



## wwPDB EM Validation Summary Report ⓘ

Mar 3, 2025 – 07:42 PM JST

PDB ID : 8X4C  
EMDB ID : EMD-38046  
Title : Cryo-EM structure of Ryanodine receptor 1 (20 uM Ca<sup>2+</sup>, 2 mM ATP)  
Authors : Chen, Q.; Hu, H.  
Deposited on : 2023-11-15  
Resolution : 3.80 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.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

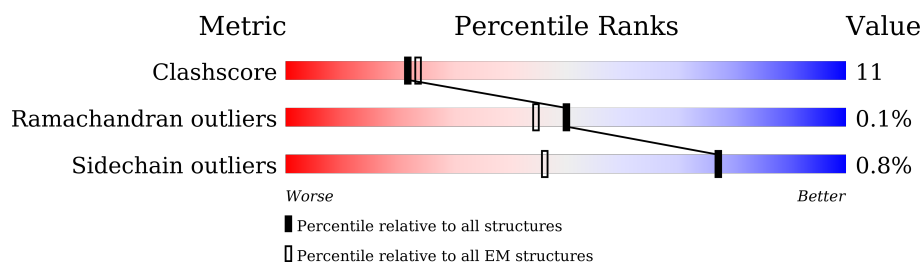
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	5037	49% 14% 37%
1	B	5037	49% 14% 37%
1	C	5037	49% 14% 37%
1	D	5037	49% 13% 37%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	5101	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	B	5101	-	-	X	-
2	ATP	D	5101	-	-	X	-

## 2 Entry composition [i](#)

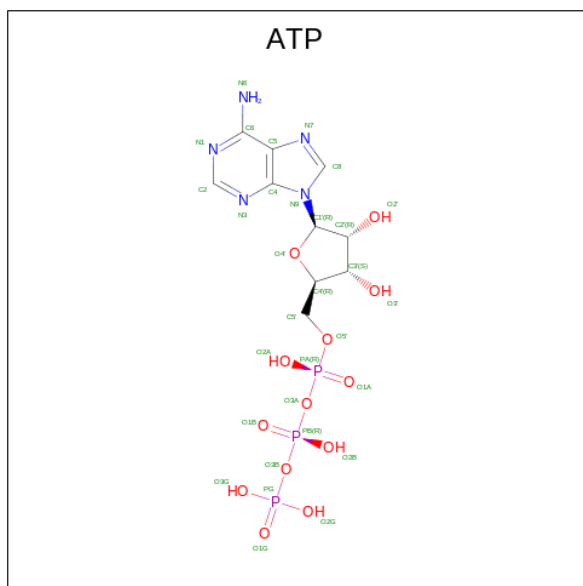
There are 3 unique types of molecules in this entry. The entry contains 95168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3155	Total	C	N	O	S	0	0
			23760	15222	4111	4274	153		
1	B	3155	Total	C	N	O	S	0	0
			23760	15222	4111	4274	153		
1	C	3155	Total	C	N	O	S	0	0
			23760	15222	4111	4274	153		
1	D	3155	Total	C	N	O	S	0	0
			23760	15222	4111	4274	153		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

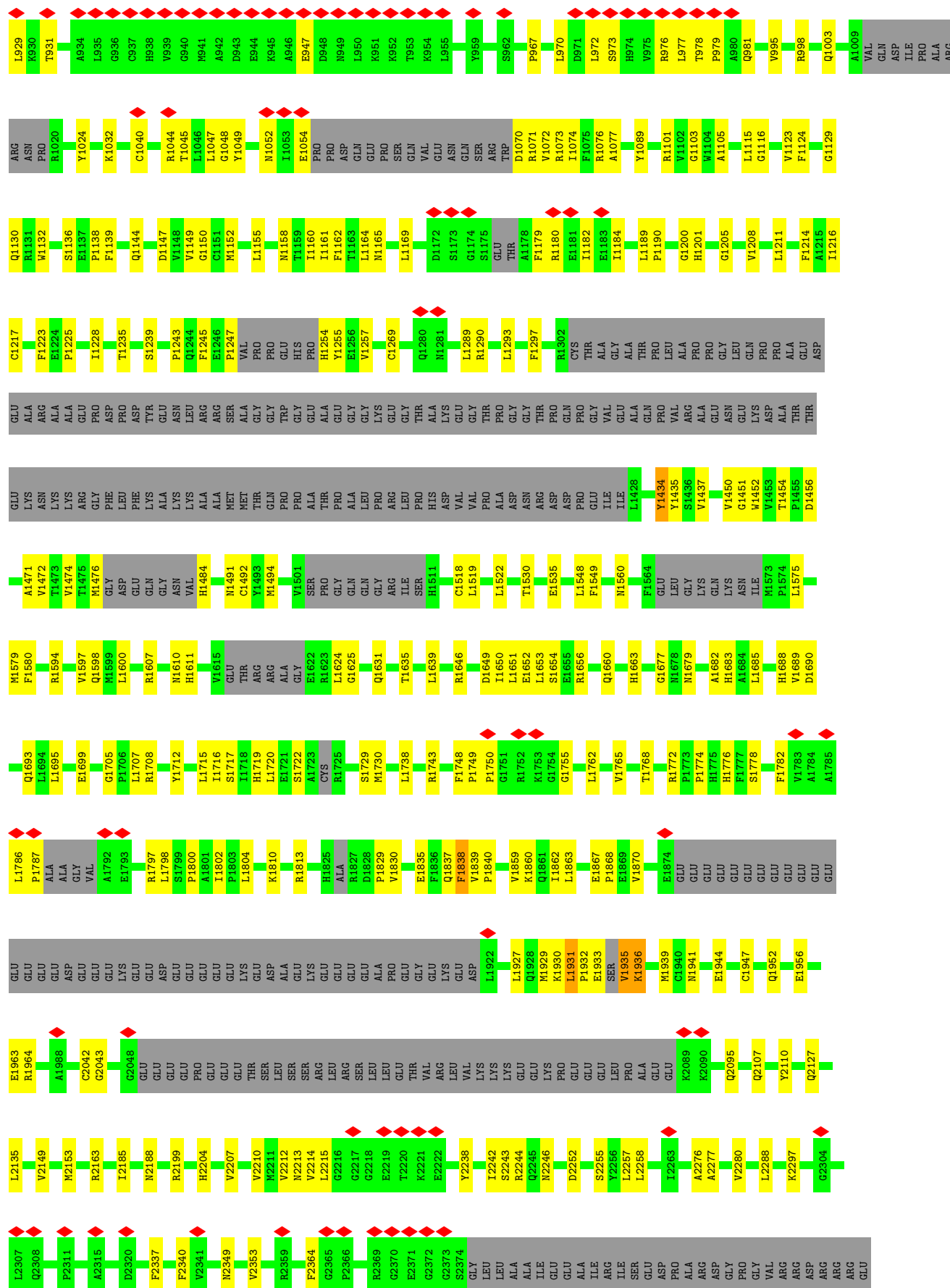
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

### 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.

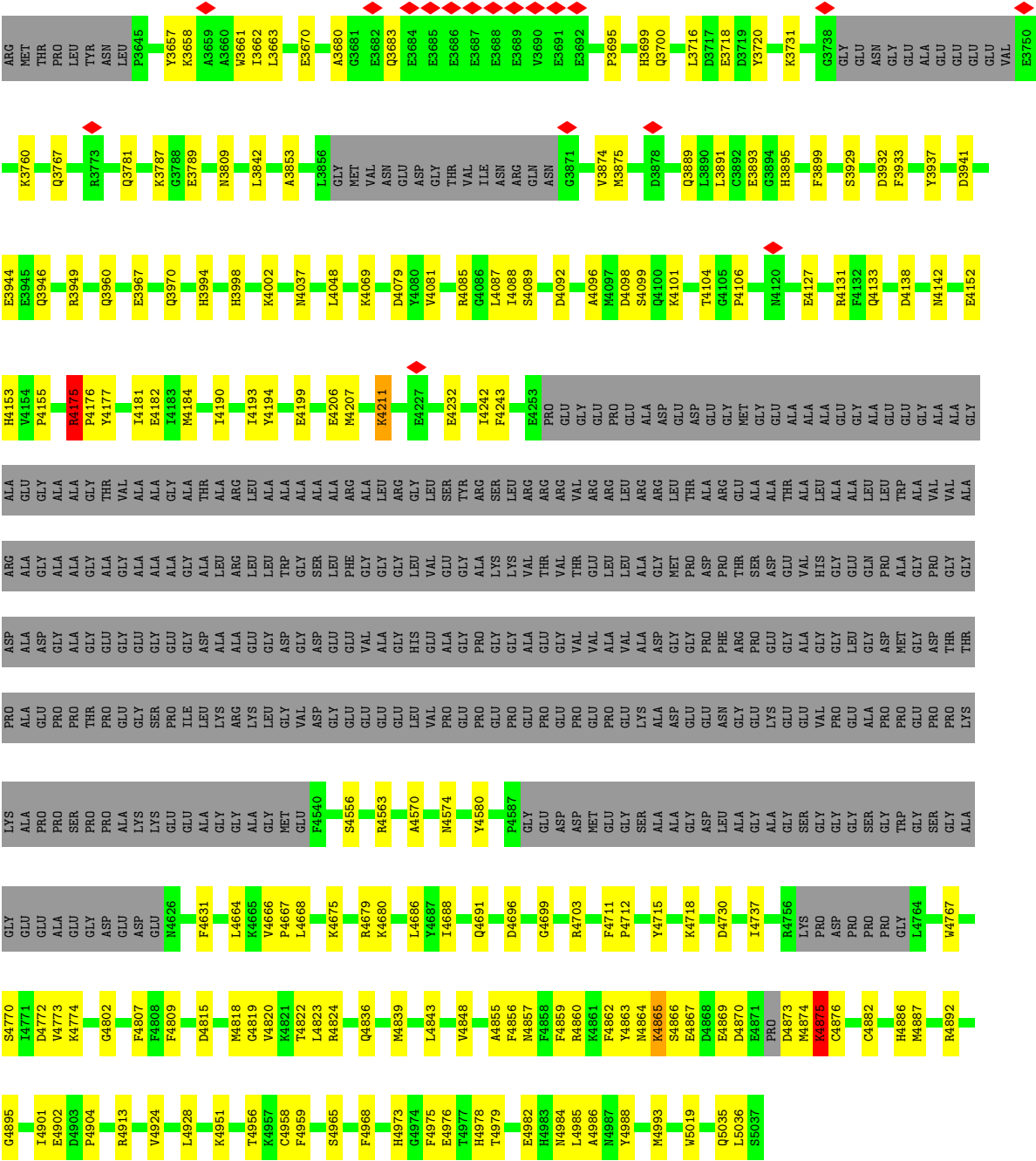
#### • Molecule 1: Ryanodine receptor 1



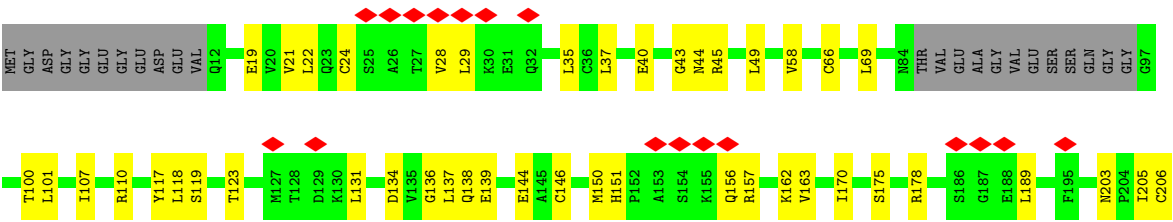








● Molecule 1: Ryanodine receptor 1





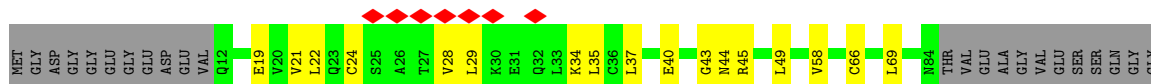














LYS	ARG	GLU	ALA	P1225	S1136	T931	SS47	S745	I638	L521	L390	F314	E211	G97
ARG	GLY	P1138	PRO	I1228	E1137	A934	P853	C746	N639	L522	T391	C315	T215	T100
PHE	LEU	F1139	ASP	T1235	F1139	L935	C854	C747	I644	Y523	C393	F316	T219	L101
LEU	LEU		ASP		Q1144	G936	P855		I645	R534	Q394	R317	V219	I107
LYS	TYR		ASP			C937	V856		R646	C537	A400	V319	L220	R110
ALA	GLU		TYR			H938	D857		N647	F540	A408	S319	L222	R110
ASN	ASN		VAL			V939	THR		N648	L544	G409	E321	F223	Y117
LYS	LYS		GLN			G940	VAL		F649	L544	L410	K322	H224	Y118
LYS	ARG		GLN			M941	THR		R652	V547	G417	L323	G225	T123
ALA	ARG		GLN			A942	V862		R660	V548	K424	D324	H226	
MET	MET		GLN			G1048	V862		R662	S549		T325	N227	
MET	ALA		GLN			G1047	V862		W662	L551		A326	D228	
THR	THR		GLN			Y1049	L867		W662	L551		P327	E229	
GLY	GLY		GLN				R869		M667	E555	S428	K328	S234	
GLN	GLY		GLN				R870		E670	A556	G429	R329	A235	
PRO	GLY		GLN				R877		V671	I560	P430	D330	A236	
PRO	GLY		GLN				R878		L675	V563	A432	V331	R242	
PRO	GLY		GLN				R879		T676	L564	P431	E332	R243	
ALA	ALA		GLN				R880		G685	V565	A434	P336	G250	
ALA	ALA		GLN				R881		W686	L568	P434	P337	H255	
PRO	LYS		GLN				L884		A687	C566	A435	E338	A256	
PRO	LYS		GLN				R886		L688	V567	L436	I339	R257	
ARG	GLY		GLN				Q889		G700	L580	V441	G342	L265	
LEU	LEU		GLN				G890		W702	E581	L442	E343	L265	
PRO	PRO		GLN				R891		T702	H582	D447	S344	H273	
PRO	PRO		GLN				R892		N705	I583	H461	L345	L274	
ASP	ASP		GLN				G894		D709	L590	K464	G346	R275	
GLY	GLY		GLN				R897		Y712	G594	Q465	E347	P279	
GLY	GLY		GLN				R897		Y713	L606	F478	H550	H284	
GLY	GLY		GLN				R900		Y714	C609	A360	Y359	V285	
GLY	GLY		GLN				R901		Y715	N610	A361	A362	T286	
GLY	GLY		GLN				R902		D717	V614	L484	P362	T287	
GLY	GLY		GLN				R903		G718	R615	S485	D363	G988	
GLY	GLY		GLN				R907		L719	S616	V487	D363	R289	
GLY	GLY		GLN				R908		H725	N617	L488	P364	A292	
GLY	GLY		GLN				R911		R728	L620	L494	K365	T294	
GLY	GLY		GLN				R912		P729	P627	R495	A366	T296	
GLY	GLY		GLN				R913		W730	G628	V496	L367	D296	
GLY	GLY		GLN				R914		W731	R629	Y497	R368	V300	
GLY	GLY		GLN				R917		S732	E330	A501	L369	V301	
GLY	GLY		GLN				R920		S732	F503	H502	G370	V302	
GLY	GLY		GLN				R923		Q735	L631	A504	V371	G305	
GLY	GLY		GLN				R927		W743	L632		L372	K306	
GLY	GLY		GLN				R928		W744	L633		A376		
GLY	GLY		GLN				R929			Q634		Q380	A311	
GLY	GLY		GLN				R930			T635		E381	S313	
GLY	GLY		GLN				R931							
GLY	GLY		GLN				R932							
GLY	GLY		GLN				R933							
GLY	GLY		GLN				R934							
GLY	GLY		GLN				R935							
GLY	GLY		GLN				R936							
GLY	GLY		GLN				R937							
GLY	GLY		GLN				R938							
GLY	GLY		GLN				R939							
GLY	GLY		GLN				R940							
GLY	GLY		GLN				R941							
GLY	GLY		GLN				R942							
GLY	GLY		GLN				R943							
GLY	GLY		GLN				R944							
GLY	GLY		GLN				R945							
GLY	GLY		GLN				R946							
GLY	GLY		GLN				R947							
GLY	GLY		GLN				R948							
GLY	GLY		GLN				R949							
GLY	GLY		GLN				R950							
GLY	GLY		GLN				R951							
GLY	GLY		GLN				R952							
GLY	GLY		GLN				R953							
GLY	GLY		GLN				R954							
GLY	GLY		GLN				R955							
GLY	GLY		GLN				R956							
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GLY	GLY		GLN				R958							
GLY	GLY		GLN				R959							
GLY	GLY		GLN				R960							
GLY	GLY		GLN				R961							
GLY	GLY		GLN				R962							
GLY	GLY		GLN				R963							
GLY	GLY		GLN				R964							
GLY	GLY		GLN				R965							
GLY	GLY		GLN				R966							
GLY	GLY		GLN				R967							
GLY	GLY		GLN				R968							
GLY	GLY		GLN				R969							
GLY	GLY		GLN				R970							
GLY	GLY		GLN				R971							
GLY	GLY		GLN				R972							
GLY	GLY		GLN				R973							
GLY	GLY		GLN				R974							
GLY	GLY		GLN				R975							
GLY	GLY		GLN				R976							
GLY	GLY		GLN				R977							
GLY	GLY		GLN				R978							
GLY	GLY		GLN				R979							
GLY	GLY		GLN				R980							
GLY	GLY		GLN				R981							
GLY	GLY		GLN				R982							
GLY	GLY		GLN				R983							
GLY	GLY		GLN				R984							
GLY	GLY		GLN				R985							
GLY	GLY		GLN				R986							
GLY	GLY		GLN				R987							
GLY	GLY		GLN				R988							
GLY	GLY		GLN				R989							
GLY	GLY		GLN				R990							
GLY	GLY		GLN				R991							
GLY	GLY		GLN				R992							
GLY	GLY		GLN				R993							
GLY	GLY		GLN				R994							
GLY	GLY		GLN				R995							
GLY	GLY		GLN				R996							
GLY	GLY		GLN				R997							
GLY	GLY		GLN				R998							
GLY	GLY		GLN				R999							
GLY	GLY		GLN				R1000							
GLY	GLY		GLN				R1001							
GLY	GLY		GLN				R1002							
GLY	GLY		GLN				R1003							
GLY	GLY		GLN				R1004							
GLY	GLY		GLN				R1005							
GLY	GLY		GLN				R1006							
GLY	GLY		GLN				R1007							
GLY	GLY		GLN				R1008							
GLY	GLY		GLN				R1009							
GLY	GLY		GLN				R1010							
GLY	GLY		GLN				R1011							
GLY	GLY		GLN				R1012							
GLY	GLY		GLN				R1013							
GLY	GLY		GLN				R1014							
GLY	GLY		GLN				R1015							
GLY	GLY		GLN				R1016							
GLY	GLY		GLN				R1017							
GLY	GLY		GLN				R1018							
GLY	GLY		GLN				R1019							
GLY	GLY		GLN				R1020							
GLY	GLY		GLN				R1021							
GLY	GLY		GLN				R1022							
GLY	GLY		GLN				R1023							
GLY	GLY		GLN				R1024							
GLY	GLY		GLN				R1025							
GLY	GLY		GLN				R1026							







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114423	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	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.212	Depositor
Minimum map value	-2.365	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.591	Depositor
Map size (Å)	523.2, 523.2, 523.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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: ATP, CA

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	0.28	0/24282	0.43	0/32988
1	B	0.28	0/24282	0.43	0/32988
1	C	0.28	0/24282	0.43	0/32988
1	D	0.28	0/24282	0.43	0/32988
All	All	0.28	0/97128	0.43	0/131952

There are no bond length outliers.

There are no bond angle outliers.

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	A	23760	0	22500	538	0
1	B	23760	0	22500	533	0
1	C	23760	0	22500	531	0
1	D	23760	0	22500	528	0
2	A	31	0	12	9	0
2	B	31	0	12	9	0
2	C	31	0	12	8	0
2	D	31	0	12	9	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	95168	0	90048	2114	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 11.

The worst 5 of 2114 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:A:1708:ARG:NE	1:A:1830:VAL:HG11	1.59	1.18
1:D:1708:ARG:NE	1:D:1830:VAL:HG11	1.59	1.17
1:C:1708:ARG:NE	1:C:1830:VAL:HG11	1.59	1.16
1:B:1708:ARG:NE	1:B:1830:VAL:HG11	1.59	1.16
1:B:721:LEU:HD21	1:B:1474:VAL:CG2	1.83	1.08

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3101/5037 (62%)	2823 (91%)	274 (9%)	4 (0%)	48	79
1	B	3101/5037 (62%)	2823 (91%)	274 (9%)	4 (0%)	48	79
1	C	3101/5037 (62%)	2823 (91%)	274 (9%)	4 (0%)	48	79
1	D	3101/5037 (62%)	2823 (91%)	274 (9%)	4 (0%)	48	79
All	All	12404/20148 (62%)	11292 (91%)	1096 (9%)	16 (0%)	50	79

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4867	GLU
1	B	4867	GLU
1	C	4867	GLU
1	D	4867	GLU
1	A	4875	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2350/4276 (55%)	2332 (99%)	18 (1%)	79	84
1	B	2350/4276 (55%)	2332 (99%)	18 (1%)	79	84
1	C	2350/4276 (55%)	2332 (99%)	18 (1%)	79	84
1	D	2350/4276 (55%)	2332 (99%)	18 (1%)	79	84
All	All	9400/17104 (55%)	9328 (99%)	72 (1%)	77	84

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1434	TYR
1	D	4875	LYS
1	D	1518	CYS
1	D	1931	LEU
1	B	1549	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 182 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2127	GLN
1	D	520	ASN
1	C	3700	GLN
1	C	4133	GLN
1	D	1158	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ATP	D	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.81	7 (22%)
2	ATP	A	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.81	7 (22%)
2	ATP	C	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.81	7 (22%)
2	ATP	B	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.81	7 (22%)

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	ATP	D	5101	-	-	6/18/38/38	0/3/3/3
2	ATP	A	5101	-	-	6/18/38/38	0/3/3/3
2	ATP	C	5101	-	-	6/18/38/38	0/3/3/3
2	ATP	B	5101	-	-	6/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ATP	C5-C4	2.05	1.46	1.40
2	B	5101	ATP	C5-C4	2.05	1.46	1.40
2	C	5101	ATP	C5-C4	2.05	1.46	1.40
2	D	5101	ATP	C5-C4	2.05	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5101	ATP	PA-O3A-PB	-4.50	117.37	132.83
2	B	5101	ATP	PA-O3A-PB	-4.50	117.37	132.83
2	C	5101	ATP	PA-O3A-PB	-4.50	117.37	132.83
2	D	5101	ATP	PA-O3A-PB	-4.50	117.37	132.83
2	A	5101	ATP	PB-O3B-PG	-3.87	119.54	132.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5101	ATP	C5'-O5'-PA-O3A
2	A	5101	ATP	C4'-C5'-O5'-PA
2	B	5101	ATP	C5'-O5'-PA-O3A
2	B	5101	ATP	C4'-C5'-O5'-PA
2	C	5101	ATP	C5'-O5'-PA-O3A

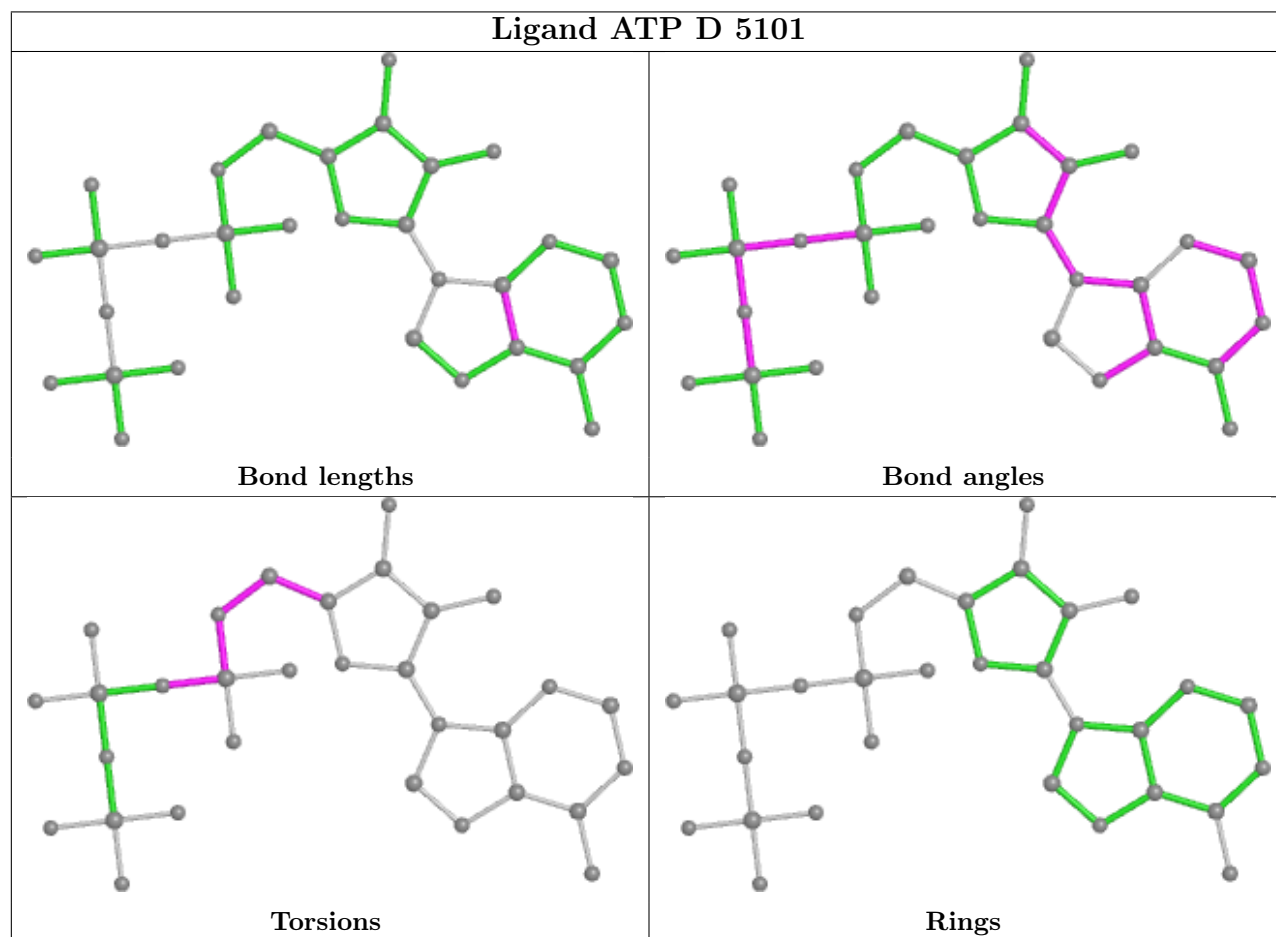
There are no ring outliers.

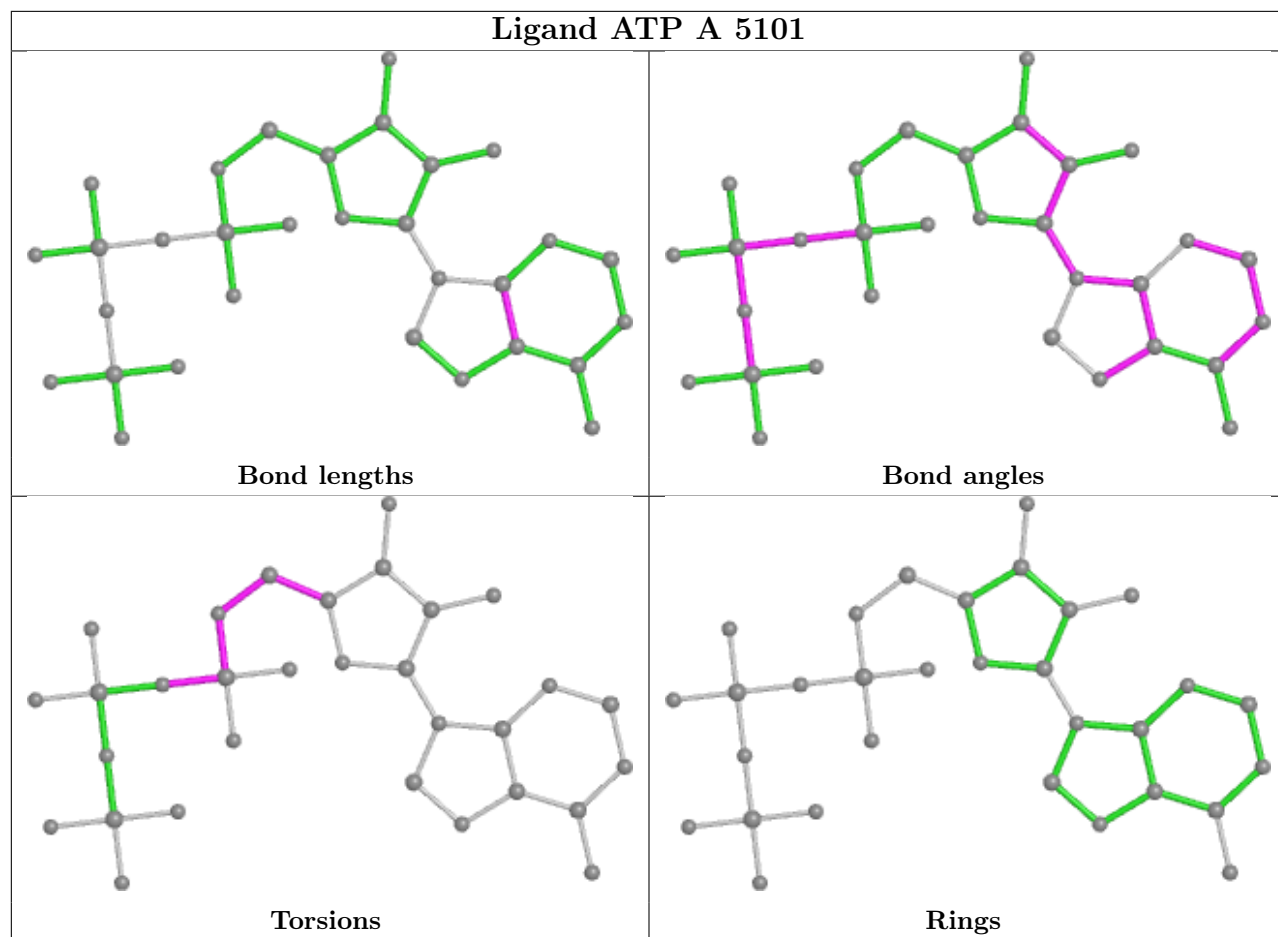
4 monomers are involved in 35 short contacts:

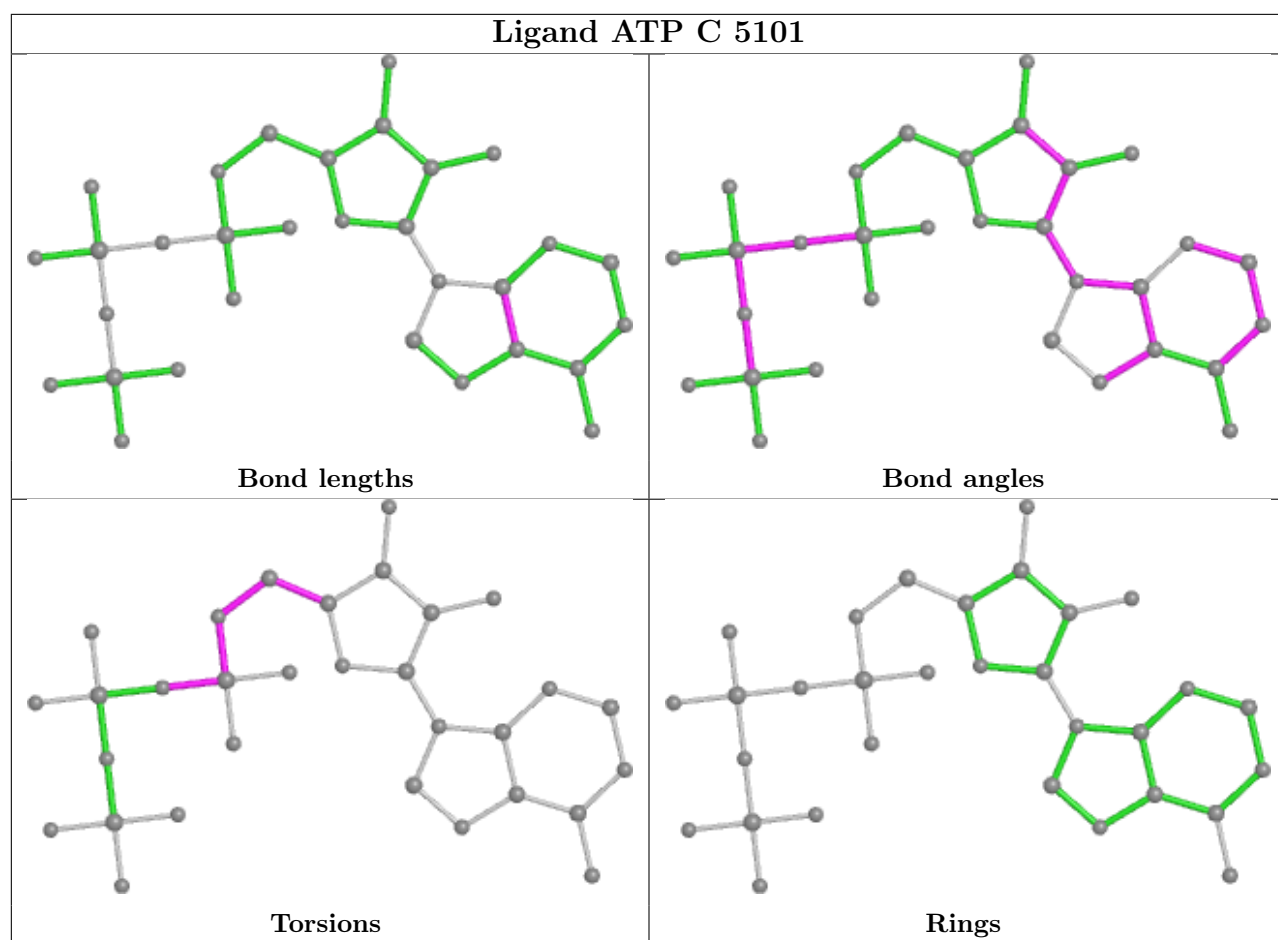
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5101	ATP	9	0
2	A	5101	ATP	9	0
2	C	5101	ATP	8	0
2	B	5101	ATP	9	0

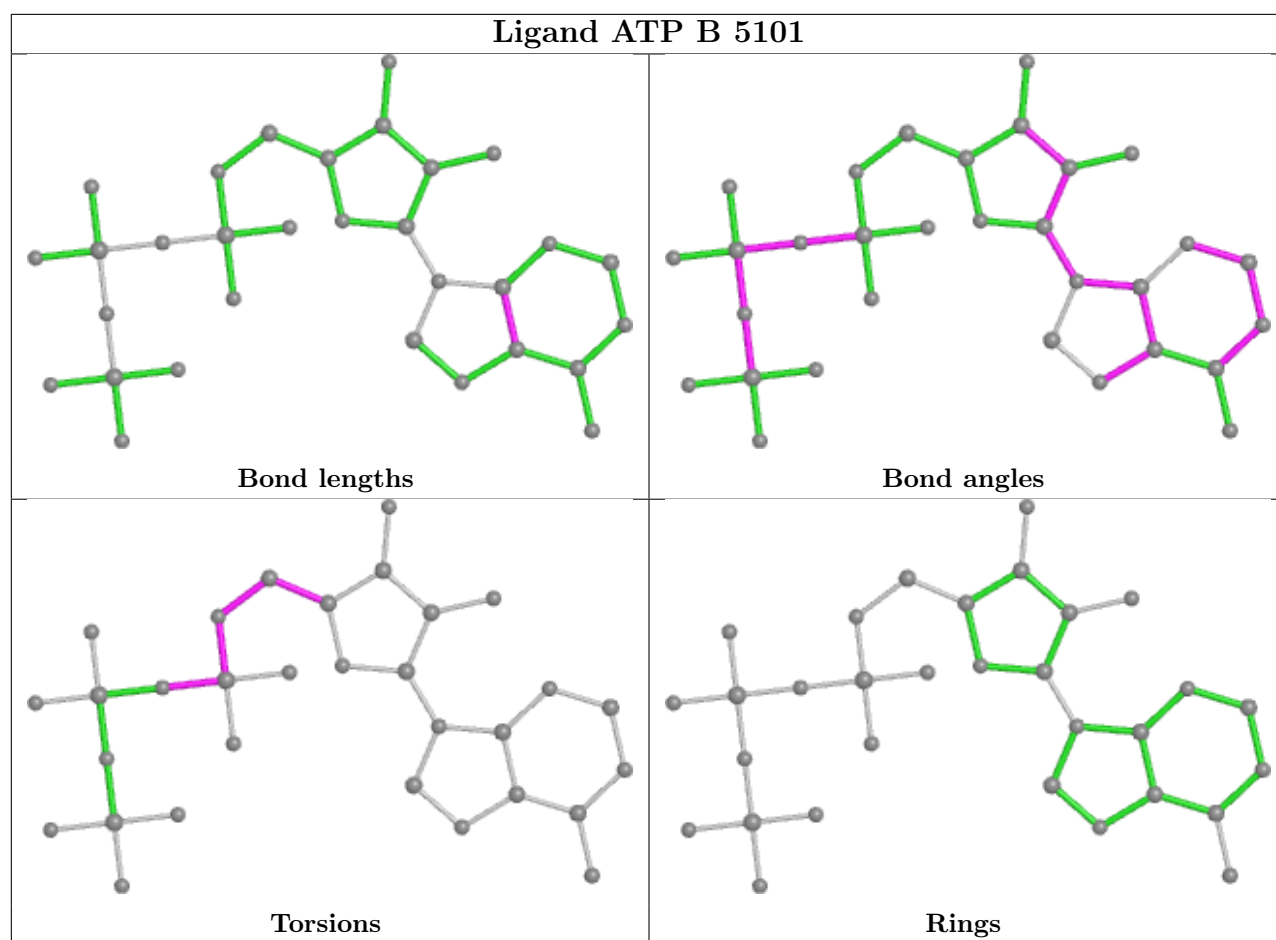
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

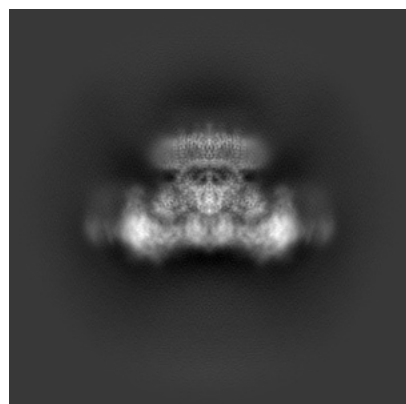
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38046. These allow visual inspection of the internal detail of the map and identification of artifacts.

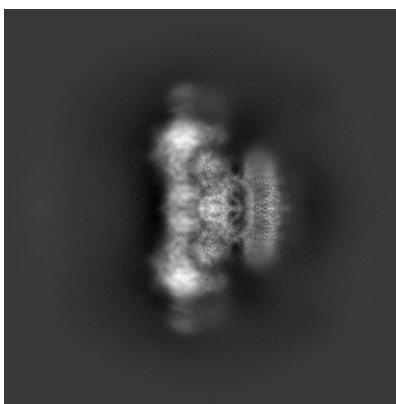
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

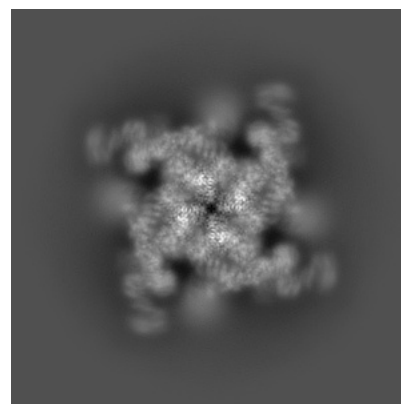
#### 6.1.1 Primary map



X

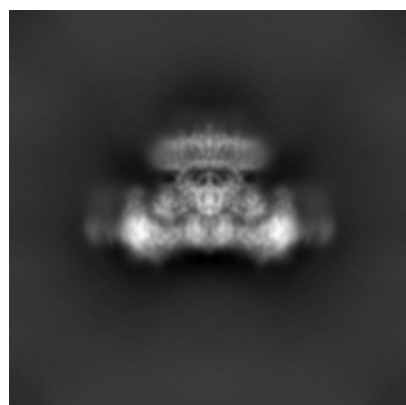


Y

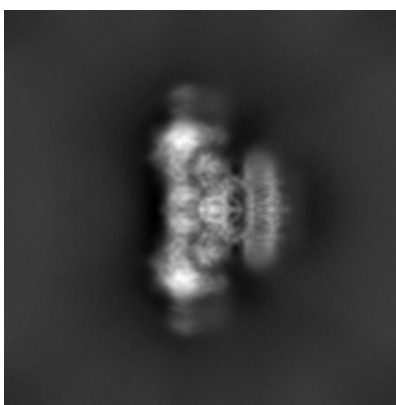


Z

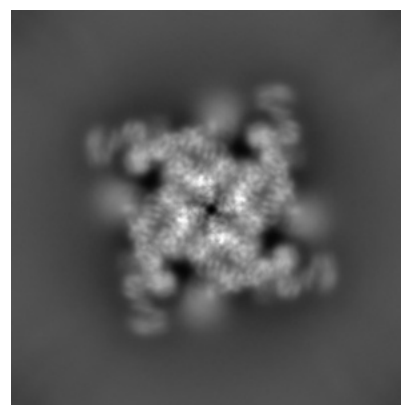
#### 6.1.2 Raw map



X



Y

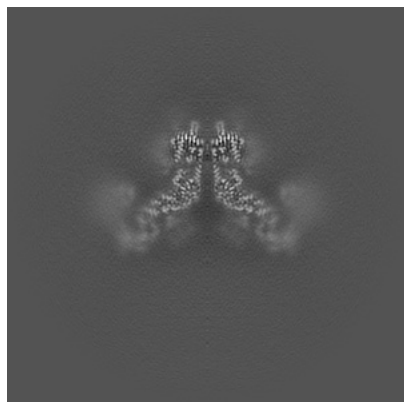


Z

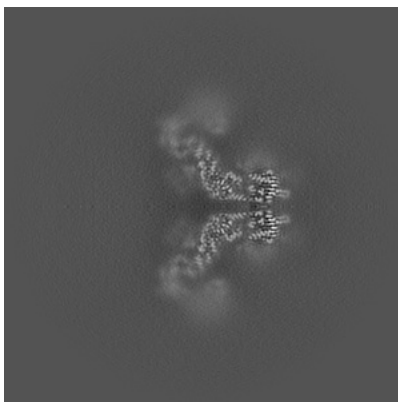
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

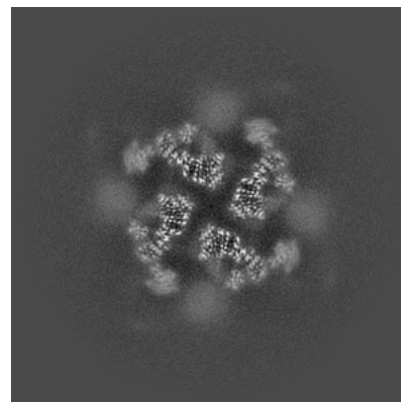
### 6.2.1 Primary map



X Index: 240

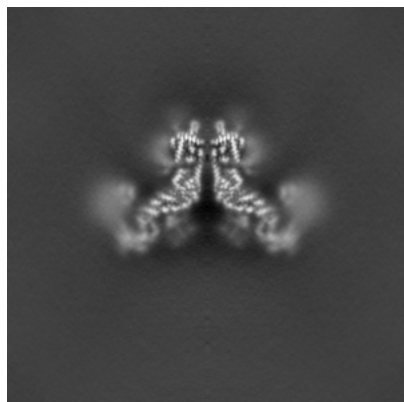


Y Index: 240

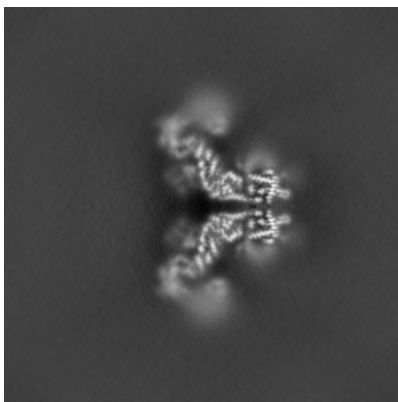


Z Index: 240

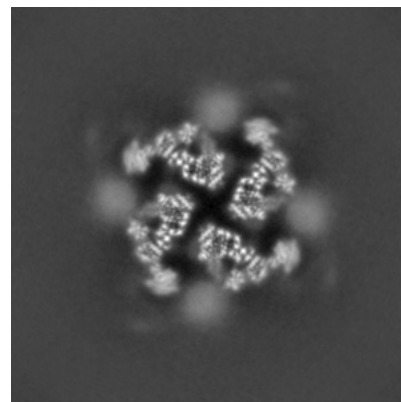
### 6.2.2 Raw map



X Index: 240



Y Index: 240



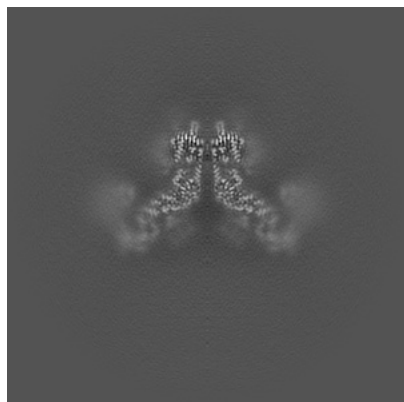
Z Index: 240

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

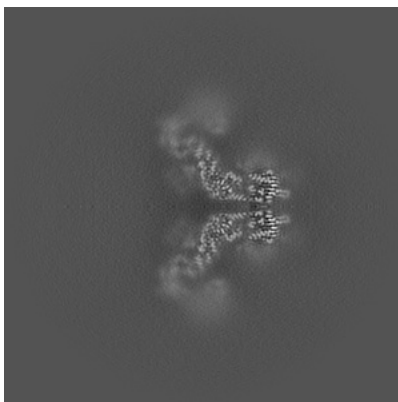


## 6.3 Largest variance slices [i](#)

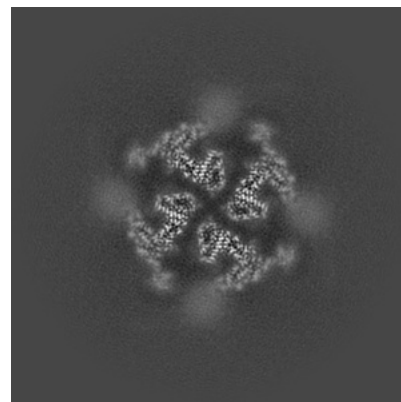
### 6.3.1 Primary map



X Index: 240

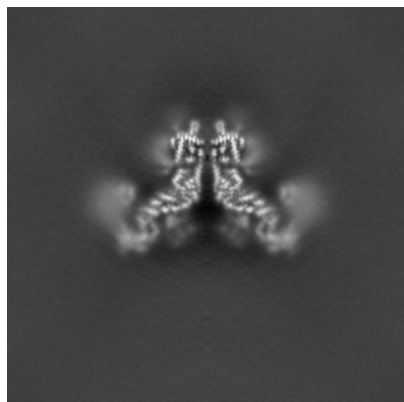


Y Index: 240

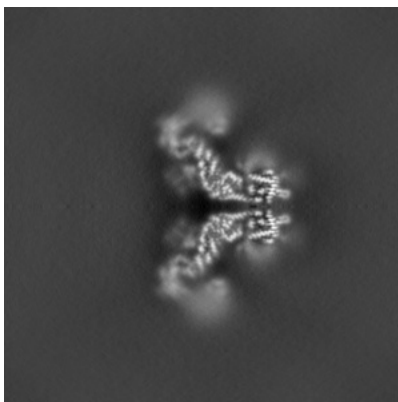


Z Index: 246

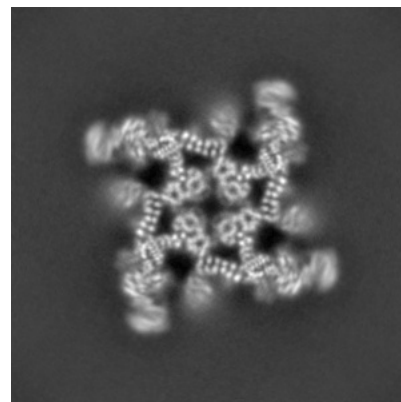
### 6.3.2 Raw map



X Index: 240



Y Index: 240

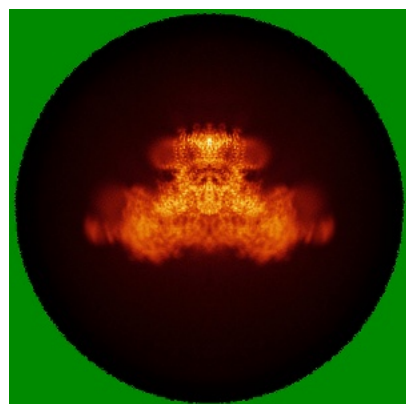


Z Index: 216

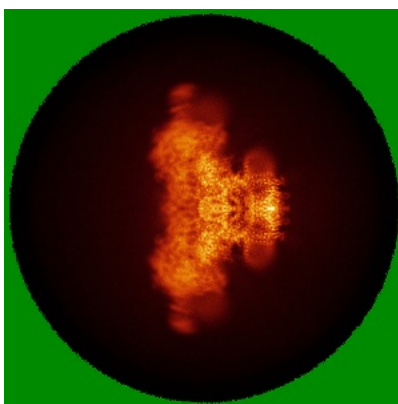
The images above show the largest variance slices of the map in three orthogonal directions.

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

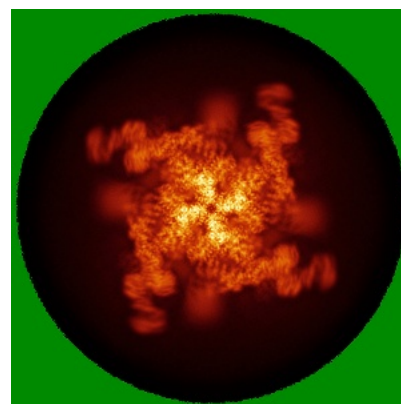
### 6.4.1 Primary map



X

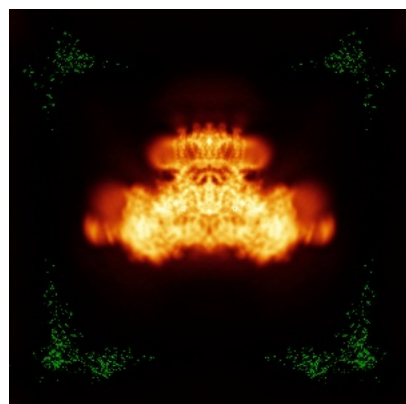


Y

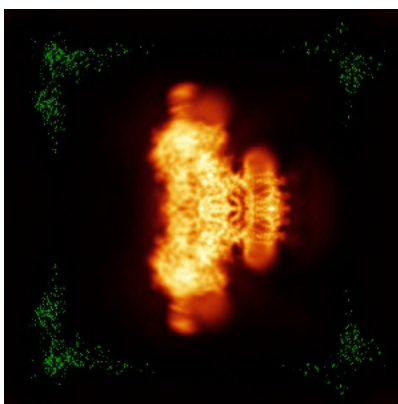


Z

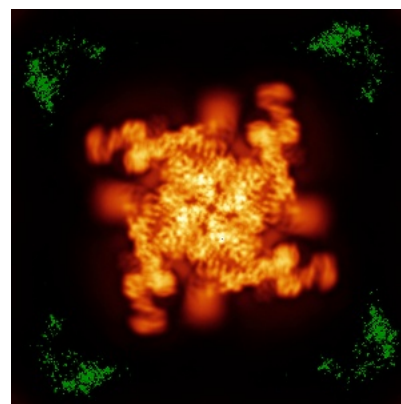
### 6.4.2 Raw map



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.

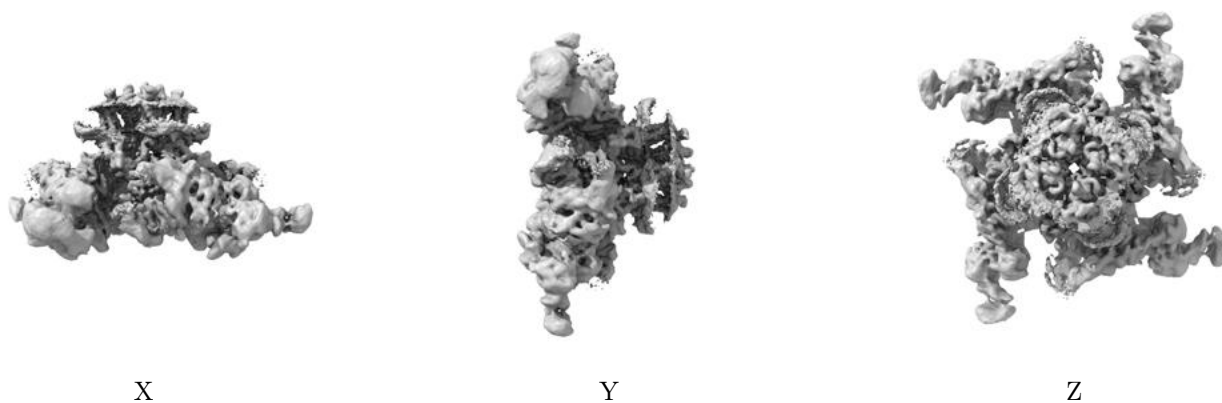
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.591. 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.

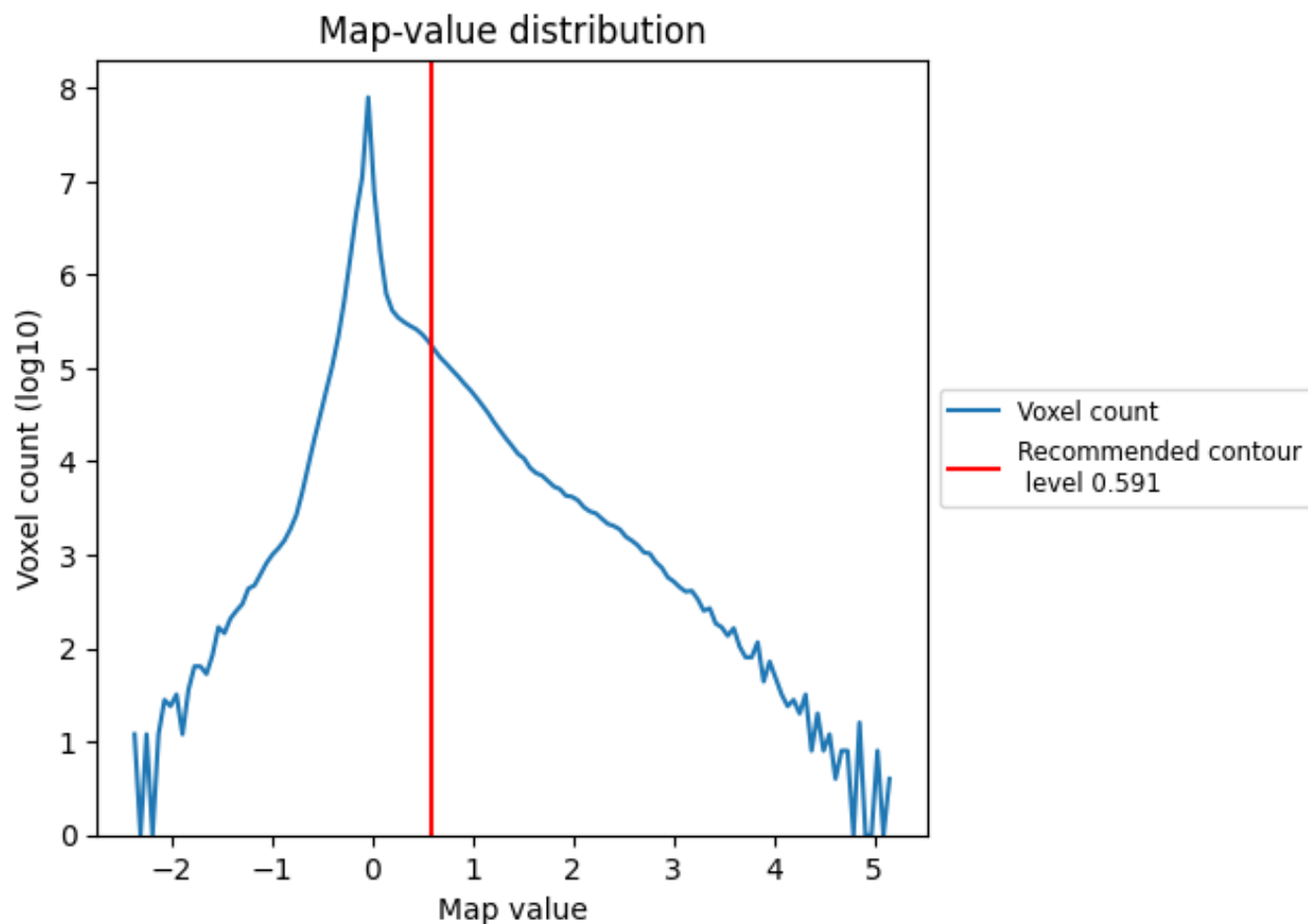
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

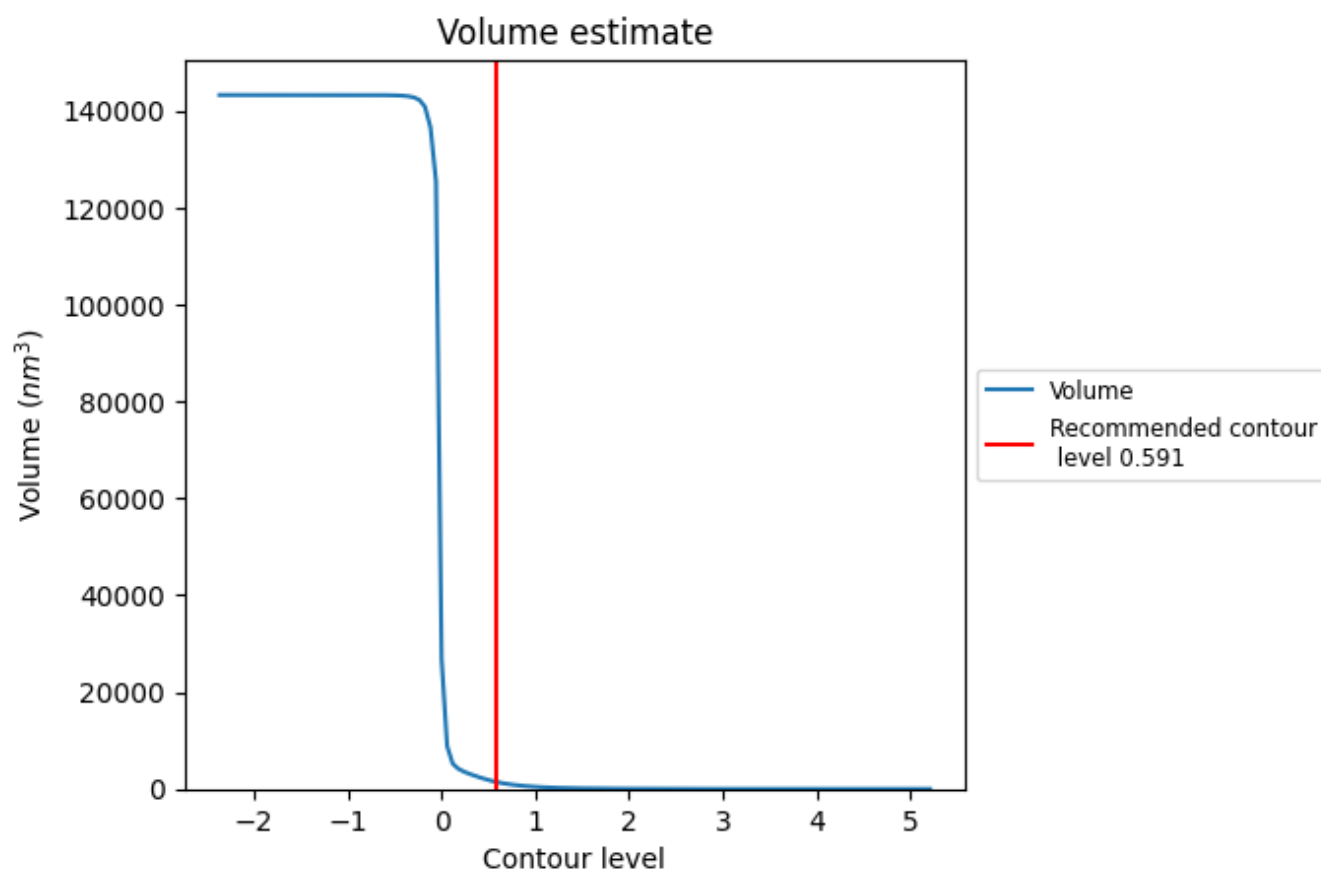
This section contains the results of statistical analysis of the map.

### 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.

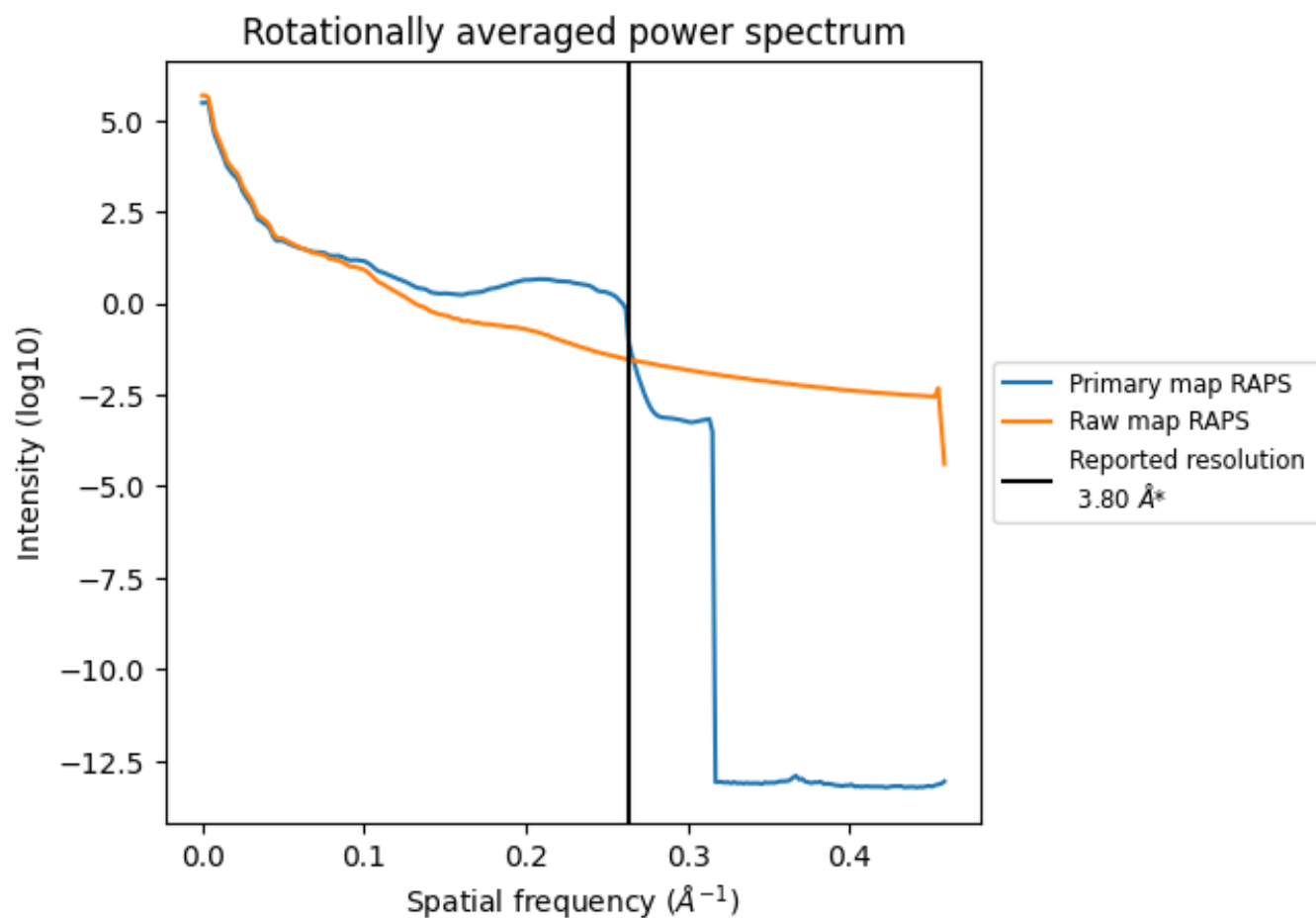
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1424 nm<sup>3</sup>; this corresponds to an approximate mass of 1286 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 ⓘ

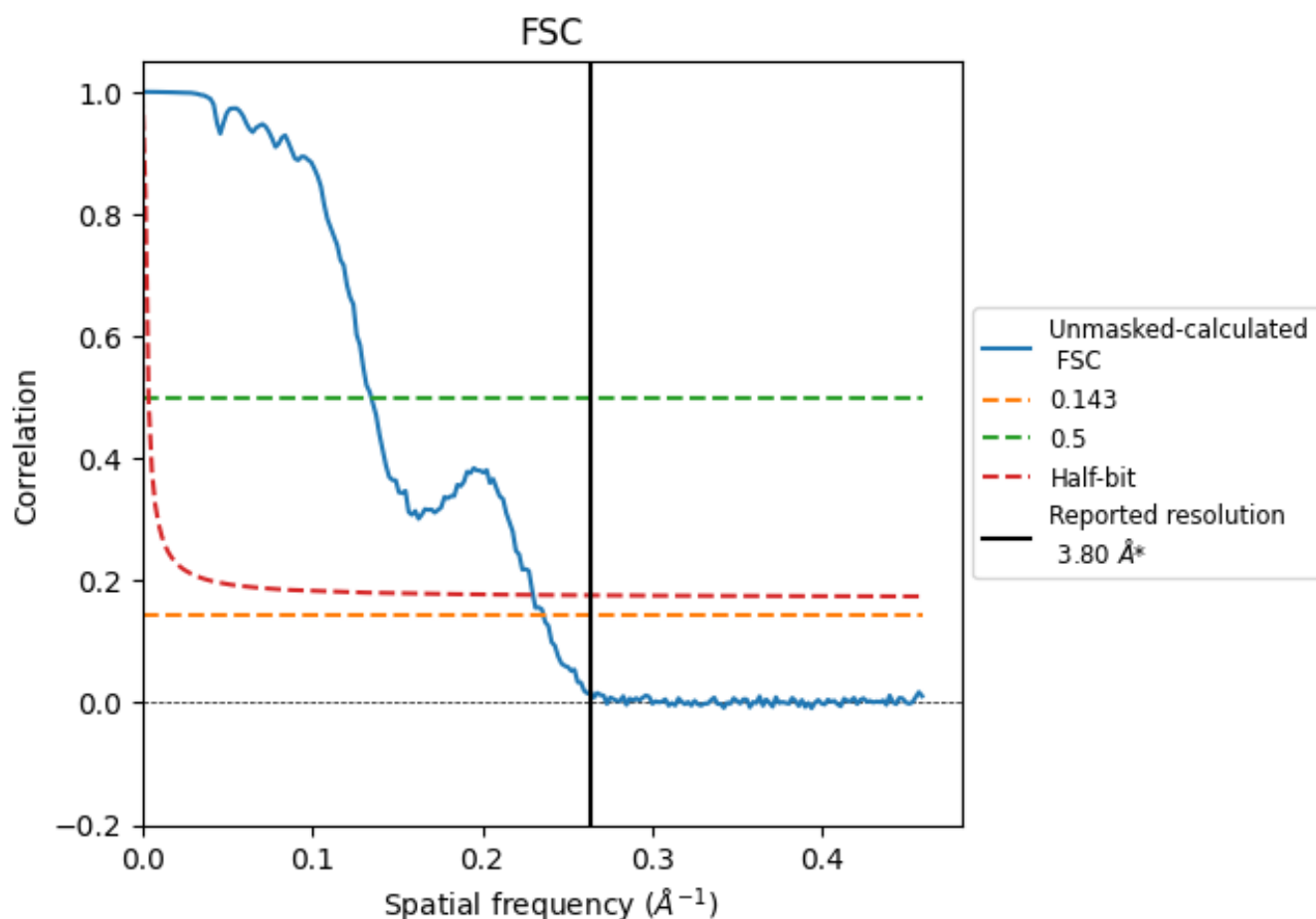


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263 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	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.43	4.35

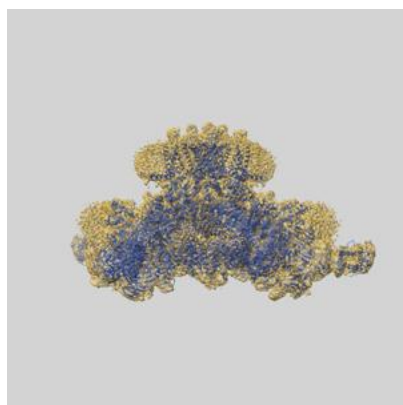
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.8 by more than 10 %



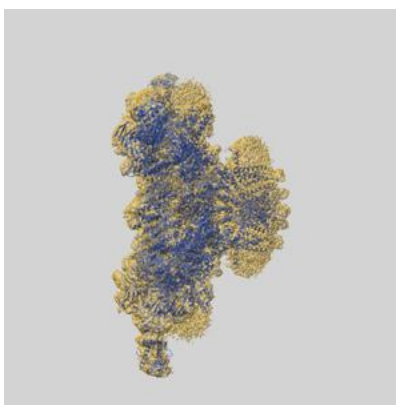
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38046 and PDB model 8X4C. Per-residue inclusion information can be found in section [3](#) on page [6](#).

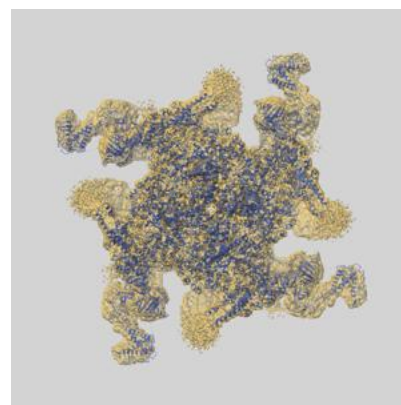
### 9.1 Map-model overlay [i](#)



X



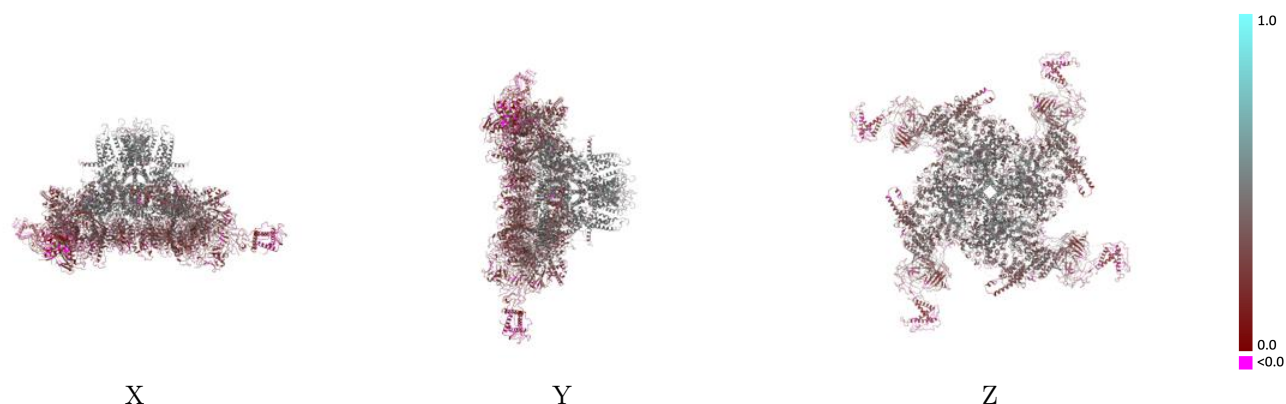
Y



Z

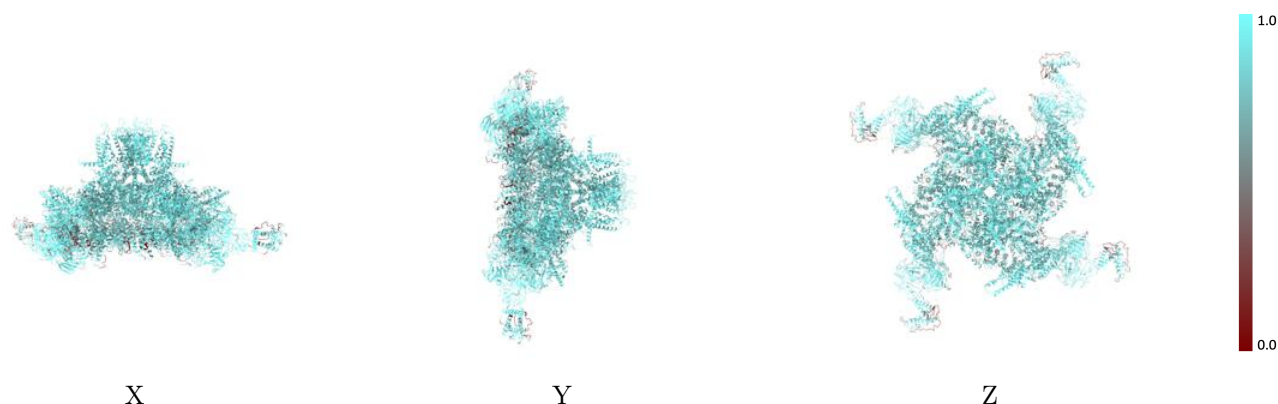
The images above show the 3D surface view of the map at the recommended contour level 0.591 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



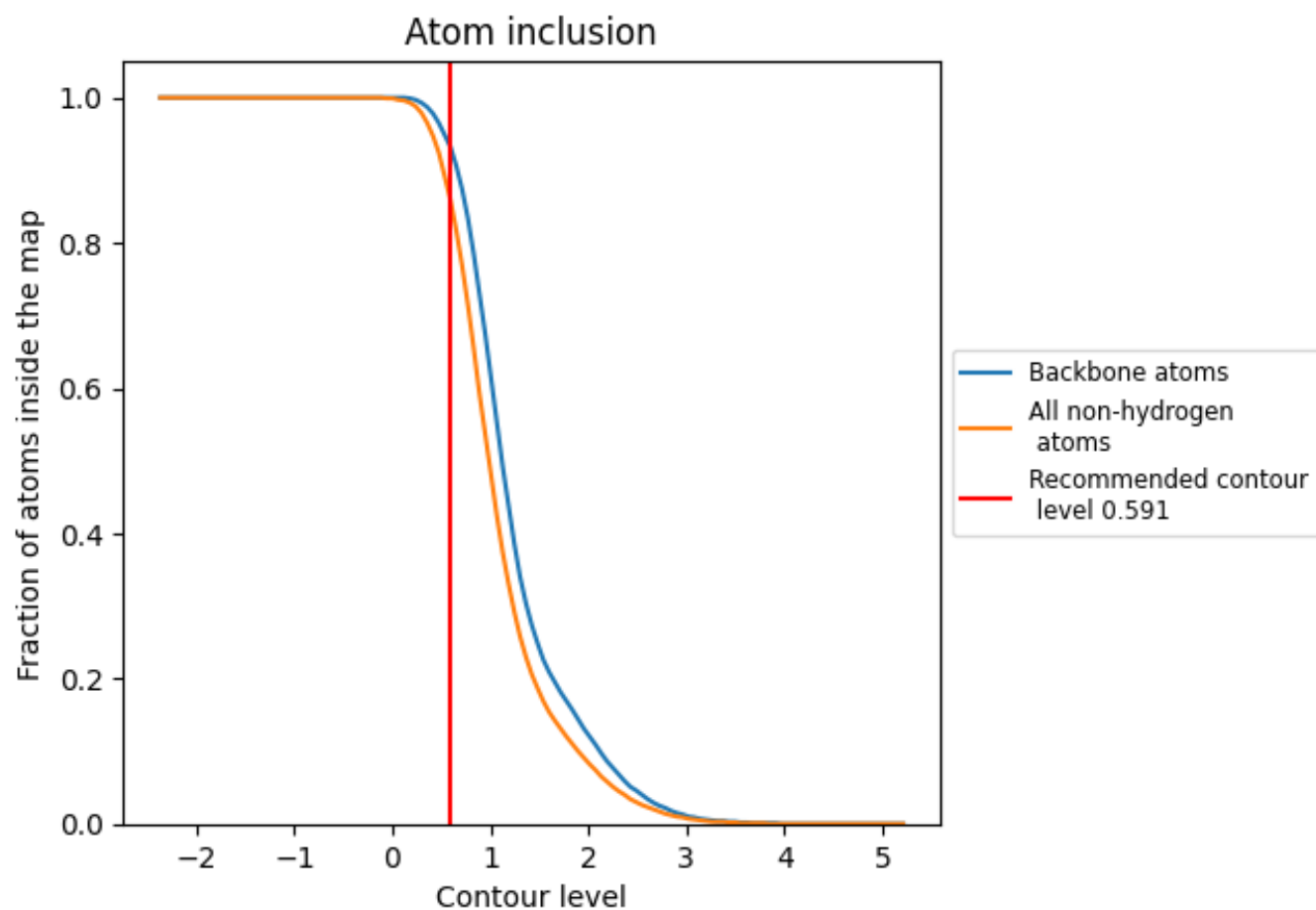
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.591).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.591) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8610	<div></div> 0.3270
A	<div></div> 0.8610	<div></div> 0.3270
B	<div></div> 0.8610	<div></div> 0.3270
C	<div></div> 0.8610	<div></div> 0.3270
D	<div></div> 0.8610	<div></div> 0.3270

