



# wwPDB EM Validation Summary Report ⓘ

Apr 20, 2026 – 01:38 PM EDT

PDB ID : 9Y04 / pdb\_00009y04  
EMDB ID : EMD-72384  
Title : Cryo-EM structure of human VCP/p97-R89W mutant bound to ATPgammaS  
Authors : Lehman, A.; Ahmed, S.; Mohajeri, A.; Yang, G.X.; Berezuk, A.M.; Mannar, D.; Cholak, S.; Tuttle, K.S.; Bennett, J.T.; Magno, J.A.; Hannibal, M.; Kovacevic, G.; Kuburovic, V.; Lewis, M.E.S.; Moldovan, O.; Nelson, Z.; Raskin, S.; Vandersteen, A.M.; Roach, J.C.; Subramaniam, S.; Patel, M.S.  
Deposited on : 2025-08-28  
Resolution : 2.55 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



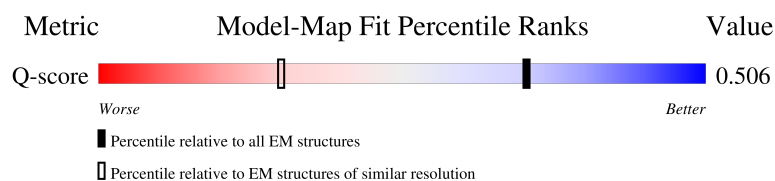
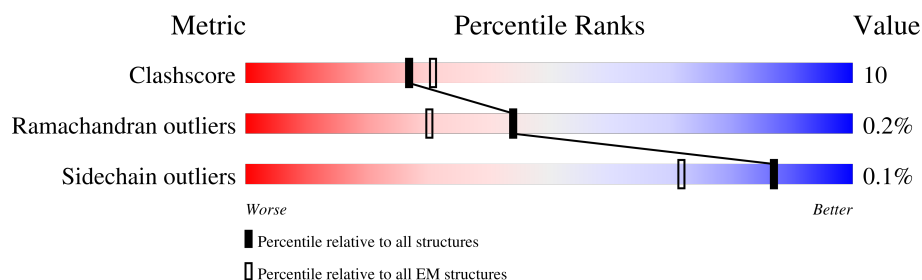
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.55 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	7475 ( 2.05 - 3.05 )




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	A	822	
1	B	822	
1	C	822	

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Mol	Chain	Length	Quality of chain
1	D	822	
1	E	822	
1	F	822	



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25998 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	B	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	C	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	D	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	E	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	F	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP P55072
A	-14	HIS	-	expression tag	UNP P55072
A	-13	HIS	-	expression tag	UNP P55072
A	-12	HIS	-	expression tag	UNP P55072
A	-11	HIS	-	expression tag	UNP P55072
A	-10	HIS	-	expression tag	UNP P55072
A	-9	SER	-	expression tag	UNP P55072
A	-8	SER	-	expression tag	UNP P55072
A	-7	GLY	-	expression tag	UNP P55072
A	-6	LEU	-	expression tag	UNP P55072
A	-5	VAL	-	expression tag	UNP P55072
A	-4	PRO	-	expression tag	UNP P55072
A	-3	ARG	-	expression tag	UNP P55072
A	-2	GLY	-	expression tag	UNP P55072
A	-1	SER	-	expression tag	UNP P55072
A	0	HIS	-	expression tag	UNP P55072
A	89	TRP	ARG	engineered mutation	UNP P55072
B	-15	HIS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P55072
B	-13	HIS	-	expression tag	UNP P55072
B	-12	HIS	-	expression tag	UNP P55072
B	-11	HIS	-	expression tag	UNP P55072
B	-10	HIS	-	expression tag	UNP P55072
B	-9	SER	-	expression tag	UNP P55072
B	-8	SER	-	expression tag	UNP P55072
B	-7	GLY	-	expression tag	UNP P55072
B	-6	LEU	-	expression tag	UNP P55072
B	-5	VAL	-	expression tag	UNP P55072
B	-4	PRO	-	expression tag	UNP P55072
B	-3	ARG	-	expression tag	UNP P55072
B	-2	GLY	-	expression tag	UNP P55072
B	-1	SER	-	expression tag	UNP P55072
B	0	HIS	-	expression tag	UNP P55072
B	89	TRP	ARG	engineered mutation	UNP P55072
C	-15	HIS	-	expression tag	UNP P55072
C	-14	HIS	-	expression tag	UNP P55072
C	-13	HIS	-	expression tag	UNP P55072
C	-12	HIS	-	expression tag	UNP P55072
C	-11	HIS	-	expression tag	UNP P55072
C	-10	HIS	-	expression tag	UNP P55072
C	-9	SER	-	expression tag	UNP P55072
C	-8	SER	-	expression tag	UNP P55072
C	-7	GLY	-	expression tag	UNP P55072
C	-6	LEU	-	expression tag	UNP P55072
C	-5	VAL	-	expression tag	UNP P55072
C	-4	PRO	-	expression tag	UNP P55072
C	-3	ARG	-	expression tag	UNP P55072
C	-2	GLY	-	expression tag	UNP P55072
C	-1	SER	-	expression tag	UNP P55072
C	0	HIS	-	expression tag	UNP P55072
C	89	TRP	ARG	engineered mutation	UNP P55072
D	-15	HIS	-	expression tag	UNP P55072
D	-14	HIS	-	expression tag	UNP P55072
D	-13	HIS	-	expression tag	UNP P55072
D	-12	HIS	-	expression tag	UNP P55072
D	-11	HIS	-	expression tag	UNP P55072
D	-10	HIS	-	expression tag	UNP P55072
D	-9	SER	-	expression tag	UNP P55072
D	-8	SER	-	expression tag	UNP P55072
D	-7	GLY	-	expression tag	UNP P55072

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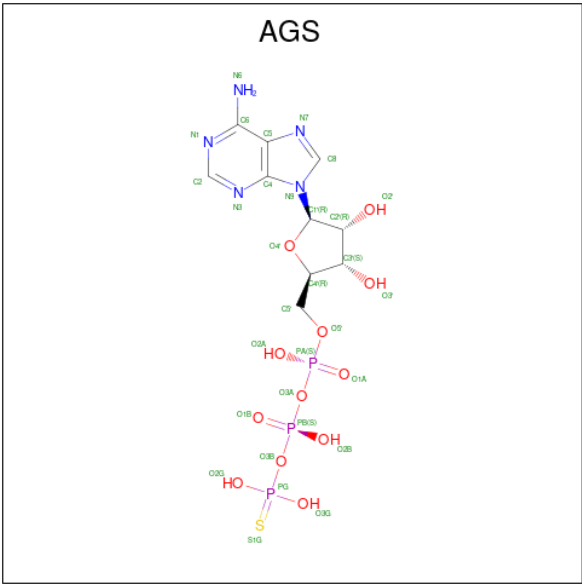


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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	LEU	-	expression tag	UNP P55072
D	-5	VAL	-	expression tag	UNP P55072
D	-4	PRO	-	expression tag	UNP P55072
D	-3	ARG	-	expression tag	UNP P55072
D	-2	GLY	-	expression tag	UNP P55072
D	-1	SER	-	expression tag	UNP P55072
D	0	HIS	-	expression tag	UNP P55072
D	89	TRP	ARG	engineered mutation	UNP P55072
E	-15	HIS	-	expression tag	UNP P55072
E	-14	HIS	-	expression tag	UNP P55072
E	-13	HIS	-	expression tag	UNP P55072
E	-12	HIS	-	expression tag	UNP P55072
E	-11	HIS	-	expression tag	UNP P55072
E	-10	HIS	-	expression tag	UNP P55072
E	-9	SER	-	expression tag	UNP P55072
E	-8	SER	-	expression tag	UNP P55072
E	-7	GLY	-	expression tag	UNP P55072
E	-6	LEU	-	expression tag	UNP P55072
E	-5	VAL	-	expression tag	UNP P55072
E	-4	PRO	-	expression tag	UNP P55072
E	-3	ARG	-	expression tag	UNP P55072
E	-2	GLY	-	expression tag	UNP P55072
E	-1	SER	-	expression tag	UNP P55072
E	0	HIS	-	expression tag	UNP P55072
E	89	TRP	ARG	engineered mutation	UNP P55072
F	-15	HIS	-	expression tag	UNP P55072
F	-14	HIS	-	expression tag	UNP P55072
F	-13	HIS	-	expression tag	UNP P55072
F	-12	HIS	-	expression tag	UNP P55072
F	-11	HIS	-	expression tag	UNP P55072
F	-10	HIS	-	expression tag	UNP P55072
F	-9	SER	-	expression tag	UNP P55072
F	-8	SER	-	expression tag	UNP P55072
F	-7	GLY	-	expression tag	UNP P55072
F	-6	LEU	-	expression tag	UNP P55072
F	-5	VAL	-	expression tag	UNP P55072
F	-4	PRO	-	expression tag	UNP P55072
F	-3	ARG	-	expression tag	UNP P55072
F	-2	GLY	-	expression tag	UNP P55072
F	-1	SER	-	expression tag	UNP P55072
F	0	HIS	-	expression tag	UNP P55072
F	89	TRP	ARG	engineered mutation	UNP P55072



- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



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



- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	Mg 2	0
3	B	2	Total 2	Mg 2	0
3	C	2	Total 2	Mg 2	0
3	D	2	Total 2	Mg 2	0
3	E	2	Total 2	Mg 2	0
3	F	2	Total 2	Mg 2	0



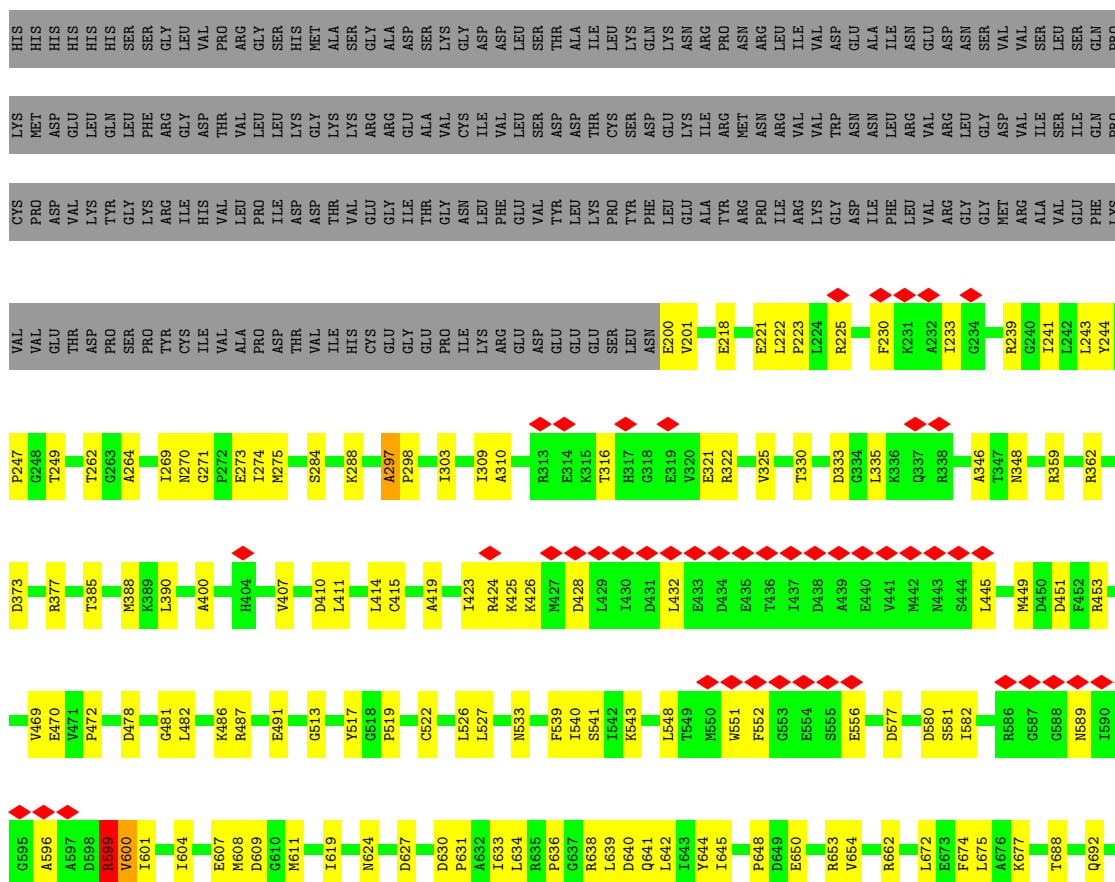




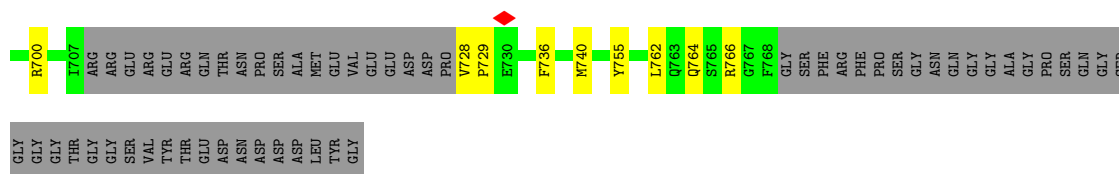




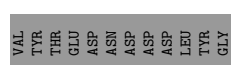
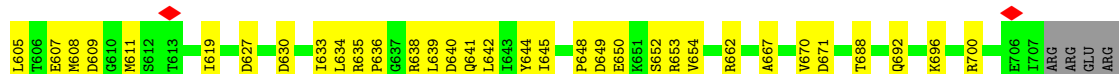
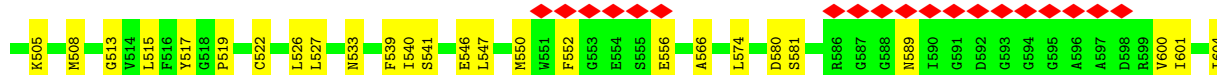
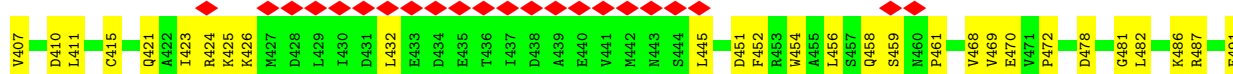
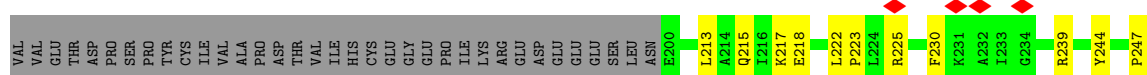
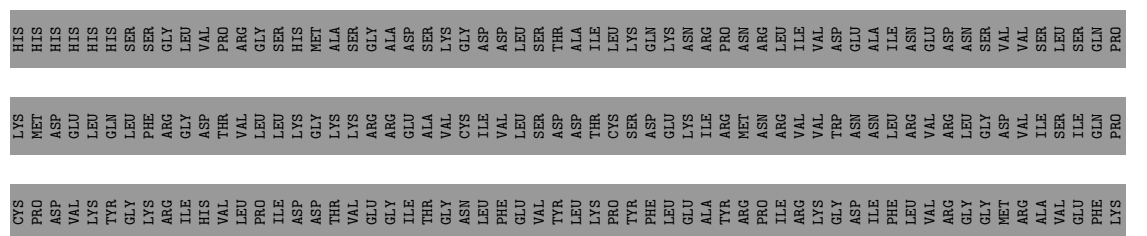
- Molecule 1: Transitional endoplasmic reticulum ATPase



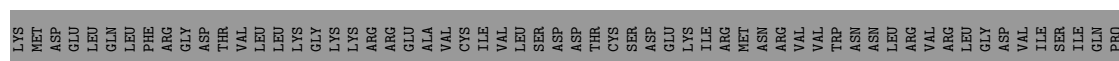
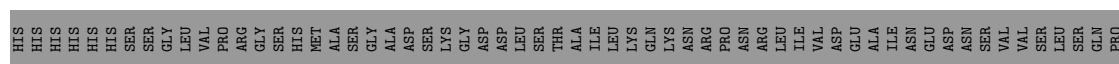




• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase





CYS	VAL	P247	C415	F516	I619	GLU
PRO	VAL	G248	A419	Y517	D627	ASP
ASP	GLU	T249	L420	G518	D630	ASP
VAL	THR		Q421	P519		PRO
LYS	ASP	T262	A422	C522		
THR	PRO	G263	I423	L526	I633	V728
GLY	SER	A264	R424	L527	L634	P729
LYS	PRO		K425	N533	R635	E730
ARG	CYS	I269	K426		P636	I731
ILE	ILE	N270	M427	F539		R732
HIS	VAL	E273	D428	I540	L639	
VAL	ALA	I274	L429	S541	Q641	D749
LEU	PRO	S282	I430	K543	L642	I752
PRO	ILE	A297	D431	E546	I643	Q764
ILE	THR	P298	L432	L547	Y644	R765
ASP	VAL	I303	E433	M550	I645	G767
ASP	HIS	D307	D434	F551	D649	F768
THR	CYS	A310	E435	F552	E650	GLY
VAL	GLU	R313	T436	G553	R651	SER
ASN	GLY	E314	I437	E554	R652	PHE
LEU	PRO	H317	D438	S555	R653	ARG
PHE	LYS	C318	A439	E556	V654	PHE
GLY	ARG	E319	E440	D577	V666	PRO
THR	GLU	R322	M441	D580	F674	SER
PRO	GLU	V325	M442	S581	K677	GLY
LEU	SER	L335	M443	K584	T688	GLM
ASN	ASN	Q337	S444	A585	Q692	GLY
ALA	V201	R338	L445	R586	R693	ALA
TYR		T347	D451	G587	L697	GLY
ARG	L213	N348	W454	N589	R700	PRO
PRO	K217	R359	L456	I590	E701	SER
ILE	E218	D368	Q458	D592	E706	GLN
ARG	E221	T385	S459	G593	I707	GLY
LYS	L222	K388	M460	G594	ARG	ARG
GLY	P223	L390	P461	A596	GLU	GLU
ASP	L224	H406	V468	A597	ARG	THR
ILE	R225	V407	E470	D598	GLN	ARG
PHE		D410	V471	R599	THR	ASN
LEU	F230	P245	P472	I601	ASN	ASP
VAL	K231		C481	L605	PRO	ASP
ARG	A232		L482	T606	ALA	ASP
GLY	I233		K486	M607	MET	LEU
GLY	G234		R487	G613	TYR	GLY
MET			E491		VAL	
ARG			M508		GLU	
ALA	R239		G513			
VAL	Y244		W514			
GLU	G245		L515			
PHE	P246					
LYS						



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	244150	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.084	Depositor
Minimum map value	-0.410	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: MG, AGS

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	0.14	0/4339	0.35	0/5855
1	B	0.14	0/4339	0.30	0/5855
1	C	0.13	0/4339	0.31	0/5855
1	D	0.17	0/4339	0.36	0/5855
1	E	0.15	0/4339	0.33	0/5855
1	F	0.13	0/4339	0.31	0/5855
All	All	0.14	0/26034	0.33	0/35130

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	599	ARG	Sidechain

### 5.2 Too-close contacts [i](#)

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



the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4269	0	4314	103	0
1	B	4269	0	4313	101	0
1	C	4269	0	4313	94	0
1	D	4269	0	4314	102	0
1	E	4269	0	4313	98	0
1	F	4269	0	4313	92	0
2	A	62	0	24	2	0
2	B	62	0	24	1	0
2	C	62	0	24	2	0
2	D	62	0	24	1	0
2	E	62	0	24	2	0
2	F	62	0	24	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	25998	0	26024	516	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 10.

The worst 5 of 516 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:TRP:HZ3	1:D:599:ARG:HB2	1.39	0.86
1:C:269:ILE:HD11	1:C:303:ILE:HG12	1.62	0.81
1:F:269:ILE:HD11	1:F:303:ILE:HG12	1.62	0.80
1:B:402:GLU:HG2	1:B:456:LEU:HD21	1.66	0.78
1:D:269:ILE:HD11	1:D:303:ILE:HG12	1.67	0.77

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	
1	A	545/822 (66%)	527 (97%)	16 (3%)	2 (0%)	30	39
1	B	545/822 (66%)	528 (97%)	16 (3%)	1 (0%)	43	56
1	C	545/822 (66%)	529 (97%)	15 (3%)	1 (0%)	43	56
1	D	545/822 (66%)	530 (97%)	14 (3%)	1 (0%)	43	56
1	E	545/822 (66%)	530 (97%)	14 (3%)	1 (0%)	43	56
1	F	545/822 (66%)	530 (97%)	14 (3%)	1 (0%)	43	56
All	All	3270/4932 (66%)	3174 (97%)	89 (3%)	7 (0%)	44	56

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	SER
1	A	297	ALA
1	B	297	ALA
1	C	297	ALA
1	D	297	ALA

### 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	455/692 (66%)	454 (100%)	1 (0%)	87	93
1	B	455/692 (66%)	455 (100%)	0	100	100
1	C	455/692 (66%)	455 (100%)	0	100	100
1	D	455/692 (66%)	452 (99%)	3 (1%)	76	85
1	E	455/692 (66%)	455 (100%)	0	100	100
1	F	455/692 (66%)	455 (100%)	0	100	100
All	All	2730/4152 (66%)	2726 (100%)	4 (0%)	87	94



All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	ASP
1	D	599	ARG
1	D	600	VAL
1	D	601	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	348	ASN
1	F	285	ASN
1	E	421	GLN
1	E	735	HIS
1	F	348	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](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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
2	AGS	B	901	3	32,33,33	0.52	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	D	902	3	32,33,33	0.50	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	E	903	3	32,33,33	0.53	1 (3%)	45,52,52	0.71	1 (2%)
2	AGS	F	904	3	32,33,33	0.50	1 (3%)	45,52,52	0.70	1 (2%)
2	AGS	E	901	3	32,33,33	0.51	1 (3%)	45,52,52	0.68	1 (2%)
2	AGS	A	902	3	32,33,33	0.52	1 (3%)	45,52,52	0.66	1 (2%)
2	AGS	A	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	C	901	3	32,33,33	0.50	0	45,52,52	0.69	1 (2%)
2	AGS	D	904	3	32,33,33	0.51	1 (3%)	45,52,52	0.66	1 (2%)
2	AGS	C	903	3	32,33,33	0.56	1 (3%)	45,52,52	0.65	1 (2%)
2	AGS	F	903	3	32,33,33	0.53	1 (3%)	45,52,52	0.72	1 (2%)
2	AGS	B	904	3	32,33,33	0.52	1 (3%)	45,52,52	0.68	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
2	AGS	B	901	3	-	9/21/38/38	0/3/3/3
2	AGS	D	902	3	-	10/21/38/38	0/3/3/3
2	AGS	E	903	3	-	4/21/38/38	0/3/3/3
2	AGS	F	904	3	-	8/21/38/38	0/3/3/3
2	AGS	E	901	3	-	9/21/38/38	0/3/3/3
2	AGS	A	902	3	-	3/21/38/38	0/3/3/3
2	AGS	A	901	3	-	10/21/38/38	0/3/3/3
2	AGS	C	901	3	-	8/21/38/38	0/3/3/3
2	AGS	D	904	3	-	3/21/38/38	0/3/3/3
2	AGS	C	903	3	-	0/21/38/38	0/3/3/3
2	AGS	F	903	3	-	3/21/38/38	0/3/3/3
2	AGS	B	904	3	-	3/21/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	903	AGS	PG-S1G	2.09	1.95	1.90
2	C	903	AGS	PG-S1G	2.08	1.95	1.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	AGS	PG-S1G	2.06	1.95	1.90
2	A	902	AGS	PG-S1G	2.06	1.95	1.90
2	B	904	AGS	PG-S1G	2.05	1.95	1.90

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	903	AGS	PB-O3B-PG	-3.95	118.71	133.17
2	F	904	AGS	PB-O3B-PG	-3.89	118.93	133.17
2	E	903	AGS	PB-O3B-PG	-3.87	119.00	133.17
2	C	901	AGS	PB-O3B-PG	-3.87	119.00	133.17
2	B	901	AGS	PB-O3B-PG	-3.82	119.19	133.17

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	AGS	PB-O3B-PG-O2G
2	A	901	AGS	C5'-O5'-PA-O2A
2	A	901	AGS	C5'-O5'-PA-O3A
2	A	901	AGS	O4'-C4'-C5'-O5'
2	A	902	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

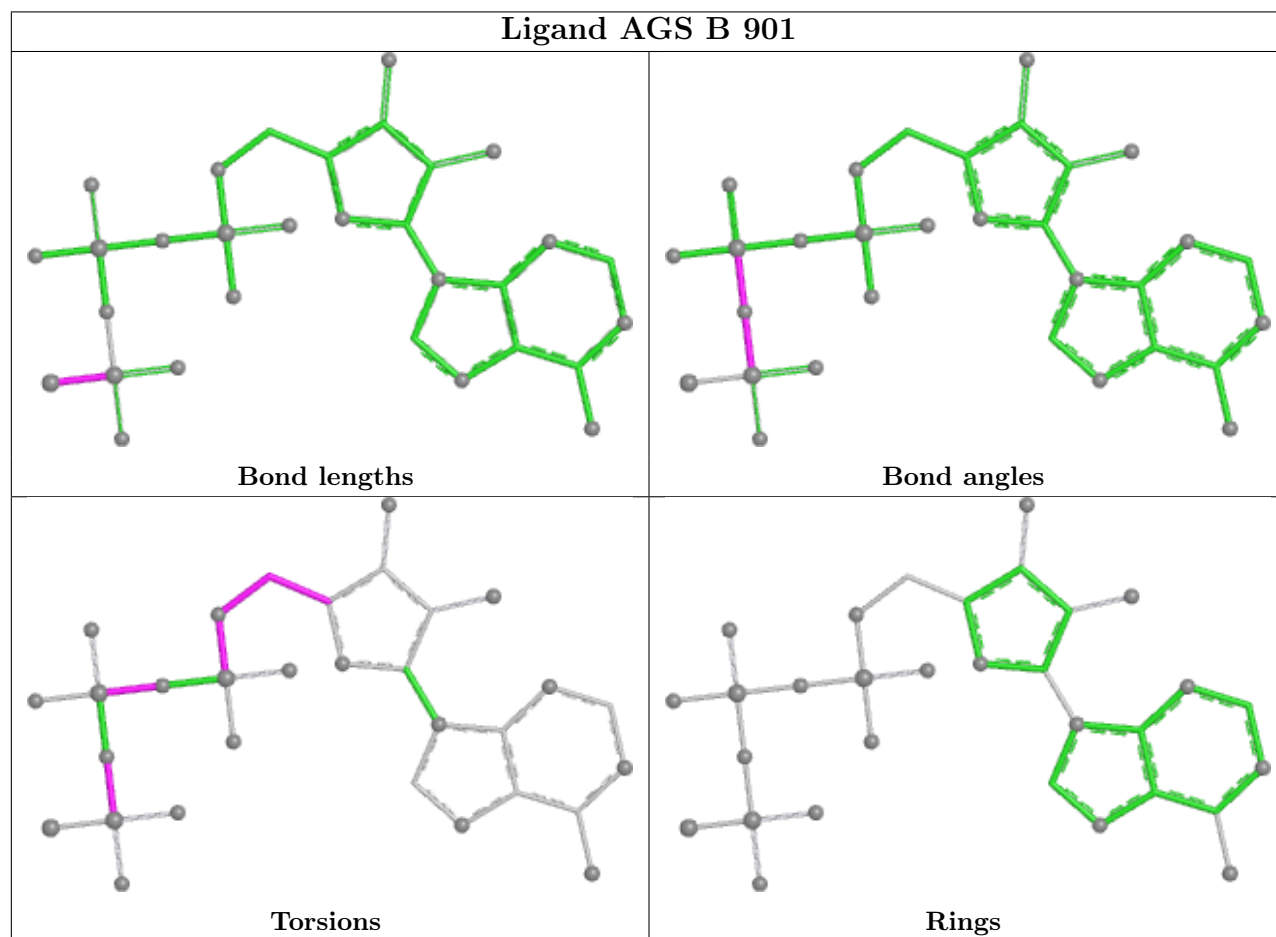
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	903	AGS	2	0
2	A	902	AGS	2	0
2	D	904	AGS	1	0
2	C	903	AGS	2	0
2	F	903	AGS	2	0
2	B	904	AGS	1	0

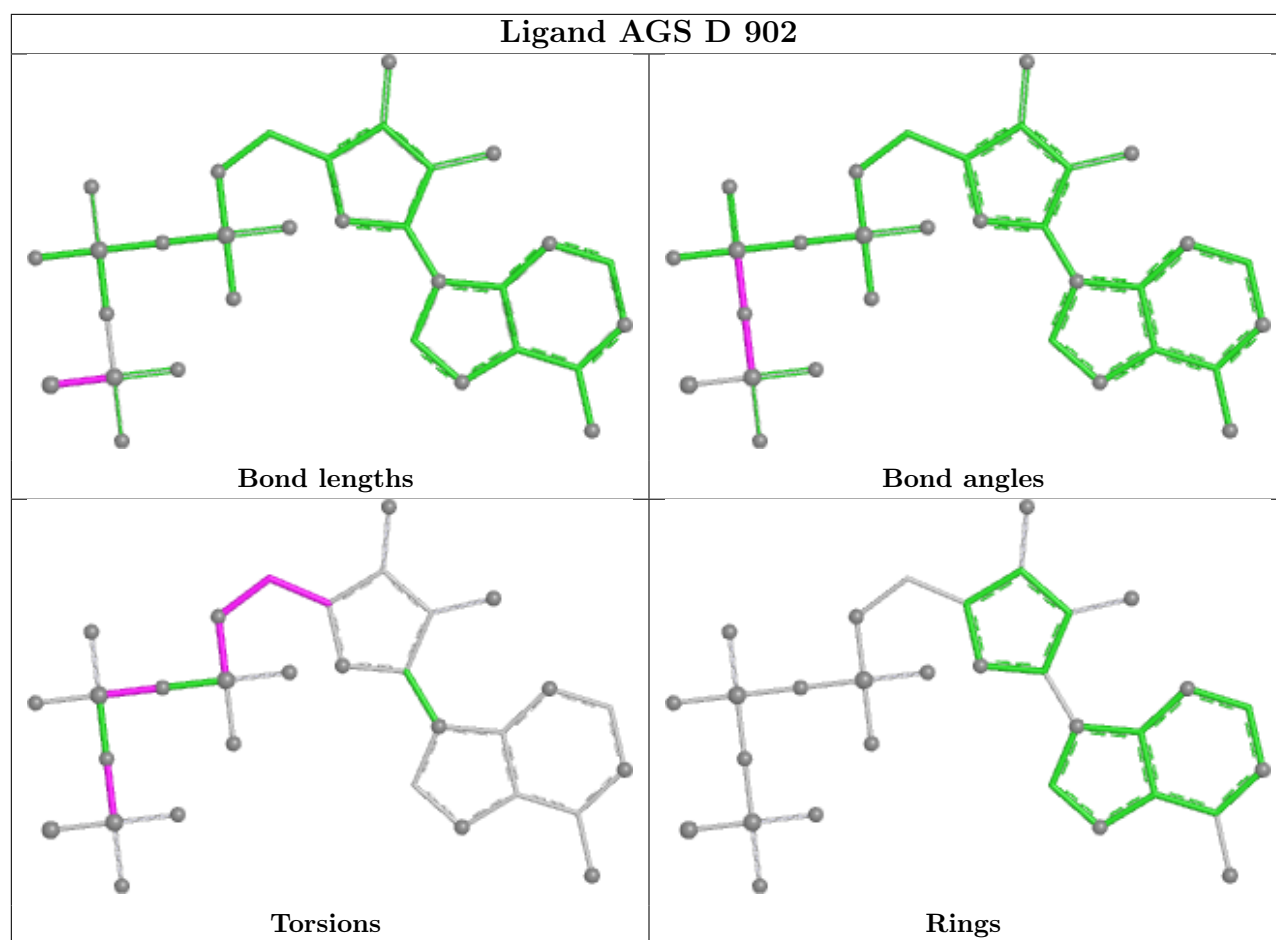
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the



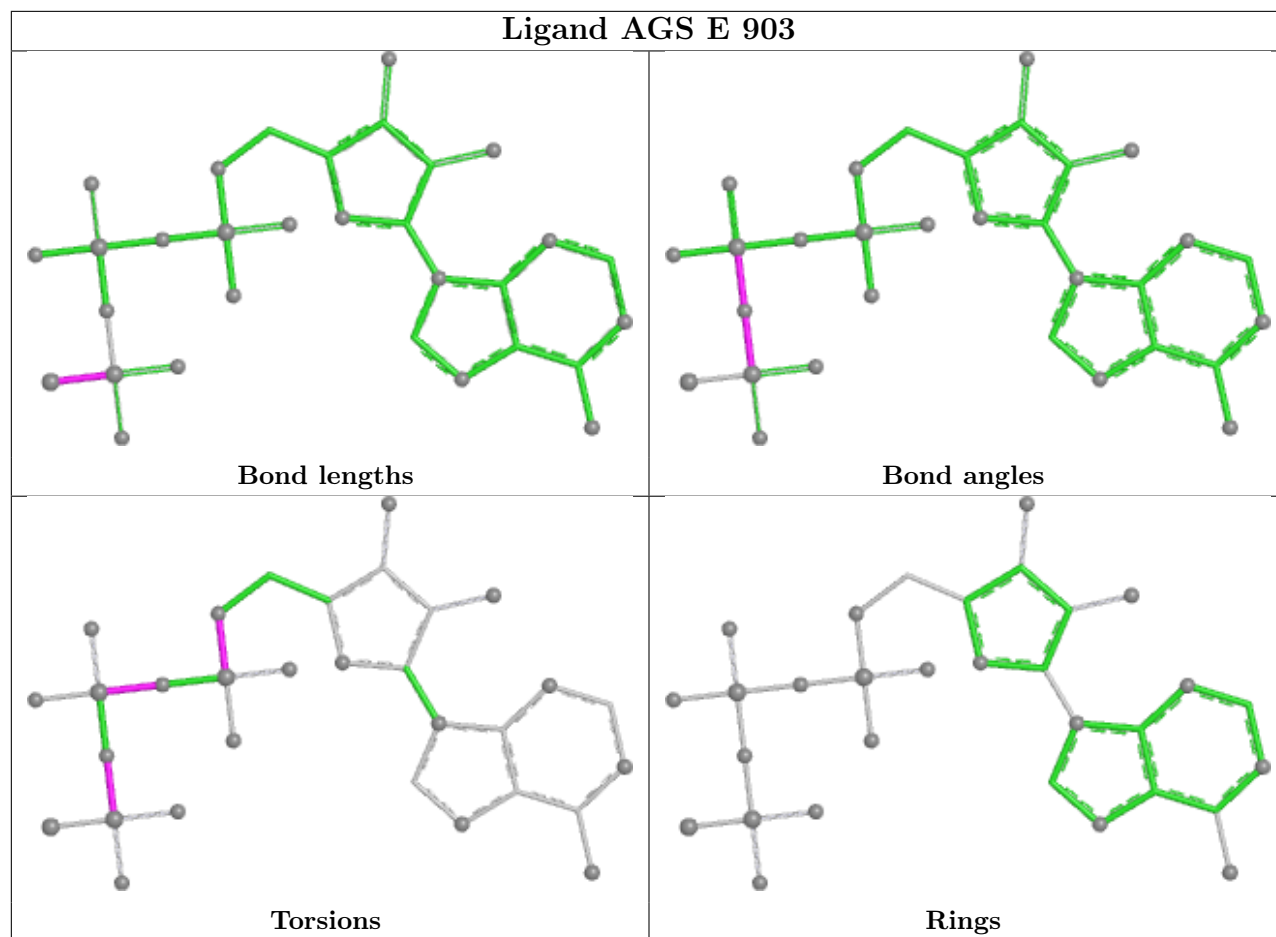
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



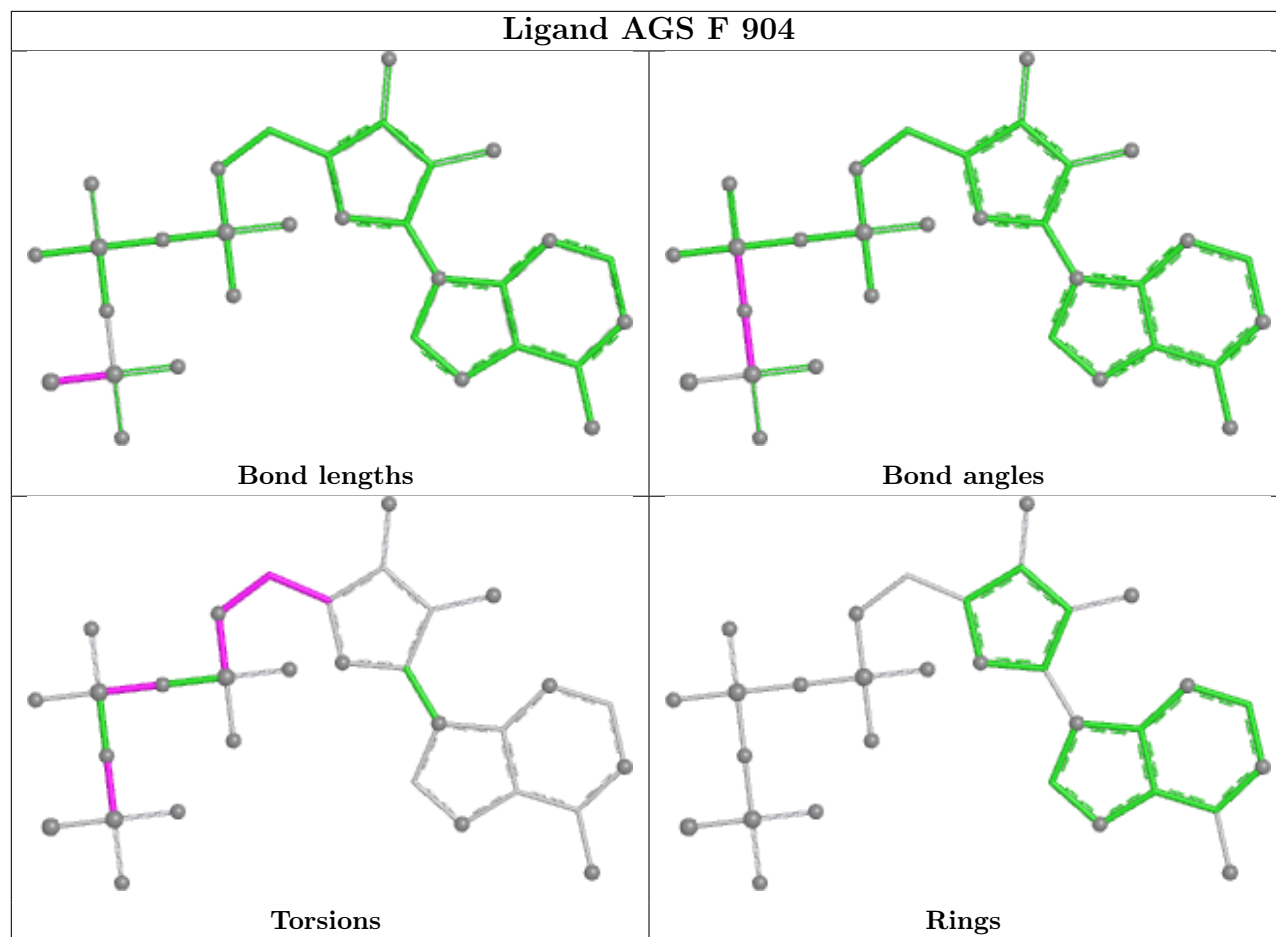




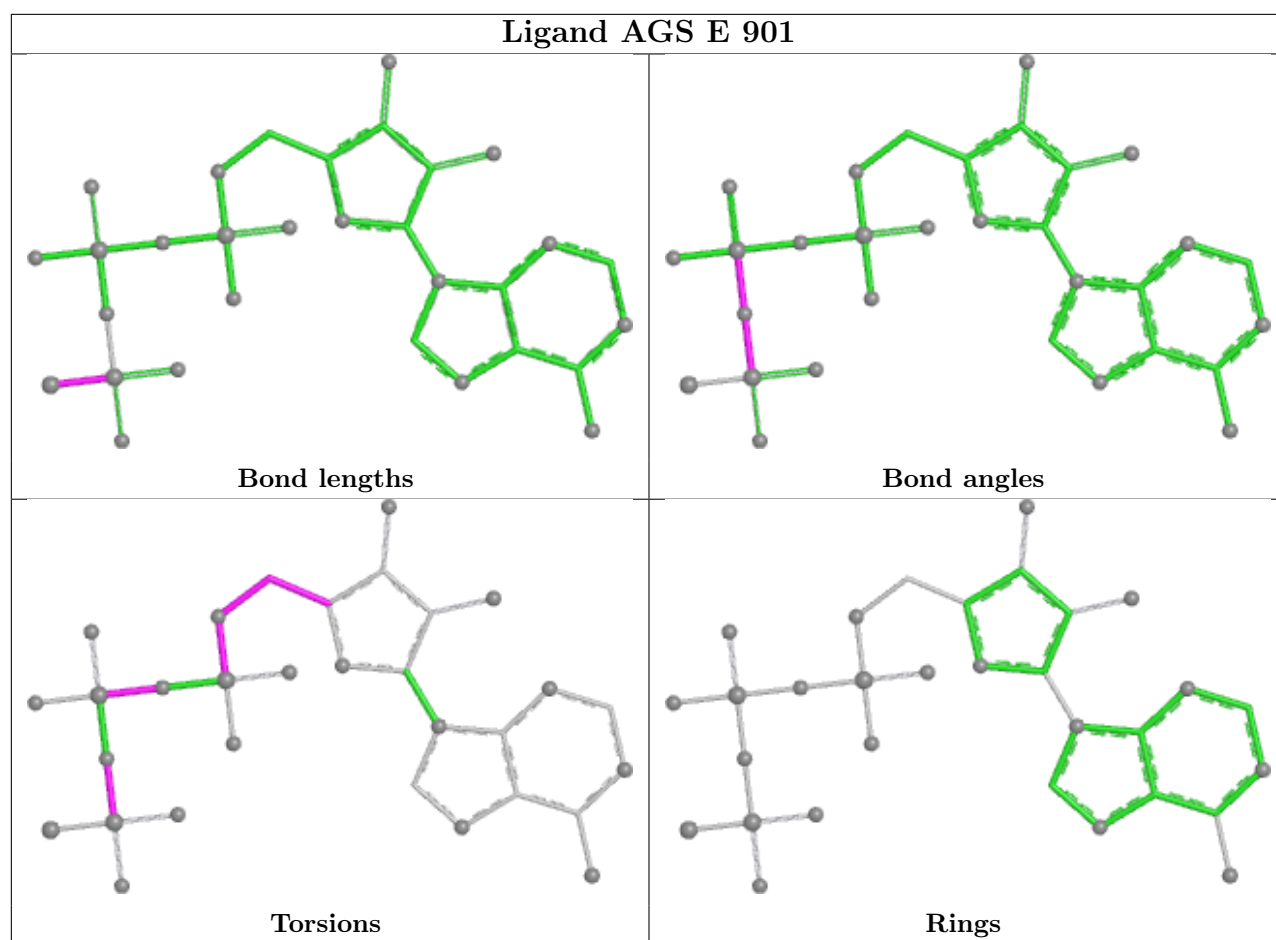




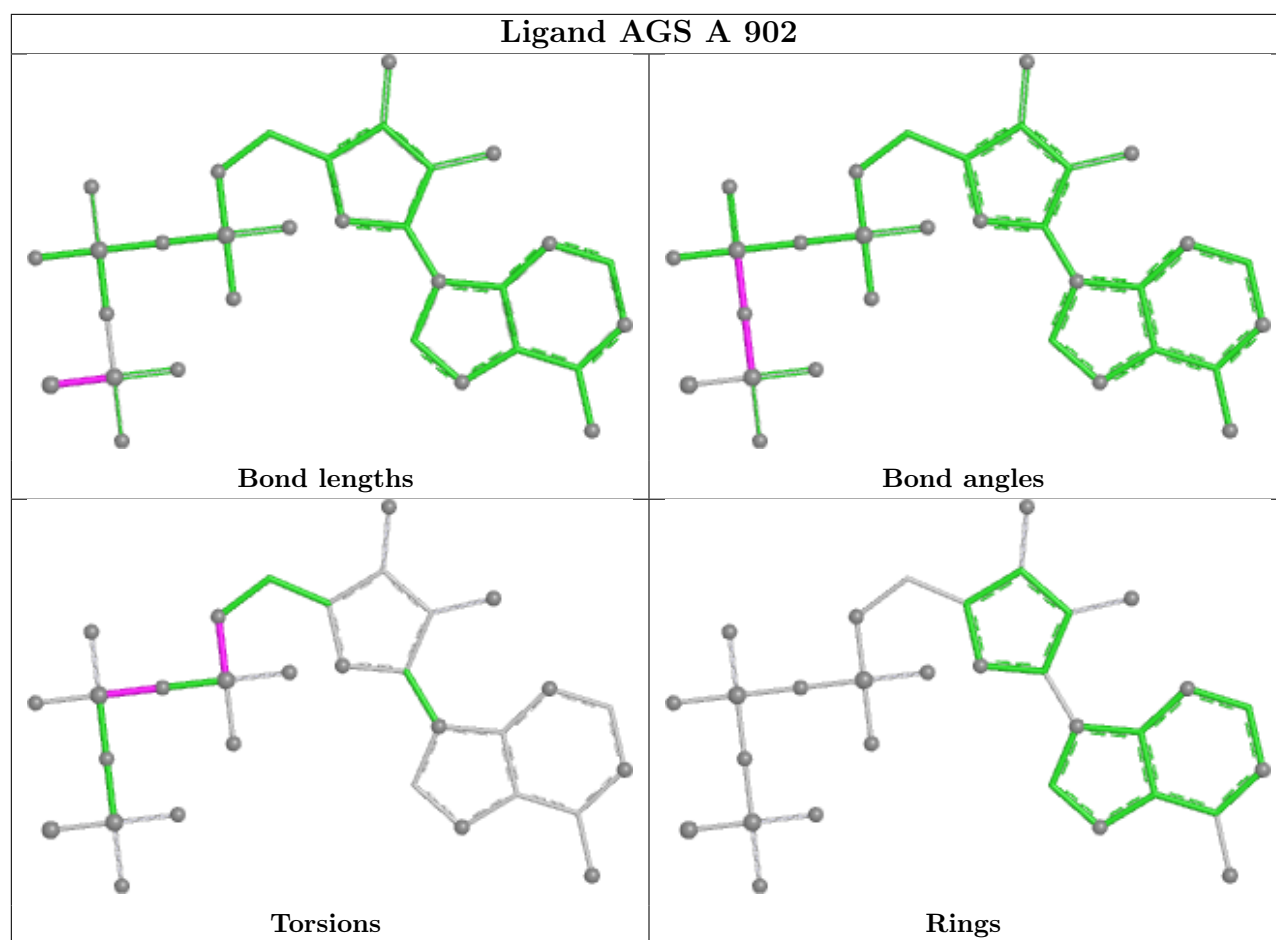




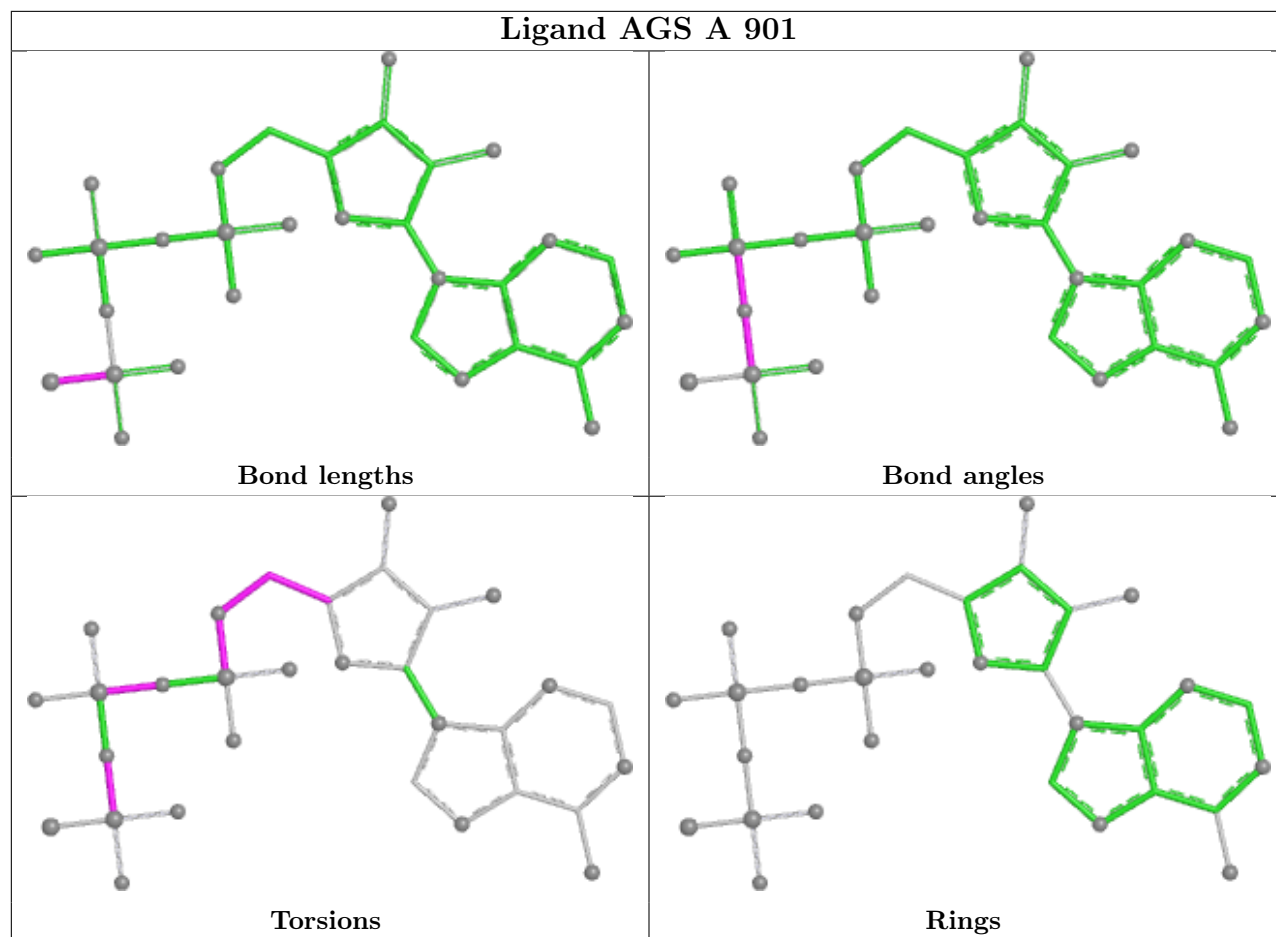




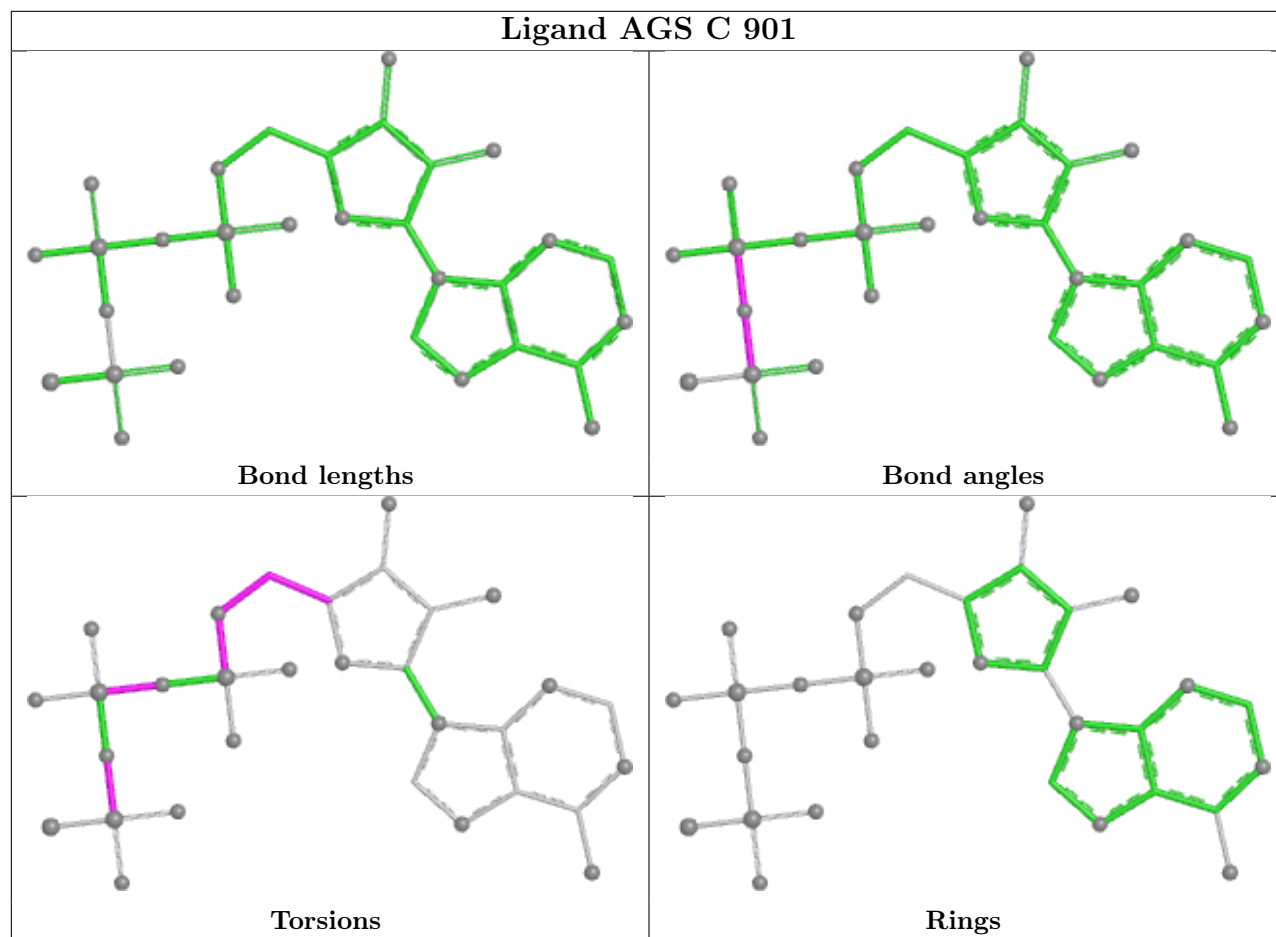




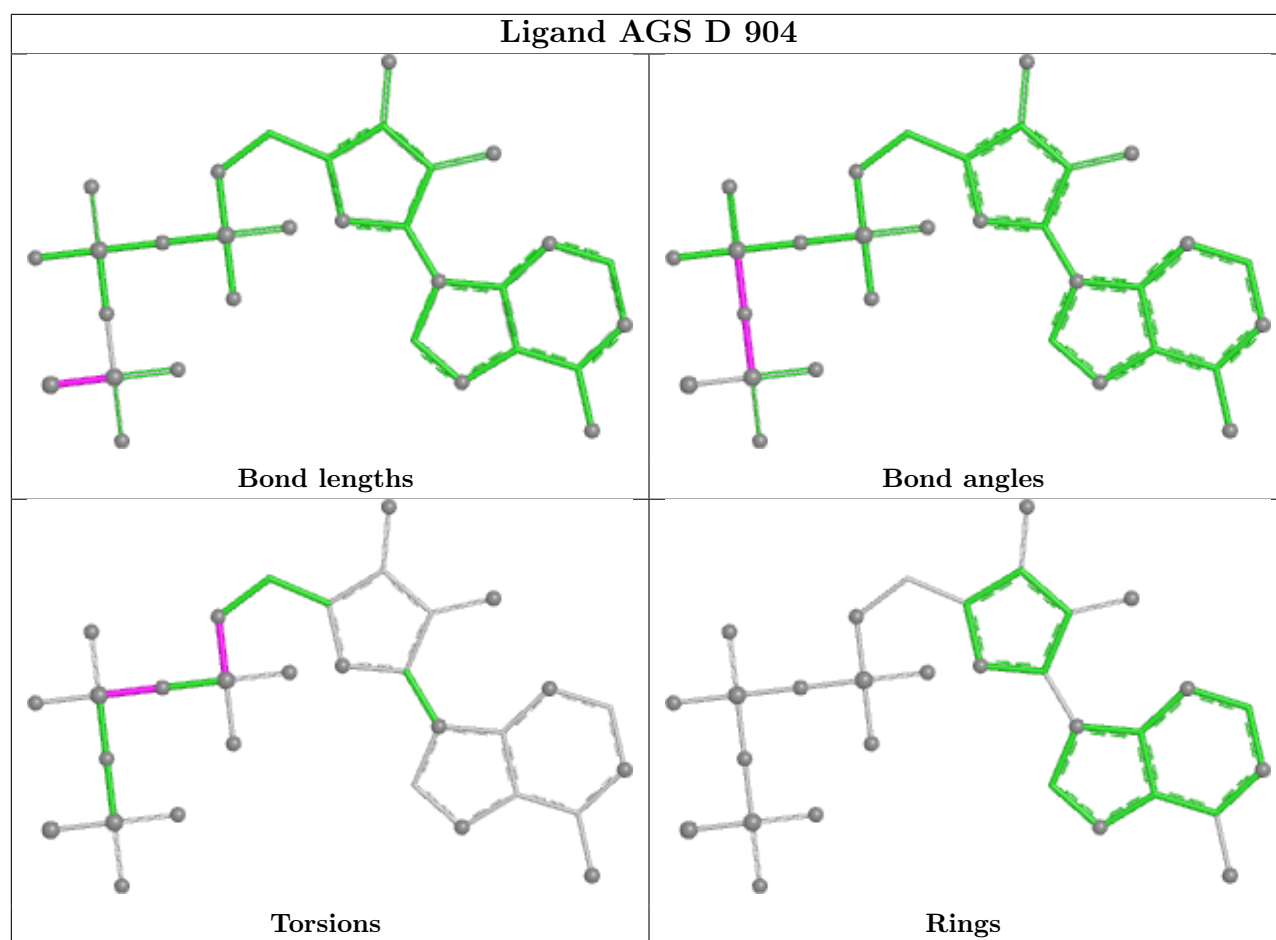




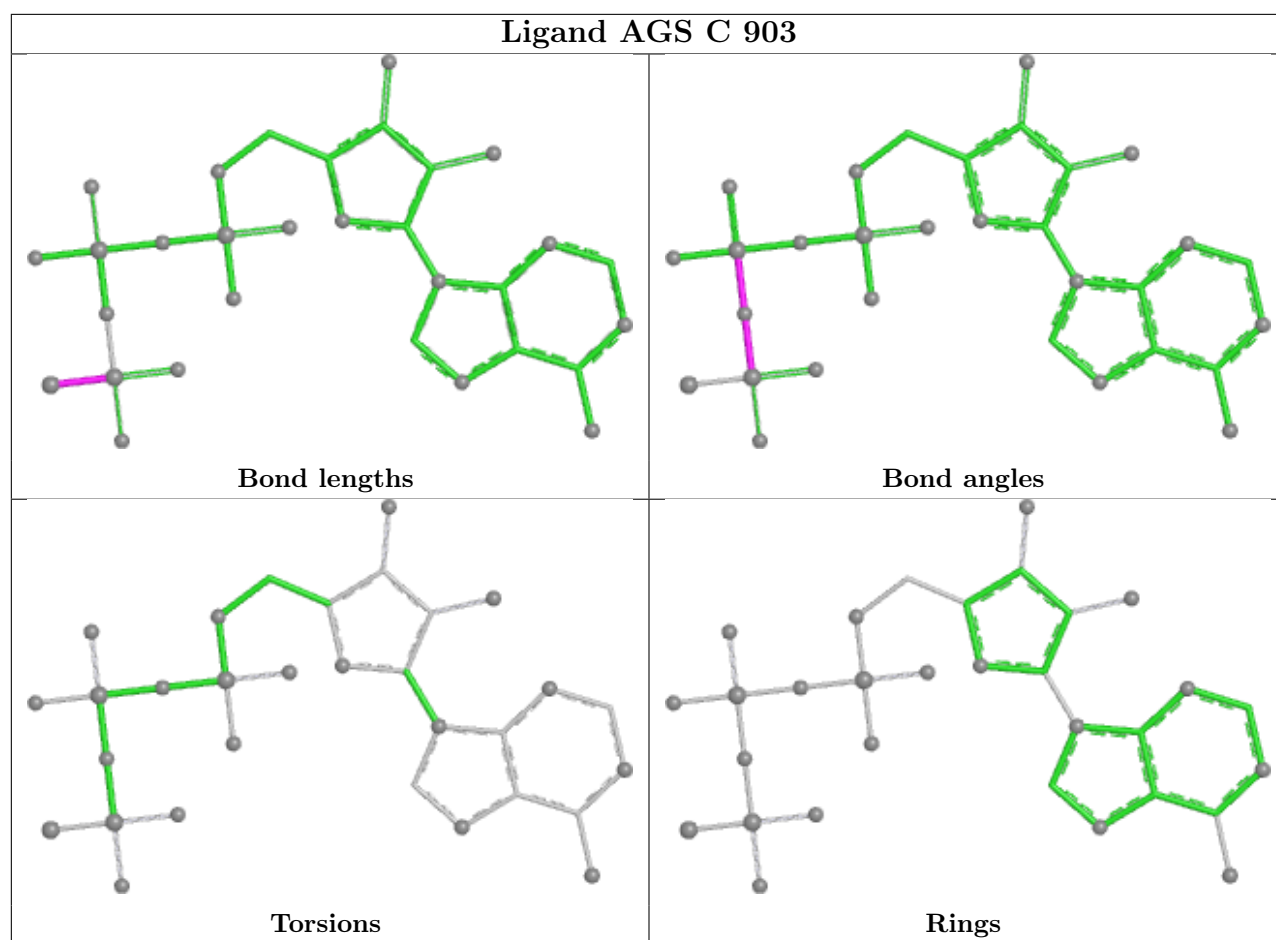






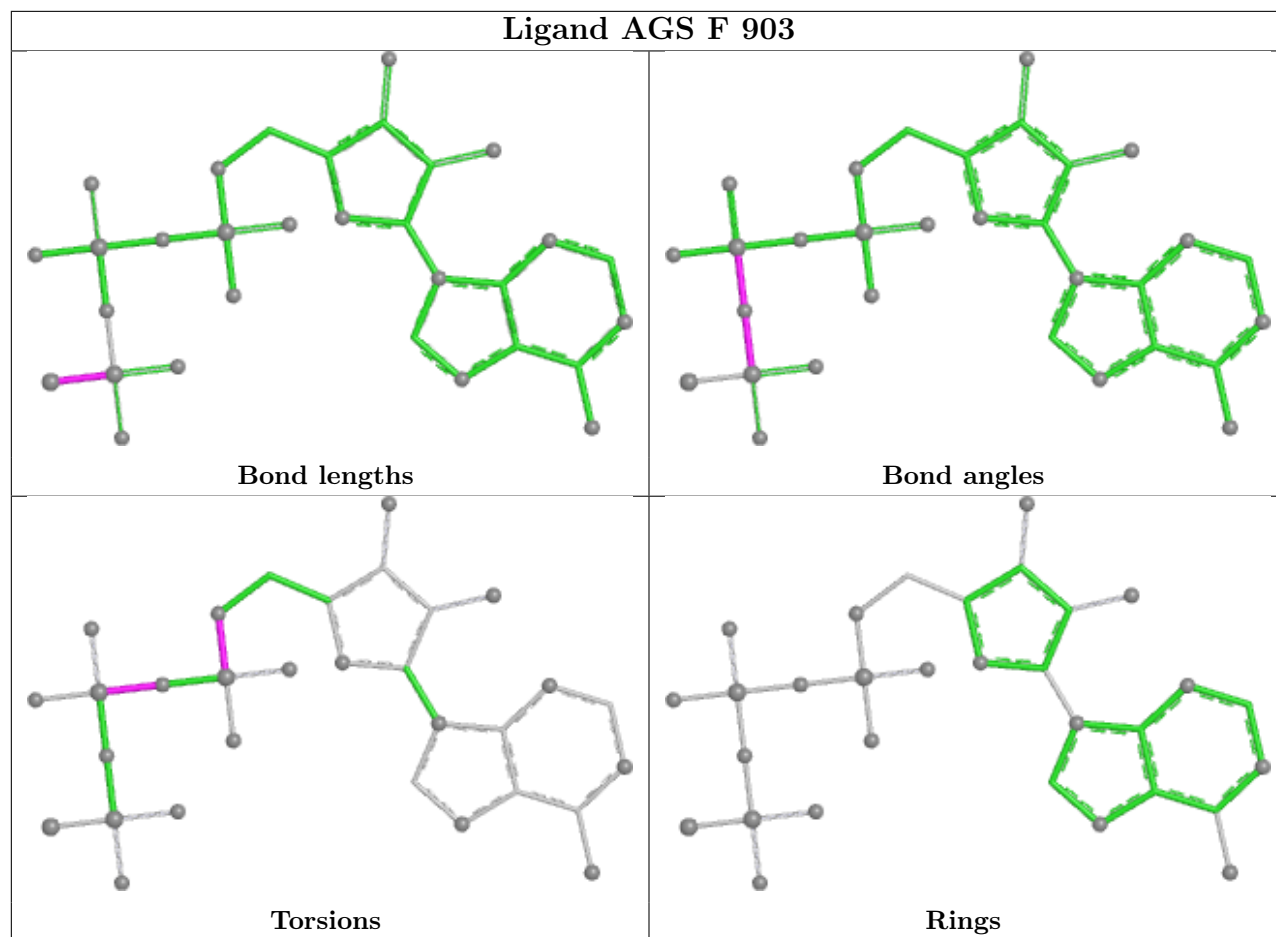




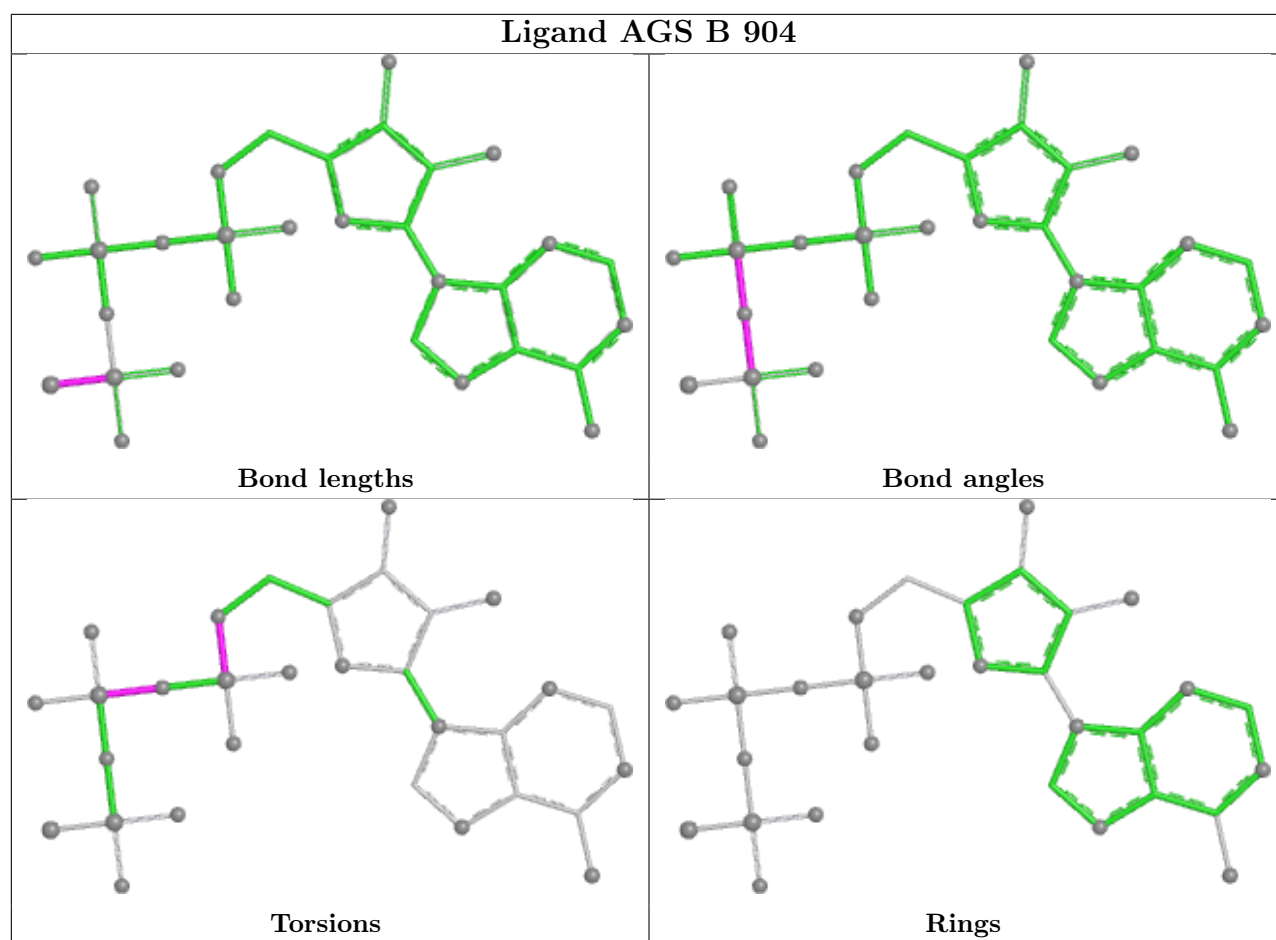




## Ligand AGS F 903







## 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.



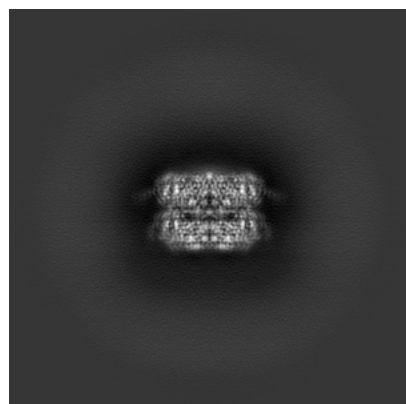
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72384. These allow visual inspection of the internal detail of the map and identification of artifacts.

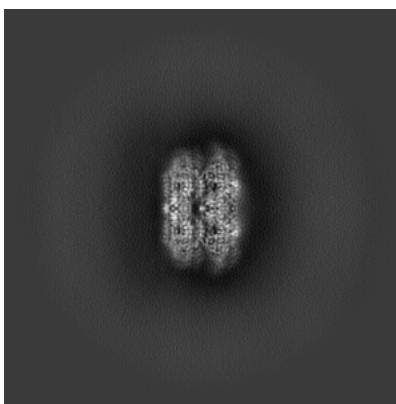
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

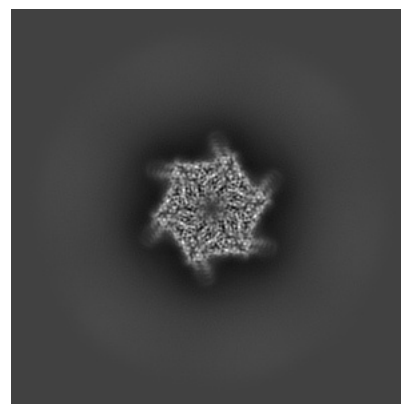
#### 6.1.1 Primary map



X

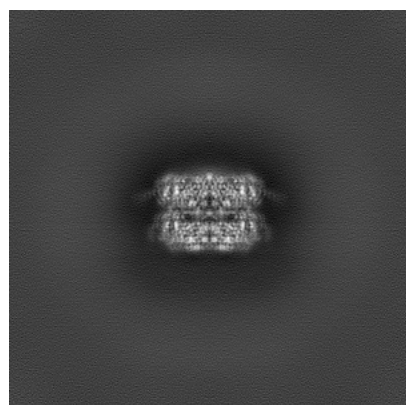


Y

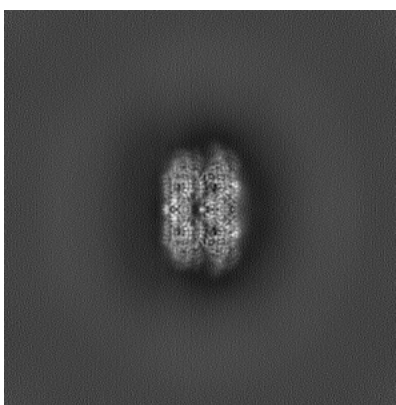


Z

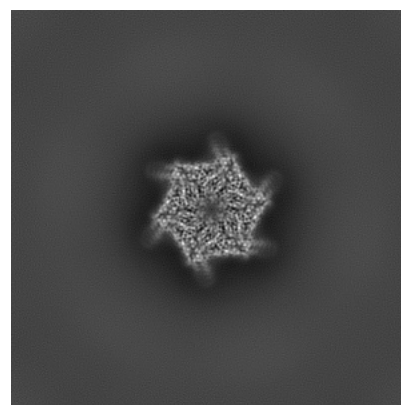
#### 6.1.2 Raw map



X



Y



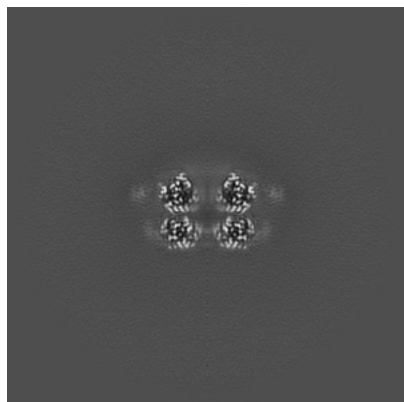
Z

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

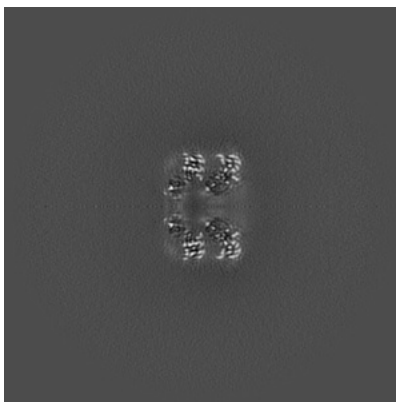


## 6.2 Central slices [i](#)

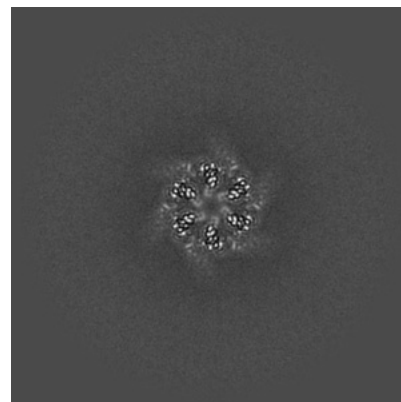
### 6.2.1 Primary map



X Index: 200

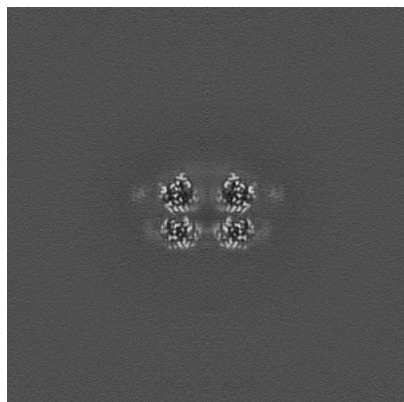


Y Index: 200

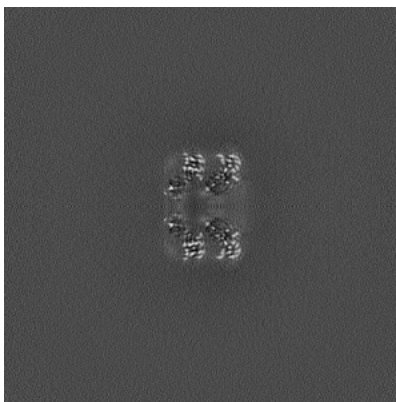


Z Index: 200

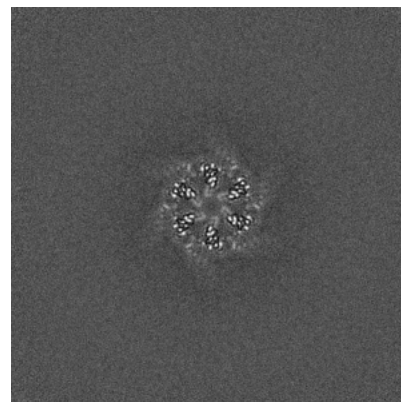
### 6.2.2 Raw map



X Index: 200



Y Index: 200



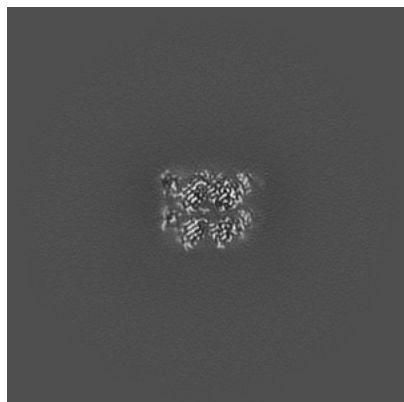
Z Index: 200

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

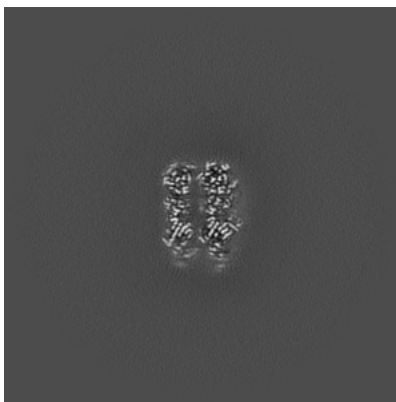


## 6.3 Largest variance slices [i](#)

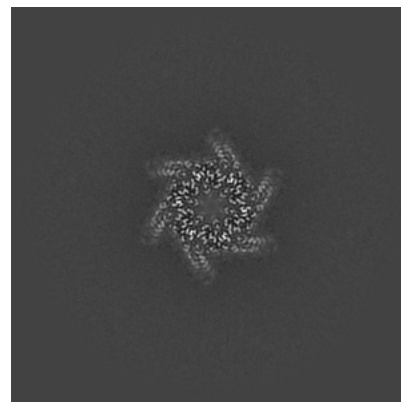
### 6.3.1 Primary map



X Index: 228

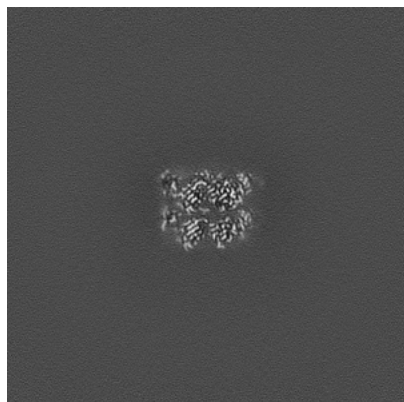


Y Index: 182

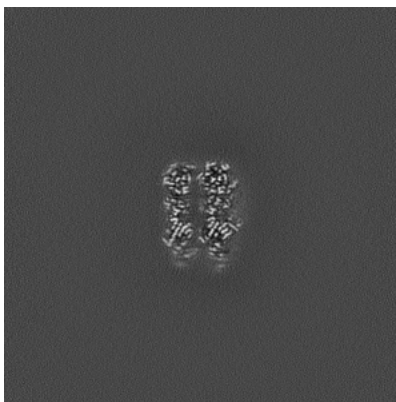


Z Index: 217

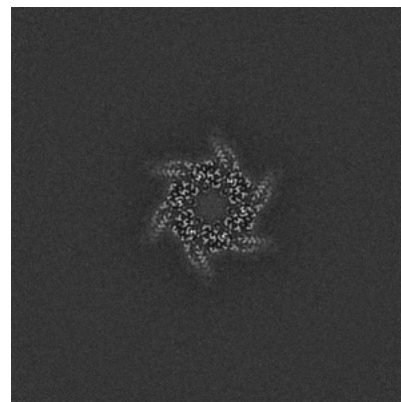
### 6.3.2 Raw map



X Index: 228



Y Index: 182



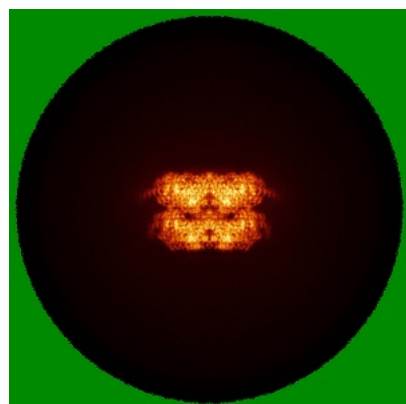
Z Index: 218

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

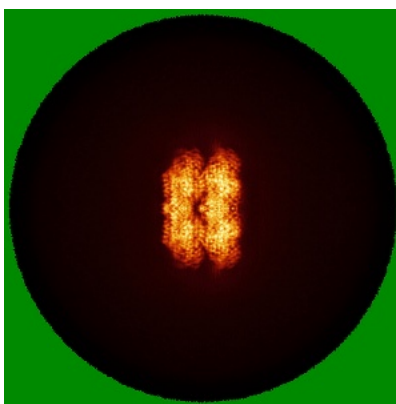


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

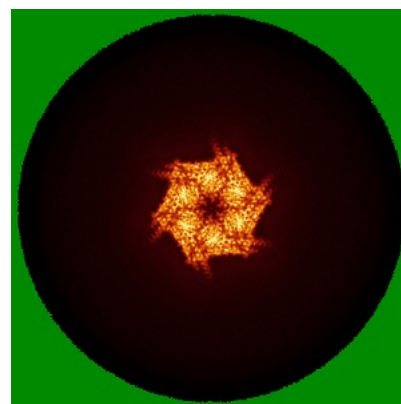
### 6.4.1 Primary map



X

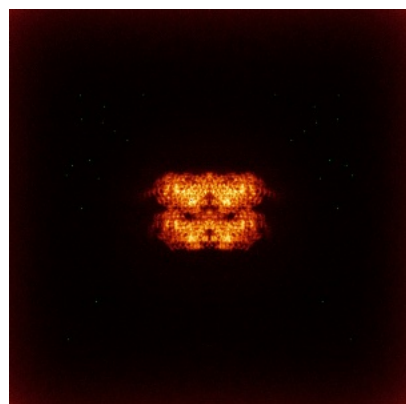


Y

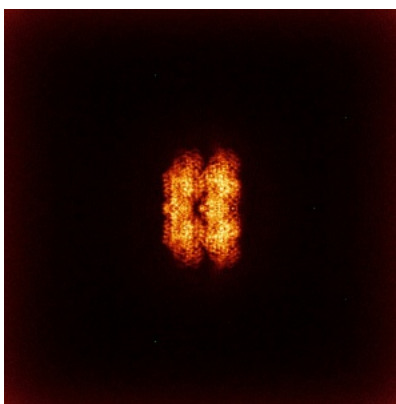


Z

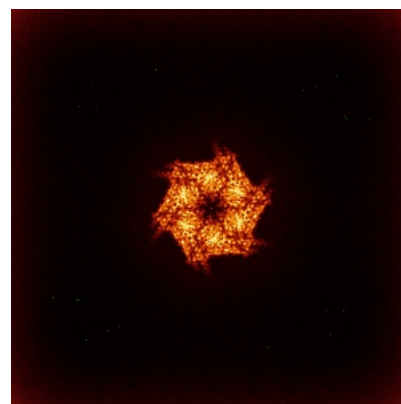
### 6.4.2 Raw map



X



Y



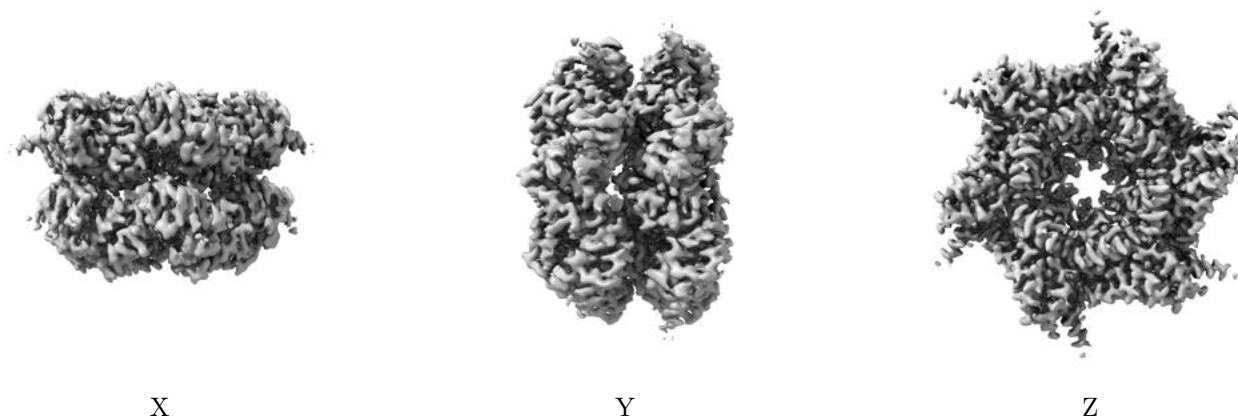
Z

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.



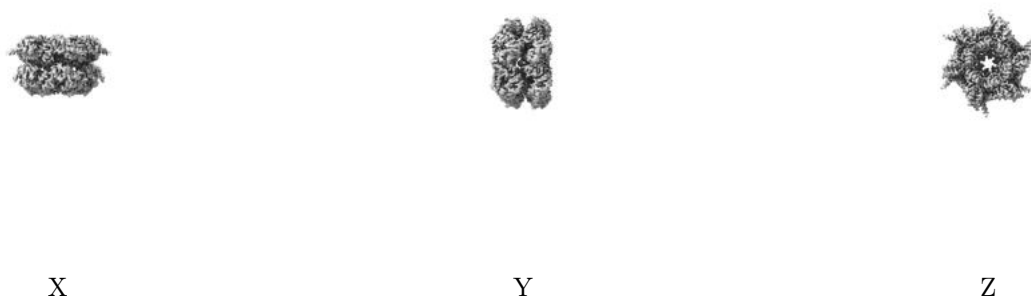
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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](#)

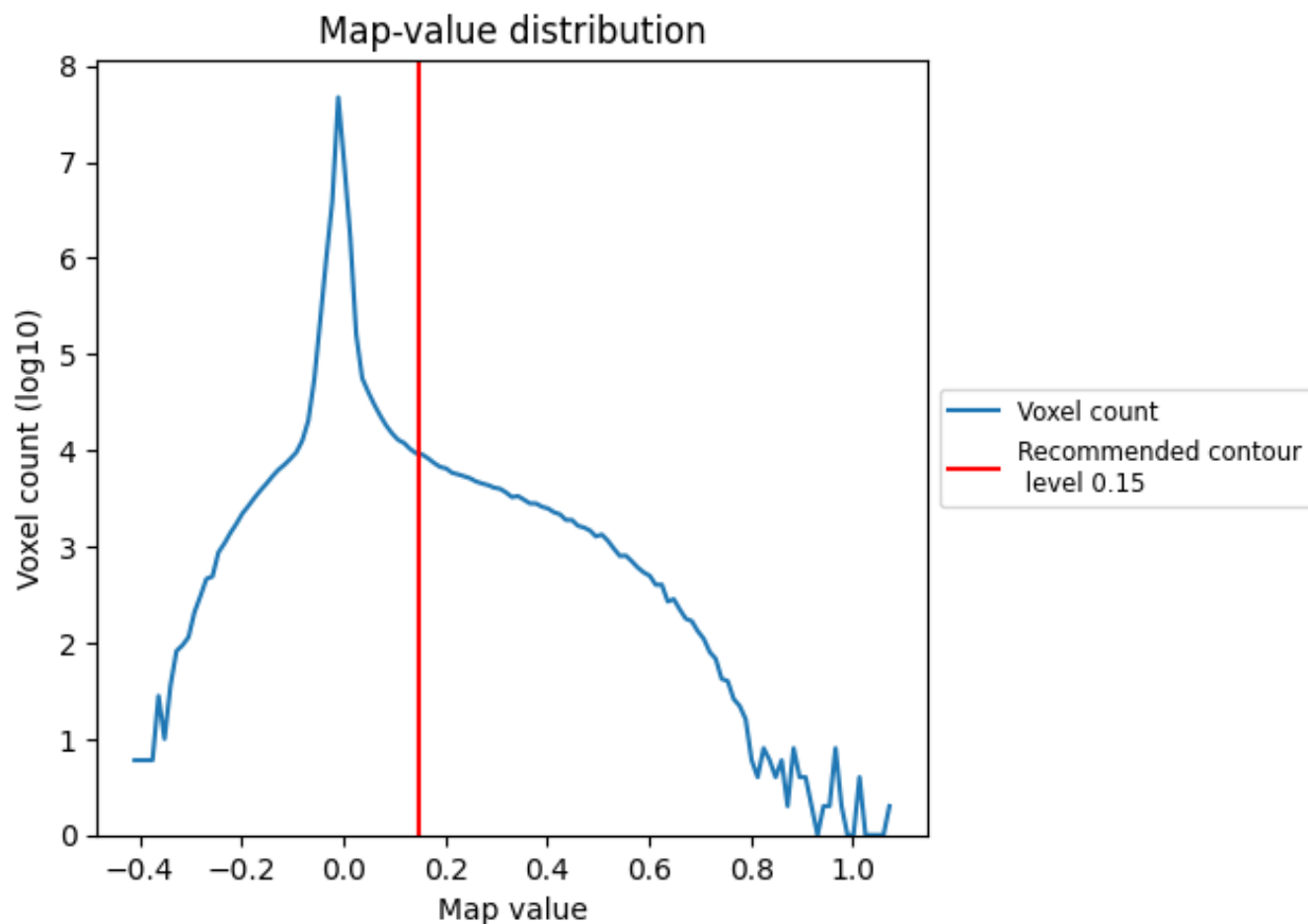
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

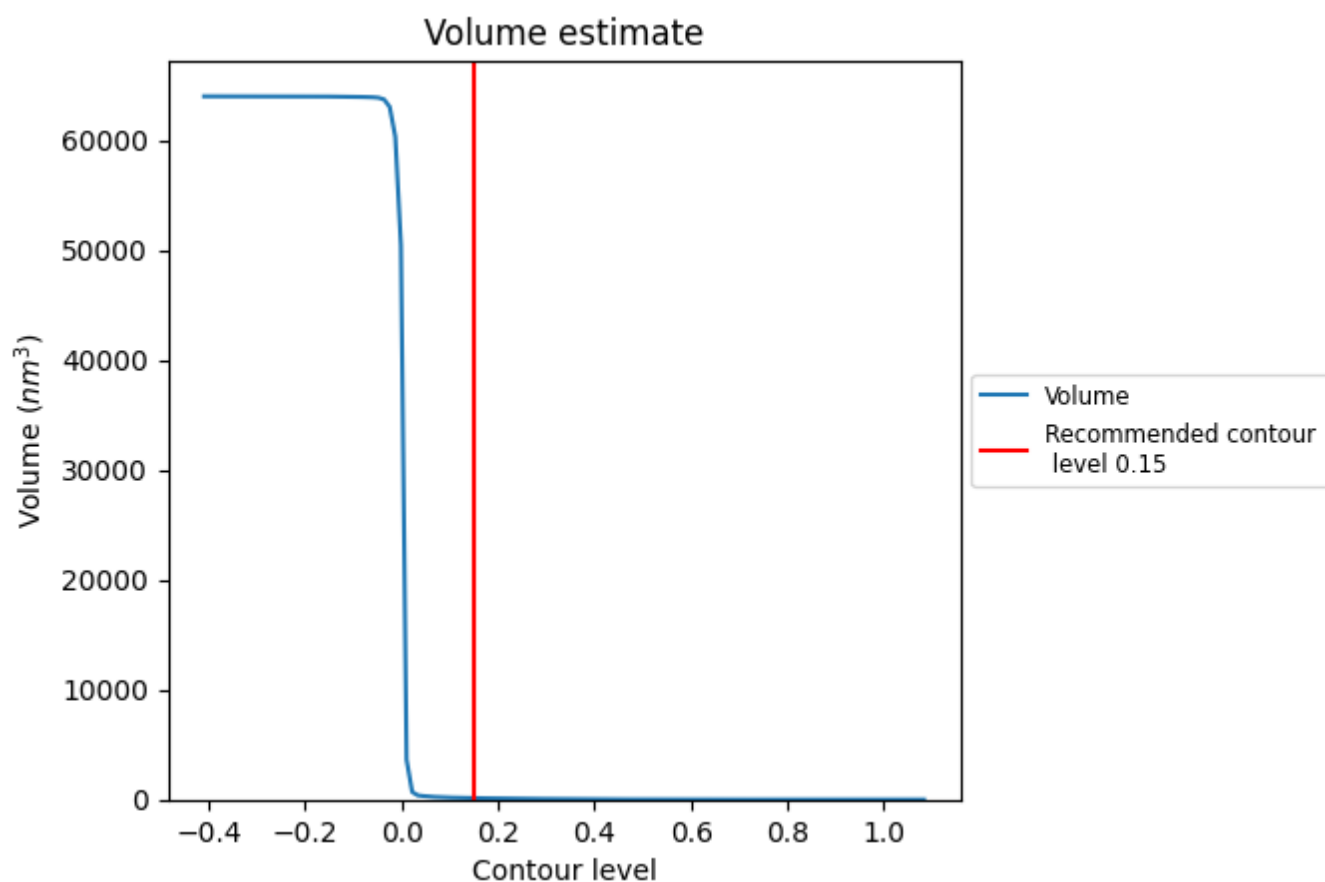
### 7.1 Map-value distribution [i](#)



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](#)

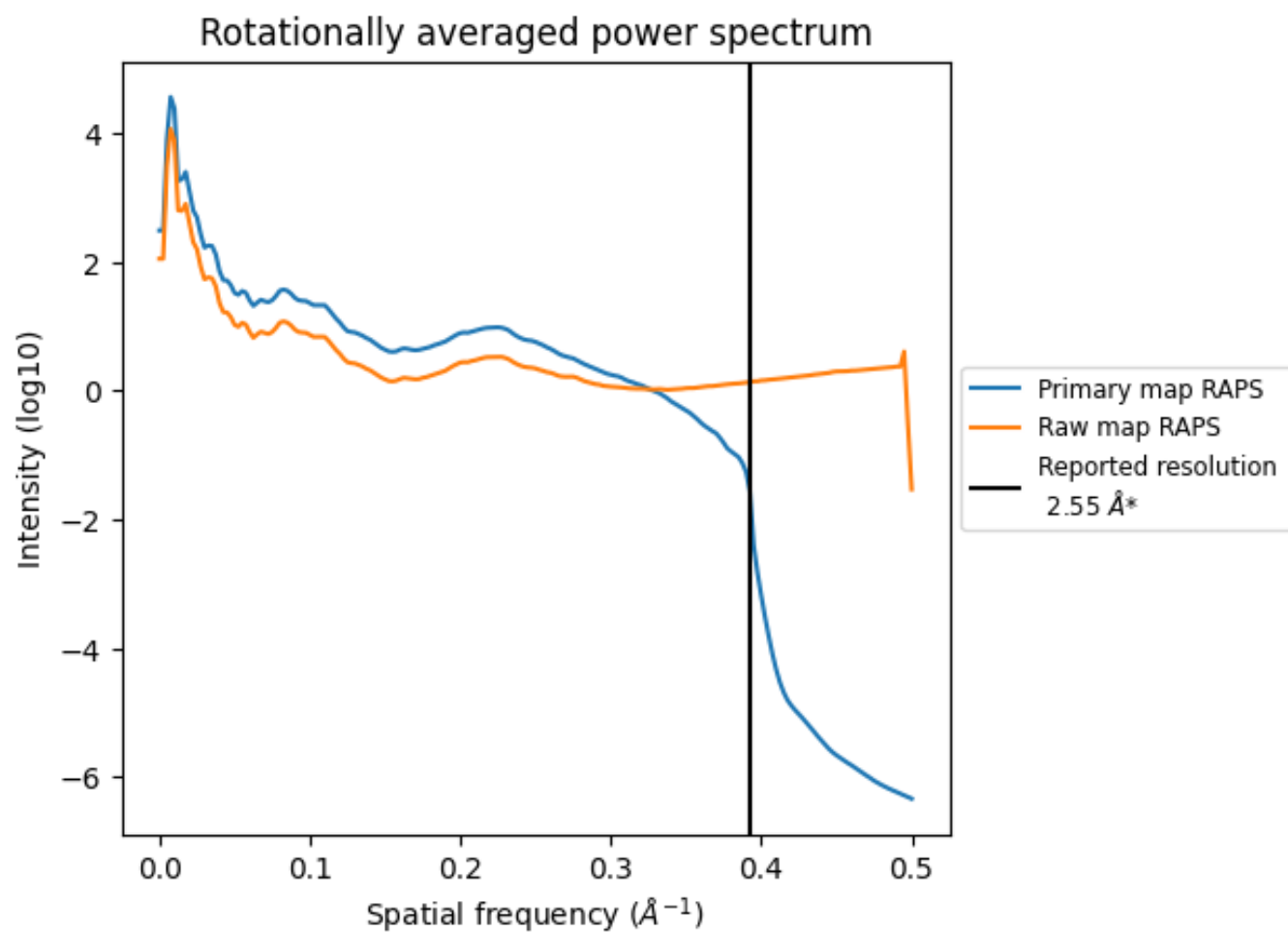


The volume at the recommended contour level is 134 nm<sup>3</sup>; this corresponds to an approximate mass of 121 kDa.

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 ⓘ



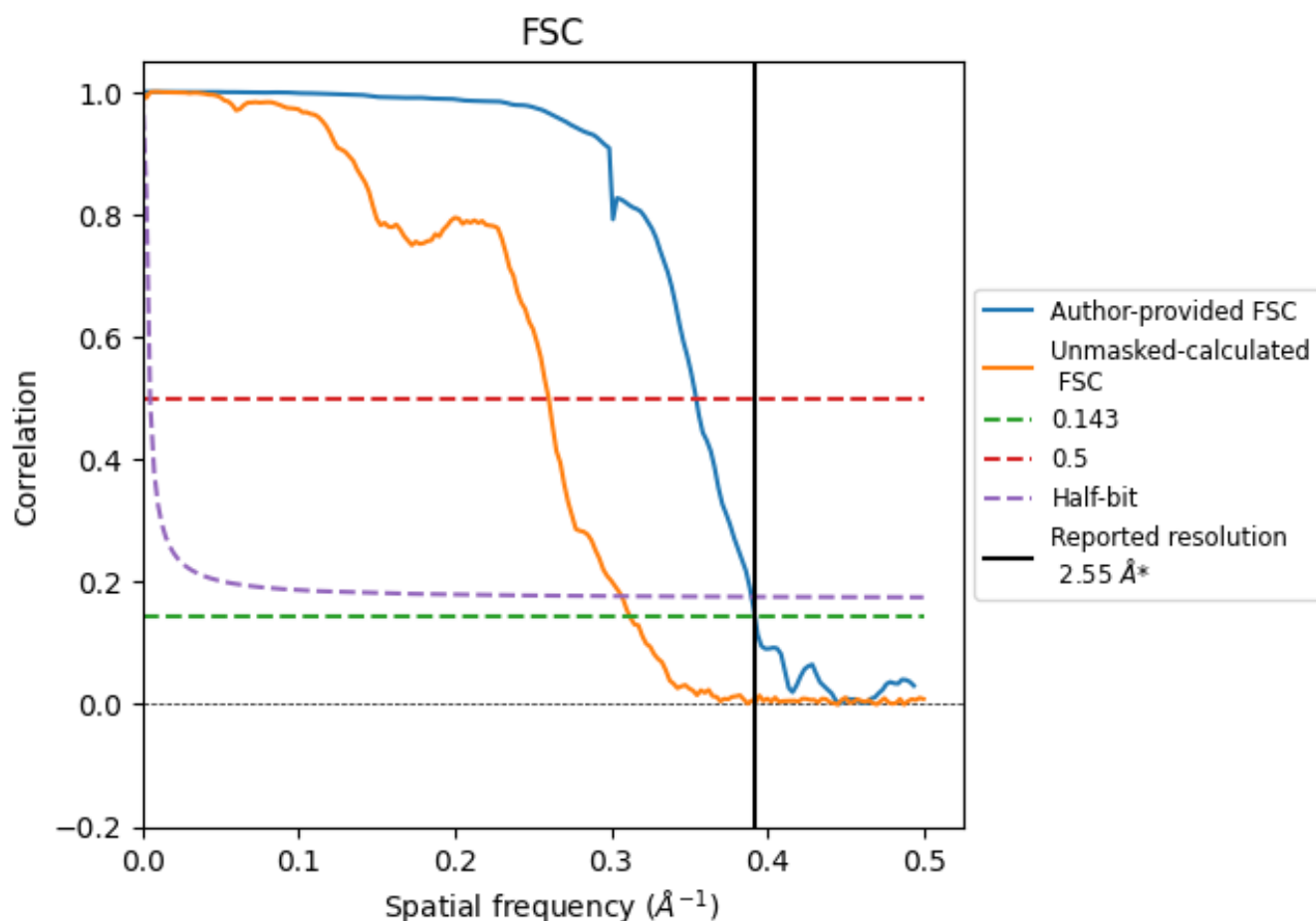
\*Reported resolution corresponds to spatial frequency of 0.392 Å<sup>-1</sup>



## 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  $0.392 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.82	2.57
Unmasked-calculated*	3.20	3.85	3.26

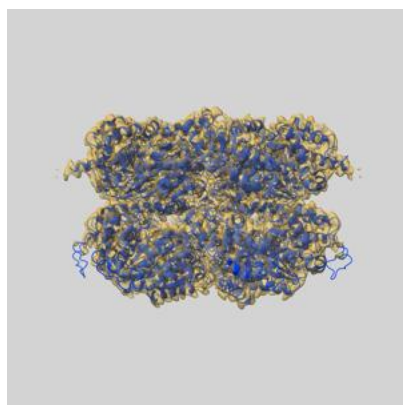
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.55 by more than 10 %



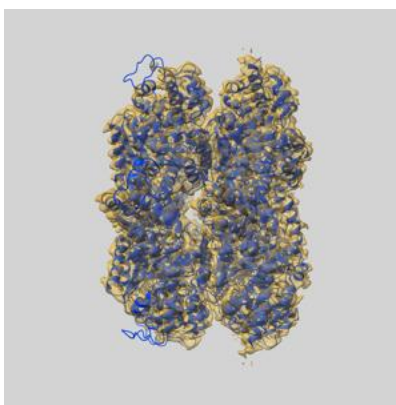
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72384 and PDB model 9Y04. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

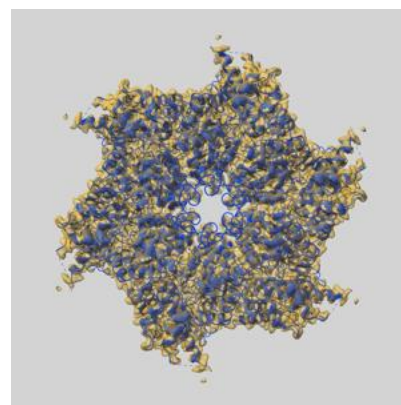
### 9.1 Map-model overlay [i](#)



X



Y

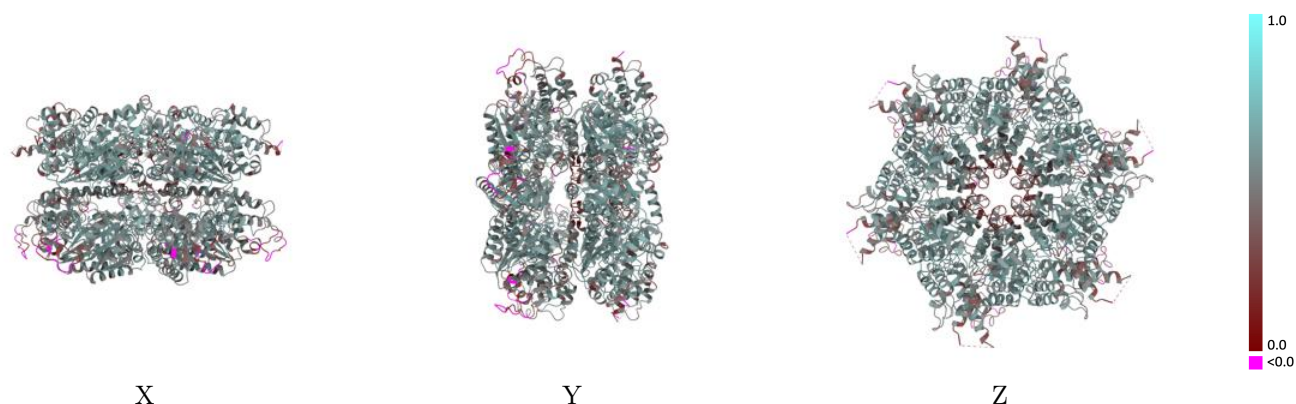


Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

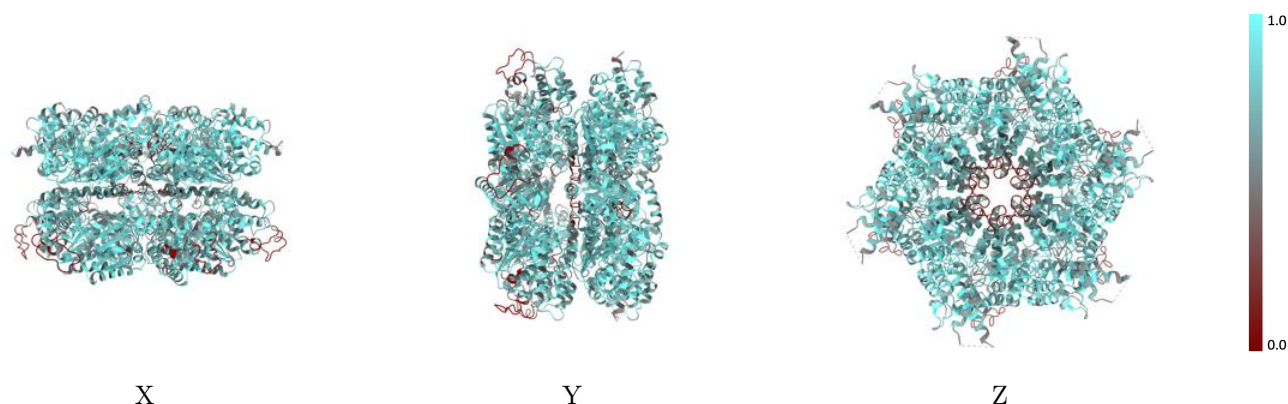


## 9.2 Q-score mapped to coordinate model [i](#)



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.

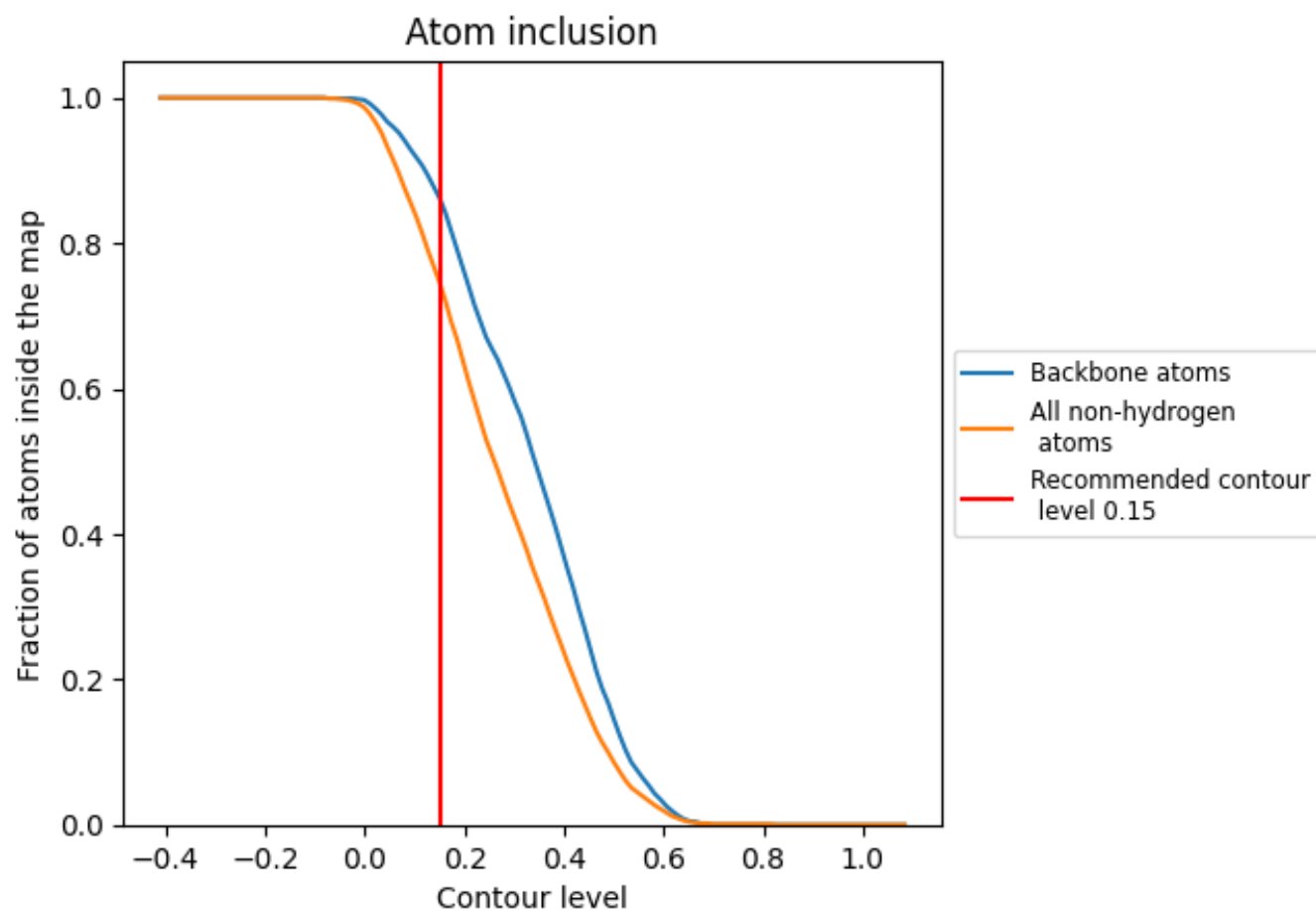
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.15).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7460</div>	<div><div></div>0.5060</div>
A	<div><div></div>0.7480</div>	<div><div></div>0.5040</div>
B	<div><div></div>0.7460</div>	<div><div></div>0.5060</div>
C	<div><div></div>0.7450</div>	<div><div></div>0.5060</div>
D	<div><div></div>0.7470</div>	<div><div></div>0.5050</div>
E	<div><div></div>0.7460</div>	<div><div></div>0.5080</div>
F	<div><div></div>0.7460</div>	<div><div></div>0.5070</div>

1.0

0.0

<0.0