



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 03:45 AM UTC

PDB ID : 9T74 / pdb\_00009t74  
EMDB ID : EMD-55625  
Title : 2'-fluoro-modified pyrimidine (FY) RNA aptamer binding to the receptor binding domain (RBD) of the SARS-CoV-2 spike protein. (focus map: RBD-aptamer)  
Authors : Kristoffersen, E.L.; Andersen, E.S.; Zwergious, N.H.  
Deposited on : 2025-11-10  
Resolution : 3.46 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

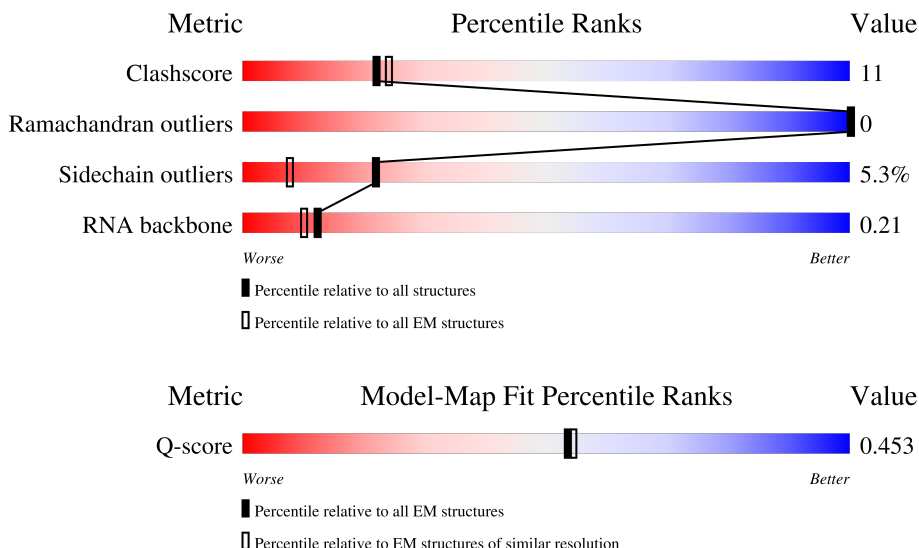
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13788 ( 2.96 - 3.96 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	51	
2	B	1134	
3	C	2	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2673 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 DNA/RNA (51-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	51	Total	C	F	N	O	P	0	0
			1084	484	26	190	333	51		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	197	Total	C	N	O	S	0	0
			1560	1001	260	291	8		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	682	SER	ARG	conflict	UNP P0DTC2
B	683	GLY	ARG	conflict	UNP P0DTC2
B	685	GLY	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	736847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.175	Depositor
Minimum map value	-0.516	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	621.12, 621.12, 621.12	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9705, 0.9705, 0.9705	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: MG, CFZ, UFT, NAG

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	0.47	2/632 (0.3%)	0.33	0/975
2	B	0.13	0/1604	0.36	0/2183
All	All	0.27	2/2236 (0.1%)	0.35	0/3158

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	UFT	O3'-P	5.33	1.61	1.56
1	A	93	UFT	O3'-P	5.24	1.61	1.56

There are no bond angle outliers.

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	1084	0	523	24	0
2	B	1560	0	1483	32	0
3	C	28	0	25	1	0
4	A	1	0	0	0	0
All	All	2673	0	2031	54	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 (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:CYS:HA	2:B:432:CYS:HB2	1.41	0.97
2:B:350:VAL:HG11	2:B:418:ILE:HD12	1.69	0.75
1:A:86:CFZ:H2'	1:A:87:G:H8	1.53	0.73
1:A:128:G:OP2	1:A:128:G:N2	2.23	0.72
2:B:418:ILE:HA	2:B:422:ASN:HB2	1.80	0.64
2:B:431:GLY:HA3	2:B:514:SER:HA	1.81	0.63
2:B:448:ASN:OD1	2:B:450:ASN:ND2	2.32	0.63
1:A:116:CFZ:H2'	1:A:117:G:H8	1.64	0.62
2:B:418:ILE:HD13	2:B:422:ASN:HD22	1.66	0.60
2:B:442:ASP:O	2:B:448:ASN:ND2	2.25	0.60
1:A:126:G:N2	2:B:489:TYR:OH	2.34	0.59
2:B:420:ASP:OD1	2:B:460:ASN:ND2	2.37	0.57
1:A:91:UFT:O2	2:B:487:ASN:ND2	2.37	0.57
1:A:133:CFZ:H5'	1:A:133:CFZ:H6	1.85	0.57
2:B:333:THR:OG1	2:B:334:ASN:N	2.38	0.56
1:A:128:G:O2'	1:A:129:G:N7	2.35	0.56
1:A:115:CFZ:H2'	1:A:116:CFZ:H6	1.88	0.54
1:A:85:G:H2'	1:A:86:CFZ:H6	1.90	0.54
2:B:454:ARG:HD3	2:B:457:ARG:HG3	1.90	0.53
1:A:116:CFZ:H2'	1:A:117:G:C8	2.43	0.53
2:B:342:PHE:HB2	3:C:1:NAG:H82	1.90	0.53
1:A:119:CFZ:H5'	1:A:119:CFZ:H6	1.92	0.52
2:B:355:ARG:HD2	2:B:396:TYR:CD1	2.44	0.52
2:B:457:ARG:NH1	2:B:467:ASP:OD2	2.41	0.52
2:B:411:ALA:HB3	2:B:414:GLN:HG3	1.92	0.51
1:A:89:CFZ:H2'	1:A:90:A:C8	2.45	0.51
1:A:122:G:H2'	1:A:123:A:C8	2.47	0.50
2:B:395:VAL:HG22	2:B:515:PHE:HD1	1.76	0.50
2:B:336:CYS:HB2	2:B:337:PRO:CD	2.42	0.50
1:A:91:UFT:H2'	1:A:92:UFT:O4'	2.12	0.49
1:A:99:UFT:H2'	1:A:100:CFZ:H6	1.93	0.49
2:B:363:ALA:N	2:B:525:CYS:O	2.37	0.49
2:B:402:ILE:HD11	2:B:510:VAL:HG21	1.94	0.49
1:A:101:CFZ:H2'	1:A:102:UFT:H6	1.96	0.48
2:B:385:THR:HG1	2:B:386:LYS:HZ2	1.57	0.48
2:B:347:PHE:CE1	2:B:399:SER:HB2	2.48	0.48
1:A:86:CFZ:H2'	1:A:87:G:C8	2.42	0.47
1:A:100:CFZ:H2'	1:A:101:CFZ:H6	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:CFZ:H2'	1:A:120:A:C8	2.50	0.47
2:B:332:ILE:HD12	2:B:527:PRO:HB3	1.97	0.46
1:A:123:A:H2'	1:A:124:CFZ:O4'	2.16	0.46
2:B:419:ALA:O	2:B:424:LYS:HB2	2.17	0.45
1:A:101:CFZ:H6	1:A:101:CFZ:H5'	2.00	0.43
1:A:93:UFT:H2'	1:A:94:G:C8	2.53	0.43
2:B:350:VAL:O	2:B:353:TRP:HD1	2.01	0.43
2:B:480:CYS:HB2	2:B:483:VAL:O	2.20	0.42
2:B:336:CYS:HB2	2:B:337:PRO:HD2	2.01	0.42
2:B:439:ASN:CG	2:B:506:GLN:HE21	2.28	0.41
2:B:456:PHE:HB3	2:B:473:TYR:CD2	2.55	0.41
2:B:339:GLY:O	2:B:343:ASN:HB2	2.21	0.41
2:B:394:ASN:OD1	2:B:516:GLU:HB2	2.20	0.41
1:A:105:A:H2'	1:A:106:CFZ:H6	2.02	0.40
1:A:115:CFZ:H2'	1:A:116:CFZ:C6	2.50	0.40
2:B:431:GLY:HA3	2:B:513:LEU:O	2.21	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	B	195/1134 (17%)	185 (95%)	10 (5%)	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	
2	B	170/983 (17%)	161 (95%)	9 (5%)	20	48

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	332	ILE
2	B	350	VAL
2	B	390	LEU
2	B	402	ILE
2	B	415	THR
2	B	430	THR
2	B	433	VAL
2	B	441	LEU
2	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	370	ASN
2	B	450	ASN
2	B	506	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	16/51 (31%)	7 (43%)	3 (18%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	88	A
1	A	97	A
1	A	104	G
1	A	105	A
1	A	109	A
1	A	121	G
1	A	129	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	96	A
1	A	103	G
1	A	108	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	UFT	A	113	1	18,21,22	2.63	9 (50%)	25,30,33	1.94	5 (20%)
1	UFT	A	99	1	18,21,22	2.63	10 (55%)	25,30,33	2.11	8 (32%)
1	UFT	A	93	1	18,21,22	2.67	10 (55%)	25,30,33	2.12	7 (28%)
1	CFZ	A	89	1	18,21,22	2.59	7 (38%)	25,30,33	1.15	2 (8%)
1	UFT	A	102	1	18,21,22	2.61	10 (55%)	25,30,33	2.07	8 (32%)
1	CFZ	A	119	1	18,21,22	2.52	6 (33%)	25,30,33	1.52	3 (12%)
1	UFT	A	110	1	18,21,22	2.61	10 (55%)	25,30,33	2.21	8 (32%)
1	CFZ	A	124	1	18,21,22	2.54	7 (38%)	25,30,33	1.43	3 (12%)
1	UFT	A	131	1	18,21,22	2.61	10 (55%)	25,30,33	2.08	8 (32%)
1	CFZ	A	107	1	18,21,22	2.53	7 (38%)	25,30,33	1.18	2 (8%)
1	UFT	A	118	1	18,21,22	2.61	9 (50%)	25,30,33	2.00	7 (28%)
1	UFT	A	95	1,4	18,21,22	2.61	10 (55%)	25,30,33	2.05	8 (32%)
1	CFZ	A	86	1	18,21,22	2.55	6 (33%)	25,30,33	1.21	2 (8%)
1	UFT	A	92	1	18,21,22	2.64	9 (50%)	25,30,33	1.93	6 (24%)
1	UFT	A	130	1	18,21,22	2.70	10 (55%)	25,30,33	2.15	6 (24%)
1	UFT	A	91	1	18,21,22	2.64	9 (50%)	25,30,33	2.08	7 (28%)
1	CFZ	A	100	1	18,21,22	2.51	7 (38%)	25,30,33	1.37	3 (12%)
1	CFZ	A	115	1	18,21,22	2.56	7 (38%)	25,30,33	1.20	2 (8%)
1	CFZ	A	134	1	18,21,22	2.51	7 (38%)	25,30,33	1.34	3 (12%)
1	UFT	A	114	1	18,21,22	2.63	10 (55%)	25,30,33	2.02	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CFZ	A	106	1	18,21,22	2.51	6 (33%)	25,30,33	1.50	3 (12%)
1	CFZ	A	116	1	18,21,22	2.53	7 (38%)	25,30,33	1.11	2 (8%)
1	CFZ	A	133	1	18,21,22	2.50	7 (38%)	25,30,33	1.49	2 (8%)
1	UFT	A	98	1	18,21,22	2.60	10 (55%)	25,30,33	2.17	7 (28%)
1	CFZ	A	112	1	18,21,22	2.52	7 (38%)	25,30,33	1.14	2 (8%)
1	CFZ	A	101	1	18,21,22	2.53	6 (33%)	25,30,33	1.61	3 (12%)

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
1	UFT	A	113	1	-	7/7/25/26	0/2/2/2
1	UFT	A	99	1	-	0/7/25/26	0/2/2/2
1	UFT	A	93	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	89	1	-	2/7/25/26	0/2/2/2
1	UFT	A	102	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	119	1	-	2/7/25/26	0/2/2/2
1	UFT	A	110	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	124	1	-	0/7/25/26	0/2/2/2
1	UFT	A	131	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	107	1	-	2/7/25/26	0/2/2/2
1	UFT	A	118	1	-	2/7/25/26	0/2/2/2
1	UFT	A	95	1,4	-	1/7/25/26	0/2/2/2
1	CFZ	A	86	1	-	0/7/25/26	0/2/2/2
1	UFT	A	92	1	-	1/7/25/26	0/2/2/2
1	UFT	A	130	1	-	0/7/25/26	0/2/2/2
1	UFT	A	91	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	100	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	115	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	134	1	-	2/7/25/26	0/2/2/2
1	UFT	A	114	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	106	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	116	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	133	1	-	2/7/25/26	0/2/2/2
1	UFT	A	98	1	-	6/7/25/26	0/2/2/2
1	CFZ	A	112	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	101	1	-	2/7/25/26	0/2/2/2

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	UFT	C2-N1	4.95	1.46	1.38
1	A	92	UFT	C2-N1	4.86	1.46	1.38
1	A	99	UFT	C2-N1	4.82	1.46	1.38
1	A	112	CFZ	C4-N4	4.81	1.45	1.33
1	A	134	CFZ	C4-N4	4.81	1.45	1.33
1	A	116	CFZ	C4-N4	4.81	1.45	1.33
1	A	118	UFT	C2-N1	4.81	1.46	1.38
1	A	89	CFZ	C4-N4	4.79	1.45	1.33
1	A	107	CFZ	C4-N4	4.79	1.45	1.33
1	A	124	CFZ	C4-N4	4.78	1.45	1.33
1	A	133	CFZ	C4-N4	4.78	1.45	1.33
1	A	115	CFZ	C4-N4	4.78	1.45	1.33
1	A	115	CFZ	C2'-C3'	-4.77	1.46	1.52
1	A	107	CFZ	C2'-C3'	-4.76	1.46	1.52
1	A	131	UFT	C2-N1	4.76	1.45	1.38
1	A	89	CFZ	C2'-C3'	-4.75	1.46	1.52
1	A	101	CFZ	C4-N4	4.74	1.45	1.33
1	A	86	CFZ	C4-N4	4.74	1.45	1.33
1	A	95	UFT	C2-N1	4.73	1.45	1.38
1	A	91	UFT	C2-N1	4.72	1.45	1.38
1	A	113	UFT	C2-N1	4.71	1.45	1.38
1	A	86	CFZ	C2'-C3'	-4.71	1.46	1.52
1	A	100	CFZ	C4-N4	4.71	1.45	1.33
1	A	114	UFT	C2-N1	4.71	1.45	1.38
1	A	116	CFZ	C2'-C3'	-4.70	1.46	1.52
1	A	119	CFZ	C4-N4	4.69	1.45	1.33
1	A	98	UFT	C2-N1	4.69	1.45	1.38
1	A	106	CFZ	C4-N4	4.68	1.45	1.33
1	A	93	UFT	C2-N1	4.66	1.45	1.38
1	A	110	UFT	C2-N1	4.64	1.45	1.38
1	A	98	UFT	C6-N1	4.64	1.49	1.38
1	A	91	UFT	C6-N1	4.62	1.49	1.38
1	A	92	UFT	C6-N1	4.62	1.49	1.38
1	A	102	UFT	C2-N1	4.60	1.45	1.38
1	A	112	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	110	UFT	C6-N1	4.60	1.49	1.38
1	A	124	CFZ	C2'-C3'	-4.59	1.46	1.52
1	A	113	UFT	C6-N1	4.59	1.49	1.38
1	A	100	CFZ	C2'-C3'	-4.59	1.46	1.52
1	A	118	UFT	C6-N1	4.57	1.49	1.38
1	A	134	CFZ	C2'-C3'	-4.56	1.46	1.52
1	A	101	CFZ	C2'-C3'	-4.55	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	UFT	C6-N1	4.52	1.48	1.38
1	A	131	UFT	C6-N1	4.52	1.48	1.38
1	A	130	UFT	C6-N1	4.52	1.48	1.38
1	A	95	UFT	C6-N1	4.51	1.48	1.38
1	A	100	CFZ	C2-N3	4.51	1.45	1.36
1	A	102	UFT	C6-N1	4.48	1.48	1.38
1	A	114	UFT	C6-N1	4.48	1.48	1.38
1	A	133	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	119	CFZ	C2-N3	4.46	1.45	1.36
1	A	119	CFZ	C2'-C3'	-4.45	1.46	1.52
1	A	101	CFZ	C2-N3	4.40	1.45	1.36
1	A	93	UFT	C6-N1	4.40	1.48	1.38
1	A	86	CFZ	C2-N3	4.40	1.45	1.36
1	A	106	CFZ	C2-N3	4.37	1.45	1.36
1	A	113	UFT	C5-C4	4.33	1.53	1.43
1	A	106	CFZ	C2'-C3'	-4.33	1.47	1.52
1	A	89	CFZ	C2-N3	4.31	1.44	1.36
1	A	134	CFZ	C2-N3	4.31	1.44	1.36
1	A	115	CFZ	C2-N3	4.31	1.44	1.36
1	A	133	CFZ	C2-N3	4.31	1.44	1.36
1	A	131	UFT	C5-C4	4.31	1.53	1.43
1	A	91	UFT	C5-C4	4.30	1.53	1.43
1	A	98	UFT	C5-C4	4.30	1.53	1.43
1	A	124	CFZ	C2-N3	4.29	1.44	1.36
1	A	99	UFT	C5-C4	4.29	1.53	1.43
1	A	110	UFT	C5-C4	4.29	1.53	1.43
1	A	102	UFT	C5-C4	4.27	1.53	1.43
1	A	95	UFT	C5-C4	4.25	1.52	1.43
1	A	93	UFT	C2'-C3'	-4.24	1.47	1.52
1	A	130	UFT	C2'-C3'	-4.24	1.47	1.52
1	A	118	UFT	C5-C4	4.21	1.52	1.43
1	A	93	UFT	C5-C4	4.20	1.52	1.43
1	A	92	UFT	C5-C4	4.18	1.52	1.43
1	A	112	CFZ	C2-N3	4.17	1.44	1.36
1	A	130	UFT	C5-C4	4.16	1.52	1.43
1	A	116	CFZ	C2-N3	4.16	1.44	1.36
1	A	114	UFT	C5-C4	4.15	1.52	1.43
1	A	118	UFT	C2'-C3'	-4.13	1.47	1.52
1	A	114	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	107	CFZ	C2-N3	4.10	1.44	1.36
1	A	92	UFT	C2'-C3'	-4.05	1.47	1.52
1	A	113	UFT	C2'-C3'	-3.97	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	110	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	131	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	99	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	102	UFT	C2'-C3'	-3.87	1.47	1.52
1	A	98	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	89	CFZ	C2'-C1'	-3.65	1.48	1.53
1	A	119	CFZ	O2-C2	3.64	1.30	1.23
1	A	91	UFT	C2'-C3'	-3.63	1.47	1.52
1	A	106	CFZ	O2-C2	3.60	1.30	1.23
1	A	89	CFZ	O2-C2	3.58	1.30	1.23
1	A	112	CFZ	O2-C2	3.56	1.30	1.23
1	A	86	CFZ	O2-C2	3.56	1.30	1.23
1	A	124	CFZ	O2-C2	3.56	1.30	1.23
1	A	115	CFZ	O2-C2	3.56	1.30	1.23
1	A	100	CFZ	O2-C2	3.55	1.30	1.23
1	A	124	CFZ	C2'-C1'	-3.55	1.48	1.53
1	A	101	CFZ	O2-C2	3.54	1.30	1.23
1	A	107	CFZ	O2-C2	3.53	1.30	1.23
1	A	116	CFZ	O2-C2	3.52	1.30	1.23
1	A	133	CFZ	O2-C2	3.50	1.30	1.23
1	A	93	UFT	C2'-C1'	-3.49	1.48	1.53
1	A	134	CFZ	O2-C2	3.43	1.30	1.23
1	A	106	CFZ	C2'-C1'	-3.38	1.49	1.53
1	A	115	CFZ	C2'-C1'	-3.34	1.49	1.53
1	A	89	CFZ	O4'-C1'	3.33	1.49	1.42
1	A	119	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	112	CFZ	C2'-C1'	-3.29	1.49	1.53
1	A	86	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	115	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	116	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	101	CFZ	C2'-C1'	-3.21	1.49	1.53
1	A	101	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	107	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	106	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	134	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	107	CFZ	C2'-C1'	-3.19	1.49	1.53
1	A	86	CFZ	C2'-C1'	-3.18	1.49	1.53
1	A	102	UFT	C2'-C1'	-3.17	1.49	1.53
1	A	116	CFZ	C2'-C1'	-3.16	1.49	1.53
1	A	100	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	133	CFZ	O4'-C1'	3.12	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	124	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	112	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	134	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	133	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	114	UFT	O4-C4	-3.00	1.18	1.24
1	A	95	UFT	O4-C4	-2.97	1.18	1.24
1	A	130	UFT	O4-C4	-2.96	1.18	1.24
1	A	99	UFT	O4-C4	-2.92	1.18	1.24
1	A	102	UFT	O4-C4	-2.92	1.18	1.24
1	A	93	UFT	O4-C4	-2.91	1.18	1.24
1	A	92	UFT	O4-C4	-2.90	1.18	1.24
1	A	91	UFT	O4-C4	-2.89	1.18	1.24
1	A	113	UFT	C2'-C1'	-2.89	1.49	1.53
1	A	131	UFT	O4-C4	-2.89	1.18	1.24
1	A	91	UFT	C2'-C1'	-2.87	1.49	1.53
1	A	113	UFT	O4-C4	-2.87	1.18	1.24
1	A	110	UFT	O4-C4	-2.87	1.18	1.24
1	A	130	UFT	C2'-C1'	-2.86	1.49	1.53
1	A	100	CFZ	C2'-C1'	-2.85	1.49	1.53
1	A	118	UFT	O4-C4	-2.80	1.19	1.24
1	A	98	UFT	O4-C4	-2.79	1.19	1.24
1	A	114	UFT	C2'-C1'	-2.74	1.49	1.53
1	A	130	UFT	C2-N3	2.74	1.42	1.38
1	A	118	UFT	C2'-C1'	-2.72	1.49	1.53
1	A	91	UFT	O4'-C1'	2.71	1.48	1.42
1	A	92	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	91	UFT	C2-N3	2.65	1.42	1.38
1	A	110	UFT	C2-N3	2.64	1.42	1.38
1	A	99	UFT	C2-N3	2.64	1.42	1.38
1	A	99	UFT	O4'-C1'	2.64	1.48	1.42
1	A	110	UFT	C2'-C1'	-2.63	1.49	1.53
1	A	98	UFT	C2-N3	2.61	1.42	1.38
1	A	131	UFT	C2-N3	2.61	1.42	1.38
1	A	130	UFT	O4'-C1'	2.61	1.48	1.42
1	A	131	UFT	O4'-C1'	2.60	1.48	1.42
1	A	114	UFT	O4'-C1'	2.60	1.48	1.42
1	A	92	UFT	C2-N3	2.59	1.42	1.38
1	A	114	UFT	C2-N3	2.58	1.42	1.38
1	A	92	UFT	O4'-C1'	2.57	1.47	1.42
1	A	93	UFT	C2-N3	2.56	1.42	1.38
1	A	93	UFT	O4'-C1'	2.55	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	UFT	C2-N3	2.53	1.42	1.38
1	A	99	UFT	C2'-C1'	-2.52	1.50	1.53
1	A	113	UFT	C2-N3	2.52	1.42	1.38
1	A	95	UFT	C2'-C1'	-2.51	1.50	1.53
1	A	98	UFT	C2'-C1'	-2.51	1.50	1.53
1	A	102	UFT	C2-N3	2.50	1.42	1.38
1	A	118	UFT	O4'-C1'	2.49	1.47	1.42
1	A	110	UFT	O4'-C1'	2.47	1.47	1.42
1	A	98	UFT	O4'-C1'	2.47	1.47	1.42
1	A	113	UFT	O4'-C1'	2.45	1.47	1.42
1	A	102	UFT	O4'-C1'	2.42	1.47	1.42
1	A	95	UFT	O4'-C1'	2.41	1.47	1.42
1	A	131	UFT	C2'-C1'	-2.41	1.50	1.53
1	A	91	UFT	O2-C2	-2.40	1.18	1.23
1	A	118	UFT	C2-N3	2.36	1.42	1.38
1	A	110	UFT	O2-C2	-2.36	1.18	1.23
1	A	99	UFT	O2-C2	-2.35	1.18	1.23
1	A	95	UFT	O2-C2	-2.34	1.18	1.23
1	A	131	UFT	O2-C2	-2.34	1.18	1.23
1	A	102	UFT	O2-C2	-2.31	1.19	1.23
1	A	98	UFT	O2-C2	-2.30	1.19	1.23
1	A	113	UFT	O2-C2	-2.30	1.19	1.23
1	A	130	UFT	C4-N3	2.29	1.42	1.38
1	A	114	UFT	O2-C2	-2.29	1.19	1.23
1	A	93	UFT	O2-C2	-2.27	1.19	1.23
1	A	130	UFT	O2-C2	-2.25	1.19	1.23
1	A	118	UFT	O2-C2	-2.24	1.19	1.23
1	A	116	CFZ	C6-C5	2.16	1.40	1.35
1	A	112	CFZ	C6-C5	2.14	1.40	1.35
1	A	107	CFZ	C6-C5	2.14	1.40	1.35
1	A	92	UFT	O2-C2	-2.12	1.19	1.23
1	A	134	CFZ	C6-C5	2.12	1.40	1.35
1	A	95	UFT	C4-N3	2.12	1.42	1.38
1	A	110	UFT	C4-N3	2.08	1.42	1.38
1	A	93	UFT	C4-N3	2.06	1.42	1.38
1	A	114	UFT	C4-N3	2.06	1.42	1.38
1	A	89	CFZ	C6-C5	2.06	1.39	1.35
1	A	99	UFT	C4-N3	2.05	1.42	1.38
1	A	133	CFZ	C6-C5	2.04	1.39	1.35
1	A	115	CFZ	C6-C5	2.04	1.39	1.35
1	A	124	CFZ	C6-C5	2.03	1.39	1.35
1	A	98	UFT	C4-N3	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	UFT	C4-N3	2.01	1.42	1.38
1	A	100	CFZ	C6-C5	2.01	1.39	1.35
1	A	102	UFT	C4-N3	2.01	1.42	1.38

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	UFT	C4-N3-C2	-5.97	119.20	126.61
1	A	99	UFT	C4-N3-C2	-5.72	119.51	126.61
1	A	93	UFT	C4-N3-C2	-5.70	119.53	126.61
1	A	91	UFT	C4-N3-C2	-5.59	119.68	126.61
1	A	110	UFT	C4-N3-C2	-5.58	119.69	126.61
1	A	131	UFT	C4-N3-C2	-5.51	119.77	126.61
1	A	95	UFT	C4-N3-C2	-5.50	119.78	126.61
1	A	102	UFT	C4-N3-C2	-5.46	119.83	126.61
1	A	98	UFT	C4-N3-C2	-5.33	119.99	126.61
1	A	114	UFT	C4-N3-C2	-5.32	120.01	126.61
1	A	113	UFT	C4-N3-C2	-5.29	120.04	126.61
1	A	92	UFT	C4-N3-C2	-4.92	120.51	126.61
1	A	118	UFT	C4-N3-C2	-4.76	120.71	126.61
1	A	101	CFZ	C3'-C2'-C1'	4.49	108.31	103.10
1	A	92	UFT	C2'-C1'-N1	-4.44	107.45	114.27
1	A	91	UFT	N3-C2-N1	4.34	120.55	114.89
1	A	99	UFT	N3-C2-N1	4.20	120.36	114.89
1	A	98	UFT	N3-C2-N1	4.15	120.29	114.89
1	A	130	UFT	C5-C4-N3	4.13	120.59	114.80
1	A	110	UFT	N3-C2-N1	4.09	120.22	114.89
1	A	113	UFT	N3-C2-N1	4.06	120.18	114.89
1	A	130	UFT	N3-C2-N1	4.04	120.15	114.89
1	A	118	UFT	C3'-C2'-C1'	4.02	107.77	103.10
1	A	131	UFT	N3-C2-N1	4.01	120.11	114.89
1	A	98	UFT	C3'-C2'-C1'	4.00	107.74	103.10
1	A	102	UFT	N3-C2-N1	3.99	120.09	114.89
1	A	133	CFZ	C2'-C3'-C4'	3.98	107.68	102.43
1	A	124	CFZ	C3'-C2'-C1'	3.97	107.70	103.10
1	A	93	UFT	N3-C2-N1	3.94	120.02	114.89
1	A	130	UFT	O4-C4-C5	-3.93	118.39	125.16
1	A	133	CFZ	C3'-C2'-C1'	3.92	107.65	103.10
1	A	101	CFZ	C2'-C3'-C4'	3.90	107.57	102.43
1	A	95	UFT	N3-C2-N1	3.88	119.94	114.89
1	A	93	UFT	C5-C4-N3	3.84	120.18	114.80
1	A	114	UFT	N3-C2-N1	3.80	119.84	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	UFT	C5-C4-N3	3.80	120.12	114.80
1	A	110	UFT	C2'-C3'-C4'	3.79	107.42	102.43
1	A	99	UFT	C5-C4-N3	3.76	120.06	114.80
1	A	119	CFZ	C2'-C3'-C4'	3.75	107.38	102.43
1	A	110	UFT	C3'-C2'-C1'	3.74	107.44	103.10
1	A	110	UFT	C5-C4-N3	3.73	120.03	114.80
1	A	131	UFT	C5-C4-N3	3.73	120.03	114.80
1	A	114	UFT	C5-C4-N3	3.73	120.03	114.80
1	A	106	CFZ	C2'-C3'-C4'	3.71	107.31	102.43
1	A	118	UFT	N3-C2-N1	3.70	119.71	114.89
1	A	98	UFT	C2'-C3'-C4'	3.69	107.30	102.43
1	A	102	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	106	CFZ	C3'-C2'-C1'	3.67	107.36	103.10
1	A	91	UFT	C5-C4-N3	3.65	119.91	114.80
1	A	92	UFT	C5-C4-N3	3.65	119.91	114.80
1	A	100	CFZ	C3'-C2'-C1'	3.58	107.25	103.10
1	A	114	UFT	C2'-C1'-N1	-3.55	108.81	114.27
1	A	113	UFT	C5-C4-N3	3.54	119.77	114.80
1	A	92	UFT	N3-C2-N1	3.53	119.49	114.89
1	A	119	CFZ	C3'-C2'-C1'	3.52	107.18	103.10
1	A	98	UFT	C5-C4-N3	3.50	119.70	114.80
1	A	93	UFT	C3'-C2'-C1'	3.42	107.06	103.10
1	A	102	UFT	C2'-C3'-C4'	3.41	106.93	102.43
1	A	118	UFT	C5-C4-N3	3.40	119.56	114.80
1	A	134	CFZ	C3'-C2'-C1'	3.39	107.03	103.10
1	A	114	UFT	O4-C4-C5	-3.24	119.58	125.16
1	A	95	UFT	C3'-C2'-C1'	3.23	106.85	103.10
1	A	118	UFT	C2'-C1'-N1	-3.23	109.31	114.27
1	A	100	CFZ	C2'-C3'-C4'	3.12	106.54	102.43
1	A	99	UFT	C3'-C2'-C1'	3.04	106.63	103.10
1	A	93	UFT	C2'-C3'-C4'	3.04	106.44	102.43
1	A	110	UFT	O4-C4-C5	-3.01	119.97	125.16
1	A	131	UFT	O4-C4-C5	-3.01	119.98	125.16
1	A	124	CFZ	C2'-C3'-C4'	3.00	106.38	102.43
1	A	95	UFT	O4-C4-C5	-3.00	120.00	125.16
1	A	102	UFT	C3'-C2'-C1'	2.99	106.58	103.10
1	A	102	UFT	O4-C4-C5	-2.99	120.01	125.16
1	A	93	UFT	O4-C4-C5	-2.98	120.03	125.16
1	A	99	UFT	O4-C4-C5	-2.94	120.10	125.16
1	A	130	UFT	C2'-C1'-N1	-2.93	109.76	114.27
1	A	91	UFT	O4-C4-C5	-2.90	120.17	125.16
1	A	107	CFZ	C2'-C1'-N1	-2.89	109.83	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	UFT	O4-C4-C5	-2.87	120.21	125.16
1	A	131	UFT	C2'-C1'-N1	-2.85	109.90	114.27
1	A	116	CFZ	C2'-C1'-N1	-2.79	109.98	114.27
1	A	98	UFT	O4-C4-C5	-2.78	120.36	125.16
1	A	131	UFT	C3'-C2'-C1'	2.77	106.31	103.10
1	A	112	CFZ	C2'-C3'-C4'	2.76	106.07	102.43
1	A	106	CFZ	C2'-C1'-N1	-2.73	110.07	114.27
1	A	113	UFT	O4-C4-C5	-2.73	120.46	125.16
1	A	118	UFT	O4-C4-C5	-2.67	120.55	125.16
1	A	86	CFZ	C3'-C2'-C1'	2.63	106.15	103.10
1	A	115	CFZ	C3'-C2'-C1'	2.62	106.15	103.10
1	A	134	CFZ	C2'-C3'-C4'	2.58	105.84	102.43
1	A	89	CFZ	C3'-C2'-C1'	2.54	106.05	103.10
1	A	91	UFT	O2-C2-N1	-2.54	119.49	122.80
1	A	99	UFT	C2'-C1'-N1	-2.51	110.41	114.27
1	A	115	CFZ	C2'-C1'-N1	-2.47	110.47	114.27
1	A	91	UFT	C2'-C1'-N1	-2.47	110.48	114.27
1	A	98	UFT	O2-C2-N1	-2.39	119.68	122.80
1	A	110	UFT	O2-C2-N1	-2.39	119.68	122.80
1	A	95	UFT	C2'-C3'-C4'	2.37	105.56	102.43
1	A	118	UFT	C2'-C3'-C4'	2.35	105.53	102.43
1	A	107	CFZ	C3'-C2'-C1'	2.34	105.82	103.10
1	A	124	CFZ	C2'-C1'-N1	-2.34	110.68	114.27
1	A	99	UFT	C4'-O4'-C1'	-2.33	104.33	109.47
1	A	100	CFZ	C2'-C1'-N1	-2.32	110.71	114.27
1	A	131	UFT	O2-C2-N1	-2.25	119.86	122.80
1	A	95	UFT	C2'-C1'-N1	-2.25	110.81	114.27
1	A	99	UFT	O2-C2-N1	-2.22	119.91	122.80
1	A	102	UFT	O2-C2-N1	-2.21	119.92	122.80
1	A	113	UFT	O2-C2-N1	-2.20	119.94	122.80
1	A	91	UFT	O3'-C3'-C2'	2.15	119.75	111.85
1	A	134	CFZ	C2'-C1'-N1	-2.15	110.97	114.27
1	A	93	UFT	O2-C2-N1	-2.15	120.00	122.80
1	A	131	UFT	C4'-O4'-C1'	-2.14	104.73	109.47
1	A	130	UFT	O2-C2-N1	-2.14	120.01	122.80
1	A	116	CFZ	C3'-C2'-C1'	2.13	105.57	103.10
1	A	95	UFT	O2-C2-N1	-2.13	120.03	122.80
1	A	112	CFZ	C3'-C2'-C1'	2.11	105.54	103.10
1	A	119	CFZ	C5'-C4'-C3'	-2.06	107.78	115.21
1	A	114	UFT	C3'-C2'-C1'	2.04	105.47	103.10
1	A	92	UFT	C3'-C2'-C1'	2.04	105.46	103.10
1	A	101	CFZ	O2-C2-N3	-2.02	119.15	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	UFT	C2'-C1'-N1	-2.02	111.17	114.27
1	A	102	UFT	C4'-O4'-C1'	-2.01	105.02	109.47
1	A	86	CFZ	C2'-C3'-C4'	2.01	105.08	102.43
1	A	89	CFZ	C2'-C3'-C4'	2.00	105.07	102.43

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	98	UFT	C2'-C1'-N1-C6
1	A	98	UFT	C2'-C1'-N1-C2
1	A	100	CFZ	C3'-C4'-C5'-O5'
1	A	100	CFZ	O4'-C4'-C5'-O5'
1	A	107	CFZ	C3'-C4'-C5'-O5'
1	A	107	CFZ	O4'-C4'-C5'-O5'
1	A	113	UFT	C2'-C1'-N1-C6
1	A	113	UFT	C2'-C1'-N1-C2
1	A	114	UFT	O4'-C4'-C5'-O5'
1	A	134	CFZ	C3'-C4'-C5'-O5'
1	A	134	CFZ	O4'-C4'-C5'-O5'
1	A	101	CFZ	C3'-C4'-C5'-O5'
1	A	114	UFT	C3'-C4'-C5'-O5'
1	A	118	UFT	O4'-C4'-C5'-O5'
1	A	119	CFZ	C3'-C4'-C5'-O5'
1	A	133	CFZ	C3'-C4'-C5'-O5'
1	A	113	UFT	C4'-C5'-O5'-P
1	A	98	UFT	O4'-C4'-C5'-O5'
1	A	101	CFZ	O4'-C4'-C5'-O5'
1	A	98	UFT	C3'-C4'-C5'-O5'
1	A	113	UFT	C3'-C4'-C5'-O5'
1	A	89	CFZ	O4'-C4'-C5'-O5'
1	A	118	UFT	C3'-C4'-C5'-O5'
1	A	119	CFZ	O4'-C4'-C5'-O5'
1	A	133	CFZ	O4'-C4'-C5'-O5'
1	A	89	CFZ	C3'-C4'-C5'-O5'
1	A	113	UFT	O4'-C1'-N1-C2
1	A	113	UFT	O4'-C1'-N1-C6
1	A	113	UFT	O4'-C4'-C5'-O5'
1	A	98	UFT	O4'-C1'-N1-C6
1	A	114	UFT	C4'-C5'-O5'-P
1	A	92	UFT	C3'-C4'-C5'-O5'
1	A	110	UFT	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	98	UFT	O4'-C1'-N1-C2
1	A	95	UFT	C2'-C1'-N1-C2

There are no ring outliers.

15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	99	UFT	1	0
1	A	93	UFT	1	0
1	A	89	CFZ	1	0
1	A	102	UFT	1	0
1	A	119	CFZ	2	0
1	A	124	CFZ	1	0
1	A	86	CFZ	3	0
1	A	92	UFT	1	0
1	A	91	UFT	2	0
1	A	100	CFZ	2	0
1	A	115	CFZ	2	0
1	A	106	CFZ	1	0
1	A	116	CFZ	4	0
1	A	133	CFZ	1	0
1	A	101	CFZ	3	0

## 5.5 Carbohydrates

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	C	1	3,2	14,14,15	0.72	0	17,19,21	0.86	0
3	NAG	C	2	3	14,14,15	0.72	0	17,19,21	0.83	0

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
3	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

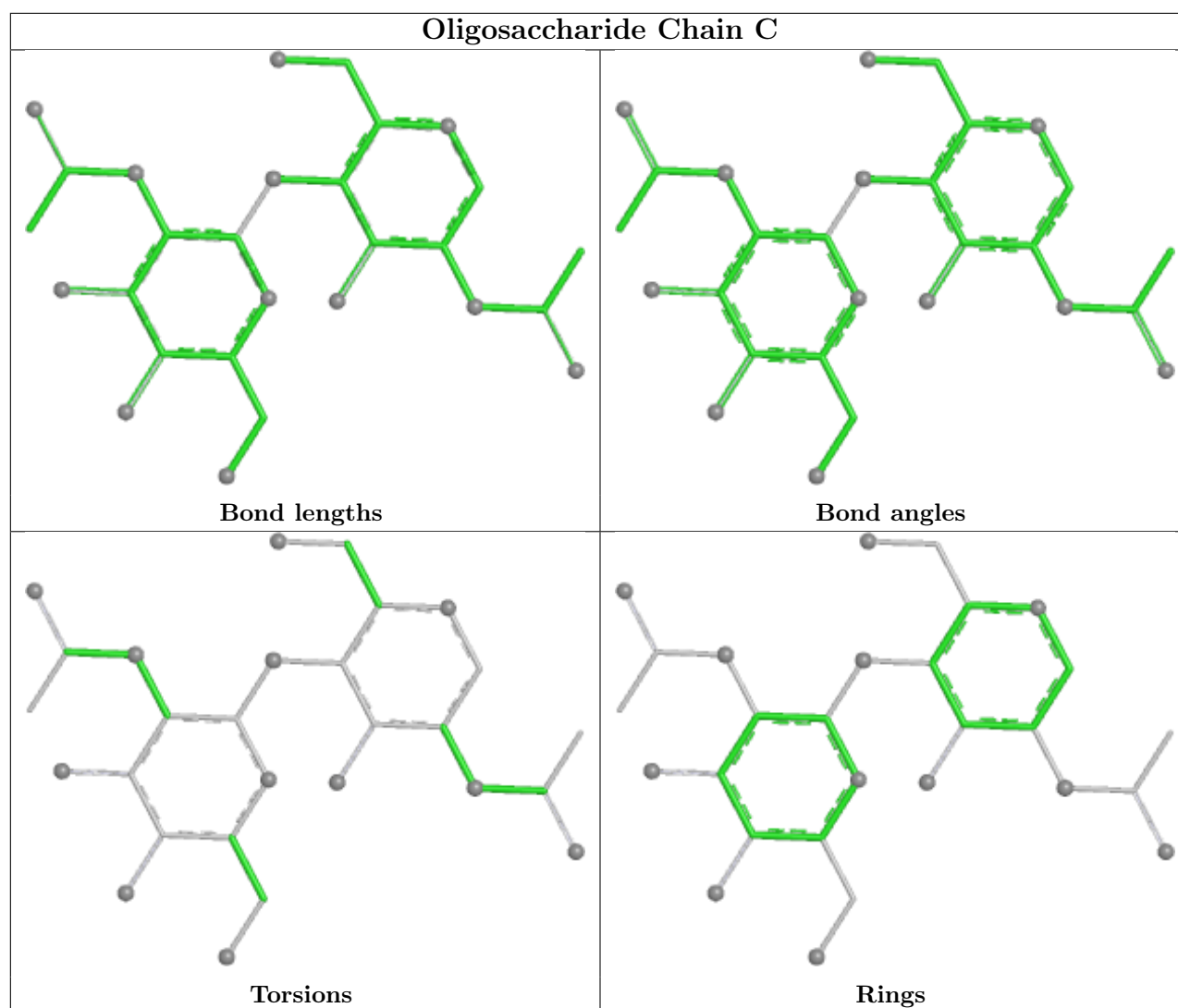
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	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 oligosaccharide.





## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

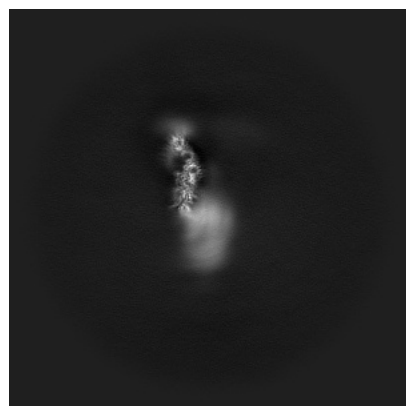
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55625. These allow visual inspection of the internal detail of the map and identification of artifacts.

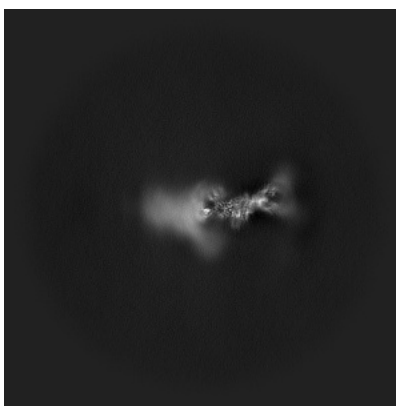
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

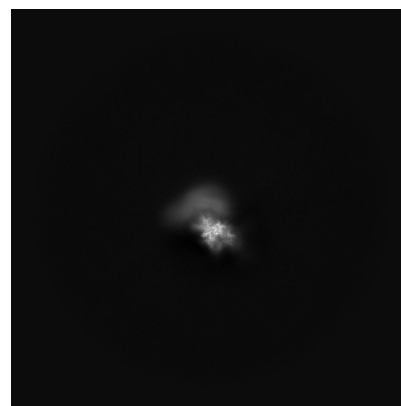
#### 6.1.1 Primary map



X



Y



Z

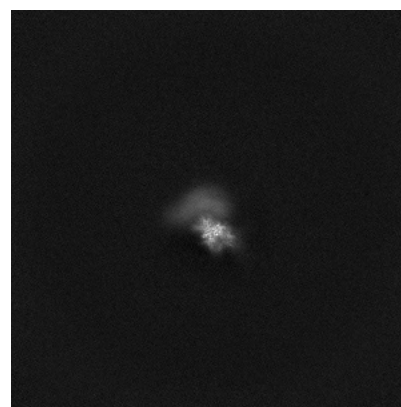
#### 6.1.2 Raw map



X



Y



Z

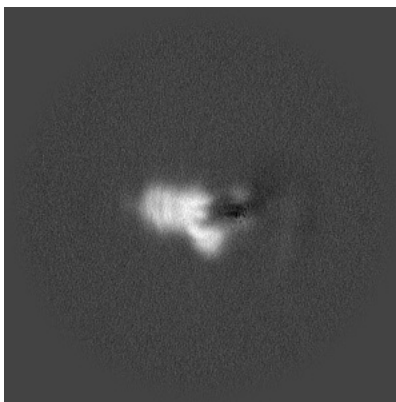
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 320



Y Index: 320

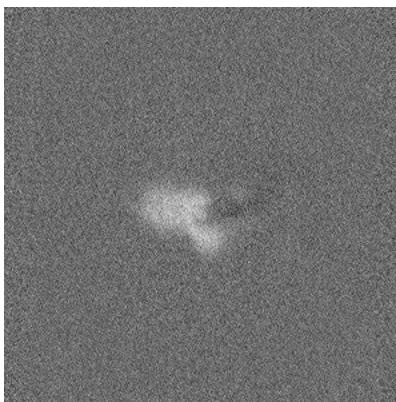


Z Index: 320

### 6.2.2 Raw map



X Index: 320



Y Index: 320



Z Index: 320

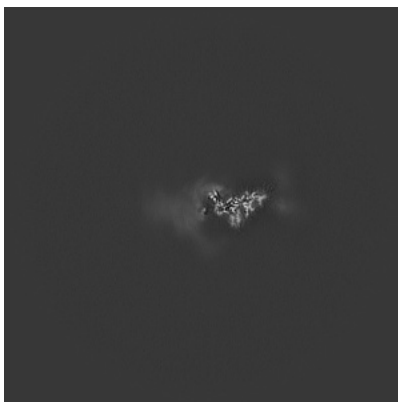
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

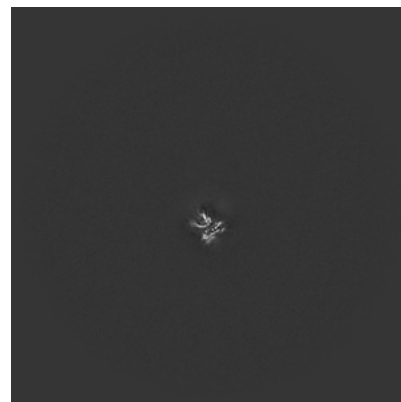
### 6.3.1 Primary map



X Index: 318

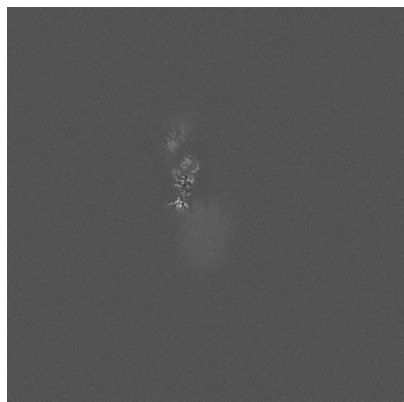


Y Index: 290

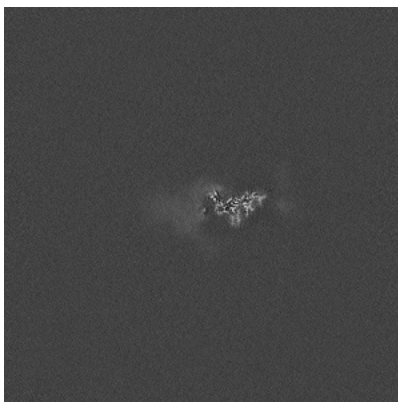


Z Index: 376

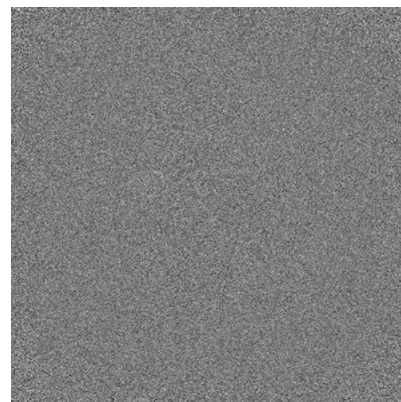
### 6.3.2 Raw map



X Index: 318



Y Index: 290

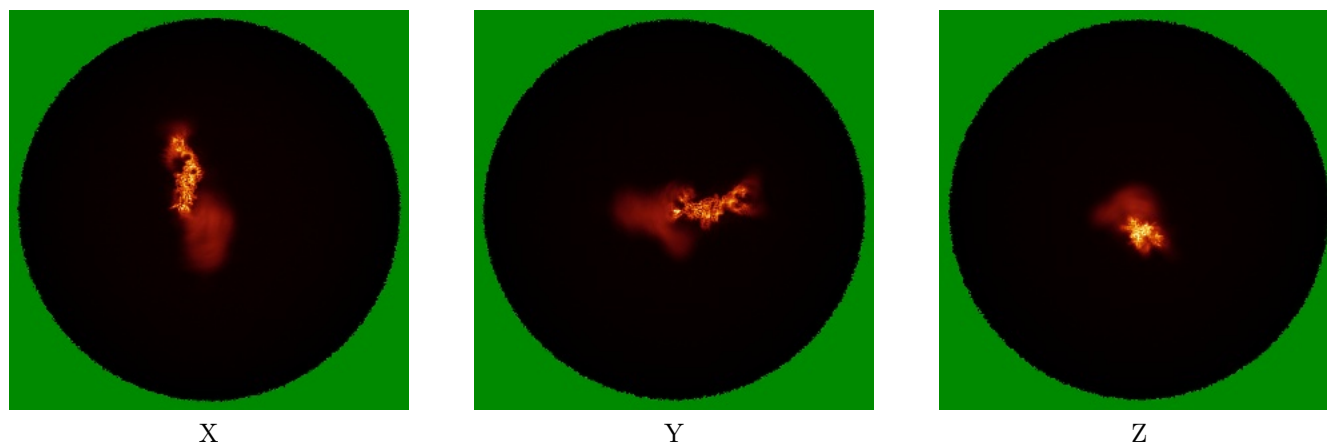


Z Index: 0

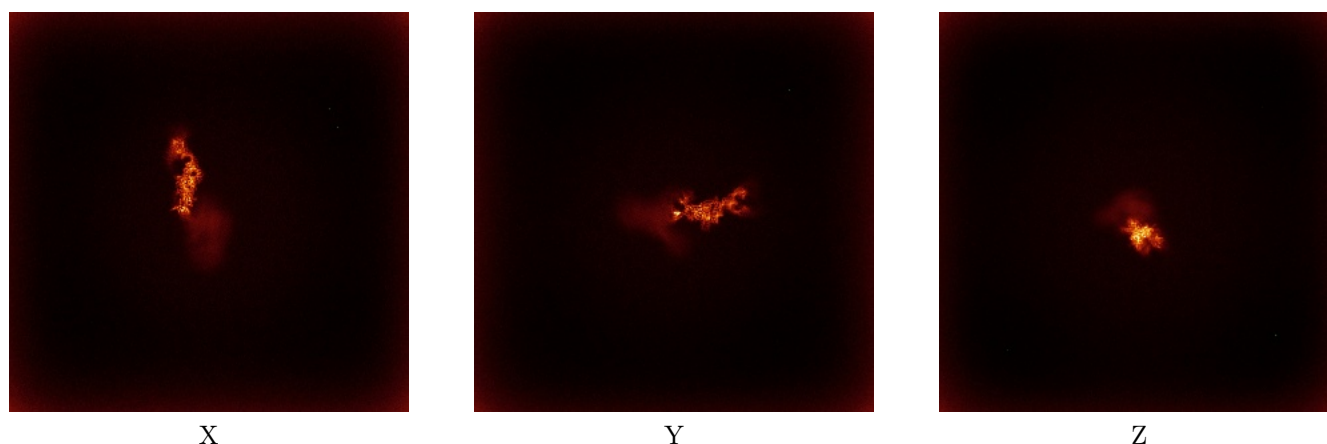
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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

## 6.5 Orthogonal surface views [i](#)

This section was not generated.

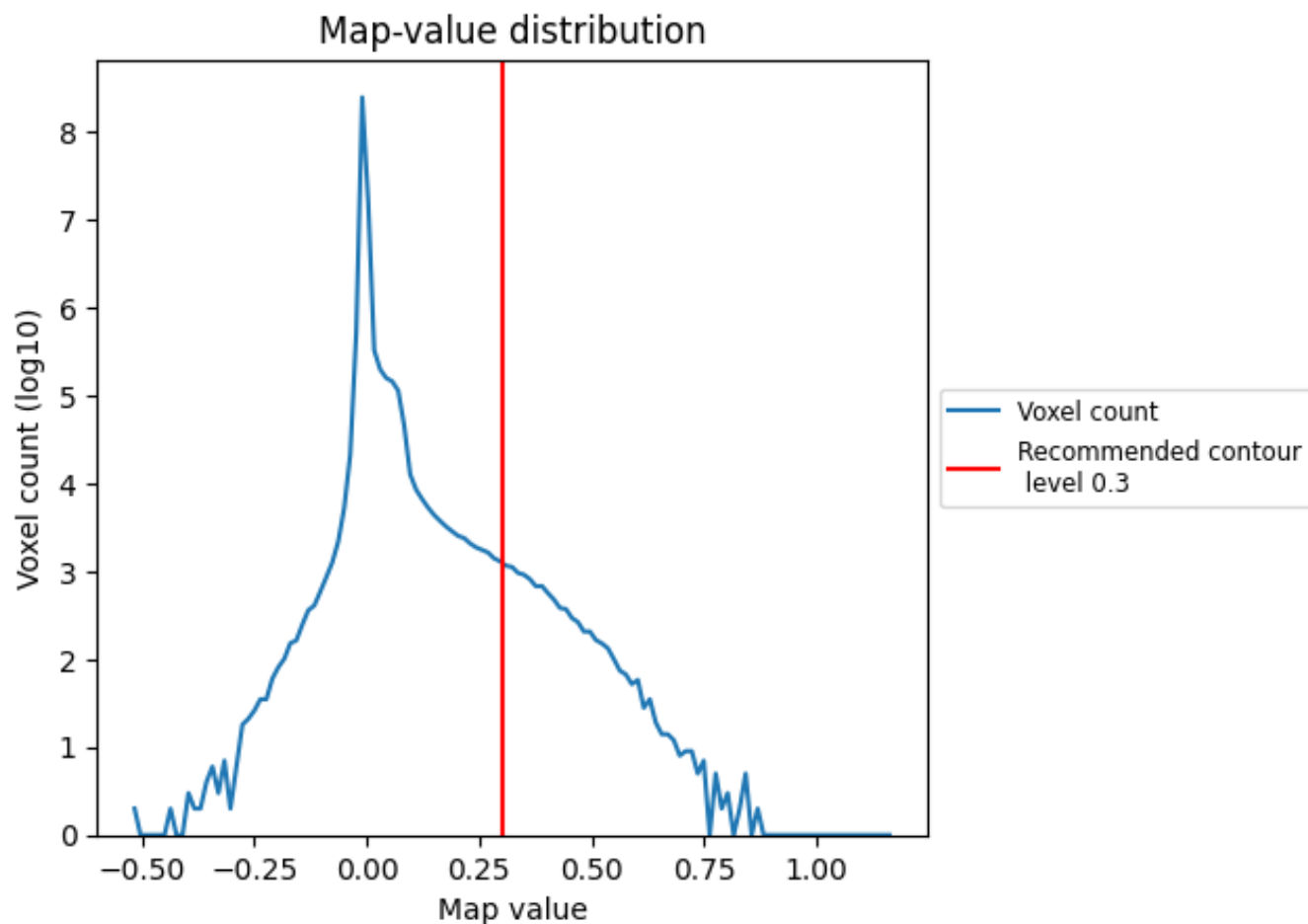
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

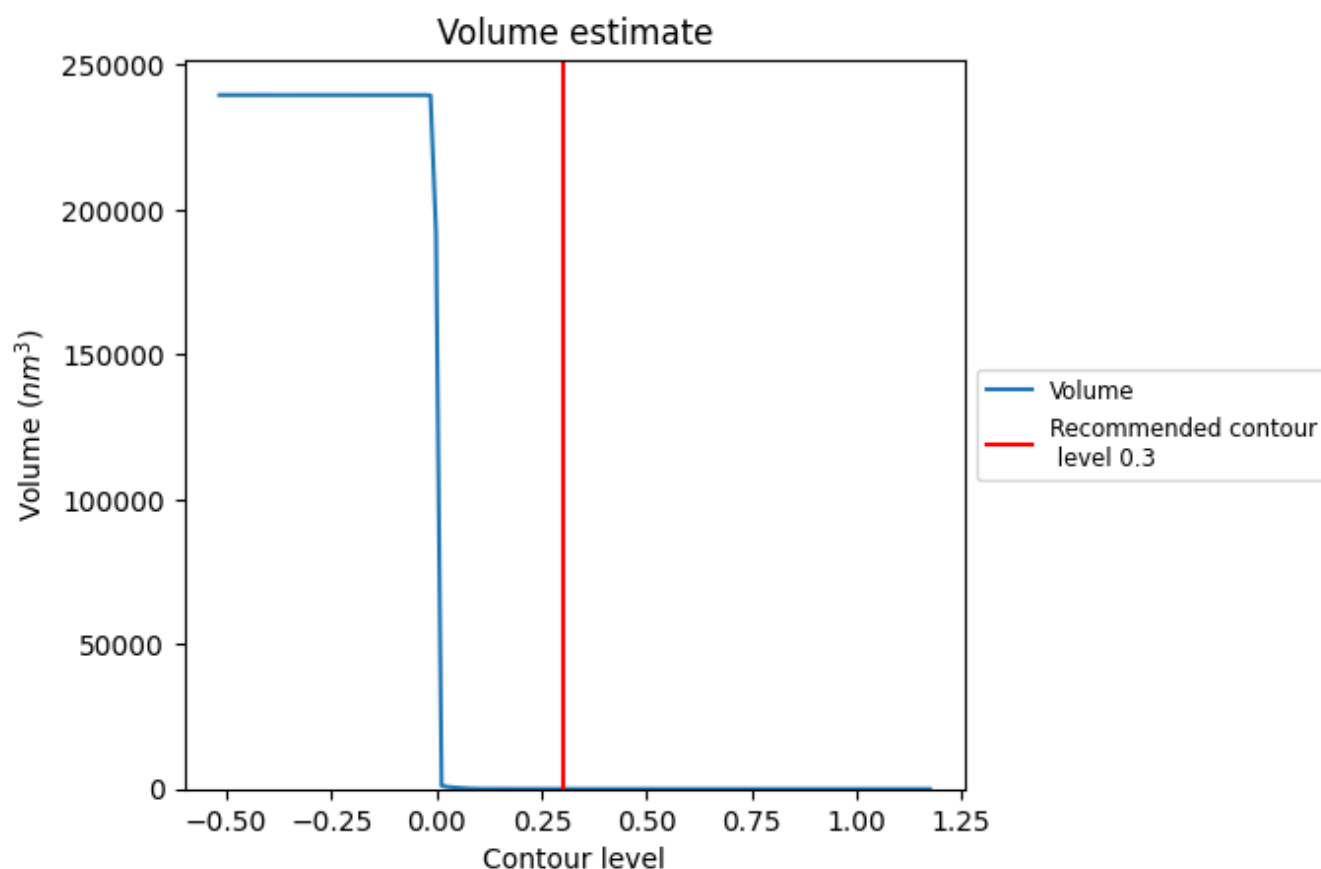
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

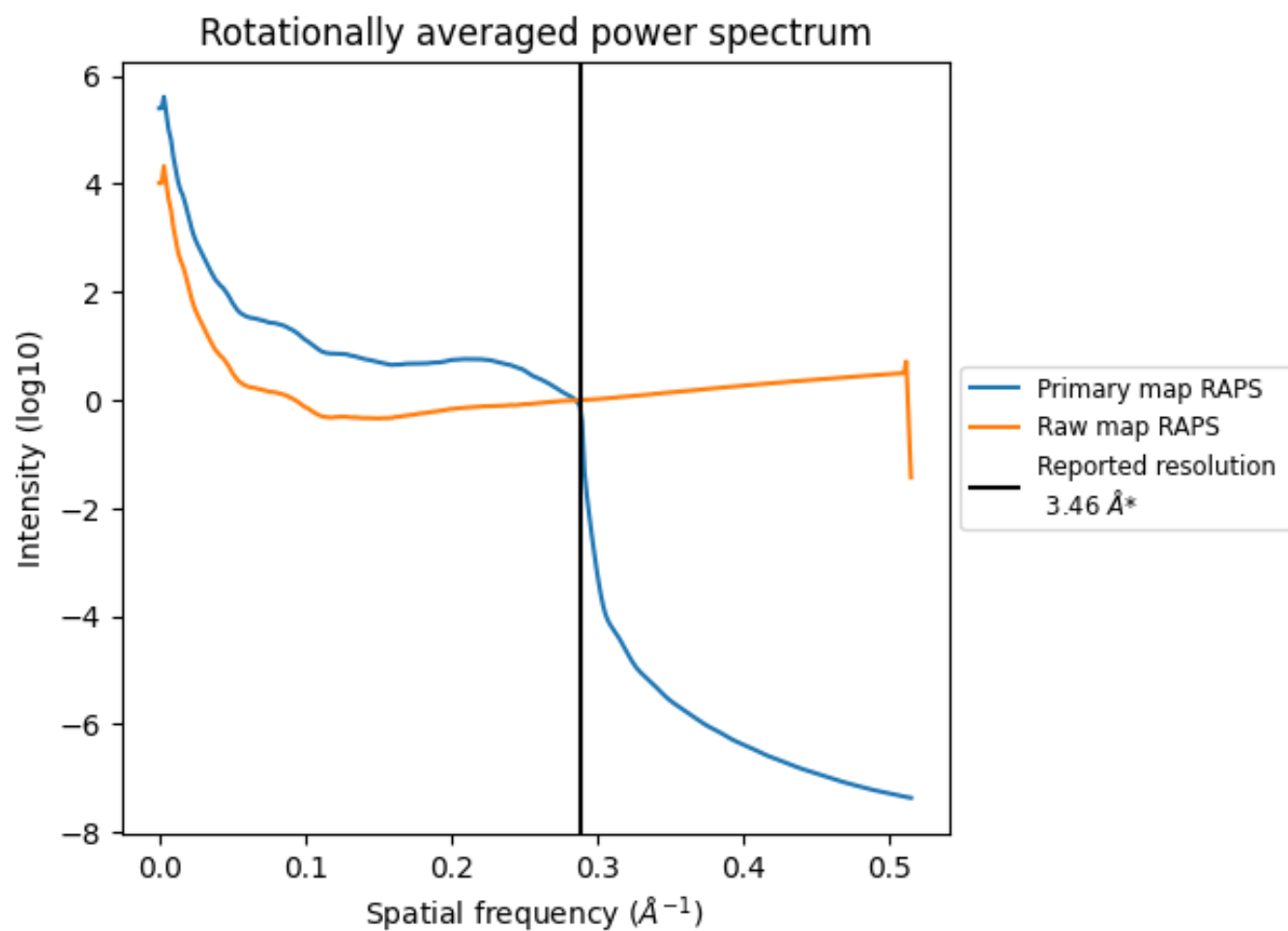


The volume at the recommended contour level is 10  $\text{nm}^3$ ; this corresponds to an approximate mass of 9 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

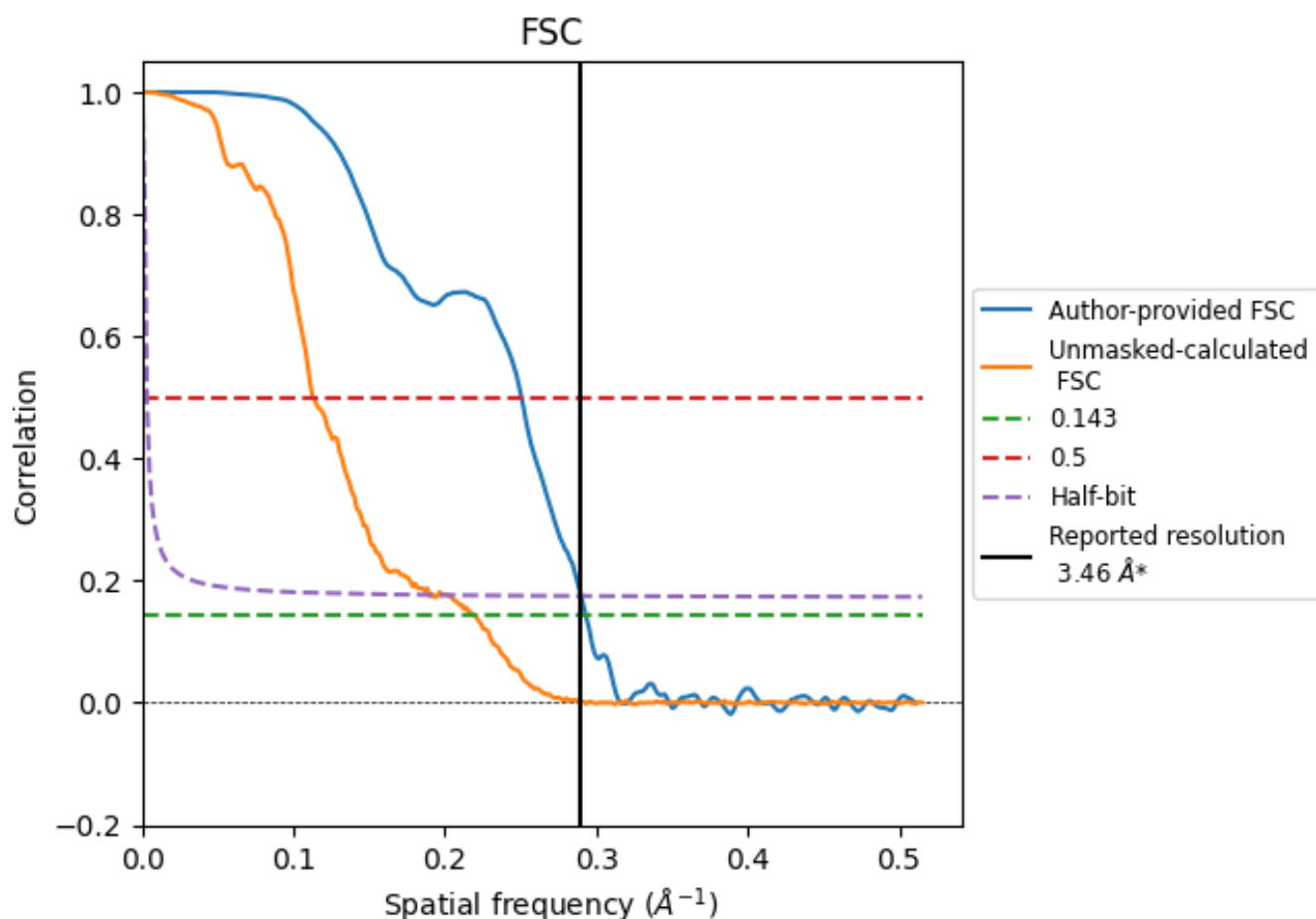


\*Reported resolution corresponds to spatial frequency of 0.289 Å<sup>-1</sup>

## 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 0.289 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

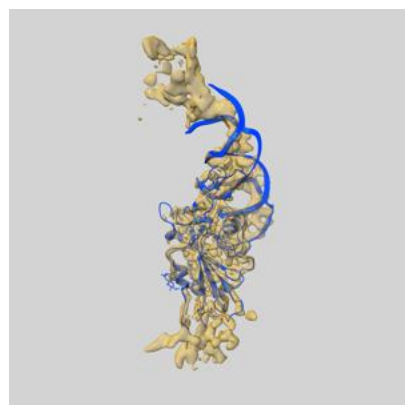
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.41	3.99	3.45
Unmasked-calculated*	4.57	8.88	5.27

\*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 4.57 differs from the reported value 3.46 by more than 10 %

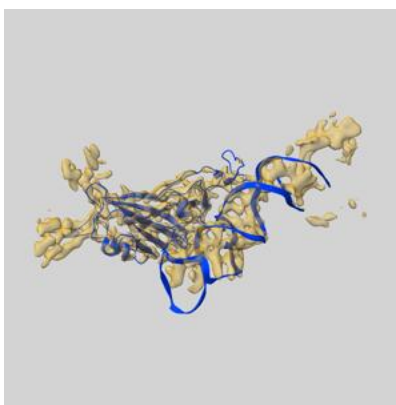
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-55625 and PDB model 9T74. Per-residue inclusion information can be found in section [3](#) on page [5](#).

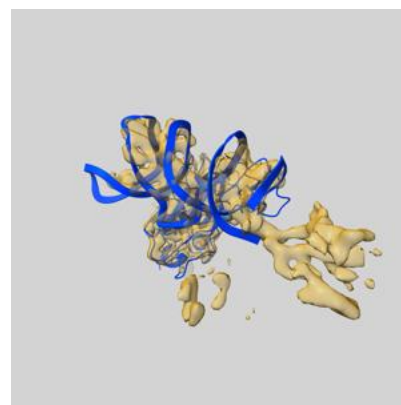
### 9.1 Map-model overlay [i](#)



X



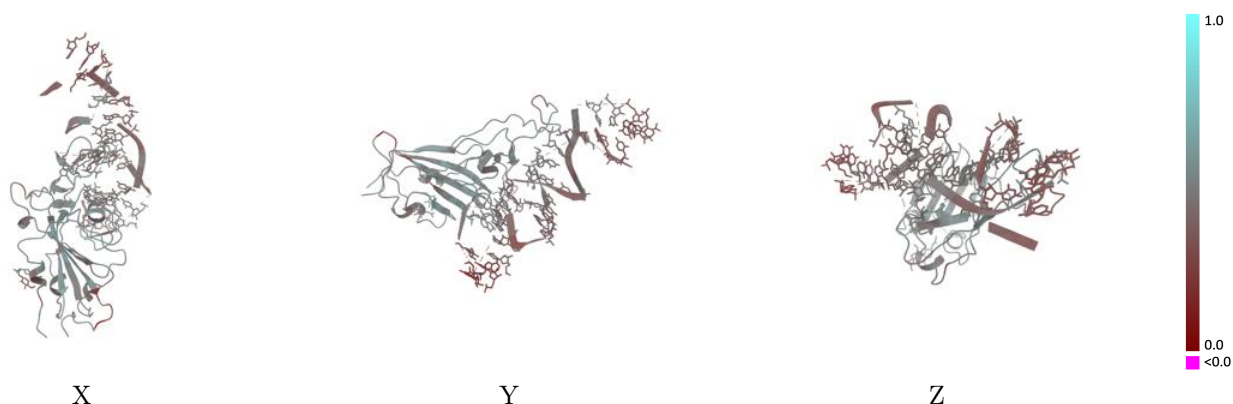
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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](#)

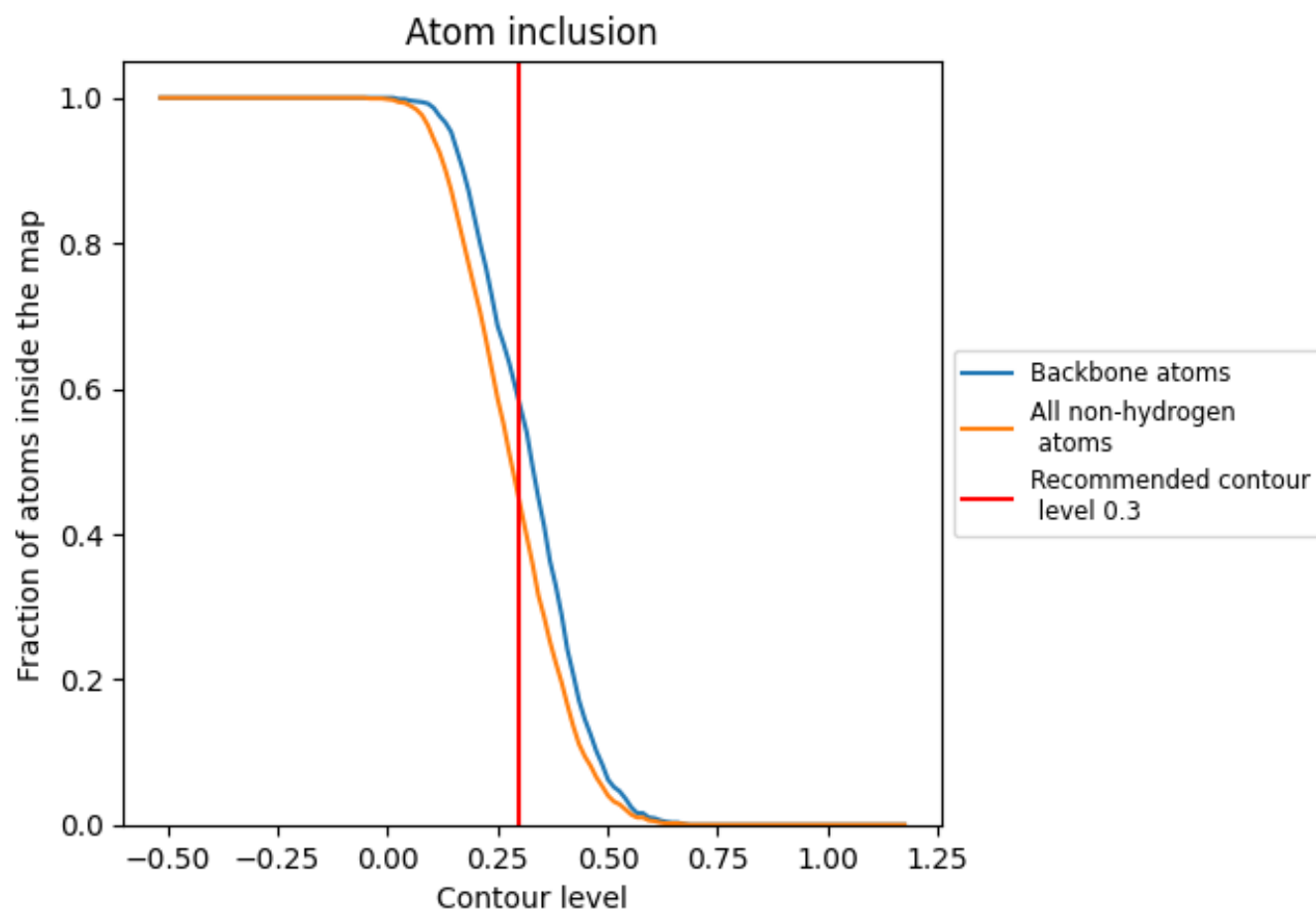


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 44% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4430	<div></div> 0.4530
A	<div></div> 0.4260	<div></div> 0.3950
B	<div></div> 0.4590	<div></div> 0.4950
C	<div></div> 0.2500	<div></div> 0.4300

