



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 11:22 AM JST

PDB ID : 7YG5
EMDB ID : EMD-33808
Title : Structure of human R-type voltage-gated CaV2.3-alpha2/delta1-beta1 channel complex in the topiramate-bound state
Authors : Gao, Y.; Zhao, Y.
Deposited on : 2022-07-11
Resolution : 3.00 Å(reported)
Based on initial model : 7VFS

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 : 1.8.5 (274361), CSD as541be (2020)
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

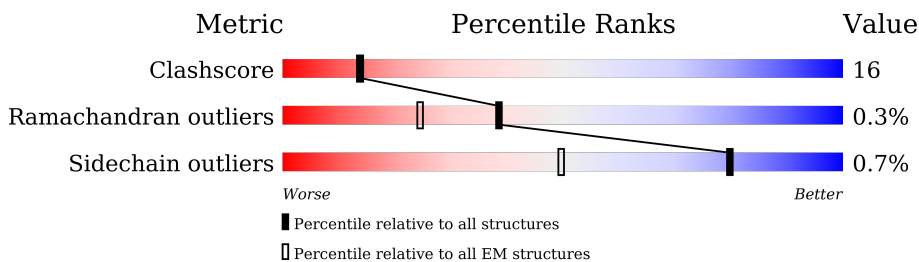
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	2313	<div> <div>9%</div> <div>39%</div> <div>17%</div> <div>•</div> <div>43%</div> </div>
2	B	598	<div> <div>22%</div> <div>16%</div> <div>11%</div> <div>73%</div> </div>
3	D	1103	<div> <div>14%</div> <div>59%</div> <div>28%</div> <div>13%</div> </div>
4	C	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
4	E	3	<div> <div>33%</div> <div>67%</div> </div>
5	F	3	<div> <div>67%</div> <div>33%</div> <div>33%</div> </div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 20308 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 R-type calcium channel subunit alpha-1E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1319	Total	C	N	O	S	0	0
			10674	7007	1761	1830	76		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1269	813	217	234	5		

- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	955	Total	C	N	O	S	0	0
			7637	4842	1281	1483	31		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



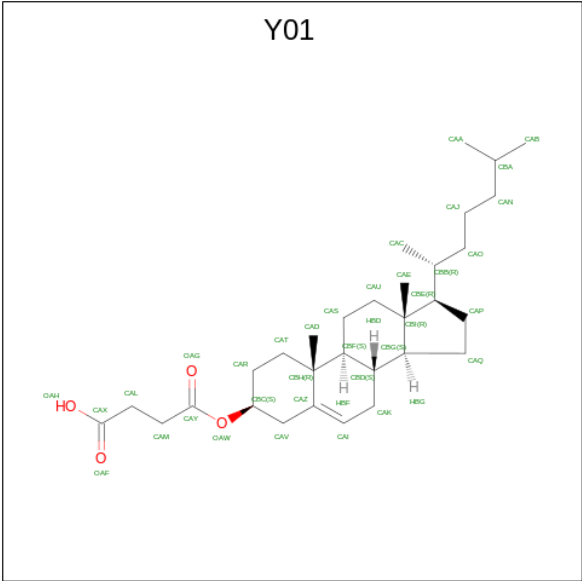
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



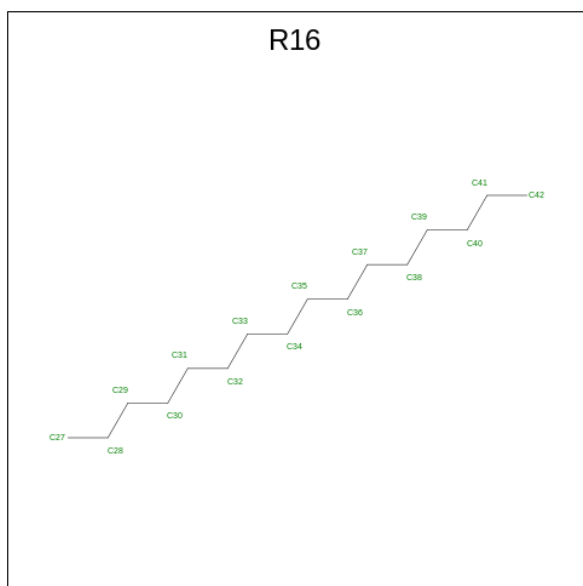
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	

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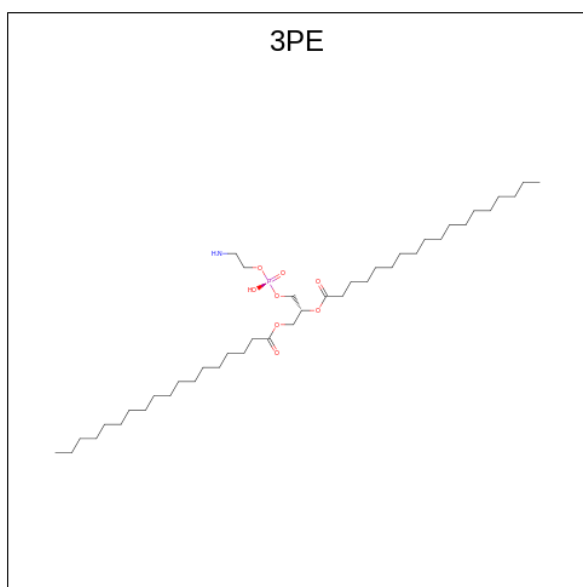
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			35	31	4	

- Molecule 7 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	C	0
			10	10	
7	A	1	Total	C	0
			16	16	
7	A	1	Total	C	0
			16	16	
7	A	1	Total	C	0
			13	13	
7	A	1	Total	C	0
			9	9	
7	A	1	Total	C	0
			16	16	

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).

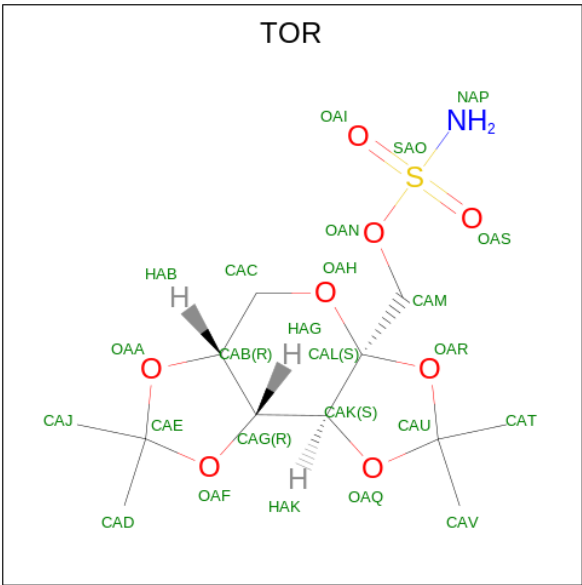


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
8	A	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

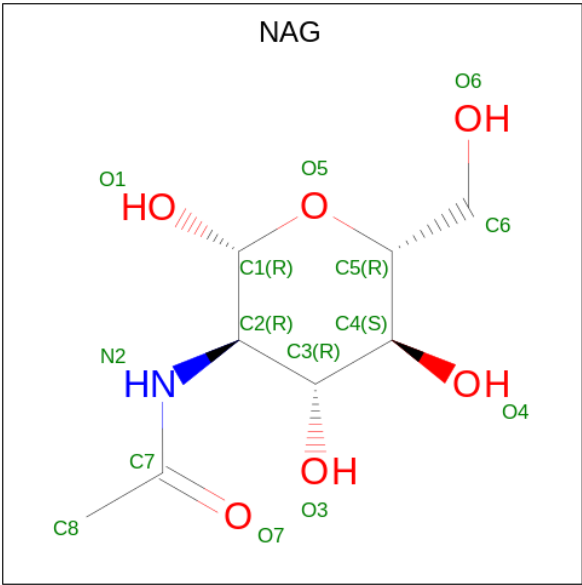
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Ca	0
			1	1	
9	D	1	Total	Ca	0
			1	1	

- Molecule 10 is [(3aS,5aR,8aR,8bS)-2,2,7,7-tetramethyltetrahydro-3aH-bis[1,3]dioxolo[4,5-b:4',5'-d]pyran-3a-yl]methyl sulfamate (three-letter code: TOR) (formula: C₁₂H₂₁NO₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
10	A	1	22	12	1	8	1	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	D	1	14	8	1	5	0
11	D	1	14	8	1	5	0

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Mol	Chain	Residues	Atoms				AltConf
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	



[illegible]

- Molecule 2: Voltage-dependent L-type calcium channel subunit beta-1

[illegible]

LEU	GLY	SER	SER	LYS	SER	GLY	ASP	ASN	SER	SER	SER	SER	LEU	GLY	ASP	VAL	VAL	THR	GLY	THR	ARG	ARG	ARG	PRO	THR	PRO	PRO	ALA	ALA	LYS	GLN	LYS	GLN	LYS	SER	THR	GLU	HIS	VAL	PRO	PRO	TYR	ASP	VAL	VAL	P227	P228	M229	R230	P231	T232	T233	L234	V235	G236	P237	S238	L239	G240
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	G241	Y242	E243	V244	T245	D246	M247	M248	A251	L252	F253	D254	F255	L256	K257	H258	R259	F260	D261	K262	R263	I264	S265	L266	T267	R268	V269	T270	A271	D272	T273	S274	L275	A276	LYS	ARG	SER	VAL	LEU	ASN	ASN	PRO	SER	LYS	HIS	ILE	ILE	ILE	GLU	ARG	SER	ASN	THR	ARG	SER	SER	LEU	ALA	ASP
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V302	Q303	S304	E305	T306	E307	R308	T309	F310	E311	L312	A313	R314	T315	L316	Q317	L318	V319	A320	L321	D322	A323	D324	T325	T326	N327	H328	P329	A330	Q331	L332	S333	K334	T335	T336	L337	A338	P339	T340	T341	V342	V343	T344	K345	T346	T347	S348	P349	K350	V351	L352	Q353	R354	L355	L356	K357	S358	R359	G360	T361
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S362	S363	S364	K365	H366	L367	V368	V369	Q370	I371	A372	K376	L377	A378	Q379	C380	P381	P382	S383	C384	F385	D386	L387	L388	L389	D390	E391	N392	Q393	L394	E395	D396	A397	C398	E399	H400	L401	A402	E403	Y404	L405	E406	A407	Y408	W409	K410	A411	T412	HIS	PRO	PRO	PRO	SER	SER	THR	PRO	PRO	ASN	PRO	EU
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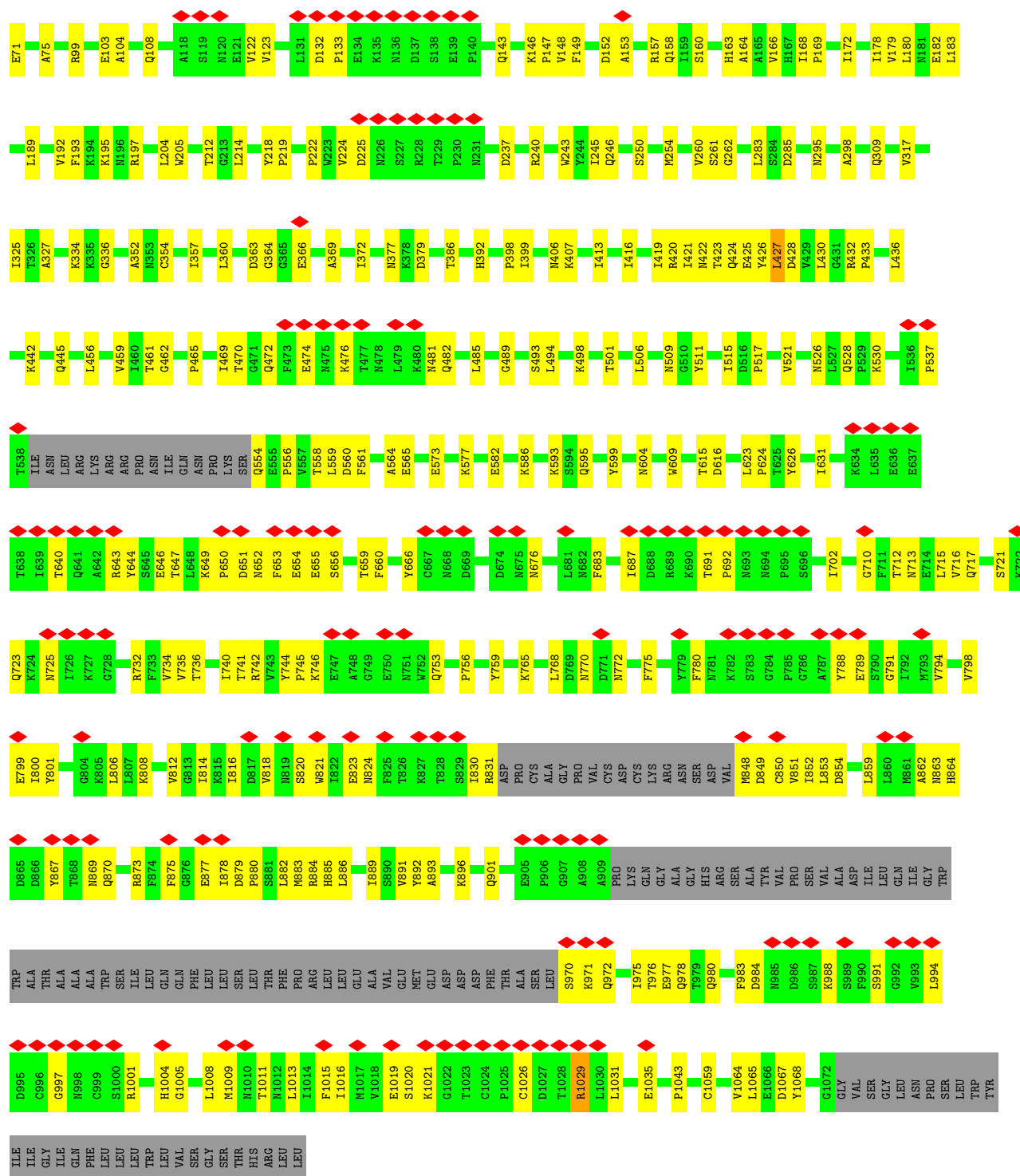
[illegible]

ARG	GLN	GLY	SER	TRP	TRP	GLU	ASP	GLU	GLU	GLU	GLU	ASP	TYR	ASP	GLU	GLU	GLU	GLU	LEU	THR	THR	ASN	ASN	ARG	ARG	ARG	ARG	GLY	GLY	ASN	LYS	ALA	ALA	ALA	GLU	GLY	GLY	GLY	PRO	PRO	VAL	VAL	LEU	LEU	GLY	GLY	ARG	ASN	ASN	LYS	LYS	GLU	GLU	LEU	GLU	GLY	TRP	TRP	GLY	GLY	ARG	GLY	VAL	VAL	TYR	TYR	ILE	ILE	ARG	ARG
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- Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1



NET	ALA	ALA	GLY	CYS	LEU	LEU	ALA	THR	THR	THR	PHE	GLN	SER	SER	GLU	GLU	PRO	F27	P28	S29	T32	I33	K34	S35	W36	V37	D38	K39	M40	Q41	E42	D43	L44	A51	S52	G53	V54	M55	L56	L57	V58	D59	I60	D66	L67	V68	T69
NET	ALA	ALA	GLY	CYS	LEU	LEU	ALA	THR	THR	THR	PHE	GLN	SER	SER	GLU	GLU	PRO	F27	P28	S29	T32	I33	K34	S35	W36	V37	D38	K39	M40	Q41	E42	D43	L44	A51	S52	G53	V54	M55	L56	L57	V58	D59	I60	D66	L67	V68	T69



● Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 



- Molecule 5: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68522	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	135000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.883	Depositor
Minimum map value	-2.363	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TOR, R16, NAG, BMA, 3PE, CA, Y01

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	0.68	2/10939 (0.0%)	0.62	3/14805 (0.0%)
2	B	0.31	0/1290	0.51	0/1744
3	D	0.66	0/7799	0.59	1/10578 (0.0%)
All	All	0.65	2/20028 (0.0%)	0.60	4/27127 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	CYS	CB-SG	-6.26	1.71	1.82
1	A	268	CYS	CB-SG	-5.39	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1356	ASP	CB-CA-C	-5.74	98.92	110.40
1	A	706	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	268	CYS	CA-CB-SG	5.61	124.09	114.00
3	D	427	LEU	CB-CG-CD1	-5.43	101.77	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10674	0	10813	342	0
2	B	1269	0	1290	57	0
3	D	7637	0	7426	225	0
4	C	39	0	34	4	0
4	E	39	0	34	0	0
5	F	39	0	34	2	0
6	A	315	0	441	34	0
7	A	80	0	163	3	0
8	A	80	0	108	0	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	A	22	0	18	5	0
11	D	112	0	104	2	0
All	All	20308	0	20465	631	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 16.

The worst 5 of 631 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:1466:THR:HB	1:A:1470:ARG:NH2	1.63	1.12
10:A:2416:TOR:OAA	10:A:2416:TOR:CAB	1.64	1.11
1:A:1759:ILE:HG13	1:A:1763:GLU:HB2	1.32	1.06
1:A:89:PRO:HB2	1:A:90:PRO:HD3	1.35	1.01
1:A:1466:THR:HB	1:A:1470:ARG:HH21	1.27	0.98

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	1309/2313 (57%)	1136 (87%)	165 (13%)	8 (1%)	22	57
2	B	158/598 (26%)	144 (91%)	14 (9%)	0	100	100
3	D	947/1103 (86%)	864 (91%)	83 (9%)	0	100	100
All	All	2414/4014 (60%)	2144 (89%)	262 (11%)	8 (0%)	38	70

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1504	CYS
1	A	1761	TYR
1	A	1682	THR
1	A	690	GLY
1	A	674	SER

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	1160/2023 (57%)	1147 (99%)	13 (1%)	70	87
2	B	136/510 (27%)	136 (100%)	0	100	100
3	D	846/971 (87%)	845 (100%)	1 (0%)	92	98
All	All	2142/3504 (61%)	2128 (99%)	14 (1%)	80	91

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	695	LEU
1	A	696	ASN
3	D	1029	ARG
1	A	1467	PHE
1	A	1760	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	108	GLN
3	D	246	GLN
3	D	980	GLN
3	D	676	ASN
3	D	870	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

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	$\# Z > 2$
4	NAG	C	1	4,3	14,14,15	0.84	1 (7%)	17,19,21	0.62	0
4	NAG	C	2	4	14,14,15	0.28	0	17,19,21	0.65	0
4	BMA	C	3	4	11,11,12	0.70	0	15,15,17	0.94	1 (6%)
4	NAG	E	1	4,3	14,14,15	0.71	1 (7%)	17,19,21	0.68	0
4	NAG	E	2	4	14,14,15	0.37	0	17,19,21	0.37	0
4	BMA	E	3	4	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
5	NAG	F	1	5,3	14,14,15	0.83	1 (7%)	17,19,21	1.18	1 (5%)
5	NAG	F	2	5	14,14,15	0.17	0	17,19,21	0.53	0
5	BMA	F	3	5	11,11,12	0.61	0	15,15,17	0.81	1 (6%)

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
4	NAG	C	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,3	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	-2.99	1.38	1.43
5	F	1	NAG	O5-C1	2.95	1.48	1.43
4	E	1	NAG	O5-C1	-2.27	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	4.61	118.44	112.19
4	E	3	BMA	C1-O5-C5	2.35	115.37	112.19
5	F	3	BMA	O2-C2-C3	-2.23	105.67	110.14
4	C	3	BMA	O2-C2-C3	-2.09	105.96	110.14
4	E	3	BMA	O2-C2-C3	-2.02	106.10	110.14

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

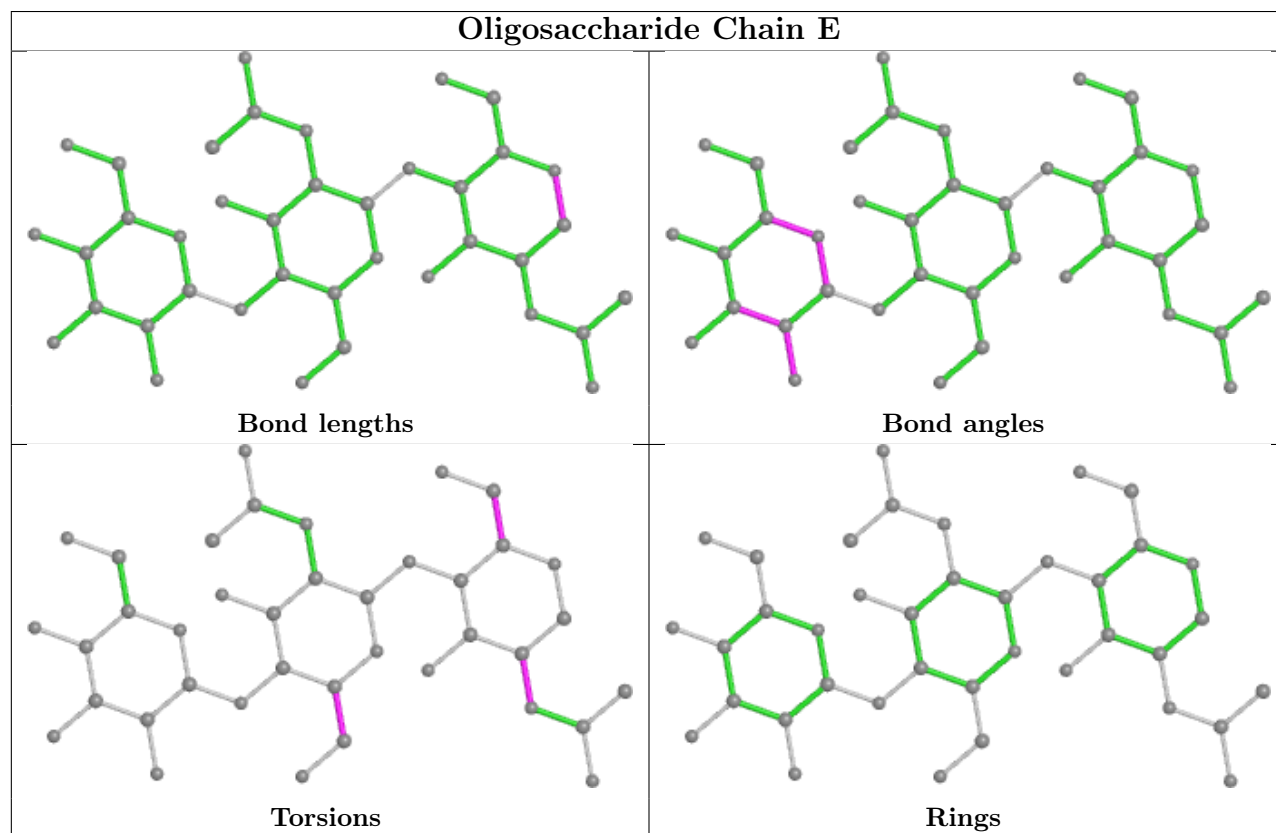
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6

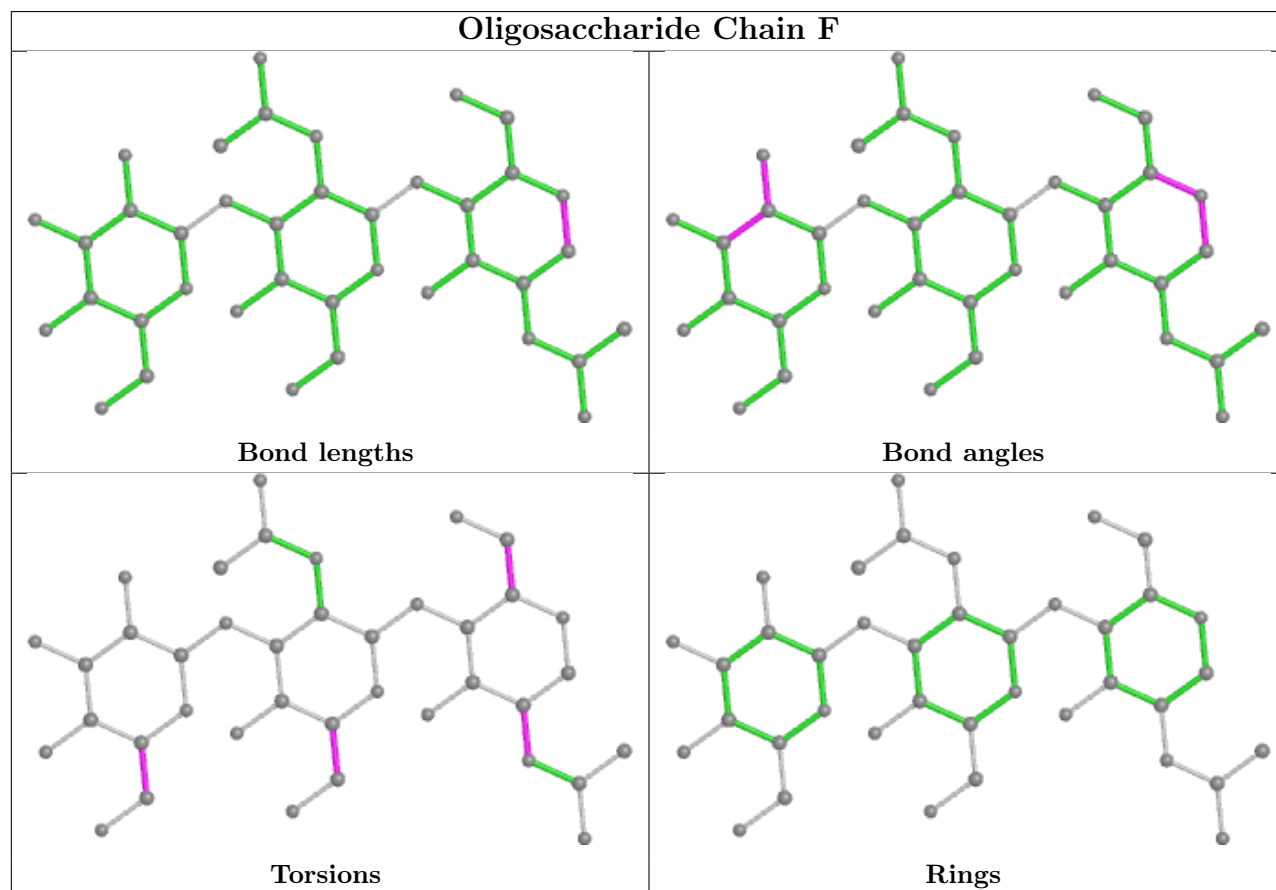
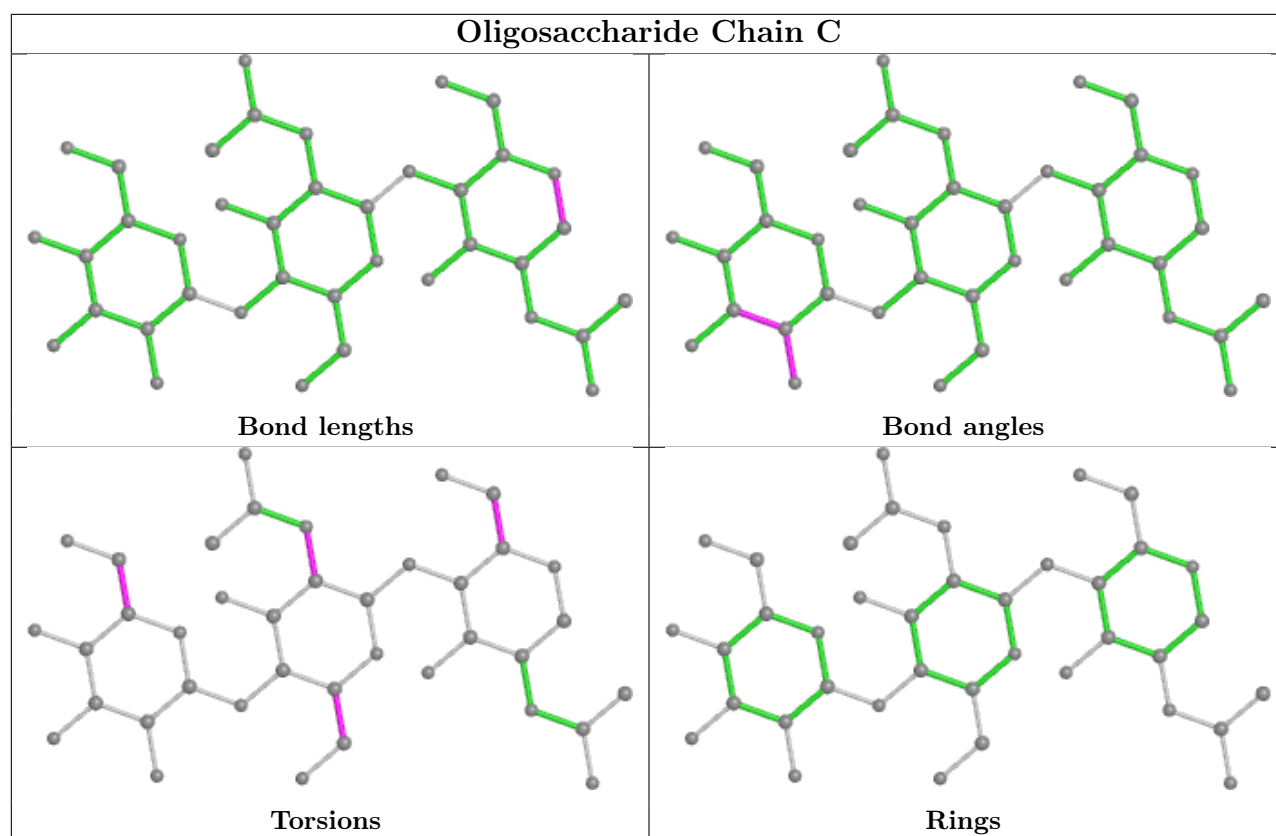
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	2	0
4	C	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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	$\# Z > 2$
8	3PE	A	2404	-	39,39,50	0.30	0	42,44,55	0.37	0
11	NAG	D	1204	3	14,14,15	0.23	0	17,19,21	0.67	0
11	NAG	D	1203	3	14,14,15	0.45	0	17,19,21	0.47	0
11	NAG	D	1206	3	14,14,15	0.22	0	17,19,21	0.53	0
6	Y01	A	2401	-	38,38,38	0.43	0	57,57,57	0.47	0
6	Y01	A	2408	-	38,38,38	0.44	0	57,57,57	0.77	1 (1%)
11	NAG	D	1207	3	14,14,15	0.24	0	17,19,21	0.50	0
6	Y01	A	2414	-	38,38,38	0.45	0	57,57,57	0.74	0
6	Y01	A	2406	-	38,38,38	0.52	0	57,57,57	0.94	3 (5%)
7	R16	A	2407	-	15,15,15	0.20	0	14,14,14	0.17	0
7	R16	A	2409	-	12,12,15	0.17	0	11,11,14	0.13	0
6	Y01	A	2412	-	38,38,38	0.46	0	57,57,57	0.97	3 (5%)
11	NAG	D	1209	3	14,14,15	0.19	0	17,19,21	0.57	0
7	R16	A	2402	-	9,9,15	0.16	0	8,8,14	0.15	0
6	Y01	A	2411	-	38,38,38	0.43	0	57,57,57	0.80	3 (5%)
11	NAG	D	1202	3	14,14,15	0.17	0	17,19,21	0.47	0
11	NAG	D	1205	3	14,14,15	0.46	0	17,19,21	0.46	0
7	R16	A	2418	-	8,8,15	0.12	0	7,7,14	0.07	0
7	R16	A	2403	-	15,15,15	0.16	0	14,14,14	0.23	0
8	3PE	A	2405	-	39,39,50	0.30	0	42,44,55	0.37	0
7	R16	A	2419	-	15,15,15	0.09	0	14,14,14	0.20	0
11	NAG	D	1208	3	14,14,15	0.32	0	17,19,21	0.60	0
10	TOR	A	2416	-	24,24,24	12.63	19 (79%)	37,41,41	2.64	10 (27%)
6	Y01	A	2413	-	38,38,38	0.53	0	57,57,57	0.80	1 (1%)
6	Y01	A	2410	-	38,38,38	0.53	0	57,57,57	1.08	3 (5%)
6	Y01	A	2417	-	38,38,38	0.45	0	57,57,57	1.06	5 (8%)

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
8	3PE	A	2404	-	-	8/43/43/54	-
11	NAG	D	1204	3	-	2/6/23/26	0/1/1/1
11	NAG	D	1203	3	-	4/6/23/26	0/1/1/1
11	NAG	D	1206	3	-	0/6/23/26	0/1/1/1
6	Y01	A	2401	-	-	10/19/77/77	0/4/4/4
6	Y01	A	2408	-	-	9/19/77/77	0/4/4/4
11	NAG	D	1207	3	-	2/6/23/26	0/1/1/1
6	Y01	A	2414	-	-	15/19/77/77	0/4/4/4
6	Y01	A	2406	-	-	13/19/77/77	0/4/4/4
7	R16	A	2407	-	-	1/13/13/13	-
7	R16	A	2409	-	-	1/10/10/13	-
6	Y01	A	2412	-	-	8/19/77/77	0/4/4/4
11	NAG	D	1209	3	-	0/6/23/26	0/1/1/1
7	R16	A	2402	-	-	0/7/7/13	-
6	Y01	A	2411	-	-	9/19/77/77	0/4/4/4
11	NAG	D	1202	3	-	0/6/23/26	0/1/1/1
11	NAG	D	1205	3	-	4/6/23/26	0/1/1/1
7	R16	A	2418	-	-	0/6/6/13	-
7	R16	A	2403	-	-	3/13/13/13	-
8	3PE	A	2405	-	-	3/43/43/54	-
7	R16	A	2419	-	-	1/13/13/13	-
11	NAG	D	1208	3	-	3/6/23/26	0/1/1/1
10	TOR	A	2416	-	-	7/7/48/48	0/3/3/3
6	Y01	A	2413	-	-	13/19/77/77	0/4/4/4
6	Y01	A	2410	-	-	10/19/77/77	0/4/4/4
6	Y01	A	2417	-	-	12/19/77/77	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2416	TOR	OAI-SAO	28.50	1.65	1.42
10	A	2416	TOR	OAS-SAO	28.36	1.65	1.42
10	A	2416	TOR	CAL-CAK	-26.70	1.11	1.54
10	A	2416	TOR	OAQ-CAU	-17.01	1.10	1.43
10	A	2416	TOR	OAR-CAL	-14.39	1.16	1.42

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2416	TOR	OAI-SAO-OAS	-10.24	110.28	119.97
10	A	2416	TOR	OAA-CAB-CAC	-5.45	100.26	110.45
10	A	2416	TOR	CAM-CAL-CAK	-5.43	103.84	115.42
10	A	2416	TOR	OAH-CAL-OAR	3.80	117.79	109.54
10	A	2416	TOR	CAU-OAQ-CAK	-3.77	101.46	108.73

There are no chirality outliers.

5 of 138 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2401	Y01	OAG-CAY-OAW-CBC
6	A	2401	Y01	CAM-CAY-OAW-CBC
6	A	2406	Y01	CAR-CBC-OAW-CAY
6	A	2406	Y01	CAM-CAY-OAW-CBC
6	A	2410	Y01	CAO-CBB-CBE-CBI

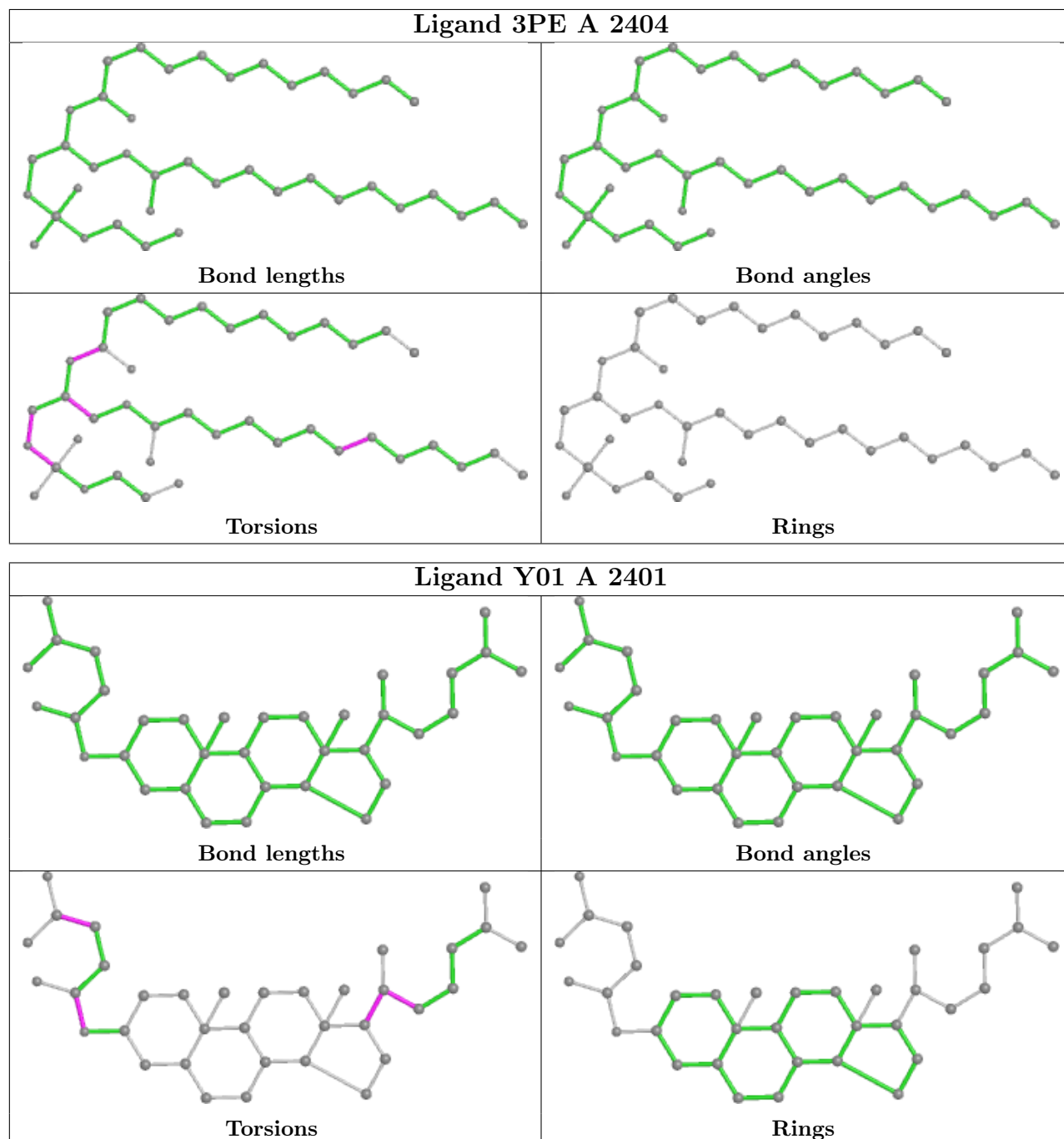
There are no ring outliers.

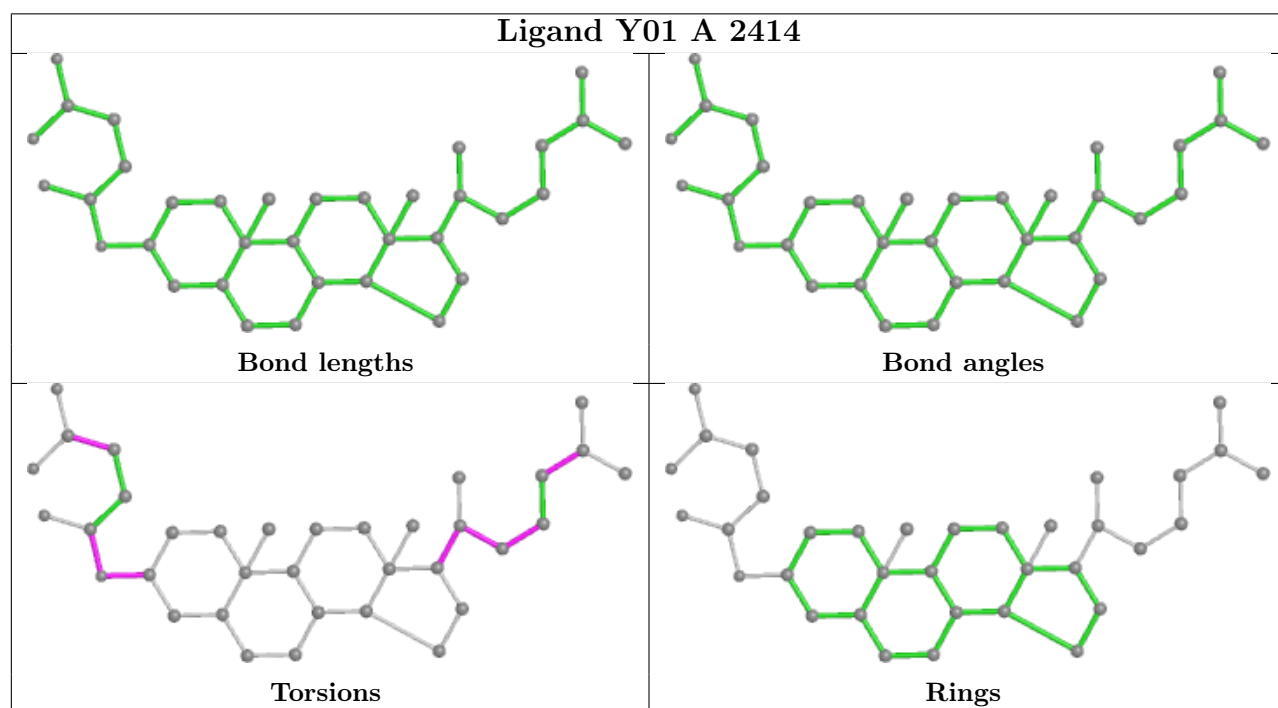
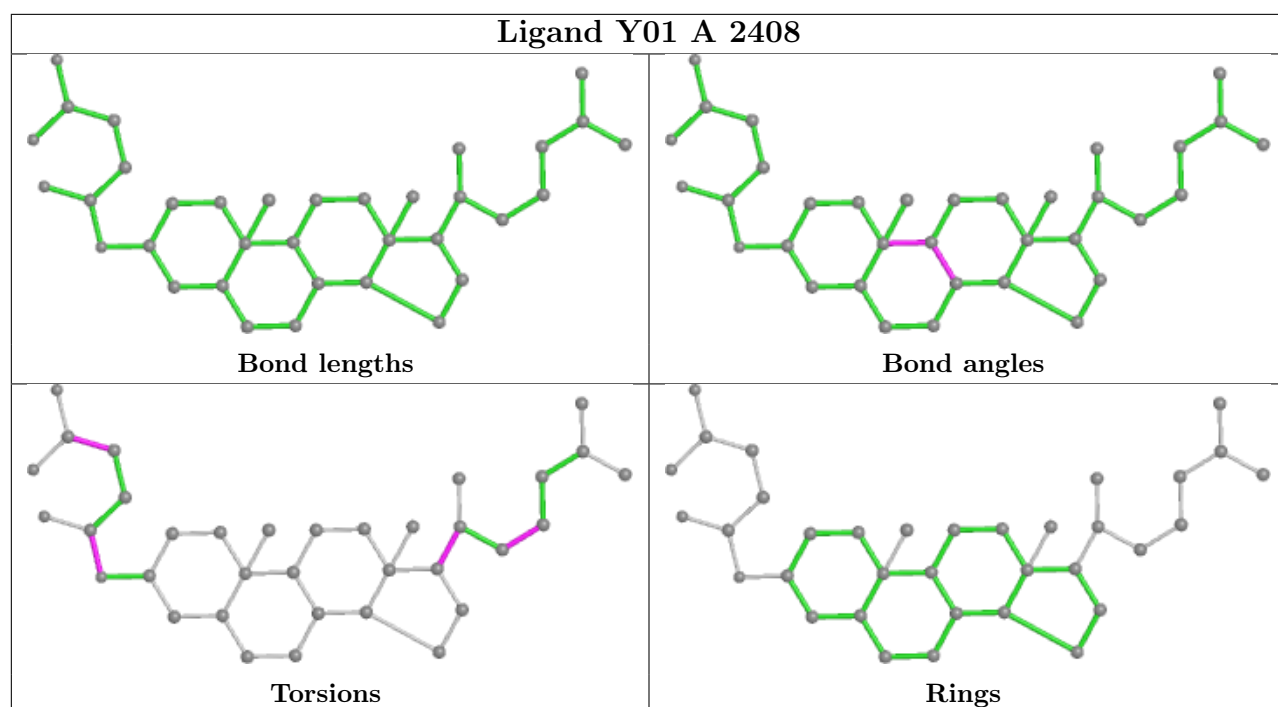
15 monomers are involved in 44 short contacts:

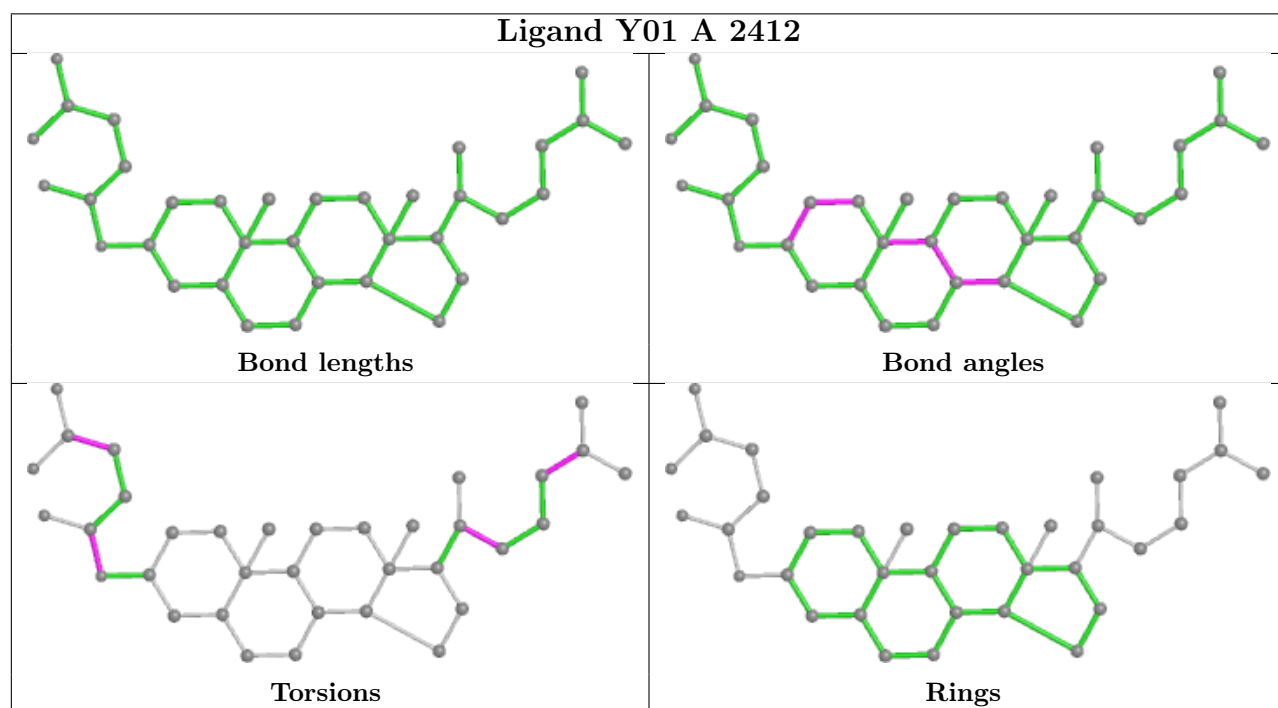
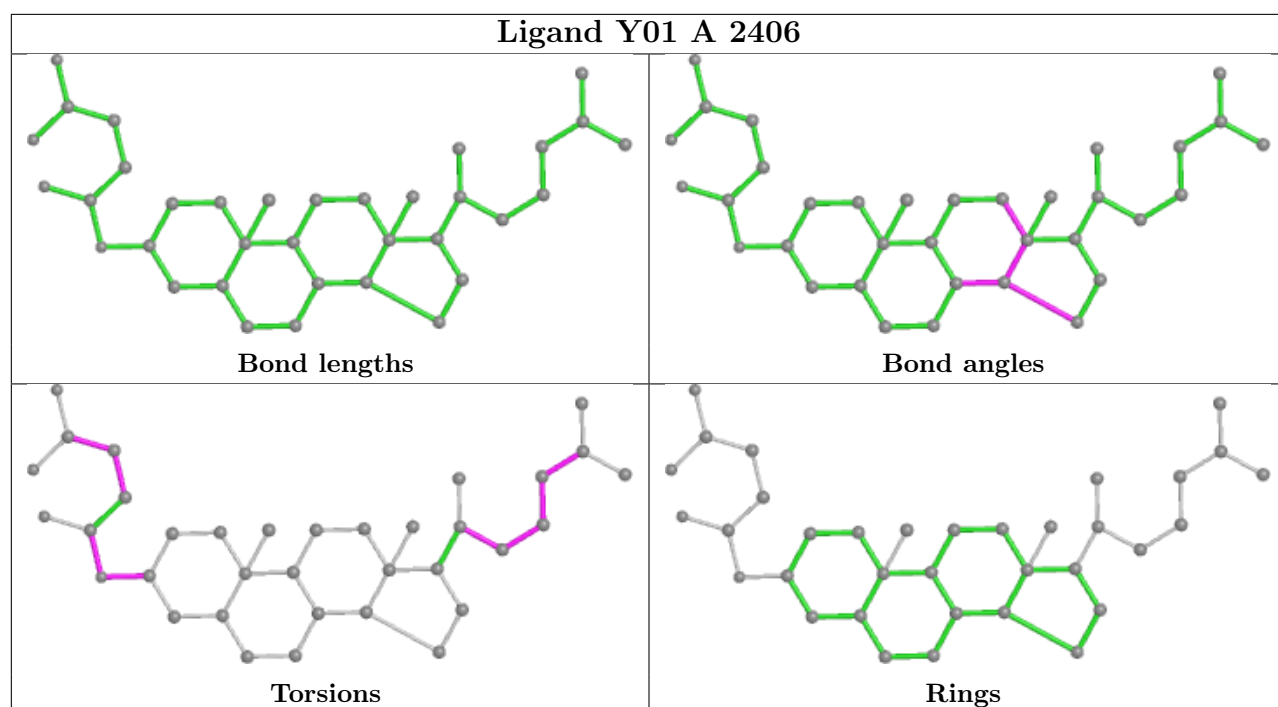
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1203	NAG	1	0
6	A	2401	Y01	6	0
6	A	2408	Y01	2	0
6	A	2414	Y01	1	0
6	A	2406	Y01	7	0
7	A	2407	R16	1	0
7	A	2409	R16	1	0
6	A	2412	Y01	6	0
6	A	2411	Y01	2	0
11	D	1205	NAG	1	0
7	A	2419	R16	1	0
10	A	2416	TOR	5	0
6	A	2413	Y01	4	0
6	A	2410	Y01	6	0
6	A	2417	Y01	5	0

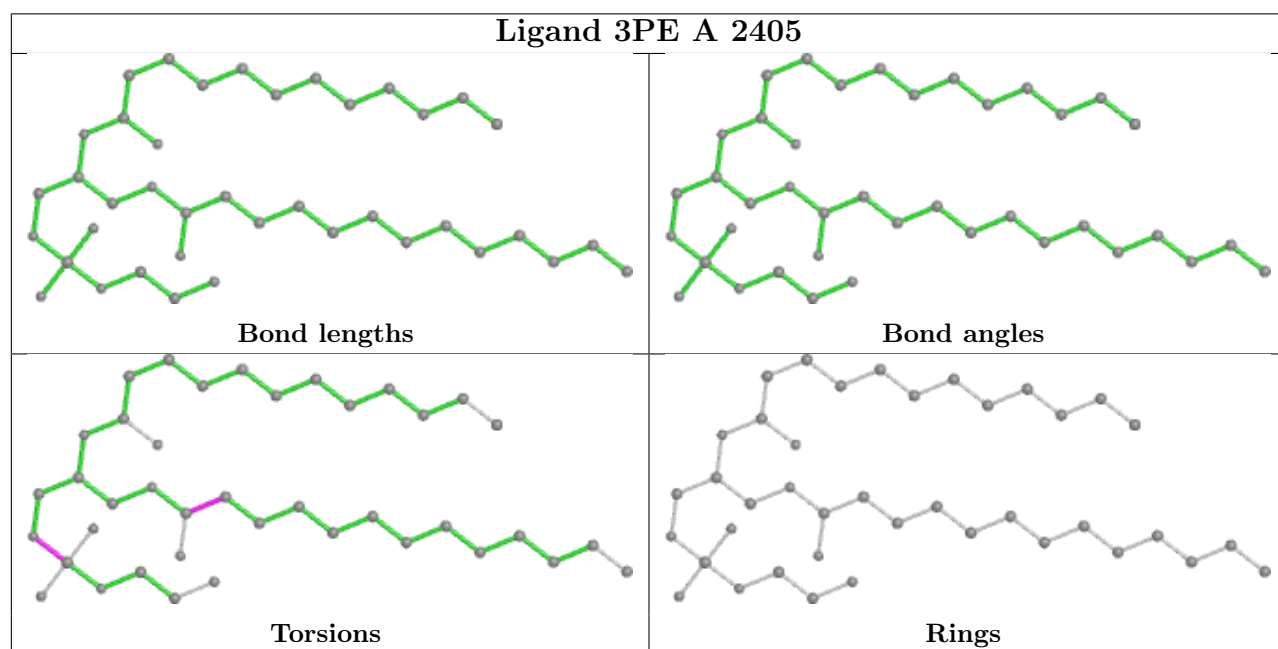
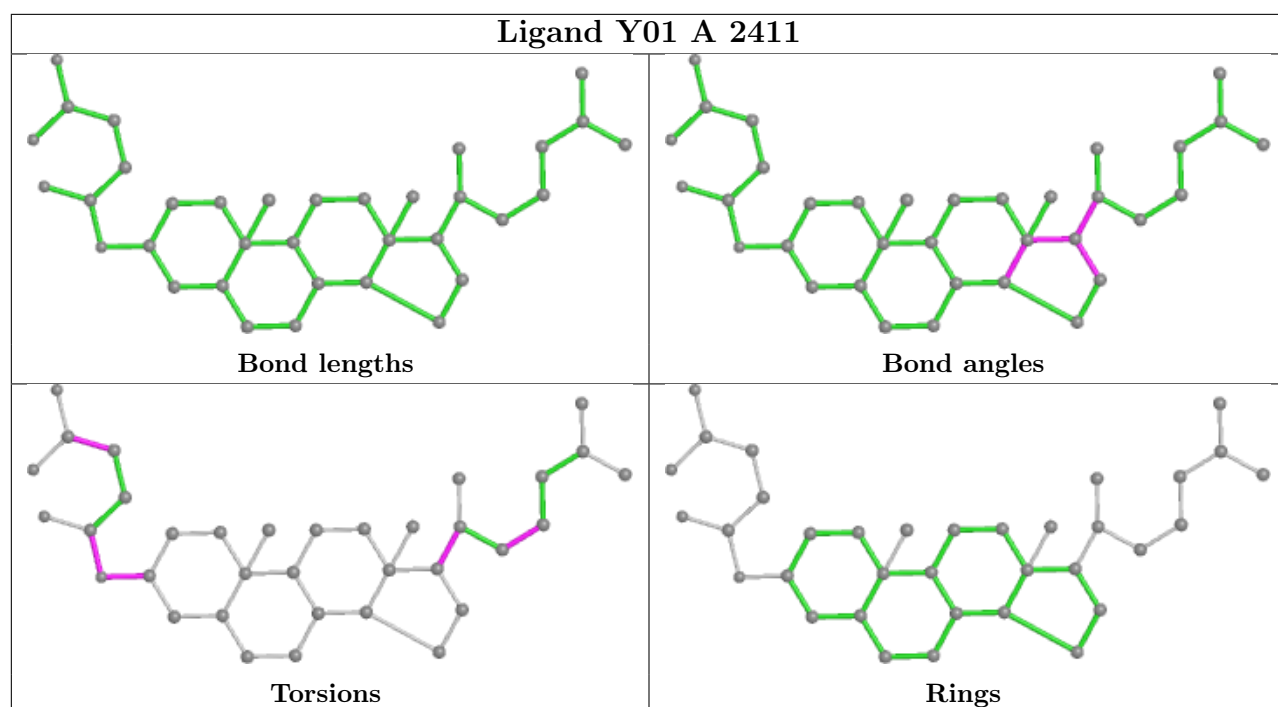
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

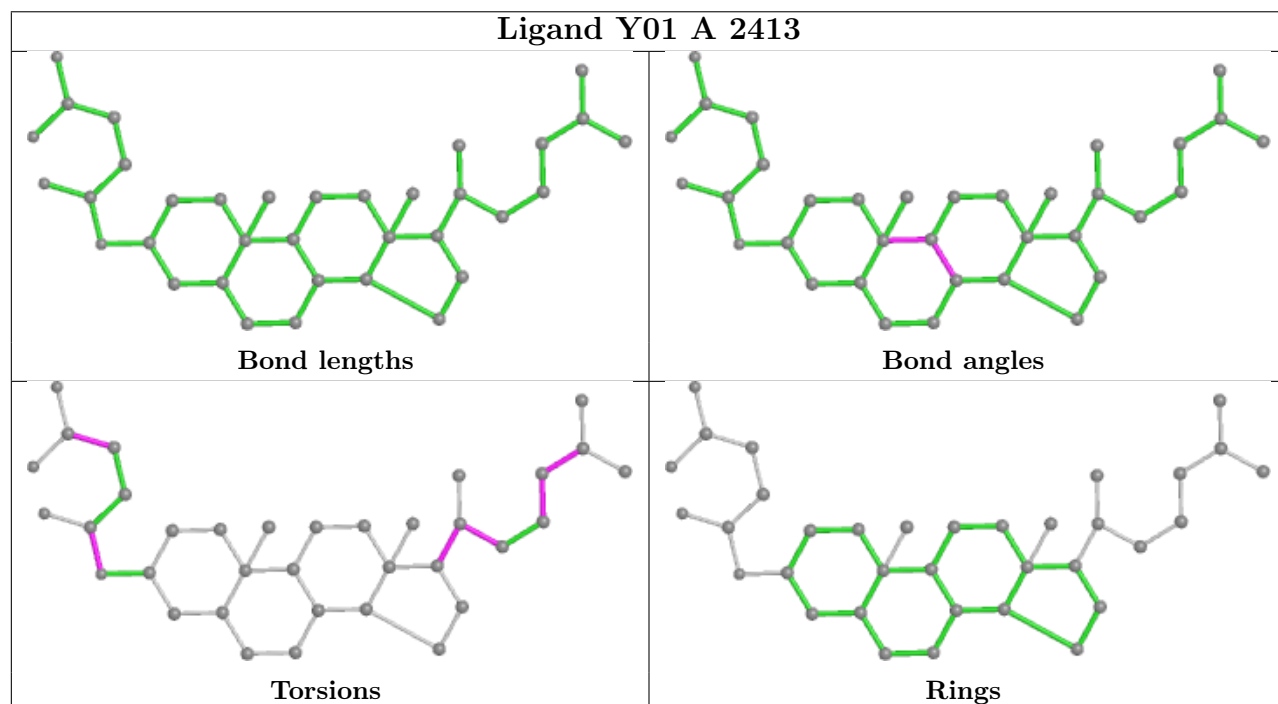
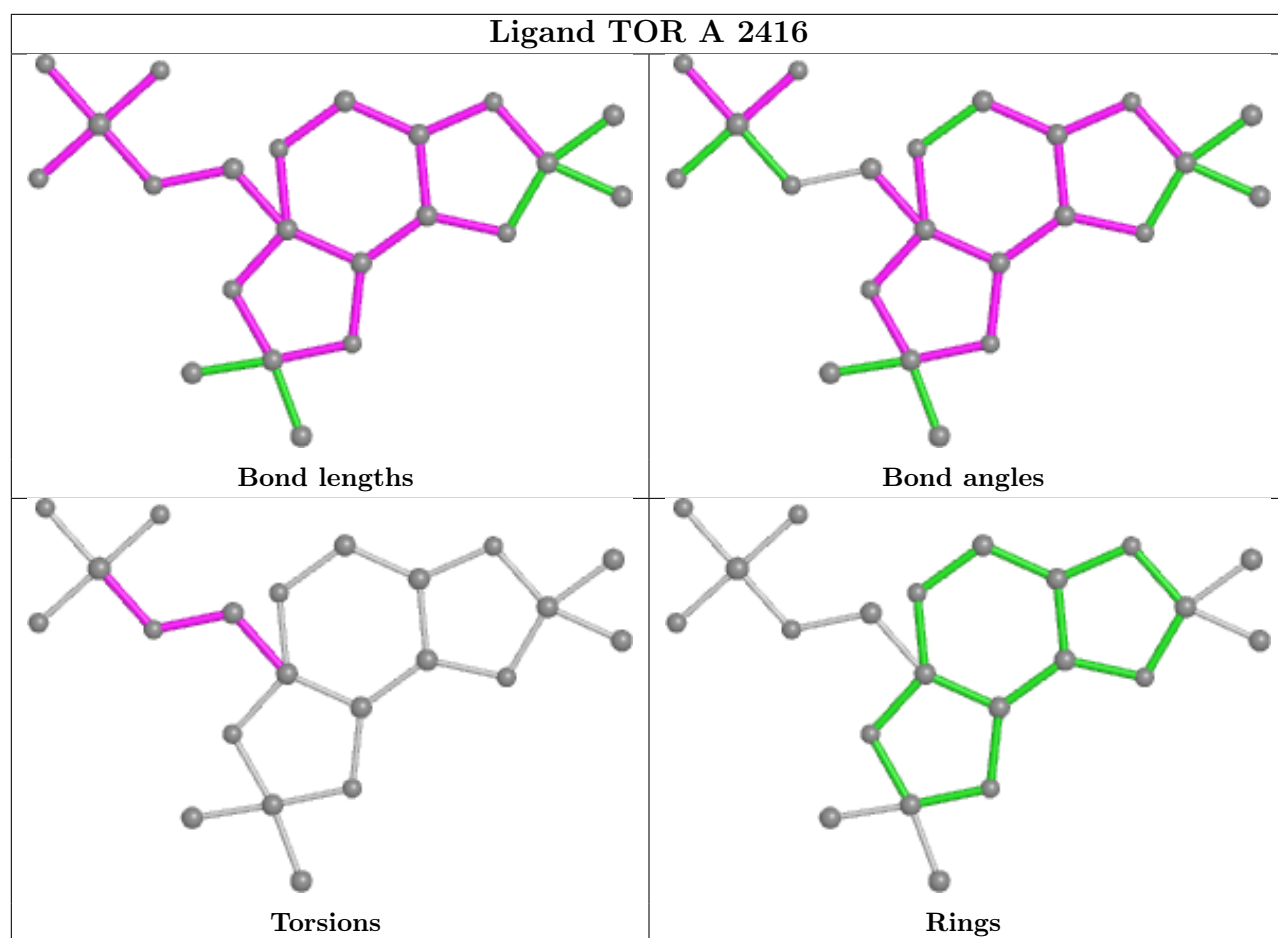
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

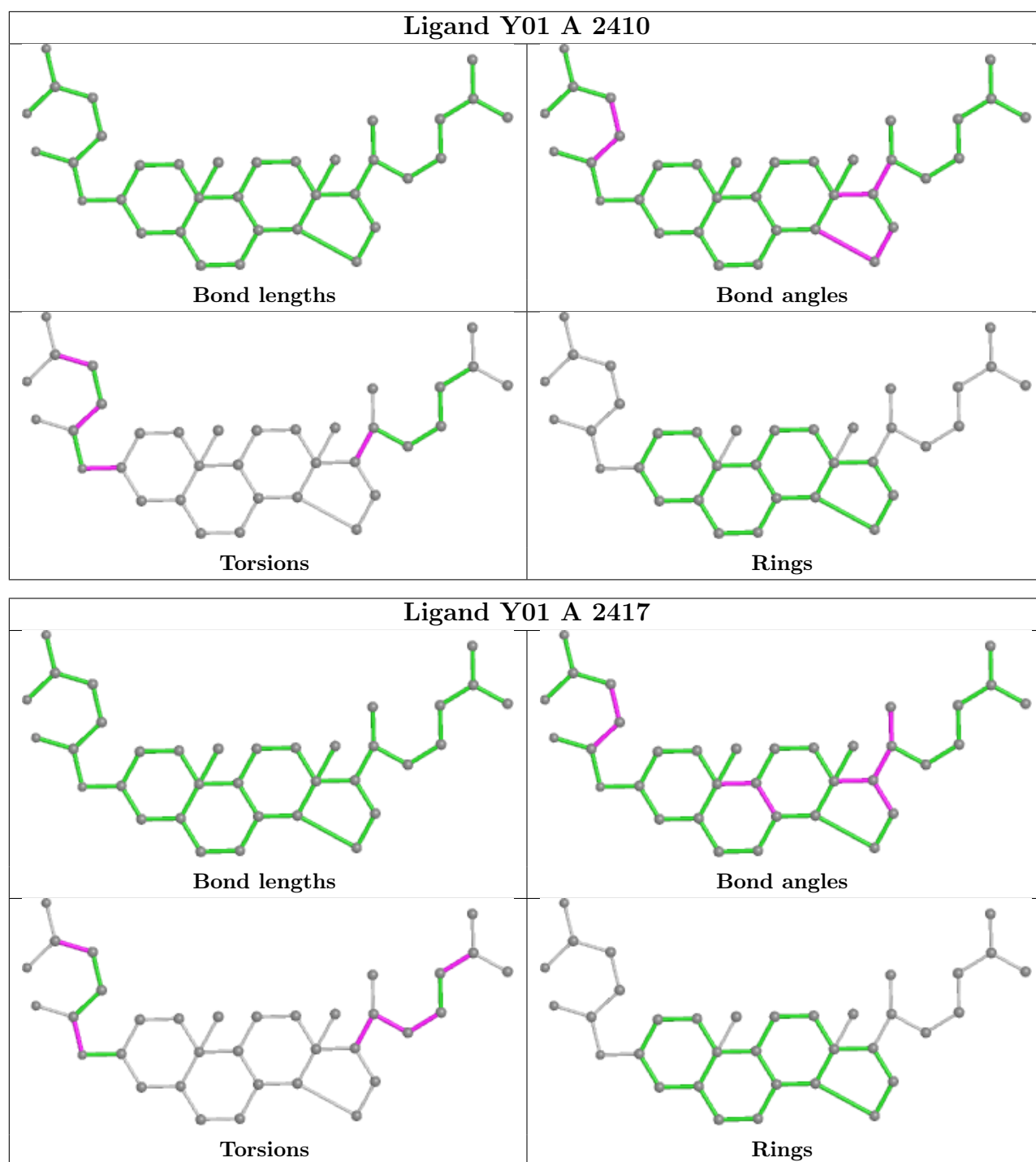












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

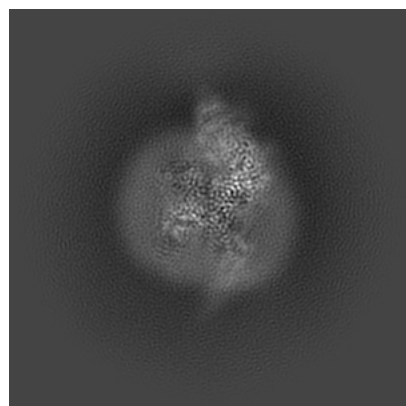
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33808. These allow visual inspection of the internal detail of the map and identification of artifacts.

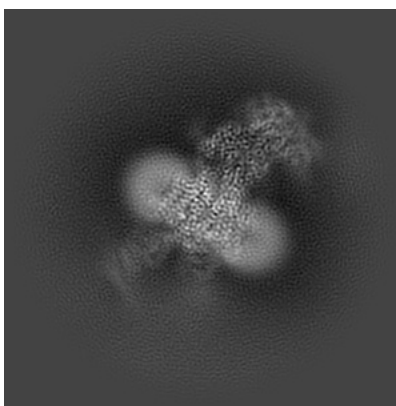
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

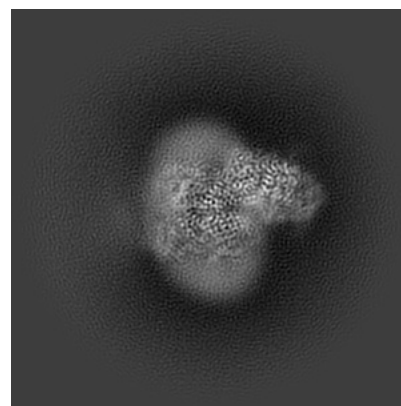
6.1.1 Primary map



X

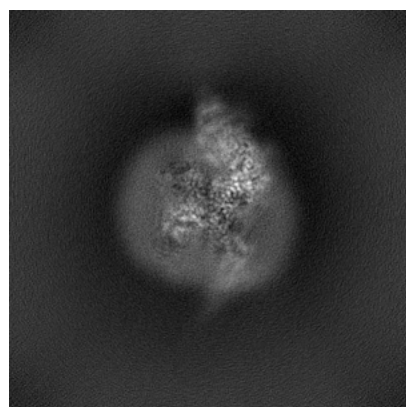


Y

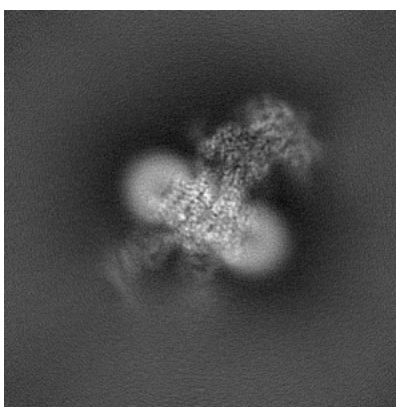


Z

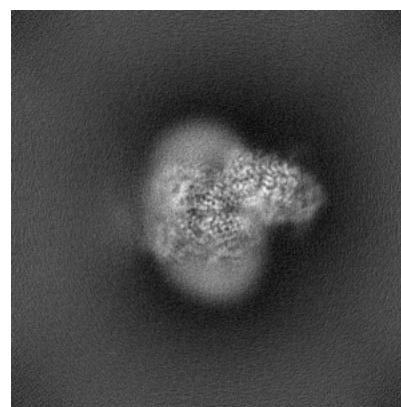
6.1.2 Raw map



X



Y

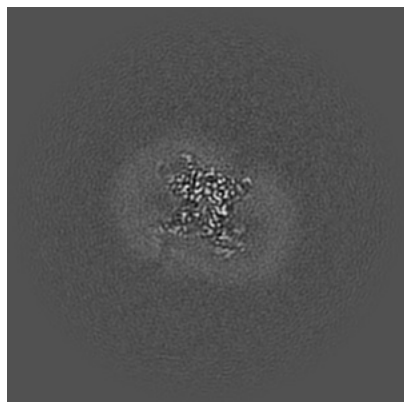


Z

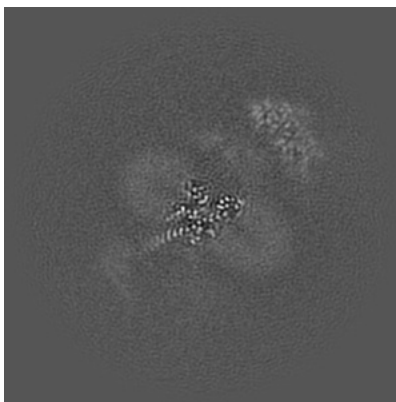
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

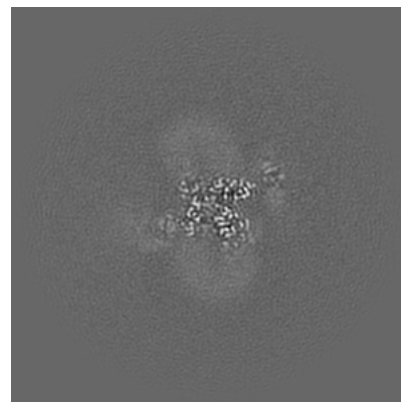
6.2.1 Primary map



X Index: 160

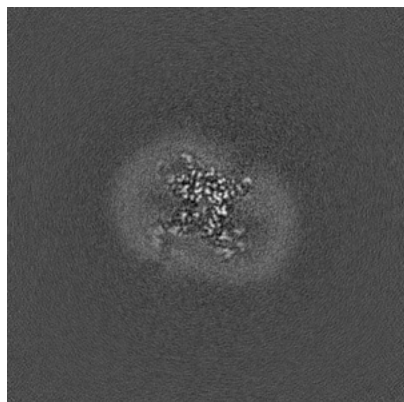


Y Index: 160

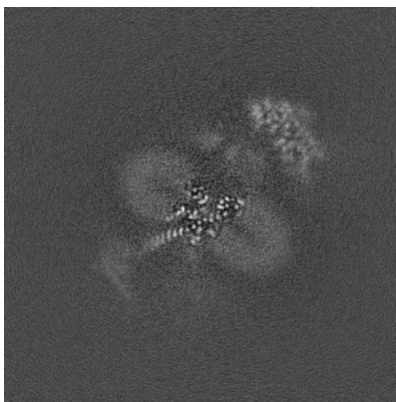


Z Index: 160

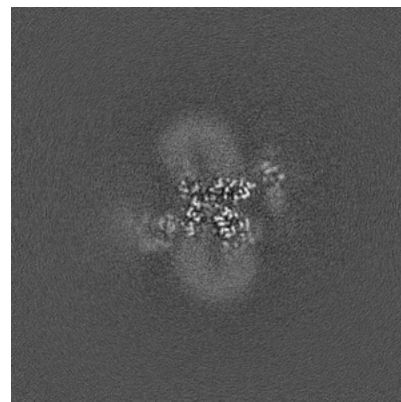
6.2.2 Raw map



X Index: 160



Y Index: 160

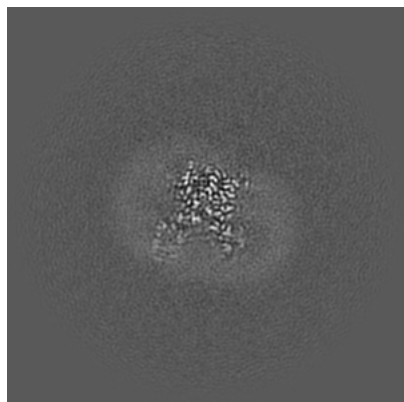


Z Index: 160

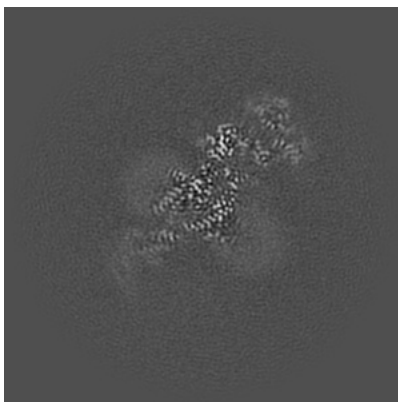
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

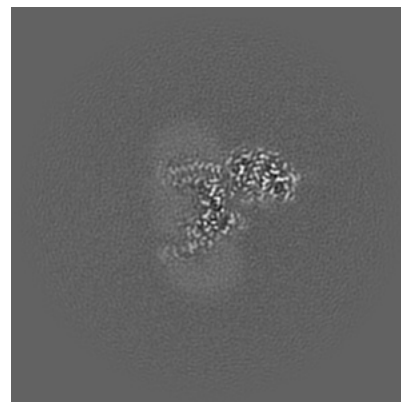
6.3.1 Primary map



X Index: 163

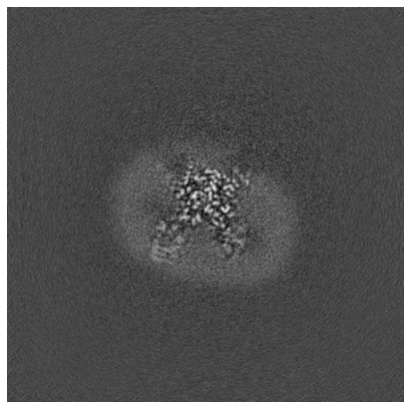


Y Index: 175

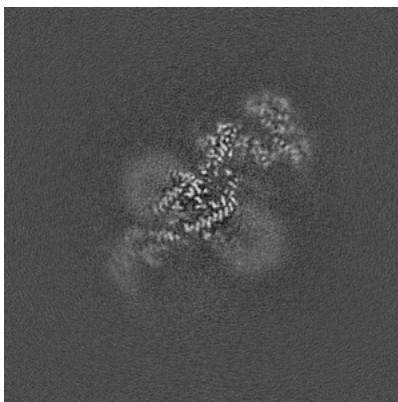


Z Index: 180

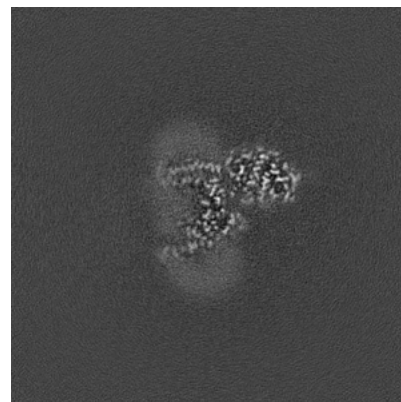
6.3.2 Raw map



X Index: 164



Y Index: 174

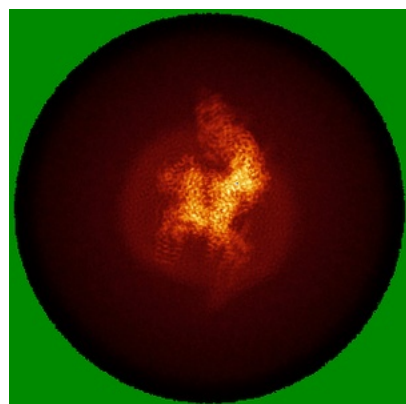


Z Index: 180

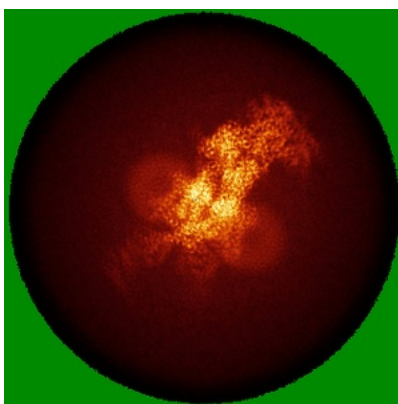
The images above show the largest variance slices of the map in three orthogonal directions.

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

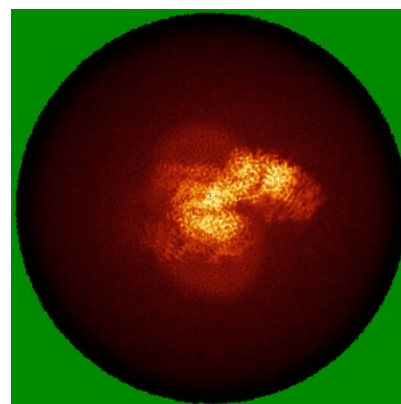
6.4.1 Primary map



X

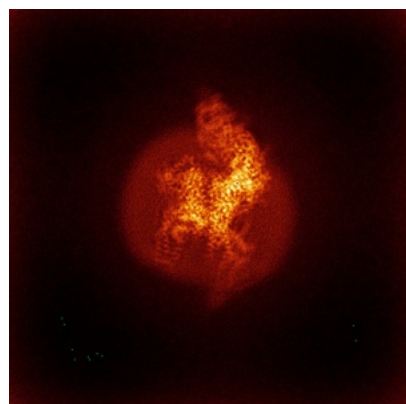


Y

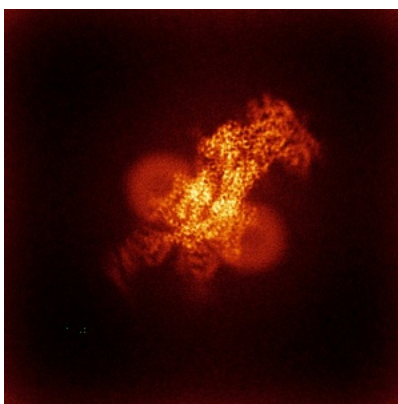


Z

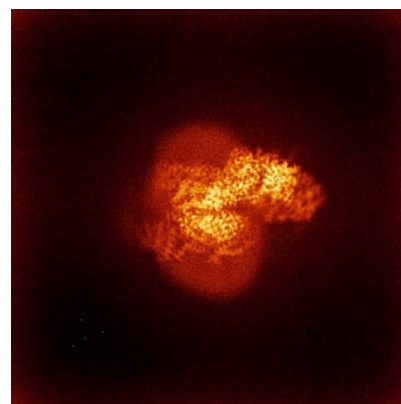
6.4.2 Raw map



X



Y

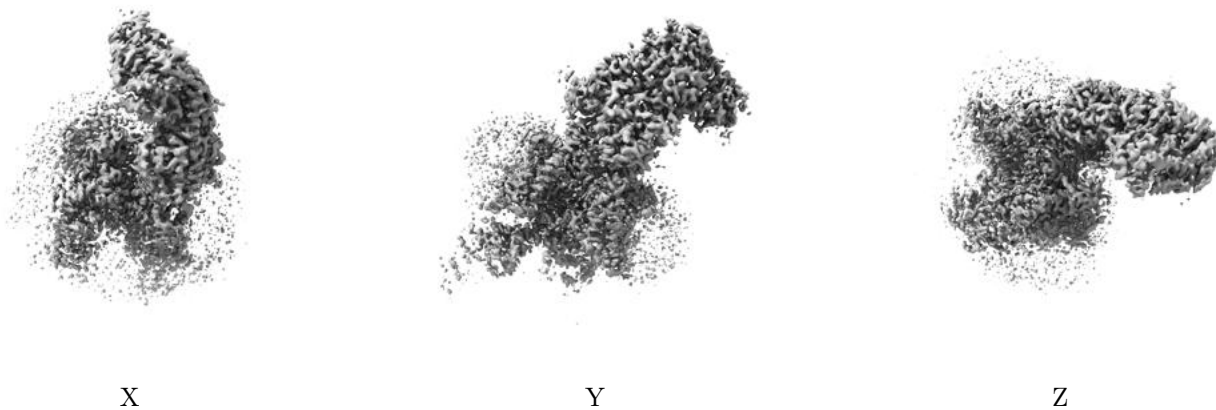


Z

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.

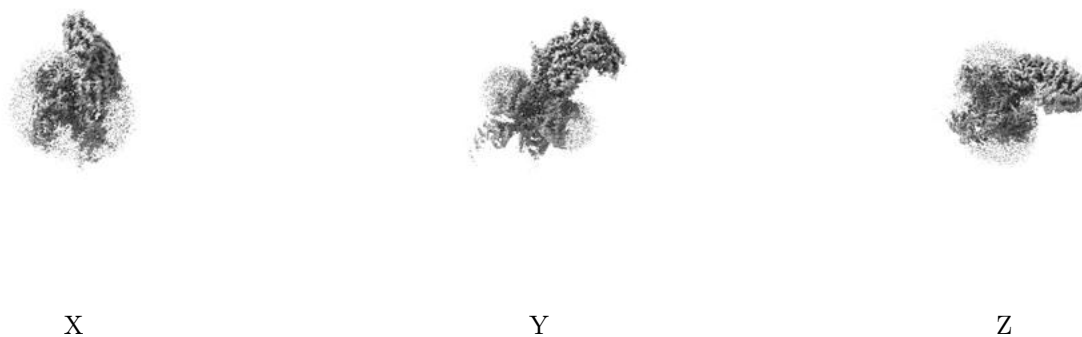
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

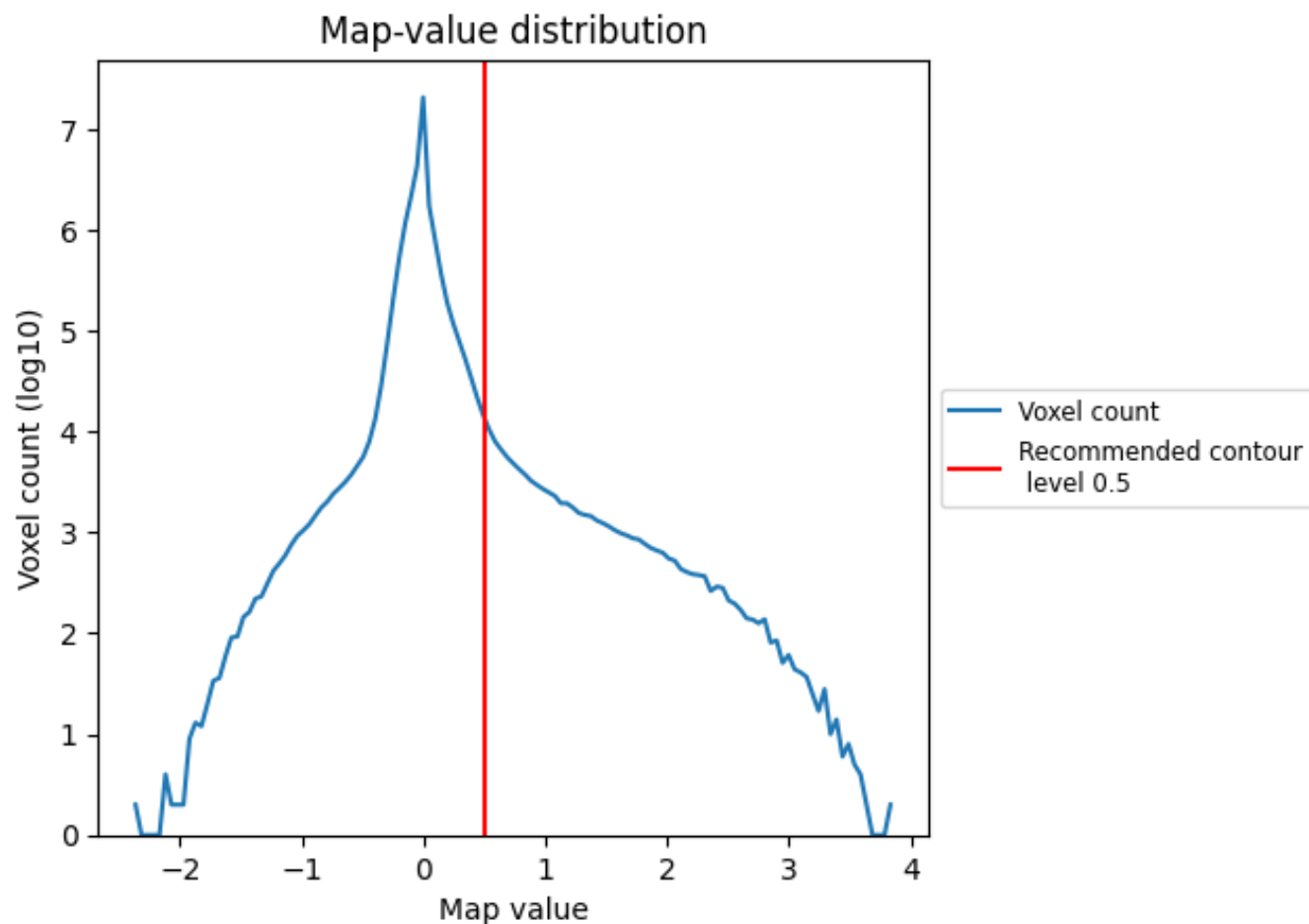
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

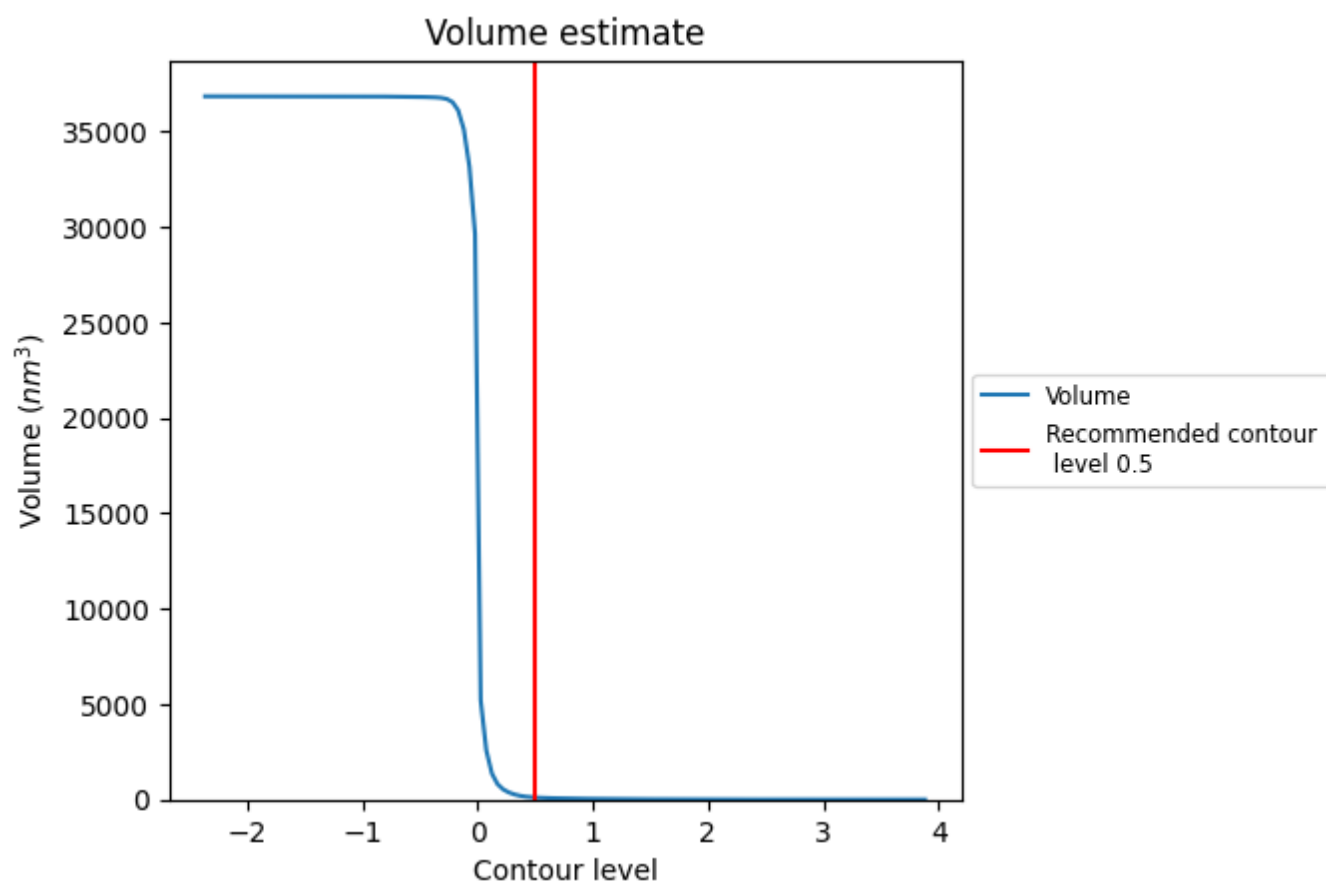
This section contains the results of statistical analysis of the map.

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.

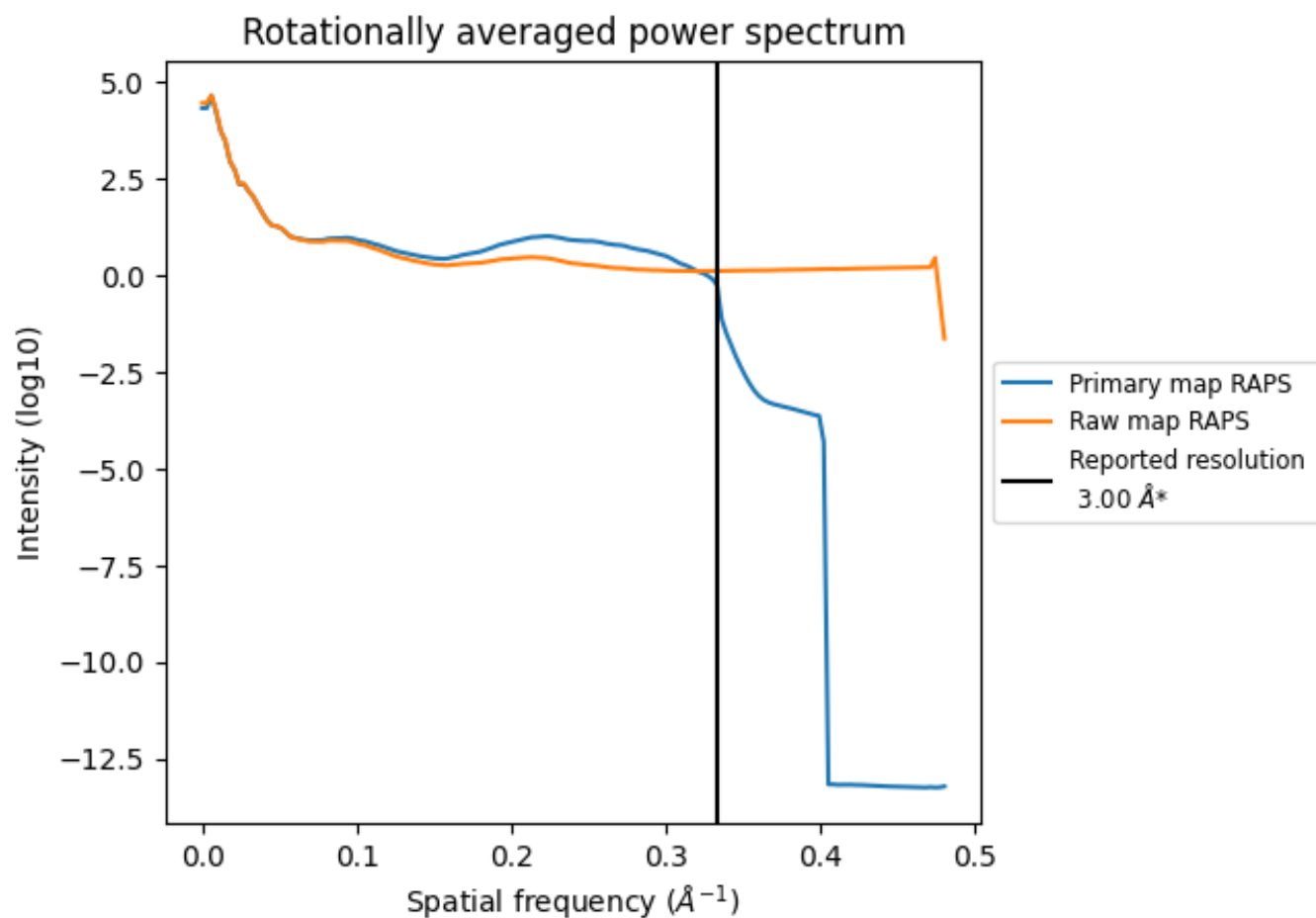
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 98 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 ⓘ

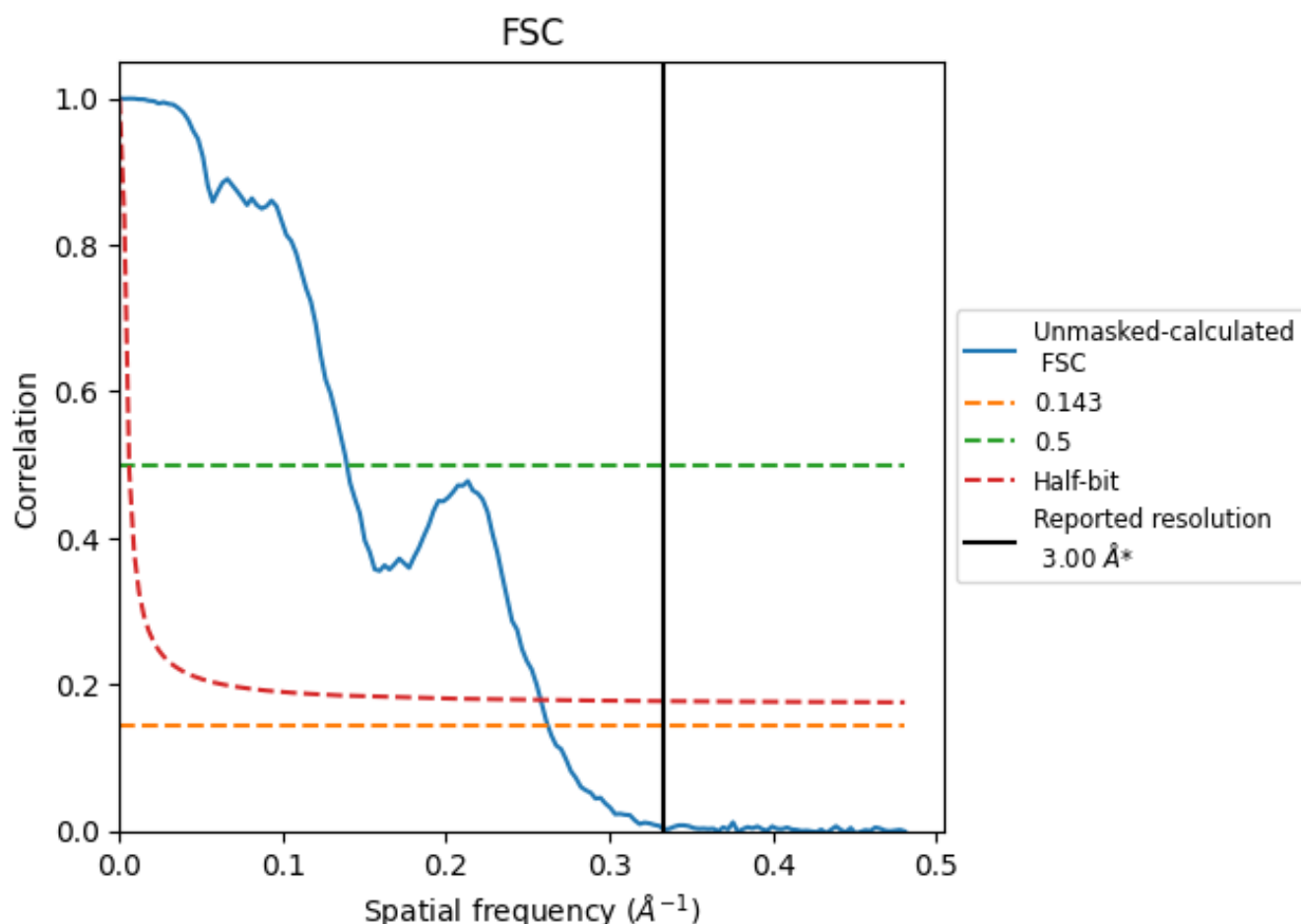


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

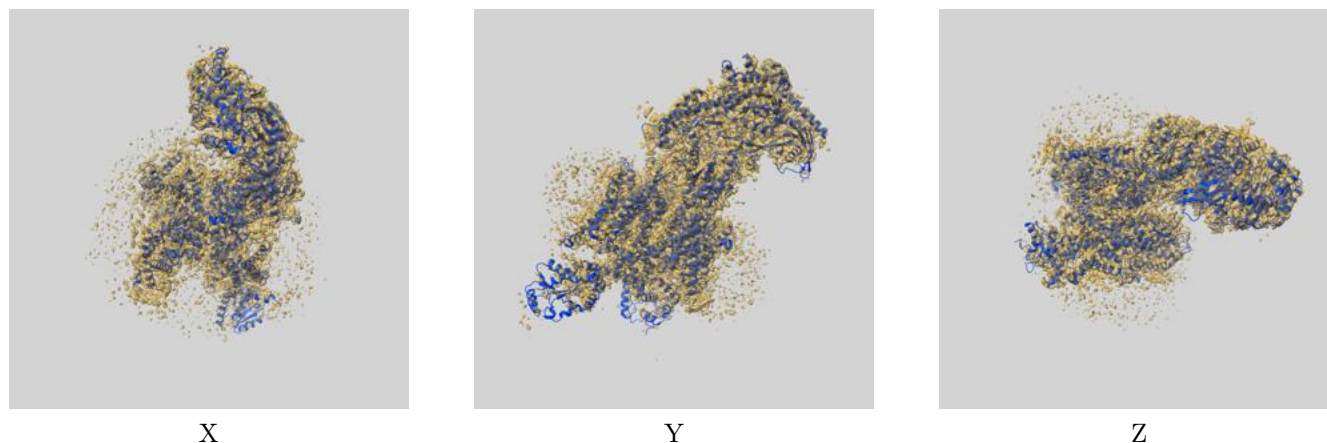
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	7.18	3.88

*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 3.81 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

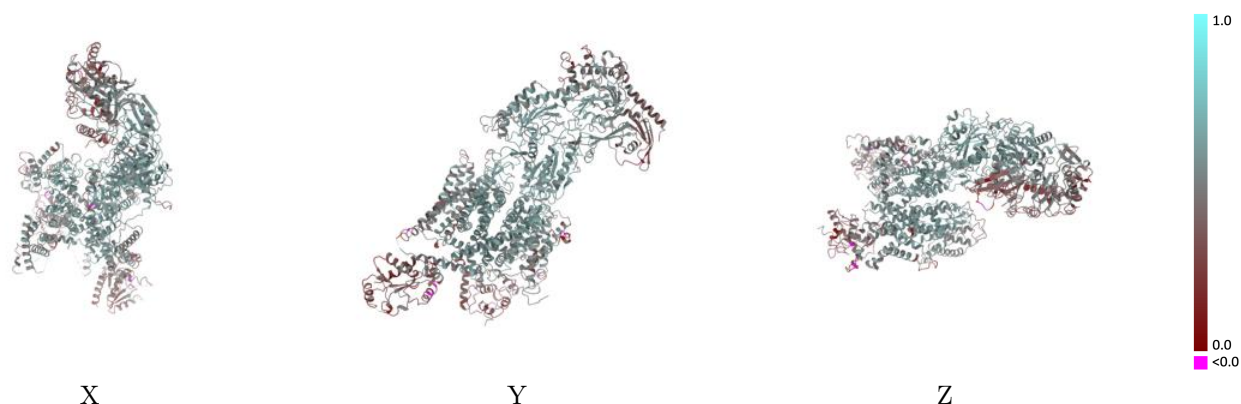
This section contains information regarding the fit between EMDB map EMD-33808 and PDB model 7YG5. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



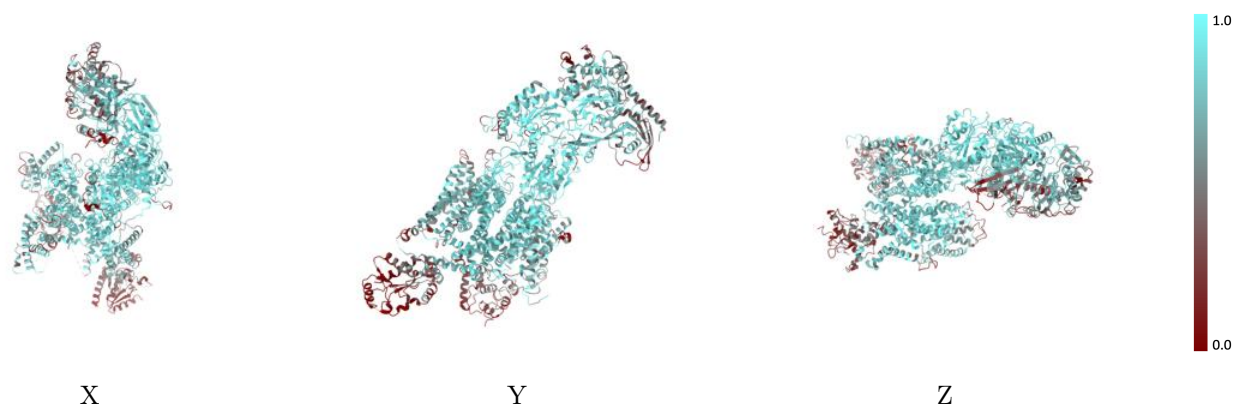
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



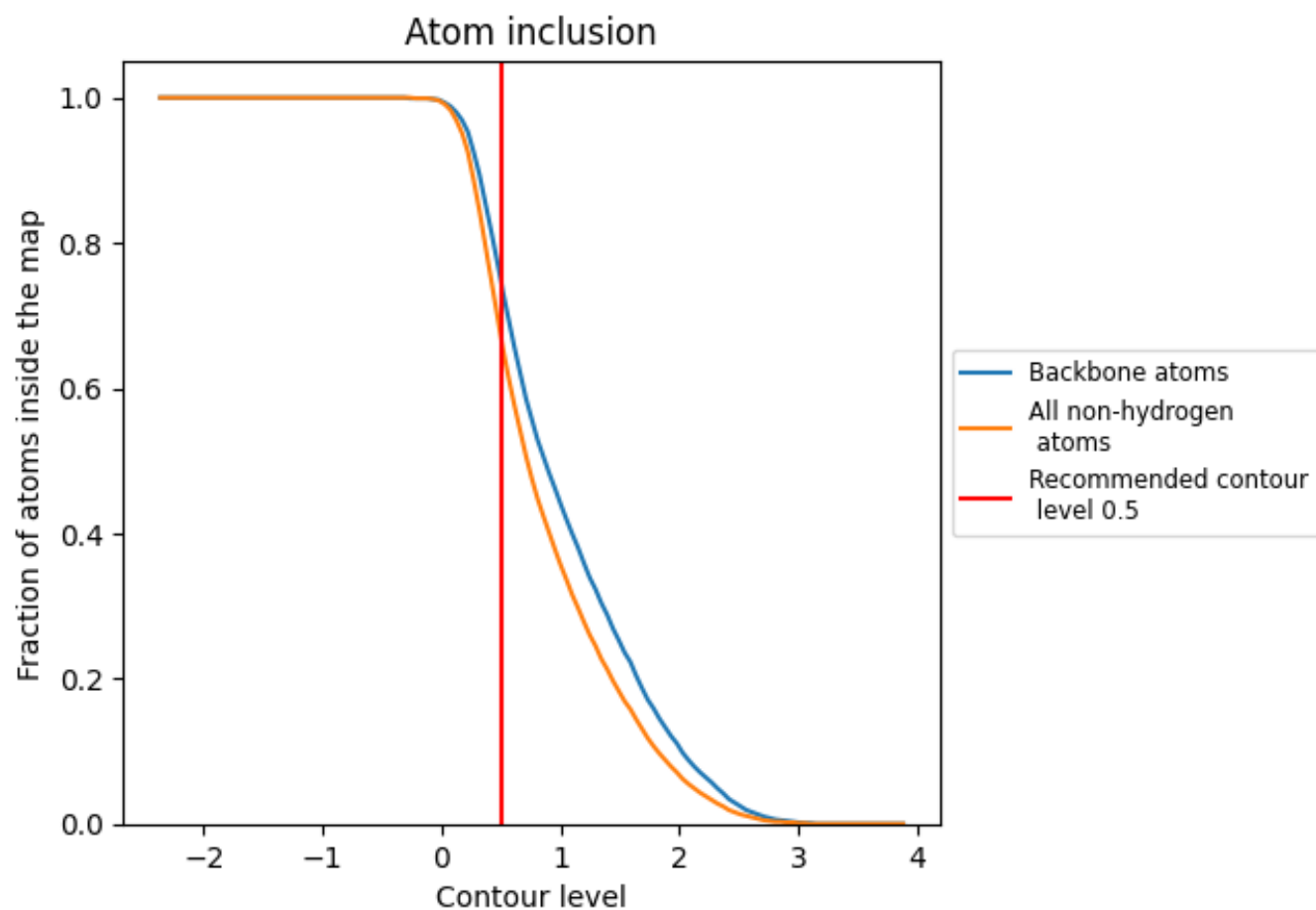
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6720	<div></div> 0.4910
A	<div></div> 0.6960	<div></div> 0.5030
B	<div></div> 0.2200	<div></div> 0.3230
C	<div></div> 0.8720	<div></div> 0.5560
D	<div></div> 0.7140	<div></div> 0.5040
E	<div></div> 0.4620	<div></div> 0.4030
F	<div></div> 0.1790	<div></div> 0.3500

1.0

0.0

<0.0