYS:HB2	2:B:746:TYR:CE1	2.54	0.42
6:R:-7:U:H2'	6:R:-6:U:C6	2.54	0.42
7:B1:1020:LEU:HD23	7:B1:1020:LEU:HA	1.88	0.42
13:A1:284:THR:HG23	14:A2:182:LYS:HB3	2.01	0.42
14:A2:154:ALA:HB1	14:A2:163:ASP:H	1.84	0.42
1:A:666:GLN:HA	1:A:672:HIS:CD2	2.53	0.42
1:A:799:TYR:O	1:A:803:VAL:HG23	2.20	0.42
7:B1:1110:VAL:O	7:B1:1114:VAL:HG23	2.19	0.42
7:B1:1115:ALA:O	7:B1:1119:VAL:HG12	2.19	0.42
9:B3:45:PRO:HA	9:B3:346:PHE:HE2	1.84	0.42
9:B3:675:LEU:HD23	9:B3:686:LEU:HD12	2.00	0.42
14:A2:170:LEU:HG	14:A2:180:ALA:HB2	2.01	0.42
5:H:22:LEU:HD22	5:H:26:CYS:HB3	2.01	0.42
7:B1:765:TYR:O	7:B1:769:VAL:HG23	2.19	0.42
11:B5:50:LEU:HD21	11:B5:65:ARG:HG3	2.01	0.42
10:B4:78:LYS:H	10:B4:78:LYS:HG2	1.70	0.42
2:B:273:MET:HE3	2:B:528:MET:HE3	2.00	0.42
7:B1:661:ARG:O	7:B1:665:ILE:HG13	2.19	0.42
8:B2:495:ARG:HG3	9:B3:1007:GLU:OE2	2.20	0.42
8:B2:511:LEU:HD23	8:B2:511:LEU:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B3:397:LEU:HD12	9:B3:398:VAL:H	1.85	0.42
14:A2:69:TYR:O	14:A2:73:THR:HG23	2.19	0.42
7:B1:1109:ARG:O	7:B1:1113:THR:HG23	2.20	0.42
8:B2:706:THR:HA	8:B2:707:PRO:HD2	1.89	0.42
9:B3:1005:VAL:O	9:B3:1032:TRP:HA	2.19	0.42
15:A3:174:PRO:HD2	15:A3:177:ARG:HD2	2.02	0.42
7:B1:1129:LEU:HA	7:B1:1129:LEU:HD23	1.82	0.42
8:B2:583:LYS:HB2	8:B2:583:LYS:HE2	1.78	0.42
3:C:560:MET:HE3	3:C:600:ASP:CB	2.50	0.42
3:C:612:ALA:HB3	7:B1:901:GLN:HG3	2.02	0.42
9:B3:126:LYS:HA	9:B3:126:LYS:HD3	1.84	0.42
9:B3:551:GLN:HB2	9:B3:595:VAL:HB	2.01	0.42
9:B3:609:LEU:HD22	9:B3:615:ARG:NH2	2.35	0.42
9:B3:1012:VAL:HG22	9:B3:1023:ILE:HG12	2.02	0.42
2:B:137:LEU:HD13	2:B:165:GLY:HA3	2.02	0.42
2:B:223:PHE:CE2	2:B:660:VAL:HG22	2.55	0.42
2:B:356:LEU:HD12	2:B:362:ILE:HA	2.01	0.42
2:B:243:ARG:NH2	2:B:566:PRO:HA	2.35	0.42
3:C:560:MET:HE1	3:C:597:LEU:O	2.19	0.42
9:B3:964:GLY:C	9:B3:966:LEU:H	2.28	0.42
11:B5:50:LEU:HD12	11:B5:50:LEU:HA	1.79	0.42
13:A1:176:ARG:HE	15:A3:76:SER:HB3	1.85	0.42
8:B2:586:ILE:HG23	8:B2:588:GLY:H	1.85	0.41
8:B2:613:LEU:O	8:B2:617:LEU:HD12	2.19	0.41
10:B4:130:PRO:HB3	10:B4:147:ILE:HG12	2.01	0.41
15:A3:163:TYR:O	15:A3:167:PHE:HB3	2.20	0.41
15:A3:384:PRO:HG3	15:A3:417:ARG:NH1	2.33	0.41
3:C:616:ARG:HD2	7:B1:938:TRP:CD1	2.54	0.41
9:B3:280:ASP:HB3	9:B3:283:ARG:HG3	2.01	0.41
14:A2:88:LYS:O	14:A2:92:GLU:HG2	2.20	0.41
2:B:388:LEU:HB3	2:B:420:SER:HB2	2.01	0.41
3:C:641:LEU:HD23	3:C:641:LEU:H	1.85	0.41
7:B1:388:TRP:HA	7:B1:391:GLU:OE1	2.20	0.41
8:B2:638:ARG:HE	10:B4:212:ALA:HA	1.85	0.41
8:B2:661:CYS:HB3	8:B2:670:TRP:NE1	2.36	0.41
13:A1:164:LEU:HD11	13:A1:168:LYS:HE3	2.02	0.41
1:A:768:GLY:HA3	2:B:530:PRO:HB2	2.01	0.41
2:B:241:LEU:HB3	2:B:272:LEU:HD11	2.01	0.41
2:B:446:VAL:HA	2:B:504:ARG:HB2	2.02	0.41
2:B:516:LYS:HA	2:B:555:LEU:HD22	2.02	0.41
2:B:634:PHE:CD1	2:B:654:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2:41:PSU:H2'	4:2:42:G:C8	2.56	0.41
9:B3:1013:ARG:HH11	9:B3:1015:LYS:HG2	1.85	0.41
9:B3:1201:PRO:N	9:B3:1202:PRO:HD2	2.35	0.41
10:B4:71:ILE:HD13	10:B4:71:ILE:HA	1.92	0.41
1:A:814:MET:HE2	7:B1:573:LYS:HD3	2.03	0.41
2:B:567:LEU:HD13	2:B:591:THR:HG21	2.02	0.41
2:B:719:VAL:HG12	2:B:745:ASN:HB3	2.00	0.41
8:B2:614:ARG:HB3	8:B2:619:MET:HE3	2.03	0.41
9:B3:930:LEU:HD12	9:B3:930:LEU:HA	1.79	0.41
7:B1:939:ARG:HE	7:B1:947:VAL:HG13	1.86	0.41
9:B3:181:MET:HE2	9:B3:181:MET:HB3	1.94	0.41
7:B1:1106:ARG:HG3	7:B1:1107:GLN:N	2.36	0.41
15:A3:379:ASN:HA	15:A3:380:PRO:HD3	1.96	0.41
4:2:39:PSU:H2'	4:2:40:OMC:C6	2.56	0.41
7:B1:717:THR:HA	7:B1:718:PRO:HA	1.92	0.41
7:B1:1120:ALA:HB2	7:B1:1128:VAL:HG11	2.02	0.41
9:B3:212:GLU:CD	9:B3:223:LYS:HD2	2.45	0.41
9:B3:896:PHE:HB2	9:B3:899:THR:HG22	2.03	0.41
11:B5:59:GLU:H	11:B5:59:GLU:HG2	1.70	0.41
2:B:267:LEU:O	2:B:271:ILE:HG12	2.21	0.41
6:R:20:U:H2'	6:R:21:U:C6	2.55	0.41
7:B1:424:ILE:HD12	12:B6:44:PRO:HG2	2.03	0.41
7:B1:1026:ASN:HD22	7:B1:1031:VAL:HG11	1.85	0.41
9:B3:550:ASN:ND2	9:B3:602:SER:HB2	2.35	0.41
9:B3:831:GLU:HG2	9:B3:833:GLU:H	1.86	0.41
14:A2:93:ALA:HB3	14:A2:94:PRO:HD3	2.03	0.41
3:C:592:ILE:HD11	3:C:646:PHE:CD1	2.56	0.41
3:C:660:TRP:HB3	7:B1:938:TRP:CZ3	2.55	0.41
1:A:666:GLN:HG2	1:A:672:HIS:CE1	2.56	0.40
2:B:456:LEU:O	2:B:742:THR:HA	2.21	0.40
2:B:622:GLY:HA3	2:B:751:THR:HA	2.03	0.40
7:B1:574:ILE:O	7:B1:578:ILE:HG12	2.21	0.40
7:B1:706:ALA:HB3	7:B1:745:ALA:HB1	2.03	0.40
9:B3:960:LEU:HD12	9:B3:960:LEU:HA	1.76	0.40
9:B3:984:LYS:HD2	15:A3:469:GLU:O	2.20	0.40
9:B3:1200:THR:HG23	9:B3:1203:GLU:H	1.86	0.40
2:B:342:ILE:HD12	2:B:437:ILE:HD11	2.03	0.40
7:B1:1066:LEU:HD23	7:B1:1066:LEU:HA	1.89	0.40
7:B1:1245:ARG:HA	7:B1:1245:ARG:HD3	1.72	0.40
7:B1:1281:ILE:CD1	11:B5:39:SER:HA	2.51	0.40
13:A1:172:GLN:HG3	13:A1:215:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B1:1013:ILE:HD13	7:B1:1049:TYR:HD2	1.87	0.40
10:B4:204:ALA:O	10:B4:207:PRO:HD2	2.21	0.40
1:A:695:ARG:O	1:A:698:GLU:HG2	2.22	0.40
9:B3:605:LEU:HB2	9:B3:619:LEU:HD11	2.02	0.40
10:B4:68:ASP:O	10:B4:72:LYS:HG3	2.21	0.40
10:B4:79:LEU:HD12	10:B4:79:LEU:HA	1.86	0.40
7:B1:464:LEU:HD13	7:B1:502:LEU:HD23	2.04	0.40
7:B1:680:LEU:HB3	7:B1:681:PRO:HD3	2.04	0.40
9:B3:537:LYS:HA	9:B3:537:LYS:HD3	1.84	0.40
9:B3:1059:PRO:O	9:B3:1062:THR:HG23	2.22	0.40
12:B6:14:PRO:HA	12:B6:15:PRO:HD3	1.96	0.40
15:A3:493:GLU:O	15:A3:497:ARG:HG2	2.21	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	A	131/824 (16%)	130 (99%)	1 (1%)	0	100	100
2	B	670/795 (84%)	662 (99%)	8 (1%)	0	100	100
3	C	150/1029 (15%)	149 (99%)	1 (1%)	0	100	100
5	H	101/110 (92%)	92 (91%)	9 (9%)	0	100	100
7	B1	891/1304 (68%)	862 (97%)	29 (3%)	0	100	100
8	B2	246/895 (28%)	232 (94%)	14 (6%)	0	100	100
9	B3	1192/1217 (98%)	1128 (95%)	64 (5%)	0	100	100
10	B4	201/424 (47%)	197 (98%)	4 (2%)	0	100	100
11	B5	73/86 (85%)	70 (96%)	3 (4%)	0	100	100
12	B6	96/125 (77%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	A1	157/793 (20%)	154 (98%)	3 (2%)	0	100	100
14	A2	195/464 (42%)	188 (96%)	7 (4%)	0	100	100
15	A3	382/501 (76%)	378 (99%)	4 (1%)	0	100	100
All	All	4485/8567 (52%)	4336 (97%)	149 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/704 (16%)	113 (100%)	0	100	100
2	B	599/704 (85%)	599 (100%)	0	100	100
3	C	135/934 (14%)	135 (100%)	0	100	100
5	H	89/95 (94%)	89 (100%)	0	100	100
7	B1	775/1104 (70%)	775 (100%)	0	100	100
8	B2	201/776 (26%)	200 (100%)	1 (0%)	81	82
9	B3	1037/1051 (99%)	1036 (100%)	1 (0%)	88	90
10	B4	167/336 (50%)	167 (100%)	0	100	100
11	B5	66/77 (86%)	66 (100%)	0	100	100
12	B6	84/109 (77%)	84 (100%)	0	100	100
13	A1	144/709 (20%)	144 (100%)	0	100	100
14	A2	174/382 (46%)	174 (100%)	0	100	100
15	A3	350/446 (78%)	350 (100%)	0	100	100
All	All	3934/7427 (53%)	3932 (100%)	2 (0%)	87	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	B2	712	GLU

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Mol	Chain	Res	Type
9	B3	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	468	GLN
2	B	495	GLN
2	B	582	ASN
2	B	737	ASN
3	C	565	ASN
3	C	604	ASN
3	C	631	ASN
7	B1	662	HIS
7	B1	842	ASN
7	B1	1218	ASN
8	B2	637	GLN
9	B3	219	HIS
9	B3	422	GLN
9	B3	666	ASN
9	B3	861	GLN
9	B3	932	ASN
9	B3	1160	HIS
11	B5	8	HIS
11	B5	36	HIS
14	A2	209	GLN
15	A3	8	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	2	36/37 (97%)	7 (19%)	1 (2%)
6	R	43/44 (97%)	21 (48%)	1 (2%)
All	All	79/81 (97%)	28 (35%)	2 (2%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	2	30	A
4	2	31	G
4	2	43	PSU

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Mol	Chain	Res	Type
4	2	44	PSU
4	2	46	U
4	2	47	OMC
4	2	65	U
6	R	-17	U
6	R	-16	U
6	R	-15	U
6	R	-14	U
6	R	-13	U
6	R	-8	U
6	R	0	A
6	R	1	U
6	R	3	U
6	R	4	U
6	R	5	U
6	R	6	U
6	R	8	U
6	R	9	U
6	R	12	U
6	R	13	U
6	R	18	U
6	R	19	U
6	R	20	U
6	R	22	U
6	R	25	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	2	44	PSU
6	R	18	U

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection.

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	2	37	4	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
4	OMC	2	47	4	19,22,23	0.51	0	25,31,34	1.02	2 (8%)
4	PSU	2	58	4	18,21,22	1.09	1 (5%)	21,30,33	1.73	4 (19%)
4	PSU	2	54	4	18,21,22	1.14	1 (5%)	21,30,33	1.93	4 (19%)
4	PSU	2	44	4	18,21,22	1.11	1 (5%)	21,30,33	1.76	4 (19%)
4	PSU	2	39	4,6	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
4	OMC	2	40	4,6	19,22,23	0.50	0	25,31,34	0.72	0
4	PSU	2	41	4,6	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
4	OMC	2	61	4	19,22,23	0.49	0	25,31,34	0.69	0
4	PSU	2	43	4	18,21,22	1.11	1 (5%)	21,30,33	1.70	4 (19%)
4	PSU	2	34	4,6	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)

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
4	PSU	2	37	4	-	0/7/25/26	0/2/2/2
4	OMC	2	47	4	-	6/9/27/28	0/2/2/2
4	PSU	2	58	4	-	3/7/25/26	0/2/2/2
4	PSU	2	54	4	-	0/7/25/26	0/2/2/2
4	PSU	2	44	4	-	3/7/25/26	0/2/2/2
4	PSU	2	39	4,6	-	0/7/25/26	0/2/2/2
4	OMC	2	40	4,6	-	0/9/27/28	0/2/2/2
4	PSU	2	41	4,6	-	0/7/25/26	0/2/2/2
4	OMC	2	61	4	-	0/9/27/28	0/2/2/2
4	PSU	2	43	4	-	6/7/25/26	0/2/2/2
4	PSU	2	34	4,6	-	0/7/25/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	43	PSU	C6-C5	3.91	1.39	1.35
4	2	44	PSU	C6-C5	3.84	1.39	1.35
4	2	58	PSU	C6-C5	3.74	1.39	1.35
4	2	54	PSU	C6-C5	3.70	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	39	PSU	C6-C5	3.66	1.39	1.35
4	2	41	PSU	C6-C5	3.61	1.39	1.35
4	2	34	PSU	C6-C5	3.61	1.39	1.35
4	2	37	PSU	C6-C5	3.47	1.39	1.35

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	37	PSU	C4-N3-C2	-4.97	119.52	126.37
4	2	37	PSU	N1-C2-N3	4.88	120.32	115.17
4	2	54	PSU	N1-C2-N3	4.82	120.25	115.17
4	2	54	PSU	C4-N3-C2	-4.81	119.75	126.37
4	2	41	PSU	N1-C2-N3	4.79	120.22	115.17
4	2	39	PSU	C4-N3-C2	-4.77	119.81	126.37
4	2	39	PSU	N1-C2-N3	4.75	120.18	115.17
4	2	41	PSU	C4-N3-C2	-4.75	119.83	126.37
4	2	34	PSU	N1-C2-N3	4.66	120.08	115.17
4	2	34	PSU	C4-N3-C2	-4.65	119.97	126.37
4	2	44	PSU	N1-C2-N3	4.63	120.05	115.17
4	2	43	PSU	N1-C2-N3	4.47	119.88	115.17
4	2	44	PSU	C4-N3-C2	-4.41	120.29	126.37
4	2	43	PSU	C4-N3-C2	-4.35	120.38	126.37
4	2	58	PSU	N1-C2-N3	4.34	119.74	115.17
4	2	58	PSU	C4-N3-C2	-4.23	120.55	126.37
4	2	41	PSU	O2-C2-N1	-3.06	119.64	122.79
4	2	47	OMC	C1'-N1-C2	2.95	124.96	118.44
4	2	44	PSU	O2-C2-N1	-2.94	119.75	122.79
4	2	54	PSU	O2-C2-N1	-2.90	119.80	122.79
4	2	37	PSU	O2-C2-N1	-2.84	119.86	122.79
4	2	34	PSU	O2-C2-N1	-2.82	119.88	122.79
4	2	39	PSU	O2-C2-N1	-2.72	119.99	122.79
4	2	58	PSU	C6-N1-C2	-2.71	120.17	122.69
4	2	43	PSU	C6-N1-C2	-2.69	120.19	122.69
4	2	44	PSU	C6-N1-C2	-2.69	120.20	122.69
4	2	58	PSU	O2-C2-N1	-2.63	120.08	122.79
4	2	43	PSU	O2-C2-N1	-2.60	120.10	122.79
4	2	54	PSU	C6-N1-C2	-2.59	120.28	122.69
4	2	41	PSU	C6-N1-C2	-2.51	120.36	122.69
4	2	34	PSU	C6-N1-C2	-2.50	120.37	122.69
4	2	37	PSU	C6-N1-C2	-2.40	120.46	122.69
4	2	39	PSU	C6-N1-C2	-2.37	120.49	122.69
4	2	47	OMC	C1'-N1-C6	-2.32	115.82	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	2	37	PSU	C6-C5-C4	2.31	119.73	118.17

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	2	43	PSU	C2'-C1'-C5-C4
4	2	43	PSU	O4'-C1'-C5-C4
4	2	43	PSU	O4'-C1'-C5-C6
4	2	43	PSU	C3'-C4'-C5'-O5'
4	2	43	PSU	O4'-C4'-C5'-O5'
4	2	44	PSU	O4'-C1'-C5-C4
4	2	44	PSU	O4'-C1'-C5-C6
4	2	58	PSU	C2'-C1'-C5-C4
4	2	58	PSU	O4'-C1'-C5-C4
4	2	58	PSU	O4'-C1'-C5-C6
4	2	47	OMC	O4'-C4'-C5'-O5'
4	2	47	OMC	C3'-C4'-C5'-O5'
4	2	47	OMC	C4'-C5'-O5'-P
4	2	47	OMC	O4'-C1'-N1-C6
4	2	44	PSU	O4'-C4'-C5'-O5'
4	2	43	PSU	C2'-C1'-C5-C6
4	2	47	OMC	C2'-C1'-N1-C6
4	2	47	OMC	O4'-C1'-N1-C2

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	2	37	PSU	1	0
4	2	47	OMC	1	0
4	2	58	PSU	1	0
4	2	39	PSU	2	0
4	2	40	OMC	4	0
4	2	41	PSU	3	0
4	2	43	PSU	1	0
4	2	34	PSU	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

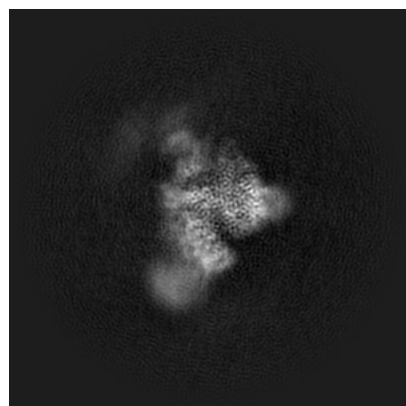
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74090. These allow visual inspection of the internal detail of the map and identification of artifacts.

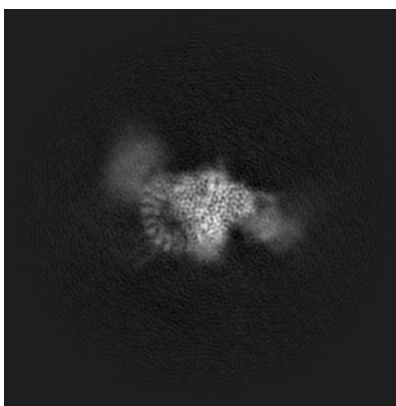
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

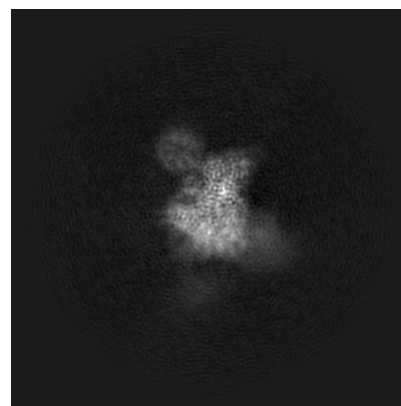
6.1.1 Primary map



X

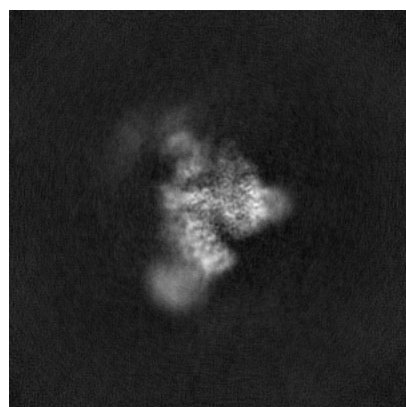


Y

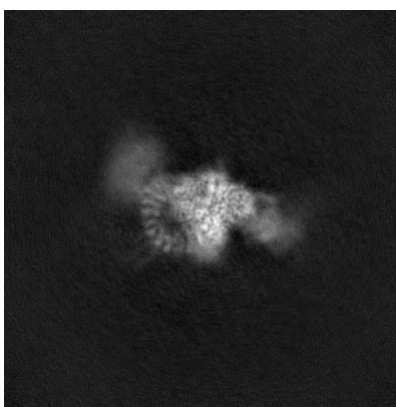


Z

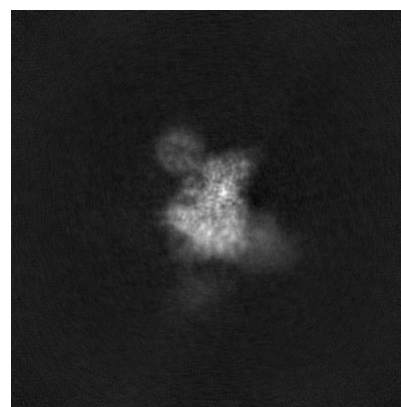
6.1.2 Raw map



X



Y

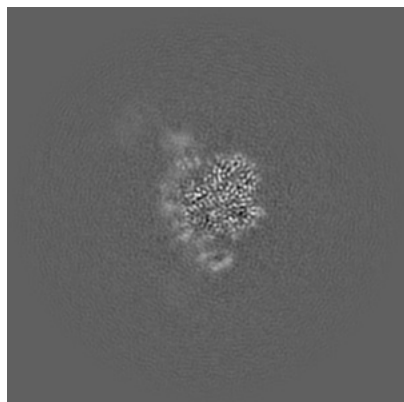


Z

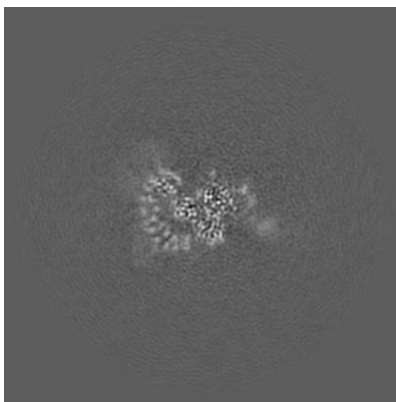
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

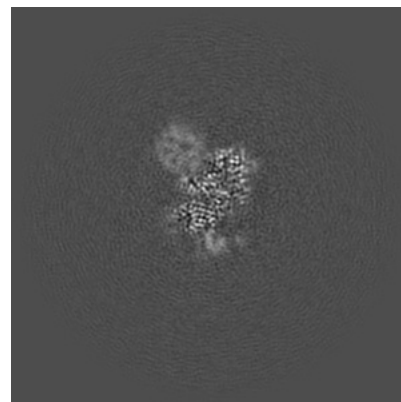
6.2.1 Primary map



X Index: 192

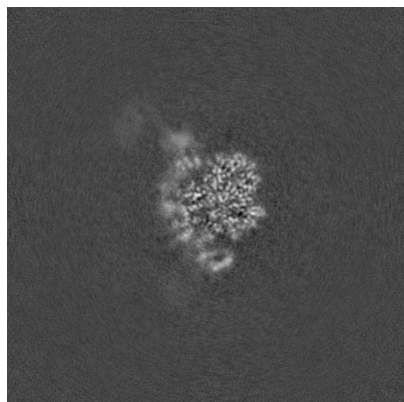


Y Index: 192

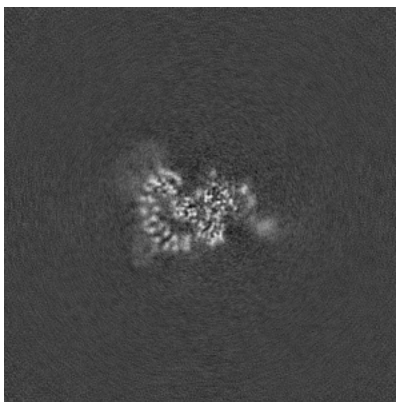


Z Index: 192

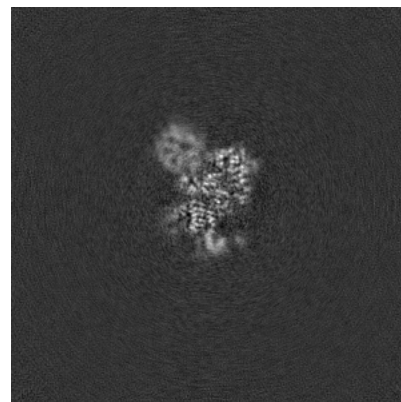
6.2.2 Raw map



X Index: 192



Y Index: 192

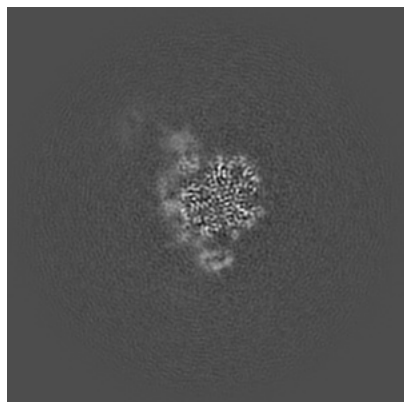


Z Index: 192

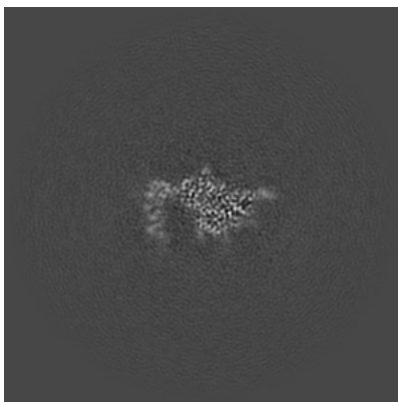
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

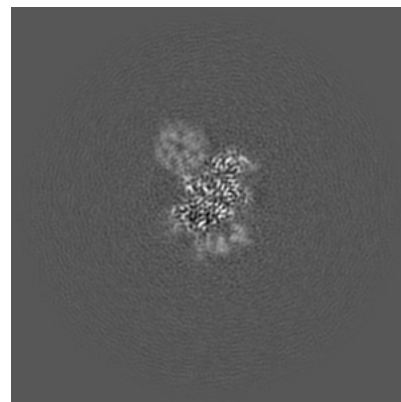
6.3.1 Primary map



X Index: 190

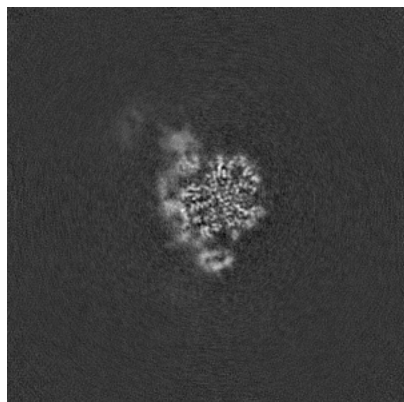


Y Index: 208

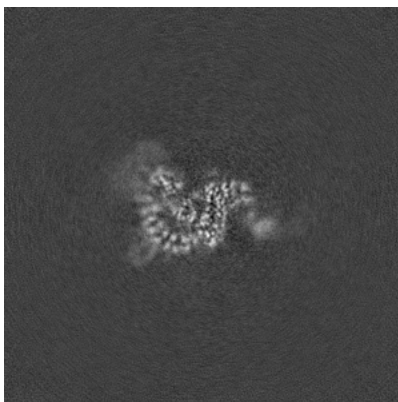


Z Index: 197

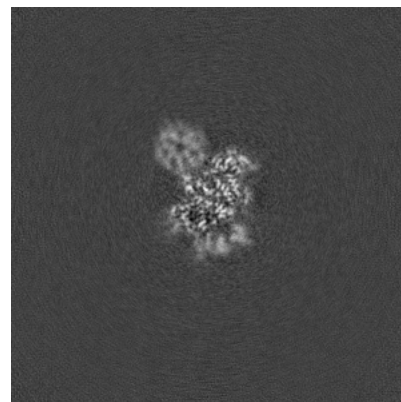
6.3.2 Raw map



X Index: 190



Y Index: 189

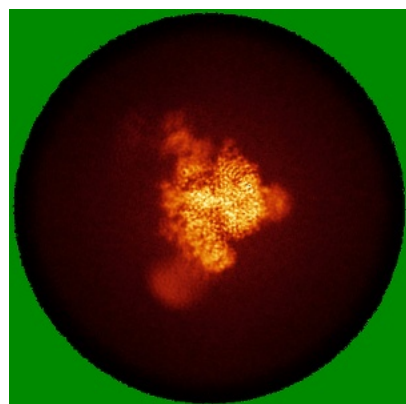


Z Index: 197

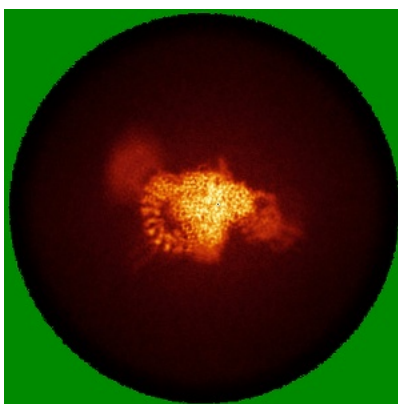
The images above show the largest variance slices of the map in three orthogonal directions.

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

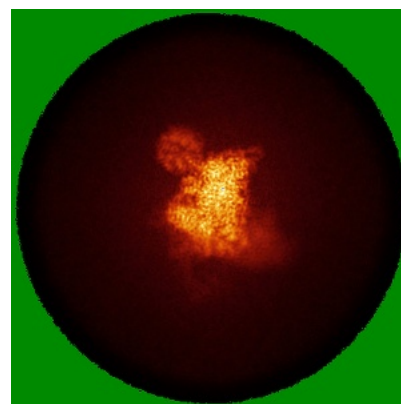
6.4.1 Primary map



X

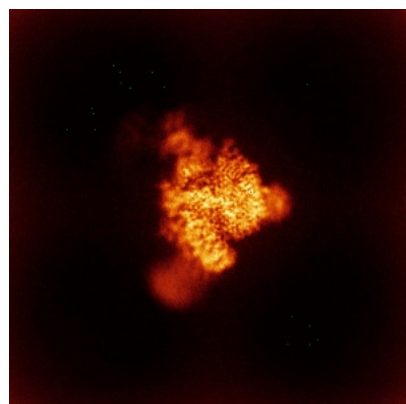


Y

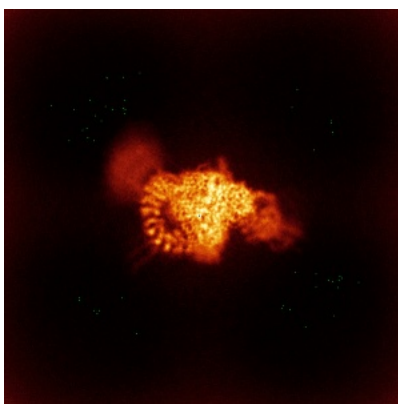


Z

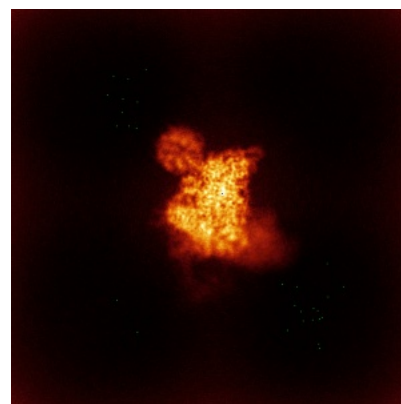
6.4.2 Raw map



X



Y

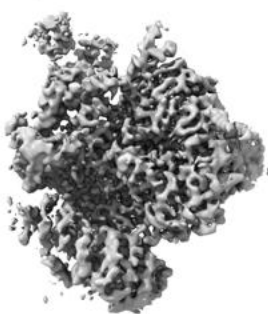


Z

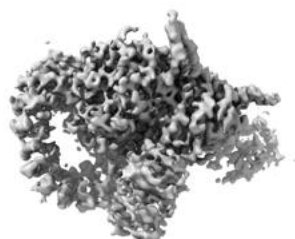
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

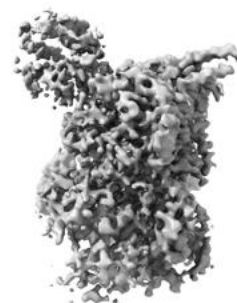
6.5.1 Primary map



X



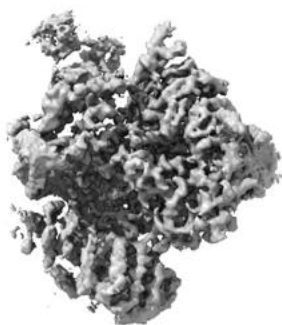
Y



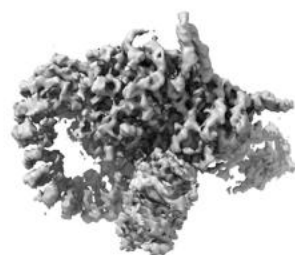
Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

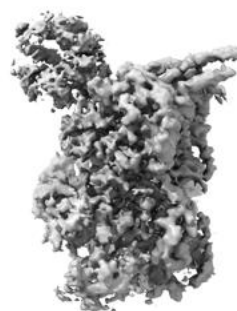
6.5.2 Raw map



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.

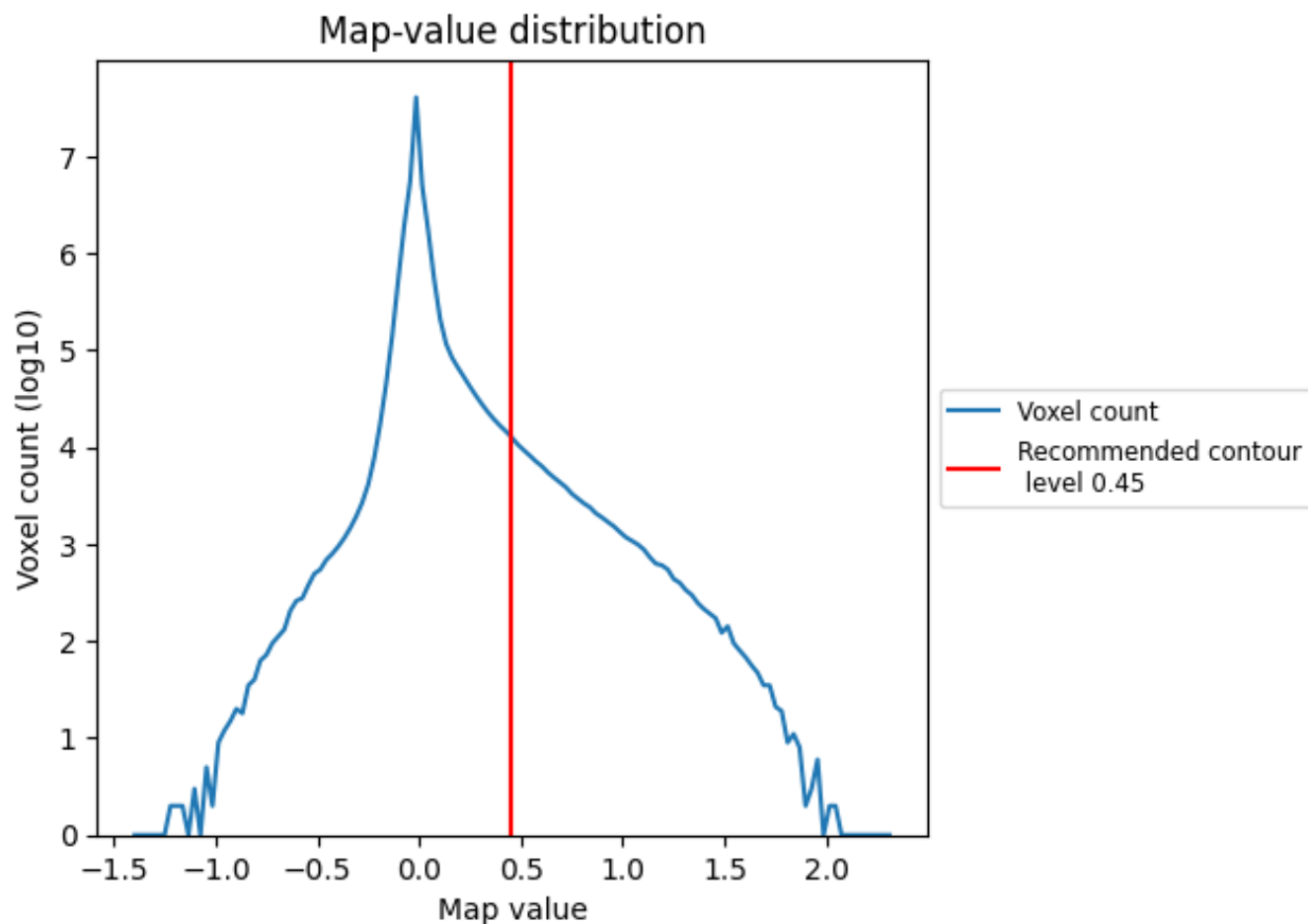
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

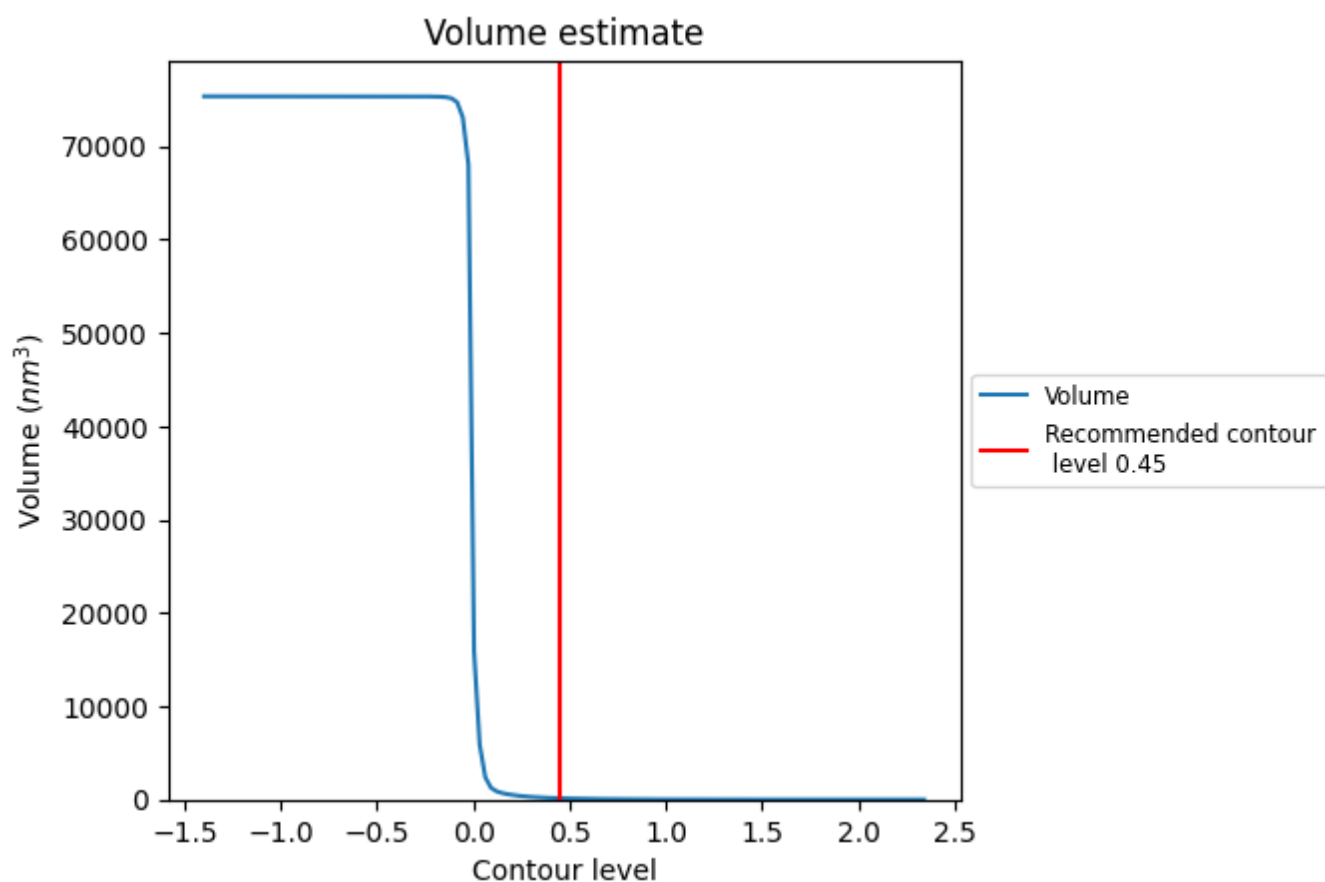
This section contains the results of statistical analysis of the map.

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.

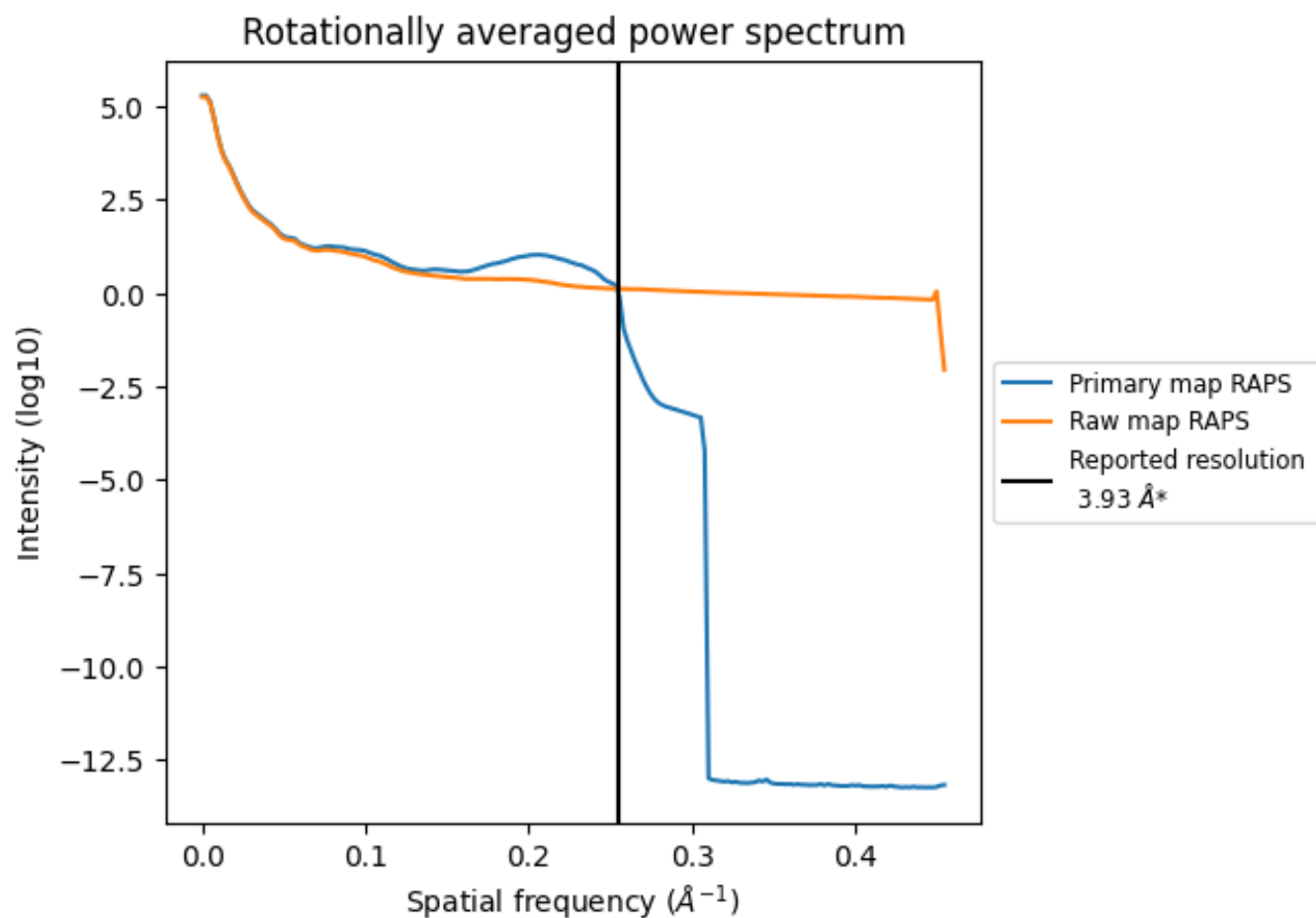
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 126 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 ⓘ

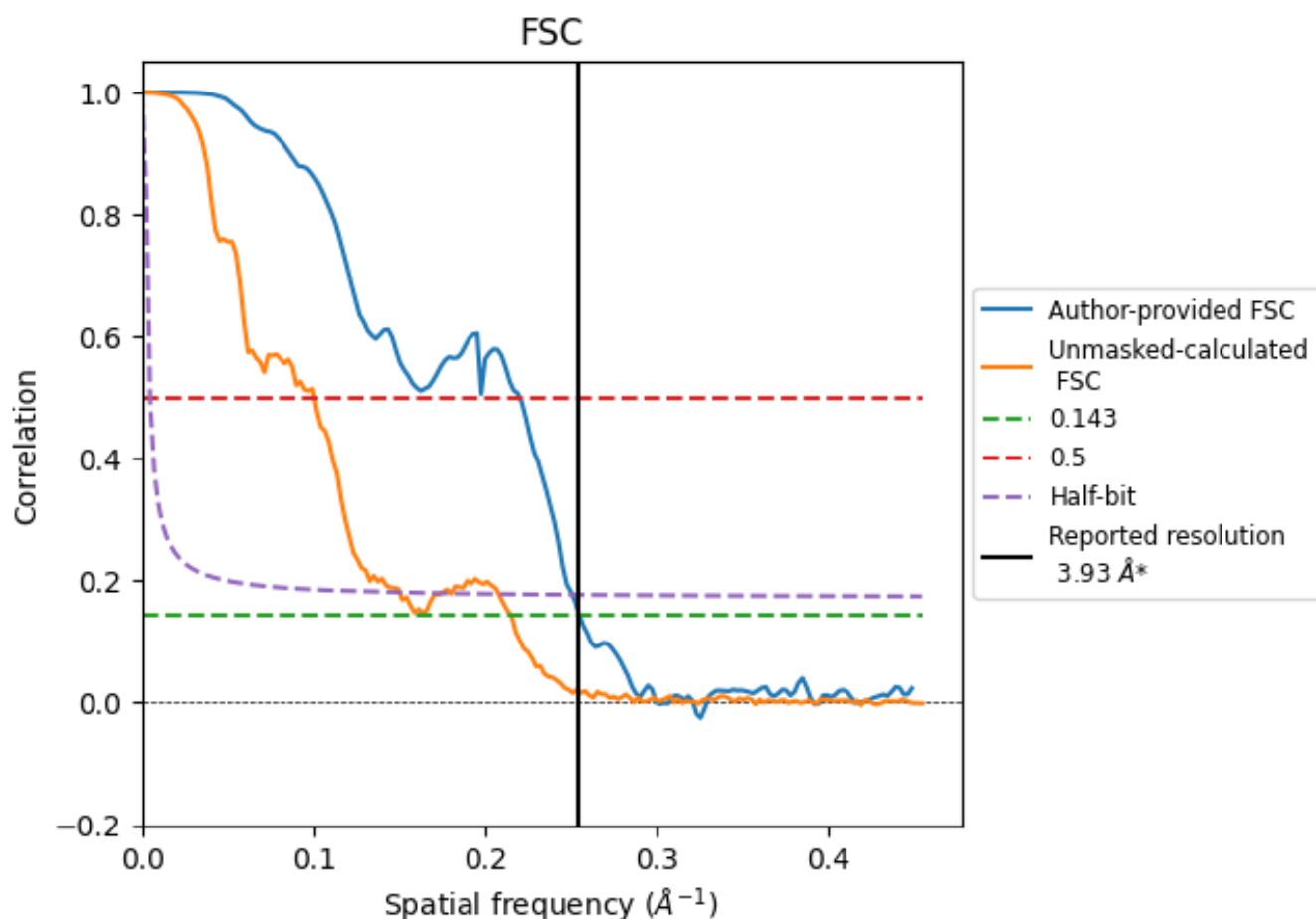


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

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 0.254 \AA^{-1}

8.2 Resolution estimates [i](#)

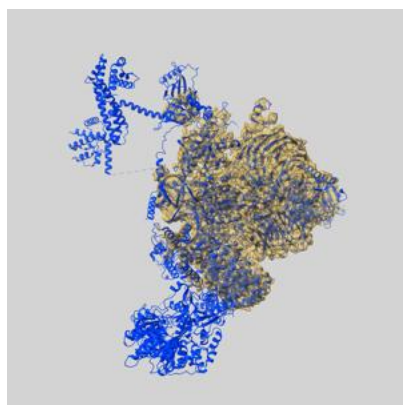
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.93	4.54	3.99
Unmasked-calculated*	4.65	9.97	6.67

*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 4.65 differs from the reported value 3.93 by more than 10 %

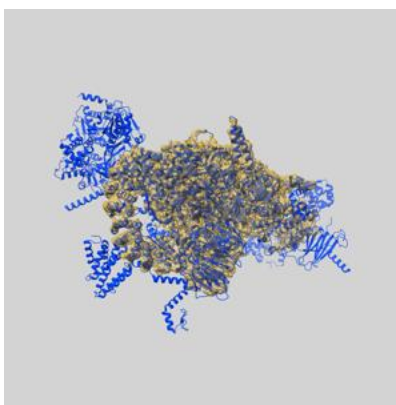
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74090 and PDB model 9ZE3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

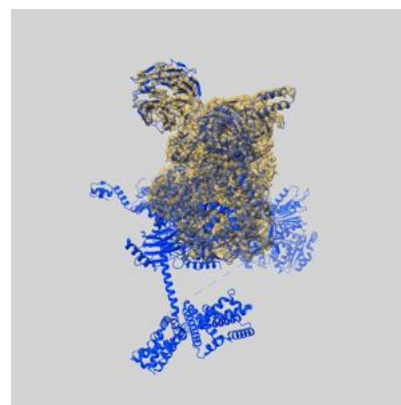
9.1 Map-model overlay [i](#)



X



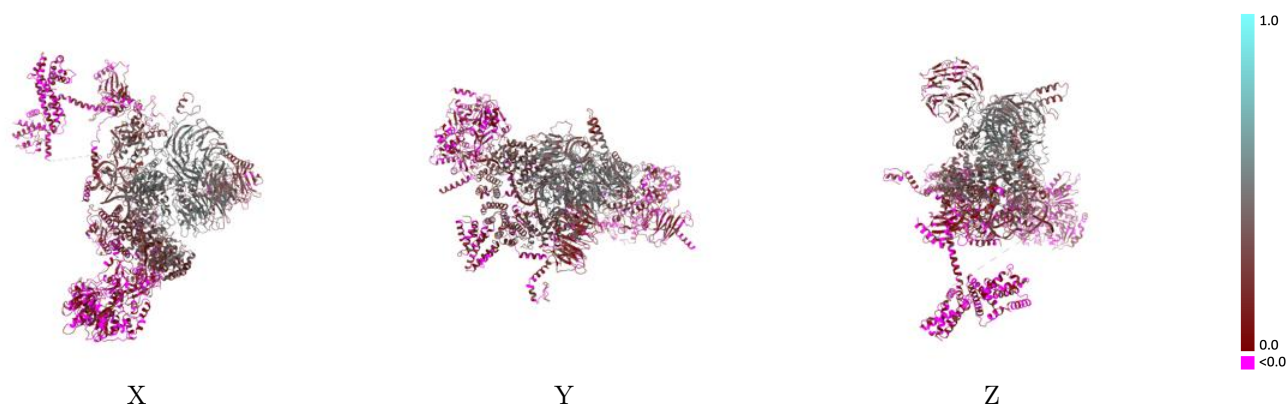
Y



Z

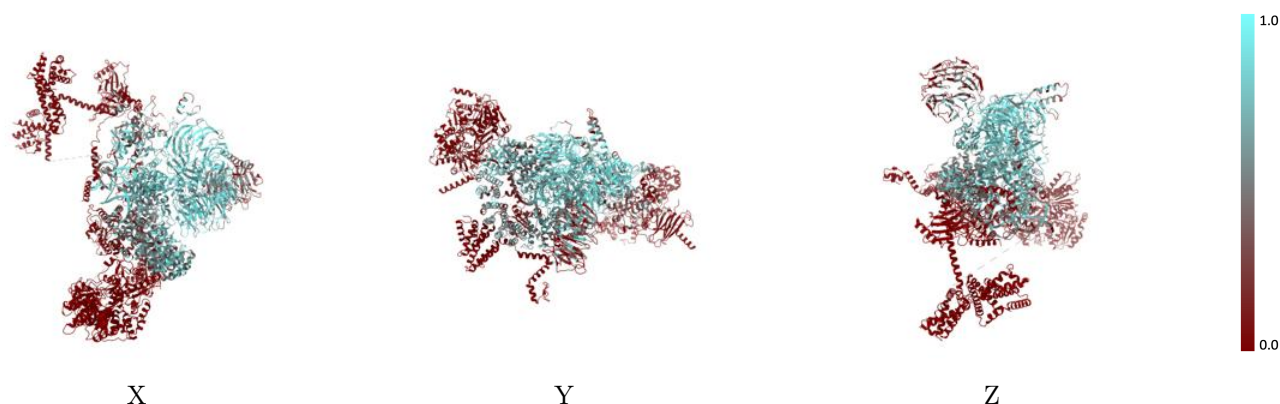
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



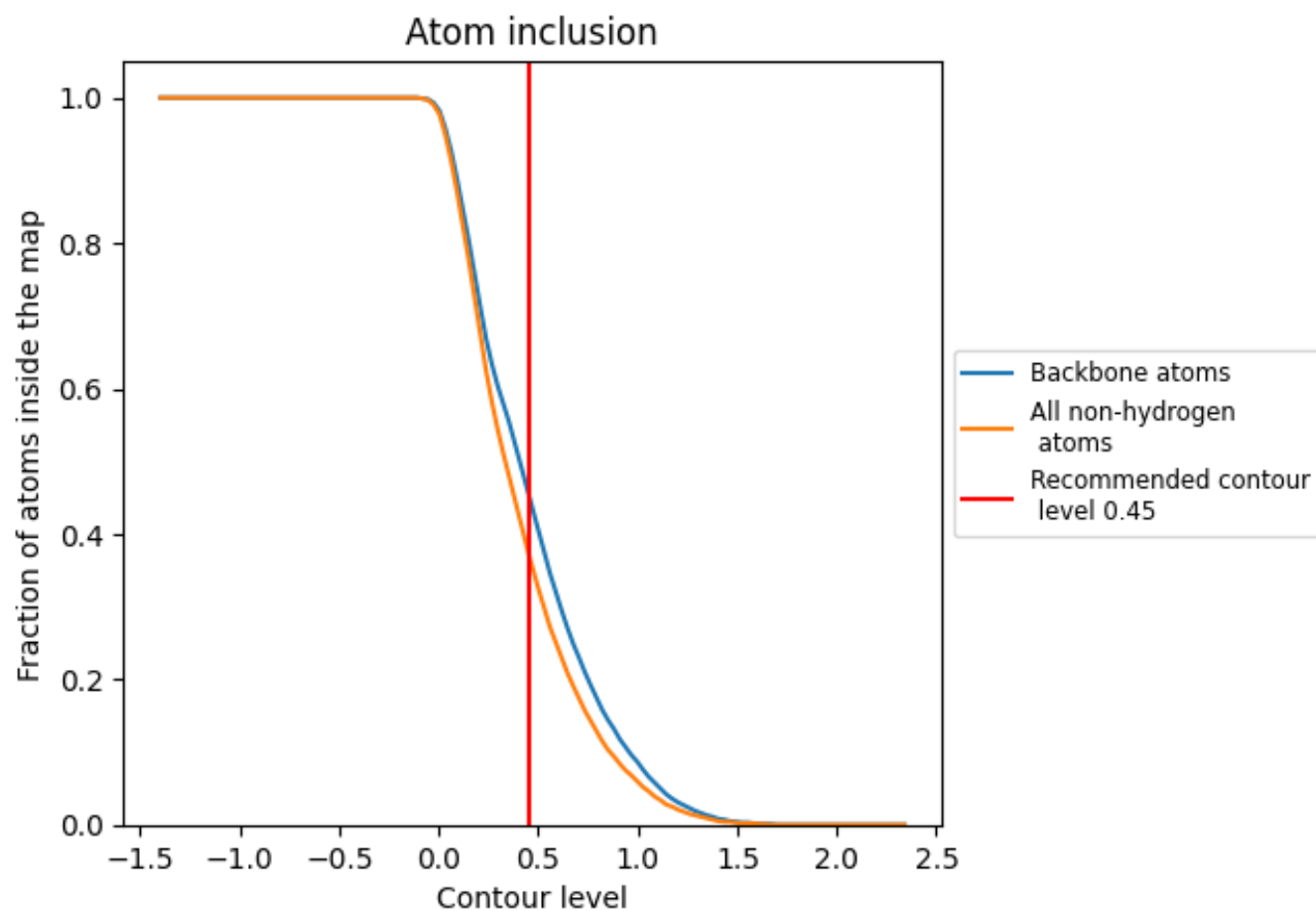
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.45).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 37% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3740	 0.2290
2	 0.6670	 0.2830
A	 0.0470	 0.0630
A1	 0.0010	 0.0460
A2	 0.0600	 0.1230
A3	 0.1880	 0.1130
B	 0.0000	 0.0270
B1	 0.5740	 0.3160
B2	 0.4830	 0.2980
B3	 0.6400	 0.3740
B4	 0.2510	 0.1910
B5	 0.7710	 0.4560
B6	 0.0080	 0.0910
C	 0.0030	 0.0790
H	 0.7540	 0.4360
R	 0.4080	 0.2090

