



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 04:24 AM UTC

PDB ID : 9C9G / pdb_00009c9g
EMDB ID : EMD-45361
Title : S.c INO80 in complex with S.c 0/80 nucleosome
Authors : Wu, H.; Kaur, U.; Narlikar, G.J.; Cheng, Y.F.
Deposited on : 2024-06-13
Resolution : 2.91 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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<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

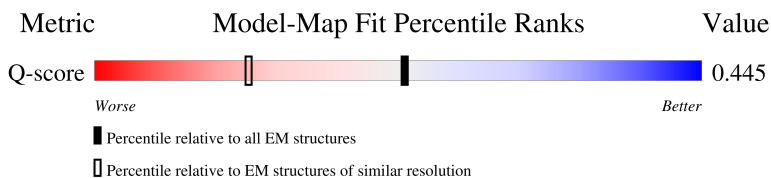
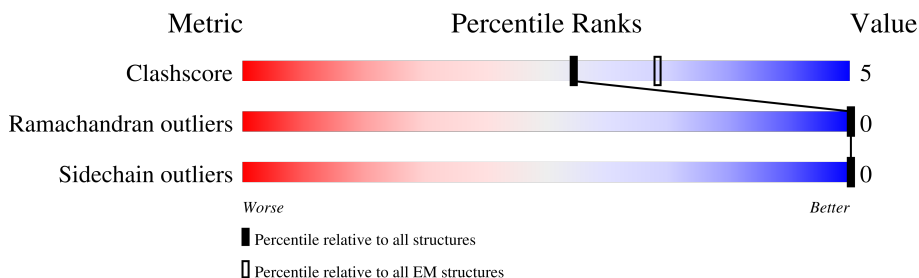
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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.










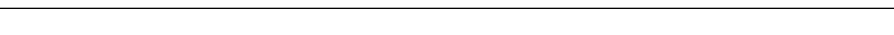
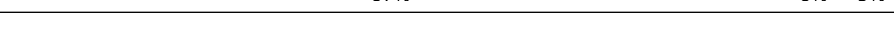
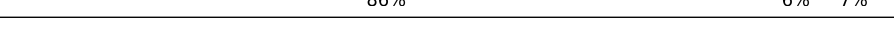
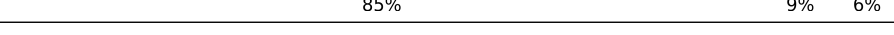





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12972 (2.41 - 3.41)

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	136	
1	E	136	
2	C	132	
2	G	132	

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Mol	Chain	Length	Quality of chain
3	D	131	
3	H	131	
4	Q	1489	
5	R	755	
6	S	166	
7	T	463	
7	V	463	
7	X	463	
8	U	471	
8	W	471	
8	Y	471	
9	Z	320	
10	B	103	
10	F	103	
11	J	227	
12	I	227	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 43020 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 Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	95	Total	C	N	O	0	0
			784	497	151	136		
1	E	95	Total	C	N	O	0	0
			784	497	151	136		

- Molecule 2 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	104	Total	C	N	O	0	0
			804	505	158	141		
2	G	104	Total	C	N	O	0	0
			795	496	157	142		

- Molecule 3 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	93	Total	C	N	O	S	0	0
			722	454	127	140	1		
3	H	93	Total	C	N	O	S	0	0
			726	456	127	142	1		

- Molecule 4 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	660	Total	C	N	O	S	0	0
			5289	3383	903	979	24		

- Molecule 5 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	552	Total	C	N	O	S	0	0
			4097	2590	708	788	11		

- Molecule 6 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	125	Total	C	N	O	S	0	0
			1014	647	189	176	2		

- Molecule 7 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	435	Total	C	N	O	S	0	0
			3339	2107	575	647	10		
7	V	443	Total	C	N	O	S	0	0
			3404	2149	585	660	10		
7	X	442	Total	C	N	O	S	0	0
			3397	2144	584	659	10		

- Molecule 8 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	436	Total	C	N	O	S	0	0
			3350	2098	583	658	11		
8	W	442	Total	C	N	O	S	0	0
			3398	2123	590	673	12		
8	Y	445	Total	C	N	O	S	0	0
			3418	2136	594	677	11		

- Molecule 9 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	57	Total	C	N	O	S	0	0
			392	244	74	72	2		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	79	Total	C	N	O	S	0	0
			621	391	121	108	1		
10	F	79	Total	C	N	O	S	0	0
			620	389	120	110	1		

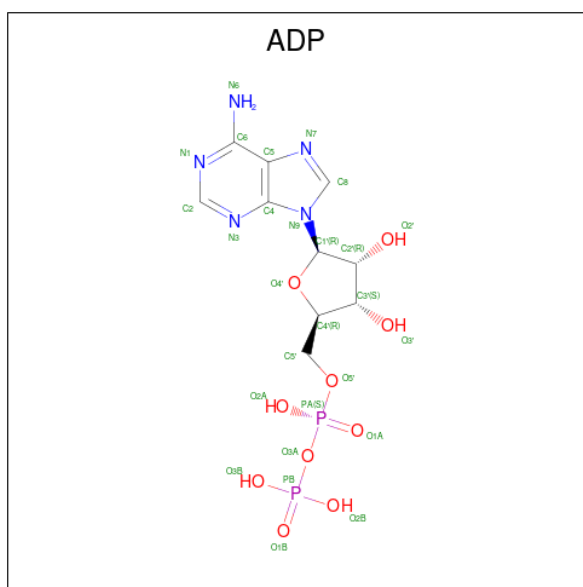
- Molecule 11 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	144	Total	C	N	O	P	0	0
			2969	1405	557	863	144		

- Molecule 12 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	144	Total	C	N	O	P	0	0
			2935	1394	532	865	144		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



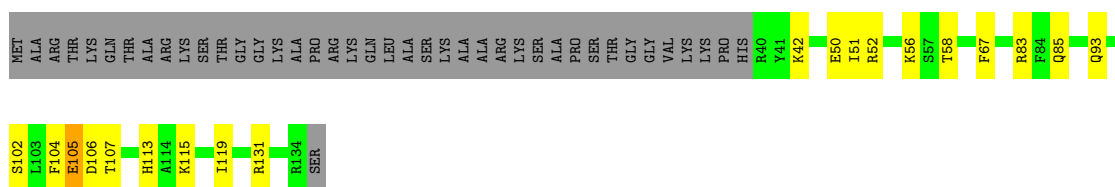
Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots [i](#)

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.

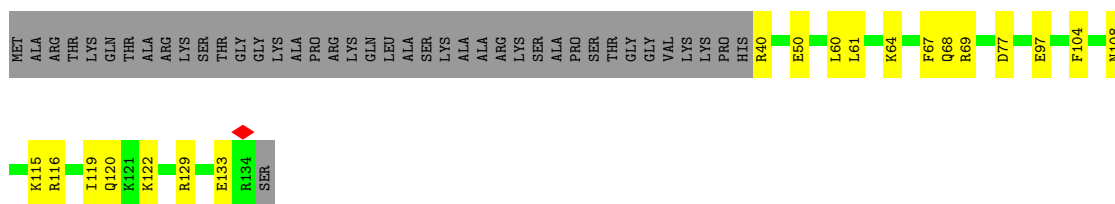
• Molecule 1: Histone H3

Chain A: 



• Molecule 1: Histone H3

Chain E: 



• Molecule 2: Histone H2A.1

Chain C: 

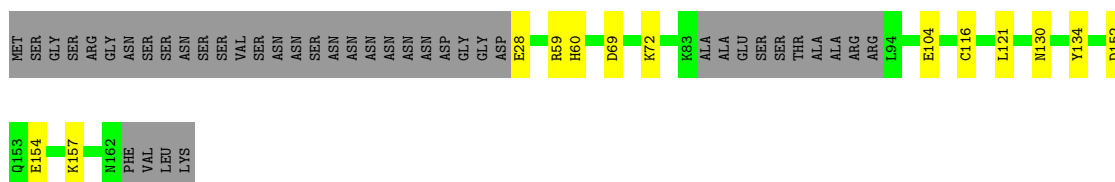


• Molecule 2: Histone H2A.1

Chain G: 

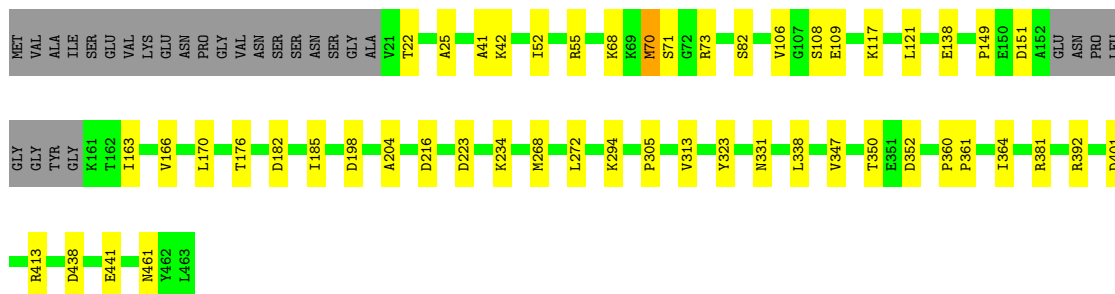


THR	ASN	ALA	GLU	VAL	SER	ASN	GLN	TRP	LYS	MET
THR	ASN	ALA	GLU	VAL	SER	ASN	GLN	TRP	LYS	MET
ASN	PHE	ARG	SER	THR	SER	GLU	LYS	ALA	ARG	SER
TRP	GLU	ASP	HIS	TYR	SER	ASN	SER	GLU	ARG	LEU
LYS	LYS	SER	LYS	ASN	SER	ASN	LYS	GLN	ASP	VAL
ASN	GLU	THR	ARG	PRO	SER	ASP	LYS	SER	ILE	LEU
GLU	ASN	LYS	LYS	ILE	THR	ASN	ASP	PHE	GLU	LEU
ASN	ARG	MET	LEU	ASP	LYS	ASN	ALA	LYS	GLN	ASN
VAL	GLU	SER	ASN	SER	LEU	SER	ALA	ALA	LEU	LYS
GLU	GLU	ARG	ASN	LYS	LEU	ASP	ALA	ALA	TYR	GLU
SER	ARG	LEU	ASN	LYS	MET	ASN	ALA	ASN	GLN	ASP
ASN	ASP	VAL	THR	ASN	ASN	ASP	ALA	LEU	ASP	LYS
LEU	LEU	GLN	ALA	ILE	SER	ASP	ALA	SER	TRP	ASP
SER	LYS	GLN	ASN	ILE	LEU	GLU	ILE	ILE	LYS	ILE
GLU	LYS	GLN	GLY	THR	SER	GLU	GLY	ASP	PHE	SER
GLN	ILE	SER	ALA	THR	LEU	GLU	LYS	ILE	ASN	PHE
LYS	GLU	ILE	ASP	GLN	THR	GLU	ILE	GLU	LEU	SER
ASN	LYS	ARG	ALA	LYS	SER	GLU	LYS	LYS	GLN	LYS
ILE	GLU	SER	ASN	TYR	LYS	GLU	ASP	ASP	GLU	THR
ASP	ALA	THR	LYS	HIS	ILE	ASN	LYS	ALA	PHE	ALA
VAL	MET	ASN	ARG	VAL	ILE	GLU	GLN	ASP	GLU	ALA
GLU	GLU	PHE	LYS	LYS	ASN	GLU	THR	GLU	LEU	GLY
SER	GLU	ARG	PHE	ARG	LYS	GLU	HIS	GLU	ASP	LYS
ALA	GLN	LYS	ASN	LEU	ASN	GLU	ALA	GLU	ASP	SER
LEU	ALA	THR	ASN	ARG	ASN	GLU	VAL	GLU	ILE	LYS
ALA	LYS	THR	ARG	LEU	ILE	GLU	ASP	GLU	GLU	ALA
PRO	LYS	SER	THR	LYS	ILE	GLU	VAL	GLU	TRP	LYS
ASN	GLU	SER	HIS	ILE	ASN	ASP	VAL	GLU	ASN	GLN
GLU	GLU	LEU	GLY	ILE	ASN	ASP	VAL	GLY	GLN	ASN
ASN	GLU	CYS	LEU	ILE	SER	LEU	THR	GLU	GLN	SER
ASP	GLU	ALA	PRO	ASP	ASP	ASP	VAL	GLU	SER	ARG
PHE	LYS	ARG	THR	ALA	ARG	GLU	ASN	LEU	LYS	GLU
HIS	GLU	GLU	TYR	LYS	PRO	GLU	GLY	GLU	ASP	ARG
ALA	SER	ALA	GLY	ARG	LYS	GLU	VAL	VAL	TRP	ARG
LYS	ARG	LYS	MET	GLU	ILE	PHE	GLU	GLY	GLN	ALA
ASP	GLN	TRP	MET	LYS	ARG	ALA	ASN	GLU	PHE	VAL
ASP	ALA	GLN	ASN	ARG	GLU	ALA	GLU	GLU	ASP	ASN
VAL	ASN	LYS	LYS	GLU	VAL	ALA	GLU	GLU	ASP	VAL
ALA	LYS	SER	ASN	ARG	GLU	PHE	ASP	ASP	ASN	ALA
ASN	LYS	SER	ALA	LYS	GLU	GLU	ASP	MET	THR	THR
GLU	LYS	ILE	LYS	VAL	ILE	GLU	GLY	GLY	THR	LYS
GLU	THR	LYS	GLN	GLN	ASN	ASN	ASN	ASN	GLN	GLN
GLU	GLN	GLN	ILE	VAL	CYS	GLU	GLY	GLY	ASP	LEU
THR	LEU	THR	ARG	LYS	THR	GLU	GLU	GLU	GLN	GLU
ALA	LEU	ARG	ALA	LYS	GLN	GLU	GLU	ALA	ASP	ASP
ALA	LEU	THR	ALA	ASN	THR	ASN	GLU	GLU	ASP	GLU
GLU	THR	ALA	ALA	ASN	ILE	ASN	ASP	ALA	ASP	ASN
ASN	SER	ALA	THR	THR	GLN	ASN	GLU	GLU	GLN	LYS
THR	PHE	ARG	HIS	LEU	GLN	PHE	ASN	HIS	LYS	LYS
ALA	GLU	PHE	TYR	ASP	THR	GLN	ASN	ARG	ARG	GLN
GLU	GLU	GLN	ASN	GLY	GLN	ASN	ASN	GLY	PHE	GLN
THR	GLU	THR	THR	LEU	HIS	GLU	ASN	ARG	LYS	ALA
ALA	GLU	GLN	TTR	ASP	GLN	PHE	ASN	HIS	LYS	LYS
ALA	LEU	THR	ASN	GLY	ASN	ASN	ASP	THR	THR	LEU
GLU	ASN	ARG	ASN	ASN	ILE	ASN	ASP	THR	LEU	S



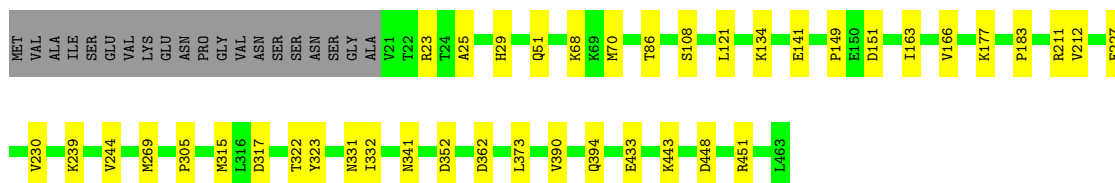
• Molecule 7: RuvB-like protein 1

Chain T: 83% 11% 6%



• Molecule 7: RuvB-like protein 1

Chain V: 87% 9% 4%



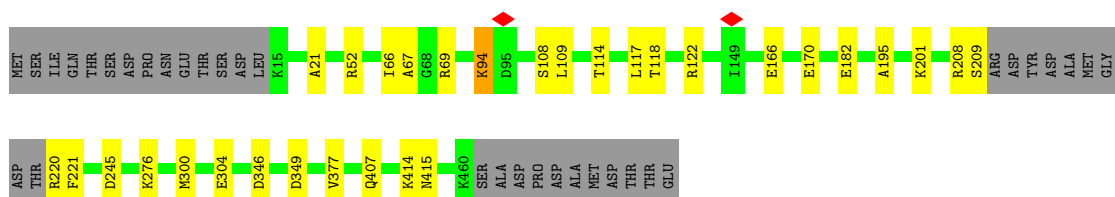
• Molecule 7: RuvB-like protein 1

Chain X: 87% 8% 5%



• Molecule 8: RuvB-like protein 2

Chain U: 86% 6% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.304	Depositor
Minimum map value	-0.351	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.153	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/793	0.69	2/1060 (0.2%)
1	E	0.33	0/793	0.89	2/1060 (0.2%)
2	C	0.32	0/815	0.88	3/1102 (0.3%)
2	G	0.33	0/806	0.80	1/1091 (0.1%)
3	D	0.32	0/732	0.88	4/986 (0.4%)
3	H	0.39	0/736	0.98	2/991 (0.2%)
4	Q	0.23	0/5408	0.52	4/7340 (0.1%)
5	R	0.20	0/4186	0.39	1/5711 (0.0%)
6	S	0.27	0/1036	0.60	0/1392
7	T	0.24	0/3378	0.46	3/4569 (0.1%)
7	V	0.24	0/3446	0.45	2/4662 (0.0%)
7	X	0.24	0/3439	0.46	2/4652 (0.0%)
8	U	0.24	0/3386	0.46	1/4561 (0.0%)
8	W	0.24	0/3436	0.40	1/4632 (0.0%)
8	Y	0.24	0/3456	0.42	0/4659
9	Z	0.20	0/397	0.47	0/536
10	B	0.30	0/628	0.84	1/840 (0.1%)
10	F	0.35	0/627	0.98	2/840 (0.2%)
11	J	0.23	0/3334	0.44	0/5148
12	I	0.23	0/3288	0.43	0/5068
All	All	0.25	0/44120	0.52	31/60900 (0.1%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	63	GLU	CA-CB-CG	6.90	127.90	114.10
1	A	105	GLU	CA-CB-CG	6.36	126.82	114.10
3	D	82	LYS	CA-CB-CG	6.32	126.74	114.10
8	U	94	LYS	CB-CG-CD	5.93	124.93	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	LYS	CA-CB-CG	5.92	125.94	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	784	0	836	23	0
1	E	784	0	836	19	0
2	C	804	0	847	27	0
2	G	795	0	821	21	0
3	D	722	0	744	32	0
3	H	726	0	748	10	0
4	Q	5289	0	5195	77	0
5	R	4097	0	3678	36	0
6	S	1014	0	1050	11	0
7	T	3339	0	3468	37	0
7	V	3404	0	3540	30	0
7	X	3397	0	3533	30	0
8	U	3350	0	3444	25	0
8	W	3398	0	3470	32	0
8	Y	3418	0	3492	36	0
9	Z	392	0	303	3	0
10	B	621	0	652	12	0
10	F	620	0	643	22	0
11	J	2969	0	1616	29	0
12	I	2935	0	1617	17	0
13	T	27	0	12	0	0
13	U	27	0	12	0	0
13	V	27	0	12	1	0
13	W	27	0	12	4	0
13	X	27	0	12	0	0
13	Y	27	0	12	0	0
All	All	43020	0	40605	420	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 5.

The worst 5 of 420 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:ARG:NH1	3:H:38:GLU:OE1	1.65	1.28
4:Q:767:LEU:HD22	4:Q:817:VAL:CG1	1.65	1.25
1:A:58:THR:HB	2:G:82:ARG:NH2	1.59	1.16
4:Q:1131:LEU:HD12	4:Q:1165:LEU:HD22	1.26	1.16
4:Q:767:LEU:CD2	4:Q:817:VAL:CG1	2.25	1.15

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	93/136 (68%)	93 (100%)	0	0	100	100
1	E	93/136 (68%)	91 (98%)	2 (2%)	0	100	100
2	C	102/132 (77%)	96 (94%)	6 (6%)	0	100	100
2	G	102/132 (77%)	99 (97%)	3 (3%)	0	100	100
3	D	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
3	H	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
4	Q	652/1489 (44%)	615 (94%)	37 (6%)	0	100	100
5	R	544/755 (72%)	535 (98%)	9 (2%)	0	100	100
6	S	121/166 (73%)	112 (93%)	9 (7%)	0	100	100
7	T	431/463 (93%)	422 (98%)	9 (2%)	0	100	100
7	V	441/463 (95%)	424 (96%)	17 (4%)	0	100	100
7	X	440/463 (95%)	423 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	U	432/471 (92%)	416 (96%)	16 (4%)	0	100	100
8	W	440/471 (93%)	425 (97%)	15 (3%)	0	100	100
8	Y	443/471 (94%)	422 (95%)	21 (5%)	0	100	100
9	Z	53/320 (17%)	52 (98%)	1 (2%)	0	100	100
10	B	77/103 (75%)	74 (96%)	3 (4%)	0	100	100
10	F	77/103 (75%)	72 (94%)	5 (6%)	0	100	100
All	All	4723/6536 (72%)	4551 (96%)	172 (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	83/113 (74%)	83 (100%)	0	100	100
1	E	83/113 (74%)	83 (100%)	0	100	100
2	C	83/99 (84%)	83 (100%)	0	100	100
2	G	81/99 (82%)	81 (100%)	0	100	100
3	D	80/109 (73%)	80 (100%)	0	100	100
3	H	81/109 (74%)	81 (100%)	0	100	100
4	Q	583/1350 (43%)	583 (100%)	0	100	100
5	R	394/682 (58%)	394 (100%)	0	100	100
6	S	109/142 (77%)	109 (100%)	0	100	100
7	T	367/391 (94%)	367 (100%)	0	100	100
7	V	375/391 (96%)	375 (100%)	0	100	100
7	X	374/391 (96%)	374 (100%)	0	100	100
8	U	371/403 (92%)	371 (100%)	0	100	100
8	W	375/403 (93%)	375 (100%)	0	100	100
8	Y	377/403 (94%)	377 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Z	27/285 (10%)	27 (100%)	0	100	100
10	B	62/79 (78%)	62 (100%)	0	100	100
10	F	62/79 (78%)	62 (100%)	0	100	100
All	All	3967/5641 (70%)	3967 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
8	Y	34	ASN
8	Y	144	GLN
10	B	93	GLN
5	R	109	ASN
5	R	78	ASN

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](#)

6 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
13	ADP	V	501	-	28,29,29	1.38	5 (17%)	43,45,45	1.84	7 (16%)
13	ADP	T	501	-	28,29,29	1.36	5 (17%)	43,45,45	1.83	9 (20%)
13	ADP	Y	501	-	28,29,29	1.36	5 (17%)	43,45,45	1.85	9 (20%)
13	ADP	U	501	-	28,29,29	1.38	5 (17%)	43,45,45	1.81	7 (16%)
13	ADP	X	501	-	28,29,29	1.36	5 (17%)	43,45,45	1.82	9 (20%)
13	ADP	W	501	-	28,29,29	1.35	3 (10%)	43,45,45	1.88	7 (16%)

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
13	ADP	V	501	-	-	4/16/32/32	0/3/3/3
13	ADP	T	501	-	-	3/16/32/32	0/3/3/3
13	ADP	Y	501	-	-	6/16/32/32	0/3/3/3
13	ADP	U	501	-	-	2/16/32/32	0/3/3/3
13	ADP	X	501	-	-	3/16/32/32	0/3/3/3
13	ADP	W	501	-	-	3/16/32/32	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	501	ADP	C5-C4	4.36	1.46	1.39
13	U	501	ADP	C5-C4	4.33	1.46	1.39
13	V	501	ADP	C5-C4	4.32	1.46	1.39
13	Y	501	ADP	C5-C4	4.23	1.46	1.39
13	X	501	ADP	C5-C4	4.19	1.46	1.39

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	W	501	ADP	C5-C4-N3	-6.35	117.98	126.72
13	V	501	ADP	C5-C4-N3	-6.01	118.45	126.72
13	Y	501	ADP	C5-C4-N3	-5.86	118.65	126.72
13	T	501	ADP	C5-C4-N3	-5.85	118.66	126.72
13	U	501	ADP	C5-C4-N3	-5.83	118.69	126.72

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

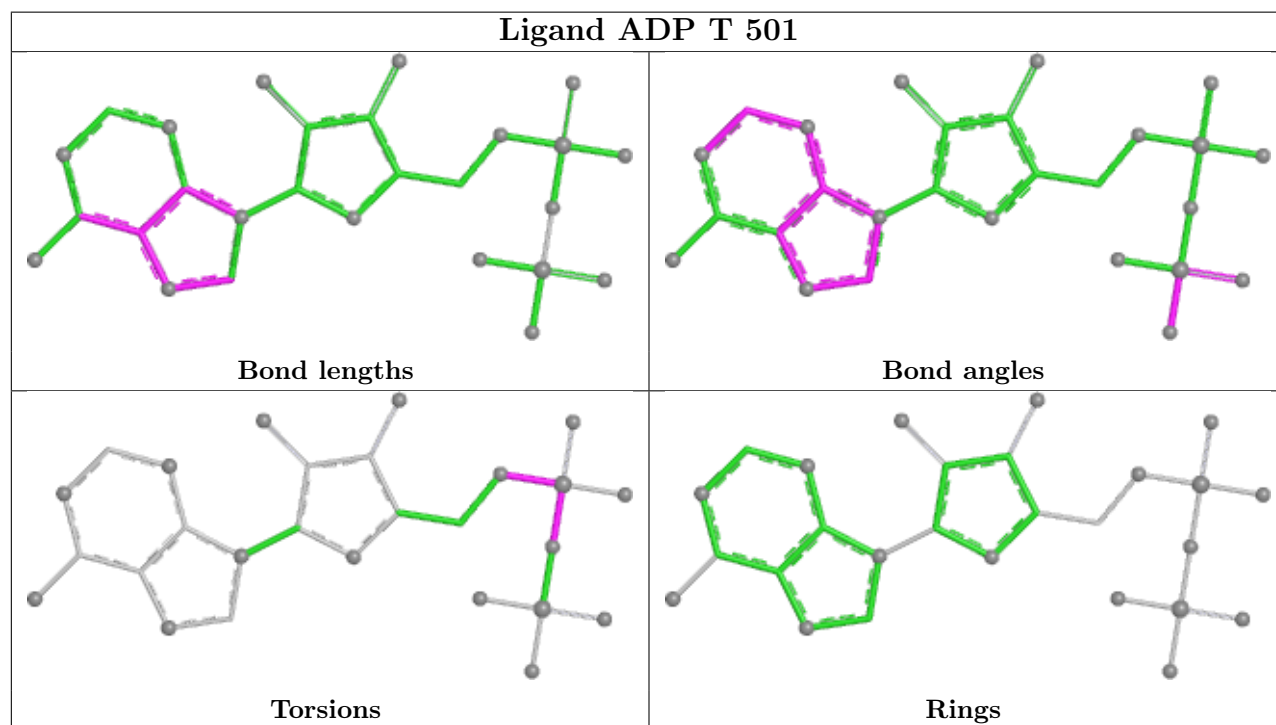
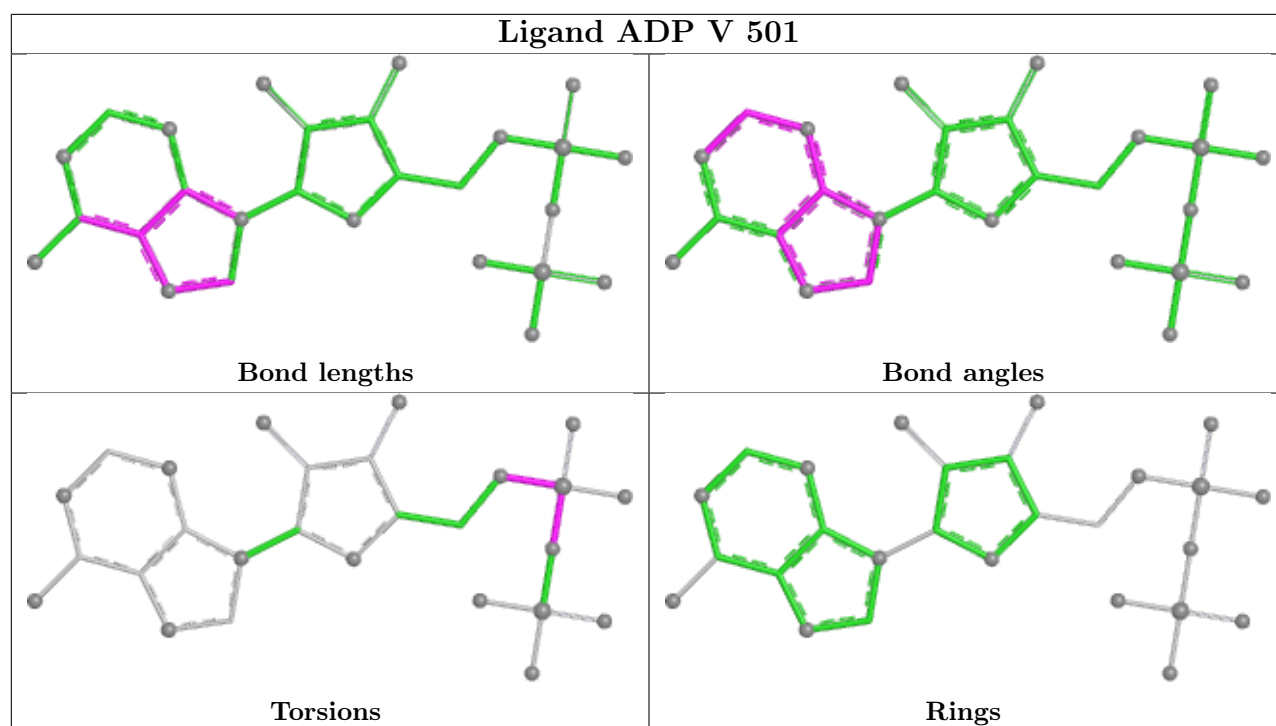
Mol	Chain	Res	Type	Atoms
13	V	501	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O2A
13	V	501	ADP	C5'-O5'-PA-O3A
13	W	501	ADP	C5'-O5'-PA-O2A
13	X	501	ADP	C5'-O5'-PA-O2A

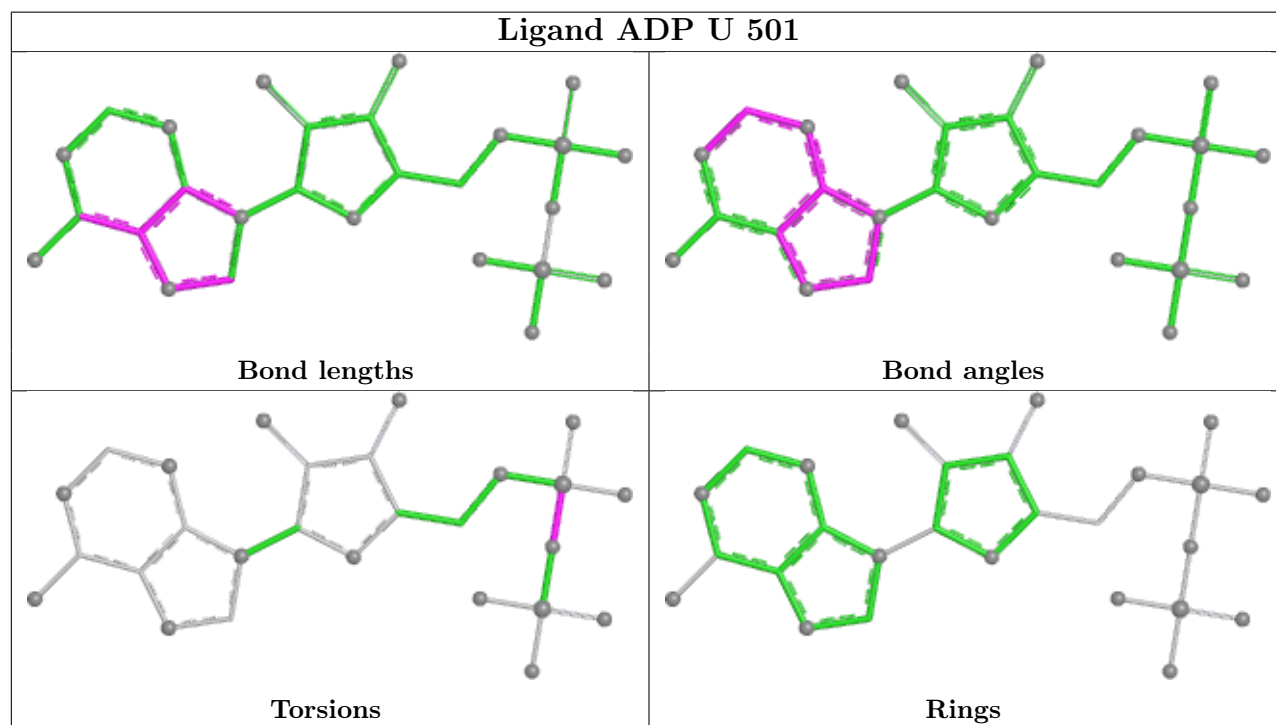
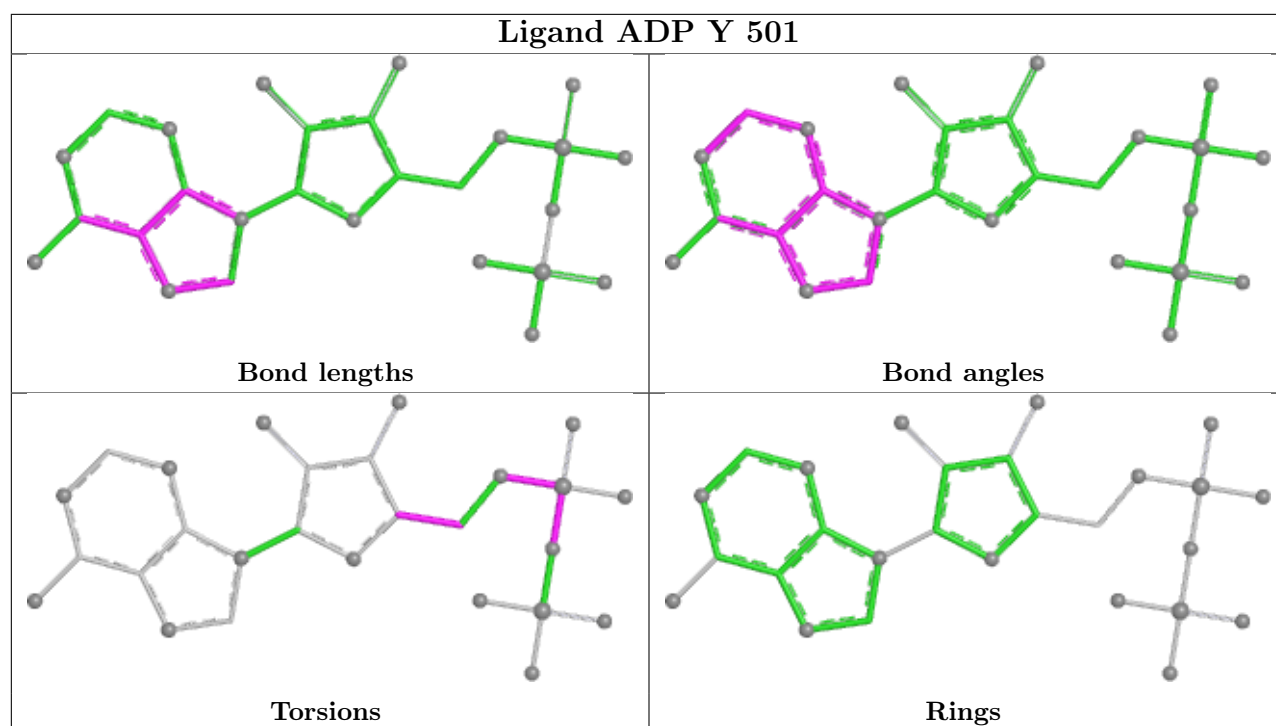
There are no ring outliers.

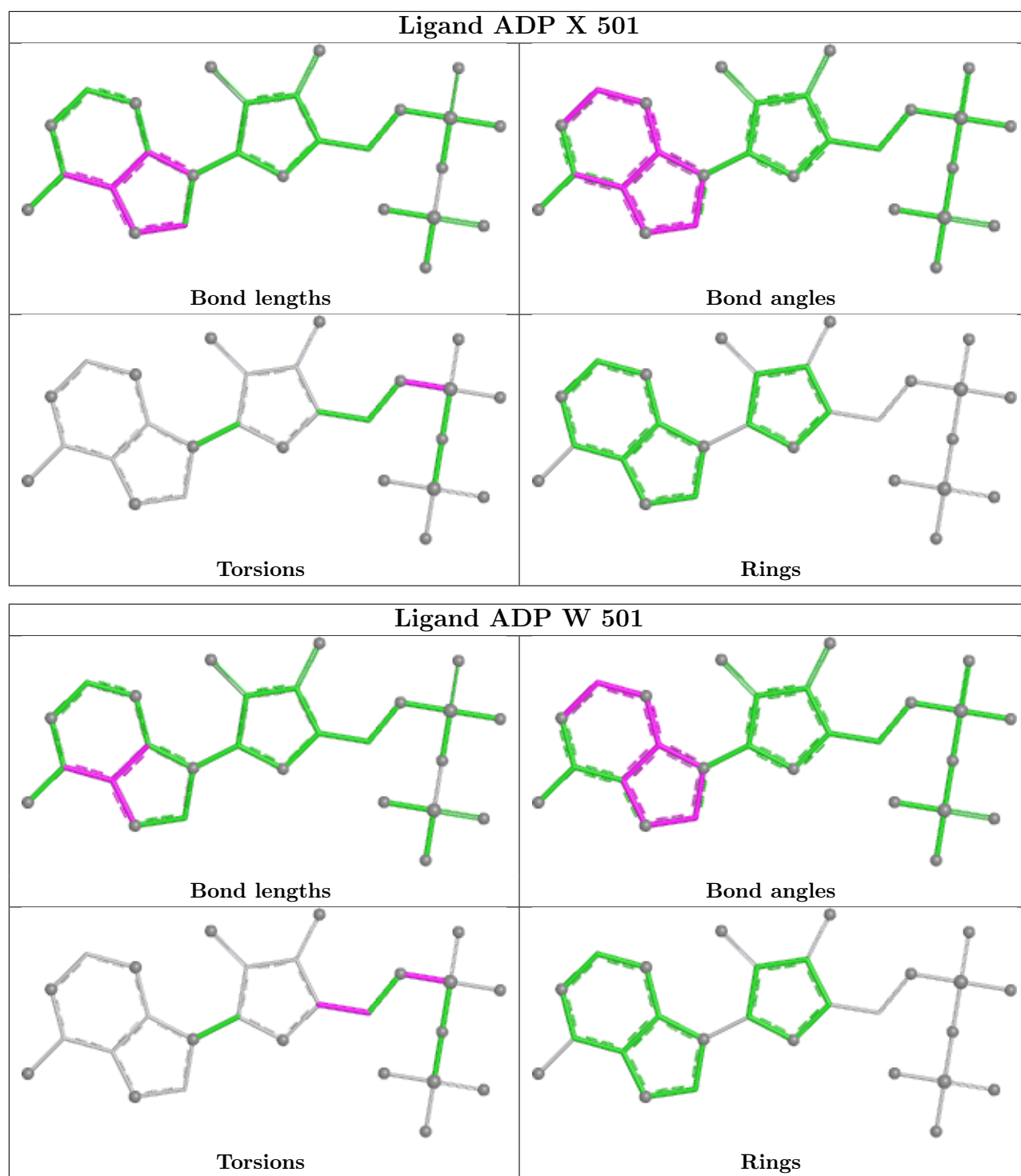
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	V	501	ADP	1	0
13	W	501	ADP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

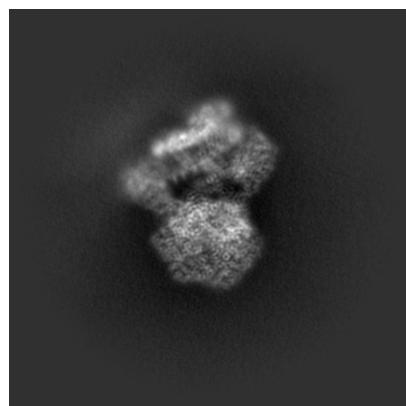
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45361. These allow visual inspection of the internal detail of the map and identification of artifacts.

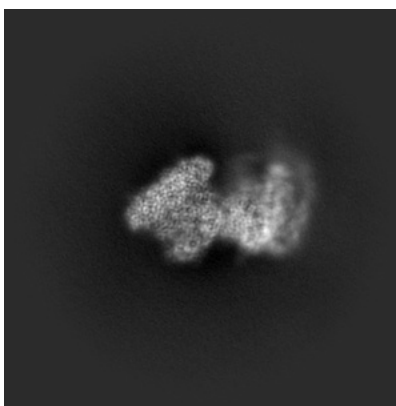
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

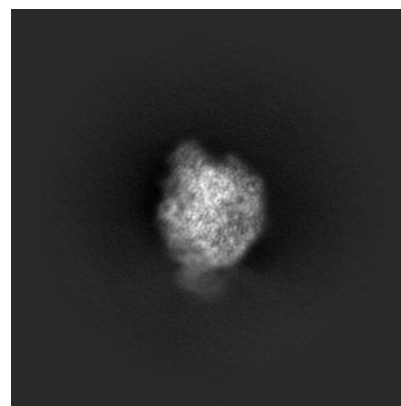
6.1.1 Primary map



X

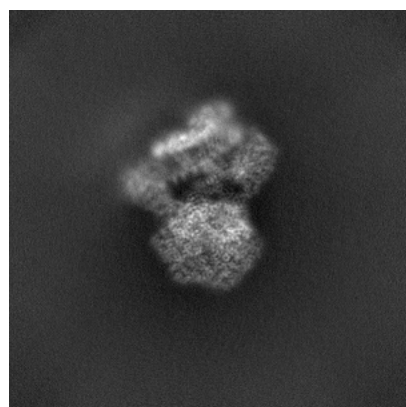


Y

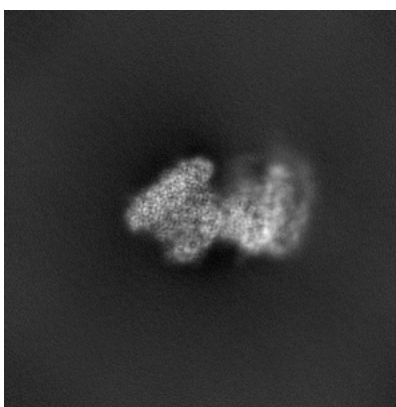


Z

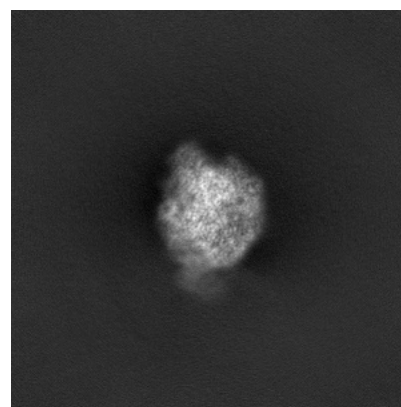
6.1.2 Raw map



X



Y

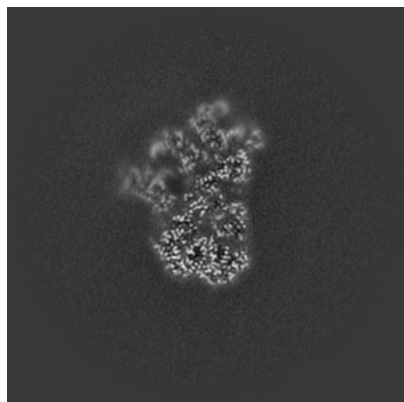


Z

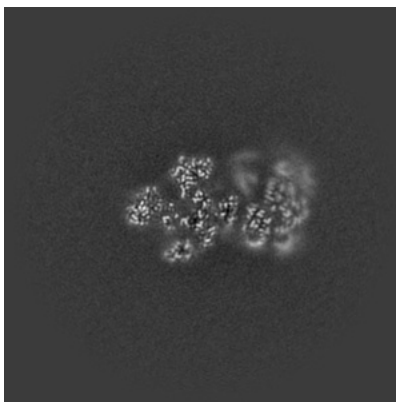
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

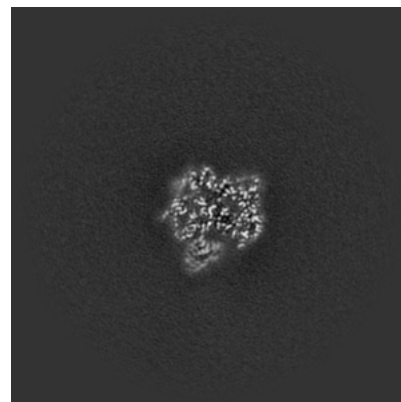
6.2.1 Primary map



X Index: 256

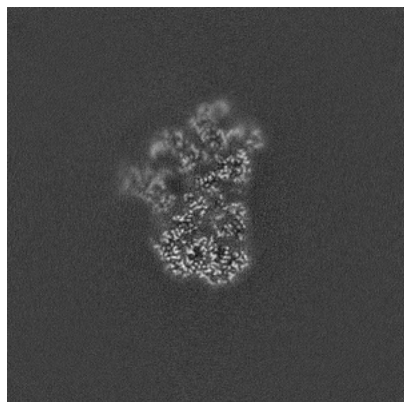


Y Index: 256

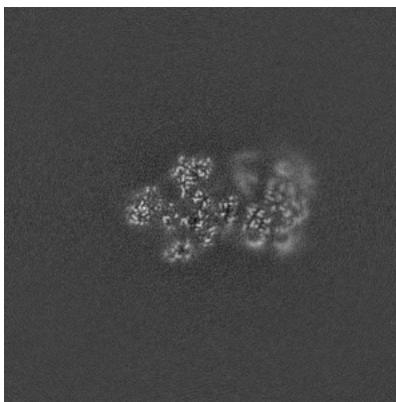


Z Index: 256

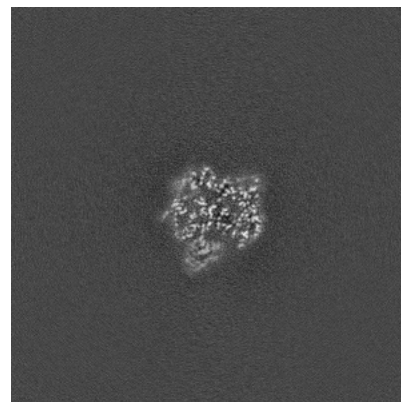
6.2.2 Raw map



X Index: 256



Y Index: 256

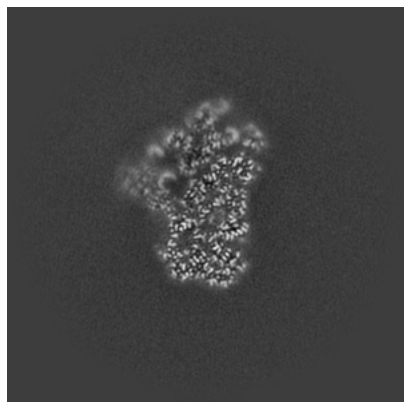


Z Index: 256

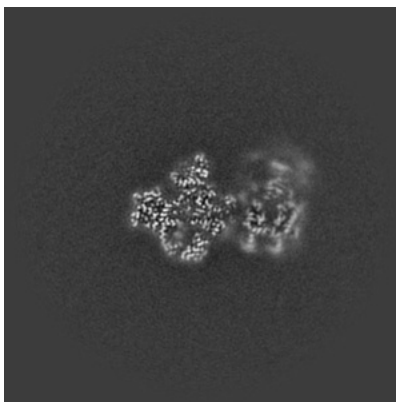
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

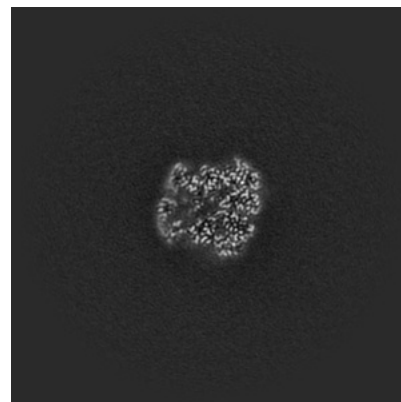
6.3.1 Primary map



X Index: 249

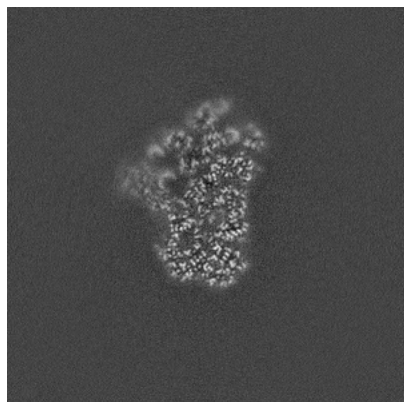


Y Index: 245

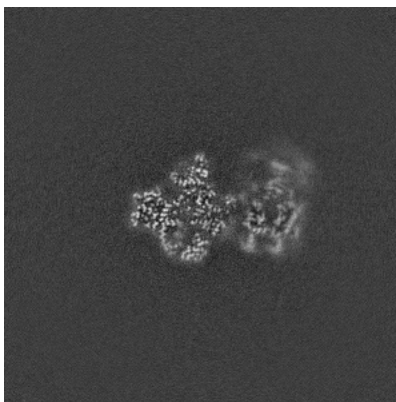


Z Index: 230

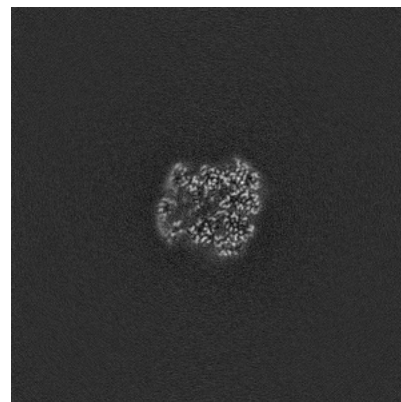
6.3.2 Raw map



X Index: 250



Y Index: 245

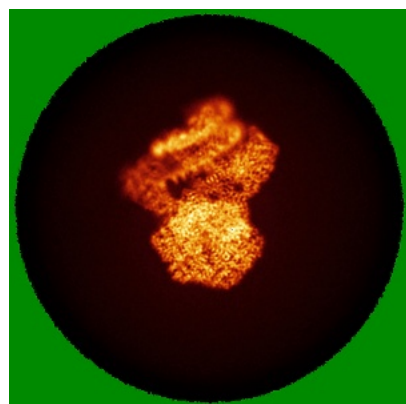


Z Index: 230

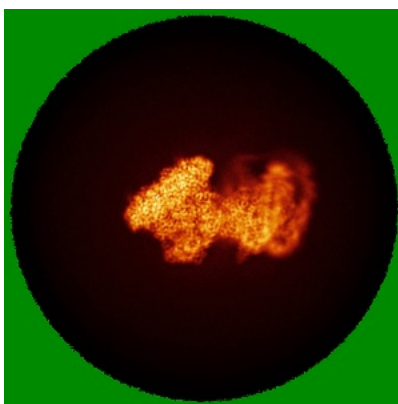
The images above show the largest variance slices of the map in three orthogonal directions.

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

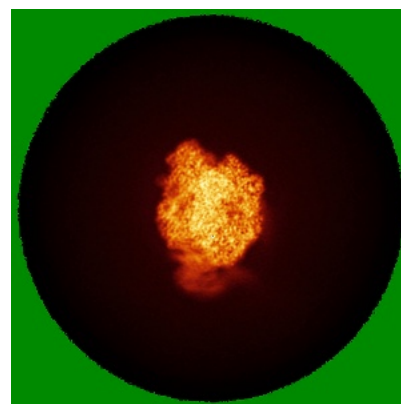
6.4.1 Primary map



X

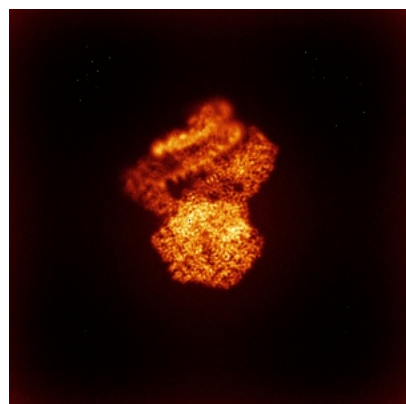


Y

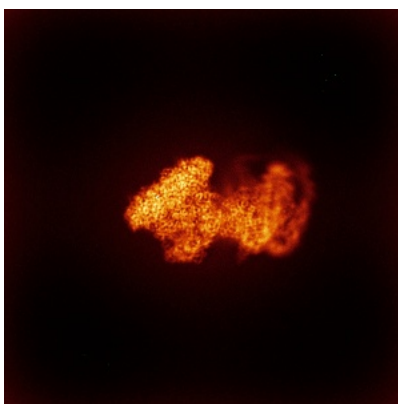


Z

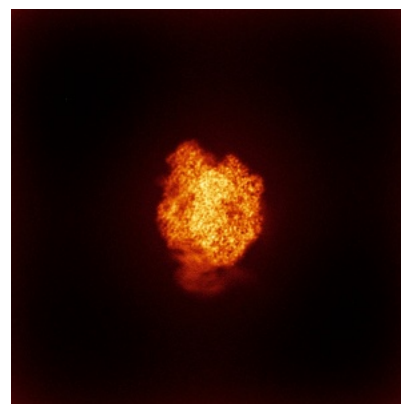
6.4.2 Raw map



X



Y



Z

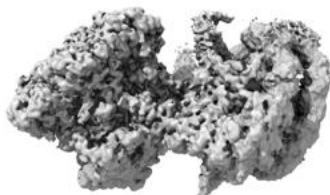
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.153. 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



X



Y



Z

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.

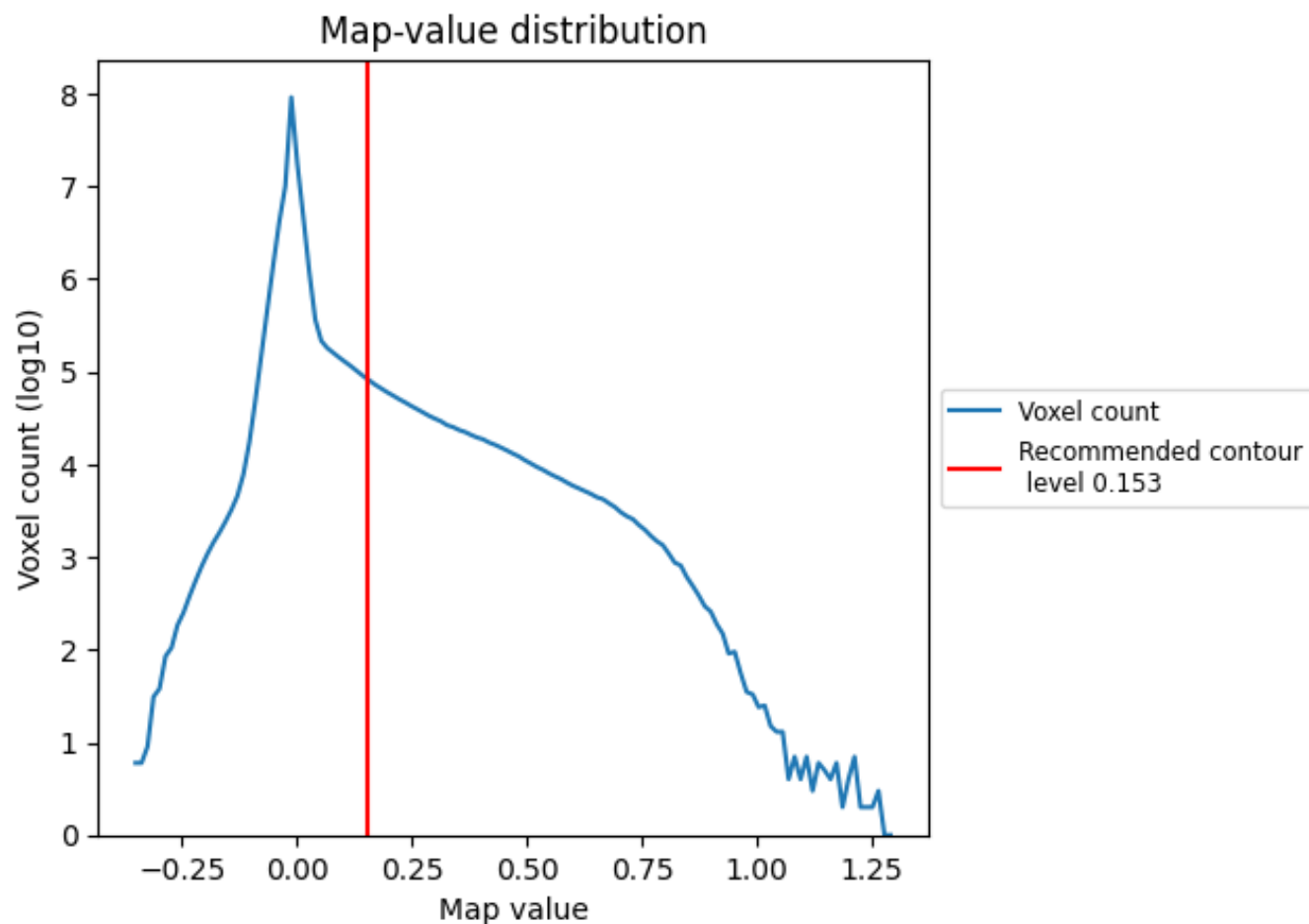
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

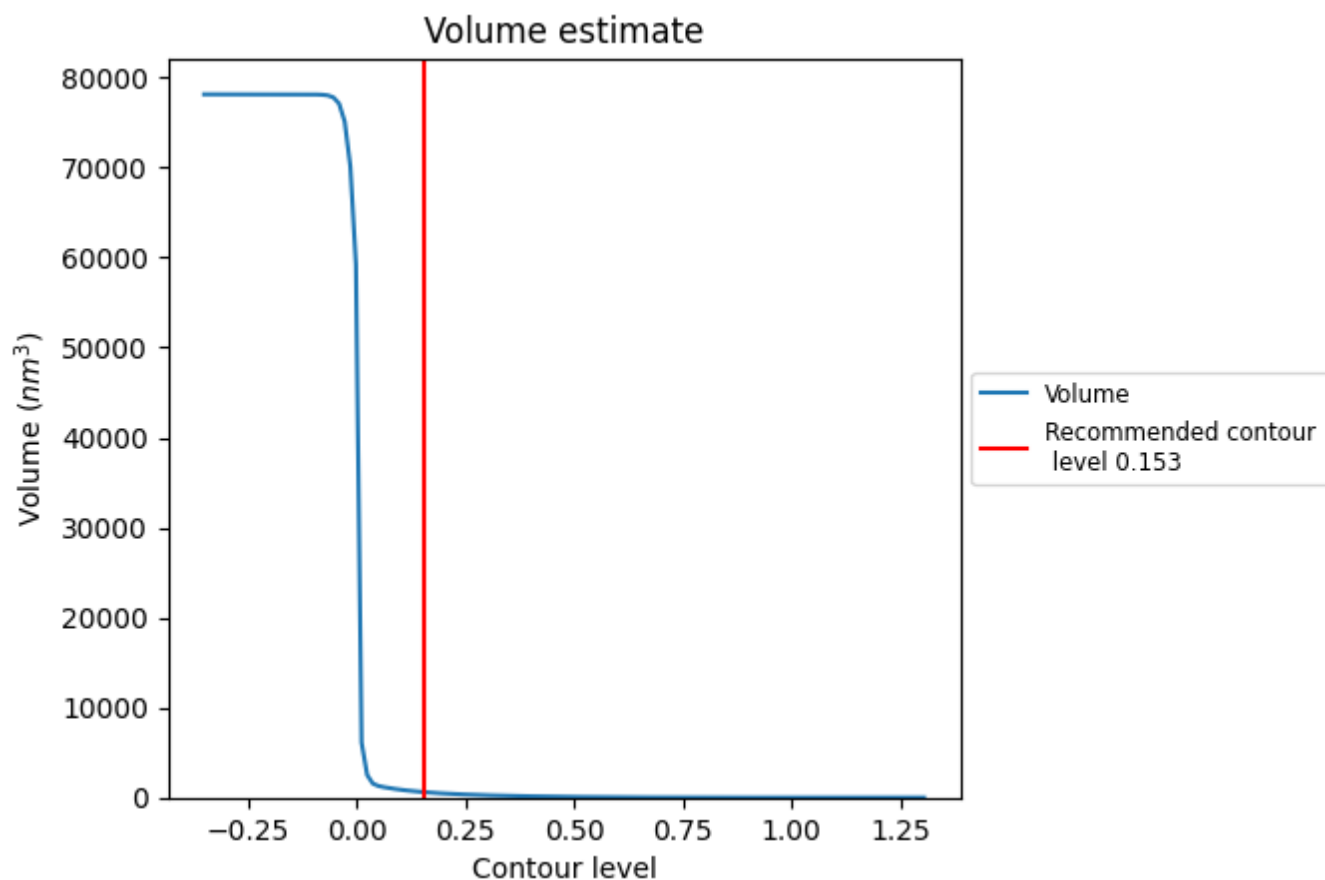
This section contains the results of statistical analysis of the map.

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.

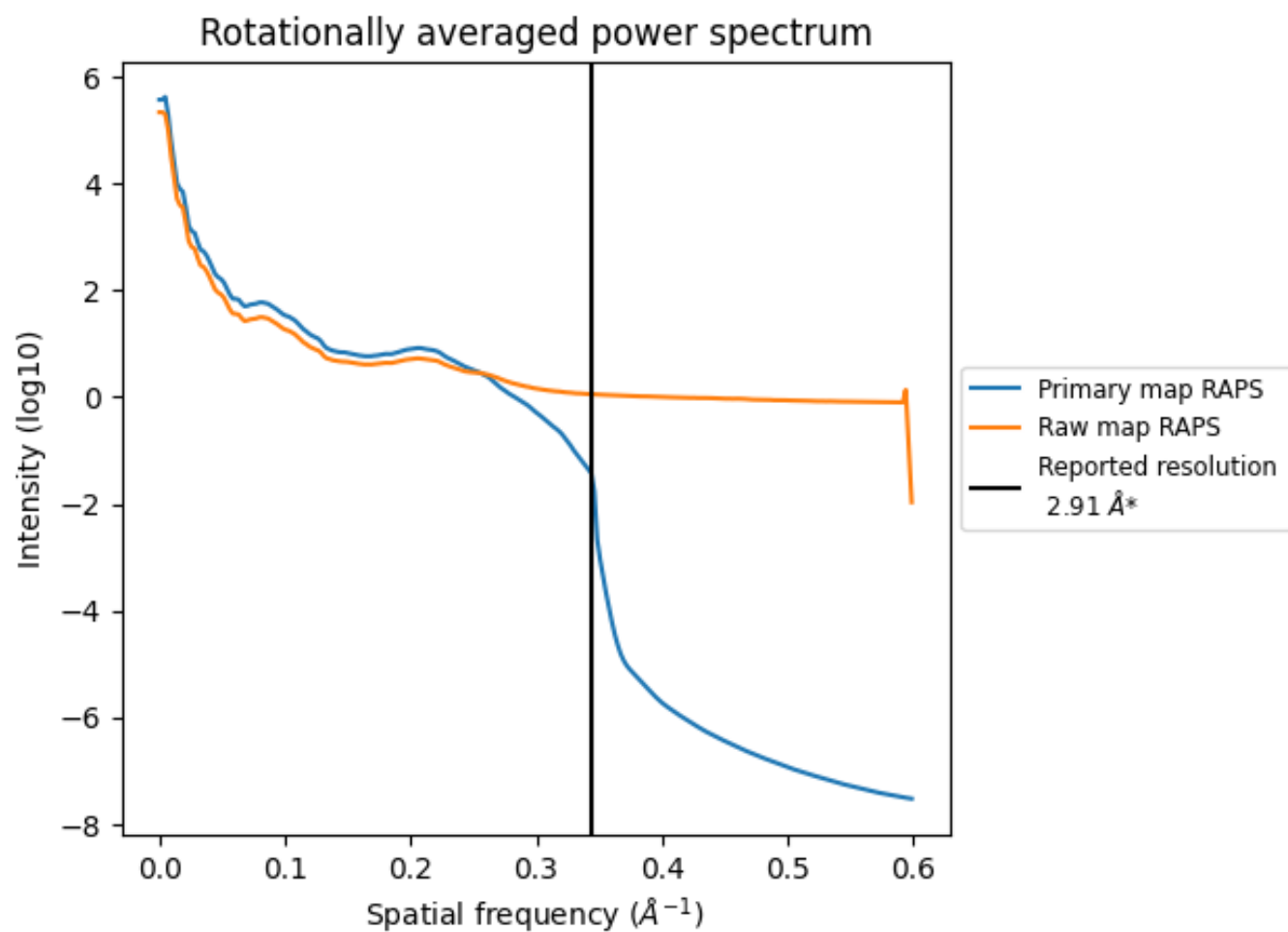
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 608 nm^3 ; this corresponds to an approximate mass of 549 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 ⓘ

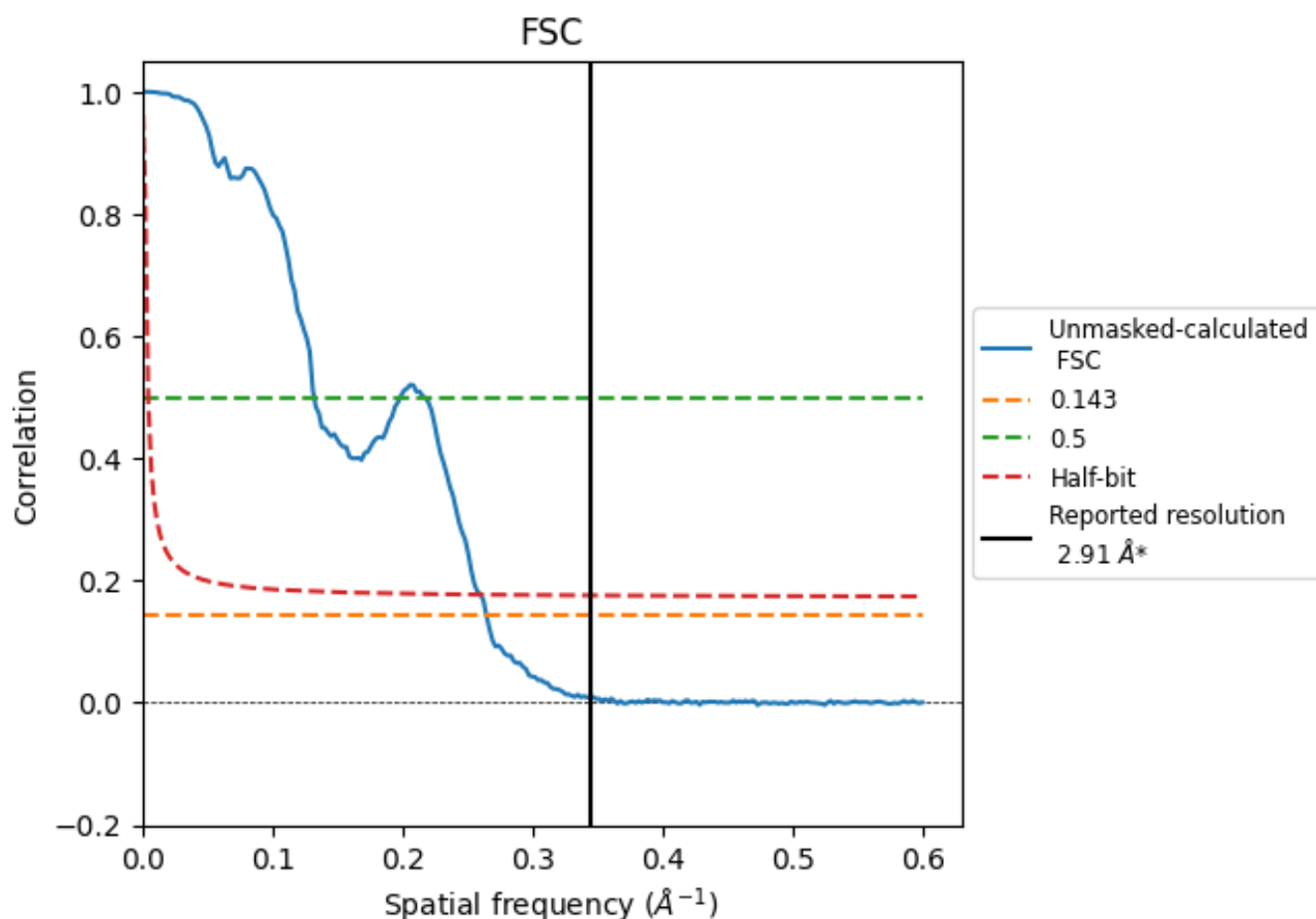


*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

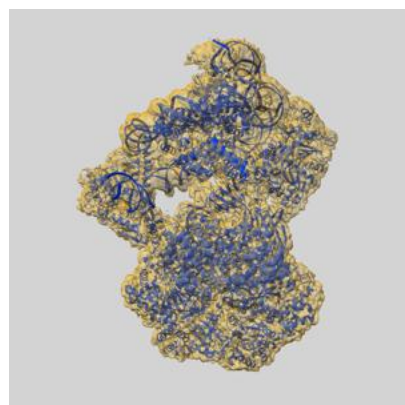
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	7.58	3.85

*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 3.78 differs from the reported value 2.91 by more than 10 %

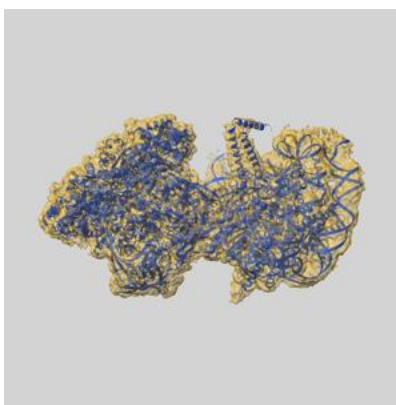
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45361 and PDB model 9C9G. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

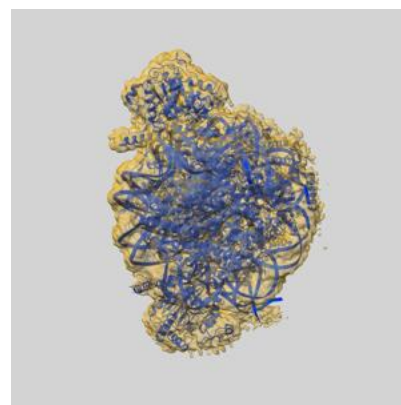
9.1 Map-model overlay [i](#)



X



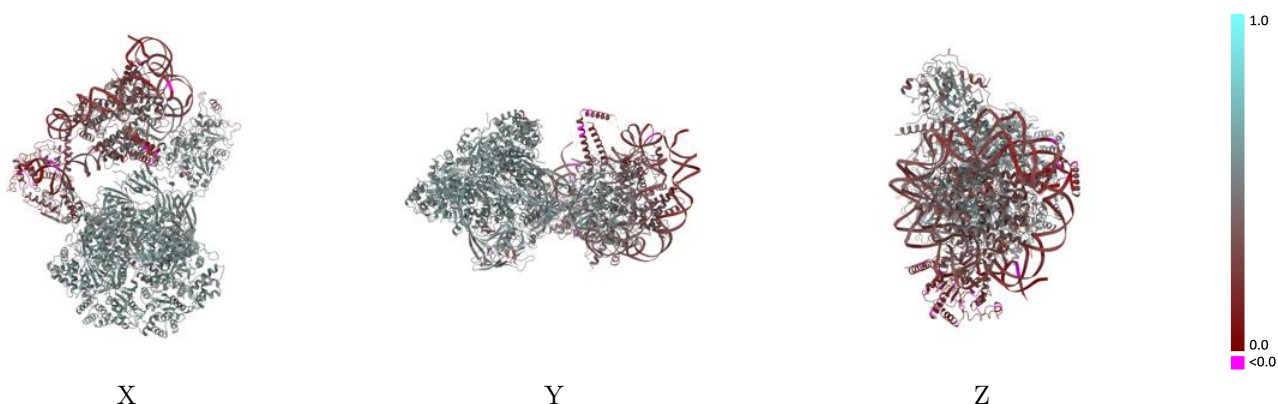
Y



Z

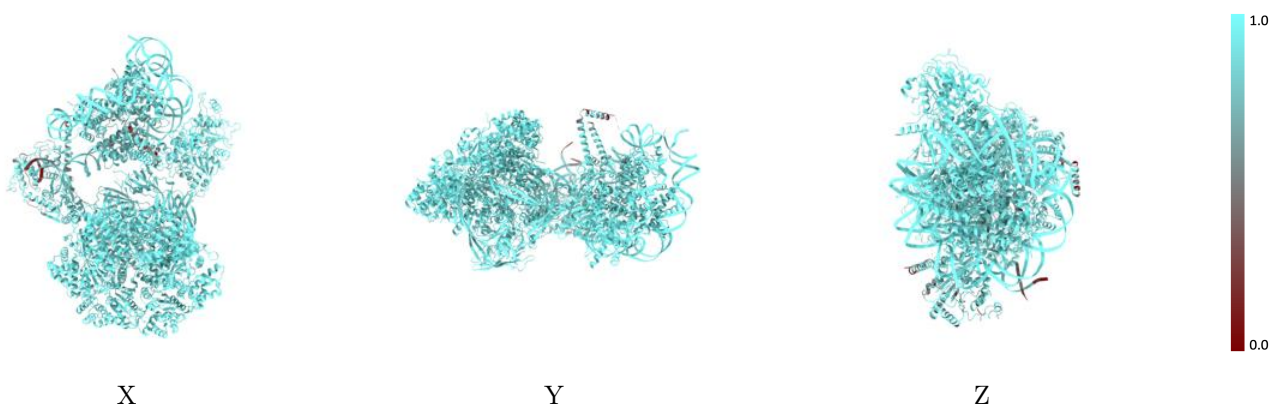
The images above show the 3D surface view of the map at the recommended contour level 0.153 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



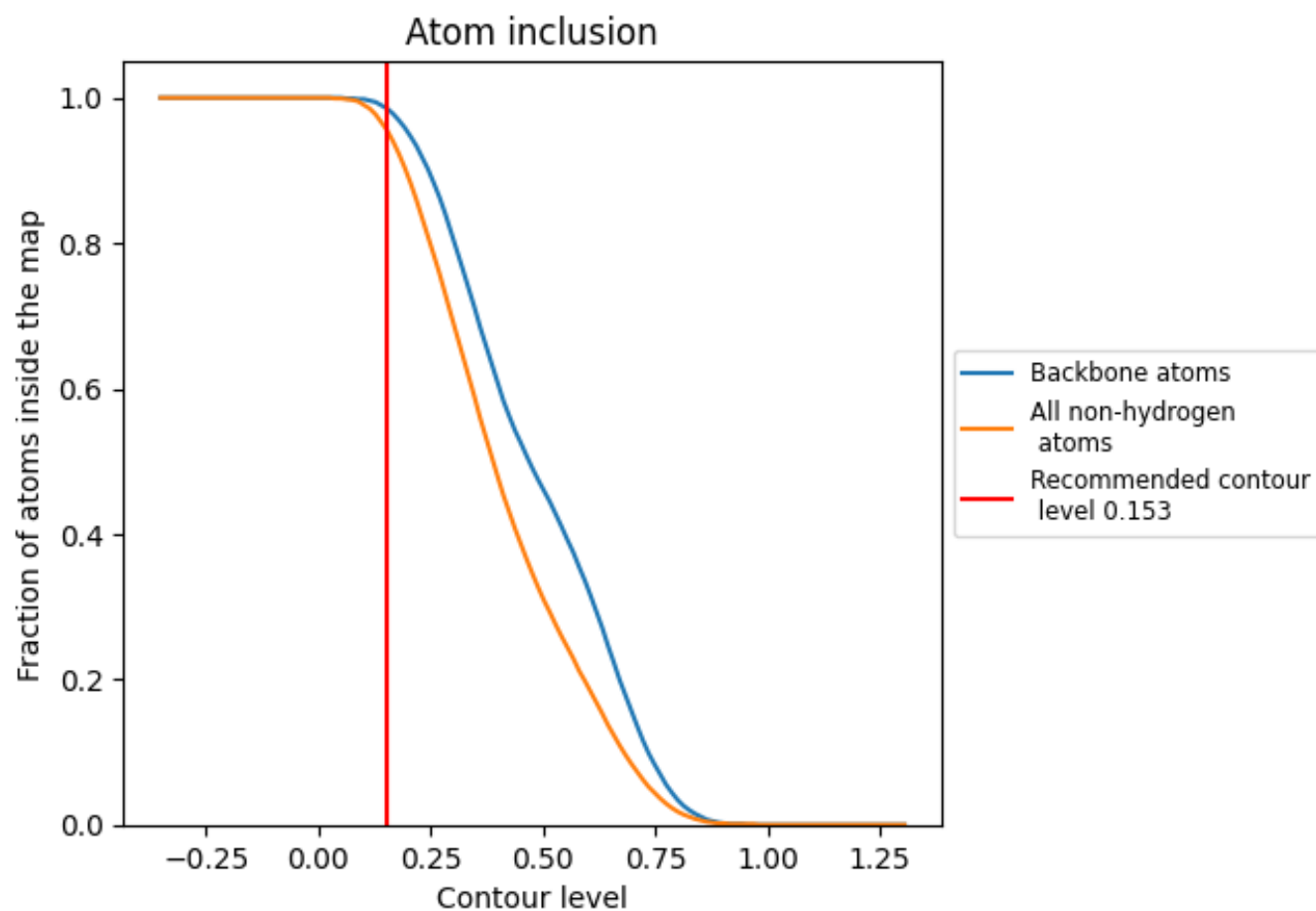
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.153).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.4450
A	 0.9700	 0.3640
B	 0.9720	 0.3810
C	 0.9600	 0.3420
D	 0.9560	 0.3580
E	 0.9250	 0.3400
F	 0.9130	 0.3770
G	 0.9200	 0.4510
H	 0.9280	 0.4570
I	 0.9540	 0.2560
J	 0.9570	 0.2580
Q	 0.8990	 0.3630
R	 0.9580	 0.4590
S	 0.9810	 0.4700
T	 0.9690	 0.5380
U	 0.9620	 0.5390
V	 0.9720	 0.5450
W	 0.9780	 0.5380
X	 0.9760	 0.5210
Y	 0.9790	 0.5300
Z	 0.8630	 0.3870

