



Full wwPDB EM Validation Report ⓘ

Jun 9, 2026 – 04:36 pm BST

PDB ID : 9RIA / pdb_00009ria
EMDB ID : EMD-53991
Title : Cryo-EM structure of tomato NRC3-AVRcap1b complex
Authors : Seager, B.A.; Kamoun, S.; Madhuprakash, J.
Deposited on : 2025-06-11
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

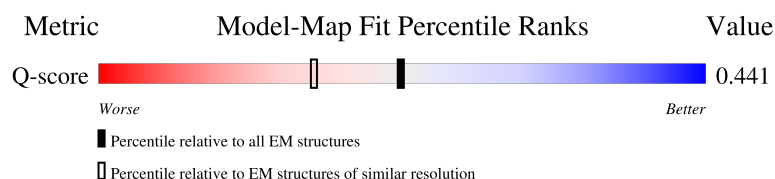
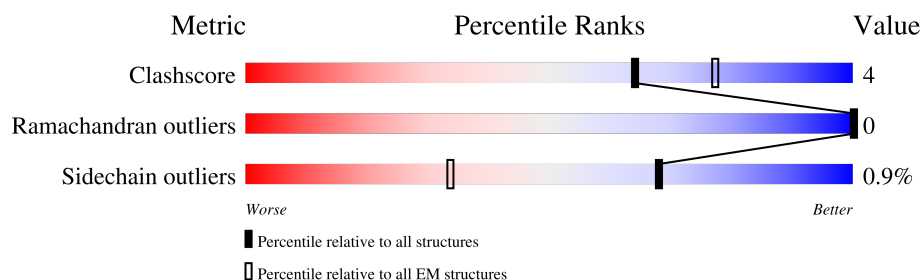
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	919	16% 81% 11% 8%
1	B	919	10% 81% 11% 8%
1	C	919	20% 81% 11% 8%
2	G	684	7% 71% 8% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24721 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 NRC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	845	Total	C	N	O	S	0	0
			6757	4305	1169	1253	30		
1	B	845	Total	C	N	O	S	0	0
			6758	4303	1170	1255	30		
1	C	843	Total	C	N	O	S	0	0
			6738	4291	1164	1253	30		

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
A	13	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
A	17	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
A	892	SER	-	expression tag	UNP A0A3Q7GDL1
A	893	ASP	-	expression tag	UNP A0A3Q7GDL1
A	894	TYR	-	expression tag	UNP A0A3Q7GDL1
A	895	LYS	-	expression tag	UNP A0A3Q7GDL1
A	896	ASP	-	expression tag	UNP A0A3Q7GDL1
A	897	HIS	-	expression tag	UNP A0A3Q7GDL1
A	898	ASP	-	expression tag	UNP A0A3Q7GDL1
A	899	GLY	-	expression tag	UNP A0A3Q7GDL1
A	900	ASP	-	expression tag	UNP A0A3Q7GDL1
A	901	TYR	-	expression tag	UNP A0A3Q7GDL1
A	902	LYS	-	expression tag	UNP A0A3Q7GDL1
A	903	ASP	-	expression tag	UNP A0A3Q7GDL1
A	904	HIS	-	expression tag	UNP A0A3Q7GDL1
A	905	ASP	-	expression tag	UNP A0A3Q7GDL1
A	906	LEU	-	expression tag	UNP A0A3Q7GDL1
A	907	ASP	-	expression tag	UNP A0A3Q7GDL1
A	908	ALA	-	expression tag	UNP A0A3Q7GDL1
A	909	ALA	-	expression tag	UNP A0A3Q7GDL1
A	910	ALA	-	expression tag	UNP A0A3Q7GDL1
A	911	ALA	-	expression tag	UNP A0A3Q7GDL1
A	912	ASP	-	expression tag	UNP A0A3Q7GDL1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	913	TYR	-	expression tag	UNP A0A3Q7GDL1
A	914	LYS	-	expression tag	UNP A0A3Q7GDL1
A	915	ASP	-	expression tag	UNP A0A3Q7GDL1
A	916	ASP	-	expression tag	UNP A0A3Q7GDL1
A	917	ASP	-	expression tag	UNP A0A3Q7GDL1
A	918	ASP	-	expression tag	UNP A0A3Q7GDL1
A	919	LYS	-	expression tag	UNP A0A3Q7GDL1
B	9	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
B	13	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
B	17	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
B	892	SER	-	expression tag	UNP A0A3Q7GDL1
B	893	ASP	-	expression tag	UNP A0A3Q7GDL1
B	894	TYR	-	expression tag	UNP A0A3Q7GDL1
B	895	LYS	-	expression tag	UNP A0A3Q7GDL1
B	896	ASP	-	expression tag	UNP A0A3Q7GDL1
B	897	HIS	-	expression tag	UNP A0A3Q7GDL1
B	898	ASP	-	expression tag	UNP A0A3Q7GDL1
B	899	GLY	-	expression tag	UNP A0A3Q7GDL1
B	900	ASP	-	expression tag	UNP A0A3Q7GDL1
B	901	TYR	-	expression tag	UNP A0A3Q7GDL1
B	902	LYS	-	expression tag	UNP A0A3Q7GDL1
B	903	ASP	-	expression tag	UNP A0A3Q7GDL1
B	904	HIS	-	expression tag	UNP A0A3Q7GDL1
B	905	ASP	-	expression tag	UNP A0A3Q7GDL1
B	906	LEU	-	expression tag	UNP A0A3Q7GDL1
B	907	ASP	-	expression tag	UNP A0A3Q7GDL1
B	908	ALA	-	expression tag	UNP A0A3Q7GDL1
B	909	ALA	-	expression tag	UNP A0A3Q7GDL1
B	910	ALA	-	expression tag	UNP A0A3Q7GDL1
B	911	ALA	-	expression tag	UNP A0A3Q7GDL1
B	912	ASP	-	expression tag	UNP A0A3Q7GDL1
B	913	TYR	-	expression tag	UNP A0A3Q7GDL1
B	914	LYS	-	expression tag	UNP A0A3Q7GDL1
B	915	ASP	-	expression tag	UNP A0A3Q7GDL1
B	916	ASP	-	expression tag	UNP A0A3Q7GDL1
B	917	ASP	-	expression tag	UNP A0A3Q7GDL1
B	918	ASP	-	expression tag	UNP A0A3Q7GDL1
B	919	LYS	-	expression tag	UNP A0A3Q7GDL1
C	9	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
C	13	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
C	17	GLU	LEU	engineered mutation	UNP A0A3Q7GDL1
C	892	SER	-	expression tag	UNP A0A3Q7GDL1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	893	ASP	-	expression tag	UNP A0A3Q7GDL1
C	894	TYR	-	expression tag	UNP A0A3Q7GDL1
C	895	LYS	-	expression tag	UNP A0A3Q7GDL1
C	896	ASP	-	expression tag	UNP A0A3Q7GDL1
C	897	HIS	-	expression tag	UNP A0A3Q7GDL1
C	898	ASP	-	expression tag	UNP A0A3Q7GDL1
C	899	GLY	-	expression tag	UNP A0A3Q7GDL1
C	900	ASP	-	expression tag	UNP A0A3Q7GDL1
C	901	TYR	-	expression tag	UNP A0A3Q7GDL1
C	902	LYS	-	expression tag	UNP A0A3Q7GDL1
C	903	ASP	-	expression tag	UNP A0A3Q7GDL1
C	904	HIS	-	expression tag	UNP A0A3Q7GDL1
C	905	ASP	-	expression tag	UNP A0A3Q7GDL1
C	906	LEU	-	expression tag	UNP A0A3Q7GDL1
C	907	ASP	-	expression tag	UNP A0A3Q7GDL1
C	908	ALA	-	expression tag	UNP A0A3Q7GDL1
C	909	ALA	-	expression tag	UNP A0A3Q7GDL1
C	910	ALA	-	expression tag	UNP A0A3Q7GDL1
C	911	ALA	-	expression tag	UNP A0A3Q7GDL1
C	912	ASP	-	expression tag	UNP A0A3Q7GDL1
C	913	TYR	-	expression tag	UNP A0A3Q7GDL1
C	914	LYS	-	expression tag	UNP A0A3Q7GDL1
C	915	ASP	-	expression tag	UNP A0A3Q7GDL1
C	916	ASP	-	expression tag	UNP A0A3Q7GDL1
C	917	ASP	-	expression tag	UNP A0A3Q7GDL1
C	918	ASP	-	expression tag	UNP A0A3Q7GDL1
C	919	LYS	-	expression tag	UNP A0A3Q7GDL1

- Molecule 2 is a protein called RxLR effector protein PITG_16705.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	542	Total	C	N	O	S	0	0
			4375	2810	738	816	11		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	61	MET	-	initiating methionine	UNP D0NVF3
G	92	GLU	PRO	engineered mutation	UNP D0NVF3
G	679	TYR	-	expression tag	UNP D0NVF3
G	680	SER	-	expression tag	UNP D0NVF3
G	681	TYR	-	expression tag	UNP D0NVF3

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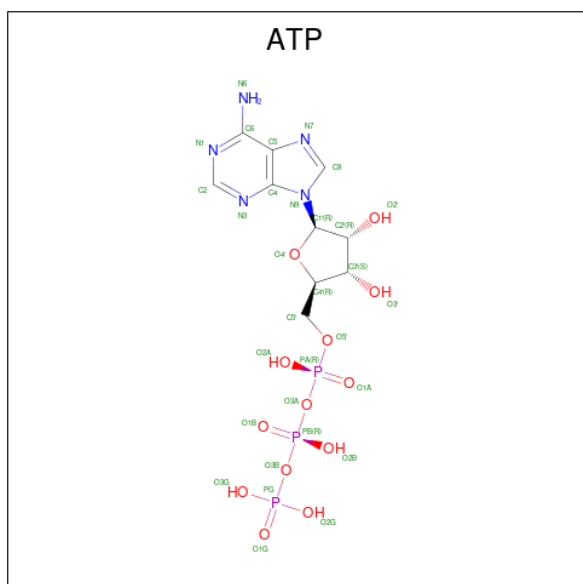
Chain	Residue	Modelled	Actual	Comment	Reference
G	682	PRO	-	expression tag	UNP D0NVF3
G	683	TYR	-	expression tag	UNP D0NVF3
G	684	ASP	-	expression tag	UNP D0NVF3
G	685	VAL	-	expression tag	UNP D0NVF3
G	686	PRO	-	expression tag	UNP D0NVF3
G	687	ASP	-	expression tag	UNP D0NVF3
G	688	TYR	-	expression tag	UNP D0NVF3
G	689	ALA	-	expression tag	UNP D0NVF3
G	690	GLY	-	expression tag	UNP D0NVF3
G	691	TYR	-	expression tag	UNP D0NVF3
G	692	PRO	-	expression tag	UNP D0NVF3
G	693	TYR	-	expression tag	UNP D0NVF3
G	694	ASP	-	expression tag	UNP D0NVF3
G	695	VAL	-	expression tag	UNP D0NVF3
G	696	PRO	-	expression tag	UNP D0NVF3
G	697	ASP	-	expression tag	UNP D0NVF3
G	698	TYR	-	expression tag	UNP D0NVF3
G	699	ALA	-	expression tag	UNP D0NVF3
G	700	GLY	-	expression tag	UNP D0NVF3
G	701	LEU	-	expression tag	UNP D0NVF3
G	702	TYR	-	expression tag	UNP D0NVF3
G	703	PRO	-	expression tag	UNP D0NVF3
G	704	TYR	-	expression tag	UNP D0NVF3
G	705	ASP	-	expression tag	UNP D0NVF3
G	706	VAL	-	expression tag	UNP D0NVF3
G	707	PRO	-	expression tag	UNP D0NVF3
G	708	ASP	-	expression tag	UNP D0NVF3
G	709	TYR	-	expression tag	UNP D0NVF3
G	710	ALA	-	expression tag	UNP D0NVF3
G	711	THR	-	expression tag	UNP D0NVF3
G	712	ARG	-	expression tag	UNP D0NVF3
G	713	ALA	-	expression tag	UNP D0NVF3
G	714	ALA	-	expression tag	UNP D0NVF3
G	715	TYR	-	expression tag	UNP D0NVF3
G	716	PRO	-	expression tag	UNP D0NVF3
G	717	TYR	-	expression tag	UNP D0NVF3
G	718	ASP	-	expression tag	UNP D0NVF3
G	719	VAL	-	expression tag	UNP D0NVF3
G	720	PRO	-	expression tag	UNP D0NVF3
G	721	ASP	-	expression tag	UNP D0NVF3
G	722	TYR	-	expression tag	UNP D0NVF3
G	723	ALA	-	expression tag	UNP D0NVF3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	724	GLY	-	expression tag	UNP D0NVF3
G	725	TYR	-	expression tag	UNP D0NVF3
G	726	PRO	-	expression tag	UNP D0NVF3
G	727	TYR	-	expression tag	UNP D0NVF3
G	728	ASP	-	expression tag	UNP D0NVF3
G	729	VAL	-	expression tag	UNP D0NVF3
G	730	PRO	-	expression tag	UNP D0NVF3
G	731	ASP	-	expression tag	UNP D0NVF3
G	732	TYR	-	expression tag	UNP D0NVF3
G	733	ALA	-	expression tag	UNP D0NVF3
G	734	GLY	-	expression tag	UNP D0NVF3
G	735	LEU	-	expression tag	UNP D0NVF3
G	736	TYR	-	expression tag	UNP D0NVF3
G	737	PRO	-	expression tag	UNP D0NVF3
G	738	TYR	-	expression tag	UNP D0NVF3
G	739	ASP	-	expression tag	UNP D0NVF3
G	740	VAL	-	expression tag	UNP D0NVF3
G	741	PRO	-	expression tag	UNP D0NVF3
G	742	ASP	-	expression tag	UNP D0NVF3
G	743	TYR	-	expression tag	UNP D0NVF3
G	744	ALA	-	expression tag	UNP D0NVF3

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

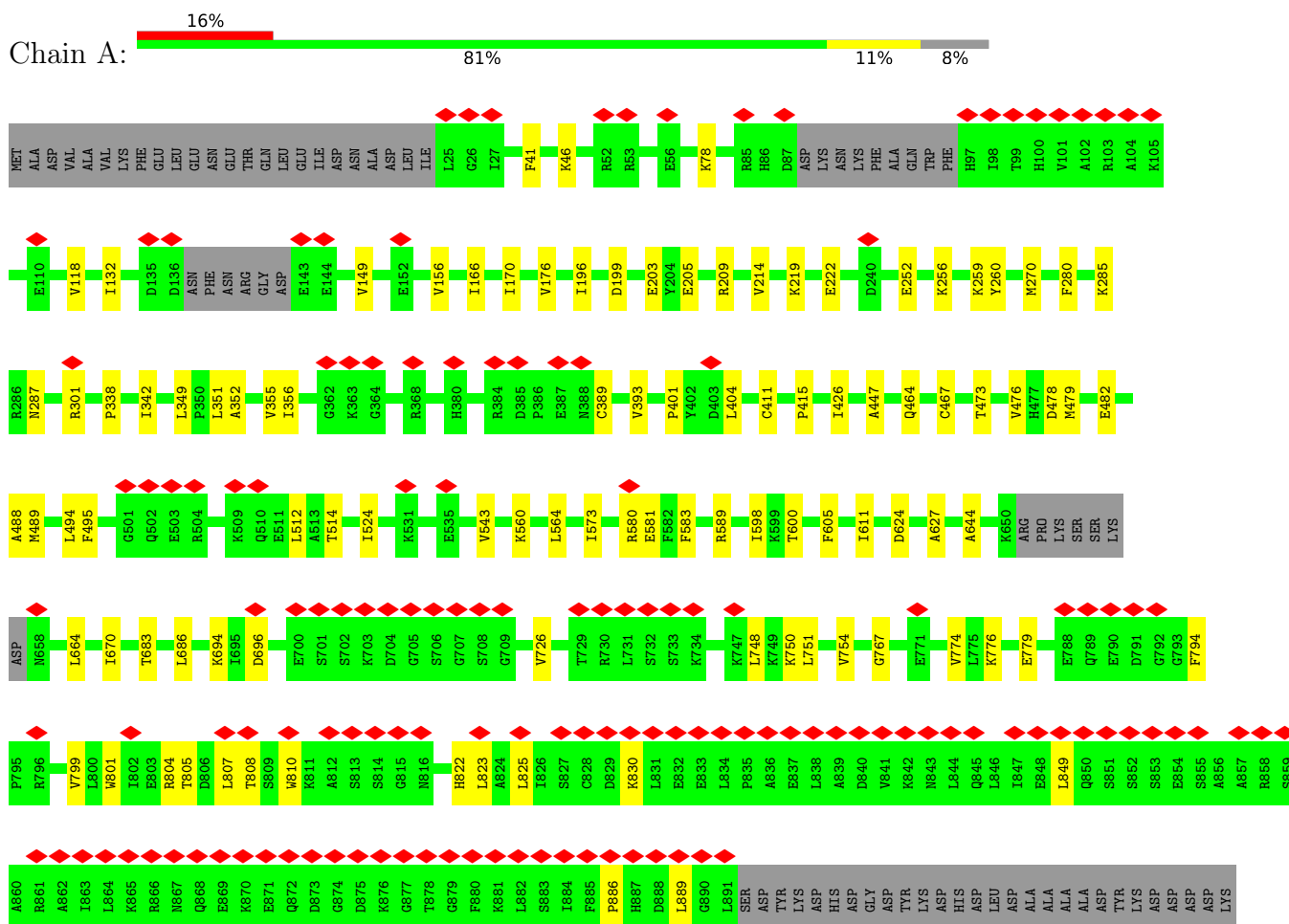


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0

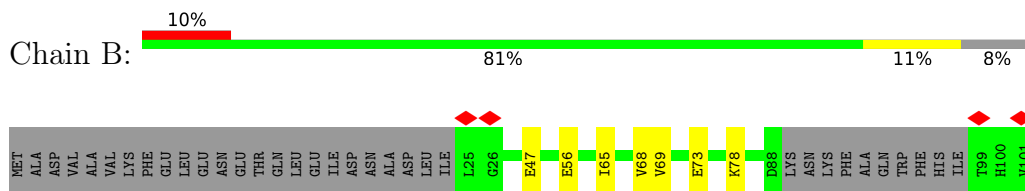
3 Residue-property plots

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.

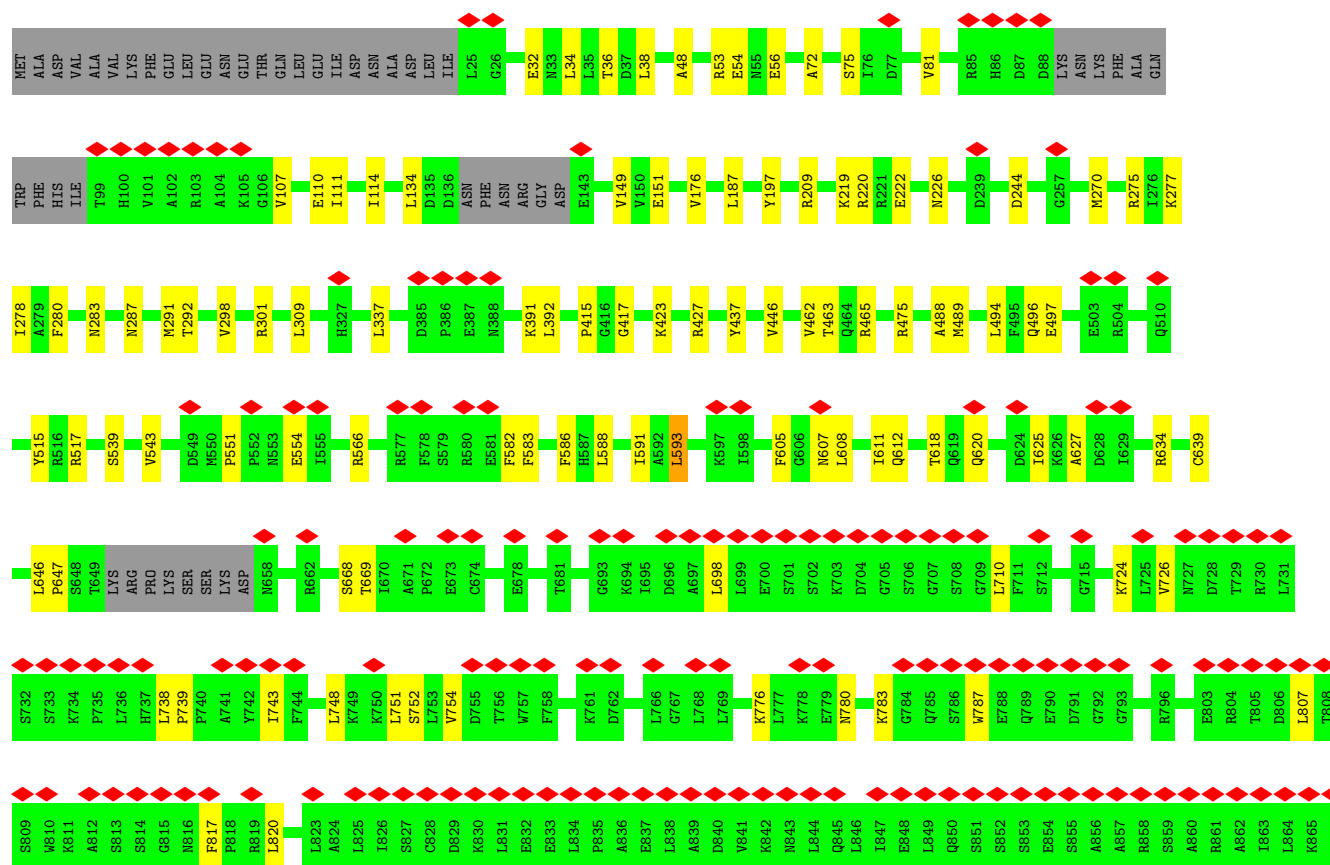
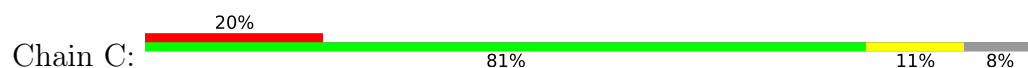
• Molecule 1: NRC3

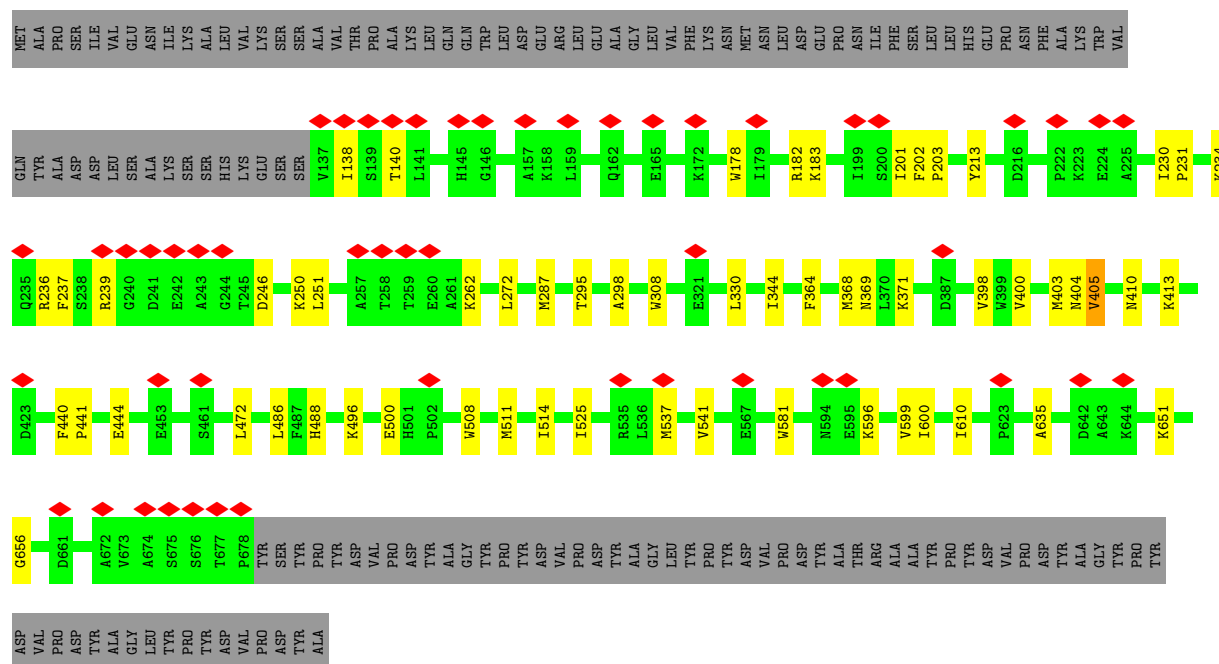


• Molecule 1: NRC3



- Molecule 1: NRC3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	267047	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.13	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.202	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size ($\text{\AA}$)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	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: ATP

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	0.13	0/6885	0.30	0/9287
1	B	0.11	0/6885	0.30	0/9286
1	C	0.11	0/6865	0.30	0/9261
2	G	0.13	0/4478	0.32	0/6064
All	All	0.12	0/25113	0.30	0/33898

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	ARG	Sidechain

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	6757	0	6877	57	0
1	B	6758	0	6876	56	0
1	C	6738	0	6850	62	0
2	G	4375	0	4381	40	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
All	All	24721	0	25020	205	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 4.

All (205) 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:C:582:PHE:HD2	1:C:583:PHE:CE1	1.92	0.88
2:G:178:TRP:HD1	2:G:183:LYS:HZ3	1.26	0.81
1:C:582:PHE:CD2	1:C:583:PHE:CE1	2.72	0.76
1:C:219:LYS:HB2	1:C:222:GLU:HG2	1.67	0.76
2:G:404:ASN:HD22	2:G:440:PHE:HB3	1.54	0.73
1:A:750:LYS:HG3	1:A:774:VAL:HB	1.73	0.70
1:A:355:VAL:HG21	1:A:389:CYS:HB2	1.75	0.69
1:B:419:GLN:HE22	1:B:475:ARG:HD3	1.57	0.69
1:C:618:THR:HG22	1:C:620:GLN:H	1.58	0.68
1:C:726:VAL:HG22	1:C:754:VAL:HB	1.74	0.68
1:C:612:GLN:HG2	1:C:634:ARG:HG3	1.76	0.68
1:A:774:VAL:HG13	1:A:799:VAL:HB	1.77	0.66
1:B:467:CYS:HB3	1:B:799:VAL:HG21	1.78	0.66
2:G:231:PRO:HA	2:G:234:LYS:HD3	1.79	0.64
1:A:270:MET:HE2	1:A:301:ARG:HB2	1.80	0.64
1:B:618:THR:HG22	1:B:620:GLN:H	1.62	0.63
2:G:511:MET:HE3	2:G:511:MET:HA	1.80	0.63
1:A:46:LYS:HD2	1:B:56:GLU:HG2	1.80	0.63
1:B:47:GLU:HG3	1:B:132:ILE:HG23	1.80	0.62
1:C:748:LEU:HD21	1:C:751:LEU:HG	1.81	0.62
1:B:219:LYS:HB2	1:B:222:GLU:HG2	1.80	0.62
1:A:176:VAL:HG22	1:A:287:ASN:HB2	1.82	0.61
1:A:351:LEU:HD23	1:A:479:MET:HE1	1.82	0.61
1:C:417:GLY:HA2	1:C:475:ARG:HH22	1.66	0.61
1:B:581:GLU:HA	1:B:584:LYS:HD2	1.81	0.61
1:B:825:LEU:HD21	1:B:828:CYS:HB2	1.83	0.60
1:A:393:VAL:HG22	1:A:479:MET:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:O	1:C:114:ILE:HD12	2.01	0.59
2:G:410:ASN:HB3	2:G:413:LYS:HE3	1.85	0.59
1:B:78:LYS:HE3	1:B:564:LEU:HD11	1.84	0.59
1:B:761:LYS:HD3	1:B:761:LYS:N	2.18	0.58
1:B:207:PHE:HB2	2:G:610:ILE:HD12	1.86	0.57
1:A:776:LYS:HA	1:A:801:TRP:HB3	1.85	0.57
1:C:591:ILE:HD11	1:C:593:LEU:HD23	1.86	0.57
1:B:176:VAL:HG22	1:B:287:ASN:HB2	1.88	0.56
1:C:134:LEU:HD12	2:G:239:ARG:HH11	1.71	0.55
1:C:669:THR:HG22	1:C:724:LYS:HZ1	1.71	0.55
1:C:489:MET:HE2	1:C:497:GLU:H	1.72	0.55
1:C:48:ALA:HA	1:C:53:ARG:HH21	1.72	0.54
1:C:724:LYS:HE2	1:C:726:VAL:HG23	1.89	0.54
1:B:699:LEU:HD13	1:B:739:PRO:HD3	1.89	0.54
2:G:344:ILE:HD11	2:G:398:VAL:HG11	1.88	0.54
1:B:278:ILE:HD11	1:C:149:VAL:HG12	1.90	0.54
1:C:582:PHE:HD2	1:C:583:PHE:CD1	2.26	0.54
1:C:739:PRO:HB2	1:C:743:ILE:HD11	1.90	0.54
2:G:178:TRP:CD1	2:G:183:LYS:HZ3	2.17	0.54
1:C:646:LEU:HD13	1:C:647:PRO:HD2	1.90	0.53
2:G:236:ARG:HG3	2:G:237:PHE:CD1	2.42	0.53
1:A:683:THR:HG22	1:A:686:LEU:HB2	1.91	0.53
1:A:825:LEU:HB2	1:A:849:LEU:HD21	1.90	0.52
1:B:321:LEU:HD11	1:B:360:LEU:HD12	1.91	0.52
1:B:588:LEU:HD21	1:B:591:ILE:HB	1.91	0.52
1:B:738:LEU:HB3	1:B:765:ILE:HD11	1.91	0.52
2:G:138:ILE:HG22	2:G:140:THR:H	1.74	0.52
1:A:488:ALA:HB1	1:A:494:LEU:HB3	1.92	0.52
1:A:779:GLU:HB3	1:A:804:ARG:HB2	1.92	0.52
2:G:182:ARG:HH11	2:G:182:ARG:HG2	1.75	0.52
2:G:364:PHE:HB3	2:G:405:VAL:HG11	1.92	0.52
2:G:400:VAL:HA	2:G:403:MET:HG3	1.92	0.52
1:A:805:THR:HG23	1:A:807:LEU:H	1.76	0.51
1:A:726:VAL:HG22	1:A:754:VAL:HB	1.92	0.51
2:G:295:THR:HG23	2:G:298:ALA:H	1.75	0.51
1:B:65:ILE:HA	1:B:68:VAL:HG12	1.94	0.50
1:C:415:PRO:HD3	1:C:543:VAL:HB	1.94	0.50
1:C:423:LYS:O	1:C:427:ARG:HG3	2.12	0.50
1:A:219:LYS:HB2	1:A:222:GLU:HG3	1.93	0.50
1:A:415:PRO:HD3	1:A:543:VAL:HB	1.94	0.50
1:B:69:VAL:O	1:B:73:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:PRO:HA	1:B:390:LYS:HB2	1.93	0.49
1:A:524:ILE:HD13	1:A:573:ILE:HD11	1.94	0.49
1:C:463:THR:HG23	1:C:475:ARG:HG2	1.95	0.49
1:A:799:VAL:HG13	1:A:822:HIS:HB3	1.95	0.49
1:A:196:ILE:HA	1:A:199:ASP:OD2	2.12	0.49
1:C:270:MET:HE2	1:C:301:ARG:HB3	1.93	0.48
1:A:560:LYS:HG3	1:A:581:GLU:HG2	1.95	0.48
2:G:182:ARG:HG2	2:G:182:ARG:O	2.12	0.48
1:C:787:TRP:HE3	1:C:807:LEU:HD22	1.77	0.48
2:G:441:PRO:HA	2:G:444:GLU:HG3	1.95	0.48
1:A:252:GLU:HG2	1:A:256:LYS:HE2	1.96	0.48
1:B:419:GLN:NE2	1:B:475:ARG:HD3	2.28	0.48
1:B:767:GLY:HA2	1:B:794:PHE:CD1	2.49	0.48
1:C:738:LEU:HG	1:C:739:PRO:HD2	1.94	0.48
1:A:748:LEU:HD21	1:A:751:LEU:HD13	1.95	0.48
1:C:488:ALA:HB1	1:C:494:LEU:HB3	1.96	0.47
2:G:287:MET:HE1	2:G:330:LEU:HD13	1.96	0.47
1:C:588:LEU:HD23	1:C:611:ILE:HD11	1.96	0.47
1:A:349:LEU:HD23	1:A:352:ALA:H	1.78	0.47
1:A:301:ARG:NH2	1:B:324:LYS:NZ	2.63	0.47
1:B:670:ILE:HD11	1:B:689:LEU:HD11	1.97	0.47
1:C:582:PHE:CD2	1:C:583:PHE:CD1	3.03	0.47
1:A:203:GLU:HB3	2:G:514:ILE:HG23	1.98	0.46
1:A:478:ASP:O	1:A:482:GLU:HG2	2.13	0.46
1:C:605:PHE:HB3	1:C:627:ALA:HB2	1.96	0.46
1:C:496:GLN:HG3	1:C:515:TYR:CD1	2.49	0.46
1:A:467:CYS:HB3	1:A:799:VAL:HG21	1.97	0.46
1:B:778:LYS:HG2	1:B:803:GLU:OE1	2.16	0.46
2:G:246:ASP:O	2:G:250:LYS:HG2	2.16	0.46
1:B:285:LYS:HE2	2:G:656:GLY:HA3	1.97	0.46
1:C:752:SER:HB3	1:C:776:LYS:HE2	1.98	0.46
1:B:747:LYS:HD2	1:B:747:LYS:N	2.31	0.46
1:C:462:VAL:HG11	1:C:465:ARG:HG3	1.97	0.46
2:G:488:HIS:CE1	2:G:537:MET:HE1	2.51	0.46
1:B:838:LEU:HB2	1:B:863:ILE:HD13	1.99	0.45
1:A:767:GLY:HA2	1:A:794:PHE:CD1	2.50	0.45
1:A:808:THR:HG22	1:A:830:LYS:HB3	1.98	0.45
1:A:41:PHE:HE2	1:A:118:VAL:HG22	1.79	0.45
1:C:551:PRO:HG2	1:C:554:GLU:HG2	1.97	0.45
1:B:787:TRP:NE1	1:B:789:GLN:HG2	2.32	0.45
2:G:581:TRP:HZ3	2:G:599:VAL:HG13	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:HD23	1:C:309:LEU:HB3	1.97	0.45
1:A:489:MET:HG2	1:A:495:PHE:O	2.17	0.45
1:A:683:THR:HG21	1:A:686:LEU:HD13	1.99	0.45
2:G:202:PHE:HB2	2:G:203:PRO:HD3	1.99	0.45
1:A:338:PRO:O	1:A:342:ILE:HG13	2.17	0.45
1:A:401:PRO:HD2	1:A:404:LEU:HD12	1.98	0.45
1:A:810:TRP:HH2	1:A:823:LEU:HD21	1.82	0.45
1:B:524:ILE:HD13	1:B:573:ILE:HD11	1.99	0.45
1:C:176:VAL:HG22	1:C:287:ASN:ND2	2.32	0.45
1:C:291:MET:HE1	1:C:298:VAL:HG12	1.98	0.45
1:C:391:LYS:HD2	1:C:392:LEU:HD12	1.99	0.45
2:G:182:ARG:HG2	2:G:182:ARG:NH1	2.32	0.44
1:B:589:ARG:HA	1:B:611:ILE:HA	1.98	0.44
2:G:525:ILE:HG12	2:G:541:VAL:HG13	1.99	0.44
1:C:107:VAL:O	1:C:111:ILE:HG12	2.18	0.44
1:C:197:TYR:CE1	1:C:209:ARG:HB3	2.52	0.44
1:B:748:LEU:HD21	1:B:751:LEU:HD13	1.99	0.44
1:A:259:LYS:HG2	1:A:285:LYS:O	2.18	0.44
1:C:724:LYS:HD3	1:C:724:LYS:C	2.42	0.44
1:C:72:ALA:HB2	1:C:114:ILE:HG21	1.98	0.44
1:C:517:ARG:HB3	1:C:539:SER:HB2	1.99	0.44
1:C:669:THR:HG22	1:C:724:LYS:NZ	2.32	0.44
1:A:589:ARG:HA	1:A:611:ILE:HA	2.00	0.44
2:G:472:LEU:HD22	2:G:486:LEU:HD21	2.00	0.44
1:B:844:LEU:HD21	1:B:847:ILE:HD11	2.00	0.43
1:C:220:ARG:HH21	1:C:278:ILE:HG21	1.82	0.43
2:G:287:MET:HB2	2:G:308:TRP:NE1	2.33	0.43
1:B:270:MET:HG2	1:B:301:ARG:HD2	2.01	0.43
1:B:415:PRO:HD3	1:B:543:VAL:HB	1.99	0.43
1:B:825:LEU:HD11	1:B:831:LEU:HD22	2.00	0.43
2:G:596:LYS:HB3	2:G:596:LYS:HE2	1.88	0.43
1:A:411:CYS:HB3	1:A:476:VAL:HG21	2.00	0.43
2:G:508:TRP:HH2	2:G:541:VAL:HA	1.84	0.43
1:A:389:CYS:O	1:A:393:VAL:HG23	2.18	0.43
1:B:436:GLN:OE1	1:B:436:GLN:HA	2.19	0.43
1:A:301:ARG:NH2	1:B:324:LYS:HZ2	2.17	0.43
1:A:644:ALA:HB3	1:A:670:ILE:HG22	2.00	0.43
1:C:197:TYR:HE1	1:C:209:ARG:HB3	1.84	0.43
1:A:589:ARG:HG3	1:A:589:ARG:HH11	1.83	0.43
2:G:496:LYS:O	2:G:500:GLU:HG3	2.19	0.43
1:B:126:ALA:HA	1:B:129:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:GLN:HG2	1:B:543:VAL:HG23	2.01	0.43
1:B:601:ILE:HD11	1:B:616:VAL:HG21	2.00	0.43
1:C:32:GLU:O	1:C:36:THR:HG23	2.19	0.43
1:C:698:LEU:HD12	1:C:710:LEU:HB2	2.01	0.43
1:A:260:TYR:OH	1:A:280:PHE:HB3	2.19	0.42
1:A:598:ILE:H	1:A:598:ILE:HG13	1.68	0.42
1:B:539:SER:HB2	1:B:567:VAL:HB	2.00	0.42
1:C:277:LYS:HA	1:C:280:PHE:CD2	2.54	0.42
1:A:600:THR:HG22	1:A:624:ASP:HB3	2.01	0.42
1:B:242:PRO:HG3	1:C:226:ASN:CG	2.44	0.42
1:B:816:ASN:HD22	1:B:816:ASN:HA	1.67	0.42
2:G:230:ILE:HG13	2:G:272:LEU:HA	2.01	0.42
1:A:694:LYS:HG2	1:A:696:ASP:OD1	2.19	0.42
1:B:638:VAL:HB	1:B:667:LEU:HD23	2.02	0.42
1:B:777:LEU:HD13	1:B:782:PHE:HD2	1.83	0.42
1:B:246:LEU:O	1:B:250:VAL:HG23	2.20	0.42
1:B:314:LYS:HD3	1:B:314:LYS:HA	1.59	0.42
2:G:262:LYS:HE3	2:G:262:LYS:HB2	1.83	0.42
1:C:34:LEU:O	1:C:38:LEU:HG	2.20	0.42
1:B:726:VAL:HG13	1:B:754:VAL:HB	2.02	0.42
1:C:54:GLU:CD	1:C:54:GLU:H	2.27	0.41
2:G:251:LEU:HD23	2:G:251:LEU:HA	1.85	0.41
2:G:369:ASN:C	2:G:371:LYS:H	2.28	0.41
1:A:170:ILE:HD12	1:A:205:GLU:HG2	2.01	0.41
1:A:580:ARG:HA	1:A:583:PHE:CD2	2.55	0.41
1:A:464:GLN:HB2	1:A:473:THR:HB	2.02	0.41
1:B:210:VAL:HG13	1:B:230:LYS:HE2	2.02	0.41
1:C:639:CYS:HA	1:C:668:SER:HB2	2.00	0.41
1:C:220:ARG:HD2	1:C:275:ARG:HD2	2.02	0.41
1:A:605:PHE:HB3	1:A:627:ALA:HB2	2.01	0.41
1:A:166:ILE:HD11	1:A:199:ASP:OD2	2.21	0.41
1:B:777:LEU:HD13	1:B:782:PHE:CD2	2.56	0.41
1:C:437:TYR:CD2	1:C:446:VAL:HG21	2.55	0.41
1:C:586:PHE:CZ	1:C:607:ASN:HB3	2.56	0.41
2:G:230:ILE:N	2:G:231:PRO:HD2	2.36	0.41
2:G:651:LYS:HE3	2:G:651:LYS:HB2	1.85	0.41
1:A:78:LYS:HE2	1:A:564:LEU:HD21	2.03	0.41
1:B:277:LYS:HA	1:B:280:PHE:CD2	2.56	0.41
1:B:708:SER:HB2	1:B:712:SER:HB3	2.02	0.41
1:C:566:ARG:O	1:C:588:LEU:HD12	2.21	0.41
1:C:780:ASN:HD21	1:C:783:LYS:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:817:PHE:HB3	1:C:820:LEU:HB2	2.03	0.41
1:B:556:PRO:O	1:B:560:LYS:HG3	2.20	0.40
1:C:151:GLU:HG2	3:C:1001:ATP:O2'	2.21	0.40
1:C:625:ILE:O	1:C:647:PRO:HD3	2.21	0.40
1:A:664:LEU:HD23	1:A:683:THR:OG1	2.21	0.40
2:G:178:TRP:HB3	2:G:213:TYR:CE1	2.56	0.40
1:B:496:GLN:HG3	1:B:515:TYR:CD1	2.57	0.40
1:C:81:VAL:HG11	1:C:586:PHE:HB3	2.02	0.40
1:A:352:ALA:O	1:A:356:ILE:HG12	2.21	0.40
1:A:426:ILE:HG23	1:A:447:ALA:HB3	2.02	0.40
1:A:886:PRO:HD2	1:A:889:LEU:HD21	2.03	0.40
1:B:47:GLU:HB2	1:C:56:GLU:HB2	2.03	0.40
2:G:364:PHE:O	2:G:368:MET:HG2	2.22	0.40
2:G:600:ILE:HG21	2:G:635:ALA:HB1	2.03	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	837/919 (91%)	822 (98%)	15 (2%)	0	100	100
1	B	837/919 (91%)	825 (99%)	12 (1%)	0	100	100
1	C	835/919 (91%)	826 (99%)	9 (1%)	0	100	100
2	G	540/684 (79%)	531 (98%)	9 (2%)	0	100	100
All	All	3049/3441 (89%)	3004 (98%)	45 (2%)	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	746/810 (92%)	740 (99%)	6 (1%)	73	82
1	B	746/810 (92%)	736 (99%)	10 (1%)	61	78
1	C	744/810 (92%)	737 (99%)	7 (1%)	70	81
2	G	473/594 (80%)	471 (100%)	2 (0%)	84	86
All	All	2709/3024 (90%)	2684 (99%)	25 (1%)	68	81

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ILE
1	A	149	VAL
1	A	156	VAL
1	A	214	VAL
1	A	512	LEU
1	A	514	THR
1	B	132	ILE
1	B	182	VAL
1	B	292	THR
1	B	356	ILE
1	B	389	CYS
1	B	475	ARG
1	B	553	ASN
1	B	600	THR
1	B	649	THR
1	B	660	VAL
1	C	75	SER
1	C	244	ASP
1	C	283	ASN
1	C	292	THR
1	C	337	LEU
1	C	593	LEU
1	C	608	LEU
2	G	201	ILE
2	G	405	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	456	ASN
1	A	727	ASN
1	A	816	ASN
1	B	383	ASN
1	B	464	GLN
1	B	536	HIS
1	B	610	ASN
1	C	327	HIS
1	C	458	ASN
1	C	486	HIS
1	C	587	HIS
2	G	193	ASN
2	G	266	ASN
2	G	404	ASN
2	G	498	ASN
2	G	505	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	B	1001	-	29,33,33	0.29	0	44,52,52	0.52	1 (2%)
3	ATP	C	1001	-	29,33,33	0.30	0	44,52,52	0.50	1 (2%)
3	ATP	A	1001	-	29,33,33	0.30	0	44,52,52	0.50	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	1001	-	-	2/22/38/38	0/3/3/3
3	ATP	C	1001	-	-	1/22/38/38	0/3/3/3
3	ATP	A	1001	-	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	ATP	PB-O3B-PG	2.07	139.91	132.83
3	A	1001	ATP	PB-O3B-PG	2.04	139.84	132.83
3	C	1001	ATP	PB-O3B-PG	2.03	139.80	132.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

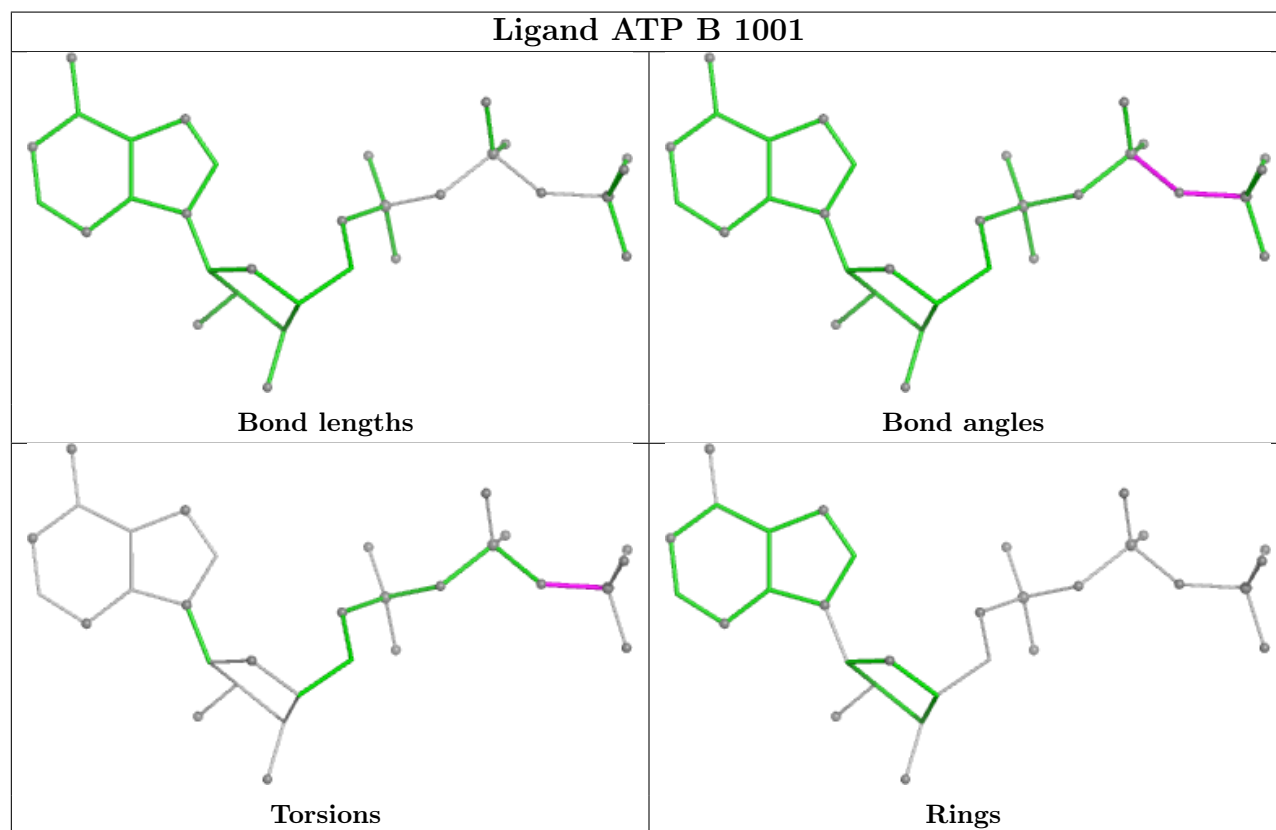
Mol	Chain	Res	Type	Atoms
3	A	1001	ATP	PB-O3B-PG-O1G
3	B	1001	ATP	PB-O3B-PG-O1G
3	A	1001	ATP	PB-O3B-PG-O2G
3	B	1001	ATP	PB-O3B-PG-O2G
3	C	1001	ATP	PG-O3B-PB-O2B

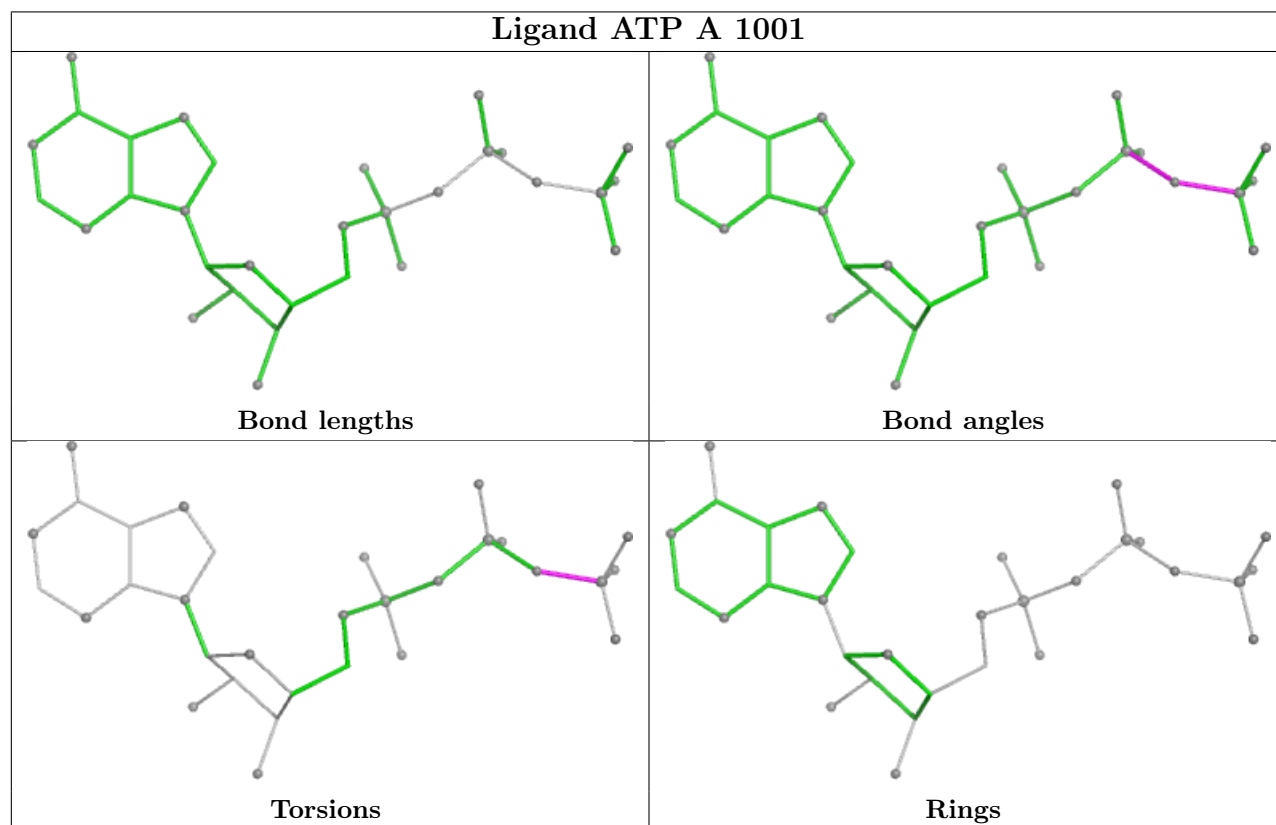
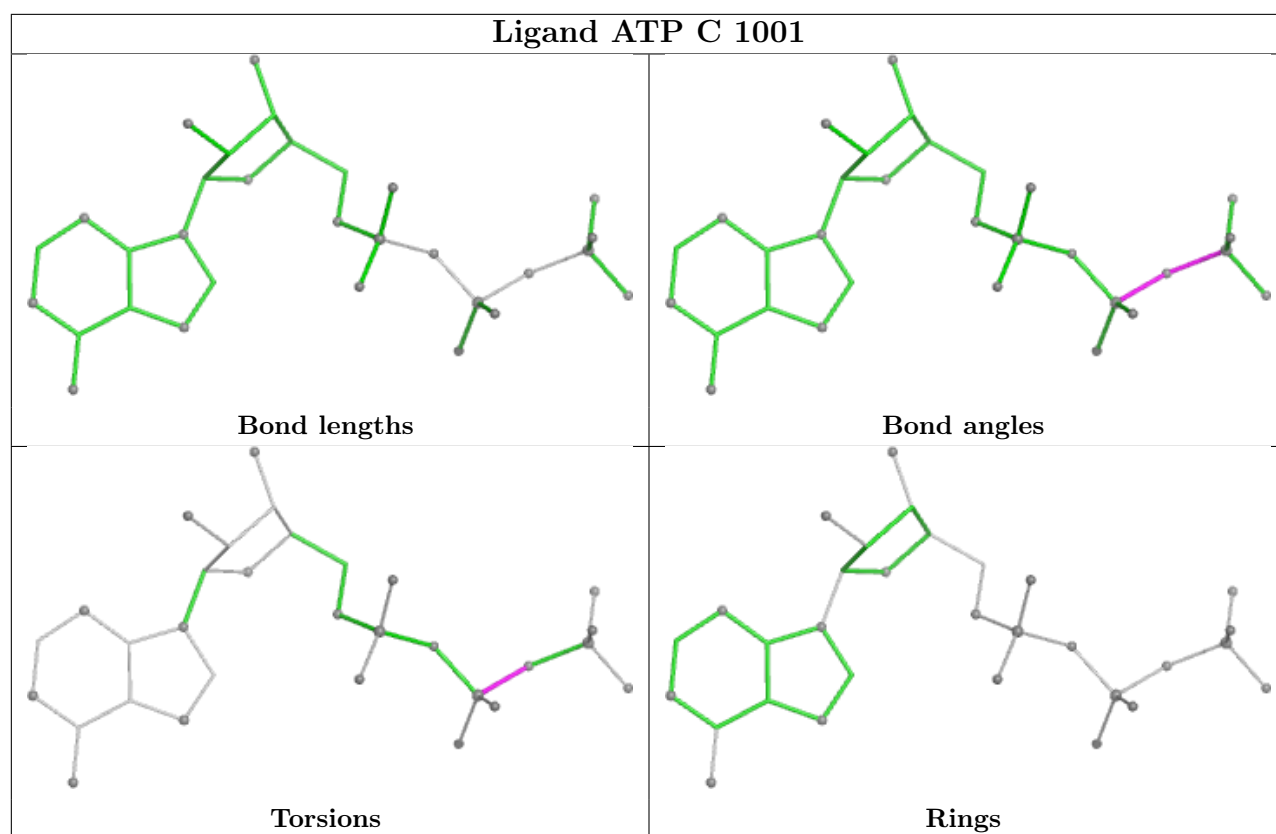
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	ATP	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

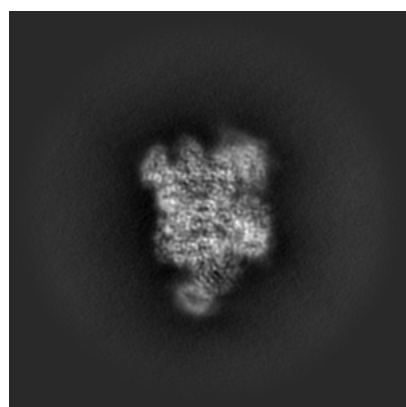
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53991. These allow visual inspection of the internal detail of the map and identification of artifacts.

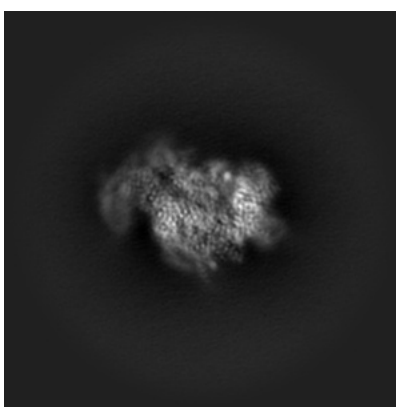
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

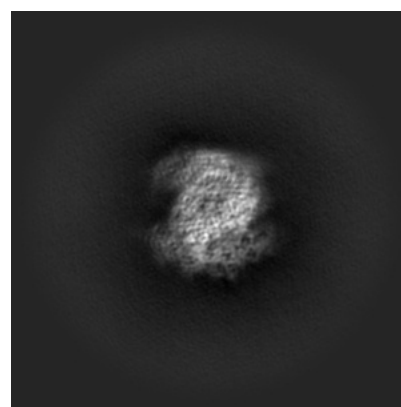
6.1.1 Primary map



X



Y

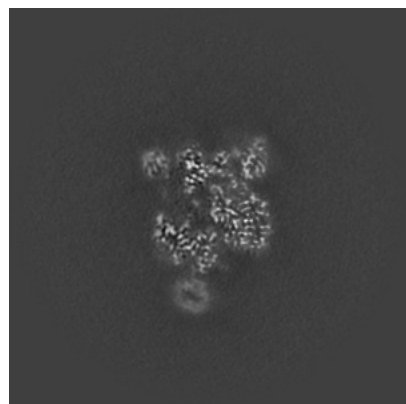


Z

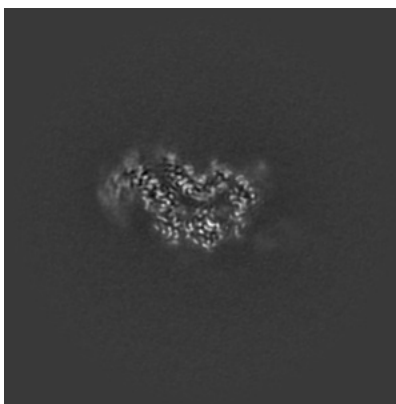
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

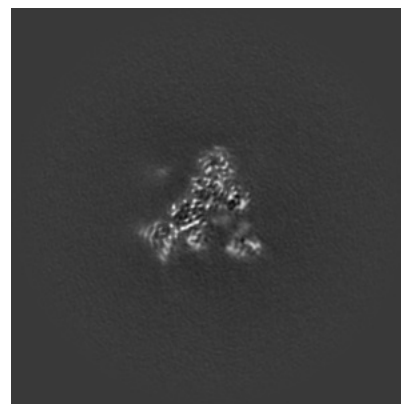
6.2.1 Primary map



X Index: 200



Y Index: 200

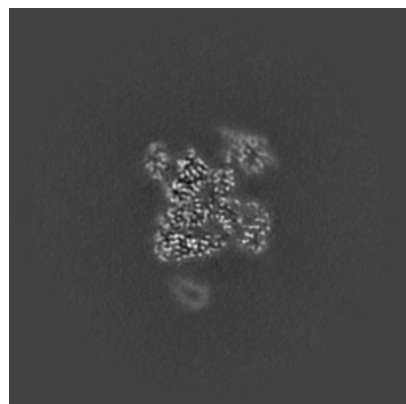


Z Index: 200

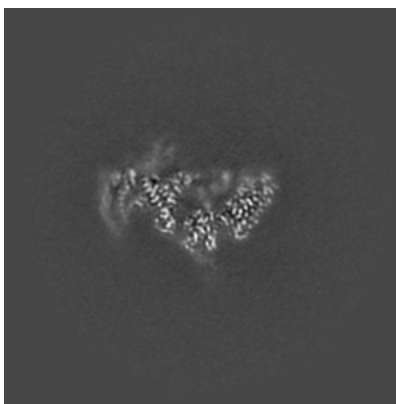
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

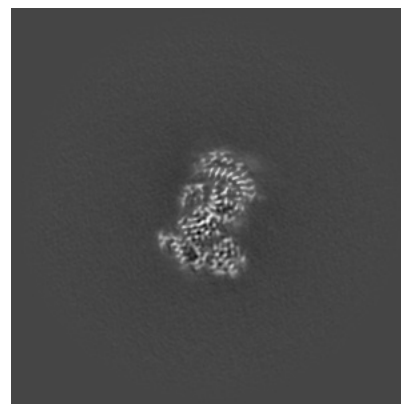
6.3.1 Primary map



X Index: 190



Y Index: 187

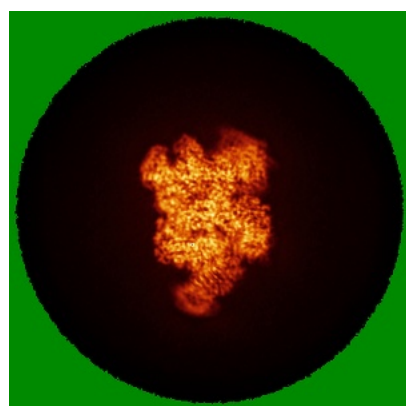


Z Index: 236

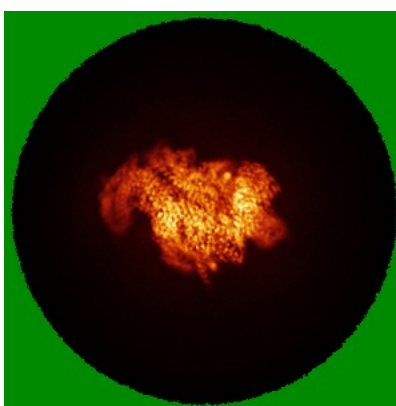
The images above show the largest variance slices of the map in three orthogonal directions.

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

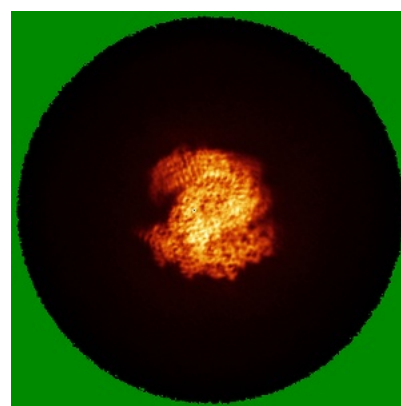
6.4.1 Primary map



X



Y

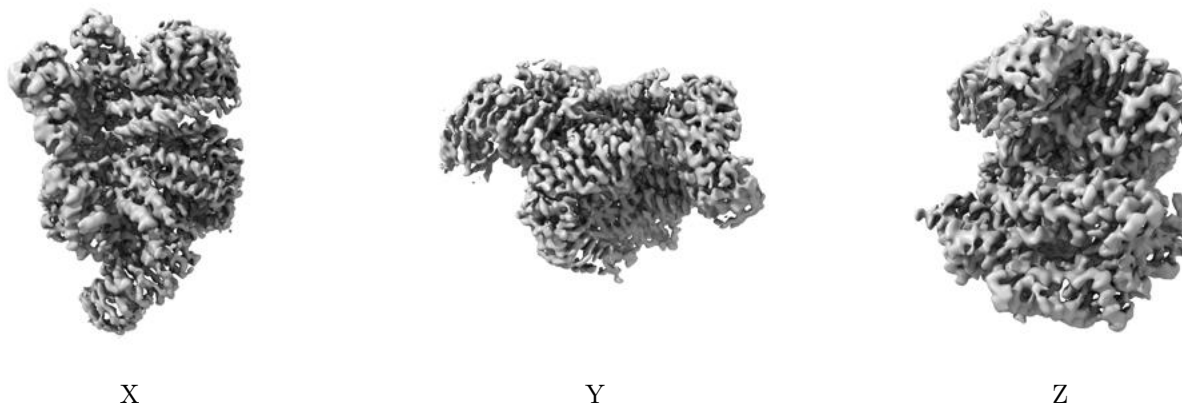


Z

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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

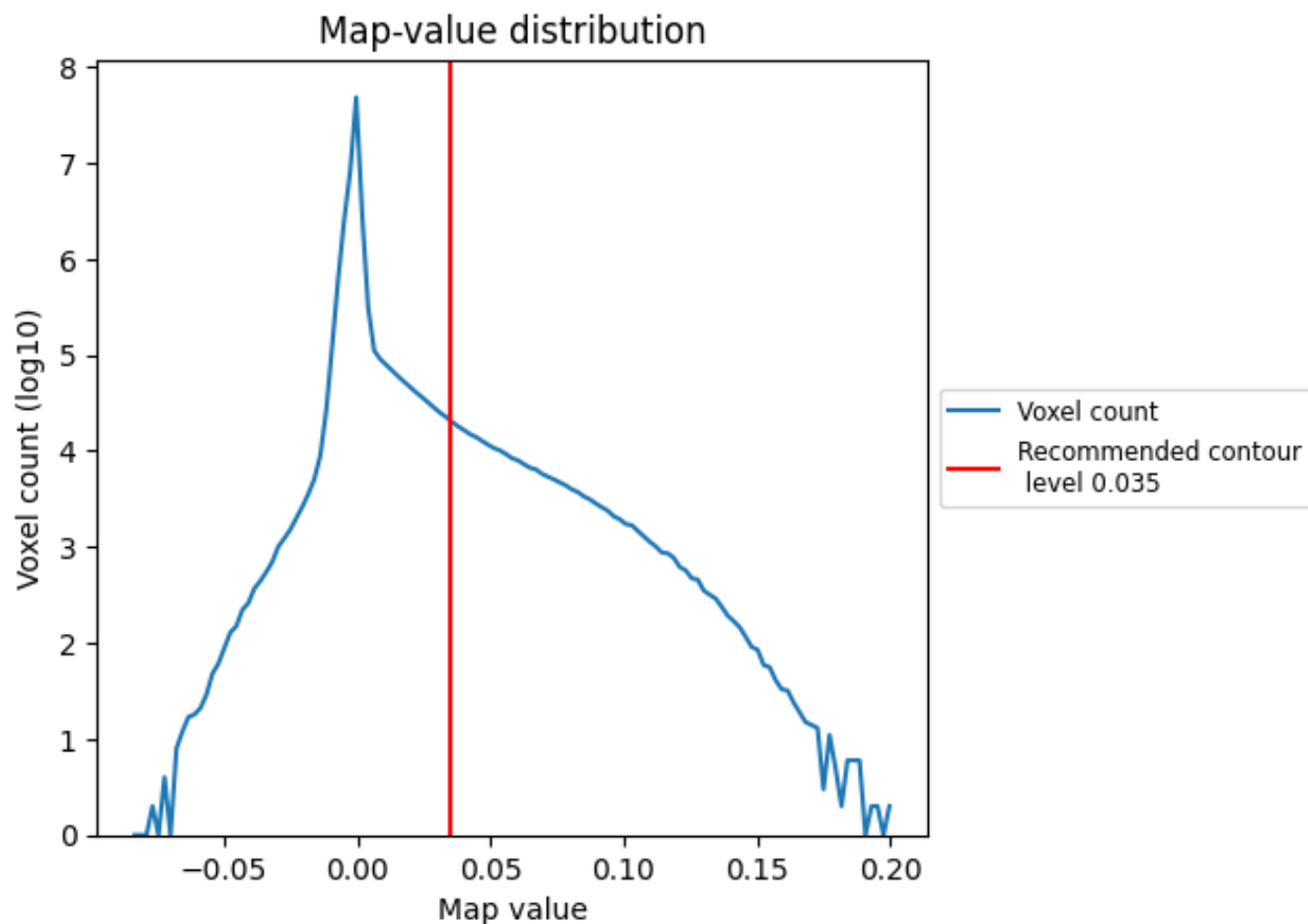
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

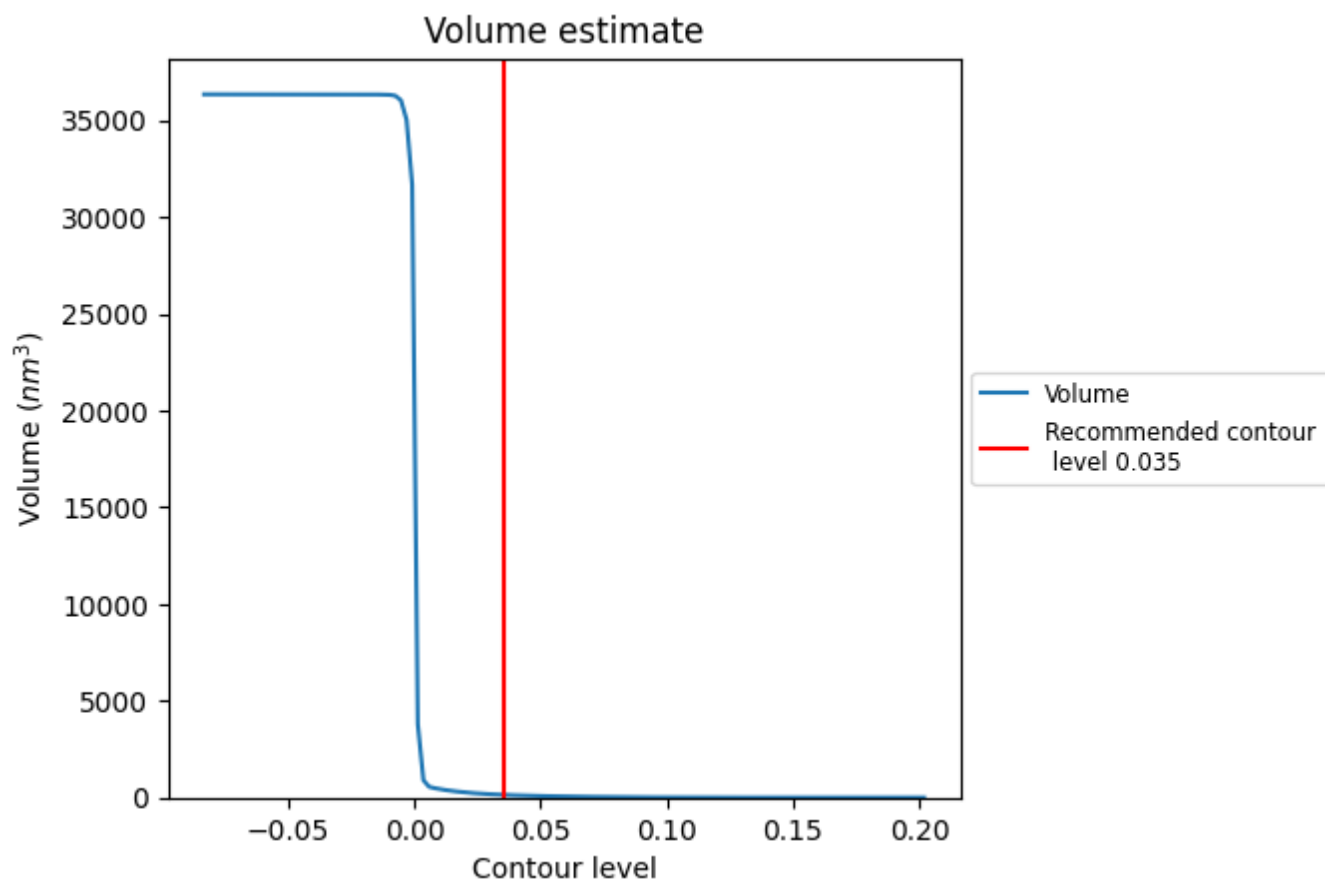
This section contains the results of statistical analysis of the map.

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.

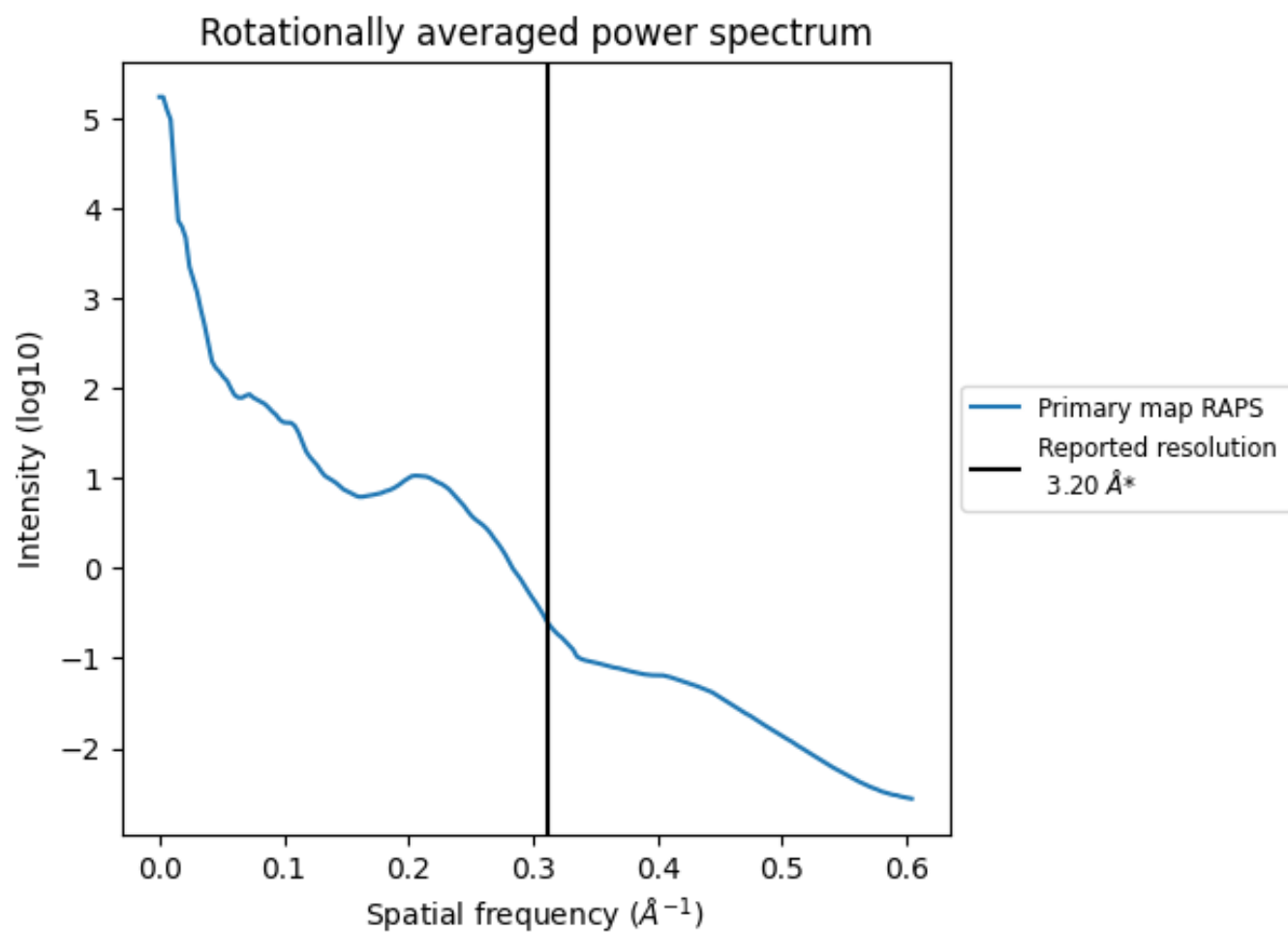
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 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 0.312 Å⁻¹

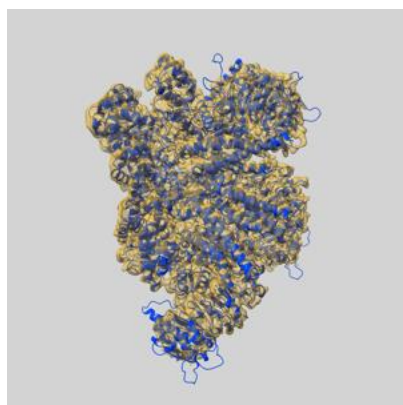
8 Fourier-Shell correlation

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

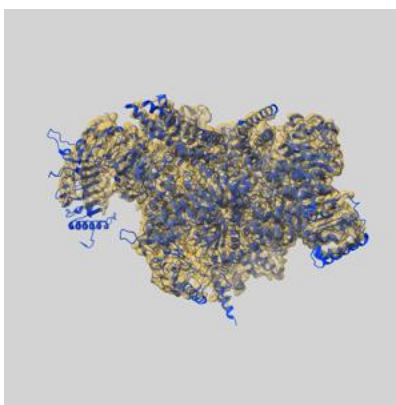
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53991 and PDB model 9RIA. Per-residue inclusion information can be found in section [3](#) on page [9](#).

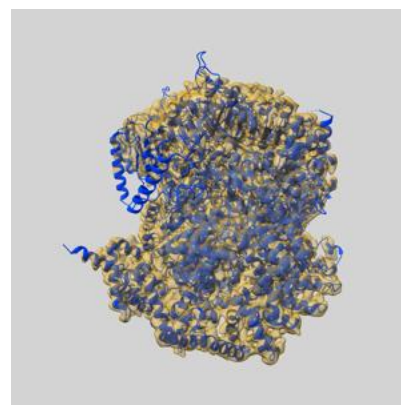
9.1 Map-model overlay [i](#)



X



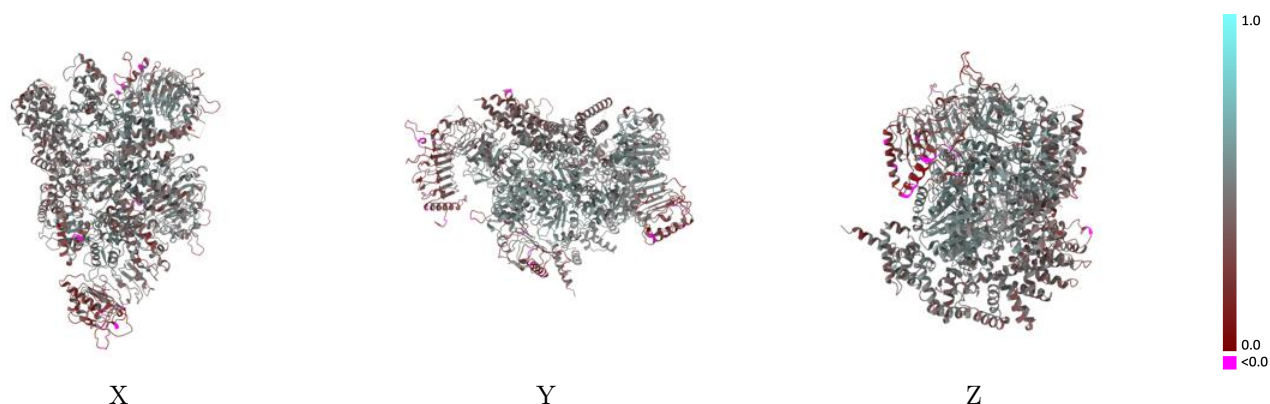
Y



Z

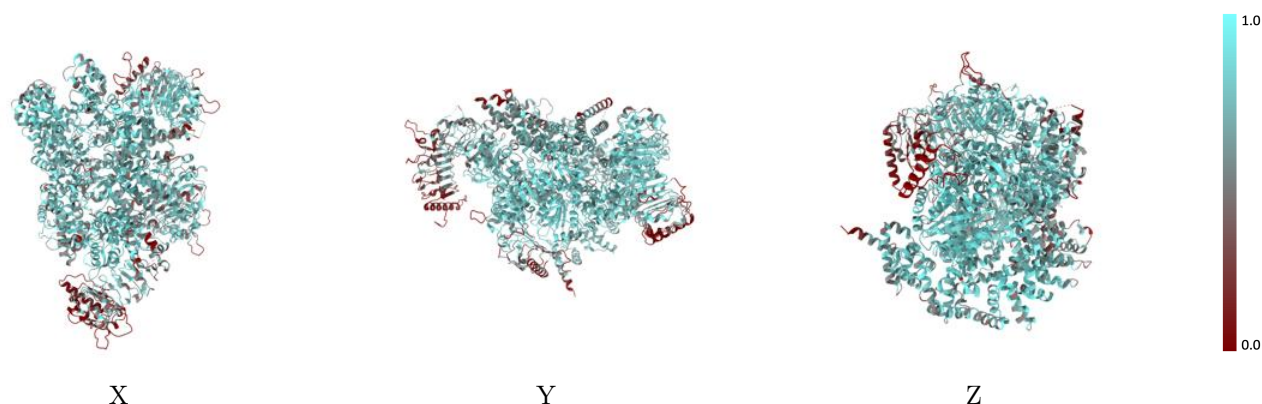
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



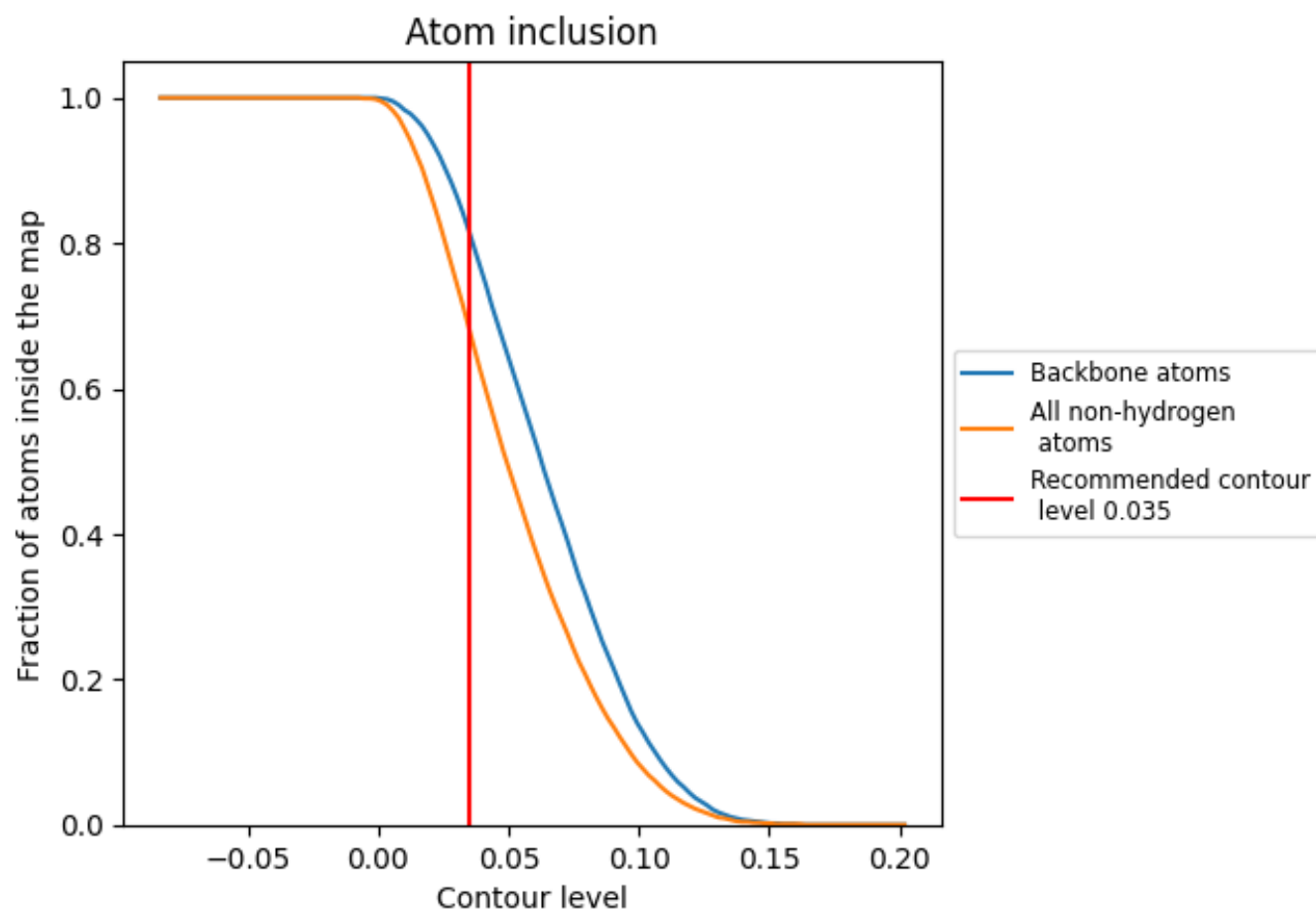
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 68% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6810	0.4410
A	0.6790	0.4440
B	0.7280	0.4790
C	0.6240	0.4170
G	0.7030	0.4170

