



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:15 PM UTC

PDB ID : 8SXT / pdb_00008sxt
EMDB ID : EMD-40858
Title : Structure of LINE-1 ORF2p with template:primer hybrid
Authors : van Eeuwen, T.; Taylor, M.S.; Rout, M.P.
Deposited on : 2023-05-24
Resolution : 3.30 Å(reported)
Based on initial model : 8C8J

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:

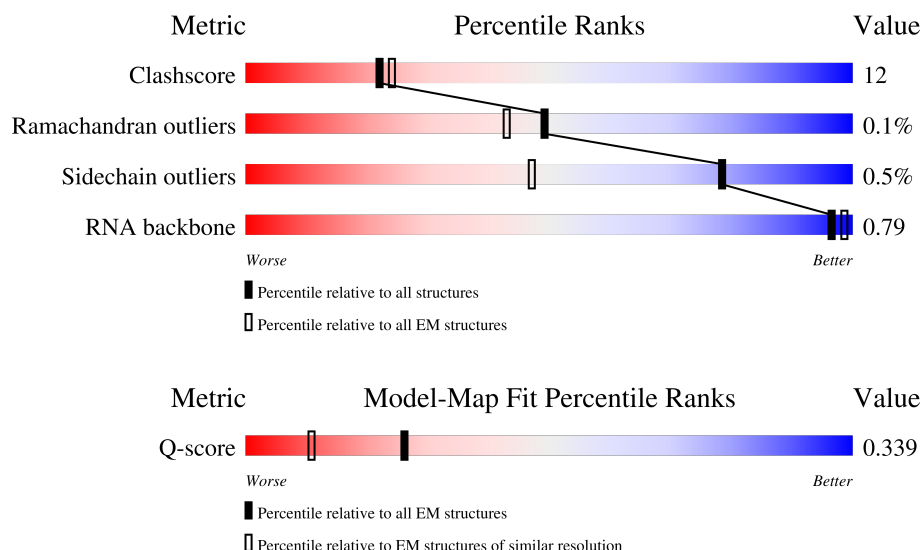
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	B	13	
2	C	17	
3	A	1275	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6382 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 DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	7	Total	C	N	O	P	0	0
			140	68	22	43	7		

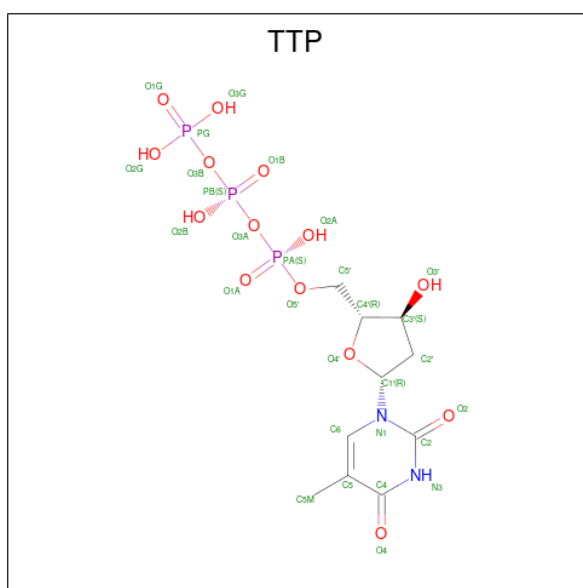
- Molecule 2 is a RNA chain called RNA template.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	11	Total	C	N	O	P	0	0
			225	102	42	71	10		

- Molecule 3 is a protein called LINE-1 retrotransposable element ORF2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	726	Total	C	N	O	S	0	0
			5987	3881	1014	1072	20		

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			29	10	2	14	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

ASN	THR	LYS	CYS	L1013	K928	E839	M754	N644	F530	L433	PHE
	MET	SER	SER	I1014	D929	L840	G755	G645	R531	D434	GLU
	ASP	VAL	SER	K1015		E841	E756	Q646	P532		ARG
	TRP	ARG	LEU	L1016	L947	K942	L757	K647	I533	M442	ILE
	ILE	PHE	ALA	K1017	K948	K942	P758	K654	N537	Q443	ASN
	LYS	LEU	ILE	L949	L949	L845	I761	K654	N537	E444	LYS
	LYS	ARG	ARG		F952	K846	L769	R658	A540	E445	ILE
	MET	ASP	GLU	T1021		F847	L789	Q659	A540	V446	ASP
	TRP	LEU	MET	A1022	I959	I848	G770	Q659	N544	E447	ARG
	HIS	GLU	GLN	K1023	N960	M849	I771	S664	N544	S448	PRO
	TYR	LEU	ILE	E1024	S961	N850	R775	P665	L547	L449	ALA
	TYR	GLU	LYS		R962	Q851	D776	L666	R550	M450	ARG
	THR	ILE	THR	I1027		K852	V777	L666	I551	R451	LEU
	MET	PRO	MET			R853	K778	E673	L558	I453	ILE
	GLU	ASP	ARG	E1037	K965	R853	D778	E673	L558	E457	LYS
	TYR	PRO	TYR	K1038	D966	A854	D779	R677	D562	I458	LYS
	ALA	ALA	HIS		L967	R855	L780	R677	D562	V459	ARG
	ALA	ILE	LEU		N968	I856	F781	R880	K578	A460	GLU
	ILE	PRO	LEU	T1042	V969	A857	K782	R880	K578	L465	LYS
	LYS	LEU	VAL	Y1043	K970	N784	E783	K683	N581	D474	ASN
	ASN	LEU	VAL	S1044	P971	K858	Y785	E684	V582		ILE
	ASP	GLY	ARG		K972	S859		I685			ASP
	GLU	ILE	MET	K1047	T973	T860	L788	K686	N587	A478	THR
	PHE	TYR	ALA		K975	L861	L789	K692	R588	E479	
	ILE	PRO	ILE	I1050	T976	S862	K790	K692	V595	Q482	
	SER	LYS	ILE	I1060	L977	Q863	E791	D702		R483	
	VAL	TYR	LYS	Y1061	E978	K864	I792			Y484	
	GLY	LYS	SER	LYS	E979	N865	K793	E709	D600	E486	
	THR	ASN	GLY	LYS	N865	K866	E794	N710	A601	E487	
	TRP	ASN	ASN	THR	L981	A867	E794	P711	E502		
	LYS	ASN	CYS	ASN	C982	G868	N797	I712	K607		
	LEU	ASN	TRP	PRO	I983	G869	K798	I713			
	GLU	LYS	ARG	ILE	T984	I870	N801	Q716	P611		
	THR	LYS	CYS	ILE	Q985	T871	I802	L719	F612		
	ILE	TRP	GLY	ALA	D987		P803	L719	M613		
	GLY	ALA	GLY	LYS	I988	K876	C904	I722	K615		
	ILE	ASP	ILE	ASP	G981	K885			T616		
	ALA	THR	THR	MET		D897	R809	F725	L620		
	ALA	LEU	VAL	ASN	F994		I810		E500		
	GLN	ARG	VAL	ARG	M995		N811	I733	K501		
	GLN	HIS	HIS	PHE	S996		I812	N734	E502		
	LYS	THR	CYS	THR	K997	E906	V813	V735	S508		
	THR	ILE	TRP	SER	T998	I907	K614	Q736			
	LYS	LYS	TRP	LYS	P999	N908	M815	I629	I517		
	ARG	ASP	CYS	ASP	K1000	P909	A816	I630	P518		
	ILE	ILE	LYS	ILE	A1001	H910	I817		K519		
	LEU	VAL	LEU	TYR	M1002	I911	K820	F741	P520		
	VAL	ALA	GLN	ALA	A1003	Y912	I828	L742	K521		
	PRO	ASN	PRO	ALA	T1004	N913	P829	N746	G521		
	ASN	ASN	ASN	LYS	K1005		I830	R747	R522		
	GLY	CYS	LEU	LYS	D1006	K919		Q748	D523		
	PRO	PRO	TRP	MET	K1007	P920	M834	T749	N640		
				LYS	I1008	E921	T835	E750	K526		
				LYS	D1009	K922	S751		K527		
					K1010	N923	F836	Q752	E528		
					W1011	K924		I753	T431		
					D1012	Q925			F432		
						N926					
						G927					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	430198	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.972	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.281	Depositor
Map size ($\text{\AA}$)	206.40001, 206.40001, 206.40001	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	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: TTP, MG

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	B	0.17	0/155	0.35	0/236
2	C	0.08	0/252	0.14	0/392
3	A	0.13	0/6118	0.39	2/8257 (0.0%)
All	All	0.13	0/6525	0.38	2/8885 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	517	ILE	CA-C-N	14.52	135.51	119.83
3	A	517	ILE	C-N-CA	14.52	135.51	119.83

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	B	140	0	79	4	0
2	C	225	0	113	10	0
3	A	5987	0	6190	134	0
4	C	29	0	13	4	0
5	A	1	0	0	0	0
All	All	6382	0	6395	147	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 12.

All (147) 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)
3:A:1013:LEU:O	3:A:1017:LYS:HG2	1.70	0.90
3:A:269:GLU:HA	3:A:272:MET:SD	2.17	0.84
3:A:268:ALA:O	3:A:272:MET:HG2	1.81	0.81
3:A:269:GLU:O	3:A:272:MET:HG3	1.82	0.79
3:A:519:LYS:HG2	3:A:520:PRO:HD2	1.65	0.77
3:A:1014:ILE:HA	3:A:1017:LYS:HD2	1.68	0.74
3:A:1014:ILE:HA	3:A:1017:LYS:CD	2.19	0.72
3:A:587:ASN:HD21	3:A:776:ASP:HA	1.56	0.70
3:A:519:LYS:HG2	3:A:520:PRO:CD	2.21	0.70
3:A:780:LEU:O	3:A:784:ASN:HB2	1.93	0.67
3:A:269:GLU:HA	3:A:272:MET:CG	2.24	0.67
3:A:921:GLU:HG3	3:A:962:ARG:HH12	1.60	0.67
3:A:459:VAL:HA	3:A:485:LYS:HZ1	1.60	0.66
3:A:792:ILE:HD12	3:A:817:ILE:HD11	1.76	0.65
3:A:1014:ILE:HA	3:A:1017:LYS:CG	2.26	0.65
3:A:578:LYS:O	3:A:582:VAL:HG23	1.96	0.65
3:A:449:LEU:HD12	3:A:550:ARG:HG2	1.78	0.64
3:A:442:ASN:ND2	3:A:445:GLU:OE2	2.31	0.63
3:A:748:GLN:O	3:A:752:GLN:NE2	2.30	0.63
3:A:268:ALA:O	3:A:272:MET:CG	2.48	0.62
3:A:811:ASN:O	3:A:815:MET:HG2	2.00	0.62
3:A:457:GLU:OE1	3:A:550:ARG:NH2	2.33	0.62
3:A:792:ILE:HG23	3:A:817:ILE:HD11	1.82	0.62
3:A:508:SER:O	3:A:537:ASN:ND2	2.29	0.61
3:A:1014:ILE:O	3:A:1017:LYS:HG3	2.00	0.61
3:A:1013:LEU:O	3:A:1017:LYS:CG	2.44	0.61
3:A:788:LEU:O	3:A:792:ILE:HG12	2.00	0.61
3:A:496:PHE:HA	3:A:499:ILE:HD12	1.84	0.60
3:A:742:LEU:HD21	3:A:753:ILE:HG21	1.83	0.60
3:A:588:ARG:NH2	3:A:929:ASP:OD1	2.35	0.60
2:C:0:A:N1	4:C:101:TTP:N3	2.38	0.59
3:A:750:GLU:O	3:A:754:MET:HG3	2.03	0.59
3:A:269:GLU:C	3:A:272:MET:HG3	2.28	0.59
3:A:517:ILE:HG23	3:A:518:PRO:HD2	1.84	0.58
3:A:432:PHE:HE2	3:A:725:PHE:HD1	1.50	0.58
3:A:587:ASN:HD22	3:A:777:VAL:HG22	1.68	0.58
3:A:804:CYS:SG	3:A:809:ARG:NH1	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:533:ILE:HA	3:A:659:GLN:HE21	1.70	0.57
3:A:523:ASP:N	3:A:523:ASP:OD1	2.35	0.56
4:C:101:TTP:H2'2	3:A:531:ARG:HH22	1.68	0.56
3:A:496:PHE:O	3:A:500:GLU:HG3	2.06	0.56
3:A:487:GLU:N	3:A:487:GLU:OE1	2.37	0.56
3:A:947:LEU:HB3	3:A:949:LEU:HD23	1.88	0.56
3:A:635:ASP:OD2	3:A:636:LYS:NZ	2.38	0.56
3:A:625:MET:HE3	3:A:625:MET:C	2.31	0.56
3:A:828:ILE:HG22	3:A:830:ILE:HG12	1.87	0.56
1:B:9:DC:H2'	1:B:10:DG:H8	1.71	0.55
3:A:742:LEU:O	3:A:775:ARG:NH2	2.39	0.55
3:A:834:MET:SD	3:A:876:LYS:NZ	2.79	0.55
3:A:920:PRO:HD3	3:A:952:PHE:HB3	1.88	0.55
3:A:927:GLY:O	3:A:929:ASP:N	2.40	0.54
3:A:809:ARG:HG2	3:A:847:PHE:HE2	1.72	0.54
3:A:742:LEU:HD13	3:A:750:GLU:HG3	1.89	0.54
3:A:722:ILE:HG21	3:A:733:ILE:HD13	1.89	0.54
3:A:845:LEU:HD12	3:A:849:TRP:HE1	1.72	0.54
3:A:523:ASP:O	3:A:529:ASN:ND2	2.38	0.54
3:A:532:PRO:O	3:A:659:GLN:NE2	2.41	0.53
3:A:540:ALA:O	3:A:544:ASN:ND2	2.30	0.53
4:C:101:TTP:H5'2	3:A:702:ASP:OD2	2.08	0.53
3:A:259:ASP:HB3	3:A:262:VAL:HB	1.90	0.53
3:A:459:VAL:HA	3:A:485:LYS:NZ	2.24	0.53
3:A:558:LEU:HD22	3:A:620:LEU:HD13	1.91	0.53
3:A:1014:ILE:C	3:A:1017:LYS:HG3	2.34	0.53
3:A:960:ASN:O	3:A:965:LYS:NZ	2.33	0.53
3:A:640:ASN:OD1	3:A:647:LYS:NZ	2.42	0.52
1:B:10:DG:H4'	3:A:769:LEU:HB3	1.91	0.51
3:A:595:VAL:HG11	3:A:711:PRO:HB3	1.91	0.51
3:A:519:LYS:HG3	3:A:531:ARG:HG2	1.92	0.51
3:A:285:GLN:OE1	3:A:285:GLN:N	2.40	0.51
3:A:523:ASP:OD1	3:A:529:ASN:ND2	2.44	0.50
3:A:845:LEU:HD12	3:A:849:TRP:NE1	2.26	0.50
3:A:562:ASP:OD2	3:A:680:ARG:NH1	2.44	0.50
3:A:742:LEU:HD12	3:A:761:ILE:HG12	1.94	0.50
3:A:425:ASN:ND2	3:A:428:GLU:OE1	2.43	0.49
3:A:492:LEU:HD23	3:A:495:LEU:HD23	1.94	0.49
3:A:277:ASN:OD1	3:A:277:ASN:N	2.46	0.49
2:C:5:A:H2'	2:C:6:A:H8	1.77	0.49
3:A:528:GLU:N	3:A:528:GLU:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:968:ASN:N	3:A:968:ASN:OD1	2.46	0.49
2:C:3:G:H2'	2:C:4:A:H8	1.78	0.48
3:A:519:LYS:CG	3:A:520:PRO:HD2	2.40	0.48
1:B:11:DC:H2'	4:C:101:TTP:H5'1	1.95	0.48
3:A:479:GLU:HA	3:A:482:GLN:HB2	1.96	0.48
3:A:451:ARG:NH1	3:A:457:GLU:OE2	2.47	0.48
3:A:789:LEU:HD13	3:A:839:GLU:OE1	2.14	0.47
3:A:393:ILE:HG22	3:A:407:ILE:HG22	1.96	0.47
1:B:9:DC:H2'	1:B:10:DG:C8	2.48	0.47
3:A:994:PHE:HD1	3:A:995:MET:HE3	1.79	0.47
3:A:258:ASN:HA	3:A:483:ARG:NH1	2.29	0.46
3:A:735:VAL:HG11	3:A:758:PRO:HB2	1.96	0.46
3:A:270:ILE:HG23	3:A:291:PHE:HE2	1.79	0.46
3:A:785:TYR:OH	3:A:828:ILE:O	2.34	0.46
3:A:501:LYS:HA	3:A:501:LYS:HE2	1.98	0.46
3:A:813:VAL:O	3:A:817:ILE:HG22	2.16	0.46
3:A:994:PHE:O	3:A:995:MET:HG2	2.14	0.46
3:A:547:LEU:O	3:A:551:ILE:HG22	2.15	0.46
3:A:630:ILE:O	3:A:633:ILE:HG22	2.16	0.45
3:A:492:LEU:HD22	3:A:496:PHE:CE2	2.52	0.45
2:C:2:C:H2'	2:C:3:G:C8	2.52	0.45
3:A:445:GLU:OE1	3:A:445:GLU:N	2.48	0.45
3:A:643:LEU:HD23	3:A:644:ASN:HB2	1.99	0.45
3:A:1014:ILE:HA	3:A:1017:LYS:HG2	1.98	0.45
3:A:971:PRO:HA	3:A:974:ILE:HD12	1.98	0.45
3:A:975:LYS:HA	3:A:978:GLU:HB2	2.00	0.44
3:A:987:ASP:OD1	3:A:988:ILE:N	2.51	0.44
3:A:611:PRO:O	3:A:615:LYS:HG3	2.17	0.44
3:A:664:SER:OG	3:A:665:PRO:HD3	2.18	0.44
3:A:527:LYS:HE3	3:A:527:LYS:HB2	1.73	0.44
3:A:453:ILE:HG13	3:A:550:ARG:HH22	1.83	0.43
3:A:712:ILE:HG23	3:A:713:VAL:HG13	1.99	0.43
3:A:519:LYS:CG	3:A:520:PRO:CD	2.93	0.43
3:A:686:LYS:HB2	3:A:686:LYS:HE3	1.68	0.43
3:A:517:ILE:HA	3:A:518:PRO:HD3	1.41	0.43
3:A:959:ILE:HG12	3:A:983:ILE:O	2.18	0.43
3:A:1060:ILE:HG22	3:A:1061:TYR:CD1	2.53	0.43
3:A:266:MET:O	3:A:270:ILE:HG12	2.19	0.43
3:A:620:LEU:HD23	3:A:620:LEU:HA	1.88	0.42
3:A:799:TRP:CD1	3:A:802:ILE:HD11	2.54	0.42
3:A:497:GLN:HA	3:A:500:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:517:ILE:O	3:A:531:ARG:N	2.39	0.42
3:A:269:GLU:CA	3:A:272:MET:CG	2.97	0.42
3:A:465:LEU:HD23	3:A:478:ALA:HB1	2.01	0.42
3:A:519:LYS:CB	3:A:520:PRO:CD	2.97	0.42
3:A:809:ARG:HG2	3:A:847:PHE:CE2	2.51	0.42
3:A:897:ASP:O	3:A:901:ARG:NH2	2.52	0.42
3:A:1017:LYS:HB2	3:A:1017:LYS:HE2	1.52	0.42
3:A:453:ILE:HD12	3:A:500:GLU:OE2	2.19	0.42
2:C:5:A:H2'	2:C:6:A:C8	2.54	0.42
3:A:885:LYS:HD3	3:A:1050:ILE:HG13	2.00	0.42
3:A:771:ILE:HD13	3:A:771:ILE:HA	1.91	0.41
3:A:1024:GLU:HA	3:A:1027:ILE:HG12	2.02	0.41
3:A:613:MET:HA	3:A:616:THR:HG22	2.03	0.41
3:A:1047:LYS:HB3	3:A:1047:LYS:HE3	1.63	0.41
2:C:2:C:H2'	2:C:3:G:H8	1.85	0.41
2:C:3:G:H2'	2:C:4:A:C8	2.55	0.41
2:C:1:G:H2'	2:C:2:C:H6	1.86	0.41
3:A:267:LYS:NZ	3:A:487:GLU:OE1	2.54	0.41
3:A:519:LYS:HG2	3:A:520:PRO:HD3	1.99	0.41
3:A:625:MET:HE3	3:A:626:TYR:N	2.35	0.41
3:A:685:ILE:H	3:A:685:ILE:HG12	1.70	0.41
2:C:1:G:H2'	2:C:2:C:C6	2.55	0.40
3:A:820:LYS:HB2	3:A:820:LYS:HE3	1.89	0.40
3:A:266:MET:HE2	3:A:266:MET:HB2	1.92	0.40
3:A:406:GLU:O	3:A:410:THR:HG22	2.21	0.40
3:A:959:ILE:HD13	3:A:985:ILE:HD12	2.04	0.40
2:C:4:A:H2'	2:C:5:A:H8	1.86	0.40
3:A:782:LYS:HE2	3:A:782:LYS:HB2	1.83	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
3	A	722/1275 (57%)	694 (96%)	27 (4%)	1 (0%)	48 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	928	LYS

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
3	A	663/1170 (57%)	660 (100%)	3 (0%)	81 83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	272	MET
3	A	741	PHE
3	A	1017	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	581	ASN
3	A	587	ASN
3	A	659	GLN
3	A	986	GLN
3	A	1055	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	10/17 (58%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	-1	G

There are no RNA pucker outliers to report.

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
4	TTP	C	101	5	29,30,30	1.33	6 (20%)	43,47,47	1.76	6 (13%)

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
4	TTP	C	101	5	-	4/22/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	101	TTP	C6-C5	2.72	1.39	1.34
4	C	101	TTP	C4-N3	-2.59	1.34	1.38
4	C	101	TTP	C4-C5	2.34	1.48	1.44
4	C	101	TTP	C6-N1	-2.27	1.34	1.38
4	C	101	TTP	C2-N3	-2.06	1.34	1.38
4	C	101	TTP	PB-O3A	2.01	1.61	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	101	TTP	C4-N3-C2	-5.08	120.67	127.34
4	C	101	TTP	N3-C2-N1	4.87	121.23	114.89
4	C	101	TTP	C5-C4-N3	4.40	119.15	115.32
4	C	101	TTP	O4-C4-C5	-3.98	120.37	124.92
4	C	101	TTP	C5-C6-N1	-3.64	119.36	123.31
4	C	101	TTP	O2-C2-N1	-2.80	119.15	122.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	101	TTP	C3'-C4'-C5'-O5'
4	C	101	TTP	O4'-C4'-C5'-O5'
4	C	101	TTP	C5'-O5'-PA-O3A
4	C	101	TTP	PB-O3A-PA-O2A

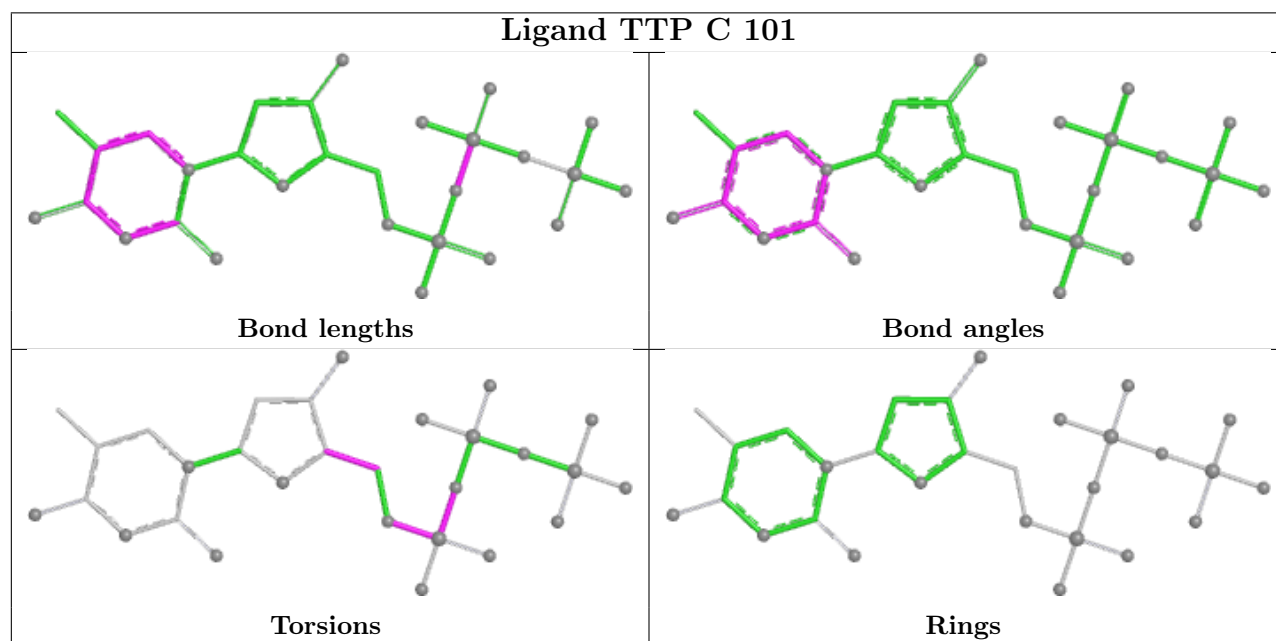
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	101	TTP	4	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.

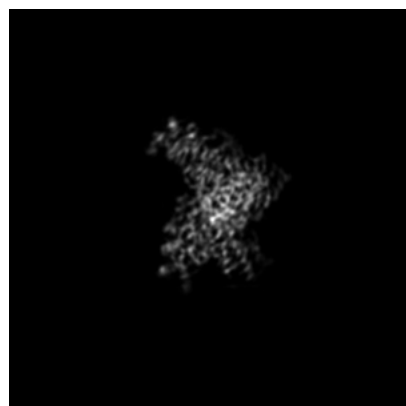
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40858. These allow visual inspection of the internal detail of the map and identification of artifacts.

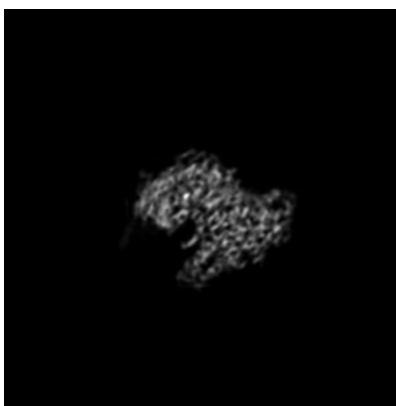
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

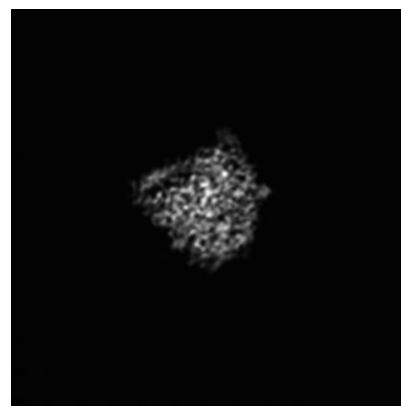
6.1.1 Primary map



X

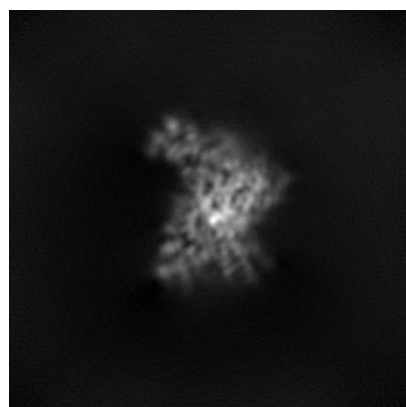


Y

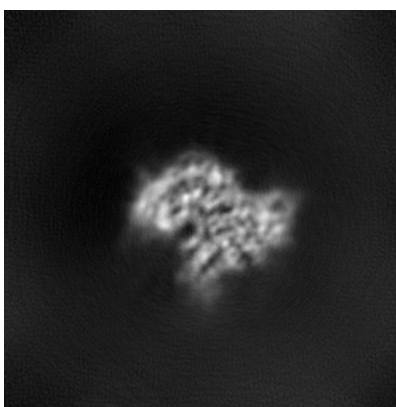


Z

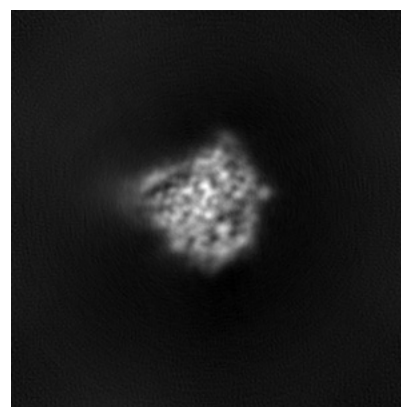
6.1.2 Raw map



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: 120

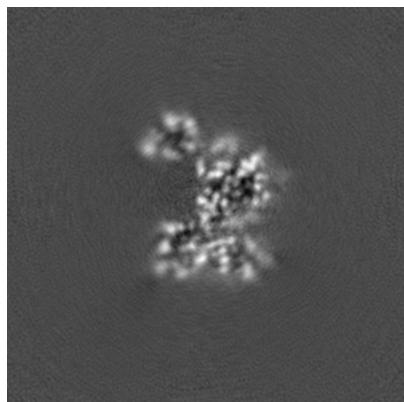


Y Index: 120

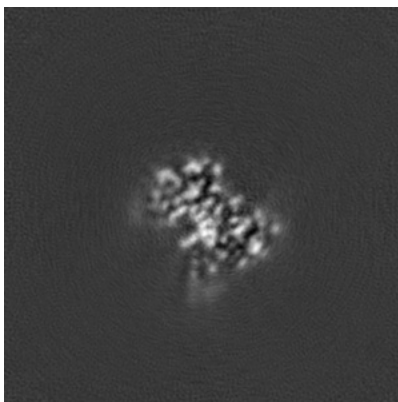


Z Index: 120

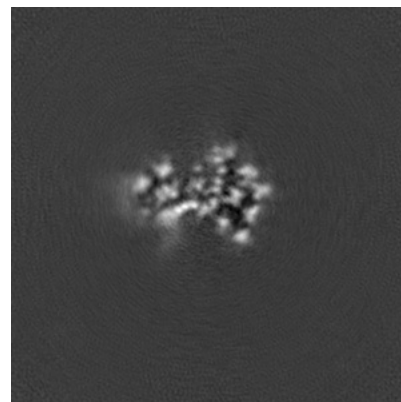
6.2.2 Raw map



X Index: 120



Y Index: 120



Z Index: 120

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: 117

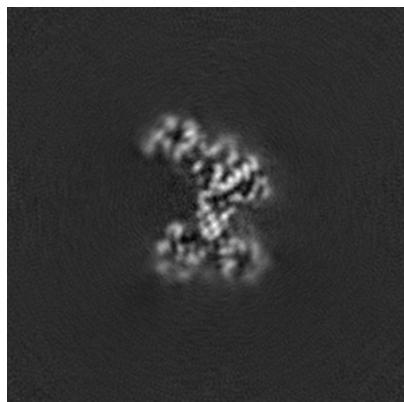


Y Index: 130

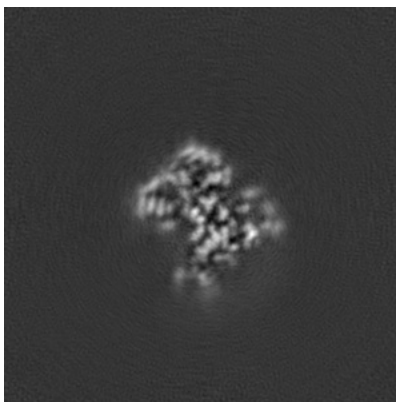


Z Index: 127

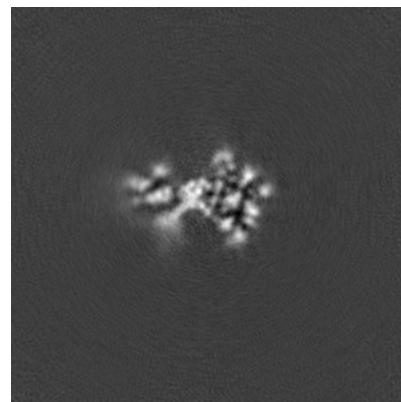
6.3.2 Raw map



X Index: 116



Y Index: 130

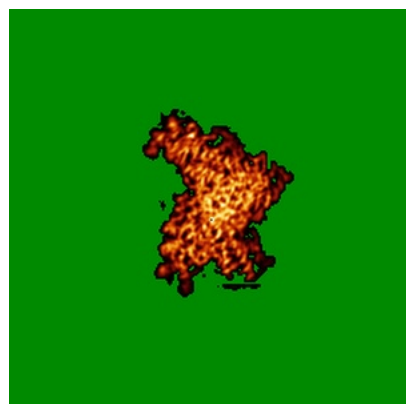


Z Index: 117

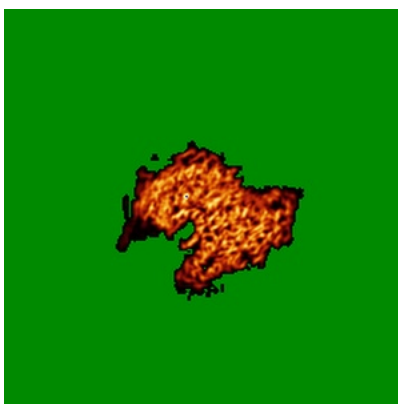
The images above show the largest variance slices of the map in three orthogonal directions.

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

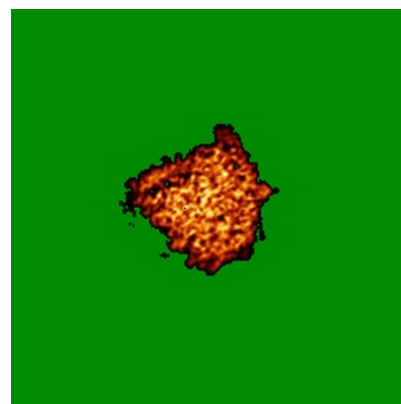
6.4.1 Primary map



X

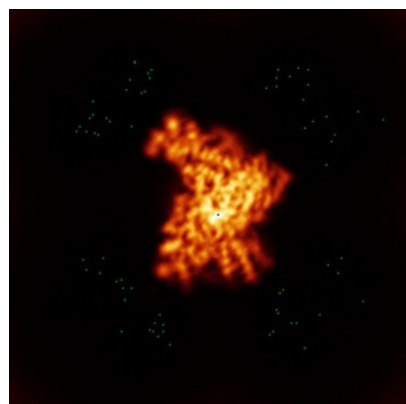


Y

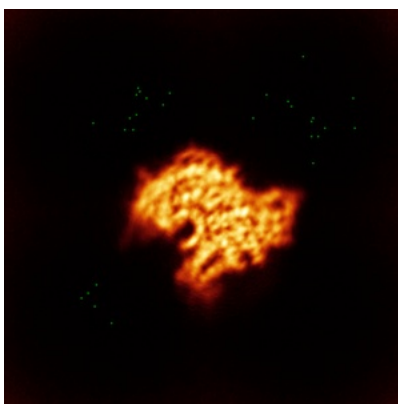


Z

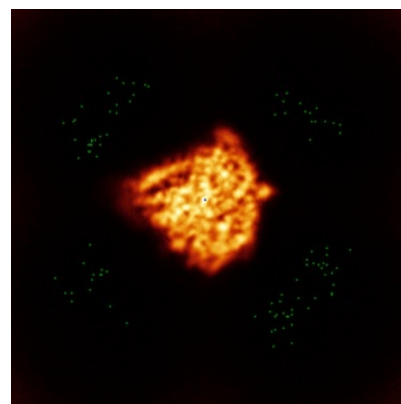
6.4.2 Raw map



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 0.281. 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.

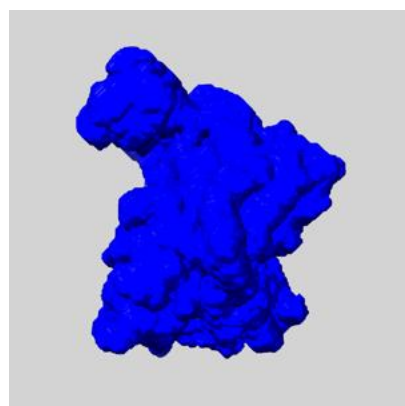
6.6 Mask visualisation [i](#)

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

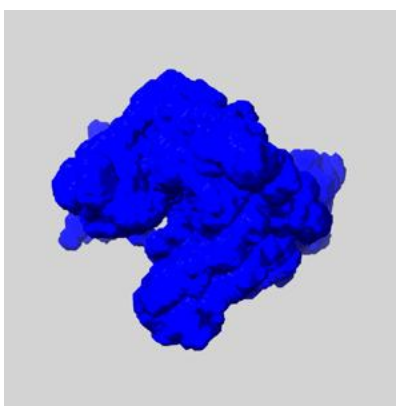
A mask typically either:

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

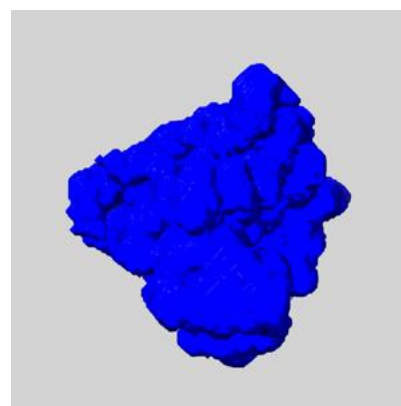
6.6.1 emd_40858_msk_1.map [i](#)



X



Y

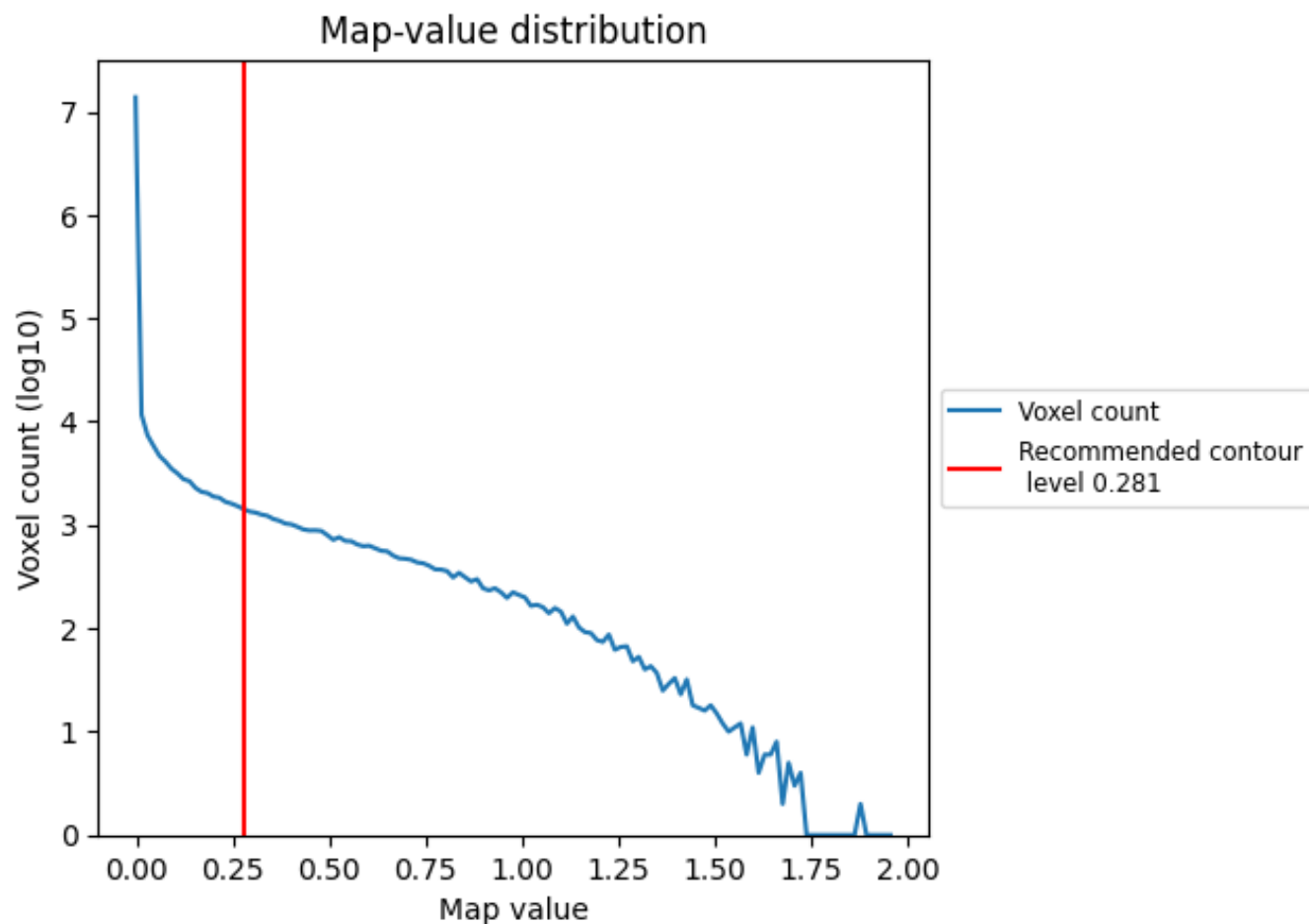


Z

7 Map analysis [i](#)

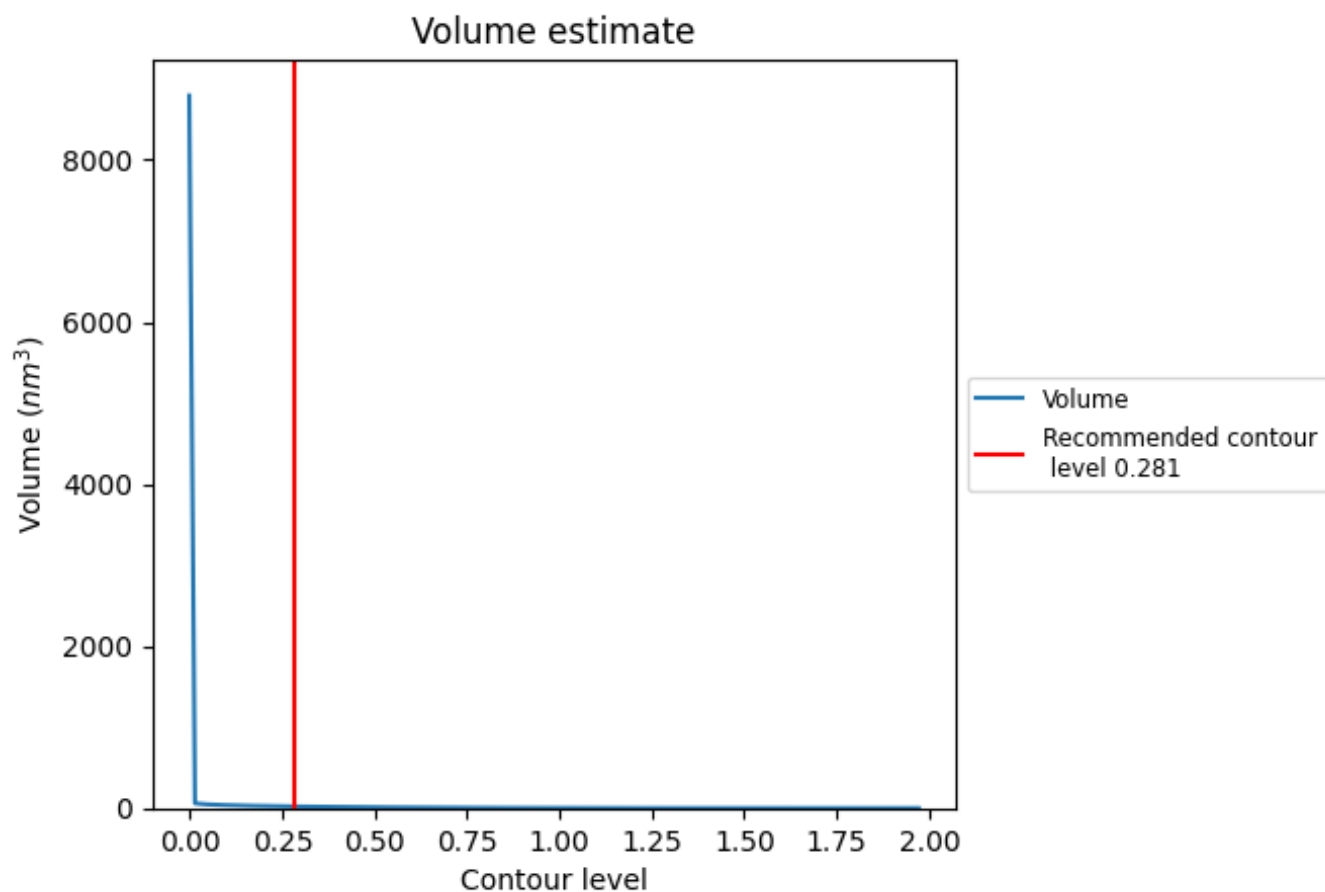
This section contains the results of statistical analysis of the map.

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.

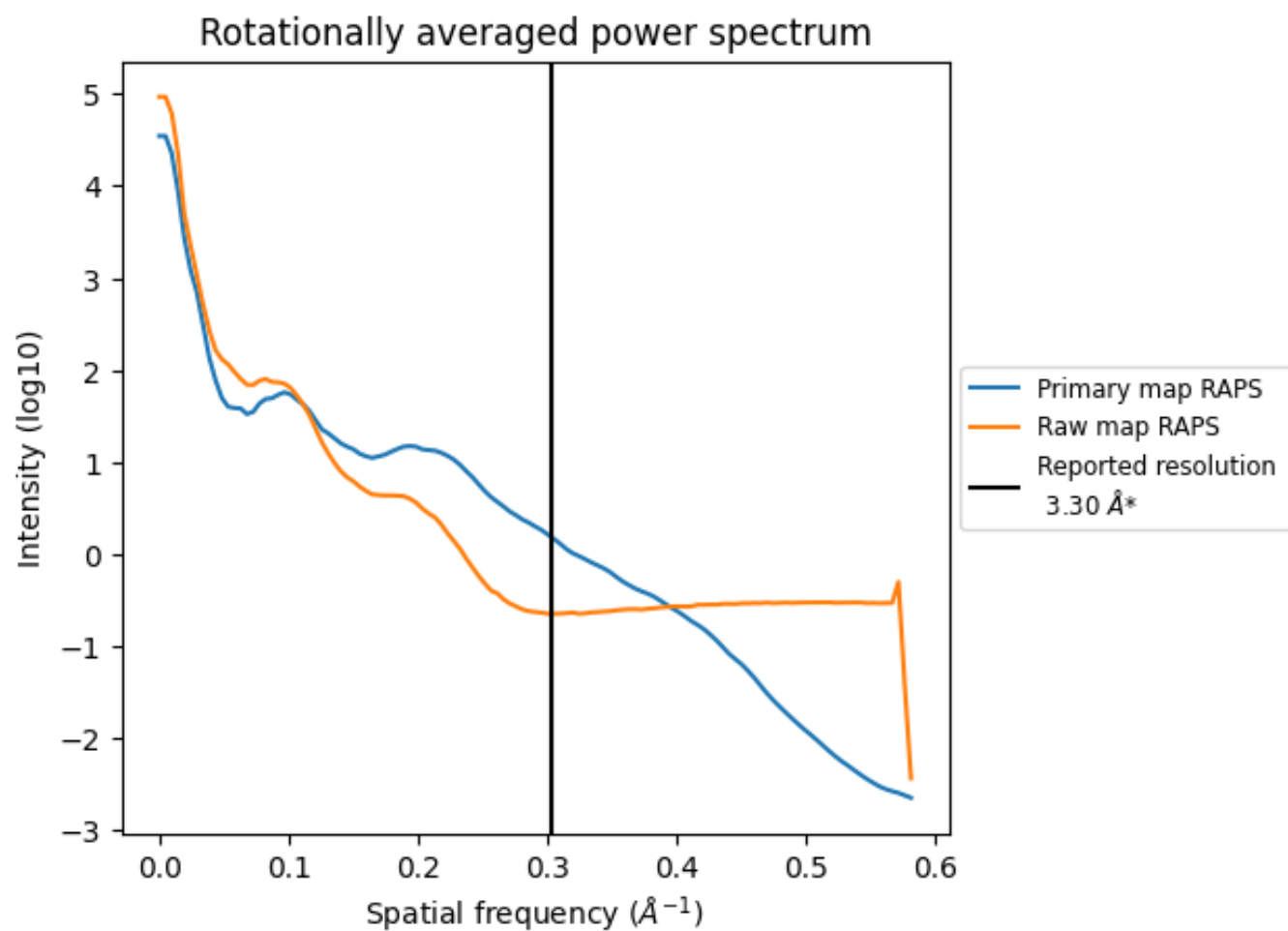
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21 nm³; this corresponds to an approximate mass of 19 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 ⓘ

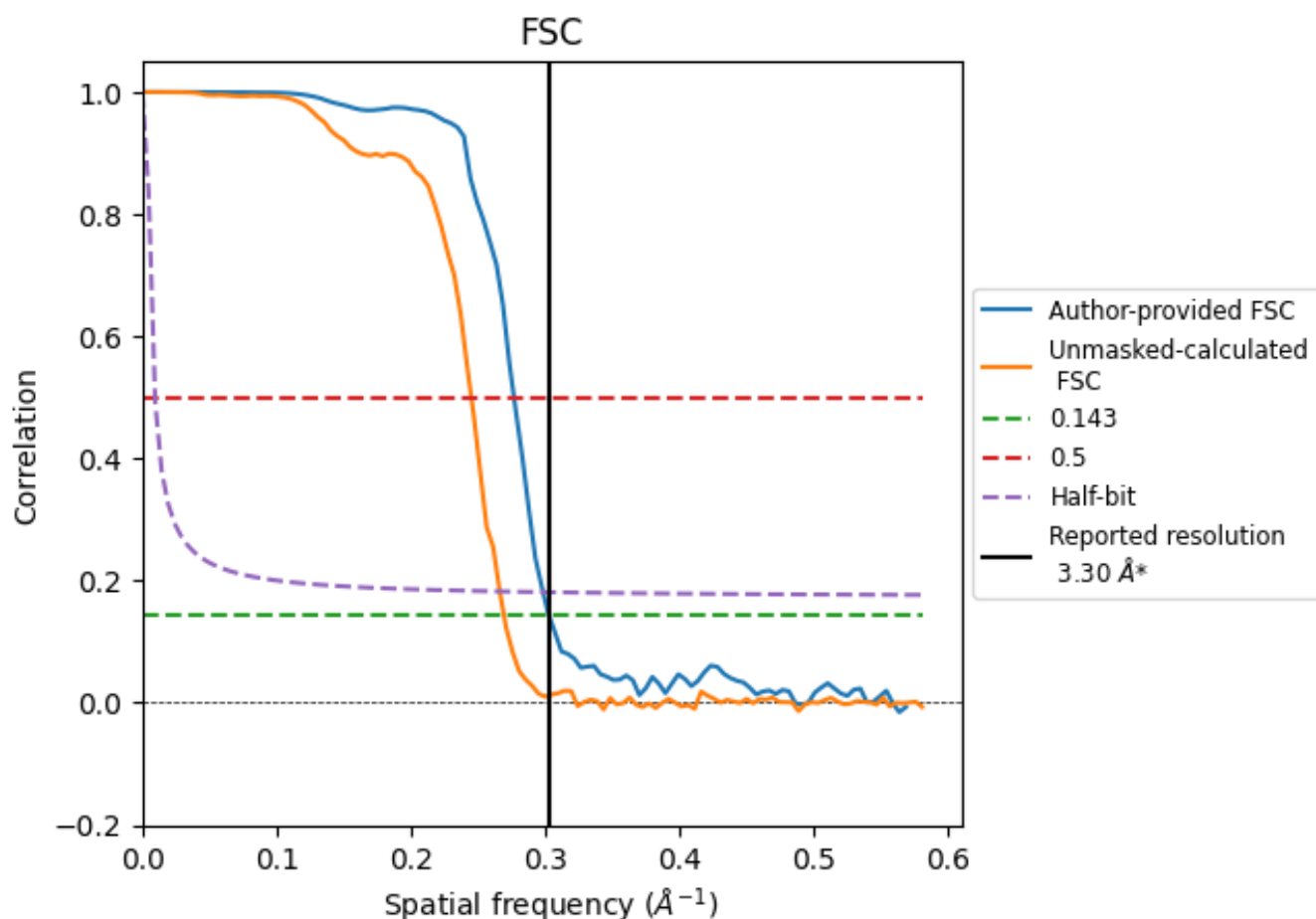


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

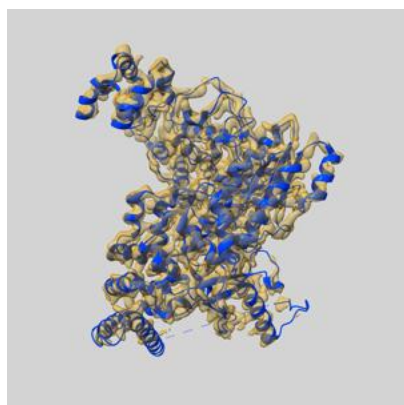
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.61	3.35
Unmasked-calculated*	3.71	4.08	3.75

*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 3.71 differs from the reported value 3.3 by more than 10 %

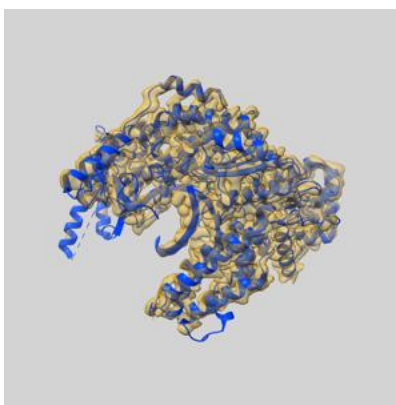
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40858 and PDB model 8SXT. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

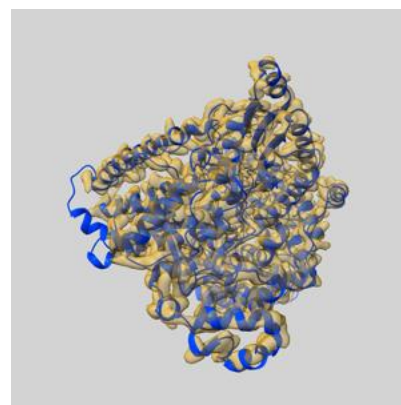
9.1 Map-model overlay [i](#)



X



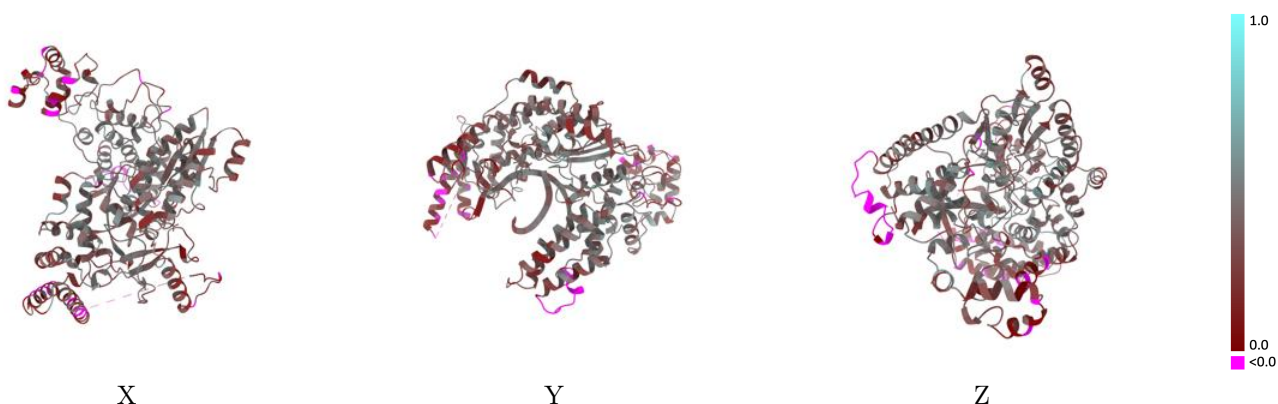
Y



Z

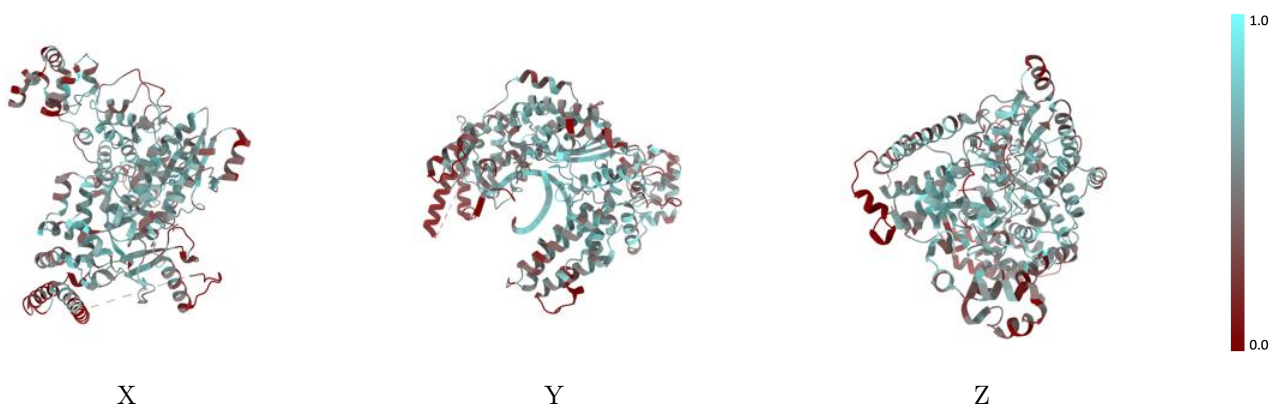
The images above show the 3D surface view of the map at the recommended contour level 0.281 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



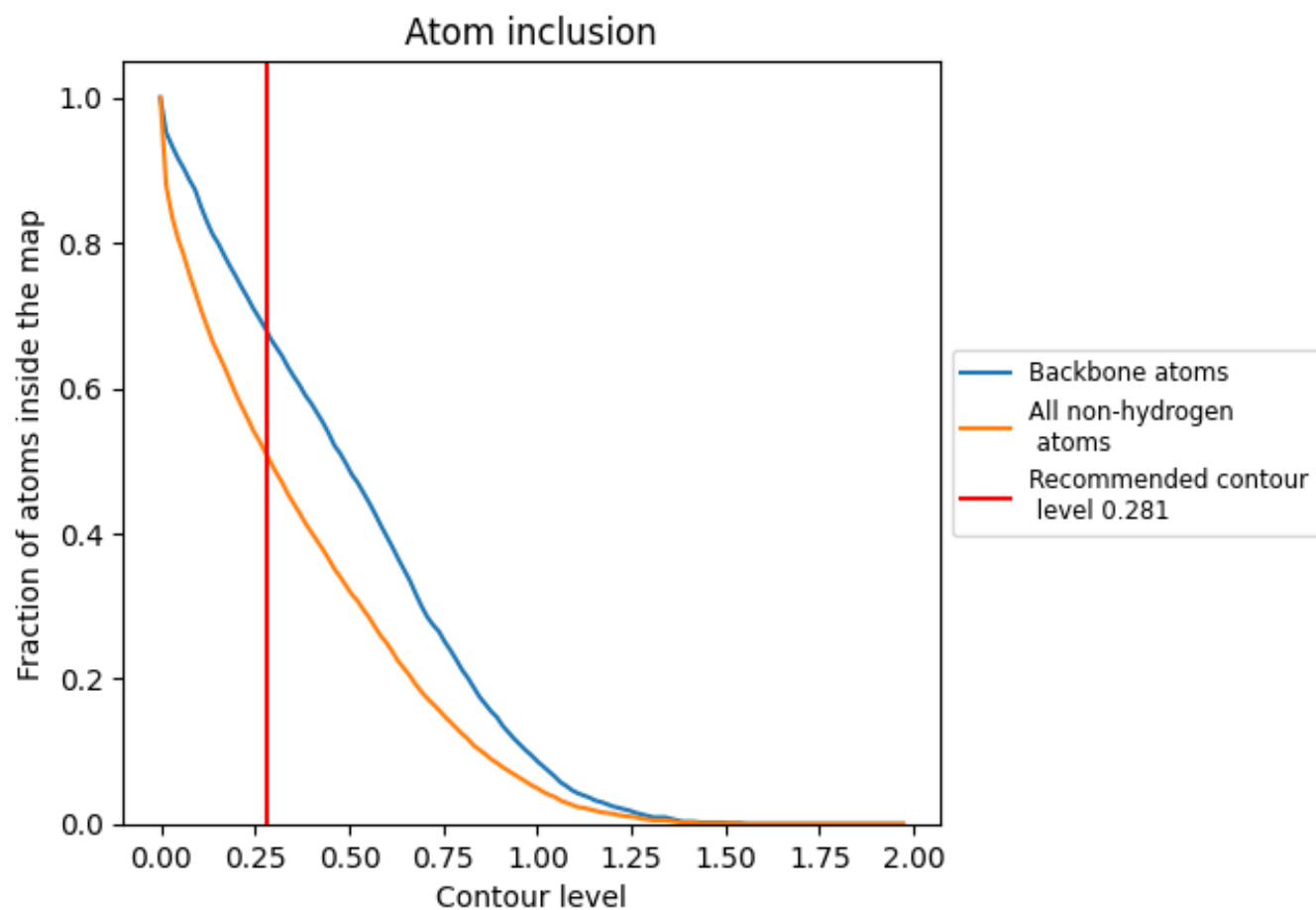
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.281).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 51% 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 (0.281) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5080	0.3390
A	0.5000	0.3370
B	0.6000	0.3480
C	0.6340	0.3900

