



# wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 06:00 PM EDT

PDB ID : 9AYJ  
EMDB ID : EMD-43993  
Title : Cryo-EM structure of human Cav3.2 with TTA-P2  
Authors : Fan, X.; Huang, J.; Yan, N.  
Deposited on : 2024-03-07  
Resolution : 3.20 Å(reported)

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

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<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

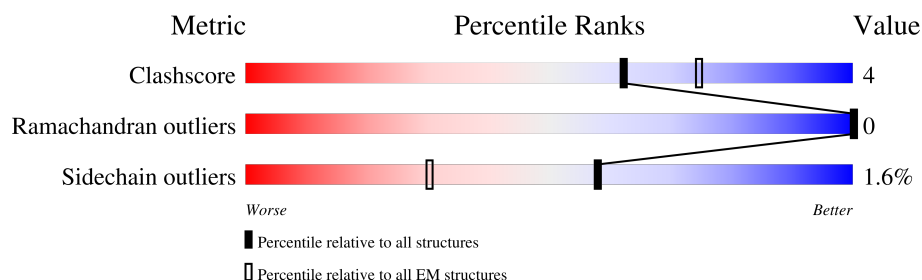
# 1 Overall quality at a glance

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	2116	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8855 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 Voltage-dependent T-type calcium channel subunit alpha-1H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1056	8473	5565	1402	1436	70	0	0

There are 43 discrepancies between the modelled and reference sequences:

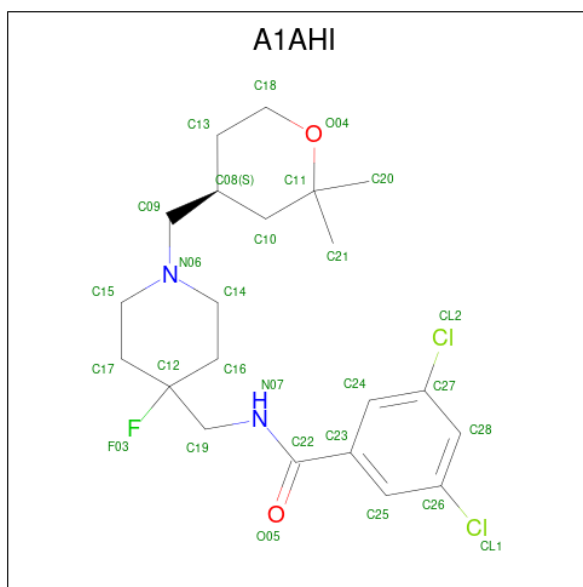
Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP O95180
A	-41	ALA	-	expression tag	UNP O95180
A	-40	SER	-	expression tag	UNP O95180
A	-39	TRP	-	expression tag	UNP O95180
A	-38	SER	-	expression tag	UNP O95180
A	-37	HIS	-	expression tag	UNP O95180
A	-36	PRO	-	expression tag	UNP O95180
A	-35	GLN	-	expression tag	UNP O95180
A	-34	PHE	-	expression tag	UNP O95180
A	-33	GLU	-	expression tag	UNP O95180
A	-32	LYS	-	expression tag	UNP O95180
A	-31	GLY	-	expression tag	UNP O95180
A	-30	GLY	-	expression tag	UNP O95180
A	-29	GLY	-	expression tag	UNP O95180
A	-28	ALA	-	expression tag	UNP O95180
A	-27	ARG	-	expression tag	UNP O95180
A	-26	GLY	-	expression tag	UNP O95180
A	-25	GLY	-	expression tag	UNP O95180
A	-24	SER	-	expression tag	UNP O95180
A	-23	GLY	-	expression tag	UNP O95180
A	-22	GLY	-	expression tag	UNP O95180
A	-21	GLY	-	expression tag	UNP O95180
A	-20	SER	-	expression tag	UNP O95180
A	-19	TRP	-	expression tag	UNP O95180
A	-18	SER	-	expression tag	UNP O95180
A	-17	HIS	-	expression tag	UNP O95180
A	-16	PRO	-	expression tag	UNP O95180
A	-15	GLN	-	expression tag	UNP O95180

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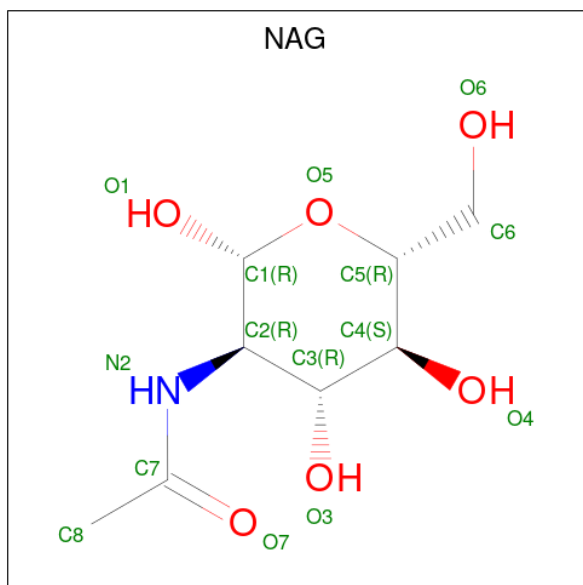
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP O95180
A	-13	GLU	-	expression tag	UNP O95180
A	-12	LYS	-	expression tag	UNP O95180
A	-11	GLY	-	expression tag	UNP O95180
A	-10	PHE	-	expression tag	UNP O95180
A	-9	ASP	-	expression tag	UNP O95180
A	-8	TYR	-	expression tag	UNP O95180
A	-7	LYS	-	expression tag	UNP O95180
A	-6	ASP	-	expression tag	UNP O95180
A	-5	ASP	-	expression tag	UNP O95180
A	-4	ASP	-	expression tag	UNP O95180
A	-3	ASP	-	expression tag	UNP O95180
A	-2	LYS	-	expression tag	UNP O95180
A	-1	GLY	-	expression tag	UNP O95180
A	0	THR	-	expression tag	UNP O95180

- Molecule 2 is 3,5-dichloro-N-[(1-{[(4S)-2,2-dimethyloxan-4-yl]methyl}-4-fluoropiperidin-4-yl)methyl]benzamide (three-letter code: A1AHI) (formula: C<sub>21</sub>H<sub>29</sub>Cl<sub>2</sub>FN<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	Cl	F	N	O	0
			28	21	2	1	2	2	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

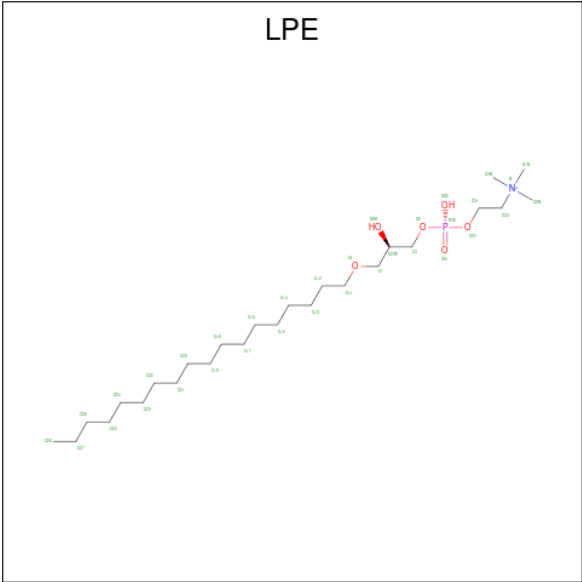


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

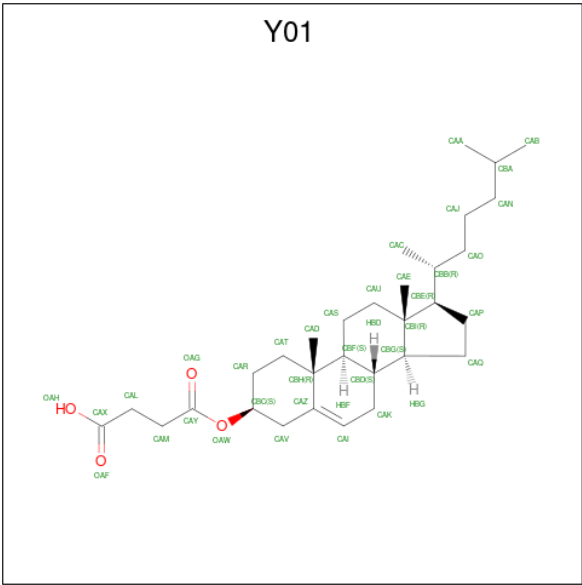
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

- Molecule 5 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: C<sub>26</sub>H<sub>57</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	19	1	6	1	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



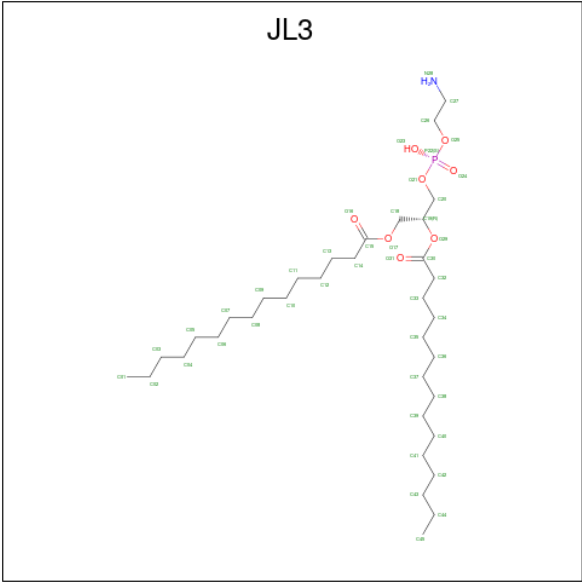
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	

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Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			35	31	4	

- Molecule 7 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-pentadecanoyloxy-propyl] pentadecanoate (three-letter code: JL3) (formula: C<sub>35</sub>H<sub>70</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
7	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	A	1	Total	C	N	O	P	0
			35	25	1	8	1	





GLU	PRO	LYS	PRO	PRO	PRO	ALA	ALA	HIS	MET	G1695	ARG	K1390	CYS
PRO	ALA	LYS	VAL	ALA	ALA	SER	ARG	PRO	ALA	I1696	ARG	I1391	LEU
PRO	ALA	LYS	GLY	GLY	VAL	SER	ARG	PRO	GLY	E1700	THR	L1395	LEU
SER	GLY	SER	GLY	GLY	THR	ARG	LEU	GLN	GLY	I1701	PHE	L1425	HIS
GLU	GLU	PRO	GLU	GLY	THR	LEU	GLY	GLN	GLY	E1702	PRO	S1425	LYS
PRO	ARG	PRO	ASP	ASP	ARG	SER	GLU	GLU	SER	A1705	GLU	I1443	VAL
PRO	TRP	ILE	LEU	HIS	THR	HIS	VAL	VAL	ARG	A1706	ALA	E1460	LEU
PRO	GLN	VAL	ARG	THR	LEU	CYS	GLY	GLU	VAL	L1707	GLN	D1463	PRO
GLY	SER	GLU	LEU	ARG	THR	ARG	THR	ASP	ASP	P1708	ARG	D1463	LYS
ASP	CYS	PRO	TYR	TYR	GLN	GLN	GLY	GLY	ASP	I1709	ARG	T1464	PRO
PRO	ARG	ALA	VAL	CYS	ALA	ALA	ALA	ARG	ARG	M1710	TYR	R1465	TRP
GLU	GLU	GLY	VAL	VAL	HIS	VAL	GLY	PRO	PRO	L1720	TYR	M1466	CYS
LYS	HIS	ASP	ALA	SER	THR	THR	PRO	PRO	ASP	L1720	ALA	R1479	ARG
ARG	LEU	GLY	GLN	SER	ASP	ASP	LEU	LEU	TYR	M1731	ASP	L1500	SER
GLY	THR	GLY	ARG	ARG	THR	THR	PRO	GLN	TYR	L1746	ASP	L1500	ARG
GLY	VAL	SER	PHE	PRO	ASP	LEU	GLY	GLN	GLN	P1605	GLN	D1504	GLU
LEU	PRO	ALA	LEU	ALA	GLY	ALA	SER	SER	GLY	T1606	ALA	D1504	ALA
TYR	SER	ARG	ASP	ALA	GLU	VAL	VAL	VAL	PRO	Y1618	ALA	L1544	ALA
LEU	PHE	PRO	LYS	PRO	GLY	GLY	ALA	GLY	GLY	Y1618	ALA	L1544	LEU
THR	ALA	SER	PRO	GLY	LYS	SER	VAL	ALA	ALA	L1619	ALA	V1519	TYR
VAL	PHE	ALA	GLY	GLY	ILE	VAL	VAL	ALA	ASP	D1620	ALA	D1520	LEU
PRO	GLU	ALA	ARG	GLU	SER	HIS	ASP	ASP	ASP	D1779	ALA	D1520	PHE
GLN	LEU	GLY	GLY	GLU	PRO	PRO	PRO	ALA	ALA	E1783	ALA	P1529	SER
LEU	LEU	SER	GLN	GLU	ALA	ALA	ALA	ASN	ASN	N1630	ALA	P1529	PRO
GLY	GLY	THR	TRP	SER	THR	THR	GLY	LEU	VAL	N1640	ALA	L1532	GLN
LYS	VAL	THR	ARG	ASP	LEU	SER	SER	VAL	VAL	N1611	ALA	L1539	ASN
PRO	PRO	LEU	PRO	PRO	ASP	CYS	CYS	ALA	ALA	D1816	ALA	L1539	GLU
GLY	SER	ARG	SER	ALA	PRO	ALA	ALA	ARG	ARG	E1647	ALA	L1547	GLU
PRO	GLY	ARG	ALA	ASP	ALA	SER	LYS	VAL	LYS	R1819	ALA	L1547	GLU
SER	PRO	ARG	GLY	GLY	GLY	GLY	LEU	VAL	VAL	Y1654	ALA	H1559	GLU
THR	THR	THR	LEU	GLY	PRO	PRO	GLN	SER	SER	R1823	ALA	H1559	GLU
ALA	PHE	PRO	GLY	VAL	VAL	VAL	ILE	VAL	VAL	E1824	ALA	R1562	GLU
THR	LEU	SER	SER	SER	GLY	GLY	PRO	SER	SER	D1825	ALA	Q1563	GLU
PRO	ALA	CYS	GLY	HIS	LYS	LYS	LEU	LEU	ARG	K1826	ALA	H1564	GLU
ALA	GLY	GLY	GLU	ILE	THR	THR	ALA	MET	MET	K1667	ALA	H1564	GLU
PRO	SER	ALA	PRO	THR	THR	THR	VAL	LEU	LEU	H1827	ALA	G1336	GLU
GLY	HIS	THR	GLY	SER	VAL	VAL	SER	SER	SER	V1855	ALA	T1336	GLU
GLY	VAL	PRO	GLY	SER	ARG	ARG	SER	LEU	LEU	F1673	ALA	V1347	GLU
GLY	VAL	HIS	ALA	ALA	PRO	ALA	PRO	PRO	ASN	R1674	ALA	V1347	GLU
ASP	THR	ARG	CYS	CYS	VAL	VAL	ALA	ASN	ASP	S1866	ALA	G1351	GLU
PRO	PRO	ASP	PRO	THR	THR	THR	ARG	ASP	ASP	ASN	ALA	G1351	GLU
SER	SER	SER	TRP	PRO	GLN	GLY	GLY	SER	LYS	F1677	ARG	E1356	GLU
LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY	TYR	TYR	K1678	ARG	E1356	GLU
GLU	ARG	GLU	PRO	THR	GLY	GLY	PRO	MET	ALA	D1679	ARG	Q1361	GLU
THR	ALA	THR	GLU	ALA	LEU	ALA	ARG	ARG	ALA	R1680	GLU	Q1361	GLU
SER	SER	SER	GLU	GLU	GLN	GLN	HIS	PRO	PRO	ASP	LYS	V1381	LYS
SER	GLY	GLY	PRO	PRO	SER	VAL	ALA	VAL	VAL	Q1683	ARG	V1381	ARG
GLY	ALA	GLY	ALA	GLY	PRO	PRO	LEU	PRO	PRO	GLU	LEU	A1382	LEU
ALA	ILE	ALA	GLY	PRO	ARG	ARG	SER	ASP	ASP	L1686	ARG	A1382	ARG
VAL	VAL	GLY	GLY	GLY	GLU	GLU	ARG	SER	ALA	A1687	ARG	M1383	ARG
PRO	PRO	GLY	ARG	ALA	PRO	ALA	GLY	SER	ALA	I1688	LEU	A1384	SER
PRO	PRO	GLY	ARG	ALA	PRO	PRO	GLY	ALA	ALA	V1689	GLU	A1384	GLY
ASP	LEU	ASP	ARG	SER	ARG	SER	THR	PRO	PRO	L1690	ARG	G1388	GLY
										L1690	ARG	G1388	ARG
										L1691	ARG	A1389	ARG
										S1692	ARG	A1389	ARG
										L1693	ARG	A1389	ARG
										M1694	ARG	A1389	ARG

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113396	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.827	Depositor
Minimum map value	-1.388	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.18	Depositor
Map size ( $\text{\AA}$ )	265.216, 265.216, 265.216	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.036, 1.036, 1.036	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: Y01, NAG, JL3, LPE, CA, A1AH1

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	0/8662	0.46	0/11741

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	8473	0	8661	69	0
2	A	28	0	0	0	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	27	0	39	1	0
6	A	140	0	196	2	0
7	A	158	0	0	0	0
All	All	8855	0	8922	72	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 4.

The worst 5 of 72 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:891:VAL:HG21	1:A:1443:ILE:HD11	1.50	0.93
1:A:294:ARG:NE	1:A:294:ARG:O	2.15	0.79
1:A:112:LEU:HD22	1:A:143:ILE:HD11	1.65	0.78
1:A:1816:ASP:O	1:A:1819:ARG:NH1	2.25	0.69
1:A:1514:LEU:HD21	1:A:1532:LEU:HD12	1.76	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1038/2116 (49%)	1021 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	939/1793 (52%)	924 (98%)	15 (2%)	58	79

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	796	SER
1	A	1646	ASP

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Mol	Chain	Res	Type
1	A	1425	SER
1	A	1811	ASN
1	A	1630	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	HIS
1	A	1357	HIS
1	A	1748	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 13 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
7	JL3	A	2411	-	34,34,44	0.61	0	37,39,49	0.61	1 (2%)
6	Y01	A	2413	-	38,38,38	0.44	0	57,57,57	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	JL3	A	2409	-	41,41,44	0.56	0	44,46,49	0.54	1 (2%)
5	LPE	A	2405	-	26,26,33	0.28	0	30,32,39	0.41	0
3	NAG	A	2403	-	14,14,15	0.27	0	17,19,21	0.52	0
6	Y01	A	2408	-	38,38,38	0.46	0	57,57,57	0.80	2 (3%)
6	Y01	A	2412	-	38,38,38	0.46	0	57,57,57	0.56	0
6	Y01	A	2406	-	38,38,38	0.49	0	57,57,57	0.69	0
3	NAG	A	2402	-	14,14,15	0.26	0	17,19,21	0.62	0
2	A1AHI	A	2401	-	30,30,30	2.67	8 (26%)	39,44,44	1.73	8 (20%)
7	JL3	A	2410	-	35,35,44	0.60	0	38,40,49	0.62	1 (2%)
7	JL3	A	2407	-	44,44,44	0.54	0	47,49,49	0.54	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
7	JL3	A	2411	-	-	16/38/38/48	-
6	Y01	A	2413	-	-	8/19/77/77	0/4/4/4
7	JL3	A	2409	-	-	19/45/45/48	-
5	LPE	A	2405	-	-	9/27/27/34	-
3	NAG	A	2403	-	-	0/6/23/26	0/1/1/1
6	Y01	A	2408	-	-	8/19/77/77	0/4/4/4
6	Y01	A	2412	-	-	6/19/77/77	0/4/4/4
6	Y01	A	2406	-	-	3/19/77/77	0/4/4/4
3	NAG	A	2402	-	-	0/6/23/26	0/1/1/1
2	A1AHI	A	2401	-	-	6/13/38/38	2/3/3/3
7	JL3	A	2410	-	-	20/39/39/48	-
7	JL3	A	2407	-	-	21/48/48/48	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	A1AHI	C09-N06	-7.77	1.31	1.47
2	A	2401	A1AHI	O04-C11	-6.06	1.41	1.45
2	A	2401	A1AHI	C14-N06	-5.78	1.31	1.46
2	A	2401	A1AHI	C15-N06	-5.68	1.31	1.46
2	A	2401	A1AHI	C22-N07	4.07	1.42	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	A1AHI	C14-C16-C12	-5.10	108.56	112.38
2	A	2401	A1AHI	C14-N06-C15	3.51	116.41	108.84
2	A	2401	A1AHI	C08-C09-N06	-3.01	109.28	114.06
2	A	2401	A1AHI	C23-C22-N07	3.01	123.37	117.12
2	A	2401	A1AHI	C15-C17-C12	-2.88	110.22	112.38

There are no chirality outliers.

5 of 116 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2401	A1AHI	C10-C08-C09-N06
2	A	2401	A1AHI	C13-C08-C09-N06
2	A	2401	A1AHI	C17-C12-C19-N07
2	A	2401	A1AHI	C16-C12-C19-N07
5	A	2405	LPE	C1-C2-C3-O3

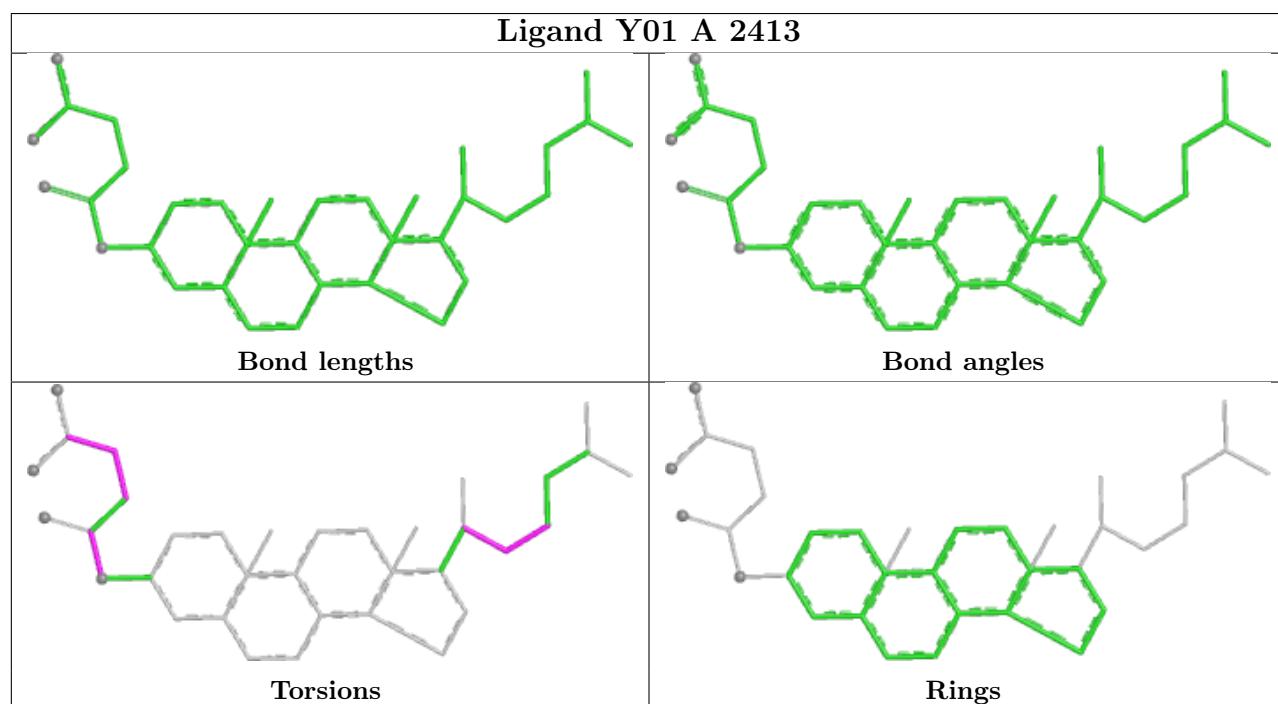
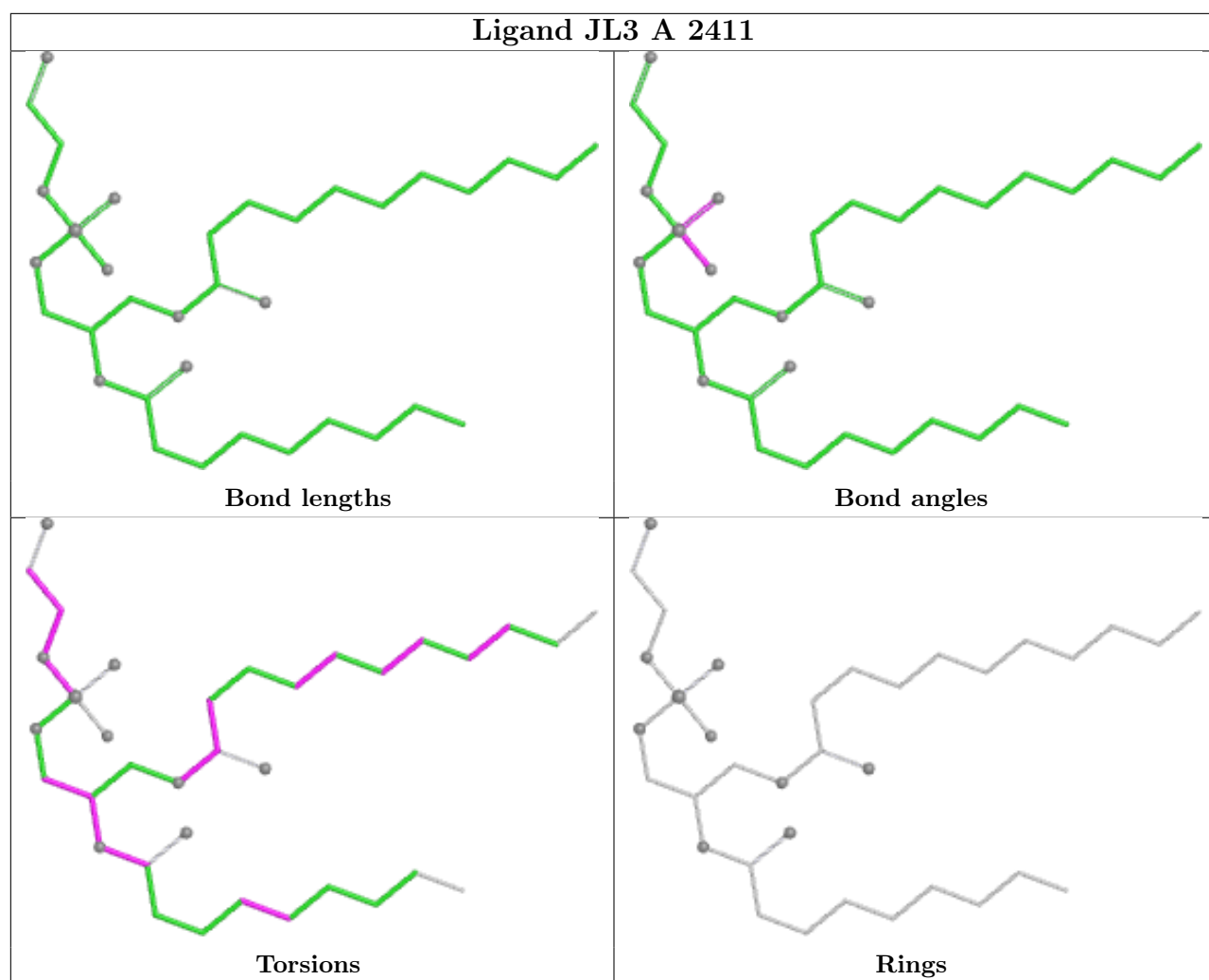
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2401	A1AHI	C08-C10-C11-C13-C18-O04
2	A	2401	A1AHI	C12-C14-C15-C16-C17-N06

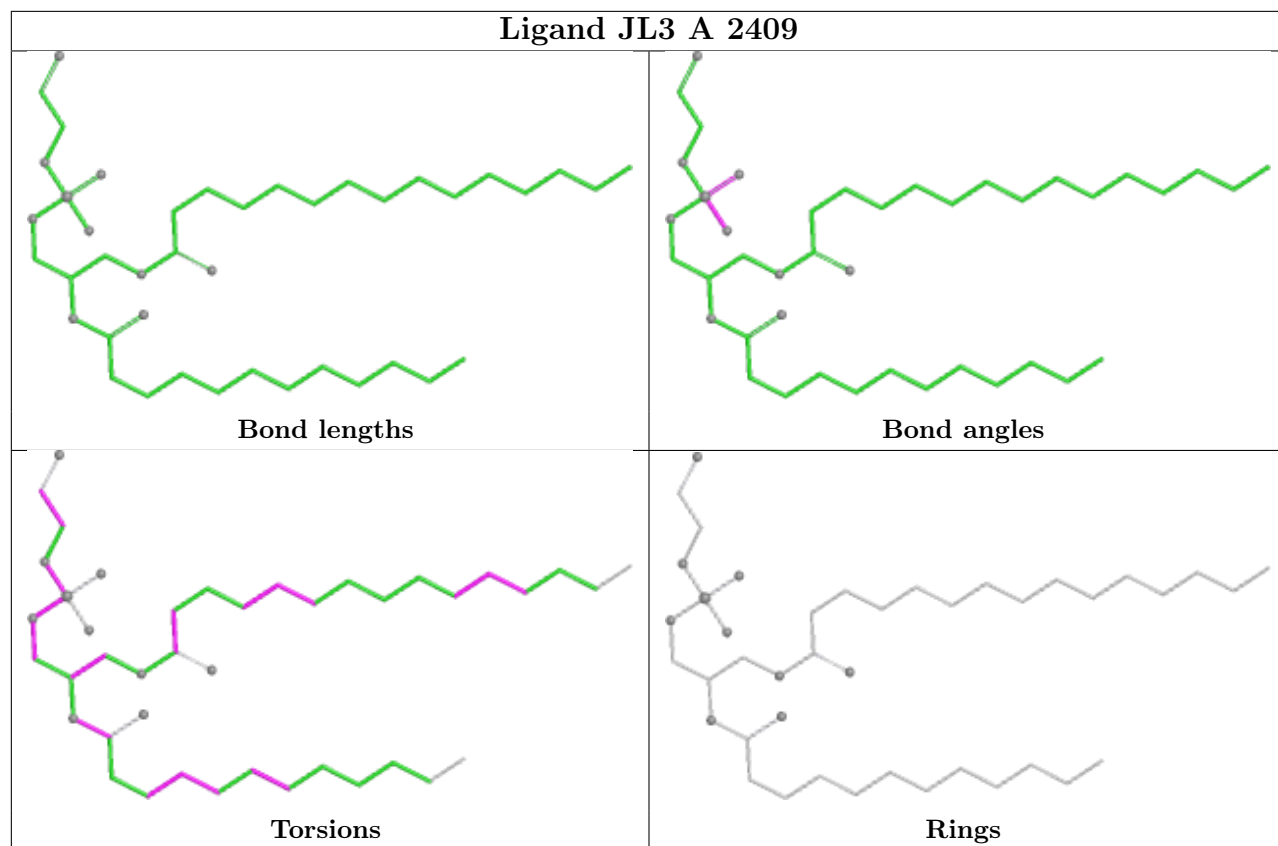
3 monomers are involved in 3 short contacts:

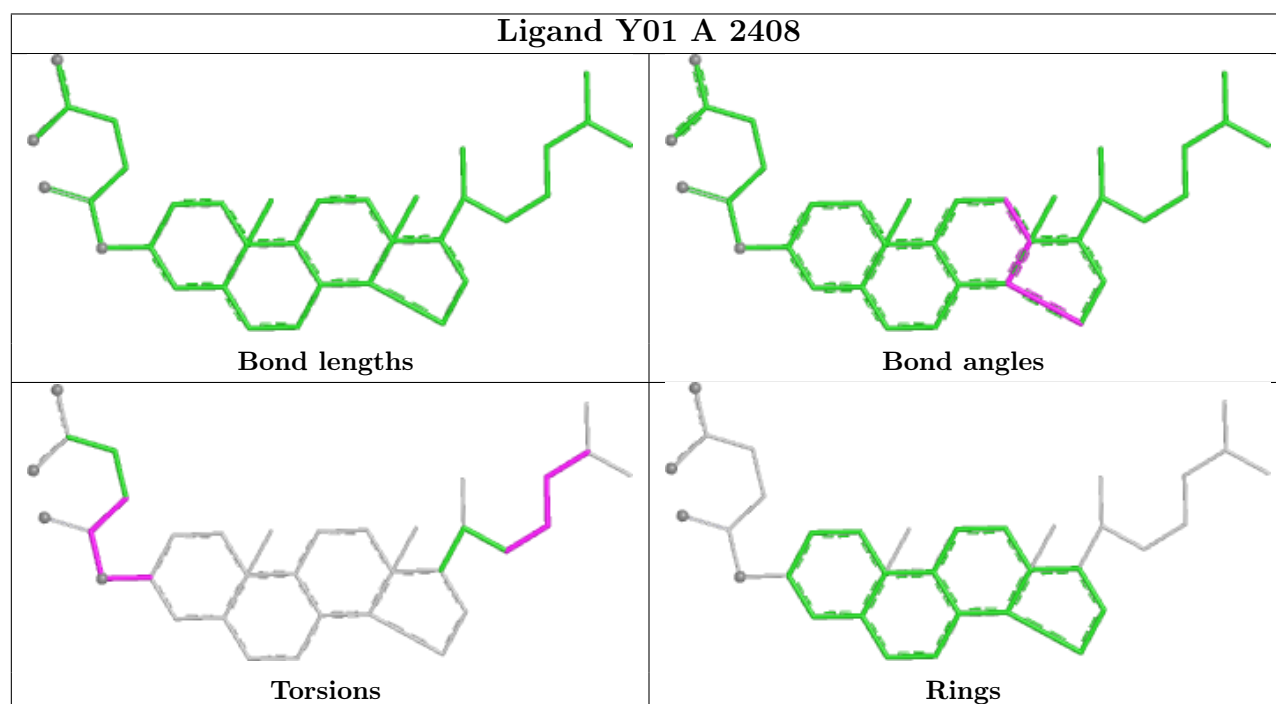
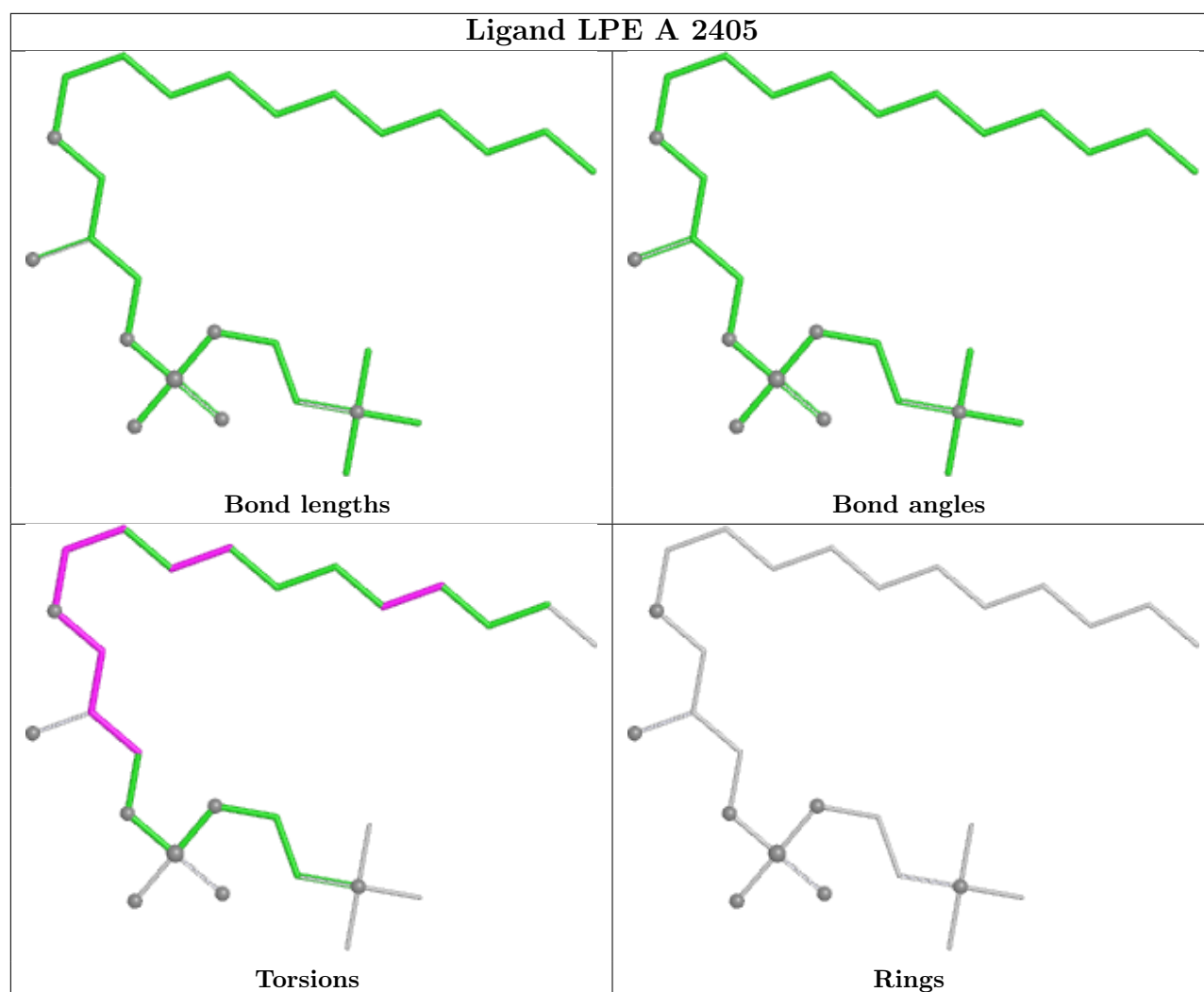
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2413	Y01	1	0
5	A	2405	LPE	1	0
6	A	2412	Y01	1	0

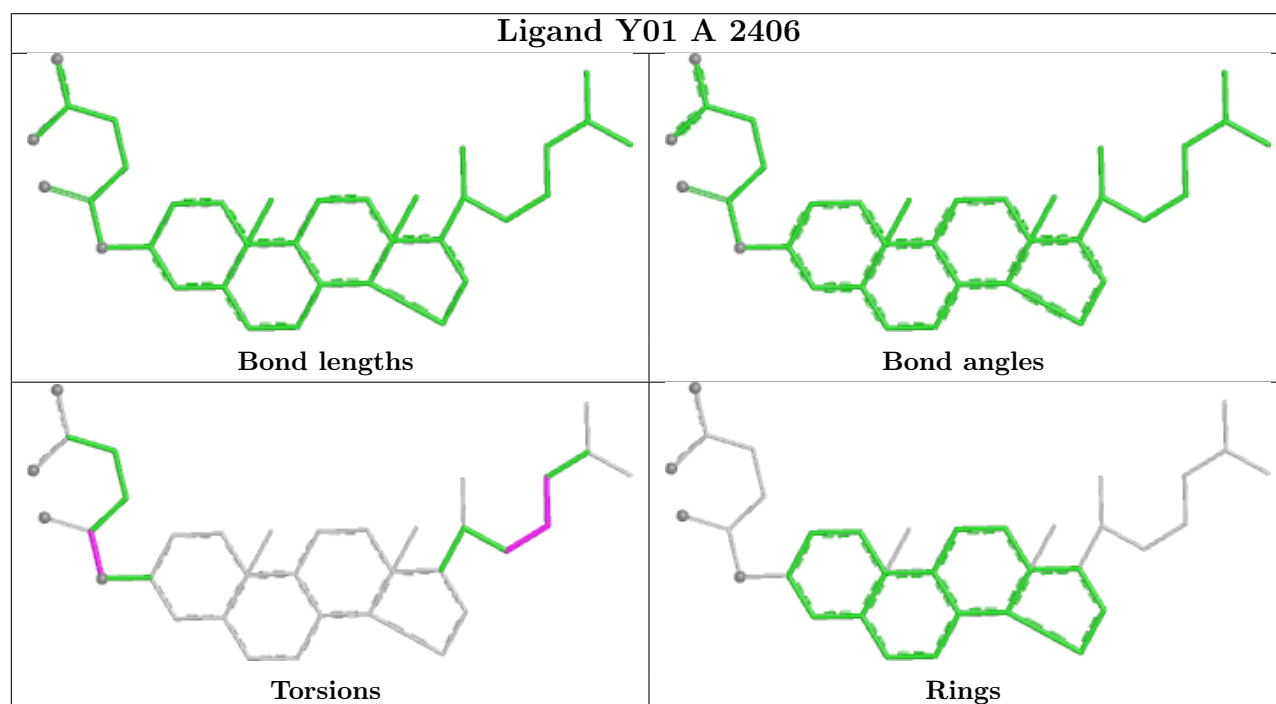
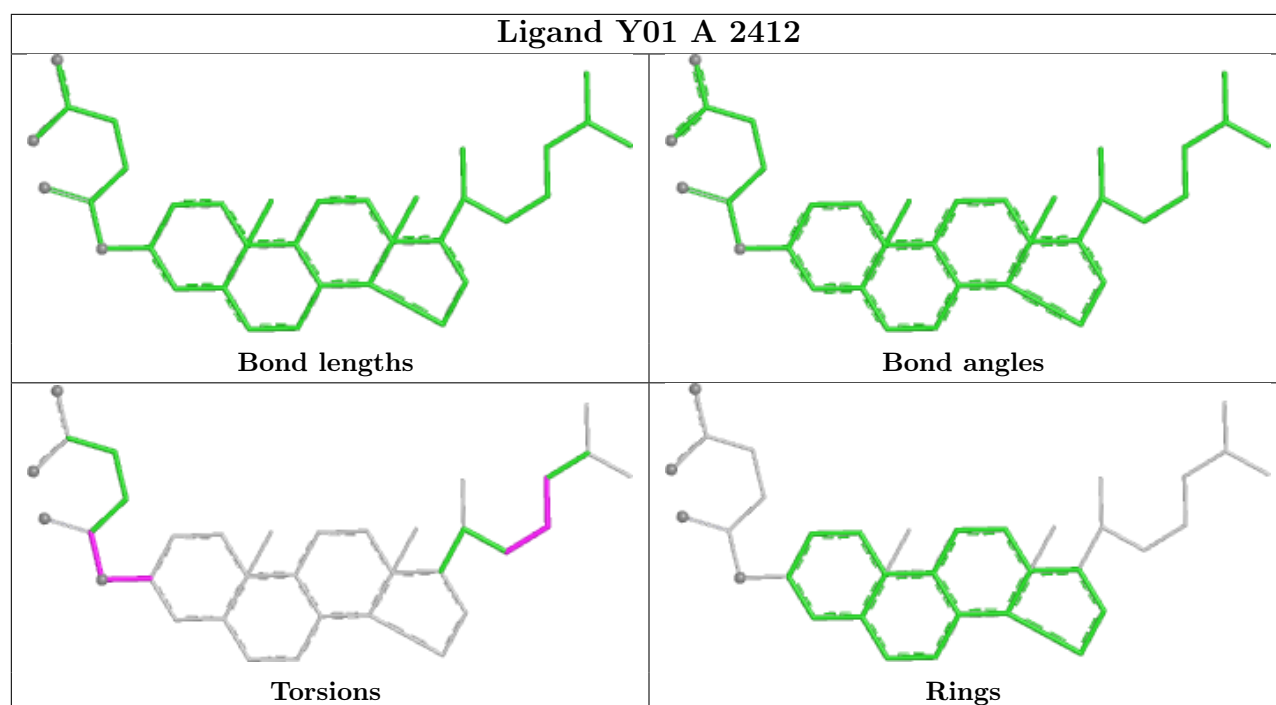
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

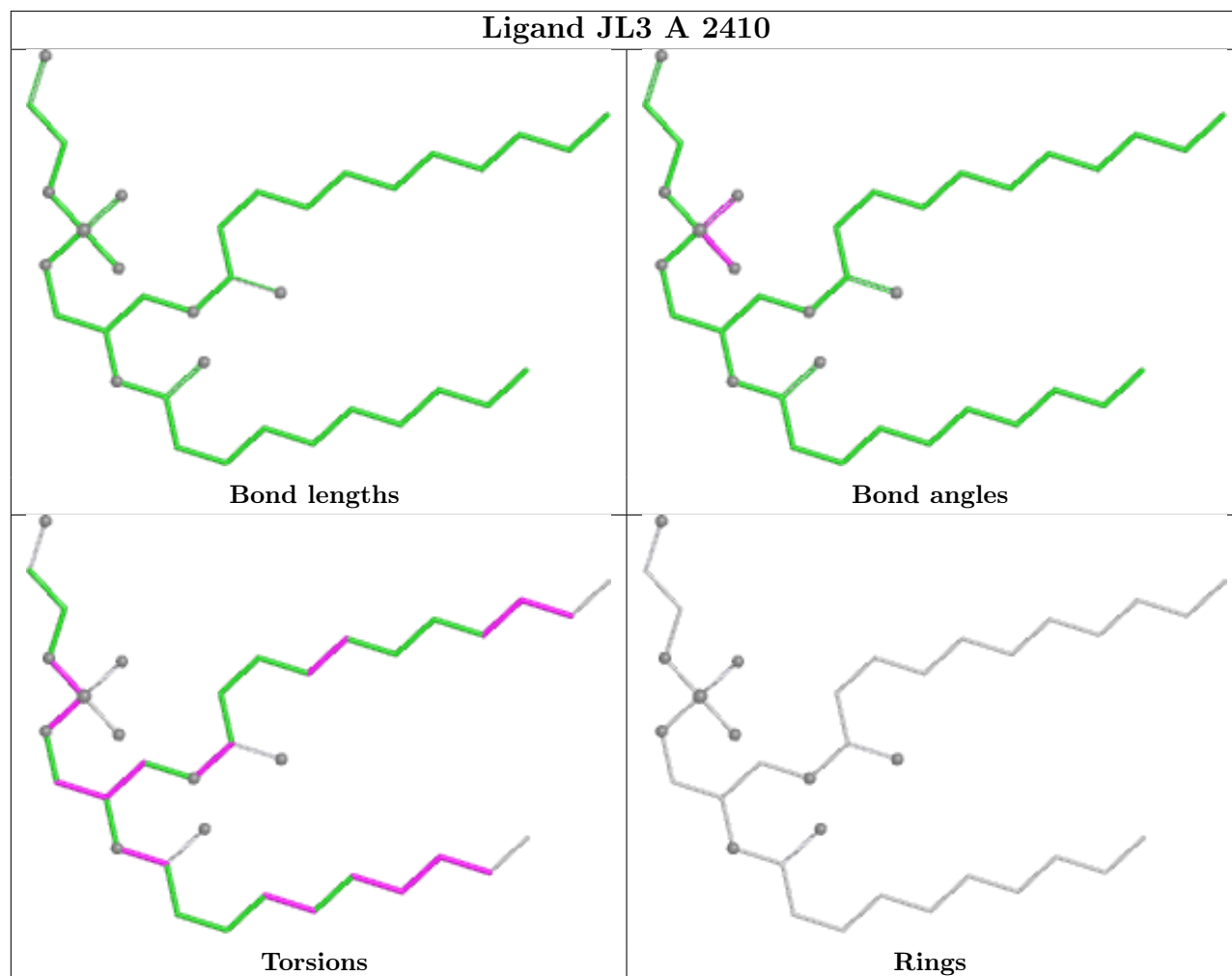
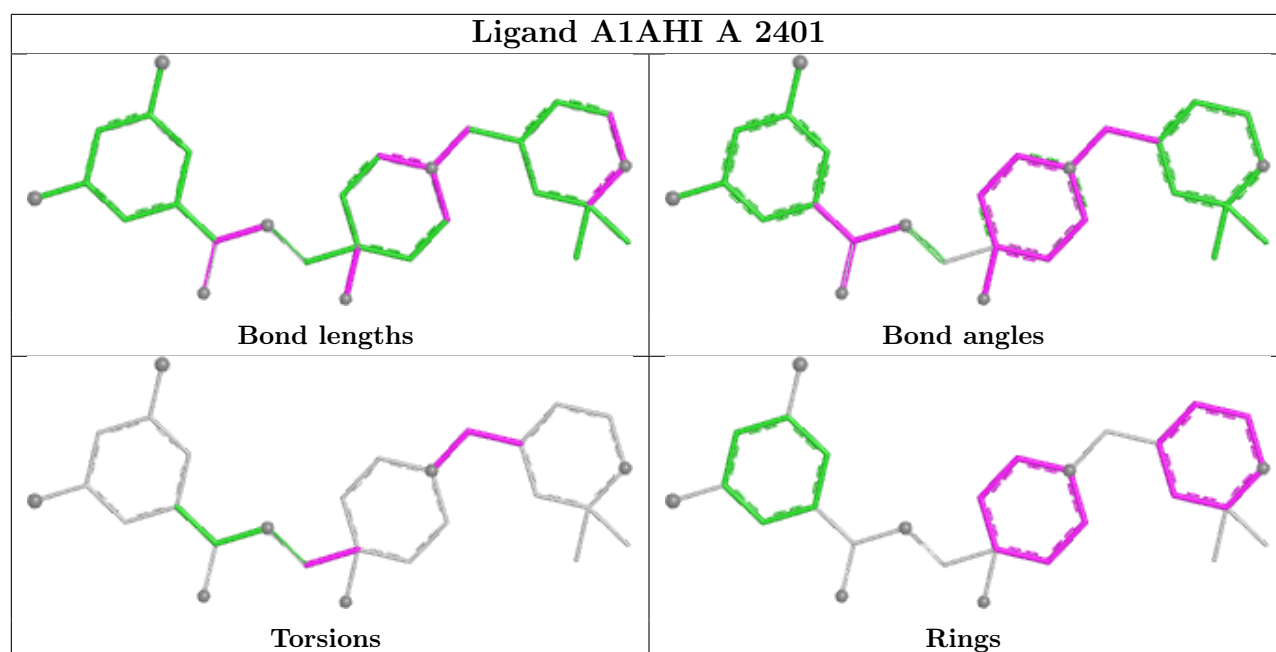


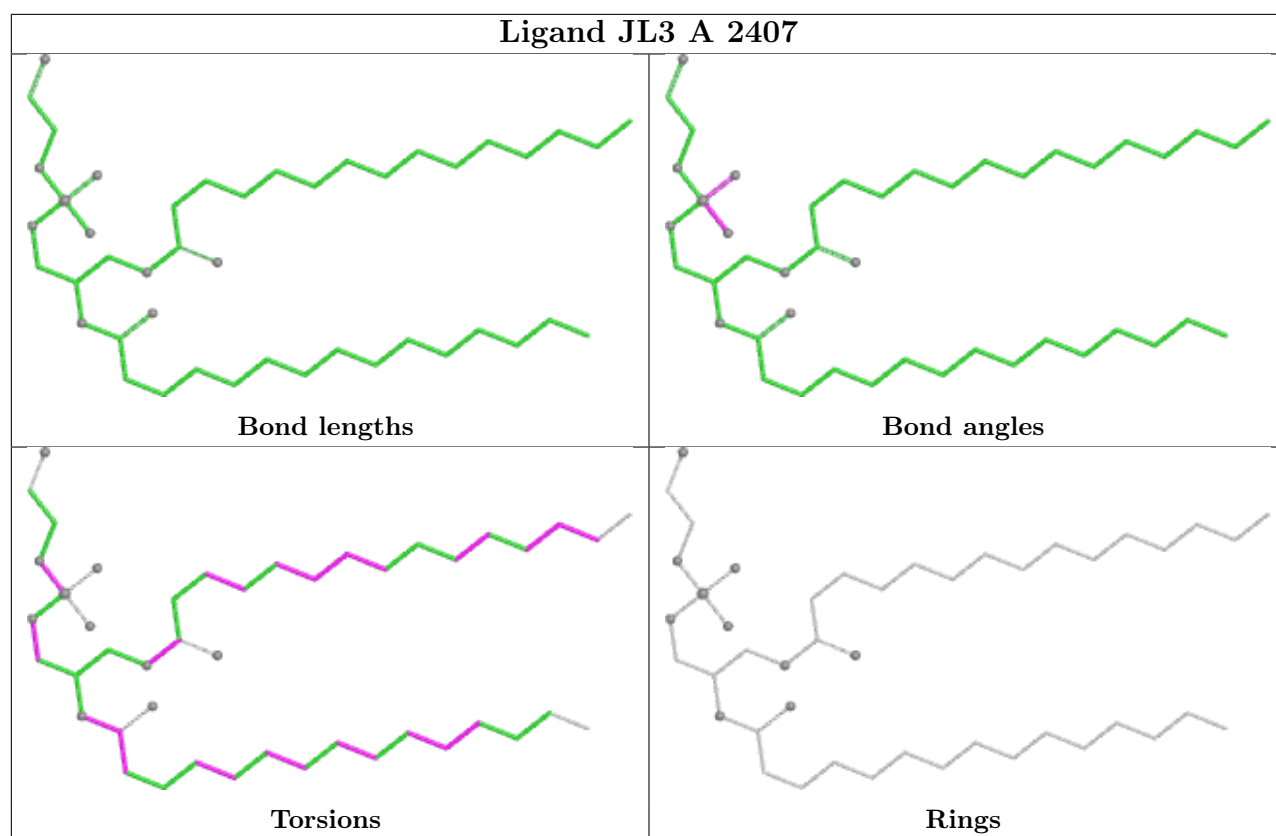












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

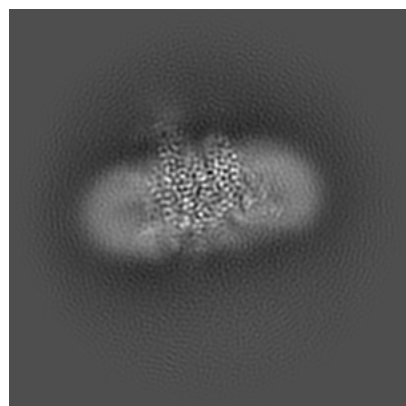
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43993. These allow visual inspection of the internal detail of the map and identification of artifacts.

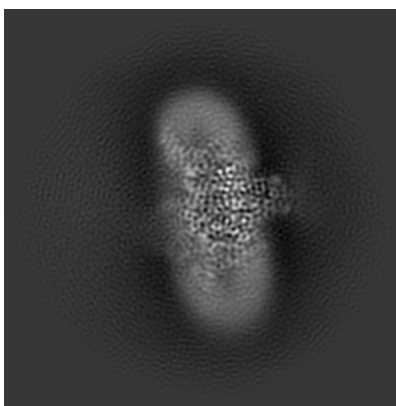
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

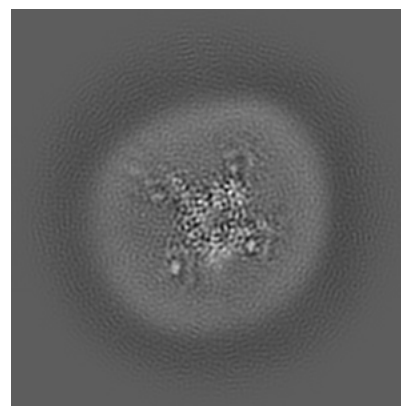
#### 6.1.1 Primary map



X

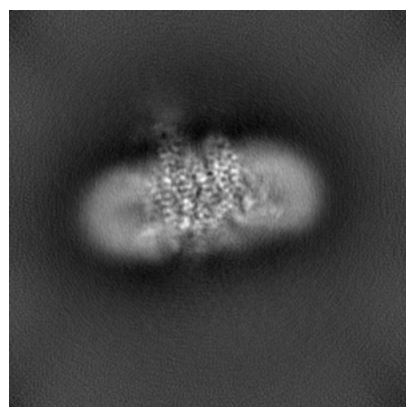


Y

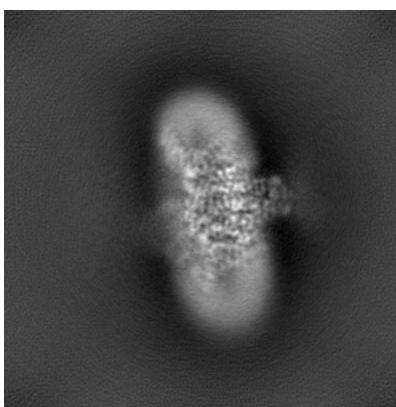


Z

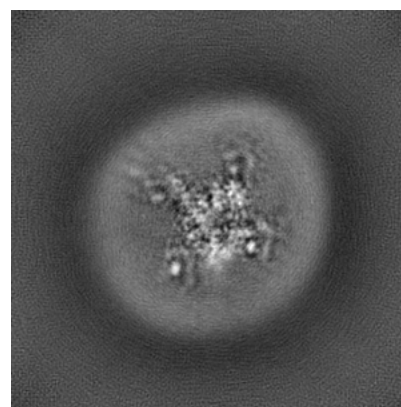
#### 6.1.2 Raw map



X



Y

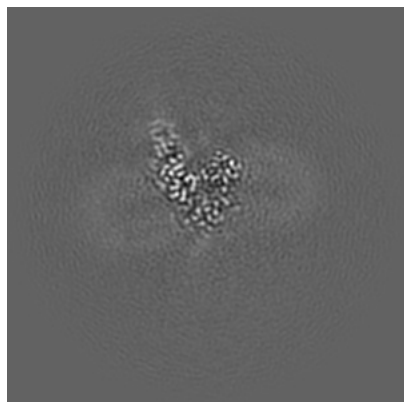


Z

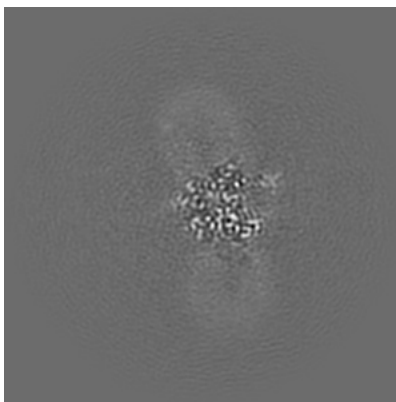
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

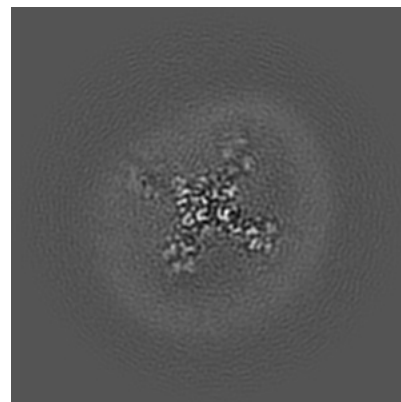
### 6.2.1 Primary map



X Index: 128

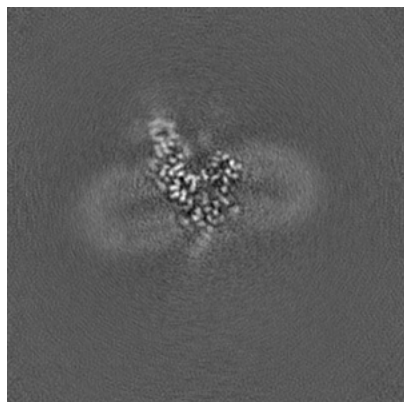


Y Index: 128

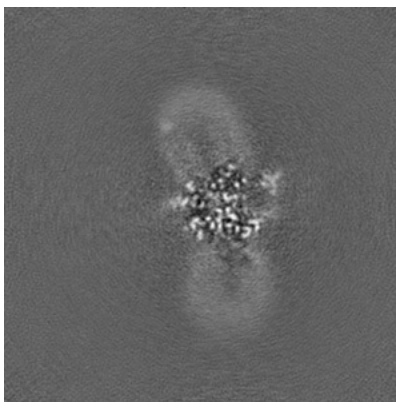


Z Index: 128

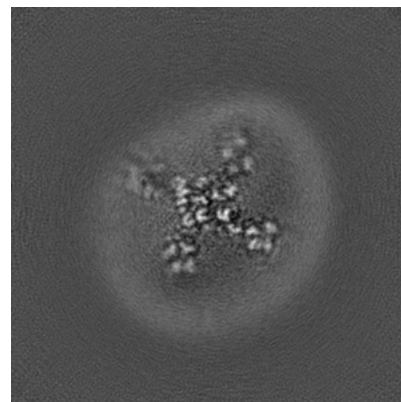
### 6.2.2 Raw map



X Index: 128



Y Index: 128

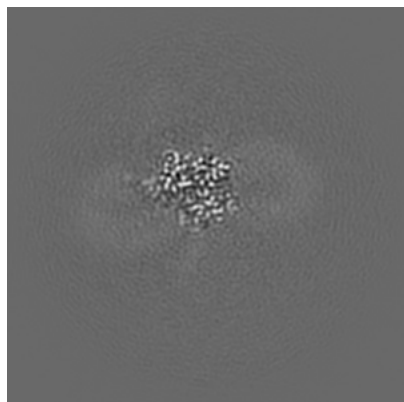


Z Index: 128

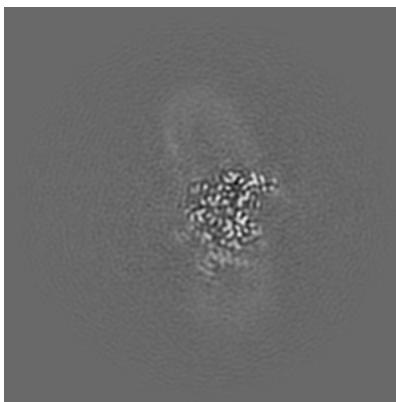
The images above show central slices of the map in three orthogonal directions.

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

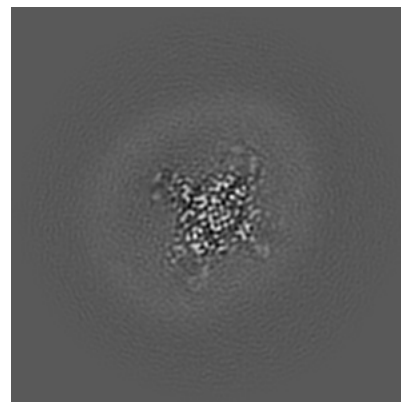
### 6.3.1 Primary map



X Index: 120

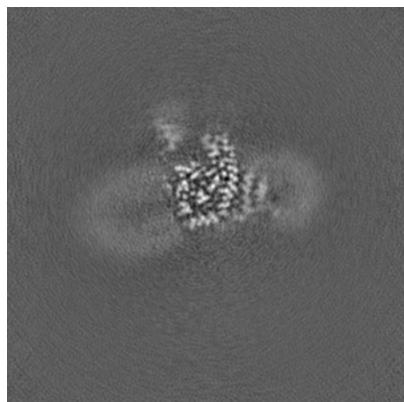


Y Index: 136

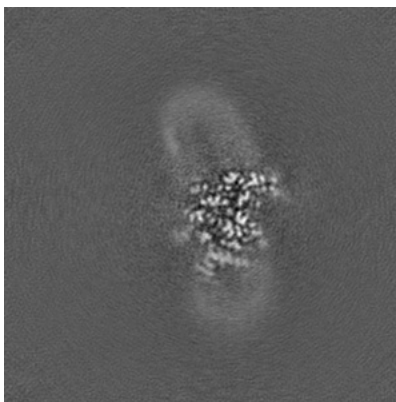


Z Index: 146

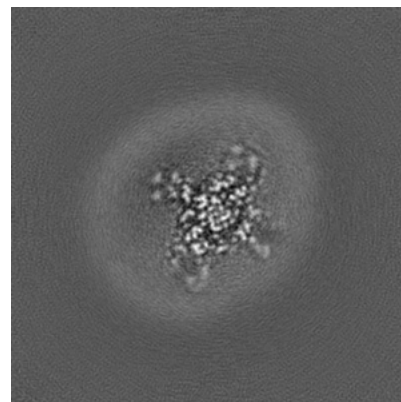
### 6.3.2 Raw map



X Index: 141



Y Index: 136



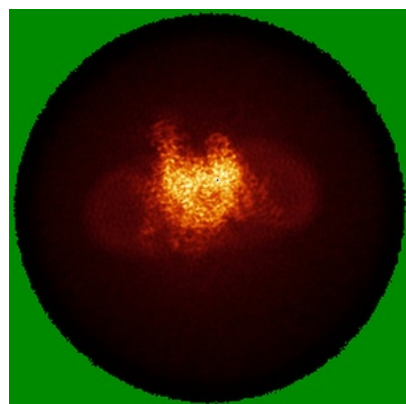
Z Index: 146

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

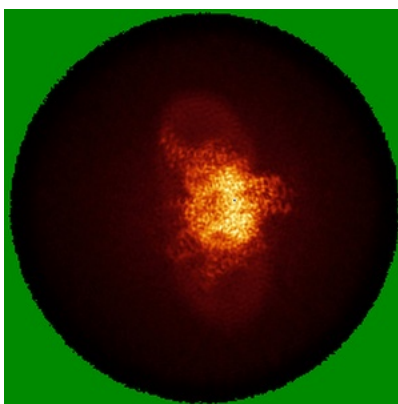


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

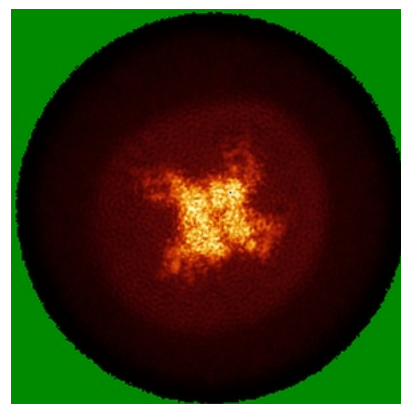
### 6.4.1 Primary map



X

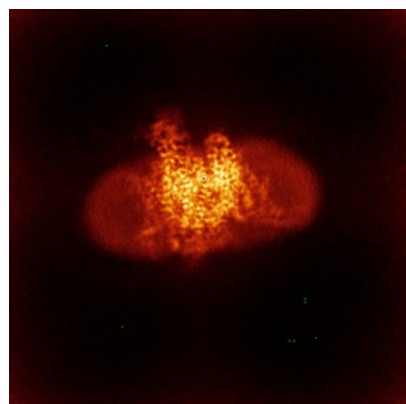


Y

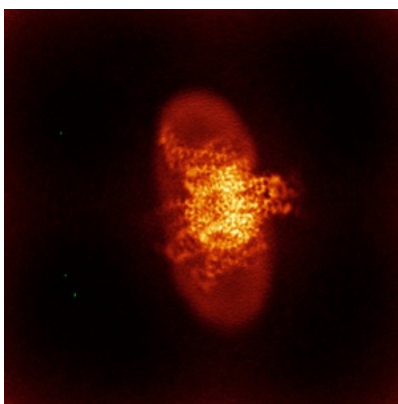


Z

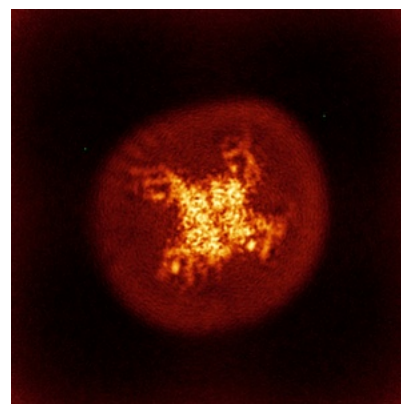
### 6.4.2 Raw map



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 0.18. 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.

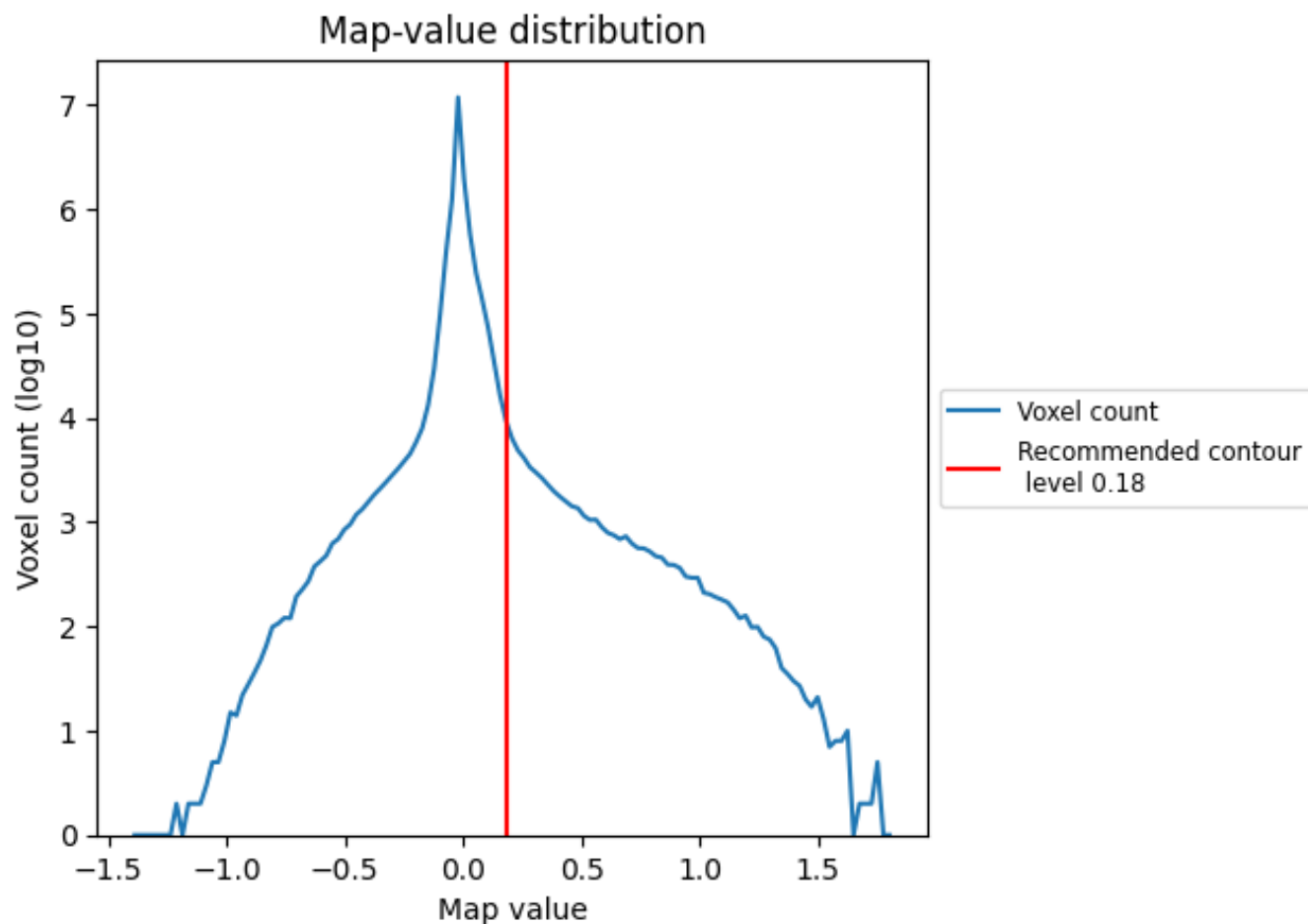
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

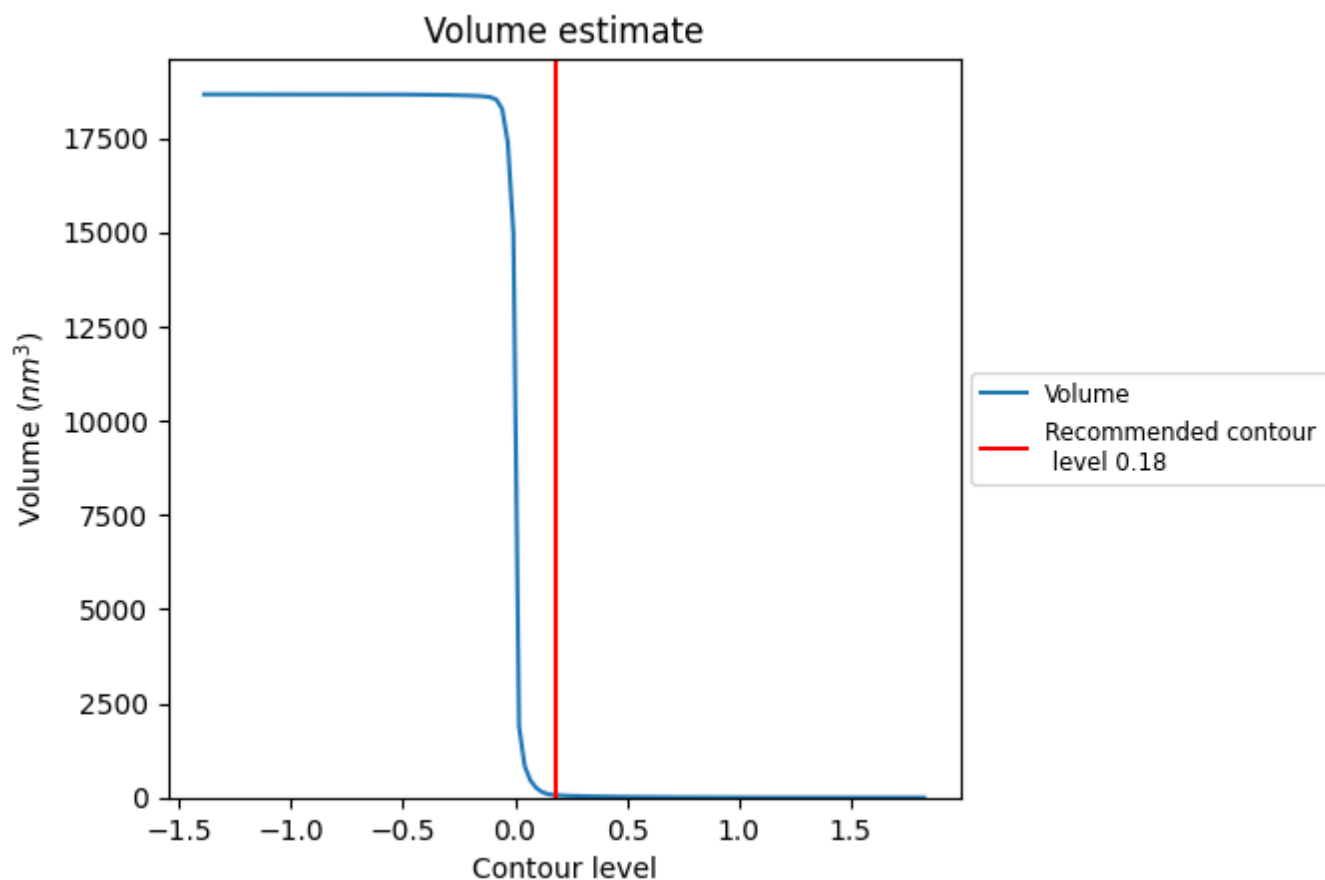
This section contains the results of statistical analysis of the map.

### 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.

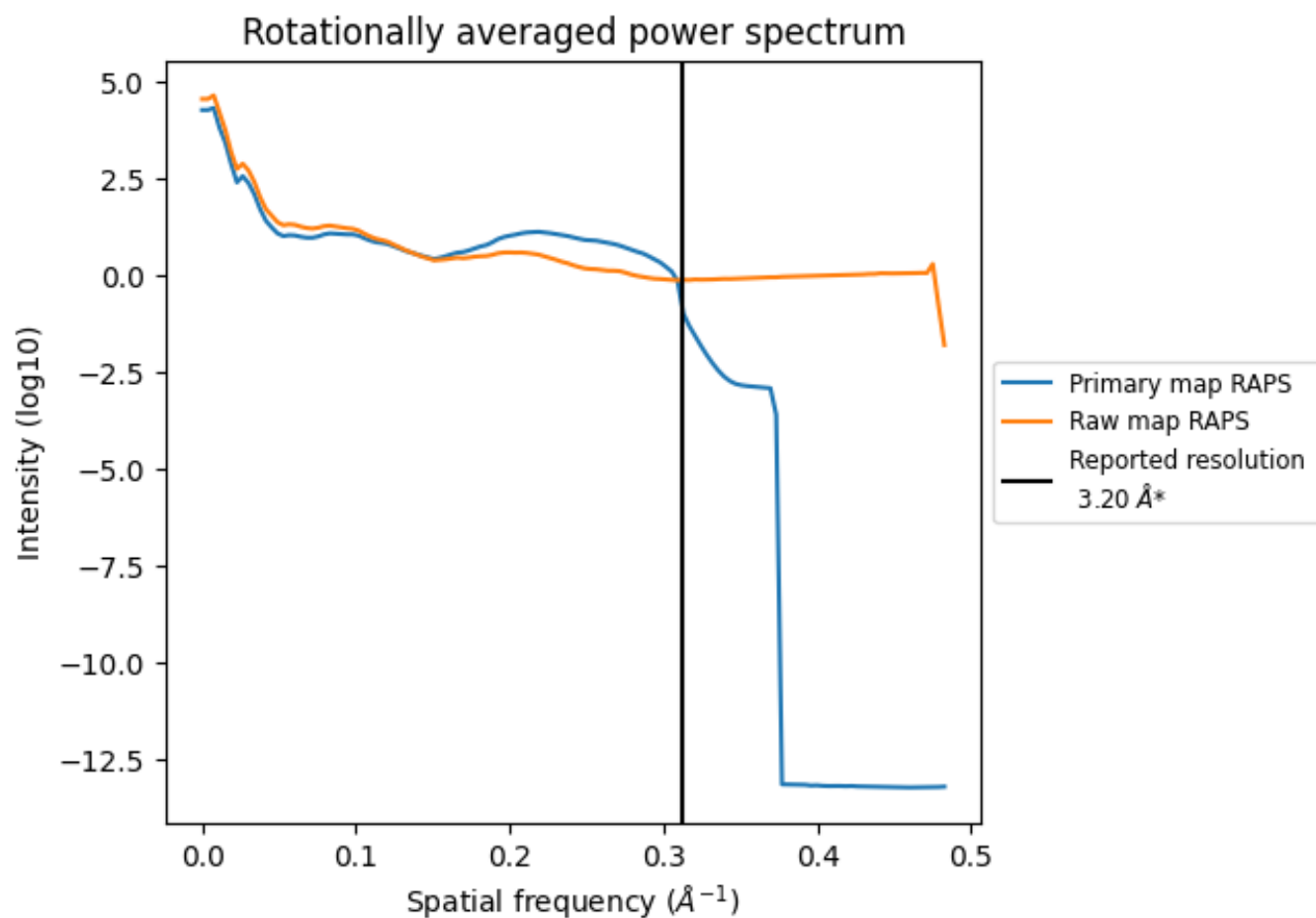
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm<sup>3</sup>; this corresponds to an approximate mass of 60 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 ⓘ

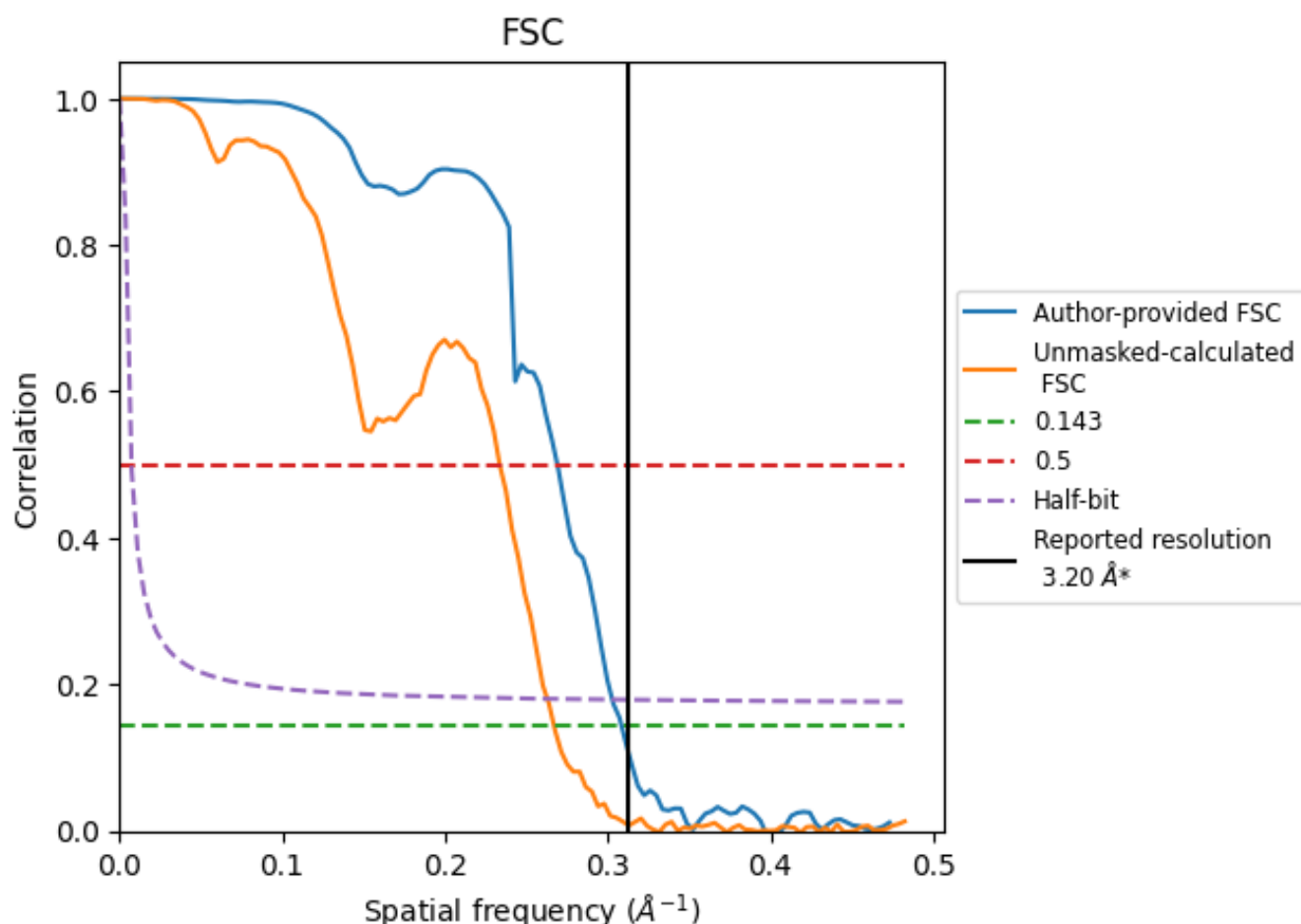


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

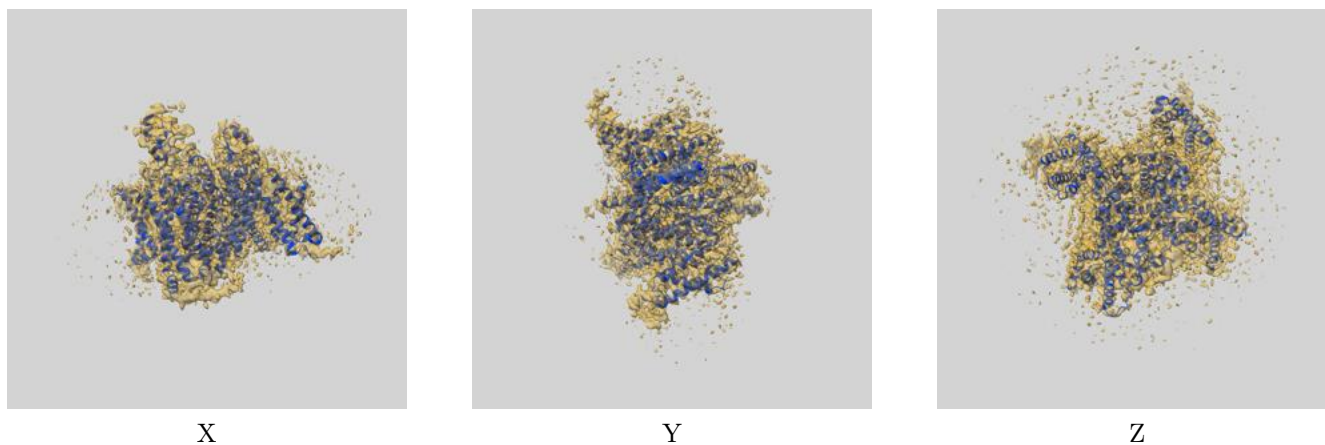
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.24	3.72	3.30
Unmasked-calculated*	3.74	4.28	3.80

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 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-43993 and PDB model 9AYJ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

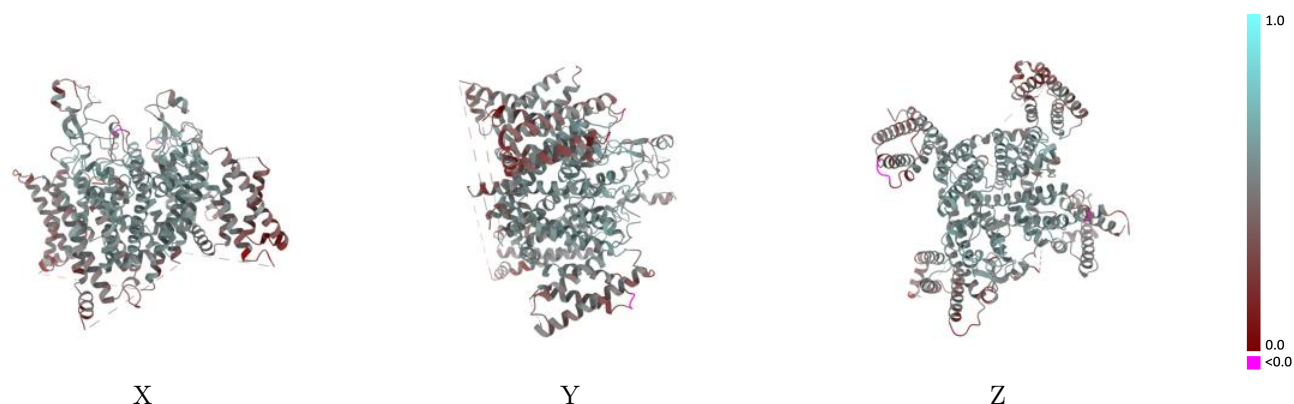
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

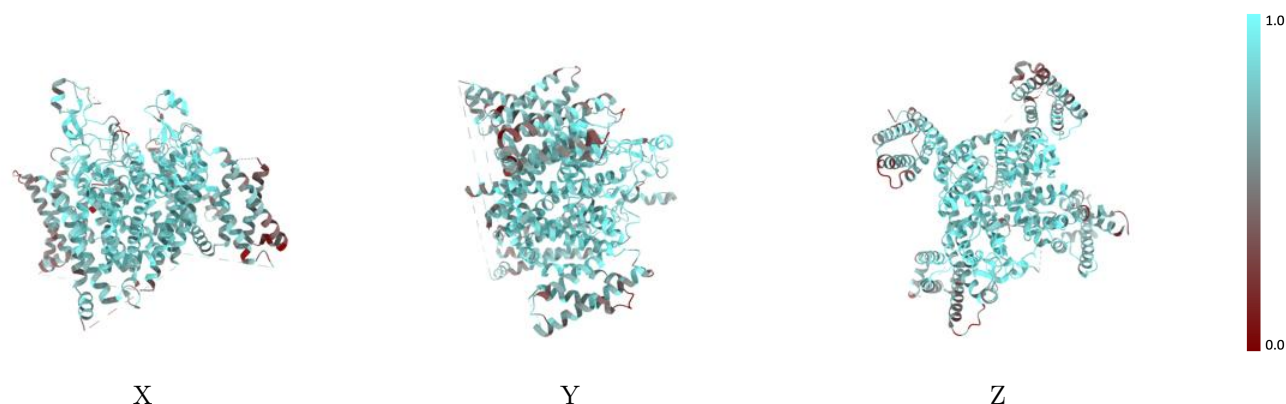


## 9.2 Q-score mapped to coordinate model [i](#)



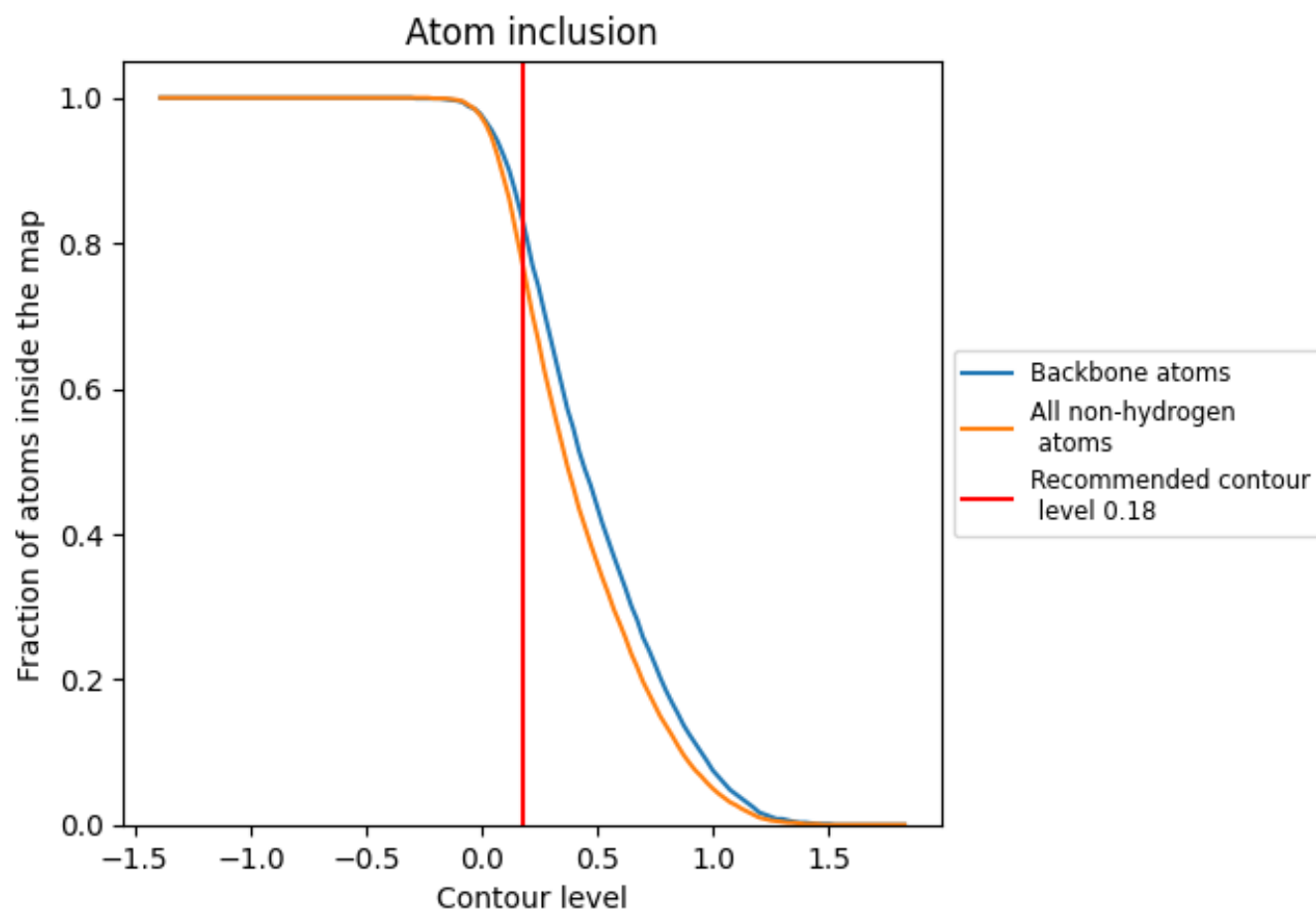
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7660	<div></div> 0.4840
A	<div></div> 0.7660	<div></div> 0.4840

