



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 07:01 PM EST

PDB ID : 7U9R  
EMDB ID : EMD-26407  
Title : Structure of PKA phosphorylated human RyR2 in the open state  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2022-03-11  
Resolution : 3.69 Å(reported)  
Based on initial model : 7U9Q

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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.39

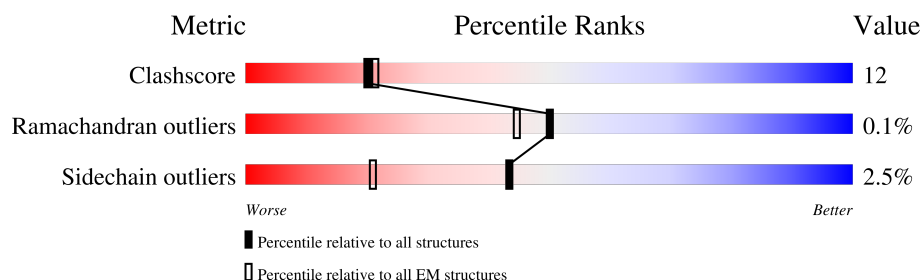
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.69 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	E	108	
1	F	108	
1	G	108	
1	H	108	
2	A	4967	
2	B	4967	
2	C	4967	
2	D	4967	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 138656 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

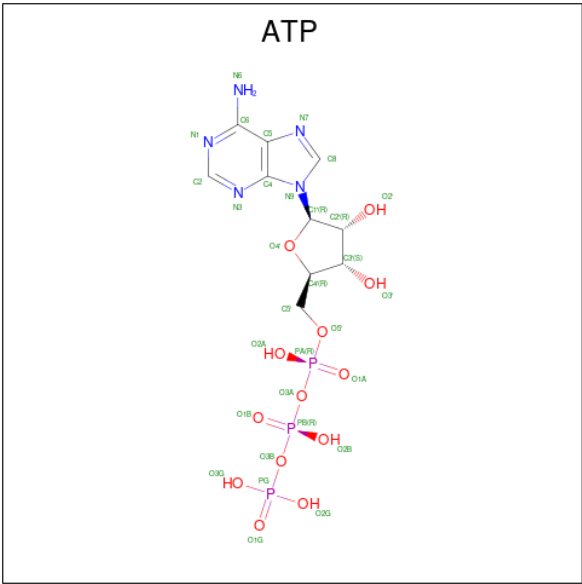
- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

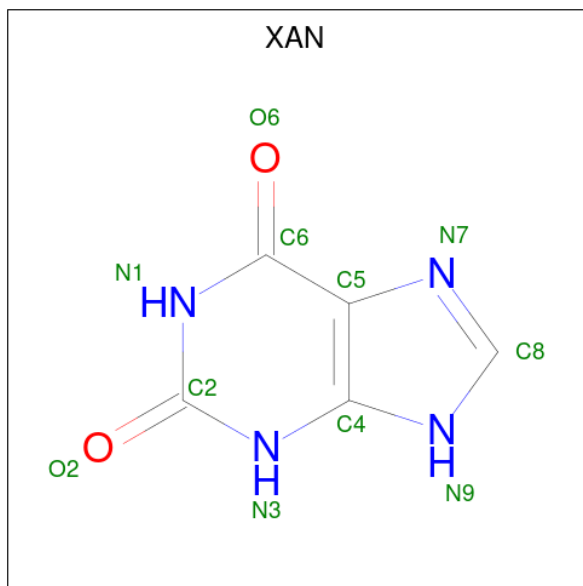
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	

- Molecule 6 is XANTHINE (three-letter code: XAN) (formula:  $C_5H_4N_4O_2$ ) (labeled as "Ligand of Interest" by depositor).

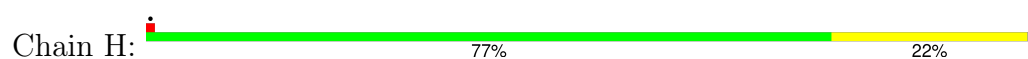


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			11	5	4	2	
6	D	1	Total	C	N	O	0
			11	5	4	2	
6	B	1	Total	C	N	O	0
			11	5	4	2	
6	C	1	Total	C	N	O	0
			11	5	4	2	

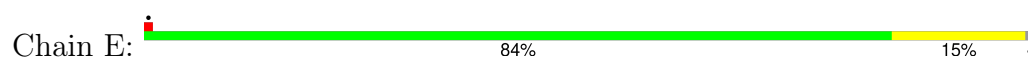
### 3 Residue-property plots [i](#)

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

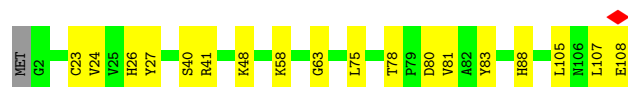
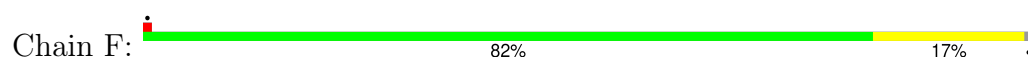
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



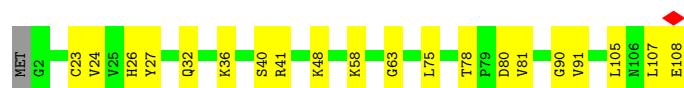
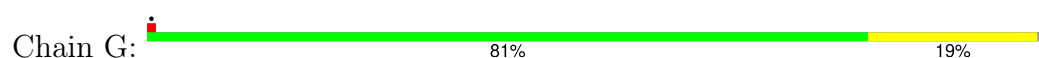
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



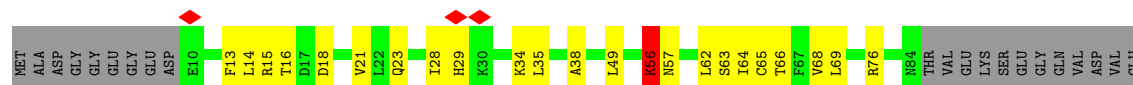
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 2









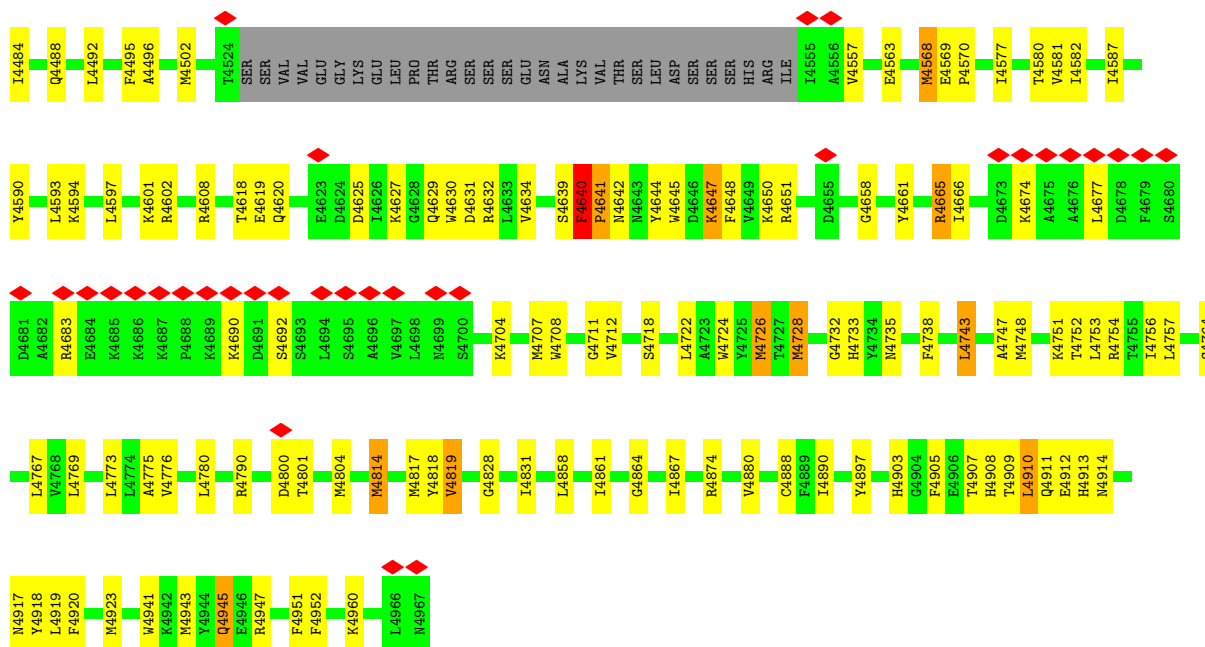
E4194	K4085	K3981	Q3656	GLU	GLY	ASP	ARG	V3168	THR	E2988
D4195	R4086	L3982	K3679	HIS	LYS	ARG	MET	L3171	ARG	F2989
T4196	L3983	L3982	C3680	PRO	LEU	TYR	ALA	E3172	ASN	L2990
I4197	K4092	E3987	K3681	GLN	ASP	MET	GLU	T3173	GLN	R2998
F4198	L4101	G3986	L3682	SER	PRO	GLN	THR	H3178	VAL	K2999
E4199	L4101	G3986	L3687	LYS	ILE	SER	ILE	N3179	ALA	E3000
M4200	E4107	M3999	M3695	ALA	TRP	LEU	TRP	I3183	ALA	K3001
A4203	M4108	V4000	A3696	ALA	TRP	ILE	TRP	Y3184	ALA	E3002
T4206	M4109	D4001	K3697	TRP	GLN	VAL	SER	S3270	ASP	M3003
S4207	T4113	M4002	H3700	HIS	MET	ALA	LYS	N3185	ASP	V3004
E4208	Q4116	L4014	D3701	LEU	ALA	ALA	SER	E3271	ASP	T3005
S4209	T4117	M4019	E3702	LEU	TYR	LEU	HIS	K3187	GLU	L3014
LEU	F4118	M4019	GLU	LEU	LYS	ASN	ALA	S3188	ALA	V3015
ASN	L4119	K4022	ASP	SER	ASP	ILE	PHE	L3197	GLU	R3016
GLU	E4120	L4023	ASP	GLN	ASP	LEU	LYS	L3197	LEU	P3103
ARG	L4121	F3854	ASP	ARG	PRO	LEU	ARG	V3201	LEU	M3104
SER	A4122	L3858	GLY	LYS	ASN	ILE	GLU	C3205	ILE	R3018
ALA	E4123	L3858	ARG	ARG	ARG	GLN	GLU	Y3285	LEU	I3019
ASN	F4129	D4030	V3599	ALA	THR	LEU	ASN	L3288	ASP	S3020
LYS	K4033	K4033	V3600	ASP	ASP	LEU	PHE	I3208	GLU	L3021
GLU	E4034	Y4035	R3604	THR	THR	ILE	THR	G3289	THR	A3026
SER	Y4035	K3712	F3605	SER	ASP	VAL	VAL	S3210	F3117	V3030
LYS	G4039	E3715	A3606	ILE	ASP	VAL	VAL	L3211	L3121	R3034
ARG	K4040	E3716	P3607	CYS	THR	GLN	GLN	E3212	I3122	I3035
PRO	R4045	K3717	L3608	ALA	PRO	GLY	ASP	R3213	R3123	L3036
GLU	R4046	M3719	Y3609	LEU	THR	LEU	ASN	M3215	E3124	G3037
GLN	D4047	Q3722	N3610	ILE	VAL	LEU	MET	E3216	D3125	Q3038
GLY	F4048	Q3722	V3617	ARG	ARG	ALA	PHE	E3217	Q3127	T3039
PRO	A4051	A3729	L3621	LEU	VAL	LEU	ALA	S3219	V3128	L3040
ARG	K4050	R3730	E3637	LEU	ASP	LEU	ILE	E3220	C3130	R3041
ALA	M4052	H3732	K3639	ASN	ILE	LYS	THR	L3221	A3042	A3042
PHE	H4055	V3755	D3638	ASN	ASP	ASN	ASP	A3222	R3043	T3044
PHE	R4056	I3763	K3641	VAL	ASN	THR	THR	E3223	V3045	V3045
S4237	H4057	T3772	E3642	LEU	VAL	SER	SER	S3224	R3046	K3047
I4238	Y4058	T3772	D3643	HIS	PHE	LYS	MET	G3225	T3048	G3049
L4239	S4061	L3778	K3646	LEU	THR	ASP	LYS	R3227	G3141	D3062
R4242	E4062	D3779	E3650	GLU	THR	GLU	ALA	T3229	S3145	D3067
L4245	T4063	Y3780	P3651	GLN	ASP	ASP	VAL	Q3230	I3146	B3070
F4246	E4064	K3784	F3652	LYS	VAL	VAL	SER	M3231	V3147	R3071
A4247	F4065	F3790	E3654	ARG	ARG	ASP	GLN	V3234	E3149	T3071
L4248	L4066	F3790	D3655	GLY	ILE	ASP	GLN	M3235	R3150	K3072
R4249	T4072	L3793	E3656	ARG	VAL	ILE	GLU	E3236	Q3151	E3073
Y4250	D4073	A3794	E3657	ARG	ARG	ILE	ASP	V3237	R3152	N3074
N4251	E4074	L3805	T3658	LYS	GLY	ARG	LYS	I3238	G3156	L3075
I4252	L4078	L3975	R3659	HIS	THR	SER	LYS	M3241	L3159	K3076
L4253	D4079	Q3975	V3660	LYS	CYS	ILE	MET	Y3245	Q3077	G3078
T4254	N4191	L3975	V3661	ASN	GLY	HIS	LYS	K3246	F3162	Q3079
L4255	N4191	Q3975	V3661	GLN	VAL	GLY	GLY	R3248	F3166	F3080
M4256	R4257	Q3975	V3661	GLN	VAL	GLY	GLY	E3336	P3167	T3081



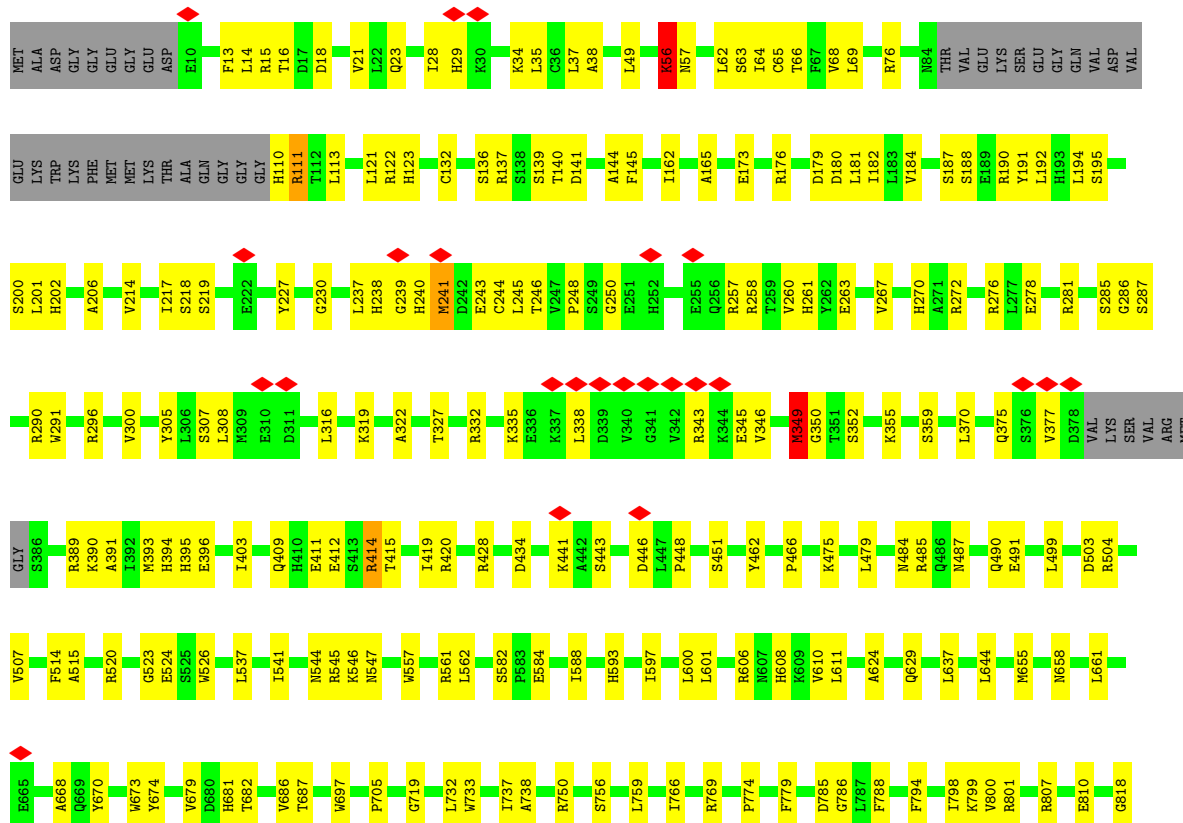








• Molecule 2: Ryanodine receptor 2

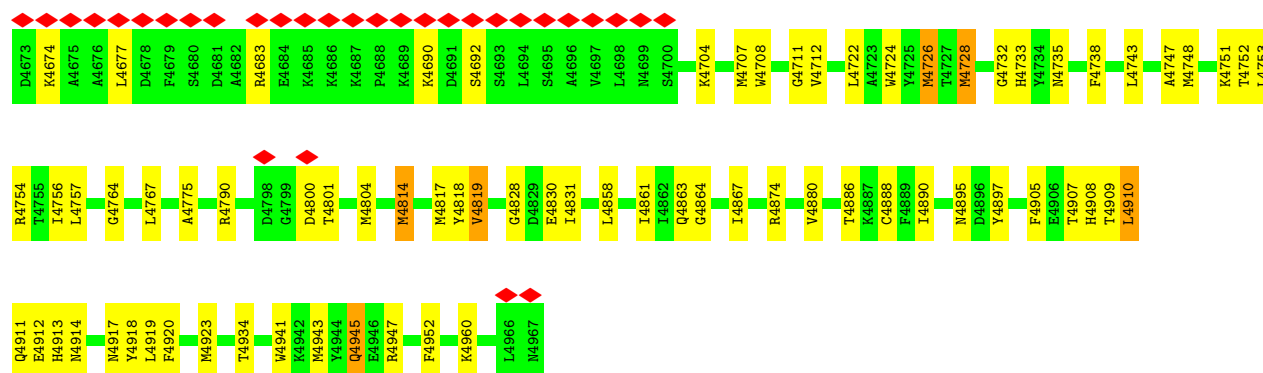




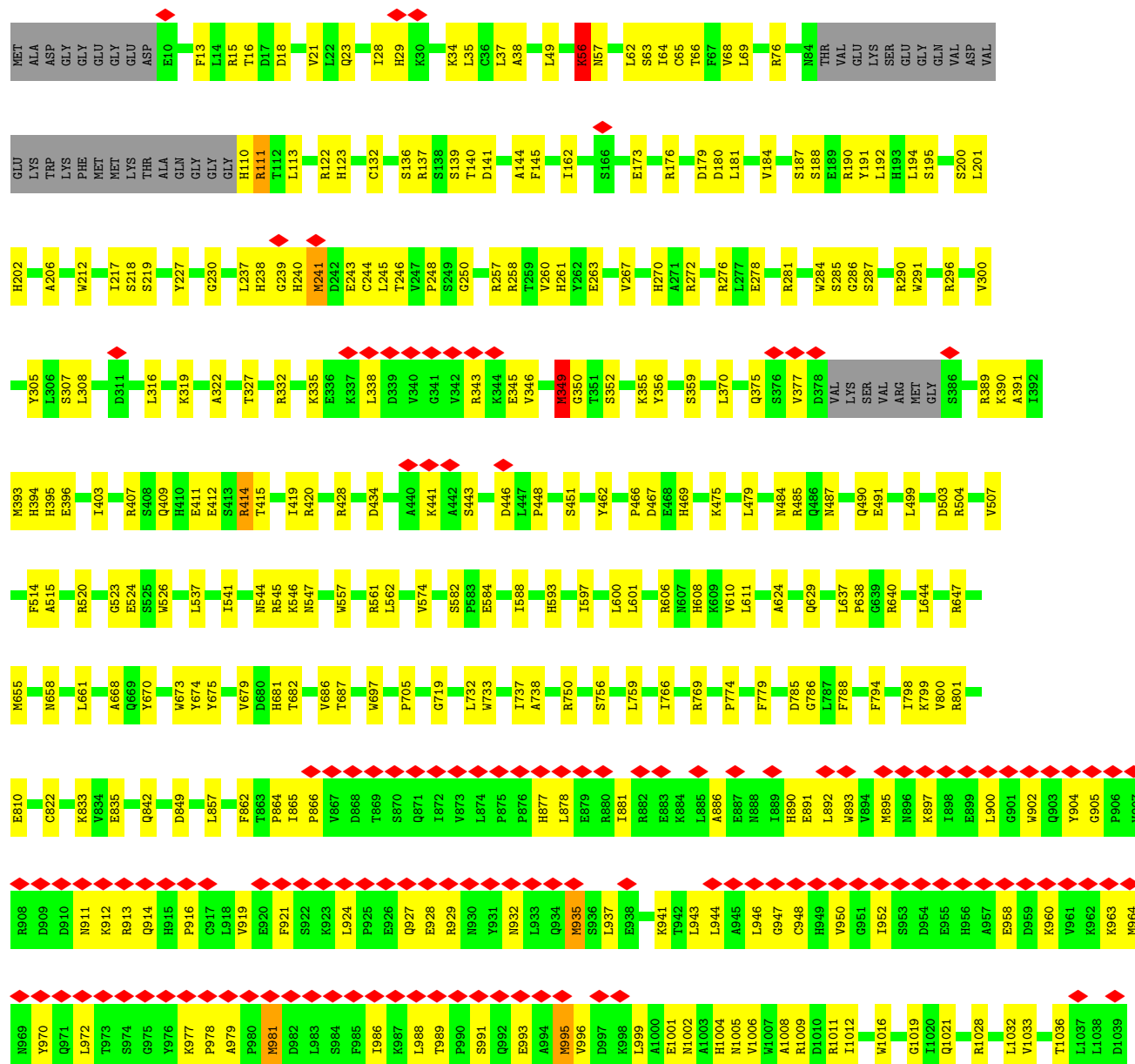








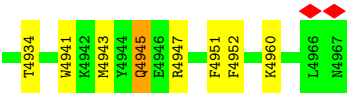
• Molecule 2: Ryanodine receptor 2











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20156	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 ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.629	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, ATP, XAN

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	E	0.27	0/834	0.50	0/1123
1	F	0.26	0/834	0.50	0/1123
1	G	0.26	0/834	0.50	0/1123
1	H	0.27	0/834	0.50	0/1123
2	A	0.27	0/34511	0.54	30/46614 (0.1%)
2	B	0.27	0/34511	0.54	30/46614 (0.1%)
2	C	0.27	0/34511	0.54	29/46614 (0.1%)
2	D	0.27	0/34511	0.54	30/46614 (0.1%)
All	All	0.27	0/141380	0.54	119/190948 (0.1%)

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
2	A	0	3
2	B	0	3
2	C	0	3
2	D	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2800	LEU	CA-CB-CG	13.22	145.71	115.30
2	D	2800	LEU	CA-CB-CG	13.22	145.71	115.30
2	B	2800	LEU	CA-CB-CG	13.22	145.70	115.30
2	A	2800	LEU	CA-CB-CG	13.21	145.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4242	ARG	CA-CB-CG	9.30	133.86	113.40

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	111	ARG	Sidechain
2	A	1614	ARG	Sidechain
2	A	4640	PHE	Peptide
2	D	111	ARG	Sidechain
2	D	1614	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	818	0	821	12	0
1	F	818	0	821	14	0
1	G	818	0	821	17	0
1	H	818	0	821	20	0
2	A	33771	0	33453	849	0
2	B	33771	0	33453	836	0
2	C	33771	0	33453	823	0
2	D	33771	0	33453	858	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	5	0
4	B	62	0	24	5	0
4	C	62	0	24	5	0
4	D	62	0	24	5	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	D	1	0	0	1	0
6	A	11	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	11	0	4	0	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
All	All	138656	0	137208	3337	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 12.

The worst 5 of 3337 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2844:MET:O	2:C:2848:TYR:HB2	1.61	1.01
2:A:2844:MET:O	2:A:2848:TYR:HB2	1.61	1.00
2:D:2844:MET:O	2:D:2848:TYR:HB2	1.61	0.99
2:B:2844:MET:O	2:B:2848:TYR:HB2	1.61	0.99
2:A:143:LEU:HD21	2:D:2325:ILE:HD11	1.44	0.99

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	A	4198/4967 (84%)	4091 (98%)	103 (2%)	4 (0%)	48	78
2	B	4198/4967 (84%)	4092 (98%)	102 (2%)	4 (0%)	48	78
2	C	4198/4967 (84%)	4091 (98%)	103 (2%)	4 (0%)	48	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	4198/4967 (84%)	4092 (98%)	102 (2%)	4 (0%)	48	78
All	All	17212/20300 (85%)	16778 (98%)	418 (2%)	16 (0%)	50	78

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1553	PHE
2	A	4641	PRO
2	A	4819	VAL
2	D	1553	PHE
2	D	4641	PRO

### 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	E	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	G	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
2	A	3708/4358 (85%)	3615 (98%)	93 (2%)	42	62
2	B	3708/4358 (85%)	3615 (98%)	93 (2%)	42	62
2	C	3708/4358 (85%)	3615 (98%)	93 (2%)	42	62
2	D	3708/4358 (85%)	3615 (98%)	93 (2%)	42	62
All	All	15184/17788 (85%)	14812 (98%)	372 (2%)	43	63

5 of 372 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2783	LEU
2	C	937	LEU
2	B	2863	LYS
2	B	3981	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	1614	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	2118	ASN
2	C	2899	ASN
2	D	544	ASN
2	D	487	ASN
2	C	2978	HIS

### 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 20 ligands modelled in this entry, 8 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
6	XAN	D	5004	-	7,12,12	1.69	1 (14%)	6,17,17	5.53	2 (33%)
6	XAN	A	5004	-	7,12,12	1.69	1 (14%)	6,17,17	5.49	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	XAN	C	5004	-	7,12,12	1.68	1 (14%)	6,17,17	5.50	2 (33%)
4	ATP	D	5005	-	28,33,33	0.73	0	34,52,52	0.72	1 (2%)
6	XAN	B	5004	-	7,12,12	1.70	1 (14%)	6,17,17	5.51	2 (33%)
4	ATP	A	5002	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	B	5002	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	B	5005	-	28,33,33	0.73	0	34,52,52	0.72	1 (2%)
4	ATP	C	5002	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	A	5005	-	28,33,33	0.73	0	34,52,52	0.72	1 (2%)
4	ATP	D	5002	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	C	5005	-	28,33,33	0.74	0	34,52,52	0.72	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
6	XAN	D	5004	-	-	-	0/2/2/2
6	XAN	A	5004	-	-	-	0/2/2/2
6	XAN	C	5004	-	-	-	0/2/2/2
4	ATP	D	5005	-	-	8/18/38/38	0/3/3/3
6	XAN	B	5004	-	-	-	0/2/2/2
4	ATP	A	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5005	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	A	5005	-	-	8/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	C	5005	-	-	8/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5004	XAN	C6-N1	4.14	1.40	1.33
6	D	5004	XAN	C6-N1	4.10	1.40	1.33
6	A	5004	XAN	C6-N1	4.10	1.40	1.33
6	C	5004	XAN	C6-N1	4.09	1.40	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	D	5004	XAN	C2-N1-C6	11.36	124.68	115.09
6	B	5004	XAN	C2-N1-C6	11.31	124.64	115.09
6	C	5004	XAN	C2-N1-C6	11.29	124.63	115.09
6	A	5004	XAN	C2-N1-C6	11.27	124.61	115.09
6	D	5004	XAN	C5-C6-N1	-6.91	114.18	123.42

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5005	ATP	PB-O3B-PG-O2G
4	A	5005	ATP	C5'-O5'-PA-O1A
4	A	5005	ATP	C5'-O5'-PA-O2A
4	A	5005	ATP	C5'-O5'-PA-O3A
4	D	5005	ATP	PB-O3B-PG-O2G

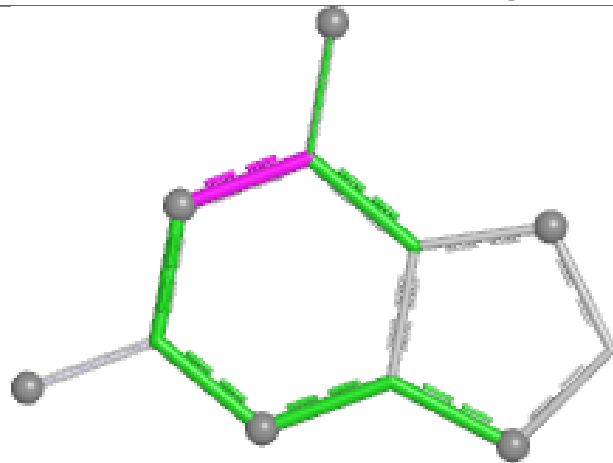
There are no ring outliers.

4 monomers are involved in 20 short contacts:

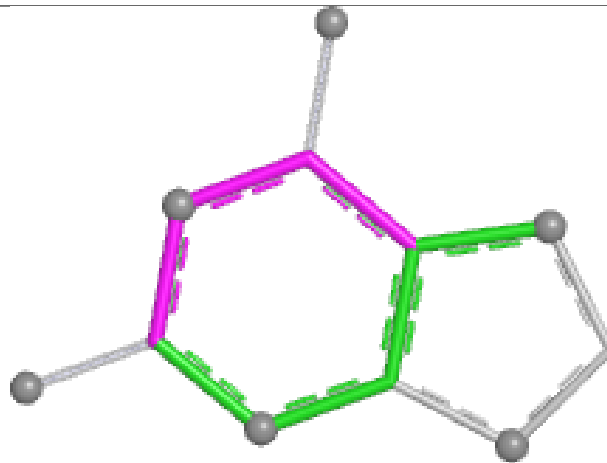
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5002	ATP	5	0
4	B	5002	ATP	5	0
4	C	5002	ATP	5	0
4	D	5002	ATP	5	0

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.

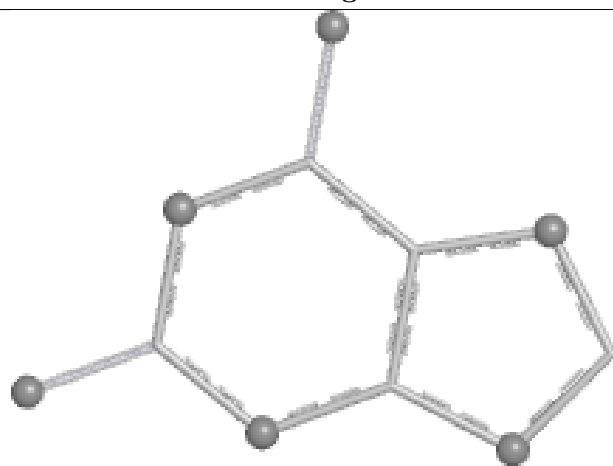
## Ligand XAN D 5004



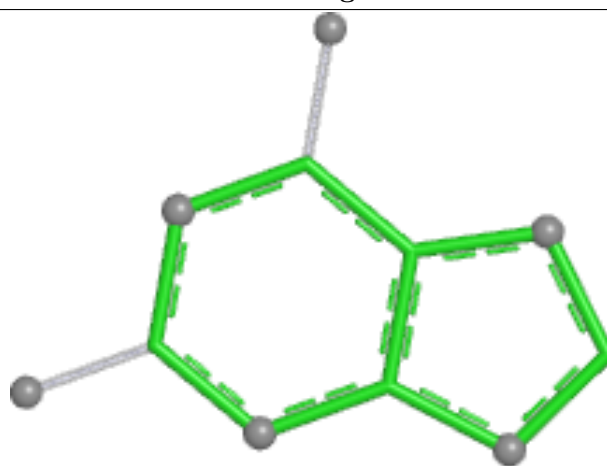
Bond lengths



Bond angles

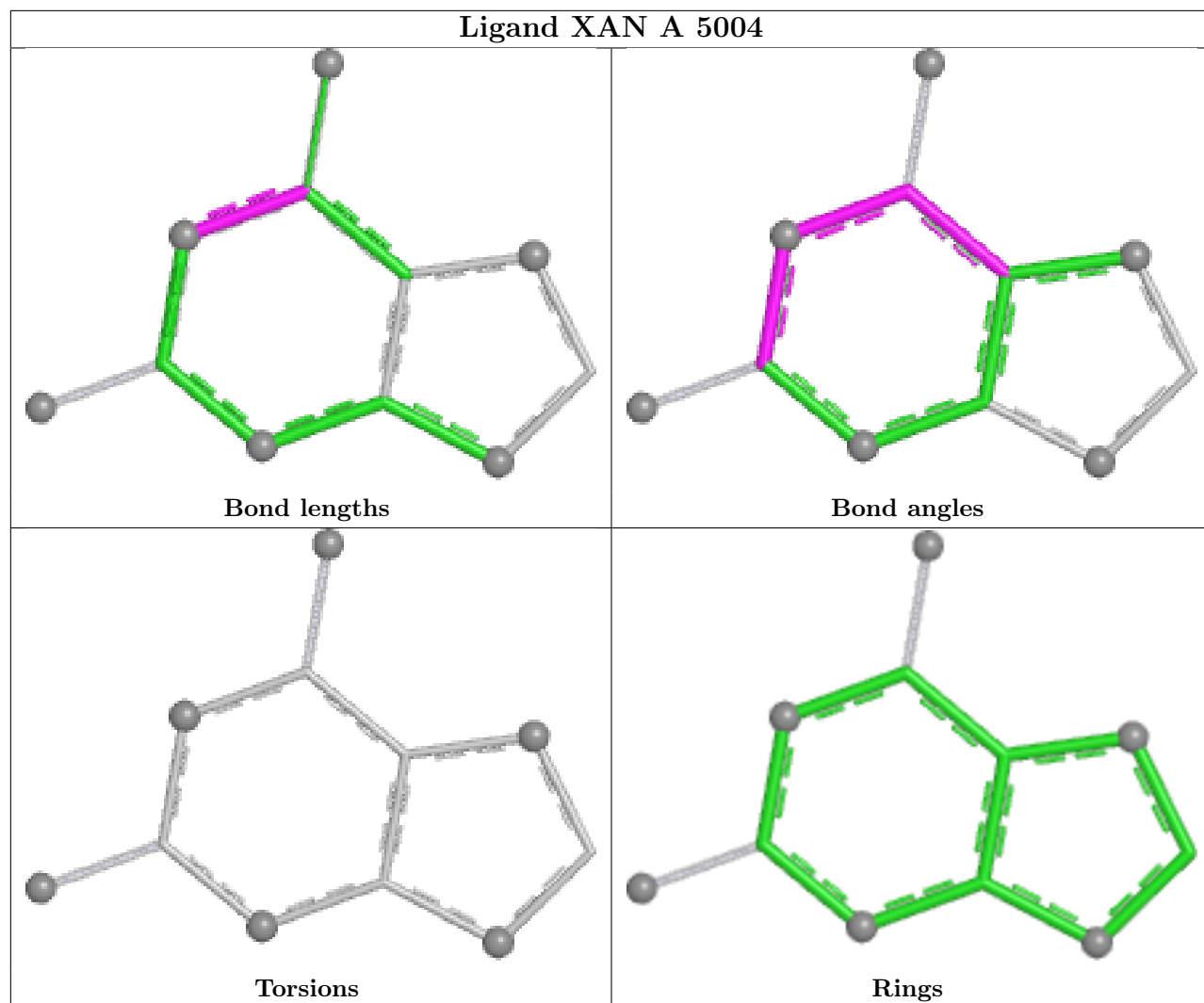


Torsions

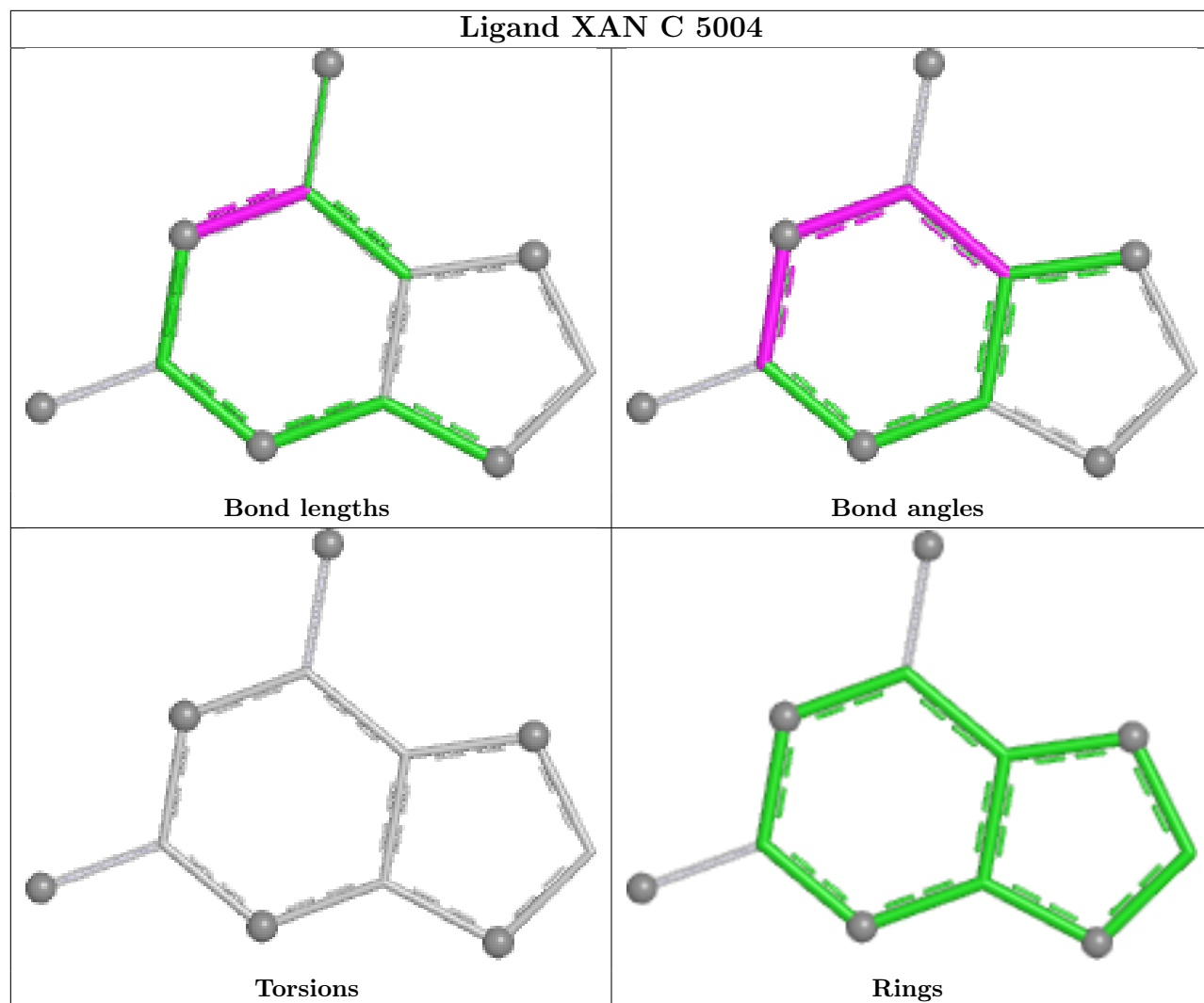


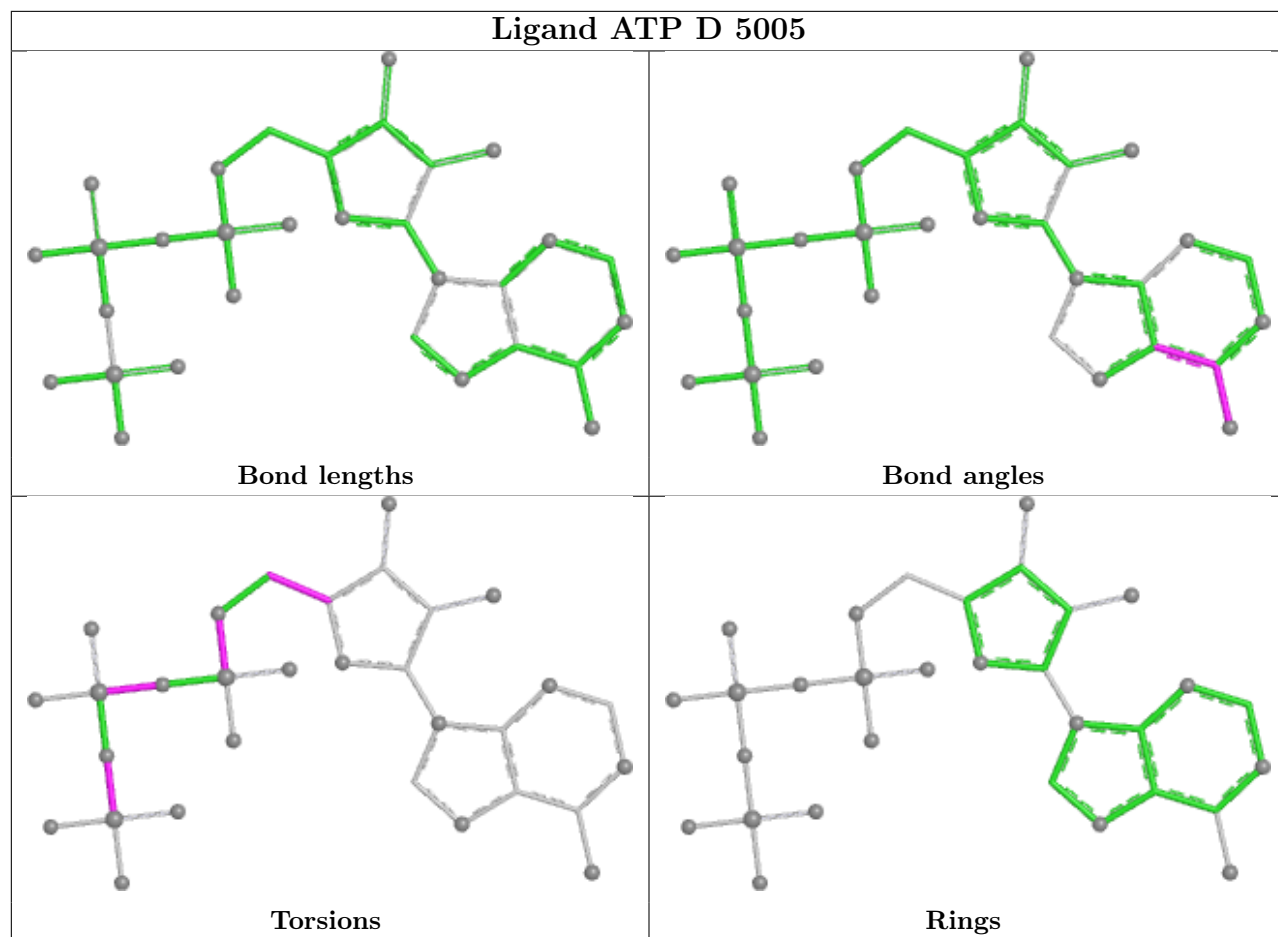
Rings

## Ligand XAN A 5004

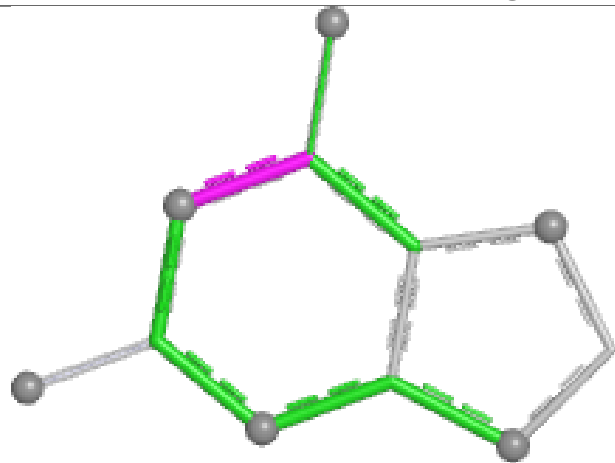




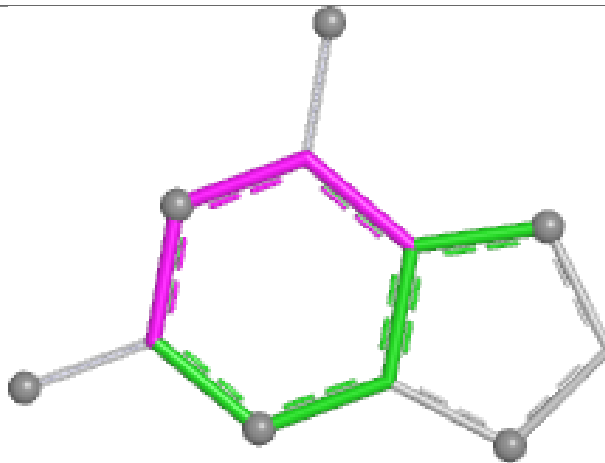




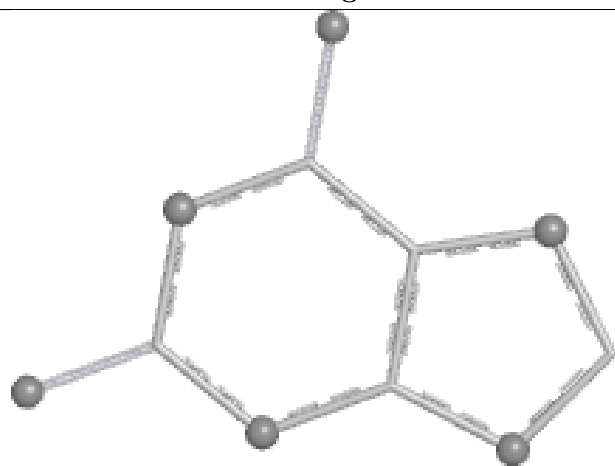
## Ligand XAN B 5004



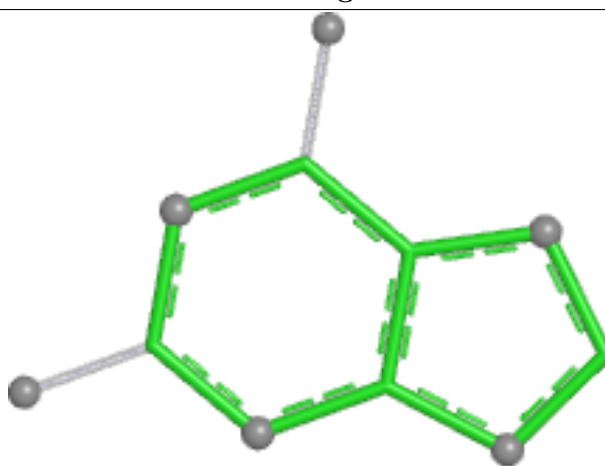
Bond lengths



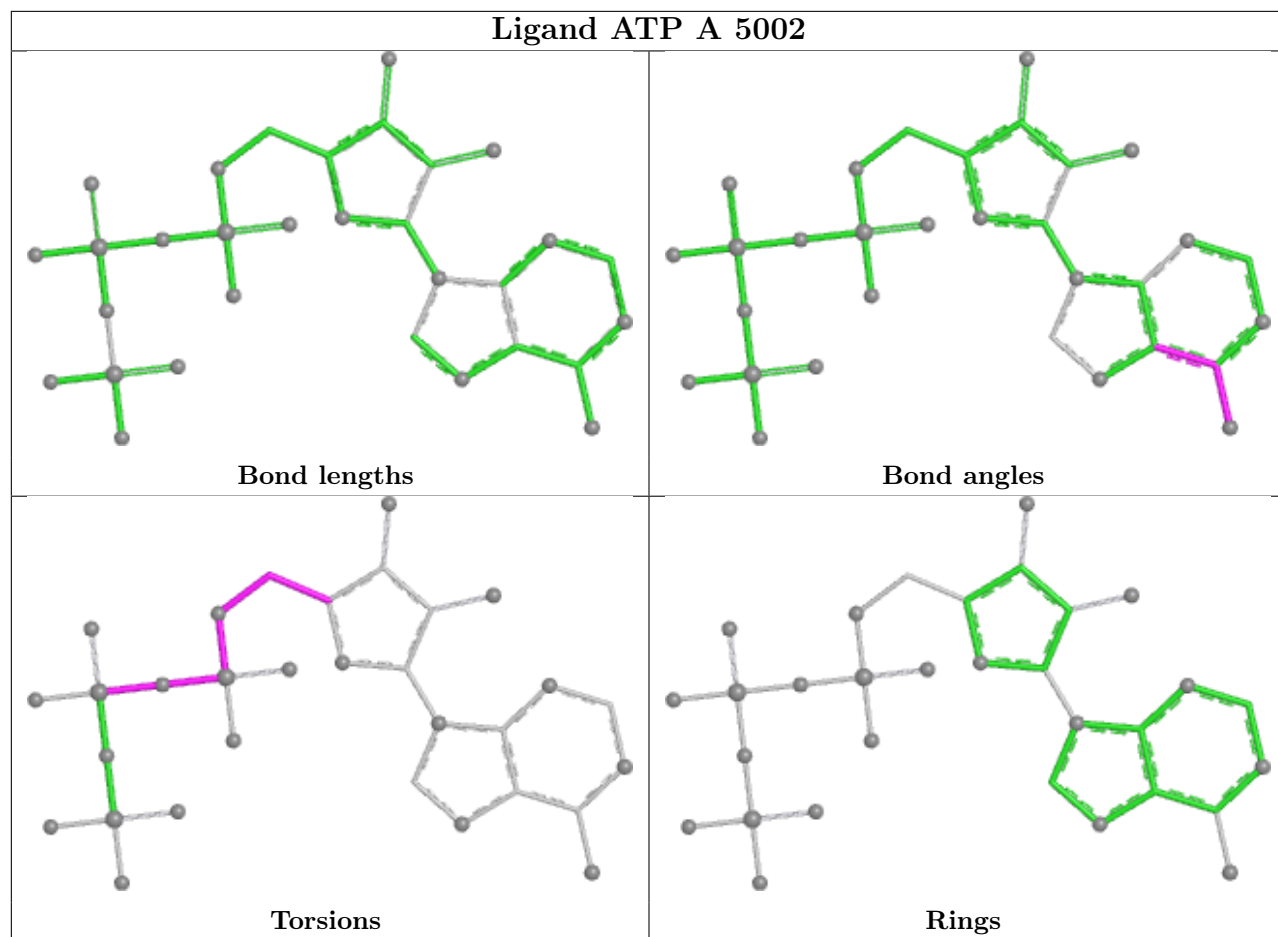
Bond angles

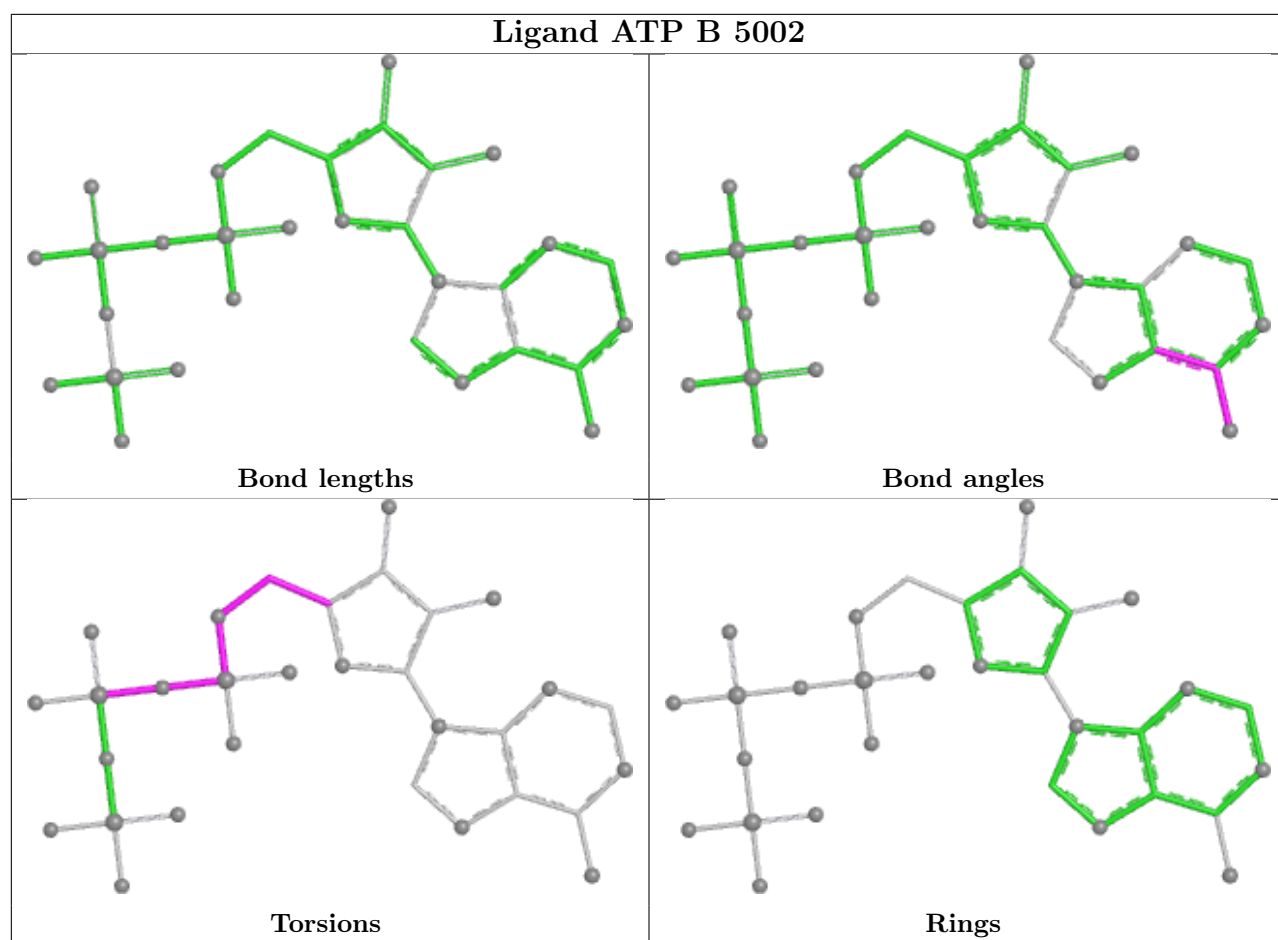


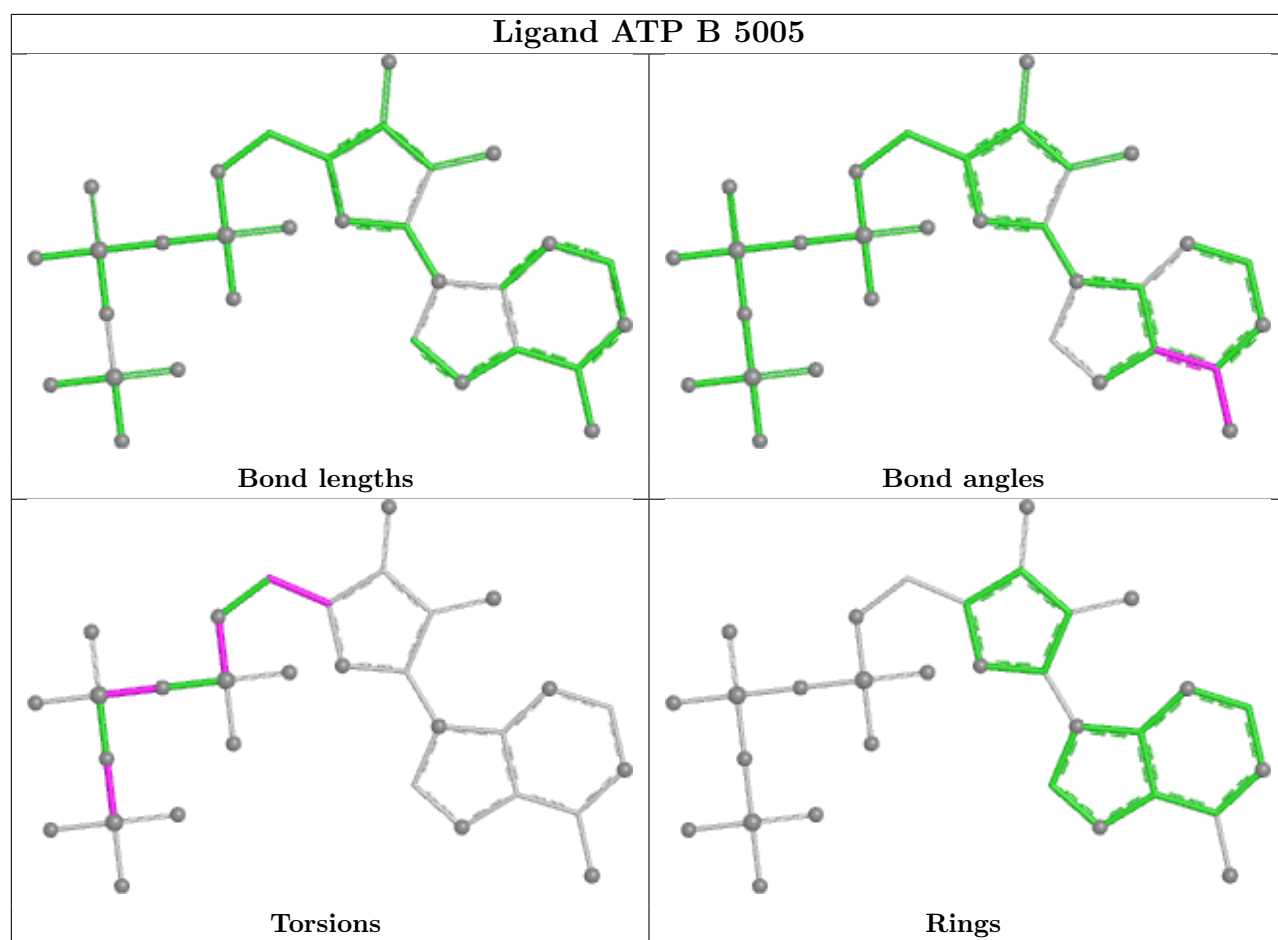
Torsions

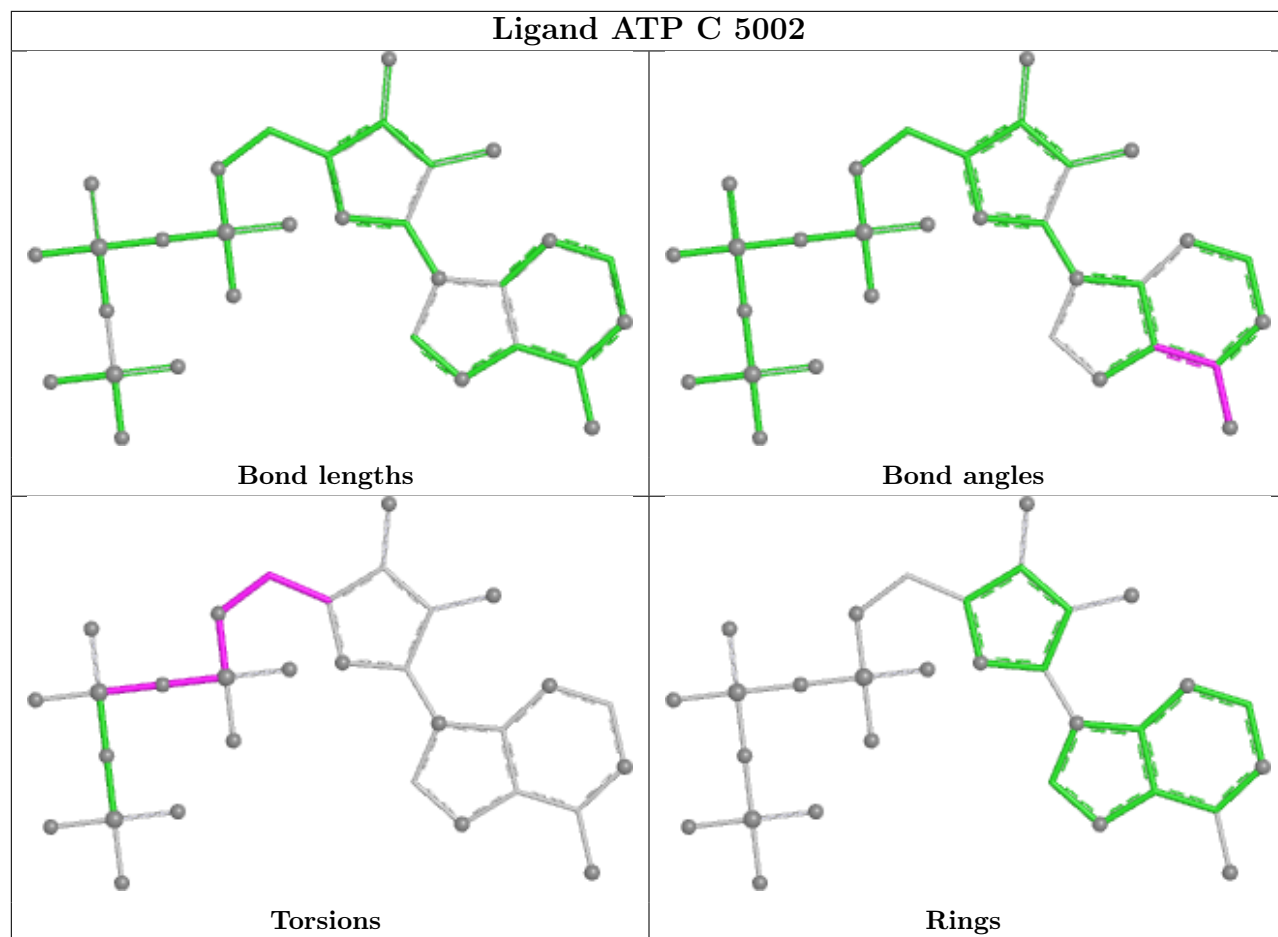


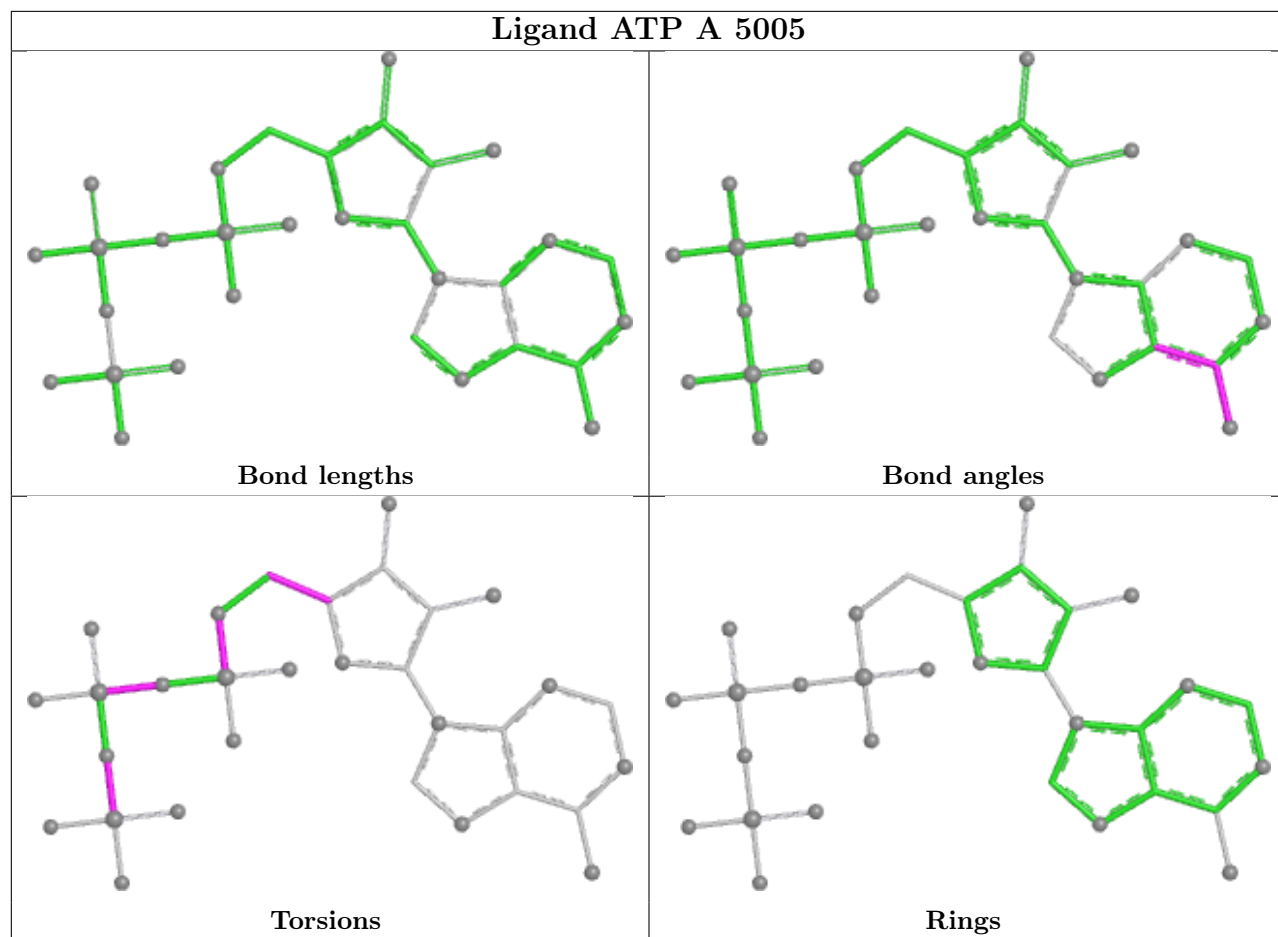
Rings



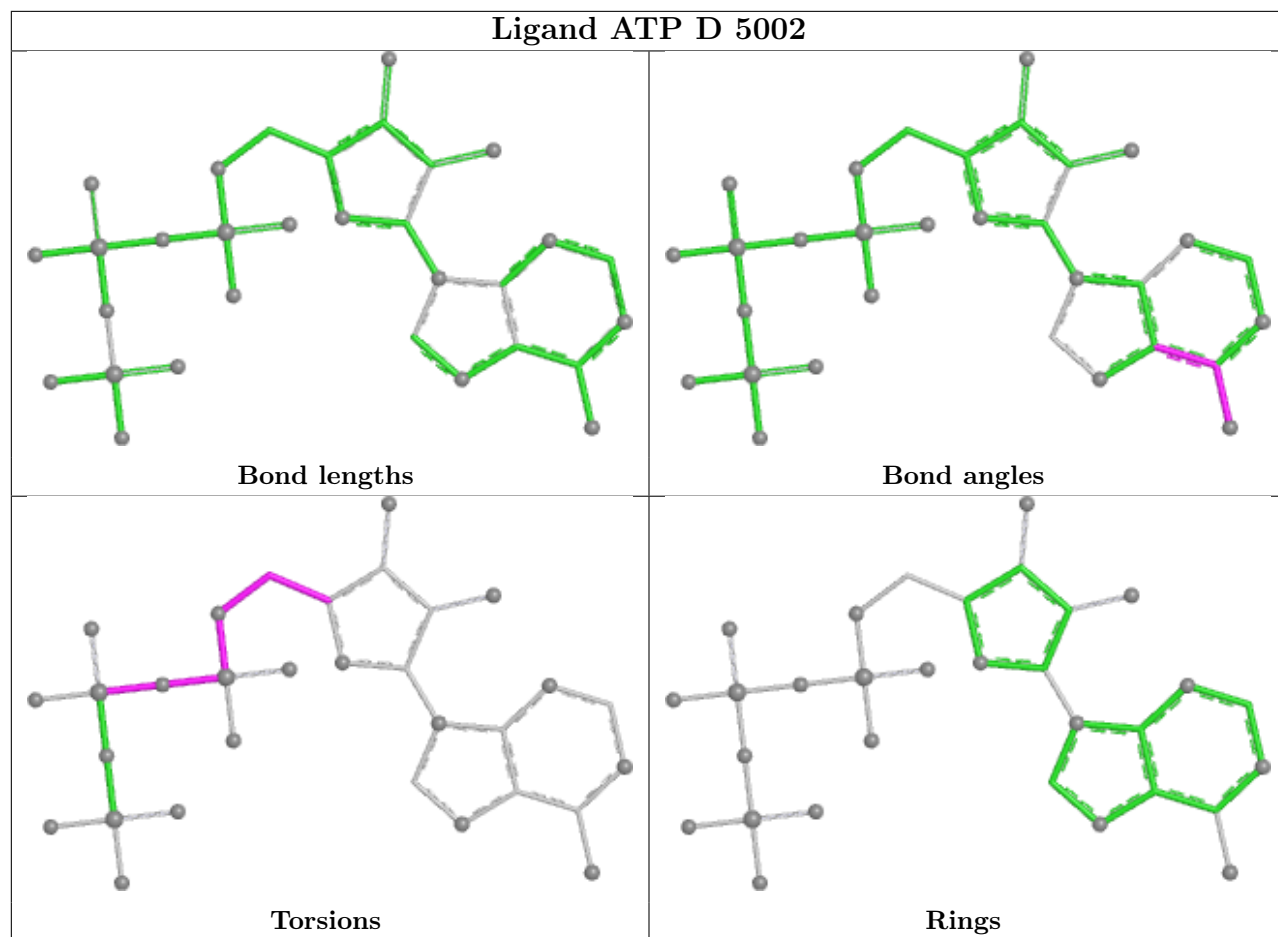


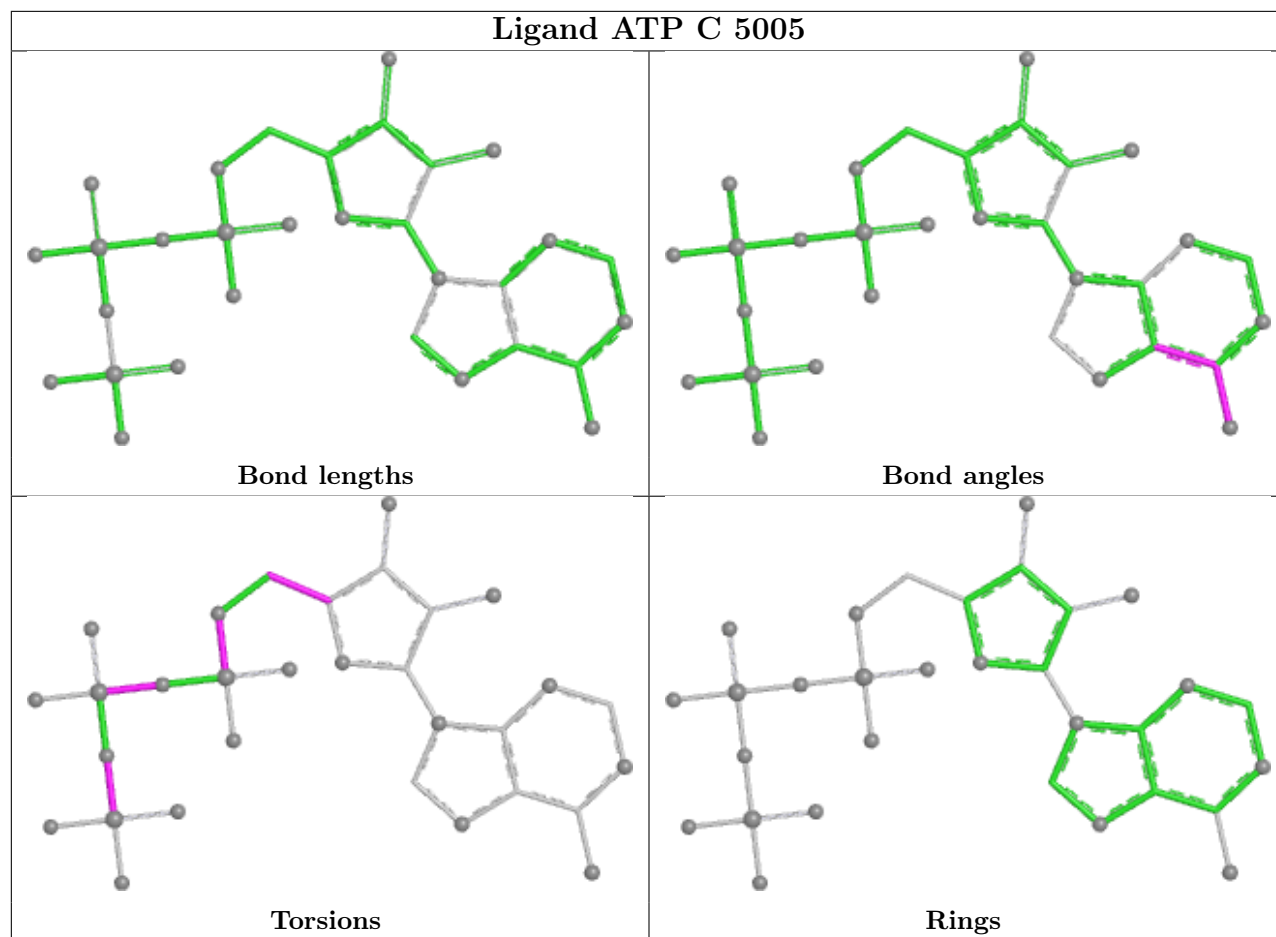












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

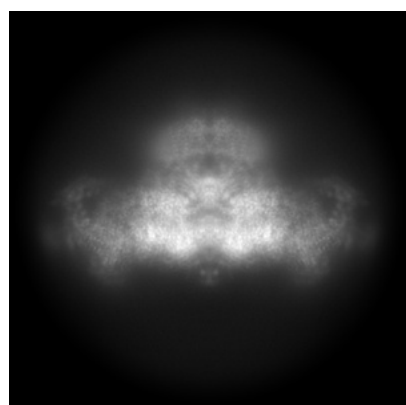
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26407. These allow visual inspection of the internal detail of the map and identification of artifacts.

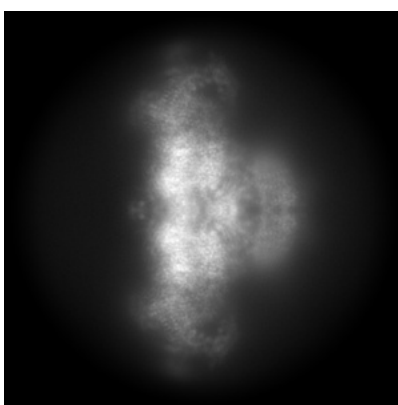
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

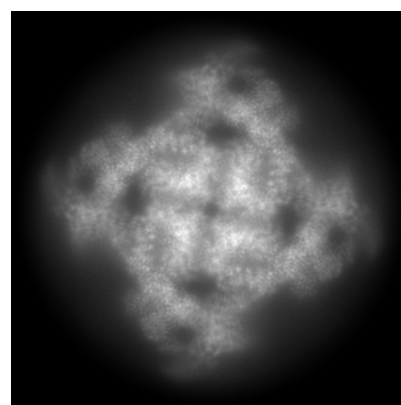
#### 6.1.1 Primary map



X



Y

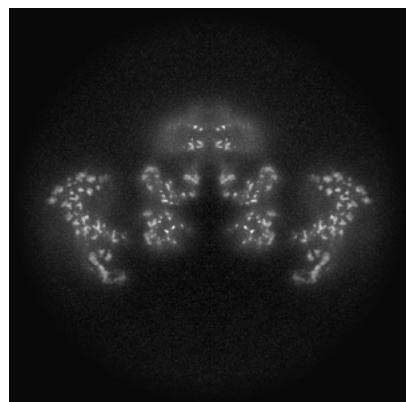


Z

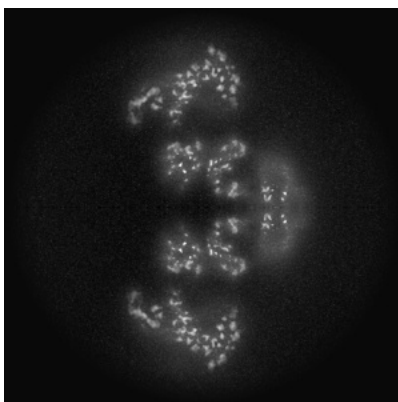
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

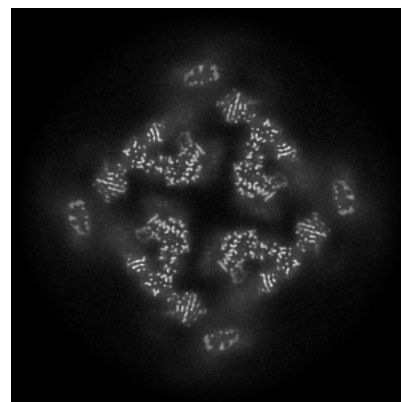
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

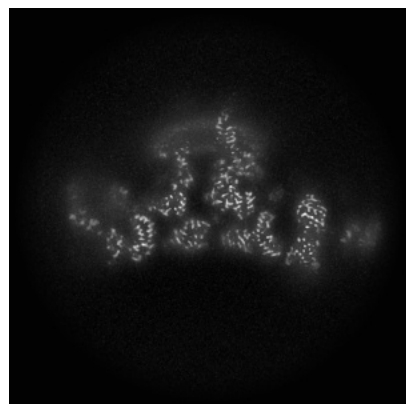


Z Index: 256

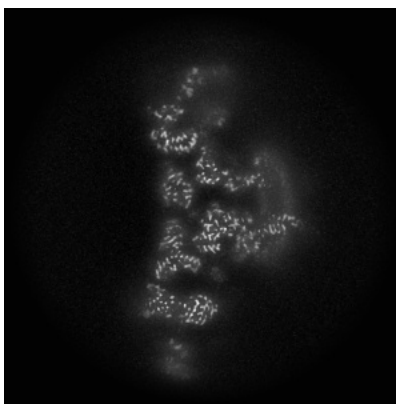
The images above show central slices of the map in three orthogonal directions.

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

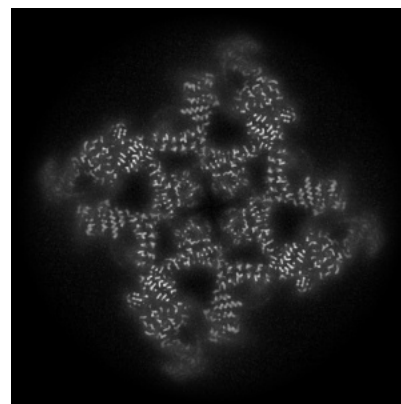
### 6.3.1 Primary map



X Index: 292



Y Index: 292

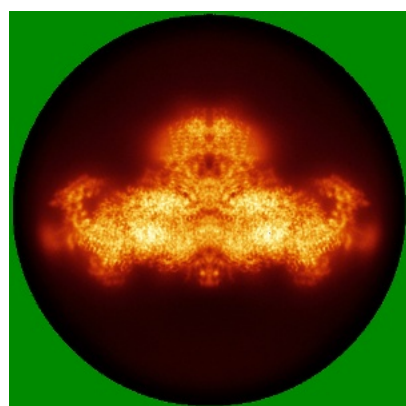


Z Index: 227

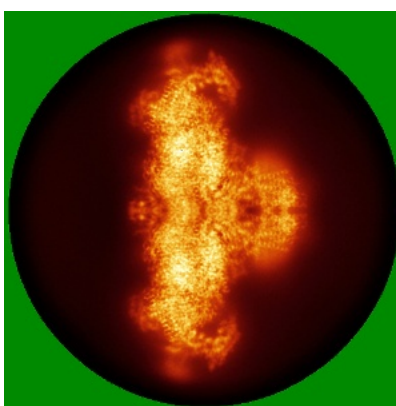
The images above show the largest variance slices of the map in three orthogonal directions.

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

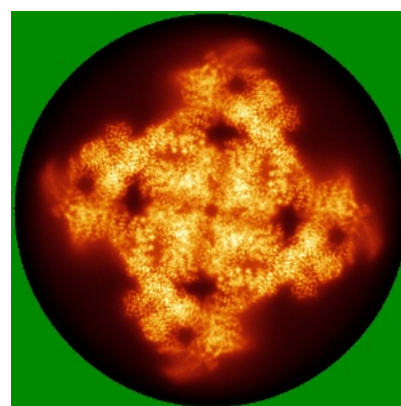
### 6.4.1 Primary map



X



Y

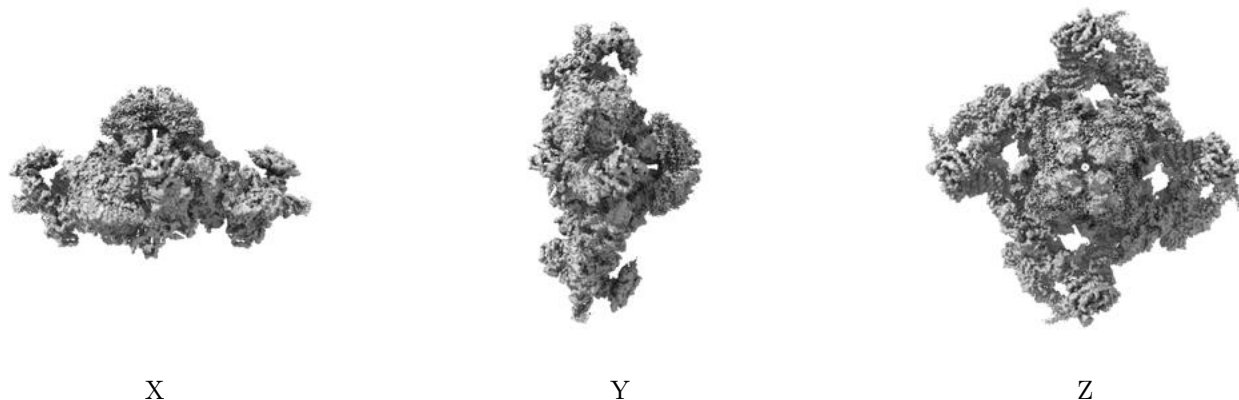


Z

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 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

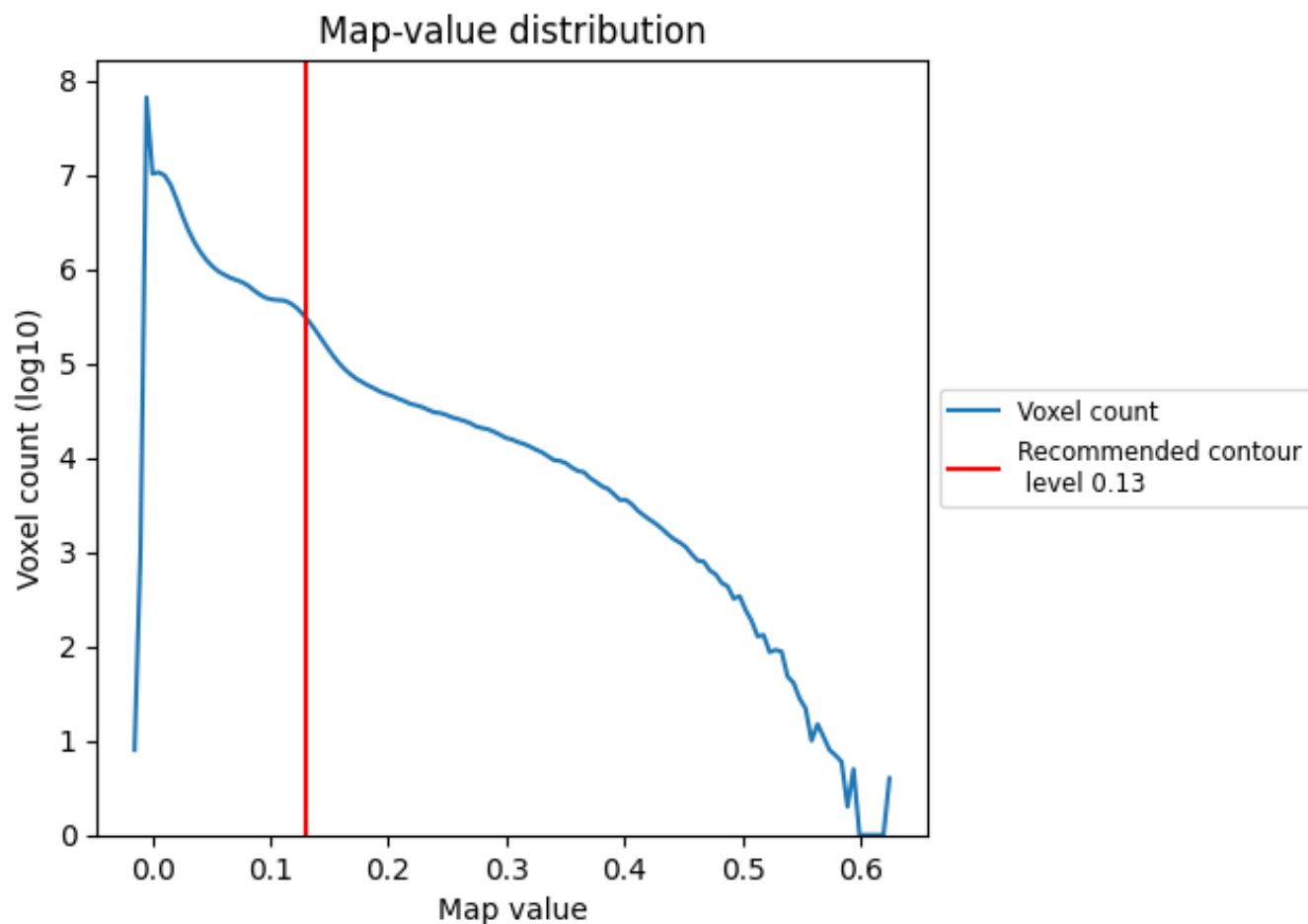
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

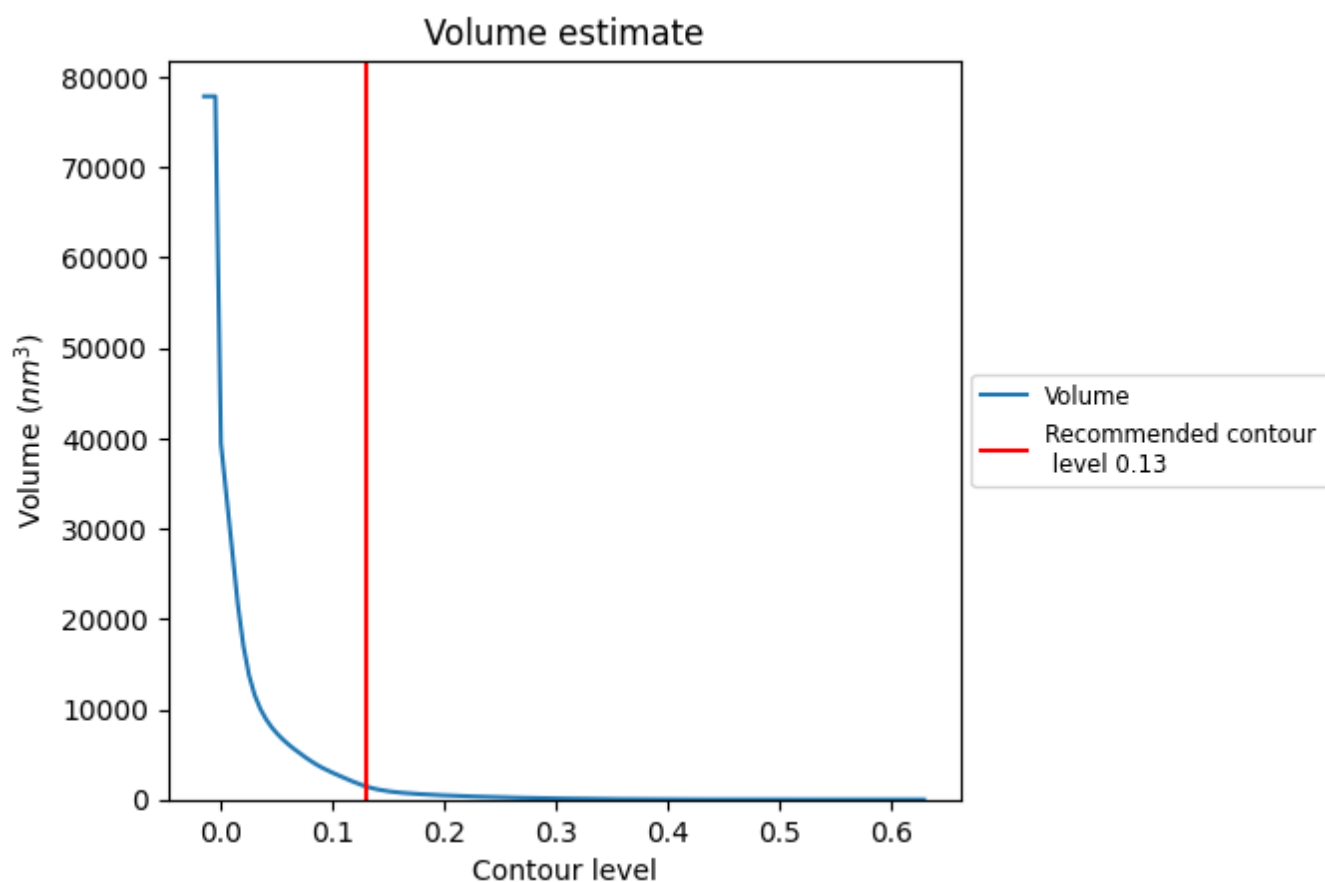
This section contains the results of statistical analysis of the map.

### 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.

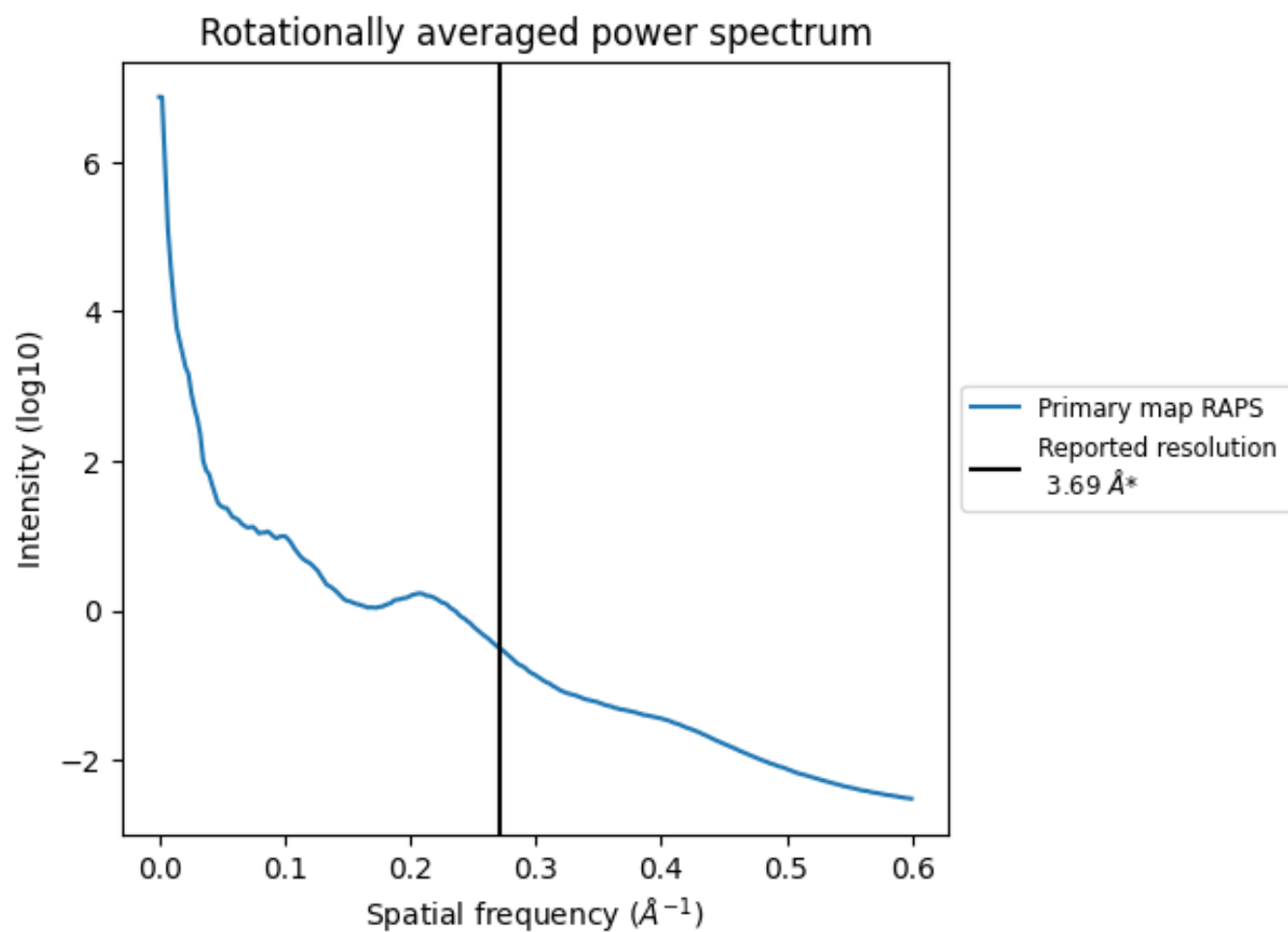
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $1461 \text{ nm}^3$ ; this corresponds to an approximate mass of 1320 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 0.271 Å<sup>-1</sup>



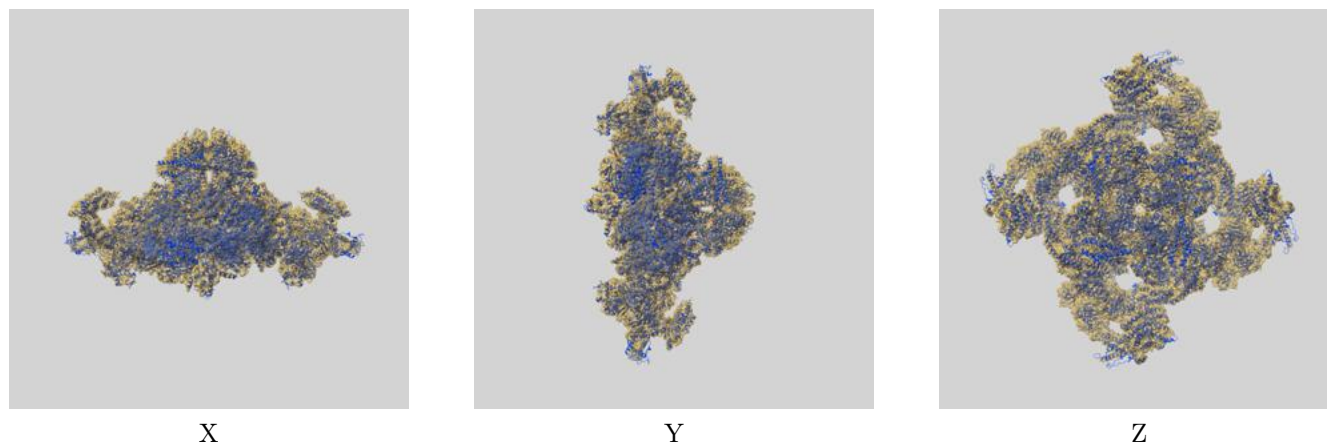
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

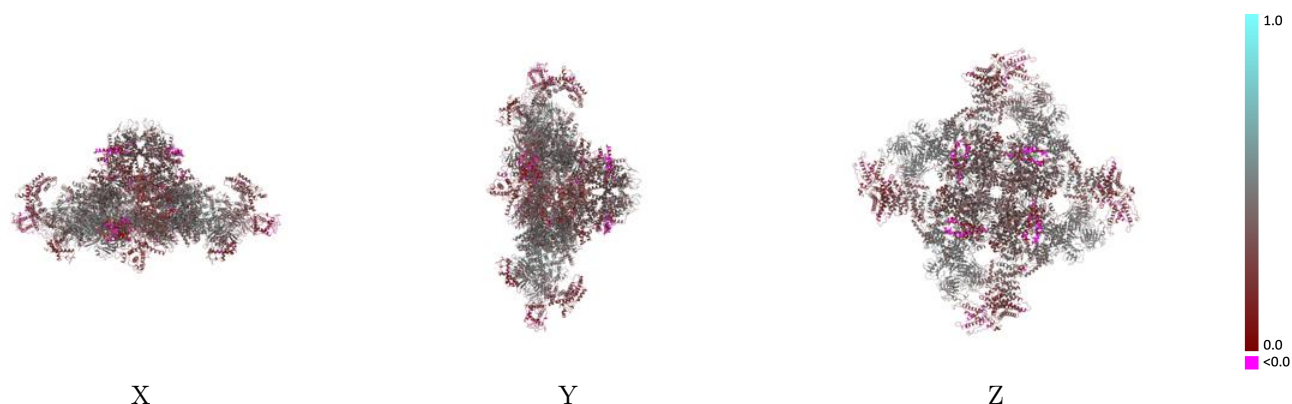
This section contains information regarding the fit between EMDB map EMD-26407 and PDB model 7U9R. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



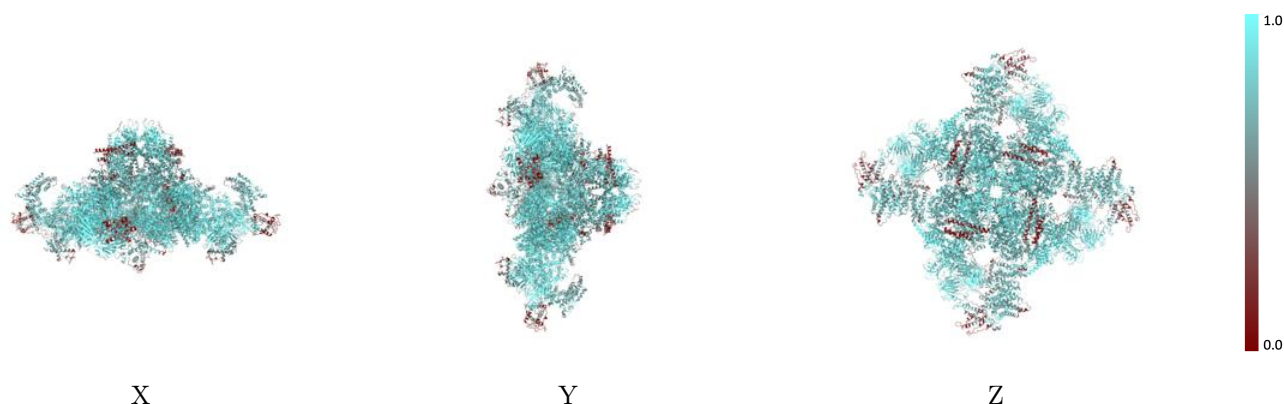
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



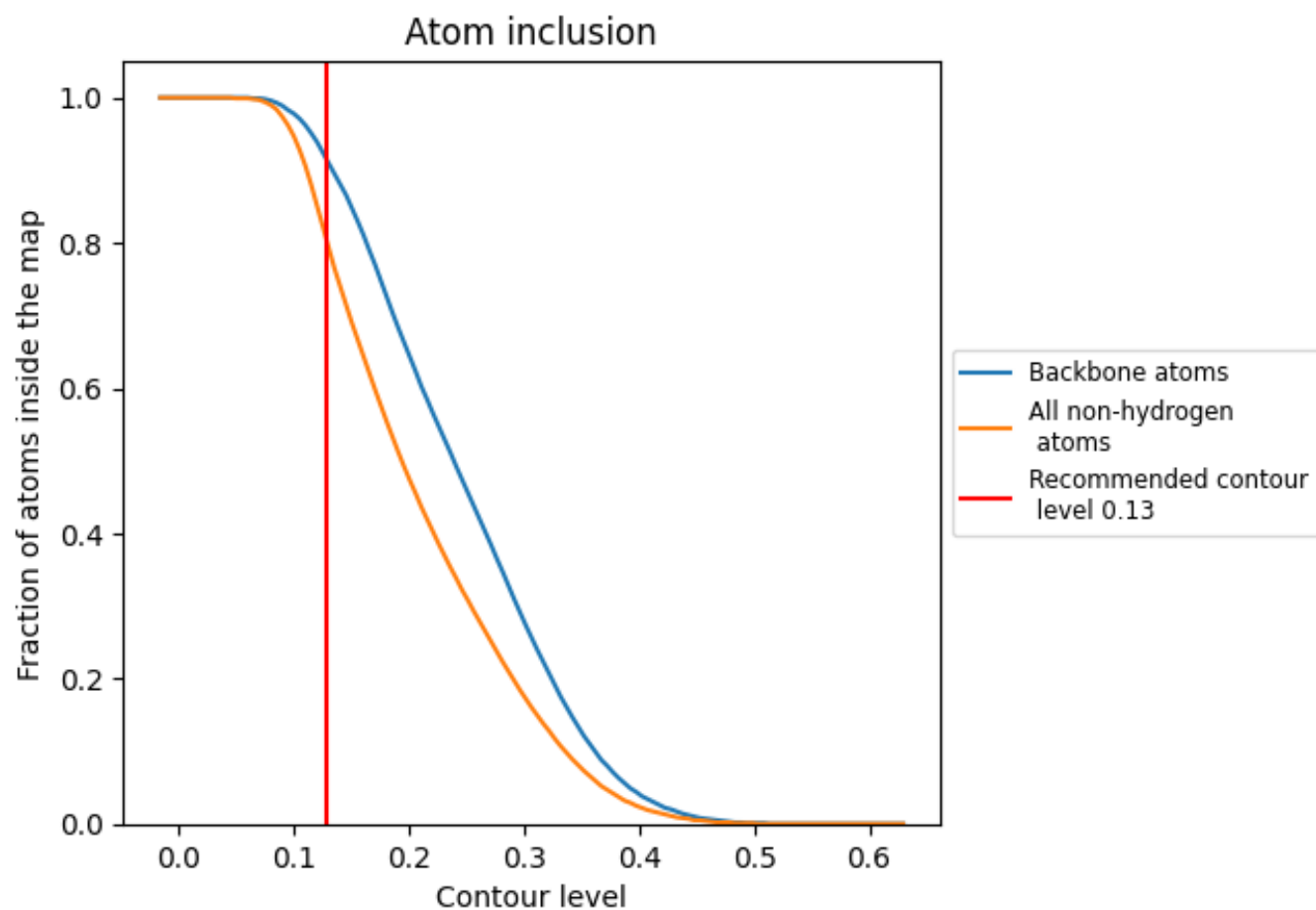
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 80% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7980	<div><div></div></div> 0.3530
A	<div><div></div></div> 0.7990	<div><div></div></div> 0.3650
B	<div><div></div></div> 0.7930	<div><div></div></div> 0.3440
C	<div><div></div></div> 0.7910	<div><div></div></div> 0.3410
D	<div><div></div></div> 0.7960	<div><div></div></div> 0.3510
E	<div><div></div></div> 0.9170	<div><div></div></div> 0.4850
F	<div><div></div></div> 0.9190	<div><div></div></div> 0.4720
G	<div><div></div></div> 0.9120	<div><div></div></div> 0.4770
H	<div><div></div></div> 0.9090	<div><div></div></div> 0.4720

1.0

0.0

<0.0