



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 09:22 PM UTC

PDB ID : 9OB1 / pdb\_00009ob1  
EMDB ID : EMD-70289  
Title : S.c INO80 in complex with Yeast 0/80 nucleosome, Apo State  
Authors : Wu, H.; Kaur, U.; Narlikar, G.J.; Cheng, Y.F.  
Deposited on : 2025-04-21  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

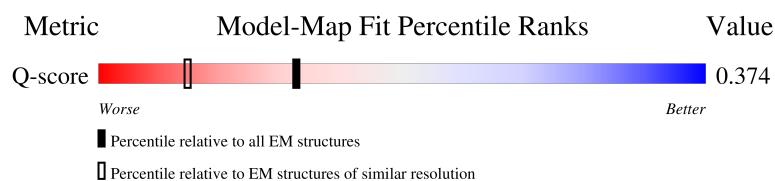
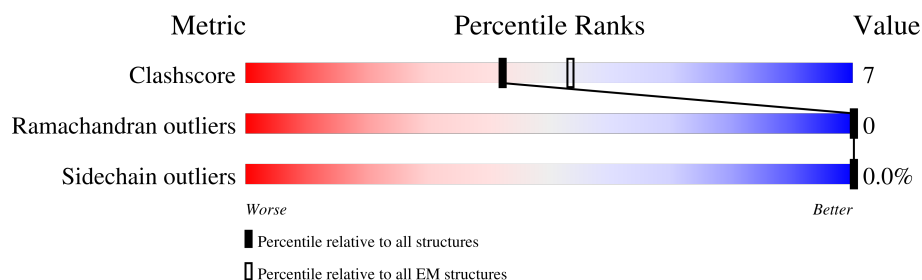
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.20 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.



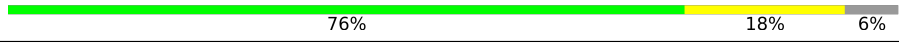



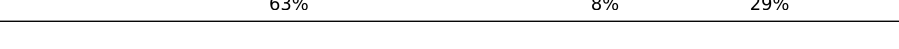







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	227	
2	J	227	
3	Q	1489	
4	R	755	

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Mol	Chain	Length	Quality of chain
5	S	166	
6	T	463	
6	V	463	
6	X	463	
7	U	471	
7	W	471	
7	Y	471	
8	Z	320	
9	A	136	
9	E	136	
10	B	103	
10	F	103	
11	C	132	
11	G	132	
12	D	131	
12	H	131	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 40498 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 (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	145	Total	C	N	O	P	0	0
			2954	1404	537	869	144		

- Molecule 2 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	145	Total	C	N	O	P	0	0
			2985	1414	560	867	144		

- Molecule 3 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	419	Total	C	N	O	S	0	0
			3372	2143	565	649	15		

- Molecule 4 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	442	Total	C	N	O	S	0	0
			3512	2235	591	675	11		

- Molecule 5 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	128	Total	C	N	O	S	0	0
			1015	652	184	177	2		

- Molecule 6 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	437	Total	C	N	O	S	0	0
			3351	2111	578	652	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	442	Total	C	N	O	S	0	0
			3394	2141	584	659	10		
6	X	443	Total	C	N	O	S	0	0
			3404	2149	585	660	10		

- Molecule 7 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	445	Total	C	N	O	S	0	0
			3421	2138	594	677	12		
7	W	442	Total	C	N	O	S	0	0
			3398	2123	590	673	12		
7	Y	436	Total	C	N	O	S	0	0
			3351	2097	583	660	11		

- Molecule 8 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	28	Total	C	N	O	S	0	0
			245	155	45	43	2		

- Molecule 9 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	97	Total	C	N	O		0	0
			801	508	155	138			
9	E	97	Total	C	N	O		0	0
			794	502	155	137			

- 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	389	121	110	1		
10	F	79	Total	C	N	O	S	0	0
			620	389	120	110	1		

- Molecule 11 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	106	Total	C	N	O		0	0
			819	514	161	144			

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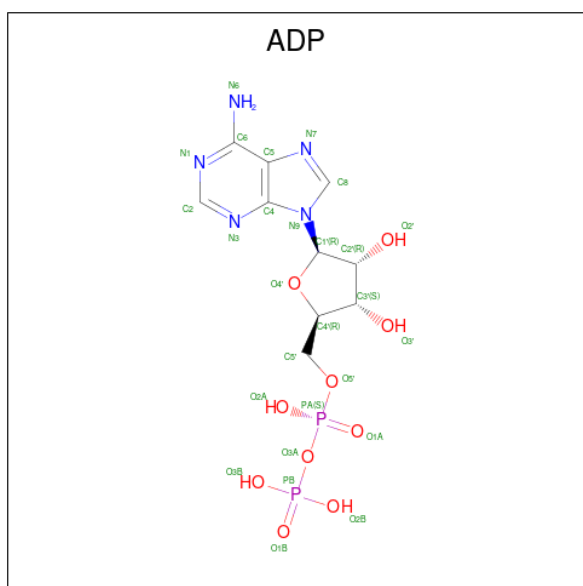
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Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	108	Total	C	N	O	0	0
			827	517	164	146		

- Molecule 12 is a protein called Histone H2B.1.

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

- 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).



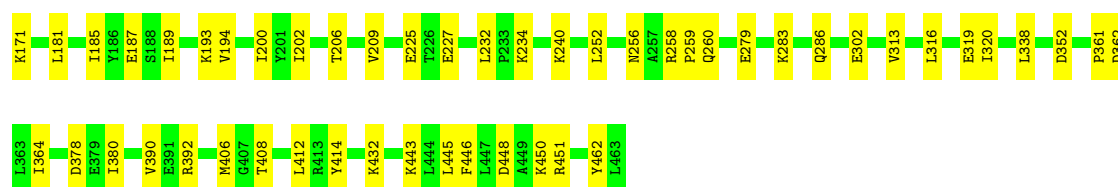
Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	





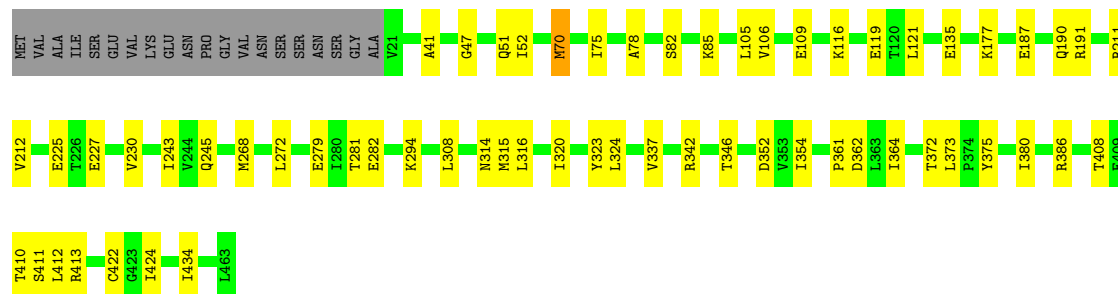






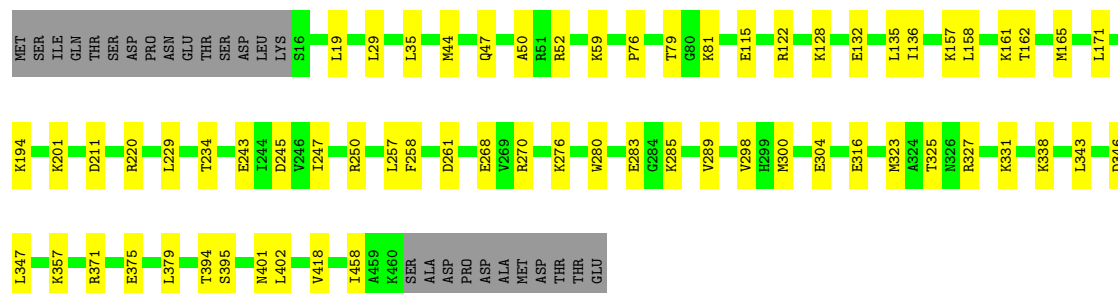
• Molecule 6: RuvB-like protein 1

Chain X: 83% 13% .



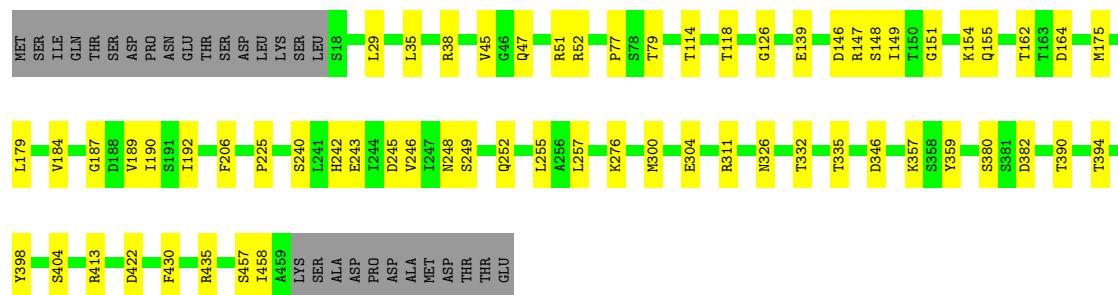
• Molecule 7: RuvB-like protein 2

Chain U: 81% 14% 6%



• Molecule 7: RuvB-like protein 2

Chain W: 80% 13% 6%



• Molecule 7: RuvB-like protein 2

Chain Y: 81% 11% 7%

- Molecule 8: Ino eighty subunit 2

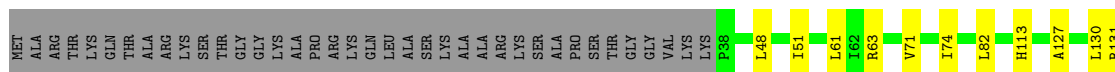
Chain Z:  8% 91%



F320

- Molecule 9: Histone H3

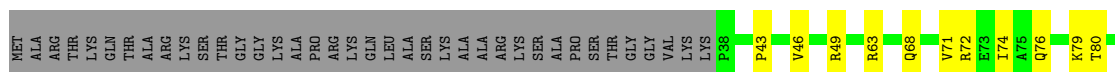
Chain A:  63% 8% 29%



R134  
SER

- Molecule 9: Histone H3

Chain E:  53% 18% 29%



- Molecule 10: Histone H4

R93	Q94	G95	R96	T97	L98	G100	F101	G102	G103																										
MET	SER	GLY	ARG	GLY	LYS	GLY	GLY	GLY	LEU	LEU	ARG	D25	I30	T31	K32	R37	R41	K45	Y52	R56	G57	V58	V61	N65	H76	A77	K78	R79	V82	T83	A84	M85	D86	Y89	K90

- Molecule 10: Histone H4

MET	SER	GLY	ARG	GLY	LYS	GLY	GLY	LYS	GLY	LEU	GLY	LYS	GLY	GLY	ALA	LYS	ARG	HIS	ARG	LYS	VAL	LEU	ARG	D25	D26	D27	D28	D29	I30	I31	I32	R37	R41	R56	K60	V61	F62	L63	V71	T72	E75	R79	T83	L91	R96	G102	G103
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- Molecule 11: Histone H2A.1

[illegible]

- Molecule 11: Histone H2A.1

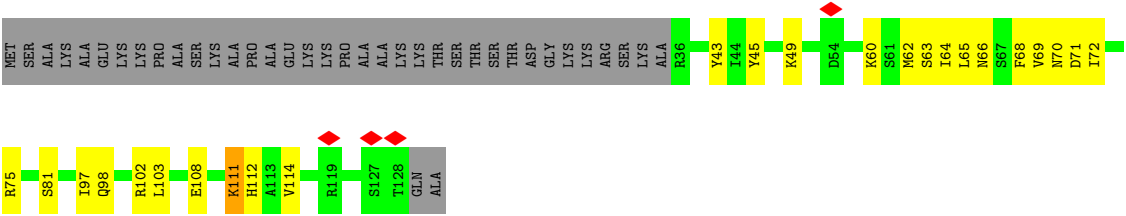
ALA	LYS	ALA	THR	LYS	ALA	SER	GLN	GLU	LEU	ALA	ALA	ALA	K13	A14	S15	Q16	S17	R18	S19	A20	K21	L24	R30	R36	Y40	S46	Y51	L56	E57	L66	R78	I79	I80	P81	R82	A87	I88	R89	N90	D91	L94	N95	L98	K119	K120	SER
MET	SER	GLY	GLY	LYS	GLY	GLY	LYS	ALA	SER	SER	ALA	K13	A14	S15	Q16	S17	R18	S19	A20	K21	L24	R30	R36	Y40	S46	Y51	L56	E57	L66	R78	I79	I80	P81	R82	A87	I88	R89	N90	D91	L94	N95	L98	K119	K120	SER	

- Molecule 12: Histone H2B.1

F68	SER	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	R36
K82	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	R37
Y86	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	T39
I92	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	Y40
T99	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	S41
L103	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	Y45
P106	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	L48
E116	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	K49
G117	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	D54
T118	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	T55
R119	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	O56
A120	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	M57
V121	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	S58
T122	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	O59
K123	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	M62
T128	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	L65
G1N	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	M66
ALA	ALA	LYS	GLU	LYS	PRO	ALA	SER	LYS	ALA	PRO	GLU	LYS	PRO	ALA	LYS	LYS	THR	SER	THR	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	N69

- Molecule 12: Histone H2B.1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47.7	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	0.929	Depositor
Minimum map value	-0.412	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	366.8672, 366.8672, 366.8672	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8189, 0.8189, 0.8189	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: 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	I	0.20	0/3310	0.41	0/5103
2	J	0.19	0/3352	0.40	0/5176
3	Q	0.24	0/3436	0.54	1/4660 (0.0%)
4	R	0.22	0/3602	0.56	5/4903 (0.1%)
5	S	0.26	0/1037	0.63	1/1397 (0.1%)
6	T	0.22	0/3390	0.46	1/4585 (0.0%)
6	V	0.22	0/3436	0.49	0/4648
6	X	0.25	0/3446	0.53	2/4662 (0.0%)
7	U	0.21	0/3459	0.42	0/4662
7	W	0.21	0/3436	0.43	2/4632 (0.0%)
7	Y	0.20	0/3387	0.44	0/4562
8	Z	0.22	0/251	0.43	0/334
9	A	0.21	0/812	0.50	0/1086
9	E	0.18	0/804	0.43	0/1075
10	B	0.25	0/628	0.68	2/840 (0.2%)
10	F	0.29	0/627	0.70	1/840 (0.1%)
11	C	0.21	0/830	0.54	0/1121
11	G	0.26	0/838	0.64	0/1131
12	D	0.25	0/736	0.72	0/991
12	H	0.28	0/736	0.70	1/991 (0.1%)
All	All	0.22	0/41553	0.50	16/57399 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	45	PRO	CA-N-CD	-6.56	102.81	112.00
6	T	70	MET	CB-CG-SD	6.18	131.23	112.70
12	H	111	LYS	CA-CB-CG	6.14	126.38	114.10
10	F	41	ARG	CA-CB-CG	5.95	126.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	89	TYR	CA-CB-CG	5.93	124.57	113.90

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	I	2954	0	1629	23	0
2	J	2985	0	1628	16	0
3	Q	3372	0	3339	62	0
4	R	3512	0	3374	43	0
5	S	1015	0	1033	9	0
6	T	3351	0	3464	59	0
6	V	3394	0	3524	52	0
6	X	3404	0	3542	42	0
7	U	3421	0	3499	46	0
7	W	3398	0	3470	43	0
7	Y	3351	0	3439	41	0
8	Z	245	0	233	3	0
9	A	801	0	851	16	0
9	E	794	0	844	34	0
10	B	621	0	645	22	0
10	F	620	0	643	21	0
11	C	819	0	865	25	0
11	G	827	0	865	16	0
12	D	726	0	748	29	0
12	H	726	0	748	16	0
13	T	27	0	12	3	0
13	U	27	0	12	0	0
13	V	27	0	12	2	0
13	W	27	0	12	2	0
13	X	27	0	12	2	0
13	Y	27	0	12	2	0
All	All	40498	0	38455	498	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 7.

The worst 5 of 498 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)
9:E:96:VAL:CG1	10:F:63:LEU:HD21	1.59	1.29
9:E:96:VAL:HG12	10:F:63:LEU:HD21	1.10	1.06
9:A:113:HIS:HB2	9:E:126:LEU:HD22	1.37	1.02
6:V:35:LEU:CD2	6:V:41:ALA:HB2	1.89	1.01
9:A:113:HIS:CB	9:E:126:LEU:HD22	1.91	0.99

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	Q	407/1489 (27%)	386 (95%)	21 (5%)	0	100	100
4	R	438/755 (58%)	418 (95%)	20 (5%)	0	100	100
5	S	124/166 (75%)	117 (94%)	7 (6%)	0	100	100
6	T	433/463 (94%)	421 (97%)	12 (3%)	0	100	100
6	V	440/463 (95%)	421 (96%)	19 (4%)	0	100	100
6	X	441/463 (95%)	425 (96%)	16 (4%)	0	100	100
7	U	443/471 (94%)	430 (97%)	13 (3%)	0	100	100
7	W	440/471 (93%)	426 (97%)	14 (3%)	0	100	100
7	Y	432/471 (92%)	412 (95%)	20 (5%)	0	100	100
8	Z	26/320 (8%)	26 (100%)	0	0	100	100
9	A	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
9	E	95/136 (70%)	95 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	B	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
10	F	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
11	C	104/132 (79%)	100 (96%)	4 (4%)	0	100	100
11	G	106/132 (80%)	102 (96%)	4 (4%)	0	100	100
12	D	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
12	H	91/131 (70%)	86 (94%)	5 (6%)	0	100	100
All	All	4360/6536 (67%)	4200 (96%)	160 (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	
3	Q	387/1350 (29%)	387 (100%)	0	100	100
4	R	386/682 (57%)	386 (100%)	0	100	100
5	S	106/142 (75%)	105 (99%)	1 (1%)	70	81
6	T	367/391 (94%)	367 (100%)	0	100	100
6	V	373/391 (95%)	373 (100%)	0	100	100
6	X	375/391 (96%)	375 (100%)	0	100	100
7	U	378/403 (94%)	378 (100%)	0	100	100
7	W	375/403 (93%)	375 (100%)	0	100	100
7	Y	371/403 (92%)	371 (100%)	0	100	100
8	Z	26/285 (9%)	26 (100%)	0	100	100
9	A	85/113 (75%)	85 (100%)	0	100	100
9	E	84/113 (74%)	84 (100%)	0	100	100
10	B	62/79 (78%)	62 (100%)	0	100	100
10	F	62/79 (78%)	62 (100%)	0	100	100
11	C	85/99 (86%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	G	84/99 (85%)	84 (100%)	0	100	100
12	D	81/109 (74%)	81 (100%)	0	100	100
12	H	81/109 (74%)	81 (100%)	0	100	100
All	All	3768/5641 (67%)	3767 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
5	S	125	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
6	V	190	GLN
7	W	441	GLN
12	H	52	HIS
6	V	256	ASN
6	V	417	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](#)

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	W	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	8 (18%)
13	ADP	Y	501	-	28,29,29	1.37	5 (17%)	43,45,45	1.82	8 (18%)
13	ADP	T	501	-	28,29,29	1.34	5 (17%)	43,45,45	1.87	9 (20%)
13	ADP	V	501	-	28,29,29	1.39	5 (17%)	43,45,45	1.83	10 (23%)
13	ADP	U	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.89	8 (18%)
13	ADP	X	501	-	28,29,29	1.37	5 (17%)	43,45,45	1.84	8 (18%)

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	W	501	-	-	2/16/32/32	0/3/3/3
13	ADP	Y	501	-	-	3/16/32/32	0/3/3/3
13	ADP	T	501	-	-	3/16/32/32	0/3/3/3
13	ADP	V	501	-	-	3/16/32/32	0/3/3/3
13	ADP	U	501	-	-	3/16/32/32	0/3/3/3
13	ADP	X	501	-	-	6/16/32/32	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	4.54	1.47	1.39
13	U	501	ADP	C5-C4	4.48	1.47	1.39
13	X	501	ADP	C5-C4	4.37	1.46	1.39
13	V	501	ADP	C5-C4	4.35	1.46	1.39
13	Y	501	ADP	C5-C4	4.31	1.46	1.39

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	501	ADP	C5-C4-N3	-6.14	118.27	126.72
13	T	501	ADP	C5-C4-N3	-5.97	118.49	126.72
13	W	501	ADP	C5-C4-N3	-5.92	118.57	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	501	ADP	C5-C4-N3	-5.90	118.59	126.72
13	Y	501	ADP	C5-C4-N3	-5.64	118.96	126.72

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

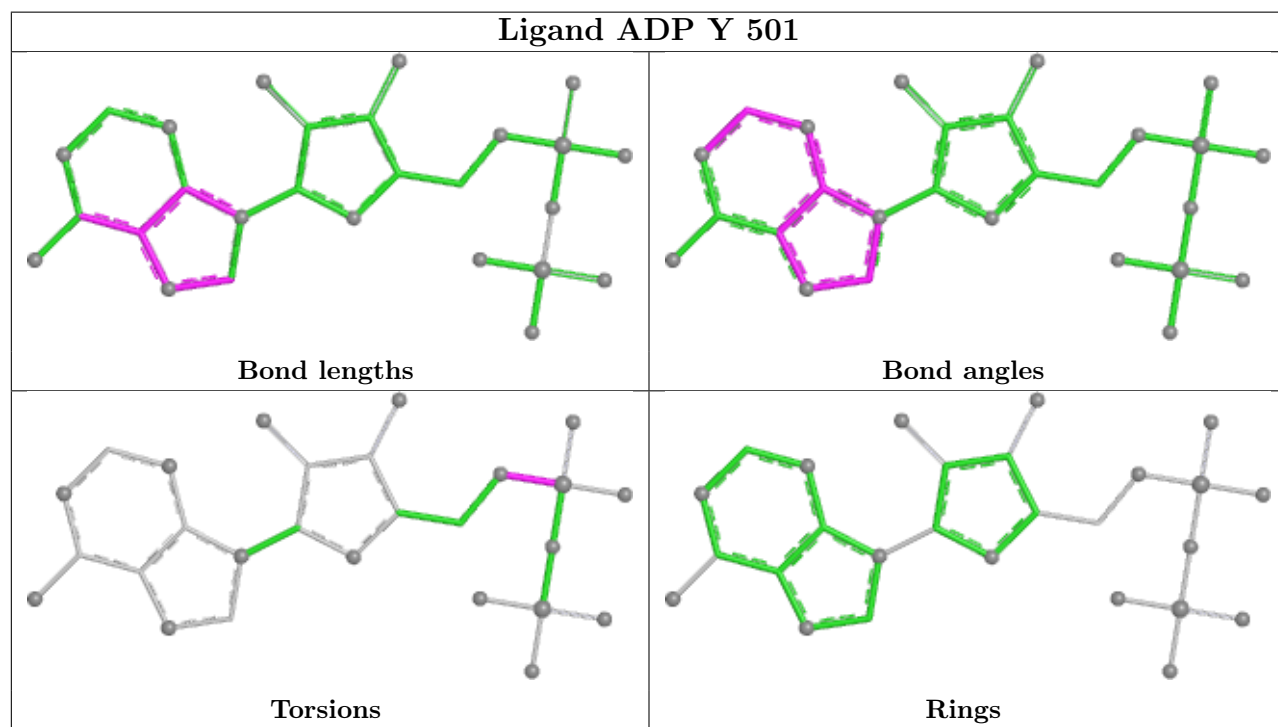
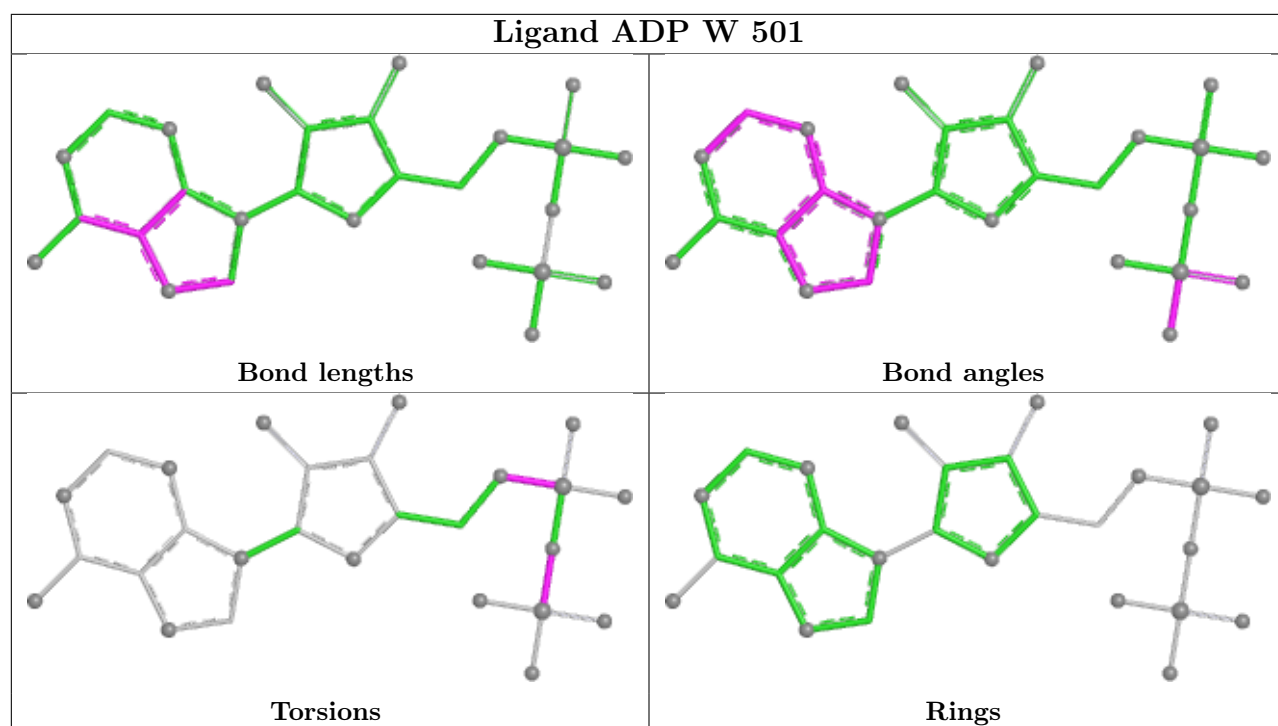
Mol	Chain	Res	Type	Atoms
13	T	501	ADP	C5'-O5'-PA-O1A
13	T	501	ADP	C5'-O5'-PA-O2A
13	T	501	ADP	C5'-O5'-PA-O3A
13	U	501	ADP	C5'-O5'-PA-O2A
13	V	501	ADP	C5'-O5'-PA-O1A

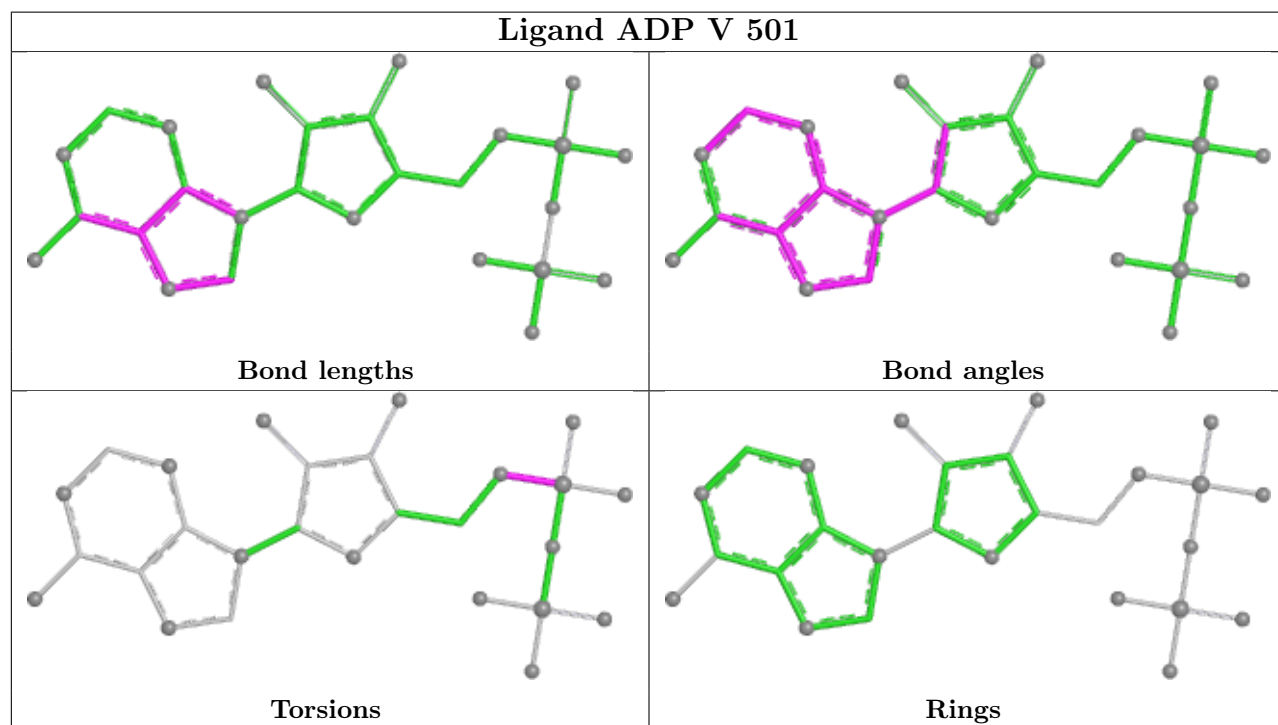
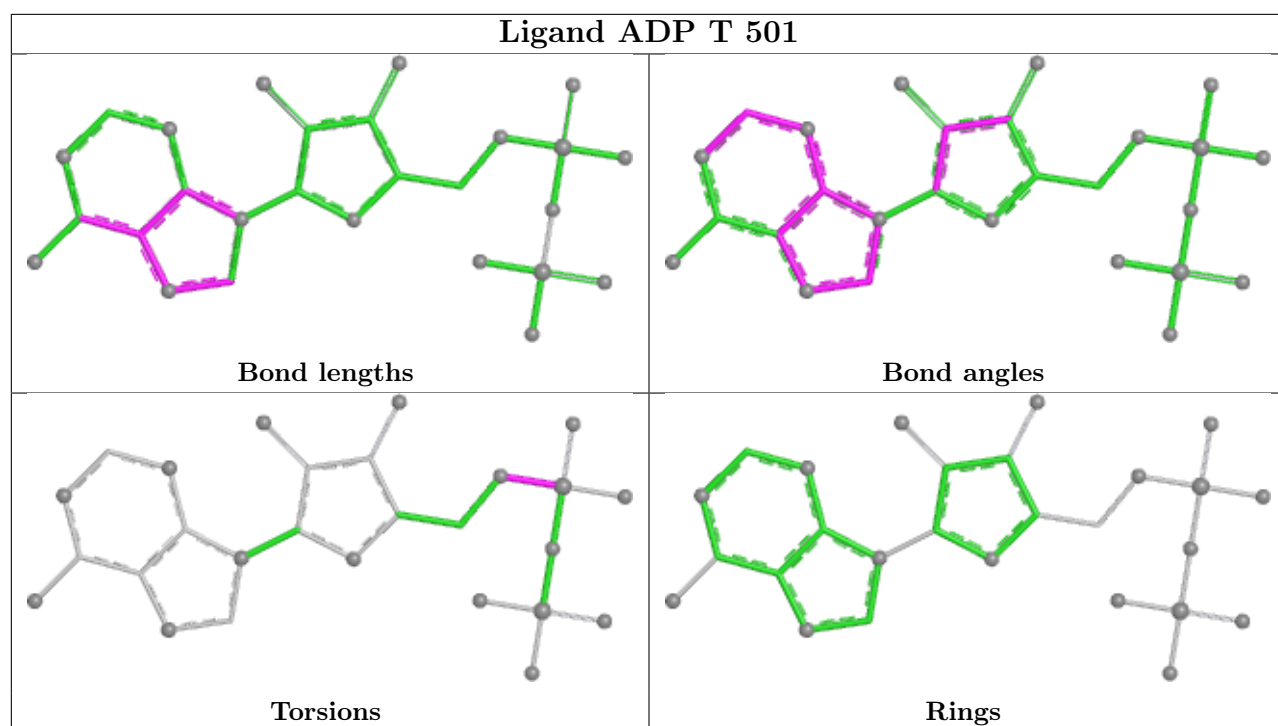
There are no ring outliers.

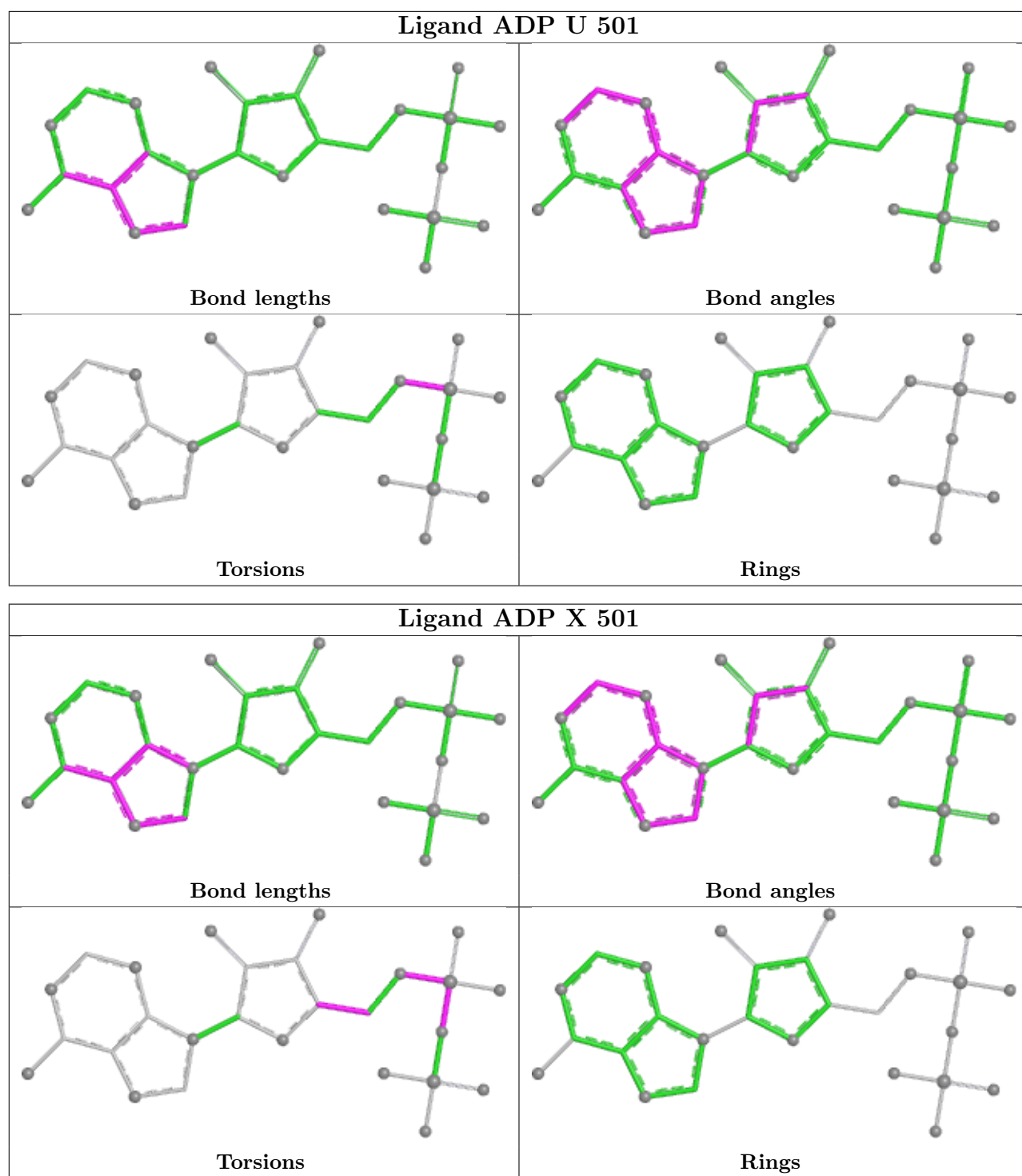
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	W	501	ADP	2	0
13	Y	501	ADP	2	0
13	T	501	ADP	3	0
13	V	501	ADP	2	0
13	X	501	ADP	2	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.

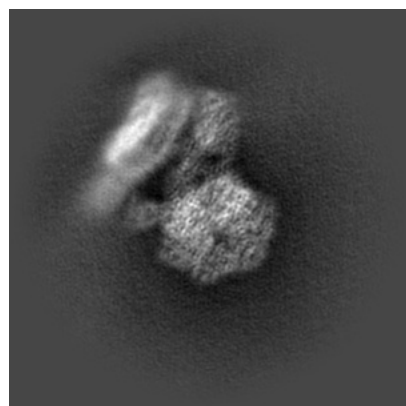
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70289. These allow visual inspection of the internal detail of the map and identification of artifacts.

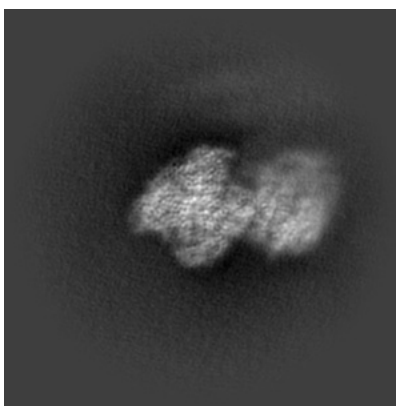
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

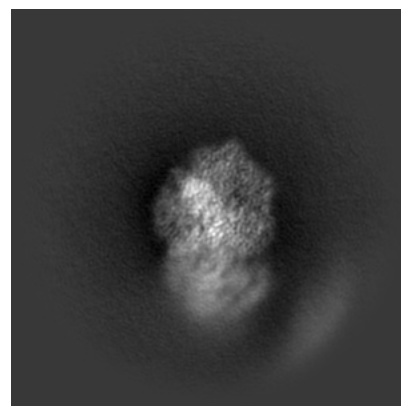
#### 6.1.1 Primary map



X

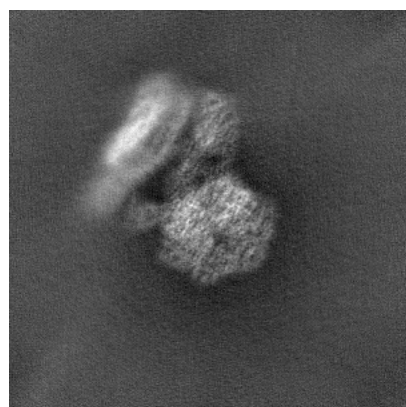


Y

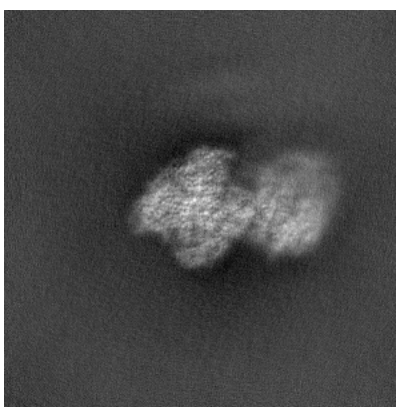


Z

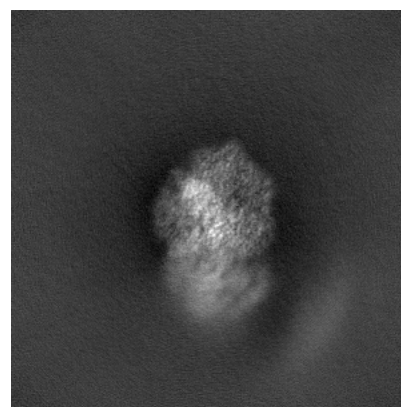
#### 6.1.2 Raw map



X



Y

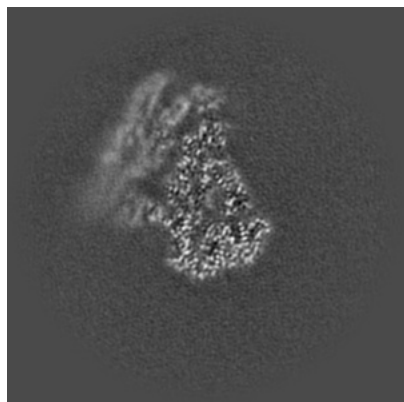


Z

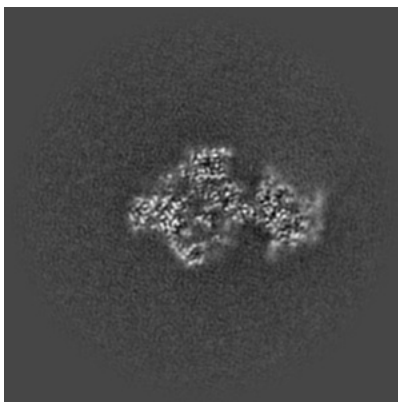
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

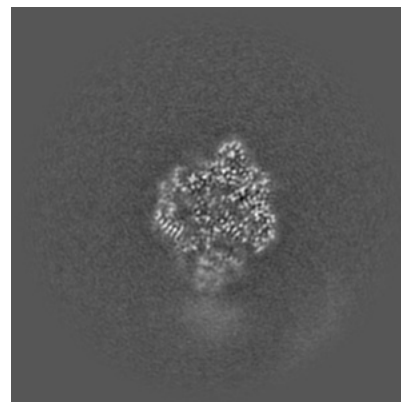
### 6.2.1 Primary map



X Index: 224

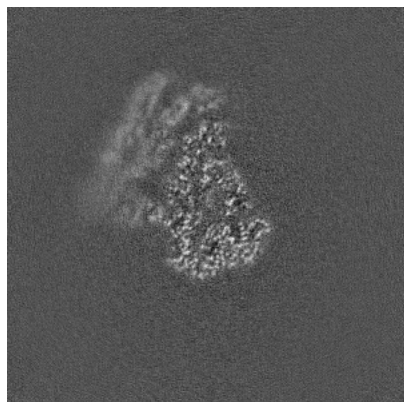


Y Index: 224

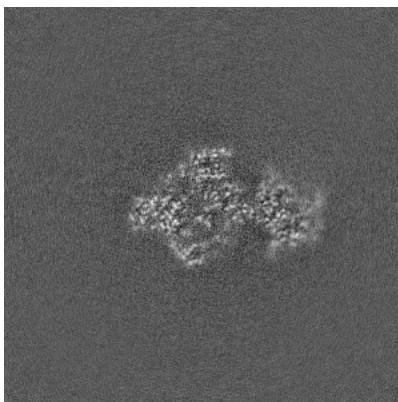


Z Index: 224

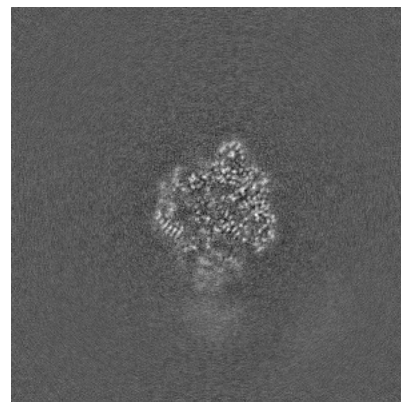
### 6.2.2 Raw map



X Index: 224



Y Index: 224

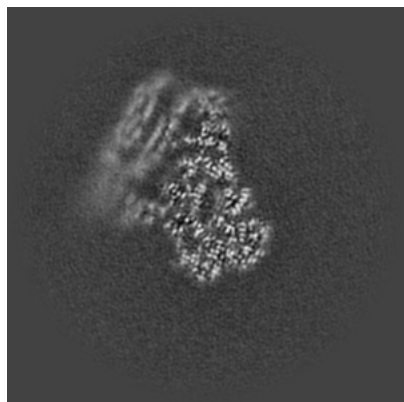


Z Index: 224

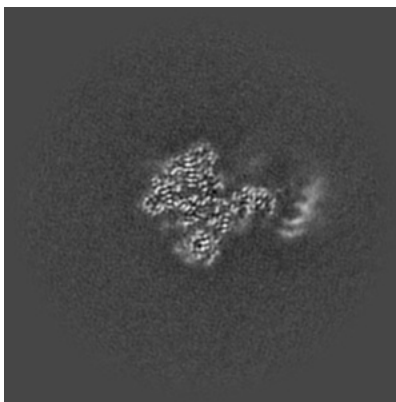
The images above show central slices of the map in three orthogonal directions.

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

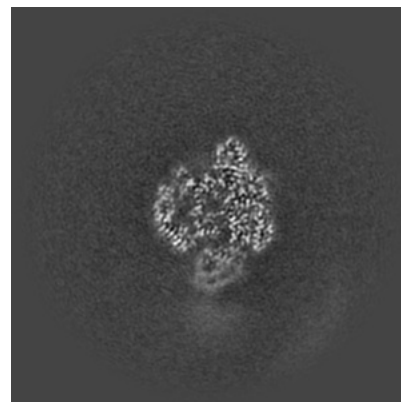
### 6.3.1 Primary map



X Index: 218

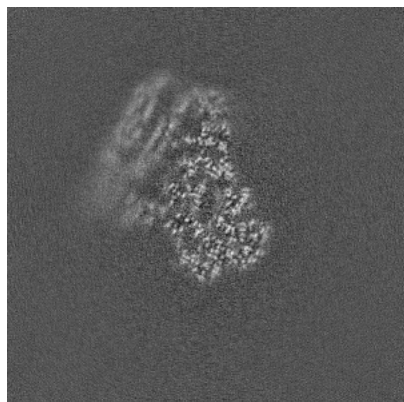


Y Index: 199

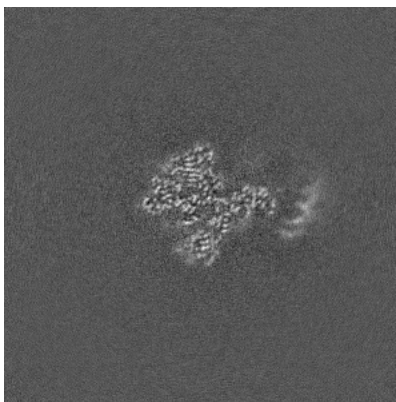


Z Index: 219

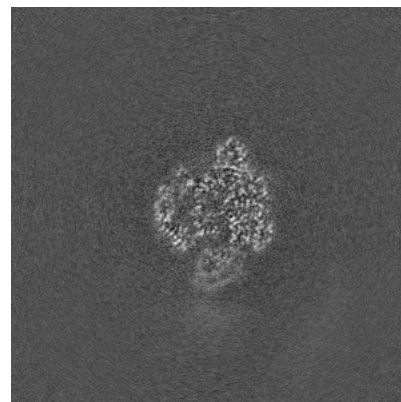
### 6.3.2 Raw map



X Index: 218



Y Index: 200

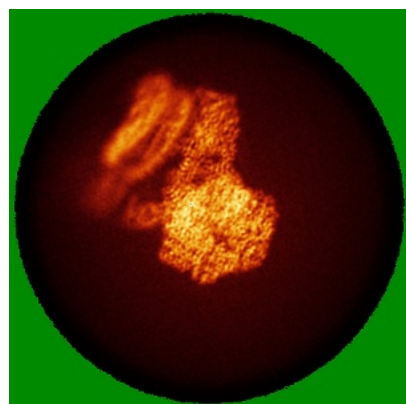


Z Index: 219

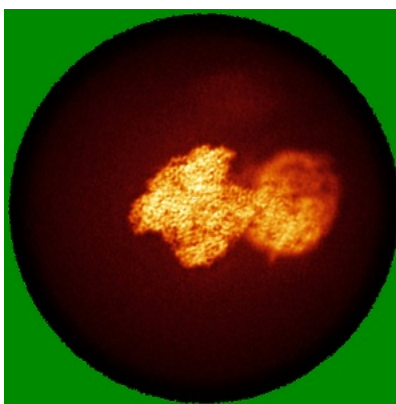
The images above show the largest variance slices of the map in three orthogonal directions.

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

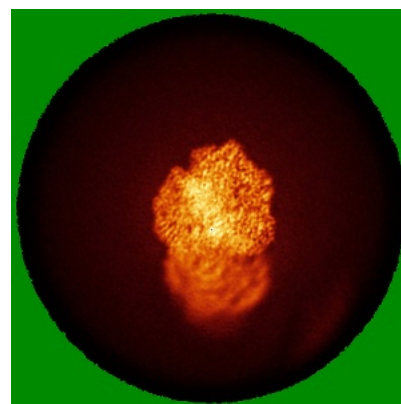
### 6.4.1 Primary map



X

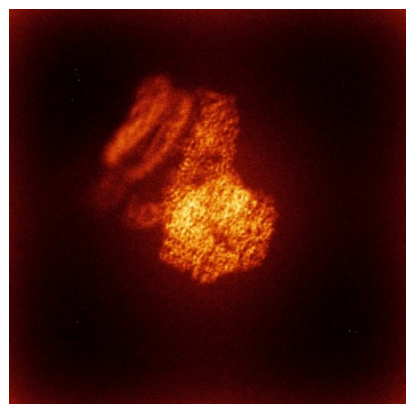


Y

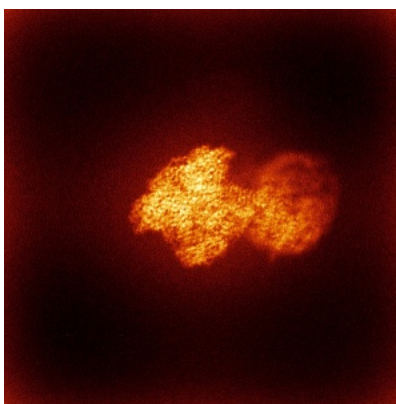


Z

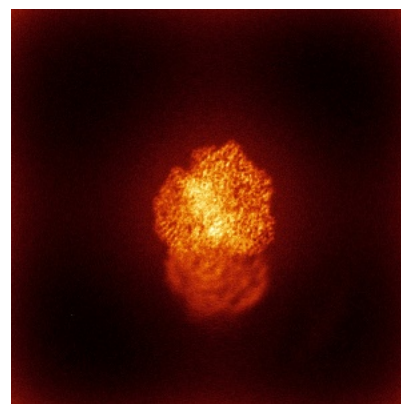
### 6.4.2 Raw map



X



Y



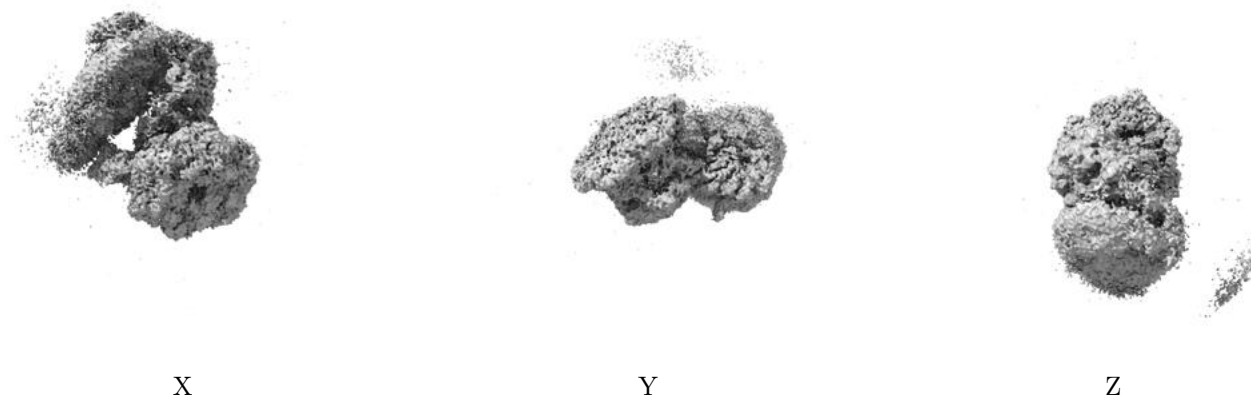
Z

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.



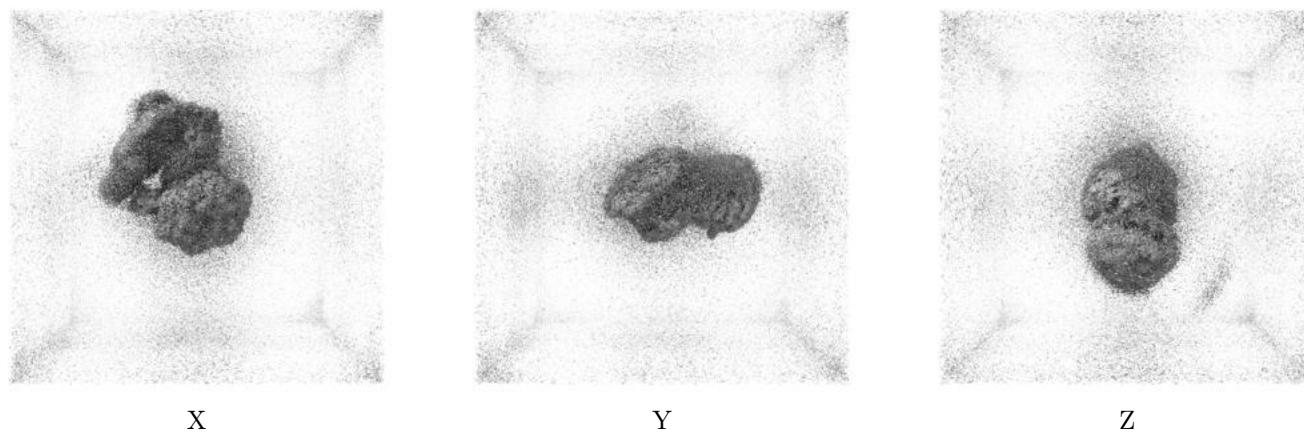
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

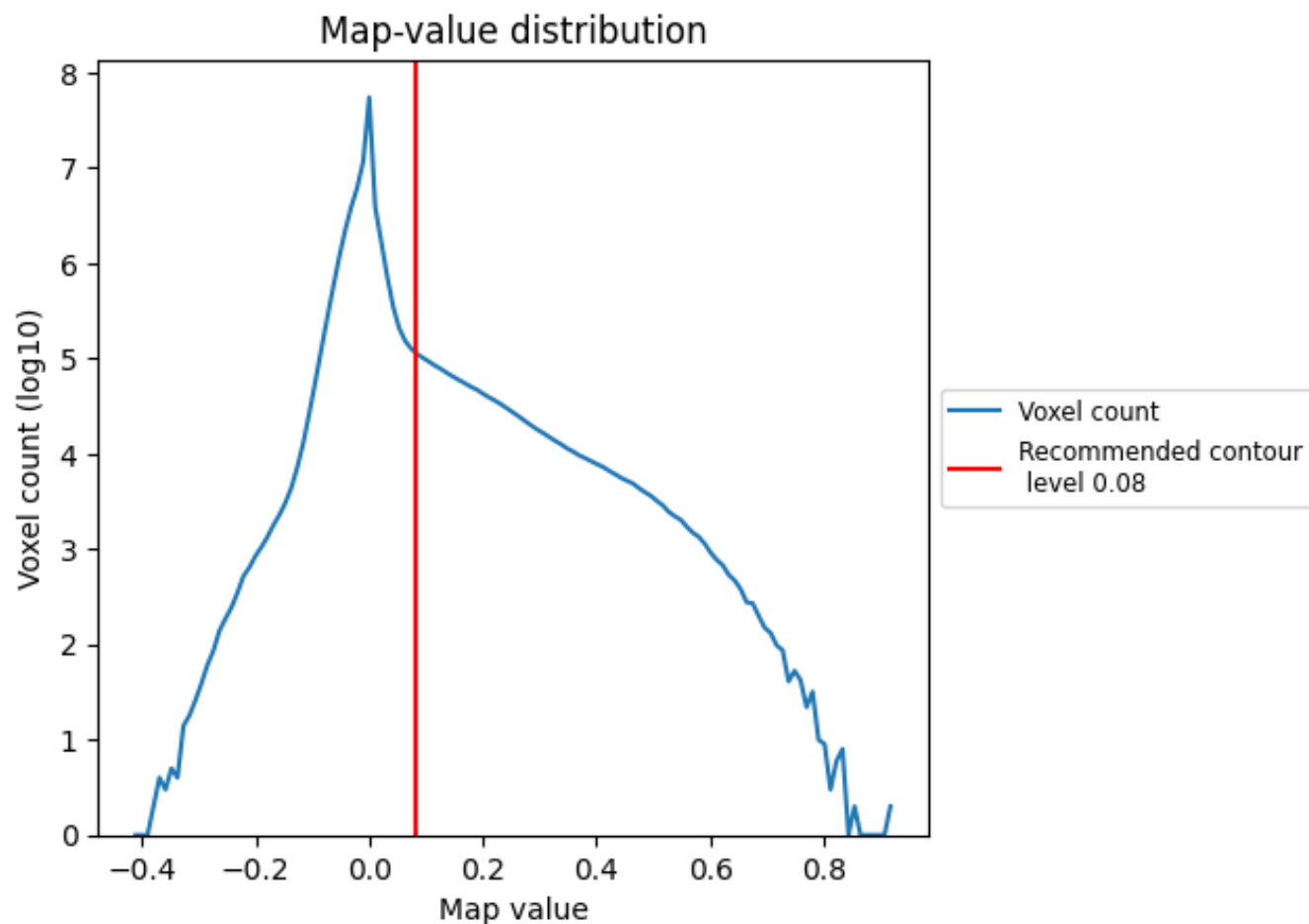
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

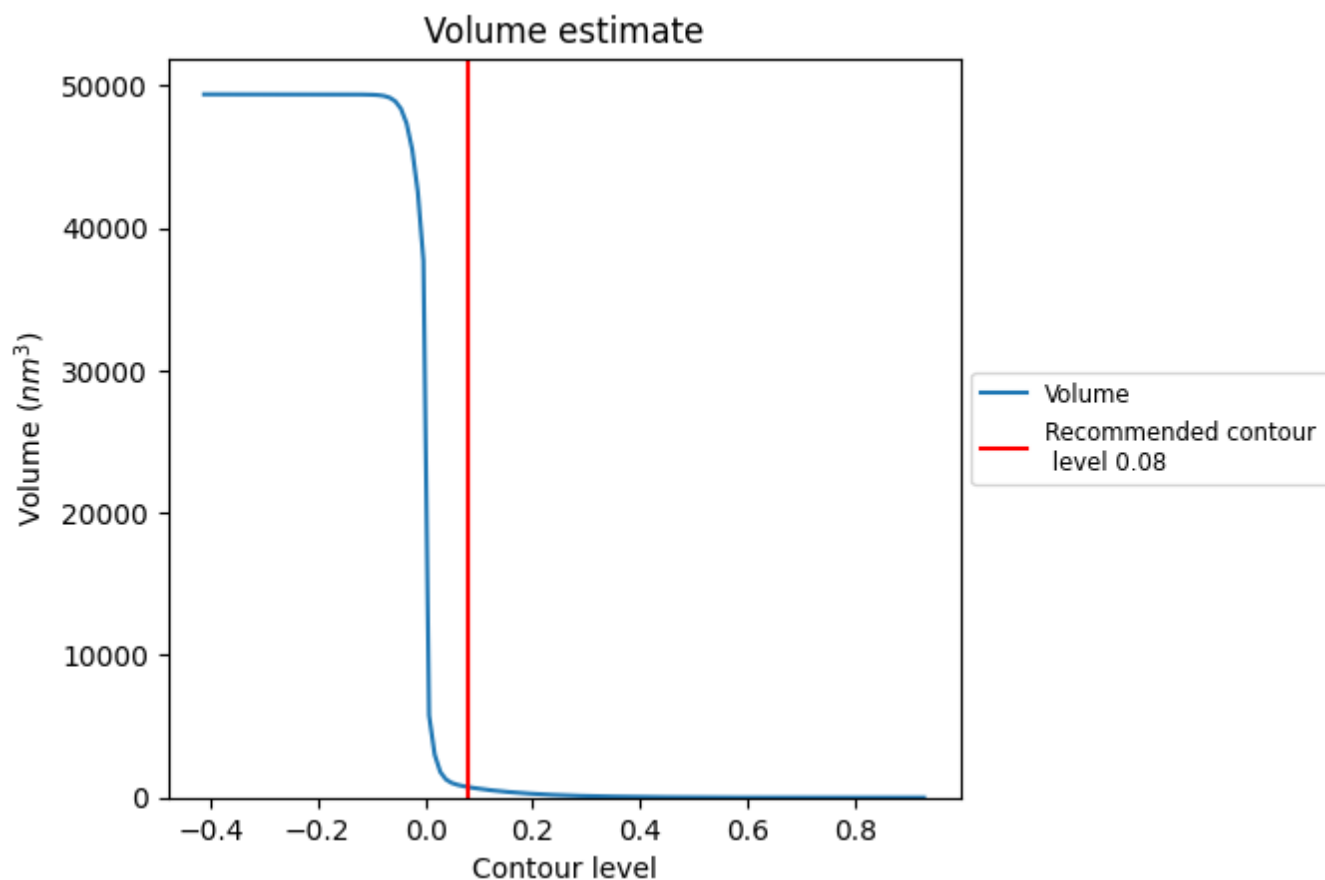
This section contains the results of statistical analysis of the map.

### 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](#)

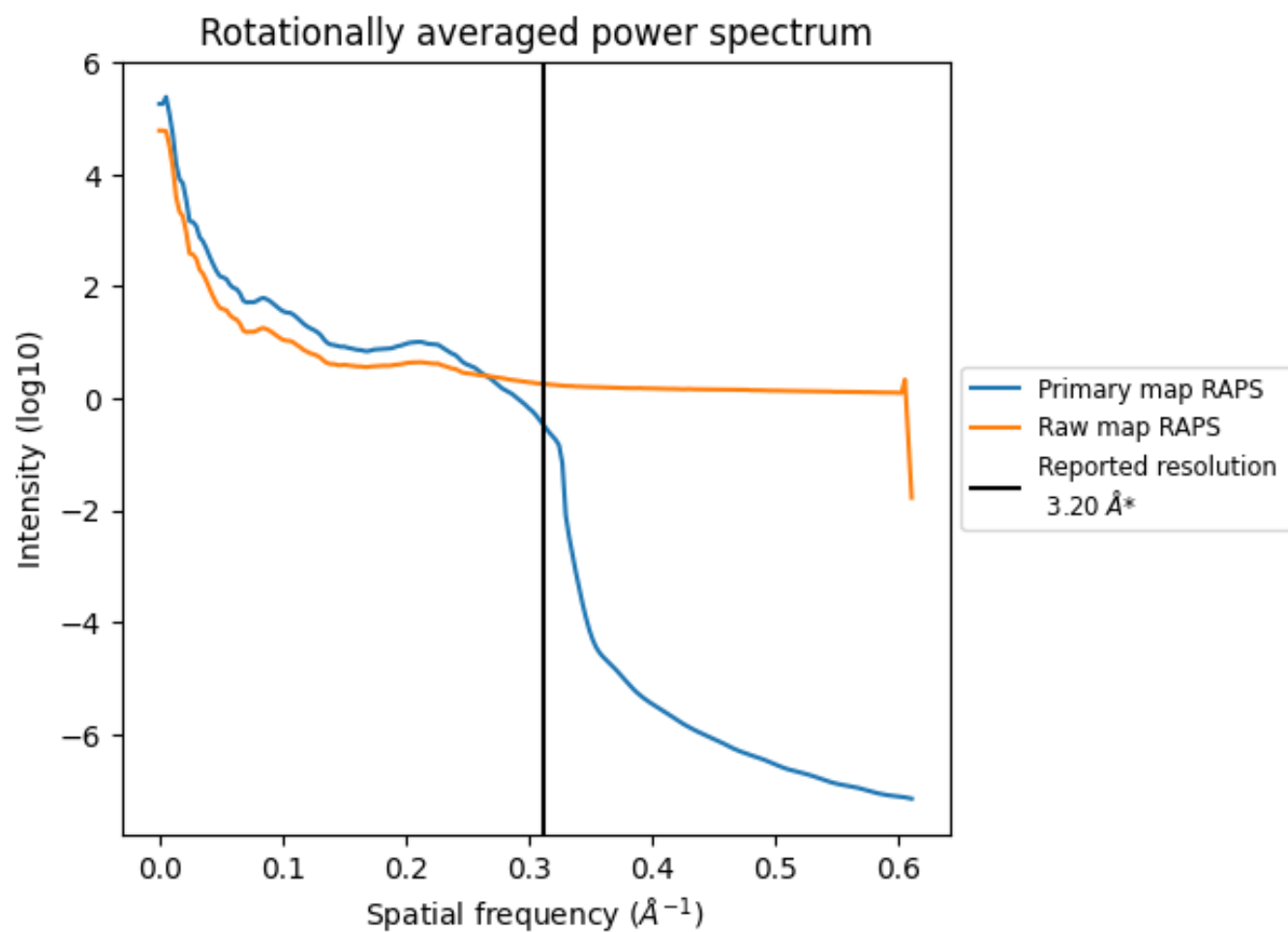


The volume at the recommended contour level is 738 nm<sup>3</sup>; this corresponds to an approximate mass of 667 kDa.

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 ⓘ

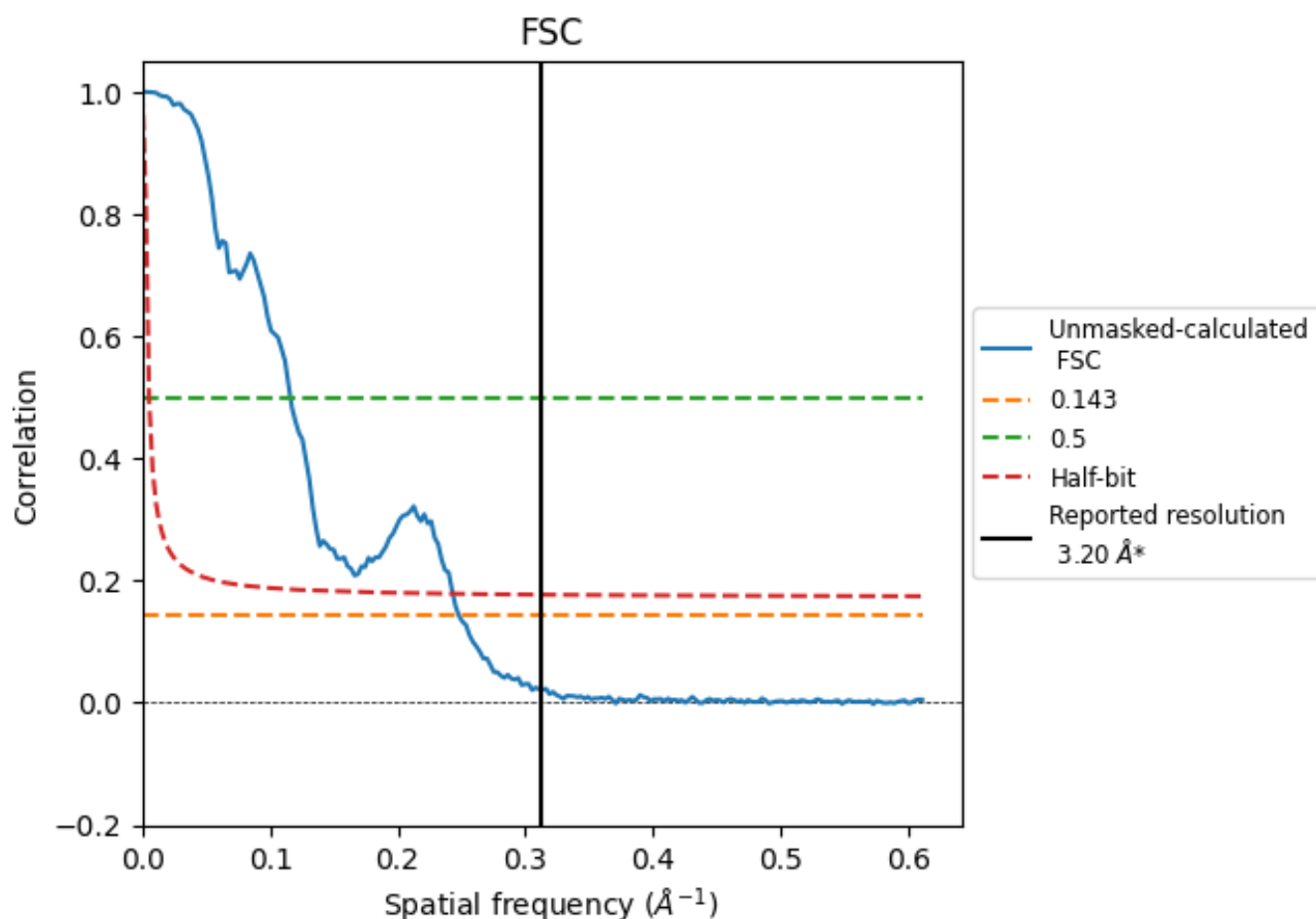


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

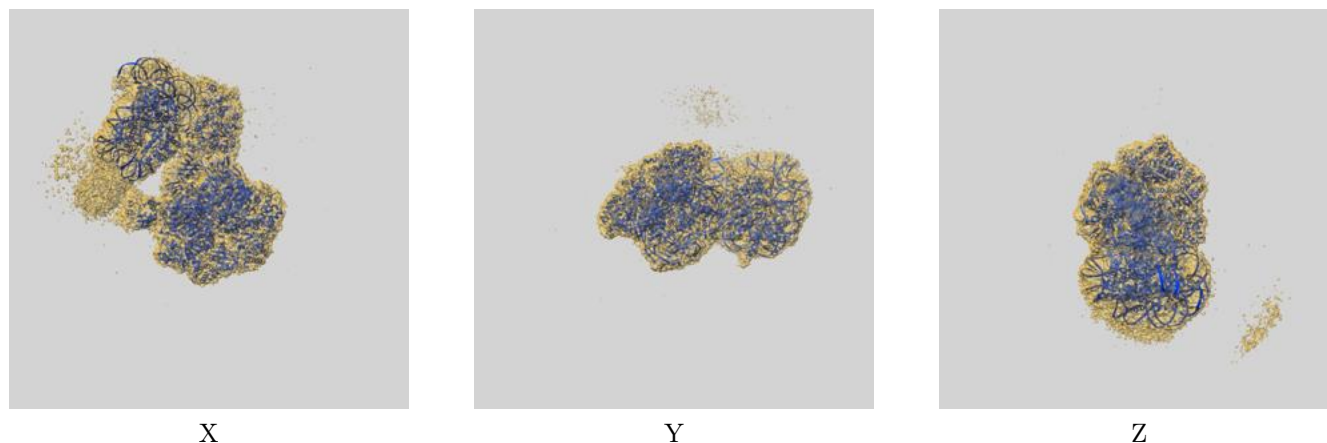
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	8.62	4.11

\*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 4.03 differs from the reported value 3.2 by more than 10 %

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

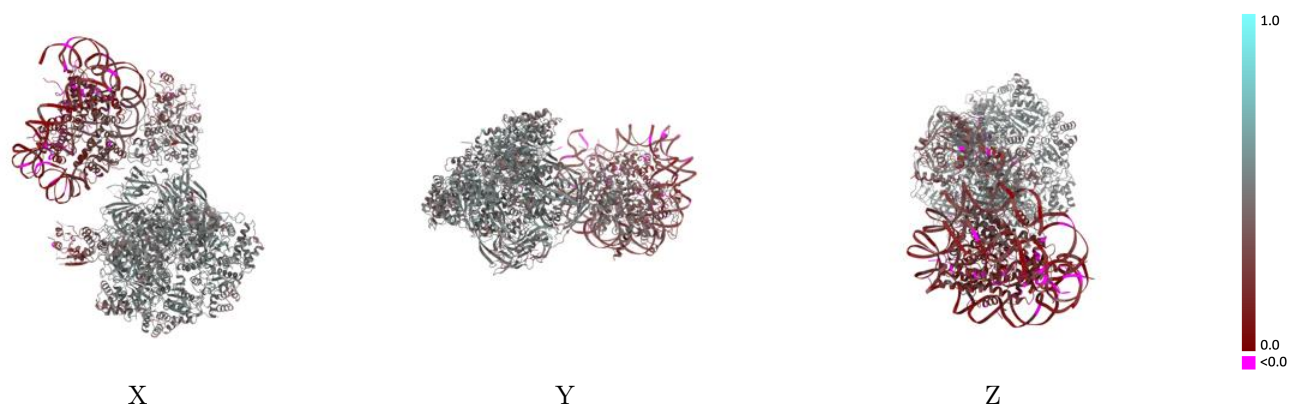
This section contains information regarding the fit between EMDB map EMD-70289 and PDB model 9OB1. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



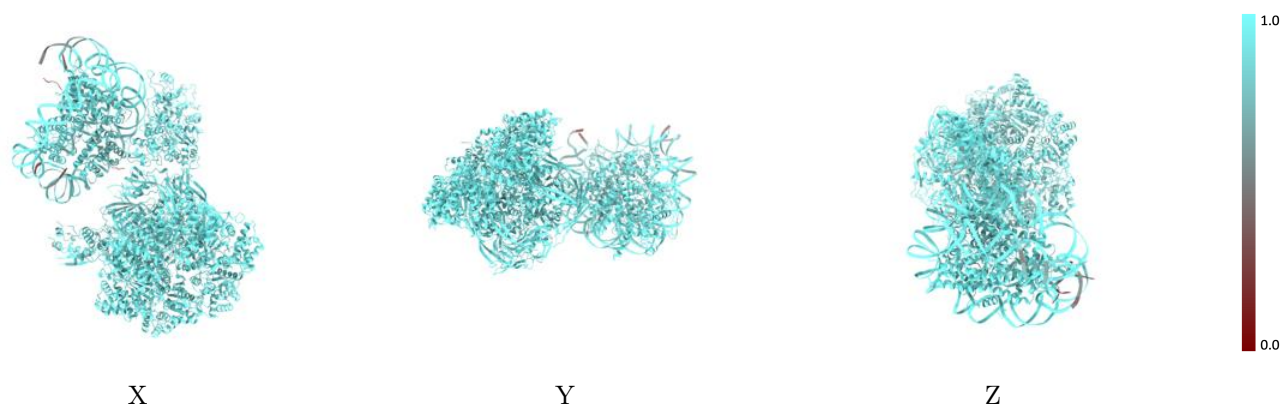
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



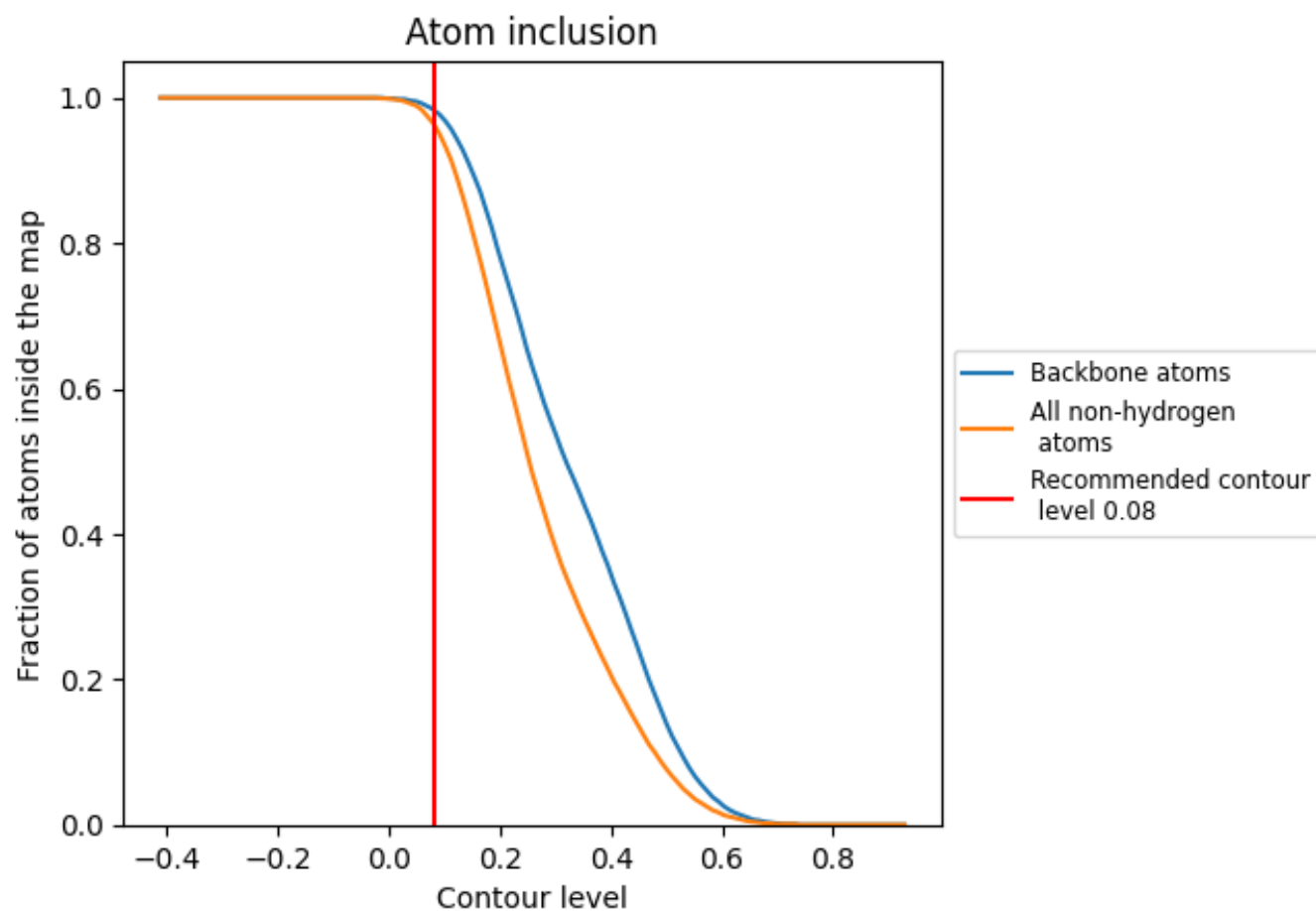
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).











































## 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.3740
A	 0.9860	 0.1490
B	 0.9750	 0.1590
C	 0.9280	 0.1630
D	 0.9730	 0.1810
E	 0.9350	 0.1530
F	 0.9530	 0.2400
G	 0.8980	 0.2400
H	 0.9010	 0.2520
I	 0.9330	 0.1700
J	 0.9390	 0.1620
Q	 0.9460	 0.4000
R	 0.9530	 0.3760
S	 0.9720	 0.3850
T	 0.9830	 0.4840
U	 0.9890	 0.4810
V	 0.9880	 0.4640
W	 0.9880	 0.4820
X	 0.9780	 0.4910
Y	 0.9710	 0.4790
Z	 1.0000	 0.4860

