



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:57 PM UTC

PDB ID : 5LJ5 / pdb_00005lj5
EMDB ID : EMD-4057
Title : Overall structure of the yeast spliceosome immediately after branching.
Authors : Galej, W.P.; Wilkinson, M.F.; Fica, S.M.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on : 2016-07-17
Resolution : 10.00 Å(reported)

This is a wwPDB EM Validation Summary 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

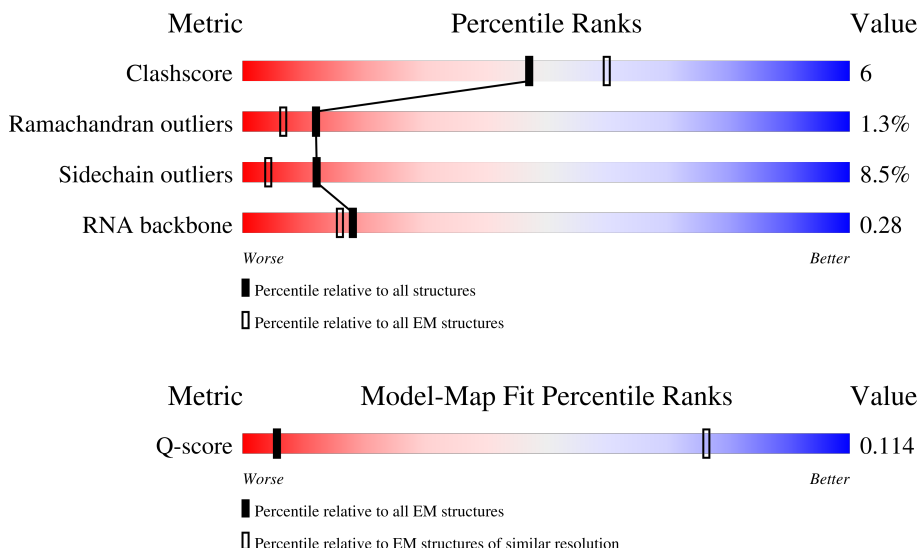
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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.



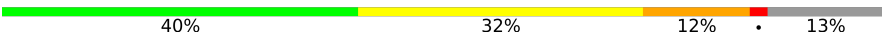
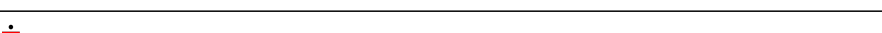
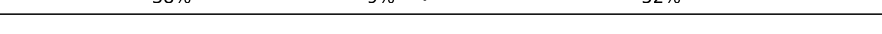
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	147 (9.50 - 10.50)

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	U	179	32% 36% 10% 21%
2	E	16	25% 56% 19%
3	I	76	22% 18% 57%

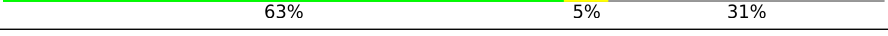
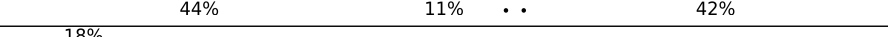
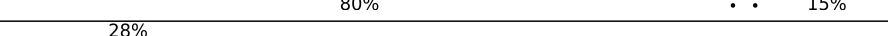
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Mol	Chain	Length	Quality of chain
4	Z	1175	
5	V	112	
6	A	2413	
7	B	2163	
8	D	278	
9	F	179	
10	C	1008	
11	G	235	
12	H	591	
13	J	451	
14	K	379	
15	L	157	
16	M	339	
17	N	364	
18	O	590	
19	P	175	
20	R	135	
21	S	687	
22	T	859	
23	b	196	
23	k	196	
24	d	101	
24	n	101	
25	e	94	
25	p	94	

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Mol	Chain	Length	Quality of chain
26	f	86	
26	q	86	
27	g	77	
27	r	77	
28	h	146	
28	l	146	
29	j	110	
29	m	110	
30	W	238	
31	Y	111	
32	Q	1071	
33	t	503	
33	u	503	
33	v	503	
33	w	503	
34	s	175	
35	x	188	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	ZN	N	401	-	-	X	-
37	ZN	N	402	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 85476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U5 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

- Molecule 2 is a RNA chain called Exon 1 (5' exon) of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	16	Total	C	N	O	P	0	0
			346	155	66	109	16		

- Molecule 3 is a RNA chain called Intron of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	33	Total	C	N	O	P	0	0
			693	312	116	232	33		

- Molecule 4 is a RNA chain called U2 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	171	Total	C	N	O	P	0	0
			3610	1614	604	1221	171		

- Molecule 5 is a RNA chain called U6 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	97	Total	C	N	O	P	0	0
			2066	925	368	676	97		

- Molecule 6 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	2168	Total	C	N	O	S	0	0
			16919	10835	2966	3060	58		

- Molecule 7 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	1707	Total	C	N	O	1	0
			8462	5048	1707	1707		

- Molecule 8 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	114	Total	C	N	O	S	0	0
			912	577	165	162	8		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	F	46	Total	C	N	O	0	0
			321	203	61	57		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	882	Total	C	N	O	S	0	0
			6756	4393	1133	1203	27		

- Molecule 11 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	97	Total	C	N	O	S	0	0
			823	513	154	155	1		

- Molecule 12 is a protein called CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	399	Total	C	N	O	S	0	0
			2639	1657	468	506	8		

- Molecule 13 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	326	Total	C	N	O	S	0	0
			2556	1616	454	476	10		

- Molecule 14 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	163	Total	C	N	O	S	0	0
			1289	808	236	240	5		

- Molecule 15 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1270	797	238	225	10		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	252	Total	C	N	O	S	0	0
			2012	1277	354	370	11		

- Molecule 17 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	209	Total	C	N	O	S	0	0
			1658	1055	287	301	15		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	283	Total	C	N	O	S	0	0
			2068	1285	385	392	6		

- Molecule 19 is a protein called CWC15.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	P	36	Total	C	N	O	0	0
			275	176	53	46		

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	97	Total	C	N	O	0	0
			544	325	106	113		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	464	Total	C	N	O	S	0	0
			3121	1949	581	584	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	592	Total	C	N	O	0	0
			2946	1762	592	592		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
23	k	80	Total	C	N	O		0	0
			396	236	80	80			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
24	n	82	Total	C	N	O		0	0
			404	240	82	82			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
25	p	75	Total	C	N	O		0	0
			369	219	75	75			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
26	q	72	Total	C	N	O		0	0
			354	210	72	72			

- Molecule 27 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
27	r	69	Total	C	N	O		0	0
			340	202	69	69			

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
28	l	79	Total	C	N	O		0	0
			392	234	79	79			

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
29	m	94	Total	C	N	O		0	0
			467	279	94	94			

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	W	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Y	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 32 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Q	619	Total	C	N	O	0	0
			3066	1828	619	619		

- Molecule 33 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	t	438	Total	C	N	O	0	0
			2171	1295	438	438		
33	u	437	Total	C	N	O	0	0
			2166	1292	437	437		
33	v	426	Total	C	N	O	0	0
			2111	1259	426	426		
33	w	435	Total	C	N	O	0	0
			2156	1286	435	435		

- Molecule 34 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	110	Total	C	N	O	0	0
			548	328	110	110		

- Molecule 35 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	132	Total	C	N	O	0	0
			660	396	132	132		

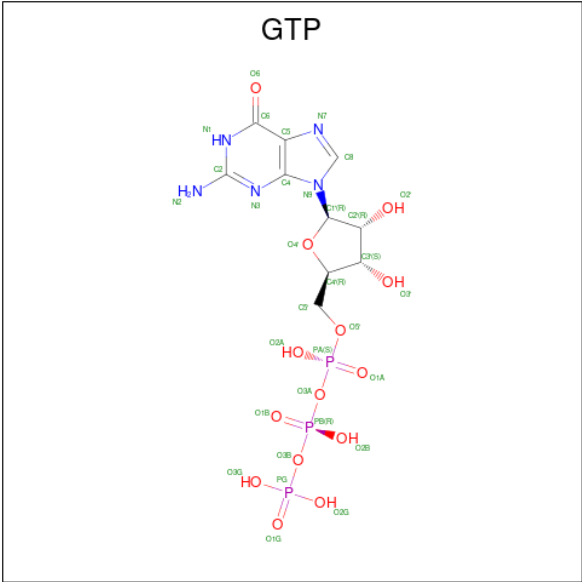
- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	E	1	Total	Mg	0
			1	1	
36	V	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	D	1	Total	Zn	0
			1	1	
37	L	3	Total	Zn	0
			3	3	
37	M	1	Total	Zn	0
			1	1	
37	N	2	Total	Zn	0
			2	2	

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

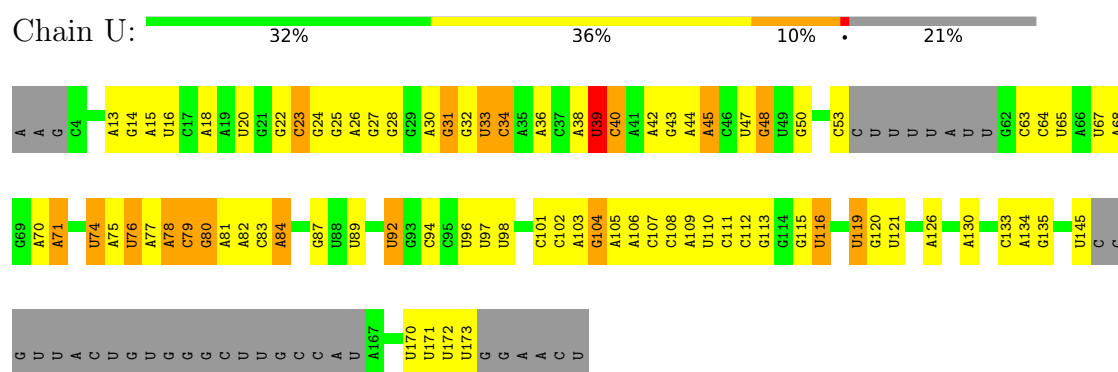


Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

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.

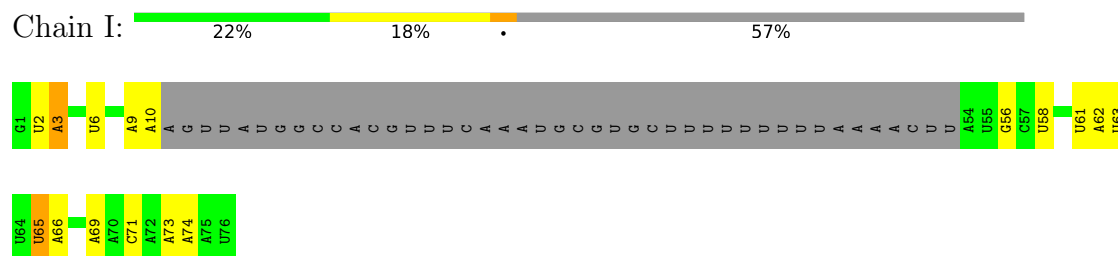
- Molecule 1: U5 snRNA (small nuclear RNA)



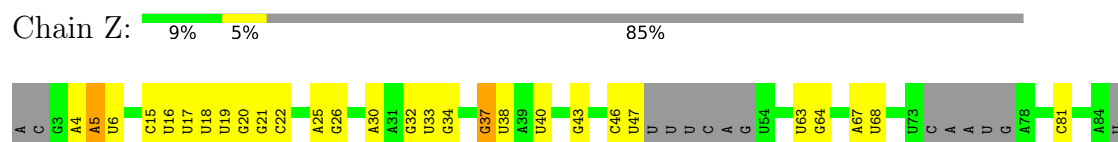
- Molecule 2: Exon 1 (5' exon) of UBC4 pre-mRNA



- Molecule 3: Intron of UBC4 pre-mRNA

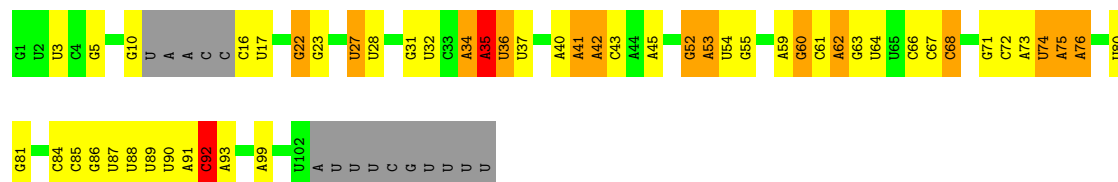


- Molecule 4: U2 snRNA (small nuclear RNA)



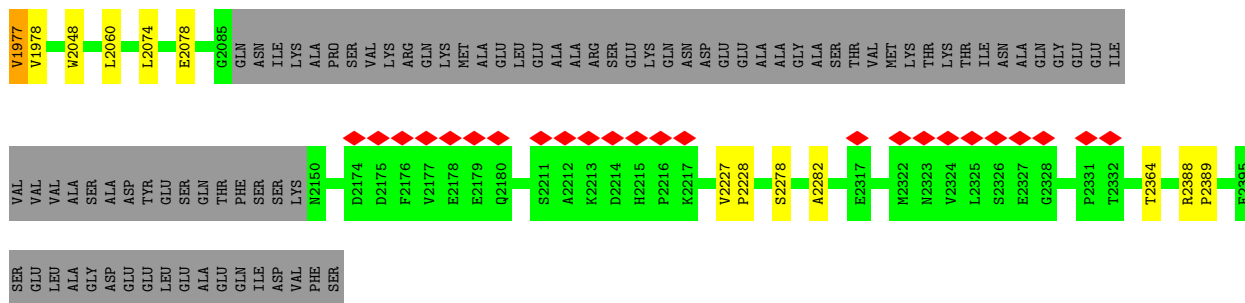


- Chain V: 40% 32% 12% • 13%

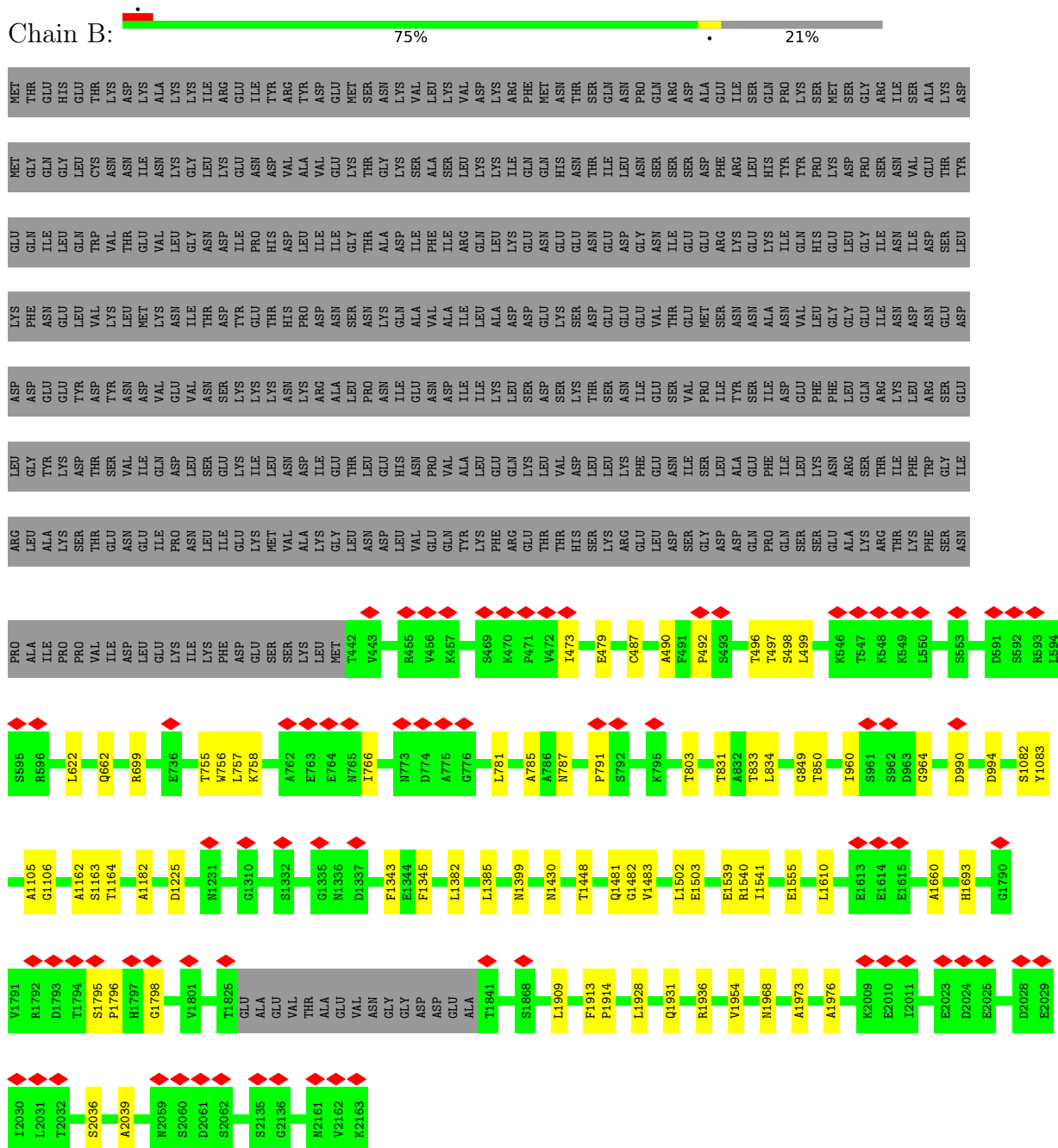


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- Molecule 7: Pre-mRNA-splicing helicase BRR2



- Molecule 8: Protein CWC16

Chain D: 

MET	S2	E3	N8	Y11	L23	S24	R25	L31	M34	L43	F47	S46	M49	R50	C51	I58	K63	L71	L76	I79	I86	S87	C88	T99	D100	P101	R114	N115	THR	VAL	PRO	GLN	ASP	LYS	PRO	ASN	ASP	LEU	ASN	ALA	LYS	THR	ALA	VAL							
GLU	SER	ILE	ASP	THR	LEU	GLN	ARG	GLY	LYS	GLY	ASN	GLU	LYS	THR	GLY	ILE	GLY	GLN	ASP	LYS	ASP	LEU	GLY	ARG	LEU	ALA	LYS	ILE	GLN	GLY	GLU	GLN	GLU	GLN	ASP	ASP	GLY	GLU	ASP	GLN	THR	LYS	ARG	LYS	THR	ALA	VAL				
GLU	MET	SER	GLN	ARG	ALA	GLY	MET	ILE	ASN	ARG	SER	LYS	HIS	ALA	GLN	GLY	LEU	THR	VAL	LYS	VAL	THR	GLY	ARG	THR	LYS	ASN	LYS	PRO	ASN	THR	GLY	ASP	GLY	GLU	ASP	GLY	GLU	ASP	GLY	GLU	ASP	GLY	GLU	ASP	GLY	GLU	ASP	GLY	GLU	
THR	LYS	GLY	LYS	ILE	GLN	LYS	LYS	LYS	SER	SER	ARG	THR	ASN	ASN	PRO	GLY	LEU	THR	VAL	ILE	LYS	VAL	THR	GLY	ARG	THR	LYS	ASN	LYS	PRO	ASN	THR	GLY	ASP	GLY	GLU	ASP	GLY	GLU	ASP	GLY	GLU	ASP	GLY	GLU	ASP	GLY	GLU	ASP	GLY	GLU

- Molecule 9: Pre-mRNA-splicing factor CWC25

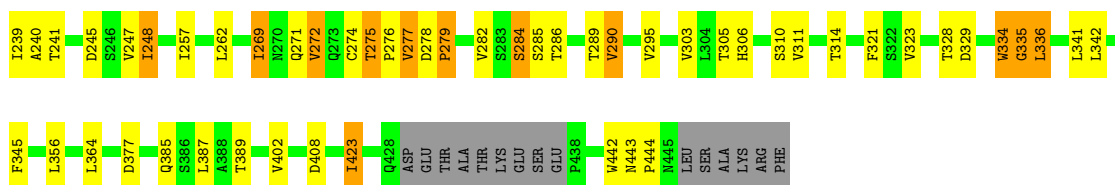
Chain F: 

ARG	ARG	THR	PRO	ASP	SER	THR	LYS	LYS	ARG	ALA	MET	SER	SER	GLN	ARG	GLY	LYS	PRO	PRO	LEU	SER	LYS	PRO	ALA	PRO	ASP	LEU	ASP	TYR																								
TYR	LEU	GLY	LYS	LYS	LEU	SER	ILE	ASN	GLN	PRO	ALA	THR	PRO	VAL	ARG	ALA	ALA	THR	THR	ILE	SER	ALA	SER	GLY	ALA	ALA	THR	SER	ILE	SER	SER	GLN	LYS	LYS	LYS	SER	LEU	GLU	TRP	MET	TYR	GLN	ASP	ALA	LYS	LEU	SER	ASP	GLU	LYS	GLU		
MET	S3	L6	R20	V23	E27	I31	Q34	R48	GLU	LEU	ASN	GLU	LEU	LEU	ASN	GLU	THR	LYS	LYS	PRO	GLY	ASP	LEU	ALA	LYS	LYS	SER	GLY	GLU	GLU	TRP	MET	TYR	GLN	ASP	ALA	LYS	LEU	SER	ASP	GLU	LYS	GLU	GLU									

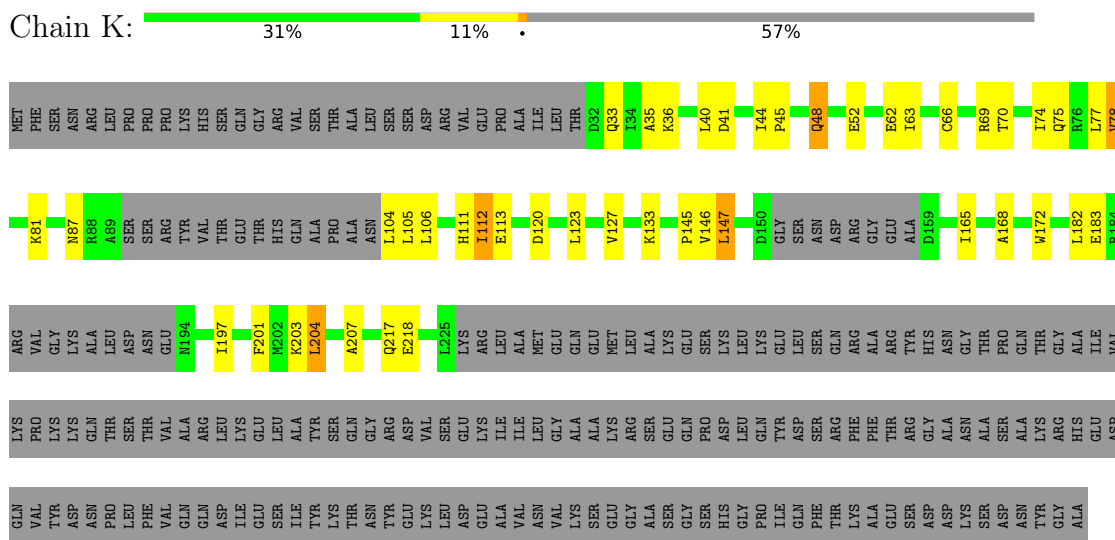
- Molecule 10: Pre-mRNA-splicing factor SNU114

Chain C: 

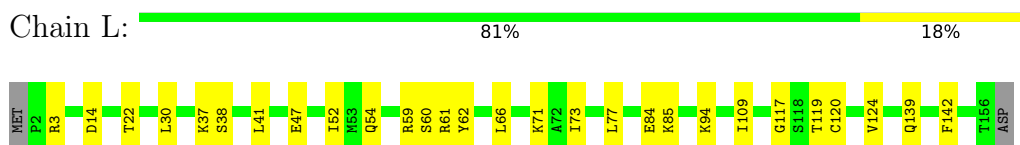
MET	GLU	GLY	ASP	LEU	PHE	ASP	GLY	PHE	ASN	ILE	GLY	VAL	ASP	PRO	PHE	ASP	SER	ASP	GLU	GLY	GLU	GLN	THR	ASN	THR	PHE	GLY	SER	GLY	ASN	ASN	ASN	ASN	GLU	ILE	GLU	TRP	MET	GLN	ASP	GLY	LEU	SER	VAL	THR	GLY	SER	LYS	
	GLU	LEU	GLY	ILE	SER	LEU	GLU	HIS	PRO	GLY	G71	V76	L77	M78	E92	P93	V94	L100	H103	T104	I105	F106	T107	Q108	L109	T116	R117	S125	M126	A127	N128	I129	R132	I133	V136	G137	V138	I139	L152	L153	D156	W172	I185	I191	K192				
	L193	C200	T201	S207	R208	M209	L210	N211	F212	L213	V219	R220	F221	D223	M222	E224	T225	A226	V227	A228	L229	E230	A231	L234	V235	L236	V241	V242	Q251	L252	Q255	N259	V261	C264	F265	V266	I267	N268	K269	L270	D271	L272	L274	L277	K287	I291			
	G301	I311	I312	F313	A314	S315	L318	G319	F320	T321	F322	T323	V328	S335	I336	T345	N358	I379	F380	L381	I384	F385	L389	S390	N391	L399	L400	R401	V406	N407	L408	Q418	P419	F420	L421	V424	L427	Q431	Q432	L435	V436	Q560	D437	A438					
	I439	Q444	P445	E446	T447	L448	W449	A470	H471	V472	L473	K474	T475	V486	R487	L488	L492	L493	V499	R500	I501	T504	I518	SER	LYS	THR	THR	THR	THR	ASN	GLY	ASP	GLU	ASP	M652	D653	C654	L655	L656	F657	D658	F663	G664	L665	L666	Q660	I670		
	V562	F677	N693	ILE	SER	ARG	LEU	GLY	GLU	GLU	ASN	LEU	PRO	GLY	LEU	SER	LEU	W708	S709	V710	R725	ASN	THR	LEU	GLY	GLY	GLN	ASN	CYS	LEU	ASP	ILE	GLY	ASP	ASP	F744	K749	T753	L760	V766	S767	F768	Y769	N770	GLY	ASN	VAL	L774	S784



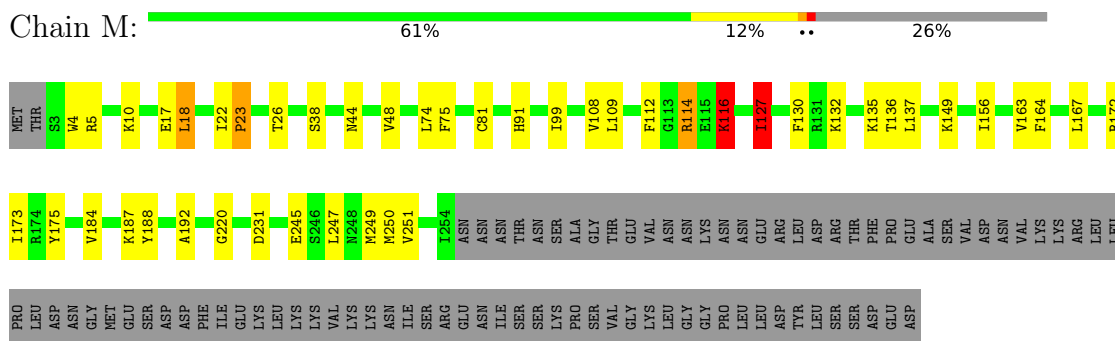
• Molecule 14: Pre-mRNA-processing protein 45



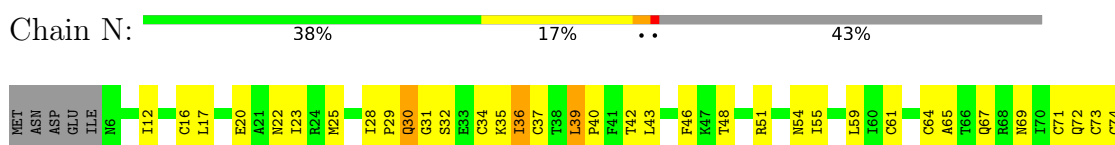
• Molecule 15: Pre-mRNA-splicing factor BUD31

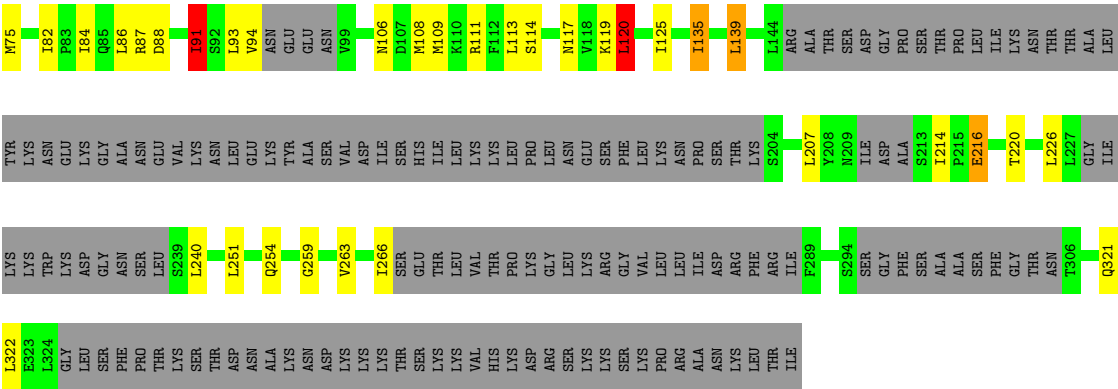


• Molecule 16: Pre-mRNA-splicing factor CWC2

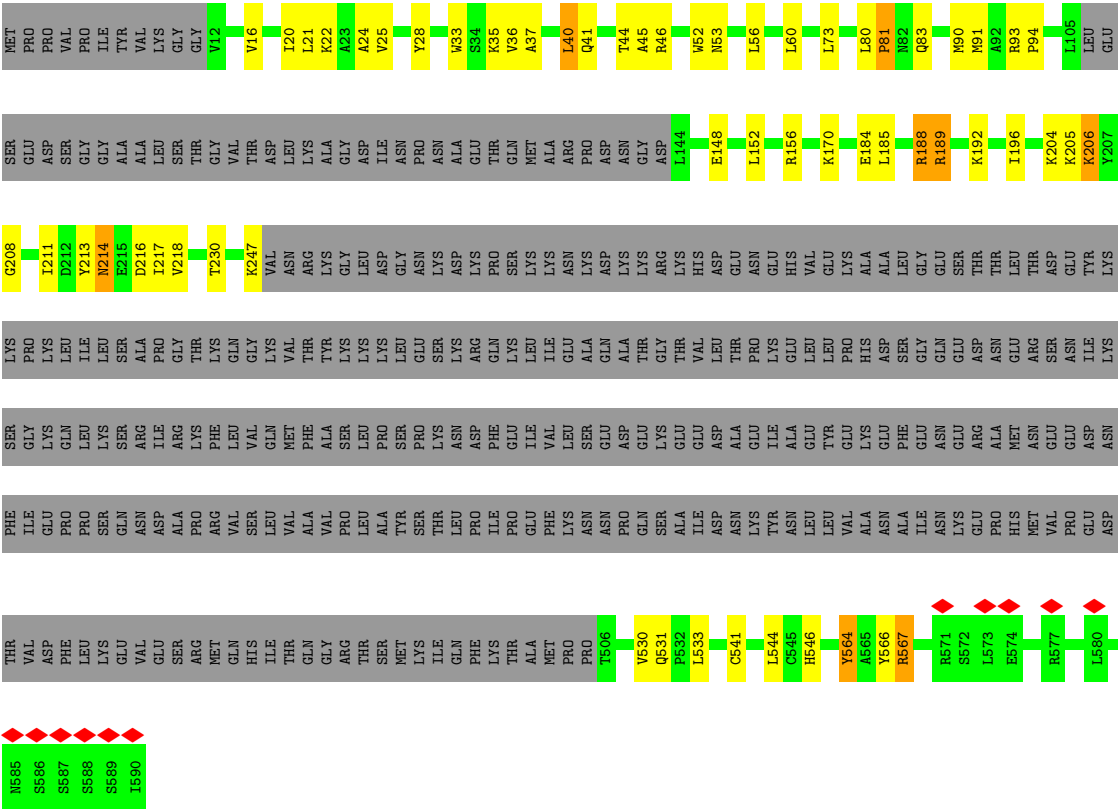
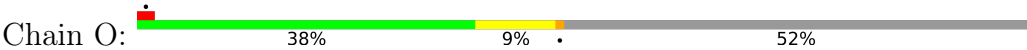


• Molecule 17: Pre-mRNA-splicing factor SLT11

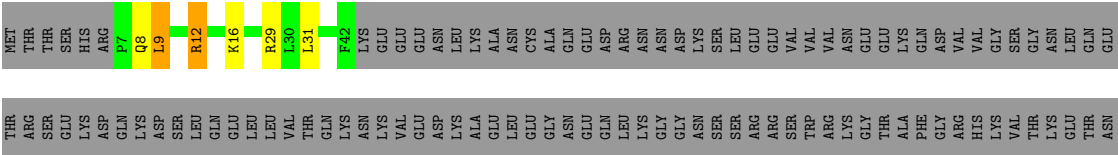




● Molecule 18: Pre-mRNA-splicing factor CEF1



● Molecule 19: CWC15



ILE
LYS
GLU
HIS
ALA
THR
LYS
LYS
SER
SER
ALA
SER
GLY
TVR
ILE
ILE
ASN
ASP
MET
THR
THR
LYS
SER
SER
GLU
HIS
HIS
HIS
VAL
ARG

• Molecule 20: Pre-mRNA-splicing factor CWC21

Chain R: 59% 10% 28%

MET
S2
I6
G7
L8
K12
G13
S14
S15
T16
N28
R31
P32
Q33
G34
S35
Q36
Q37
Q38
R39
Q40
Q41
S50
HIS
ASP
HIS
LYS
ALA
LYS
SER
ARG
PRO
PRO
LEU
ALA
VAL
GLN
LYS
GLN
I64
Q111
GLU
GLN
GLN
ARG
MET
SER
SER
LEU
TYR
THR
PRO
LYS
ALA
ARG
LEU

THR
GLU
GLU
GLN
HIS
ARG
HIS
GLU

• Molecule 21: Pre-mRNA-splicing factor CLF1

Chain S: 57% 8% 32%

MET
ASP
THR
LEU
GLU
PRO
THR
ALA
VAL
ASP
THR
HIS
VAL
SER
ALA
GLU
GLN
ILE
LEU
ARG
ASP
VAL
TVR
LYS
LYS
GLY
GLN
ALA
ARG
GLY
SER
THR
ASN
ILE
ASP
ASP
I37
R44
R48
Y57
R60
Q67
A72
E77
Q78
M81
R82
R83
I87
F88
E89

L92
I99
P100
V112
K113
C114
I115
N116
H117
A118
R119
M122
V132
L140
I141
V142
E143
E144
V149
V152
L155
Y156
T157
K158
W159
C160
V169
F172
V173
G184
T188
Y189
Y192
V193
M199
W202
E209
E216
F217
T218
L224

A225
I226
D227
T228
V229
N234
I237
W238
V243
L246
Q257
Y260
S263
L266
I271
E272
K273
TRP
PRO
PRO
SER
N277
F291
GLY
ASP
ASP
N295
W315
ASN
ALA
TYR
ASP
Y320
L329
E332
F334
P335
I338
S349
ARG
PRO
LYS
GLU
LEU
SER

K356
E377
LEU
ASN
S381
I395
ILE
PRO
HIS
HIS
HIS
PHE
THR
F403
R416
ASP
D419
V420
G432
LEU
CYS
PRO
LYS
SER
ALA
LYS
T439
L450
E452
Q467
PRO
SER
D470
L471
M483
LEU
G485
E500
ASN
SER
ASP
PHE
LEU
THR
K507
E521
THR
PHE
GLU
SER

GLN
GLU
PHE
GLU
GLU
ASP
A630
N641
GLN
TYR
SER
P645
T656
SER
PRO
THR
THR
GLU
GLN
GLN
LEU
LEU
ASP
LEU
ALA
LYS
LEU
VAL
PHE
GLU
PHE
ILE
LYS
VAL
GLU
ASP
GLU
SER
GLU
ASN
LYS
LEU
GLU
ASN
LYS
LEU
GLU
PHE
GLU
GLU
VAL
PHE
GLU
PHE
GLU
PHE

LYS
GLU
LYS
ASP
ASP
LYS
LYS
GLY
ARG
LEU
SER
ILE
ILE
PHE
ASN
VAL
GLU
ALA
LYS
LYS
ASP
TVR
GLU
GLU
THR
GLY
THR
GLU
LEU
ALA
LYS
GLN
GLN
GLN
ALA
LEU

ASP
ILE
ASP
ASP
ASP
LYS
PRO
LYS
PRO
GLY
PRO
SER
LYS
PHE
PHE
LEU
GLU
LEU
ALA
LYS
LYS
TRP
LYS
GLN
GLU
GLN
ALA
LEU

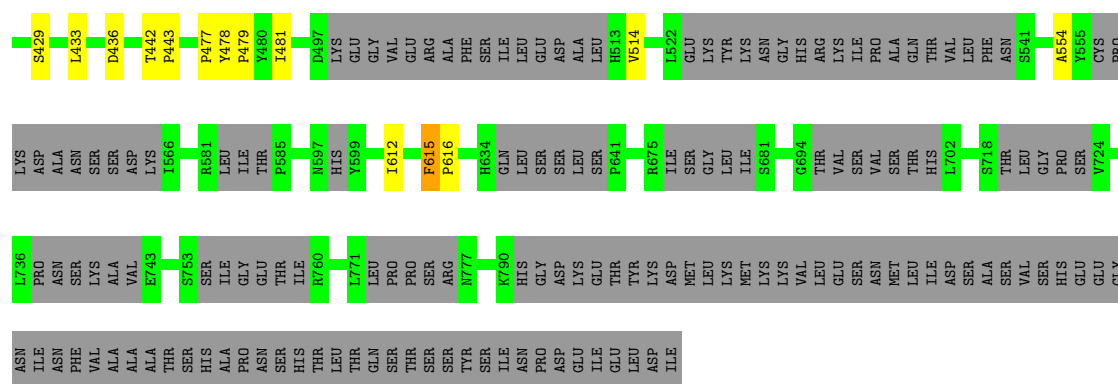
• Molecule 22: Pre-mRNA-splicing factor SYF1

Chain T: 66% 31%

MET
SER
ALA
TYR
ILE
ALA
MET
LYS
LYS
GLY
VAL
ILE
THR
ASN
VAL
ASP
GLU
GLU
ASN
ASN
ASN
ASN
I21
I37
K48
GLU
GLY
GLY
ARG
THR
D54
S63
THR
LYS
GLU
VAL
VAL
VAL
E69
A119
I120
E121
GLN
TYR
ASP
LEU
ALA
M127
I128
E140
ARG
M143
Y159
LEU
PRO
PRO
LEU

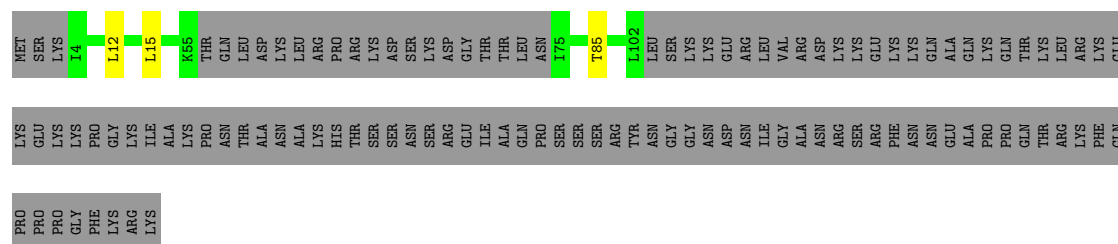
THR
GLN
ASP
LEU
SER
GLN
GLU
GLU
GLU
E174
T191
LYS
GLY
GLY
PHE
PHE
ILE
SER
SER
GLU
ILE
SER
GLU
ASN
THR
Q209
Y218
LYS
LYS
VAL
VAL
ALA
PRO
Q224
R238
I120
ASP
N240
L251
PRO
GLN
ASP
GLU
ASN
SER
GLY
LYS
TVR
LEU
PRO
SER
SER
SER
LEU

LEU
PRO
PHE
GLU
L270
G282
LEU
D284
G296
ILE
TVR
P299
D300
F304
G314
SER
ARG
G317
Q332
THR
LEU
ARG
TYR
SER
SER
ASP
F339
I342
K360
D365
SER
LYS
PHE
PHE
ASN
GLN
LYS
D373
H381
L391
N397
A400
S405
ASN
L407
S420
A421



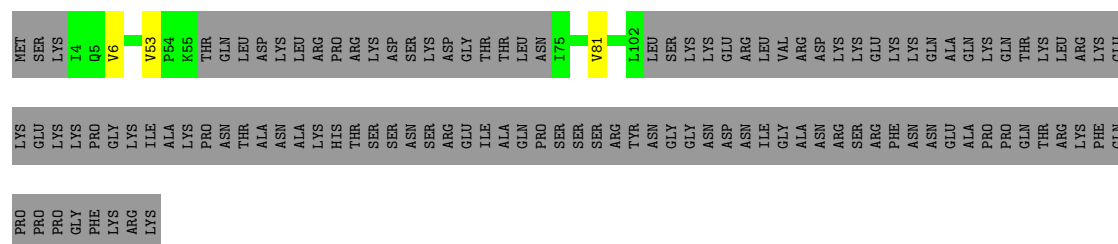
• Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain b: 39% 59%



• Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain k: 39% 59%



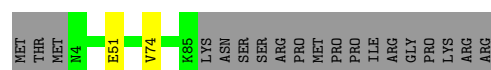
• Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain d: 69% 10% 19%



• Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain n: 79% 19%



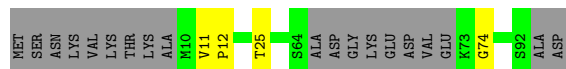
- Molecule 25: Small nuclear ribonucleoprotein E

Chain e:  64% 16% 20%



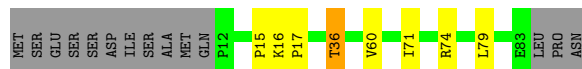
- Molecule 25: Small nuclear ribonucleoprotein E

Chain p:  76% • 20%



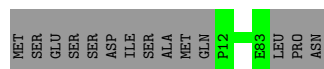
- Molecule 26: Small nuclear ribonucleoprotein F

Chain f:  74% 8% • 16%



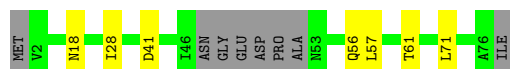
- Molecule 26: Small nuclear ribonucleoprotein F

Chain q:  84% 16%



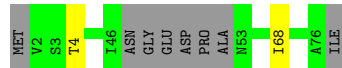
- Molecule 27: Small nuclear ribonucleoprotein G

Chain g:  81% 9% 10%



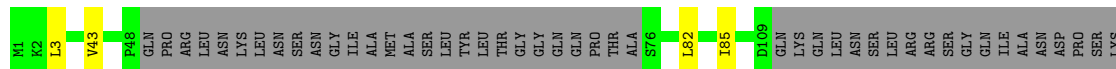
- Molecule 27: Small nuclear ribonucleoprotein G

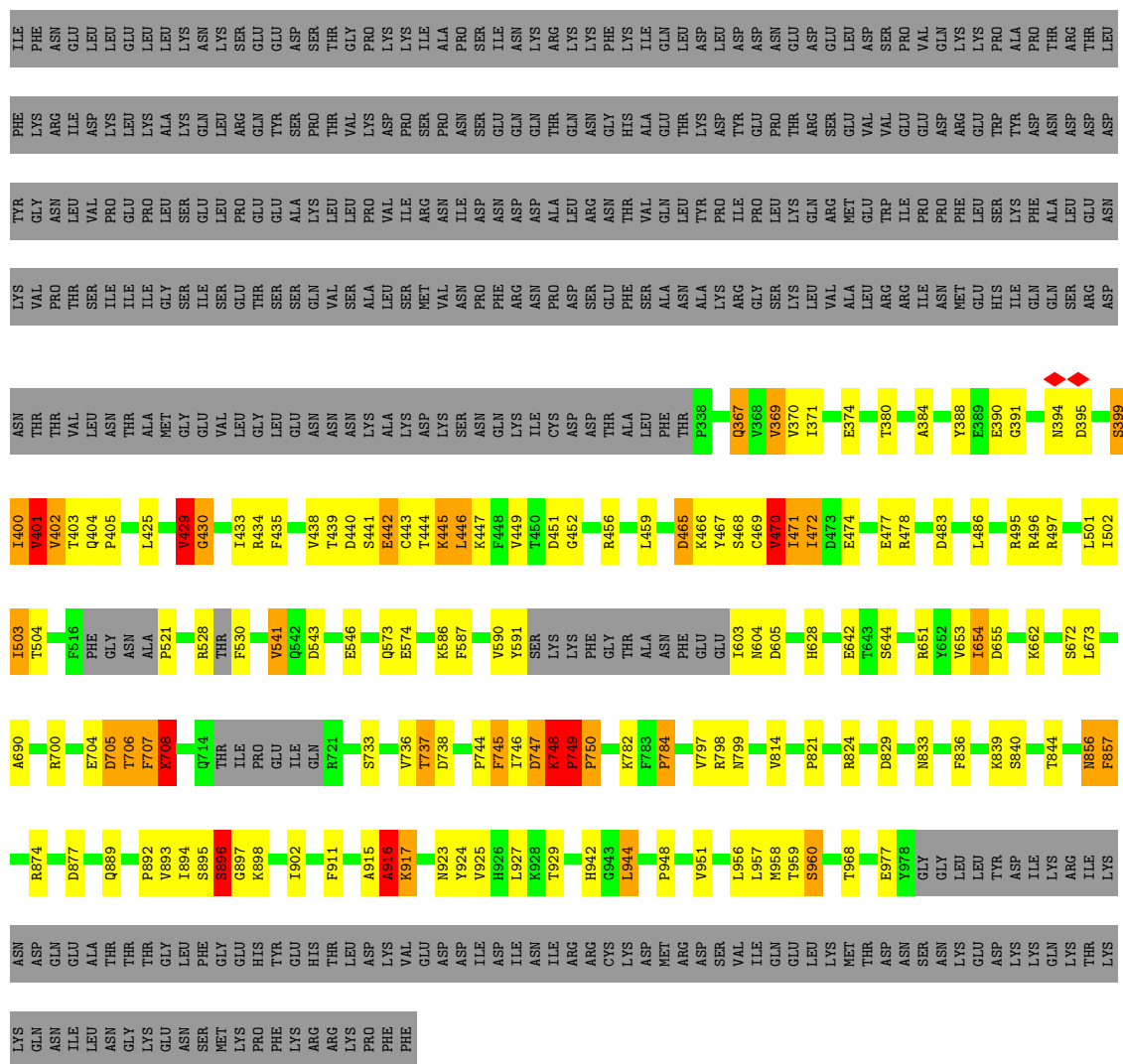
Chain r:  87% • 10%



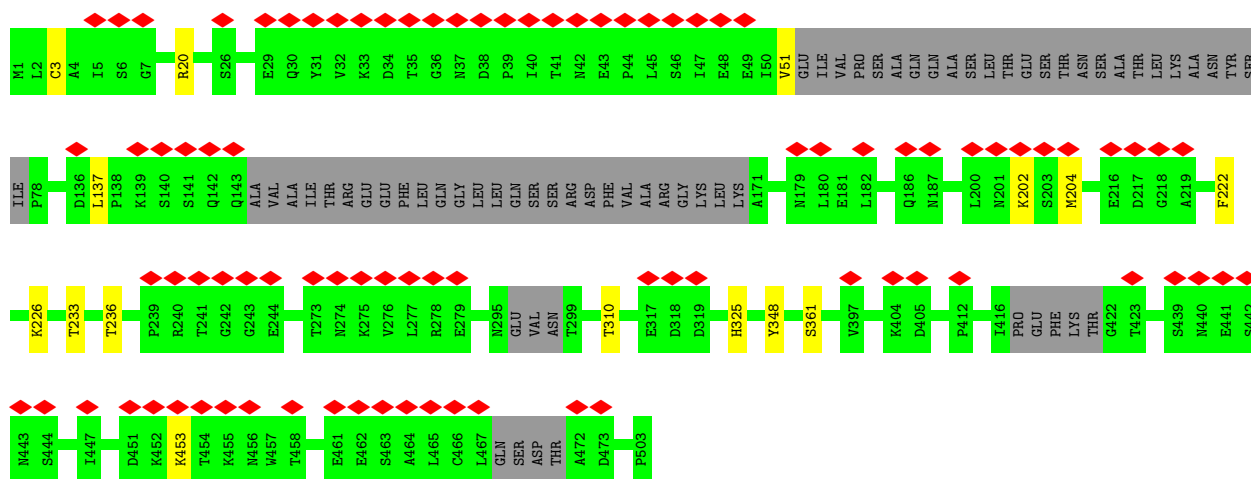
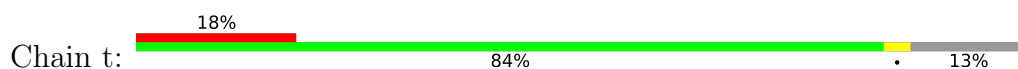
- Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain h:  53% • 44%



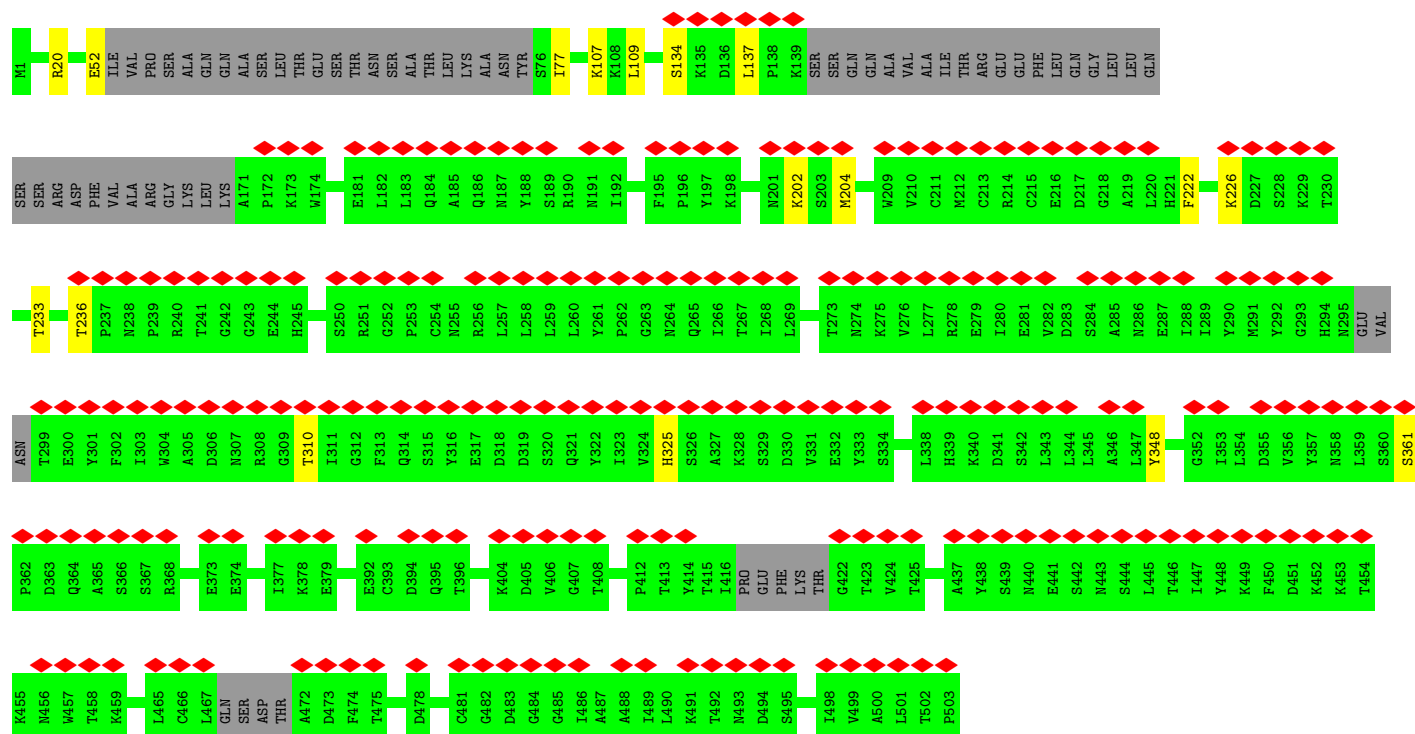


• Molecule 33: Pre-mRNA-processing factor 19

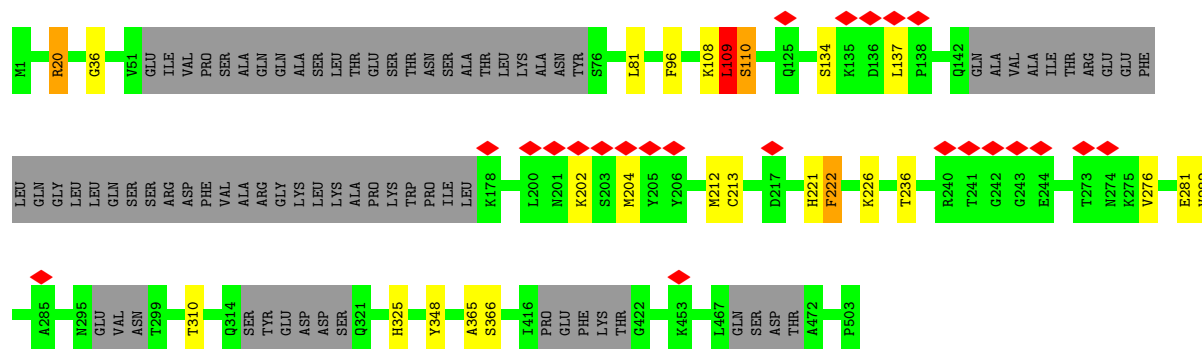


• Molecule 33: Pre-mRNA-processing factor 19

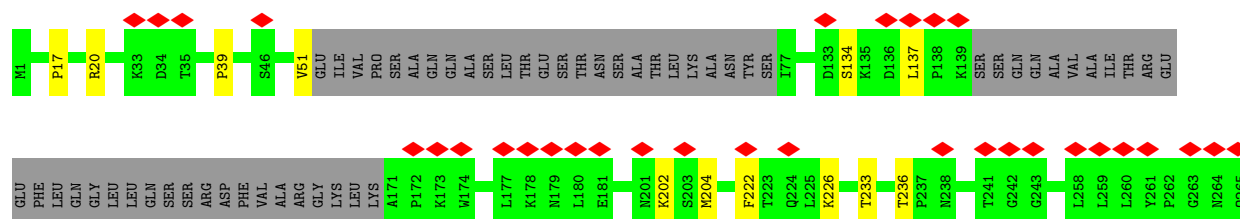
Chain u:



Chain v:



Chain w



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15872	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	589.16, 589.16, 589.16	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	U	0.41	0/3351	0.88	5/5213 (0.1%)
2	E	0.42	0/388	0.80	1/603 (0.2%)
3	I	0.40	0/772	0.81	1/1195 (0.1%)
4	Z	0.40	0/4018	0.76	1/6233 (0.0%)
5	V	0.41	0/2310	0.87	9/3594 (0.3%)
6	A	0.58	1/17321 (0.0%)	1.06	26/23534 (0.1%)
7	B	0.88	0/8463	1.19	17/11800 (0.1%)
8	D	0.49	0/929	0.81	0/1243
9	F	0.53	0/325	1.20	0/442
10	C	0.55	0/6902	1.02	7/9386 (0.1%)
11	G	0.52	0/839	1.10	0/1126
12	H	0.55	0/2667	1.35	4/3630 (0.1%)
13	J	0.59	0/2613	0.88	2/3551 (0.1%)
14	K	0.53	0/1308	1.05	4/1765 (0.2%)
15	L	0.52	0/1294	1.05	2/1732 (0.1%)
16	M	0.51	0/2058	0.97	2/2769 (0.1%)
17	N	0.55	0/1680	1.03	2/2258 (0.1%)
18	O	0.70	0/2091	1.28	6/2824 (0.2%)
19	P	0.61	0/282	0.88	1/380 (0.3%)
20	R	0.52	0/545	1.35	3/748 (0.4%)
21	S	0.53	0/3155	1.32	2/4298 (0.0%)
22	T	0.48	0/2918	1.49	12/4032 (0.3%)
23	b	0.53	0/636	0.71	0/856
23	k	0.49	0/394	0.99	2/546 (0.4%)
24	d	0.53	0/634	0.88	2/859 (0.2%)
24	n	0.48	0/403	1.14	4/559 (0.7%)
25	e	0.61	0/585	0.84	0/795
25	p	0.49	0/367	1.28	6/507 (1.2%)
26	f	0.57	0/585	0.85	0/791
26	q	0.50	0/353	1.01	0/489
27	g	0.55	0/532	0.76	0/715
27	r	0.48	0/338	0.90	2/467 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	h	0.50	0/649	0.77	0/880
28	l	0.52	0/390	1.23	4/541 (0.7%)
29	j	0.55	0/753	0.89	0/1013
29	m	0.50	0/466	1.18	4/649 (0.6%)
30	W	0.50	0/814	1.18	10/1134 (0.9%)
31	Y	0.49	0/415	1.08	0/577
32	Q	0.88	1/3061 (0.0%)	1.89	81/4260 (1.9%)
33	t	0.76	0/2165	1.14	10/3010 (0.3%)
33	u	0.81	1/2160 (0.0%)	1.15	11/3003 (0.4%)
33	v	0.84	2/2104 (0.1%)	1.23	14/2923 (0.5%)
33	w	0.76	0/2150	1.12	9/2989 (0.3%)
34	s	0.98	1/546 (0.2%)	1.45	11/760 (1.4%)
All	All	0.62	6/86729 (0.0%)	1.12	277/120679 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	A	0	2
11	G	0	1
16	M	0	1
18	O	0	2
21	S	0	1
32	Q	0	45
33	t	0	1
33	v	0	1
33	w	0	1
34	s	0	2
All	All	0	57

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	v	109	LEU	C-N	8.00	1.44	1.33
33	v	134	SER	C-O	-5.76	1.17	1.24
34	s	133	PRO	CA-C	5.59	1.60	1.52
32	Q	708	LYS	N-CA	5.22	1.52	1.46
33	u	77	ILE	C-N	5.14	1.40	1.33

The worst 5 of 277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Q	403	THR	N-CA-C	15.89	128.68	111.36
32	Q	404	GLN	N-CA-C	15.28	121.67	108.07
32	Q	402	VAL	N-CA-C	14.99	125.99	107.70
12	H	87	ILE	CA-C-N	14.31	134.45	118.85
12	H	87	ILE	C-N-CA	14.31	134.45	118.85

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
11	G	3	ARG	Peptide
16	M	231	ASP	Peptide
18	O	83	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	2999	0	1515	23	0
2	E	346	0	173	5	0
3	I	693	0	351	3	0
4	Z	3610	0	1831	16	0
5	V	2066	0	1042	23	0
6	A	16919	0	16184	261	0
7	B	8462	0	3706	35	0
8	D	912	0	936	12	0
9	F	321	0	282	6	0
10	C	6756	0	6801	122	0
11	G	823	0	808	29	0
12	H	2639	0	2073	26	0
13	J	2556	0	2551	60	0
14	K	1289	0	1309	20	0
15	L	1270	0	1294	13	0
16	M	2012	0	1968	33	0
17	N	1658	0	1712	65	0
18	O	2068	0	1853	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	275	0	283	4	0
20	R	544	0	345	18	0
21	S	3121	0	2399	59	0
22	T	2946	0	1252	16	0
23	b	631	0	670	2	0
23	k	396	0	169	0	0
24	d	625	0	647	6	0
24	n	404	0	180	0	0
25	e	575	0	597	7	0
25	p	369	0	152	0	0
26	f	573	0	572	4	0
26	q	354	0	153	0	0
27	g	529	0	557	3	0
27	r	340	0	152	0	0
28	h	644	0	686	3	0
28	l	392	0	165	0	0
29	j	741	0	778	3	0
29	m	467	0	199	0	0
30	W	816	0	341	1	0
31	Y	416	0	182	0	0
32	Q	3066	0	1345	53	0
33	t	2171	0	945	5	0
33	u	2166	0	942	5	0
33	v	2111	0	917	32	0
33	w	2156	0	938	3	0
34	s	548	0	219	10	0
35	x	660	0	142	7	0
36	E	1	0	0	0	0
36	V	1	0	0	0	0
37	D	1	0	0	1	0
37	L	3	0	0	0	0
37	M	1	0	0	0	0
37	N	2	0	0	5	0
38	C	32	0	12	0	0
All	All	85476	0	62328	882	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 6.

The worst 5 of 882 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)
11:G:22:SER:HB2	33:v:276:VAL:N	1.39	1.36
32:Q:434:ARG:O	32:Q:874:ARG:HA	1.26	1.35
17:N:34:CYS:SG	17:N:37:CYS:SG	1.35	1.34
20:R:36:GLN:O	20:R:40:GLN:N	1.60	1.32
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30

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	
6	A	2160/2413 (90%)	1997 (92%)	152 (7%)	11 (0%)	24	63
7	B	1704/2163 (79%)	1585 (93%)	111 (6%)	8 (0%)	24	63
8	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	6	34
9	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100
10	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	8	40
11	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	11	46
12	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	12	49
13	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	2	20
14	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	21	59
15	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	9	42
16	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	10	44
17	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	8	40
18	O	277/590 (47%)	248 (90%)	24 (9%)	5 (2%)	6	34
19	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	3	23
20	R	93/135 (69%)	81 (87%)	11 (12%)	1 (1%)	11	46
21	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	T	536/859 (62%)	506 (94%)	21 (4%)	9 (2%)	7	36
23	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
23	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	4	25
24	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	9	42
24	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
25	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
25	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	9	40
26	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	9	40
26	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	8	40
28	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
28	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	4	25
29	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
29	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
30	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	1	16
31	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
32	Q	609/1071 (57%)	486 (80%)	73 (12%)	50 (8%)	0	9
33	t	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
33	u	425/503 (84%)	413 (97%)	12 (3%)	0	100	100
33	v	412/503 (82%)	403 (98%)	6 (2%)	3 (1%)	18	56
33	w	423/503 (84%)	414 (98%)	7 (2%)	2 (0%)	24	63
34	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	14
All	All	11527/16230 (71%)	10551 (92%)	821 (7%)	155 (1%)	12	42

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP
6	A	737	ARG
7	B	766	ILE
12	H	414	PRO
16	M	127	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	1701/2182 (78%)	1567 (92%)	134 (8%)	11	32
8	D	100/256 (39%)	90 (90%)	10 (10%)	7	24
9	F	26/163 (16%)	25 (96%)	1 (4%)	29	50
10	C	722/910 (79%)	662 (92%)	60 (8%)	10	30
11	G	89/216 (41%)	83 (93%)	6 (7%)	15	36
12	H	185/552 (34%)	167 (90%)	18 (10%)	8	24
13	J	283/397 (71%)	248 (88%)	35 (12%)	4	17
14	K	143/328 (44%)	119 (83%)	24 (17%)	2	10
15	L	138/141 (98%)	128 (93%)	10 (7%)	13	35
16	M	213/296 (72%)	196 (92%)	17 (8%)	11	31
17	N	194/332 (58%)	170 (88%)	24 (12%)	4	17
18	O	174/525 (33%)	156 (90%)	18 (10%)	7	23
19	P	26/152 (17%)	22 (85%)	4 (15%)	2	12
20	R	23/121 (19%)	19 (83%)	4 (17%)	2	9
21	S	208/633 (33%)	184 (88%)	24 (12%)	5	18
23	b	70/176 (40%)	70 (100%)	0	100	100
24	d	69/89 (78%)	67 (97%)	2 (3%)	37	58
25	e	65/83 (78%)	61 (94%)	4 (6%)	16	38
26	f	63/77 (82%)	61 (97%)	2 (3%)	34	56
27	g	58/66 (88%)	56 (97%)	2 (3%)	32	54
28	h	77/129 (60%)	77 (100%)	0	100	100
29	j	79/103 (77%)	76 (96%)	3 (4%)	29	50
All	All	4706/7927 (59%)	4304 (92%)	402 (8%)	12	29

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	J	147	ILE
14	K	217	GLN
29	j	48	LEU
13	J	202	GLU
13	J	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
13	J	273	GLN
18	O	72	GLN
13	J	317	HIS
15	L	46	ASN
21	S	167	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	138/179 (77%)	68 (49%)	13 (9%)
2	E	15/16 (93%)	10 (66%)	2 (13%)
3	I	31/76 (40%)	15 (48%)	0
4	Z	162/1175 (13%)	58 (35%)	11 (6%)
5	V	96/112 (85%)	36 (37%)	6 (6%)
All	All	442/1558 (28%)	187 (42%)	32 (7%)

5 of 187 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	13	A
1	U	14	G
1	U	15	A
1	U	16	U
1	U	18	A

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	V	60	G
5	V	74	U
1	U	172	U
1	U	96	U

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Mol	Chain	Res	Type
5	V	84	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](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	GTP	C	1101	-	33,34,34	1.09	3 (9%)	50,54,54	1.77	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GTP	C	1101	-	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	C	1101	GTP	C5-C4	2.70	1.46	1.38
38	C	1101	GTP	C5-N7	-2.61	1.33	1.39
38	C	1101	GTP	C6-N1	-2.39	1.34	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	1101	GTP	C5-C4-N3	-5.96	118.91	128.39
38	C	1101	GTP	C2-N3-C4	5.05	121.00	112.30
38	C	1101	GTP	N9-C4-N3	4.57	135.08	125.95
38	C	1101	GTP	C6-C5-N7	3.18	136.08	130.29
38	C	1101	GTP	O6-C6-C5	-2.83	119.07	126.53

There are no chirality outliers.

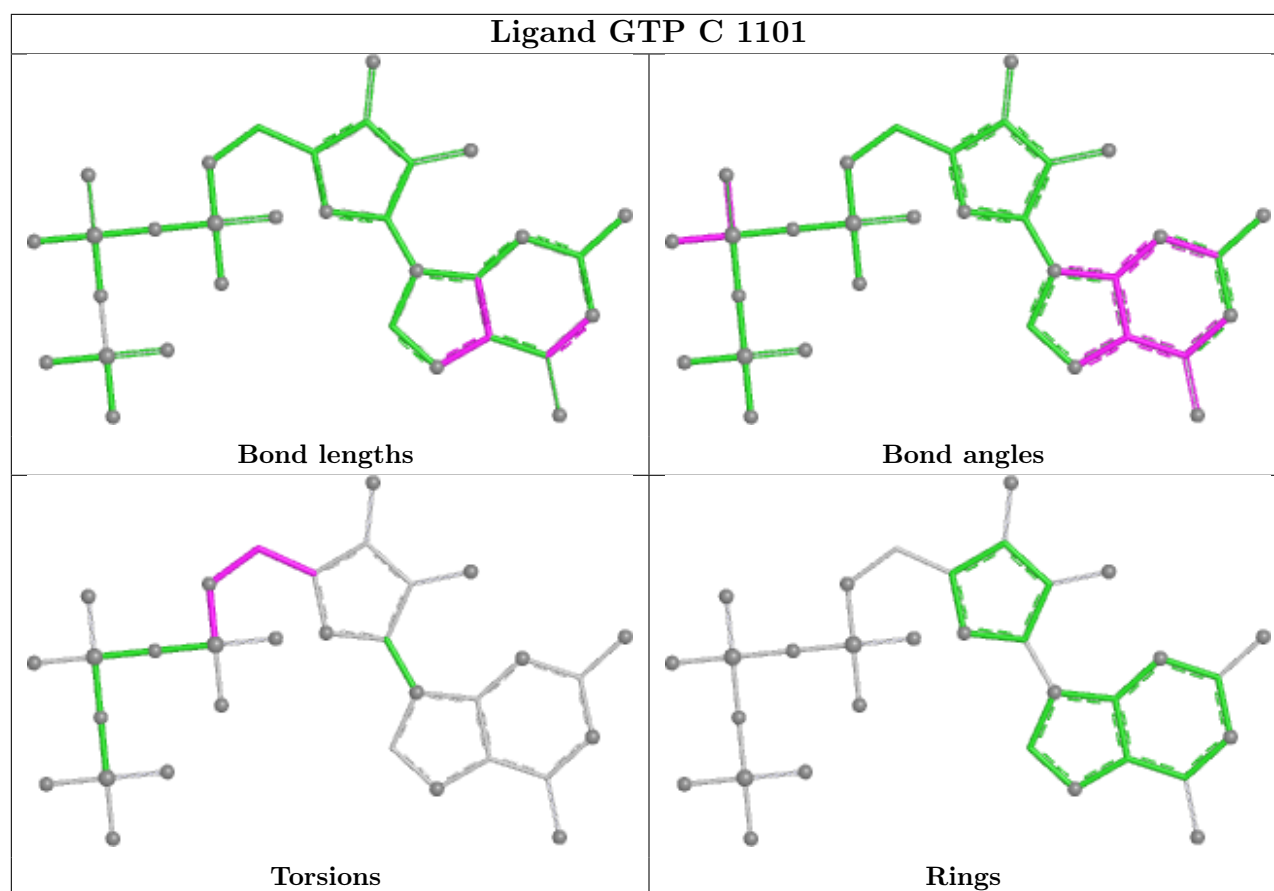
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	C	1101	GTP	C5'-O5'-PA-O3A
38	C	1101	GTP	C5'-O5'-PA-O1A
38	C	1101	GTP	C3'-C4'-C5'-O5'
38	C	1101	GTP	O4'-C4'-C5'-O5'
38	C	1101	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	x	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	54:UNK	C	55:UNK	N	111.76
1	x	110:UNK	C	111:UNK	N	53.94
1	x	36:UNK	C	37:UNK	N	49.39
1	x	87:UNK	C	88:UNK	N	31.03

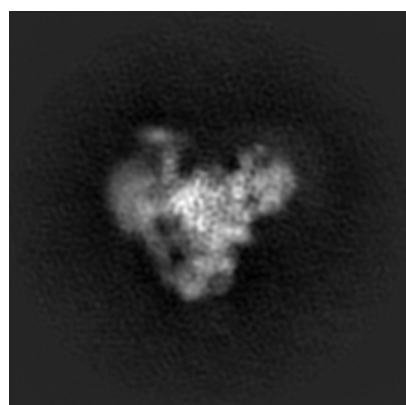
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4057. These allow visual inspection of the internal detail of the map and identification of artifacts.

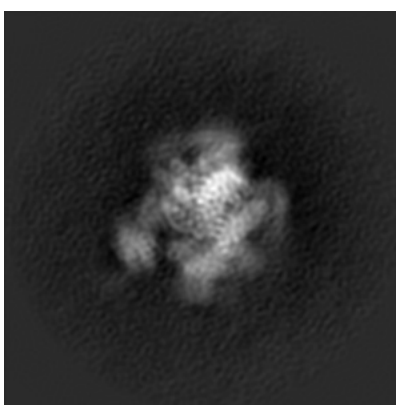
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

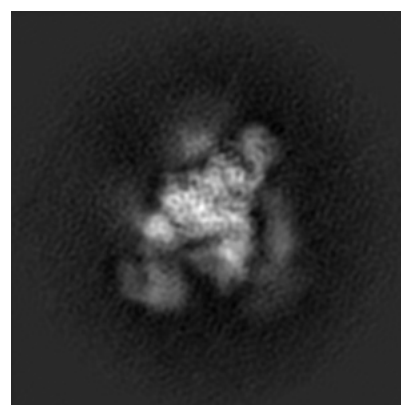
6.1.1 Primary map



X



Y

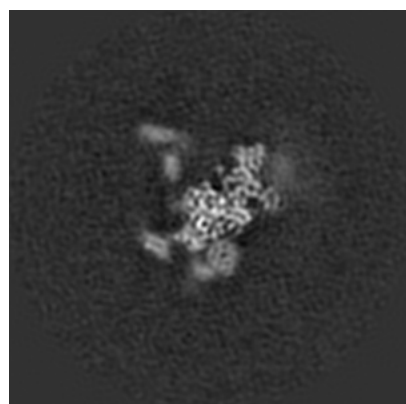


Z

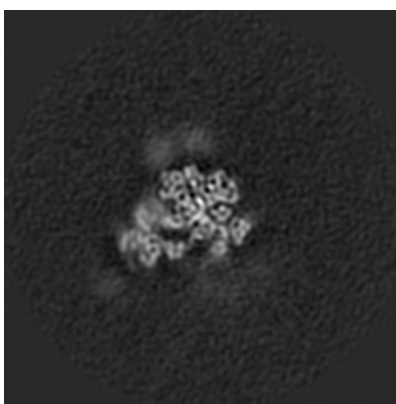
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

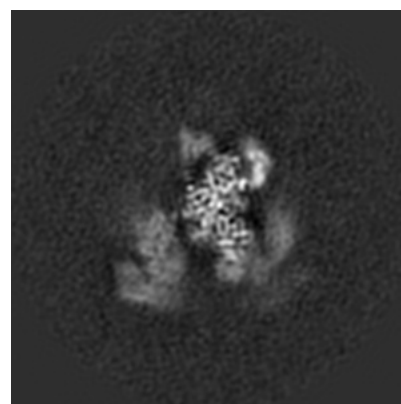
6.2.1 Primary map



X Index: 206



Y Index: 206

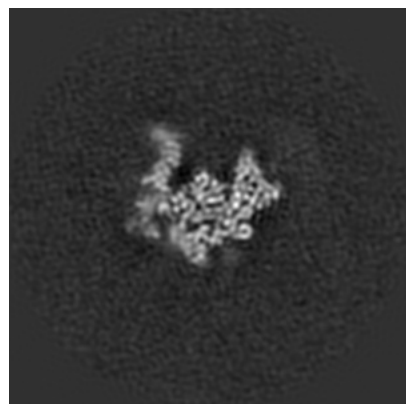


Z Index: 206

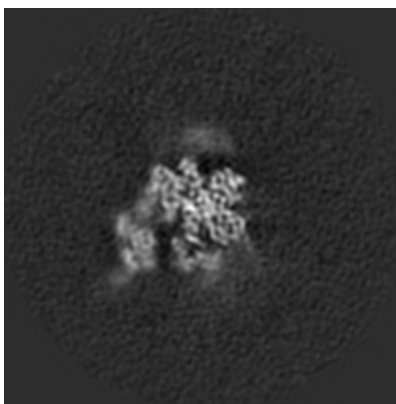
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

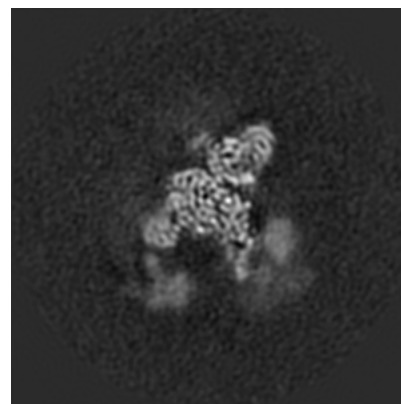
6.3.1 Primary map



X Index: 228



Y Index: 196

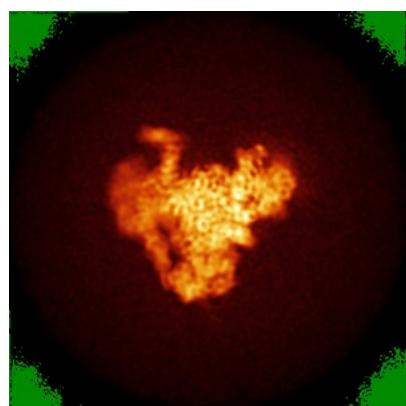


Z Index: 221

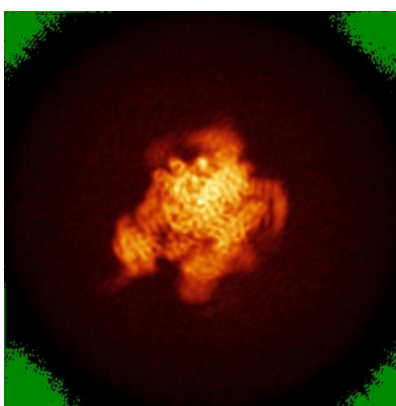
The images above show the largest variance slices of the map in three orthogonal directions.

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

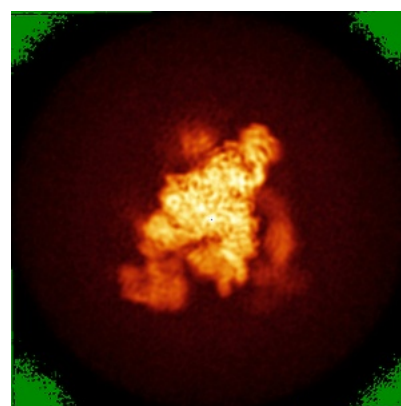
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

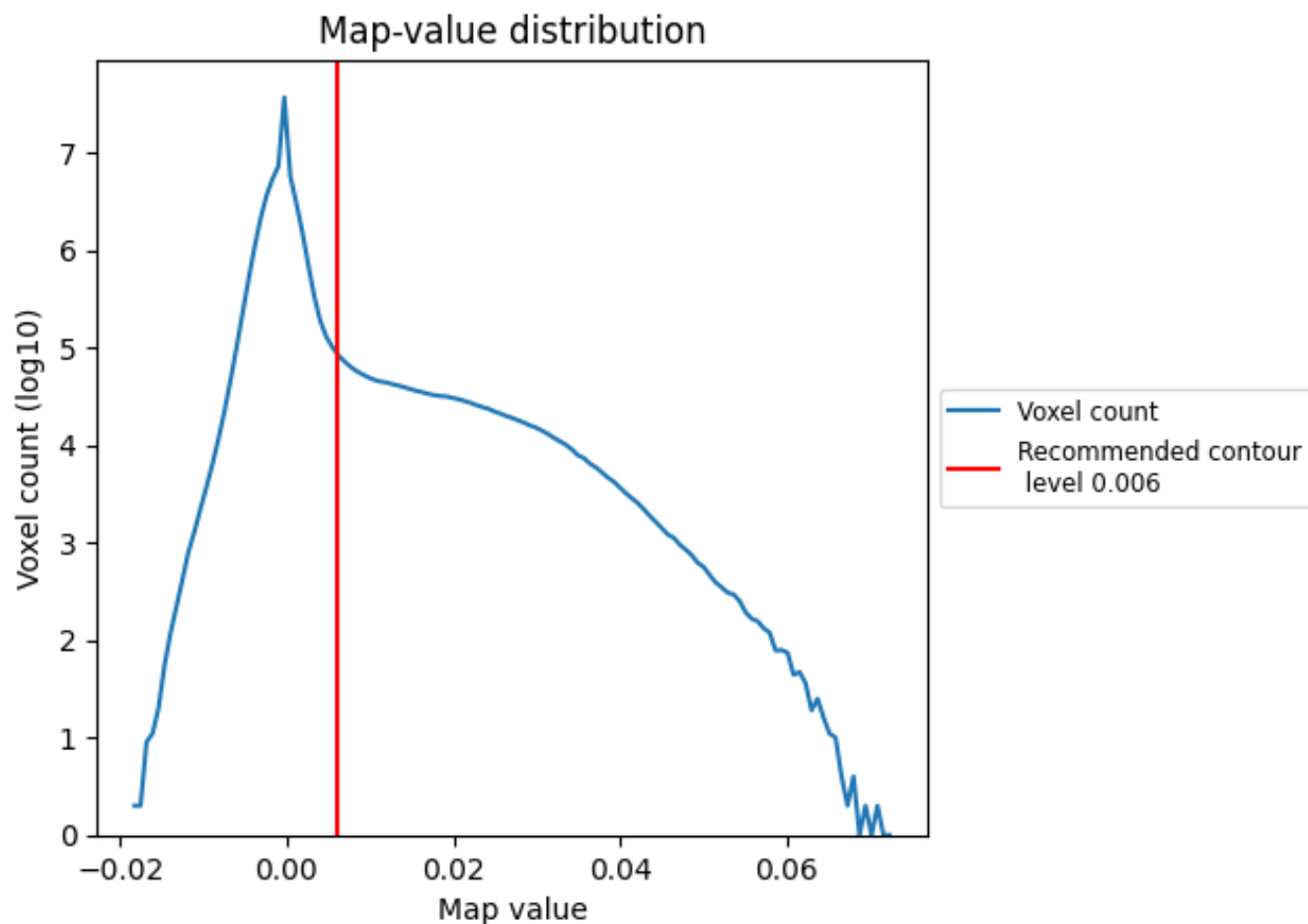
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

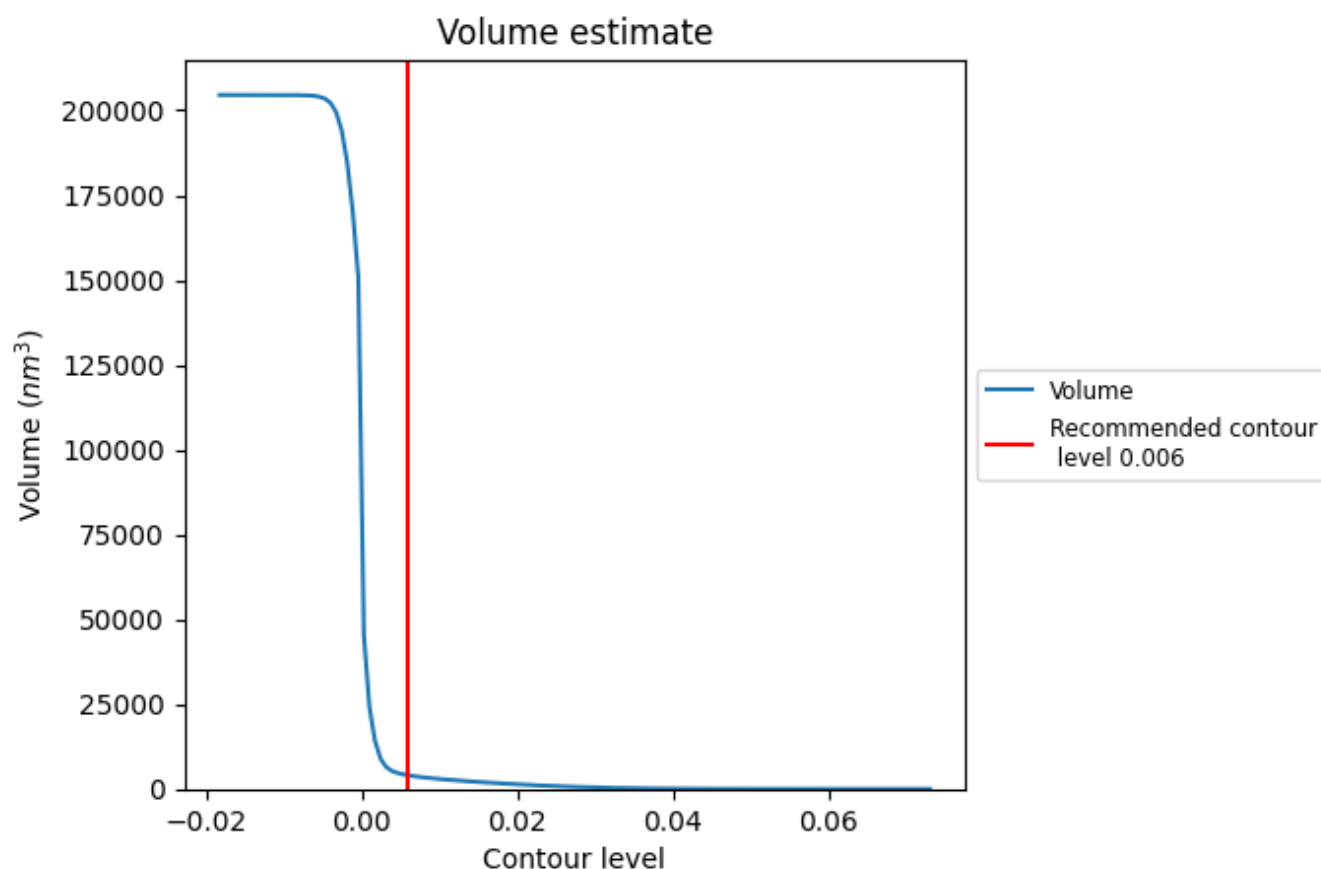
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

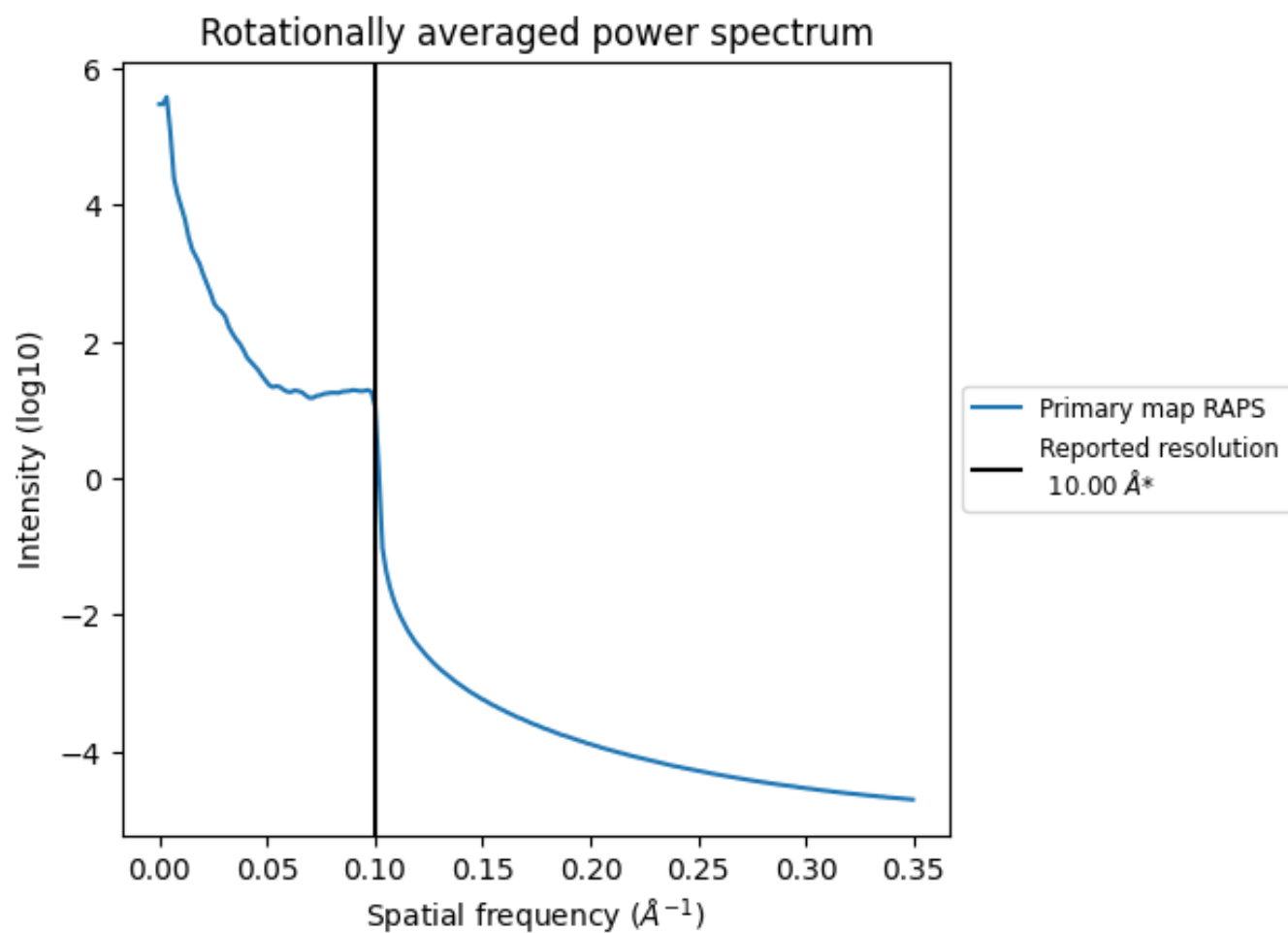
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4018 nm³; this corresponds to an approximate mass of 3629 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 ⓘ

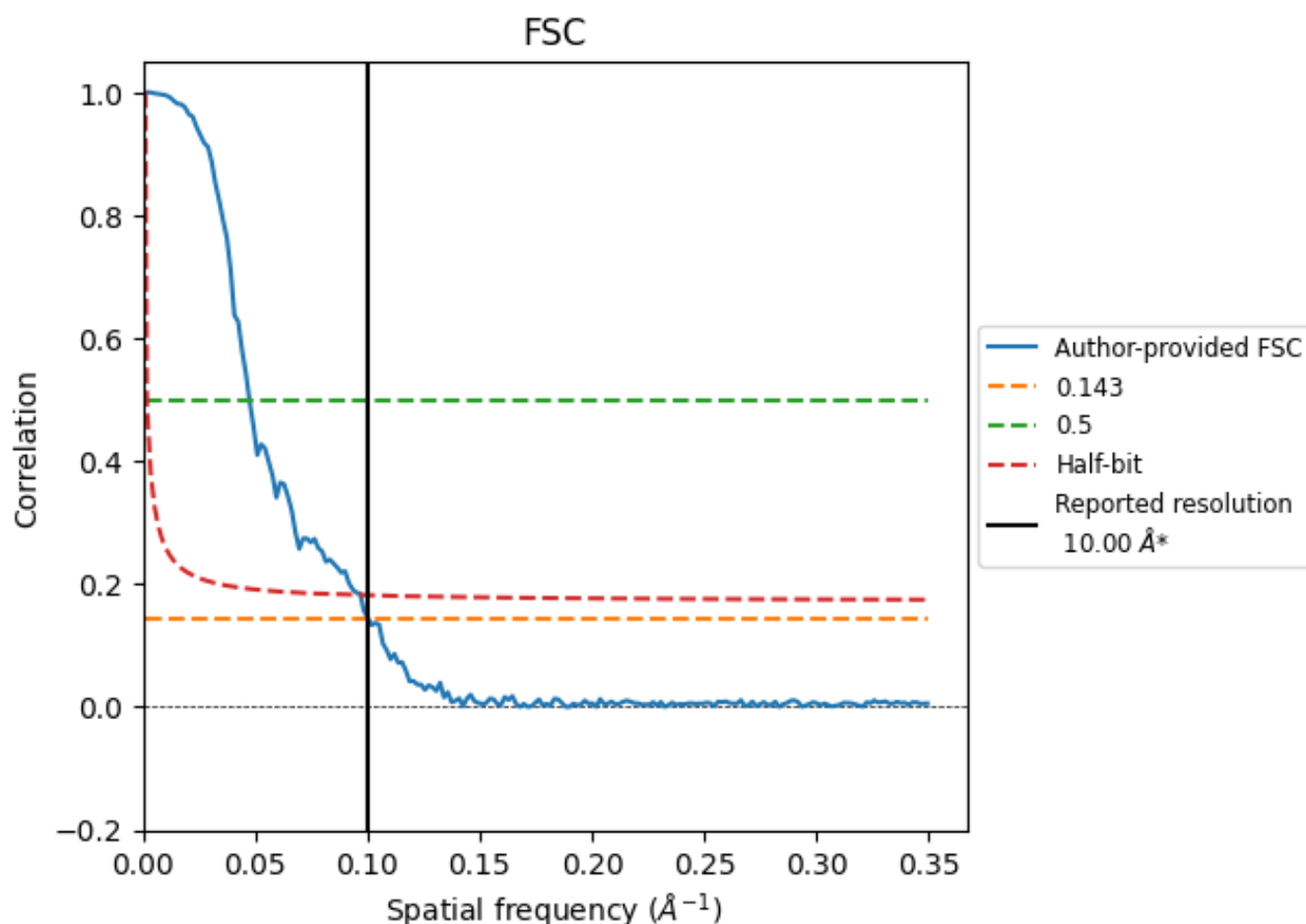


*Reported resolution corresponds to spatial frequency of 0.100 $\text{\AA}^{-1}$

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 0.100 Å⁻¹

8.2 Resolution estimates [i](#)

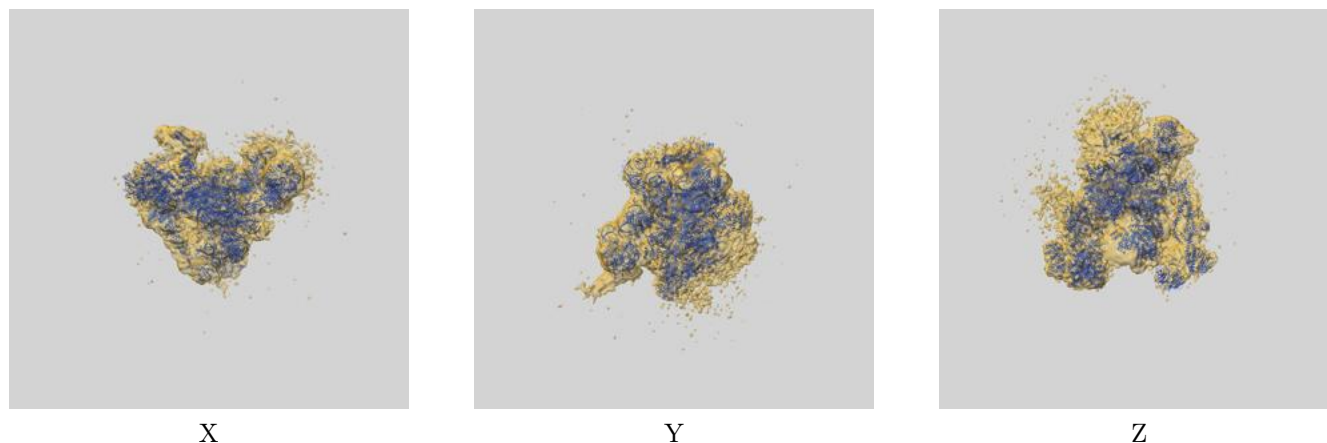
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.95	21.10	10.32
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

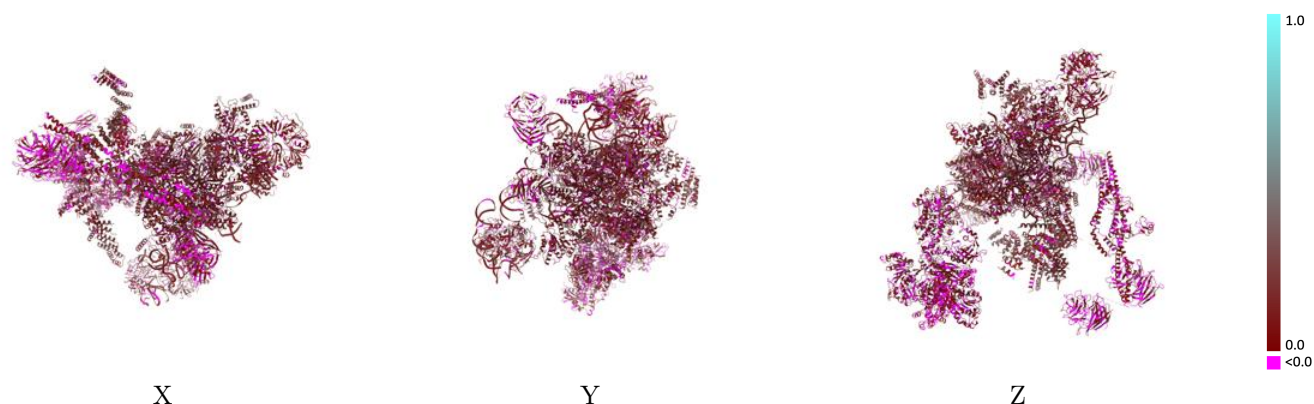
This section contains information regarding the fit between EMDB map EMD-4057 and PDB model 5LJ5. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

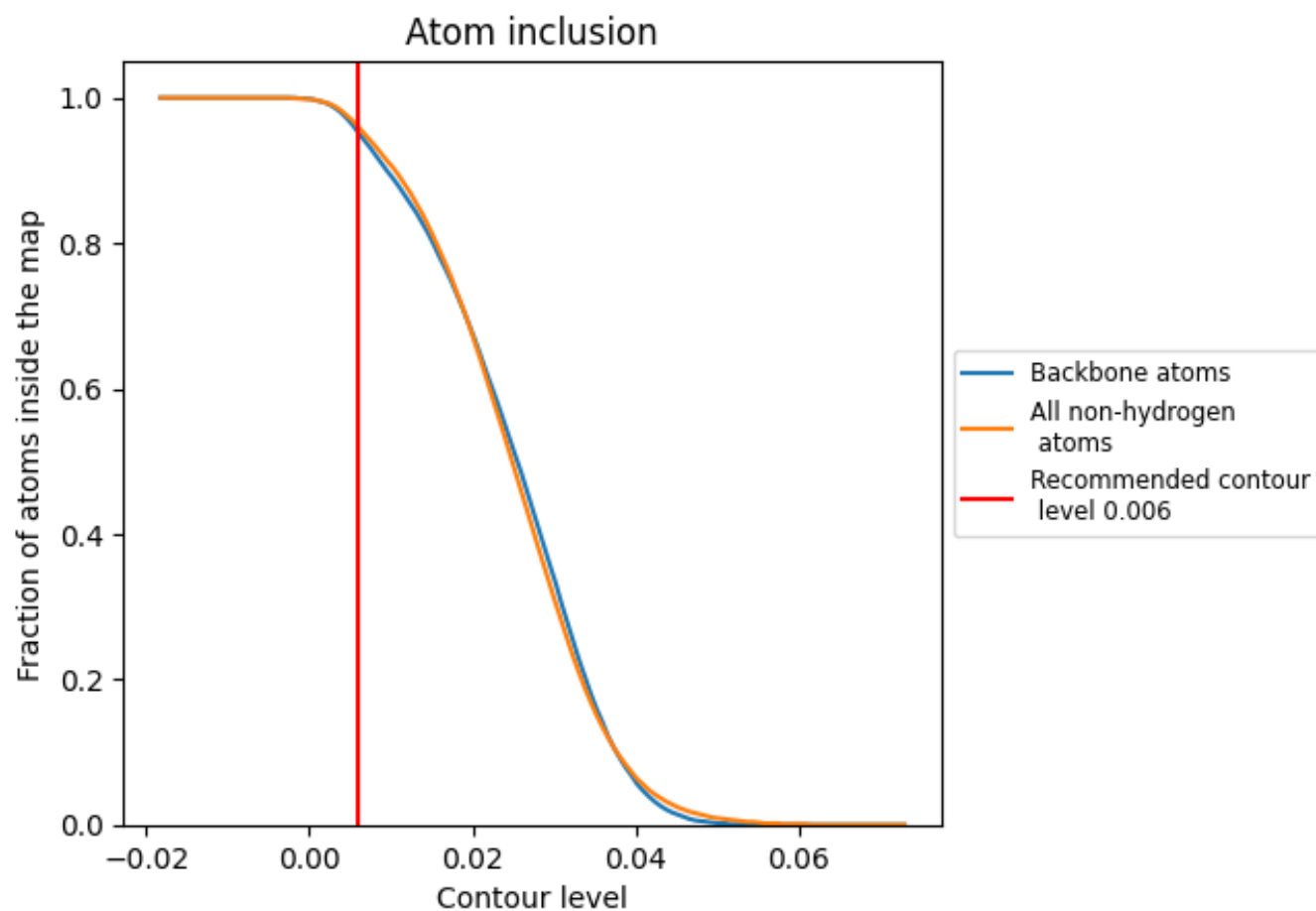


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.1140
A	 0.9820	 0.1130
B	 0.9520	 0.0430
C	 0.9890	 0.1230
D	 0.9820	 0.1110
E	 1.0000	 0.1490
F	 0.9910	 0.1550
G	 0.9910	 0.1270
H	 0.9960	 0.1600
I	 1.0000	 0.1410
J	 0.9900	 0.1030
K	 0.9870	 0.1390
L	 0.9990	 0.1210
M	 0.9880	 0.1220
N	 0.9910	 0.1370
O	 0.9600	 0.1170
P	 0.9890	 0.0910
Q	 0.9970	 0.0980
R	 0.9980	 0.2170
S	 0.9940	 0.1570
T	 1.0000	 0.2110
U	 1.0000	 0.1590
V	 1.0000	 0.1670
W	 0.9990	 0.1180
Y	 1.0000	 0.1230
Z	 1.0000	 0.1350
b	 1.0000	 0.1000
d	 1.0000	 0.1240
e	 1.0000	 0.1180
f	 0.9980	 0.1080
g	 0.9940	 0.1040
h	 0.9980	 0.1150
j	 0.9990	 0.1240
k	 1.0000	 0.1330
l	 1.0000	 0.1610



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Chain	Atom inclusion	Q-score
m	 1.0000	 0.1750
n	 1.0000	 0.1600
p	 1.0000	 0.1770
q	 1.0000	 0.1890
r	 0.9970	 0.1630
s	 0.9640	 0.0670
t	 0.7890	 0.0310
u	 0.4930	 0.0330
v	 0.9440	 0.0720
w	 0.6830	 0.0100
x	 1.0000	 0.2770