



## Full wwPDB EM Validation Report ⓘ

Nov 25, 2025 – 04:53 PM EST

PDB ID : 9ZC8 / pdb\_00009zc8  
EMDB ID : EMD-70036  
Title : 5-methyl-cytidine RNA origami 6-helix bundle type-1 dimer  
Authors : McRae, E.K.S.  
Deposited on : 2025-11-22  
Resolution : 12.10 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.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

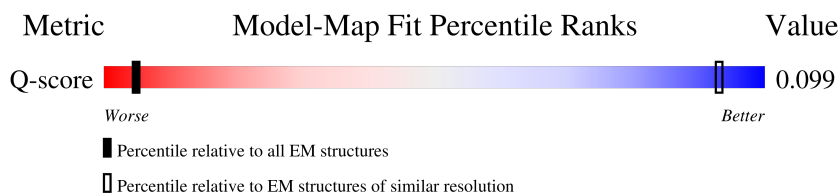
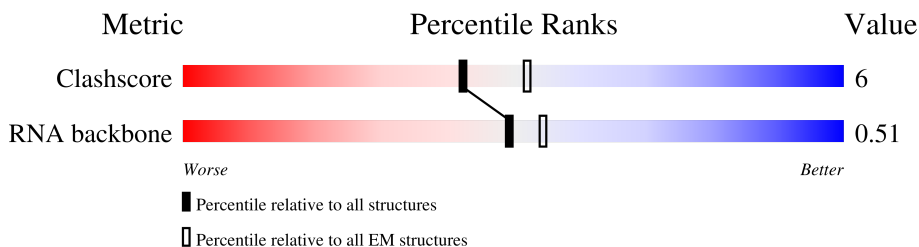
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



The reported resolution of this entry is 12.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
RNA backbone	6643	2191	-
Q-score	-	25397	85 ( 11.60 - 12.60 )

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	720	 60% 33% 7%
1	B	720	 58% 33% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5MC	A	369	-	-	X	-

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31034 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.

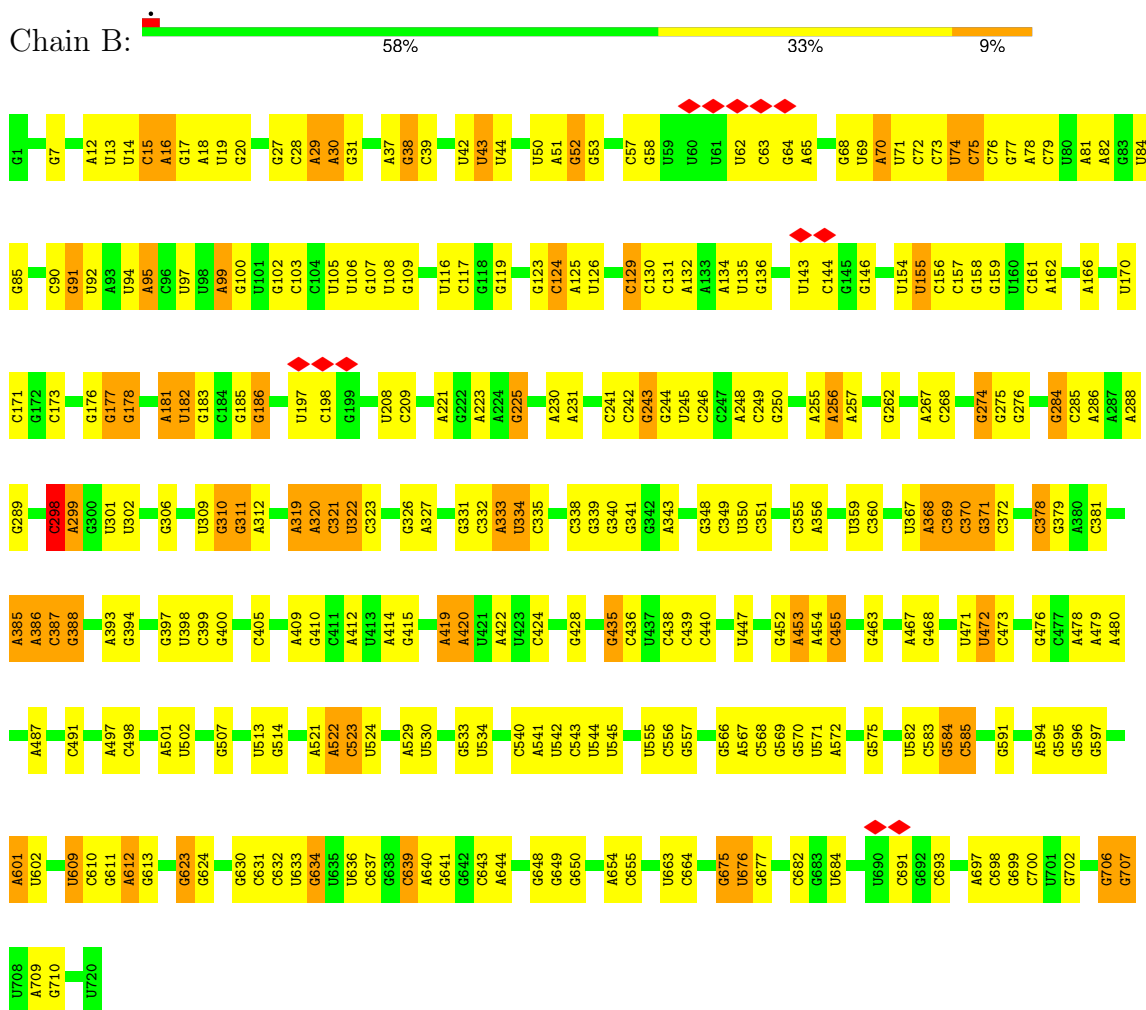
- Molecule 1 is a RNA chain called 5-methyl-cytidine RNA origami 6-helix bundle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	720	Total	C	N	O	P	0	0
			15517	7022	2708	5067	720		
1	A	720	Total	C	N	O	P	0	0
			15517	7022	2708	5067	720		

### 3 Residue-property plots

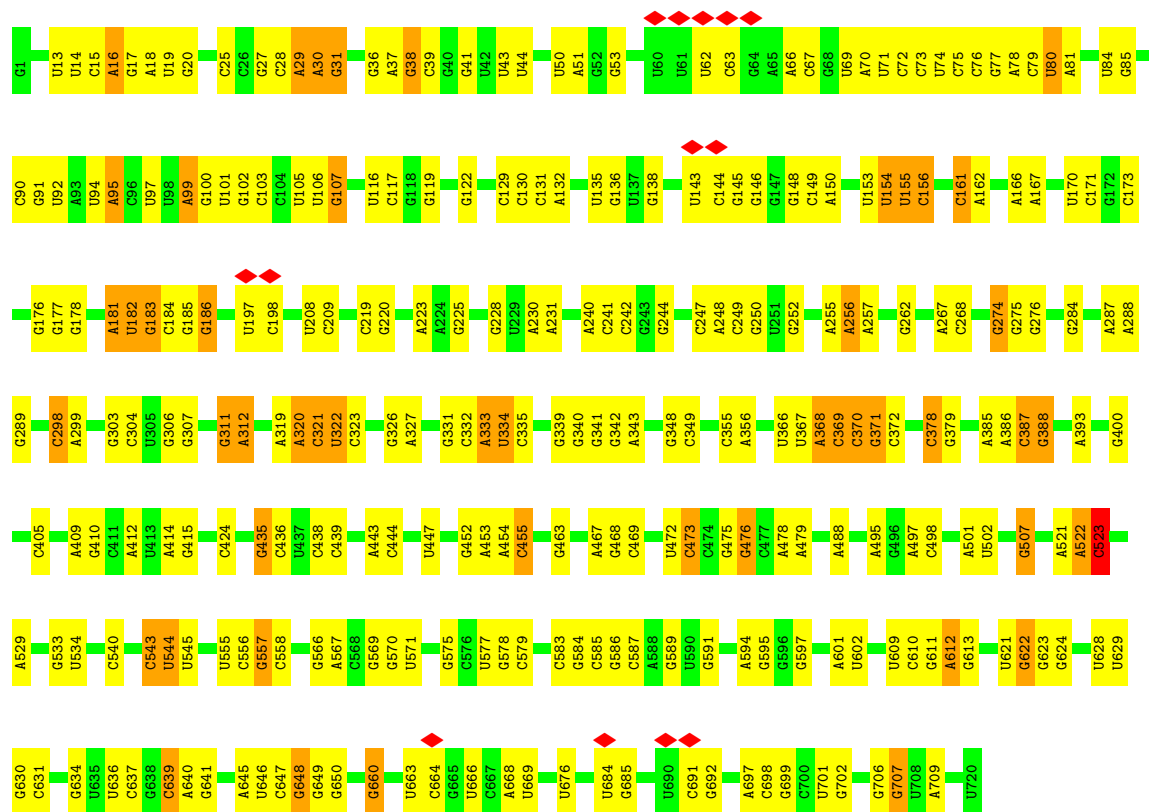
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 5-methyl-cytidine RNA origami 6-helix bundle



- Molecule 1: 5-methyl-cytidine RNA origami 6-helix bundle





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	2616	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.845	Depositor
Minimum map value	-0.457	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	1	Depositor
Map size (Å)	662.4, 662.4, 662.4	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.68, 3.68, 3.68	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC

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	0.10	0/13202	0.26	0/20627
1	B	0.11	0/13202	0.27	0/20627
All	All	0.10	0/26404	0.27	0/41254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15517	0	8101	139	0
1	B	15517	0	8101	165	0
All	All	31034	0	16202	302	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (302) 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)
1:A:369:5MC:H3'	1:A:370:5MC:HM53	1.63	0.79
1:B:369:5MC:H3'	1:B:370:5MC:HM53	1.67	0.76
1:A:369:5MC:HN41	1:A:707:G:H1	1.34	0.74
1:B:256:A:H61	1:B:455:5MC:HM52	1.57	0.69
1:B:262:G:H1	1:B:455:5MC:HN41	1.41	0.69
1:A:186:G:H1	1:A:209:5MC:HN41	1.41	0.69
1:B:440:5MC:HN41	1:B:596:G:H1	1.39	0.68
1:B:53:G:H1	1:B:72:5MC:HN41	1.41	0.66
1:A:36:G:H1	1:A:523:5MC:HN41	1.45	0.65
1:B:326:G:H1	1:B:387:5MC:HN41	1.43	0.64
1:A:78:A:C4	1:A:79:5MC:HM52	2.33	0.64
1:A:370:5MC:H5''	1:A:371:G:OP2	1.98	0.63
1:A:256:A:H61	1:A:455:5MC:HM52	1.64	0.62
1:B:78:A:C4	1:B:79:5MC:HM52	2.34	0.62
1:A:30:A:C2	1:A:523:5MC:HM52	2.34	0.62
1:A:698:5MC:H2'	1:A:699:G:H8	1.66	0.61
1:A:369:5MC:N4	1:A:707:G:H1	2.00	0.60
1:A:348:G:H2'	1:A:349:5MC:O4'	2.01	0.60
1:A:372:5MC:HN41	1:A:650:G:H1	1.51	0.59
1:B:639:5MC:H2'	1:B:640:A:H8	1.68	0.59
1:A:262:G:H1	1:A:455:5MC:HN41	1.51	0.59
1:A:30:A:N1	1:A:523:5MC:HM52	2.18	0.58
1:A:76:5MC:H2'	1:A:77:G:H8	1.69	0.58
1:A:103:5MC:HN41	1:A:307:G:H1	1.50	0.58
1:B:370:5MC:H5''	1:B:371:G:OP2	2.04	0.57
1:A:473:5MC:HN41	1:A:570:G:H1	1.53	0.57
1:B:76:5MC:H2'	1:B:77:G:H8	1.70	0.57
1:B:129:5MC:HN41	1:B:276:G:H1	1.52	0.57
1:B:491:5MC:HN41	1:A:228:G:H1	1.52	0.56
1:A:29:A:C8	1:A:523:5MC:HM53	2.41	0.56
1:B:30:A:C6	1:B:523:5MC:HM52	2.41	0.56
1:B:285:5MC:HM52	1:B:286:A:N6	2.21	0.56
1:A:697:A:H2'	1:A:698:5MC:O4'	2.06	0.56
1:A:156:5MC:H5''	1:A:274:G:H5''	1.88	0.55
1:B:630:G:H2'	1:B:631:5MC:C6	2.41	0.55
1:B:156:5MC:H5'	1:B:274:G:H5''	1.89	0.55
1:B:27:G:H2'	1:B:28:5MC:C6	2.42	0.55
1:B:186:G:H1	1:B:209:5MC:HN41	1.55	0.55
1:A:73:5MC:H4'	1:A:97:U:H5''	1.88	0.54
1:A:25:5MC:HN41	1:A:41:G:H1	1.55	0.54
1:B:372:5MC:HN41	1:B:650:G:H1	1.54	0.54
1:A:369:5MC:HM51	1:A:369:5MC:OP2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:G:H1	1:B:387:5MC:N4	2.06	0.54
1:A:36:G:H1	1:A:523:5MC:N4	2.05	0.53
1:B:570:G:H2'	1:B:571:U:C6	2.44	0.53
1:A:130:5MC:HN41	1:A:275:G:H1	1.57	0.52
1:B:71:U:H2'	1:B:72:5MC:C6	2.45	0.52
1:B:369:5MC:HN41	1:B:707:G:H1	1.55	0.52
1:A:27:G:H2'	1:A:28:5MC:C6	2.45	0.52
1:B:123:G:H3'	1:B:124:5MC:HM53	1.92	0.52
1:B:82:A:H62	1:B:91:G:H4'	1.75	0.51
1:B:348:G:H2'	1:B:349:5MC:O4'	2.10	0.51
1:B:523:5MC:H2'	1:B:524:U:C6	2.45	0.51
1:B:639:5MC:H2'	1:B:640:A:C8	2.45	0.51
1:B:320:A:H2	1:B:387:5MC:HM52	1.76	0.51
1:A:630:G:H2'	1:A:631:5MC:C6	2.46	0.51
1:A:326:G:H1	1:A:387:5MC:HN41	1.59	0.51
1:A:321:5MC:HM52	1:A:386:A:C2	2.45	0.51
1:B:76:5MC:H2'	1:B:77:G:C8	2.46	0.50
1:B:640:A:H2	1:B:641:G:O6	1.93	0.50
1:B:340:G:N2	1:B:341:G:N7	2.60	0.50
1:B:16:A:N6	1:B:51:A:C6	2.79	0.50
1:B:320:A:C2	1:B:387:5MC:HM52	2.47	0.50
1:B:311:G:H2'	1:B:312:A:H8	1.76	0.50
1:A:439:5MC:N4	1:A:597:G:H1	2.10	0.50
1:B:697:A:H2'	1:B:698:5MC:O4'	2.11	0.49
1:A:311:G:H2'	1:A:312:A:C8	2.47	0.49
1:B:439:5MC:HN41	1:B:597:G:H1	1.59	0.49
1:A:303:G:H2'	1:A:304:5MC:O4'	2.13	0.49
1:A:668:A:C2	1:A:669:U:C4	3.01	0.49
1:B:158:G:HO2'	1:B:159:G:C5'	2.26	0.49
1:B:135:U:H5'	1:B:177:G:H21	1.77	0.49
1:B:630:G:H2'	1:B:631:5MC:H6	1.78	0.49
1:A:468:G:H2'	1:A:469:5MC:C6	2.47	0.49
1:B:333:A:O2'	1:B:334:U:P	2.70	0.49
1:A:129:5MC:HN41	1:A:276:G:H1	1.61	0.49
1:A:333:A:O2'	1:A:334:U:P	2.71	0.49
1:B:369:5MC:N4	1:B:707:G:H1	2.11	0.48
1:A:69:U:C2	1:A:70:A:C8	3.01	0.48
1:A:106:U:H2'	1:A:107:G:C1'	2.42	0.48
1:A:321:5MC:C2'	1:A:322:U:H5'	2.43	0.48
1:A:248:A:H2'	1:A:249:5MC:C6	2.48	0.48
1:A:334:U:H2'	1:A:335:5MC:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:A:H61	1:B:394:G:N2	2.11	0.48
1:A:340:G:N2	1:A:341:G:N7	2.61	0.48
1:A:639:5MC:H2'	1:A:640:A:C8	2.47	0.48
1:A:355:5MC:H2'	1:A:356:A:H8	1.78	0.48
1:B:230:A:H2'	1:B:231:A:O4'	2.13	0.48
1:B:400:G:H4'	1:B:707:G:O2'	2.13	0.48
1:B:125:A:O2'	1:B:126:U:O4'	2.31	0.48
1:B:571:U:H2'	1:B:572:A:H8	1.79	0.48
1:A:368:A:C4	1:A:369:5MC:HM52	2.49	0.48
1:A:181:A:O2'	1:A:182:U:P	2.72	0.48
1:A:640:A:H2	1:A:641:G:O6	1.97	0.48
1:B:94:U:H3	1:B:95:A:H62	1.62	0.48
1:B:130:5MC:HN41	1:B:275:G:H1	1.62	0.48
1:B:73:5MC:H4'	1:B:97:U:H5''	1.97	0.47
1:A:230:A:H2'	1:A:231:A:O4'	2.15	0.47
1:B:42:U:C4	1:B:43:U:C5	3.03	0.47
1:B:208:U:H2'	1:B:209:5MC:C6	2.49	0.47
1:B:256:A:N6	1:B:455:5MC:HM52	2.27	0.47
1:A:153:U:H2'	1:A:154:U:O4'	2.14	0.47
1:B:334:U:H2'	1:B:335:5MC:C6	2.50	0.47
1:B:69:U:C2	1:B:70:A:C8	3.02	0.47
1:B:497:A:H2'	1:B:498:5MC:C6	2.50	0.47
1:A:71:U:H2'	1:A:72:5MC:C6	2.49	0.47
1:A:476:G:C6	1:A:507:G:N2	2.83	0.47
1:A:628:U:P	1:A:639:5MC:H5'	2.55	0.47
1:A:94:U:H3	1:A:95:A:H62	1.63	0.46
1:B:634:G:O6	1:B:640:A:N6	2.49	0.46
1:B:676:U:H2'	1:B:677:G:C8	2.50	0.46
1:A:414:A:C2	1:A:415:G:N7	2.83	0.46
1:B:13:U:H2'	1:B:14:U:H6	1.81	0.46
1:B:405:5MC:HN41	1:B:624:G:H1	1.63	0.46
1:B:567:A:C8	1:B:568:5MC:HM52	2.50	0.46
1:B:682:5MC:OP2	1:B:693:5MC:H5''	2.14	0.46
1:A:19:U:H2'	1:A:20:G:H8	1.80	0.46
1:B:322:U:H2'	1:B:323:5MC:C6	2.51	0.46
1:B:248:A:H2'	1:B:249:5MC:C6	2.51	0.46
1:A:267:A:H2'	1:A:268:5MC:C6	2.50	0.46
1:A:322:U:H2'	1:A:323:5MC:C6	2.50	0.46
1:A:334:U:H2'	1:A:335:5MC:C6	2.51	0.46
1:B:319:A:C4	1:B:387:5MC:HM51	2.51	0.46
1:A:409:A:H2'	1:A:410:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:A:H2'	1:B:655:5MC:C6	2.51	0.46
1:A:368:A:C2	1:A:369:5MC:C4	3.04	0.46
1:A:630:G:H2'	1:A:631:5MC:H6	1.81	0.46
1:B:467:A:H2'	1:B:468:G:O4'	2.16	0.46
1:B:79:5MC:HN41	1:B:100:G:H1	1.64	0.46
1:A:697:A:H2'	1:A:698:5MC:C6	2.51	0.45
1:B:284:G:H3'	1:B:285:5MC:HM53	1.98	0.45
1:A:369:5MC:C5	1:A:370:5MC:HM51	2.52	0.45
1:A:76:5MC:H2'	1:A:77:G:C8	2.50	0.45
1:A:326:G:C6	1:A:388:G:C6	3.04	0.45
1:B:369:5MC:HM52	1:B:676:U:C5	2.51	0.45
1:A:660:G:C6	1:A:668:A:N6	2.85	0.45
1:B:243:G:H2'	1:B:244:G:O4'	2.16	0.45
1:B:355:5MC:H2'	1:B:356:A:H8	1.82	0.45
1:B:19:U:H2'	1:B:20:G:H8	1.81	0.45
1:B:267:A:H2'	1:B:268:5MC:C6	2.52	0.45
1:B:181:A:C2'	1:B:182:U:O5'	2.65	0.45
1:A:320:A:H2	1:A:387:5MC:HM52	1.82	0.45
1:A:400:G:H4'	1:A:707:G:O2'	2.17	0.45
1:A:405:5MC:HN41	1:A:624:G:H1	1.63	0.45
1:B:135:U:C2	1:B:136:G:C8	3.06	0.44
1:B:699:G:H2'	1:B:700:5MC:C6	2.52	0.44
1:B:414:A:C2	1:B:415:G:N7	2.85	0.44
1:B:108:U:H2'	1:B:109:G:C8	2.53	0.44
1:B:419:A:O2'	1:B:420:A:O4'	2.35	0.44
1:B:331:G:H2'	1:B:332:5MC:C6	2.53	0.44
1:B:301:U:C2	1:B:302:U:C5	3.06	0.44
1:B:602:U:H5''	1:B:631:5MC:O2'	2.18	0.44
1:B:16:A:N6	1:B:51:A:N6	2.65	0.44
1:B:38:G:H2'	1:B:39:5MC:C6	2.52	0.44
1:B:156:5MC:C6	1:B:157:5MC:HM52	2.53	0.44
1:B:310:G:H2'	1:B:311:G:H8	1.82	0.44
1:B:533:G:H2'	1:B:534:U:O4'	2.18	0.44
1:A:31:G:C2	1:A:529:A:C2	3.06	0.44
1:B:15:5MC:P	1:B:74:U:H2'	2.58	0.44
1:B:30:A:N1	1:B:523:5MC:HM52	2.32	0.44
1:B:368:A:C2	1:B:369:5MC:C4	3.06	0.44
1:B:381:5MC:HN41	1:B:397:G:H1	1.66	0.44
1:B:521:A:O3'	1:B:522:A:O4'	2.35	0.44
1:A:467:A:H2'	1:A:468:G:O4'	2.18	0.43
1:A:533:G:H2'	1:A:534:U:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:A:N3	1:B:487:A:H2'	2.33	0.43
1:A:13:U:H2'	1:A:14:U:H6	1.82	0.43
1:A:252:G:O6	1:A:267:A:C6	2.71	0.43
1:A:138:G:O6	1:A:150:A:N6	2.52	0.43
1:A:166:A:C6	1:A:176:G:O6	2.72	0.43
1:A:53:G:H1	1:A:72:5MC:HN41	1.66	0.43
1:A:132:A:N6	1:A:274:G:C6	2.86	0.43
1:B:309:U:C2	1:B:310:G:C8	3.07	0.43
1:B:409:A:H2'	1:B:410:G:O4'	2.19	0.43
1:B:706:G:O6	1:B:707:G:O6	2.36	0.43
1:A:248:A:H2'	1:A:249:5MC:H6	1.83	0.43
1:B:709:A:C2	1:B:710:G:N7	2.87	0.43
1:B:158:G:C6	1:B:243:G:O6	2.72	0.43
1:B:262:G:H1	1:B:455:5MC:N4	2.11	0.43
1:B:371:G:OP2	1:B:676:U:OP2	2.36	0.43
1:A:38:G:H2'	1:A:39:5MC:C6	2.54	0.43
1:A:685:G:O6	1:A:697:A:C6	2.71	0.43
1:A:497:A:H2'	1:A:498:5MC:C6	2.53	0.43
1:A:578:G:H2'	1:A:579:5MC:C6	2.54	0.43
1:B:12:A:H2'	1:B:13:U:O4'	2.19	0.43
1:B:181:A:HO2'	1:B:182:U:P	2.42	0.43
1:B:322:U:H4'	1:B:422:A:O2'	2.19	0.43
1:B:632:5MC:HM52	1:B:633:U:C5	2.54	0.43
1:A:16:A:N6	1:A:51:A:N6	2.66	0.43
1:A:326:G:C2	1:A:327:A:N7	2.86	0.43
1:B:311:G:H2'	1:B:312:A:C8	2.54	0.43
1:A:412:A:N6	1:A:435:G:O6	2.52	0.43
1:A:611:G:C2	1:A:612:A:N7	2.86	0.43
1:B:132:A:N6	1:B:274:G:C6	2.87	0.42
1:B:321:5MC:HM53	1:B:386:A:H2	1.83	0.42
1:B:419:A:H61	1:B:428:G:N2	2.17	0.42
1:B:630:G:C6	1:B:644:A:N6	2.87	0.42
1:A:161:5MC:H2'	1:A:162:A:H8	1.83	0.42
1:A:439:5MC:HN41	1:A:597:G:H1	1.66	0.42
1:A:570:G:H2'	1:A:571:U:C6	2.54	0.42
1:B:412:A:N6	1:B:435:G:C6	2.87	0.42
1:B:29:A:C5	1:B:523:5MC:C6	3.07	0.42
1:B:698:5MC:H2'	1:B:699:G:C8	2.54	0.42
1:A:81:A:N6	1:A:99:A:N6	2.66	0.42
1:B:81:A:N6	1:B:99:A:N6	2.68	0.42
1:B:181:A:O2'	1:B:182:U:P	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:G:C2	1:B:612:A:N7	2.88	0.42
1:A:18:A:H2'	1:A:19:U:C6	2.54	0.42
1:A:148:G:H2'	1:A:149:5MC:C6	2.54	0.42
1:A:566:G:C2	1:A:567:A:N7	2.87	0.42
1:B:52:G:H2'	1:B:53:G:O4'	2.20	0.42
1:B:64:G:C2	1:B:65:A:N7	2.88	0.42
1:A:372:5MC:N4	1:A:650:G:H1	2.18	0.42
1:A:575:G:O6	1:A:591:G:C6	2.73	0.42
1:B:225:G:C2	1:A:495:A:N1	2.87	0.42
1:B:541:A:H2'	1:B:542:U:O4'	2.19	0.42
1:A:577:U:C2	1:A:589:G:N2	2.88	0.42
1:B:452:G:C6	1:B:463:G:C6	3.07	0.42
1:A:333:A:H2'	1:A:334:U:C6	2.55	0.42
1:A:602:U:H5''	1:A:631:5MC:O2'	2.19	0.42
1:A:78:A:O2'	1:A:79:5MC:H5'	2.19	0.42
1:B:134:A:H2'	1:B:135:U:H6	1.85	0.42
1:B:575:G:O6	1:B:591:G:C6	2.72	0.42
1:A:100:G:H2'	1:A:101:U:O4'	2.20	0.42
1:A:612:A:C2	1:A:613:G:N7	2.88	0.42
1:B:478:A:H2'	1:B:479:A:C8	2.55	0.42
1:B:675:G:H5'	1:B:676:U:P	2.59	0.42
1:A:247:5MC:H2'	1:A:248:A:H8	1.85	0.42
1:A:586:G:H2'	1:A:587:5MC:C6	2.55	0.42
1:B:155:U:H1'	1:B:178:G:OP1	2.20	0.41
1:B:479:A:H2'	1:B:480:A:C8	2.55	0.41
1:B:623:G:H2'	1:B:624:G:O4'	2.20	0.41
1:A:17:G:C4	1:A:18:A:C8	3.08	0.41
1:A:77:G:C2	1:A:78:A:C8	3.08	0.41
1:A:640:A:N3	1:A:640:A:H2'	2.35	0.41
1:B:75:5MC:H2'	1:B:76:5MC:C6	2.55	0.41
1:B:285:5MC:HM52	1:B:286:A:C6	2.56	0.41
1:B:319:A:N6	1:B:327:A:H61	2.18	0.41
1:B:359:U:H2'	1:B:360:5MC:O4'	2.19	0.41
1:B:601:A:H1'	1:B:643:5MC:O2'	2.20	0.41
1:A:80:U:H4'	1:A:122:G:O2'	2.20	0.41
1:A:105:U:C2	1:A:106:U:C5	3.08	0.41
1:A:340:G:C2	1:A:341:G:N7	2.88	0.41
1:A:543:5MC:H4'	1:A:544:U:OP1	2.19	0.41
1:B:333:A:H2'	1:B:334:U:C6	2.56	0.41
1:B:398:U:H2'	1:B:399:5MC:C6	2.54	0.41
1:B:501:A:H2'	1:B:502:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:G:H2'	1:A:184:5MC:C6	2.55	0.41
1:A:240:A:H2'	1:A:241:5MC:C6	2.54	0.41
1:A:501:A:H2'	1:A:502:U:C6	2.55	0.41
1:B:640:A:C2	1:B:641:G:O6	2.72	0.41
1:A:219:5MC:H2'	1:A:220:G:C8	2.55	0.41
1:A:368:A:C6	1:A:709:A:N1	2.89	0.41
1:A:443:A:H2'	1:A:444:5MC:C6	2.56	0.41
1:A:452:G:C6	1:A:463:G:C6	3.08	0.41
1:A:701:U:O2	1:A:702:G:C8	2.73	0.41
1:B:129:5MC:N4	1:B:276:G:H1	2.17	0.41
1:B:513:U:C2	1:B:514:G:C8	3.08	0.41
1:A:156:5MC:HN41	1:A:244:G:H1	1.68	0.41
1:B:609:U:H2'	1:B:611:G:C6	2.55	0.41
1:B:612:A:C2	1:B:613:G:C5	3.08	0.41
1:A:66:A:H2'	1:A:67:5MC:C6	2.55	0.41
1:A:331:G:H2'	1:A:332:5MC:C6	2.56	0.41
1:B:77:G:C6	1:B:339:G:C6	3.09	0.41
1:B:326:G:C6	1:B:388:G:C6	3.08	0.41
1:B:612:A:C2	1:B:613:G:N7	2.88	0.41
1:A:154:U:O2'	1:A:155:U:C6	2.63	0.41
1:B:17:G:C4	1:B:18:A:C8	3.09	0.41
1:B:29:A:C4	1:B:523:5MC:C5	3.09	0.41
1:B:693:5MC:O5'	1:B:693:5MC:H6	2.03	0.41
1:A:77:G:C6	1:A:339:G:C6	3.09	0.41
1:A:145:G:H4'	1:A:167:A:OP1	2.20	0.41
1:A:208:U:H2'	1:A:209:5MC:C6	2.56	0.41
1:A:366:U:H2'	1:A:367:U:C6	2.56	0.41
1:A:557:G:H2'	1:A:558:5MC:O4'	2.19	0.41
1:B:368:A:N6	1:B:709:A:C6	2.88	0.41
1:B:452:G:H3'	1:B:453:A:H2'	2.03	0.41
1:B:452:G:H5''	1:B:453:A:OP2	2.21	0.41
1:B:639:5MC:C2	1:B:640:A:N7	2.89	0.41
1:B:57:5MC:H2'	1:B:58:G:C8	2.57	0.40
1:B:350:U:H2'	1:B:351:5MC:C6	2.56	0.40
1:B:584:G:H2'	1:B:585:5MC:O4'	2.21	0.40
1:A:478:A:H2'	1:A:479:A:H8	1.86	0.40
1:A:621:U:H3'	1:A:622:G:C5'	2.51	0.40
1:B:298:5MC:H2'	1:B:299:A:C8	2.56	0.40
1:B:310:G:O2'	1:B:311:G:O5'	2.39	0.40
1:B:471:U:H2'	1:B:472:U:C6	2.56	0.40
1:B:51:A:C2	1:B:52:G:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:5MC:H2'	1:B:162:A:C8	2.56	0.40
1:B:245:U:H2'	1:B:246:5MC:C6	2.56	0.40
1:B:529:A:H2'	1:B:530:U:C6	2.56	0.40
1:A:135:U:C2	1:A:136:G:C8	3.09	0.40
1:A:628:U:H2'	1:A:629:U:C6	2.56	0.40
1:B:68:G:C4	1:B:69:U:C5	3.10	0.40
1:A:161:5MC:H2'	1:A:162:A:C8	2.57	0.40
1:A:521:A:O3'	1:A:522:A:O4'	2.39	0.40
1:B:105:U:C2	1:B:106:U:C5	3.10	0.40
1:B:176:G:H2'	1:B:177:G:O4'	2.20	0.40
1:B:640:A:H2'	1:B:640:A:N3	2.36	0.40
1:A:177:G:C2	1:A:178:G:N7	2.89	0.40
1:A:645:A:H2'	1:A:646:U:C6	2.57	0.40
1:A:647:5MC:N4	1:A:648:G:C8	2.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	719/720 (99%)	126 (17%)	8 (1%)
1	B	719/720 (99%)	135 (18%)	10 (1%)
All	All	1438/1440 (99%)	261 (18%)	18 (1%)

All (261) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	7	G
1	B	15	5MC

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Mol	Chain	Res	Type
1	B	16	A
1	B	29	A
1	B	30	A
1	B	31	G
1	B	37	A
1	B	38	G
1	B	43	U
1	B	44	U
1	B	50	U
1	B	52	G
1	B	62	U
1	B	63	5MC
1	B	70	A
1	B	74	U
1	B	75	5MC
1	B	84	U
1	B	85	G
1	B	90	5MC
1	B	91	G
1	B	92	U
1	B	95	A
1	B	99	A
1	B	102	G
1	B	103	5MC
1	B	107	G
1	B	116	U
1	B	117	5MC
1	B	119	G
1	B	124	5MC
1	B	129	5MC
1	B	131	5MC
1	B	143	U
1	B	144	5MC
1	B	146	G
1	B	154	U
1	B	155	U
1	B	166	A
1	B	170	U
1	B	171	5MC
1	B	173	5MC
1	B	177	G
1	B	178	G

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Mol	Chain	Res	Type
1	B	182	U
1	B	183	G
1	B	185	G
1	B	186	G
1	B	197	U
1	B	198	5MC
1	B	221	A
1	B	223	A
1	B	225	G
1	B	241	5MC
1	B	242	5MC
1	B	243	G
1	B	250	G
1	B	256	A
1	B	257	A
1	B	274	G
1	B	284	G
1	B	288	A
1	B	289	G
1	B	299	A
1	B	306	G
1	B	310	G
1	B	311	G
1	B	319	A
1	B	320	A
1	B	321	5MC
1	B	322	U
1	B	334	U
1	B	338	5MC
1	B	343	A
1	B	367	U
1	B	368	A
1	B	369	5MC
1	B	370	5MC
1	B	371	G
1	B	378	5MC
1	B	379	G
1	B	385	A
1	B	386	A
1	B	387	5MC
1	B	388	G
1	B	393	A

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Mol	Chain	Res	Type
1	B	419	A
1	B	420	A
1	B	424	5MC
1	B	435	G
1	B	436	5MC
1	B	438	5MC
1	B	447	U
1	B	453	A
1	B	454	A
1	B	455	5MC
1	B	473	5MC
1	B	476	G
1	B	507	G
1	B	522	A
1	B	523	5MC
1	B	540	5MC
1	B	543	5MC
1	B	544	U
1	B	545	U
1	B	555	U
1	B	556	5MC
1	B	557	G
1	B	566	G
1	B	569	G
1	B	582	U
1	B	583	5MC
1	B	584	G
1	B	585	5MC
1	B	594	A
1	B	595	G
1	B	601	A
1	B	609	U
1	B	610	5MC
1	B	612	A
1	B	623	G
1	B	634	G
1	B	636	U
1	B	637	5MC
1	B	639	5MC
1	B	648	G
1	B	649	G
1	B	663	U

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Mol	Chain	Res	Type
1	B	664	5MC
1	B	676	U
1	B	684	U
1	B	691	5MC
1	B	702	G
1	B	706	G
1	B	707	G
1	A	15	5MC
1	A	16	A
1	A	29	A
1	A	30	A
1	A	31	G
1	A	37	A
1	A	38	G
1	A	43	U
1	A	44	U
1	A	50	U
1	A	62	U
1	A	63	5MC
1	A	74	U
1	A	75	5MC
1	A	80	U
1	A	84	U
1	A	85	G
1	A	90	5MC
1	A	91	G
1	A	92	U
1	A	95	A
1	A	99	A
1	A	102	G
1	A	107	G
1	A	116	U
1	A	117	5MC
1	A	119	G
1	A	131	5MC
1	A	143	U
1	A	144	5MC
1	A	146	G
1	A	154	U
1	A	155	U
1	A	156	5MC
1	A	161	5MC

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Mol	Chain	Res	Type
1	A	170	U
1	A	171	5MC
1	A	173	5MC
1	A	182	U
1	A	183	G
1	A	185	G
1	A	186	G
1	A	197	U
1	A	198	5MC
1	A	223	A
1	A	225	G
1	A	242	5MC
1	A	250	G
1	A	256	A
1	A	257	A
1	A	274	G
1	A	284	G
1	A	287	A
1	A	288	A
1	A	289	G
1	A	299	A
1	A	306	G
1	A	311	G
1	A	312	A
1	A	319	A
1	A	320	A
1	A	321	5MC
1	A	322	U
1	A	334	U
1	A	342	G
1	A	343	A
1	A	368	A
1	A	369	5MC
1	A	370	5MC
1	A	371	G
1	A	378	5MC
1	A	379	G
1	A	385	A
1	A	387	5MC
1	A	388	G
1	A	393	A
1	A	424	5MC

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Mol	Chain	Res	Type
1	A	435	G
1	A	436	5MC
1	A	438	5MC
1	A	447	U
1	A	453	A
1	A	454	A
1	A	455	5MC
1	A	473	5MC
1	A	475	G
1	A	476	G
1	A	488	A
1	A	507	G
1	A	522	A
1	A	523	5MC
1	A	540	5MC
1	A	543	5MC
1	A	544	U
1	A	545	U
1	A	555	U
1	A	556	5MC
1	A	557	G
1	A	569	G
1	A	583	5MC
1	A	584	G
1	A	585	5MC
1	A	594	A
1	A	595	G
1	A	601	A
1	A	609	U
1	A	610	5MC
1	A	612	A
1	A	622	G
1	A	623	G
1	A	634	G
1	A	636	U
1	A	637	5MC
1	A	639	5MC
1	A	648	G
1	A	649	G
1	A	660	G
1	A	663	U
1	A	664	5MC

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Mol	Chain	Res	Type
1	A	666	U
1	A	676	U
1	A	684	U
1	A	691	5MC
1	A	692	G
1	A	706	G
1	A	707	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	181	A
1	B	255	A
1	B	298	5MC
1	B	319	A
1	B	333	A
1	B	378	5MC
1	B	419	A
1	B	472	U
1	B	584	G
1	B	675	G
1	A	181	A
1	A	255	A
1	A	298	5MC
1	A	319	A
1	A	333	A
1	A	378	5MC
1	A	472	U
1	A	543	5MC

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

358 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	5MC	B	268	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	B	469	1	19,22,23	0.26	0	26,32,35	0.42	0
1	5MC	A	473	1	19,22,23	0.28	0	26,32,35	0.41	0
1	5MC	A	511	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	679	1	19,22,23	0.27	0	26,32,35	0.45	0
1	5MC	B	26	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	378	1	19,22,23	0.27	0	26,32,35	0.71	1 (3%)
1	5MC	A	57	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	90	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	B	558	1	19,22,23	0.28	0	26,32,35	0.41	0
1	5MC	B	523	1	19,22,23	0.36	0	26,32,35	0.59	0
1	5MC	B	246	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	A	384	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	117	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	328	1	19,22,23	0.34	0	26,32,35	0.48	0
1	5MC	B	210	1	19,22,23	0.32	0	26,32,35	0.49	0
1	5MC	B	21	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	693	1	19,22,23	0.26	0	26,32,35	0.42	0
1	5MC	A	332	1	19,22,23	0.26	0	26,32,35	0.45	0
1	5MC	B	556	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	B	643	1	19,22,23	0.31	0	26,32,35	0.41	0
1	5MC	A	25	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	B	444	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	370	1	19,22,23	0.31	0	26,32,35	0.52	0
1	5MC	B	587	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	B	498	1	19,22,23	0.24	0	26,32,35	0.44	0
1	5MC	A	536	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	A	620	1	19,22,23	0.29	0	26,32,35	0.41	0
1	5MC	A	387	1	19,22,23	0.31	0	26,32,35	0.54	0
1	5MC	B	360	1	19,22,23	0.32	0	26,32,35	0.44	0
1	5MC	A	639	1	19,22,23	0.28	0	26,32,35	0.40	0
1	5MC	B	79	1	19,22,23	0.30	0	26,32,35	0.52	0
1	5MC	B	600	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	219	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	349	1	19,22,23	0.33	0	26,32,35	0.46	0
1	5MC	A	21	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	691	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	149	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	188	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	B	550	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	604	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	667	1	19,22,23	0.30	0	26,32,35	0.42	0
1	5MC	A	614	1	19,22,23	0.24	0	26,32,35	0.47	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	455	1	19,22,23	0.28	0	26,32,35	0.57	0
1	5MC	B	10	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	63	1	19,22,23	0.27	0	26,32,35	0.45	0
1	5MC	B	232	1	19,22,23	0.30	0	26,32,35	0.46	0
1	5MC	A	39	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	249	1	19,22,23	0.28	0	26,32,35	0.41	0
1	5MC	B	165	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	455	1	19,22,23	0.26	0	26,32,35	0.58	0
1	5MC	B	652	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	462	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	B	151	1	19,22,23	0.28	0	26,32,35	0.44	0
1	5MC	A	139	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	585	1	19,22,23	0.27	0	26,32,35	0.44	0
1	5MC	B	565	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	A	206	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	B	568	1	19,22,23	0.29	0	26,32,35	0.49	0
1	5MC	B	583	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	369	1	19,22,23	0.25	0	26,32,35	0.48	0
1	5MC	A	417	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	B	438	1	19,22,23	0.28	0	26,32,35	0.46	0
1	5MC	A	418	1	19,22,23	0.27	0	26,32,35	0.42	0
1	5MC	A	647	1	19,22,23	0.40	0	26,32,35	0.55	0
1	5MC	A	28	1	19,22,23	0.24	0	26,32,35	0.45	0
1	5MC	A	268	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	625	1	19,22,23	0.31	0	26,32,35	0.43	0
1	5MC	B	28	1	19,22,23	0.22	0	26,32,35	0.45	0
1	5MC	B	372	1	19,22,23	0.25	0	26,32,35	0.43	0
1	5MC	B	241	1	19,22,23	0.26	0	26,32,35	0.45	0
1	5MC	B	129	1	19,22,23	0.26	0	26,32,35	0.42	0
1	5MC	A	631	1	19,22,23	0.31	0	26,32,35	0.43	0
1	5MC	A	279	1	19,22,23	0.31	0	26,32,35	0.43	0
1	5MC	B	254	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	A	494	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	124	1	19,22,23	0.25	0	26,32,35	0.49	0
1	5MC	A	523	1	19,22,23	0.58	1 (5%)	26,32,35	0.67	0
1	5MC	A	212	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	A	210	1	19,22,23	0.31	0	26,32,35	0.46	0
1	5MC	B	407	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	511	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	76	1	19,22,23	0.30	0	26,32,35	0.47	0
1	5MC	B	620	1	19,22,23	0.29	0	26,32,35	0.41	0
1	5MC	B	486	1	19,22,23	0.32	0	26,32,35	0.46	0
1	5MC	A	446	1	19,22,23	0.29	0	26,32,35	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	682	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	A	372	1	19,22,23	0.25	0	26,32,35	0.43	0
1	5MC	A	249	1	19,22,23	0.27	0	26,32,35	0.41	0
1	5MC	B	592	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	A	528	1	19,22,23	0.30	0	26,32,35	0.42	0
1	5MC	A	73	1	19,22,23	0.30	0	26,32,35	0.48	0
1	5MC	A	382	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	130	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	565	1	19,22,23	0.31	0	26,32,35	0.45	0
1	5MC	B	353	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	387	1	19,22,23	0.27	0	26,32,35	0.54	0
1	5MC	B	604	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	568	1	19,22,23	0.24	0	26,32,35	0.45	0
1	5MC	A	34	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	B	335	1	19,22,23	0.32	0	26,32,35	0.43	0
1	5MC	B	114	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	406	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	704	1	19,22,23	0.33	0	26,32,35	0.49	0
1	5MC	B	218	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	417	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	39	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	232	1	19,22,23	0.30	0	26,32,35	0.46	0
1	5MC	A	383	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	426	1	19,22,23	0.29	0	26,32,35	0.45	0
1	5MC	A	657	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	370	1	19,22,23	0.31	0	26,32,35	0.47	0
1	5MC	A	458	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	399	1	19,22,23	0.31	0	26,32,35	0.45	0
1	5MC	B	201	1	19,22,23	0.31	0	26,32,35	0.47	0
1	5MC	B	439	1	19,22,23	0.27	0	26,32,35	0.42	0
1	5MC	B	171	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	548	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	10	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	285	1	19,22,23	0.33	0	26,32,35	0.48	0
1	5MC	A	241	1	19,22,23	0.25	0	26,32,35	0.45	0
1	5MC	B	349	1	19,22,23	0.32	0	26,32,35	0.44	0
1	5MC	B	355	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	B	528	1	19,22,23	0.27	0	26,32,35	0.41	0
1	5MC	B	198	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	B	691	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	234	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	96	1	19,22,23	0.32	0	26,32,35	0.47	0
1	5MC	A	246	1	19,22,23	0.29	0	26,32,35	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	B	96	1	19,22,23	0.32	0	26,32,35	0.47	0
1	5MC	A	360	1	19,22,23	0.32	0	26,32,35	0.44	0
1	5MC	B	614	1	19,22,23	0.23	0	26,32,35	0.46	0
1	5MC	B	373	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	149	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	651	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	B	57	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	651	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	B	369	1	19,22,23	0.22	0	26,32,35	0.44	0
1	5MC	B	698	1	19,22,23	0.33	0	26,32,35	0.44	0
1	5MC	A	637	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	B	298	1	19,22,23	0.30	0	26,32,35	0.66	1 (3%)
1	5MC	A	486	1	19,22,23	0.33	0	26,32,35	0.49	0
1	5MC	B	506	1	19,22,23	0.26	0	26,32,35	0.41	0
1	5MC	A	477	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	B	474	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	548	1	19,22,23	0.28	0	26,32,35	0.44	0
1	5MC	A	425	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	B	425	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	161	1	19,22,23	0.32	0	26,32,35	0.40	0
1	5MC	A	104	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	451	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	304	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	131	1	19,22,23	0.31	0	26,32,35	0.45	0
1	5MC	A	67	1	19,22,23	0.27	0	26,32,35	0.43	0
1	5MC	B	441	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	B	212	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	184	1	19,22,23	0.29	0	26,32,35	0.45	0
1	5MC	A	459	1	19,22,23	0.31	0	26,32,35	0.45	0
1	5MC	B	354	1	19,22,23	0.29	0	26,32,35	0.42	0
1	5MC	B	139	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	518	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	550	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	111	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	492	1	19,22,23	0.33	0	26,32,35	0.42	0
1	5MC	B	15	1	19,22,23	0.23	0	26,32,35	0.52	0
1	5MC	B	304	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	679	1	19,22,23	0.29	0	26,32,35	0.47	0
1	5MC	A	543	1	19,22,23	0.34	0	26,32,35	0.50	0
1	5MC	B	49	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	B	140	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	110	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	173	1	19,22,23	0.27	0	26,32,35	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	363	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	700	1	19,22,23	0.27	0	26,32,35	0.43	0
1	5MC	B	144	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	114	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	73	1	19,22,23	0.30	0	26,32,35	0.48	0
1	5MC	B	362	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	130	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	655	1	19,22,23	0.27	0	26,32,35	0.44	0
1	5MC	B	406	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	512	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	315	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	384	1	19,22,23	0.31	0	26,32,35	0.46	0
1	5MC	A	198	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	B	117	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	B	328	1	19,22,23	0.31	0	26,32,35	0.48	0
1	5MC	A	587	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	A	698	1	19,22,23	0.37	0	26,32,35	0.50	0
1	5MC	A	124	1	19,22,23	0.31	0	26,32,35	0.45	0
1	5MC	B	120	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	583	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	161	1	19,22,23	0.29	0	26,32,35	0.41	0
1	5MC	B	323	1	19,22,23	0.29	0	26,32,35	0.46	0
1	5MC	B	282	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	438	1	19,22,23	0.28	0	26,32,35	0.46	0
1	5MC	B	46	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	316	1	19,22,23	0.30	0	26,32,35	0.46	0
1	5MC	A	184	1	19,22,23	0.30	0	26,32,35	0.41	0
1	5MC	A	474	1	19,22,23	0.32	0	26,32,35	0.46	0
1	5MC	A	444	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	A	498	1	19,22,23	0.26	0	26,32,35	0.43	0
1	5MC	A	576	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	411	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	B	247	1	19,22,23	0.30	0	26,32,35	0.46	0
1	5MC	B	657	1	19,22,23	0.30	0	26,32,35	0.42	0
1	5MC	B	157	1	19,22,23	0.31	0	26,32,35	0.45	0
1	5MC	B	632	1	19,22,23	0.34	0	26,32,35	0.54	0
1	5MC	B	459	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	B	551	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	603	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	201	1	19,22,23	0.31	0	26,32,35	0.47	0
1	5MC	A	63	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	B	631	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	381	1	19,22,23	0.29	0	26,32,35	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	652	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	129	1	19,22,23	0.26	0	26,32,35	0.41	0
1	5MC	B	477	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	A	517	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	A	218	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	B	383	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	171	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	110	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	46	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	103	1	19,22,23	0.26	0	26,32,35	0.44	0
1	5MC	B	585	1	19,22,23	0.25	0	26,32,35	0.41	0
1	5MC	B	363	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	424	1	19,22,23	0.27	0	26,32,35	0.47	0
1	5MC	A	144	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	362	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	700	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	15	1	19,22,23	0.22	0	26,32,35	0.53	0
1	5MC	B	72	1	19,22,23	0.27	0	26,32,35	0.44	0
1	5MC	B	104	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	664	1	19,22,23	0.29	0	26,32,35	0.45	0
1	5MC	A	282	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	A	308	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	156	1	19,22,23	0.29	0	26,32,35	0.42	0
1	5MC	B	405	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	75	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	140	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	316	1	19,22,23	0.31	0	26,32,35	0.46	0
1	5MC	B	492	1	19,22,23	0.30	0	26,32,35	0.42	0
1	5MC	A	600	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	354	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	103	1	19,22,23	0.27	0	26,32,35	0.44	0
1	5MC	A	655	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	B	440	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	157	1	19,22,23	0.30	0	26,32,35	0.42	0
1	5MC	A	540	1	19,22,23	0.27	0	26,32,35	0.47	0
1	5MC	A	315	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	579	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	564	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	B	465	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	B	338	1	19,22,23	0.29	0	26,32,35	0.48	0
1	5MC	A	574	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	B	67	1	19,22,23	0.24	0	26,32,35	0.44	0
1	5MC	B	446	1	19,22,23	0.29	0	26,32,35	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	B	682	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	B	610	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	351	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	A	254	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	A	335	1	19,22,23	0.32	0	26,32,35	0.42	0
1	5MC	A	704	1	19,22,23	0.32	0	26,32,35	0.48	0
1	5MC	A	325	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	382	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	407	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	34	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	B	517	1	19,22,23	0.29	0	26,32,35	0.42	0
1	5MC	A	426	1	19,22,23	0.29	0	26,32,35	0.46	0
1	5MC	A	79	1	19,22,23	0.30	0	26,32,35	0.52	0
1	5MC	B	242	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	B	543	1	19,22,23	0.28	0	26,32,35	0.46	0
1	5MC	B	164	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	399	1	19,22,23	0.31	0	26,32,35	0.45	0
1	5MC	B	424	1	19,22,23	0.27	0	26,32,35	0.46	0
1	5MC	B	436	1	19,22,23	0.29	0	26,32,35	0.45	0
1	5MC	A	632	1	19,22,23	0.36	0	26,32,35	0.56	0
1	5MC	A	164	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	564	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	B	603	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	576	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	353	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	90	1	19,22,23	0.28	0	26,32,35	0.46	0
1	5MC	A	321	1	19,22,23	0.27	0	26,32,35	0.51	0
1	5MC	A	323	1	19,22,23	0.29	0	26,32,35	0.46	0
1	5MC	B	667	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	411	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	451	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	462	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	165	1	19,22,23	0.31	0	26,32,35	0.47	0
1	5MC	B	234	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	473	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	308	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	373	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	173	1	19,22,23	0.26	0	26,32,35	0.40	0
1	5MC	B	75	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	556	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	72	1	19,22,23	0.29	0	26,32,35	0.45	0
1	5MC	A	439	1	19,22,23	0.26	0	26,32,35	0.44	0
1	5MC	B	332	1	19,22,23	0.25	0	26,32,35	0.46	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	512	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	285	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	338	1	19,22,23	0.32	0	26,32,35	0.47	0
1	5MC	A	355	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	405	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	26	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	B	637	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	378	1	19,22,23	0.26	0	26,32,35	0.70	1 (3%)
1	5MC	A	551	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	A	120	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	A	219	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	A	558	1	19,22,23	0.29	0	26,32,35	0.41	0
1	5MC	A	156	1	19,22,23	0.29	0	26,32,35	0.42	0
1	5MC	B	321	1	19,22,23	0.32	0	26,32,35	0.40	0
1	5MC	A	441	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	579	1	19,22,23	0.27	0	26,32,35	0.44	0
1	5MC	A	440	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	381	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	643	1	19,22,23	0.29	0	26,32,35	0.42	0
1	5MC	B	404	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	A	247	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	A	592	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	B	664	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	B	639	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	B	325	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	494	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	206	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	A	209	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	B	25	1	19,22,23	0.29	0	26,32,35	0.43	0
1	5MC	A	298	1	19,22,23	0.29	0	26,32,35	0.64	1 (3%)
1	5MC	A	506	1	19,22,23	0.24	0	26,32,35	0.42	0
1	5MC	B	209	1	19,22,23	0.28	0	26,32,35	0.43	0
1	5MC	A	610	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	131	1	19,22,23	0.31	0	26,32,35	0.46	0
1	5MC	A	151	1	19,22,23	0.28	0	26,32,35	0.44	0
1	5MC	A	111	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	A	436	1	19,22,23	0.28	0	26,32,35	0.47	0
1	5MC	B	540	1	19,22,23	0.29	0	26,32,35	0.44	0
1	5MC	B	536	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	A	469	1	19,22,23	0.25	0	26,32,35	0.43	0
1	5MC	B	491	1	19,22,23	0.28	0	26,32,35	0.45	0
1	5MC	A	49	1	19,22,23	0.33	0	26,32,35	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	B	574	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	A	242	1	19,22,23	0.29	0	26,32,35	0.42	0
1	5MC	B	351	1	19,22,23	0.32	0	26,32,35	0.43	0
1	5MC	A	404	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	B	418	1	19,22,23	0.28	0	26,32,35	0.42	0
1	5MC	A	465	1	19,22,23	0.31	0	26,32,35	0.44	0
1	5MC	B	188	1	19,22,23	0.30	0	26,32,35	0.44	0
1	5MC	B	693	1	19,22,23	0.21	0	26,32,35	0.43	0
1	5MC	A	76	1	19,22,23	0.30	0	26,32,35	0.45	0
1	5MC	B	518	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	625	1	19,22,23	0.31	0	26,32,35	0.43	0
1	5MC	B	279	1	19,22,23	0.31	0	26,32,35	0.43	0
1	5MC	B	458	1	19,22,23	0.30	0	26,32,35	0.43	0
1	5MC	B	647	1	19,22,23	0.35	0	26,32,35	0.53	0
1	5MC	A	491	1	19,22,23	0.28	0	26,32,35	0.44	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
1	5MC	B	268	1	-	0/7/25/26	0/2/2/2
1	5MC	B	469	1	-	0/7/25/26	0/2/2/2
1	5MC	A	473	1	-	0/7/25/26	0/2/2/2
1	5MC	A	511	1	-	1/7/25/26	0/2/2/2
1	5MC	B	679	1	-	0/7/25/26	0/2/2/2
1	5MC	B	26	1	-	0/7/25/26	0/2/2/2
1	5MC	B	378	1	-	2/7/25/26	0/2/2/2
1	5MC	A	57	1	-	1/7/25/26	0/2/2/2
1	5MC	B	90	1	-	2/7/25/26	0/2/2/2
1	5MC	B	558	1	-	1/7/25/26	0/2/2/2
1	5MC	B	523	1	-	1/7/25/26	0/2/2/2
1	5MC	B	246	1	-	0/7/25/26	0/2/2/2
1	5MC	A	384	1	-	0/7/25/26	0/2/2/2
1	5MC	A	117	1	-	2/7/25/26	0/2/2/2
1	5MC	A	328	1	-	0/7/25/26	0/2/2/2
1	5MC	B	210	1	-	0/7/25/26	0/2/2/2
1	5MC	B	21	1	-	0/7/25/26	0/2/2/2
1	5MC	A	693	1	-	2/7/25/26	0/2/2/2
1	5MC	A	332	1	-	0/7/25/26	0/2/2/2
1	5MC	B	556	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	B	643	1	-	0/7/25/26	0/2/2/2
1	5MC	A	25	1	-	1/7/25/26	0/2/2/2
1	5MC	B	444	1	-	0/7/25/26	0/2/2/2
1	5MC	A	370	1	-	2/7/25/26	0/2/2/2
1	5MC	B	587	1	-	2/7/25/26	0/2/2/2
1	5MC	B	498	1	-	0/7/25/26	0/2/2/2
1	5MC	A	536	1	-	0/7/25/26	0/2/2/2
1	5MC	A	620	1	-	2/7/25/26	0/2/2/2
1	5MC	A	387	1	-	0/7/25/26	0/2/2/2
1	5MC	B	360	1	-	0/7/25/26	0/2/2/2
1	5MC	A	639	1	-	3/7/25/26	0/2/2/2
1	5MC	B	79	1	-	1/7/25/26	0/2/2/2
1	5MC	B	600	1	-	0/7/25/26	0/2/2/2
1	5MC	B	219	1	-	0/7/25/26	0/2/2/2
1	5MC	A	349	1	-	0/7/25/26	0/2/2/2
1	5MC	A	21	1	-	0/7/25/26	0/2/2/2
1	5MC	A	691	1	-	2/7/25/26	0/2/2/2
1	5MC	A	149	1	-	0/7/25/26	0/2/2/2
1	5MC	A	188	1	-	0/7/25/26	0/2/2/2
1	5MC	B	550	1	-	0/7/25/26	0/2/2/2
1	5MC	A	604	1	-	0/7/25/26	0/2/2/2
1	5MC	A	667	1	-	1/7/25/26	0/2/2/2
1	5MC	A	614	1	-	0/7/25/26	0/2/2/2
1	5MC	A	455	1	-	1/7/25/26	0/2/2/2
1	5MC	B	10	1	-	0/7/25/26	0/2/2/2
1	5MC	B	63	1	-	2/7/25/26	0/2/2/2
1	5MC	B	232	1	-	0/7/25/26	0/2/2/2
1	5MC	A	39	1	-	0/7/25/26	0/2/2/2
1	5MC	B	249	1	-	0/7/25/26	0/2/2/2
1	5MC	B	165	1	-	1/7/25/26	0/2/2/2
1	5MC	B	455	1	-	1/7/25/26	0/2/2/2
1	5MC	B	652	1	-	0/7/25/26	0/2/2/2
1	5MC	A	462	1	-	0/7/25/26	0/2/2/2
1	5MC	B	151	1	-	1/7/25/26	0/2/2/2
1	5MC	A	139	1	-	1/7/25/26	0/2/2/2
1	5MC	A	585	1	-	1/7/25/26	0/2/2/2
1	5MC	B	565	1	-	0/7/25/26	0/2/2/2
1	5MC	A	206	1	-	1/7/25/26	0/2/2/2
1	5MC	B	568	1	-	0/7/25/26	0/2/2/2
1	5MC	B	583	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	369	1	-	2/7/25/26	0/2/2/2
1	5MC	A	417	1	-	0/7/25/26	0/2/2/2
1	5MC	B	438	1	-	3/7/25/26	0/2/2/2
1	5MC	A	418	1	-	1/7/25/26	0/2/2/2
1	5MC	A	647	1	-	0/7/25/26	0/2/2/2
1	5MC	A	28	1	-	0/7/25/26	0/2/2/2
1	5MC	A	268	1	-	0/7/25/26	0/2/2/2
1	5MC	A	625	1	-	0/7/25/26	0/2/2/2
1	5MC	B	28	1	-	0/7/25/26	0/2/2/2
1	5MC	B	372	1	-	0/7/25/26	0/2/2/2
1	5MC	B	241	1	-	2/7/25/26	0/2/2/2
1	5MC	B	129	1	-	2/7/25/26	0/2/2/2
1	5MC	A	631	1	-	0/7/25/26	0/2/2/2
1	5MC	A	279	1	-	0/7/25/26	0/2/2/2
1	5MC	B	254	1	-	0/7/25/26	0/2/2/2
1	5MC	A	494	1	-	0/7/25/26	0/2/2/2
1	5MC	B	124	1	-	3/7/25/26	0/2/2/2
1	5MC	A	523	1	-	2/7/25/26	0/2/2/2
1	5MC	A	212	1	-	0/7/25/26	0/2/2/2
1	5MC	A	210	1	-	0/7/25/26	0/2/2/2
1	5MC	B	407	1	-	0/7/25/26	0/2/2/2
1	5MC	B	511	1	-	2/7/25/26	0/2/2/2
1	5MC	B	76	1	-	0/7/25/26	0/2/2/2
1	5MC	B	620	1	-	2/7/25/26	0/2/2/2
1	5MC	B	486	1	-	0/7/25/26	0/2/2/2
1	5MC	A	446	1	-	0/7/25/26	0/2/2/2
1	5MC	A	682	1	-	1/7/25/26	0/2/2/2
1	5MC	A	372	1	-	0/7/25/26	0/2/2/2
1	5MC	A	249	1	-	0/7/25/26	0/2/2/2
1	5MC	B	592	1	-	0/7/25/26	0/2/2/2
1	5MC	A	528	1	-	0/7/25/26	0/2/2/2
1	5MC	A	73	1	-	0/7/25/26	0/2/2/2
1	5MC	A	382	1	-	0/7/25/26	0/2/2/2
1	5MC	A	130	1	-	0/7/25/26	0/2/2/2
1	5MC	A	565	1	-	0/7/25/26	0/2/2/2
1	5MC	B	353	1	-	1/7/25/26	0/2/2/2
1	5MC	B	387	1	-	2/7/25/26	0/2/2/2
1	5MC	B	604	1	-	1/7/25/26	0/2/2/2
1	5MC	A	568	1	-	0/7/25/26	0/2/2/2
1	5MC	A	34	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	B	335	1	-	0/7/25/26	0/2/2/2
1	5MC	B	114	1	-	0/7/25/26	0/2/2/2
1	5MC	A	406	1	-	0/7/25/26	0/2/2/2
1	5MC	B	704	1	-	0/7/25/26	0/2/2/2
1	5MC	B	218	1	-	0/7/25/26	0/2/2/2
1	5MC	B	417	1	-	0/7/25/26	0/2/2/2
1	5MC	B	39	1	-	0/7/25/26	0/2/2/2
1	5MC	A	232	1	-	0/7/25/26	0/2/2/2
1	5MC	A	383	1	-	0/7/25/26	0/2/2/2
1	5MC	B	426	1	-	2/7/25/26	0/2/2/2
1	5MC	A	657	1	-	0/7/25/26	0/2/2/2
1	5MC	B	370	1	-	2/7/25/26	0/2/2/2
1	5MC	A	458	1	-	1/7/25/26	0/2/2/2
1	5MC	B	399	1	-	0/7/25/26	0/2/2/2
1	5MC	B	201	1	-	0/7/25/26	0/2/2/2
1	5MC	B	439	1	-	0/7/25/26	0/2/2/2
1	5MC	B	171	1	-	2/7/25/26	0/2/2/2
1	5MC	A	548	1	-	0/7/25/26	0/2/2/2
1	5MC	A	10	1	-	0/7/25/26	0/2/2/2
1	5MC	B	285	1	-	0/7/25/26	0/2/2/2
1	5MC	A	241	1	-	2/7/25/26	0/2/2/2
1	5MC	B	349	1	-	0/7/25/26	0/2/2/2
1	5MC	B	355	1	-	0/7/25/26	0/2/2/2
1	5MC	B	528	1	-	1/7/25/26	0/2/2/2
1	5MC	B	198	1	-	6/7/25/26	0/2/2/2
1	5MC	B	691	1	-	2/7/25/26	0/2/2/2
1	5MC	A	234	1	-	0/7/25/26	0/2/2/2
1	5MC	A	96	1	-	0/7/25/26	0/2/2/2
1	5MC	A	246	1	-	0/7/25/26	0/2/2/2
1	5MC	B	96	1	-	0/7/25/26	0/2/2/2
1	5MC	A	360	1	-	0/7/25/26	0/2/2/2
1	5MC	B	614	1	-	0/7/25/26	0/2/2/2
1	5MC	B	373	1	-	1/7/25/26	0/2/2/2
1	5MC	B	149	1	-	0/7/25/26	0/2/2/2
1	5MC	A	651	1	-	0/7/25/26	0/2/2/2
1	5MC	B	57	1	-	1/7/25/26	0/2/2/2
1	5MC	B	651	1	-	0/7/25/26	0/2/2/2
1	5MC	B	369	1	-	2/7/25/26	0/2/2/2
1	5MC	B	698	1	-	0/7/25/26	0/2/2/2
1	5MC	A	637	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	B	298	1	-	0/7/25/26	0/2/2/2
1	5MC	A	486	1	-	0/7/25/26	0/2/2/2
1	5MC	B	506	1	-	2/7/25/26	0/2/2/2
1	5MC	A	477	1	-	1/7/25/26	0/2/2/2
1	5MC	B	474	1	-	1/7/25/26	0/2/2/2
1	5MC	B	548	1	-	0/7/25/26	0/2/2/2
1	5MC	A	425	1	-	0/7/25/26	0/2/2/2
1	5MC	B	425	1	-	0/7/25/26	0/2/2/2
1	5MC	B	161	1	-	2/7/25/26	0/2/2/2
1	5MC	A	104	1	-	2/7/25/26	0/2/2/2
1	5MC	B	451	1	-	0/7/25/26	0/2/2/2
1	5MC	A	304	1	-	0/7/25/26	0/2/2/2
1	5MC	B	131	1	-	2/7/25/26	0/2/2/2
1	5MC	A	67	1	-	0/7/25/26	0/2/2/2
1	5MC	B	441	1	-	1/7/25/26	0/2/2/2
1	5MC	B	212	1	-	2/7/25/26	0/2/2/2
1	5MC	B	184	1	-	2/7/25/26	0/2/2/2
1	5MC	A	459	1	-	0/7/25/26	0/2/2/2
1	5MC	B	354	1	-	0/7/25/26	0/2/2/2
1	5MC	B	139	1	-	1/7/25/26	0/2/2/2
1	5MC	A	518	1	-	0/7/25/26	0/2/2/2
1	5MC	A	550	1	-	0/7/25/26	0/2/2/2
1	5MC	B	111	1	-	0/7/25/26	0/2/2/2
1	5MC	A	492	1	-	0/7/25/26	0/2/2/2
1	5MC	B	15	1	-	2/7/25/26	0/2/2/2
1	5MC	B	304	1	-	0/7/25/26	0/2/2/2
1	5MC	A	679	1	-	0/7/25/26	0/2/2/2
1	5MC	A	543	1	-	3/7/25/26	0/2/2/2
1	5MC	B	49	1	-	0/7/25/26	0/2/2/2
1	5MC	B	140	1	-	0/7/25/26	0/2/2/2
1	5MC	B	110	1	-	0/7/25/26	0/2/2/2
1	5MC	A	173	1	-	2/7/25/26	0/2/2/2
1	5MC	A	363	1	-	0/7/25/26	0/2/2/2
1	5MC	B	700	1	-	0/7/25/26	0/2/2/2
1	5MC	B	144	1	-	2/7/25/26	0/2/2/2
1	5MC	A	114	1	-	0/7/25/26	0/2/2/2
1	5MC	B	73	1	-	0/7/25/26	0/2/2/2
1	5MC	B	362	1	-	1/7/25/26	0/2/2/2
1	5MC	B	130	1	-	0/7/25/26	0/2/2/2
1	5MC	B	655	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	B	406	1	-	0/7/25/26	0/2/2/2
1	5MC	B	512	1	-	1/7/25/26	0/2/2/2
1	5MC	B	315	1	-	0/7/25/26	0/2/2/2
1	5MC	B	384	1	-	0/7/25/26	0/2/2/2
1	5MC	A	198	1	-	6/7/25/26	0/2/2/2
1	5MC	B	117	1	-	2/7/25/26	0/2/2/2
1	5MC	B	328	1	-	0/7/25/26	0/2/2/2
1	5MC	A	587	1	-	0/7/25/26	0/2/2/2
1	5MC	A	698	1	-	0/7/25/26	0/2/2/2
1	5MC	A	124	1	-	0/7/25/26	0/2/2/2
1	5MC	B	120	1	-	0/7/25/26	0/2/2/2
1	5MC	A	583	1	-	2/7/25/26	0/2/2/2
1	5MC	A	161	1	-	2/7/25/26	0/2/2/2
1	5MC	B	323	1	-	0/7/25/26	0/2/2/2
1	5MC	B	282	1	-	0/7/25/26	0/2/2/2
1	5MC	A	438	1	-	3/7/25/26	0/2/2/2
1	5MC	B	46	1	-	0/7/25/26	0/2/2/2
1	5MC	B	316	1	-	0/7/25/26	0/2/2/2
1	5MC	A	184	1	-	2/7/25/26	0/2/2/2
1	5MC	A	474	1	-	0/7/25/26	0/2/2/2
1	5MC	A	444	1	-	0/7/25/26	0/2/2/2
1	5MC	A	498	1	-	0/7/25/26	0/2/2/2
1	5MC	A	576	1	-	0/7/25/26	0/2/2/2
1	5MC	A	411	1	-	0/7/25/26	0/2/2/2
1	5MC	B	247	1	-	0/7/25/26	0/2/2/2
1	5MC	B	657	1	-	0/7/25/26	0/2/2/2
1	5MC	B	157	1	-	0/7/25/26	0/2/2/2
1	5MC	B	632	1	-	0/7/25/26	0/2/2/2
1	5MC	B	459	1	-	0/7/25/26	0/2/2/2
1	5MC	B	551	1	-	0/7/25/26	0/2/2/2
1	5MC	A	603	1	-	0/7/25/26	0/2/2/2
1	5MC	A	201	1	-	0/7/25/26	0/2/2/2
1	5MC	A	63	1	-	2/7/25/26	0/2/2/2
1	5MC	B	631	1	-	0/7/25/26	0/2/2/2
1	5MC	A	381	1	-	0/7/25/26	0/2/2/2
1	5MC	A	652	1	-	0/7/25/26	0/2/2/2
1	5MC	A	129	1	-	2/7/25/26	0/2/2/2
1	5MC	B	477	1	-	0/7/25/26	0/2/2/2
1	5MC	A	517	1	-	0/7/25/26	0/2/2/2
1	5MC	A	218	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	B	383	1	-	0/7/25/26	0/2/2/2
1	5MC	A	171	1	-	2/7/25/26	0/2/2/2
1	5MC	A	110	1	-	0/7/25/26	0/2/2/2
1	5MC	A	46	1	-	0/7/25/26	0/2/2/2
1	5MC	A	103	1	-	1/7/25/26	0/2/2/2
1	5MC	B	585	1	-	2/7/25/26	0/2/2/2
1	5MC	B	363	1	-	0/7/25/26	0/2/2/2
1	5MC	A	424	1	-	1/7/25/26	0/2/2/2
1	5MC	A	144	1	-	2/7/25/26	0/2/2/2
1	5MC	A	362	1	-	1/7/25/26	0/2/2/2
1	5MC	A	700	1	-	0/7/25/26	0/2/2/2
1	5MC	A	15	1	-	2/7/25/26	0/2/2/2
1	5MC	B	72	1	-	0/7/25/26	0/2/2/2
1	5MC	B	104	1	-	2/7/25/26	0/2/2/2
1	5MC	A	664	1	-	2/7/25/26	0/2/2/2
1	5MC	A	282	1	-	0/7/25/26	0/2/2/2
1	5MC	A	308	1	-	2/7/25/26	0/2/2/2
1	5MC	B	156	1	-	0/7/25/26	0/2/2/2
1	5MC	B	405	1	-	2/7/25/26	0/2/2/2
1	5MC	A	75	1	-	0/7/25/26	0/2/2/2
1	5MC	A	140	1	-	0/7/25/26	0/2/2/2
1	5MC	A	316	1	-	0/7/25/26	0/2/2/2
1	5MC	B	492	1	-	0/7/25/26	0/2/2/2
1	5MC	A	600	1	-	0/7/25/26	0/2/2/2
1	5MC	A	354	1	-	0/7/25/26	0/2/2/2
1	5MC	B	103	1	-	2/7/25/26	0/2/2/2
1	5MC	A	655	1	-	0/7/25/26	0/2/2/2
1	5MC	B	440	1	-	0/7/25/26	0/2/2/2
1	5MC	A	157	1	-	0/7/25/26	0/2/2/2
1	5MC	A	540	1	-	2/7/25/26	0/2/2/2
1	5MC	A	315	1	-	0/7/25/26	0/2/2/2
1	5MC	B	579	1	-	0/7/25/26	0/2/2/2
1	5MC	B	564	1	-	0/7/25/26	0/2/2/2
1	5MC	B	465	1	-	0/7/25/26	0/2/2/2
1	5MC	B	338	1	-	2/7/25/26	0/2/2/2
1	5MC	A	574	1	-	0/7/25/26	0/2/2/2
1	5MC	B	67	1	-	0/7/25/26	0/2/2/2
1	5MC	B	446	1	-	0/7/25/26	0/2/2/2
1	5MC	B	682	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	B	610	1	-	2/7/25/26	0/2/2/2
1	5MC	A	351	1	-	0/7/25/26	0/2/2/2
1	5MC	A	254	1	-	0/7/25/26	0/2/2/2
1	5MC	A	335	1	-	1/7/25/26	0/2/2/2
1	5MC	A	704	1	-	0/7/25/26	0/2/2/2
1	5MC	A	325	1	-	0/7/25/26	0/2/2/2
1	5MC	B	382	1	-	0/7/25/26	0/2/2/2
1	5MC	A	407	1	-	1/7/25/26	0/2/2/2
1	5MC	B	34	1	-	0/7/25/26	0/2/2/2
1	5MC	B	517	1	-	0/7/25/26	0/2/2/2
1	5MC	A	426	1	-	2/7/25/26	0/2/2/2
1	5MC	A	79	1	-	0/7/25/26	0/2/2/2
1	5MC	B	242	1	-	0/7/25/26	0/2/2/2
1	5MC	B	543	1	-	3/7/25/26	0/2/2/2
1	5MC	B	164	1	-	0/7/25/26	0/2/2/2
1	5MC	A	399	1	-	0/7/25/26	0/2/2/2
1	5MC	B	424	1	-	1/7/25/26	0/2/2/2
1	5MC	B	436	1	-	2/7/25/26	0/2/2/2
1	5MC	A	632	1	-	0/7/25/26	0/2/2/2
1	5MC	A	164	1	-	0/7/25/26	0/2/2/2
1	5MC	A	564	1	-	0/7/25/26	0/2/2/2
1	5MC	B	603	1	-	0/7/25/26	0/2/2/2
1	5MC	B	576	1	-	0/7/25/26	0/2/2/2
1	5MC	A	353	1	-	0/7/25/26	0/2/2/2
1	5MC	A	90	1	-	2/7/25/26	0/2/2/2
1	5MC	A	321	1	-	0/7/25/26	0/2/2/2
1	5MC	A	323	1	-	0/7/25/26	0/2/2/2
1	5MC	B	667	1	-	1/7/25/26	0/2/2/2
1	5MC	B	411	1	-	0/7/25/26	0/2/2/2
1	5MC	A	451	1	-	1/7/25/26	0/2/2/2
1	5MC	B	462	1	-	0/7/25/26	0/2/2/2
1	5MC	A	165	1	-	0/7/25/26	0/2/2/2
1	5MC	B	234	1	-	0/7/25/26	0/2/2/2
1	5MC	B	473	1	-	2/7/25/26	0/2/2/2
1	5MC	B	308	1	-	2/7/25/26	0/2/2/2
1	5MC	A	373	1	-	1/7/25/26	0/2/2/2
1	5MC	B	173	1	-	2/7/25/26	0/2/2/2
1	5MC	B	75	1	-	2/7/25/26	0/2/2/2
1	5MC	A	556	1	-	2/7/25/26	0/2/2/2
1	5MC	A	72	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	439	1	-	0/7/25/26	0/2/2/2
1	5MC	B	332	1	-	0/7/25/26	0/2/2/2
1	5MC	A	512	1	-	0/7/25/26	0/2/2/2
1	5MC	A	285	1	-	0/7/25/26	0/2/2/2
1	5MC	A	338	1	-	0/7/25/26	0/2/2/2
1	5MC	A	355	1	-	0/7/25/26	0/2/2/2
1	5MC	A	405	1	-	2/7/25/26	0/2/2/2
1	5MC	A	26	1	-	1/7/25/26	0/2/2/2
1	5MC	B	637	1	-	2/7/25/26	0/2/2/2
1	5MC	A	378	1	-	2/7/25/26	0/2/2/2
1	5MC	A	551	1	-	0/7/25/26	0/2/2/2
1	5MC	A	120	1	-	0/7/25/26	0/2/2/2
1	5MC	A	219	1	-	0/7/25/26	0/2/2/2
1	5MC	A	558	1	-	0/7/25/26	0/2/2/2
1	5MC	A	156	1	-	2/7/25/26	0/2/2/2
1	5MC	B	321	1	-	1/7/25/26	0/2/2/2
1	5MC	A	441	1	-	0/7/25/26	0/2/2/2
1	5MC	A	579	1	-	0/7/25/26	0/2/2/2
1	5MC	A	440	1	-	0/7/25/26	0/2/2/2
1	5MC	B	381	1	-	0/7/25/26	0/2/2/2
1	5MC	A	643	1	-	0/7/25/26	0/2/2/2
1	5MC	B	404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	247	1	-	0/7/25/26	0/2/2/2
1	5MC	A	592	1	-	0/7/25/26	0/2/2/2
1	5MC	B	664	1	-	6/7/25/26	0/2/2/2
1	5MC	B	639	1	-	3/7/25/26	0/2/2/2
1	5MC	B	325	1	-	0/7/25/26	0/2/2/2
1	5MC	B	494	1	-	0/7/25/26	0/2/2/2
1	5MC	B	206	1	-	1/7/25/26	0/2/2/2
1	5MC	A	209	1	-	0/7/25/26	0/2/2/2
1	5MC	B	25	1	-	1/7/25/26	0/2/2/2
1	5MC	A	298	1	-	0/7/25/26	0/2/2/2
1	5MC	A	506	1	-	2/7/25/26	0/2/2/2
1	5MC	B	209	1	-	0/7/25/26	0/2/2/2
1	5MC	A	610	1	-	2/7/25/26	0/2/2/2
1	5MC	A	131	1	-	2/7/25/26	0/2/2/2
1	5MC	A	151	1	-	1/7/25/26	0/2/2/2
1	5MC	A	111	1	-	0/7/25/26	0/2/2/2
1	5MC	A	436	1	-	2/7/25/26	0/2/2/2
1	5MC	B	540	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	B	536	1	-	0/7/25/26	0/2/2/2
1	5MC	A	469	1	-	0/7/25/26	0/2/2/2
1	5MC	B	491	1	-	2/7/25/26	0/2/2/2
1	5MC	A	49	1	-	1/7/25/26	0/2/2/2
1	5MC	B	574	1	-	0/7/25/26	0/2/2/2
1	5MC	A	242	1	-	1/7/25/26	0/2/2/2
1	5MC	B	351	1	-	0/7/25/26	0/2/2/2
1	5MC	A	404	1	-	0/7/25/26	0/2/2/2
1	5MC	B	418	1	-	1/7/25/26	0/2/2/2
1	5MC	A	465	1	-	0/7/25/26	0/2/2/2
1	5MC	B	188	1	-	0/7/25/26	0/2/2/2
1	5MC	B	693	1	-	0/7/25/26	0/2/2/2
1	5MC	A	76	1	-	0/7/25/26	0/2/2/2
1	5MC	B	518	1	-	0/7/25/26	0/2/2/2
1	5MC	B	625	1	-	0/7/25/26	0/2/2/2
1	5MC	B	279	1	-	0/7/25/26	0/2/2/2
1	5MC	B	458	1	-	0/7/25/26	0/2/2/2
1	5MC	B	647	1	-	0/7/25/26	0/2/2/2
1	5MC	A	491	1	-	2/7/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	523	5MC	C5-C4	-2.27	1.42	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	5MC	O3'-C3'-C2'	2.31	119.24	111.82
1	B	378	5MC	O3'-C3'-C2'	2.26	119.05	111.82
1	A	378	5MC	O3'-C3'-C2'	2.24	119.01	111.82
1	B	298	5MC	O3'-C3'-C2'	2.19	118.84	111.82

There are no chirality outliers.

All (226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	63	5MC	O4'-C4'-C5'-O5'
1	A	63	5MC	O4'-C4'-C5'-O5'
1	B	90	5MC	O4'-C4'-C5'-O5'
1	A	90	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	90	5MC	C3'-C4'-C5'-O5'
1	B	117	5MC	O4'-C4'-C5'-O5'
1	A	117	5MC	O4'-C4'-C5'-O5'
1	B	144	5MC	O4'-C4'-C5'-O5'
1	A	144	5MC	O4'-C4'-C5'-O5'
1	B	171	5MC	O4'-C4'-C5'-O5'
1	A	171	5MC	O4'-C4'-C5'-O5'
1	B	198	5MC	C2'-C1'-N1-C2
1	B	198	5MC	C2'-C1'-N1-C6
1	A	198	5MC	O4'-C4'-C5'-O5'
1	A	198	5MC	C2'-C1'-N1-C2
1	A	198	5MC	C2'-C1'-N1-C6
1	B	369	5MC	O4'-C4'-C5'-O5'
1	B	369	5MC	C3'-C4'-C5'-O5'
1	A	369	5MC	O4'-C4'-C5'-O5'
1	A	369	5MC	C3'-C4'-C5'-O5'
1	B	370	5MC	O4'-C4'-C5'-O5'
1	B	438	5MC	O4'-C4'-C5'-O5'
1	B	438	5MC	C3'-C4'-C5'-O5'
1	A	438	5MC	O4'-C4'-C5'-O5'
1	A	438	5MC	C3'-C4'-C5'-O5'
1	B	543	5MC	O4'-C4'-C5'-O5'
1	B	556	5MC	O4'-C4'-C5'-O5'
1	A	556	5MC	O4'-C4'-C5'-O5'
1	B	583	5MC	O4'-C4'-C5'-O5'
1	B	610	5MC	O4'-C4'-C5'-O5'
1	A	610	5MC	O4'-C4'-C5'-O5'
1	B	637	5MC	O4'-C4'-C5'-O5'
1	A	637	5MC	O4'-C4'-C5'-O5'
1	A	639	5MC	O4'-C4'-C5'-O5'
1	B	664	5MC	C2'-C1'-N1-C2
1	B	664	5MC	C2'-C1'-N1-C6
1	A	664	5MC	O4'-C4'-C5'-O5'
1	B	75	5MC	O4'-C4'-C5'-O5'
1	B	90	5MC	C3'-C4'-C5'-O5'
1	B	124	5MC	O4'-C4'-C5'-O5'
1	B	131	5MC	O4'-C4'-C5'-O5'
1	A	131	5MC	O4'-C4'-C5'-O5'
1	B	144	5MC	C3'-C4'-C5'-O5'
1	A	161	5MC	C3'-C4'-C5'-O5'
1	B	173	5MC	O4'-C4'-C5'-O5'
1	A	184	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	198	5MC	O4'-C4'-C5'-O5'
1	B	241	5MC	O4'-C4'-C5'-O5'
1	A	241	5MC	O4'-C4'-C5'-O5'
1	A	370	5MC	O4'-C4'-C5'-O5'
1	A	405	5MC	O4'-C4'-C5'-O5'
1	B	506	5MC	O4'-C4'-C5'-O5'
1	B	506	5MC	C3'-C4'-C5'-O5'
1	A	540	5MC	C3'-C4'-C5'-O5'
1	B	543	5MC	C3'-C4'-C5'-O5'
1	A	543	5MC	O4'-C4'-C5'-O5'
1	A	583	5MC	O4'-C4'-C5'-O5'
1	B	639	5MC	O4'-C4'-C5'-O5'
1	B	639	5MC	C3'-C4'-C5'-O5'
1	A	639	5MC	C3'-C4'-C5'-O5'
1	B	664	5MC	O4'-C4'-C5'-O5'
1	B	691	5MC	O4'-C4'-C5'-O5'
1	A	691	5MC	O4'-C4'-C5'-O5'
1	A	693	5MC	O4'-C4'-C5'-O5'
1	B	124	5MC	C3'-C4'-C5'-O5'
1	B	129	5MC	O4'-C4'-C5'-O5'
1	A	129	5MC	O4'-C4'-C5'-O5'
1	A	156	5MC	O4'-C4'-C5'-O5'
1	A	161	5MC	O4'-C4'-C5'-O5'
1	A	171	5MC	C3'-C4'-C5'-O5'
1	A	173	5MC	O4'-C4'-C5'-O5'
1	B	212	5MC	O4'-C4'-C5'-O5'
1	B	378	5MC	O4'-C4'-C5'-O5'
1	B	378	5MC	C3'-C4'-C5'-O5'
1	B	405	5MC	O4'-C4'-C5'-O5'
1	B	426	5MC	O4'-C4'-C5'-O5'
1	A	491	5MC	O4'-C4'-C5'-O5'
1	A	540	5MC	O4'-C4'-C5'-O5'
1	B	556	5MC	C3'-C4'-C5'-O5'
1	B	15	5MC	O4'-C4'-C5'-O5'
1	B	63	5MC	C3'-C4'-C5'-O5'
1	A	63	5MC	C3'-C4'-C5'-O5'
1	B	103	5MC	O4'-C4'-C5'-O5'
1	A	144	5MC	C3'-C4'-C5'-O5'
1	B	171	5MC	C3'-C4'-C5'-O5'
1	A	198	5MC	C3'-C4'-C5'-O5'
1	B	370	5MC	C3'-C4'-C5'-O5'
1	A	543	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	556	5MC	C3'-C4'-C5'-O5'
1	A	583	5MC	C3'-C4'-C5'-O5'
1	B	610	5MC	C3'-C4'-C5'-O5'
1	A	610	5MC	C3'-C4'-C5'-O5'
1	B	637	5MC	C3'-C4'-C5'-O5'
1	A	637	5MC	C3'-C4'-C5'-O5'
1	A	664	5MC	C3'-C4'-C5'-O5'
1	A	543	5MC	C4'-C5'-O5'-P
1	A	15	5MC	O4'-C4'-C5'-O5'
1	B	117	5MC	C3'-C4'-C5'-O5'
1	A	117	5MC	C3'-C4'-C5'-O5'
1	B	131	5MC	C3'-C4'-C5'-O5'
1	B	173	5MC	C3'-C4'-C5'-O5'
1	A	184	5MC	C3'-C4'-C5'-O5'
1	B	241	5MC	C3'-C4'-C5'-O5'
1	A	241	5MC	C3'-C4'-C5'-O5'
1	A	378	5MC	C3'-C4'-C5'-O5'
1	A	436	5MC	C3'-C4'-C5'-O5'
1	B	583	5MC	C3'-C4'-C5'-O5'
1	B	664	5MC	C3'-C4'-C5'-O5'
1	A	691	5MC	C3'-C4'-C5'-O5'
1	B	15	5MC	C3'-C4'-C5'-O5'
1	A	15	5MC	C3'-C4'-C5'-O5'
1	B	75	5MC	C3'-C4'-C5'-O5'
1	B	104	5MC	O4'-C4'-C5'-O5'
1	A	104	5MC	O4'-C4'-C5'-O5'
1	A	131	5MC	C3'-C4'-C5'-O5'
1	B	198	5MC	C3'-C4'-C5'-O5'
1	B	387	5MC	O4'-C4'-C5'-O5'
1	A	436	5MC	O4'-C4'-C5'-O5'
1	B	491	5MC	O4'-C4'-C5'-O5'
1	A	620	5MC	O4'-C4'-C5'-O5'
1	B	691	5MC	C3'-C4'-C5'-O5'
1	A	156	5MC	C3'-C4'-C5'-O5'
1	B	161	5MC	C3'-C4'-C5'-O5'
1	A	370	5MC	C3'-C4'-C5'-O5'
1	A	378	5MC	O4'-C4'-C5'-O5'
1	B	473	5MC	C3'-C4'-C5'-O5'
1	A	308	5MC	C3'-C4'-C5'-O5'
1	B	511	5MC	O4'-C4'-C5'-O5'
1	B	620	5MC	O4'-C4'-C5'-O5'
1	A	173	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	405	5MC	C3'-C4'-C5'-O5'
1	A	426	5MC	O4'-C4'-C5'-O5'
1	A	451	5MC	O4'-C4'-C5'-O5'
1	B	585	5MC	O4'-C4'-C5'-O5'
1	B	587	5MC	O4'-C4'-C5'-O5'
1	A	693	5MC	C3'-C4'-C5'-O5'
1	B	129	5MC	C3'-C4'-C5'-O5'
1	B	212	5MC	C3'-C4'-C5'-O5'
1	B	387	5MC	C3'-C4'-C5'-O5'
1	B	405	5MC	C3'-C4'-C5'-O5'
1	B	418	5MC	O4'-C4'-C5'-O5'
1	B	426	5MC	C3'-C4'-C5'-O5'
1	A	129	5MC	C3'-C4'-C5'-O5'
1	A	139	5MC	O4'-C4'-C5'-O5'
1	A	506	5MC	C3'-C4'-C5'-O5'
1	B	308	5MC	C3'-C4'-C5'-O5'
1	B	436	5MC	O4'-C4'-C5'-O5'
1	B	436	5MC	C3'-C4'-C5'-O5'
1	B	362	5MC	O4'-C4'-C5'-O5'
1	A	491	5MC	C3'-C4'-C5'-O5'
1	B	57	5MC	O4'-C4'-C5'-O5'
1	B	151	5MC	O4'-C4'-C5'-O5'
1	A	151	5MC	O4'-C4'-C5'-O5'
1	B	165	5MC	O4'-C4'-C5'-O5'
1	B	184	5MC	O4'-C4'-C5'-O5'
1	B	473	5MC	O4'-C4'-C5'-O5'
1	A	667	5MC	O4'-C4'-C5'-O5'
1	A	639	5MC	C4'-C5'-O5'-P
1	B	543	5MC	C4'-C5'-O5'-P
1	B	540	5MC	C3'-C4'-C5'-O5'
1	B	664	5MC	O4'-C1'-N1-C6
1	B	639	5MC	C4'-C5'-O5'-P
1	B	198	5MC	O4'-C1'-N1-C6
1	A	198	5MC	O4'-C1'-N1-C6
1	A	523	5MC	O4'-C4'-C5'-O5'
1	B	438	5MC	C4'-C5'-O5'-P
1	A	25	5MC	O4'-C4'-C5'-O5'
1	B	424	5MC	C3'-C4'-C5'-O5'
1	A	506	5MC	O4'-C4'-C5'-O5'
1	B	540	5MC	O4'-C4'-C5'-O5'
1	A	438	5MC	C4'-C5'-O5'-P
1	A	26	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	103	5MC	C3'-C4'-C5'-O5'
1	A	308	5MC	O4'-C4'-C5'-O5'
1	A	373	5MC	O4'-C4'-C5'-O5'
1	A	424	5MC	C3'-C4'-C5'-O5'
1	A	458	5MC	O4'-C4'-C5'-O5'
1	B	474	5MC	O4'-C4'-C5'-O5'
1	A	511	5MC	O4'-C4'-C5'-O5'
1	B	558	5MC	O4'-C4'-C5'-O5'
1	A	585	5MC	O4'-C4'-C5'-O5'
1	B	664	5MC	O4'-C1'-N1-C2
1	B	124	5MC	C4'-C5'-O5'-P
1	B	25	5MC	O4'-C4'-C5'-O5'
1	A	103	5MC	O4'-C4'-C5'-O5'
1	B	321	5MC	O4'-C4'-C5'-O5'
1	B	353	5MC	O4'-C4'-C5'-O5'
1	B	373	5MC	O4'-C4'-C5'-O5'
1	A	418	5MC	O4'-C4'-C5'-O5'
1	A	477	5MC	O4'-C4'-C5'-O5'
1	A	682	5MC	O4'-C4'-C5'-O5'
1	B	308	5MC	O4'-C4'-C5'-O5'
1	A	620	5MC	C3'-C4'-C5'-O5'
1	A	57	5MC	O4'-C4'-C5'-O5'
1	B	104	5MC	C3'-C4'-C5'-O5'
1	A	206	5MC	O4'-C4'-C5'-O5'
1	B	491	5MC	C3'-C4'-C5'-O5'
1	A	523	5MC	C3'-C4'-C5'-O5'
1	B	528	5MC	O4'-C4'-C5'-O5'
1	B	604	5MC	O4'-C4'-C5'-O5'
1	A	198	5MC	O4'-C1'-N1-C2
1	A	49	5MC	C3'-C4'-C5'-O5'
1	A	407	5MC	O4'-C4'-C5'-O5'
1	A	455	5MC	O4'-C4'-C5'-O5'
1	B	198	5MC	O4'-C1'-N1-C2
1	A	104	5MC	C3'-C4'-C5'-O5'
1	A	242	5MC	O4'-C4'-C5'-O5'
1	A	335	5MC	O4'-C4'-C5'-O5'
1	B	455	5MC	O4'-C4'-C5'-O5'
1	B	139	5MC	O4'-C4'-C5'-O5'
1	B	161	5MC	O4'-C4'-C5'-O5'
1	B	184	5MC	C3'-C4'-C5'-O5'
1	B	206	5MC	O4'-C4'-C5'-O5'
1	A	362	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	441	5MC	O4'-C4'-C5'-O5'
1	B	511	5MC	C3'-C4'-C5'-O5'
1	B	523	5MC	O4'-C4'-C5'-O5'
1	B	587	5MC	C3'-C4'-C5'-O5'
1	B	620	5MC	C3'-C4'-C5'-O5'
1	B	667	5MC	O4'-C4'-C5'-O5'
1	B	338	5MC	C2'-C1'-N1-C6
1	B	79	5MC	C3'-C4'-C5'-O5'
1	A	426	5MC	C3'-C4'-C5'-O5'
1	B	512	5MC	O4'-C4'-C5'-O5'
1	B	585	5MC	C3'-C4'-C5'-O5'
1	B	338	5MC	C2'-C1'-N1-C2

There are no ring outliers.

101 monomers are involved in 156 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	268	5MC	1	0
1	A	473	5MC	1	0
1	B	523	5MC	5	0
1	B	246	5MC	1	0
1	A	332	5MC	1	0
1	B	643	5MC	1	0
1	A	25	5MC	1	0
1	A	370	5MC	3	0
1	B	498	5MC	1	0
1	A	387	5MC	2	0
1	B	360	5MC	1	0
1	A	639	5MC	2	0
1	B	79	5MC	2	0
1	A	349	5MC	1	0
1	A	149	5MC	1	0
1	A	455	5MC	2	0
1	A	39	5MC	1	0
1	B	249	5MC	1	0
1	B	455	5MC	4	0
1	B	568	5MC	1	0
1	A	369	5MC	7	0
1	A	647	5MC	1	0
1	A	28	5MC	1	0
1	A	268	5MC	1	0
1	B	28	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	372	5MC	1	0
1	B	129	5MC	2	0
1	A	631	5MC	3	0
1	B	124	5MC	1	0
1	A	523	5MC	5	0
1	B	76	5MC	3	0
1	A	372	5MC	2	0
1	A	249	5MC	2	0
1	A	73	5MC	1	0
1	A	130	5MC	1	0
1	B	387	5MC	5	0
1	B	335	5MC	1	0
1	B	39	5MC	1	0
1	B	370	5MC	2	0
1	B	399	5MC	1	0
1	B	439	5MC	1	0
1	B	285	5MC	3	0
1	A	241	5MC	1	0
1	B	349	5MC	1	0
1	B	355	5MC	1	0
1	B	57	5MC	1	0
1	B	369	5MC	5	0
1	B	698	5MC	2	0
1	B	298	5MC	1	0
1	B	161	5MC	1	0
1	A	304	5MC	1	0
1	A	67	5MC	1	0
1	B	15	5MC	1	0
1	A	543	5MC	1	0
1	B	700	5MC	1	0
1	B	73	5MC	1	0
1	B	130	5MC	1	0
1	B	655	5MC	1	0
1	A	587	5MC	1	0
1	A	698	5MC	3	0
1	A	161	5MC	2	0
1	B	323	5MC	1	0
1	A	184	5MC	1	0
1	A	444	5MC	1	0
1	A	498	5MC	1	0
1	B	157	5MC	1	0
1	B	632	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	631	5MC	3	0
1	A	129	5MC	1	0
1	A	103	5MC	1	0
1	B	585	5MC	1	0
1	B	72	5MC	2	0
1	B	156	5MC	2	0
1	B	405	5MC	1	0
1	B	440	5MC	1	0
1	B	682	5MC	1	0
1	A	335	5MC	2	0
1	A	79	5MC	2	0
1	A	321	5MC	2	0
1	A	323	5MC	1	0
1	B	75	5MC	1	0
1	A	72	5MC	2	0
1	A	439	5MC	2	0
1	B	332	5MC	1	0
1	A	355	5MC	1	0
1	A	405	5MC	1	0
1	A	219	5MC	1	0
1	A	558	5MC	1	0
1	A	156	5MC	2	0
1	B	321	5MC	1	0
1	A	579	5MC	1	0
1	B	381	5MC	1	0
1	A	247	5MC	1	0
1	B	639	5MC	3	0
1	A	209	5MC	2	0
1	B	209	5MC	2	0
1	A	469	5MC	1	0
1	B	491	5MC	1	0
1	B	351	5MC	1	0
1	B	693	5MC	2	0
1	A	76	5MC	2	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

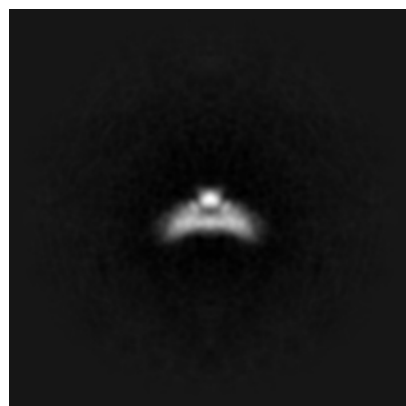
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70036. These allow visual inspection of the internal detail of the map and identification of artifacts.

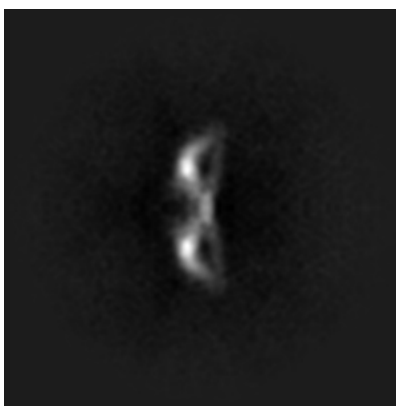
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

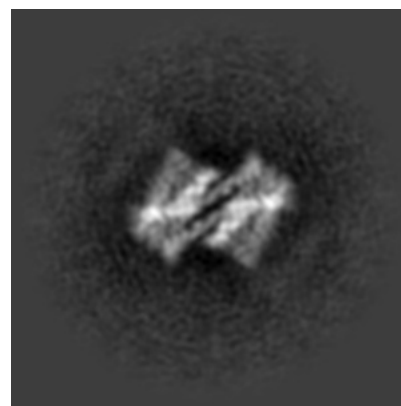
#### 6.1.1 Primary map



X

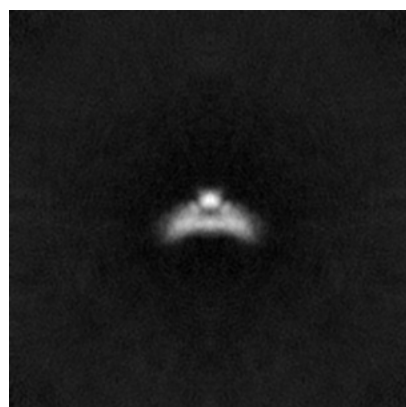


Y

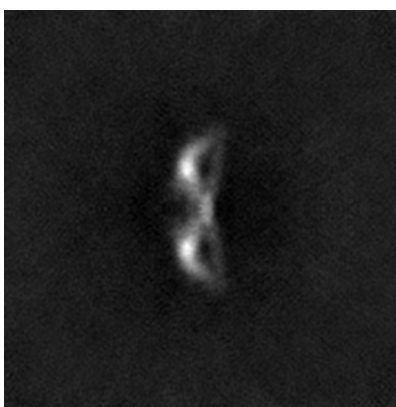


Z

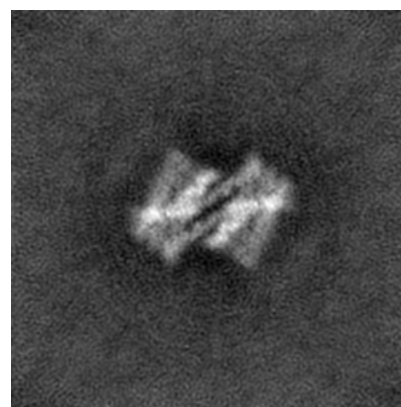
#### 6.1.2 Raw map



X



Y

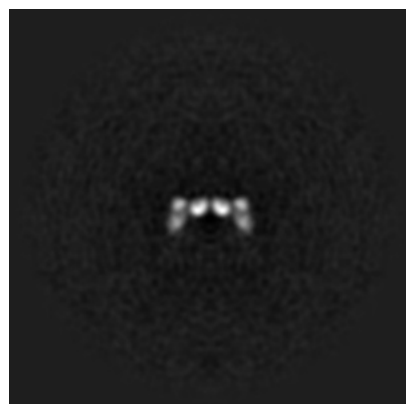


Z

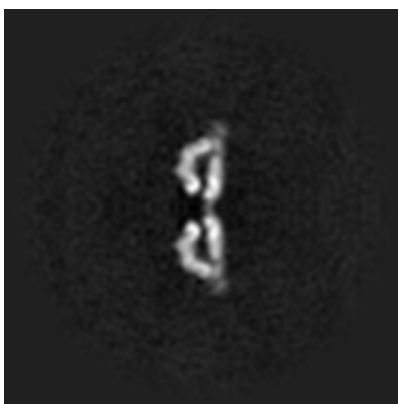
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

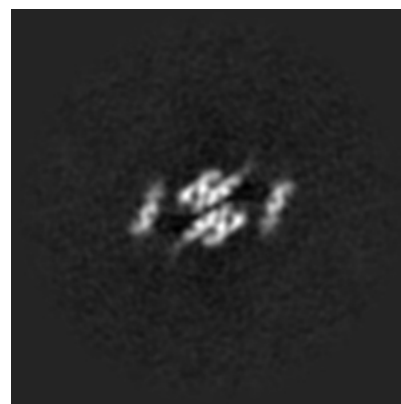
### 6.2.1 Primary map



X Index: 90

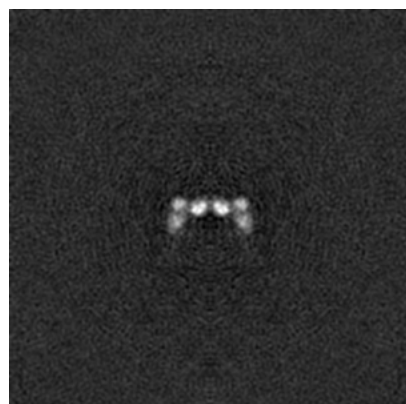


Y Index: 90

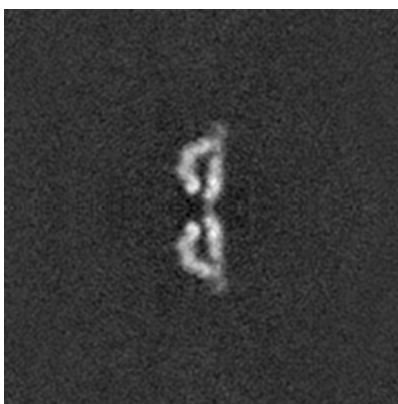


Z Index: 90

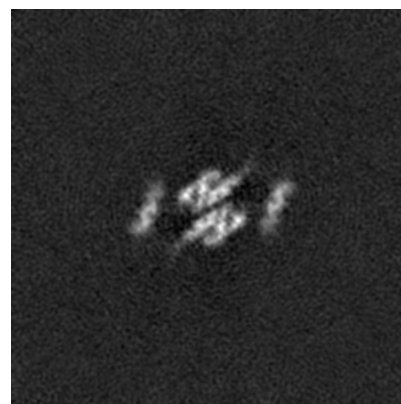
### 6.2.2 Raw map



X Index: 90



Y Index: 90



Z Index: 90

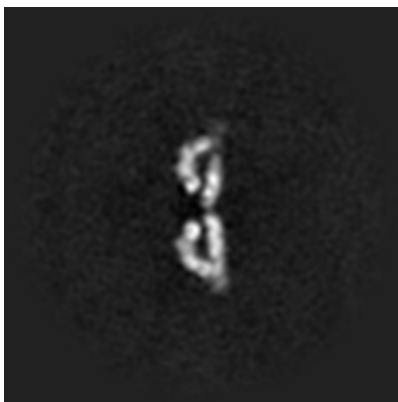
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 76



Y Index: 89



Z Index: 83

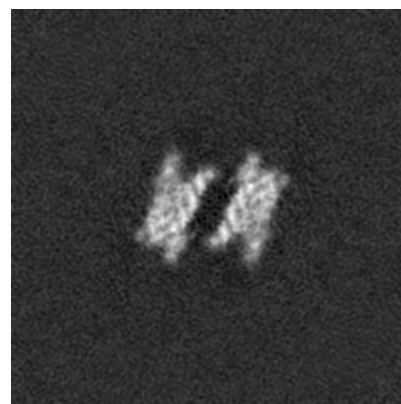
### 6.3.2 Raw map



X Index: 76



Y Index: 89

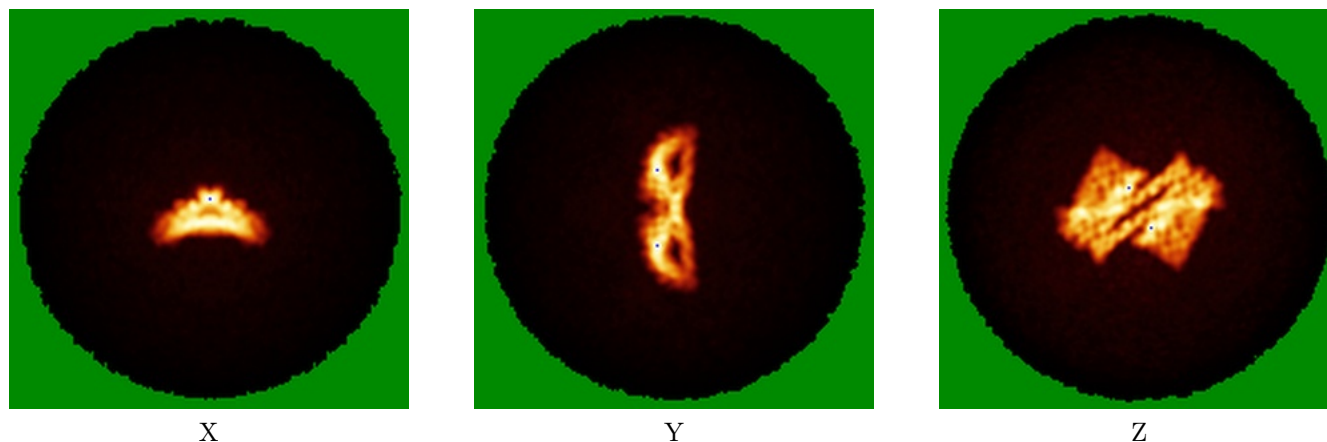


Z Index: 83

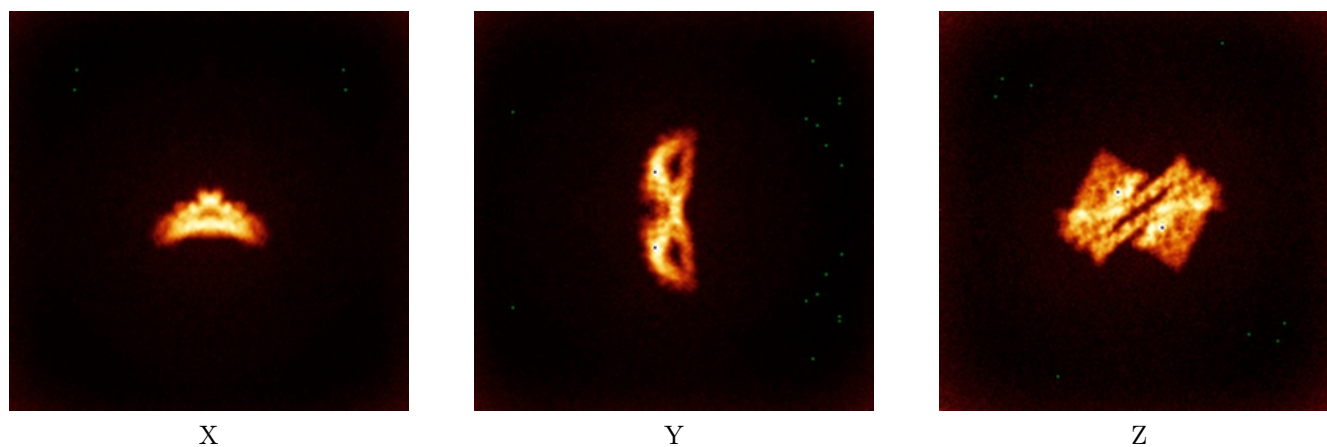
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



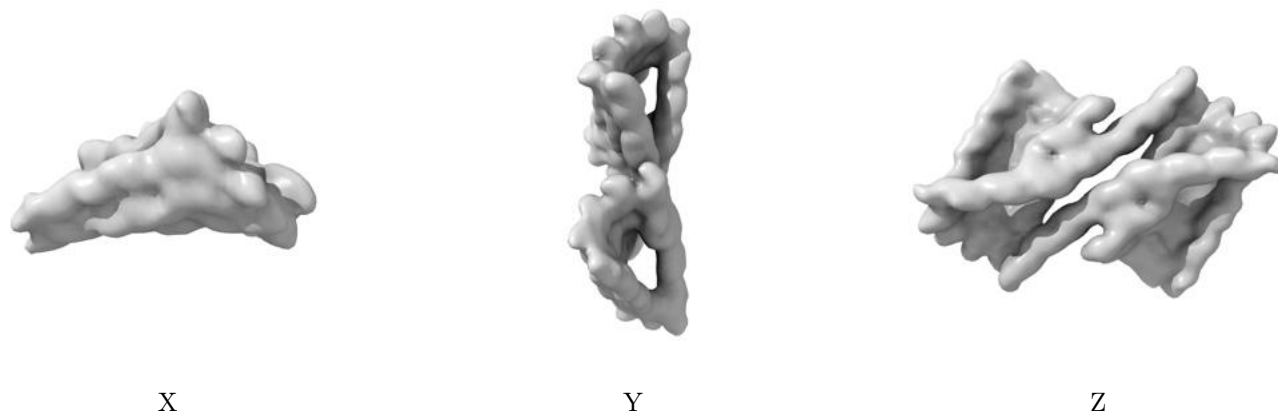
### 6.4.2 Raw map



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.

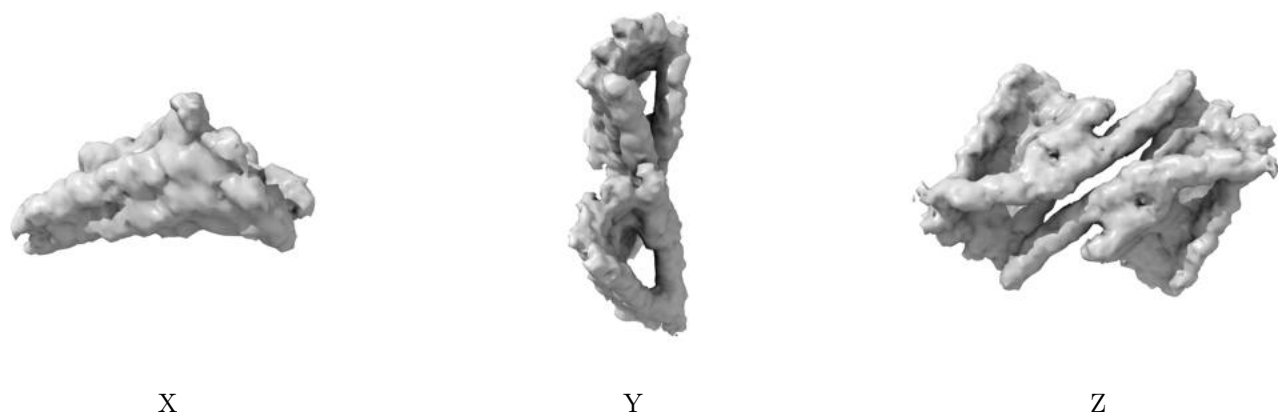
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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



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.

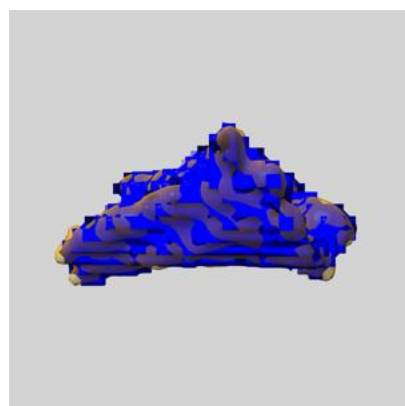
## 6.6 Mask visualisation [i](#)

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

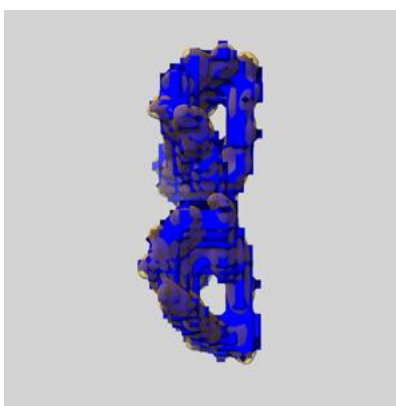
A mask typically either:

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

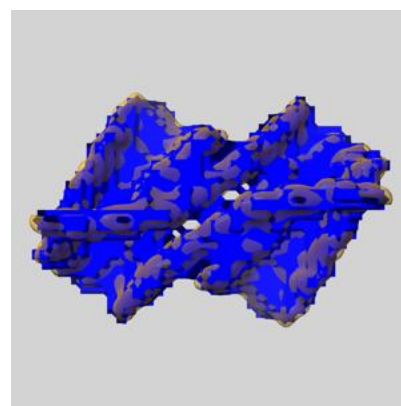
### 6.6.1 emd\_70036\_msk\_1.map [i](#)



X



Y



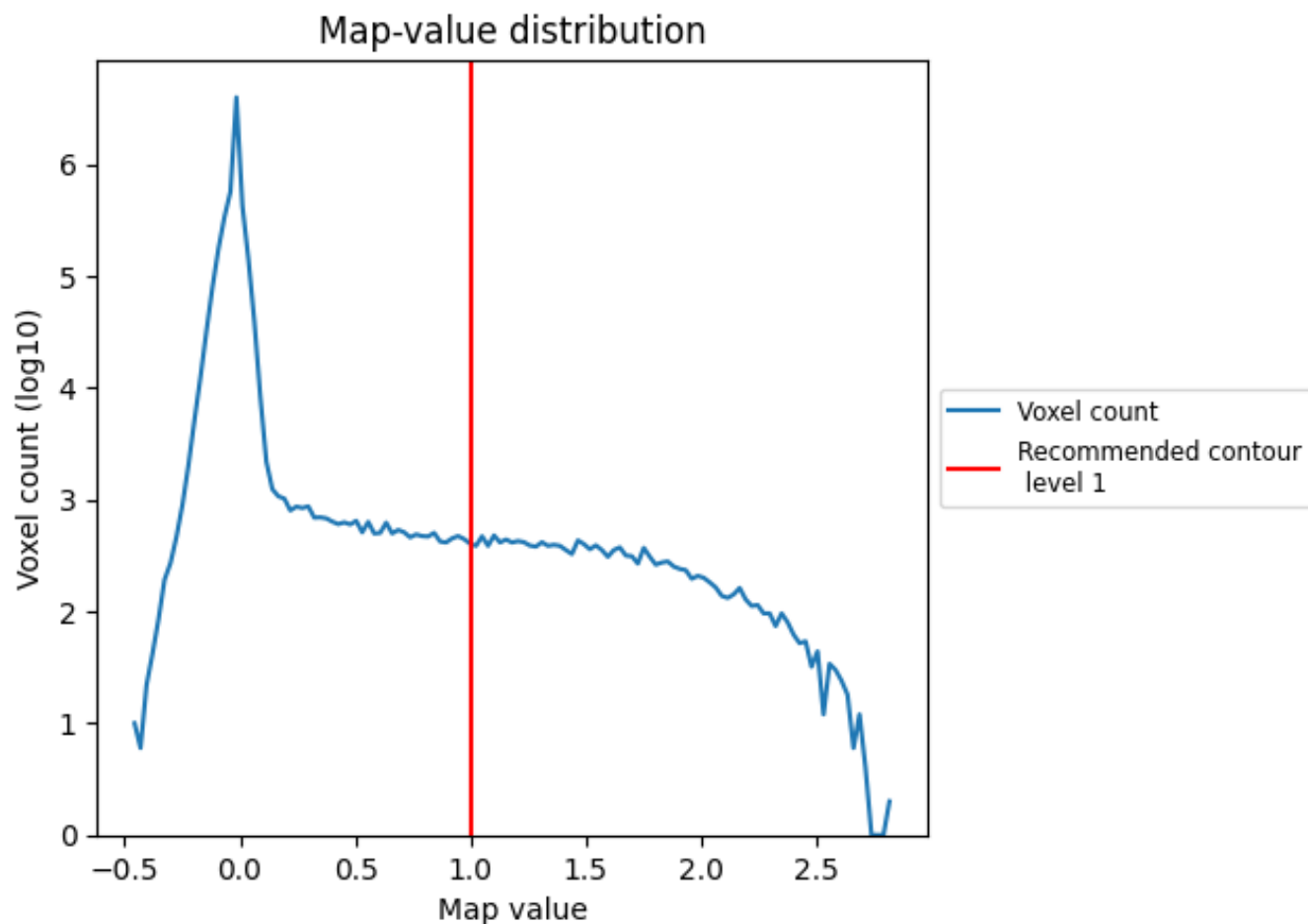
Z



## 7 Map analysis [i](#)

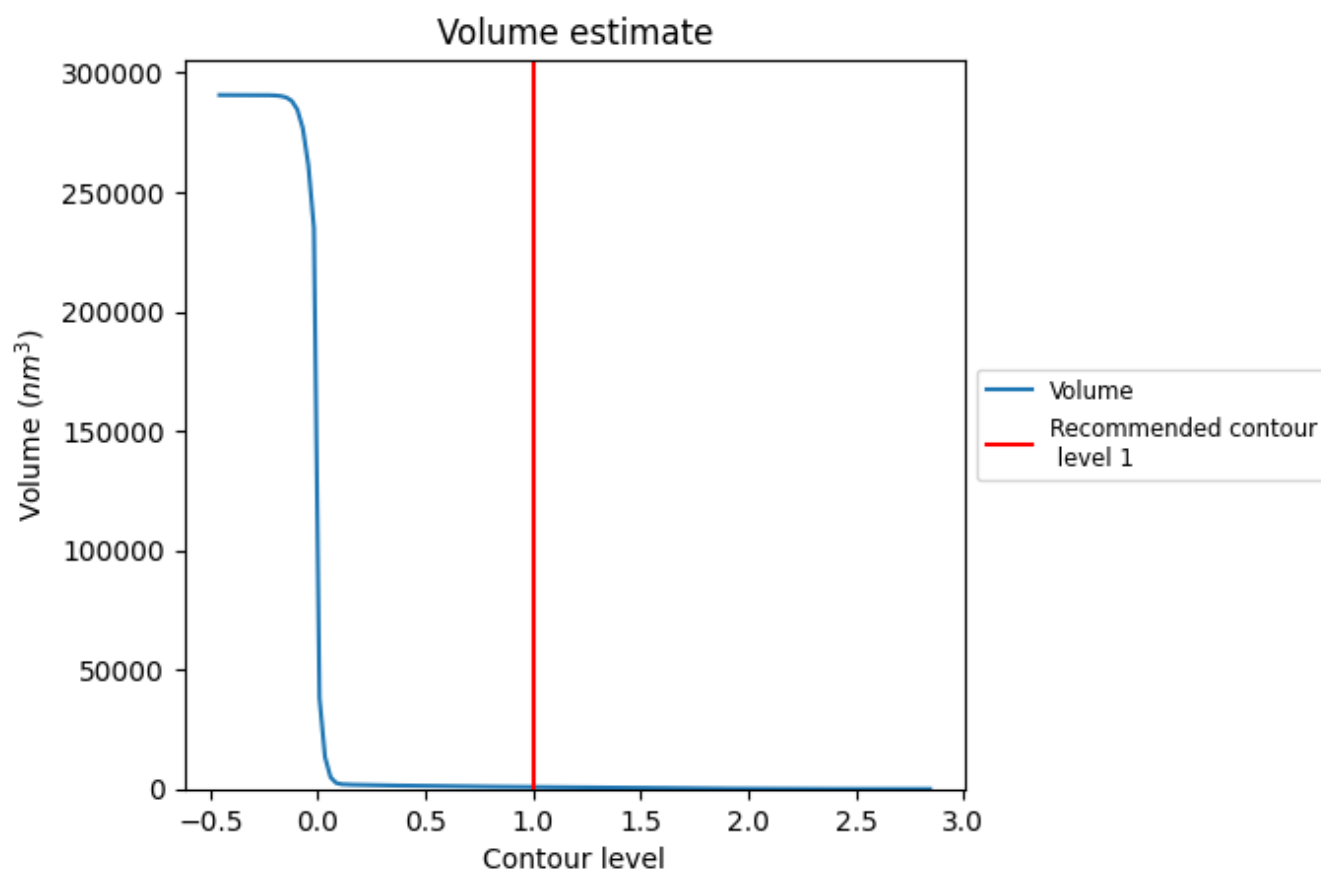
This section contains the results of statistical analysis of the map.

### 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.

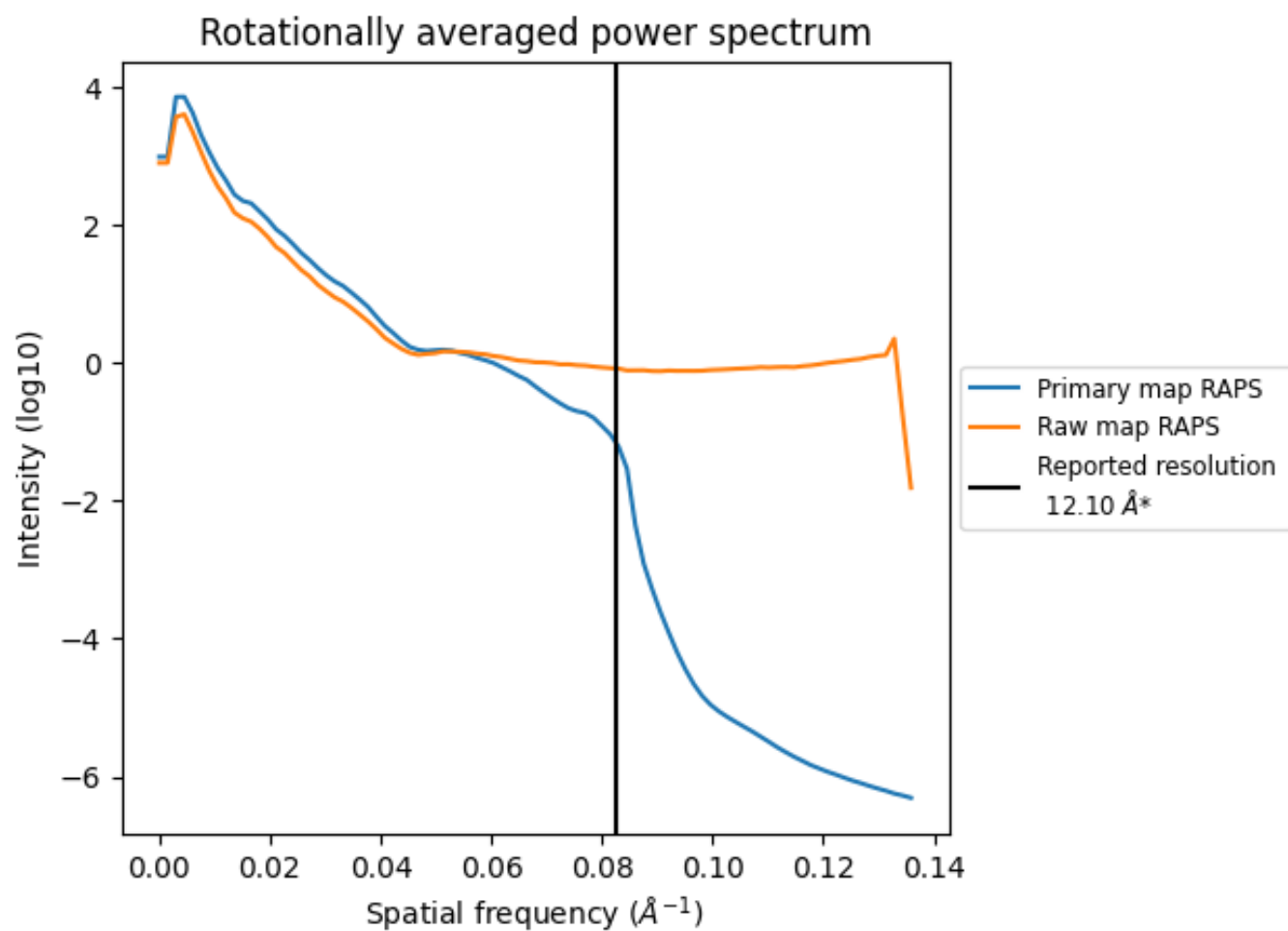
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 800  $\text{nm}^3$ ; this corresponds to an approximate mass of 722 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 ⓘ

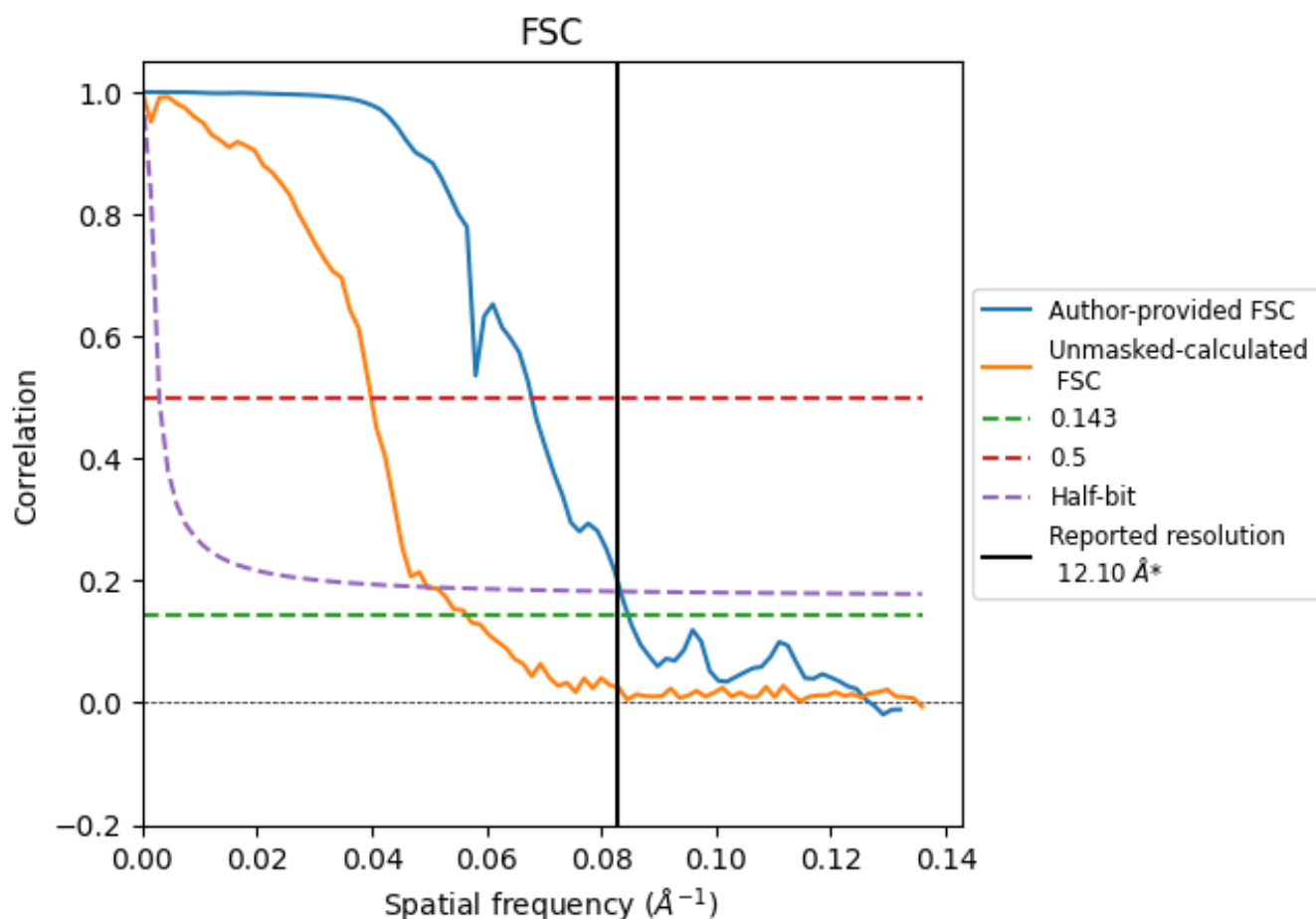


\*Reported resolution corresponds to spatial frequency of 0.083  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.083 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

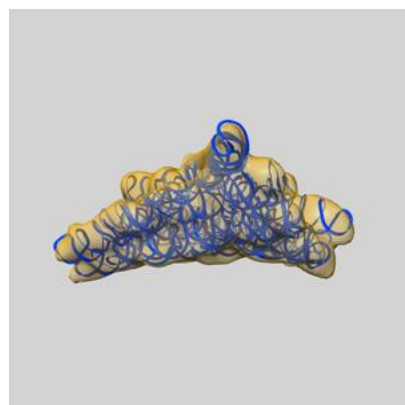
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	12.10	-	-
Author-provided FSC curve	11.81	14.75	12.00
Unmasked-calculated*	17.70	25.13	20.12

\*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 17.70 differs from the reported value 12.1 by more than 10 %

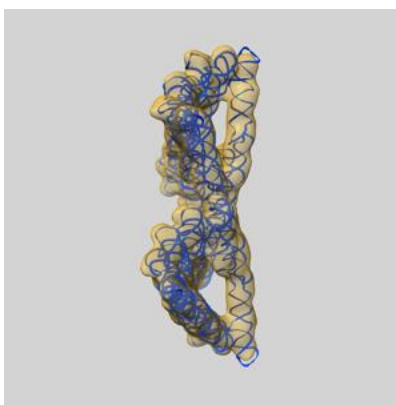
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70036 and PDB model 9ZC8. Per-residue inclusion information can be found in section [3](#) on page [5](#).

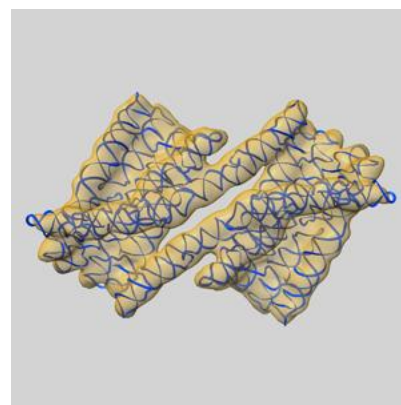
### 9.1 Map-model overlay [i](#)



X



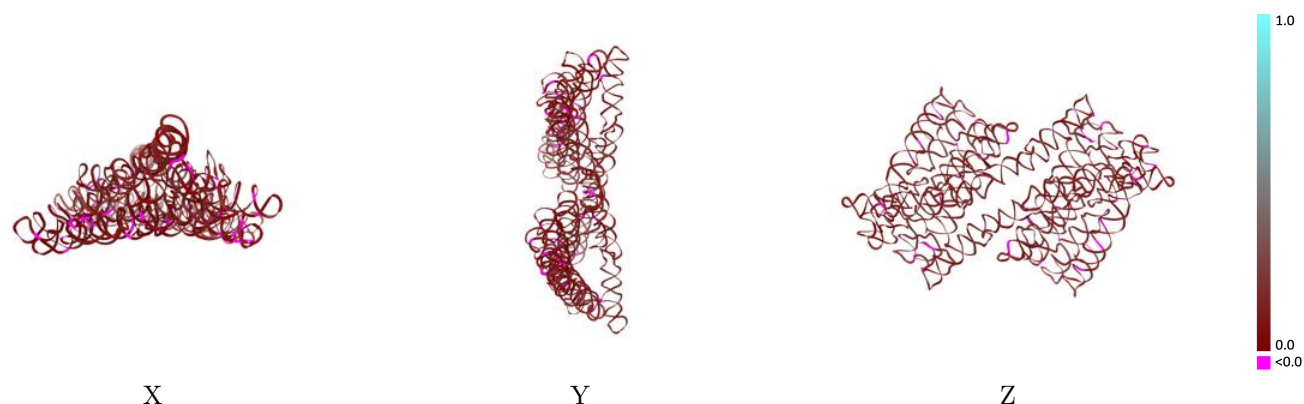
Y



Z

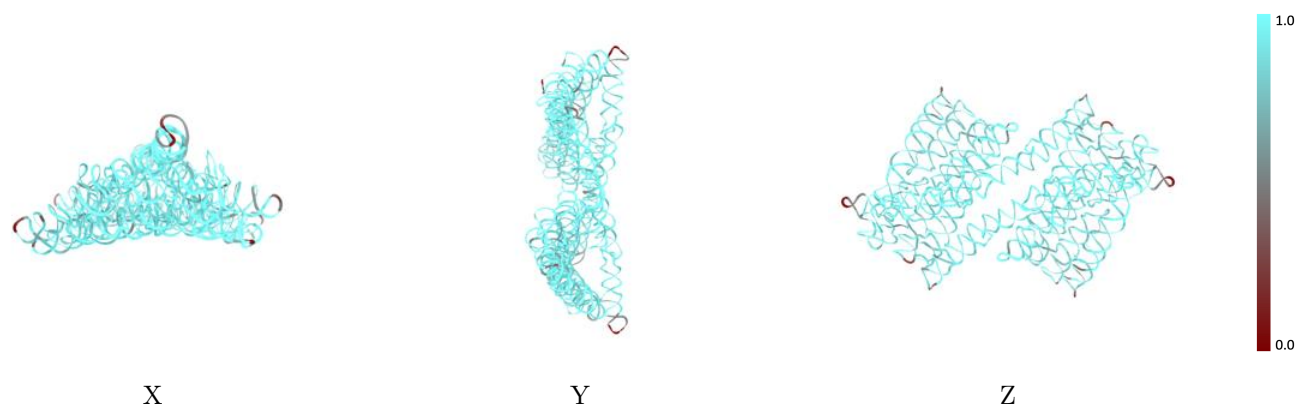
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



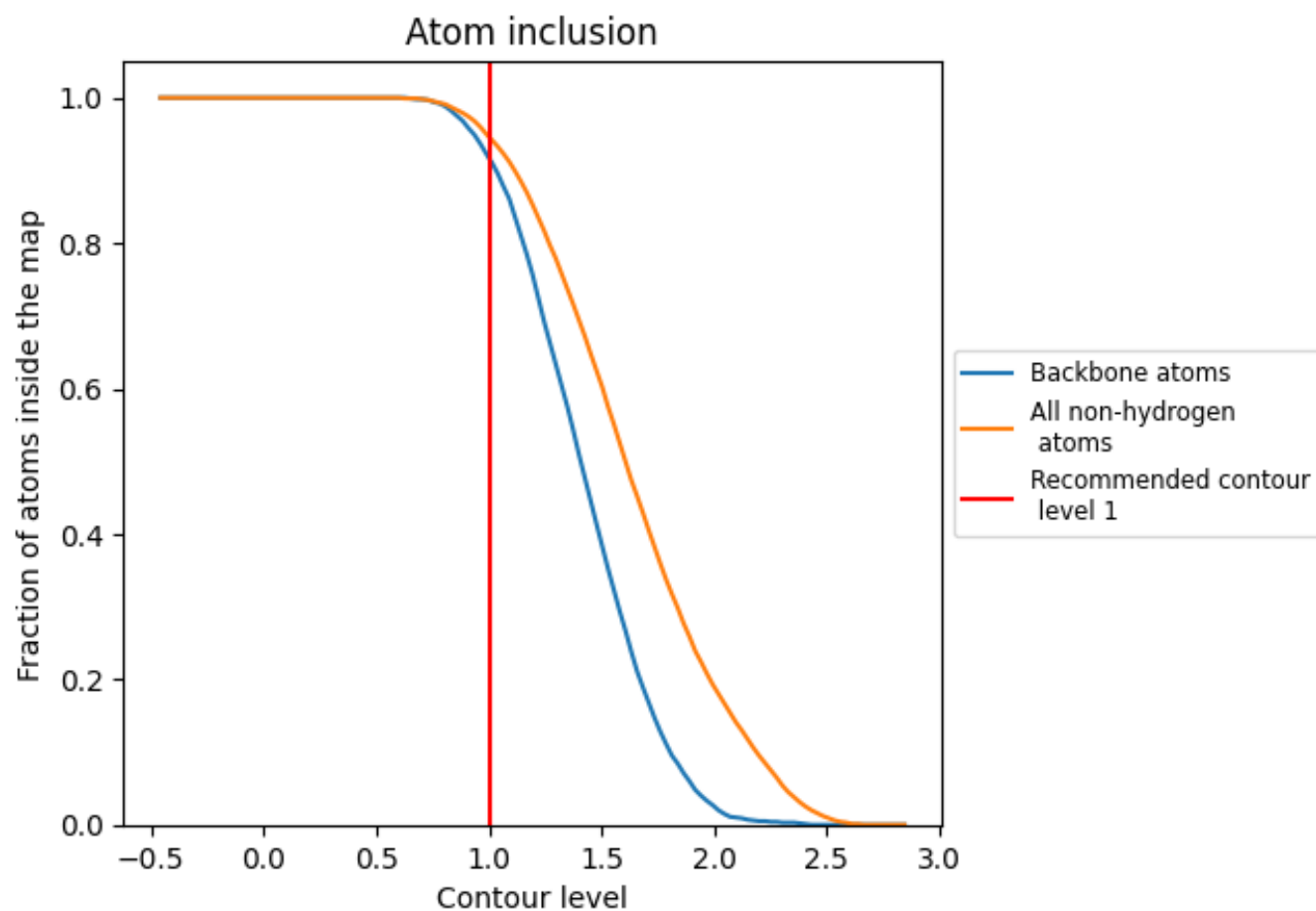
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 95% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9460	<div></div> 0.0990
A	<div></div> 0.9460	<div></div> 0.0980
B	<div></div> 0.9460	<div></div> 0.0990

