



Full wwPDB EM Validation Report ⓘ

Apr 15, 2024 – 03:39 PM EDT

PDB ID : 9AYL
EMDB ID : EMD-43995
Title : Cryo-EM structure of human Cav3.2 with ACT-709478
Authors : Fan, X.; Huang, J.; Yan, N.
Deposited on : 2024-03-08
Resolution : 2.80 Å (reported)

This is a Full wwPDB EM Validation 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>.

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

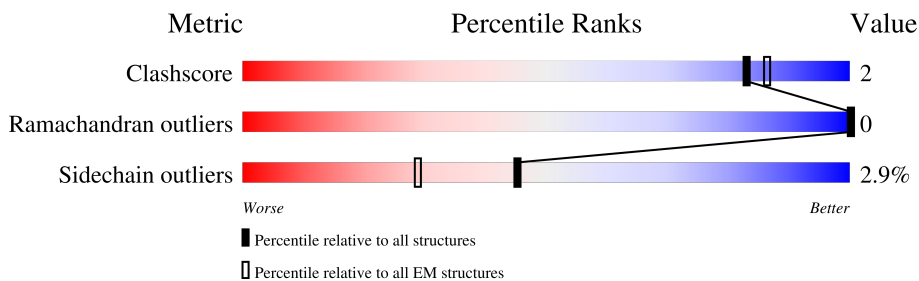
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2116	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8853 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	1055	8468	5562	1401	1435	70	0	0

There are 43 discrepancies between the modelled and reference sequences:

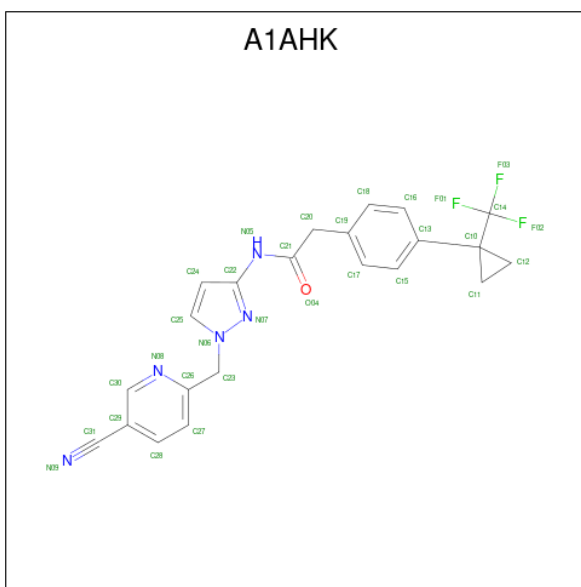
Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP O95180
A	-41	ALA	-	expression tag	UNP O95180
A	-40	SER	-	expression tag	UNP O95180
A	-39	TRP	-	expression tag	UNP O95180
A	-38	SER	-	expression tag	UNP O95180
A	-37	HIS	-	expression tag	UNP O95180
A	-36	PRO	-	expression tag	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 N-{1-[(5-cyanopyridin-2-yl)methyl]-1H-pyrazol-3-yl}-2-[4-[1-(trifluoromethyl)cyclopropyl]phenyl]acetamide (three-letter code: A1AHK) (formula: C₂₂H₁₈F₃N₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
2	A	1	31	22	3	5	1	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

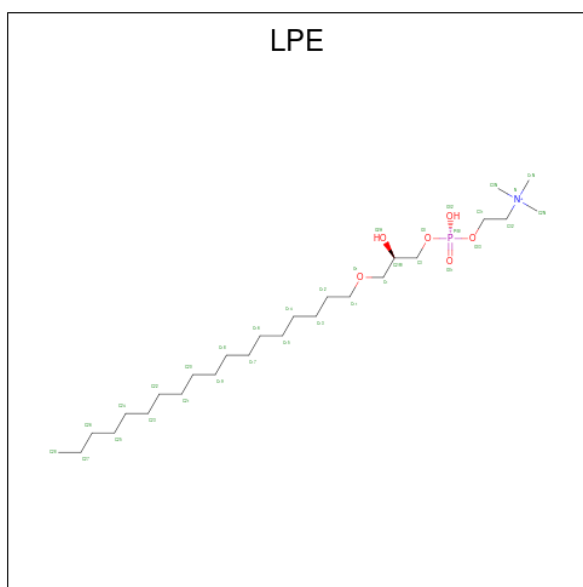


Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
3	A	1	14	8	1	5	0
3	A	1	Total	C	N	O	0
			14	8	1	5	

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

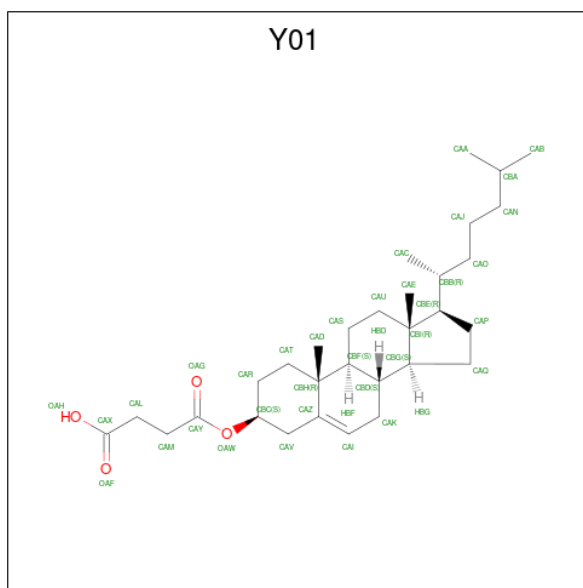
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	1	1	1	0

- Molecule 5 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: C₂₆H₅₇NO₆P).



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

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



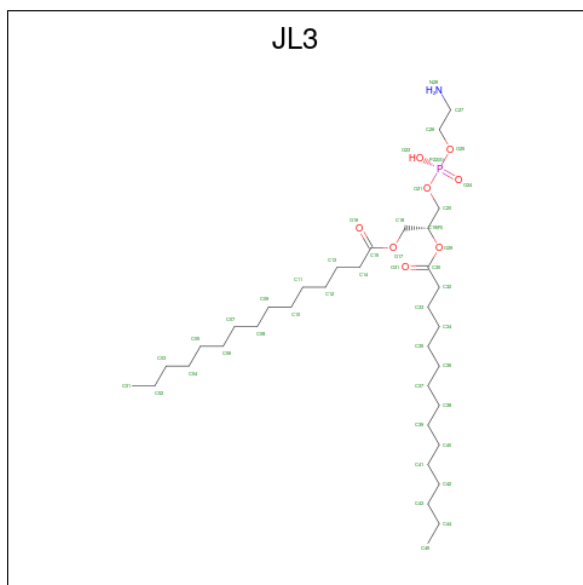
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	A	1	35	31	4	0
6	A	1	35	31	4	0
6	A	1	35	31	4	0

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

- Molecule 7 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-pentadecanoyloxy-propyl] pentadecanoate (three-letter code: JL3) (formula: C₃₅H₇₀NO₈P).

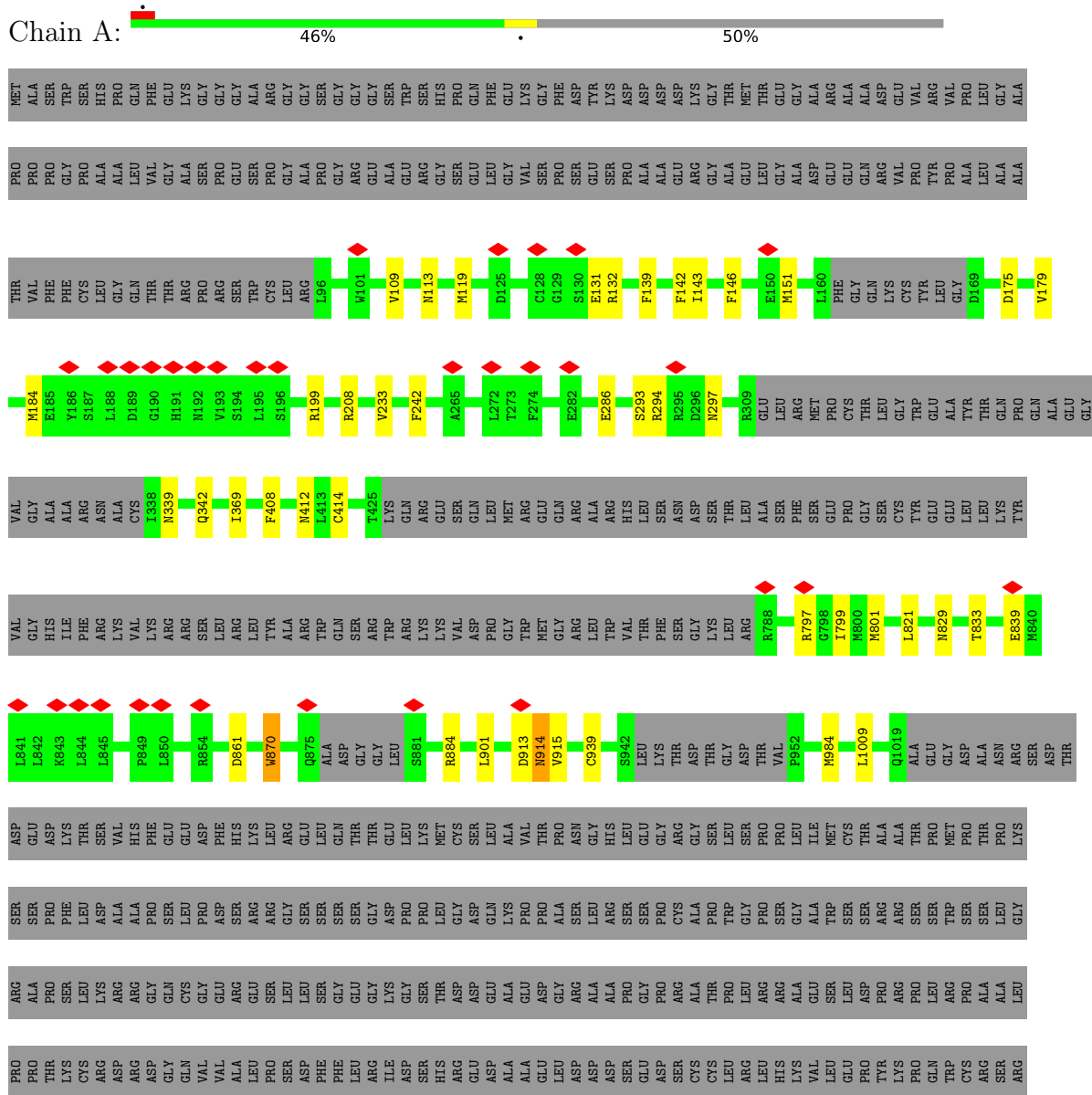


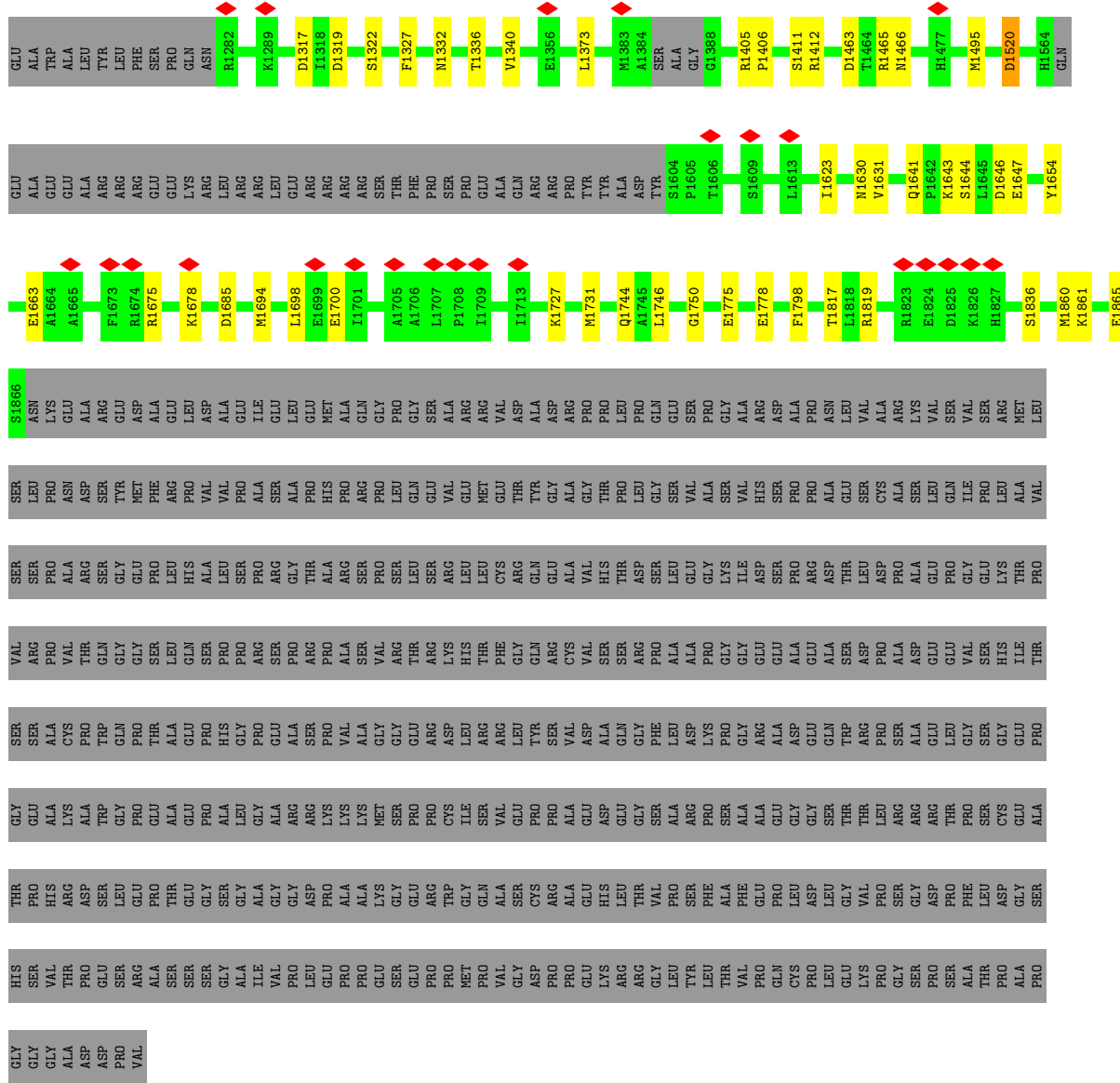
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	45	35	1	8	1	0
7	A	1	42	32	1	8	1	0
7	A	1	36	26	1	8	1	0
7	A	1	35	25	1	8	1	0

3 Residue-property plots (i)

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

- Molecule 1: Voltage-dependent T-type calcium channel subunit alpha-1H





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188950	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	2.215	Depositor
Minimum map value	-1.560	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	265.216, 265.216, 265.216	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: A1AHK, LPE, NAG, Y01, CA, JL3

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	0/8657	0.47	0/11734

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	8468	0	8656	41	0
2	A	31	0	0	0	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	27	0	39	0	0
6	A	140	0	196	2	0
7	A	158	0	0	0	0
All	All	8853	0	8917	43	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 2.

All (43) 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:829:ASN:O	1:A:833:THR:OG1	2.00	0.79
1:A:131:GLU:N	1:A:131:GLU:OE1	2.26	0.68
1:A:913:ASP:OD1	1:A:914:ASN:N	2.29	0.65
1:A:1654:TYR:OH	1:A:1700:GLU:OE2	2.18	0.61
1:A:242:PHE:CE2	1:A:1631:VAL:HG13	2.39	0.58
1:A:1685:ASP:OD1	1:A:1727:LYS:NZ	2.29	0.57
1:A:1694:MET:O	1:A:1698:LEU:HD12	2.04	0.57
1:A:1463:ASP:OD1	1:A:1465:ARG:NH1	2.37	0.56
1:A:1775:GLU:O	1:A:1819:ARG:NH2	2.38	0.56
1:A:175:ASP:OD2	1:A:208:ARG:NH1	2.41	0.54
1:A:1641:GLN:NE2	1:A:1646:ASP:OD1	2.41	0.53
6:A:2413:Y01:OAW	6:A:2413:Y01:HAD1	2.09	0.53
1:A:799:ILE:HD12	1:A:839:GLU:OE1	2.09	0.53
1:A:286:GLU:HA	1:A:286:GLU:OE1	2.09	0.52
1:A:297:ASN:OD1	1:A:297:ASN:N	2.43	0.52
1:A:1319:ASP:O	1:A:1322:SER:OG	2.28	0.50
1:A:821:LEU:O	1:A:821:LEU:HD23	2.13	0.49
1:A:1647:GLU:HA	1:A:1647:GLU:OE1	2.13	0.48
6:A:2412:Y01:HAB1	6:A:2412:Y01:HAO1	1.96	0.48
1:A:1744:GLN:O	1:A:1861:LYS:NZ	2.38	0.48
1:A:915:VAL:HG22	1:A:1009:LEU:HD11	1.97	0.47
1:A:408:PHE:O	1:A:412:ASN:ND2	2.47	0.46
1:A:1332:ASN:O	1:A:1336:THR:HG22	2.16	0.46
1:A:1520:ASP:N	1:A:1520:ASP:OD1	2.49	0.46
1:A:1411:SER:OG	1:A:1412:ARG:NH1	2.49	0.45
1:A:1860:MET:HE3	1:A:1860:MET:HA	1.99	0.45
1:A:1746:LEU:O	1:A:1750:GLY:N	2.43	0.44
1:A:339:ASN:OD1	1:A:342:GLN:NE2	2.46	0.44
1:A:109:VAL:CG1	1:A:143:ILE:HG23	2.47	0.44
1:A:233:VAL:HG11	1:A:414:CYS:SG	2.57	0.44
1:A:119:MET:O	1:A:132:ARG:NH2	2.50	0.44
1:A:294:ARG:NE	1:A:294:ARG:O	2.51	0.44
1:A:142:PHE:C	1:A:142:PHE:CD1	2.91	0.43
1:A:151:MET:CE	1:A:179:VAL:HG11	2.49	0.43
1:A:1373:LEU:C	1:A:1373:LEU:HD23	2.39	0.42
1:A:1623:ILE:HD11	1:A:1663:GLU:HG3	2.01	0.42
1:A:1322:SER:H	1:A:1322:SER:HG	1.56	0.42
1:A:1817:THR:CB	1:A:1836:SER:HG	2.33	0.41
1:A:861:ASP:OD1	1:A:861:ASP:C	2.58	0.41
1:A:1405:ARG:N	1:A:1406:PRO:CD	2.83	0.41
1:A:870:TRP:CD1	1:A:870:TRP:C	2.93	0.41
1:A:369:ILE:HD13	1:A:984:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:THR:O	1:A:1340:VAL:HG12	2.21	0.40

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	1037/2116 (49%)	1024 (99%)	13 (1%)	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%)	912 (97%)	27 (3%)	42 76

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	139	PHE
1	A	146	PHE
1	A	184	MET
1	A	199	ARG

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Mol	Chain	Res	Type
1	A	293	SER
1	A	797	ARG
1	A	801	MET
1	A	870	TRP
1	A	884	ARG
1	A	901	LEU
1	A	914	ASN
1	A	939	CYS
1	A	1317	ASP
1	A	1327	PHE
1	A	1466	ASN
1	A	1495	MET
1	A	1520	ASP
1	A	1630	ASN
1	A	1643	LYS
1	A	1644	SER
1	A	1675	ARG
1	A	1678	LYS
1	A	1731	MET
1	A	1778	GLU
1	A	1798	PHE
1	A	1865	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

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
5	LPE	A	2405	-	26,26,33	0.27	0	30,32,39	0.34	0
6	Y01	A	2412	-	38,38,38	0.45	0	57,57,57	0.58	0
7	JL3	A	2409	-	41,41,44	0.56	0	44,46,49	0.57	1 (2%)
7	JL3	A	2411	-	34,34,44	0.60	0	37,39,49	0.61	1 (2%)
3	NAG	A	2403	-	14,14,15	0.26	0	17,19,21	0.65	0
3	NAG	A	2402	-	14,14,15	0.26	0	17,19,21	0.65	0
7	JL3	A	2407	-	44,44,44	0.56	0	47,49,49	0.51	1 (2%)
6	Y01	A	2408	-	38,38,38	0.45	0	57,57,57	0.66	0
2	A1AHK	A	2401	-	29,34,34	4.85	16 (55%)	36,50,50	2.21	9 (25%)
7	JL3	A	2410	-	35,35,44	0.60	0	38,40,49	0.58	1 (2%)
6	Y01	A	2413	-	38,38,38	0.45	0	57,57,57	0.63	0
6	Y01	A	2406	-	38,38,38	0.46	0	57,57,57	0.51	0

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	LPE	A	2405	-	-	10/27/27/34	-
6	Y01	A	2412	-	-	9/19/77/77	0/4/4/4
7	JL3	A	2409	-	-	17/45/45/48	-
7	JL3	A	2411	-	-	18/38/38/48	-
3	NAG	A	2403	-	-	0/6/23/26	0/1/1/1
3	NAG	A	2402	-	-	0/6/23/26	0/1/1/1
7	JL3	A	2407	-	-	24/48/48/48	-
6	Y01	A	2408	-	-	14/19/77/77	0/4/4/4
2	A1AHK	A	2401	-	-	11/27/33/33	0/4/4/4
7	JL3	A	2410	-	-	19/39/39/48	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	Y01	A	2413	-	-	6/19/77/77	0/4/4/4
6	Y01	A	2406	-	-	10/19/77/77	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	A1AHK	C30-C29	9.19	1.52	1.39
2	A	2401	A1AHK	C16-C13	8.86	1.53	1.39
2	A	2401	A1AHK	C15-C13	8.72	1.53	1.39
2	A	2401	A1AHK	C18-C16	7.97	1.53	1.38
2	A	2401	A1AHK	C17-C15	7.80	1.53	1.38
2	A	2401	A1AHK	C18-C19	6.64	1.53	1.38
2	A	2401	A1AHK	C30-N08	6.57	1.48	1.34
2	A	2401	A1AHK	C26-N08	6.55	1.48	1.34
2	A	2401	A1AHK	C17-C19	6.49	1.52	1.38
2	A	2401	A1AHK	C27-C26	6.25	1.52	1.38
2	A	2401	A1AHK	C27-C28	5.47	1.48	1.38
2	A	2401	A1AHK	C21-N05	4.58	1.45	1.35
2	A	2401	A1AHK	C28-C29	4.47	1.48	1.39
2	A	2401	A1AHK	C29-C31	3.46	1.52	1.44
2	A	2401	A1AHK	O04-C21	-2.94	1.17	1.23
2	A	2401	A1AHK	C22-N05	2.68	1.46	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	A1AHK	C24-C22-N07	-6.64	107.23	110.92
2	A	2401	A1AHK	C11-C10-C13	5.28	131.20	119.70
2	A	2401	A1AHK	C26-C23-N06	-4.96	104.98	112.13
2	A	2401	A1AHK	C25-N06-N07	-4.17	108.18	111.45
2	A	2401	A1AHK	C28-C29-C30	2.57	120.74	117.26
2	A	2401	A1AHK	C22-N05-C21	-2.37	124.00	128.25
7	A	2411	JL3	O23-P22-O24	2.35	123.87	112.24
2	A	2401	A1AHK	C20-C19-C17	-2.31	117.59	120.89
7	A	2409	JL3	O23-P22-O24	2.29	123.54	112.24
7	A	2410	JL3	O23-P22-O24	2.28	123.52	112.24
7	A	2407	JL3	O23-P22-O24	2.27	123.45	112.24
2	A	2401	A1AHK	C29-C30-N08	-2.22	120.22	123.51
2	A	2401	A1AHK	C20-C21-N05	2.18	119.27	114.77

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2401	A1AHK	C11-C10-C14-F01
2	A	2401	A1AHK	C11-C10-C14-F02
2	A	2401	A1AHK	C11-C10-C14-F03
2	A	2401	A1AHK	C12-C10-C14-F01
2	A	2401	A1AHK	C12-C10-C14-F02
2	A	2401	A1AHK	C12-C10-C14-F03
5	A	2405	LPE	C31-O33-P-O32
6	A	2406	Y01	OAG-CAY-OAW-CBC
6	A	2406	Y01	CAM-CAY-OAW-CBC
6	A	2408	Y01	CAV-CBC-OAW-CAY
6	A	2408	Y01	CAM-CAY-OAW-CBC
6	A	2412	Y01	CAR-CBC-OAW-CAY
6	A	2413	Y01	CAM-CAY-OAW-CBC
7	A	2407	JL3	C20-O21-P22-O23
7	A	2407	JL3	C20-O21-P22-O25
7	A	2407	JL3	C26-O25-P22-O23
7	A	2407	JL3	O17-C18-C19-O29
7	A	2407	JL3	O25-C26-C27-N28
7	A	2409	JL3	O17-C18-C19-O29
7	A	2409	JL3	O25-C26-C27-N28
7	A	2410	JL3	C20-O21-P22-O23
7	A	2410	JL3	C20-O21-P22-O24
7	A	2410	JL3	C26-O25-P22-O23
7	A	2410	JL3	C26-O25-P22-O24
7	A	2410	JL3	O25-C26-C27-N28
7	A	2410	JL3	C32-C30-O29-C19
7	A	2411	JL3	O25-C26-C27-N28
7	A	2411	JL3	C32-C30-O29-C19
7	A	2407	JL3	O16-C15-O17-C18
7	A	2411	JL3	O16-C15-O17-C18
6	A	2408	Y01	OAG-CAY-OAW-CBC
6	A	2413	Y01	OAG-CAY-OAW-CBC
7	A	2410	JL3	O31-C30-O29-C19
7	A	2411	JL3	O31-C30-O29-C19
7	A	2407	JL3	C14-C15-O17-C18
7	A	2411	JL3	C14-C15-O17-C18
7	A	2407	JL3	C32-C30-O29-C19
6	A	2408	Y01	CAJ-CAO-CBB-CBE
6	A	2408	Y01	CAJ-CAO-CBB-CAC
6	A	2413	Y01	CAJ-CAO-CBB-CBE
7	A	2407	JL3	C30-C32-C33-C34
7	A	2411	JL3	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
6	A	2408	Y01	CAN-CAJ-CAO-CBB
7	A	2407	JL3	O31-C30-O29-C19
7	A	2407	JL3	C26-O25-P22-O21
7	A	2410	JL3	C20-O21-P22-O25
7	A	2410	JL3	C26-O25-P22-O21
7	A	2410	JL3	C14-C15-O17-C18
7	A	2407	JL3	C08-C09-C10-C11
7	A	2411	JL3	C35-C36-C37-C38
7	A	2409	JL3	C03-C04-C05-C06
7	A	2411	JL3	C10-C11-C12-C13
7	A	2411	JL3	C33-C34-C35-C36
7	A	2409	JL3	C32-C30-O29-C19
7	A	2407	JL3	C09-C10-C11-C12
7	A	2407	JL3	C37-C38-C39-C40
7	A	2407	JL3	C03-C04-C05-C06
6	A	2413	Y01	CAJ-CAO-CBB-CAC
7	A	2411	JL3	C06-C07-C08-C09
7	A	2410	JL3	O16-C15-O17-C18
7	A	2409	JL3	O31-C30-O29-C19
7	A	2411	JL3	C32-C33-C34-C35
7	A	2409	JL3	C30-C32-C33-C34
5	A	2405	LPE	O1-C11-C12-C13
7	A	2409	JL3	C09-C10-C11-C12
7	A	2411	JL3	C18-C19-C20-O21
7	A	2409	JL3	O17-C18-C19-C20
7	A	2410	JL3	O17-C18-C19-C20
6	A	2412	Y01	CAV-CBC-OAW-CAY
6	A	2412	Y01	CAM-CAY-OAW-CBC
5	A	2405	LPE	C12-C13-C14-C15
5	A	2405	LPE	C15-C16-C17-C18
6	A	2406	Y01	CAN-CAJ-CAO-CBB
7	A	2407	JL3	O17-C18-C19-C20
7	A	2410	JL3	C12-C13-C14-C15
7	A	2411	JL3	C07-C08-C09-C10
6	A	2408	Y01	CAC-CBB-CBE-CBI
7	A	2410	JL3	O17-C18-C19-O29
6	A	2408	Y01	CAO-CBB-CBE-CBI
6	A	2408	Y01	CAO-CBB-CBE-CAP
6	A	2412	Y01	CAO-CAJ-CAN-CBA
7	A	2409	JL3	C12-C13-C14-C15
7	A	2407	JL3	C35-C36-C37-C38
7	A	2409	JL3	C05-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
5	A	2405	LPE	C13-C14-C15-C16
2	A	2401	A1AHK	N06-C23-C26-C27
2	A	2401	A1AHK	N06-C23-C26-N08
5	A	2405	LPE	C31-O33-P-O3
5	A	2405	LPE	C16-C17-C18-C19
5	A	2405	LPE	C31-O33-P-O31
7	A	2407	JL3	C20-O21-P22-O24
7	A	2407	JL3	C04-C05-C06-C07
6	A	2408	Y01	CAC-CBB-CBE-CAP
7	A	2409	JL3	C02-C03-C04-C05
7	A	2410	JL3	C27-C26-O25-P22
2	A	2401	A1AHK	C13-C10-C14-F01
7	A	2411	JL3	O29-C19-C20-O21
7	A	2409	JL3	C10-C11-C12-C13
7	A	2409	JL3	C36-C37-C38-C39
6	A	2412	Y01	OAG-CAY-OAW-CBC
7	A	2409	JL3	C26-O25-P22-O21
7	A	2411	JL3	C26-O25-P22-O21
6	A	2408	Y01	CAO-CAJ-CAN-CBA
7	A	2409	JL3	C38-C39-C40-C41
6	A	2406	Y01	CAJ-CAO-CBB-CBE
7	A	2407	JL3	C07-C08-C09-C10
7	A	2407	JL3	C33-C34-C35-C36
6	A	2412	Y01	CAM-CAL-CAX-OAF
5	A	2405	LPE	C17-C18-C19-C20
6	A	2412	Y01	CAM-CAL-CAX-OAH
7	A	2410	JL3	O29-C19-C20-O21
6	A	2406	Y01	CAM-CAL-CAX-OAH
7	A	2410	JL3	C18-C19-C20-O21
6	A	2408	Y01	CAM-CAL-CAX-OAH
6	A	2413	Y01	CAM-CAL-CAX-OAH
7	A	2410	JL3	O29-C30-C32-C33
6	A	2408	Y01	CAR-CBC-OAW-CAY
7	A	2407	JL3	C40-C41-C42-C43
7	A	2411	JL3	C13-C14-C15-O17
6	A	2406	Y01	CAM-CAL-CAX-OAF
6	A	2413	Y01	CAM-CAL-CAX-OAF
7	A	2409	JL3	C06-C07-C08-C09
6	A	2408	Y01	CAM-CAL-CAX-OAF
7	A	2411	JL3	C13-C14-C15-O16
7	A	2410	JL3	O31-C30-C32-C33
6	A	2406	Y01	CAX-CAL-CAM-CAY

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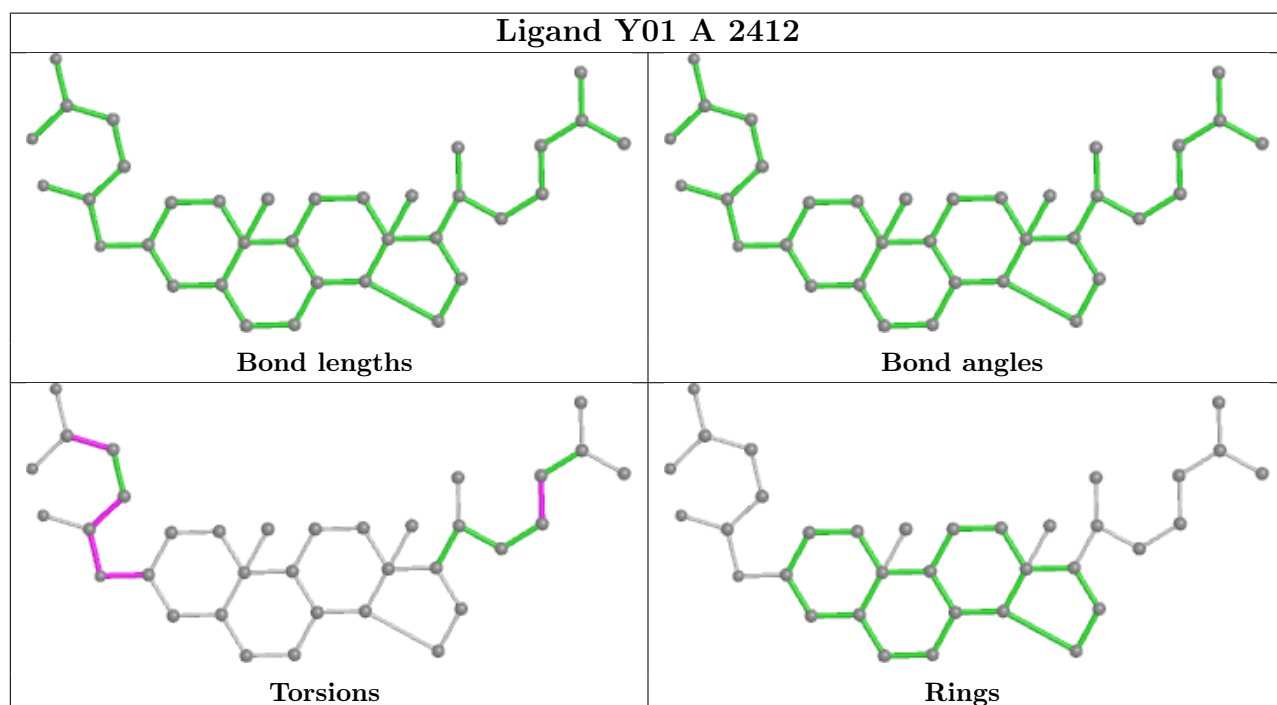
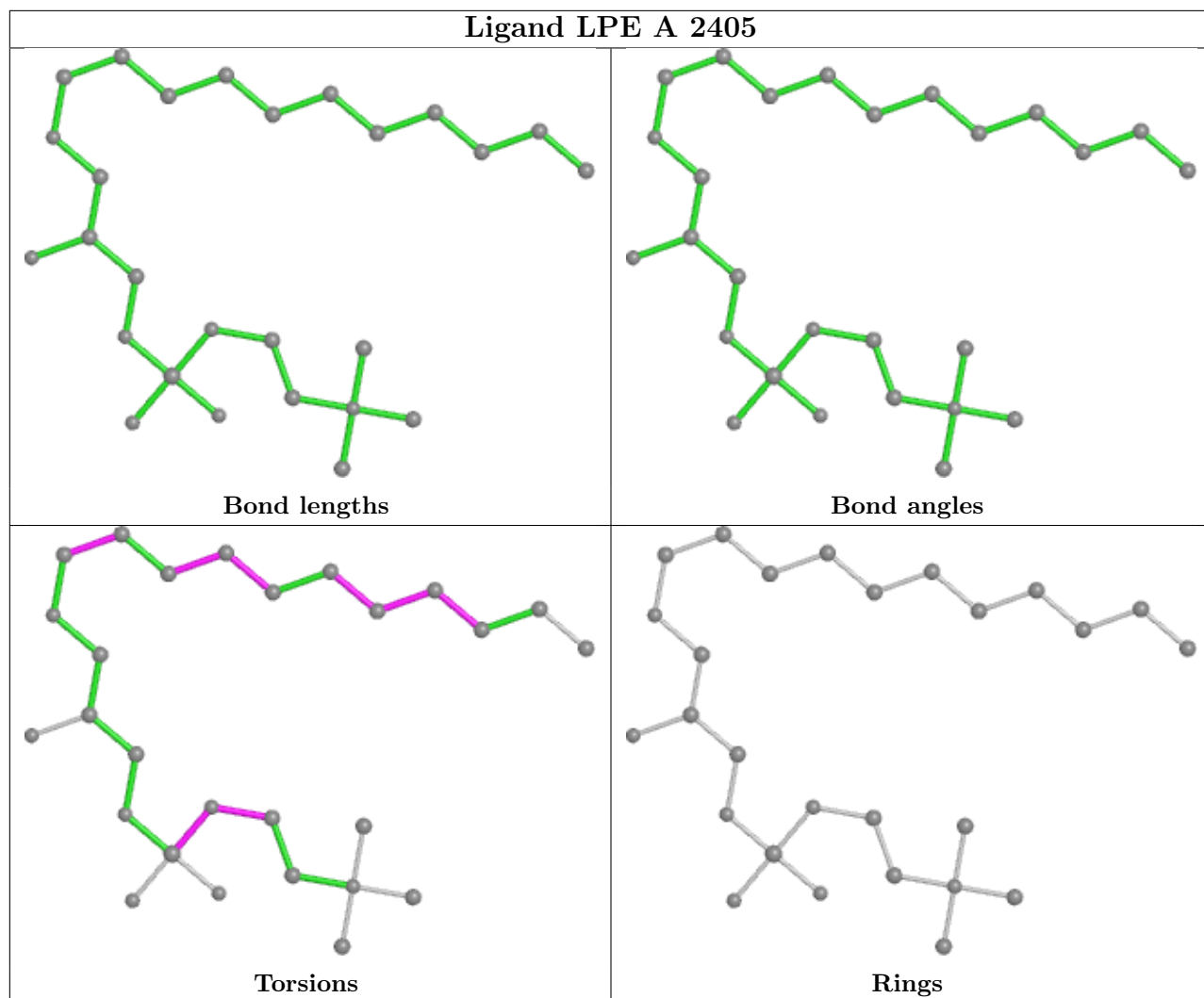
Mol	Chain	Res	Type	Atoms
7	A	2407	JL3	C10-C11-C12-C13
5	A	2405	LPE	C32-C31-O33-P
7	A	2409	JL3	C27-C26-O25-P22
7	A	2411	JL3	C27-C26-O25-P22
6	A	2406	Y01	CAL-CAM-CAY-OAG
6	A	2412	Y01	CAL-CAM-CAY-OAW
2	A	2401	A1AHK	C13-C10-C14-F02
2	A	2401	A1AHK	C13-C10-C14-F03
6	A	2406	Y01	CAL-CAM-CAY-OAW
6	A	2406	Y01	CAJ-CAO-CBB-CAC
7	A	2407	JL3	C13-C14-C15-O17
6	A	2412	Y01	CAL-CAM-CAY-OAG

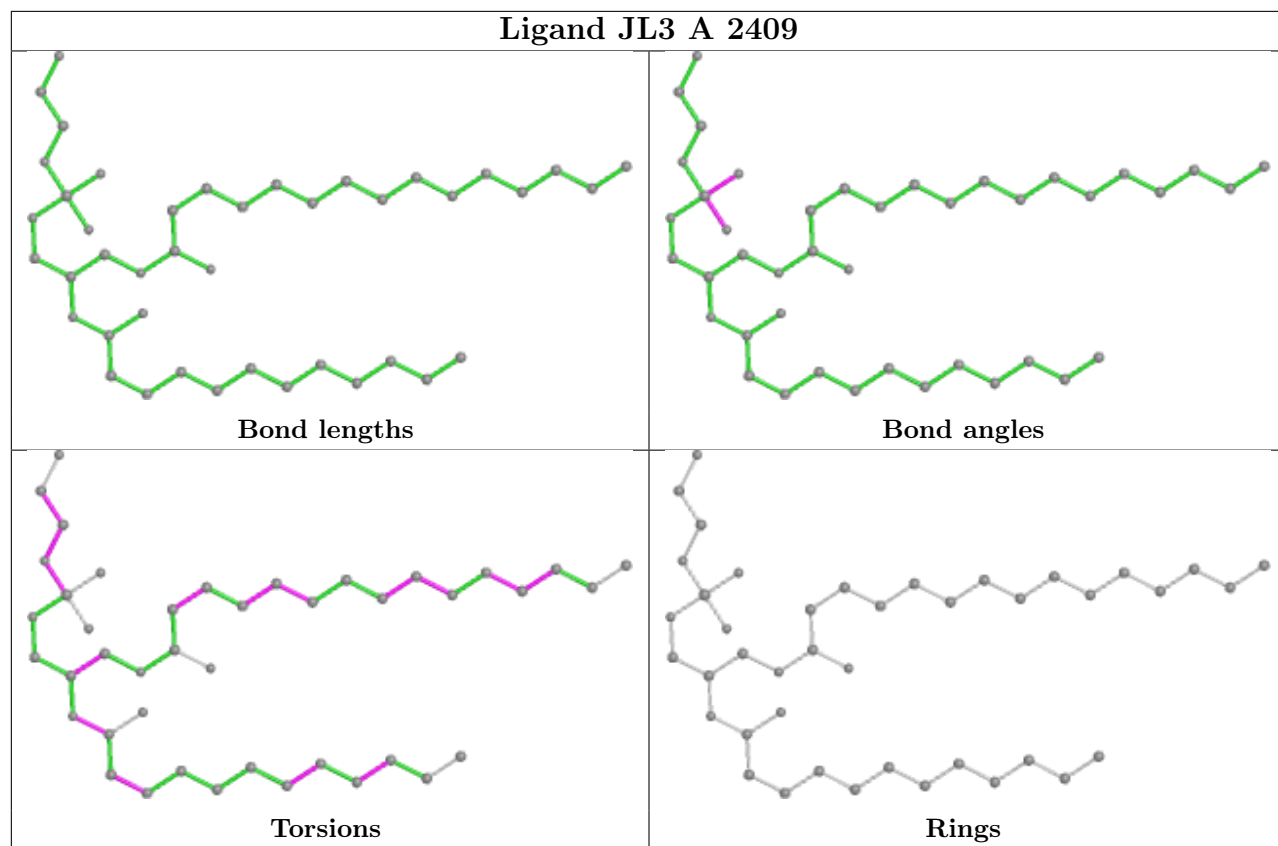
There are no ring outliers.

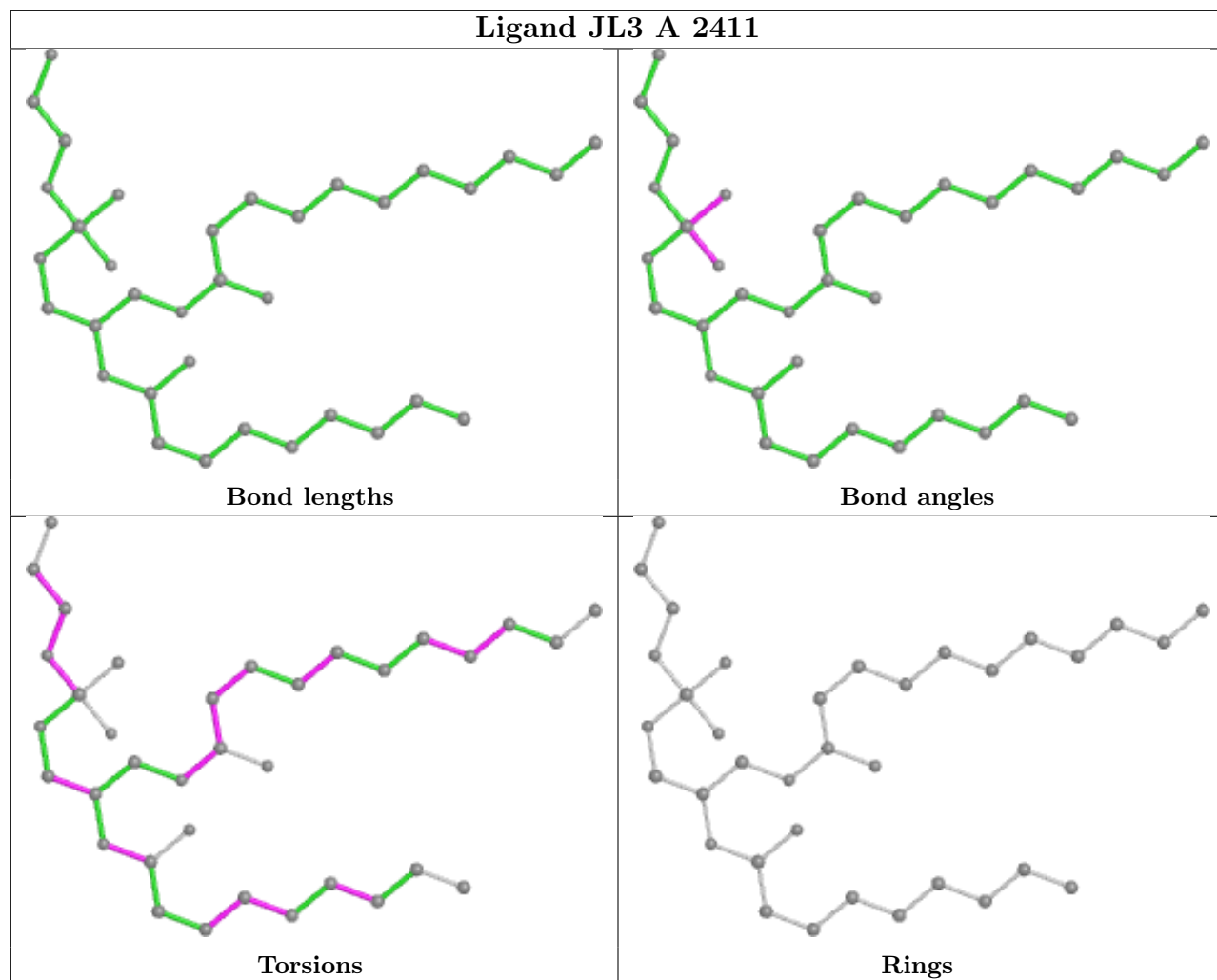
2 monomers are involved in 2 short contacts:

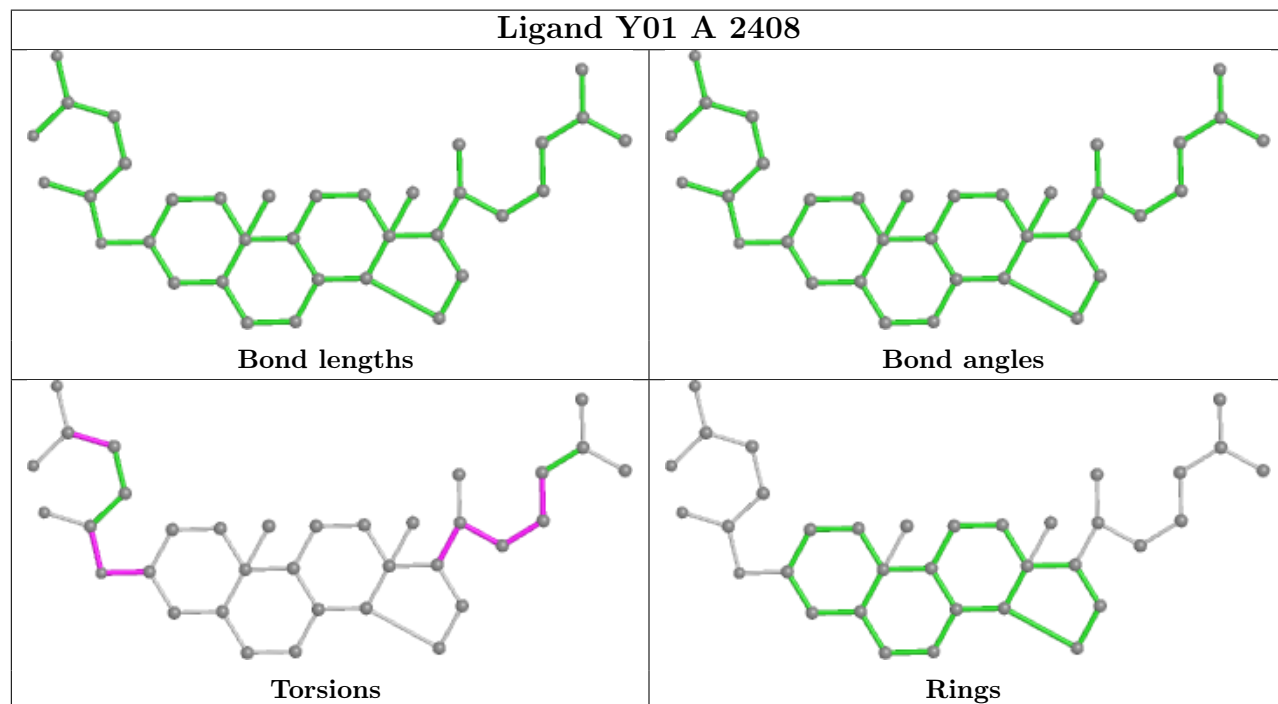
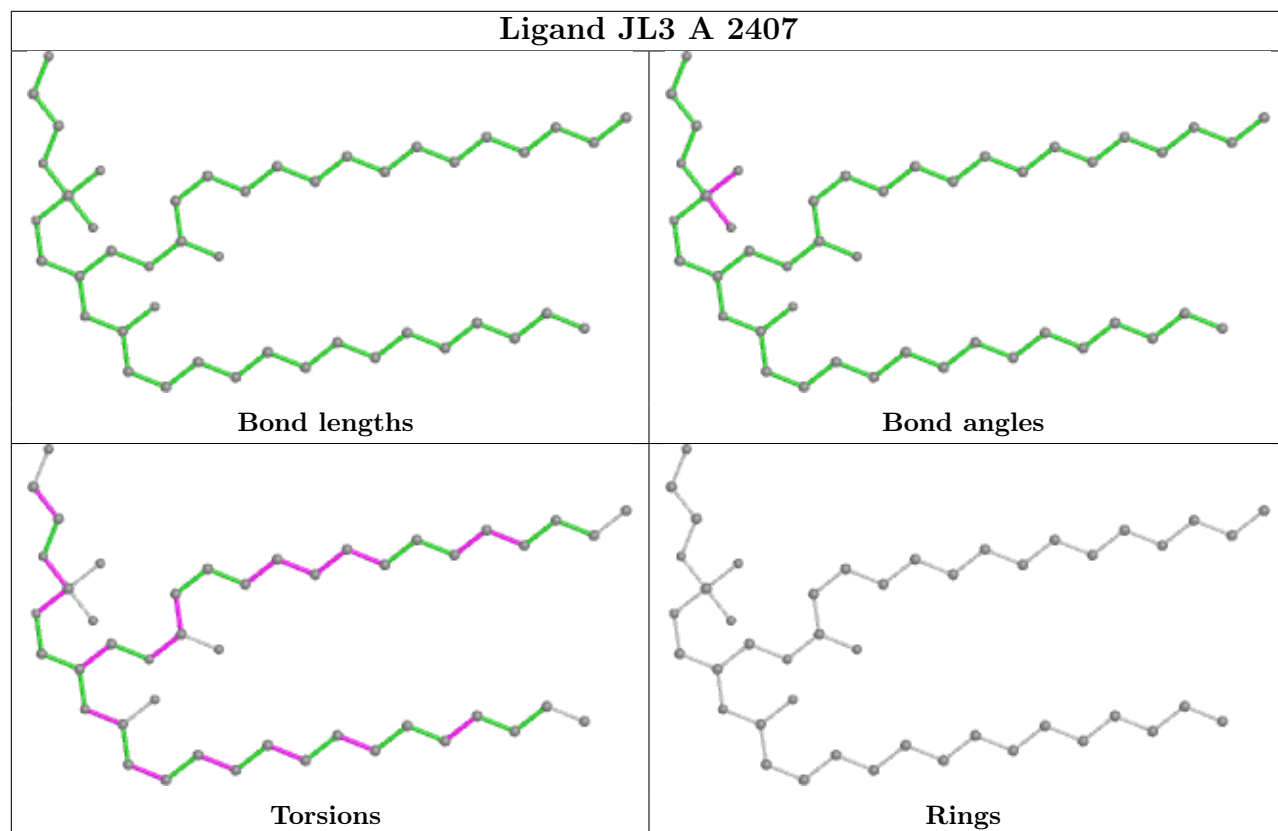
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2412	Y01	1	0
6	A	2413	Y01	1	0

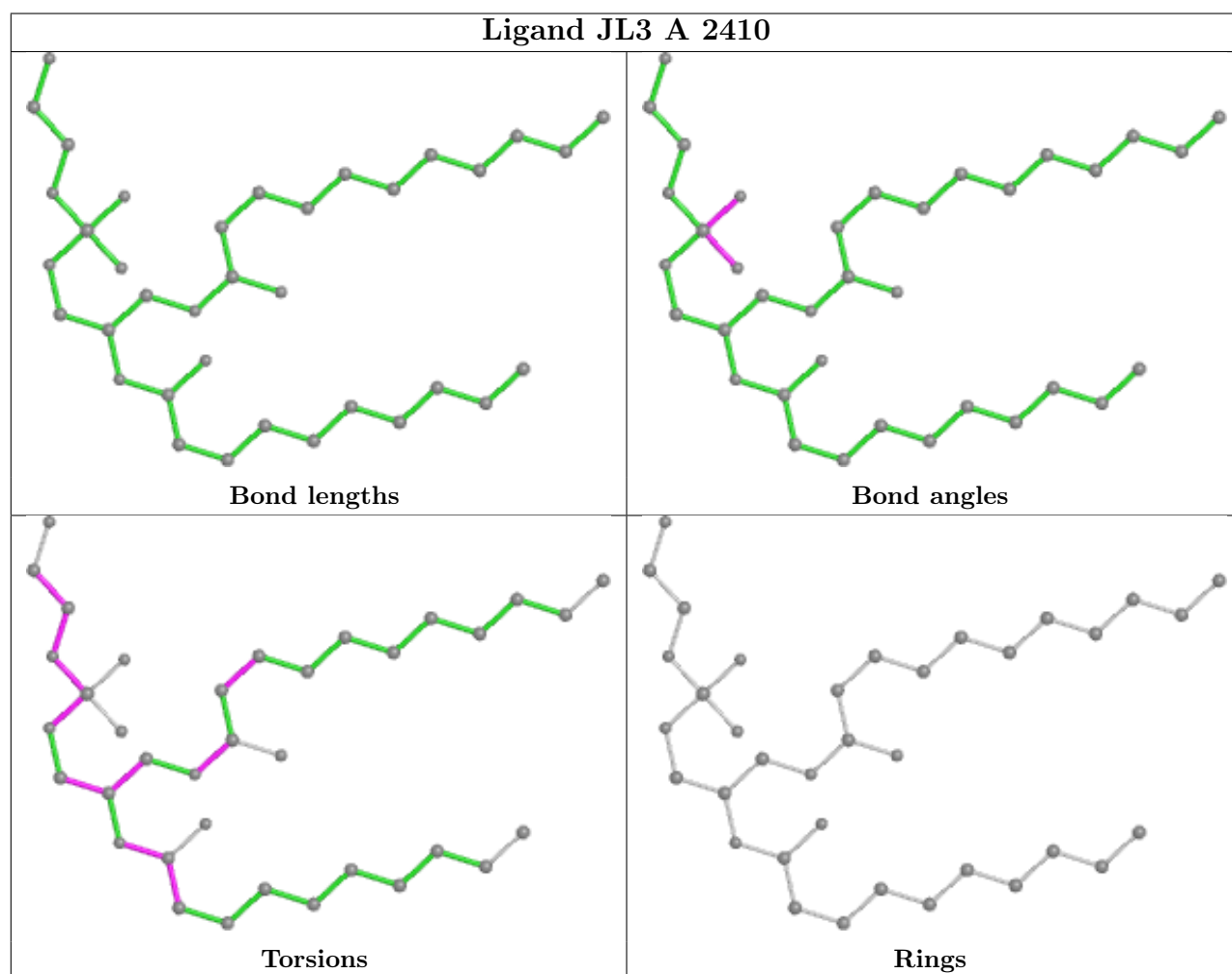
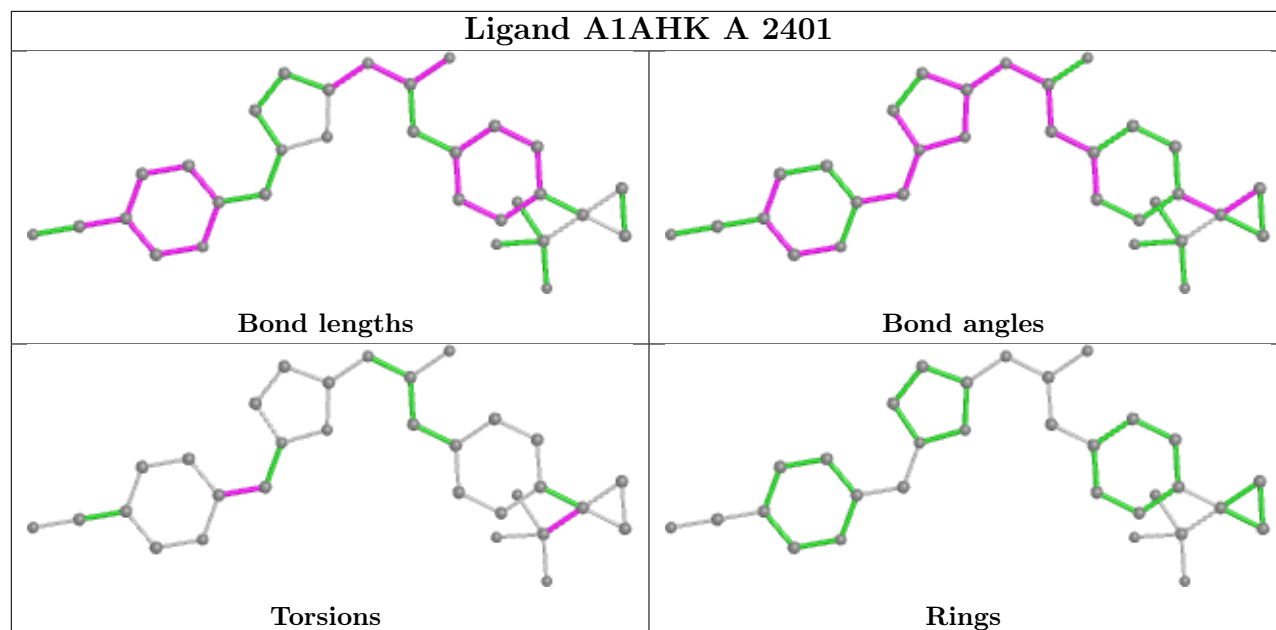
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

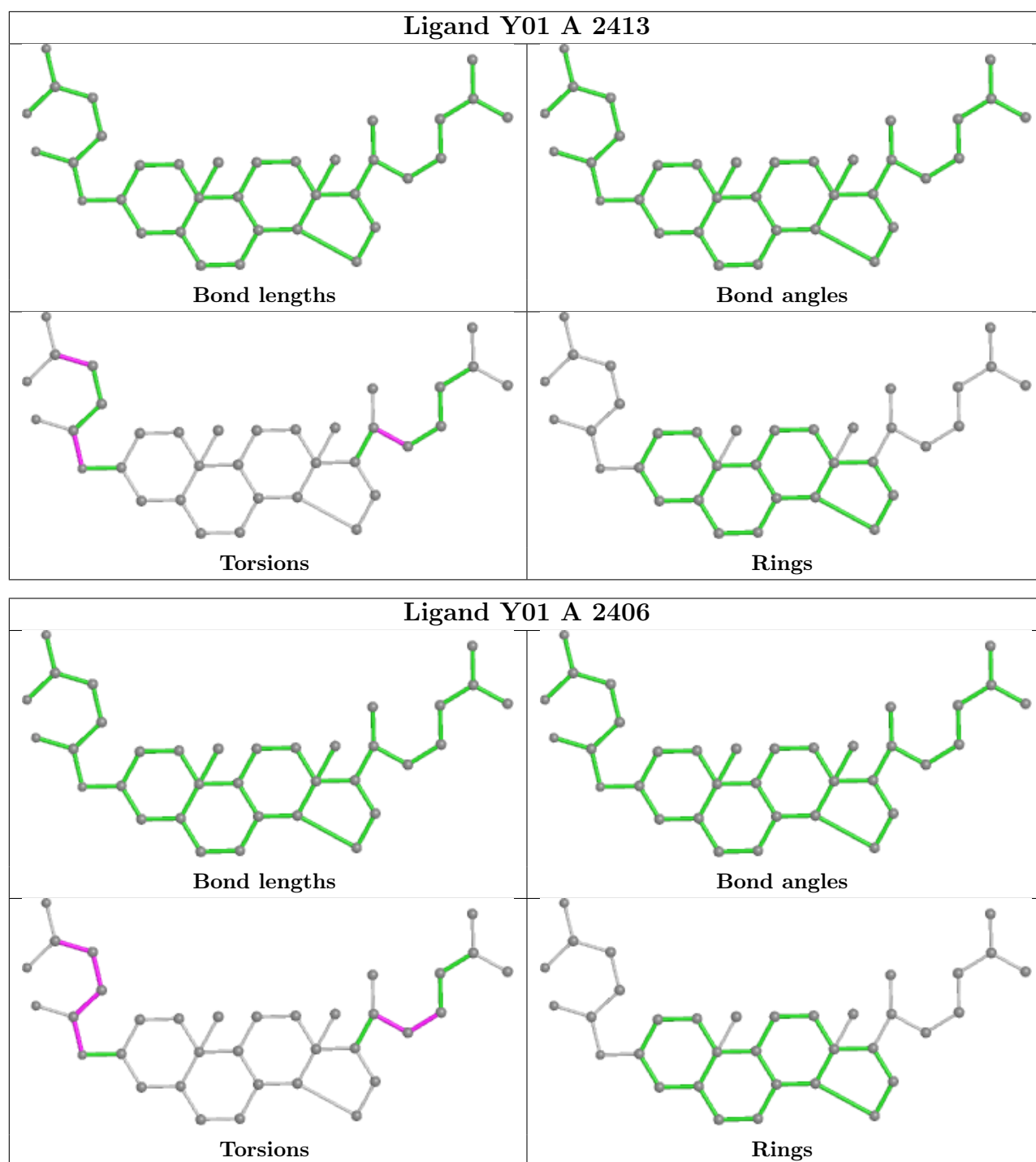












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

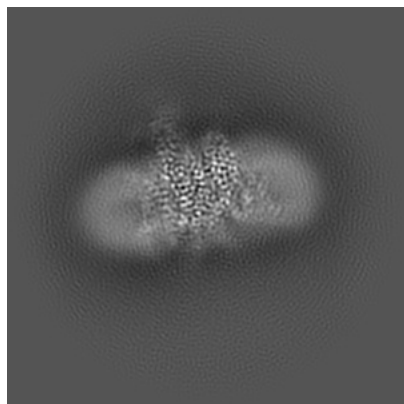
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43995. These allow visual inspection of the internal detail of the map and identification of artifacts.

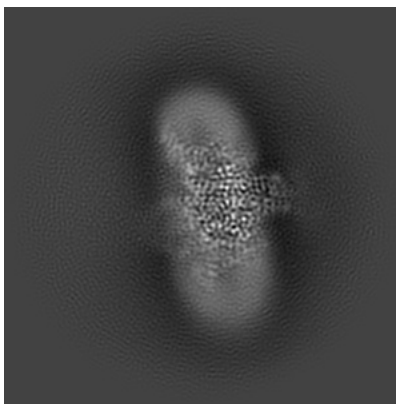
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

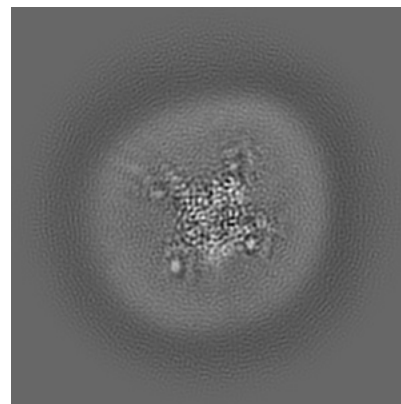
6.1.1 Primary map



X

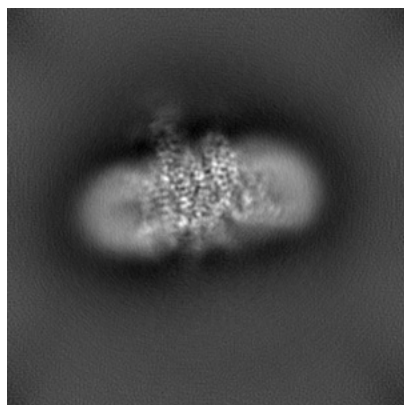


Y

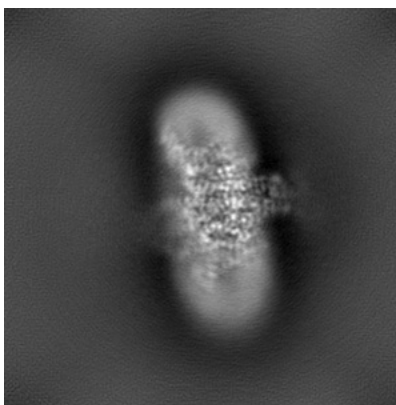


Z

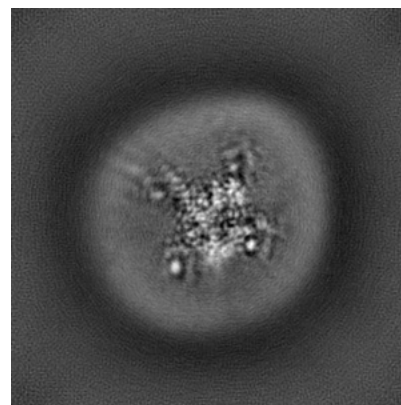
6.1.2 Raw map



X



Y

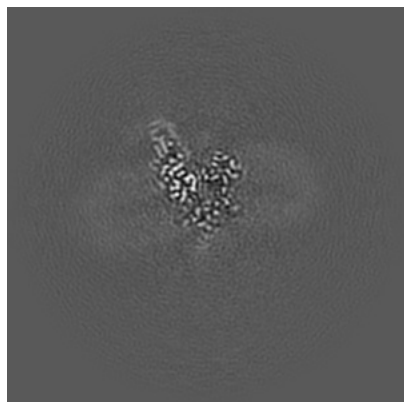


Z

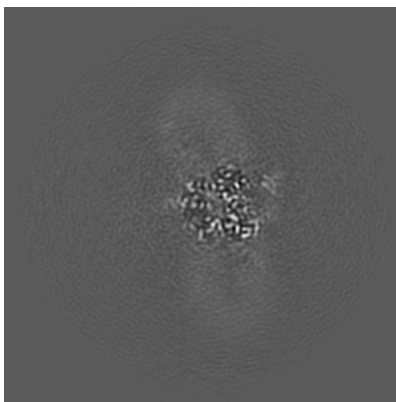
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

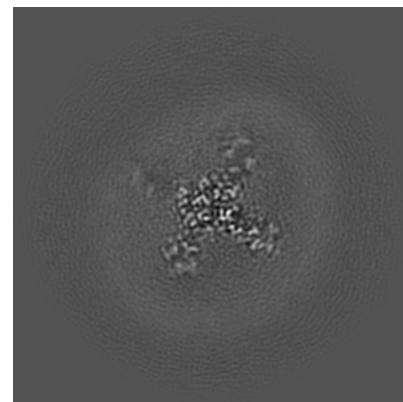
6.2.1 Primary map



X Index: 128

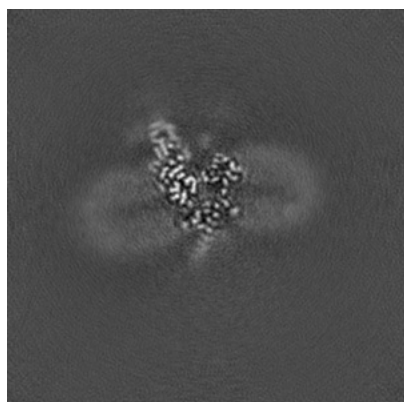


Y Index: 128

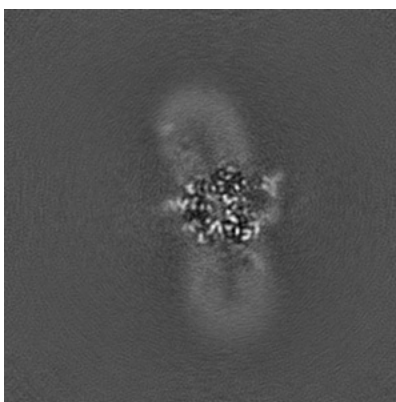


Z Index: 128

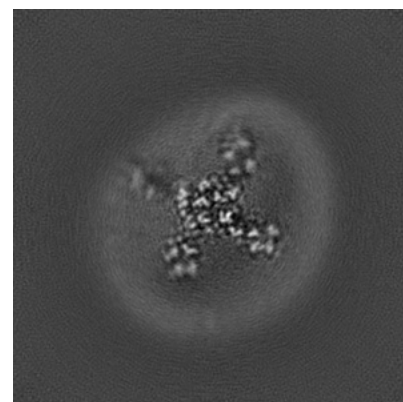
6.2.2 Raw map



X Index: 128



Y Index: 128

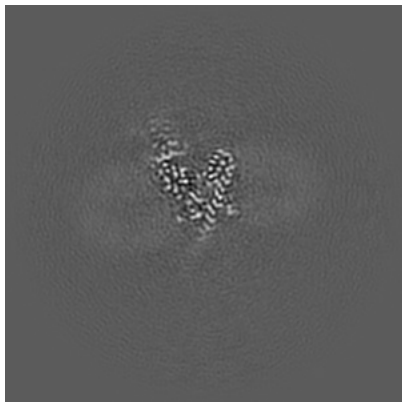


Z Index: 128

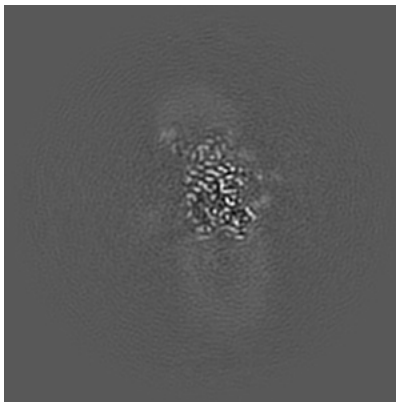
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

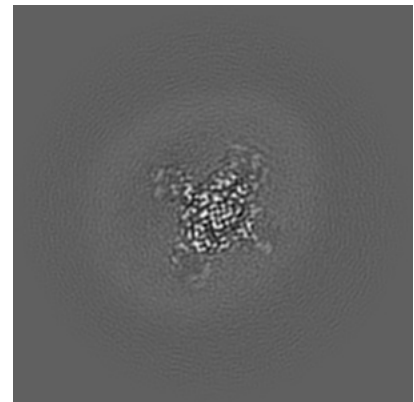
6.3.1 Primary map



X Index: 130

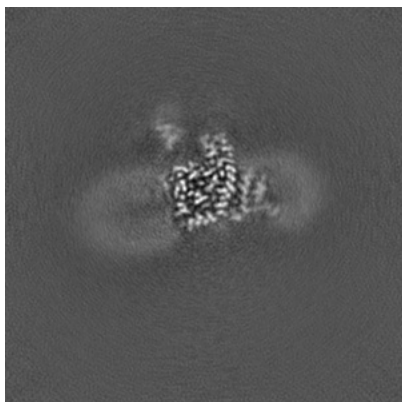


Y Index: 115

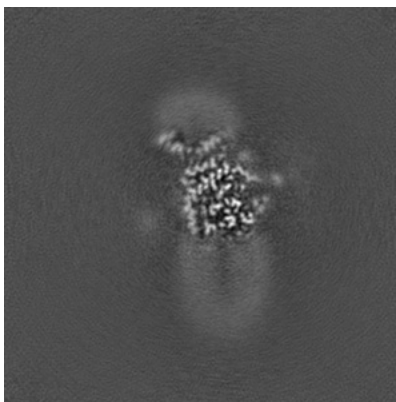


Z Index: 146

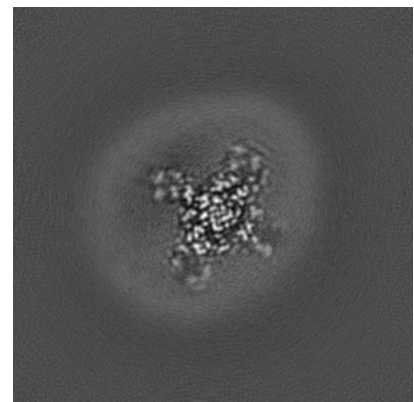
6.3.2 Raw map



X Index: 141



Y Index: 113

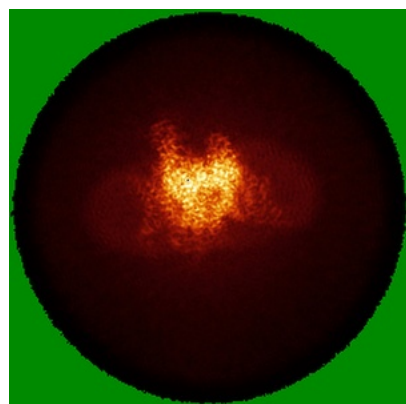


Z Index: 146

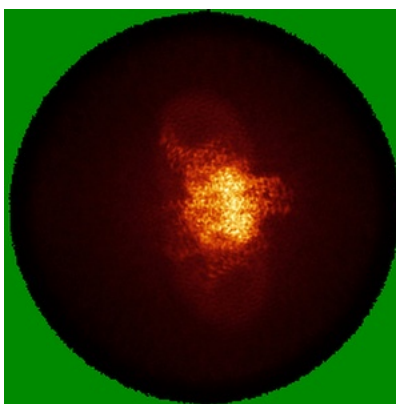
The images above show the largest variance slices of the map in three orthogonal directions.

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

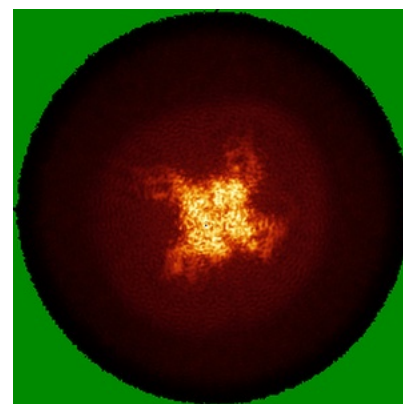
6.4.1 Primary map



X

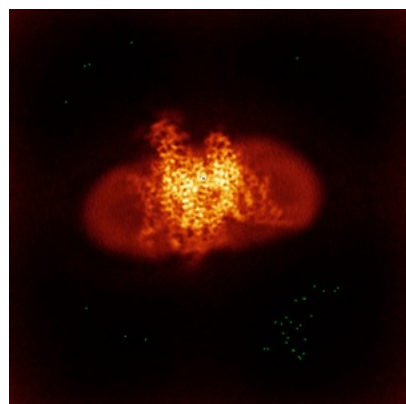


Y

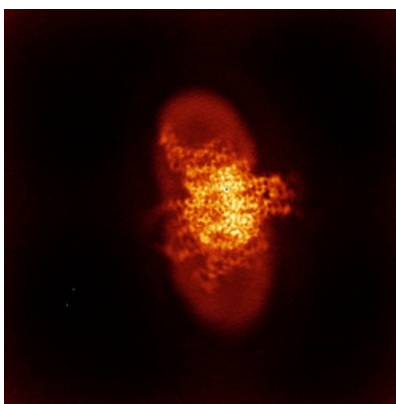


Z

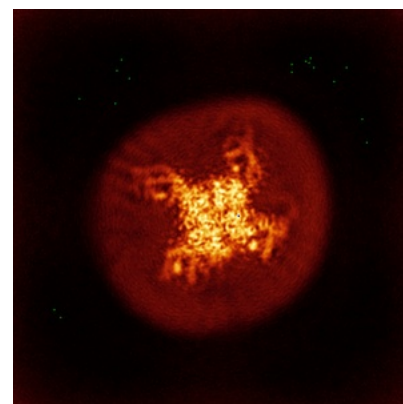
6.4.2 Raw map



X



Y

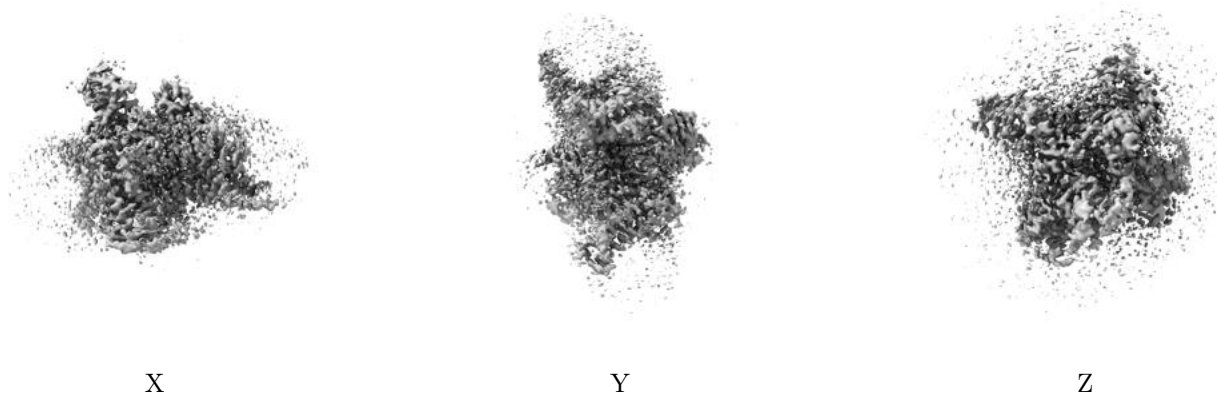


Z

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.

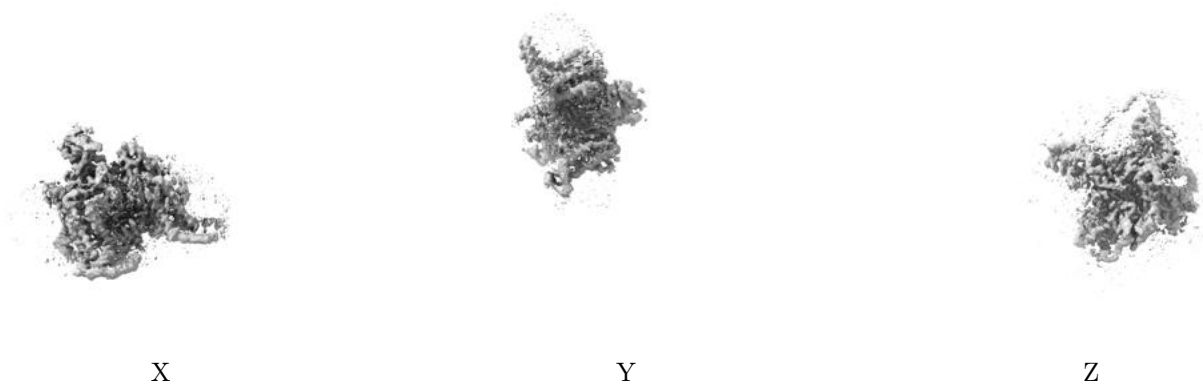
6.5 Orthogonal surface views [i](#)

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.

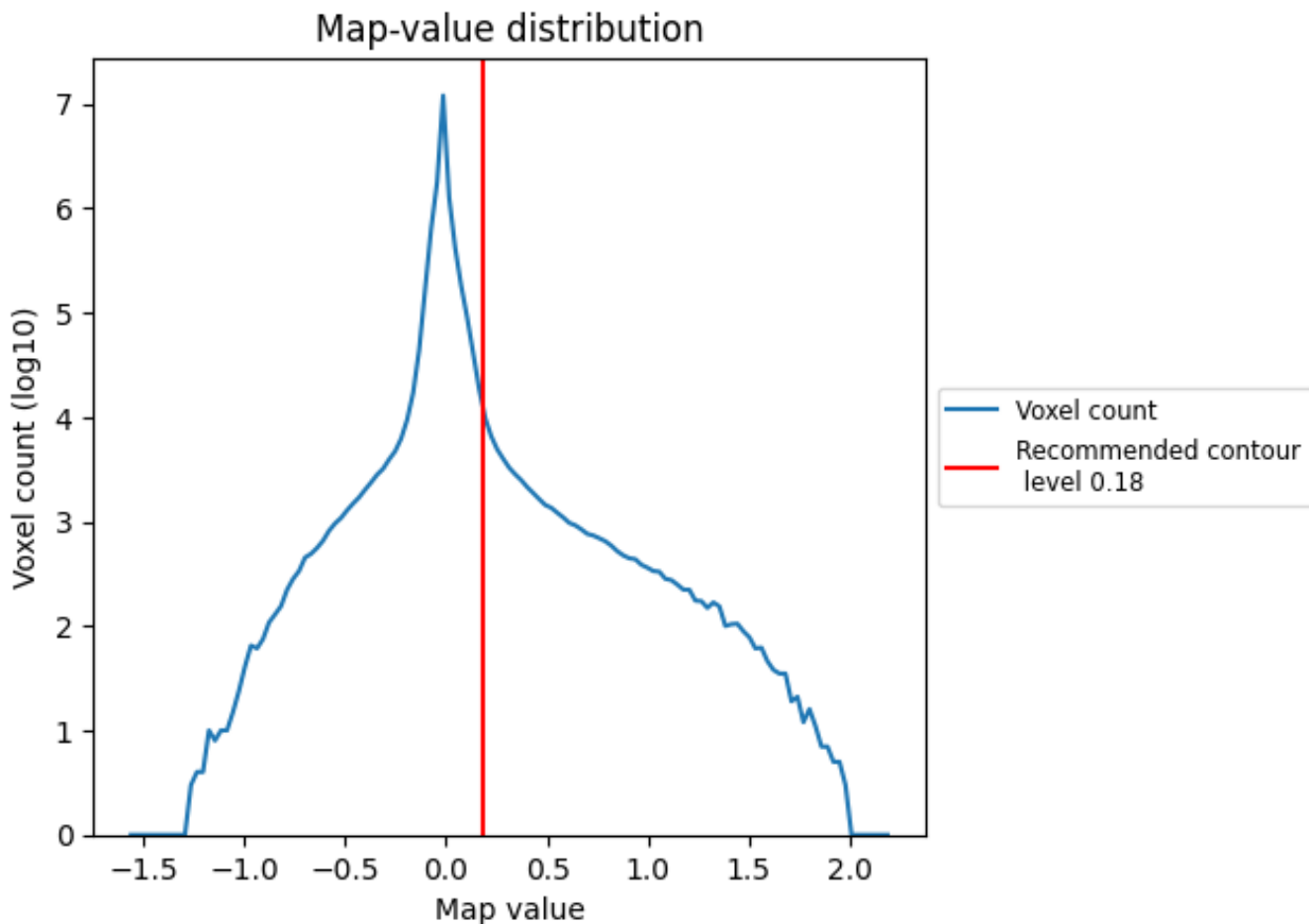
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

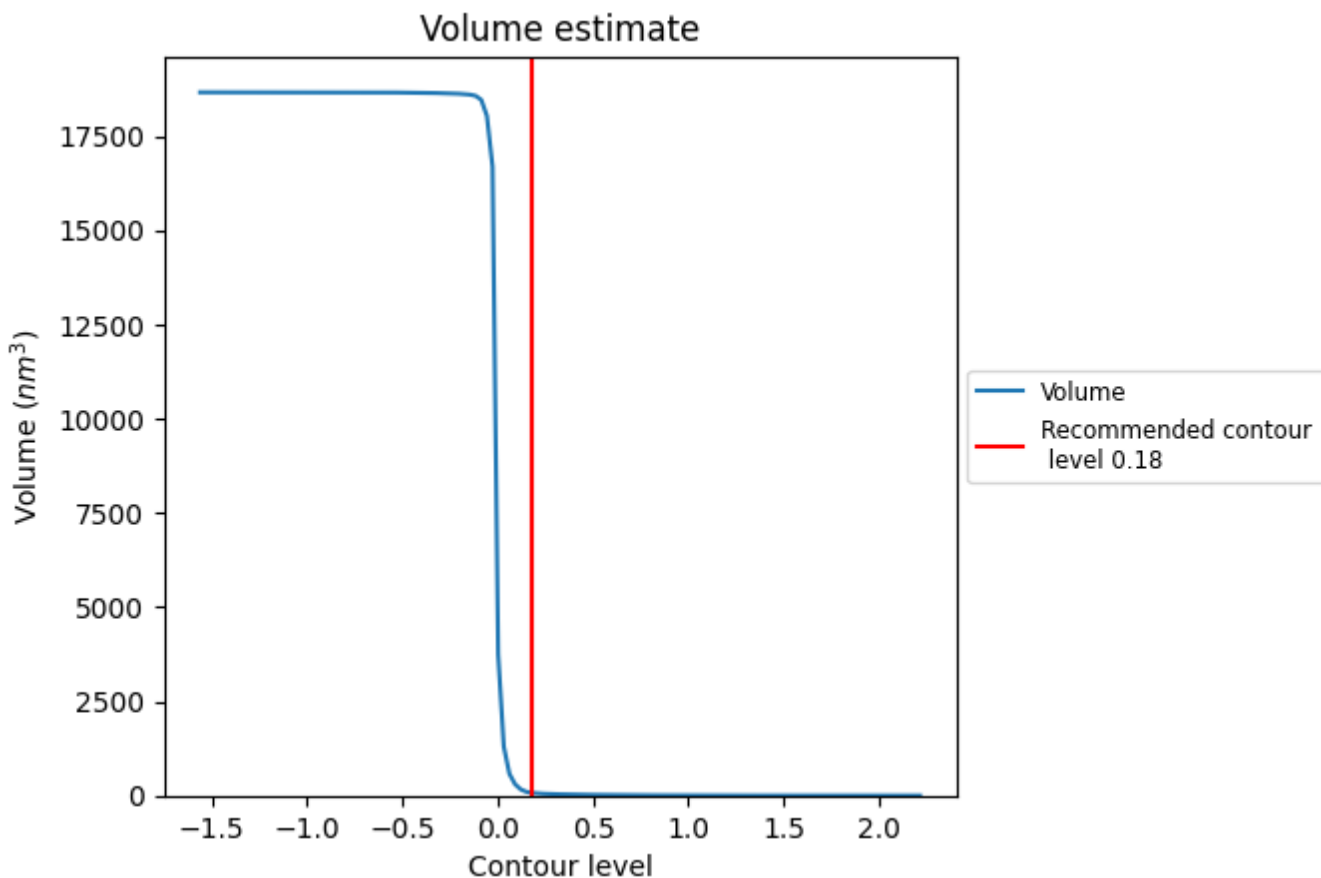
This section contains the results of statistical analysis of the map.

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.

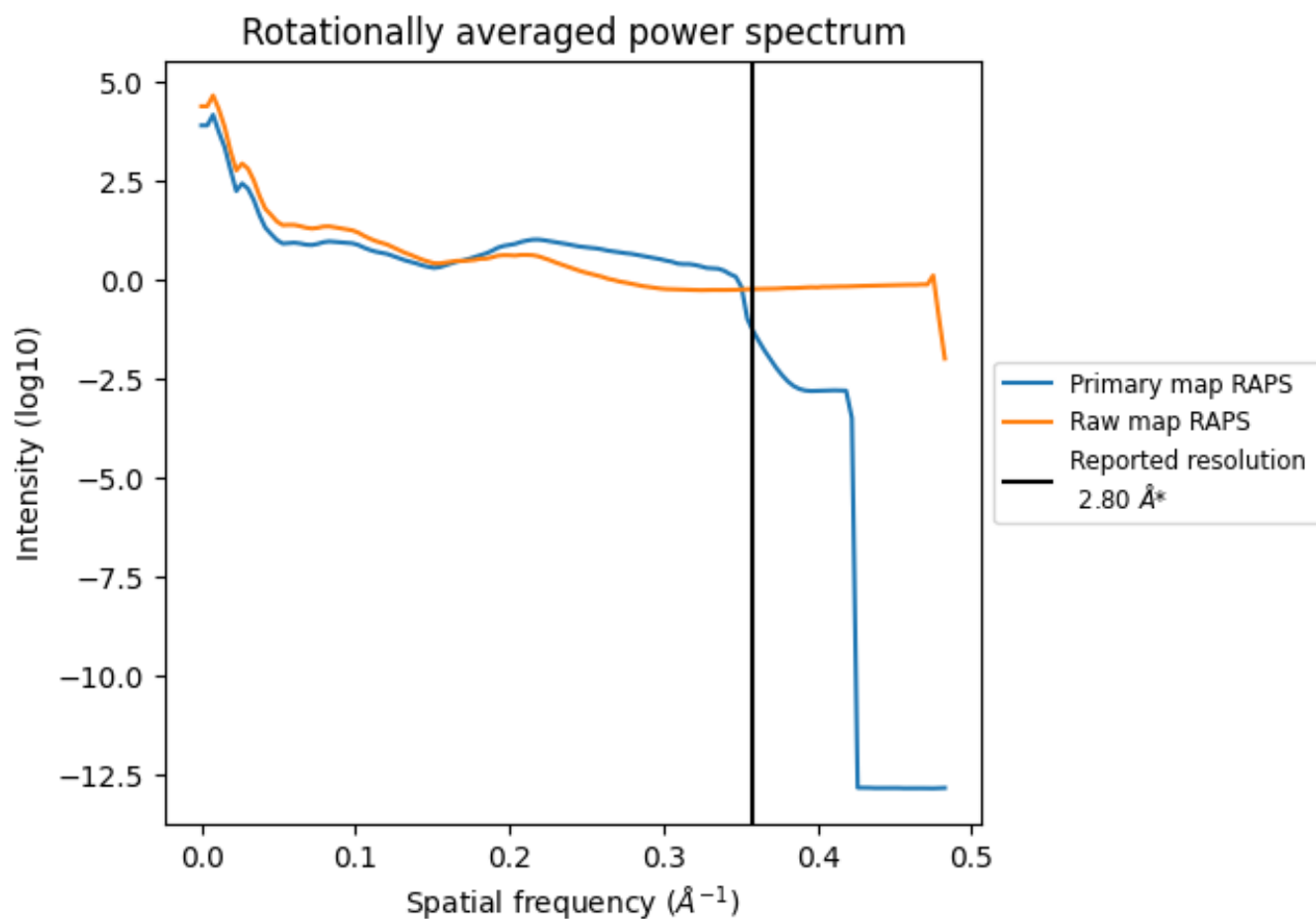
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm^3 ; this corresponds to an approximate mass of 64 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 i

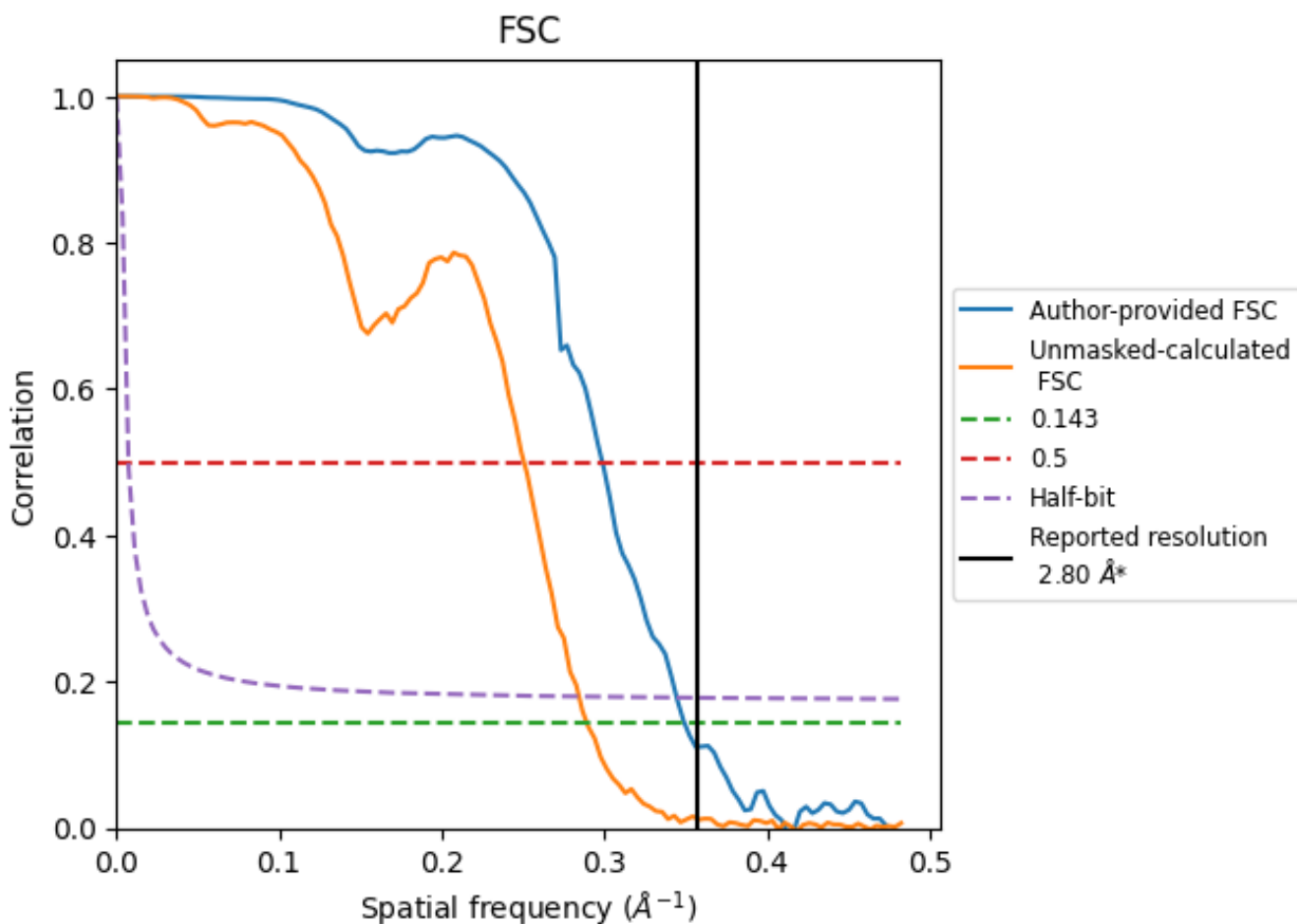


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

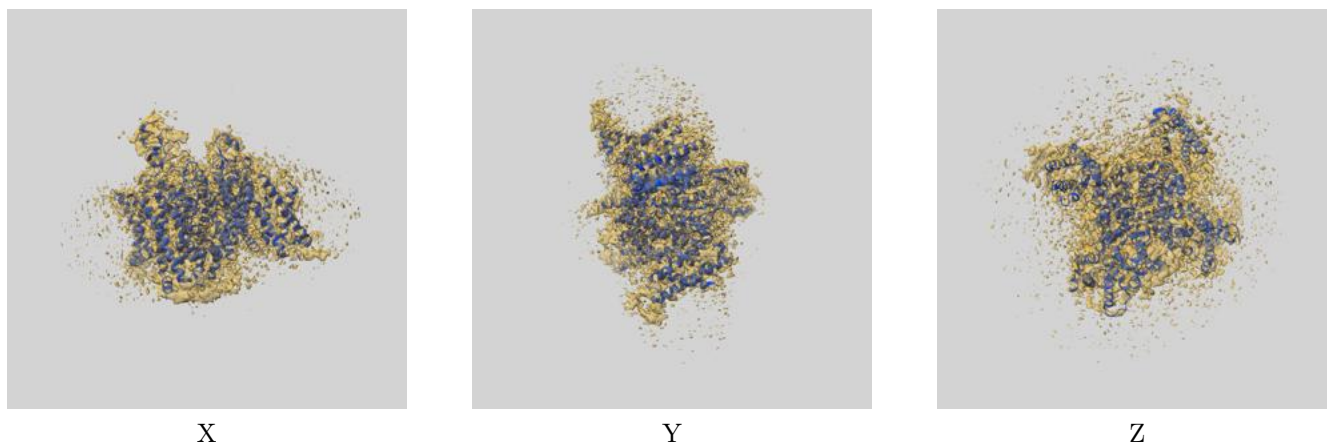
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.86	3.35	2.90
Unmasked-calculated*	3.46	3.99	3.51

*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 3.46 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

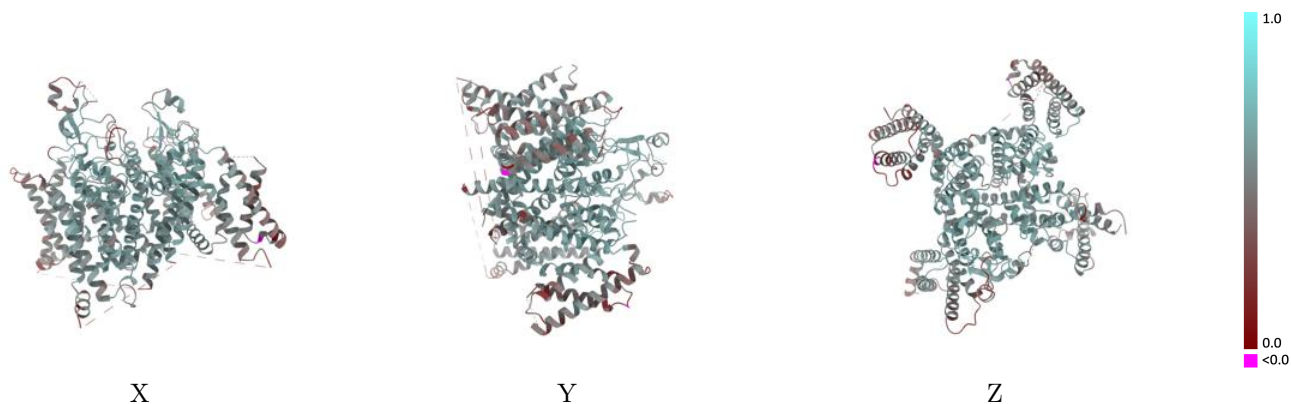
This section contains information regarding the fit between EMDB map EMD-43995 and PDB model 9AYL. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



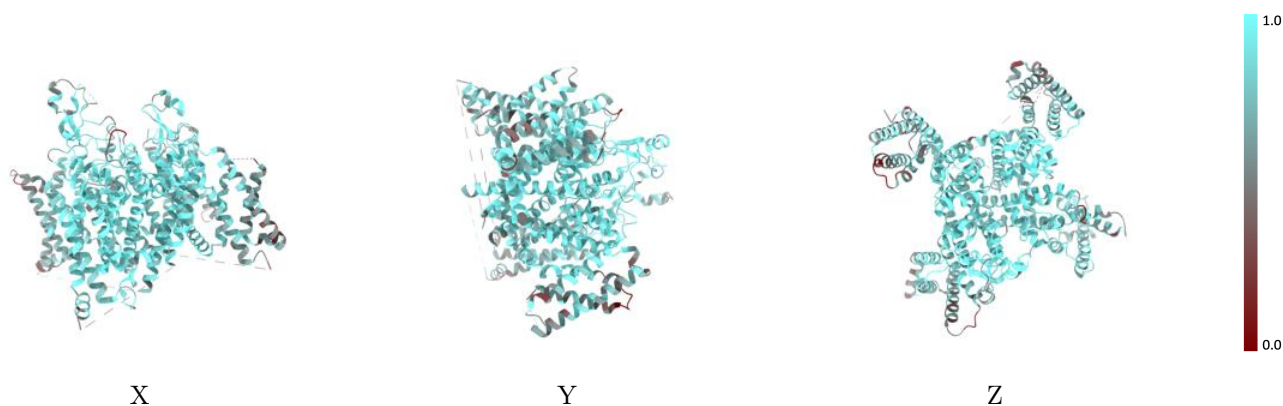
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



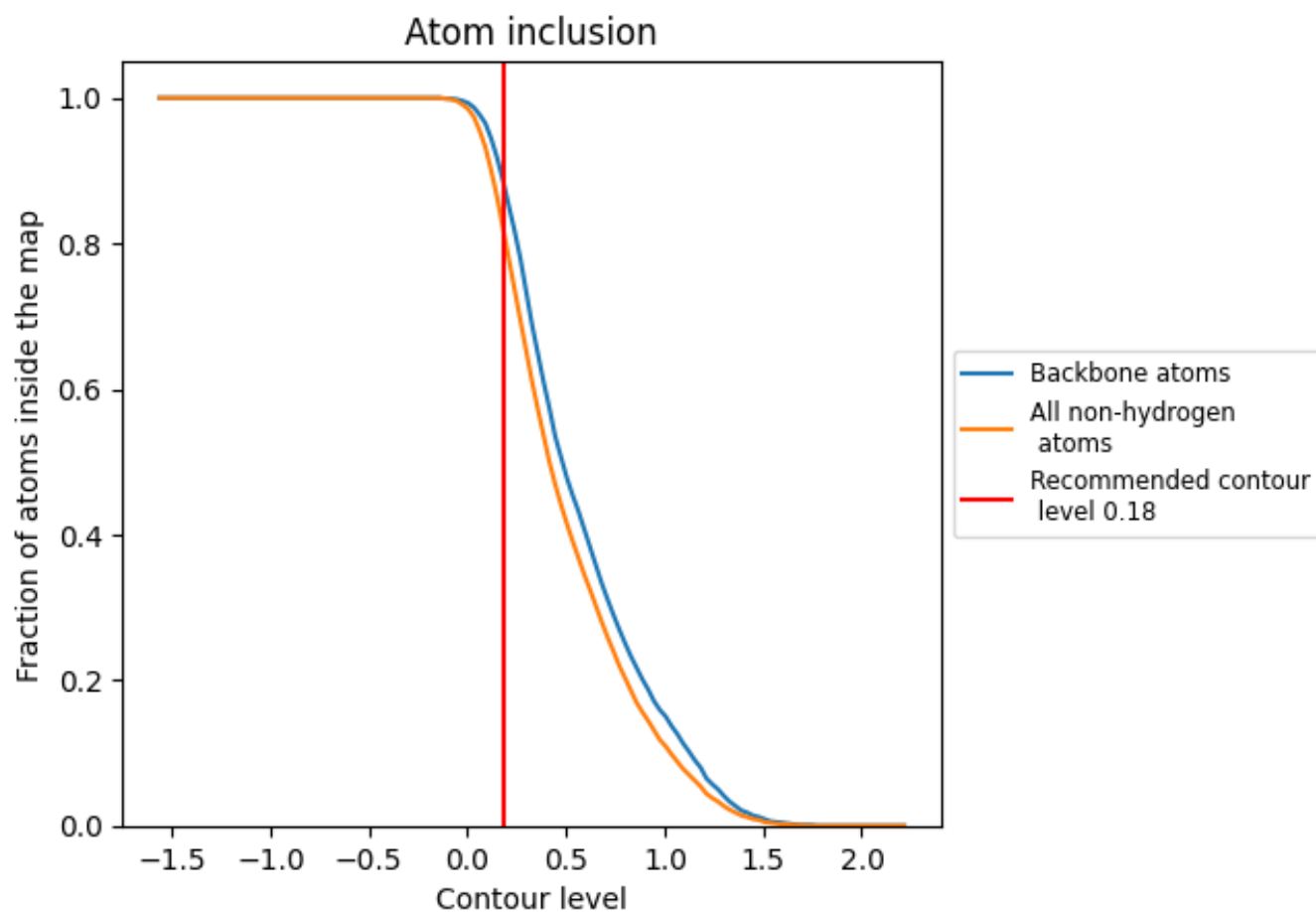
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 89% of all backbone atoms, 82% 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	 0.8220	 0.5310
A	 0.8220	 0.5310

