Full wwPDB EM Validation Report (i)

Nov 10, 2024 – 09:43 am GMT

PDB ID	:	7ONB
EMDB ID	:	EMD-12994
Title	:	Structure of the U2 5' module of the A3'-SSA complex
Authors	:	Cretu, C.; Pena, V.
Deposited on	:	2021-05-25
Resolution	:	3.10 Å(reported)
Based on initial models	:	7B9C, 6FF7, 6FF4

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 (i) 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 (1)) were used in the production of this report:

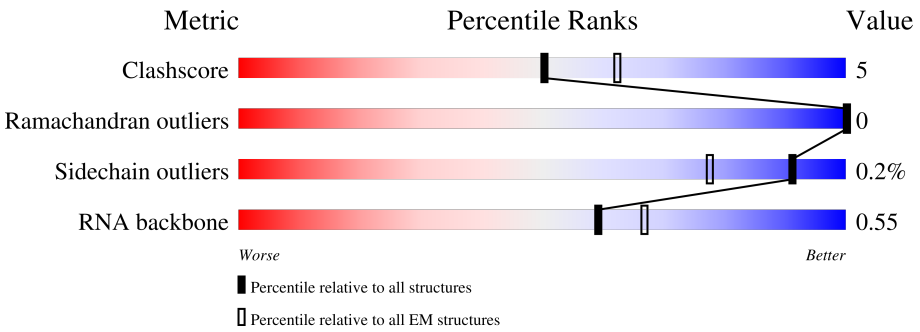
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1217	19% 85% 13% •
2	B	86	5% 72% 6% 22%
3	C	1304	13% 50% 12% 37%
4	D	110	• 72% • 26%
5	F	21	19% 95% 5%
6	G	229	• • • • 94%
7	H	188	• 10% 7% 83%

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Mol	Chain	Length	Quality of chain
8	I	895	9% 18% 80%
9	M	464	8% 90%
10	N	501	17% 81%
11	K	424	16% 16% 84%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 20140 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 Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1190	8494	5347	1494	1622	31	0	0

- Molecule 2 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	67	548	348	95	100	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	816	6493	4166	1122	1166	39	0	0

- Molecule 4 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	81	613	376	109	115	13	0	0

- Molecule 5 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	F	21	140	84	32	24	0	0

- Molecule 6 is a RNA chain called MINX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	G	14	297	133	51	99	14	0	0

- Molecule 7 is a RNA chain called RNU2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	H	32	668	300	104	232	32	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	181	1323	856	234	231	2	0	0

- Molecule 9 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	47	378	234	73	68	3	0	0

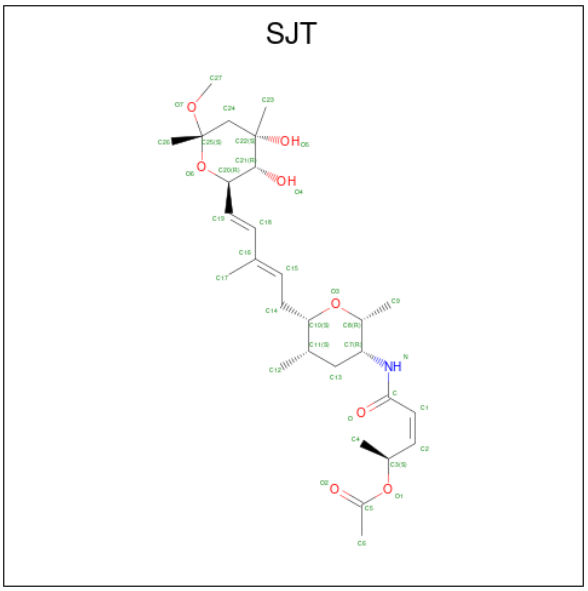
- Molecule 10 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	97	804	513	142	145	4	0	0

- Molecule 11 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	68	340	204	68	68	0	0

- Molecule 12 is spliceostatin A (form II) (three-letter code: SJT) (formula: $C_{28}H_{45}NO_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	D	1	37	28	1	8	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

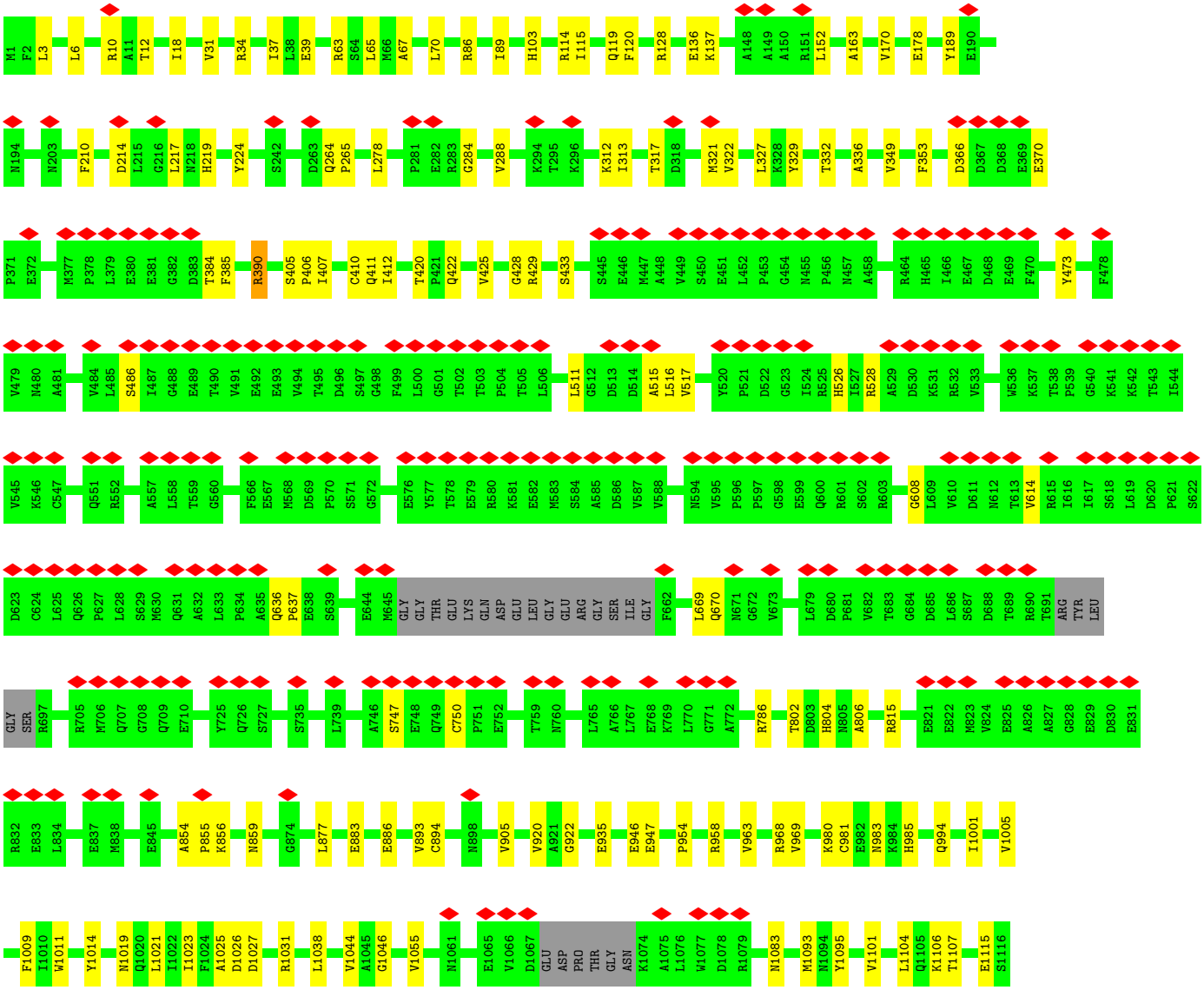
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
13	D	3	3	3	0
13	M	1	Total	Zn	0
			1	1	
13	N	1	Total	Zn	0
			1	1	

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.

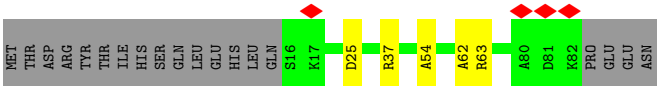
- Molecule 1: Splicing factor 3B subunit 3

Chain A:



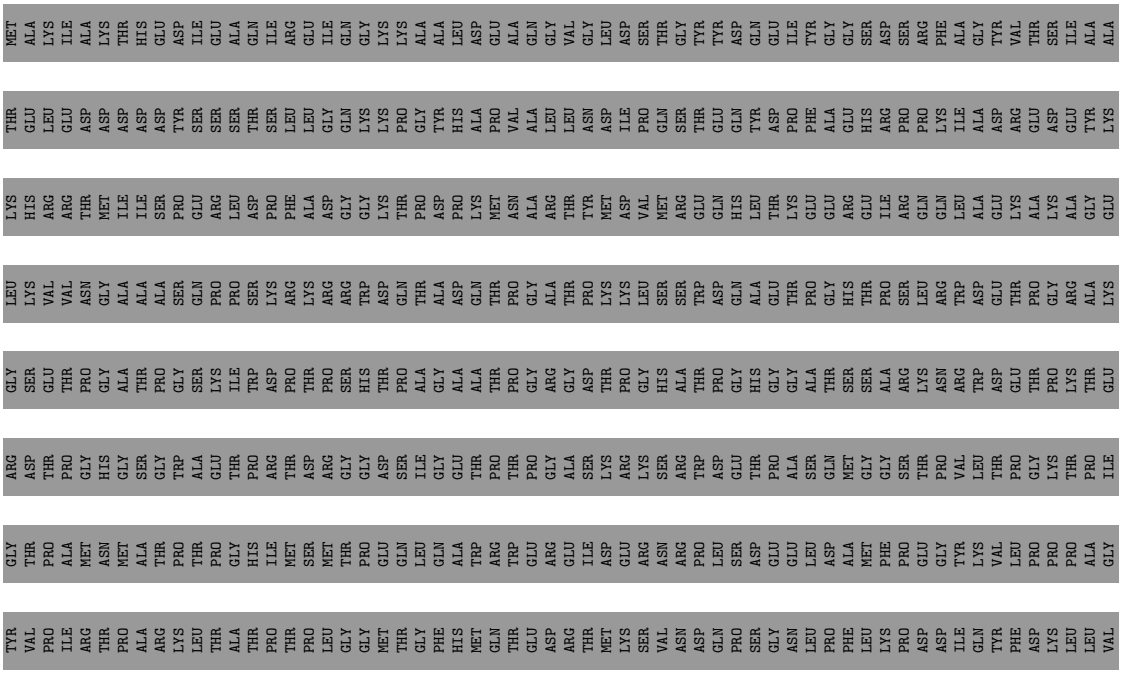
• Molecule 2: Splicing factor 3B subunit 5

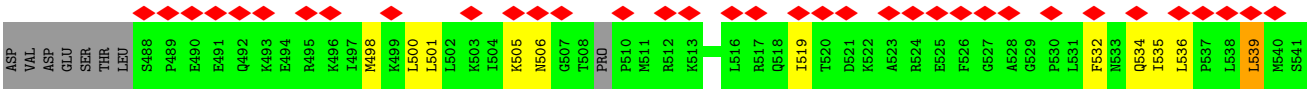
Chain B:

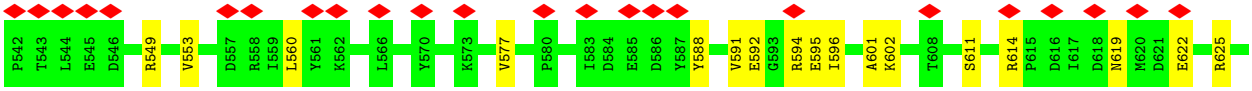


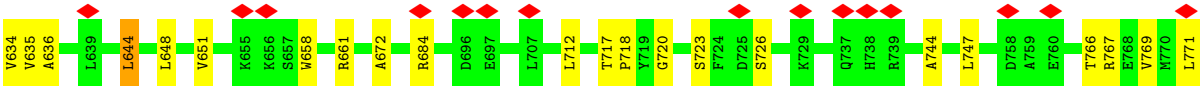
• Molecule 3: Splicing factor 3B subunit 1

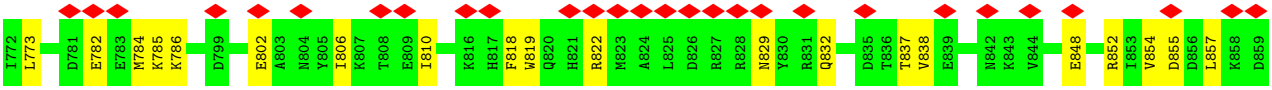
Chain C:

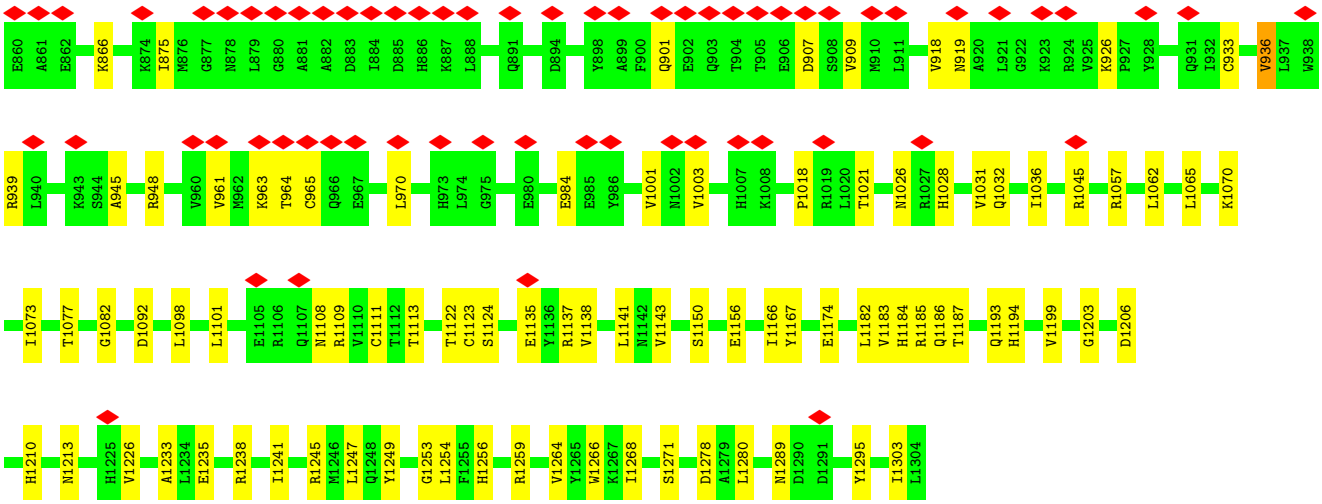






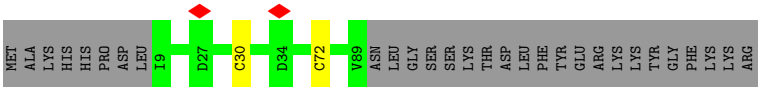






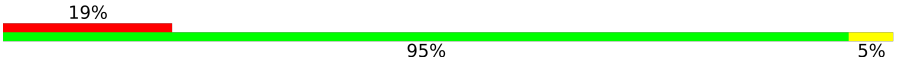
- Molecule 4: PHD finger-like domain-containing protein 5A

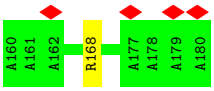
Chain D:



- Molecule 5: UNK

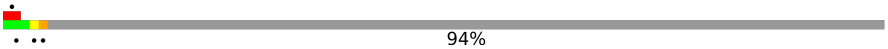
Chain F:

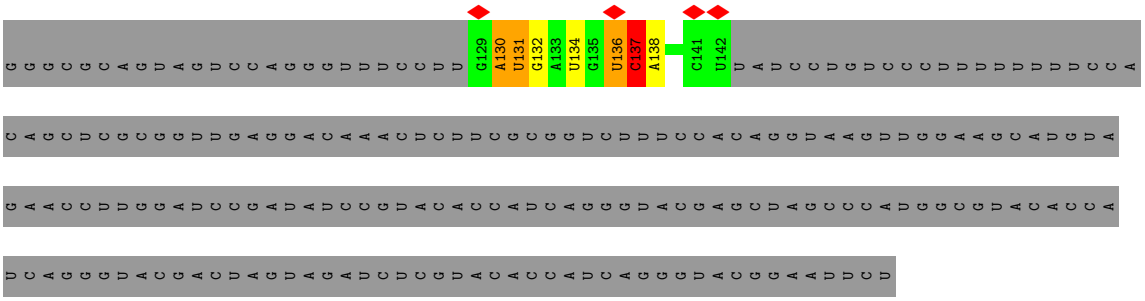




- Molecule 6: MINX

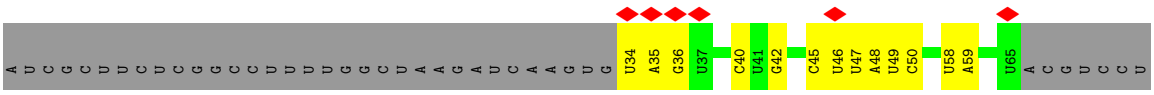
Chain G:

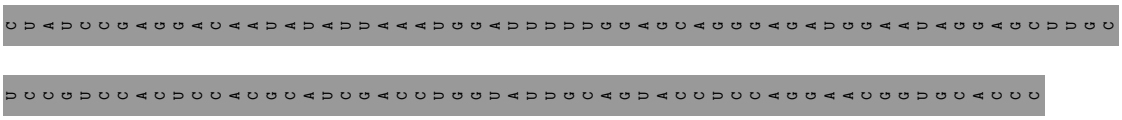




- Molecule 7: RNU2

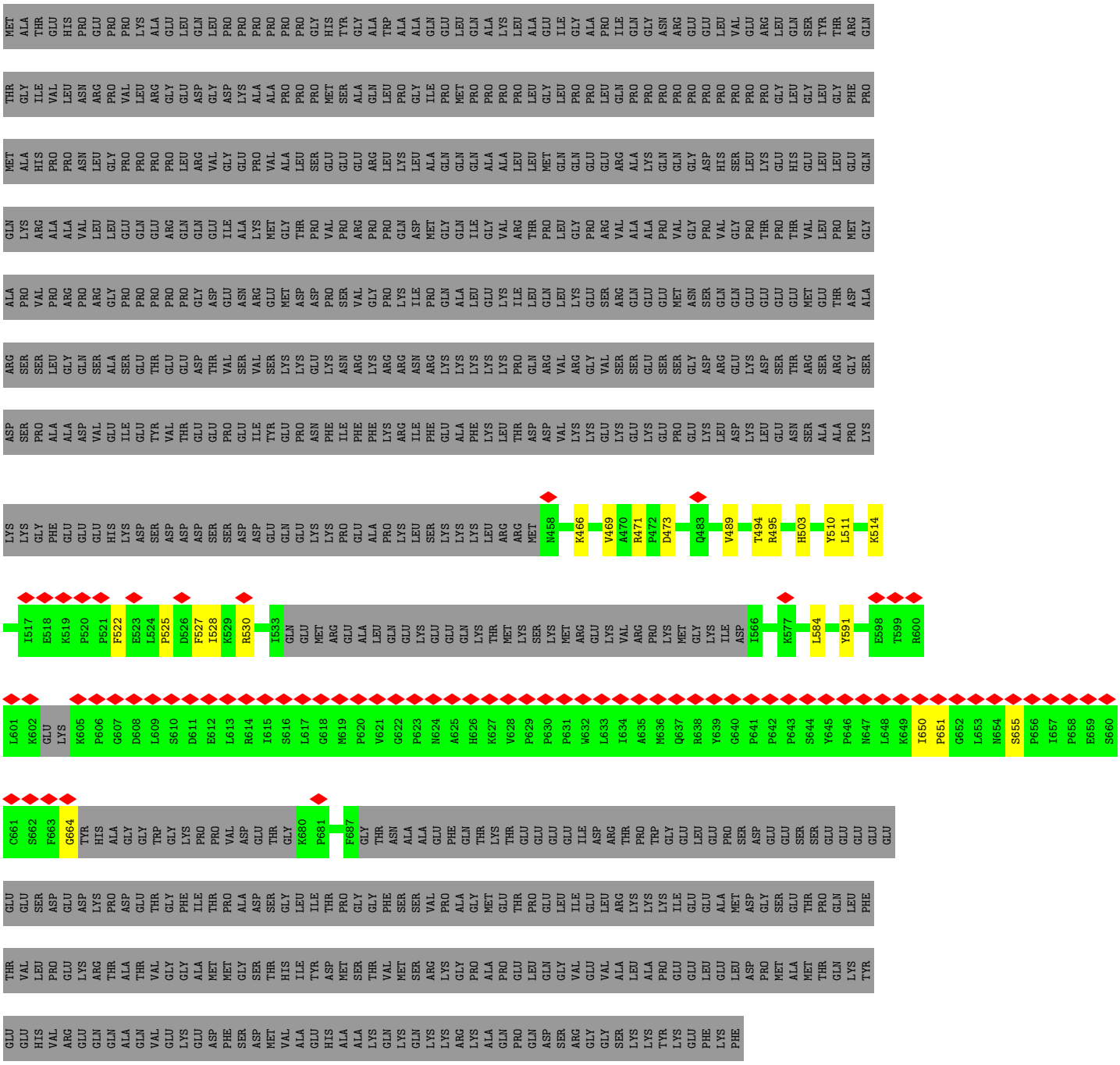
Chain H:





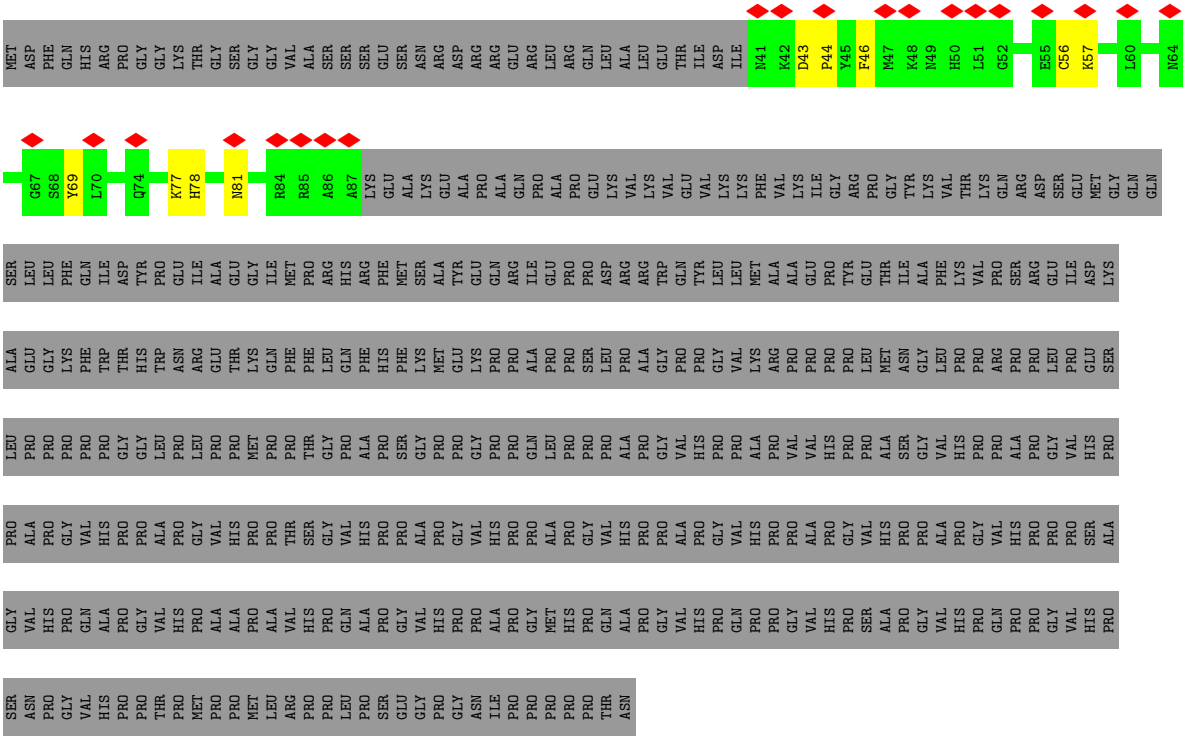
• Molecule 8: Splicing factor 3B subunit 2

Chain I: 9% 18% • 80%



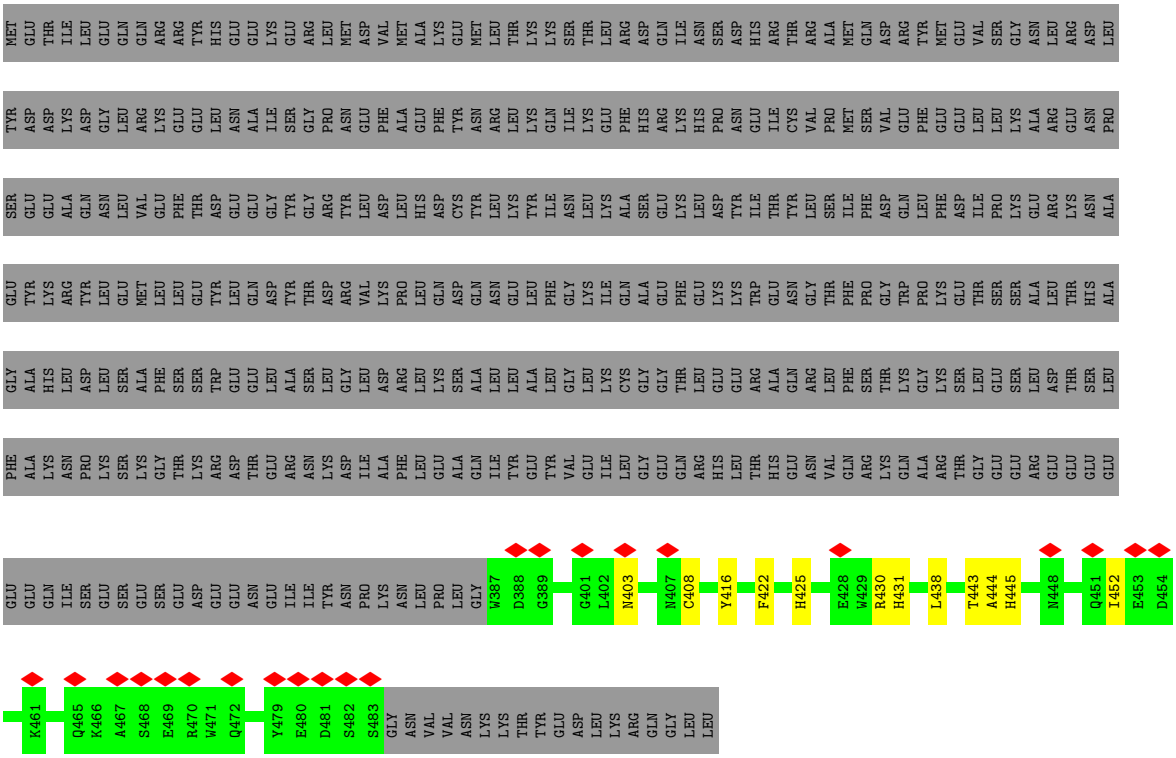
• Molecule 9: Splicing factor 3A subunit 2

Chain M: • 8% • 90%



- Molecule 10: Splicing factor 3A subunit 3

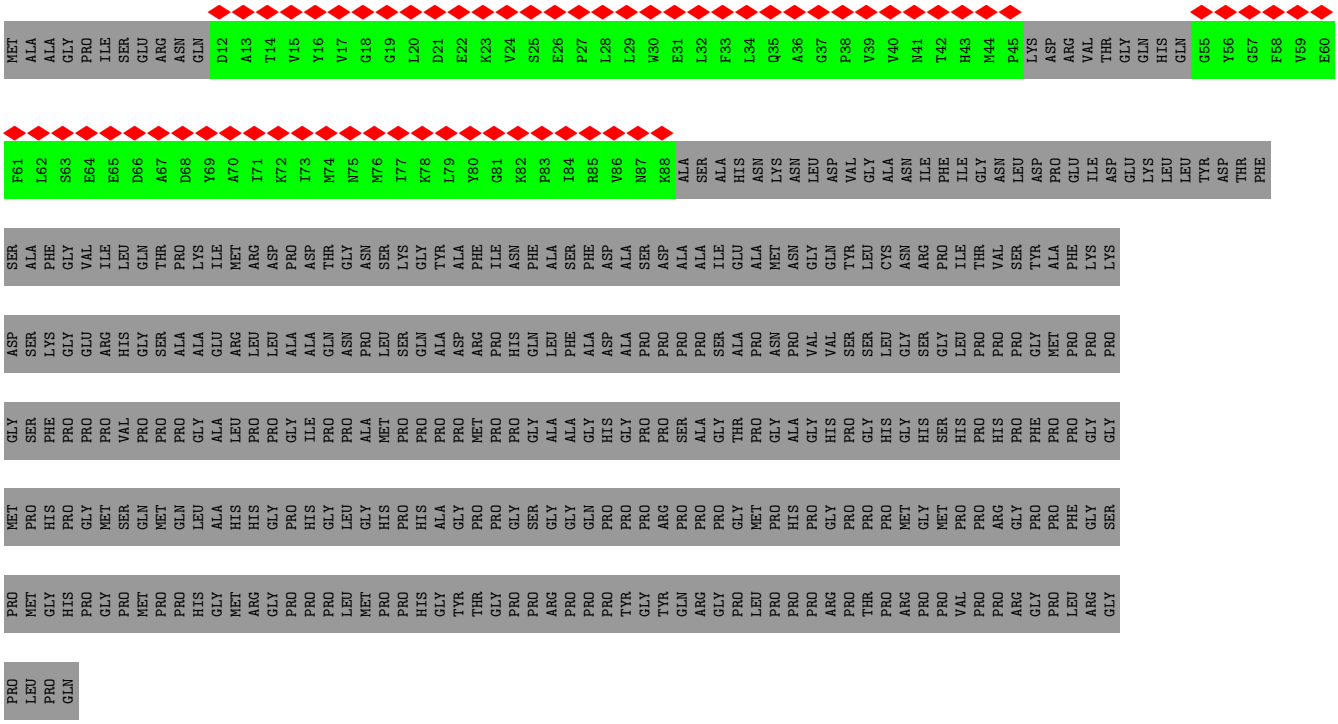
Chain N: 17% 81%



- Molecule 11: Splicing factor 3B subunit 4

Chain K:

16%
16%
84%


MET ALA ALA GLY PRO ILE SER GLU ARG ASN GLN D12 A13 T14 V15 Y16 V17 G18 G19 L20 D21 E22 K23 V24 S25 E26 P27 L28 L29 W30 E31 L32 F33 L34 Q35 A36 G37 P38 V39 V40 N41 T42 H43 M44 P45 LYS ASP ARG VAL THR GLY GLN HIS GLN G55 Y56 G57 F58 V59 E60
F61 L62 S63 E64 E65 D66 A67 D68 Y69 A70 I71 K72 I73 M74 N75 M76 I77 K78 L79 Y80 G81 K82 P83 I84 R85 V86 N87 K88 ALA SER ALA HIS ASN LYS ASN LEU ASP VAL GLY ALA ASN ILE PHE ILE GLY ASN LEU ASP PRO GLU ILE ASP GLU LYS LEU LEU TYR ASP THR PHE
SER ALA PHE GLY VAL ILE LEU GLN THR PRO LYS ILE MET ARG ASP PRO ASP THR GLY ASN SER LYS GLY TYR ALA PHE ILE ASN PHE ALA SER PHE ASP ALA SER ASP ALA ALA ILE GLU ALA MET ASN GLY GLN TYR LEU CYS ASN ARG PRO ILE THR VAL SER TYR ALA PHE LYS LYS
ASP SER LYS GLY GLU ARG HIS GLY SER ALA ALA GLU ARG LEU LEU ALA ALA GLN ASN PRO LEU SER GLN ALA ASP ARG PRO HIS GLN LEU PHE ALA ASP ALA PRO PRO PRO SER ALA PRO ASN PRO VAL VAL SER SER LEU GLY SER GLY LEU PRO PRO PRO GLY MET PRO PRO PRO
GLY SER PHE PRO PRO PRO VAL PRO PRO PRO GLY ALA LEU PRO PRO GLY ILE PRO PRO ALA MET PRO PRO PRO PRO MET PRO PRO GLY ALA ALA GLY HIS GLY PRO PRO SER ALA GLY THR PRO GLY ALA GLY HIS PRO GLY HIS GLY HIS SER HIS PRO HIS PRO PHE PRO PRO GLY GLY
MET PRO HIS PRO GLY MET SER GLN MET GLN LEU ALA HIS HIS GLY PRO HIS GLY LEU GLY HIS PRO HIS ALA GLY PRO PRO GLY SER GLY GLY GLN PRO PRO PRO ARG PRO PRO PRO GLY MET PRO HIS PRO GLY PRO PRO PRO MET GLY MET PRO PRO ARG GLY PRO PRO PHE GLY SER
PRO MET GLY HIS PRO GLY PRO MET PRO PRO HIS GLY MET ARG GLY PRO PRO PRO LEU MET PRO PRO HIS GLY TYR THR GLY PRO PRO ARG PRO PRO PRO TYR GLY TYR GLN ARG GLY PRO LEU PRO PRO PRO ARG PRO THR PRO ARG PRO PRO VAL PRO PRO ARG GLY PRO LEU ARG GLY
PRO LEU PRO GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78262	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 ($e^-/Å^2$)	41.41	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.29	0/8654	0.53	0/11799
2	B	0.32	0/564	0.62	0/761
3	C	0.35	0/6614	0.68	7/8950 (0.1%)
4	D	0.32	0/621	0.64	0/833
5	F	0.24	0/141	0.48	0/191
6	G	0.34	0/331	1.23	7/513 (1.4%)
7	H	0.30	0/743	1.12	8/1152 (0.7%)
8	I	0.28	0/1363	0.53	0/1862
9	M	0.26	0/386	0.49	0/517
10	N	0.25	0/832	0.45	0/1131
11	K	0.27	0/341	0.45	0/473
All	All	0.31	0/20590	0.64	22/28182 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	539	LEU	CA-CB-CG	8.89	135.74	115.30
7	H	34	U	O4'-C1'-N1	7.74	114.39	108.20
7	H	40	C	N1-C2-O2	6.94	123.06	118.90
7	H	34	U	OP1-P-OP2	-6.80	109.40	119.60
6	G	131	U	P-O3'-C3'	6.67	127.70	119.70
6	G	137	C	N1-C2-O2	6.63	122.88	118.90
6	G	130	A	OP1-P-OP2	-6.54	109.80	119.60
7	H	40	C	C6-N1-C2	-6.08	117.87	120.30
3	C	747	LEU	CA-CB-CG	6.04	129.21	115.30
7	H	40	C	N3-C2-O2	-5.99	117.71	121.90
7	H	58	U	N1-C2-O2	5.74	126.82	122.80
6	G	137	C	C2-N1-C1'	5.71	125.08	118.80
6	G	137	C	C6-N1-C2	-5.62	118.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	771	LEU	CA-CB-CG	5.57	128.10	115.30
3	C	644	LEU	CA-CB-CG	5.53	128.03	115.30
7	H	58	U	N3-C2-O2	-5.46	118.38	122.20
6	G	137	C	C5-C6-N1	5.41	123.71	121.00
3	C	970	LEU	CA-CB-CG	5.41	127.74	115.30
3	C	501	LEU	CA-CB-CG	5.29	127.47	115.30
7	H	40	C	C2-N1-C1'	5.24	124.56	118.80
3	C	936	VAL	CA-CB-CG2	5.08	118.52	110.90
6	G	137	C	N3-C2-O2	-5.07	118.35	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	8494	0	7601	91	0
2	B	548	0	518	5	0
3	C	6493	0	6705	94	0
4	D	613	0	594	1	0
5	F	140	0	137	1	0
6	G	297	0	150	2	0
7	H	668	0	337	2	0
8	I	1323	0	1199	15	0
9	M	378	0	366	5	0
10	N	804	0	738	9	0
11	K	340	0	166	0	0
12	D	37	0	0	0	0
13	D	3	0	0	0	0
13	M	1	0	0	0	0
13	N	1	0	0	0	0
All	All	20140	0	18511	206	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 (206) 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)
10:N:408:CYS:SG	10:N:431:HIS:HE1	2.01	0.84
9:M:56:CYS:SG	9:M:78:HIS:HE1	2.02	0.82
3:C:854:VAL:O	3:C:857:LEU:HB2	1.89	0.71
3:C:532:PHE:HA	3:C:535:ILE:HG22	1.77	0.67
1:A:3:LEU:HB2	1:A:1173:VAL:HG12	1.77	0.65
3:C:536:LEU:HA	3:C:539:LEU:HG	1.78	0.65
3:C:963:LYS:HB2	3:C:1003:VAL:HB	1.78	0.64
3:C:1098:LEU:HD13	3:C:1135:GLU:HG2	1.80	0.64
3:C:848:GLU:HG3	3:C:852:ARG:HH12	1.62	0.63
3:C:622:GLU:OE1	3:C:625:ARG:NH2	2.32	0.63
3:C:553:VAL:HG22	3:C:596:ILE:HD11	1.79	0.62
3:C:901:GLN:O	3:C:939:ARG:NH2	2.33	0.62
3:C:1182:LEU:HA	3:C:1185:ARG:HD2	1.83	0.61
1:A:1104:LEU:HD23	1:A:1117:LEU:HD21	1.83	0.61
3:C:848:GLU:O	3:C:852:ARG:NH1	2.34	0.61
1:A:1055:VAL:HB	1:A:1093:MET:HB3	1.83	0.60
3:C:1123:CYS:SG	3:C:1124:SER:N	2.74	0.60
1:A:511:LEU:H	1:A:516:LEU:HA	1.65	0.59
3:C:498:MET:SD	3:C:534:GLN:NE2	2.75	0.59
1:A:1117:LEU:HD22	1:A:1129:LEU:HD12	1.85	0.59
3:C:1113:THR:HG23	3:C:1150:SER:HA	1.85	0.58
1:A:854:ALA:HB1	1:A:856:LYS:HD2	1.86	0.57
3:C:592:GLU:HA	3:C:595:GLU:HG2	1.87	0.57
1:A:958:ARG:NH2	1:A:1014:TYR:OH	2.38	0.56
1:A:786:ARG:NH1	1:A:802:THR:O	2.39	0.56
3:C:1166:ILE:HD11	3:C:1199:VAL:HG11	1.87	0.56
1:A:806:ALA:HA	1:A:856:LYS:HB3	1.88	0.56
1:A:980:LYS:O	1:A:1019:ASN:ND2	2.39	0.55
1:A:473:TYR:HA	1:A:486:SER:HA	1.88	0.55
1:A:210:PHE:HB2	1:A:224:TYR:HB2	1.87	0.55
1:A:214:ASP:OD2	3:C:602:LYS:NZ	2.40	0.55
1:A:1158:ARG:NH1	1:A:1162:SER:OG	2.40	0.55
1:A:429:ARG:NH1	2:B:54:ALA:O	2.40	0.55
3:C:1001:VAL:O	3:C:1045:ARG:NH2	2.40	0.55
3:C:1254:LEU:O	3:C:1266:TRP:NE1	2.39	0.54
3:C:919:ASN:HA	3:C:961:VAL:HG11	1.89	0.54
3:C:838:VAL:HG22	3:C:875:ILE:HG13	1.90	0.54
1:A:6:LEU:HB2	1:A:1128:ILE:HG22	1.90	0.53
1:A:128:ARG:NH1	1:A:178:GLU:O	2.41	0.53
1:A:1026:ASP:OD2	8:I:495:ARG:NH2	2.41	0.53
3:C:855:ASP:N	3:C:855:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1070:LYS:HB3	3:C:1073:ILE:HG22	1.91	0.53
1:A:428:GLY:HA3	1:A:433:SER:HA	1.91	0.53
3:C:1137:ARG:HG2	8:I:522:PHE:HB3	1.90	0.53
1:A:278:LEU:HB2	1:A:855:PRO:HB2	1.91	0.53
3:C:648:LEU:HA	3:C:651:VAL:HG12	1.90	0.53
1:A:983:ASN:ND2	1:A:1021:LEU:O	2.42	0.53
1:A:946:GLU:OE2	1:A:968:ARG:NH2	2.42	0.52
3:C:1174:GLU:OE2	3:C:1210:HIS:NE2	2.42	0.52
3:C:619:ASN:O	3:C:625:ARG:NH1	2.36	0.52
1:A:1083:ASN:HB2	8:I:495:ARG:HA	1.90	0.52
1:A:312:LYS:NZ	1:A:366:ASP:OD1	2.43	0.52
3:C:1026:ASN:O	3:C:1032:GLN:NE2	2.42	0.52
3:C:1186:GLN:HB2	3:C:1226:VAL:HG22	1.92	0.52
3:C:1206:ASP:OD1	3:C:1206:ASP:N	2.43	0.52
9:M:44:PRO:O	9:M:57:LYS:NZ	2.43	0.52
3:C:549:ARG:NE	3:C:592:GLU:OE1	2.42	0.52
1:A:317:THR:HG22	1:A:322:VAL:HG22	1.92	0.52
3:C:766:THR:HA	3:C:769:VAL:HG12	1.92	0.52
6:G:134:U:H3	7:H:42:G:H1	1.56	0.52
1:A:114:ARG:HH22	2:B:37:ARG:HD3	1.75	0.51
3:C:505:LYS:NZ	3:C:506:ASN:OD1	2.41	0.51
1:A:10:ARG:HB3	1:A:37:ILE:HD13	1.93	0.51
1:A:114:ARG:NH2	1:A:136:GLU:OE1	2.38	0.51
1:A:1027:ASP:OD2	1:A:1031:ARG:NH1	2.43	0.51
1:A:637:PRO:HA	1:A:669:LEU:HA	1.91	0.51
1:A:353:PHE:HB3	1:A:406:PRO:HD3	1.93	0.51
3:C:785:LYS:HG3	3:C:818:PHE:HE1	1.76	0.51
1:A:10:ARG:NH1	1:A:39:GLU:OE2	2.43	0.51
1:A:985:HIS:HB2	1:A:1023:ILE:HD12	1.93	0.51
1:A:284:GLY:O	2:B:63:ARG:NH2	2.45	0.50
1:A:969:VAL:HG23	1:A:1021:LEU:HD11	1.94	0.50
3:C:1193:GLN:HB2	3:C:1233:ALA:HA	1.92	0.50
1:A:18:ILE:HD12	1:A:67:ALA:HB2	1.94	0.50
3:C:767:ARG:NH2	3:C:802:GLU:OE2	2.39	0.50
8:I:466:LYS:NZ	10:N:445:HIS:O	2.44	0.50
1:A:893:VAL:HG12	1:A:905:VAL:HG22	1.92	0.50
9:M:77:LYS:O	9:M:81:ASN:ND2	2.44	0.50
1:A:883:GLU:HB2	1:A:886:GLU:HG3	1.94	0.49
1:A:920:VAL:HG22	1:A:922:GLY:H	1.76	0.49
1:A:412:ILE:HB	1:A:1107:THR:HG21	1.95	0.49
1:A:1101:VAL:HG22	1:A:1121:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:720:GLY:O	3:C:723:SER:OG	2.31	0.49
3:C:1028:HIS:HB3	3:C:1031:VAL:HG12	1.92	0.49
3:C:1247:LEU:HD22	3:C:1280:LEU:HD22	1.94	0.49
1:A:1026:ASP:N	1:A:1026:ASP:OD1	2.44	0.49
3:C:1108:ASN:O	3:C:1111:CYS:HB2	2.13	0.49
1:A:1005:VAL:HG23	3:C:1303:ILE:HD11	1.95	0.49
3:C:1253:GLY:HA2	3:C:1256:HIS:HB2	1.94	0.48
1:A:136:GLU:OE2	1:A:189:TYR:OH	2.29	0.48
3:C:684:ARG:NH1	3:C:726:SER:OG	2.40	0.48
1:A:1001:ILE:HG12	1:A:1044:VAL:HG21	1.94	0.48
1:A:1210:ASP:OD2	1:A:1214:ARG:NH2	2.43	0.48
1:A:515:ALA:HA	1:A:528:ARG:HA	1.95	0.48
1:A:1009:PHE:HZ	1:A:1046:GLY:HA3	1.79	0.48
1:A:120:PHE:HB3	1:A:170:VAL:HG12	1.96	0.48
1:A:137:LYS:HG3	1:A:163:ALA:HA	1.97	0.47
1:A:969:VAL:HB	1:A:981:CYS:HB3	1.96	0.47
3:C:536:LEU:HD13	3:C:577:VAL:HG21	1.96	0.47
8:I:651:PRO:HD3	8:I:664:GLY:HA2	1.95	0.47
1:A:804:HIS:NE2	1:A:859:ASN:O	2.48	0.47
1:A:1150:SER:OG	1:A:1151:GLU:OE1	2.32	0.47
8:I:469:VAL:HG11	8:I:489:VAL:HG11	1.96	0.47
1:A:12:THR:O	1:A:34:ARG:NH1	2.47	0.47
3:C:500:LEU:HD23	3:C:519:ILE:HD13	1.96	0.47
3:C:1101:LEU:HD12	3:C:1109:ARG:HG2	1.95	0.47
1:A:31:VAL:HG12	1:A:65:LEU:HD21	1.95	0.47
3:C:948:ARG:NH2	3:C:984:GLU:OE1	2.46	0.47
1:A:410:CYS:SG	1:A:411:GLN:N	2.88	0.47
1:A:1187:PRO:HA	1:A:1190:GLN:HB2	1.98	0.46
3:C:961:VAL:HA	3:C:964:THR:HG22	1.98	0.46
1:A:317:THR:HA	1:A:322:VAL:HA	1.98	0.46
3:C:1241:ILE:HD13	3:C:1245:ARG:HG2	1.98	0.46
1:A:384:THR:OG1	1:A:385:PHE:N	2.49	0.46
1:A:1083:ASN:ND2	8:I:494:THR:O	2.49	0.46
7:H:59:A:OP1	10:N:403:ASN:ND2	2.49	0.46
9:M:43:ASP:OD1	9:M:43:ASP:N	2.42	0.46
1:A:329:TYR:OH	1:A:332:THR:OG1	2.27	0.46
3:C:1182:LEU:HG	3:C:1226:VAL:HG21	1.98	0.46
3:C:1141:LEU:HG	3:C:1184:HIS:HE1	1.82	0.45
1:A:994:GLN:HB3	1:A:1038:LEU:HD11	1.99	0.45
3:C:1235:GLU:OE1	3:C:1271:SER:OG	2.35	0.45
3:C:588:TYR:HA	3:C:591:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:636:ALA:HB2	3:C:644:LEU:HD13	1.98	0.45
1:A:70:LEU:HD11	1:A:152:LEU:HD13	1.98	0.45
3:C:782:GLU:OE1	3:C:829:ASN:ND2	2.50	0.45
3:C:786:LYS:O	3:C:832:GLN:NE2	2.50	0.45
3:C:1082:GLY:HA3	3:C:1122:THR:HG21	1.99	0.45
1:A:217:LEU:HB3	1:A:219:HIS:CD2	2.51	0.45
3:C:744:ALA:HB2	3:C:784:MET:HG3	1.99	0.45
3:C:1213:ASN:OD1	3:C:1249:TYR:OH	2.30	0.45
3:C:1062:LEU:HD22	3:C:1077:THR:HG23	1.99	0.45
1:A:86:ARG:NH1	1:A:1157:GLY:O	2.51	0.44
1:A:1194:SER:HA	1:A:1197:LEU:HD12	1.97	0.44
2:B:25:ASP:OD1	3:C:1259:ARG:NH2	2.38	0.44
10:N:443:THR:HG23	10:N:445:HIS:H	1.81	0.44
8:I:503:HIS:CG	8:I:510:TYR:HB2	2.53	0.44
1:A:313:ILE:HG12	1:A:327:LEU:HG	2.00	0.44
3:C:658:TRP:HA	3:C:661:ARG:HD3	1.98	0.44
3:C:1235:GLU:OE2	3:C:1238:ARG:NH2	2.45	0.44
10:N:422:PHE:O	10:N:425:HIS:ND1	2.45	0.44
8:I:525:PRO:HG2	8:I:528:ILE:HD12	2.00	0.43
1:A:264:GLN:NE2	1:A:265:PRO:O	2.46	0.43
3:C:1289:ASN:OD1	3:C:1295:TYR:N	2.47	0.43
1:A:114:ARG:HG3	1:A:115:ILE:HG23	2.00	0.43
3:C:1138:VAL:HG23	3:C:1143:VAL:HG21	2.01	0.43
1:A:407:ILE:HG23	1:A:425:VAL:HG13	2.00	0.43
3:C:1264:VAL:O	3:C:1268:ILE:HG13	2.19	0.43
8:I:527:PHE:HA	8:I:530:ARG:HH11	1.83	0.43
3:C:1167:TYR:HE1	8:I:584:LEU:HD11	1.83	0.43
1:A:1095:TYR:HB2	1:A:1173:VAL:HG21	2.00	0.43
3:C:717:THR:HA	3:C:718:PRO:HA	1.86	0.43
8:I:471:ARG:HH21	8:I:473:ASP:HB3	1.84	0.43
10:N:438:LEU:HD11	10:N:452:ILE:HG23	2.00	0.43
1:A:370:GLU:OE2	1:A:390:ARG:NE	2.42	0.43
1:A:336:ALA:HB2	1:A:349:VAL:HG13	2.01	0.42
3:C:918:VAL:HG12	3:C:961:VAL:HG21	2.00	0.42
1:A:877:LEU:HD13	1:A:935:GLU:HG2	2.01	0.42
3:C:1185:ARG:NH2	8:I:511:LEU:HB2	2.34	0.42
3:C:1156:GLU:HB2	3:C:1194:HIS:CG	2.54	0.42
1:A:89:ILE:HB	1:A:103:HIS:HB2	2.00	0.42
1:A:321:MET:H	1:A:321:MET:HG3	1.75	0.42
3:C:611:SER:HA	3:C:614:ARG:HE	1.85	0.42
3:C:773:LEU:HA	3:C:773:LEU:HD23	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:866:LYS:HG3	3:C:909:VAL:HG11	2.02	0.42
1:A:1011:TRP:HB2	1:A:1025:ALA:HB3	2.01	0.42
3:C:601:ALA:HB2	3:C:635:VAL:HG22	2.02	0.42
3:C:819:TRP:HE1	3:C:837:THR:HG21	1.84	0.42
1:A:636:GLN:O	1:A:670:GLN:N	2.53	0.42
3:C:672:ALA:HB2	3:C:712:LEU:HD23	2.02	0.42
3:C:945:ALA:HA	3:C:948:ARG:HG3	2.00	0.42
1:A:1106:LYS:HG2	1:A:1115:GLU:HG2	2.02	0.42
6:G:136:U:H2'	6:G:137:C:H4'	2.01	0.42
3:C:907:ASP:HB3	3:C:909:VAL:HG12	2.00	0.41
3:C:1183:VAL:O	3:C:1187:THR:HG22	2.20	0.41
10:N:403:ASN:N	10:N:403:ASN:OD1	2.53	0.41
1:A:288:VAL:HG12	2:B:62:ALA:HB3	2.03	0.41
1:A:608:GLY:HA2	1:A:614:VAL:HA	2.02	0.41
1:A:1166:TYR:OH	3:C:1278:ASP:OD2	2.34	0.41
3:C:560:LEU:HD23	3:C:560:LEU:HA	1.90	0.41
8:I:650:ILE:O	8:I:655:SER:N	2.51	0.41
1:A:517:VAL:HA	1:A:526:HIS:HA	2.03	0.41
3:C:926:LYS:HG3	3:C:965:CYS:HB3	2.03	0.41
3:C:933:CYS:HA	3:C:936:VAL:HG22	2.02	0.41
3:C:536:LEU:HD23	3:C:539:LEU:HD21	2.02	0.41
3:C:1057:ARG:HA	3:C:1057:ARG:HD2	1.91	0.41
3:C:1036:ILE:HD11	3:C:1065:LEU:HD13	2.01	0.41
8:I:514:LYS:NZ	8:I:591:TYR:OH	2.53	0.41
9:M:46:PHE:HB2	9:M:69:TYR:CZ	2.56	0.41
1:A:894:CYS:HB3	1:A:954:PRO:HG3	2.02	0.41
10:N:443:THR:OG1	10:N:444:ALA:N	2.54	0.41
1:A:420:THR:O	1:A:422:GLN:NE2	2.53	0.41
1:A:747:SER:N	1:A:750:CYS:O	2.48	0.41
1:A:947:GLU:HB2	1:A:963:VAL:HG12	2.02	0.41
3:C:939:ARG:HA	3:C:939:ARG:HD3	1.92	0.41
1:A:405:SER:HA	1:A:406:PRO:HA	1.80	0.41
3:C:1018:PRO:O	3:C:1021:THR:OG1	2.37	0.41
10:N:416:TYR:OH	10:N:430:ARG:NH1	2.46	0.41
1:A:1188:ASN:OD1	1:A:1188:ASN:N	2.54	0.40
3:C:500:LEU:HD12	3:C:500:LEU:HA	1.84	0.40
3:C:594:ARG:HG2	3:C:634:VAL:HG11	2.02	0.40
3:C:1092:ASP:OD1	5:F:168:ARG:NH1	2.54	0.40
3:C:806:ILE:HG12	3:C:810:ILE:HD12	2.02	0.40
1:A:1171:LYS:HG3	3:C:1203:GLY:HA2	2.03	0.40
4:D:30:CYS:HB2	4:D:72:CYS:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HH21	1:A:119:GLN:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1182/1217 (97%)	1128 (95%)	54 (5%)	0	100	100
2	B	65/86 (76%)	63 (97%)	2 (3%)	0	100	100
3	C	812/1304 (62%)	795 (98%)	17 (2%)	0	100	100
4	D	79/110 (72%)	76 (96%)	3 (4%)	0	100	100
5	F	19/21 (90%)	19 (100%)	0	0	100	100
8	I	173/895 (19%)	166 (96%)	7 (4%)	0	100	100
9	M	45/464 (10%)	44 (98%)	1 (2%)	0	100	100
10	N	95/501 (19%)	90 (95%)	5 (5%)	0	100	100
11	K	64/424 (15%)	63 (98%)	1 (2%)	0	100	100
All	All	2534/5022 (50%)	2444 (96%)	90 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	770/1051 (73%)	768 (100%)	2 (0%)	91	95
2	B	58/77 (75%)	58 (100%)	0	100	100
3	C	702/1104 (64%)	701 (100%)	1 (0%)	92	97
4	D	69/95 (73%)	69 (100%)	0	100	100
5	F	6/6 (100%)	6 (100%)	0	100	100
8	I	120/776 (16%)	120 (100%)	0	100	100
9	M	40/382 (10%)	40 (100%)	0	100	100
10	N	82/446 (18%)	82 (100%)	0	100	100
11	K	3/336 (1%)	3 (100%)	0	100	100
All	All	1850/4273 (43%)	1847 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	ARG
1	A	815	ARG
3	C	822	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	534	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	G	13/229 (5%)	5 (38%)	2 (15%)
7	H	31/188 (16%)	8 (25%)	0
All	All	44/417 (10%)	13 (29%)	2 (4%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	G	131	U
6	G	132	G
6	G	136	U
6	G	137	C

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Mol	Chain	Res	Type
6	G	138	A
7	H	35	A
7	H	36	G
7	H	45	C
7	H	46	U
7	H	47	U
7	H	48	A
7	H	49	U
7	H	50	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	G	130	A
6	G	131	U

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 6 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
12	SJT	D	1401	4	37,38,38	0.22	0	42,55,55	0.84	1 (2%)

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
12	SJT	D	1401	4	-	1/26/63/63	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	1401	SJT	C2-C1-C	4.48	133.89	122.69

There are no chirality outliers.

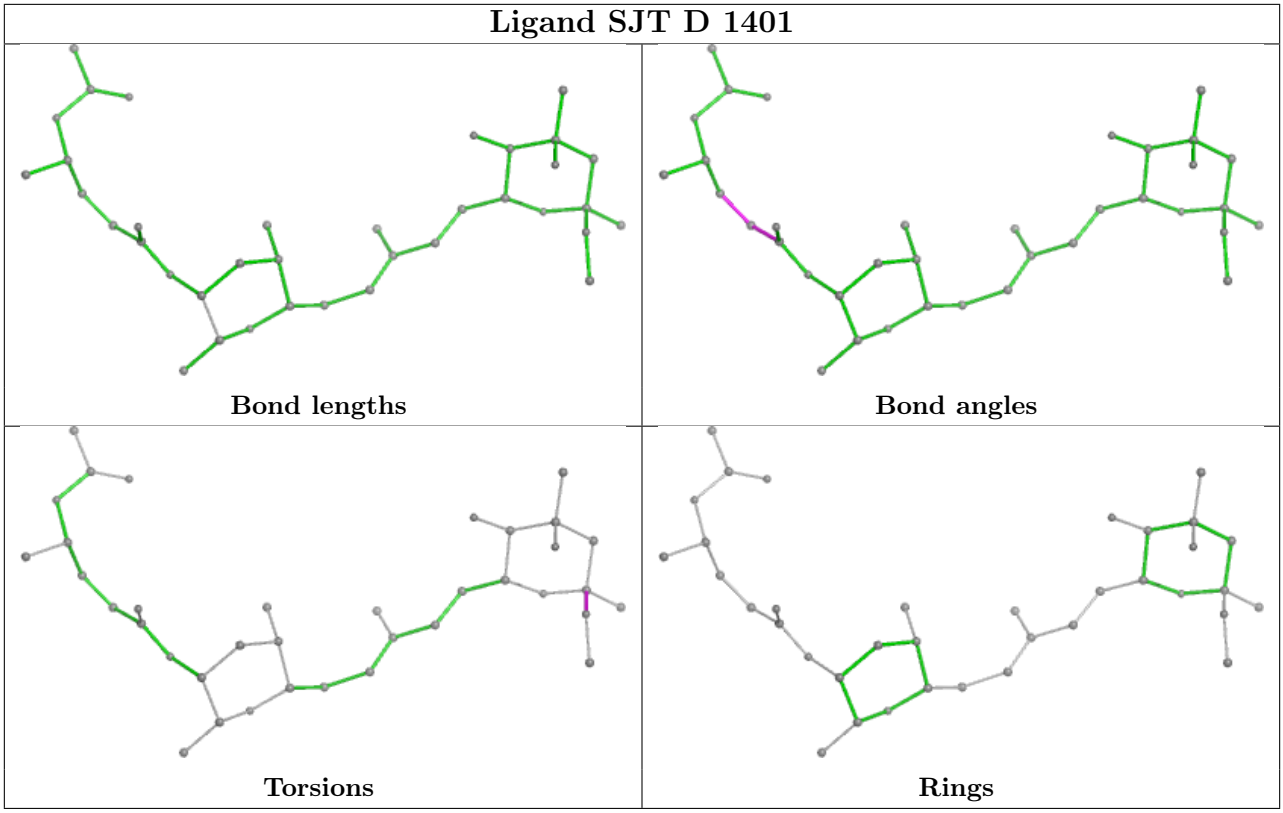
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	1401	SJT	O6-C25-O7-C27

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

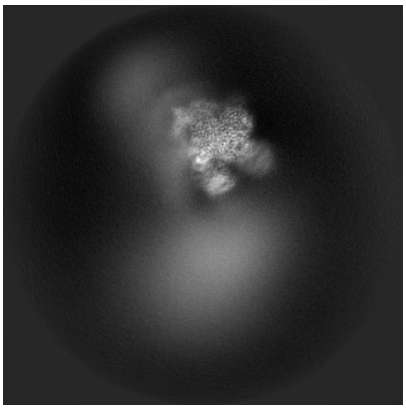
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12994. These allow visual inspection of the internal detail of the map and identification of artifacts.

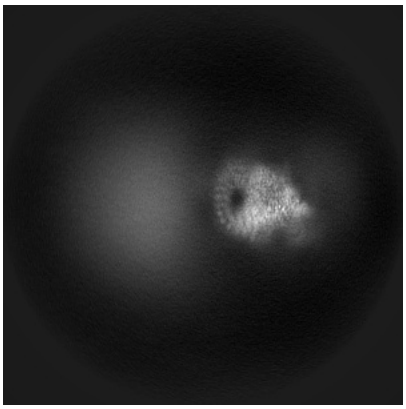
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

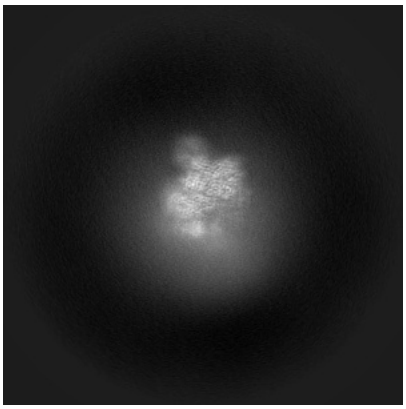
6.1.1 Primary map



X

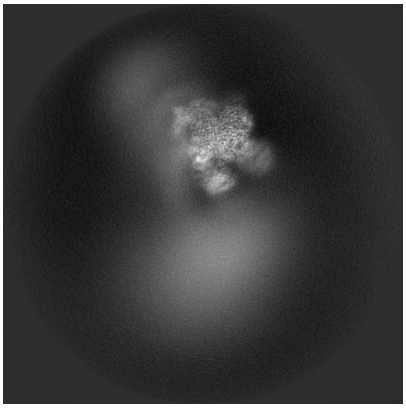


Y

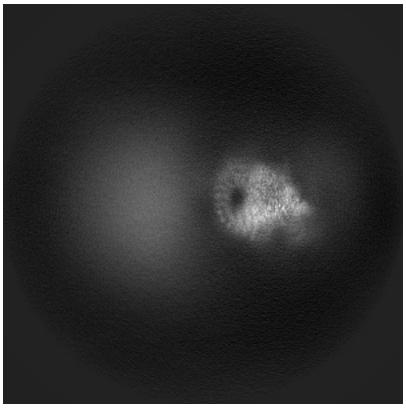


Z

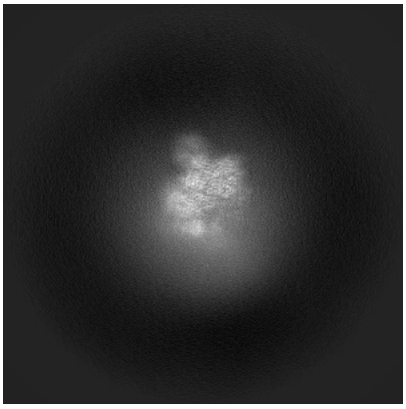
6.1.2 Raw map



X



Y

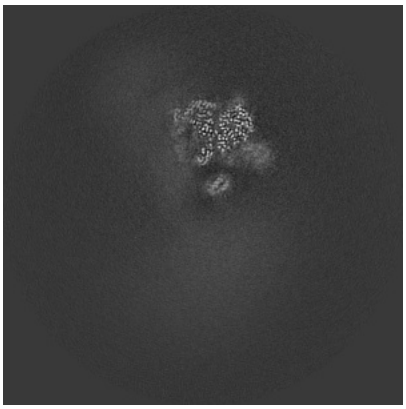


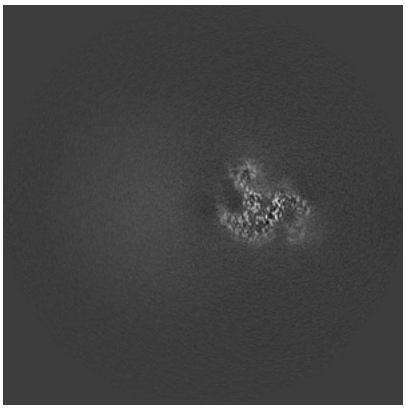
Z

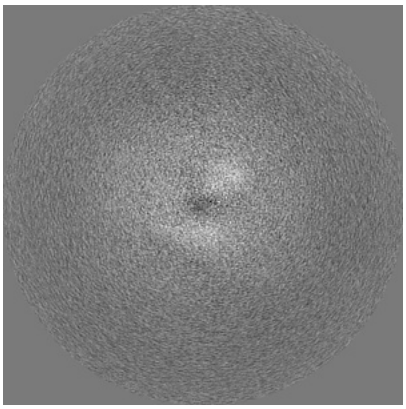
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

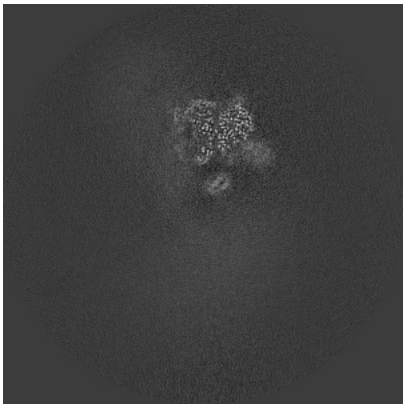
6.2.1 Primary map

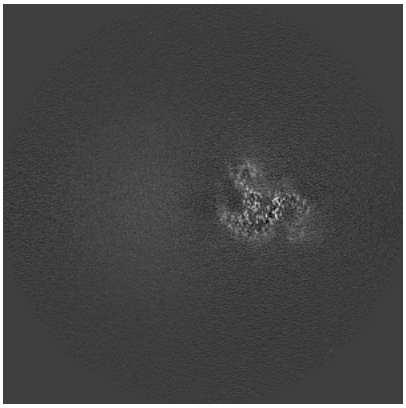

X Index: 240

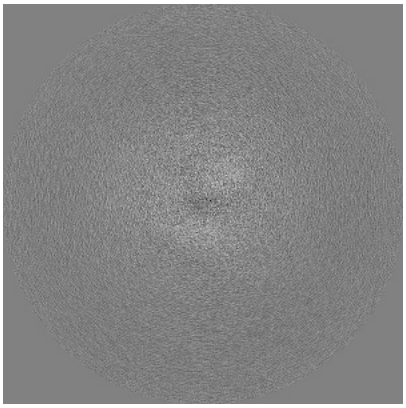

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

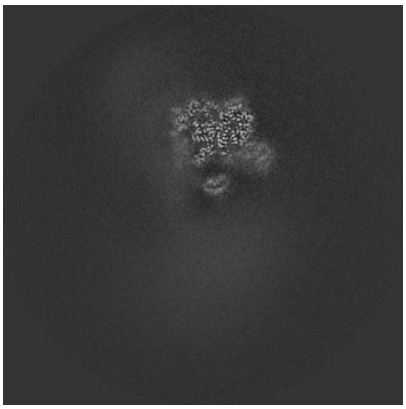

Y Index: 240

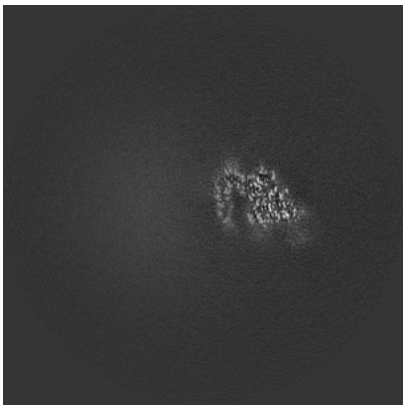

Z Index: 240

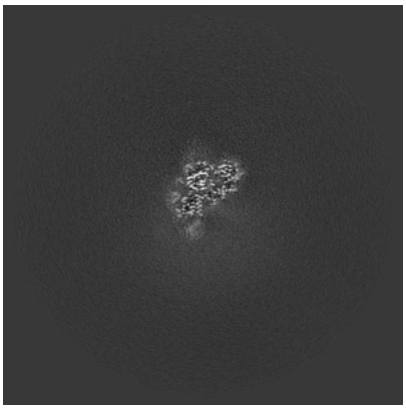
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

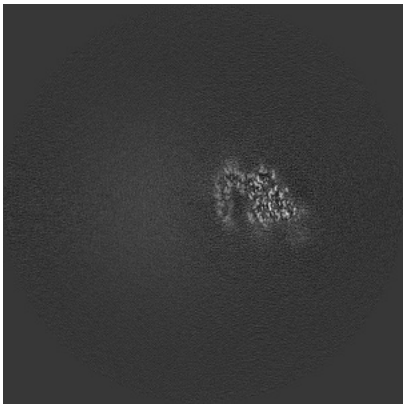

X Index: 236

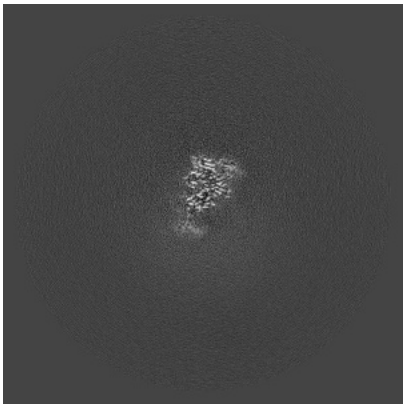

Y Index: 264


Z Index: 319

6.3.2 Raw map

X Index: 234

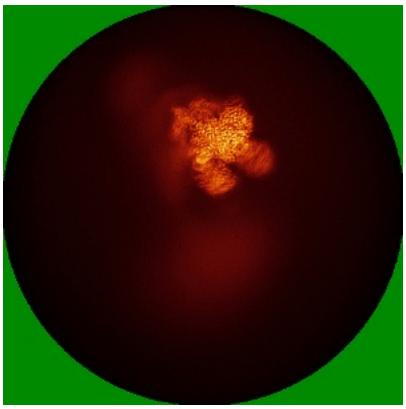

Y Index: 264

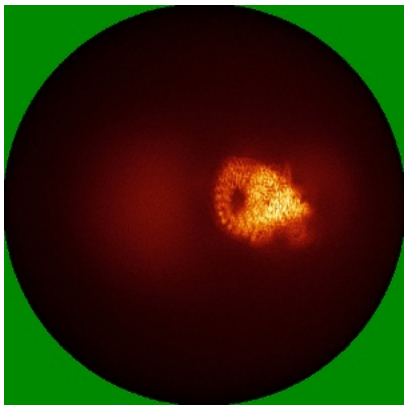

Z Index: 327

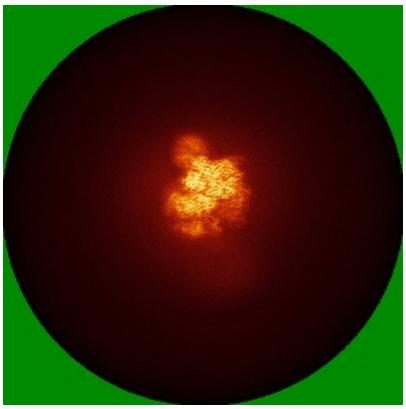
The images above show the largest variance slices of the map in three orthogonal directions.

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

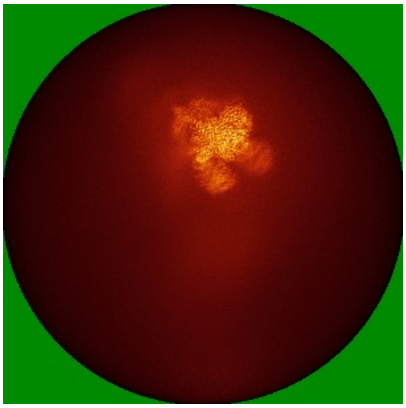
6.4.1 Primary map

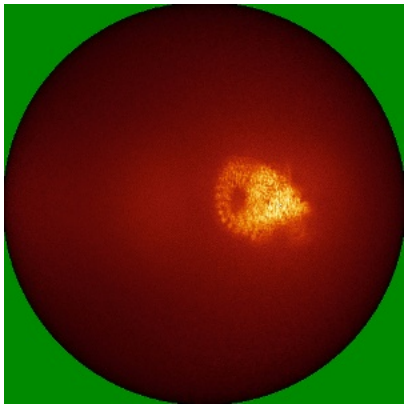

X

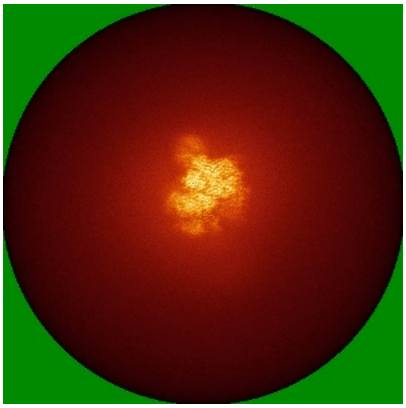

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

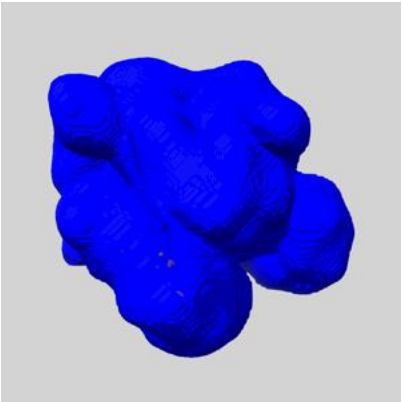
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

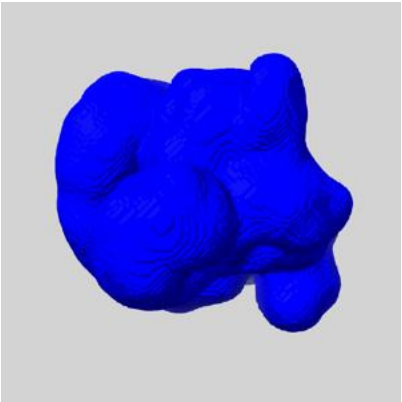
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

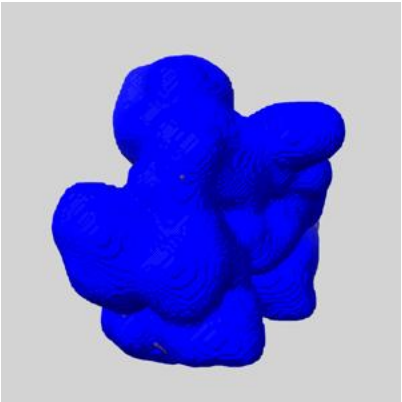
6.6.1 emd_12994_msk_1.map (i)



X



Y

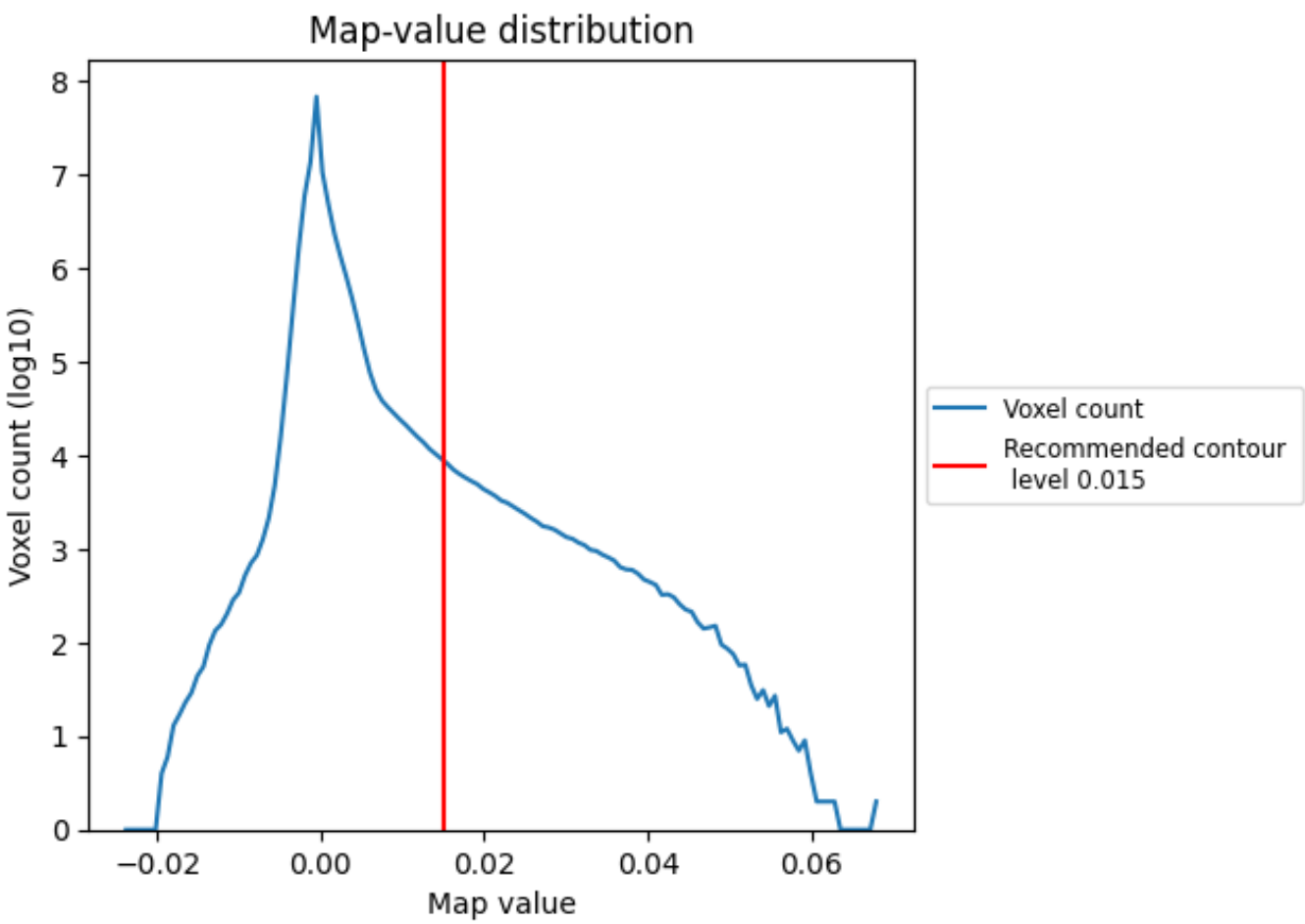


Z

7 Map analysis (i)

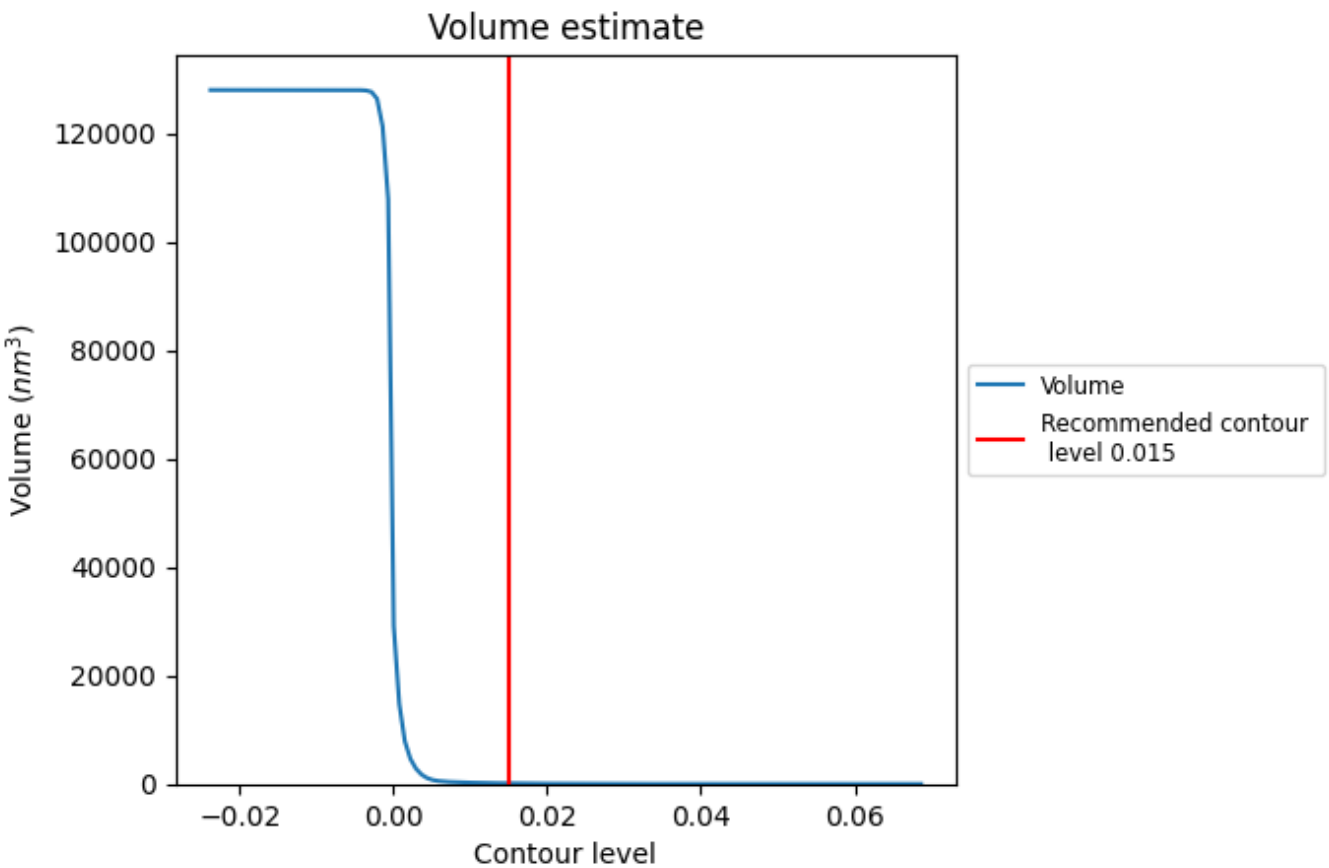
This section contains the results of statistical analysis of the map.

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.

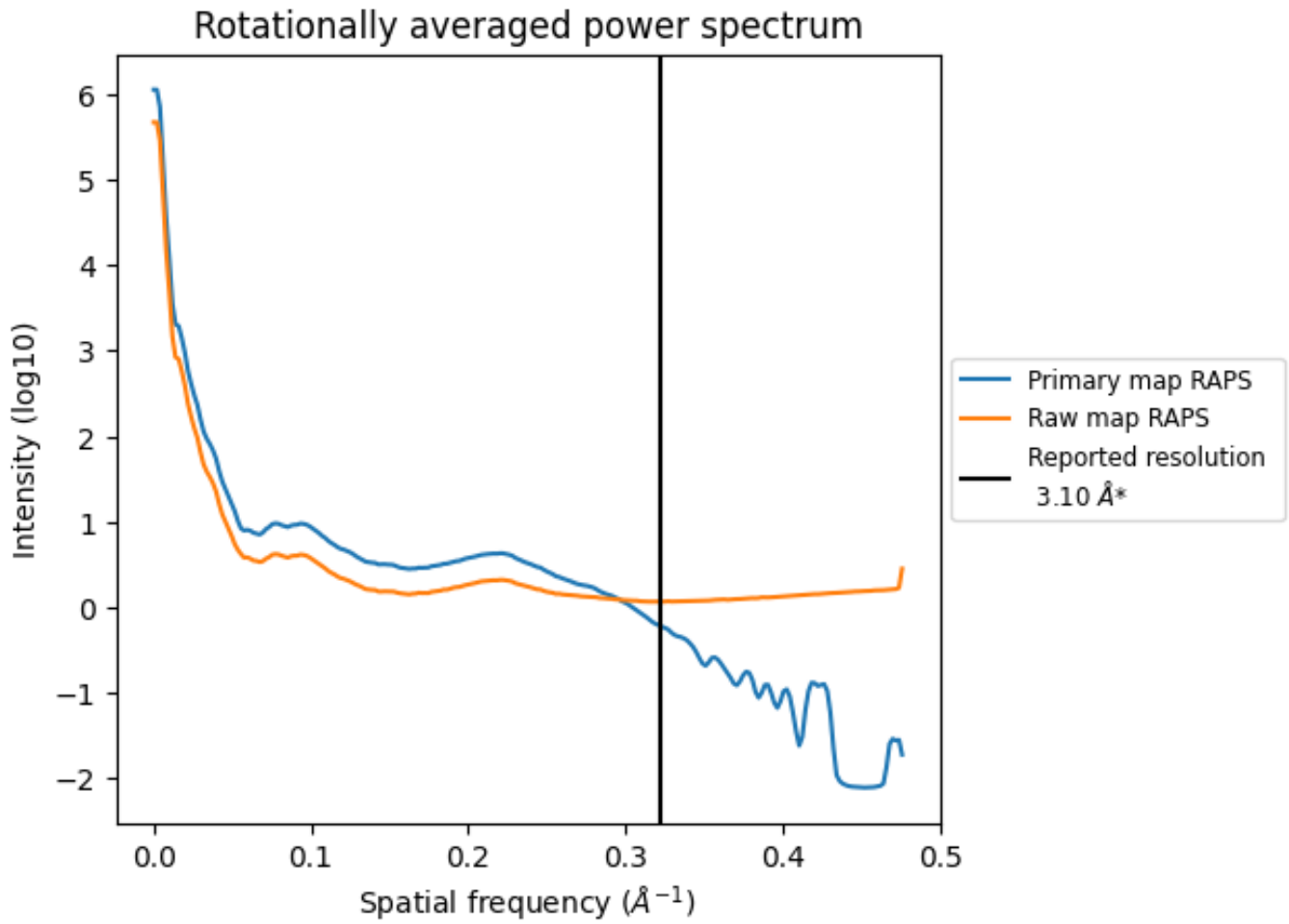
7.2 Volume estimate (i)



The volume at the recommended contour level is 112 nm^3; this corresponds to an approximate mass of 101 kDa.

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

7.3 Rotationally averaged power spectrum (i)

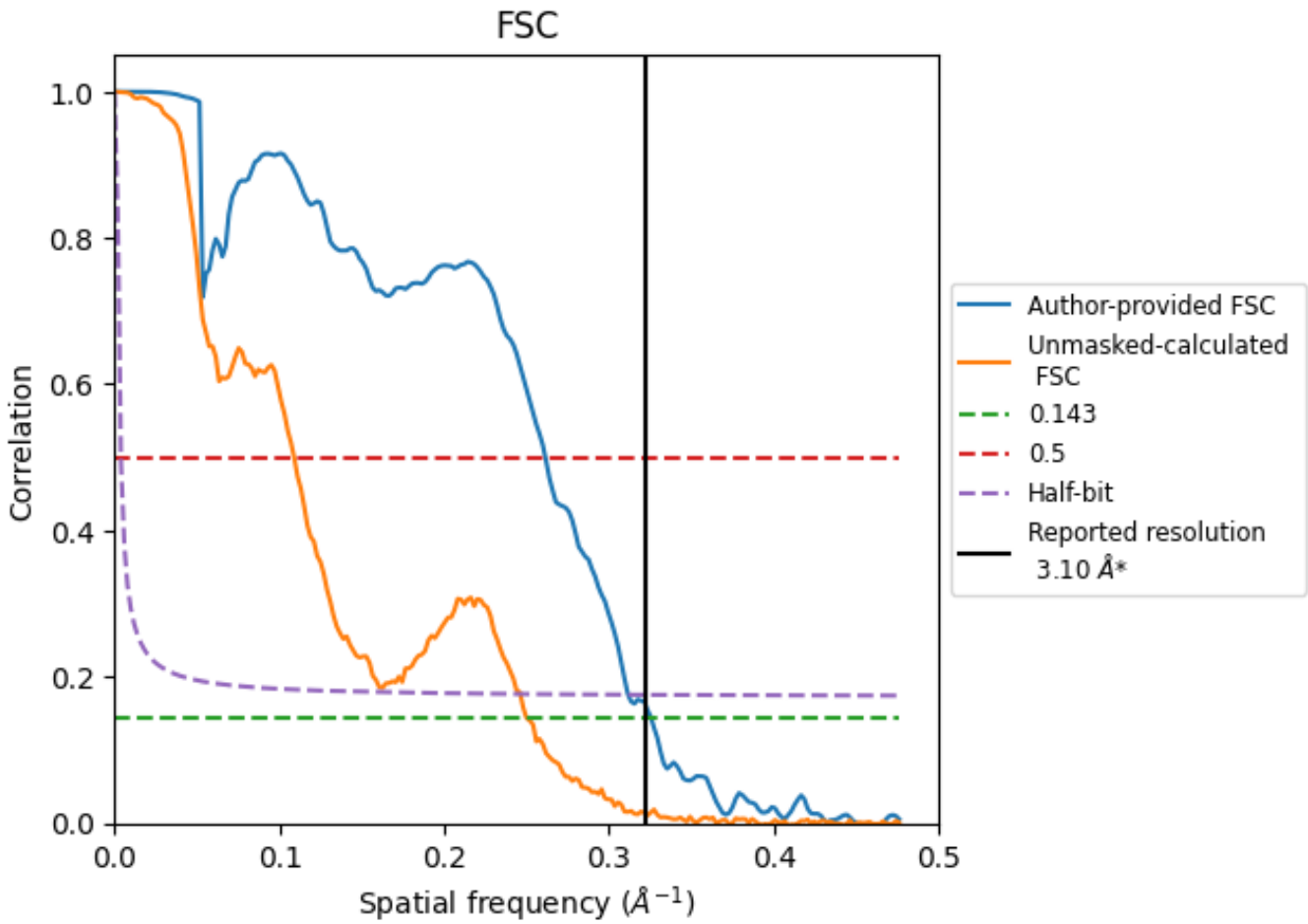


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

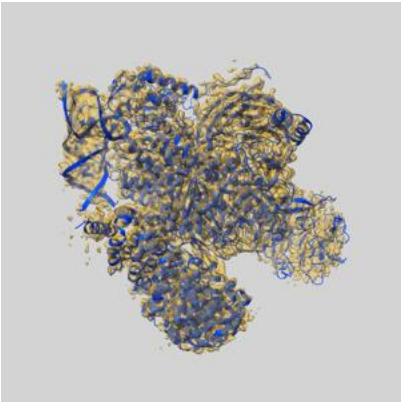
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.82	3.21
Unmasked-calculated*	4.00	9.17	4.06

*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 4.00 differs from the reported value 3.1 by more than 10 %

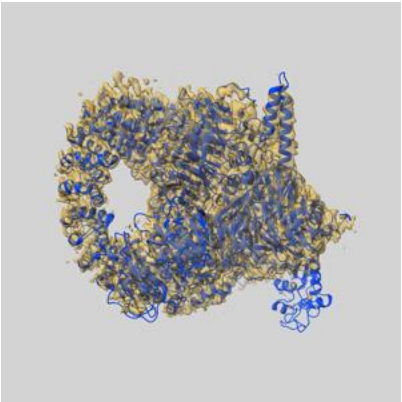
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12994 and PDB model 7ONB. Per-residue inclusion information can be found in section 3 on page 7.

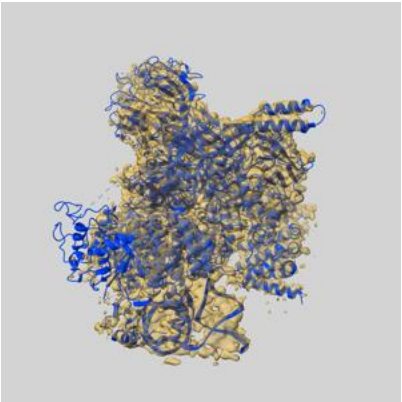
9.1 Map-model overlay (i)



X



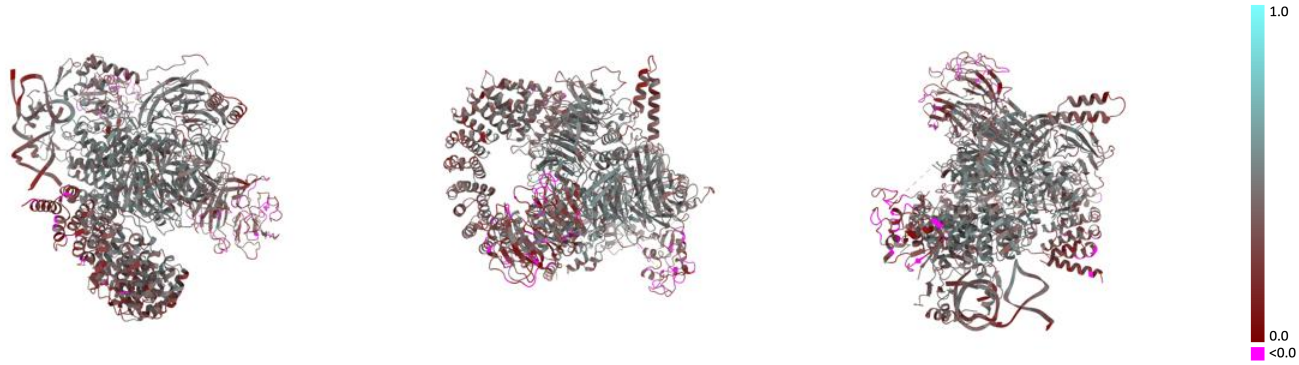
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

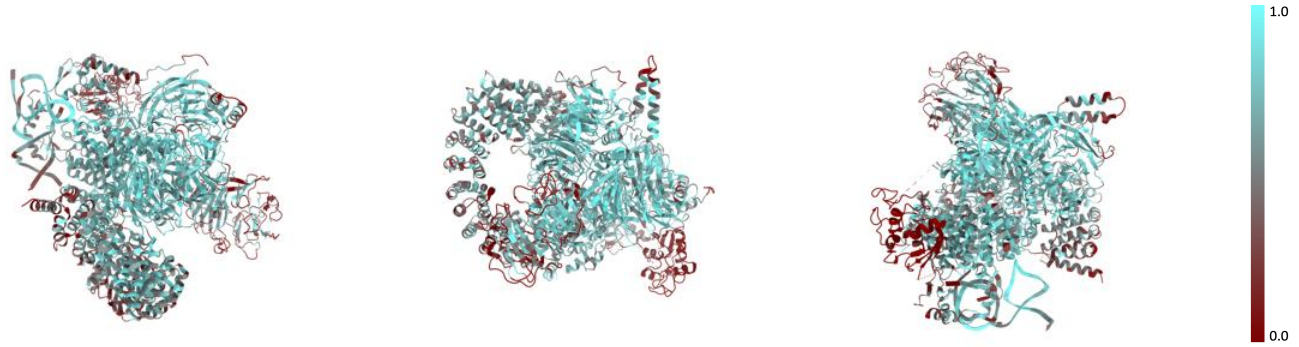
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

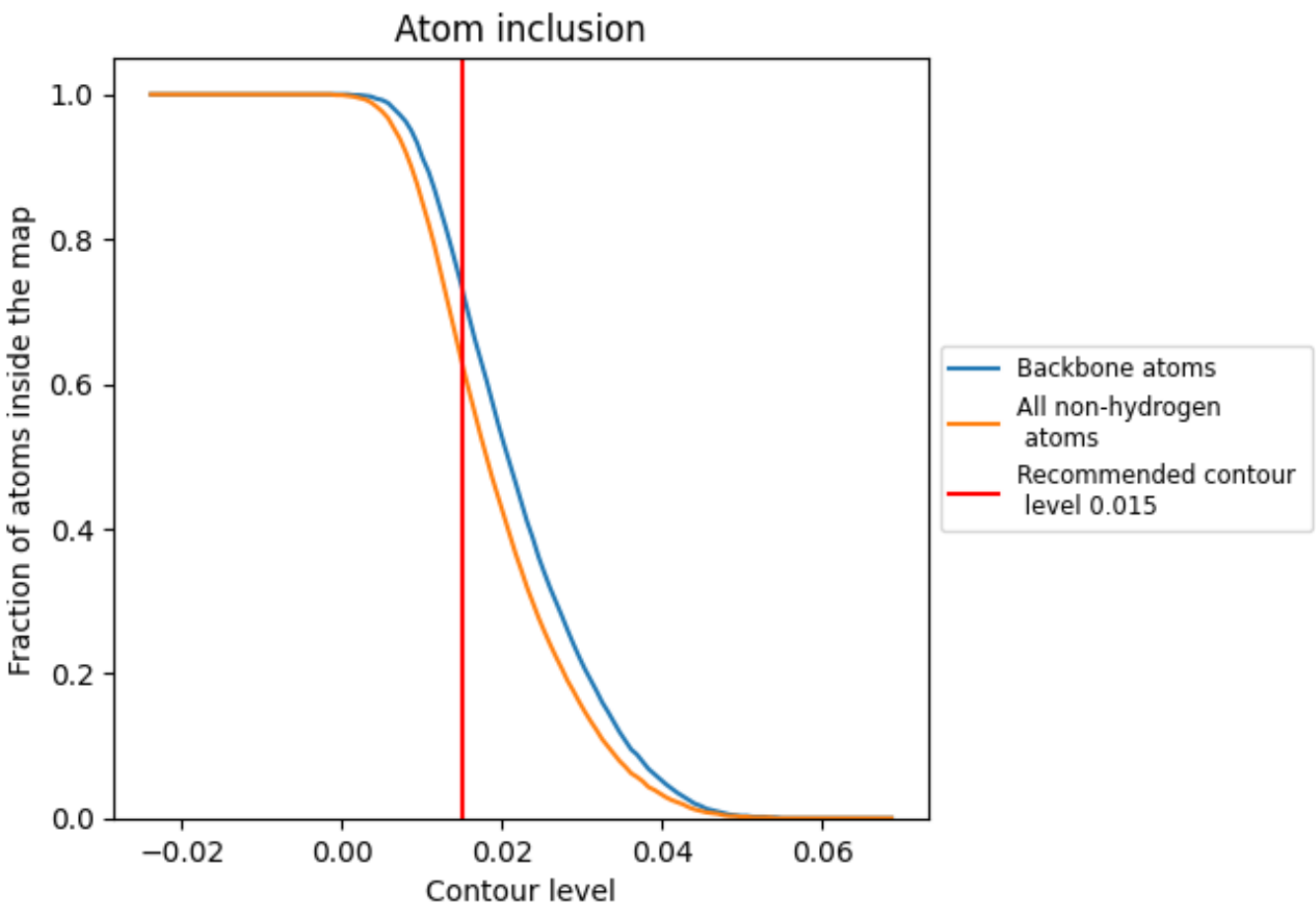
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6310	0.3890
A	0.6940	0.4120
B	0.7700	0.4490
C	0.5950	0.3660
D	0.7630	0.4560
F	0.7220	0.3700
G	0.5250	0.3200
H	0.6990	0.3460
I	0.4950	0.3640
K	0.0350	0.2610
M	0.4730	0.3790
N	0.5770	0.4080