



## Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 03:56 pm GMT

PDB ID : 9Q8Z / pdb\_00009q8z  
EMDB ID : EMD-52913  
Title : Human chondroitin sulfate polymerase complex CHSY3-CHPF  
Authors : Dutta, P.; Cordeiro, R.L.; Wild, R.  
Deposited on : 2025-02-25  
Resolution : 3.00 Å(reported)  
Based on initial model : .

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 : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
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

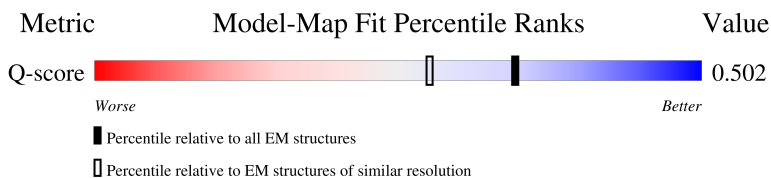
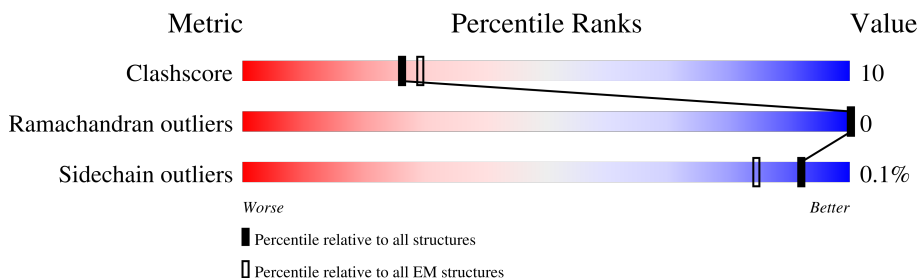
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	710	
2	B	753	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chondroitin sulfate synthase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	589	Total	C	N	O	S	2	0
			4679	2980	858	826	15		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	-	expression tag	UNP Q8IZ52
A	75	PRO	-	expression tag	UNP Q8IZ52
A	76	GLY	-	expression tag	UNP Q8IZ52
A	77	GLY	-	expression tag	UNP Q8IZ52
A	78	SER	-	expression tag	UNP Q8IZ52
A	79	THR	-	expression tag	UNP Q8IZ52
A	80	GLY	-	expression tag	UNP Q8IZ52
A	776	GLY	-	expression tag	UNP Q8IZ52
A	777	THR	-	expression tag	UNP Q8IZ52
A	778	LEU	-	expression tag	UNP Q8IZ52
A	779	GLU	-	expression tag	UNP Q8IZ52
A	780	VAL	-	expression tag	UNP Q8IZ52
A	781	LEU	-	expression tag	UNP Q8IZ52
A	782	PHE	-	expression tag	UNP Q8IZ52
A	783	GLN	-	expression tag	UNP Q8IZ52

- Molecule 2 is a protein called Chondroitin sulfate synthase 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	590	Total	C	N	O	S	0	0
			4864	3119	838	879	28		

There are 26 discrepancies between the modelled and reference sequences:

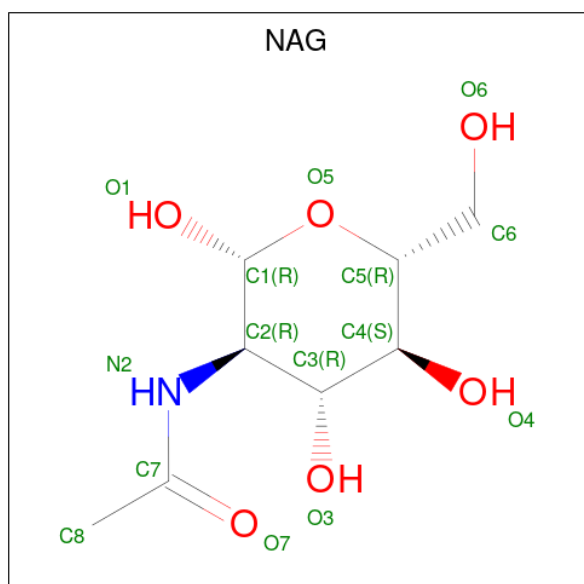
Chain	Residue	Modelled	Actual	Comment	Reference
B	150	GLY	-	expression tag	UNP Q70JA7
B	151	PRO	-	expression tag	UNP Q70JA7

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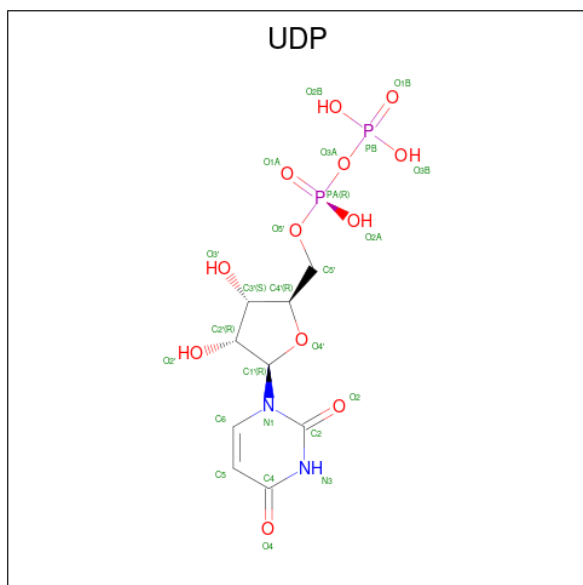
Chain	Residue	Modelled	Actual	Comment	Reference
B	152	GLY	-	expression tag	UNP Q70JA7
B	153	GLY	-	expression tag	UNP Q70JA7
B	154	SER	-	expression tag	UNP Q70JA7
B	155	THR	-	expression tag	UNP Q70JA7
B	883	GLY	-	expression tag	UNP Q70JA7
B	884	THR	-	expression tag	UNP Q70JA7
B	885	GLY	-	expression tag	UNP Q70JA7
B	886	SER	-	expression tag	UNP Q70JA7
B	887	GLY	-	expression tag	UNP Q70JA7
B	888	LEU	-	expression tag	UNP Q70JA7
B	889	ASN	-	expression tag	UNP Q70JA7
B	890	ASP	-	expression tag	UNP Q70JA7
B	891	ILE	-	expression tag	UNP Q70JA7
B	892	PHE	-	expression tag	UNP Q70JA7
B	893	GLU	-	expression tag	UNP Q70JA7
B	894	ALA	-	expression tag	UNP Q70JA7
B	895	GLN	-	expression tag	UNP Q70JA7
B	896	LYS	-	expression tag	UNP Q70JA7
B	897	ILE	-	expression tag	UNP Q70JA7
B	898	GLU	-	expression tag	UNP Q70JA7
B	899	TRP	-	expression tag	UNP Q70JA7
B	900	HIS	-	expression tag	UNP Q70JA7
B	901	GLU	-	expression tag	UNP Q70JA7
B	902	GLY	-	expression tag	UNP Q70JA7

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

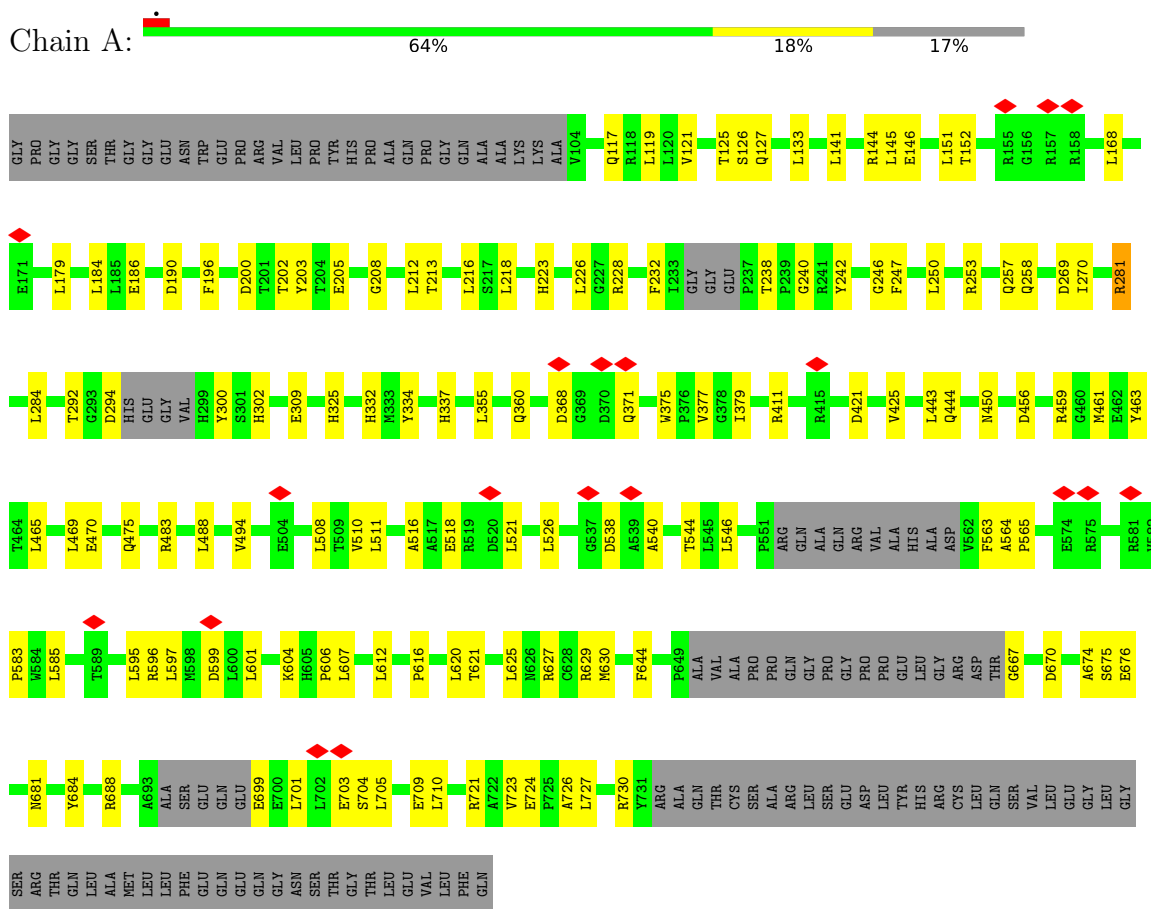
- Molecule 4 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ) (labeled as "Ligand of Interest" by depositor).



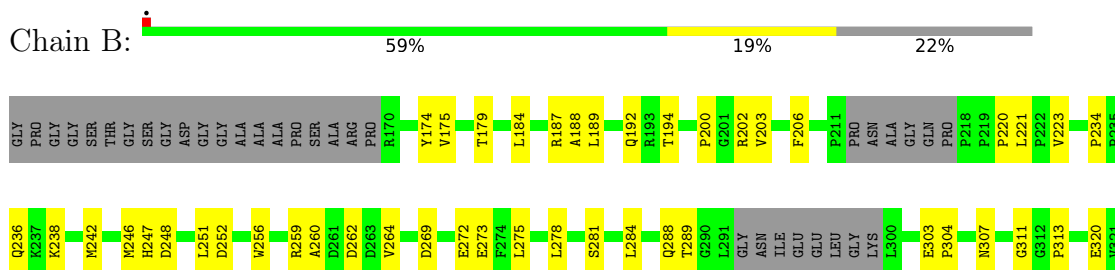
### 3 Residue-property plots

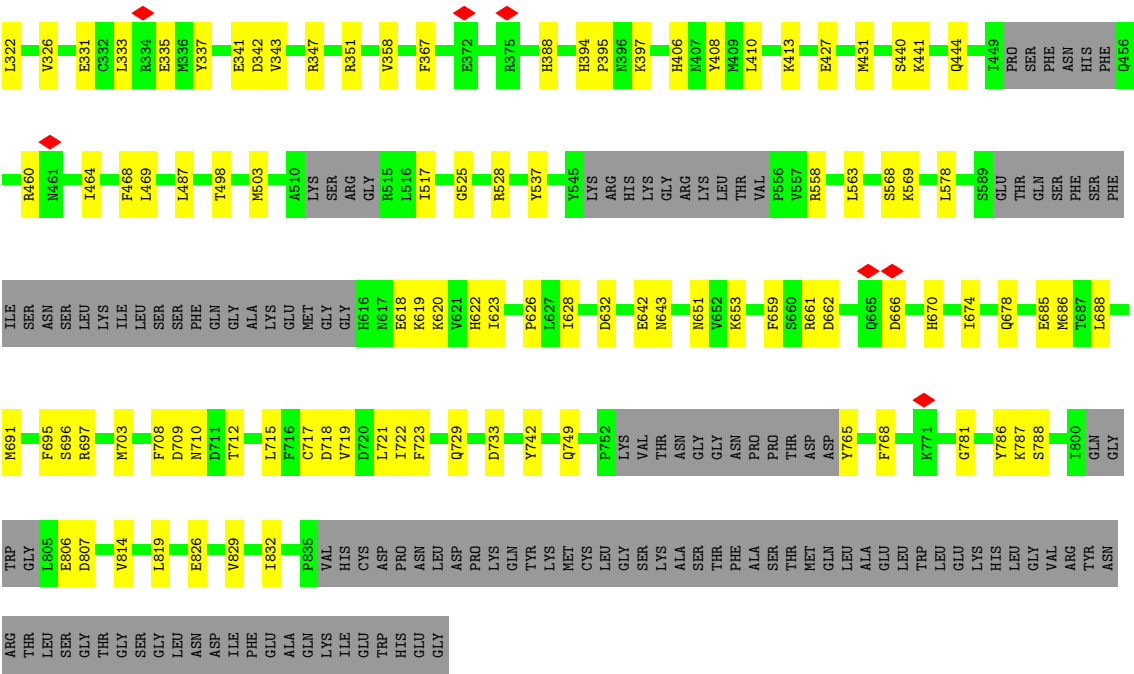
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Chondroitin sulfate synthase 2



#### • Molecule 2: Chondroitin sulfate synthase 3





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166015	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.782	Depositor
Minimum map value	-0.268	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0918	Depositor
Map size (Å)	280.32, 280.32, 280.32	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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: NAG, MN, UDP

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	0.12	0/4804	0.28	0/6537
2	B	0.12	0/4977	0.29	0/6705
All	All	0.12	0/9781	0.28	0/13242

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 [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	4679	0	4631	92	0
2	B	4864	0	4797	107	0
3	A	14	0	13	0	0
3	B	28	0	26	2	0
4	B	25	0	11	1	0
5	B	2	0	0	0	0
All	All	9612	0	9478	188	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 10.

All (188) 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:701:LEU:O	1:A:705:LEU:HB2	1.74	0.88
2:B:289:THR:HG23	2:B:307:ASN:HD22	1.48	0.78
1:A:205:GLU:HG3	1:A:208:GLY:H	1.49	0.77
1:A:595:LEU:HD11	1:A:710:LEU:HD22	1.66	0.75
2:B:247:HIS:CG	2:B:326:VAL:HG21	2.26	0.70
1:A:596:ARG:NH2	1:A:703:GLU:OE2	2.27	0.68
1:A:238:THR:HG21	1:A:284:LEU:HD21	1.75	0.67
2:B:537:TYR:HB2	2:B:563:LEU:HB2	1.74	0.67
2:B:288:GLN:NE2	2:B:367:PHE:O	2.29	0.65
1:A:475:GLN:N	1:A:475:GLN:OE1	2.28	0.65
2:B:806:GLU:N	2:B:806:GLU:OE2	2.30	0.65
1:A:375:TRP:O	1:A:459:ARG:NH2	2.30	0.64
1:A:521:LEU:HD11	1:A:616:PRO:HB2	1.80	0.64
1:A:544:THR:HG23	1:A:583:PRO:HG2	1.80	0.62
2:B:718:ASP:HB3	2:B:721:LEU:HD13	1.81	0.62
2:B:623:ILE:HG12	2:B:715:LEU:HD23	1.81	0.62
2:B:189:LEU:HD12	2:B:221:LEU:HD13	1.81	0.62
2:B:194:THR:HG23	2:B:406:HIS:HB2	1.83	0.60
2:B:678:GLN:NE2	2:B:686:MET:O	2.34	0.60
2:B:179:THR:HG22	2:B:262:ASP:HB3	1.82	0.60
2:B:342:ASP:OD1	2:B:343:VAL:N	2.34	0.60
1:A:144:ARG:NH1	2:B:427:GLU:OE1	2.35	0.60
1:A:709:GLU:OE2	2:B:460:ARG:NE	2.33	0.60
2:B:175:VAL:HG13	2:B:203:VAL:HG13	1.85	0.59
1:A:699:GLU:OE1	1:A:699:GLU:N	2.36	0.59
2:B:659:PHE:HE2	2:B:696:SER:H	1.49	0.59
1:A:606:PRO:O	1:A:681:ASN:ND2	2.33	0.59
2:B:628:ILE:HD11	2:B:661:ARG:HB2	1.84	0.59
1:A:202:THR:OG1	1:A:246:GLY:O	2.21	0.59
1:A:518:GLU:N	1:A:518:GLU:OE1	2.35	0.59
1:A:202:THR:OG1	1:A:325:HIS:ND1	2.36	0.58
2:B:729:GLN:NE2	2:B:733:ASP:OD2	2.37	0.58
1:A:516:ALA:HA	1:A:563:PHE:HZ	1.69	0.57
1:A:630:MET:HE1	2:B:558:ARG:HH22	1.69	0.57
2:B:717:CYS:SG	2:B:718:ASP:N	2.78	0.57
2:B:259:ARG:NH2	2:B:341:GLU:OE2	2.37	0.57
2:B:337:TYR:HD2	2:B:347:ARG:HH12	1.52	0.57
2:B:238:LYS:NZ	4:B:1001:UDP:O2	2.37	0.56
2:B:269:ASP:O	2:B:273:GLU:HG3	2.05	0.56
2:B:788:SER:HB2	3:B:1002:NAG:H61	1.87	0.56
1:A:540:ALA:O	1:A:629:ARG:NH1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:HIS:ND1	2:B:248:ASP:OD1	2.38	0.56
2:B:619:LYS:NZ	2:B:786:TYR:OH	2.35	0.56
1:A:675:SER:OG	1:A:676:GLU:N	2.36	0.56
2:B:431:MET:HE3	2:B:431:MET:HA	1.88	0.56
2:B:723:PHE:HB3	2:B:829:VAL:HB	1.87	0.56
1:A:494:VAL:HG21	2:B:498:THR:HG23	1.87	0.55
2:B:262:ASP:N	2:B:262:ASP:OD1	2.33	0.55
2:B:626:PRO:HG3	2:B:697:ARG:HD2	1.89	0.54
1:A:238:THR:HG22	1:A:240:GLY:H	1.71	0.54
1:A:117:GLN:NE2	1:A:146:GLU:OE2	2.40	0.54
2:B:187:ARG:NH1	2:B:397:LYS:HG3	2.23	0.54
2:B:179:THR:HG21	2:B:188:ALA:HB2	1.89	0.53
2:B:264:VAL:HG23	2:B:394:HIS:HB2	1.91	0.53
2:B:632:ASP:N	2:B:632:ASP:OD1	2.41	0.53
2:B:807:ASP:N	2:B:807:ASP:OD1	2.40	0.53
2:B:313:PRO:HB2	2:B:367:PHE:HB3	1.89	0.53
1:A:670:ASP:N	1:A:670:ASP:OD1	2.42	0.53
2:B:464:ILE:HB	2:B:528:ARG:HH11	1.73	0.53
2:B:568:SER:OG	2:B:569:LYS:N	2.39	0.53
1:A:510:VAL:HA	1:A:612:LEU:HB3	1.90	0.53
1:A:228:ARG:HD2	1:A:302:HIS:CD2	2.43	0.52
1:A:203:TYR:OH	1:A:337:HIS:ND1	2.30	0.52
2:B:247:HIS:HB2	2:B:322:LEU:HD12	1.91	0.52
2:B:620:LYS:NZ	2:B:685:GLU:OE2	2.42	0.52
2:B:200:PRO:HG2	2:B:272:GLU:HB2	1.91	0.52
1:A:141:LEU:HD11	1:A:145:LEU:HD22	1.91	0.52
1:A:444:GLN:HB2	1:A:470:GLU:HB3	1.91	0.52
2:B:289:THR:OG1	2:B:358:VAL:O	2.28	0.52
2:B:269:ASP:N	2:B:269:ASP:OD1	2.42	0.52
1:A:511:LEU:HD13	1:A:601:LEU:HD13	1.93	0.51
2:B:247:HIS:CD2	2:B:251:LEU:HD22	2.46	0.51
1:A:223:HIS:NE2	1:A:258:GLN:OE1	2.42	0.51
2:B:709:ASP:OD1	2:B:712:THR:OG1	2.29	0.51
1:A:247:PHE:O	1:A:300:TYR:OH	2.27	0.50
1:A:723:VAL:HG23	2:B:468:PHE:HB2	1.93	0.50
2:B:259:ARG:NH1	2:B:311:GLY:O	2.39	0.50
1:A:425:VAL:HG12	1:A:465:LEU:HD11	1.93	0.49
2:B:710:ASN:HB2	2:B:788:SER:HB3	1.95	0.49
1:A:585:LEU:HD22	1:A:604:LYS:HE3	1.95	0.48
1:A:595:LEU:HD12	1:A:688:ARG:HD3	1.95	0.48
2:B:674:ILE:HG13	2:B:688:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:THR:HG21	1:A:726:ALA:HB1	1.96	0.48
1:A:218:LEU:HB3	3:B:1003:NAG:H82	1.95	0.47
1:A:461:MET:HG2	1:A:463:TYR:CE1	2.49	0.47
2:B:335:GLU:OE2	2:B:351:ARG:NE	2.47	0.47
1:A:443:LEU:HD13	1:A:469:LEU:HD13	1.96	0.47
1:A:595:LEU:HD23	1:A:705:LEU:O	2.14	0.47
2:B:184:LEU:HD22	2:B:223:VAL:HG11	1.97	0.47
2:B:441:LYS:HA	2:B:444:GLN:HE21	1.80	0.47
2:B:749:GLN:OE1	2:B:765:TYR:N	2.47	0.47
2:B:192:GLN:HB2	2:B:221:LEU:HD21	1.97	0.47
1:A:186:GLU:HA	1:A:186:GLU:OE2	2.14	0.47
2:B:202:ARG:HH11	2:B:202:ARG:HG3	1.77	0.47
1:A:627:ARG:NH2	1:A:724:GLU:OE1	2.37	0.46
2:B:331:GLU:O	2:B:335:GLU:HG2	2.15	0.46
2:B:618:GLU:O	2:B:651:ASN:ND2	2.49	0.46
1:A:730:ARG:N	1:A:730:ARG:HD3	2.30	0.46
1:A:368:ASP:HB3	1:A:371:GLN:HB2	1.96	0.46
1:A:334:TYR:CD1	2:B:431:MET:HE1	2.50	0.46
2:B:256:TRP:HH2	2:B:284:LEU:HD12	1.81	0.46
1:A:232:PHE:CE2	1:A:281:ARG:HG2	2.50	0.46
1:A:604:LYS:HB2	1:A:604:LYS:HE2	1.63	0.46
1:A:212:LEU:O	1:A:216:LEU:HD12	2.16	0.46
2:B:642:GLU:HG3	2:B:643:ASN:N	2.31	0.46
1:A:355:LEU:HD22	2:B:410:LEU:HD22	1.98	0.46
1:A:411:ARG:HD2	2:B:768:PHE:HB2	1.98	0.46
2:B:234:PRO:O	2:B:236:GLN:N	2.48	0.45
2:B:247:HIS:CD2	2:B:326:VAL:HG21	2.51	0.45
2:B:620:LYS:HG2	2:B:651:ASN:HD21	1.82	0.45
2:B:174:TYR:HE2	2:B:246:MET:HG2	1.82	0.45
1:A:226:LEU:HB3	1:A:250:LEU:HB3	1.98	0.45
1:A:483:ARG:HH21	2:B:578:LEU:HB3	1.81	0.45
2:B:710:ASN:HA	2:B:787:LYS:HB3	1.99	0.45
1:A:253:ARG:O	1:A:257:GLN:HG2	2.17	0.45
1:A:151:LEU:HD12	1:A:168:LEU:HD21	1.99	0.45
1:A:456:ASP:HB3	1:A:459:ARG:HB3	1.99	0.45
1:A:607:LEU:HA	1:A:681:ASN:HD22	1.82	0.45
2:B:252:ASP:OD1	2:B:252:ASP:N	2.34	0.44
2:B:242:MET:HE2	2:B:242:MET:HB3	1.73	0.44
2:B:388:HIS:NE2	2:B:408:TYR:OH	2.35	0.44
2:B:718:ASP:OD1	2:B:719:VAL:N	2.50	0.44
2:B:722:ILE:HD13	2:B:832:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:SER:OG	1:A:127:GLN:N	2.50	0.44
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.85	0.44
1:A:701:LEU:HD22	1:A:705:LEU:HD22	1.99	0.44
2:B:413:LYS:HE3	2:B:413:LYS:HB2	1.76	0.44
1:A:337:HIS:HD2	2:B:431:MET:SD	2.40	0.44
2:B:814:VAL:HG13	2:B:819:LEU:HB2	1.99	0.44
2:B:487:LEU:HD12	2:B:487:LEU:HA	1.88	0.43
2:B:708:PHE:O	2:B:787:LYS:NZ	2.52	0.43
1:A:232:PHE:HE1	1:A:242:TYR:HB3	1.83	0.43
2:B:189:LEU:HD13	2:B:220:PRO:HB2	2.00	0.43
2:B:278:LEU:HD13	2:B:284:LEU:HD13	2.01	0.43
2:B:303:GLU:OE1	2:B:304:PRO:HD3	2.19	0.43
1:A:508:LEU:HD11	1:A:612:LEU:HD12	2.00	0.43
1:A:620:LEU:HD22	1:A:625:LEU:HD21	1.99	0.43
2:B:622:HIS:NE2	2:B:653:LYS:HD3	2.33	0.43
1:A:379:ILE:HG21	1:A:488:LEU:HD21	1.99	0.43
2:B:661:ARG:HD2	2:B:662:ASP:CG	2.44	0.43
1:A:133:LEU:HB3	1:A:200:ASP:HB2	2.00	0.43
1:A:269:ASP:OD1	1:A:270:ILE:N	2.48	0.43
2:B:260:ALA:HB1	2:B:264:VAL:HG11	2.00	0.43
2:B:395:PRO:HB2	2:B:397:LYS:HD2	1.99	0.43
2:B:659:PHE:CD2	2:B:695:PHE:HA	2.53	0.43
1:A:421:ASP:OD2	1:A:463:TYR:OH	2.37	0.42
1:A:704:SER:O	1:A:704:SER:OG	2.22	0.42
2:B:427:GLU:O	2:B:431:MET:HG2	2.20	0.42
1:A:125:THR:OG1	1:A:126:SER:N	2.53	0.42
1:A:269:ASP:OD1	1:A:270:ILE:HG23	2.18	0.42
2:B:691:MET:HE1	2:B:703:MET:CE	2.49	0.42
1:A:450:ASN:HD21	2:B:729:GLN:HE22	1.67	0.42
1:A:644:PHE:CE1	1:A:667:GLY:HA3	2.55	0.42
2:B:469:LEU:O	2:B:525:GLY:N	2.52	0.42
1:A:309:GLU:OE2	1:A:332:HIS:NE2	2.50	0.42
2:B:187:ARG:HH12	2:B:397:LYS:HG3	1.82	0.42
2:B:503:MET:HE1	2:B:517:ILE:HG22	2.02	0.42
1:A:360:GLN:HG3	1:A:377:VAL:HG21	2.02	0.42
1:A:546:LEU:HD13	1:A:597:LEU:HD12	2.00	0.42
1:A:168:LEU:HD12	1:A:179:LEU:HB3	2.00	0.41
1:A:599:ASP:OD2	1:A:684:TYR:OH	2.25	0.41
2:B:826:GLU:HG3	2:B:829:VAL:HG12	2.00	0.41
1:A:121:VAL:HG22	1:A:196:PHE:HB3	2.02	0.41
1:A:190:ASP:OD1	1:A:190:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:HD23	2:B:333:LEU:HA	1.92	0.41
2:B:697:ARG:NH2	2:B:781:GLY:O	2.53	0.41
2:B:256:TRP:CG	2:B:275:LEU:HD13	2.56	0.41
2:B:281:SER:O	2:B:320:GLU:HG3	2.20	0.41
1:A:701:LEU:HD23	1:A:701:LEU:HA	1.78	0.41
1:A:727:LEU:HD23	1:A:727:LEU:HA	1.88	0.41
2:B:440:SER:O	2:B:444:GLN:HG2	2.20	0.41
2:B:742:TYR:OH	2:B:826:GLU:OE1	2.27	0.41
1:A:564:ALA:N	1:A:565:PRO:HD2	2.36	0.41
2:B:618:GLU:OE1	2:B:618:GLU:N	2.53	0.41
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.89	0.41
1:A:674:ALA:HA	1:A:721:ARG:HH12	1.85	0.41
2:B:247:HIS:HD2	2:B:251:LEU:HD22	1.85	0.41
1:A:119:LEU:HD22	1:A:213:THR:HG21	2.03	0.41
1:A:292:THR:HG22	1:A:294:ASP:H	1.85	0.40
1:A:526:LEU:HD23	1:A:526:LEU:HA	1.86	0.40
1:A:538:ASP:OD1	1:A:538:ASP:N	2.51	0.40
1:A:644:PHE:HE1	1:A:667:GLY:HA3	1.85	0.40
2:B:691:MET:HE1	2:B:703:MET:SD	2.62	0.40
2:B:206:PHE:CG	2:B:242:MET:HG3	2.55	0.40
2:B:303:GLU:OE1	2:B:303:GLU:HA	2.21	0.40
2:B:666:ASP:HB2	2:B:670:HIS:CE1	2.56	0.40
1:A:125:THR:HG23	1:A:152:THR:HB	2.04	0.40
1:A:595:LEU:HD13	1:A:595:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	579/710 (82%)	550 (95%)	29 (5%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	572/753 (76%)	553 (97%)	19 (3%)	0	100	100
All	All	1151/1463 (79%)	1103 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	487/577 (84%)	486 (100%)	1 (0%)	92	97
2	B	534/662 (81%)	534 (100%)	0	100	100
All	All	1021/1239 (82%)	1020 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	HIS
1	A	444	GLN
1	A	713	HIS
2	B	181	GLN
2	B	288	GLN
2	B	307	ASN
2	B	365	GLN
2	B	370	ASN
2	B	402	GLN
2	B	407	ASN
2	B	444	GLN
2	B	564	GLN

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Mol	Chain	Res	Type
2	B	581	ASN
2	B	588	ASN
2	B	622	HIS
2	B	643	ASN
2	B	729	GLN
2	B	749	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	B	1003	2	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	B	1002	2	14,14,15	0.20	0	17,19,21	0.47	0
4	UDP	B	1001	5	24,26,26	0.41	0	37,40,40	0.76	2 (5%)
3	NAG	A	801	1	14,14,15	0.18	0	17,19,21	0.38	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	B	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1002	2	-	1/6/23/26	0/1/1/1
4	UDP	B	1001	5	-	5/16/32/32	0/2/2/2
3	NAG	A	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	UDP	PA-O3A-PB	-2.82	123.16	132.83
4	B	1001	UDP	O3B-PB-O3A	2.22	112.07	104.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	NAG	O5-C5-C6-O6
3	A	801	NAG	C4-C5-C6-O6
3	B	1003	NAG	O5-C5-C6-O6
3	B	1003	NAG	C4-C5-C6-O6
3	B	1002	NAG	O5-C5-C6-O6
4	B	1001	UDP	O4'-C4'-C5'-O5'
4	B	1001	UDP	O4'-C1'-N1-C6
4	B	1001	UDP	C2'-C1'-N1-C6
4	B	1001	UDP	C3'-C4'-C5'-O5'
4	B	1001	UDP	O4'-C1'-N1-C2

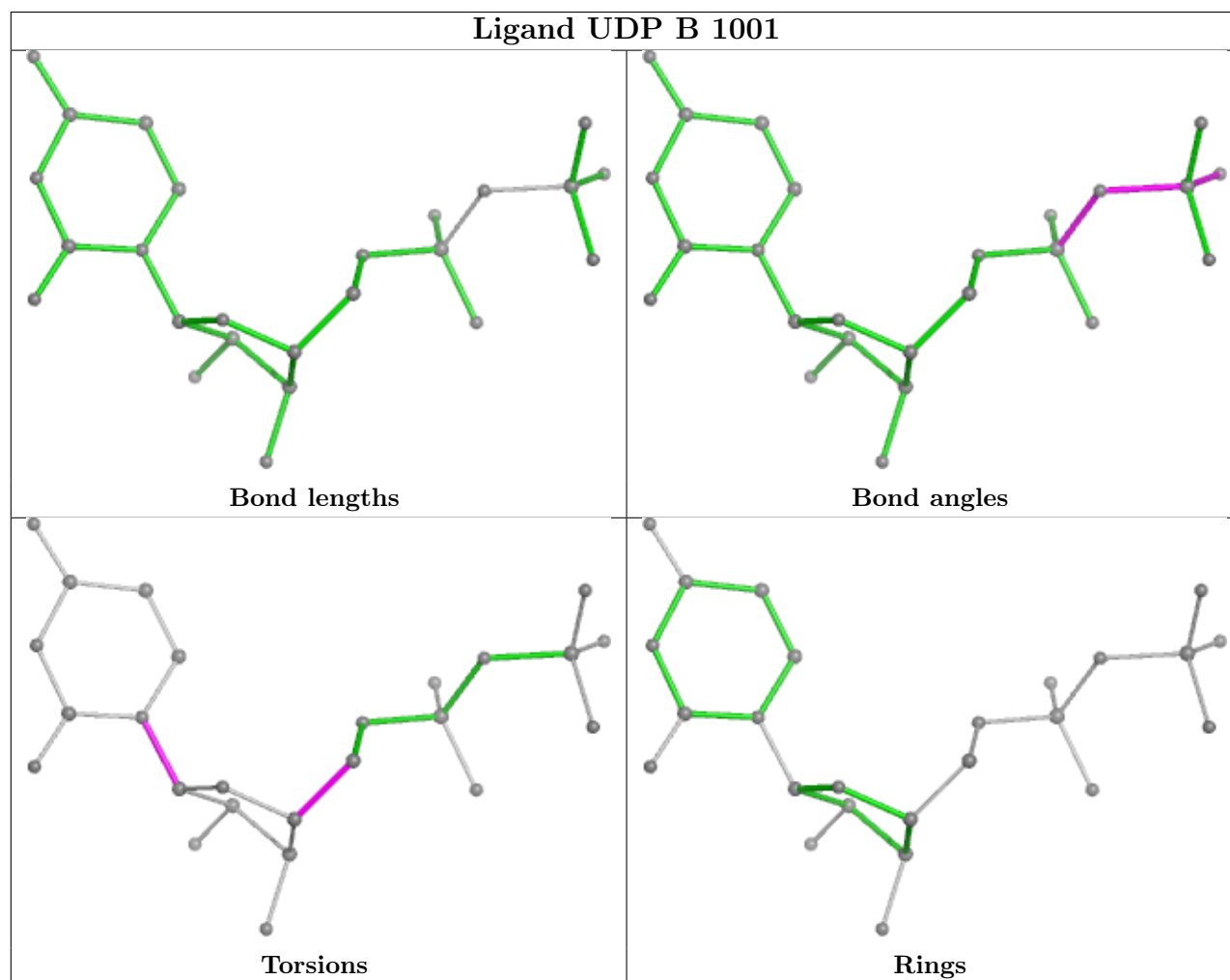
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003	NAG	1	0
3	B	1002	NAG	1	0
4	B	1001	UDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

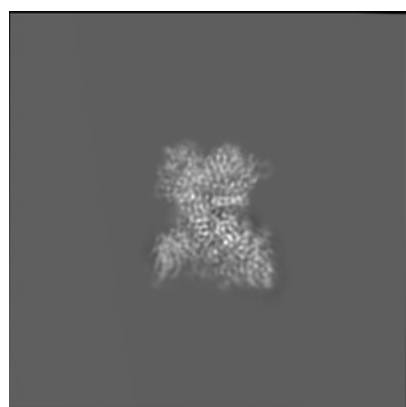
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52913. These allow visual inspection of the internal detail of the map and identification of artifacts.

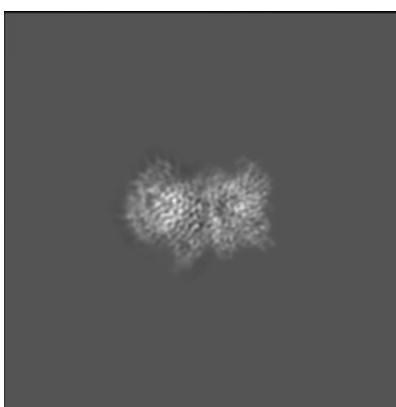
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

#### 6.1.1 Primary map



X



Y



Z

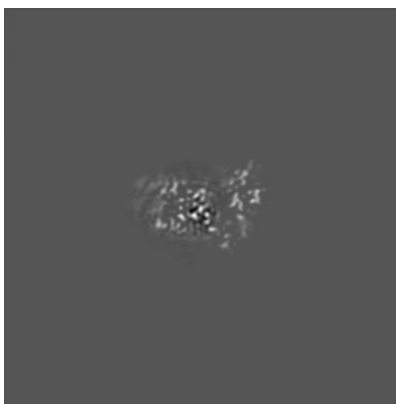
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

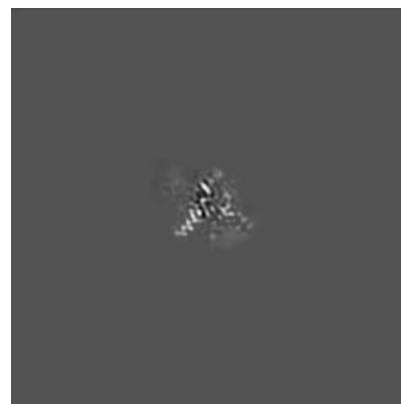
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

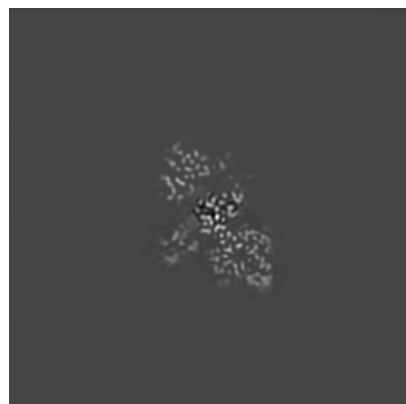


Z Index: 192

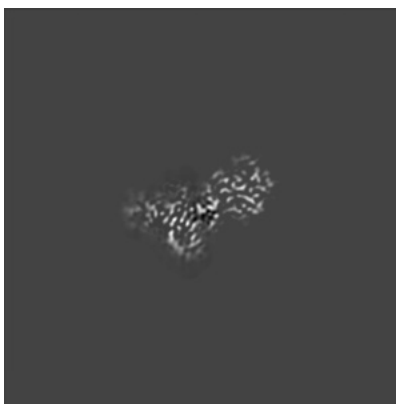
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 185



Y Index: 207

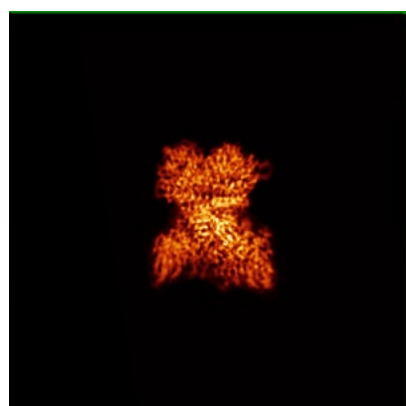


Z Index: 163

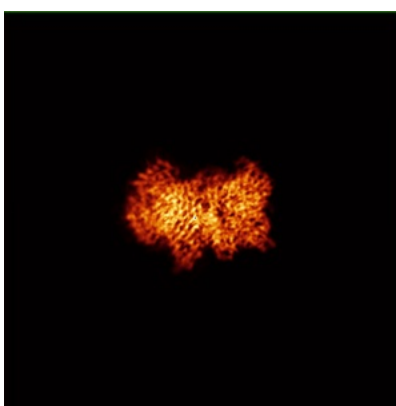
The images above show the largest variance slices of the map in three orthogonal directions.

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

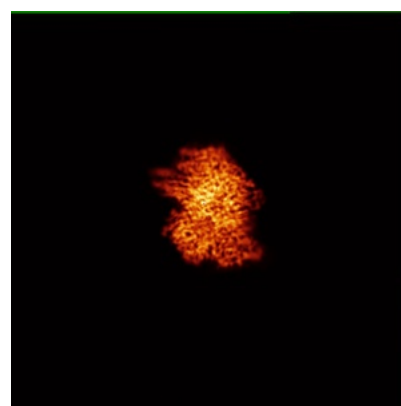
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0918. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

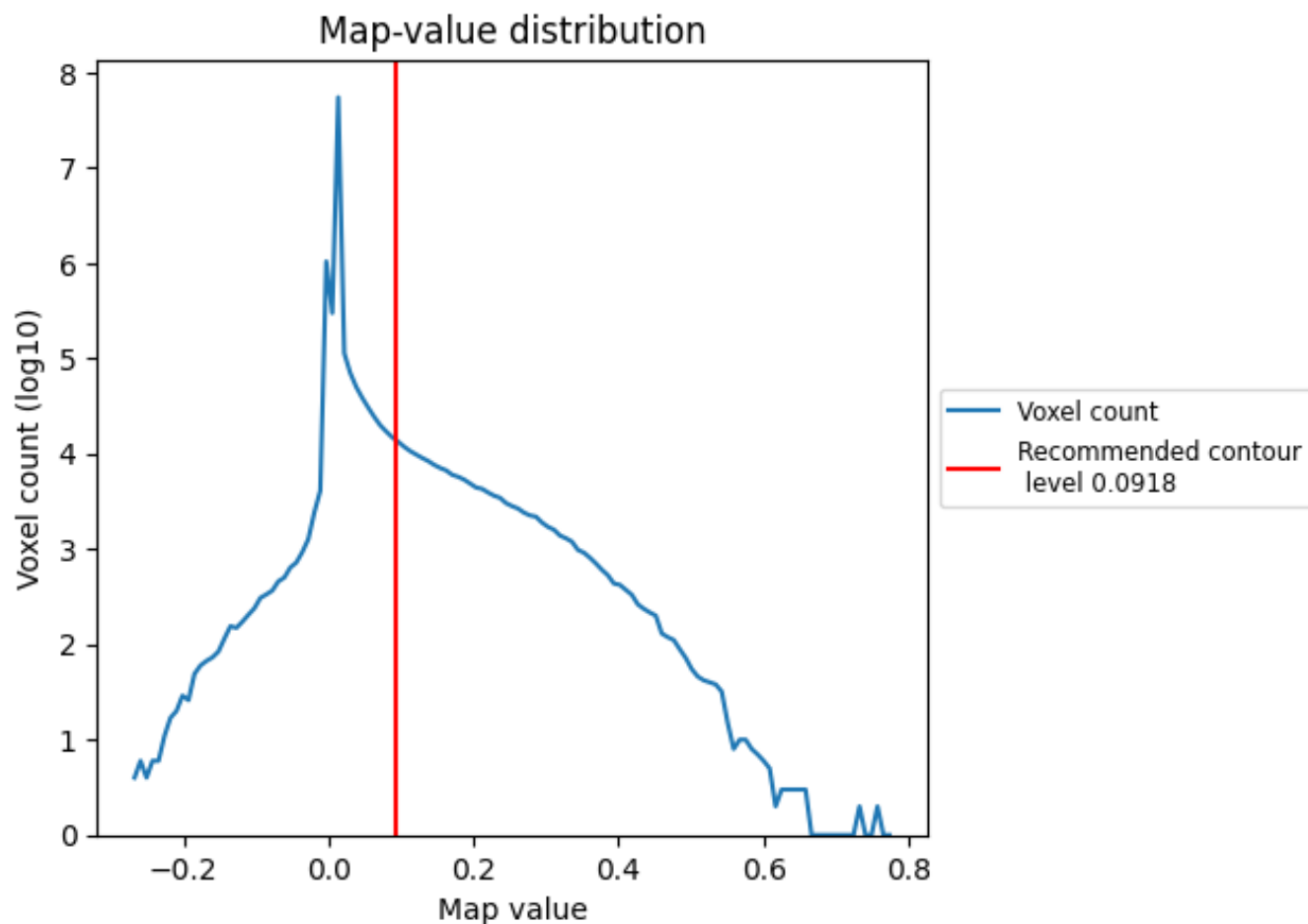
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

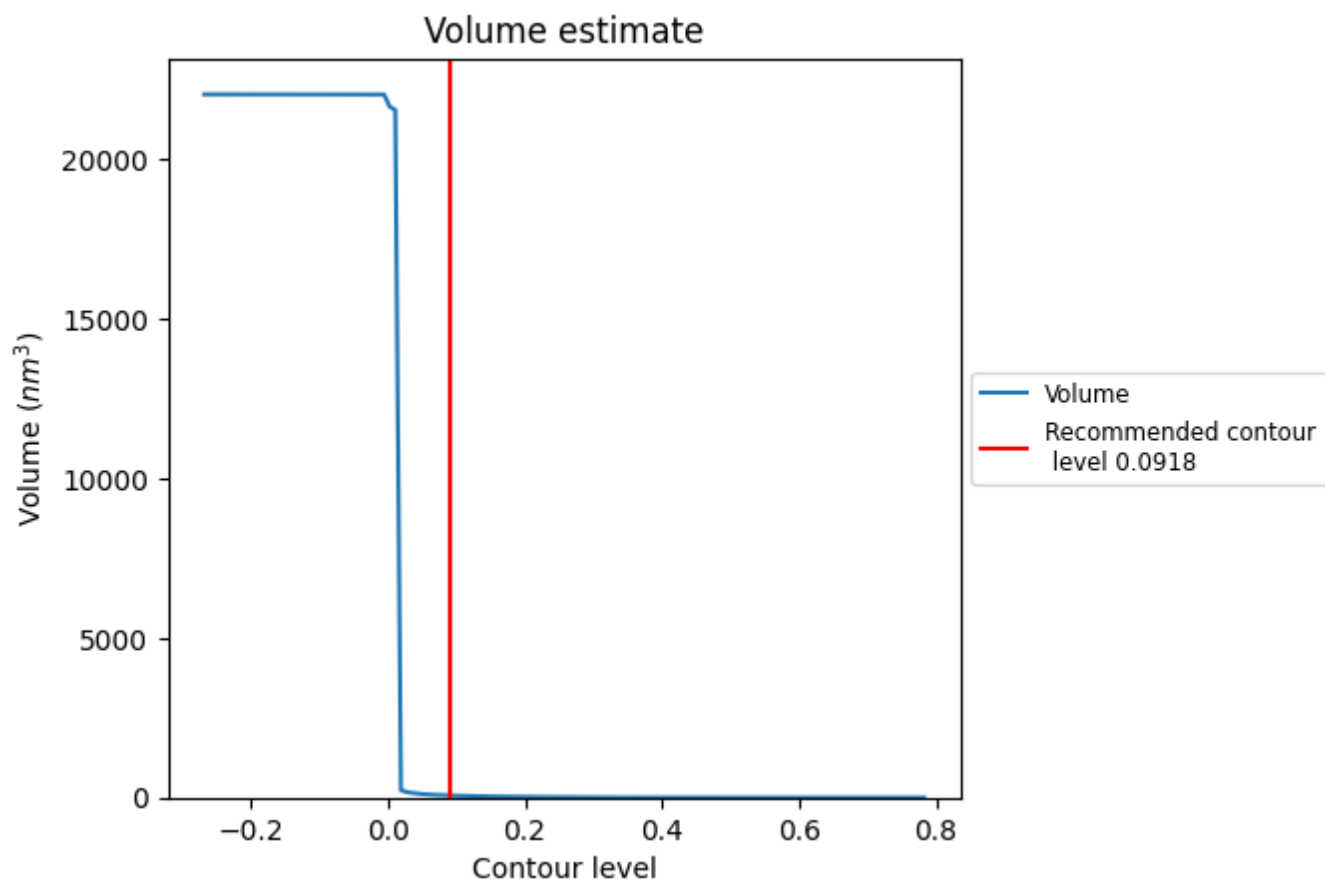
This section contains the results of statistical analysis of the map.

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



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

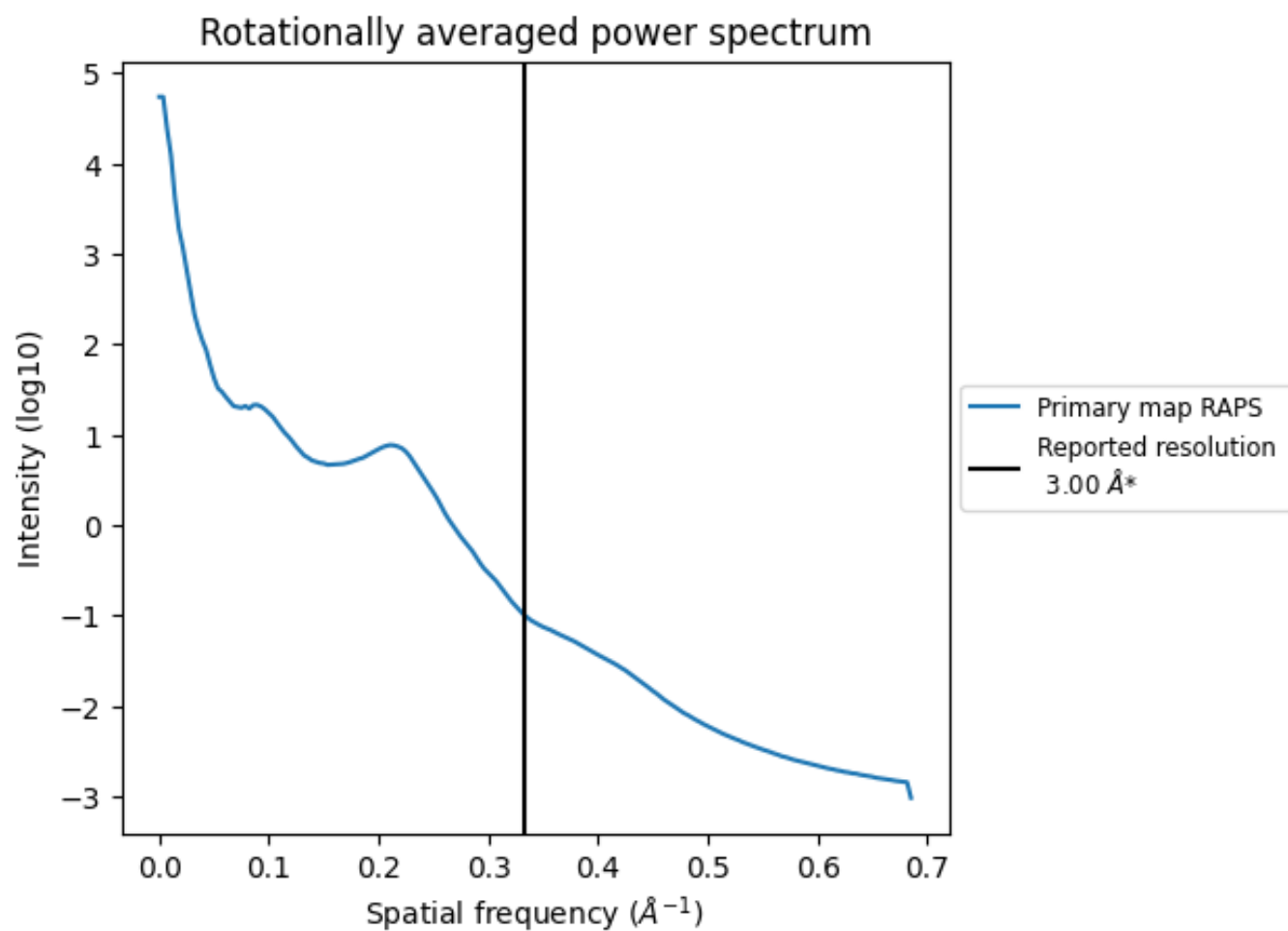
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64  $\text{nm}^3$ ; this corresponds to an approximate mass of 58 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 0.333 Å<sup>-1</sup>

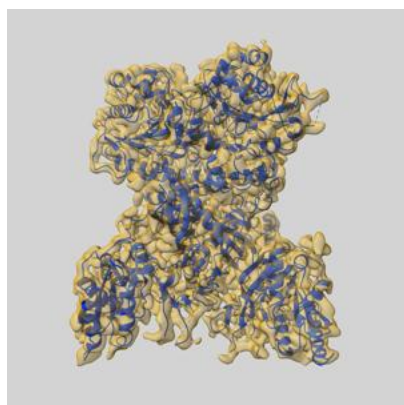
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

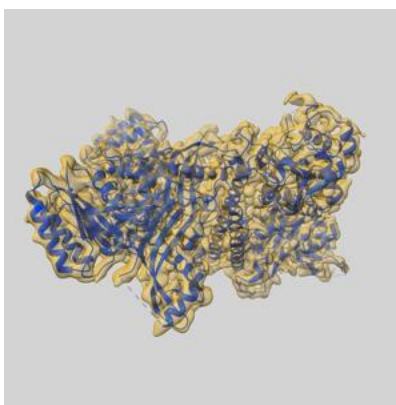
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52913 and PDB model 9Q8Z. Per-residue inclusion information can be found in section [3](#) on page [6](#).

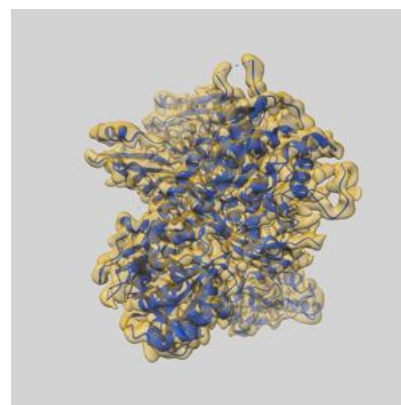
### 9.1 Map-model overlay [i](#)



X



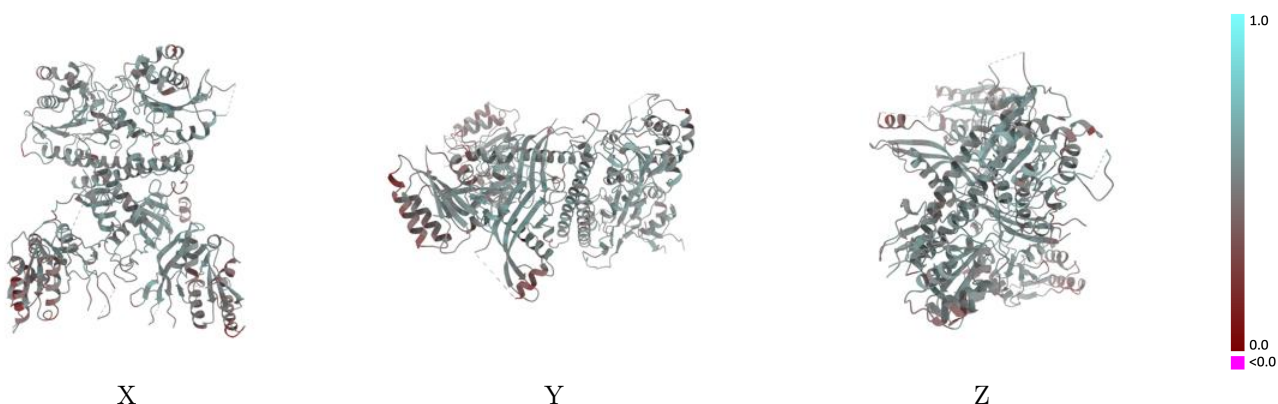
Y



Z

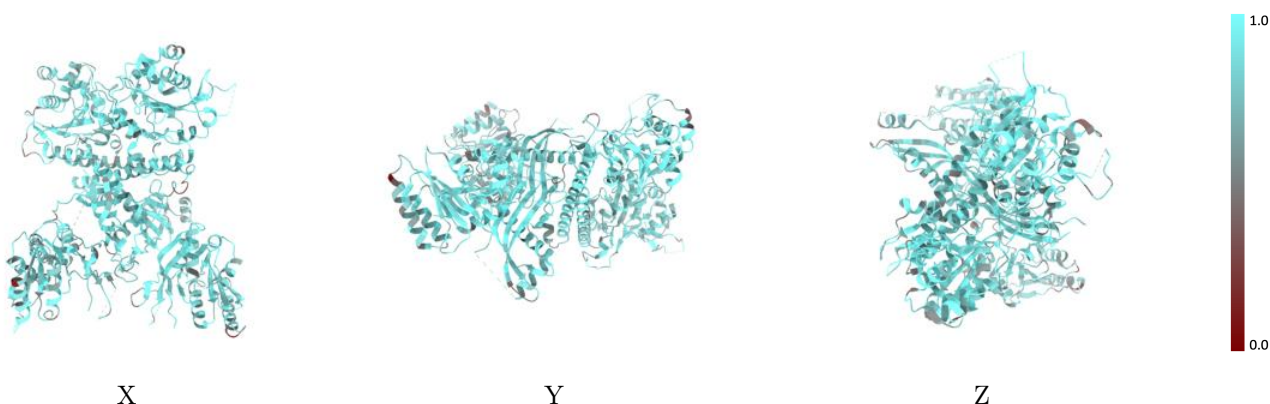
The images above show the 3D surface view of the map at the recommended contour level 0.0918 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



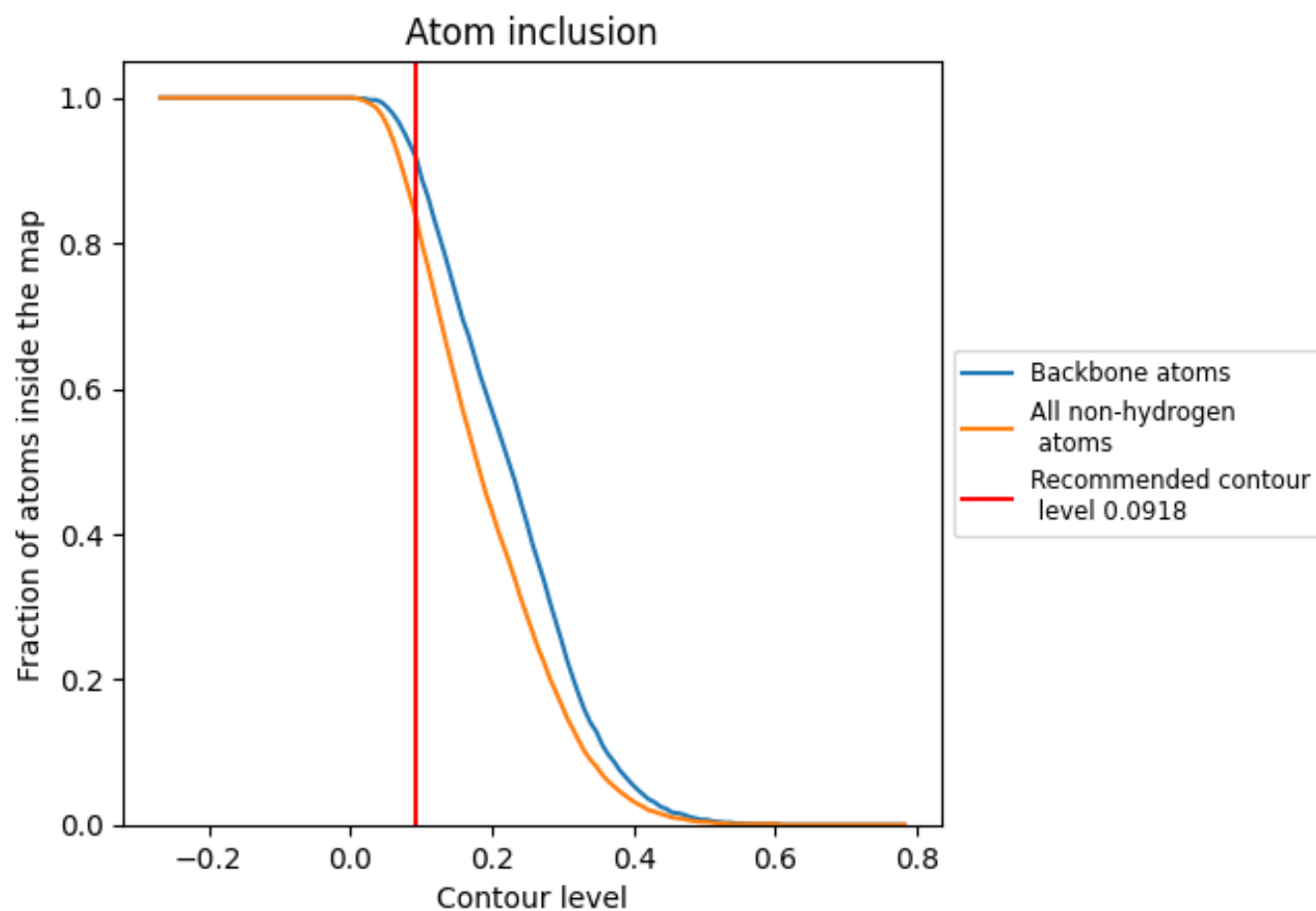
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0918).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.0918) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8380	<div></div> 0.5020
A	<div></div> 0.8260	<div></div> 0.4980
B	<div></div> 0.8490	<div></div> 0.5060

