



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 03:42 AM EDT

PDB ID : 8TLA  
EMDB ID : EMD-41366  
Title : Human Type 3 IP3 Receptor - Higher-Order Inhibited State - Symmetry Mate  
1  
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.  
Deposited on : 2023-07-26  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

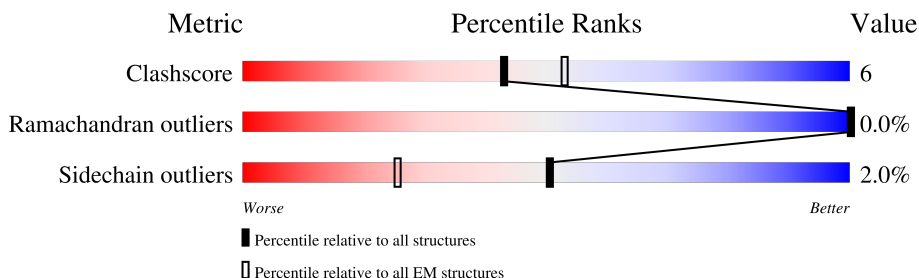
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	2671	<div> <div>30%</div> <div>61%</div> <div>13%</div> <div>26%</div> </div>
1	B	2671	<div> <div>34%</div> <div>61%</div> <div>13%</div> <div>26%</div> </div>
1	C	2671	<div> <div>17%</div> <div>65%</div> <div>10%</div> <div>25%</div> </div>
1	D	2671	<div> <div>14%</div> <div>65%</div> <div>11%</div> <div>24%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 130502 atoms, of which 65433 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.

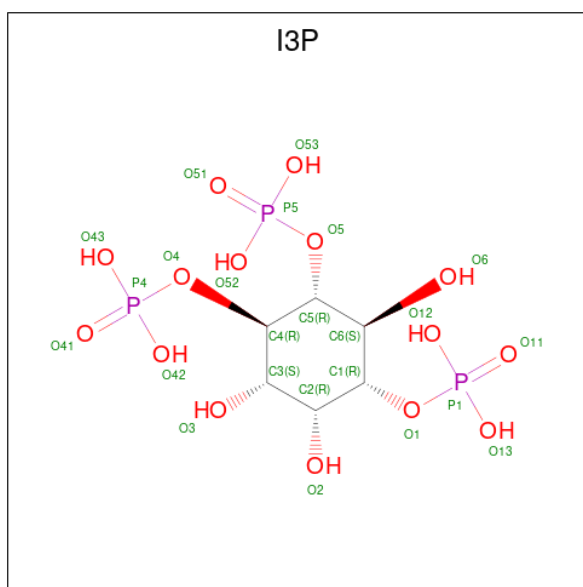
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1989	Total	C	H	N	O	S	0	0
			32350	10293	16244	2749	2960	104		
1	B	1987	Total	C	H	N	O	S	0	0
			32312	10283	16225	2743	2957	104		
1	C	2004	Total	C	H	N	O	S	0	0
			32571	10370	16344	2767	2986	104		
1	D	2034	Total	C	H	N	O	S	0	0
			32957	10480	16536	2807	3029	105		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: C<sub>6</sub>H<sub>15</sub>O<sub>15</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

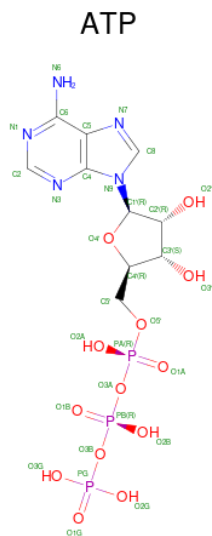


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

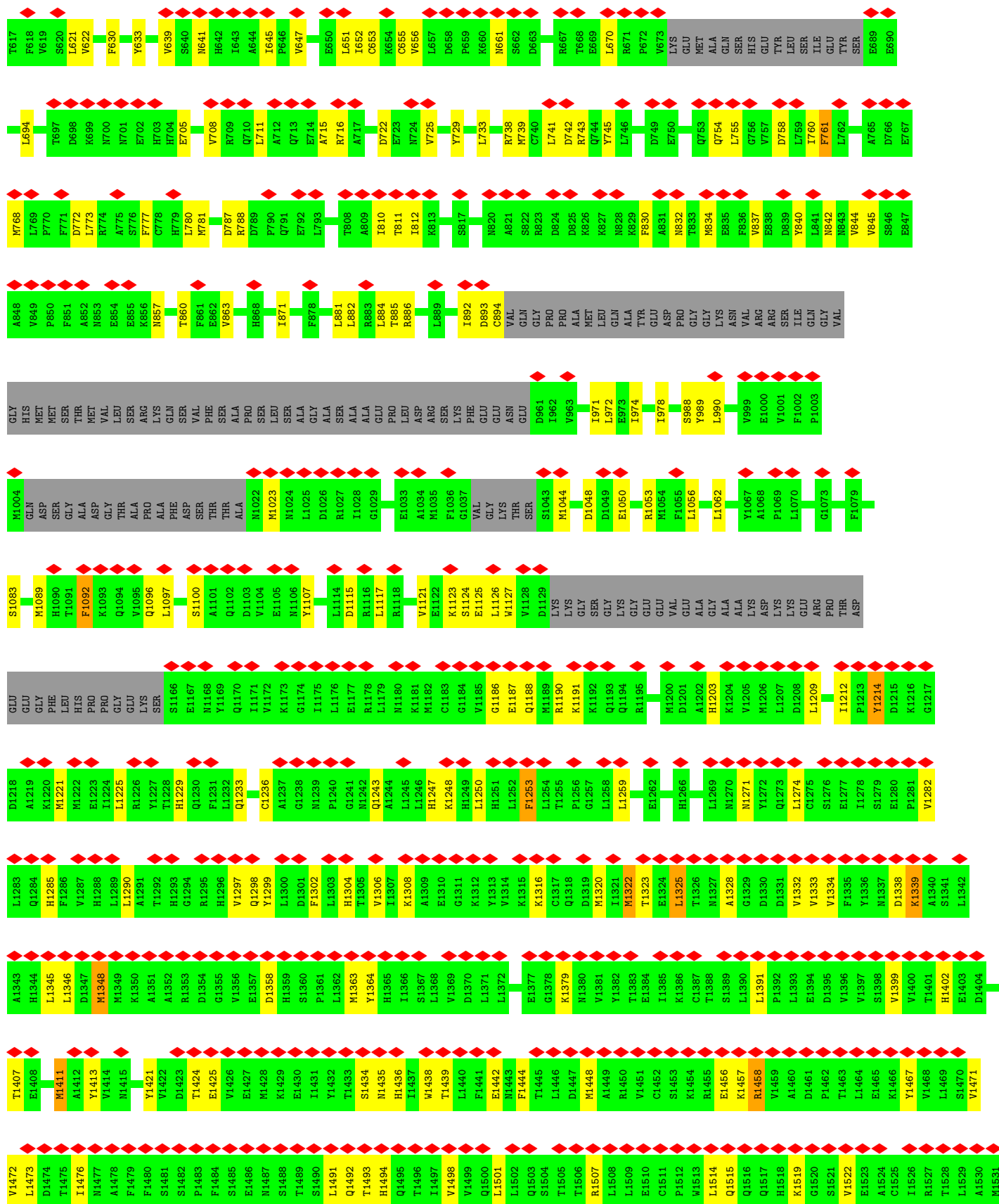
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

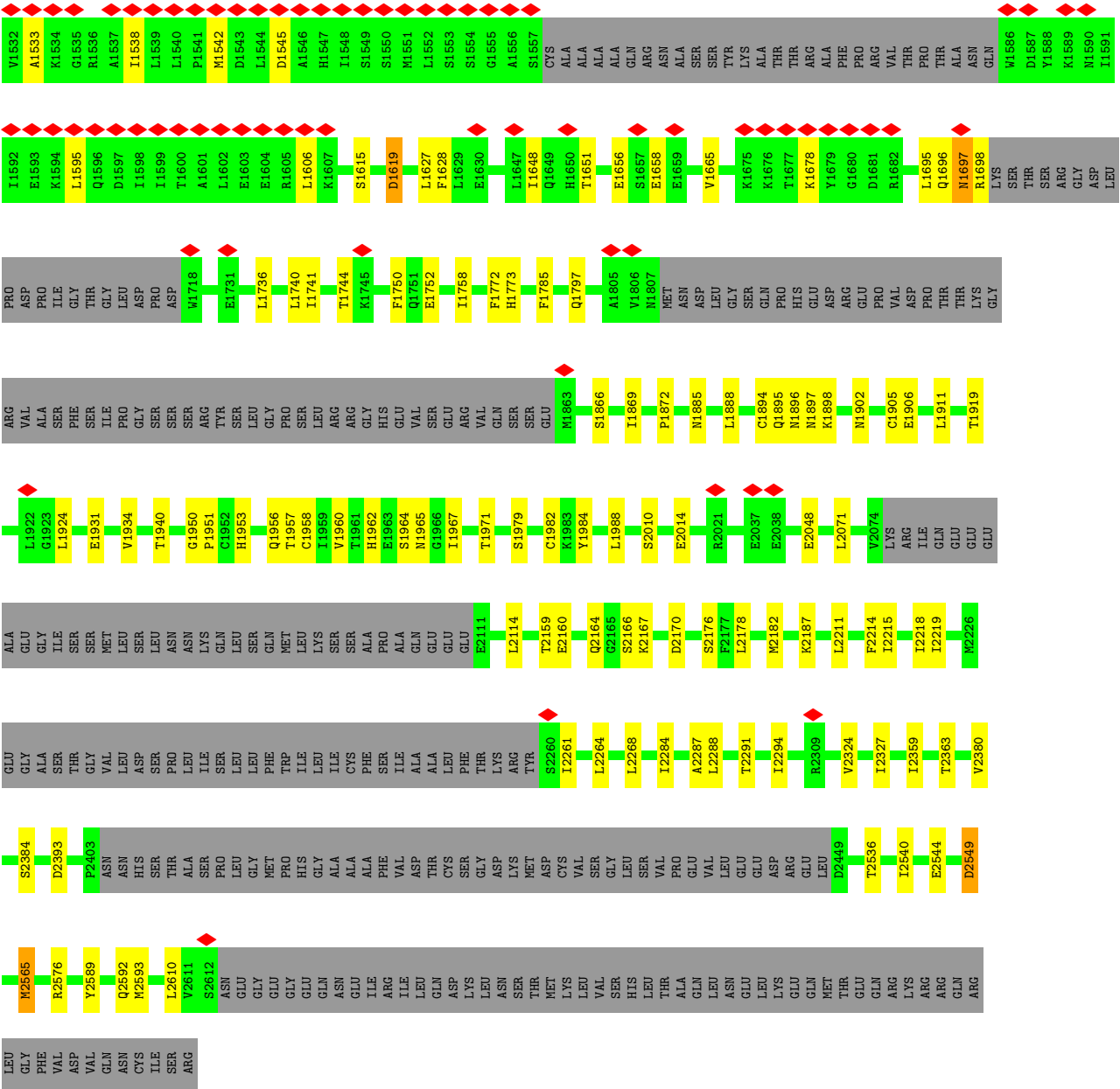
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



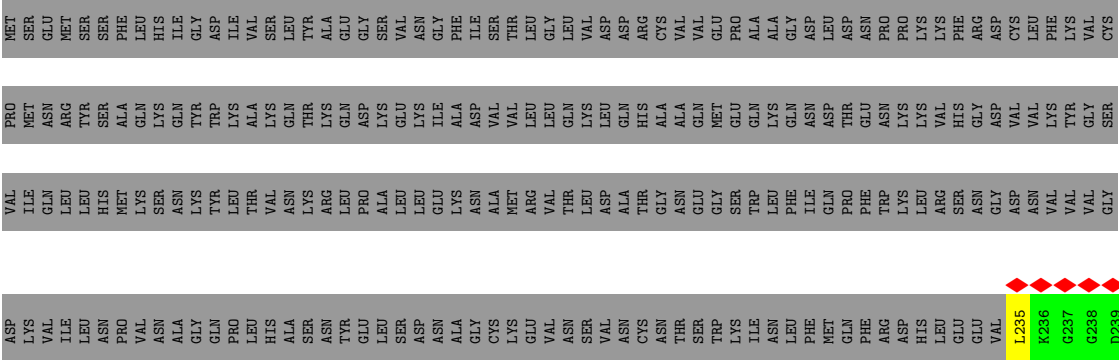
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0







● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

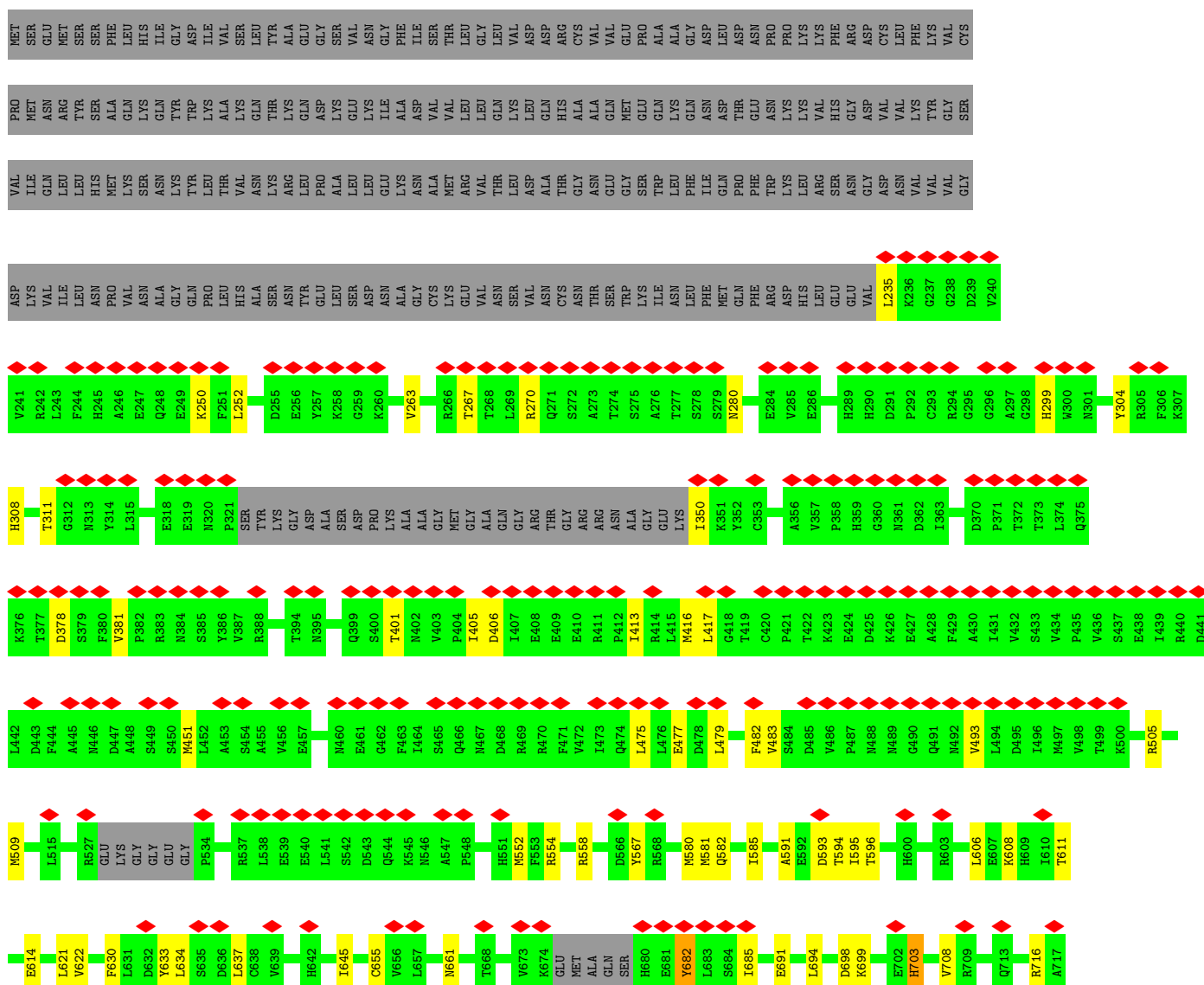




PRO	ALA	M1022	M1023	M1024	L1025	D1026	R1027	E1030	Q1031	A1032	M1035	F1036	G1037	VAL	ASN	GLY	LYS	THR	SER	M1044	S1043	M1045	L1046	V1047	D1048	D1049	E1050	G1051	M1054	F1055	L1056	R1057	V1058	Y1067	A1068	P1069	L1070	V1071	S1072	L1077	L1078	F1079	Q1086	H1090	T1091	F1092	K1093												
SER	VAL	PHE	ASP	ALA	PRO	THR	THR	ALA	L881	L884	T885	L888	L889	G890	I891	D892	K893	C894	VAL	GLN	GLY	ASN	GLU	D961	I962	V963	E966	L969	K970	I971	L972	E973	I974	I978	D984	L991	E1000	V1001	F1002	P1003	M1004	GLN	ASP	SER	GLY	VAL	LEU	SER	ARG	LYS	GLN								
N301	G302	L303	Y304	R305	F306	K307	H308	L309	A310	T311	G312	N313	Y314	L315	A316	A317	E318	E319	N320	P321	SER	LYS	TVR	GLY	ASP	SER	PRO	LYS	ALA	ALA	GLY	MET	GLY	GLY	ALA	GLN	GLY	ARG	ARG	ASN	ALA	GLY	LYS	I350	K351	Y352	V355	A356	V357	P358	H359	G360	N361						
D362	I363	A364	S365	L366	F367	E368	L369	D370	P371	T372	T373	L374	Q375	K376	T377	D378	S379	F380	V381	P382	R383	N384	Y385	S386	V387	R388	L389	R390	H391	L392	C393	T394	T396	W397	I398	Q399	S400	T401	N402	V403	P404	I405	D406	I407	E408	E409	E410	R411	P412	I413	R414	L415	M416	L417	G418	T419	C420	P421	
T422	K423	E424	D425	K426	E427	A428	F429	A430	I431	V432	S433	V434	P435	V436	S437	E438	I439	R440	D441	L442	D443	F444	A445	N446	D447	A448	S449	S450	M451	L452	A453	S454	A455	V456	E457	K458	L459	N460	E461	G462	F463	I464	S465	Q466	N467	D468	R469	R470	F471	V472	I473	Q474	L475	L476	E477	D478	L479	V480	F481
F482	V483	S484	D485	V486	P487	N488	N489	G490	Q491	N492	V493	L494	D495	I496	M497	V498	T499	K500	P501	N502	R503	E504	R505	Q506	K507	L508	M509	E511	Q512	N513	I514	L515	K516	Q517	V518	F519	G520	I521	L522	K523	A524	P525	F526	R527	GLU	LYS	GLY	GLY	GLY	P534	L535	V536	R537	L538	E539	E540	L541		
S542	D543	Q544	K545	N546	P547	K548	V549	Q550	H551	N552	F553	R554	L555	C556	Y557	R558	V559	L560	R561	H562	S563	Q564	E565	D566	Y567	R568	K569	N570	Q571	E572	H573	D574	A575	K576	Q577	F578	G579	M580	M581	Q582	S583	Q584	T585	G586	V587	D588	L589	L590	A591	E592	D593	T594	I595	T596	A597	L598	L599	H600	N601
N602	R603	K604	L605	L606	E607	K608	H609	I610	T611	K612	T613	E614	V615	E616	T617	F618	V619	S620	L621	K624	N625	R626	E627	F630	L631	D632	Y633	L634	S635	D636	L637	C638	V639	S640	N641	H642	I643	A644	I645	L646	I647	C653	D654	C655	V656	L657	D658	P659	K660	N661	S662	D663	T664	L665					
I666	R667	T668	E669	L670	R671	P672	V673	LYS	GLU	MET	GLN	SER	HIS	GLU	TVR	LEU	ILE	GLU	TVR	E689	E690	E691	V692	M693	L694	T695	N696	T697	D698	K699	N700	N701	E702	H703	H704	E705	K706	S707	V708	R709	Q710	L711	A712	Q713	E714	A715	R716	G718	N719	A720	H721	D722	E723	N724	V725				
Y726	Q732	D742	R743	Q744	Y745	L746	A747	I748	D749	E750	I751	S752	Q753	Q754	L755	G756	V757	D758	L759	I760	F761	L762	C763	D766	E767	M768	L769	P770	F771	D772	L773	R774	A775	H779	L780	H781	L782	H785	V786	Q791	E792	L793	V794	T795	F796	K798	F799	A800	R801	T804									
E805	T806	A809	I810	T811	D814	S817	N818	L819	N820	A821	S822	R823	D824	D825	K826	K827	N828	K829	N832	T833	N834	E835	Y837	E838	D839	Y840	L841	N842	N843	V844	V845	S846	E847	A848	V849	P850	F851	A852	N853	E854	E855	K856	N857	F861	E862	V863	V864	L865	A866	L867	H868	N869	L870						
I871	Y872	F873	G874	F875	Y876	S877	F878	L881	L884	T885	L888	L889	G890	I891	D892	K893	C894	VAL	GLN	GLY	ASN	GLU	D961	I962	V963	E966	L969	K970	I971	L972	E973	I974	I978	D984	L991	E1000	V1001	F1002	P1003	M1004	GLN	ASP	SER	GLY	VAL	LEU	SER	ARG	LYS	GLN									

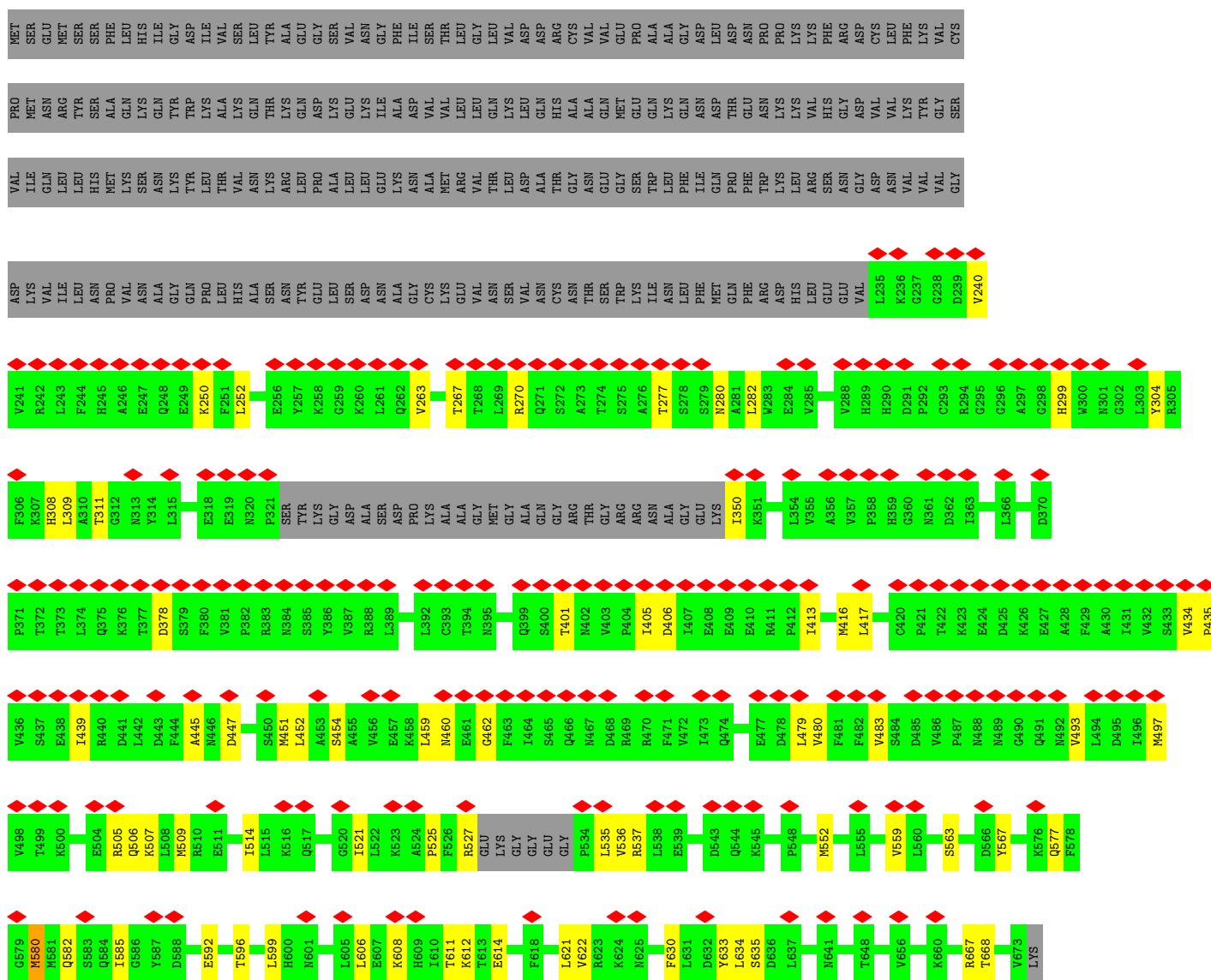


- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85139	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 ( $e^-/\text{\AA}^2$ )	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.885	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.826, 0.826, 0.826	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, ZN, CA, I3P

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	0.25	0/16403	0.46	0/22156
1	B	0.25	0/16384	0.46	0/22131
1	C	0.24	0/16528	0.45	0/22327
1	D	0.25	0/16726	0.46	0/22603
All	All	0.25	0/66041	0.46	0/89217

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	16106	16244	16243	235	0
1	B	16087	16225	16224	236	0
1	C	16227	16344	16353	178	0
1	D	16421	16536	16535	194	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	1	0
3	C	24	9	9	1	0
3	D	24	9	9	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
All	All	65069	65433	65439	837	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 6.

The worst 5 of 837 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:1962:HIS:HD1	1:D:1964:SER:HG	1.08	0.99
1:A:1962:HIS:HD1	1:A:1964:SER:HG	1.06	0.96
1:C:885:THR:HG22	1:C:978:ILE:HD13	1.48	0.93
1:A:729:TYR:CE1	1:A:733:LEU:HD21	2.04	0.92
1:C:2203:LEU:O	1:C:2207:ILE:HD12	1.73	0.89

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	1961/2671 (73%)	1930 (98%)	30 (2%)	1 (0%)	48 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1959/2671 (73%)	1933 (99%)	26 (1%)	0	100	100
1	C	1978/2671 (74%)	1951 (99%)	27 (1%)	0	100	100
1	D	2010/2671 (75%)	1979 (98%)	30 (2%)	1 (0%)	100	100
All	All	7908/10684 (74%)	7793 (98%)	113 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1514	LEU
1	A	1697	ASN

### 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	1807/2385 (76%)	1764 (98%)	43 (2%)	44	71
1	B	1805/2385 (76%)	1764 (98%)	41 (2%)	45	72
1	C	1820/2385 (76%)	1790 (98%)	30 (2%)	58	79
1	D	1838/2385 (77%)	1805 (98%)	33 (2%)	54	77
All	All	7270/9540 (76%)	7123 (98%)	147 (2%)	50	75

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	552	MET
1	D	2047	ARG
1	D	722	ASP
1	D	1364	TYR
1	B	632	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1622	HIS
1	D	1380	ASN
1	C	573	HIS
1	D	1318	GLN
1	B	2135	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
5	ATP	A	3004	-	28,33,33	0.62	0	34,52,52	0.87	1 (2%)
3	I3P	C	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	0
3	I3P	A	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	0
5	ATP	C	3004	-	28,33,33	0.63	0	34,52,52	0.90	1 (2%)
3	I3P	D	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.85	0
3	I3P	B	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	0
5	ATP	B	3004	-	28,33,33	0.62	0	34,52,52	0.87	1 (2%)
5	ATP	D	3004	-	28,33,33	0.61	0	34,52,52	0.87	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
5	ATP	A	3004	-	-	7/18/38/38	0/3/3/3
3	I3P	C	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	1/15/39/39	0/1/1/1
5	ATP	C	3004	-	-	10/18/38/38	0/3/3/3
3	I3P	D	3002	-	-	3/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	2/15/39/39	0/1/1/1
5	ATP	B	3004	-	-	6/18/38/38	0/3/3/3
5	ATP	D	3004	-	-	5/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	I3P	P4-O4	6.06	1.70	1.59
3	B	3002	I3P	P4-O4	6.06	1.70	1.59
3	A	3002	I3P	P4-O4	6.05	1.70	1.59
3	D	3002	I3P	P4-O4	6.05	1.70	1.59
3	D	3002	I3P	P5-O5	5.96	1.70	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3004	ATP	C5-C6-N6	2.34	123.88	120.31
5	B	3004	ATP	C5-C6-N6	2.32	123.85	120.31
5	A	3004	ATP	C5-C6-N6	2.32	123.85	120.31
5	C	3004	ATP	C5-C6-N6	2.32	123.85	120.31

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

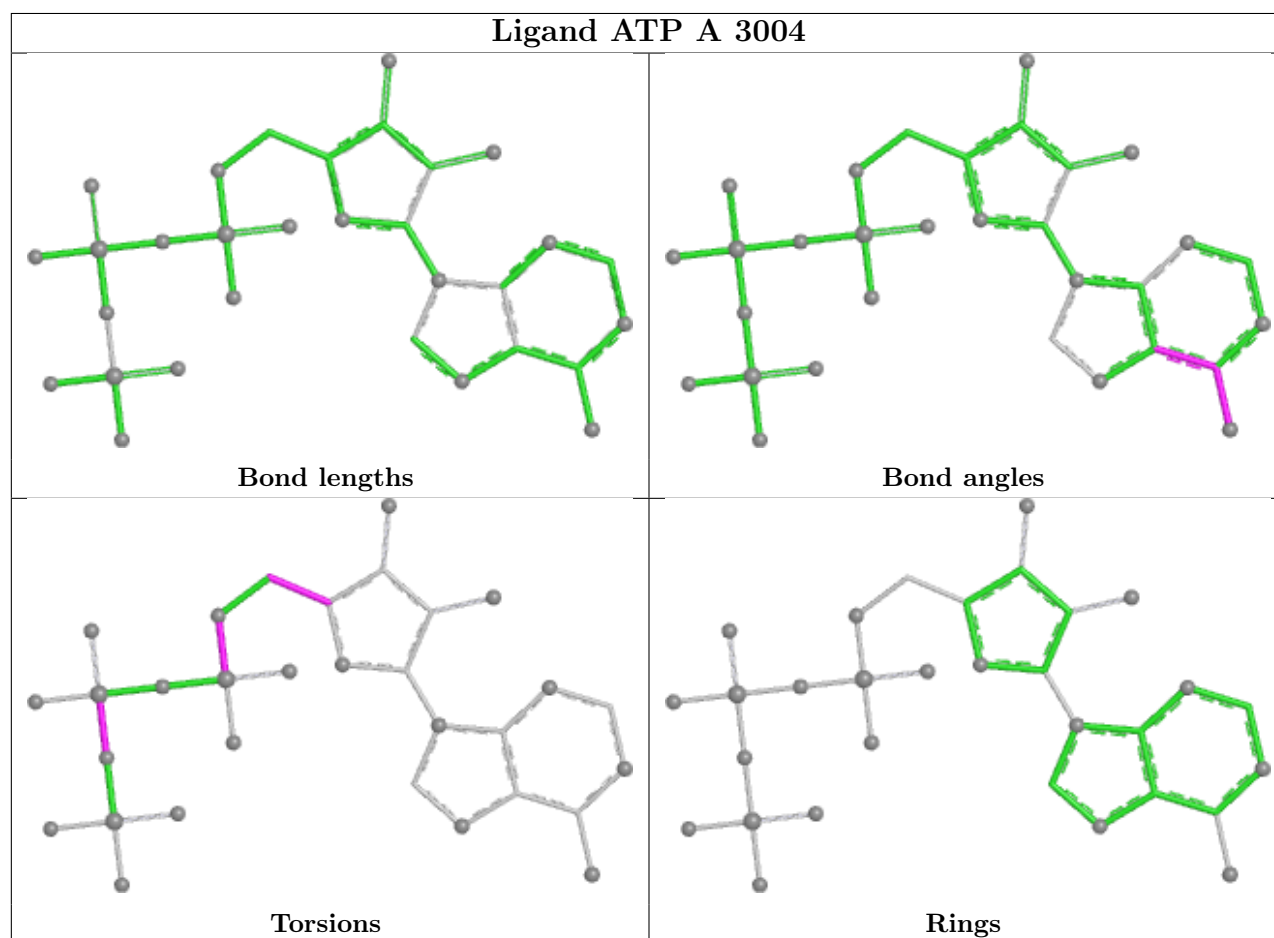
Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	C5'-O5'-PA-O2A
5	A	3004	ATP	C5'-O5'-PA-O3A
5	B	3004	ATP	C5'-O5'-PA-O2A
5	C	3004	ATP	PB-O3B-PG-O2G
5	C	3004	ATP	C5'-O5'-PA-O1A

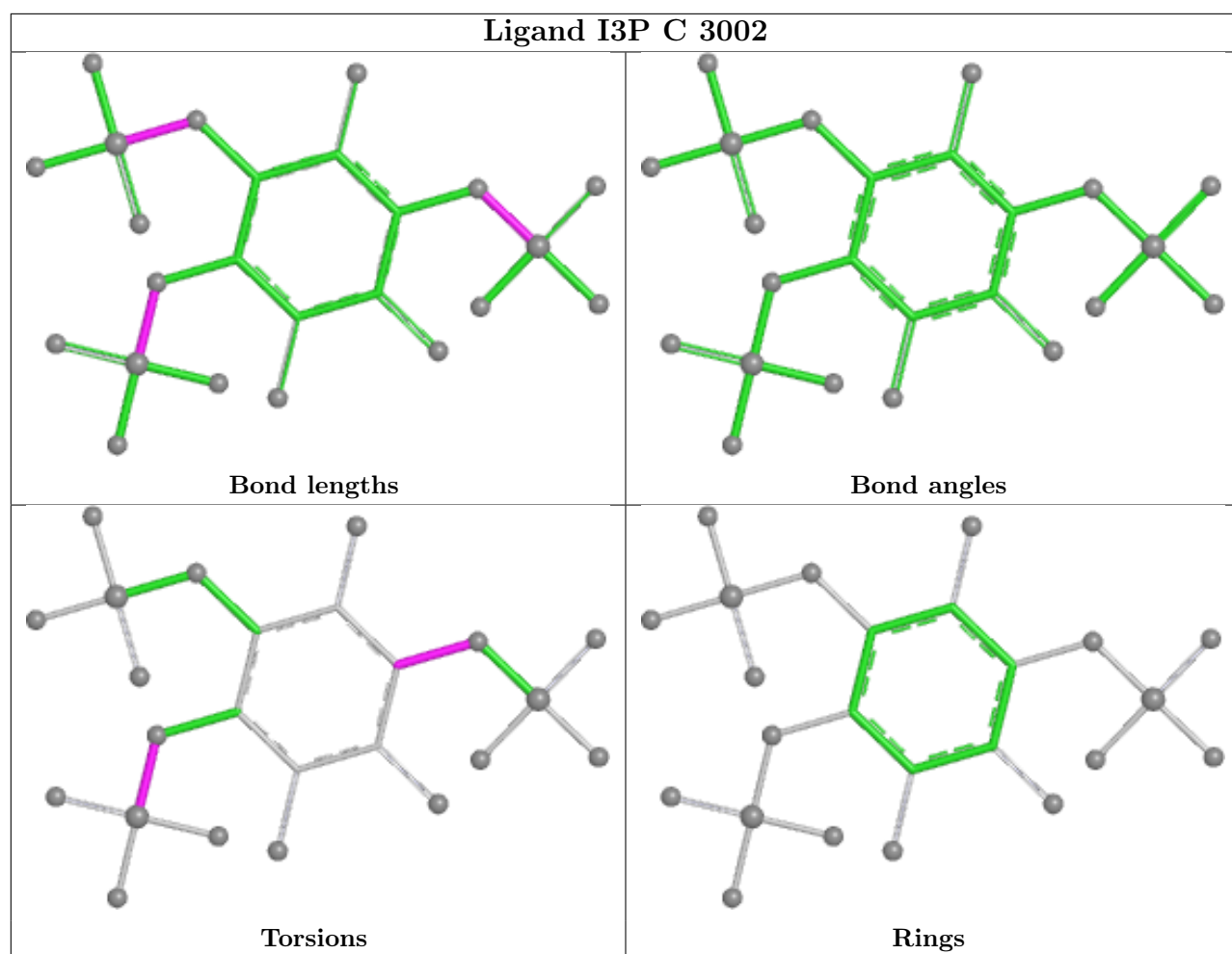
There are no ring outliers.

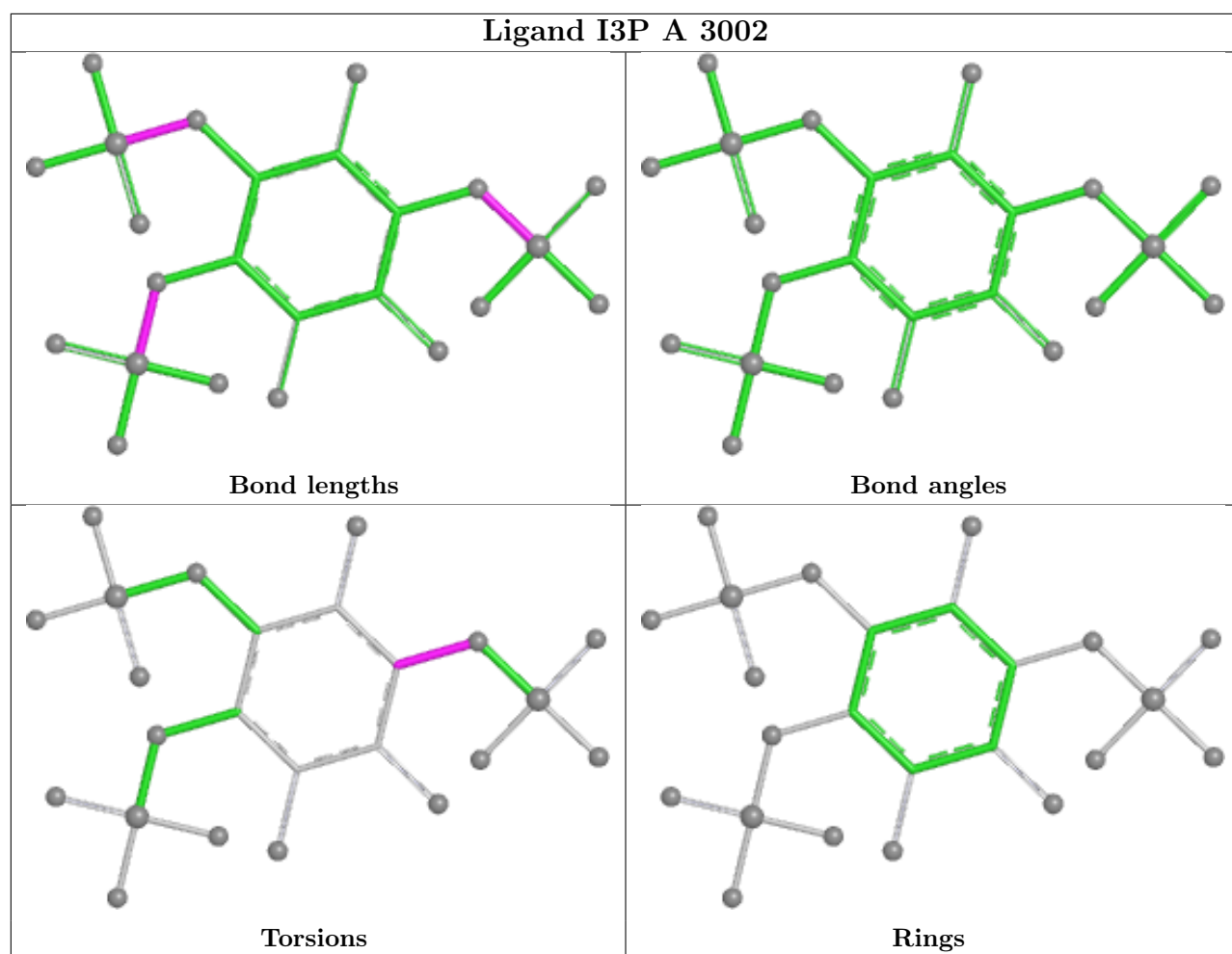
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3002	I3P	1	0
3	A	3002	I3P	1	0
3	D	3002	I3P	1	0
3	B	3002	I3P	1	0

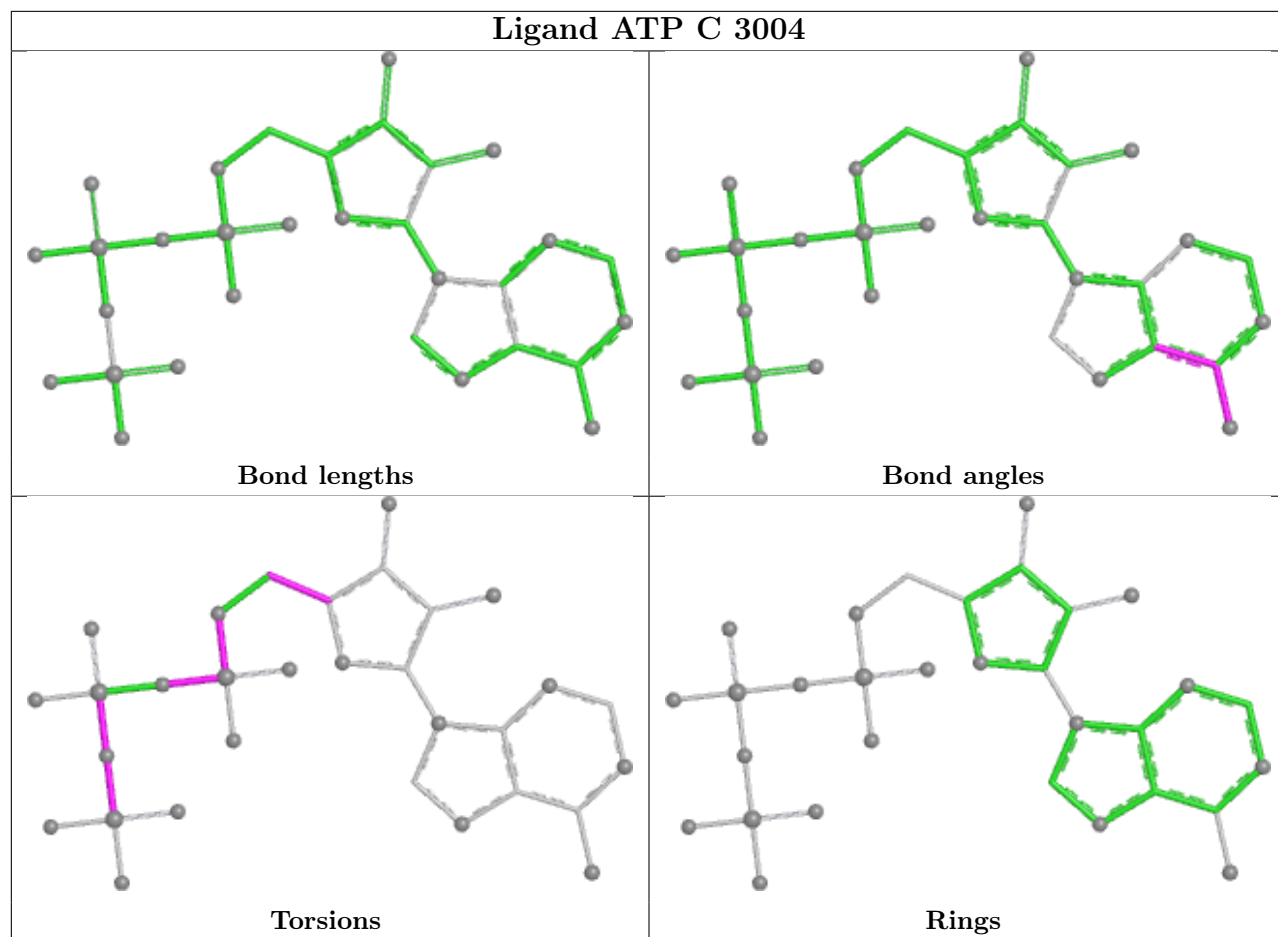
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

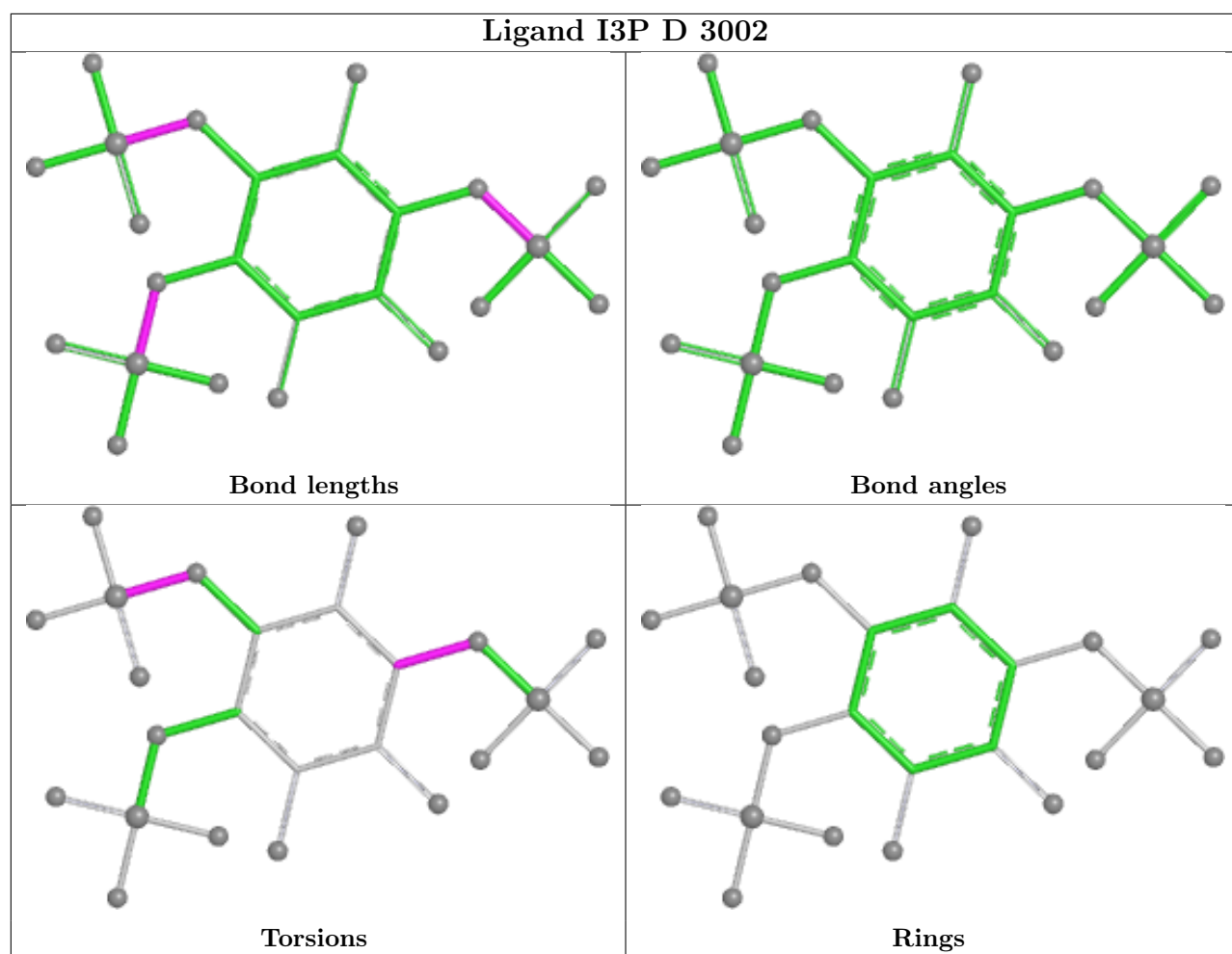


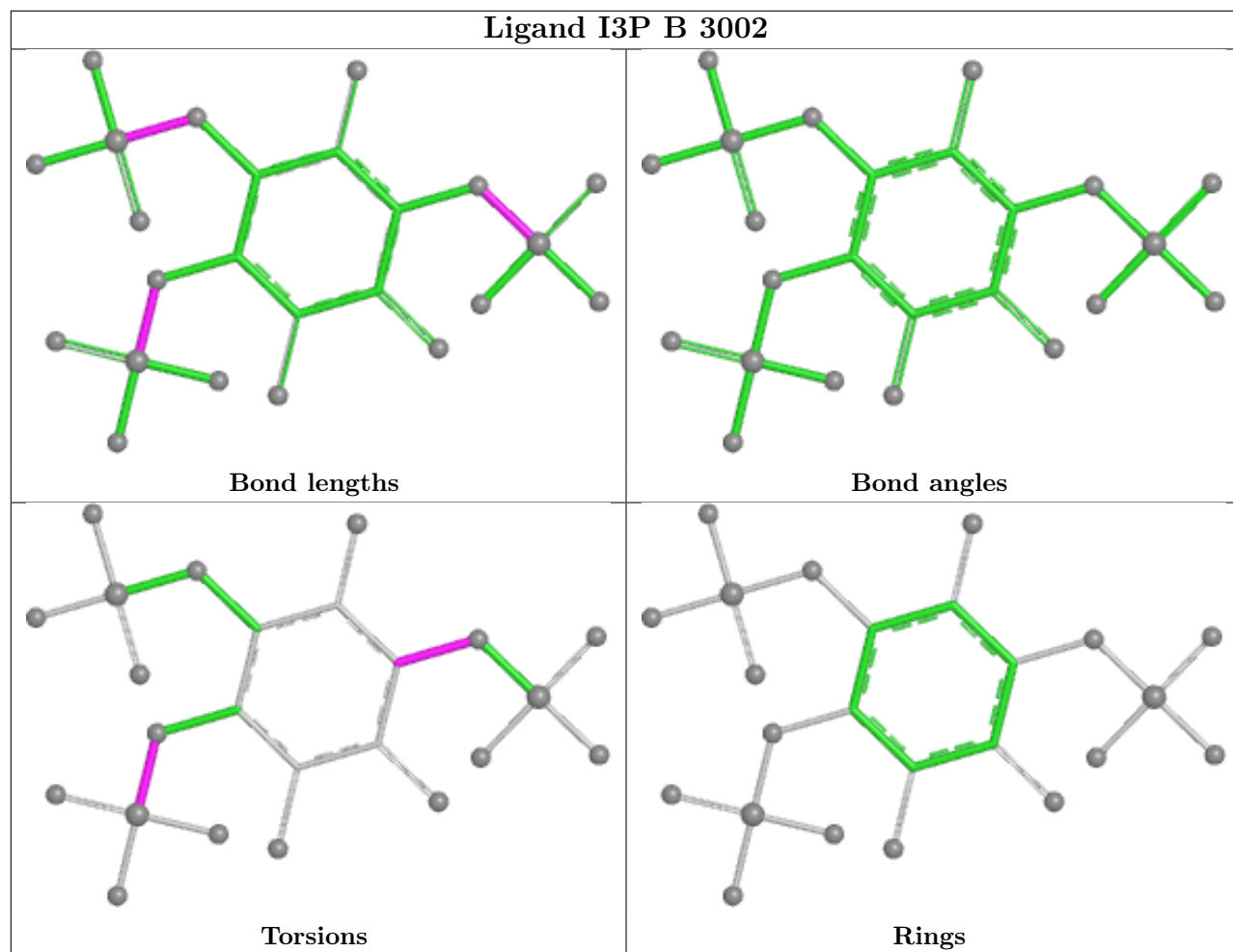


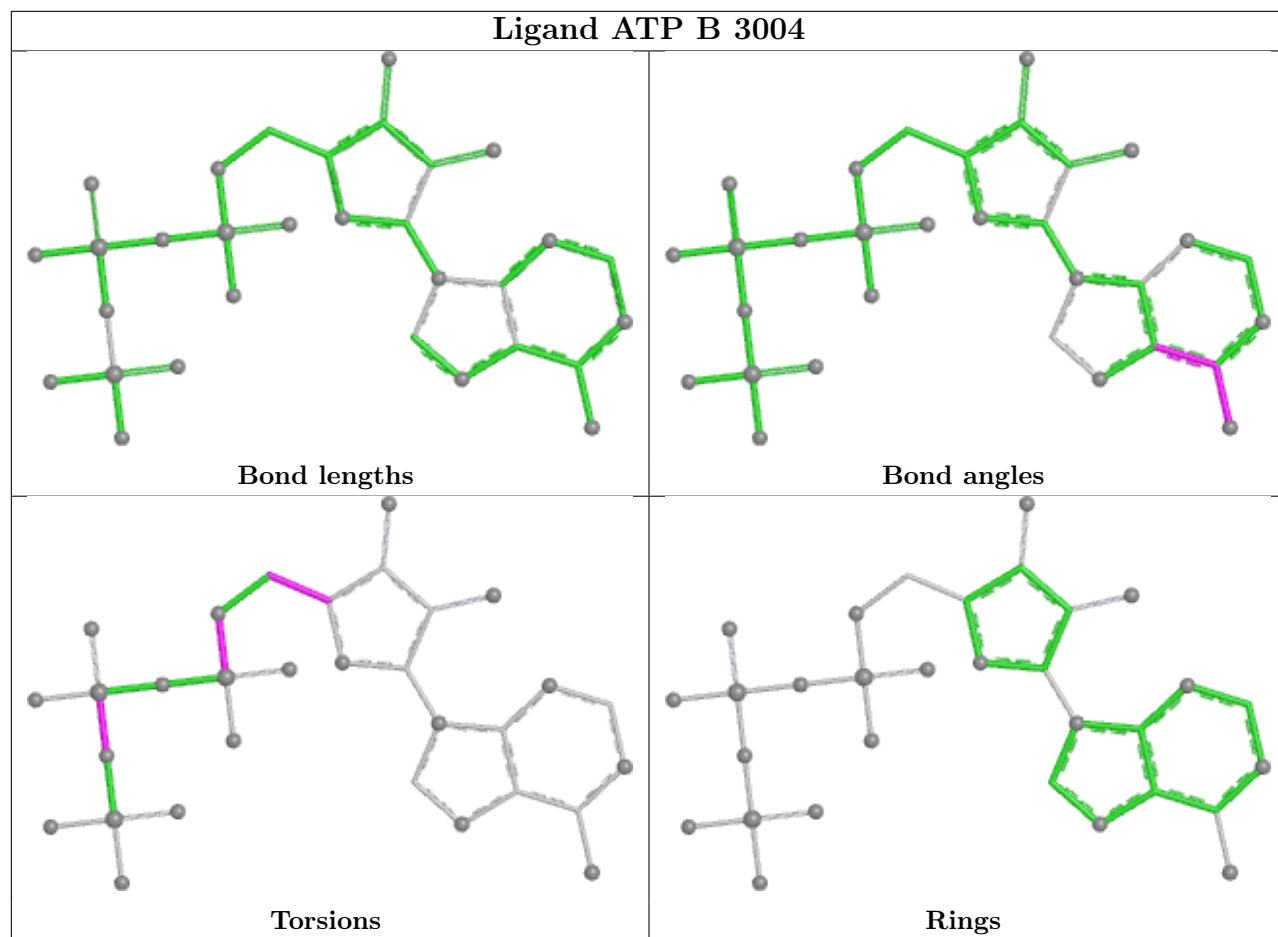


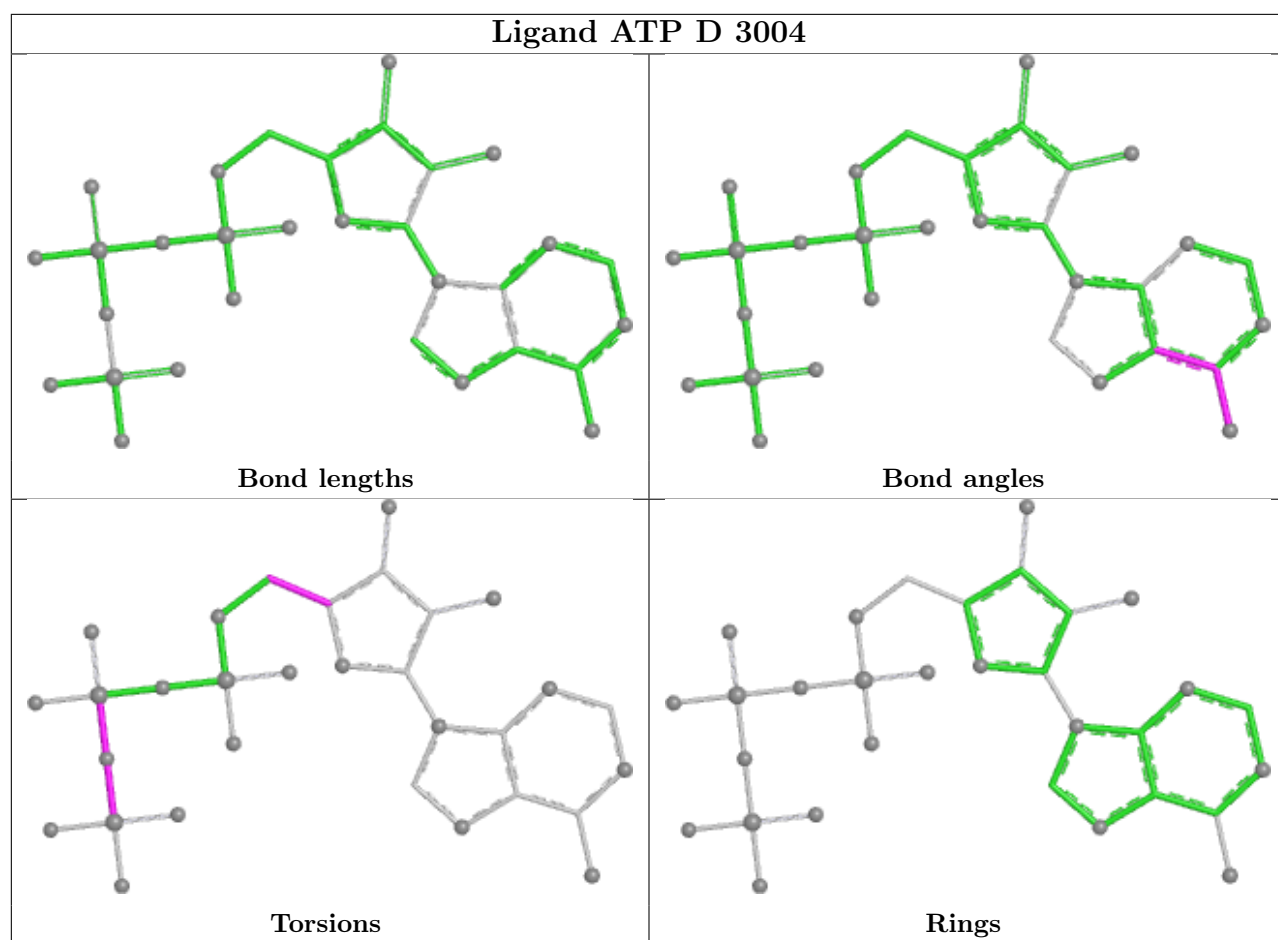












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

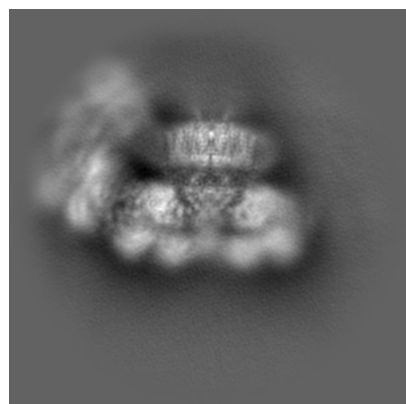
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41366. These allow visual inspection of the internal detail of the map and identification of artifacts.

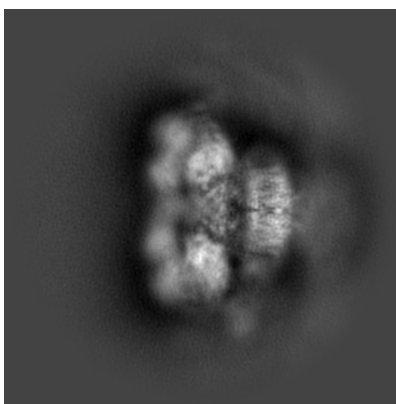
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

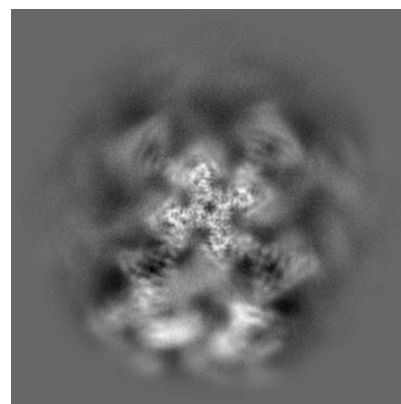
#### 6.1.1 Primary map



X

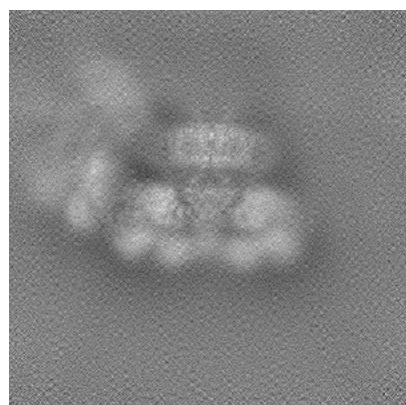


Y

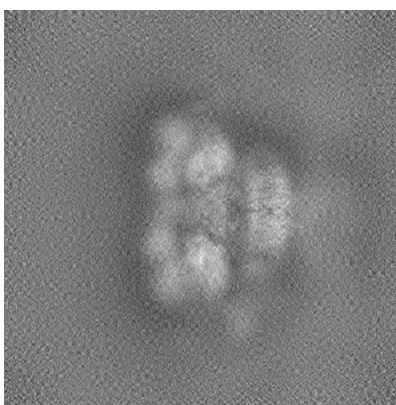


Z

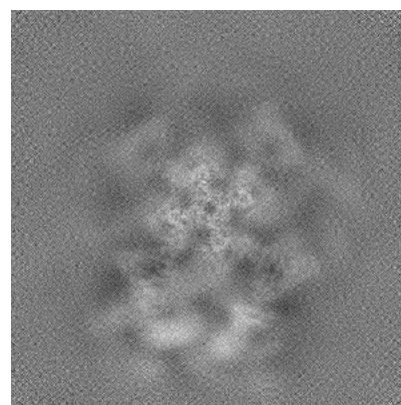
#### 6.1.2 Raw map



X



Y

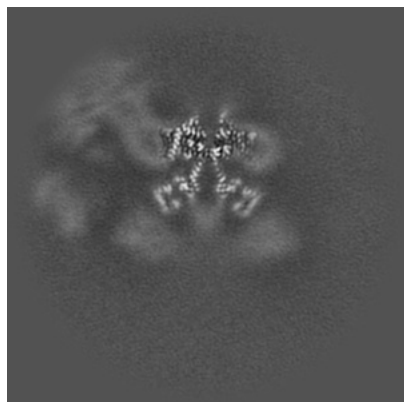


Z

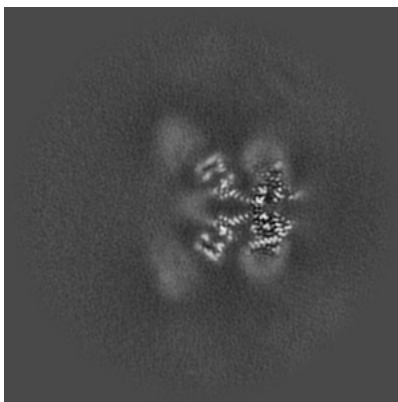
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

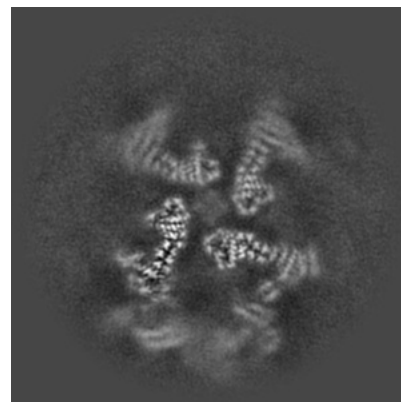
### 6.2.1 Primary map



X Index: 256

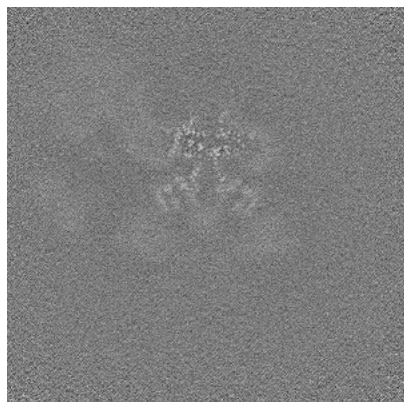


Y Index: 256



Z Index: 256

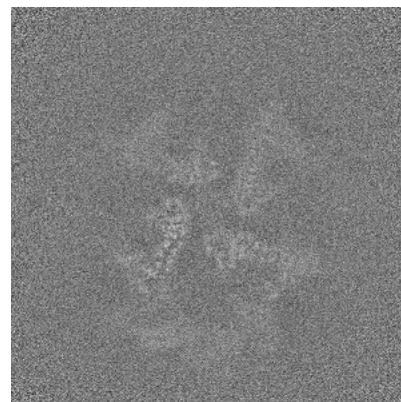
### 6.2.2 Raw map



X Index: 256



Y Index: 256



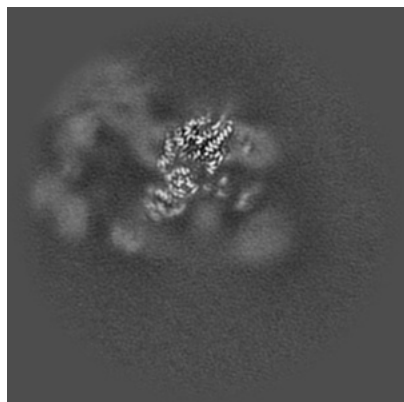
Z Index: 256

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

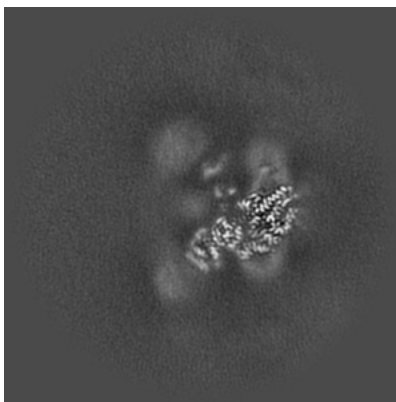


## 6.3 Largest variance slices [i](#)

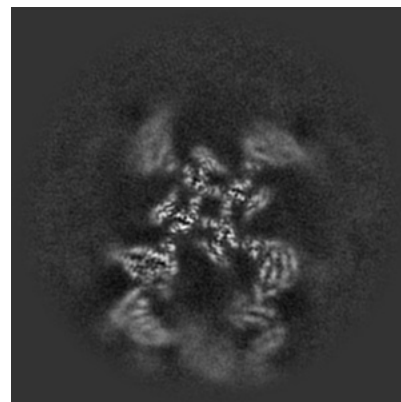
### 6.3.1 Primary map



X Index: 266

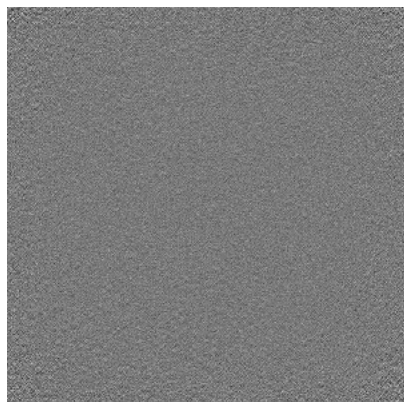


Y Index: 246

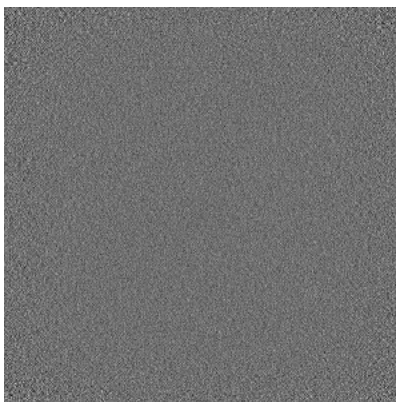


Z Index: 271

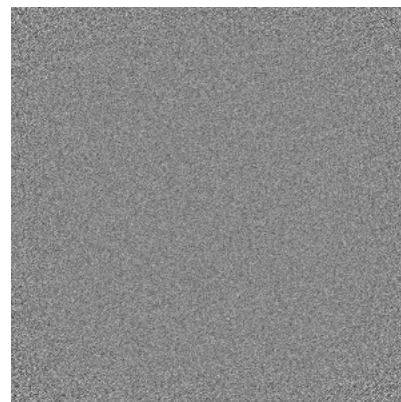
### 6.3.2 Raw map



X Index: 0



Y Index: 0



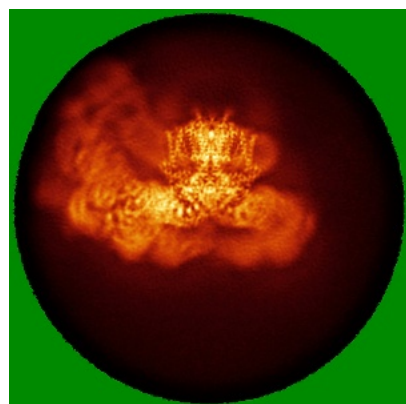
Z Index: 0

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

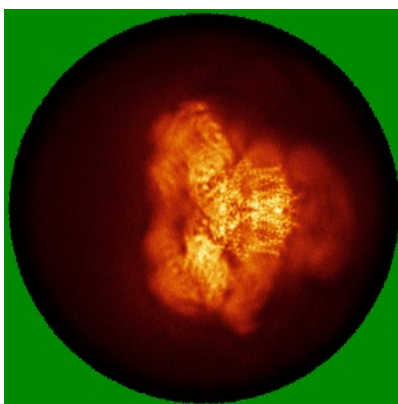


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

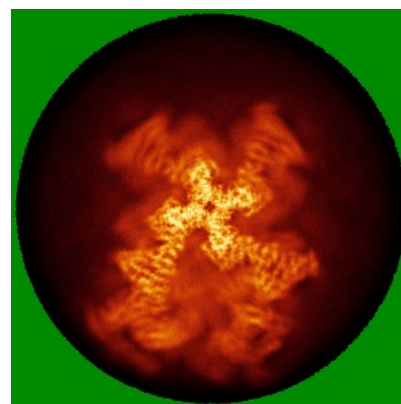
### 6.4.1 Primary map



X

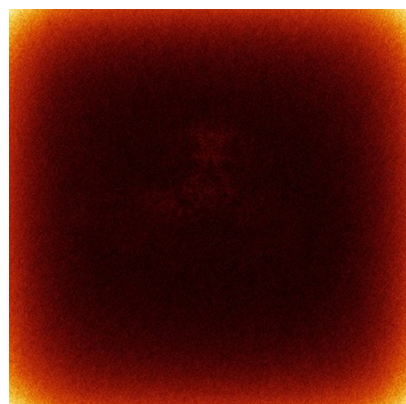


Y

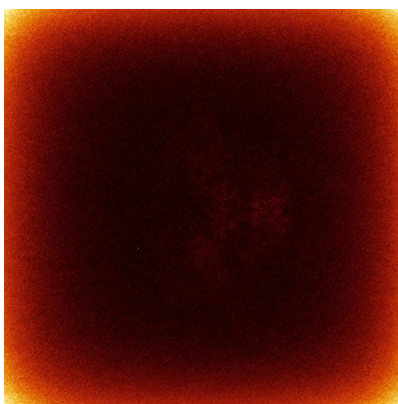


Z

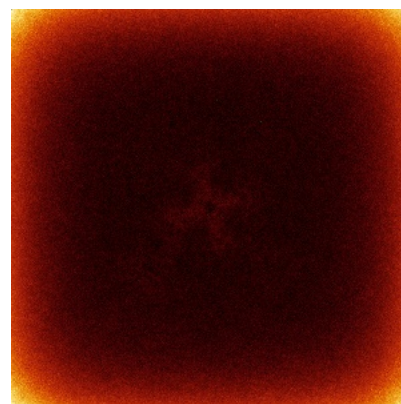
### 6.4.2 Raw map



X



Y

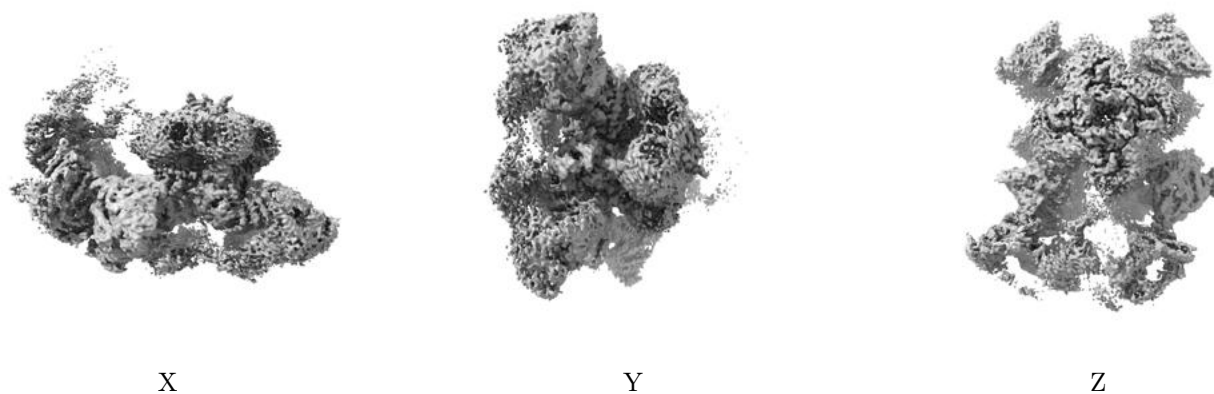


Z

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.

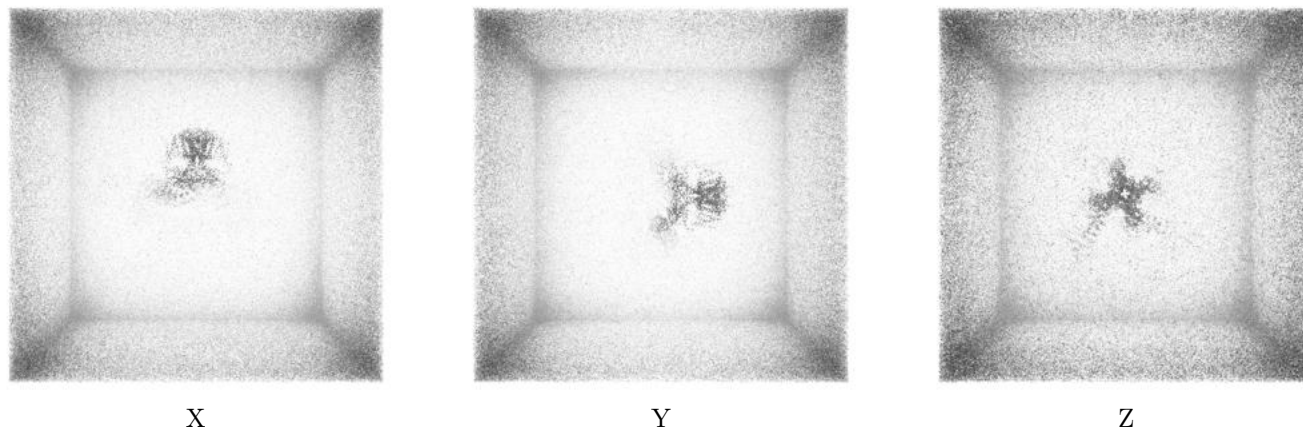
## 6.5 Orthogonal surface views [i](#)

### 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.

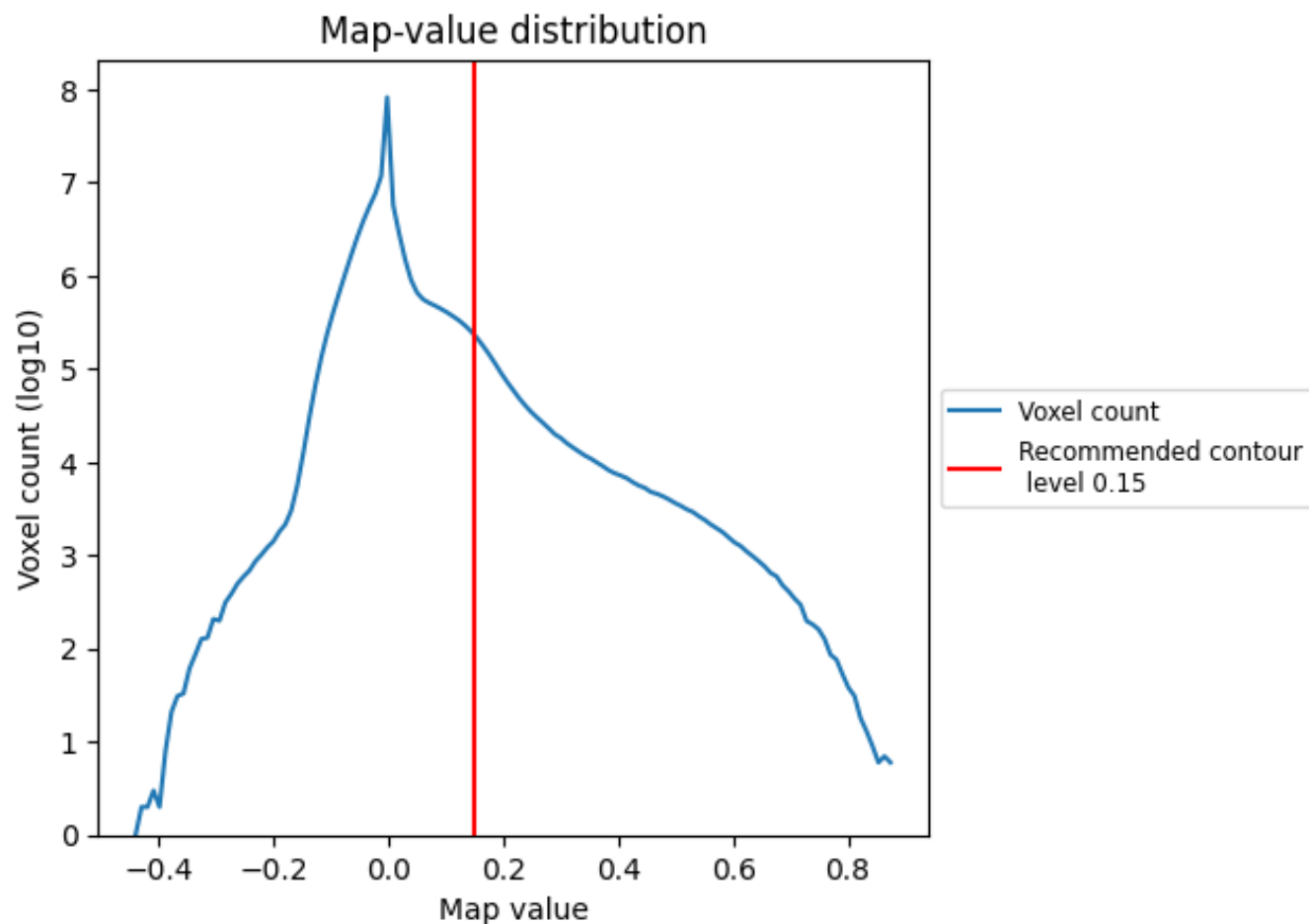
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

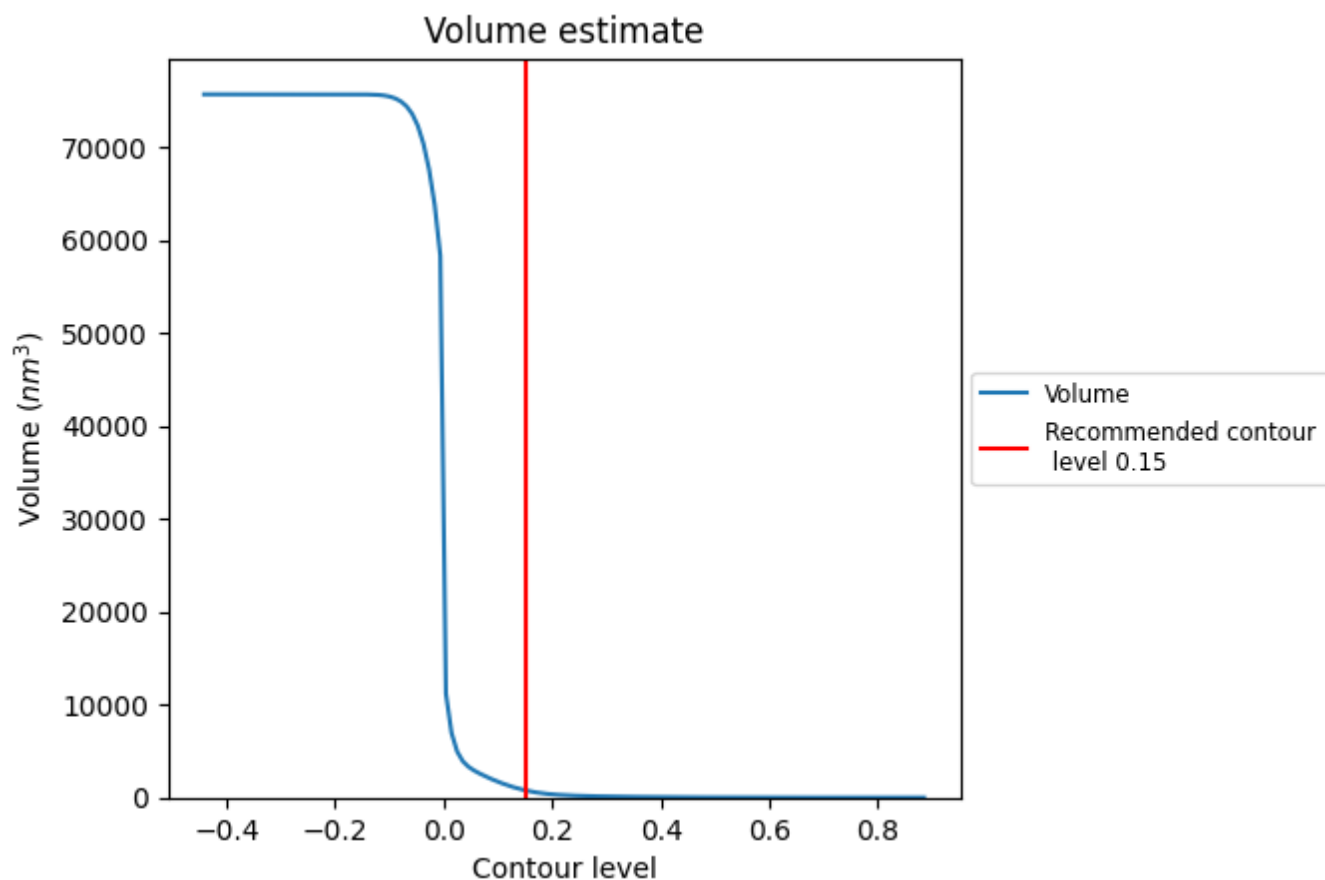
This section contains the results of statistical analysis of the map.

### 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.

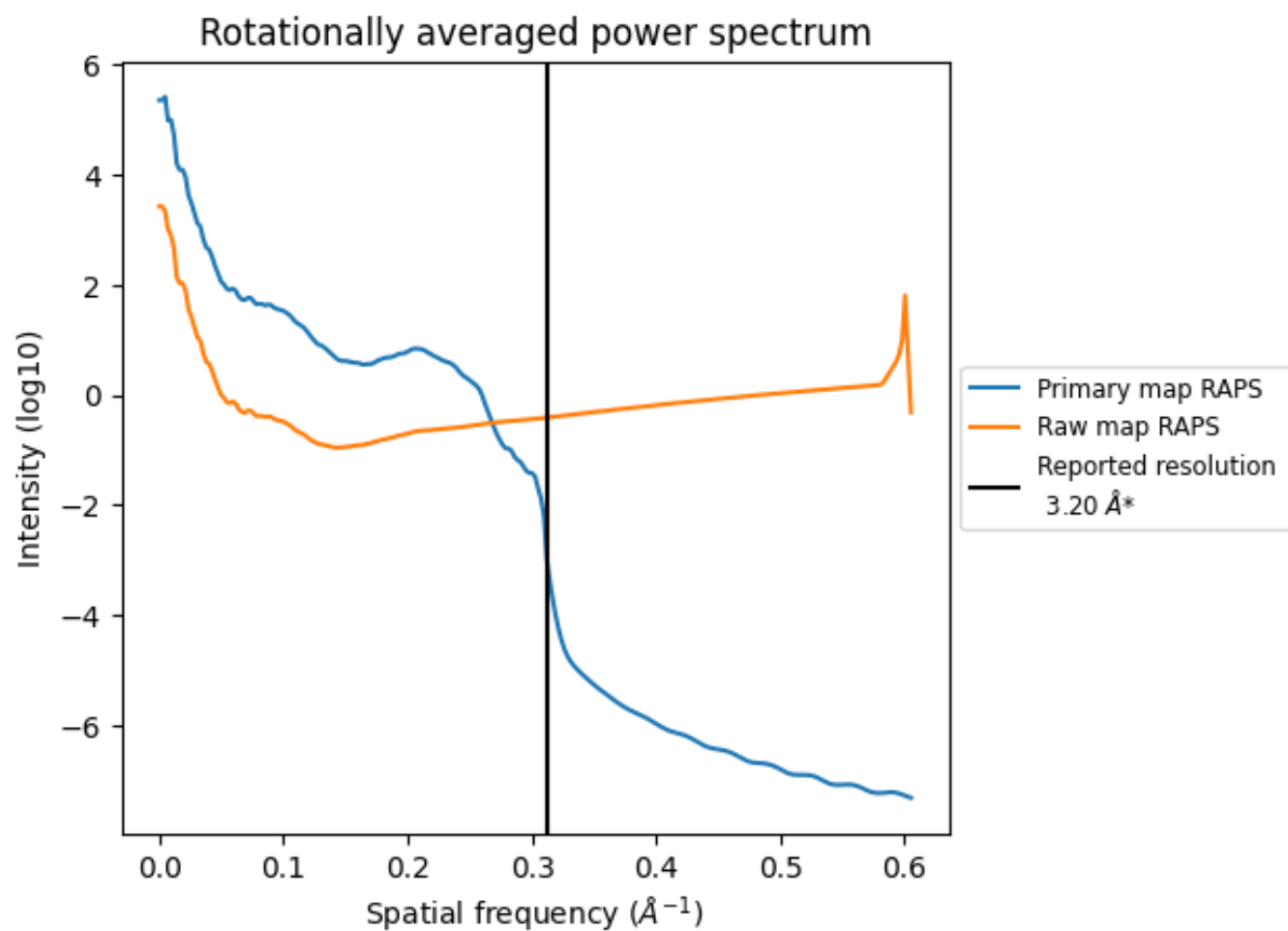
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 788 nm<sup>3</sup>; this corresponds to an approximate mass of 712 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

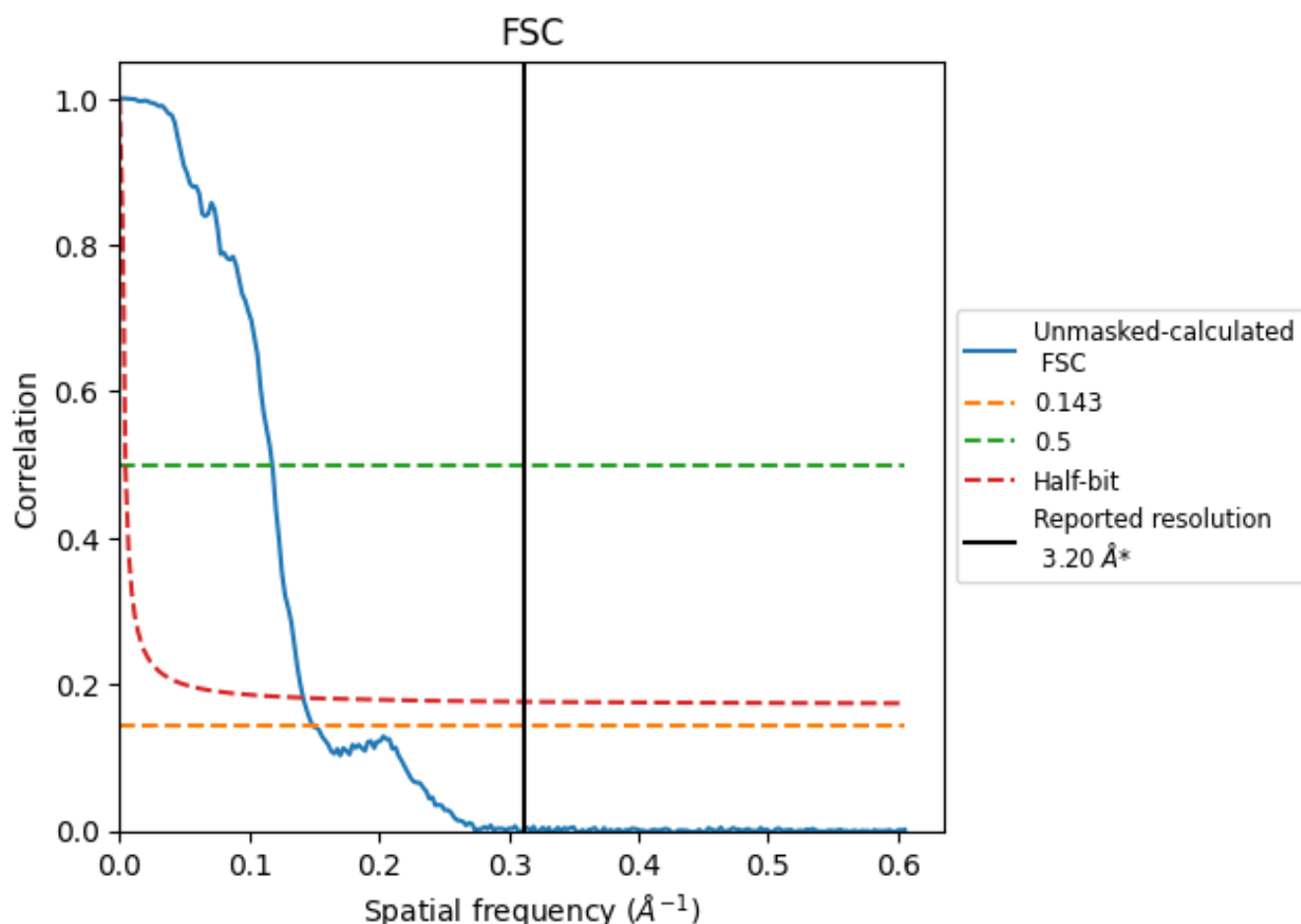


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

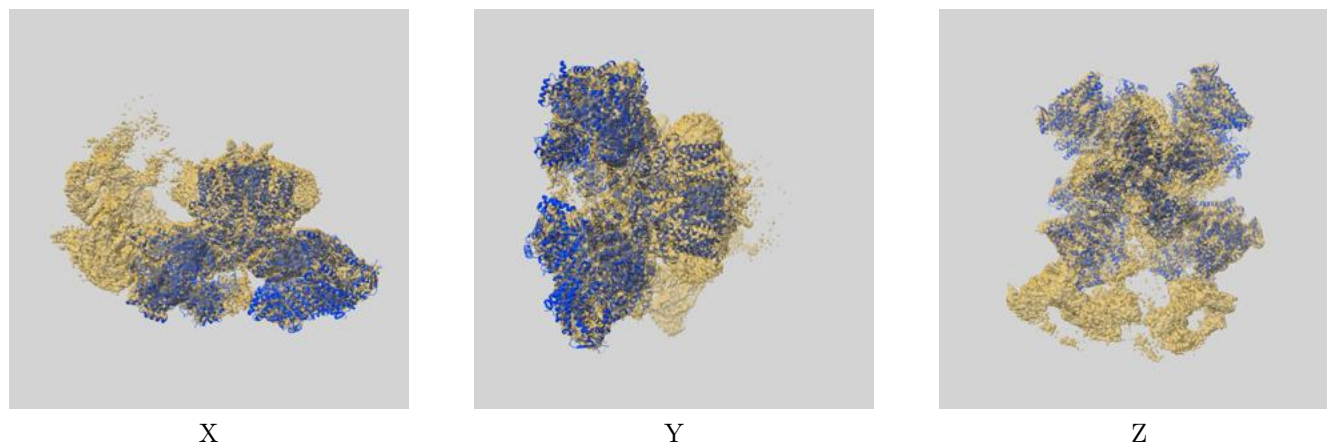
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.72	8.50	7.06

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 3.2 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-41366 and PDB model 8TLA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

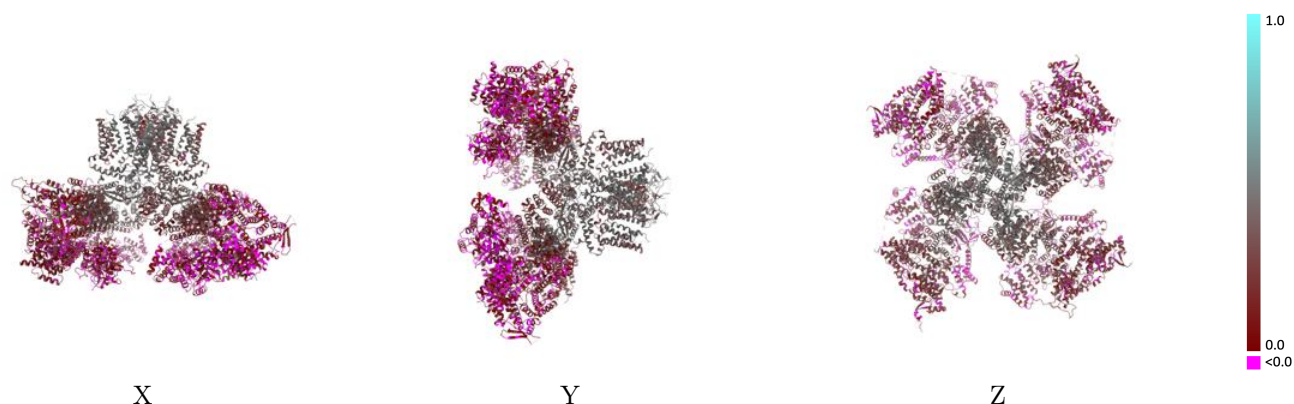
### 9.1 Map-model overlay [i](#)



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

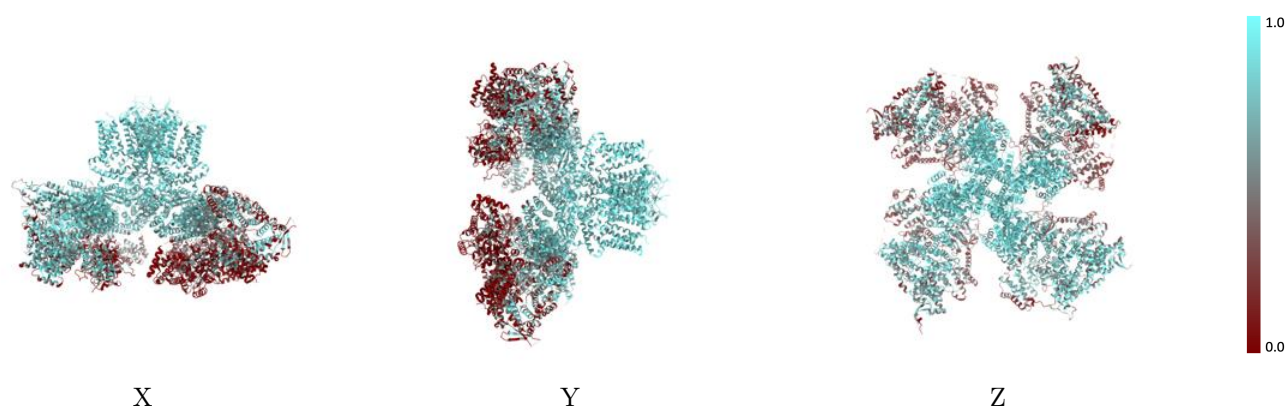


## 9.2 Q-score mapped to coordinate model [i](#)



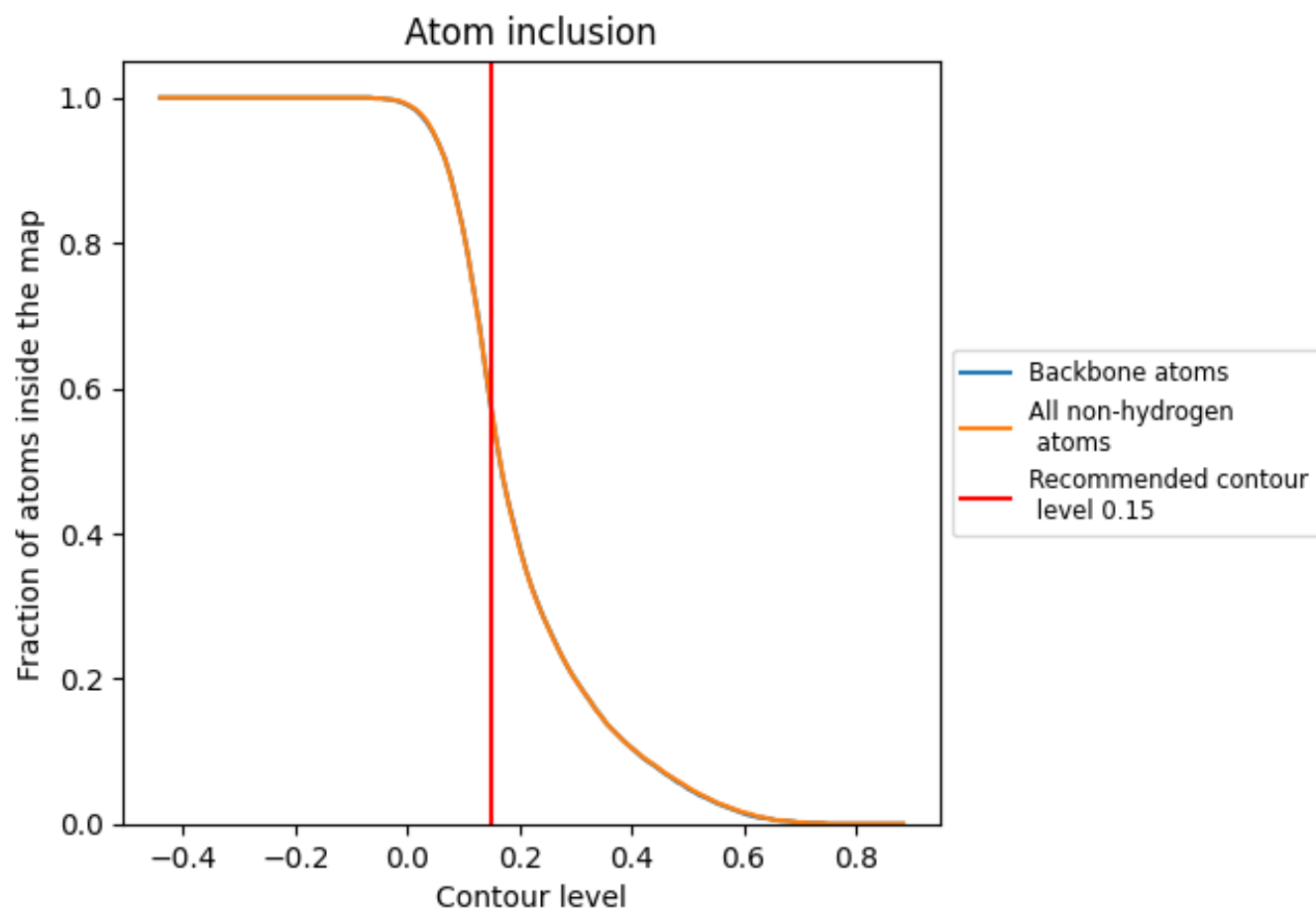
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 57% of all backbone atoms, 57% 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> 0.5720	<div></div> 0.1980
A	<div></div> 0.5100	<div></div> 0.1710
B	<div></div> 0.4700	<div></div> 0.1640
C	<div></div> 0.6520	<div></div> 0.2320
D	<div></div> 0.6740	<div></div> 0.2250

