



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 01:35 AM UTC

PDB ID : 8WW6 / pdb_00008ww6
EMDB ID : EMD-37882
Title : Structure of ATP-rs-Form AsfvPrimPol Hexamer
Authors : Shi, T.H.; Guo, Y.Y.; Yan, R.H.
Deposited on : 2023-10-25
Resolution : 3.73 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

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

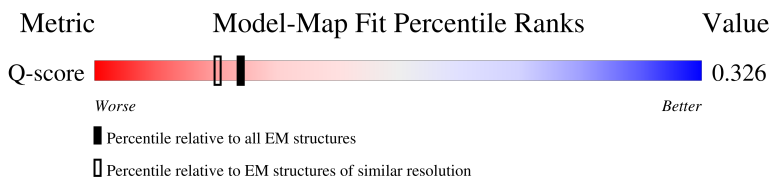
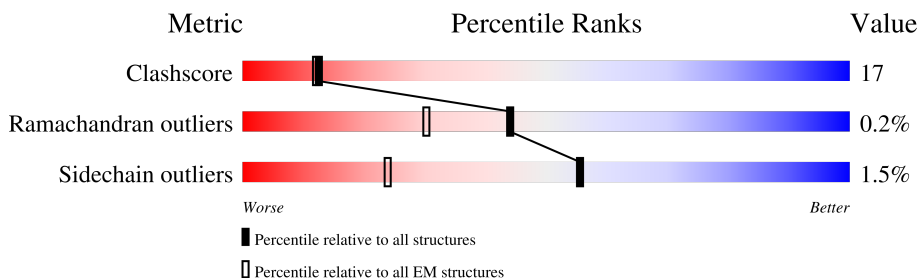
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

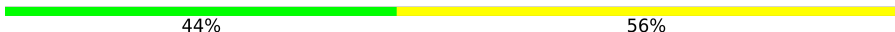
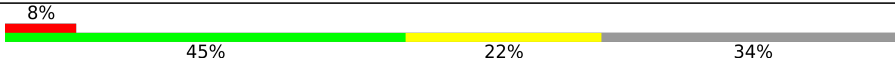
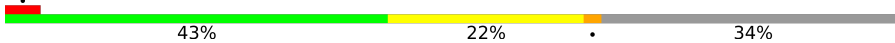
The reported resolution of this entry is 3.73 Å.

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	10415 (3.23 - 4.23)

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	H	25	
2	I	4	
3	A	972	
3	B	972	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	972	43%23%34%
3	D	972	41%24%34%
3	E	972	44%22%34%
3	F	972	44%22%34%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32825 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 (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	25	Total	C	N	O	P	0	0
			500	250	50	175	25		

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	4	Total	C	N	O	P	0	0
			84	40	20	20	4		

- Molecule 3 is a protein called Putative primase C962R.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
3	A	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
3	C	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
3	D	644	Total	C	N	O	S	0	0
			5333	3440	907	961	25		
3	E	643	Total	C	N	O	S	0	0
			5328	3436	906	960	26		
3	F	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	963	LEU	-	expression tag	UNP A0A2X0TKI6
B	964	GLU	-	expression tag	UNP A0A2X0TKI6
B	965	ASP	-	expression tag	UNP A0A2X0TKI6
B	966	TYR	-	expression tag	UNP A0A2X0TKI6
B	967	LYS	-	expression tag	UNP A0A2X0TKI6

Continued on next page...

Continued from previous page...

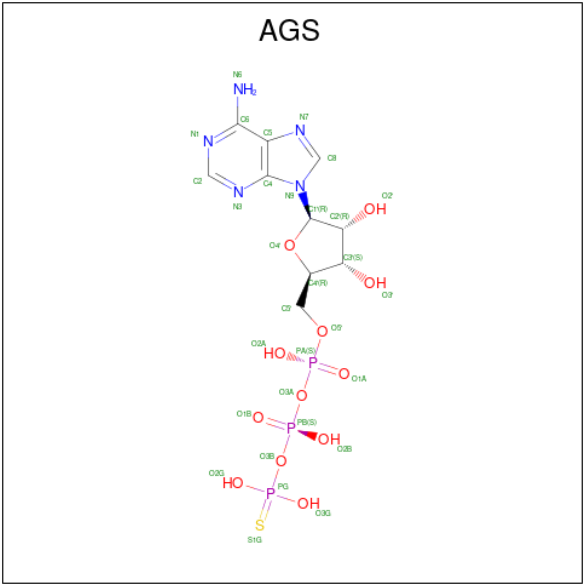
Chain	Residue	Modelled	Actual	Comment	Reference
B	968	ASP	-	expression tag	UNP A0A2X0TKI6
B	969	ASP	-	expression tag	UNP A0A2X0TKI6
B	970	ASP	-	expression tag	UNP A0A2X0TKI6
B	971	ASP	-	expression tag	UNP A0A2X0TKI6
B	972	LYS	-	expression tag	UNP A0A2X0TKI6
A	963	LEU	-	expression tag	UNP A0A2X0TKI6
A	964	GLU	-	expression tag	UNP A0A2X0TKI6
A	965	ASP	-	expression tag	UNP A0A2X0TKI6
A	966	TYR	-	expression tag	UNP A0A2X0TKI6
A	967	LYS	-	expression tag	UNP A0A2X0TKI6
A	968	ASP	-	expression tag	UNP A0A2X0TKI6
A	969	ASP	-	expression tag	UNP A0A2X0TKI6
A	970	ASP	-	expression tag	UNP A0A2X0TKI6
A	971	ASP	-	expression tag	UNP A0A2X0TKI6
A	972	LYS	-	expression tag	UNP A0A2X0TKI6
C	963	LEU	-	expression tag	UNP A0A2X0TKI6
C	964	GLU	-	expression tag	UNP A0A2X0TKI6
C	965	ASP	-	expression tag	UNP A0A2X0TKI6
C	966	TYR	-	expression tag	UNP A0A2X0TKI6
C	967	LYS	-	expression tag	UNP A0A2X0TKI6
C	968	ASP	-	expression tag	UNP A0A2X0TKI6
C	969	ASP	-	expression tag	UNP A0A2X0TKI6
C	970	ASP	-	expression tag	UNP A0A2X0TKI6
C	971	ASP	-	expression tag	UNP A0A2X0TKI6
C	972	LYS	-	expression tag	UNP A0A2X0TKI6
D	963	LEU	-	expression tag	UNP A0A2X0TKI6
D	964	GLU	-	expression tag	UNP A0A2X0TKI6
D	965	ASP	-	expression tag	UNP A0A2X0TKI6
D	966	TYR	-	expression tag	UNP A0A2X0TKI6
D	967	LYS	-	expression tag	UNP A0A2X0TKI6
D	968	ASP	-	expression tag	UNP A0A2X0TKI6
D	969	ASP	-	expression tag	UNP A0A2X0TKI6
D	970	ASP	-	expression tag	UNP A0A2X0TKI6
D	971	ASP	-	expression tag	UNP A0A2X0TKI6
D	972	LYS	-	expression tag	UNP A0A2X0TKI6
E	963	LEU	-	expression tag	UNP A0A2X0TKI6
E	964	GLU	-	expression tag	UNP A0A2X0TKI6
E	965	ASP	-	expression tag	UNP A0A2X0TKI6
E	966	TYR	-	expression tag	UNP A0A2X0TKI6
E	967	LYS	-	expression tag	UNP A0A2X0TKI6
E	968	ASP	-	expression tag	UNP A0A2X0TKI6
E	969	ASP	-	expression tag	UNP A0A2X0TKI6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	970	ASP	-	expression tag	UNP A0A2X0TKI6
E	971	ASP	-	expression tag	UNP A0A2X0TKI6
E	972	LYS	-	expression tag	UNP A0A2X0TKI6
F	963	LEU	-	expression tag	UNP A0A2X0TKI6
F	964	GLU	-	expression tag	UNP A0A2X0TKI6
F	965	ASP	-	expression tag	UNP A0A2X0TKI6
F	966	TYR	-	expression tag	UNP A0A2X0TKI6
F	967	LYS	-	expression tag	UNP A0A2X0TKI6
F	968	ASP	-	expression tag	UNP A0A2X0TKI6
F	969	ASP	-	expression tag	UNP A0A2X0TKI6
F	970	ASP	-	expression tag	UNP A0A2X0TKI6
F	971	ASP	-	expression tag	UNP A0A2X0TKI6
F	972	LYS	-	expression tag	UNP A0A2X0TKI6

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
4	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

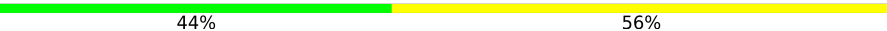
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

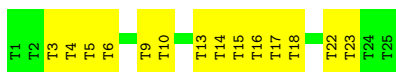
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	A	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA (25-MER)

Chain H: 



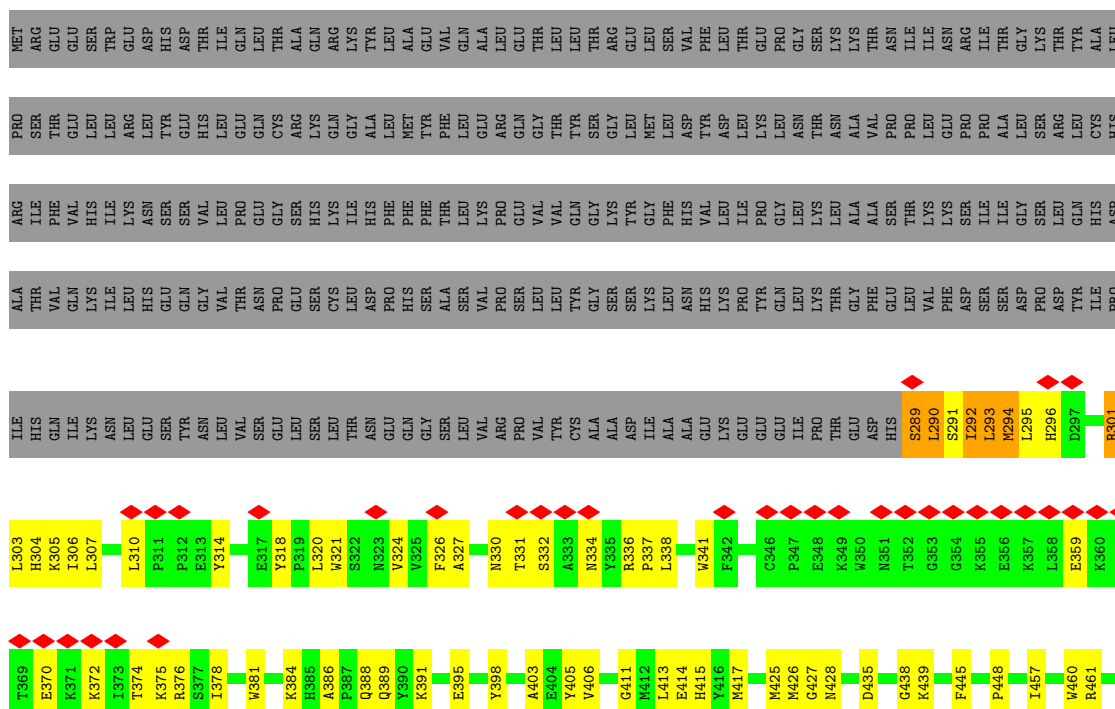
- Molecule 2: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain I: 

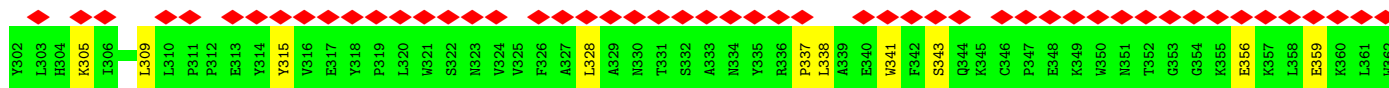
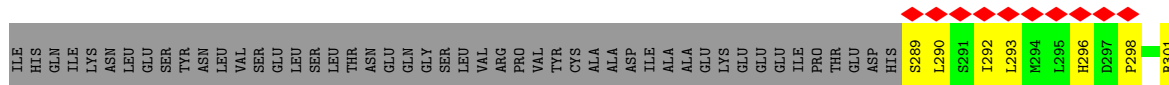
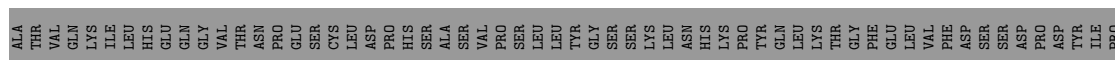
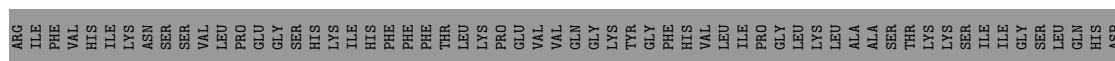
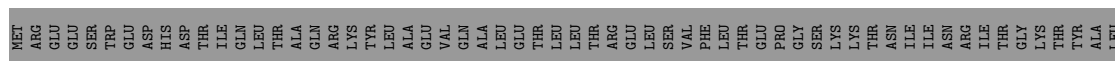


- Molecule 3: Putative primase C962R

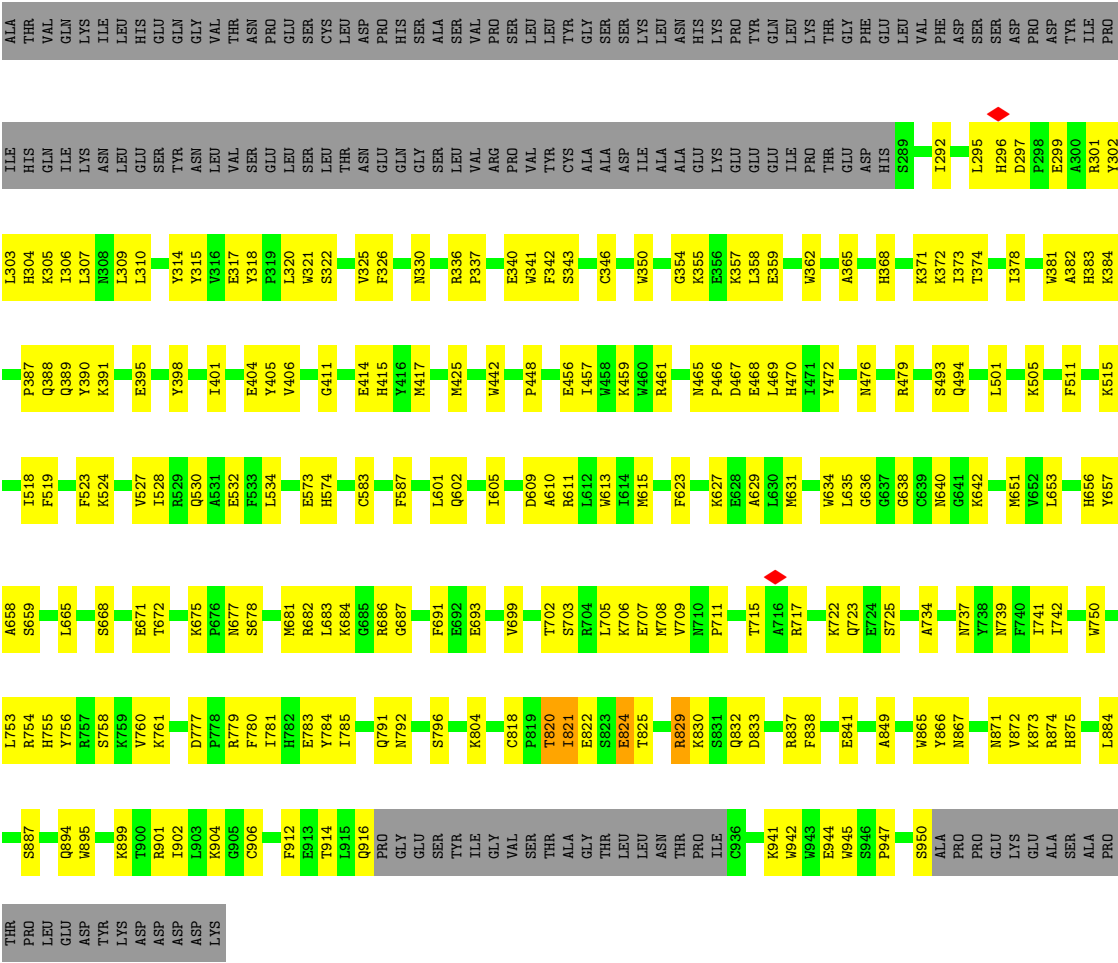
Chain B: 



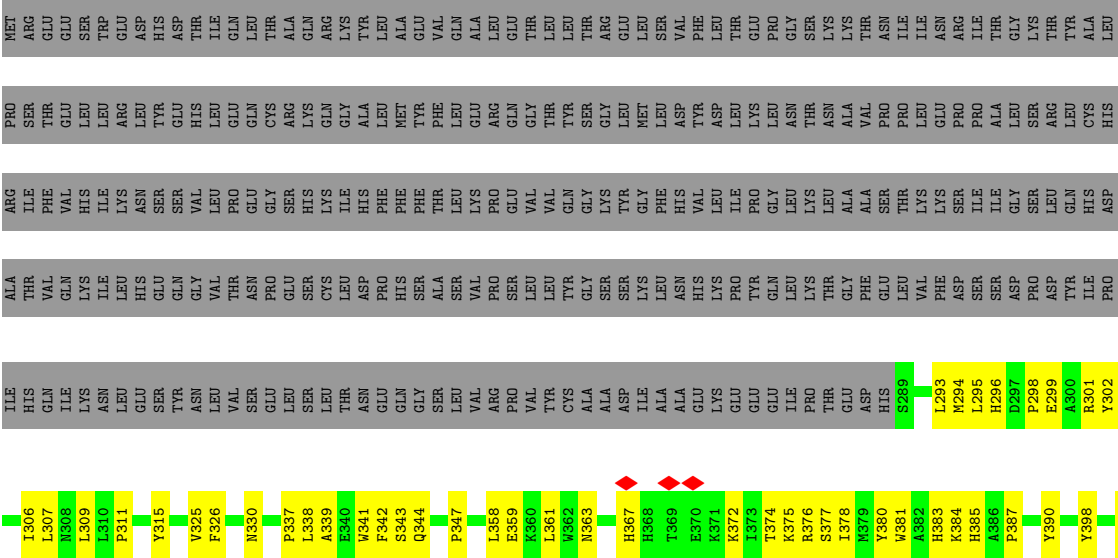
- Molecule 3: Putative primase C962R







● Molecule 3: Putative primase C962R



GLU	R874	E773	M681	F587	V406
ALA	H875	K774	K684	L601	G411
SER	L876	A877	G885	Q602	E414
ALA	L877	E776	R686	I605	H415
PRO	E878	D777	G687	D609	Y416
THR	L880	P778	F691	A610	M417
PRO	E883	R779	E692	R611	
LEU	W895	F780	E693	D609	M425
GLU	W895	E783	T694	A610	
ASP		Y784	N695	R611	
TYR		I785	S697	I614	D433
LYS	K899	Q791	E698	M615	W434
ASP	T900	S796	V699	F616	D435
ASP	R901	I797	L700	S619	
ASP	I902	L798	S703	F623	K439
ASP	L903	K804	R704	L626	P448
ASP	K904	L805	E707	K627	
ASP	G905	E808	P711	E628	M452
LYS	R907	I813	D712	A629	M453
	E913	V816	V714	L630	Q454
	Q916	I821	A716	M631	
GLU	P917	E822	R717	L632	I457
SER	G918	S823	K722	L633	W458
TYR	GLU	E824	Q723	W634	K459
ILE	SER	T825	E724	L635	W460
GLY	GLY	Y828	S725	G636	R461
VAL	VAL	F838	F726	G637	P466
SER	THR	I839	A734	E468	D467
THR	ALA	T840	A735	L469	E468
ALA	ASN	V844	S736	H470	H470
GLY	THR		N737	I471	Y472
THR	PRO	P847	F740	K642	S478
LEU	I935	S848	I741	T643	R479
LEU	P938	A849	G748	F644	
ASN	W942	V852	R751	L645	H491
THR	W945	A863	R752	M646	L492
PRO	S946	E864	L753	H656	S493
ALA	P947	W865	R754	Y657	Q494
PRO	N948	Y866	H755	L665	Y504
ALA	P949	N867	S758	L666	
ALA	S950	T868	K759	T667	F519
PRO	ALA	N869	V760	S668	N520
PRO	PRO	I870	K761	C669	
GLU	GLU	N871	F762	R670	I828
LYS	LYS	V872	N770	E671	R536
		K873		T672	Q537
				A673	R537
				E674	R538
				K675	S539
				P676	
				N677	Q542
				F680	E573

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38908	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.164	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	420.48, 420.48, 420.48	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	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: AGS, 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	H	0.22	0/549	0.55	0/846
2	I	0.13	0/95	0.19	0/144
3	A	0.12	0/5503	0.30	0/7458
3	B	0.16	0/5503	0.39	0/7458
3	C	0.15	0/5503	0.37	0/7458
3	D	0.19	0/5489	0.43	1/7439 (0.0%)
3	E	0.15	0/5483	0.37	0/7430
3	F	0.15	0/5503	0.37	1/7458 (0.0%)
All	All	0.16	0/33628	0.38	2/45691 (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	F	670	ARG	CB-CA-C	-5.29	110.46	116.54
3	D	373	ILE	N-CA-C	-5.25	108.72	113.71

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	H	500	0	301	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	84	0	45	3	0
3	A	5347	0	5216	160	0
3	B	5347	0	5217	210	0
3	C	5347	0	5217	181	0
3	D	5333	0	5202	196	0
3	E	5328	0	5196	172	0
3	F	5347	0	5217	176	0
4	A	31	0	12	7	0
4	B	31	0	12	7	0
4	C	31	0	12	6	0
4	D	31	0	12	5	0
4	E	31	0	12	6	0
4	F	31	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	32825	0	31683	1082	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 17.

The worst 5 of 1082 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:B:874:ARG:HH21	3:B:875:HIS:C	1.63	1.06
3:F:667:THR:HA	3:F:700:LEU:HB3	1.48	0.95
3:C:667:THR:HB	3:C:700:LEU:HB3	1.48	0.95
3:D:294:MET:HG3	3:D:301:ARG:HG3	1.51	0.90
3:B:294:MET:HG3	3:B:301:ARG:HG2	1.52	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	642/972 (66%)	590 (92%)	50 (8%)	2 (0%)	36	65
3	B	642/972 (66%)	585 (91%)	55 (9%)	2 (0%)	36	65
3	C	642/972 (66%)	590 (92%)	50 (8%)	2 (0%)	36	65
3	D	640/972 (66%)	578 (90%)	60 (9%)	2 (0%)	36	65
3	E	639/972 (66%)	565 (88%)	74 (12%)	0	100	100
3	F	642/972 (66%)	574 (89%)	67 (10%)	1 (0%)	43	71
All	All	3847/5832 (66%)	3482 (90%)	356 (9%)	9 (0%)	44	71

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	844	VAL
3	B	946	SER
3	A	372	LYS
3	C	388	GLN
3	C	946	SER

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	581/879 (66%)	581 (100%)	0	100	100
3	B	581/879 (66%)	565 (97%)	16 (3%)	38	58
3	C	581/879 (66%)	576 (99%)	5 (1%)	70	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	579/879 (66%)	564 (97%)	15 (3%)	40	60
3	E	579/879 (66%)	575 (99%)	4 (1%)	76	77
3	F	581/879 (66%)	570 (98%)	11 (2%)	50	65
All	All	3482/5274 (66%)	3431 (98%)	51 (2%)	55	68

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	310	LEU
3	D	708	MET
3	F	696	LYS
3	D	320	LEU
3	D	703	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	747	HIS
3	D	491	HIS
3	F	810	ASN
3	C	836	HIS
3	D	396	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

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	AGS	D	1001	5	32,33,33	2.03	7 (21%)	45,52,52	1.87	10 (22%)
4	AGS	E	1001	5	32,33,33	0.53	1 (3%)	45,52,52	0.68	1 (2%)
4	AGS	C	1001	5	32,33,33	2.04	9 (28%)	45,52,52	1.87	10 (22%)
4	AGS	A	1001	5	32,33,33	0.50	1 (3%)	45,52,52	0.68	1 (2%)
4	AGS	B	1001	5	32,33,33	2.03	7 (21%)	45,52,52	1.85	11 (24%)
4	AGS	F	1001	5	32,33,33	0.50	1 (3%)	45,52,52	0.67	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	D	1001	5	-	8/21/38/38	0/3/3/3
4	AGS	E	1001	5	-	9/21/38/38	0/3/3/3
4	AGS	C	1001	5	-	7/21/38/38	0/3/3/3
4	AGS	A	1001	5	-	11/21/38/38	0/3/3/3
4	AGS	B	1001	5	-	9/21/38/38	0/3/3/3
4	AGS	F	1001	5	-	7/21/38/38	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	AGS	PG-S1G	7.92	2.07	1.90
4	C	1001	AGS	PG-S1G	7.92	2.07	1.90
4	D	1001	AGS	PG-S1G	7.91	2.07	1.90
4	C	1001	AGS	C5-C4	4.65	1.47	1.39
4	D	1001	AGS	C5-C4	4.63	1.47	1.39

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	AGS	C5-C4-N3	-5.70	118.87	126.72
4	D	1001	AGS	C5-C4-N3	-5.66	118.93	126.72
4	B	1001	AGS	C5-C4-N3	-5.60	119.01	126.72
4	C	1001	AGS	N3-C4-N9	4.66	135.09	127.17
4	D	1001	AGS	N3-C4-N9	4.61	135.01	127.17

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

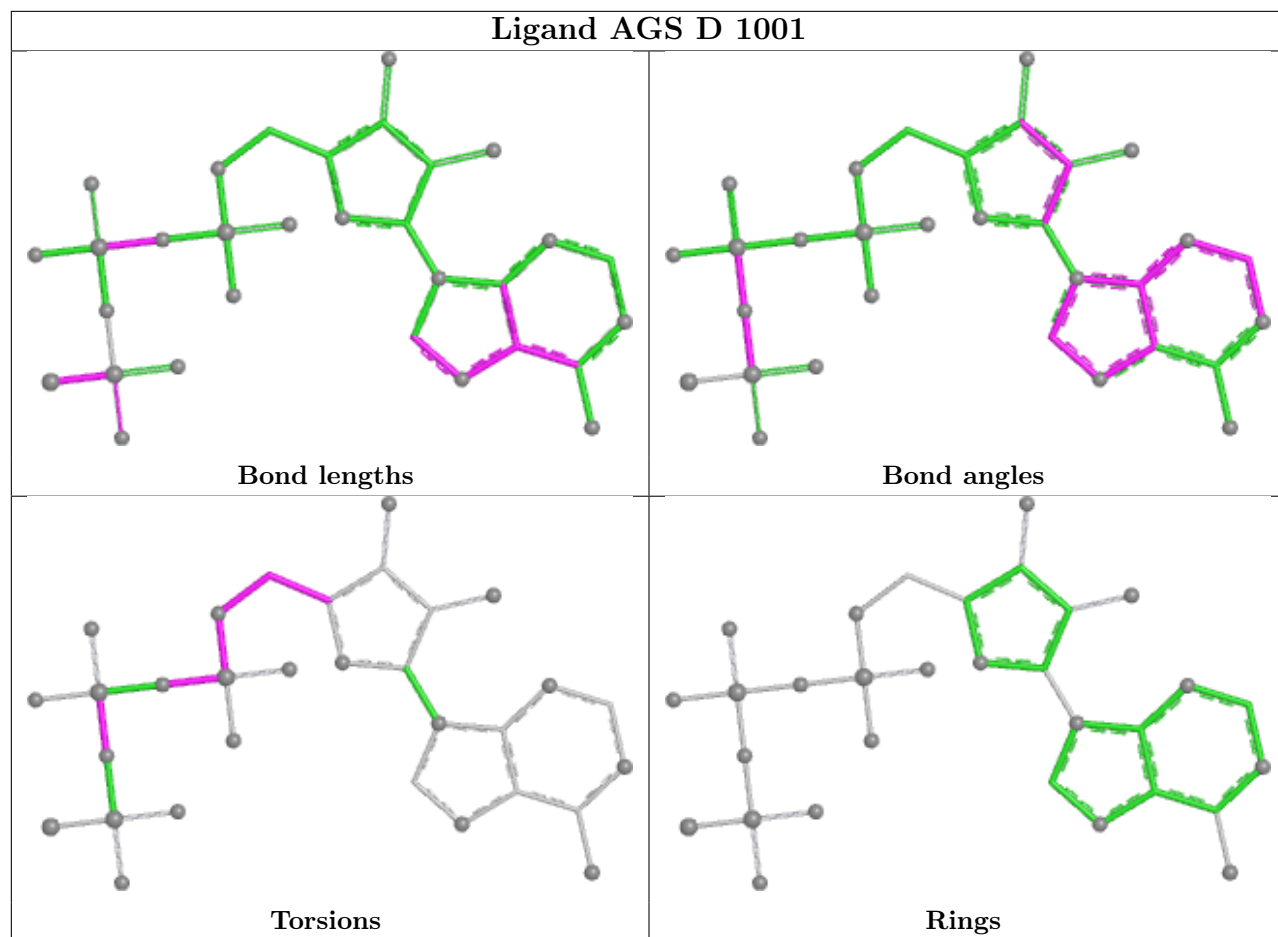
Mol	Chain	Res	Type	Atoms
4	B	1001	AGS	C5'-O5'-PA-O2A
4	B	1001	AGS	C5'-O5'-PA-O3A
4	A	1001	AGS	C5'-O5'-PA-O1A
4	A	1001	AGS	C5'-O5'-PA-O2A
4	A	1001	AGS	C5'-O5'-PA-O3A

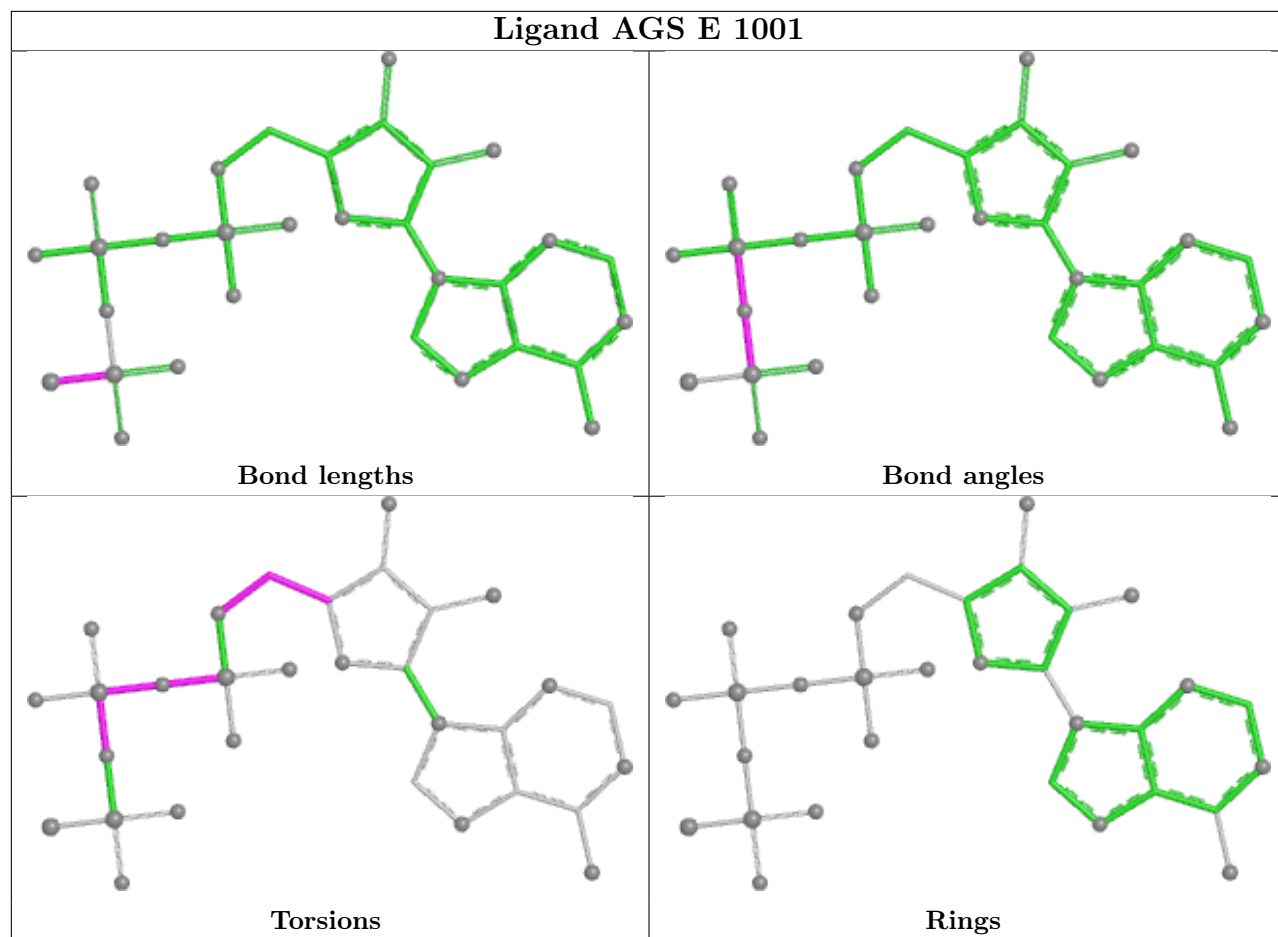
There are no ring outliers.

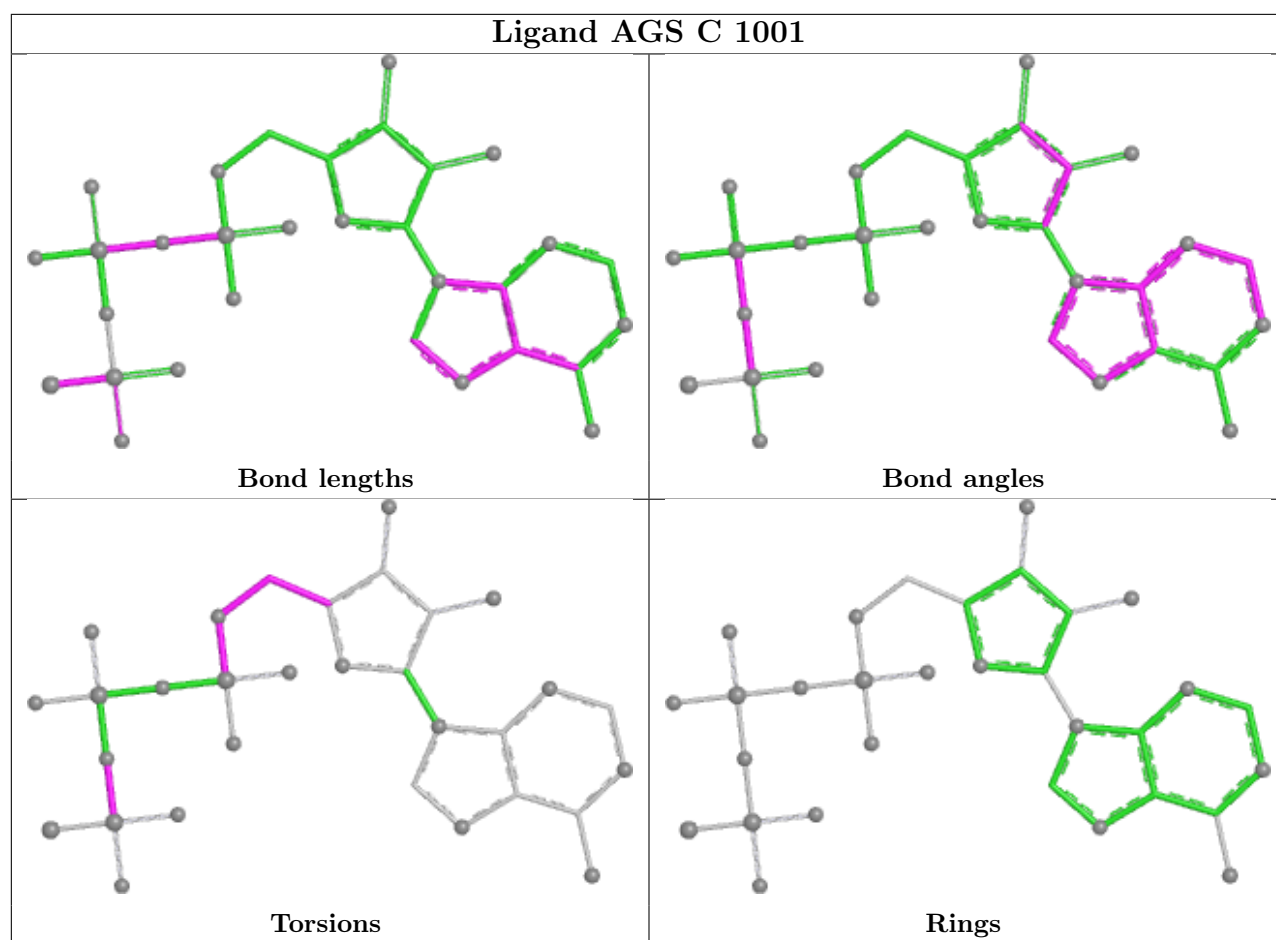
6 monomers are involved in 35 short contacts:

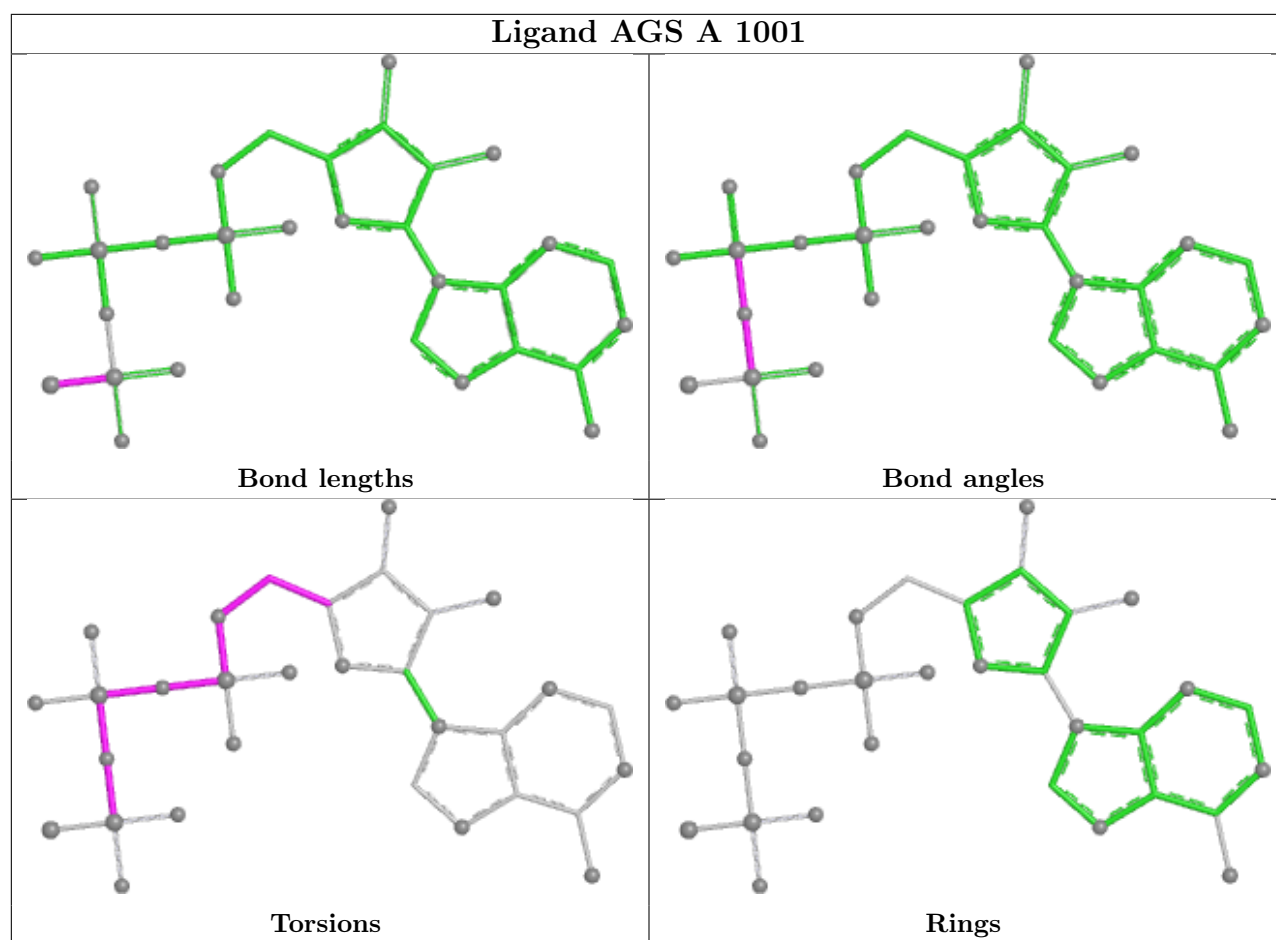
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1001	AGS	5	0
4	E	1001	AGS	6	0
4	C	1001	AGS	6	0
4	A	1001	AGS	7	0
4	B	1001	AGS	7	0
4	F	1001	AGS	4	0

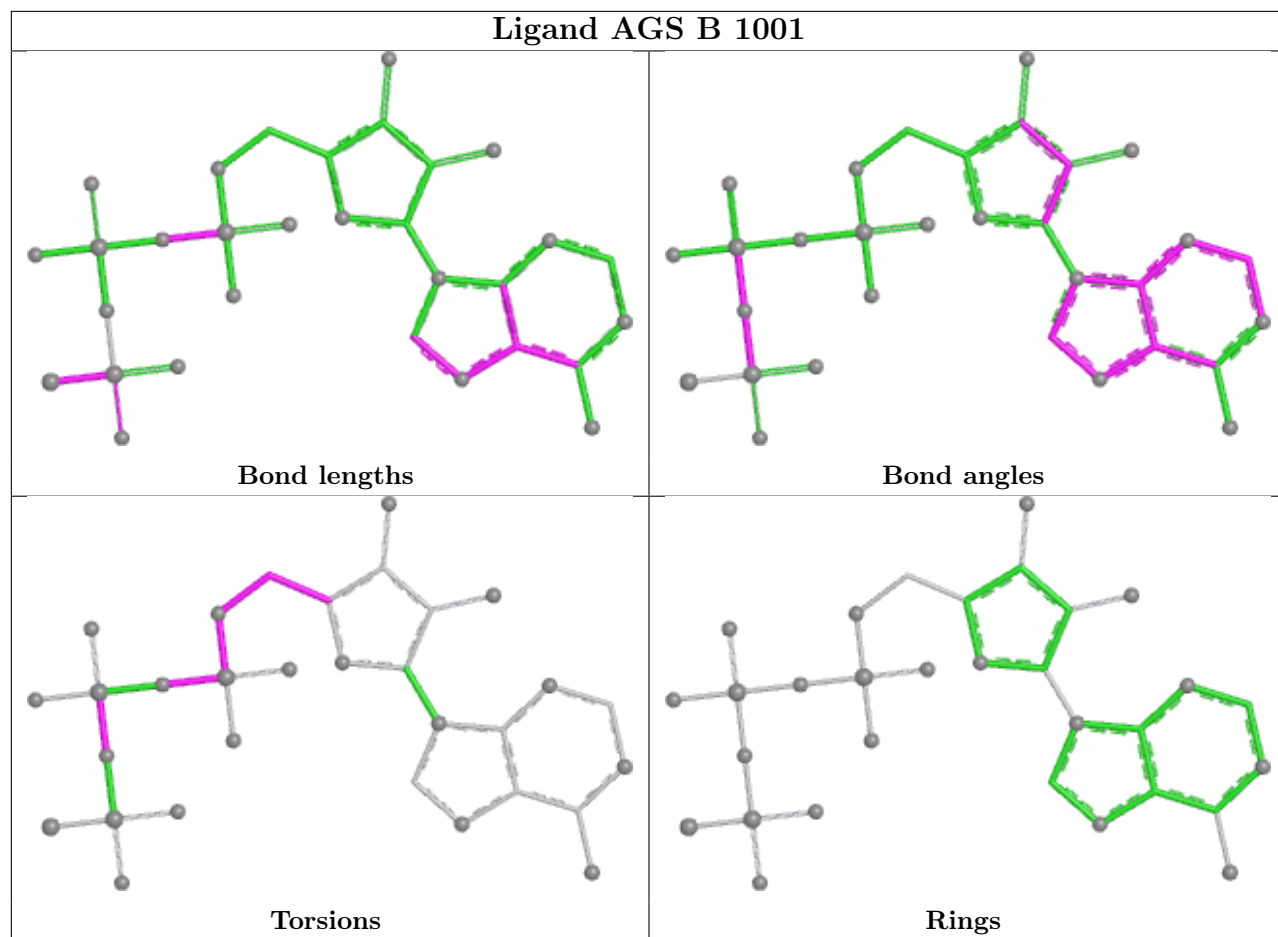
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

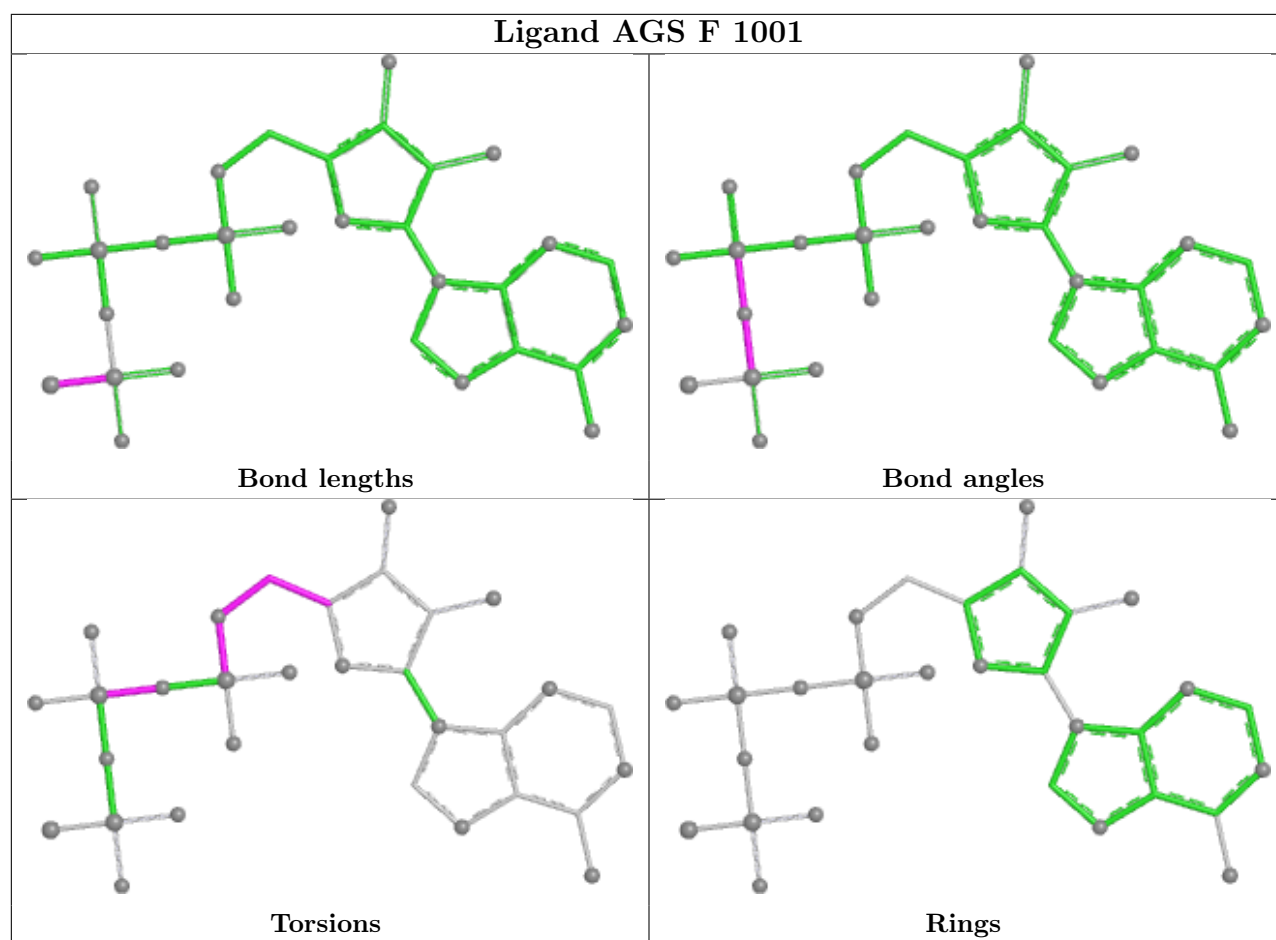












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

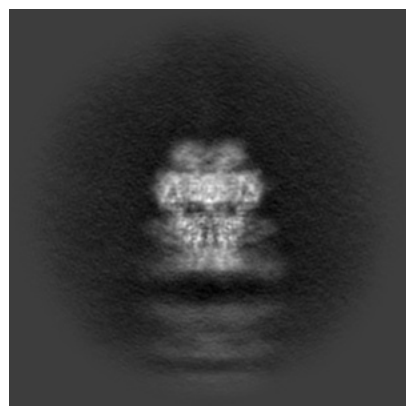
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37882. These allow visual inspection of the internal detail of the map and identification of artifacts.

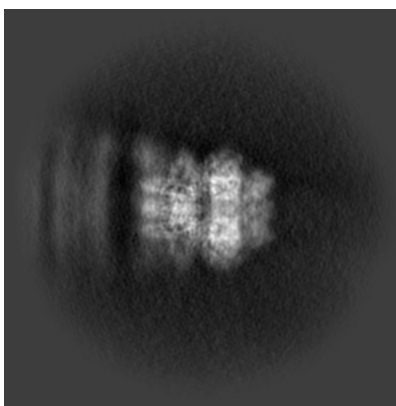
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

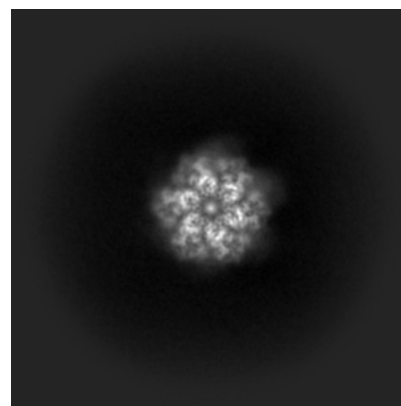
6.1.1 Primary map



X

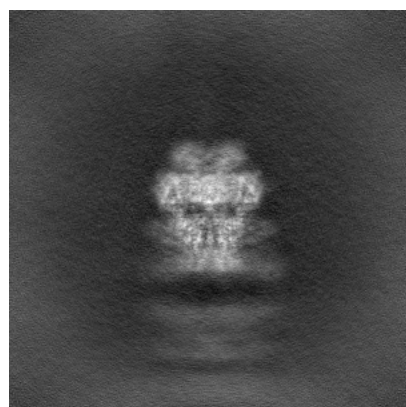


Y

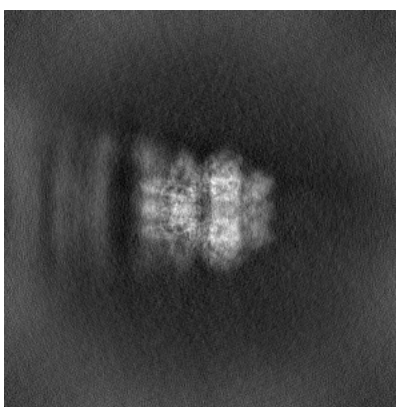


Z

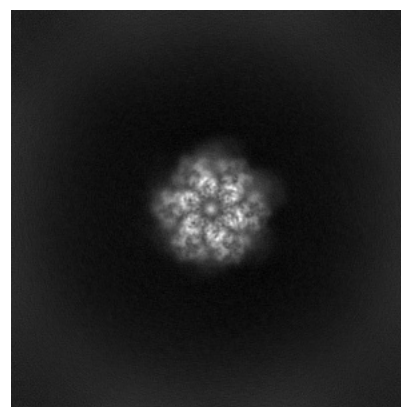
6.1.2 Raw map



X



Y

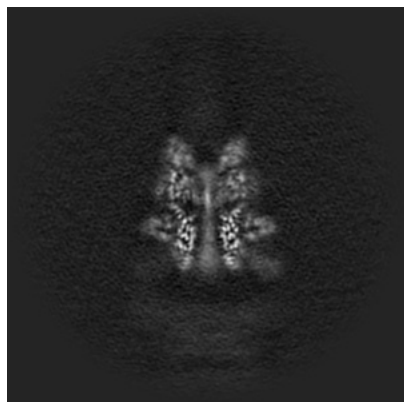


Z

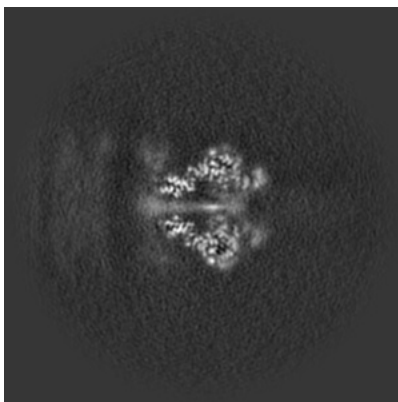
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

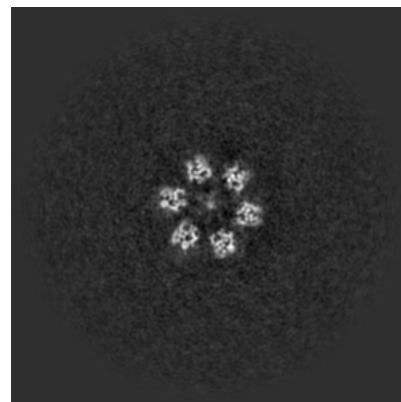
6.2.1 Primary map



X Index: 192

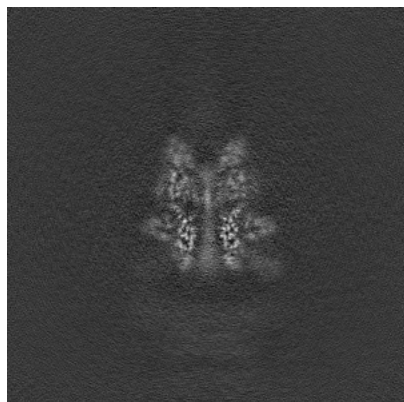


Y Index: 192

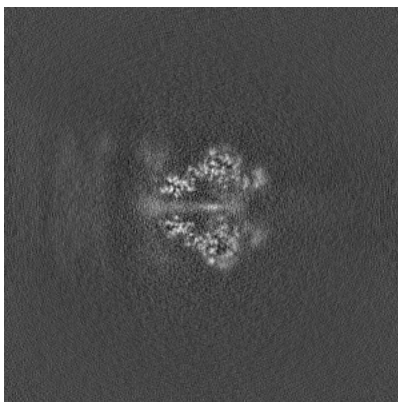


Z Index: 192

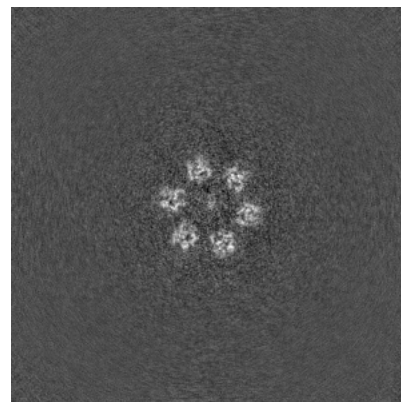
6.2.2 Raw map



X Index: 192



Y Index: 192

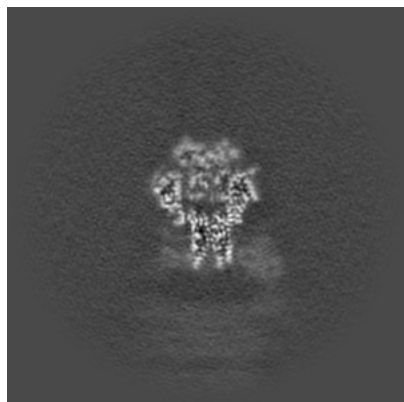


Z Index: 192

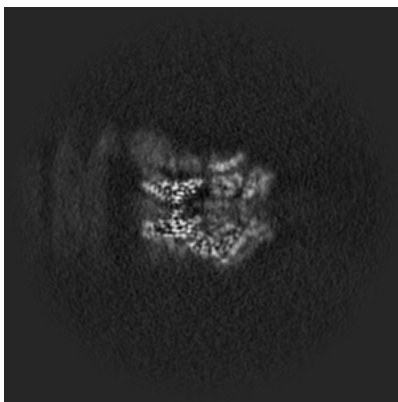
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

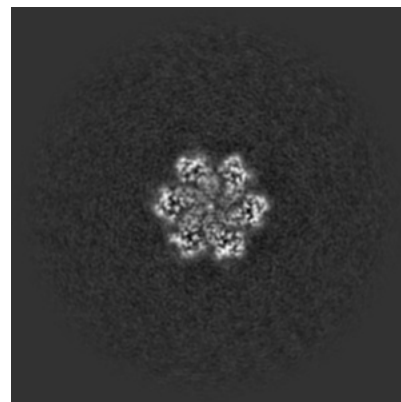
6.3.1 Primary map



X Index: 211

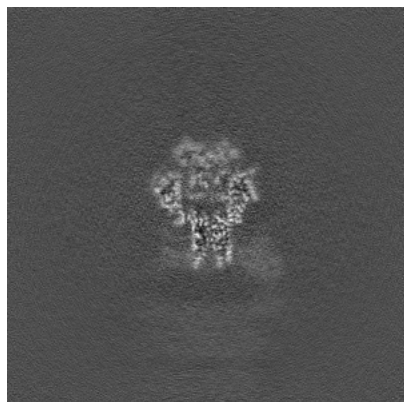


Y Index: 203



Z Index: 201

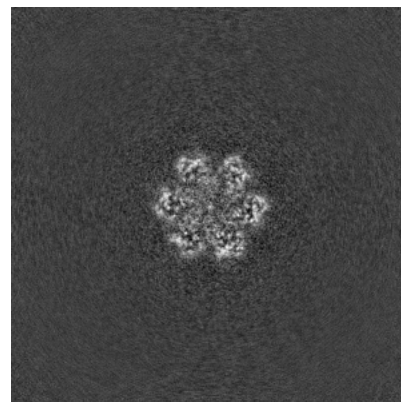
6.3.2 Raw map



X Index: 211



Y Index: 203

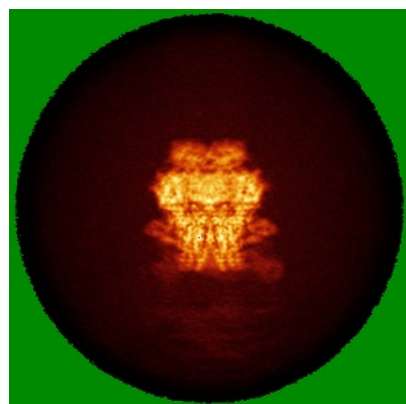


Z Index: 201

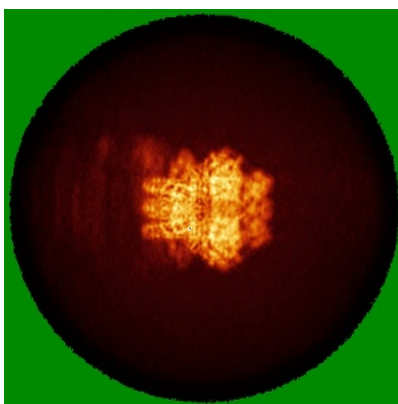
The images above show the largest variance slices of the map in three orthogonal directions.

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

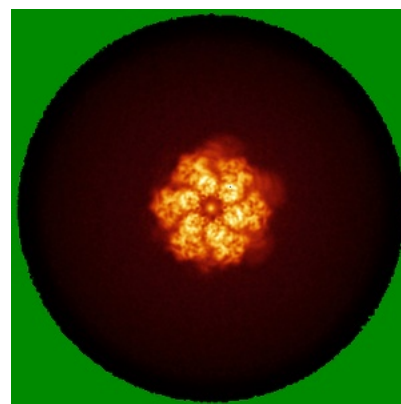
6.4.1 Primary map



X

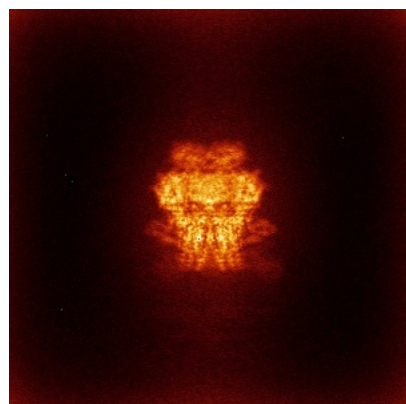


Y

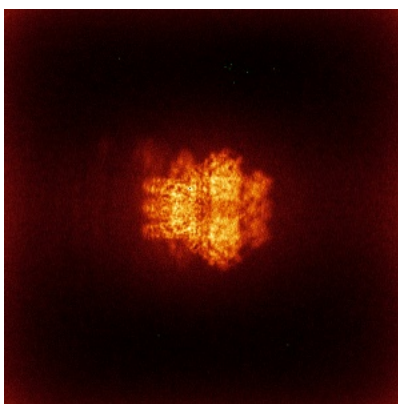


Z

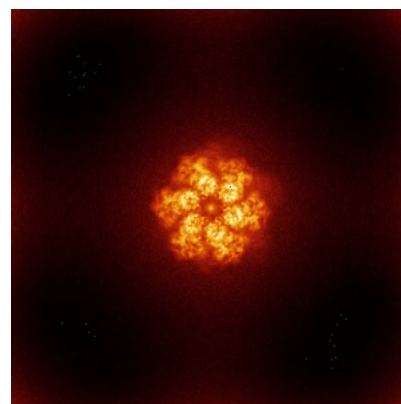
6.4.2 Raw map



X



Y

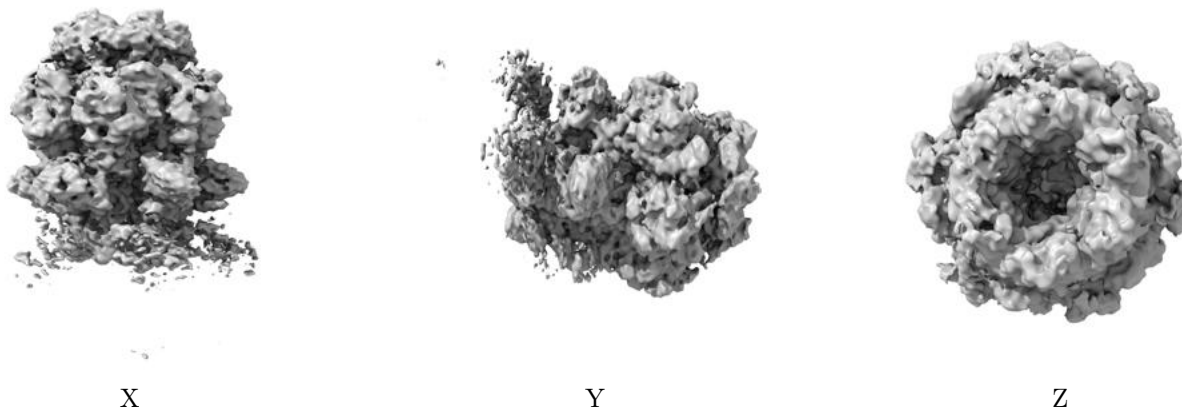


Z

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.

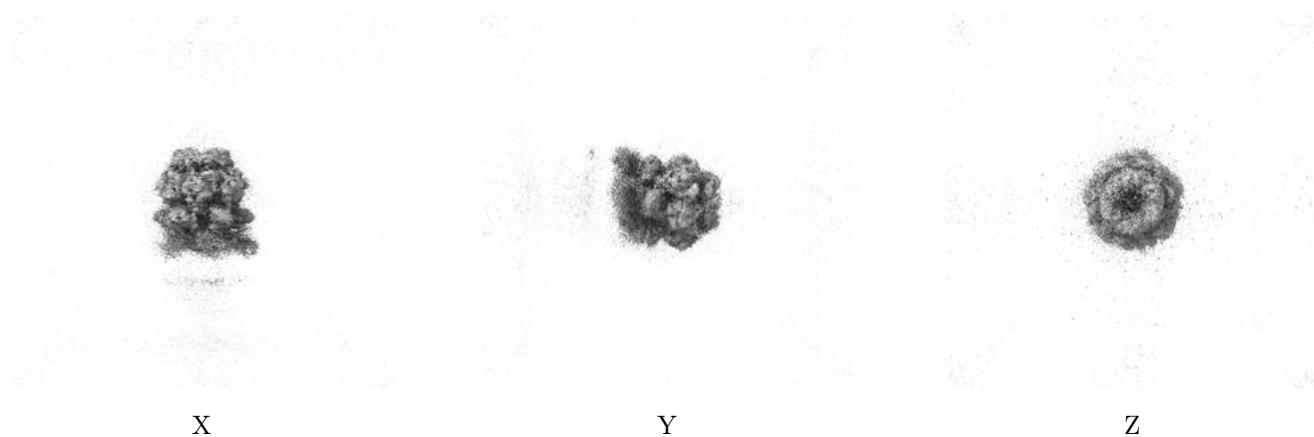
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

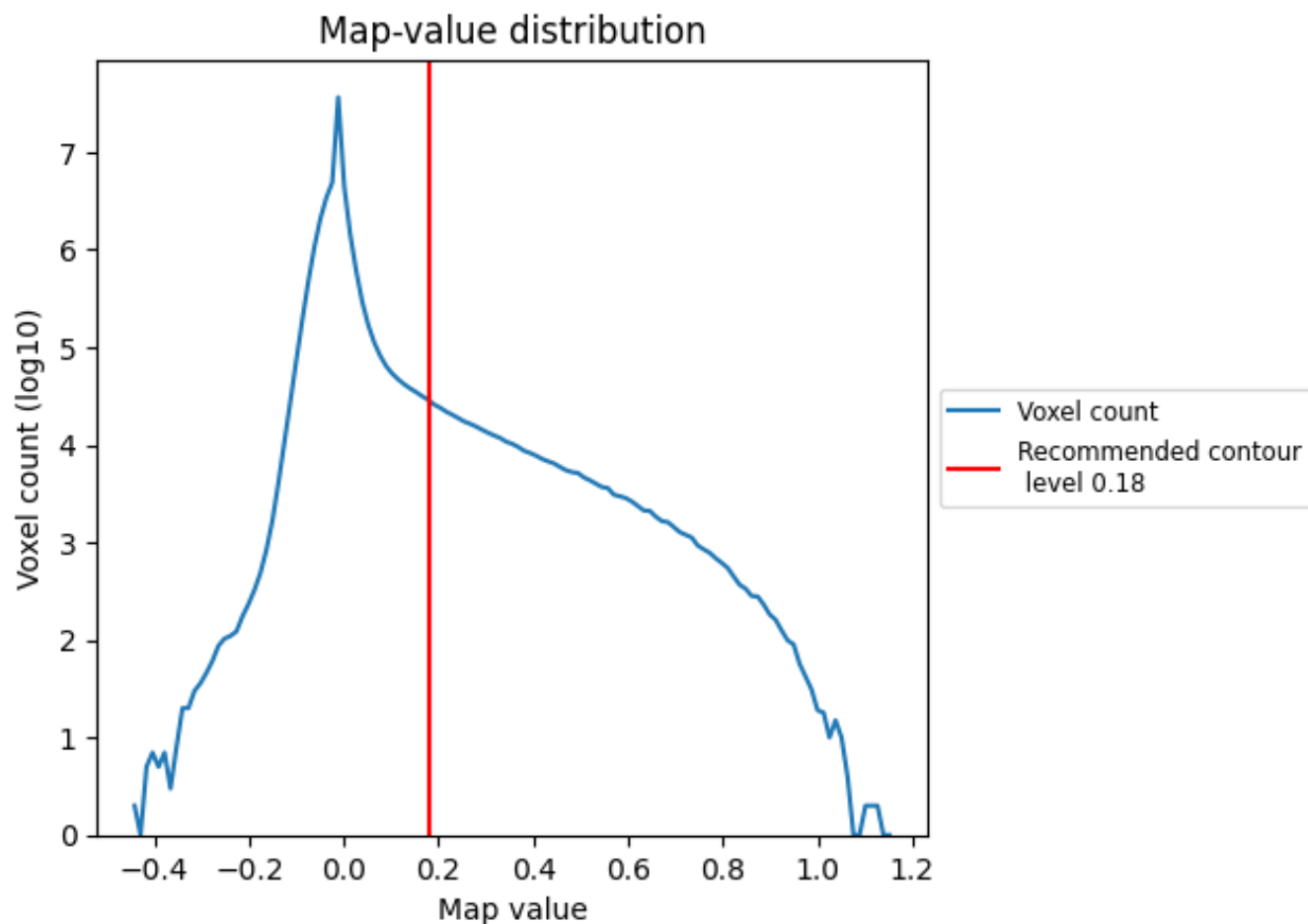
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

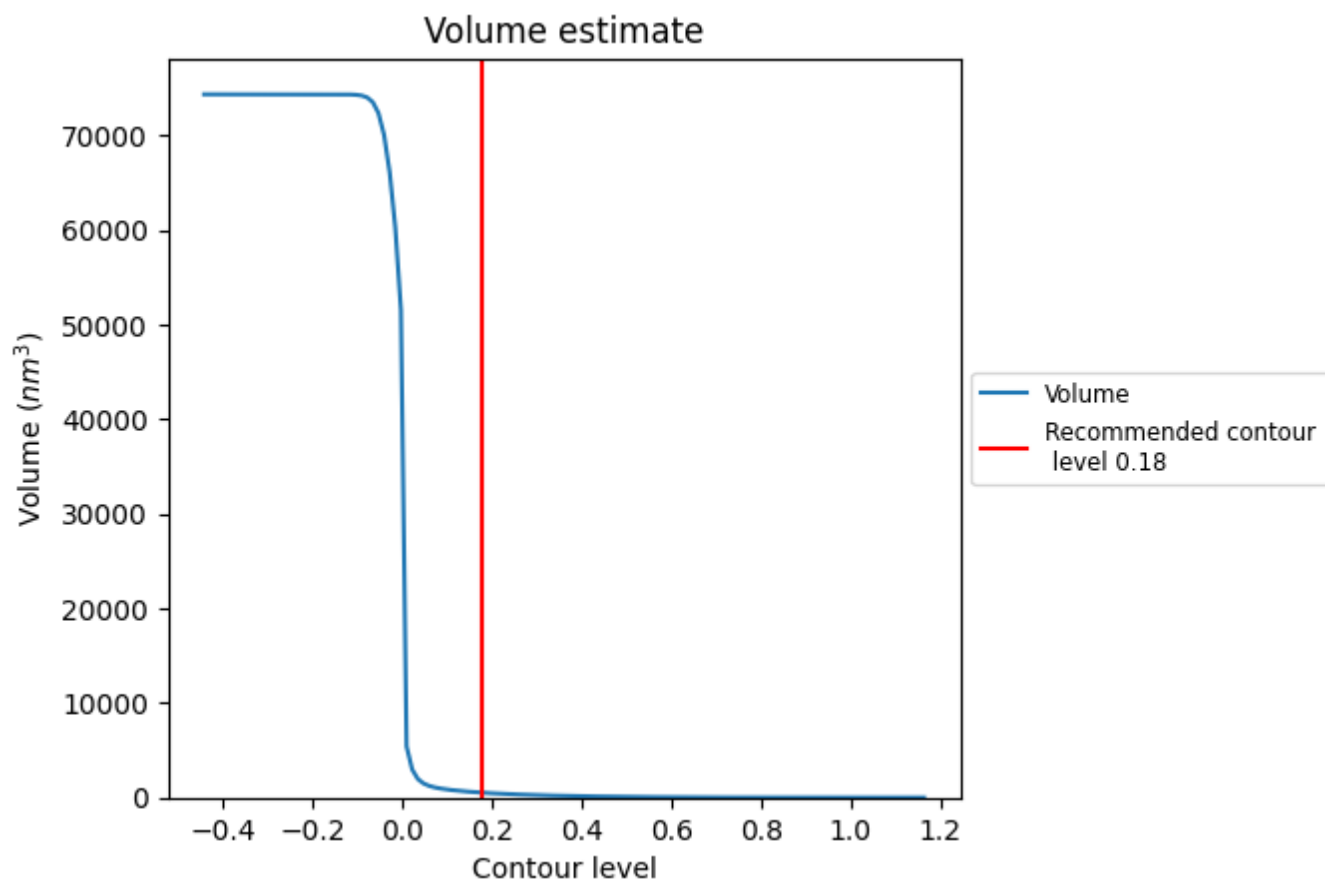
This section contains the results of statistical analysis of the map.

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.

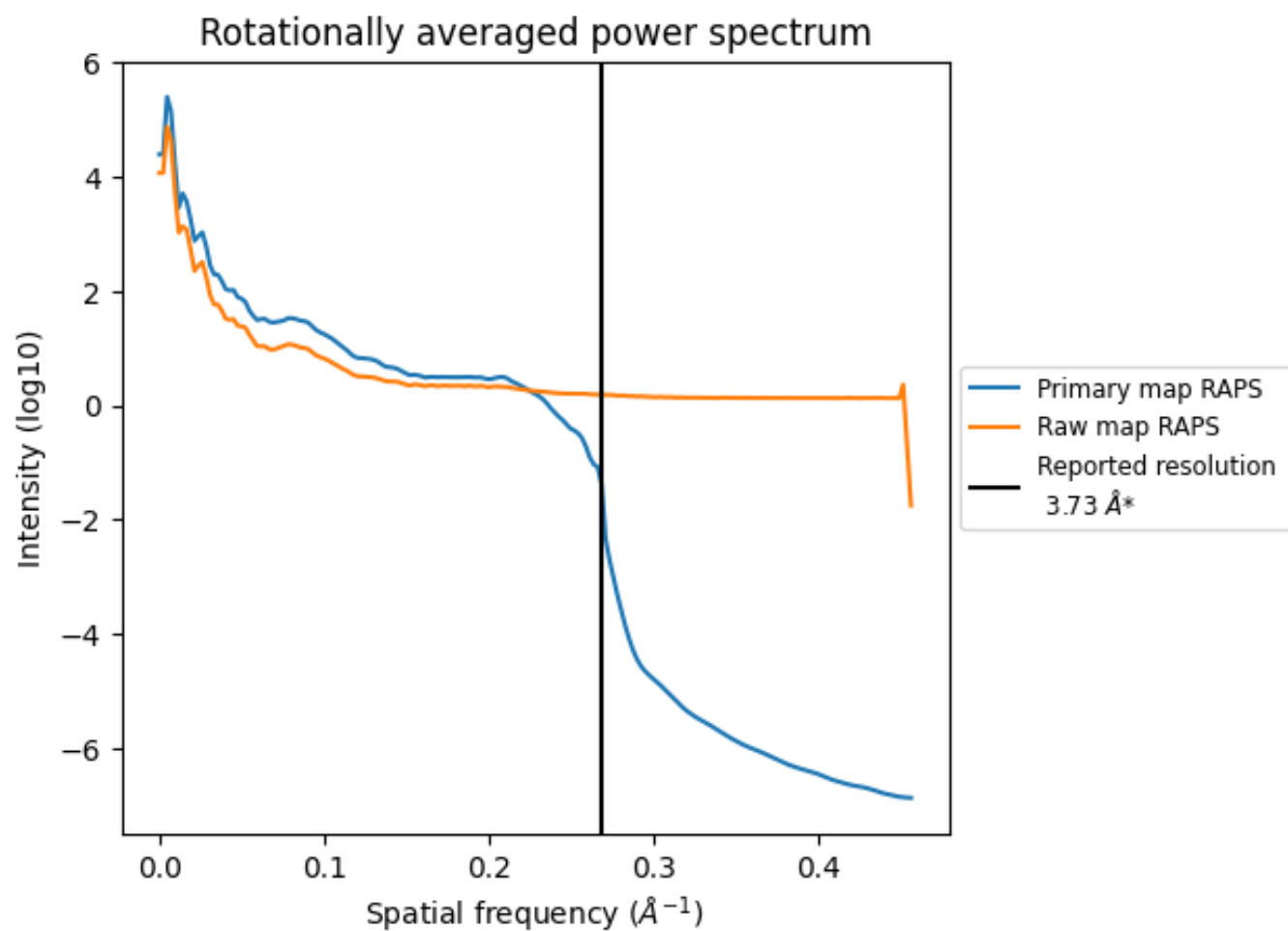
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm³; this corresponds to an approximate mass of 463 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 ⓘ

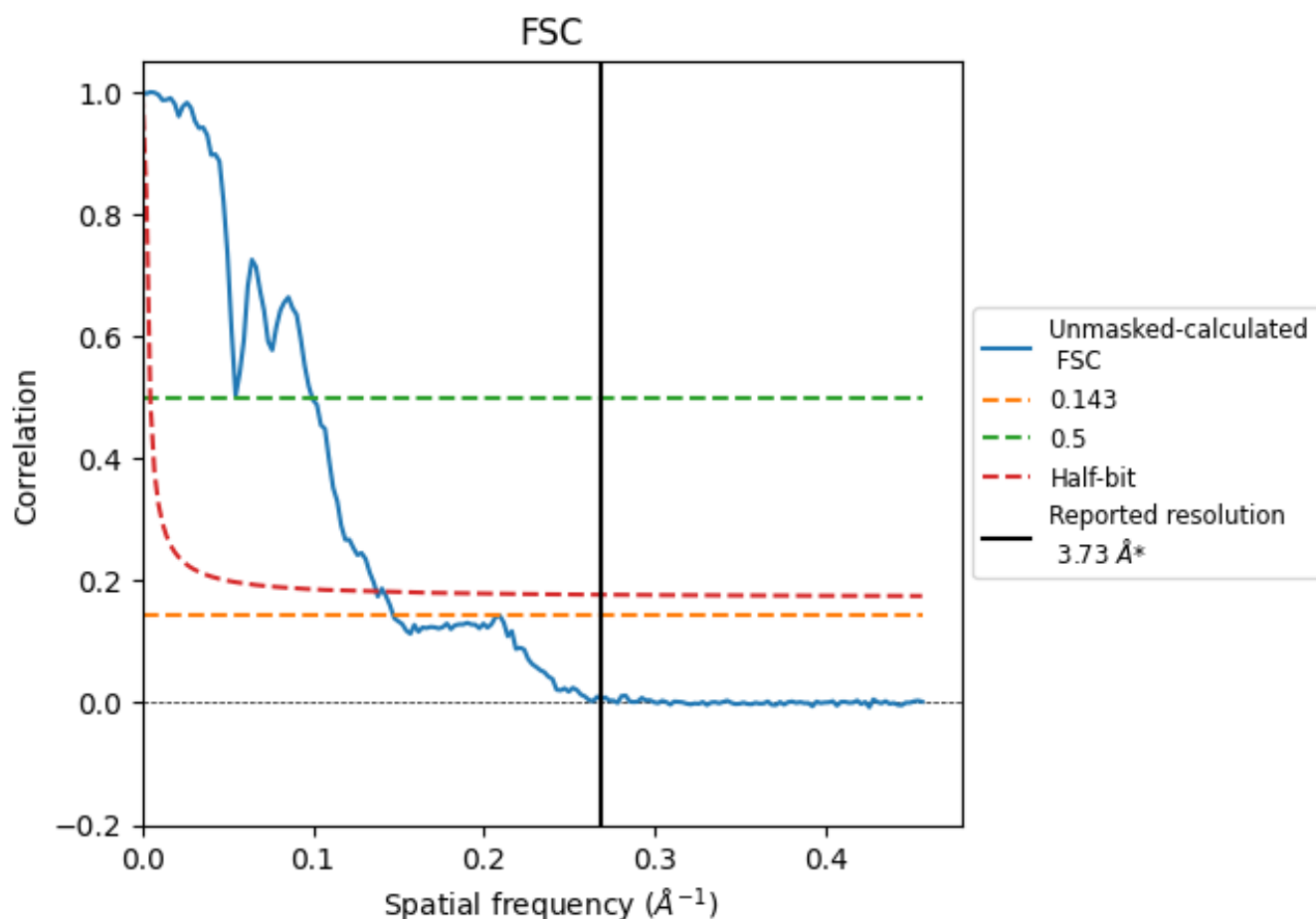


*Reported resolution corresponds to spatial frequency of 0.268 Å⁻¹

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 $0.268 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

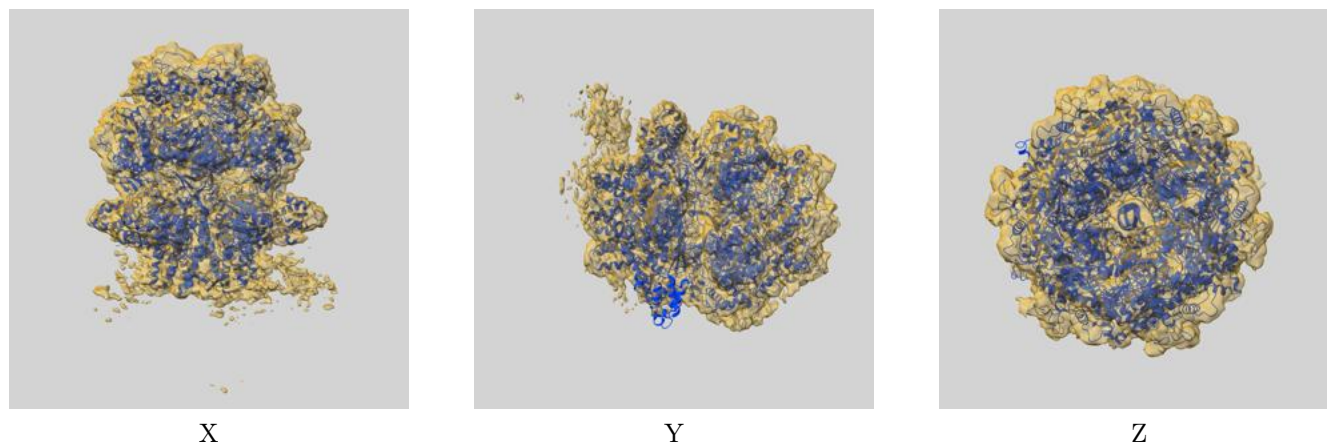
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.81	10.05	7.29

*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 6.81 differs from the reported value 3.73 by more than 10 %

9 Map-model fit [i](#)

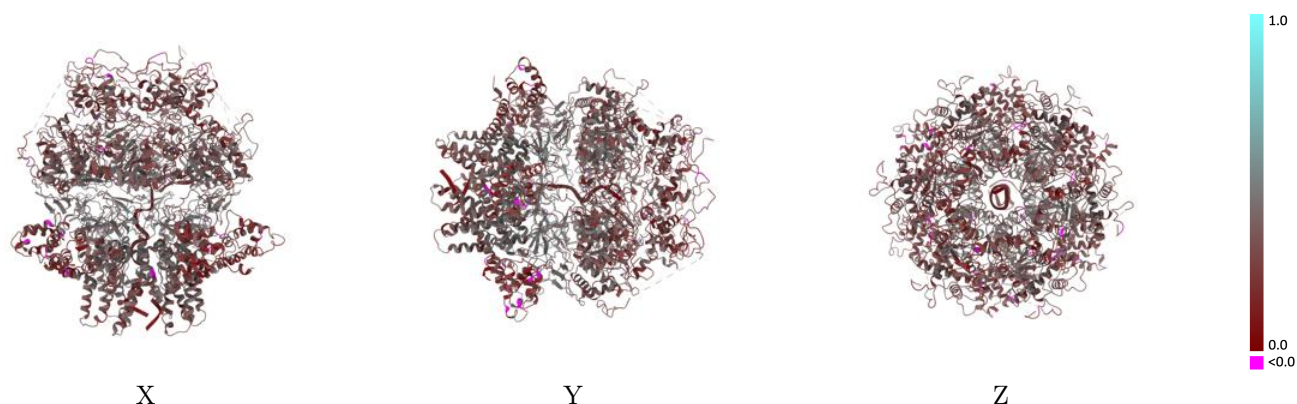
This section contains information regarding the fit between EMDB map EMD-37882 and PDB model 8WW6. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



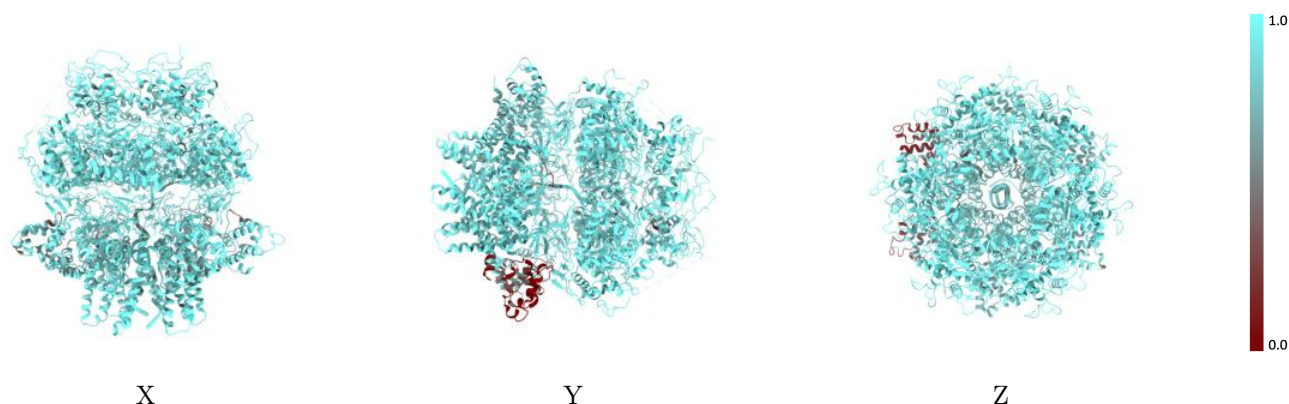
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



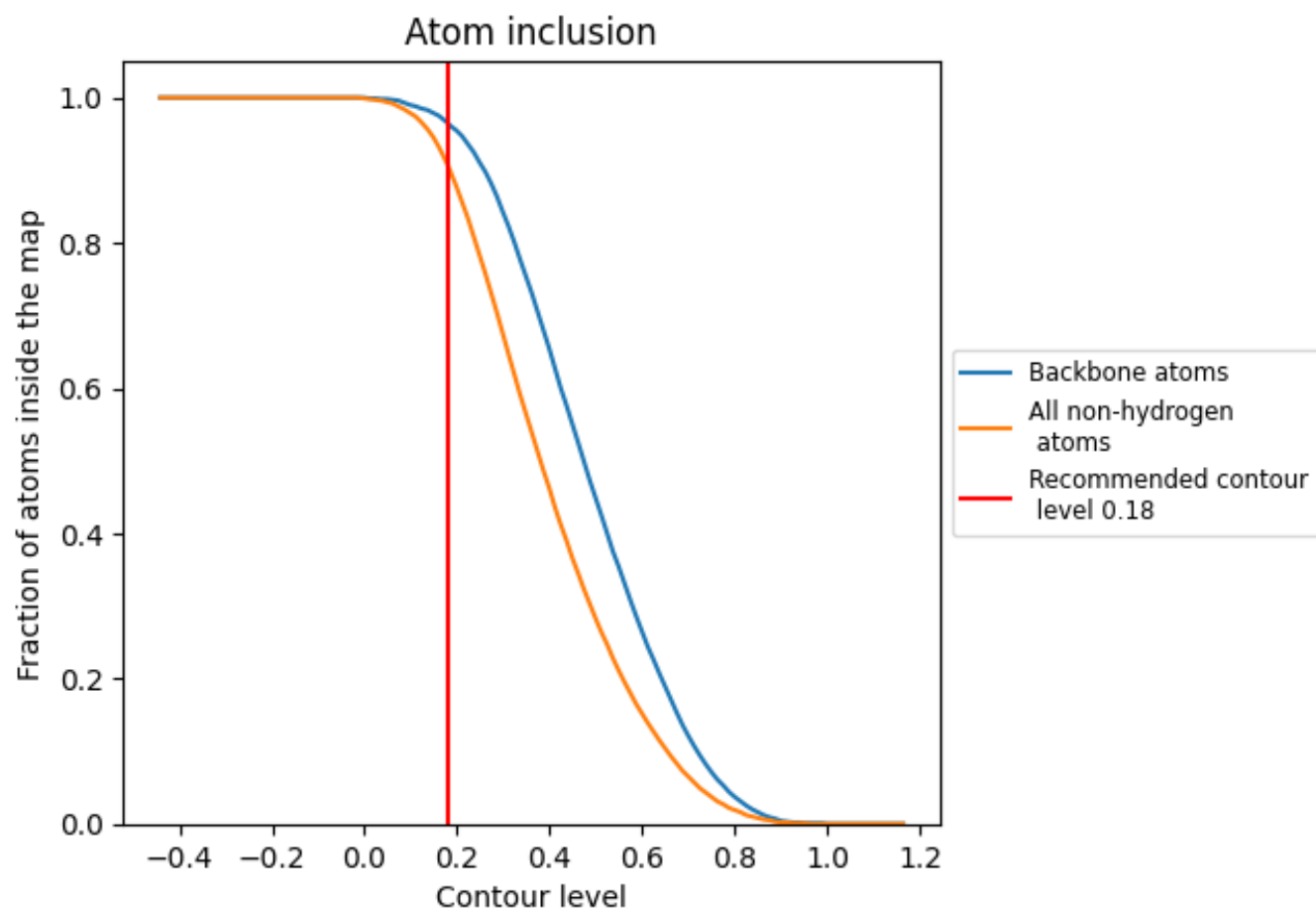
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.3260
A	0.8340	0.3170
B	0.8770	0.3250
C	0.9350	0.3340
D	0.9310	0.3390
E	0.9300	0.3360
F	0.9430	0.3270
H	0.8280	0.1500
I	0.9880	0.1090

1.0

0.0

<0.0