



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:37 am GMT

PDB ID : 5GAM
EMDB ID : EMD-8011
Title : Foot region of the yeast spliceosomal U4/U6.U5 tri-snRNP
Authors : Nguyen, T.H.D.; Galej, W.P.; Bai, X.C.; Oubridge, C.; Scheres, S.H.W.; Newman, A.J.; Nagai, K.
Deposited on : 2015-12-15
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

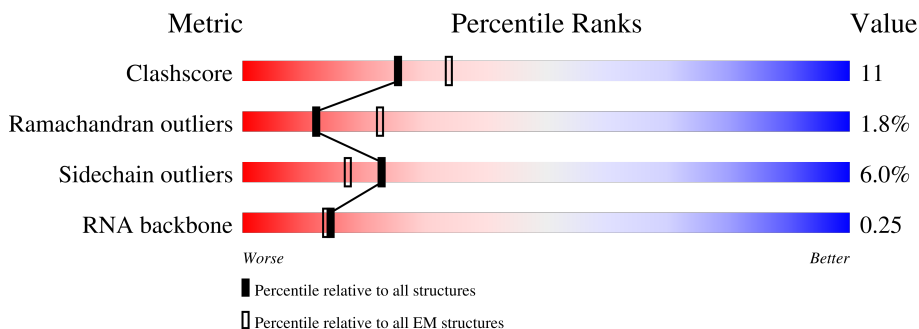
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	178	24% (green), 30% (yellow), 24% (orange), 21% (grey), 1% (red)
2	A	735	62% (green), 17% (yellow), 19% (grey), 2% (orange)
3	C	1008	57% (green), 25% (yellow), 15% (grey), 3% (orange)
4	W	31	35% (green), 32% (yellow), 13% (orange), 19% (grey)
5	b	196	41% (green), 59% (grey)
6	e	94	74% (green), 5% (yellow), 20% (grey)
7	f	86	80% (green), 16% (grey), 4% (yellow)

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Mol	Chain	Length	Quality of chain
8	g	77	 <p>87% 10%</p>
9	x	18	 <p>100%</p>
10	d	101	 <p>78% 19%</p>
11	h	146	 <p>52% 44%</p>
12	j	110	 <p>81% 5% 15%</p>

2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 19123 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.

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

- Molecule 2 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	593	4702	3052	817	817	16	0	0

- Molecule 3 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	855	6450	4195	1089	1143	23	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	530	SER	GLU	conflict	UNP P36048
C	531	LYS	ASP	conflict	UNP P36048
C	532	THR	ASP	conflict	UNP P36048

- Molecule 4 is a RNA chain called U6 snRNA, 5' end.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	W	25	532	237	91	179	25	0	0

- Molecule 5 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	b	80	631	403	114	111	3	0	0

- Molecule 6 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 9 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	x	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D1.

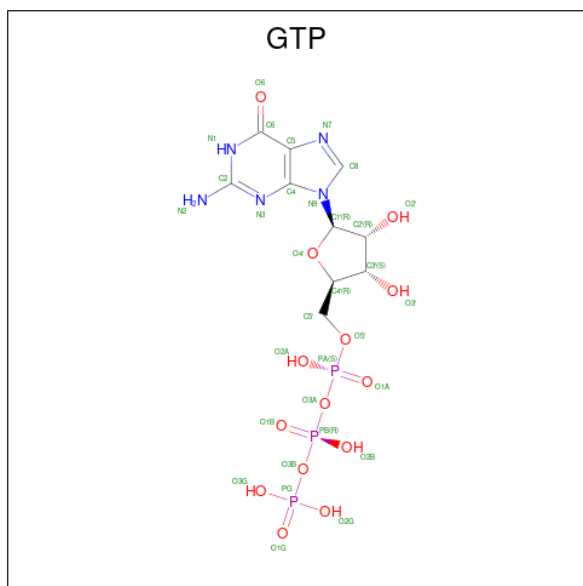
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

C₁₀H₁₆N₅O₁₄P₃).




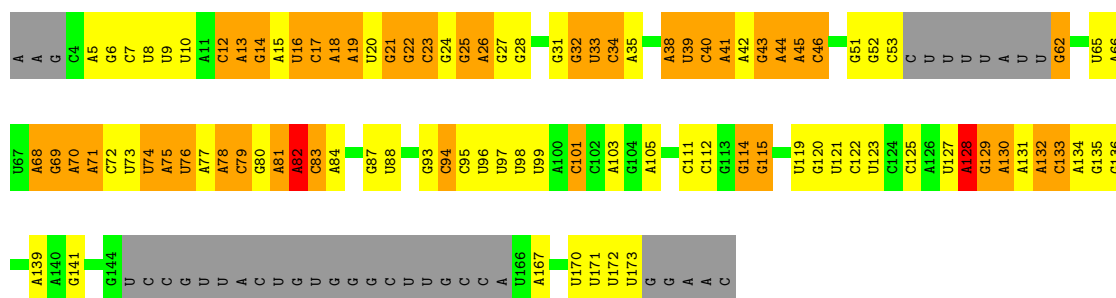
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	C	1	32	10	5	14	3	0

3 Residue-property plots [i](#)

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

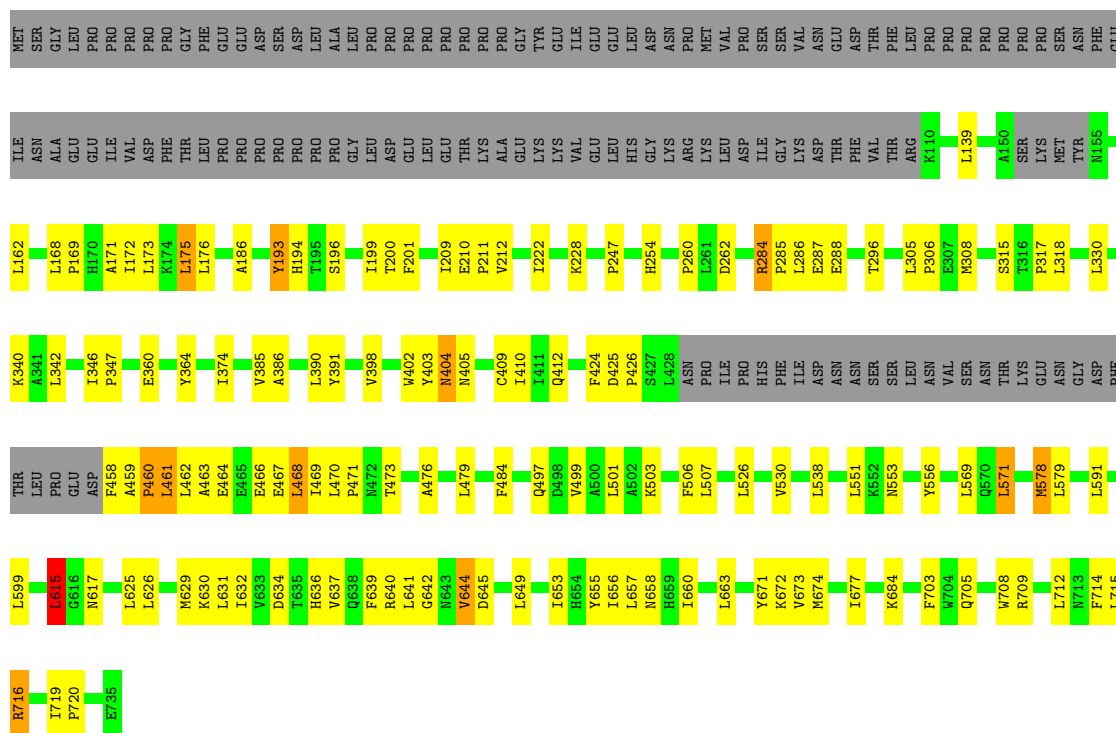
- Molecule 1: U5 snRNA

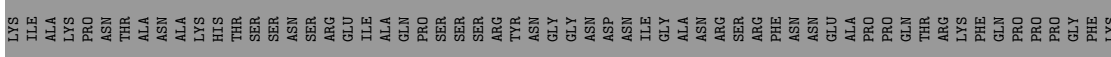
Chain U: 



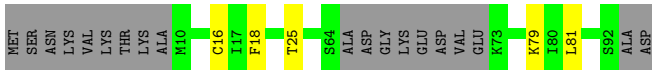
- Molecule 2: Pre-mRNA-splicing factor 8

Chain A: 

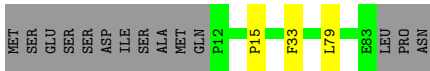
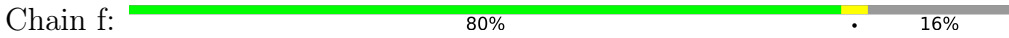




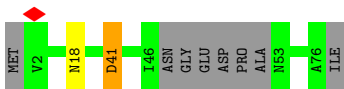
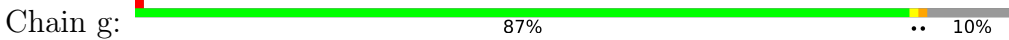
• Molecule 6: Small nuclear ribonucleoprotein E



• Molecule 7: Small nuclear ribonucleoprotein F



• Molecule 8: Small nuclear ribonucleoprotein G

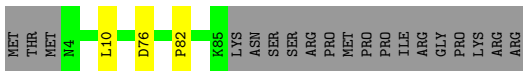
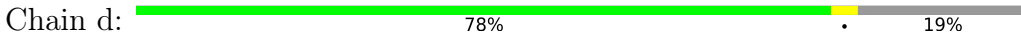


• Molecule 9: Unknown polypeptide

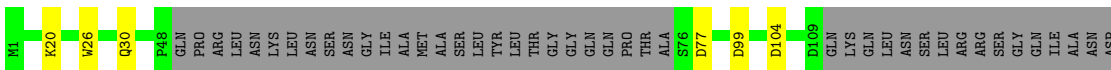


There are no outlier residues recorded for this chain.

• Molecule 10: Small nuclear ribonucleoprotein Sm D3




• Molecule 11: Small nuclear ribonucleoprotein Sm D1



PRO
SER
LYS
LYS
ARG
ARG
ARG
ASP
PHE
GLY
ALA
PRO
ALA
ASN
LYS
ARG
ARG
ARG
GLY
LEU

- Molecule 12: Small nuclear ribonucleoprotein Sm D2

Chain j:  81% 5% 15%

MET
SER
SER
GLN
ILE
ILE
ASP
ARG
ARG
PRO
LYS
HIS
GLU
LEU
SER
R15
F24
R49
T77
D99
S100
F108
VAL
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.076	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (\AA)	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: 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	0.38	0/3351	0.87	3/5213 (0.1%)
2	A	0.42	0/4840	0.74	2/6596 (0.0%)
3	C	0.44	0/6590	0.78	1/8975 (0.0%)
4	W	0.26	0/592	0.73	0/918
5	b	0.36	0/636	0.64	0/856
6	e	0.39	0/585	0.60	0/795
7	f	0.43	0/585	0.62	0/791
8	g	0.35	0/532	0.62	0/715
10	d	0.36	0/634	0.66	0/859
11	h	0.36	0/649	0.59	0/880
12	j	0.41	0/753	0.67	0/1013
All	All	0.41	0/19747	0.76	6/27611 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	5
3	C	0	4
8	g	0	1
All	All	0	10

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	82	A	C2'-C3'-O3'	7.10	125.12	109.50
1	U	128	A	C2'-C3'-O3'	6.70	124.43	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	62	G	C4'-C3'-O3'	5.50	124.01	113.00
2	A	425	ASP	CB-CG-OD2	5.26	123.03	118.30
3	C	659	LEU	CA-CB-CG	5.17	127.19	115.30
2	A	615	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	460	PRO	Peptide
2	A	464	GLU	Peptide
2	A	466	GLU	Peptide
2	A	553	ASN	Peptide
2	A	556	TYR	Peptide
3	C	498	THR	Peptide
3	C	607	LEU	Peptide
3	C	811	GLU	Peptide
3	C	958	PRO	Peptide
8	g	41	ASP	Peptide

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	U	2999	0	1515	103	0
2	A	4702	0	4527	109	0
3	C	6450	0	6420	186	0
4	W	532	0	269	4	0
5	b	631	0	670	0	0
6	e	575	0	597	0	0
7	f	573	0	572	0	0
8	g	529	0	557	0	0
9	x	90	0	20	0	0
10	d	625	0	647	0	0
11	h	644	0	686	0	0
12	j	741	0	778	0	0
13	C	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19123	0	17270	377	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 11.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:139:LEU:HD13	2:A:193:TYR:CD2	1.31	1.63
2:A:139:LEU:CD1	2:A:193:TYR:CD2	2.15	1.29
1:U:42:A:H3'	1:U:43:G:H5''	1.24	1.15
2:A:139:LEU:HD13	2:A:193:TYR:CE2	1.87	1.08
2:A:139:LEU:CD1	2:A:193:TYR:HD2	1.60	1.07
1:U:42:A:C3'	1:U:43:G:H5''	1.88	1.03
1:U:42:A:H2'	1:U:43:G:C4'	1.98	0.94
1:U:41:A:C8	1:U:75:A:C2	2.56	0.93
2:A:468:LEU:HD21	3:C:382:TYR:HB3	1.51	0.92
1:U:42:A:H3'	1:U:43:G:C5'	1.99	0.91
2:A:468:LEU:CD1	3:C:281:PRO:HG3	2.00	0.91
1:U:74:U:H2'	1:U:76:U:OP2	1.77	0.85
2:A:460:PRO:HB3	3:C:376:PHE:CD1	2.10	0.85
1:U:41:A:C8	1:U:75:A:N1	2.46	0.82
1:U:74:U:O2'	1:U:76:U:OP2	1.98	0.82
1:U:74:U:C2'	1:U:76:U:OP2	2.30	0.79
1:U:74:U:H2'	1:U:75:A:H4'	1.62	0.79
2:A:461:LEU:HD22	3:C:404:PHE:CE1	2.19	0.78
3:C:472:VAL:HG22	3:C:486:VAL:HG22	1.66	0.77
1:U:42:A:C2'	1:U:43:G:H5''	2.14	0.77
2:A:461:LEU:HD11	3:C:380:PRO:HB3	1.67	0.77
2:A:708:TRP:CE2	2:A:712:LEU:HD11	2.19	0.77
1:U:41:A:H2'	1:U:42:A:C8	2.19	0.77
3:C:387:TYR:HB3	3:C:396:LEU:HD12	1.67	0.76
3:C:324:ILE:HG23	3:C:377:ILE:HD11	1.68	0.75
1:U:43:G:H4'	1:U:43:G:OP1	1.85	0.75
2:A:658:ASN:HD22	2:A:684:LYS:HB2	1.53	0.74
3:C:836:SER:O	3:C:840:PRO:HD2	1.87	0.74
1:U:17:C:H2'	1:U:18:A:C8	2.24	0.73
1:U:42:A:C3'	1:U:43:G:C5'	2.62	0.73
3:C:200:CYS:HB3	3:C:436:VAL:HG21	1.72	0.72
2:A:469:ILE:HG23	2:A:473:THR:CG2	2.20	0.71
1:U:74:U:C2'	1:U:75:A:H4'	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:390:LEU:HD22	2:A:391:TYR:CE1	2.26	0.70
3:C:868:VAL:HG11	3:C:876:VAL:HG21	1.73	0.70
1:U:41:A:N9	1:U:75:A:C2	2.60	0.70
2:A:467:GLU:N	2:A:467:GLU:OE1	2.21	0.70
1:U:24:G:H2'	1:U:25:G:O4'	1.92	0.69
3:C:872:LEU:HD13	3:C:922:THR:HG22	1.74	0.69
1:U:45:A:N3	1:U:45:A:H2'	2.07	0.68
1:U:42:A:H2'	1:U:43:G:O4'	1.93	0.68
1:U:42:A:H2'	1:U:43:G:C5'	2.24	0.68
2:A:171:ALA:HB1	2:A:201:PHE:HB3	1.77	0.67
2:A:458:PHE:CE2	3:C:336:ILE:HD11	2.30	0.67
3:C:774:LEU:HD13	3:C:803:VAL:HG23	1.78	0.66
1:U:46:C:H4'	3:C:111:LYS:HG3	1.77	0.66
1:U:45:A:H3'	1:U:46:C:C6	2.31	0.65
2:A:462:LEU:HD23	3:C:403:ASN:HD22	1.61	0.65
3:C:236:LEU:HD11	3:C:435:LEU:HD21	1.79	0.65
3:C:761:ALA:O	3:C:765:VAL:HG13	1.97	0.65
2:A:715:LEU:O	2:A:719:ILE:HG23	1.97	0.64
3:C:345:THR:HA	3:C:348:LEU:HD12	1.78	0.64
3:C:149:LEU:HD21	3:C:435:LEU:HD11	1.77	0.64
1:U:45:A:C5'	1:U:46:C:H5	2.11	0.64
2:A:468:LEU:HD11	3:C:281:PRO:HG3	1.80	0.64
1:U:133:C:H2'	1:U:133:C:O2	1.97	0.64
3:C:360:ARG:HA	3:C:361:THR:HG22	1.79	0.64
1:U:46:C:H4'	3:C:111:LYS:CG	2.28	0.64
2:A:673:VAL:HG22	2:A:714:PHE:CE1	2.32	0.63
3:C:323:THR:HG21	3:C:438:ALA:HB2	1.78	0.63
2:A:468:LEU:HD12	3:C:281:PRO:HG3	1.79	0.63
3:C:387:TYR:CE1	3:C:399:LEU:CD1	2.82	0.63
3:C:864:VAL:HG22	3:C:930:LEU:CD2	2.27	0.63
2:A:470:LEU:HB3	2:A:471:PRO:HD2	1.81	0.62
1:U:45:A:H5''	1:U:46:C:H5	1.65	0.62
3:C:659:LEU:HD21	3:C:668:ILE:HD13	1.82	0.62
1:U:42:A:H2'	1:U:43:G:H5''	1.81	0.62
1:U:41:A:C2	1:U:42:A:C6	2.88	0.62
3:C:472:VAL:HG13	3:C:484:SER:OG	2.00	0.61
1:U:40:C:N3	1:U:115:G:C6	2.69	0.61
3:C:501:ILE:CD1	3:C:567:ILE:HG23	2.31	0.61
3:C:387:TYR:CZ	3:C:399:LEU:HD11	2.35	0.61
3:C:501:ILE:HD11	3:C:567:ILE:HD12	1.82	0.61
1:U:20:U:H2'	1:U:21:G:C1'	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:193:TYR:HB3	2:A:200:THR:HG23	1.82	0.61
1:U:128:A:H2'	1:U:129:G:O4'	2.01	0.60
3:C:857:LEU:HG	3:C:967:VAL:HG22	1.83	0.60
1:U:45:A:H3'	1:U:46:C:H6	1.65	0.60
2:A:330:LEU:HD22	2:A:385:VAL:HG23	1.84	0.60
2:A:176:LEU:HD23	2:A:715:LEU:HD12	1.84	0.60
1:U:22:G:C2	1:U:131:A:C2	2.90	0.59
3:C:235:VAL:HG23	3:C:261:VAL:HG11	1.83	0.59
3:C:387:TYR:CZ	3:C:399:LEU:CD1	2.85	0.59
3:C:762:SER:O	3:C:765:VAL:HG22	2.02	0.59
2:A:462:LEU:HD23	3:C:403:ASN:ND2	2.17	0.59
3:C:223:ASP:OD2	3:C:631:GLY:N	2.36	0.59
1:U:19:A:H2'	1:U:20:U:C1'	2.32	0.59
2:A:175:LEU:HD13	2:A:571:LEU:HD12	1.85	0.58
2:A:222:ILE:HD11	2:A:317:PRO:HG2	1.84	0.58
1:U:42:A:H2'	1:U:43:G:H4'	1.83	0.58
2:A:194:HIS:HD2	2:A:196:SER:H	1.52	0.58
3:C:193:LEU:HD11	3:C:213:LEU:HB3	1.86	0.57
3:C:605:ILE:HD13	3:C:656:LEU:HD11	1.85	0.57
1:U:25:G:H4'	1:U:26:A:O4'	2.03	0.57
2:A:403:TYR:CD2	3:C:189:LEU:HD11	2.40	0.57
1:U:33:U:O4	2:A:284:ARG:NH2	2.37	0.57
2:A:569:LEU:HD21	2:A:637:VAL:HG21	1.86	0.57
2:A:461:LEU:N	2:A:461:LEU:HD12	2.19	0.57
1:U:23:C:H2'	1:U:24:G:O4'	2.05	0.57
1:U:42:A:C2'	1:U:43:G:C5'	2.81	0.57
3:C:318:LEU:HD21	3:C:421:LEU:HD13	1.87	0.57
3:C:864:VAL:HG21	3:C:906:VAL:HG23	1.86	0.57
2:A:172:ILE:HD11	2:A:626:LEU:CD2	2.34	0.57
3:C:241:VAL:HG11	3:C:273:LEU:HD23	1.85	0.57
1:U:38:A:H2'	1:U:39:U:C6	2.40	0.57
1:U:12:C:O2'	1:U:13:A:O4'	2.23	0.56
3:C:387:TYR:CE1	3:C:399:LEU:HD12	2.40	0.56
4:W:29:U:H2'	4:W:30:G:O4'	2.04	0.56
2:A:673:VAL:HG22	2:A:714:PHE:CZ	2.40	0.56
3:C:108:GLN:O	3:C:111:LYS:HD3	2.04	0.56
2:A:459:ALA:HB1	2:A:463:ALA:CB	2.35	0.56
2:A:461:LEU:HD12	2:A:461:LEU:H	1.71	0.56
3:C:472:VAL:HG22	3:C:486:VAL:CG2	2.35	0.56
1:U:79:C:C2	1:U:114:G:N2	2.73	0.56
3:C:656:LEU:HD22	3:C:670:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:314:ALA:HB2	3:C:321:THR:HG22	1.87	0.56
3:C:723:LEU:HD12	3:C:773:VAL:HG11	1.88	0.56
2:A:656:ILE:O	2:A:660:ILE:HD12	2.06	0.56
1:U:26:A:C8	1:U:26:A:O5'	2.59	0.56
1:U:31:G:O2'	1:U:32:G:H5'	2.06	0.56
2:A:639:PHE:HA	2:A:644:VAL:HG11	1.87	0.56
3:C:133:ILE:HD13	3:C:560:GLN:HB3	1.88	0.56
3:C:234:LEU:HD13	3:C:439:ILE:HG23	1.88	0.55
2:A:199:ILE:HG23	2:A:199:ILE:O	2.06	0.55
3:C:602:VAL:HG11	3:C:908:VAL:HG21	1.88	0.55
2:A:193:TYR:CD1	2:A:193:TYR:N	2.73	0.55
2:A:193:TYR:N	2:A:193:TYR:HD1	2.05	0.55
3:C:774:LEU:HD22	3:C:803:VAL:HB	1.89	0.54
1:U:26:A:C6	1:U:129:G:H1'	2.42	0.54
3:C:152:LEU:HB2	3:C:432:GLN:HE22	1.72	0.54
3:C:710:VAL:HG22	3:C:820:LEU:HD23	1.89	0.54
3:C:626:SER:HB3	3:C:634:ILE:HD12	1.90	0.54
1:U:41:A:C4	1:U:75:A:C2	2.96	0.54
3:C:320:PHE:CE2	3:C:425:LEU:HD13	2.43	0.54
3:C:187:ARG:NH1	3:C:654:CYS:SG	2.73	0.54
1:U:20:U:H2'	1:U:21:G:O4'	2.09	0.53
3:C:688:SER:HB3	3:C:821:LEU:HD12	1.88	0.53
3:C:423:HIS:CE1	3:C:427:LEU:HD11	2.43	0.53
1:U:40:C:O2	1:U:115:G:C2	2.62	0.53
3:C:288:LEU:HD13	3:C:313:PHE:CE2	2.43	0.53
2:A:318:LEU:HD11	2:A:703:PHE:CE1	2.44	0.53
2:A:636:HIS:CE1	2:A:653:ILE:HD11	2.45	0.52
1:U:73:U:H2'	1:U:74:U:C1'	2.40	0.52
3:C:251:GLN:HG2	3:C:933:TRP:CD2	2.44	0.52
2:A:305:LEU:HD21	2:A:476:ALA:HB2	1.91	0.52
3:C:269:LYS:HA	3:C:1101:GTP:O6	2.10	0.52
3:C:241:VAL:CG1	3:C:273:LEU:HD23	2.40	0.52
3:C:774:LEU:HD21	3:C:813:ILE:HB	1.91	0.52
1:U:19:A:H2'	1:U:20:U:N1	2.24	0.52
3:C:545:LEU:HB3	3:C:546:GLY:HA3	1.90	0.52
2:A:674:MET:HA	2:A:677:ILE:HD12	1.91	0.51
3:C:862:TYR:CD2	3:C:908:VAL:HG22	2.46	0.51
1:U:18:A:H3'	1:U:19:A:H8	1.75	0.51
3:C:320:PHE:CD2	3:C:425:LEU:HD13	2.46	0.51
1:U:132:A:C2'	1:U:133:C:OP1	2.58	0.51
2:A:176:LEU:HD13	2:A:632:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:THR:O	3:C:198:LEU:HD23	2.10	0.51
1:U:22:G:N1	1:U:131:A:C2	2.79	0.51
2:A:461:LEU:CD1	3:C:380:PRO:HB3	2.40	0.51
3:C:124:LEU:HD22	3:C:553:VAL:HG11	1.93	0.51
3:C:615:LEU:N	3:C:616:PRO:HD2	2.25	0.51
2:A:497:GLN:HB3	2:A:712:LEU:HD13	1.93	0.51
3:C:675:THR:HG23	3:C:909:ILE:HG12	1.91	0.51
1:U:40:C:C2	1:U:115:G:N1	2.79	0.50
1:U:70:A:H3'	1:U:71:A:H5''	1.91	0.50
2:A:390:LEU:HG	3:C:605:ILE:HD11	1.92	0.50
2:A:459:ALA:HB1	2:A:463:ALA:HB3	1.93	0.50
2:A:139:LEU:CD1	2:A:193:TYR:CE2	2.74	0.50
3:C:138:VAL:HG12	3:C:214:ASP:HA	1.93	0.50
3:C:239:ILE:HD13	3:C:245:VAL:HG22	1.94	0.50
2:A:591:LEU:HD13	2:A:599:LEU:HD11	1.94	0.50
3:C:780:PRO:HD2	3:C:783:ILE:HD13	1.93	0.50
1:U:129:G:H4'	1:U:130:A:C4'	2.42	0.50
3:C:680:SER:O	3:C:856:ILE:N	2.45	0.50
3:C:628:TYR:O	3:C:630:PRO:HD3	2.11	0.50
1:U:74:U:H2'	1:U:76:U:P	2.52	0.50
2:A:526:LEU:O	2:A:530:VAL:HG23	2.12	0.50
3:C:255:GLN:HG3	3:C:598:ILE:HD13	1.93	0.50
3:C:314:ALA:CB	3:C:321:THR:HG22	2.42	0.49
2:A:390:LEU:HD22	2:A:391:TYR:CD1	2.47	0.49
2:A:625:LEU:HD22	2:A:715:LEU:HD21	1.94	0.49
3:C:235:VAL:CG2	3:C:261:VAL:HG11	2.42	0.49
2:A:315:SER:O	2:A:318:LEU:N	2.44	0.49
3:C:322:PHE:HE2	3:C:381:LEU:HD11	1.77	0.49
3:C:862:TYR:CE2	3:C:908:VAL:HG13	2.48	0.49
3:C:869:HIS:CD2	3:C:925:LEU:HD22	2.47	0.49
2:A:288:GLU:OE2	2:A:296:THR:HG22	2.12	0.49
3:C:208:ARG:NH1	3:C:440:THR:OG1	2.46	0.49
3:C:864:VAL:HG22	3:C:930:LEU:HD22	1.94	0.49
3:C:712:ALA:HB2	3:C:818:TYR:CD2	2.47	0.49
3:C:659:LEU:HD23	3:C:660:ARG:N	2.28	0.48
1:U:78:A:N6	1:U:81:A:C2	2.81	0.48
1:U:128:A:H2'	1:U:128:A:N3	2.28	0.48
2:A:462:LEU:CD2	3:C:403:ASN:ND2	2.77	0.48
2:A:657:LEU:HD13	2:A:708:TRP:HA	1.94	0.48
2:A:630:LYS:O	2:A:634:ASP:N	2.40	0.48
3:C:154:VAL:O	3:C:157:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:712:ALA:HB1	3:C:816:VAL:CG1	2.44	0.48
2:A:636:HIS:CD2	2:A:649:LEU:HD21	2.49	0.48
3:C:236:LEU:HD21	3:C:439:ILE:CG1	2.44	0.48
3:C:768:PHE:HB3	3:C:775:ILE:HA	1.96	0.48
3:C:288:LEU:HD13	3:C:313:PHE:HE2	1.79	0.48
2:A:194:HIS:CD2	2:A:196:SER:H	2.30	0.48
2:A:424:PHE:CZ	3:C:900:LEU:HD21	2.49	0.48
3:C:775:ILE:O	3:C:818:TYR:N	2.47	0.48
3:C:602:VAL:HG12	3:C:602:VAL:O	2.14	0.47
2:A:468:LEU:O	2:A:468:LEU:HD23	2.14	0.47
3:C:502:LEU:HD12	3:C:591:PHE:CD1	2.49	0.47
3:C:605:ILE:HD12	3:C:652:MET:HG3	1.96	0.47
1:U:13:A:H2'	1:U:14:G:C8	2.49	0.47
1:U:22:G:C5	1:U:23:C:C5	3.02	0.47
1:U:74:U:H3'	1:U:75:A:H5''	1.95	0.47
3:C:315:SER:HB3	3:C:320:PHE:CE2	2.50	0.47
2:A:172:ILE:HG23	2:A:629:MET:CG	2.45	0.47
3:C:387:TYR:CE1	3:C:399:LEU:HD11	2.48	0.47
3:C:493:LEU:HD23	3:C:542:ILE:HD11	1.97	0.47
3:C:567:ILE:HG22	3:C:571:TYR:CE1	2.50	0.47
1:U:74:U:H2'	1:U:75:A:C4'	2.38	0.47
2:A:168:LEU:HA	2:A:199:ILE:HD11	1.96	0.47
3:C:270:LEU:HD11	3:C:313:PHE:HB3	1.96	0.47
3:C:457:SER:OG	3:C:592:PHE:HA	2.15	0.47
3:C:873:LEU:HD22	3:C:900:LEU:HD13	1.96	0.47
3:C:934:HIS:O	3:C:935:LYS:CB	2.63	0.47
3:C:988:THR:HB	3:C:989:LEU:CB	2.45	0.47
1:U:25:G:H2'	1:U:25:G:N3	2.30	0.47
2:A:460:PRO:HB3	3:C:376:PHE:CE1	2.47	0.47
3:C:361:THR:O	3:C:361:THR:HG23	2.15	0.47
2:A:644:VAL:HG22	2:A:645:ASP:H	1.80	0.47
2:A:719:ILE:N	2:A:720:PRO:CD	2.78	0.47
3:C:236:LEU:HD21	3:C:439:ILE:HG12	1.97	0.47
3:C:567:ILE:HG22	3:C:571:TYR:CD1	2.49	0.47
2:A:507:LEU:HD23	2:A:526:LEU:CD2	2.46	0.46
1:U:21:G:C2	1:U:132:A:C2	3.03	0.46
3:C:873:LEU:N	3:C:874:PRO:CD	2.77	0.46
1:U:75:A:H5'	1:U:76:U:C5	2.50	0.46
3:C:324:ILE:HD13	3:C:324:ILE:N	2.29	0.46
3:C:944:VAL:HG23	3:C:967:VAL:HG21	1.98	0.46
3:C:223:ASP:OD2	3:C:630:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:470:ALA:HB3	3:C:577:LEU:HD11	1.98	0.46
3:C:492:LEU:HD12	3:C:492:LEU:O	2.15	0.46
1:U:26:A:N6	1:U:129:G:H1'	2.30	0.46
1:U:115:G:H2'	1:U:115:G:N3	2.31	0.46
2:A:709:ARG:HA	2:A:712:LEU:HD12	1.97	0.46
3:C:154:VAL:HG11	3:C:177:TYR:CD2	2.51	0.46
3:C:360:ARG:HA	3:C:361:THR:CG2	2.46	0.46
2:A:330:LEU:HD21	2:A:386:ALA:HB2	1.98	0.46
3:C:816:VAL:HG11	3:C:818:TYR:CE1	2.50	0.46
3:C:866:ILE:HD13	3:C:918:LEU:HD11	1.96	0.46
3:C:582:SER:OG	3:C:583:LYS:N	2.48	0.46
1:U:87:G:H2'	1:U:88:U:C6	2.51	0.46
3:C:191:ILE:HG22	3:C:192:LYS:HG3	1.98	0.46
3:C:242:VAL:HG21	3:C:272:ARG:HG2	1.97	0.45
2:A:209:ILE:HB	2:A:212:VAL:HB	1.97	0.45
2:A:499:VAL:HG12	2:A:501:LEU:HD21	1.98	0.45
3:C:470:ALA:HB3	3:C:577:LEU:CD1	2.46	0.45
3:C:879:LEU:HD11	3:C:921:SER:OG	2.17	0.45
3:C:408:LEU:HD11	3:C:424:VAL:HG22	1.99	0.45
3:C:152:LEU:HD11	3:C:319:GLY:HA2	1.97	0.45
3:C:856:ILE:HD13	3:C:939:LYS:HG3	1.97	0.45
1:U:38:A:H2'	1:U:39:U:C5	2.52	0.45
3:C:324:ILE:HG23	3:C:377:ILE:CD1	2.44	0.45
3:C:625:ILE:HG22	3:C:634:ILE:HD11	1.97	0.45
3:C:866:ILE:HB	3:C:902:VAL:HG13	1.97	0.45
2:A:469:ILE:HG23	2:A:473:THR:HG23	1.99	0.45
1:U:101:C:OP1	2:A:672:LYS:N	2.46	0.45
3:C:655:LEU:C	3:C:655:LEU:HD23	2.37	0.45
4:W:27:U:H2'	4:W:28:U:C6	2.51	0.45
2:A:458:PHE:CG	2:A:458:PHE:O	2.70	0.45
2:A:168:LEU:N	2:A:169:PRO:HD2	2.32	0.45
1:U:21:G:N2	1:U:132:A:N3	2.65	0.44
2:A:631:LEU:HD21	2:A:663:LEU:HD13	1.99	0.44
3:C:632:VAL:HG22	3:C:651:TYR:HE2	1.82	0.44
1:U:101:C:OP1	2:A:671:TYR:N	2.51	0.44
2:A:458:PHE:O	2:A:458:PHE:CD2	2.70	0.44
1:U:41:A:N7	1:U:75:A:N1	2.65	0.44
2:A:168:LEU:CD2	2:A:578:MET:HG2	2.48	0.44
2:A:172:ILE:HG23	2:A:629:MET:HG3	1.99	0.44
2:A:199:ILE:HG13	2:A:201:PHE:HD2	1.82	0.44
2:A:578:MET:HG3	2:A:579:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:5:G:C6	4:W:6:C:N4	2.85	0.44
1:U:74:U:H3'	1:U:75:A:C5'	2.48	0.44
3:C:133:ILE:HA	3:C:209:MET:O	2.17	0.44
3:C:572:ILE:HG22	3:C:573:LYS:HG3	1.99	0.44
4:W:5:G:C2	4:W:6:C:C2	3.05	0.44
1:U:18:A:H2'	1:U:19:A:H5'	1.99	0.44
1:U:19:A:H2'	1:U:20:U:O4'	2.18	0.44
2:A:210:GLU:N	2:A:211:PRO:HD2	2.32	0.44
3:C:129:ILE:HG22	3:C:130:PRO:O	2.17	0.44
3:C:385:PHE:CE1	3:C:425:LEU:HD11	2.53	0.44
1:U:41:A:C2	1:U:42:A:N1	2.86	0.44
2:A:172:ILE:HD11	2:A:626:LEU:HD21	2.00	0.44
2:A:459:ALA:HB1	2:A:460:PRO:HD2	2.00	0.44
2:A:538:LEU:HD12	2:A:538:LEU:N	2.32	0.44
1:U:18:A:H3'	1:U:19:A:C8	2.51	0.44
3:C:324:ILE:HD12	3:C:377:ILE:HD13	2.00	0.43
2:A:458:PHE:CZ	3:C:336:ILE:HD11	2.54	0.43
3:C:416:ASP:HB3	3:C:417:PRO:HD2	2.01	0.43
3:C:918:LEU:HD22	3:C:926:GLY:O	2.18	0.43
3:C:862:TYR:CG	3:C:908:VAL:HG22	2.53	0.43
3:C:577:LEU:C	3:C:577:LEU:HD12	2.39	0.43
1:U:32:G:C2	1:U:34:C:C2	3.06	0.43
1:U:44:A:C2	1:U:70:A:N6	2.87	0.43
1:U:19:A:C2'	1:U:20:U:O4'	2.67	0.43
1:U:32:G:C6	1:U:34:C:C4	3.06	0.43
2:A:484:PHE:CD1	2:A:484:PHE:C	2.90	0.43
3:C:468:LEU:C	3:C:468:LEU:HD12	2.38	0.43
3:C:883:ARG:NH2	3:C:914:PHE:CG	2.87	0.43
1:U:93:G:C6	1:U:94:C:N4	2.86	0.43
2:A:404:ASN:CG	2:A:405:ASN:N	2.72	0.43
3:C:285:TYR:HB2	3:C:374:VAL:HG22	2.01	0.43
1:U:93:G:C2	1:U:94:C:N3	2.87	0.43
1:U:98:U:C4	1:U:99:U:C5	3.07	0.43
3:C:629:TYR:HB3	3:C:651:TYR:OH	2.19	0.43
3:C:142:LEU:HD22	3:C:143:HIS:N	2.33	0.43
3:C:242:VAL:HG22	3:C:277:LEU:HD11	2.00	0.43
1:U:42:A:C5	1:U:43:G:C8	3.06	0.43
2:A:308:MET:HG3	2:A:479:LEU:HD11	2.00	0.43
2:A:461:LEU:O	3:C:403:ASN:ND2	2.48	0.43
3:C:360:ARG:HD3	3:C:361:THR:HG22	2.01	0.43
3:C:597:TYR:O	3:C:599:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:186:ALA:HB2	2:A:640:ARG:HH12	1.84	0.42
3:C:138:VAL:HG22	3:C:146:LYS:HB2	2.01	0.42
1:U:74:U:C2	1:U:75:A:H4'	2.54	0.42
3:C:444:GLN:N	3:C:445:PRO:HA	2.34	0.42
3:C:864:VAL:HG21	3:C:906:VAL:CG2	2.49	0.42
2:A:172:ILE:HA	2:A:571:LEU:HD11	2.02	0.42
3:C:957:ALA:HB1	3:C:961:SER:OG	2.20	0.42
2:A:342:LEU:HD11	2:A:398:VAL:HG21	2.00	0.42
3:C:567:ILE:O	3:C:568:SER:CB	2.67	0.42
3:C:866:ILE:HG22	3:C:868:VAL:CG1	2.49	0.42
1:U:82:A:C2'	1:U:83:C:OP1	2.68	0.42
3:C:191:ILE:HG23	3:C:221:PHE:CE2	2.55	0.42
1:U:111:C:N3	2:A:716:ARG:NH1	2.67	0.42
2:A:503:LYS:HA	2:A:506:PHE:CE2	2.54	0.42
3:C:306:PRO:HG2	3:C:349:TRP:CE3	2.55	0.42
3:C:911:SER:O	3:C:912:ALA:C	2.58	0.42
3:C:962:LEU:HD11	3:C:966:PHE:CZ	2.54	0.42
2:A:173:LEU:HA	2:A:715:LEU:HD13	2.01	0.42
1:U:42:A:C6	1:U:43:G:C5	3.07	0.42
1:U:68:A:O2'	1:U:69:G:H8	2.02	0.42
3:C:472:VAL:HB	3:C:575:ALA:HB3	2.02	0.42
3:C:617:LYS:CB	3:C:666:ILE:HD11	2.50	0.42
1:U:79:C:N4	1:U:114:G:C6	2.88	0.42
2:A:284:ARG:N	2:A:285:PRO:HA	2.34	0.42
2:A:631:LEU:HD23	2:A:656:ILE:HG23	2.00	0.42
1:U:43:G:C2'	1:U:44:A:H5'	2.49	0.41
1:U:79:C:C4	1:U:114:G:N1	2.88	0.41
3:C:379:ILE:N	3:C:380:PRO:HD2	2.34	0.41
3:C:629:TYR:CE2	3:C:655:LEU:HA	2.55	0.41
3:C:888:ILE:HG23	3:C:902:VAL:HG23	2.01	0.41
3:C:142:LEU:HD21	3:C:189:LEU:HD22	2.02	0.41
1:U:25:G:H4'	1:U:26:A:C5'	2.51	0.41
3:C:472:VAL:N	3:C:575:ALA:O	2.54	0.41
3:C:774:LEU:HD13	3:C:803:VAL:CG2	2.47	0.41
2:A:346:ILE:O	2:A:347:PRO:C	2.58	0.41
3:C:869:HIS:HB2	3:C:872:LEU:HD12	2.03	0.41
2:A:305:LEU:N	2:A:306:PRO:CD	2.84	0.41
2:A:719:ILE:N	2:A:720:PRO:HD3	2.36	0.41
3:C:500:ARG:HB3	3:C:578:TYR:CZ	2.55	0.41
1:U:18:A:C2'	1:U:19:A:H5'	2.50	0.41
1:U:74:U:N1	1:U:75:A:H4'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:ILE:N	3:C:129:ILE:HD12	2.35	0.41
3:C:412:ALA:HA	3:C:415:TYR:CE1	2.56	0.41
1:U:31:G:H2'	1:U:32:G:C8	2.55	0.41
2:A:641:LEU:HD12	2:A:642:GLY:O	2.21	0.41
2:A:708:TRP:NE1	2:A:712:LEU:HD11	2.35	0.41
3:C:195:GLY:O	3:C:478:TYR:OH	2.39	0.41
3:C:780:PRO:HD2	3:C:783:ILE:HG21	2.02	0.41
3:C:138:VAL:CG1	3:C:214:ASP:HA	2.50	0.41
1:U:16:U:H3'	1:U:17:C:C6	2.56	0.40
1:U:46:C:H4'	3:C:111:LYS:HG2	2.01	0.40
1:U:132:A:H2'	1:U:133:C:OP1	2.21	0.40
2:A:410:ILE:HG23	2:A:412:GLN:HE21	1.85	0.40
3:C:539:VAL:HG13	3:C:564:ILE:HG23	2.02	0.40
3:C:797:GLN:HA	3:C:800:TYR:CD2	2.55	0.40
3:C:245:VAL:HG21	3:C:295:ILE:HG13	2.03	0.40
3:C:774:LEU:HD11	3:C:813:ILE:C	2.41	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	
2	A	587/735 (80%)	511 (87%)	67 (11%)	9 (2%)	10	44
3	C	847/1008 (84%)	730 (86%)	93 (11%)	24 (3%)	5	33
5	b	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
6	e	71/94 (76%)	66 (93%)	5 (7%)	0	100	100
7	f	70/86 (81%)	62 (89%)	6 (9%)	2 (3%)	4	32
8	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
10	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
12	j	92/110 (84%)	86 (94%)	6 (6%)	0	100	100
All	All	1966/2553 (77%)	1734 (88%)	196 (10%)	36 (2%)	12	41

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	247	PRO
2	A	615	LEU
3	C	269	LYS
3	C	356	LYS
3	C	367	VAL
3	C	369	LYS
3	C	371	PRO
3	C	432	GLN
3	C	568	SER
3	C	912	ALA
3	C	935	LYS
2	A	404	ASN
2	A	644	VAL
3	C	428	ILE
3	C	446	PHE
3	C	535	PRO
3	C	884	ARG
7	f	33	PHE
2	A	286	LEU
2	A	360	GLU
3	C	598	ILE
3	C	767	SER
3	C	886	SER
2	A	262	ASP
2	A	426	PRO
3	C	180	ASN
3	C	309	ASN
3	C	361	THR
3	C	596	ASP
3	C	370	TYR
7	f	15	PRO
10	d	82	PRO
2	A	260	PRO
3	C	458	ILE

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Mol	Chain	Res	Type
3	C	464	PRO
3	C	951	ILE

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	
2	A	482/677 (71%)	460 (95%)	22 (5%)	27	57
3	C	673/910 (74%)	618 (92%)	55 (8%)	11	41
5	b	70/176 (40%)	70 (100%)	0	100	100
6	e	65/83 (78%)	60 (92%)	5 (8%)	13	43
7	f	63/77 (82%)	62 (98%)	1 (2%)	62	80
8	g	58/66 (88%)	56 (97%)	2 (3%)	37	64
10	d	69/89 (78%)	67 (97%)	2 (3%)	42	66
11	h	77/129 (60%)	71 (92%)	6 (8%)	12	42
12	j	79/103 (77%)	74 (94%)	5 (6%)	18	49
All	All	1636/2310 (71%)	1538 (94%)	98 (6%)	23	50

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	162	LEU
2	A	175	LEU
2	A	193	TYR
2	A	228	LYS
2	A	254	HIS
2	A	284	ARG
2	A	287	GLU
2	A	340	LYS
2	A	364	TYR
2	A	374	ILE
2	A	402	TRP
2	A	409	CYS

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Mol	Chain	Res	Type
2	A	461	LEU
2	A	468	LEU
2	A	551	LEU
2	A	571	LEU
2	A	578	MET
2	A	615	LEU
2	A	617	ASN
2	A	655	TYR
2	A	705	GLN
2	A	716	ARG
3	C	111	LYS
3	C	112	ASN
3	C	113	ILE
3	C	160	ARG
3	C	173	LYS
3	C	176	ARG
3	C	179	ASP
3	C	183	GLN
3	C	207	SER
3	C	211	ASN
3	C	219	VAL
3	C	255	GLN
3	C	260	ASN
3	C	327	PHE
3	C	342	ASP
3	C	347	ARG
3	C	359	PHE
3	C	361	THR
3	C	400	LEU
3	C	406	VAL
3	C	421	LEU
3	C	431	GLN
3	C	468	LEU
3	C	469	TRP
3	C	475	THR
3	C	476	VAL
3	C	478	TYR
3	C	534	THR
3	C	537	CYS
3	C	576	THR
3	C	577	LEU
3	C	590	LYS

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Mol	Chain	Res	Type
3	C	658	ASP
3	C	659	LEU
3	C	674	LEU
3	C	678	SER
3	C	707	SER
3	C	723	LEU
3	C	760	LEU
3	C	762	SER
3	C	770	ASN
3	C	772	ASN
3	C	784	SER
3	C	791	TYR
3	C	851	LEU
3	C	861	ILE
3	C	869	HIS
3	C	883	ARG
3	C	902	VAL
3	C	922	THR
3	C	928	CYS
3	C	933	TRP
3	C	961	SER
3	C	971	ARG
3	C	988	THR
6	e	16	CYS
6	e	18	PHE
6	e	25	THR
6	e	79	LYS
6	e	81	LEU
7	f	79	LEU
8	g	18	ASN
8	g	41	ASP
10	d	10	LEU
10	d	76	ASP
11	h	20	LYS
11	h	26	TRP
11	h	30	GLN
11	h	77	ASP
11	h	99	ASP
11	h	104	ASP
12	j	24	PHE
12	j	49	ARG
12	j	77	THR

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Mol	Chain	Res	Type
12	j	99	ASP
12	j	100	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	146	HIS
2	A	194	HIS
2	A	310	ASN
2	A	326	ASN
2	A	344	ASN
2	A	392	ASN
2	A	404	ASN
2	A	412	GLN
2	A	558	GLN
2	A	559	GLN
2	A	576	HIS
2	A	617	ASN
2	A	658	ASN
3	C	112	ASN
3	C	260	ASN
3	C	289	ASN
3	C	418	GLN
3	C	423	HIS
3	C	431	GLN
3	C	776	ASN
6	e	34	GLN
7	f	77	ASN
8	g	66	ASN
11	h	30	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	139/178 (78%)	81 (58%)	23 (16%)
4	W	24/31 (77%)	11 (45%)	4 (16%)
All	All	163/209 (77%)	92 (56%)	27 (16%)

All (92) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	5	A
1	U	7	C
1	U	8	U
1	U	9	U
1	U	10	U
1	U	12	C
1	U	13	A
1	U	14	G
1	U	15	A
1	U	16	U
1	U	17	C
1	U	18	A
1	U	19	A
1	U	22	G
1	U	23	C
1	U	25	G
1	U	26	A
1	U	27	G
1	U	28	G
1	U	32	G
1	U	34	C
1	U	35	A
1	U	38	A
1	U	39	U
1	U	40	C
1	U	41	A
1	U	43	G
1	U	44	A
1	U	45	A
1	U	46	C
1	U	51	G
1	U	52	G
1	U	53	C
1	U	65	U
1	U	66	A
1	U	68	A
1	U	69	G
1	U	70	A
1	U	71	A
1	U	72	C
1	U	74	U
1	U	75	A
1	U	76	U

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Mol	Chain	Res	Type
1	U	77	A
1	U	78	A
1	U	79	C
1	U	80	G
1	U	81	A
1	U	82	A
1	U	83	C
1	U	84	A
1	U	94	C
1	U	95	C
1	U	96	U
1	U	97	U
1	U	101	C
1	U	103	A
1	U	105	A
1	U	112	C
1	U	115	G
1	U	119	U
1	U	120	G
1	U	121	U
1	U	122	C
1	U	123	U
1	U	125	C
1	U	127	U
1	U	128	A
1	U	129	G
1	U	130	A
1	U	133	C
1	U	134	A
1	U	135	G
1	U	136	G
1	U	139	A
1	U	141	G
1	U	167	A
1	U	170	U
1	U	171	U
1	U	172	U
1	U	173	U
4	W	2	U
4	W	7	G
4	W	8	A
4	W	17	U

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Mol	Chain	Res	Type
4	W	25	C
4	W	26	A
4	W	27	U
4	W	28	U
4	W	29	U
4	W	30	G
4	W	31	G

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	U	6	G
1	U	7	C
1	U	21	G
1	U	25	G
1	U	26	A
1	U	27	G
1	U	33	U
1	U	38	A
1	U	40	C
1	U	51	G
1	U	62	G
1	U	68	A
1	U	78	A
1	U	82	A
1	U	83	C
1	U	95	C
1	U	114	G
1	U	127	U
1	U	128	A
1	U	129	G
1	U	132	A
1	U	133	C
1	U	172	U
4	W	16	C
4	W	25	C
4	W	26	A
4	W	27	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	GTP	C	1101	-	26,34,34	0.84	1 (3%)	32,54,54	1.61	5 (15%)

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
13	GTP	C	1101	-	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	1101	GTP	C6-N1	-2.10	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	1101	GTP	PB-O3B-PG	-4.25	118.24	132.83
13	C	1101	GTP	PA-O3A-PB	-3.93	119.33	132.83
13	C	1101	GTP	O6-C6-C5	-3.22	118.08	124.37
13	C	1101	GTP	C5-C6-N1	2.94	119.14	113.95
13	C	1101	GTP	O3G-PG-O2G	2.09	115.63	107.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

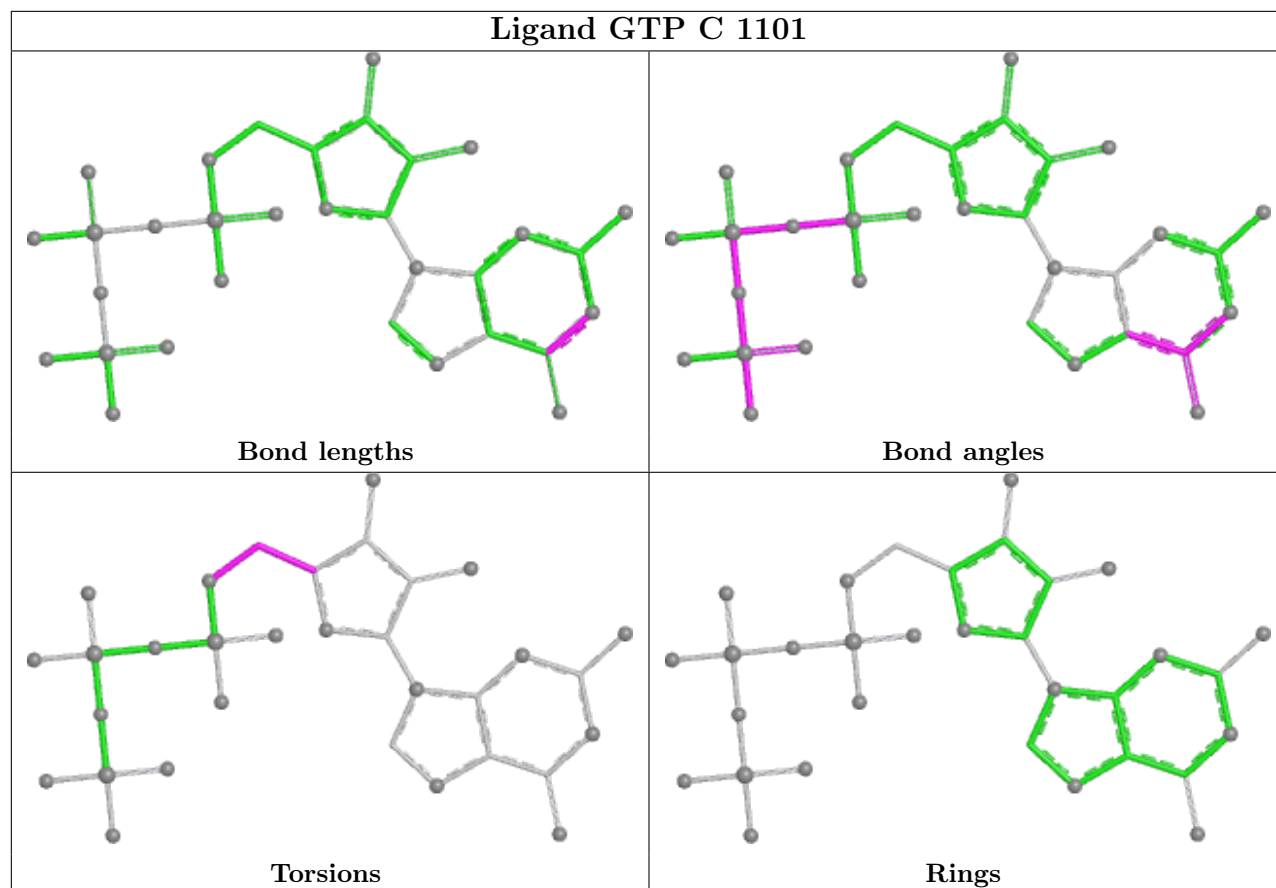
Mol	Chain	Res	Type	Atoms
13	C	1101	GTP	O4'-C4'-C5'-O5'
13	C	1101	GTP	C3'-C4'-C5'-O5'
13	C	1101	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	1101	GTP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

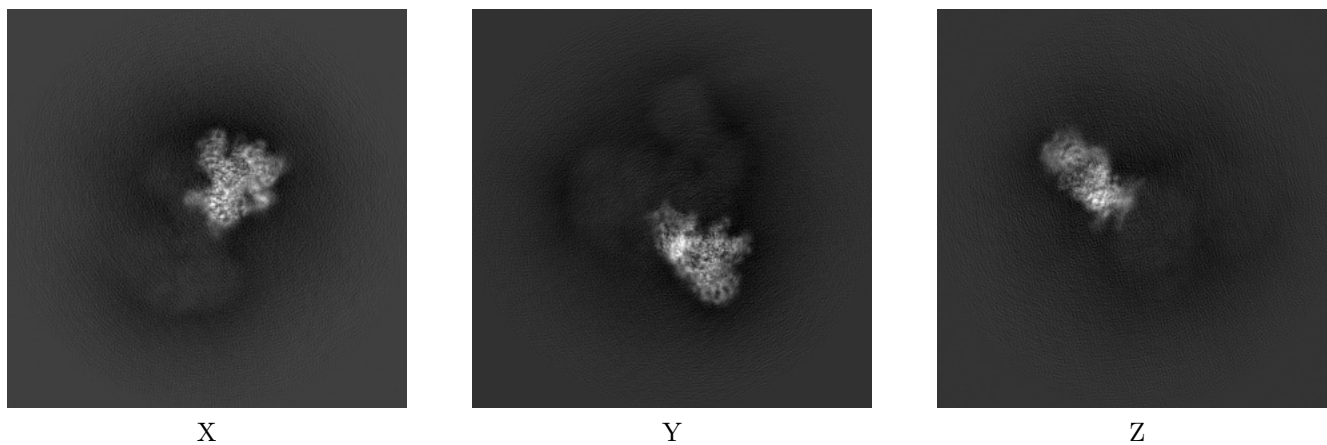
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8011. 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](#)

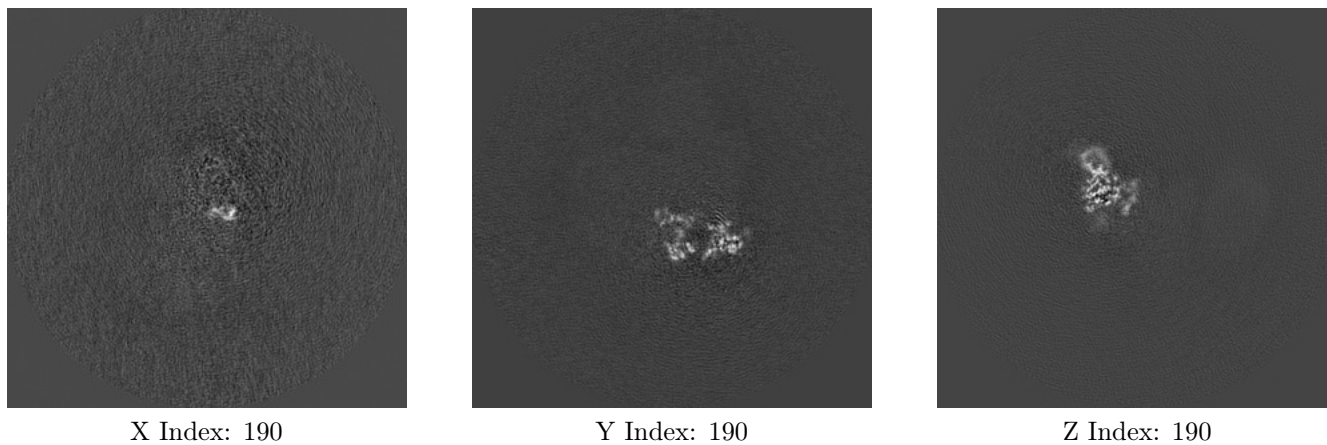
6.1.1 Primary map



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

6.2 Central slices [i](#)

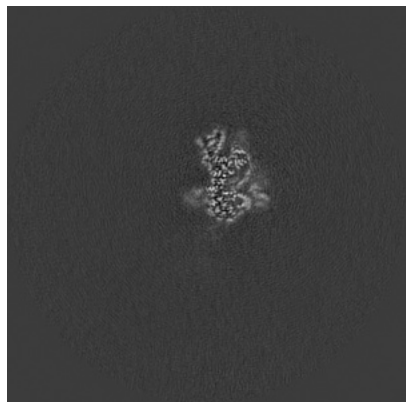
6.2.1 Primary map



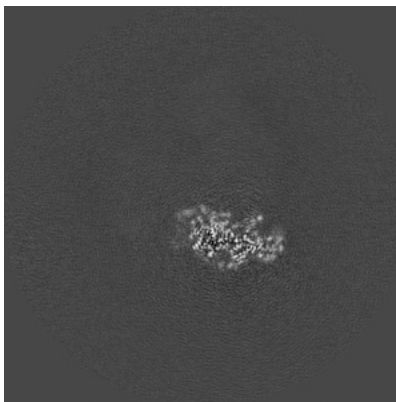
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

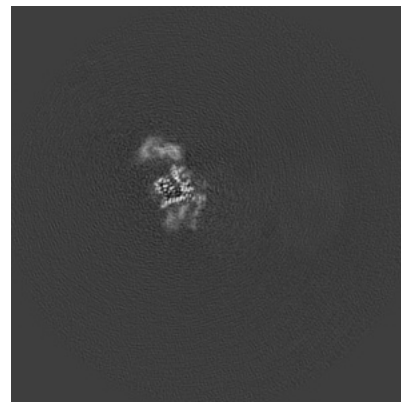
6.3.1 Primary map



X Index: 156



Y Index: 198



Z Index: 199

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

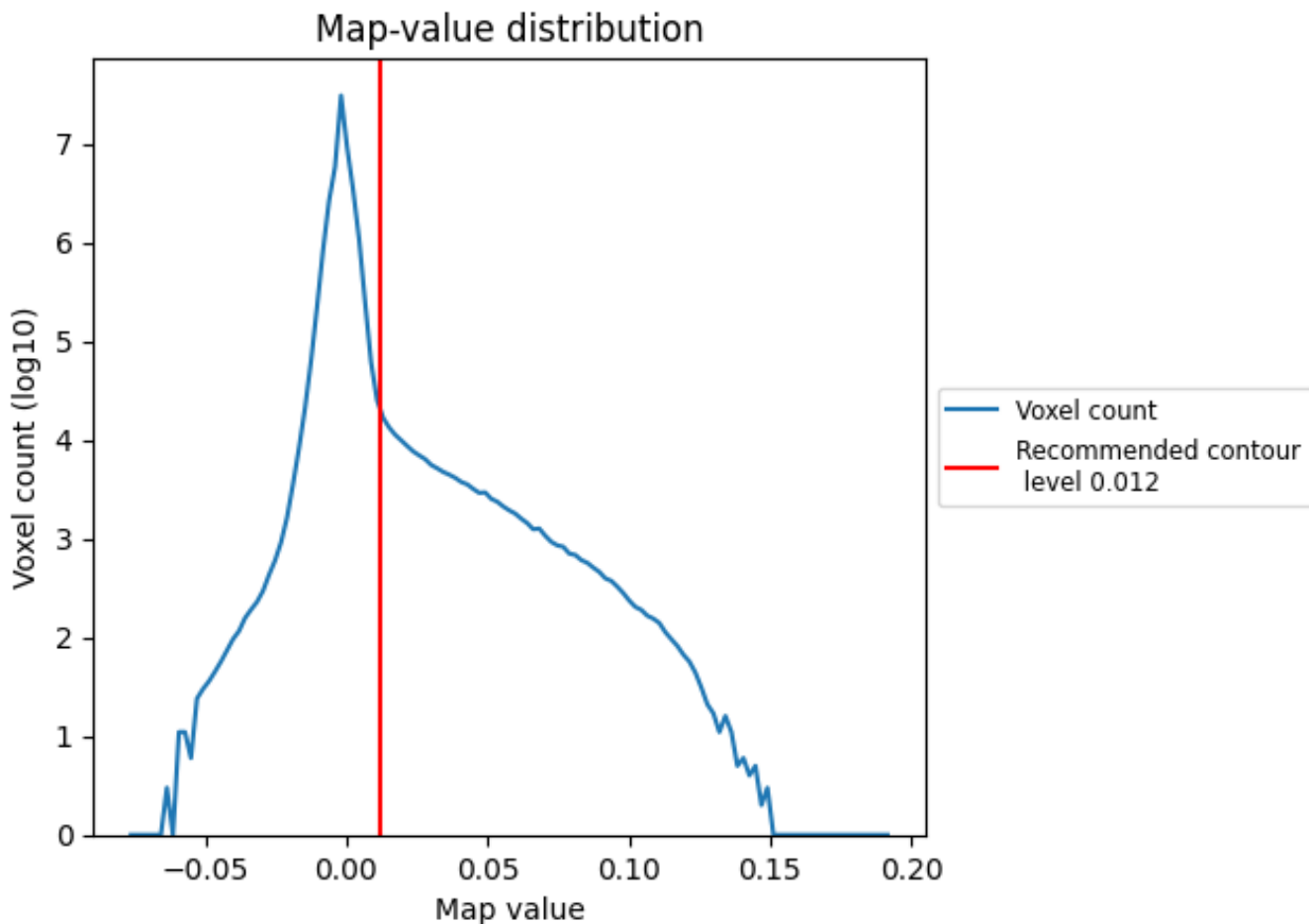
6.5 Mask visualisation

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

7 Map analysis [i](#)

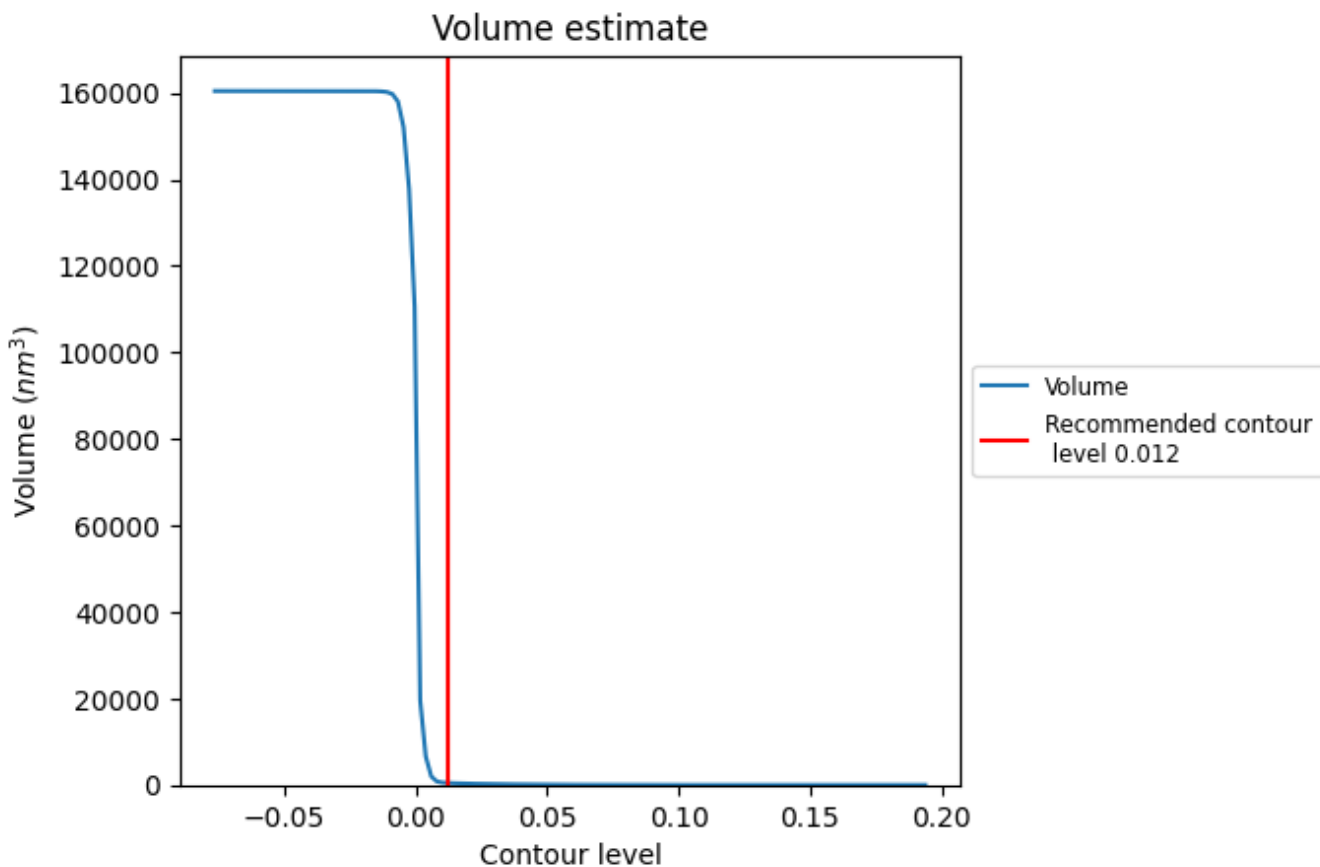
This section contains the results of statistical analysis of the map.

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.

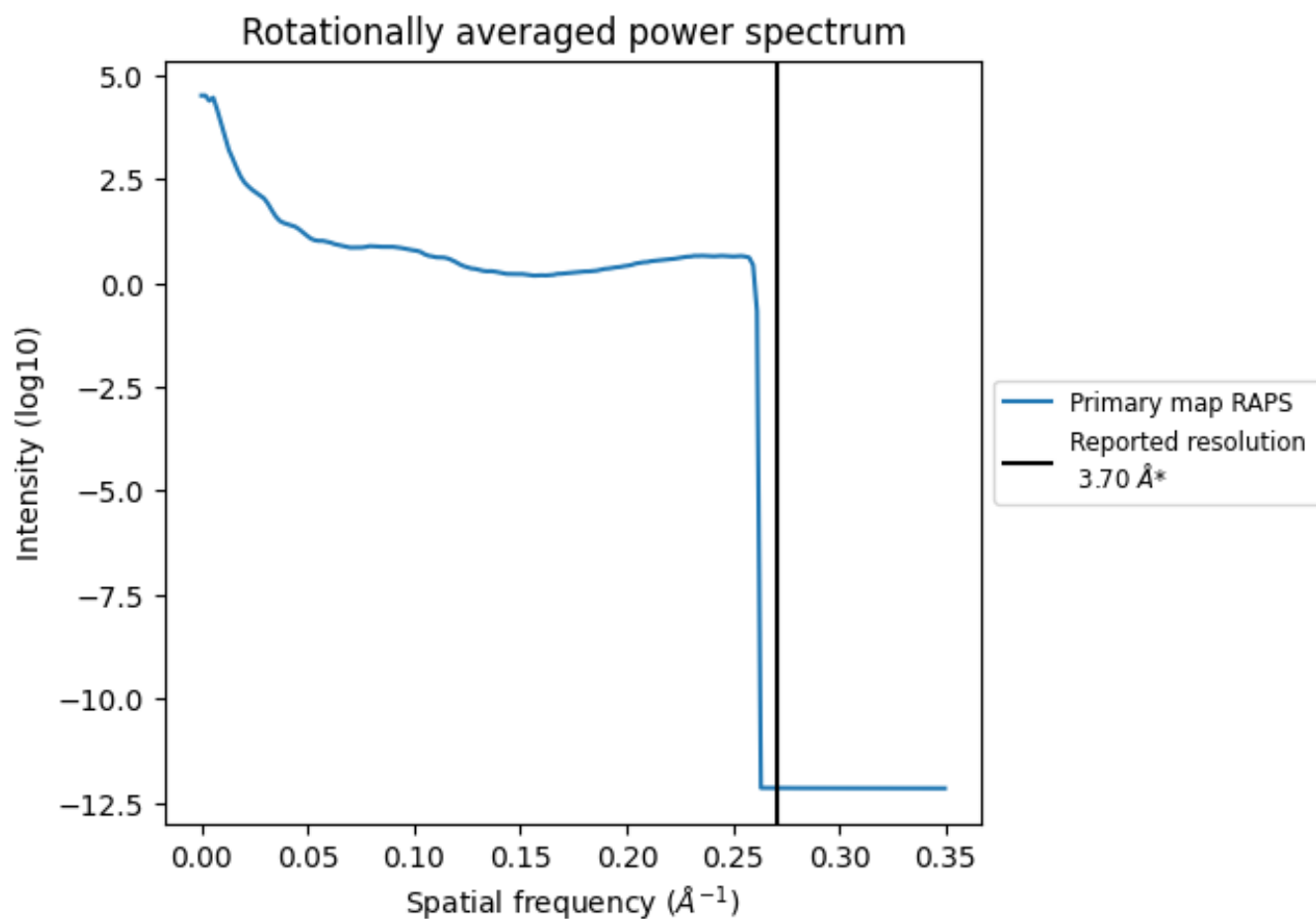
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 467 nm³; this corresponds to an approximate mass of 422 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](#)

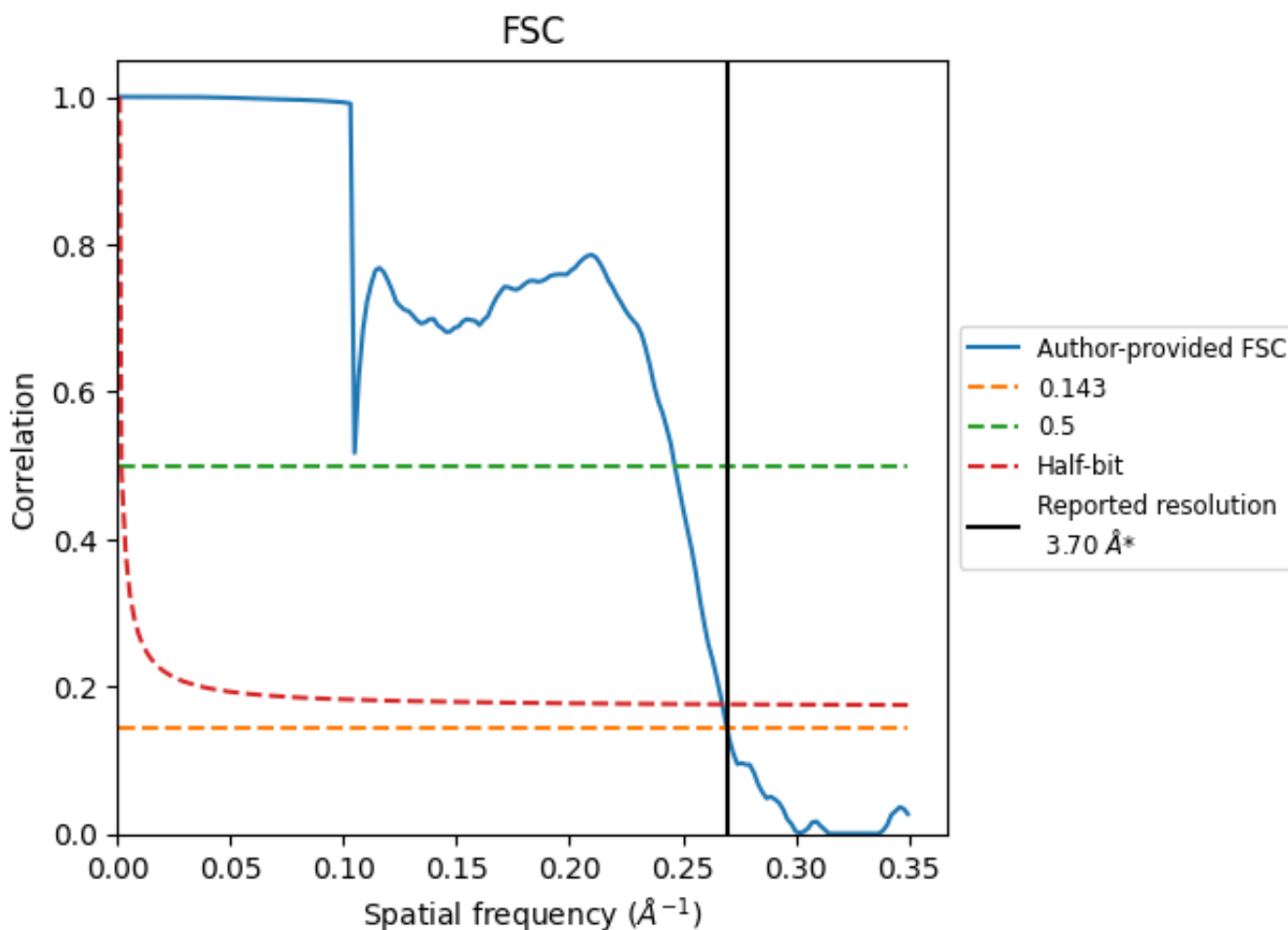


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270\AA^{-1}

8.2 Resolution estimates [i](#)

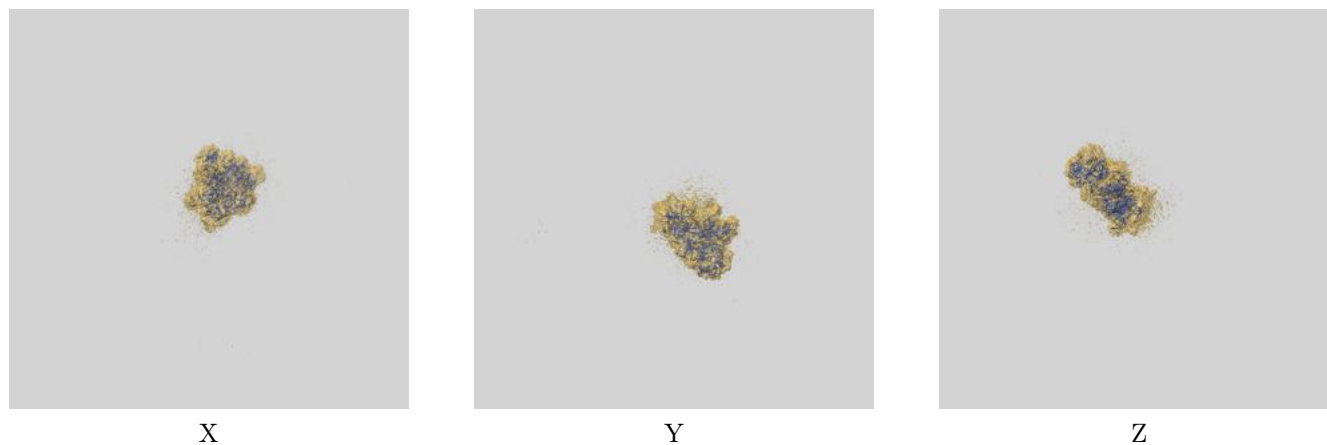
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.06	3.74
Unmasked-calculated*	-	-	-

*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-8011 and PDB model 5GAM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



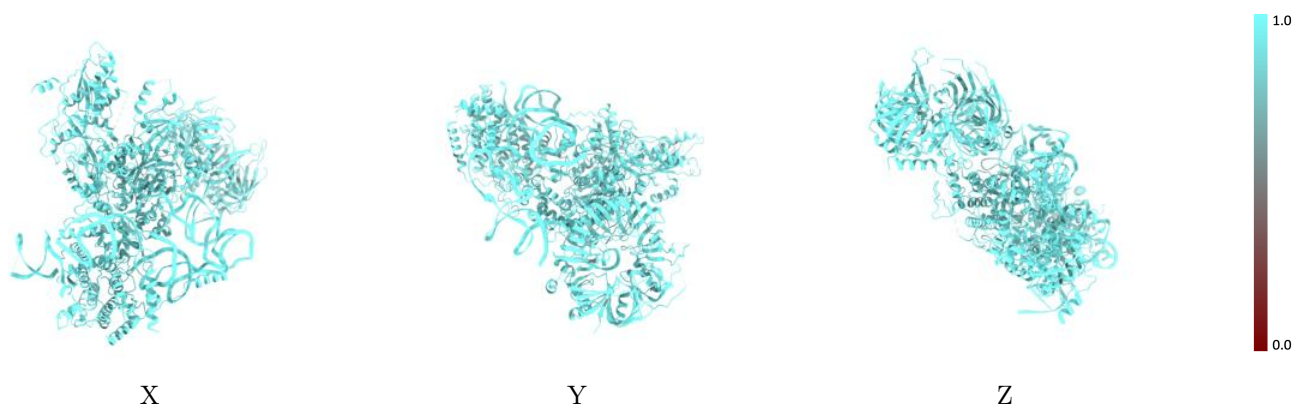
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



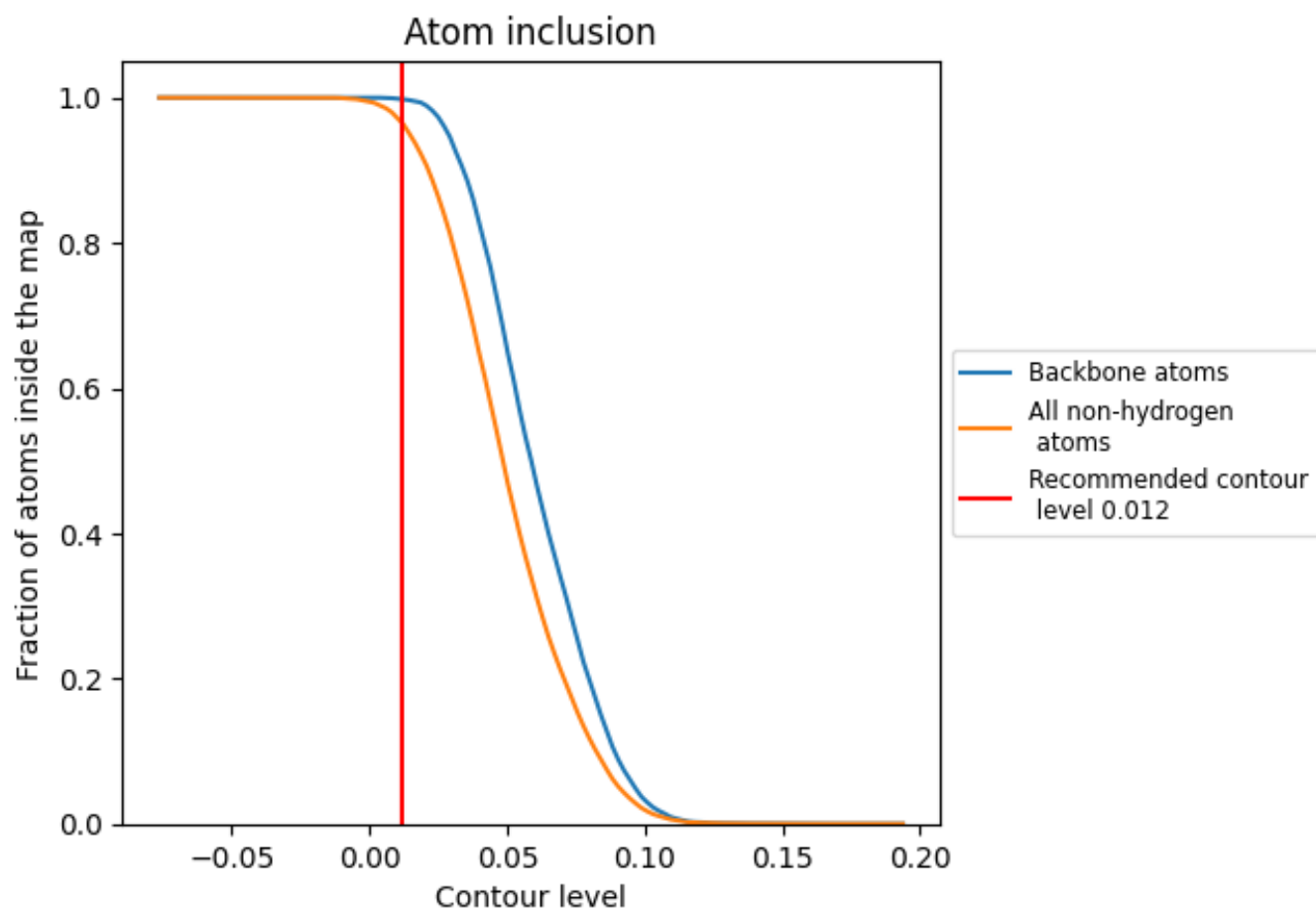
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 100% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9646	 0.3630
A	 0.9589	 0.3960
C	 0.9627	 0.4090
U	 0.9927	 0.2850
W	 0.9962	 0.2480
b	 0.9271	 0.3790
d	 0.9466	 0.4150
e	 0.9510	 0.2850
f	 0.9680	 0.2620
g	 0.9539	 0.3430
h	 0.9324	 0.2970
j	 0.9641	 0.2950
x	 1.0000	 0.3890

