



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 08:02 PM EDT

PDB ID : 8TL9
EMDB ID : EMD-41365
Title : Human Type 3 IP3 Receptor - Resting State (+IP3/ATP)
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on : 2023-07-26
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

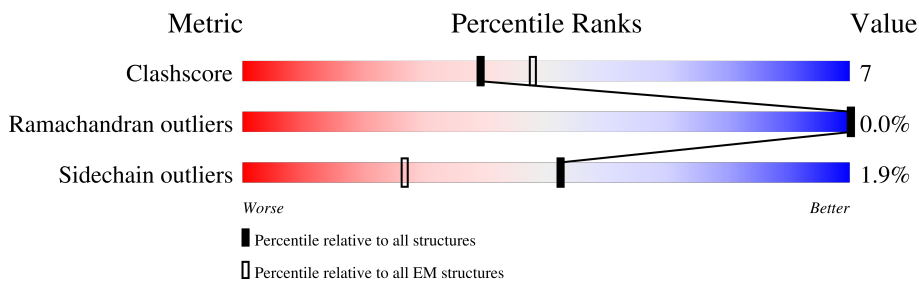
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 ≥ 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	
1	B	2671	
1	C	2671	
1	D	2671	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 130518 atoms, of which 65442 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.

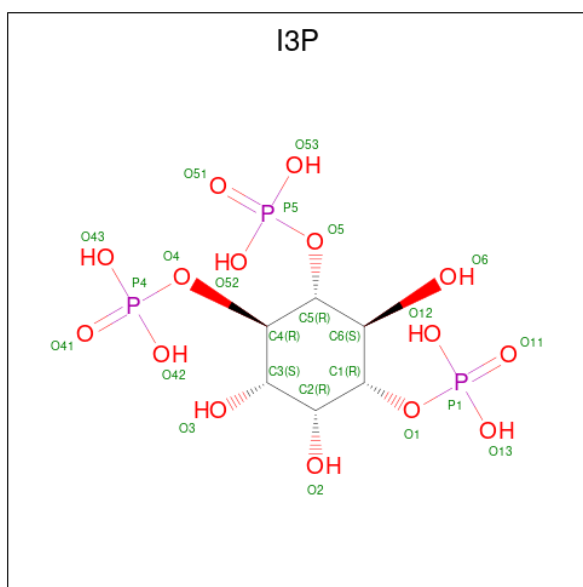
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

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	2005	Total	C	H	N	O	S	0	0
			32587	10375	16353	2768	2987	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: C₆H₁₅O₁₅P₃) (labeled as "Ligand of Interest" by depositor).

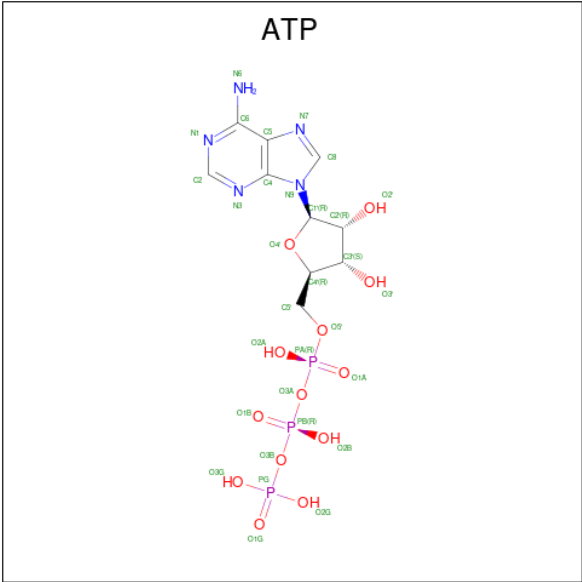


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- 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	

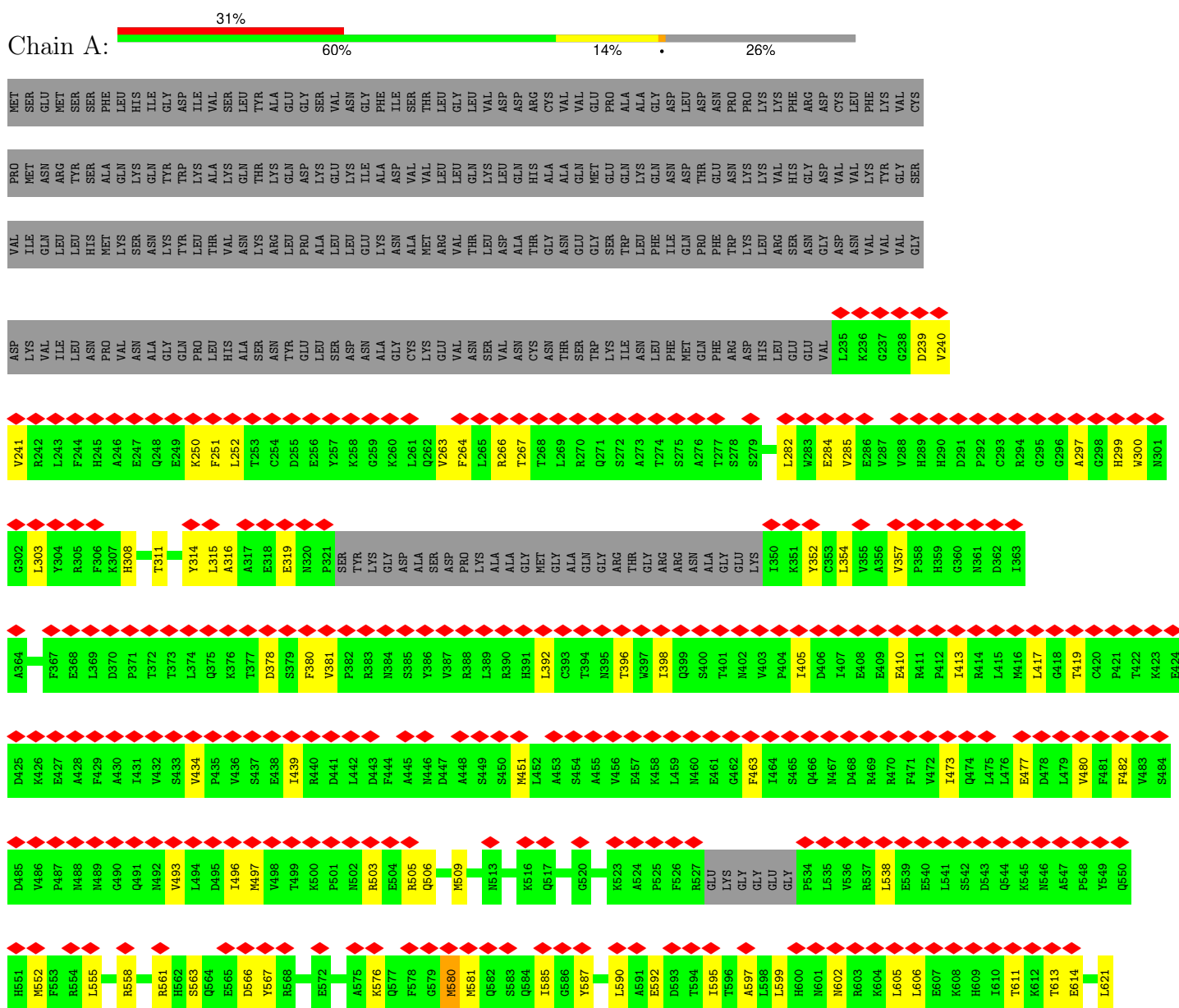
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



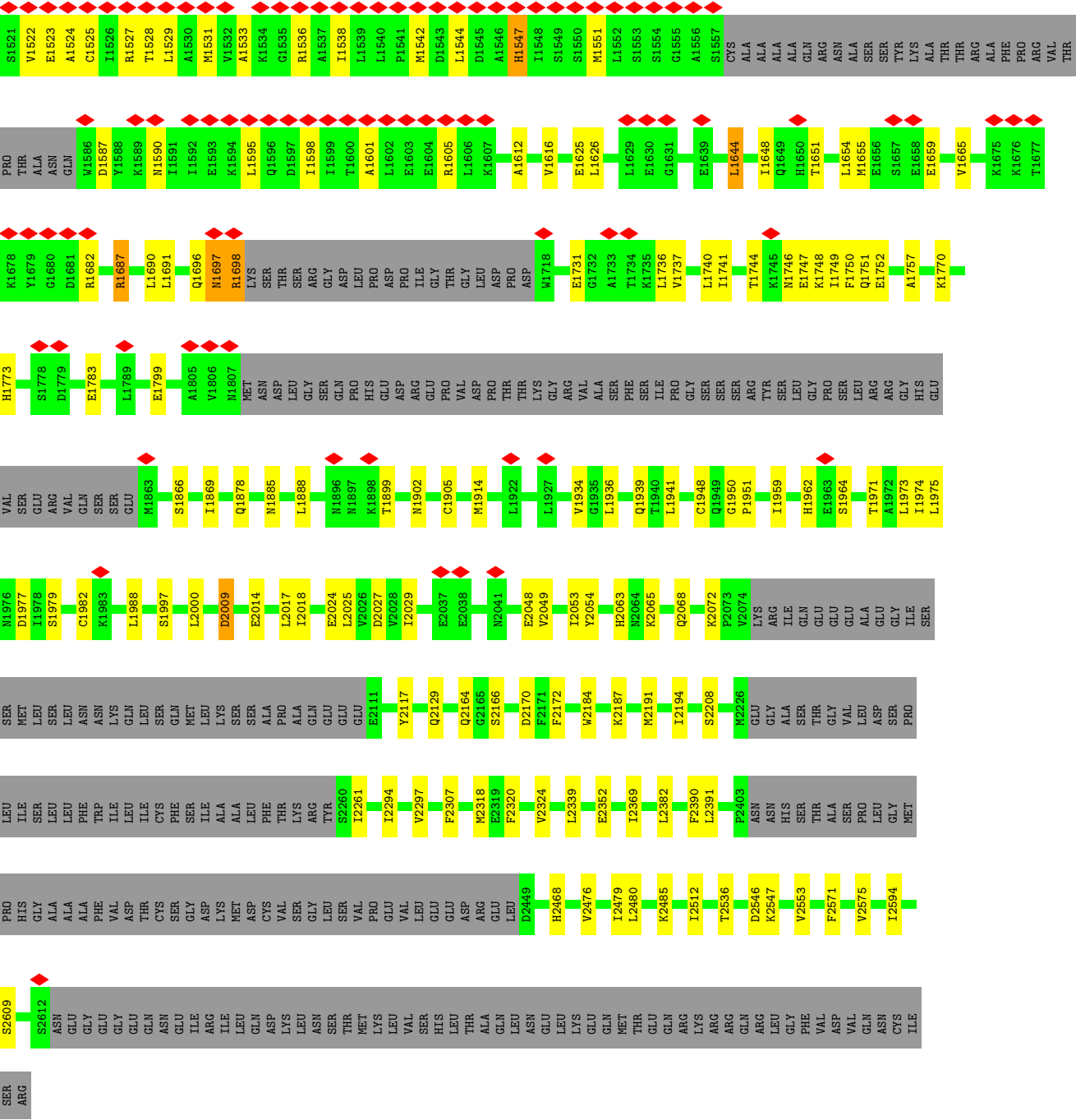
3 Residue-property plots

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.

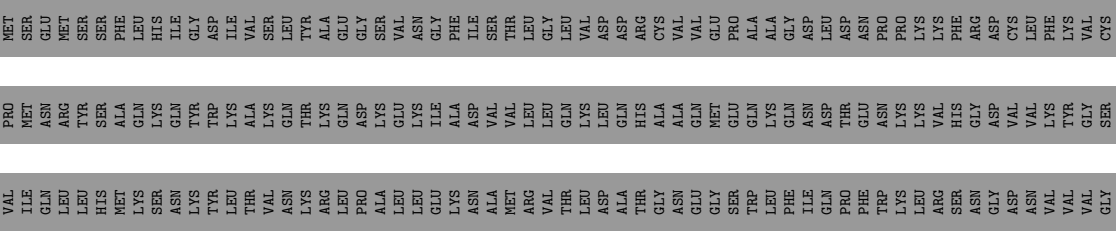
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





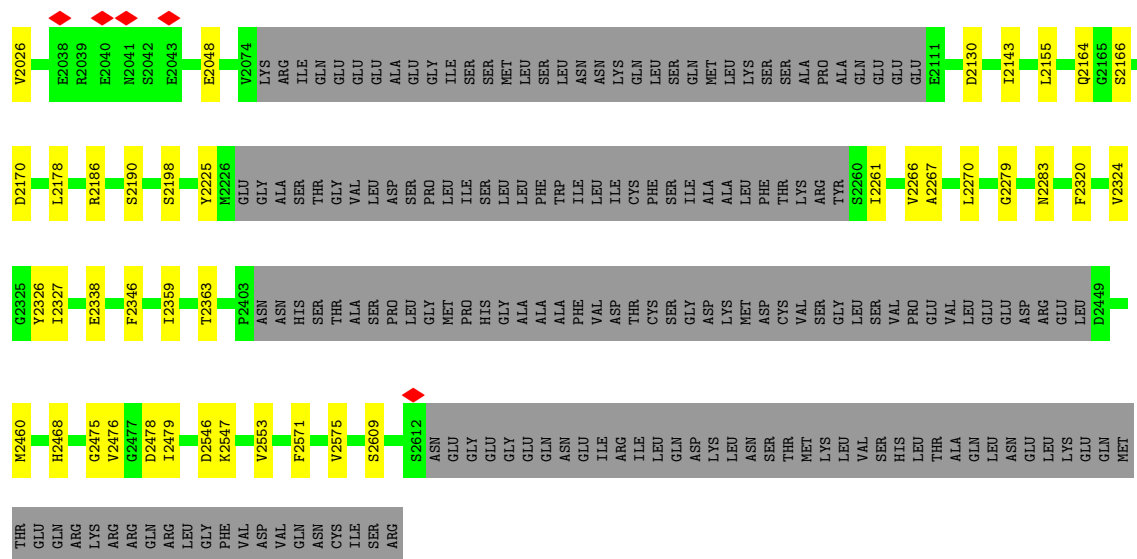


● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

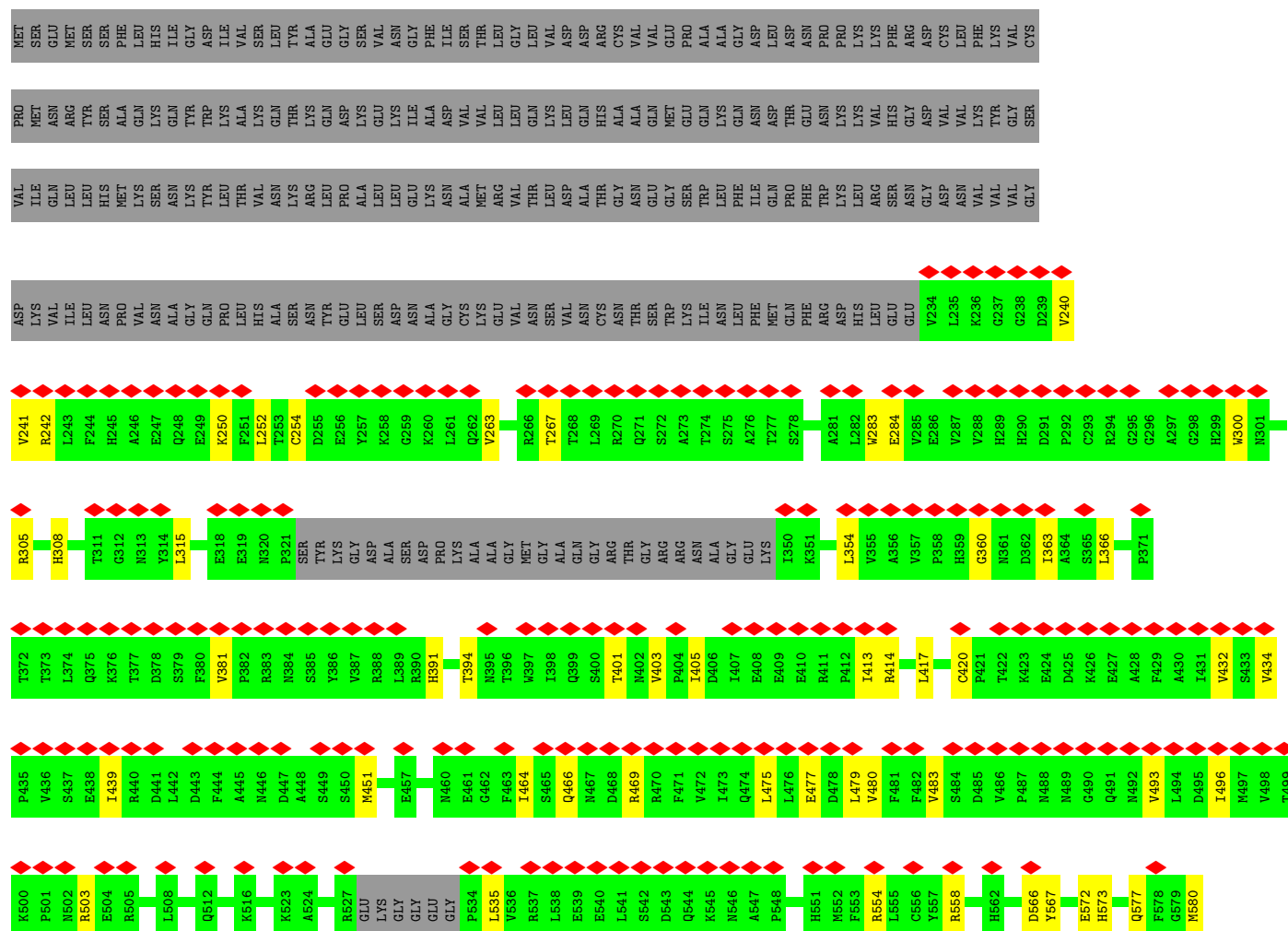






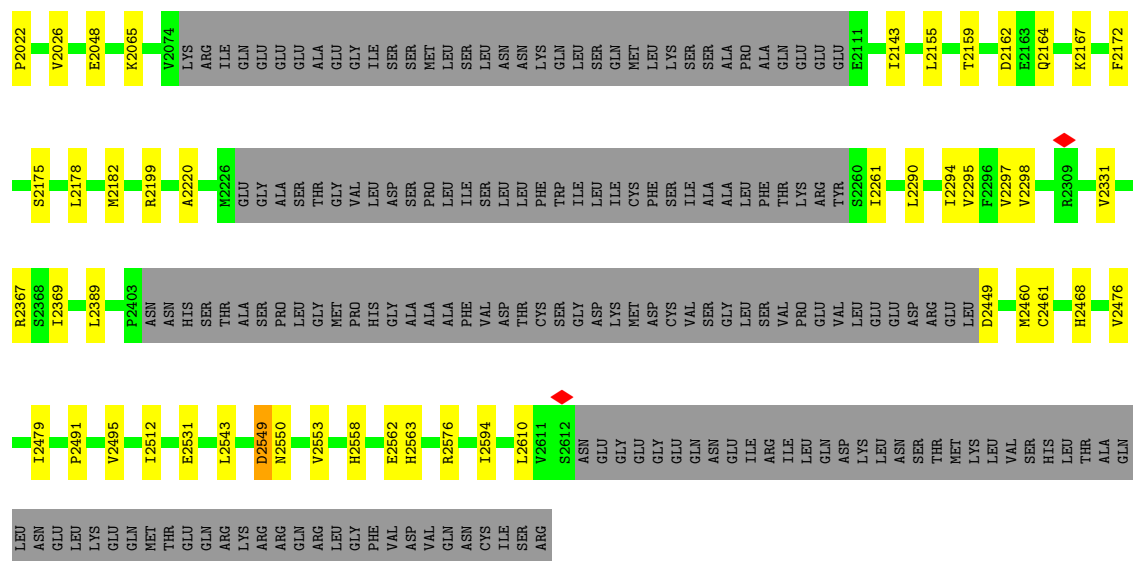


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





LEU	ARG	ARG	GLY	HIS	GLU	VAL	SER	GLU	ARG	VAL	GLN	SER	GLU	M1863	G1864	L1868	Q1871	P1872	N1885	L1888	C1894	Q1895	M1896	Y1901	C1905	E1906	T1919	L1922	G1923	L1924	E1931	V1934	C1948	Q1949	G1950	P1951	I1959	H1962	E1963	S1964	N1965	L1988																
F1750	A1757	H1773	S1782	F1785	V1788	D1791	E1799	T1803	V1806	N1807	MET	ASN	ASP	LEU	GLY	SER	GLN	PRO	HIS	GLU	ASP	ARG	GLU	PRO	VAL	ASP	PRO	THR	THR	LYS	GLY	ARG	VAL	SER	SER	SER	ILE	PRO	SER	ARG	TTR	SER	N1964	N1965	L1988													
V1610	D1619	V1620	L1621	L1626	F1643	L1644	T1648	K1652	D1681	Q1685	L1686	R1687	M1697	R1698	LYS	SER	THR	SER	GLN	PRO	HIS	GLU	ASP	LEU	PRO	VAL	ASP	PRO	THR	THR	LYS	GLY	ARG	VAL	SER	SER	SER	ILE	PRO	SER	ARG	TTR	SER	N1964	N1965	L1988												
E1486	N1487	S1488	T1489	Q1492	I1497	L1502	T1505	E1510	W1513	L1514	Q1515	H1518	K1519	I1526	L1529	A1530	K1534	L1539	M1542	D1543	H1547	M1551	L1552	S1553	S1554	G1555	A1556	S1557	C1558	A1559	A1560	R1564	A1571	T1572	T1573	R1574	A1575	F1576	P1577	R1578	P1581																	
C1236	L1246	F1253	T1263	L1269	Q1273	E1277	Q1284	F1286	H1288	L1289	R1295	T1305	K1315	Q1318	D1319	M1322	T1326	N1327	A1328	G1329	D1330	D1331	V1332	V1333	K1339	A1340	H1344	L1345	L1346	D1347	M1348	A1351	A1352	R1353	D1354	G1355	D1358	L1368																				
N1380	Y1381	Y1382	T1383	E1384	I1385	T1388	L1391	P1392	L1393	V1396	V1397	V1400	T1401	H1402	C1405	I1406	T1407	V1417	Y1421	V1426	E1427	H1436	T1437	W1438	T1439	L1440	F1441	F1444	T1445	M1448	R1455	E1456	K1457	R1458	V1459	A1460	D1461	L1464	E1465	V1468	L1469	S1470	S1485															
G1037	VAL	LYS	THR	SER	S1043	M1044	V1047	D1048	D1049	H1065	D1066	R1085	D1129	LYS	GLY	SER	GLY	GLY	ALA	VAL	GLU	ALA	ALA	GLY	ALA	ALA	LYS	ASP	LYS	GLU	ARG	PHE	GLU	GLU	ASN	ASP	GLU	GLY	PHE	GLN	ALA	TTR	GLU	ASP	PRO	GLY	V1001	F1002	D1006	S1007	M1035	F1036						
L759	L760	M768	L769	D772	L773	C778	M781	R788	D789	L819	N832	T833	M834	K858	E862	I871	Y876	L882	R883	L884	T885	R886	D893	C894	VAL	GLN	GLY	PRO	PRO	ALA	ALA	MET	LEU	GLN	ALA	TTR	GLU	ASP	PRO	GLY	V1001	F1002	D1006	S1007	M1035	F1036												
A591	I595	T596	L599	L606	E614	L621	V622	F630	L633	L634	E650	K654	T668	V673	LYS	GLU	GLY	MET	ALA	GLN	SER	HIS	GLU	TYR	LEU	SER	ILE	GLU	TYR	SER	E689	M693	L694	N700	N719	D722	V725	Y745	I748	L755																		
Q506	M509	I514	G520	I521	L522	K523	A524	P525	F526	R527	GLU	LYS	GLY	GLY	GLY	P534	L535	V536	R537	L538	E539	Q544	K545	M552	F553	R554	L555	C556	Y557	R558	V559	S563	D566	Y567	R568	E572	K576	Q577	F578	M581	Q582	S583	Q584	I585	G586	Y587	L590											
D441	L442	D443	F444	A445	M446	D447	S450	M451	L452	A453	S454	E457	K458	L459	M460	E461	Q462	F463	Q466	M467	D468	R469	R470	F471	V472	I473	Q474	L475	L476	E477	D478	L479	V480	V483	S484	D485	V486	P487	M488	M489	G490	Q491	M492	V493	L494	D495	I496	M497	V498	T499	K500	R503	E504	R505				
F380	V381	P382	R383	N384	S385	Y386	V387	R388	L389	R390	H391	L392	C393	T394	N395	T396	V397	I398	Q399	S400	T401	M402	V403	P404	I405	D406	I407	E408	E409	E410	R411	P412	I413	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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88082	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	0.869	Depositor
Minimum map value	-0.421	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN, ATP, 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	0.47	0/22156
1	B	0.25	0/16384	0.46	0/22131
1	C	0.25	0/16535	0.46	0/22337
1	D	0.25	0/16726	0.46	0/22603
All	All	0.25	0/66048	0.46	0/89227

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	255	0
1	B	16087	16225	16224	248	0
1	C	16234	16353	16362	210	0
1	D	16421	16536	16535	203	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	0	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	0	0
3	D	24	9	9	0	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	65076	65442	65448	911	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 7.

The worst 5 of 911 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:1962:HIS:HD1	1:A:1964:SER:HG	0.98	0.96
1:B:1799:GLU:OE1	1:B:1866:SER:OG	1.91	0.89
1:C:354:LEU:HD12	1:C:417:LEU:HD12	1.55	0.87
1:D:1510:GLU:OE2	1:D:1547:HIS:NE2	2.08	0.84
1:A:1262:GLU:O	1:A:1266:HIS:ND1	2.11	0.83

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 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1959/2671 (73%)	1937 (99%)	22 (1%)	0	100	100
1	C	1979/2671 (74%)	1948 (98%)	31 (2%)	0	100	100
1	D	2010/2671 (75%)	1975 (98%)	35 (2%)	0	100	100
All	All	7909/10684 (74%)	7790 (98%)	118 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	1760 (97%)	47 (3%)	41	66
1	B	1805/2385 (76%)	1758 (97%)	47 (3%)	41	66
1	C	1821/2385 (76%)	1803 (99%)	18 (1%)	73	84
1	D	1838/2385 (77%)	1811 (98%)	27 (2%)	60	77
All	All	7271/9540 (76%)	7132 (98%)	139 (2%)	52	72

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	778	CYS
1	D	1043	SER
1	D	1894	CYS
1	B	444	PHE
1	B	251	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2292	ASN
1	C	1622	HIS
1	D	1622	HIS
1	C	1065	HIS
1	C	2598	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
3	I3P	B	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.92	0
5	ATP	C	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	0.87	0
3	I3P	A	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.87	0
5	ATP	B	3004	-	28,33,33	0.62	0	34,52,52	0.86	1 (2%)
5	ATP	D	3004	-	28,33,33	0.62	0	34,52,52	0.87	1 (2%)
3	I3P	D	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.85	0
5	ATP	A	3004	-	28,33,33	0.61	0	34,52,52	0.86	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
3	I3P	B	3002	-	-	1/15/39/39	0/1/1/1
5	ATP	C	3004	-	-	2/18/38/38	0/3/3/3
3	I3P	C	3002	-	-	1/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	0/15/39/39	0/1/1/1
5	ATP	B	3004	-	-	4/18/38/38	0/3/3/3
5	ATP	D	3004	-	-	2/18/38/38	0/3/3/3
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1
5	ATP	A	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	A	3002	I3P	P4-O4	6.06	1.70	1.59
3	B	3002	I3P	P4-O4	6.06	1.70	1.59
3	C	3002	I3P	P4-O4	6.06	1.70	1.59
3	D	3002	I3P	P4-O4	6.05	1.70	1.59
3	C	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	A	3004	ATP	C5'-C6-N6	2.33	123.86	120.31
5	B	3004	ATP	C5'-C6-N6	2.33	123.86	120.31
5	C	3004	ATP	C5'-C6-N6	2.32	123.85	120.31
5	D	3004	ATP	C5'-C6-N6	2.32	123.85	120.31

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

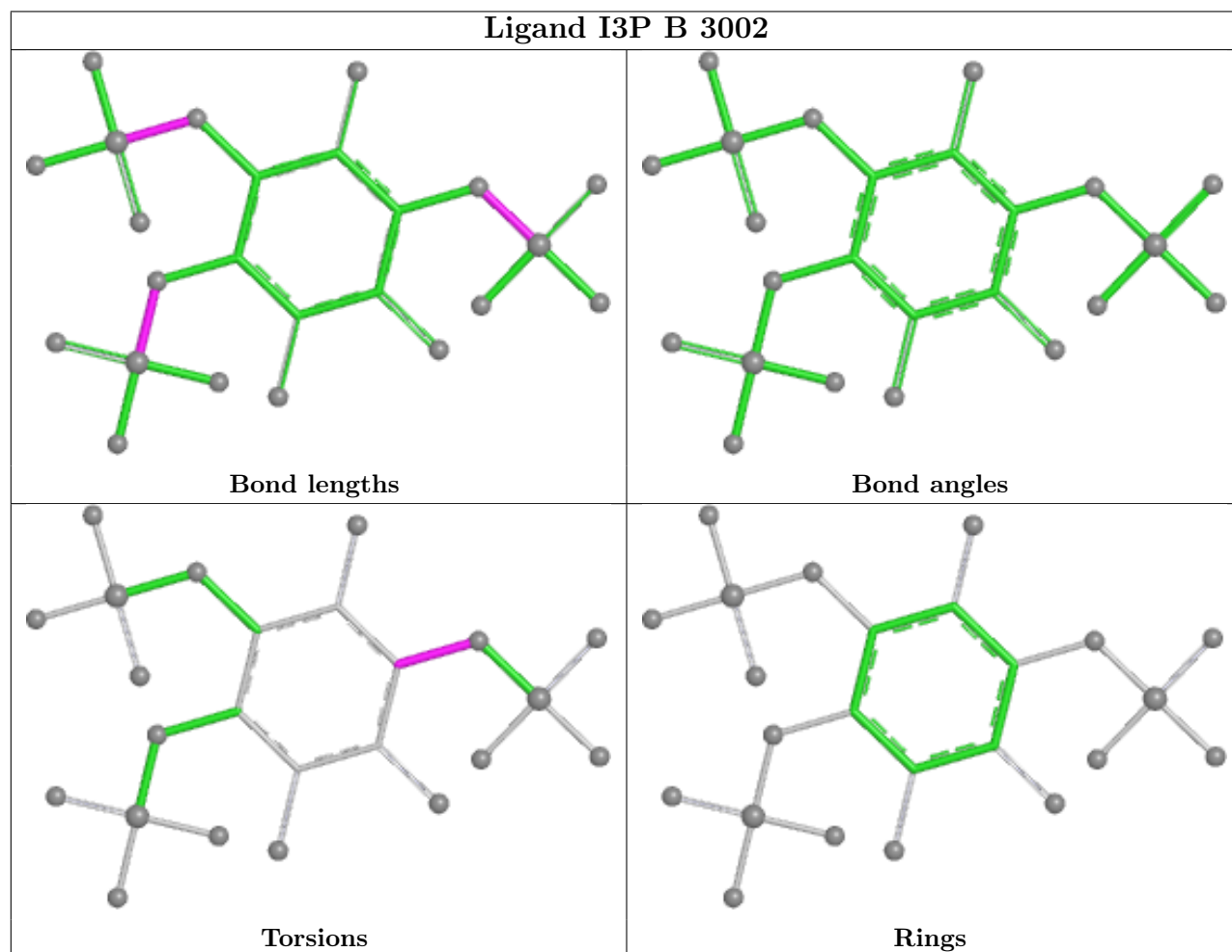
Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	C5'-O5'-PA-O2A
5	A	3004	ATP	C3'-C4'-C5'-O5'
5	A	3004	ATP	O4'-C4'-C5'-O5'
5	D	3004	ATP	O4'-C4'-C5'-O5'
5	D	3004	ATP	C3'-C4'-C5'-O5'

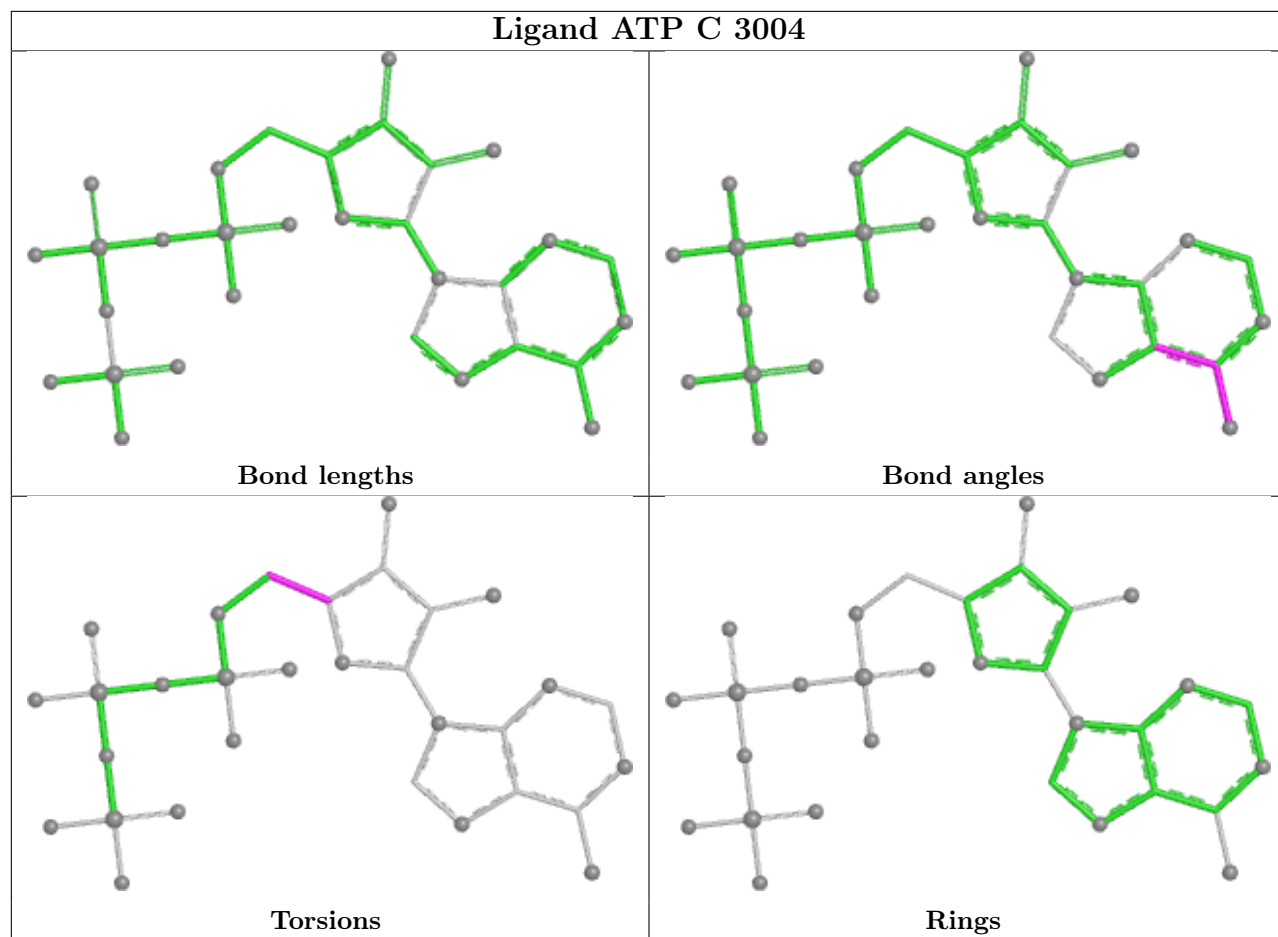
There are no ring outliers.

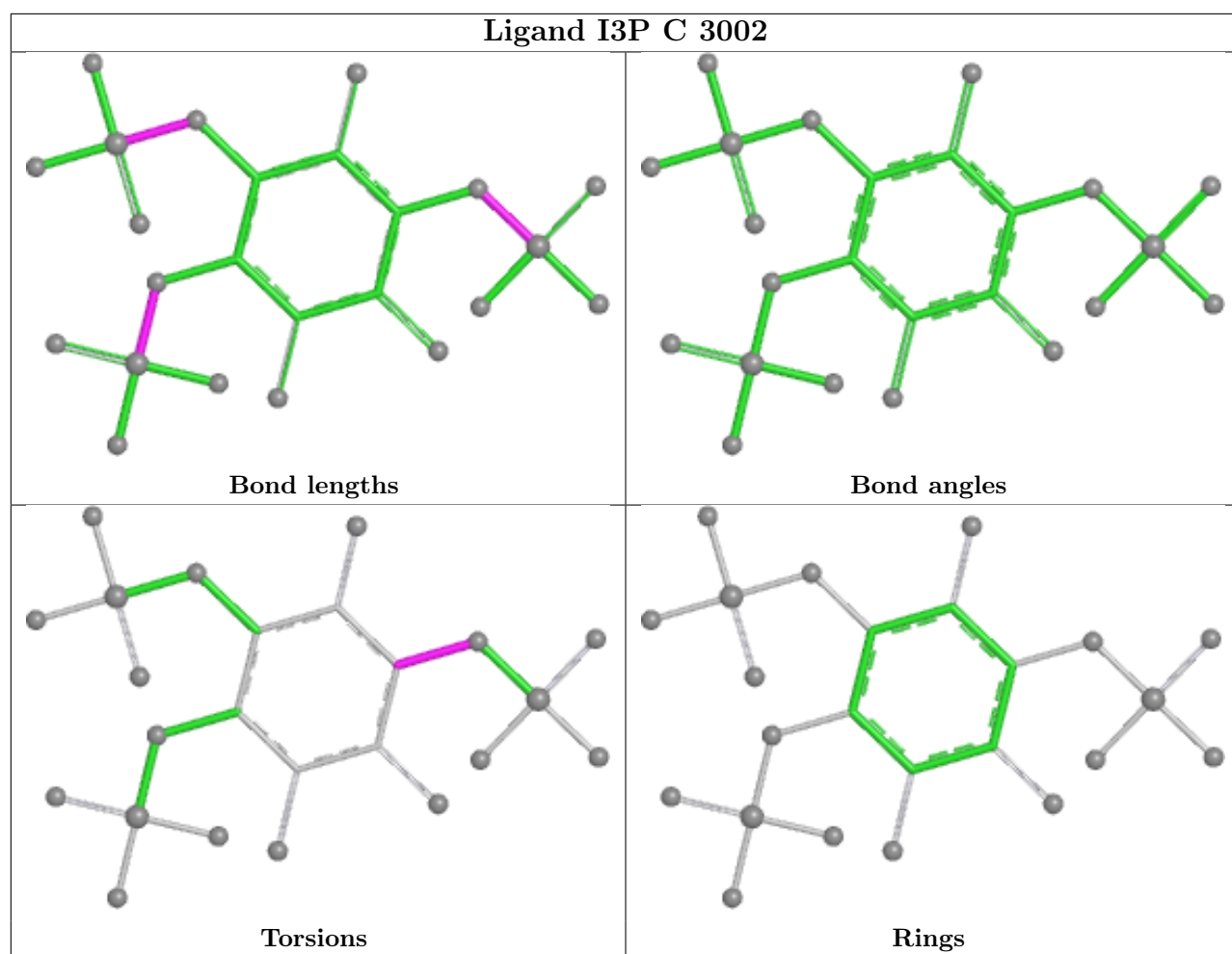
1 monomer is involved in 1 short contact:

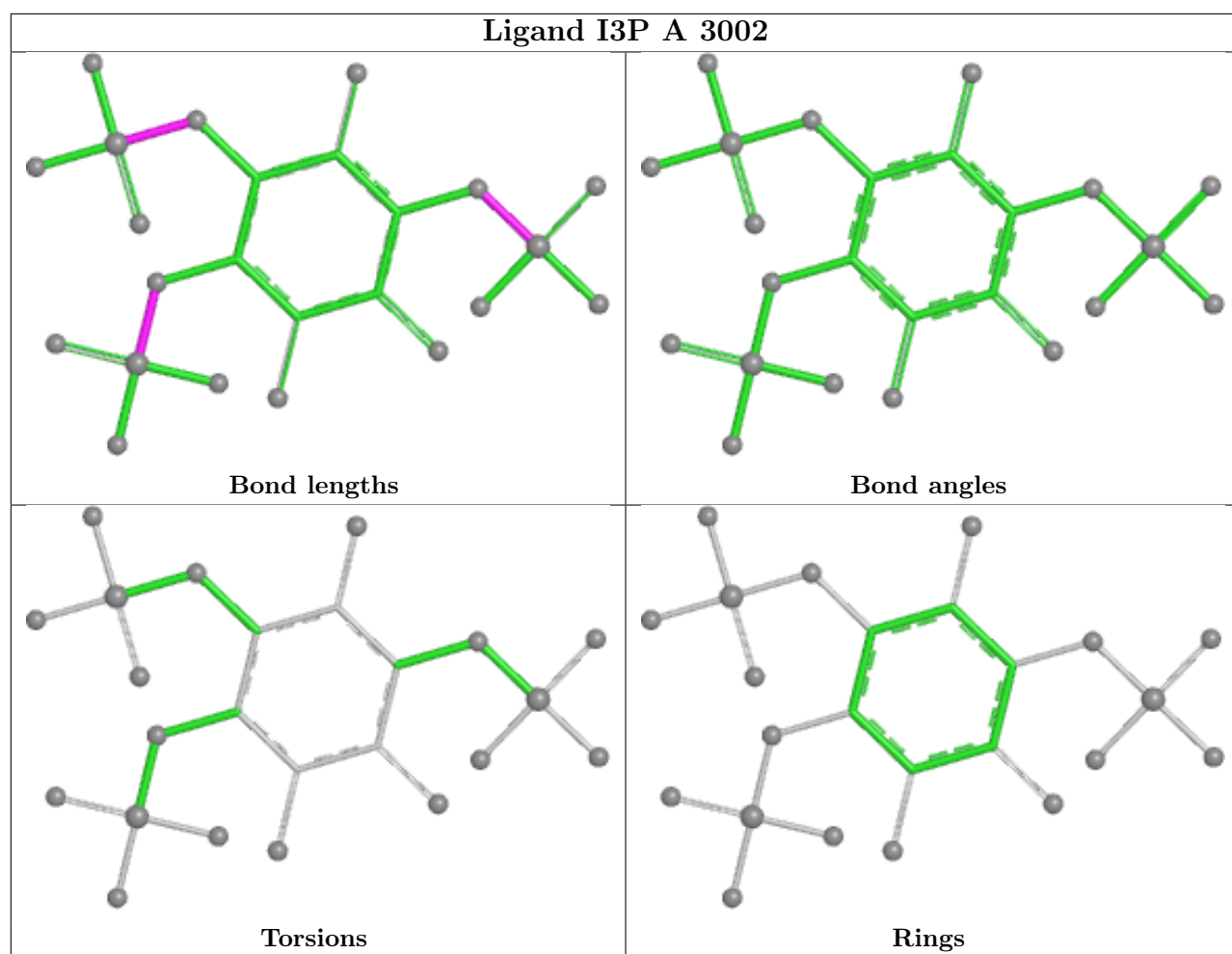
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3002	I3P	1	0

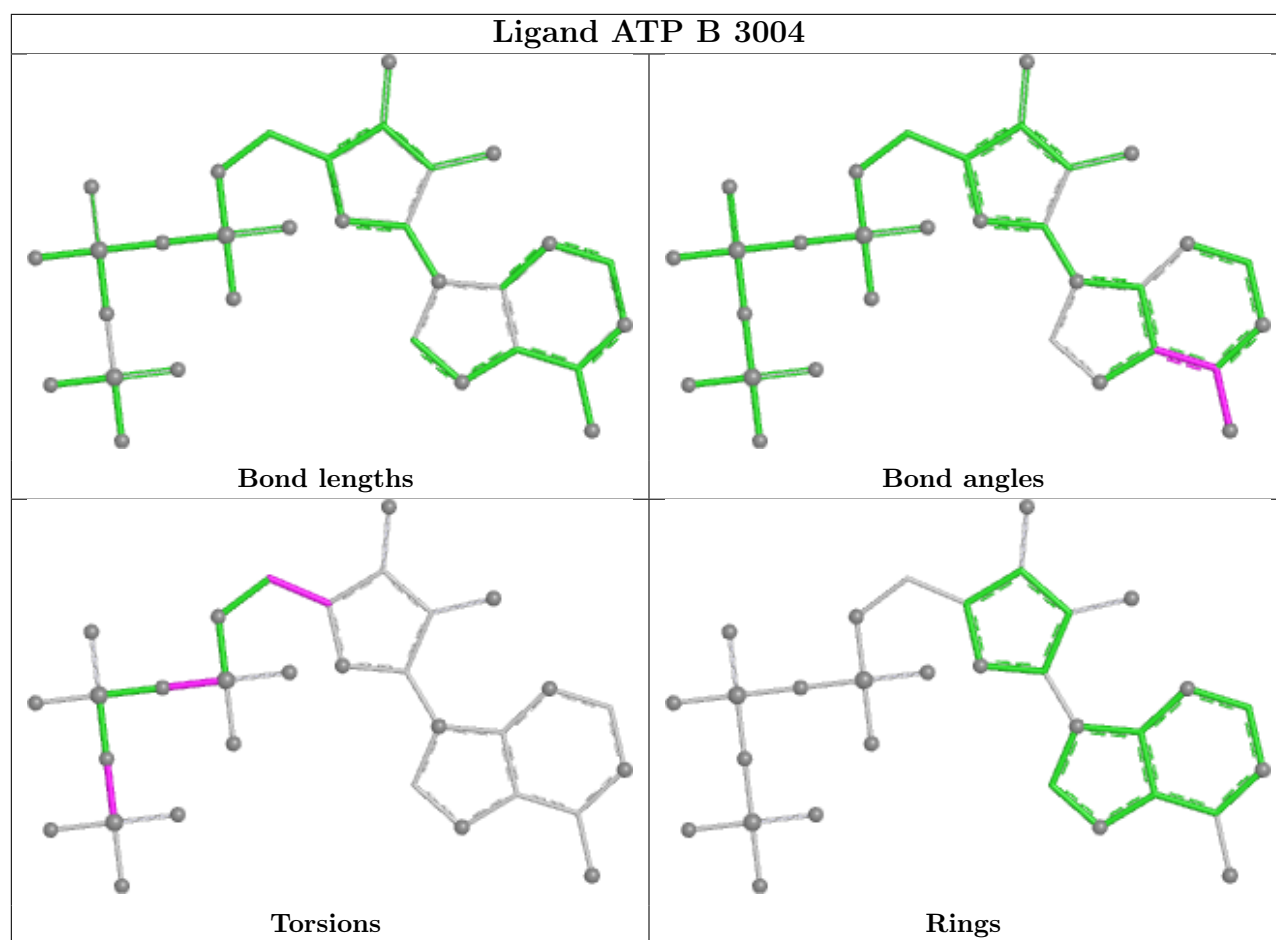
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

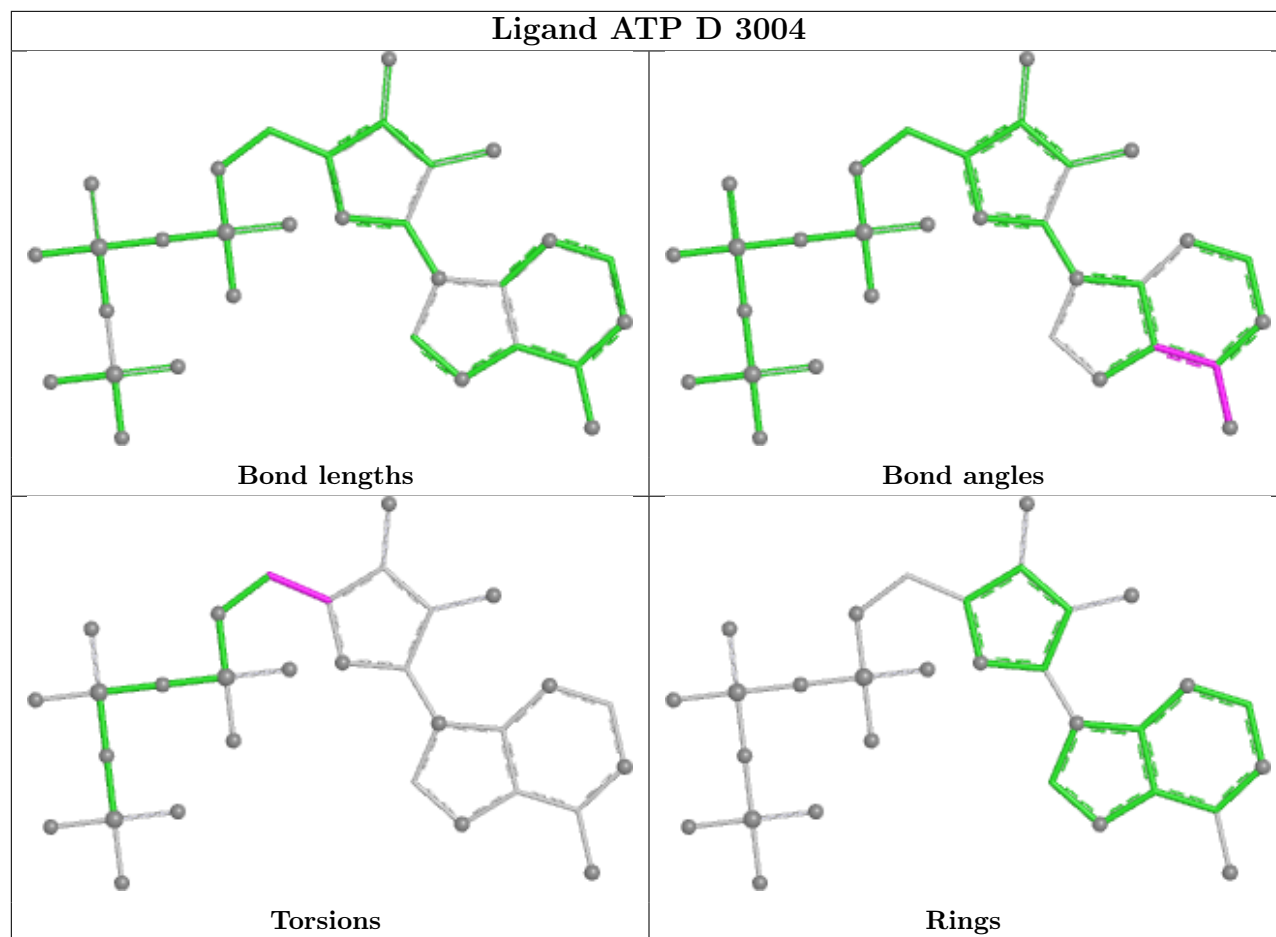


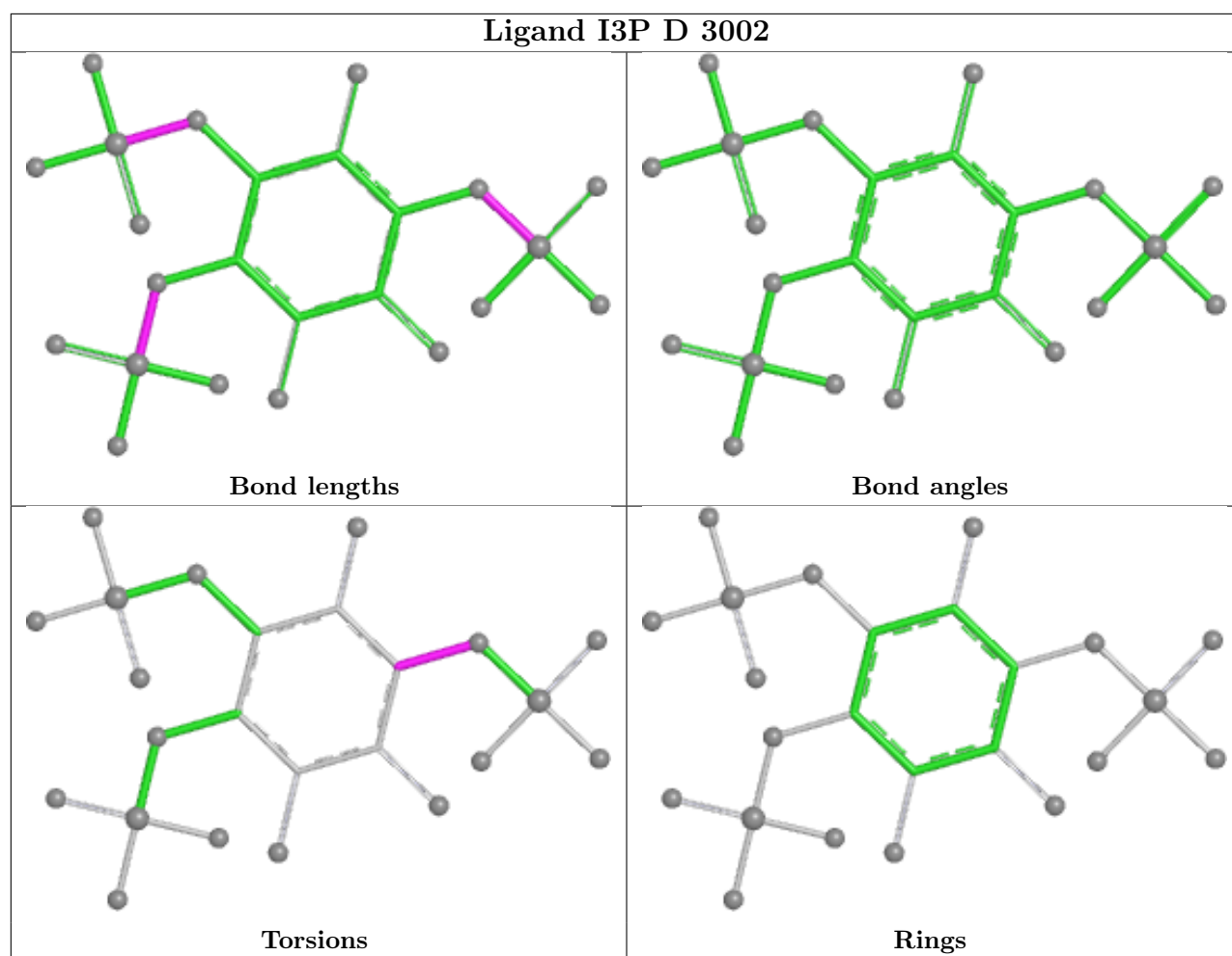


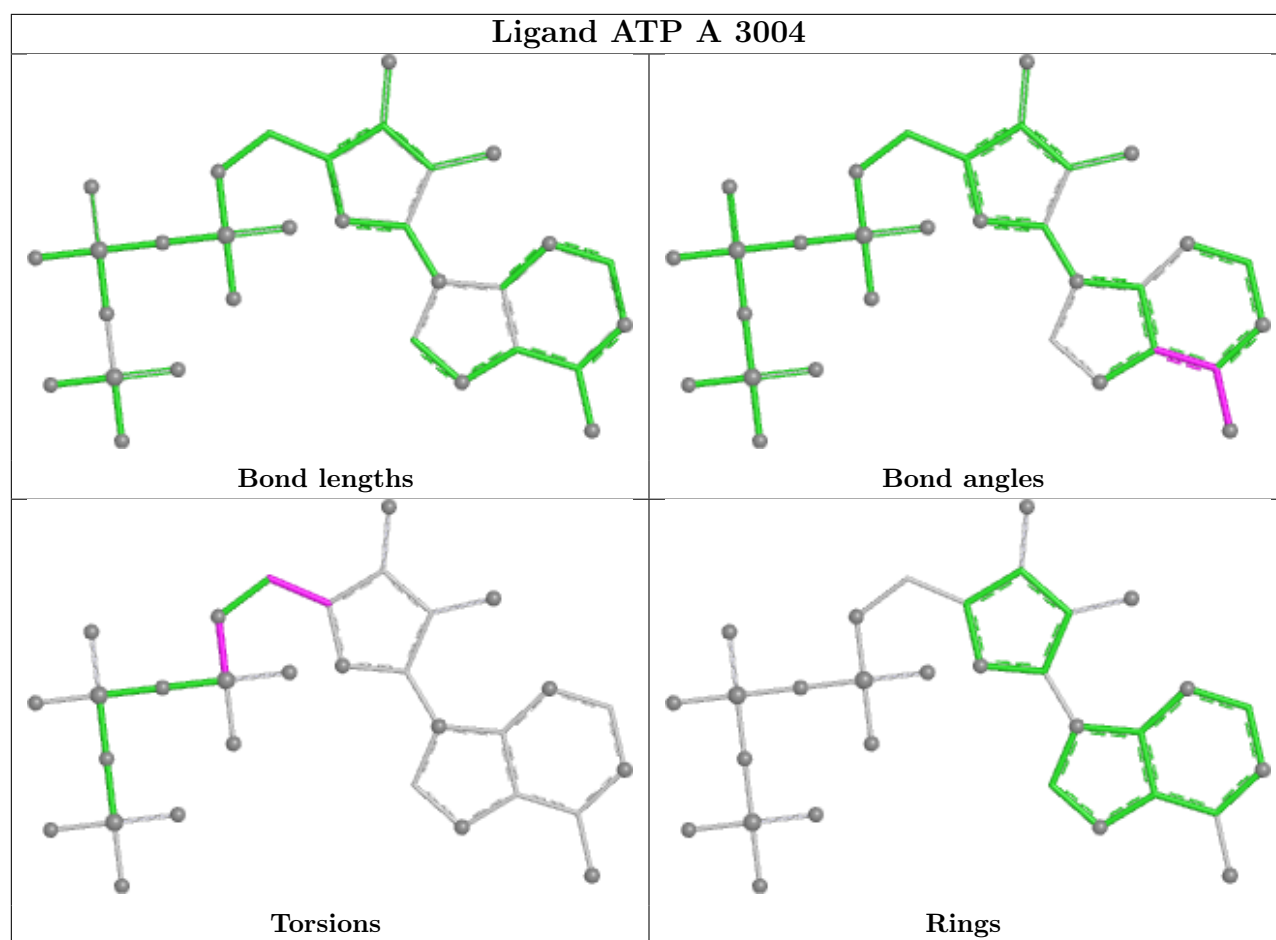












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

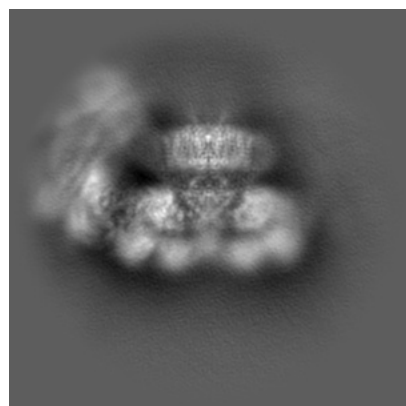
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41365. These allow visual inspection of the internal detail of the map and identification of artifacts.

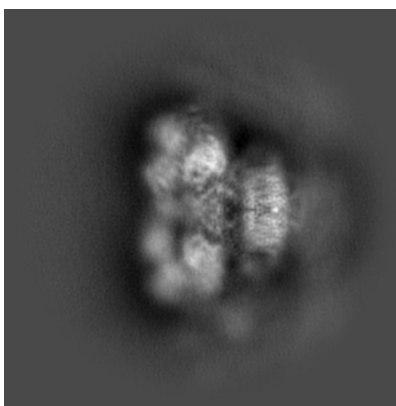
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

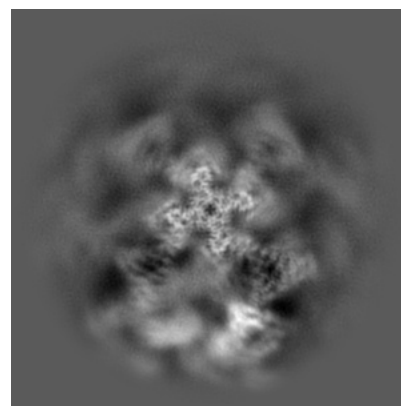
6.1.1 Primary map



X

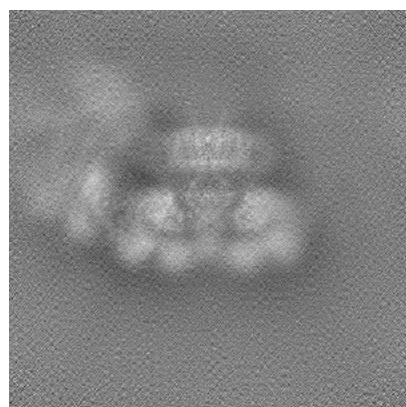


Y

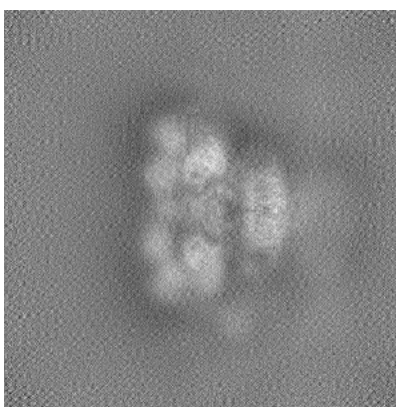


Z

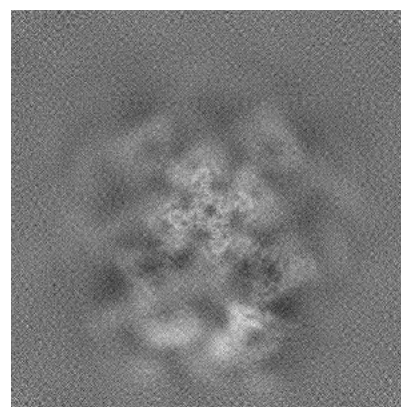
6.1.2 Raw map



X



Y

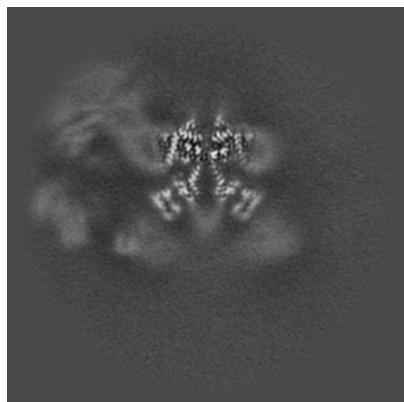


Z

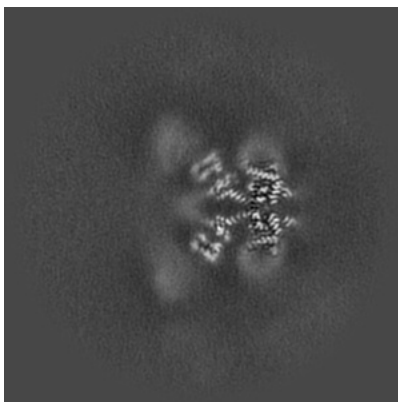
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

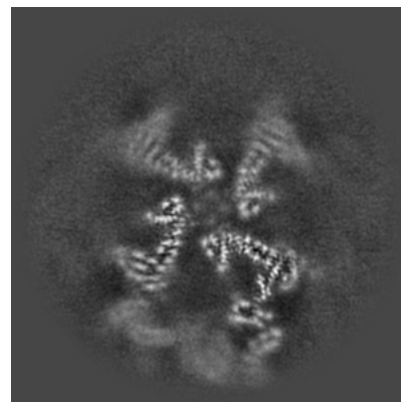
6.2.1 Primary map



X Index: 256

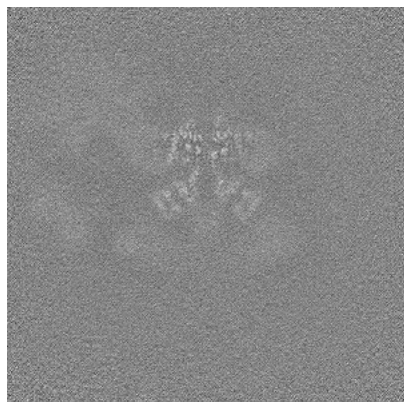


Y Index: 256



Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

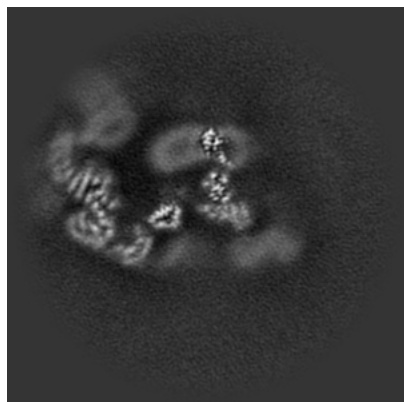


Z Index: 256

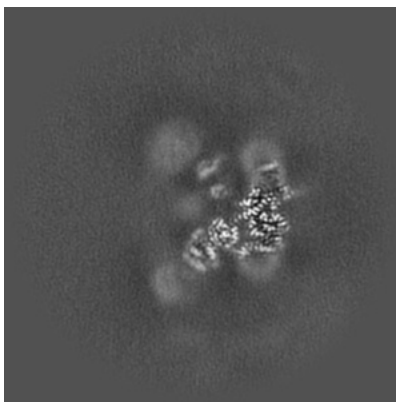
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

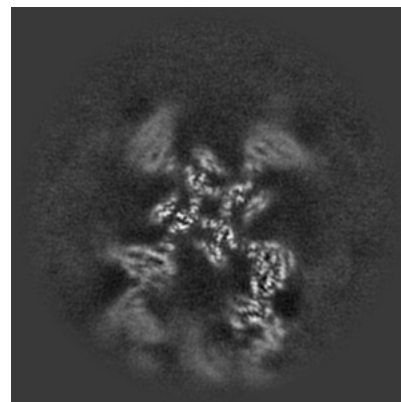
6.3.1 Primary map



X Index: 293

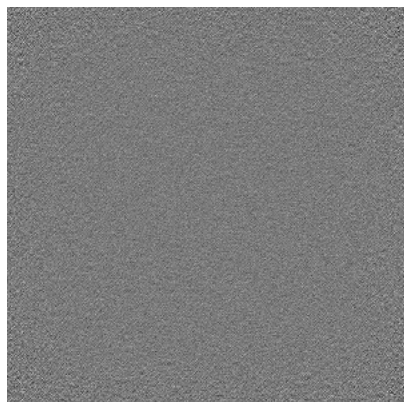


Y Index: 247

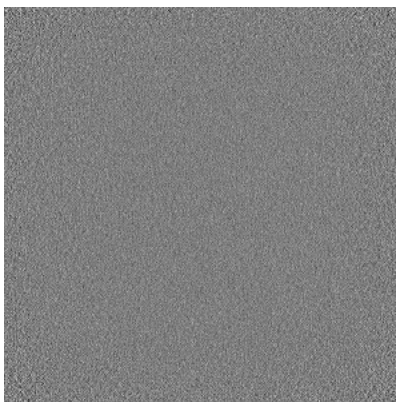


Z Index: 266

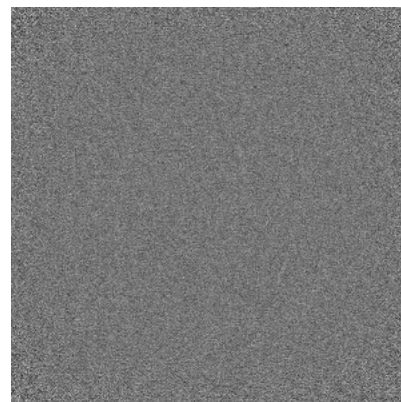
6.3.2 Raw map



X Index: 0



Y Index: 0

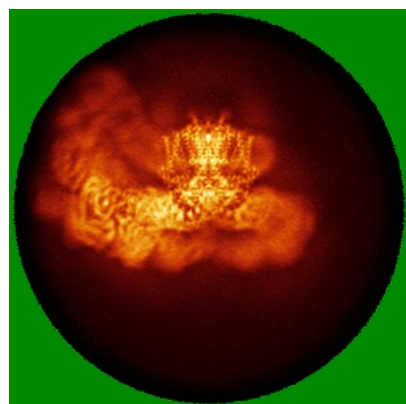


Z Index: 0

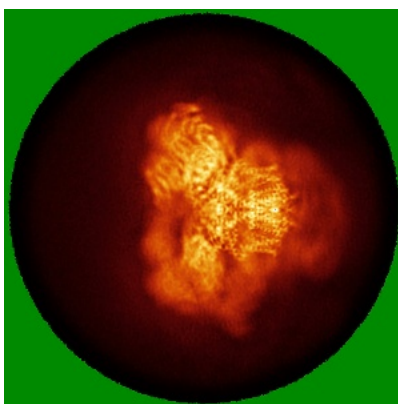
The images above show the largest variance slices of the map in three orthogonal directions.

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

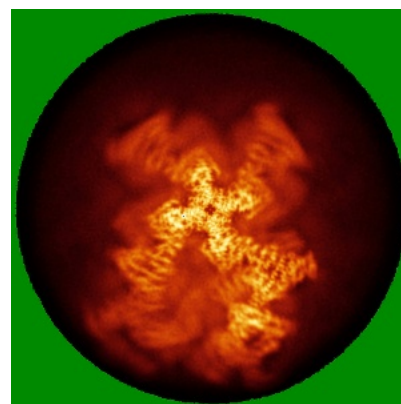
6.4.1 Primary map



X

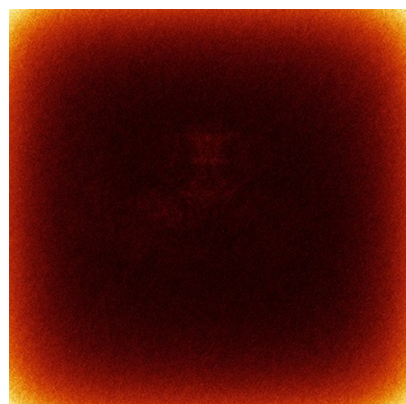


Y

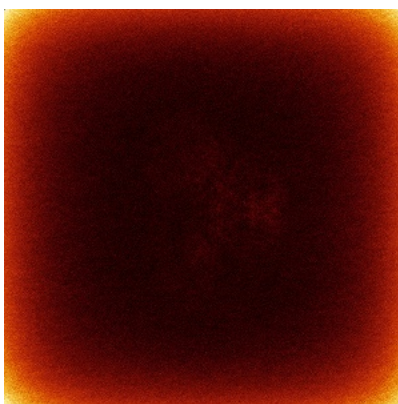


Z

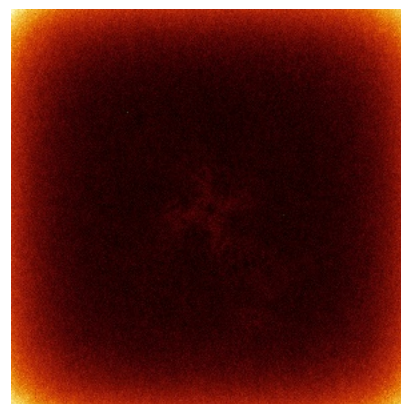
6.4.2 Raw map



X



Y

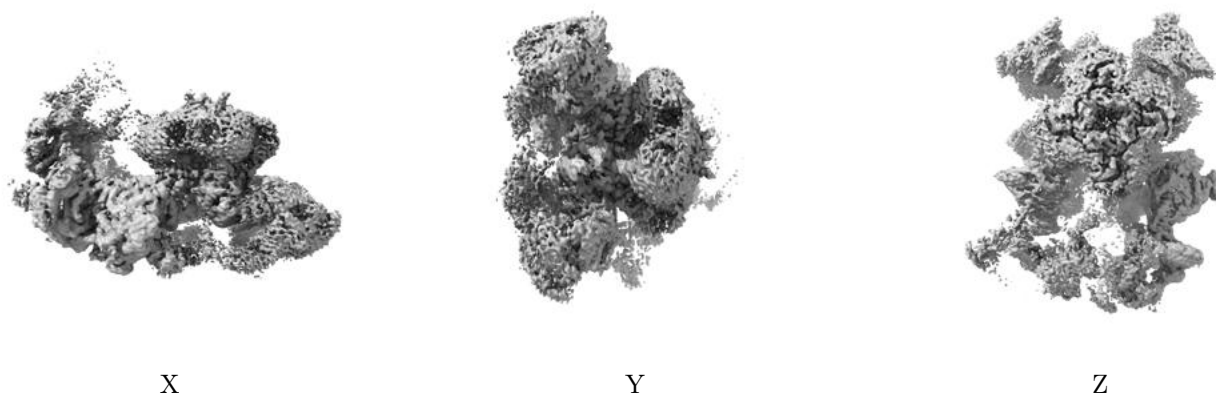


Z

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.

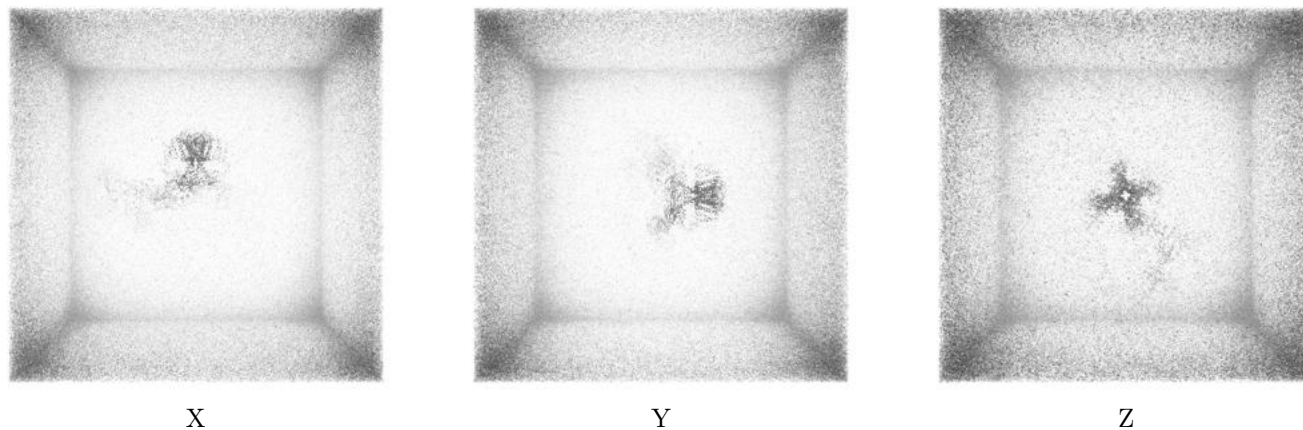
6.5 Orthogonal surface views [i](#)

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.

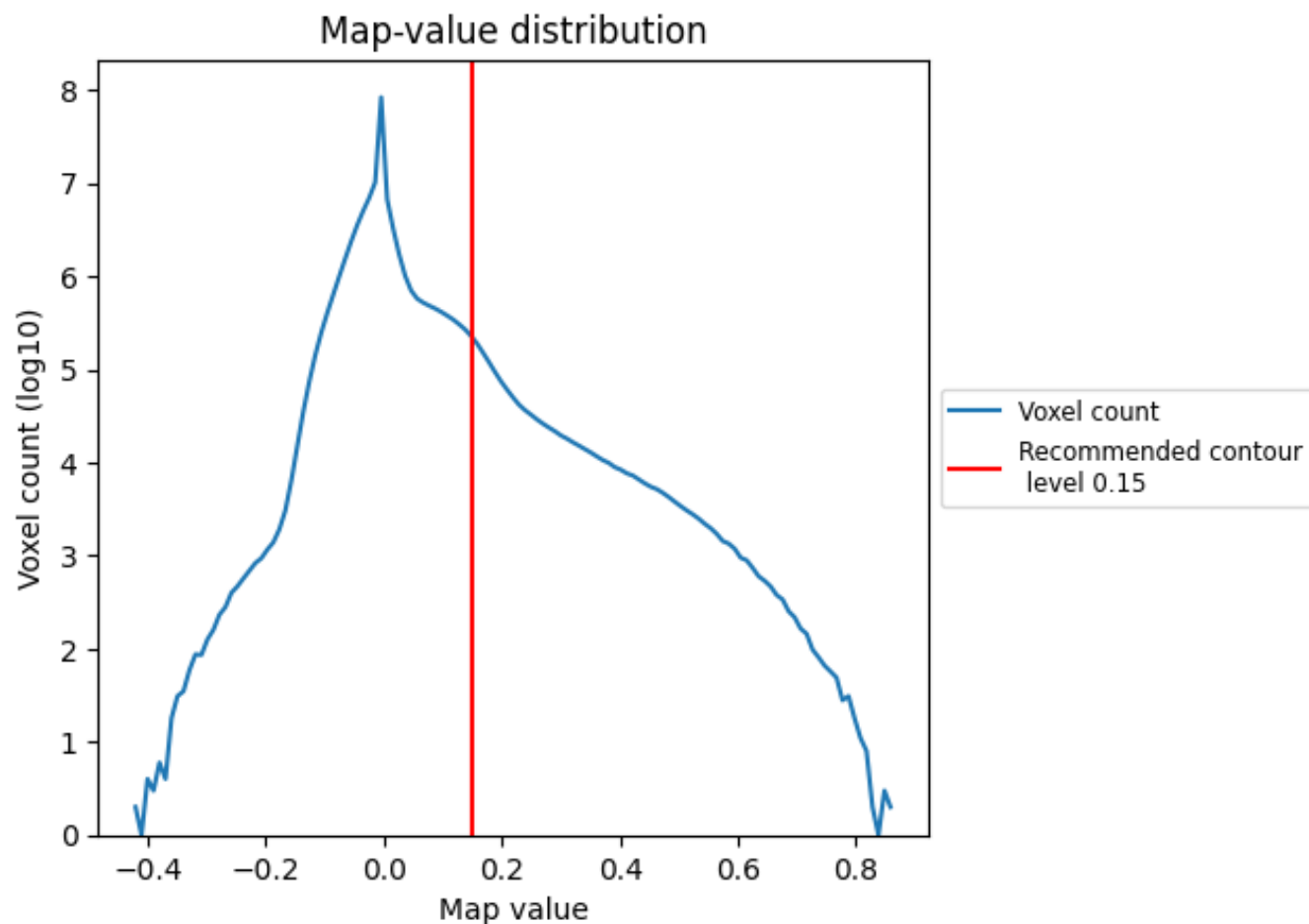
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

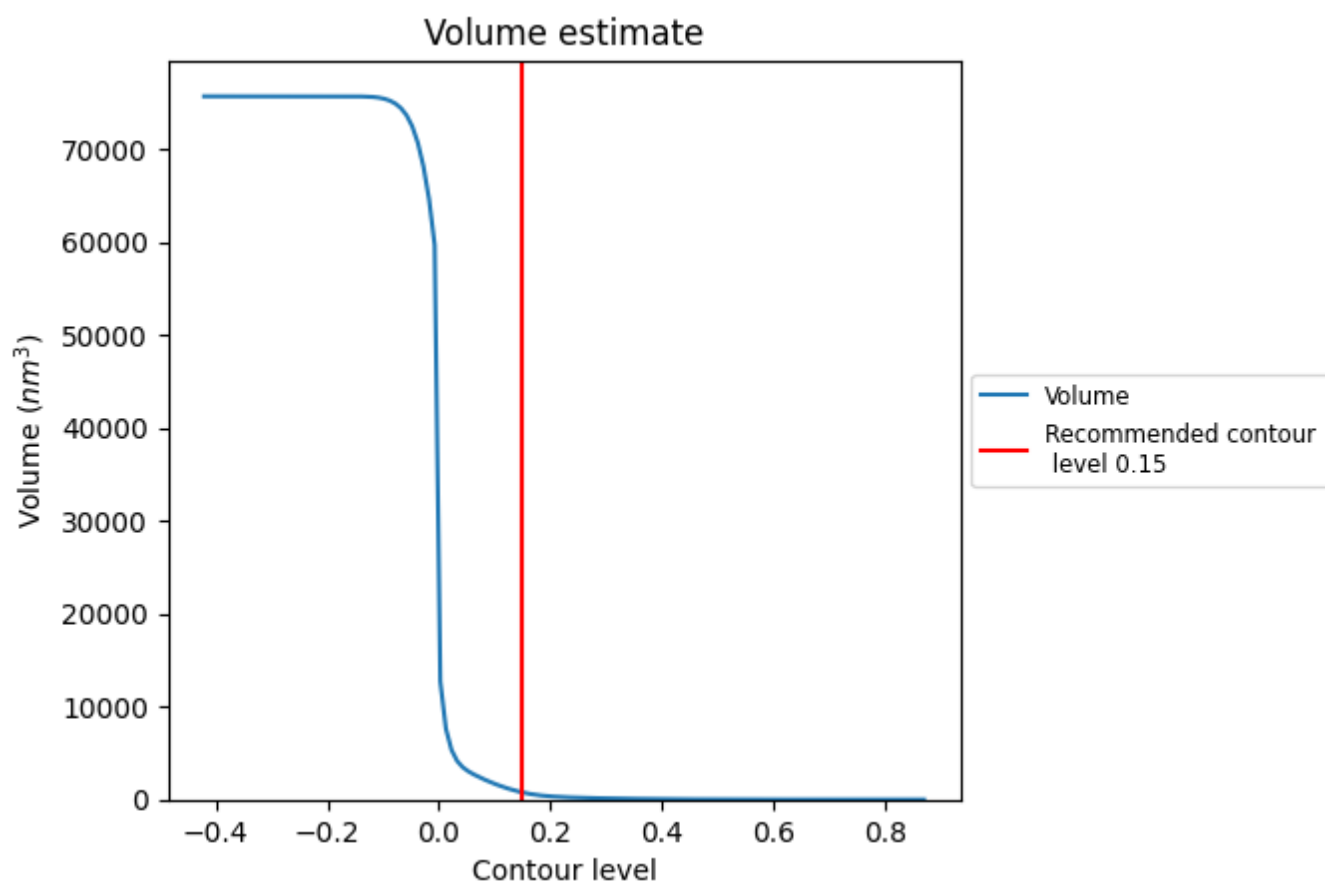
This section contains the results of statistical analysis of the map.

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.

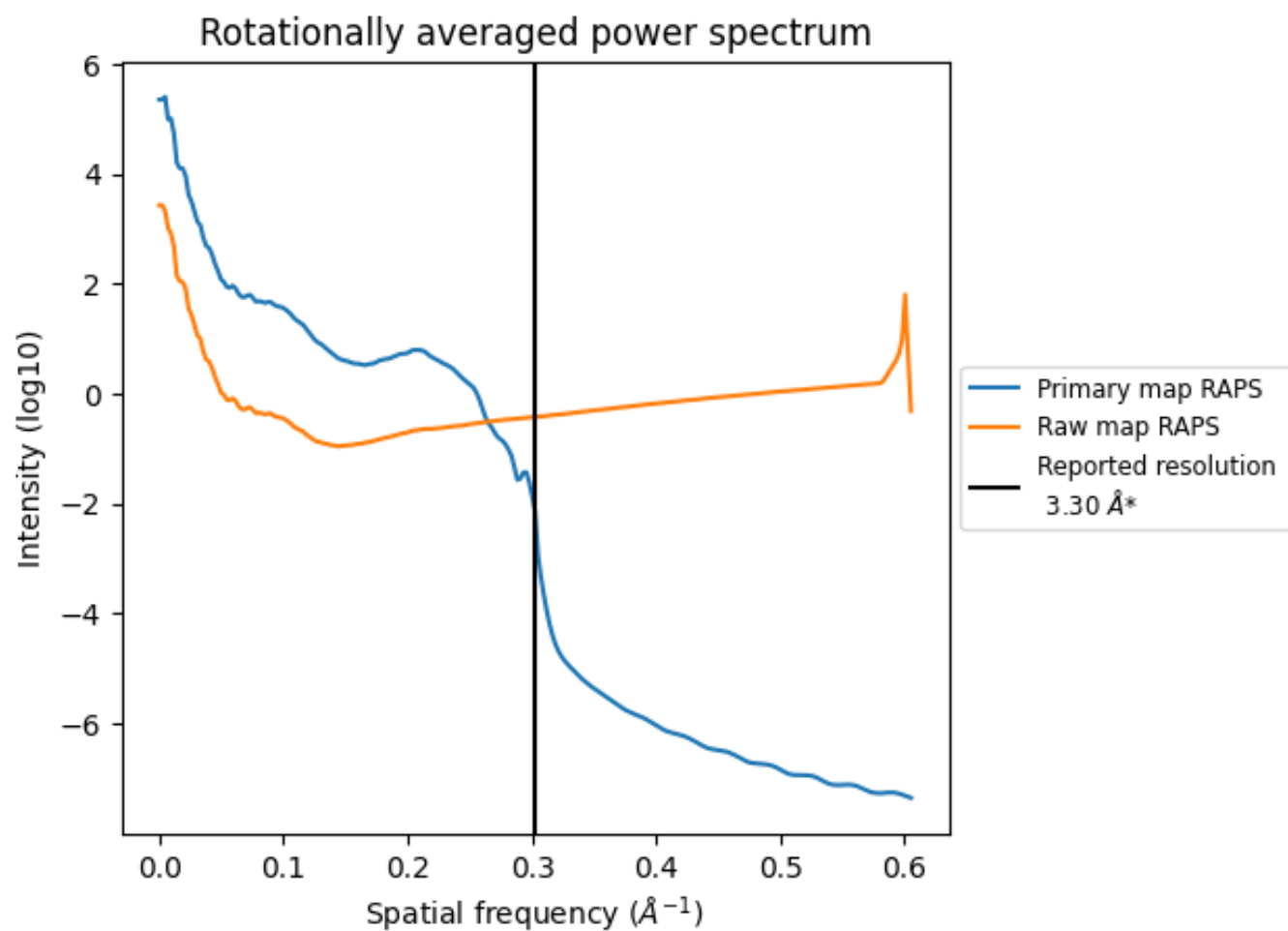
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 764 nm³; this corresponds to an approximate mass of 690 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 ⓘ

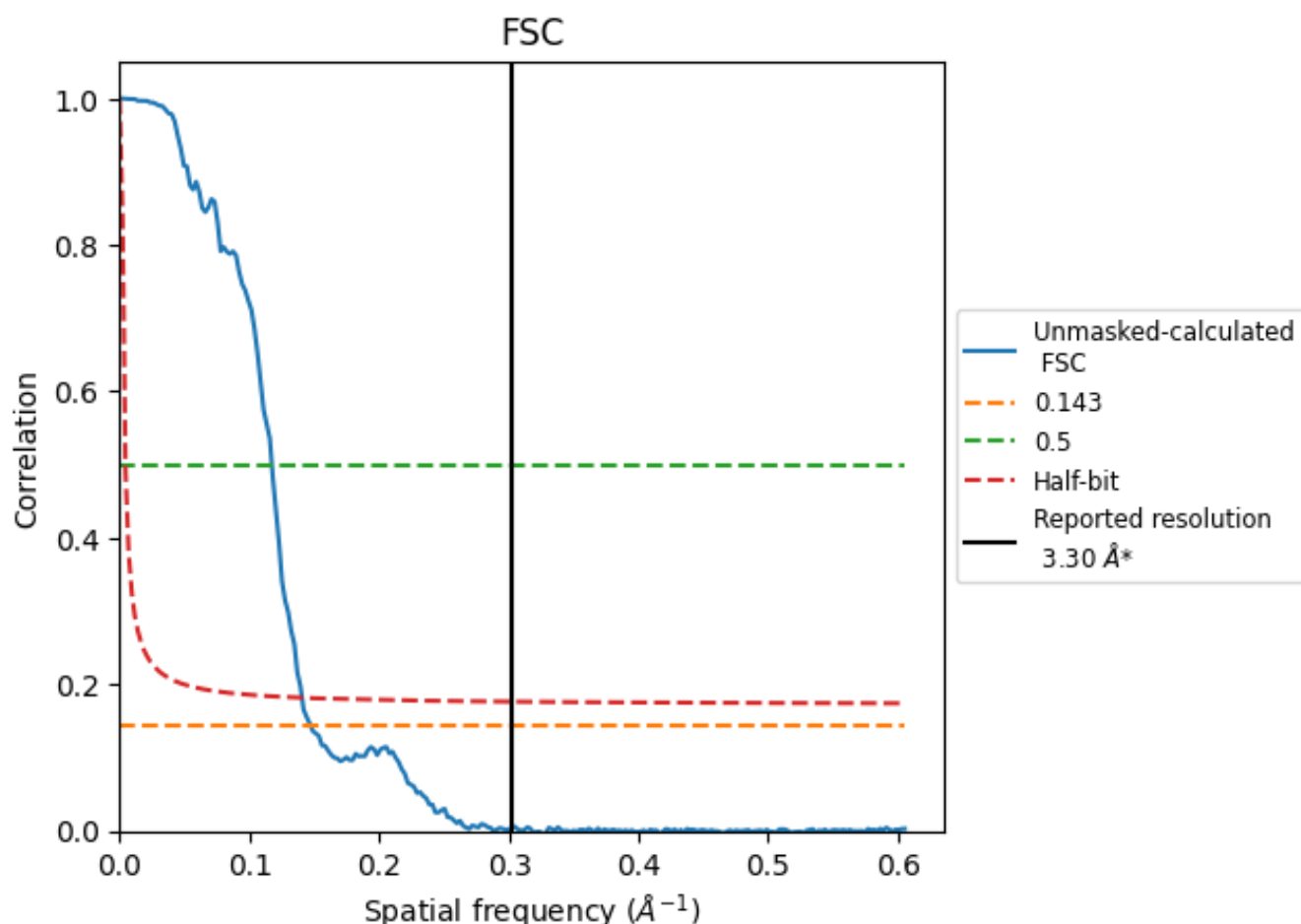


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

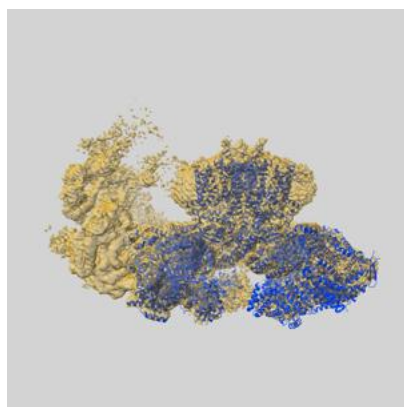
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.78	8.52	7.11

*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 6.78 differs from the reported value 3.3 by more than 10 %

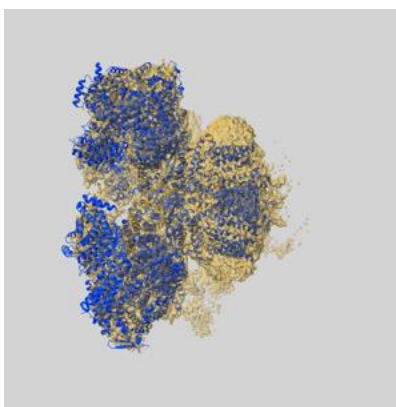
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41365 and PDB model 8TL9. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

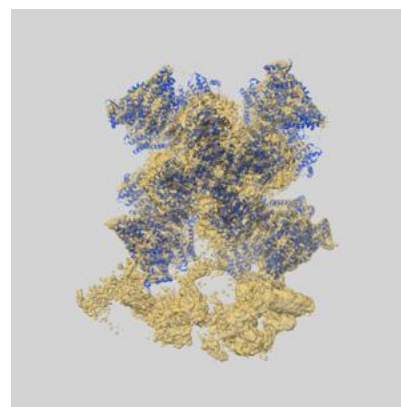
9.1 Map-model overlay [i](#)



X



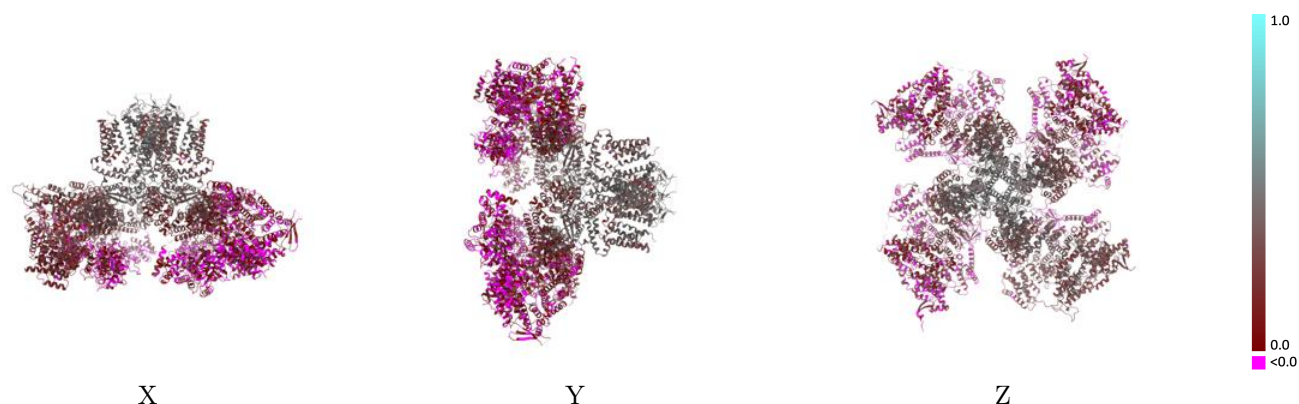
Y



Z

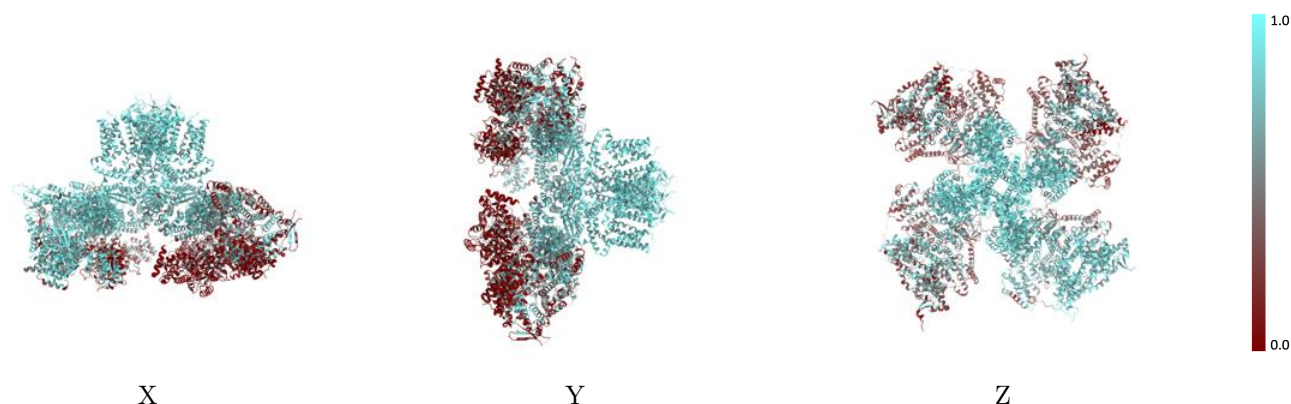
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



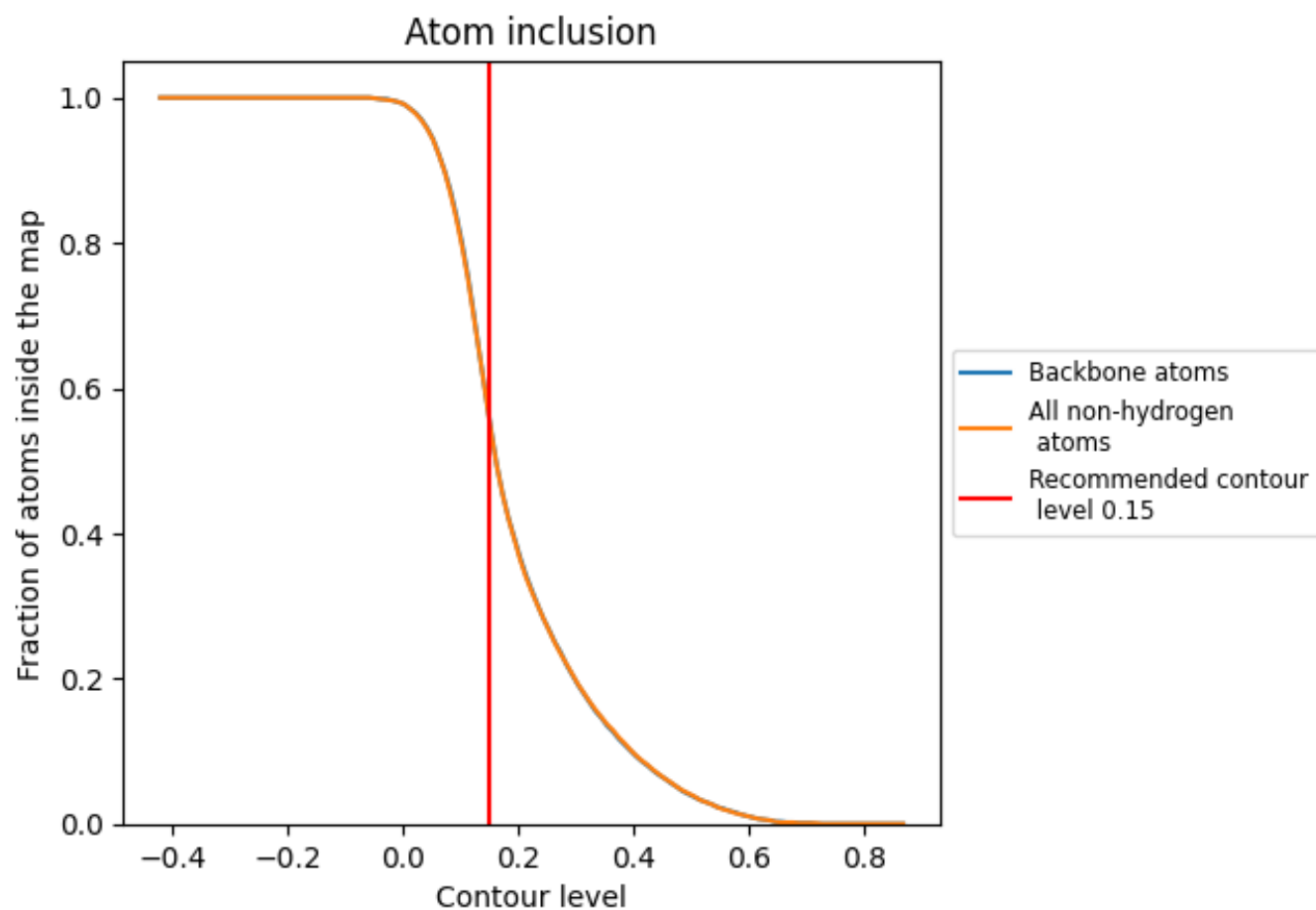
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 56% of all backbone atoms, 56% 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> 0.5580	<div></div> 0.1960
A	<div></div> 0.4890	<div></div> 0.1590
B	<div></div> 0.4520	<div></div> 0.1630
C	<div></div> 0.5790	<div></div> 0.1900
D	<div></div> 0.7300	<div></div> 0.2700

