



## wwPDB EM Validation Summary Report ⓘ

Aug 6, 2025 – 11:29 AM EDT

PDB ID : 9N2D / pdb\_00009n2d  
EMDB ID : EMD-48835  
Title : Cryo-EM structure of an extended F. johnsoniae BAM complex, composite map  
Authors : Deme, J.C.; Lea, S.M.  
Deposited on : 2025-01-28  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

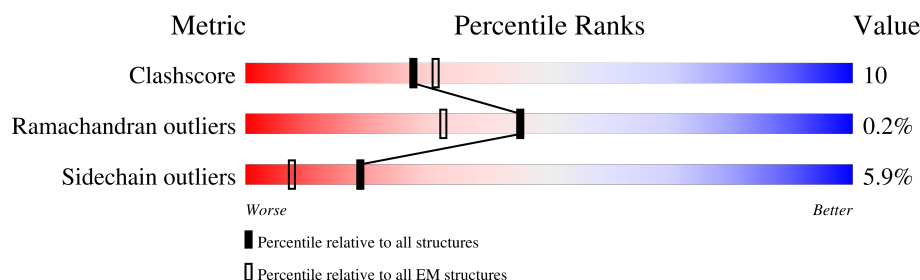
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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	F	264	<div> <div>5%</div> <div>68%</div> <div>22%</div> <div>8%</div> </div>
2	A	900	<div> <div>54%</div> <div>14%</div> <div>31%</div> </div>
3	C	517	<div> <div>73%</div> <div>23%</div> </div>
4	B	409	<div> <div>75%</div> <div>19%</div> <div>5%</div> </div>
5	D	388	<div> <div>5%</div> <div>69%</div> <div>25%</div> <div>5%</div> </div>
6	E	249	<div> <div>41%</div> <div>15%</div> <div>41%</div> </div>
7	J	3	<div> <div>67%</div> <div>33%</div> </div>
8	G	2	<div> <div>50%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GCU	J	2	X	-	-	-
7	MAN	J	3	X	-	-	-
8	GCU	G	2	X	-	-	-

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 18488 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 Bam D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	244	Total	C	N	O	S	0	0
			1979	1276	317	381	5		

- Molecule 2 is a protein called Bam A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	618	Total	C	N	O	S	1	0
			4936	3161	816	954	5		

- Molecule 3 is a protein called Bam H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	517	Total	C	N	O	S	0	0
			4024	2537	660	820	7		

- Molecule 4 is a protein called Bam G.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	390	Total	C	N	O	S	0	0
			2995	1916	488	586	5		

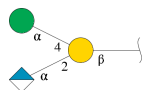
- Molecule 5 is a protein called Bam M.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	369	Total	C	N	O	S	0	0
			2947	1871	462	607	7		

- Molecule 6 is a protein called Bam P.

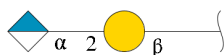
Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	146	Total	C	N	O	S	0	0
			1155	735	194	222	4		

- Molecule 7 is an oligosaccharide called alpha-D-glucopyranuronic acid-(1-2)-[alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose.



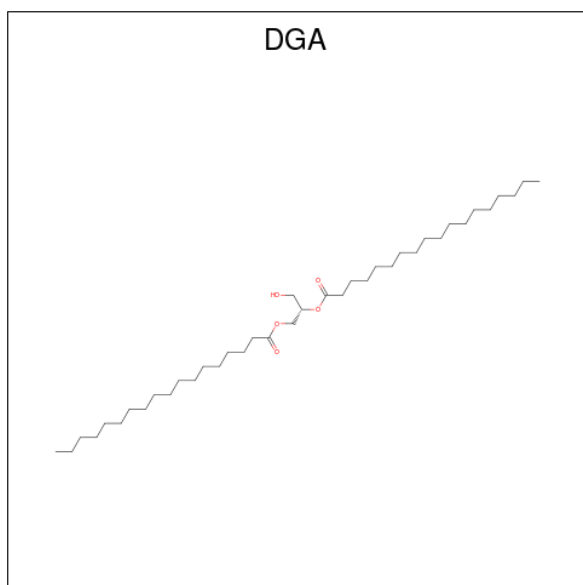
Mol	Chain	Residues	Atoms			AltConf	Trace
7	J	3	Total	C	O	0	0
			34	18	16		

- Molecule 8 is an oligosaccharide called alpha-D-glucopyranuronic acid-(1-2)-beta-D-galactopyranose.



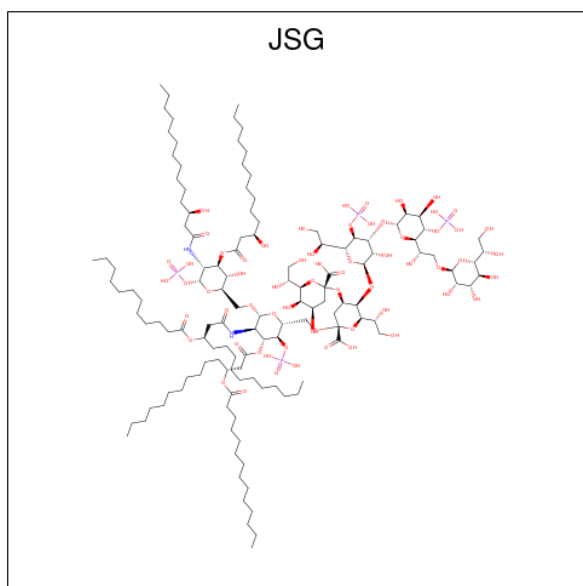
Mol	Chain	Residues	Atoms			AltConf	Trace
8	G	2	Total	C	O	0	0
			23	12	11		

- Molecule 9 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



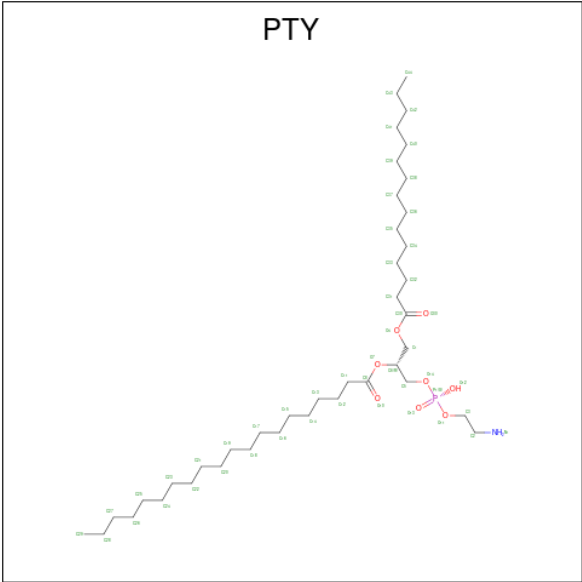
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			44	39	5	

- Molecule 10 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[(2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-5-[(2 {S},3 {S},4 {R},5 {R},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-4-[(2 {R},3 {S},4 {R},5 {S},6 {R})-6-[(1 {S})-2-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-1-oxidanyl-ethyl]-3,4-bis(oxidanyl)-5-phosphonoxy-oxan-2-yl]oxy-3-oxidanyl-5-phosphonoxy-oxan-2-yl]oxy-2-carboxy-2-[(2 {R},3 {S},4 {R},5 {R},6 {R})-5-[(3 {R})-3-dodecanoyloxytetradecanoyl]amino]-6-[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[(3 {R})-3-oxidanyltetradecanoyl]amino]-4-[(3 {R})-3-oxidanyltetradecanoyl]oxy-6-phosphonoxy-oxan-2-yl]methoxy]-3-phosphonoxy-4-[(3 {R})-3-tetradecanoyloxytetradecanoyl]oxy-oxan-2-yl]methoxy]oxan-4-yl]oxy-4,5-bis(oxidanyl)oxane-2-carboxylic acid (CCD ID: JSG) (formula:  $C_{131}H_{240}N_2O_{63}P_4$ ).



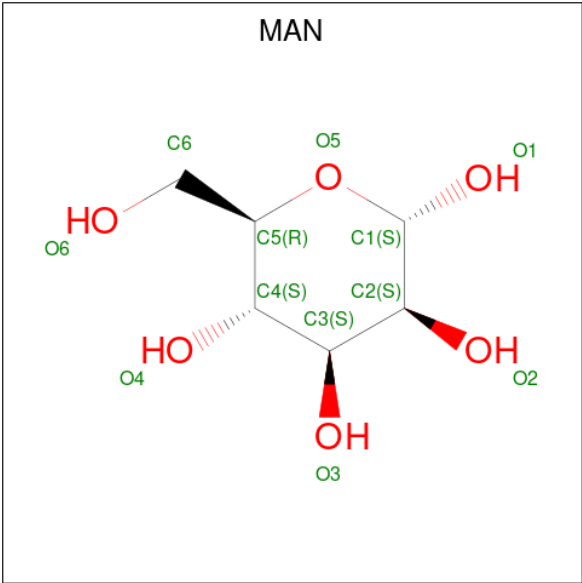
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	A	1	200	131	2	63	4	0

- Molecule 11 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



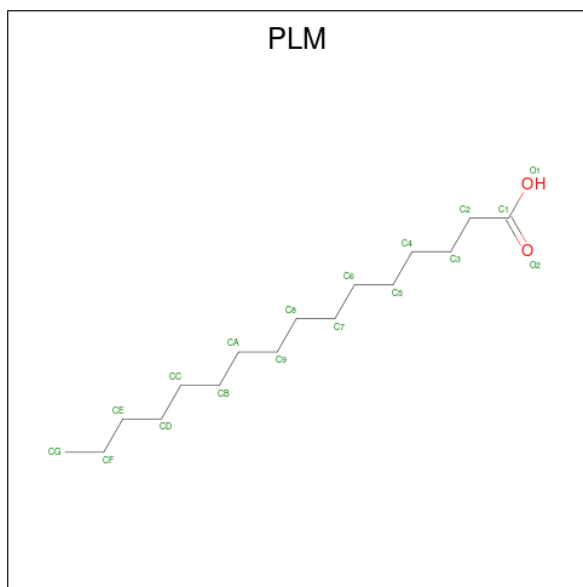
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
11	A	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 12 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			11	6	5	

- Molecule 13 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			17	16	1	

- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

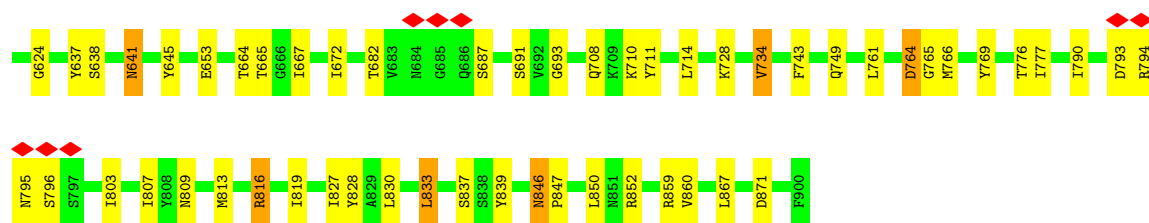
Mol	Chain	Residues	Atoms		AltConf
14	D	7	Total	Ca	0
			7	7	

- Molecule 15 is water.

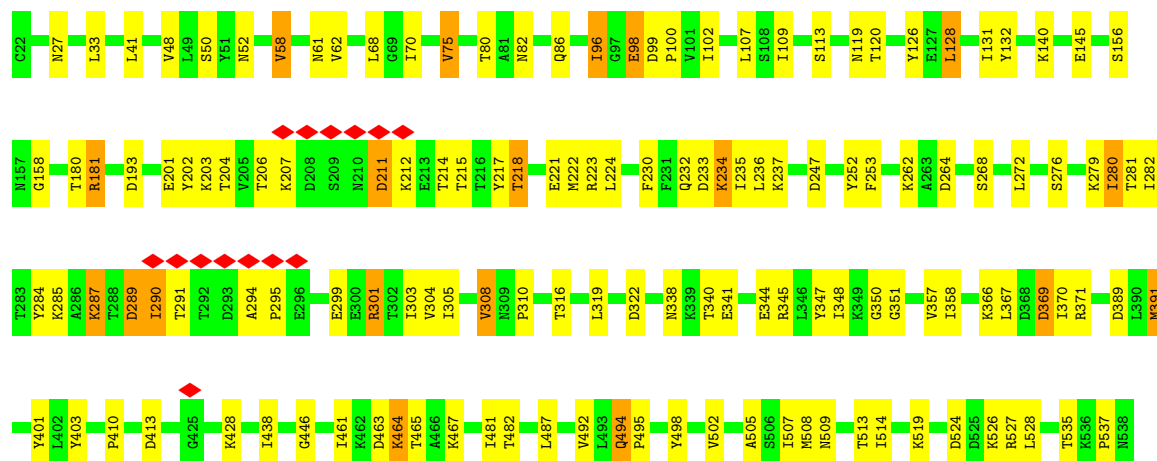
Mol	Chain	Residues	Atoms		AltConf
15	A	6	Total	O	0
			6	6	
15	C	8	Total	O	0
			8	8	
15	B	1	Total	O	0
			1	1	
15	D	1	Total	O	0
			1	1	



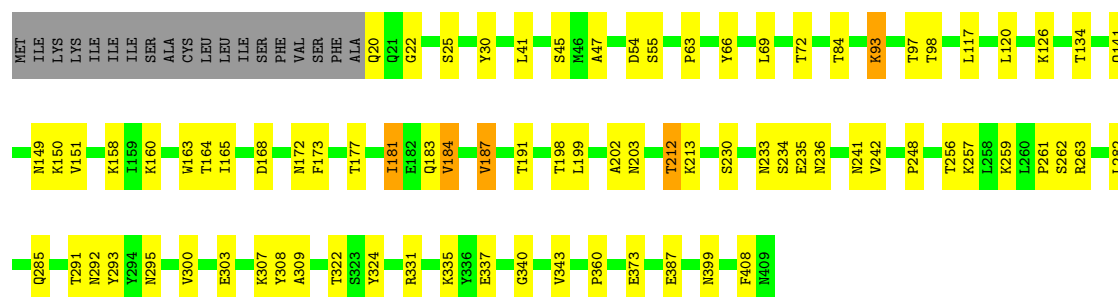




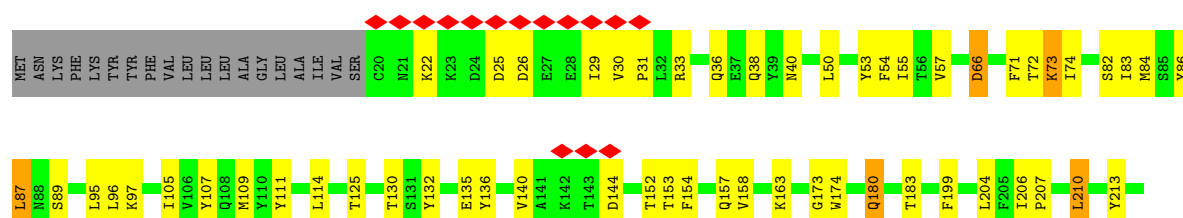
• Molecule 3: Bam H

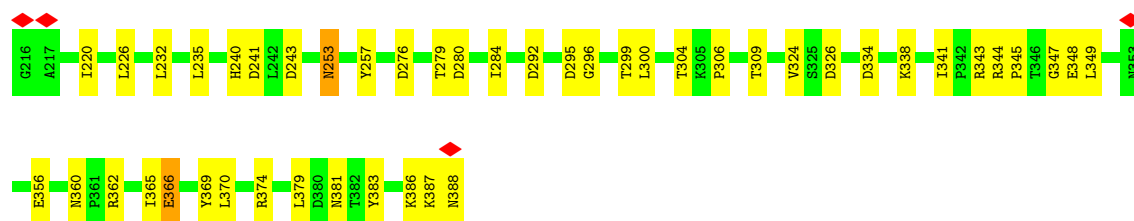


• Molecule 4: Bam G

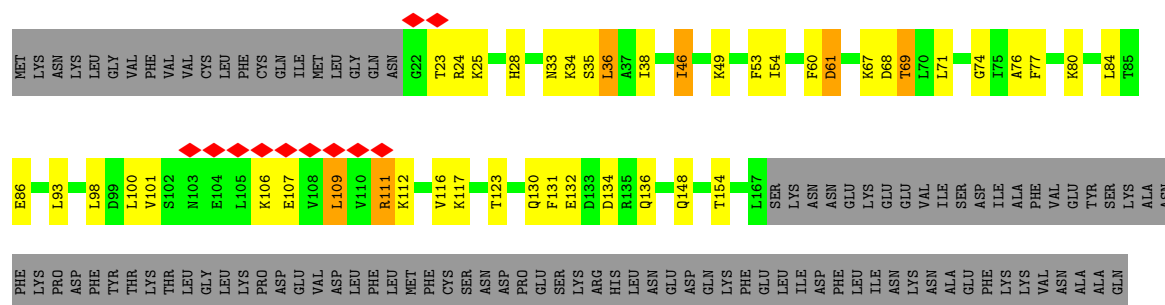


• Molecule 5: Bam M





• Molecule 6: Bam P



• Molecule 7: alpha-D-glucopyranuronic acid-(1-2)-[alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose



• Molecule 8: alpha-D-glucopyranuronic acid-(1-2)-beta-D-galactopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	16.665	Depositor
Minimum map value	-1.207	Depositor
Average map value	0.114	Depositor
Map value standard deviation	0.382	Depositor
Recommended contour level	2.75	Depositor
Map size (Å)	374.784, 374.784, 374.784	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.732, 0.732, 0.732	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: DGA, PLM, GCU, PTY, GAL, JSG, MAN, CA

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	F	0.11	0/2024	0.28	0/2725
2	A	0.14	0/5062	0.39	0/6849
3	C	0.15	0/4101	0.39	0/5565
4	B	0.14	0/3062	0.40	0/4148
5	D	0.15	0/3028	0.40	0/4127
6	E	0.12	0/1169	0.33	0/1569
All	All	0.14	0/18446	0.38	0/24983

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	F	1979	0	1945	40	0
2	A	4936	0	4765	97	0
3	C	4024	0	3931	80	0
4	B	2995	0	2937	48	0
5	D	2947	0	2753	66	0
6	E	1155	0	1198	26	0
7	J	34	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	23	0	15	3	0
9	A	44	0	75	3	0
10	A	200	0	0	2	0
11	A	100	0	158	1	0
12	C	11	0	10	3	0
13	C	17	0	31	4	0
14	D	7	0	0	0	0
15	A	6	0	0	2	0
15	B	1	0	0	0	0
15	C	8	0	0	1	0
15	D	1	0	0	0	0
All	All	18488	0	17843	345	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 10.

The worst 5 of 345 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)
12:C:601:MAN:C1	8:G:1:GAL:O4	1.65	1.43
12:C:601:MAN:O5	8:G:1:GAL:O4	1.75	1.03
3:C:206:THR:HG1	3:C:214:THR:HG1	1.23	0.81
1:F:212:LEU:HG	1:F:224:ARG:HD3	1.63	0.81
4:B:261:PRO:O	4:B:263:ARG:NH1	2.17	0.77

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	F	242/264 (92%)	230 (95%)	12 (5%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	617/900 (69%)	599 (97%)	17 (3%)	1 (0%)	44	68
3	C	515/517 (100%)	490 (95%)	23 (4%)	2 (0%)	30	55
4	B	388/409 (95%)	378 (97%)	10 (3%)	0	100	100
5	D	367/388 (95%)	345 (94%)	21 (6%)	1 (0%)	37	61
6	E	144/249 (58%)	135 (94%)	9 (6%)	0	100	100
All	All	2273/2727 (83%)	2177 (96%)	92 (4%)	4 (0%)	45	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	488	PRO
3	C	211	ASP
5	D	366	GLU
3	C	290	ILE

### 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	F	205/223 (92%)	196 (96%)	9 (4%)	24	51
2	A	529/783 (68%)	505 (96%)	24 (4%)	23	50
3	C	446/446 (100%)	411 (92%)	35 (8%)	10	26
4	B	323/340 (95%)	307 (95%)	16 (5%)	20	46
5	D	324/340 (95%)	308 (95%)	16 (5%)	21	47
6	E	133/228 (58%)	117 (88%)	16 (12%)	4	10
All	All	1960/2360 (83%)	1844 (94%)	116 (6%)	19	38

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	369	ASP
6	E	109	LEU

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Mol	Chain	Res	Type
4	B	165	ILE
6	E	93	LEU
5	D	324	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	407	ASN
6	E	130	GLN
4	B	162	HIS
5	D	359	ASN
3	C	489	ASN

### 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 ⓘ

5 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	$\# Z  > 2$
8	GAL	G	1	8	11,11,12	0.92	0	15,15,17	1.74	3 (20%)
8	GCU	G	2	8	12,12,13	1.13	2 (16%)	14,17,19	1.39	1 (7%)
7	GAL	J	1	7	11,11,12	0.78	0	15,15,17	1.10	1 (6%)
7	GCU	J	2	7	12,12,13	1.11	1 (8%)	14,17,19	0.96	0
7	MAN	J	3	7	11,11,12	0.84	1 (9%)	15,15,17	1.05	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
8	GAL	G	1	8	-	2/2/19/22	0/1/1/1
8	GCU	G	2	8	1/1/5/6	1/4/21/24	0/1/1/1
7	GAL	J	1	7	-	2/2/19/22	0/1/1/1
7	GCU	J	2	7	1/1/5/6	2/4/21/24	0/1/1/1
7	MAN	J	3	7	1/1/4/5	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	2	GCU	O6B-C6	-2.25	1.23	1.30
8	G	2	GCU	O6B-C6	-2.22	1.23	1.30
7	J	3	MAN	O5-C1	-2.10	1.40	1.43
8	G	2	GCU	O5-C1	-2.01	1.40	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1	GAL	O4-C4-C5	4.25	119.80	109.32
8	G	2	GCU	C1-C2-C3	3.30	114.45	109.64
8	G	1	GAL	C1-C2-C3	-2.78	105.60	109.64
8	G	1	GAL	O5-C1-C2	-2.72	104.31	110.79
7	J	1	GAL	C1-C2-C3	-2.26	106.35	109.64

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	J	2	GCU	C1
7	J	3	MAN	C1
8	G	2	GCU	C1

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	2	GCU	C4-C5-C6-O6A
7	J	2	GCU	C4-C5-C6-O6B
7	J	1	GAL	O5-C5-C6-O6
7	J	1	GAL	C4-C5-C6-O6

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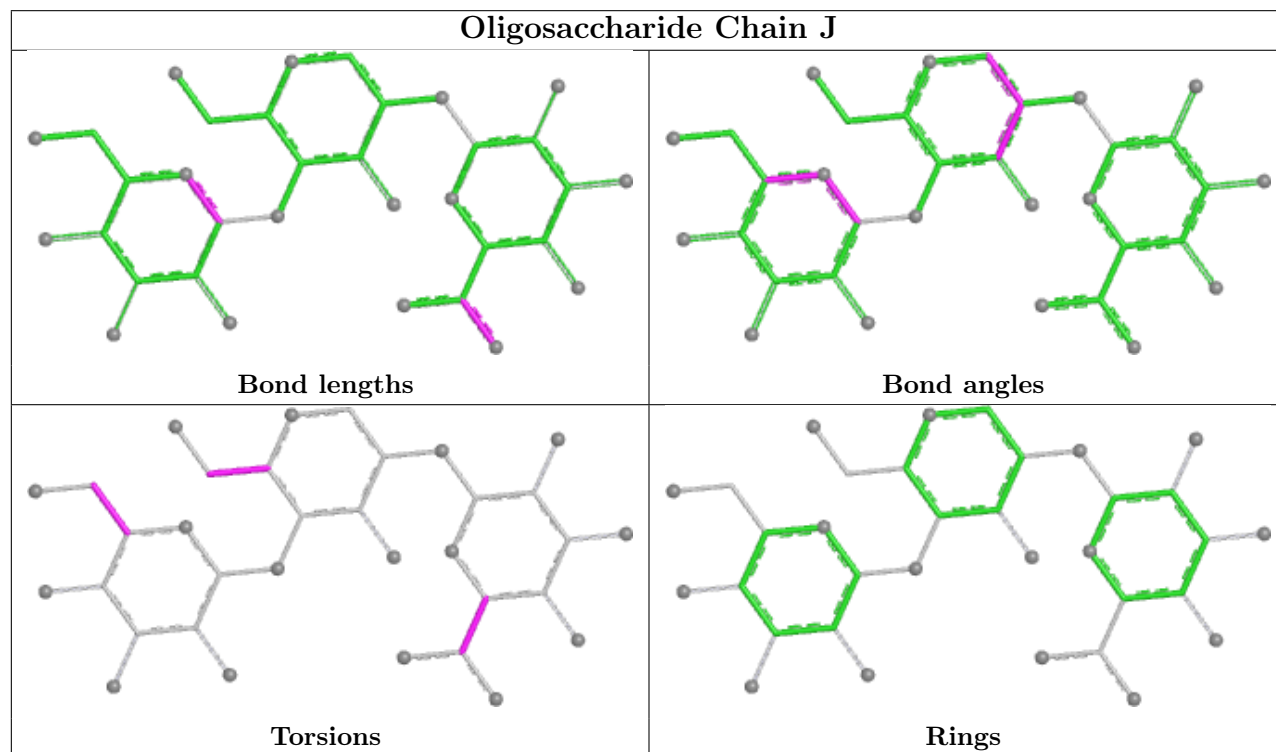
Mol	Chain	Res	Type	Atoms
8	G	1	GAL	C4-C5-C6-O6

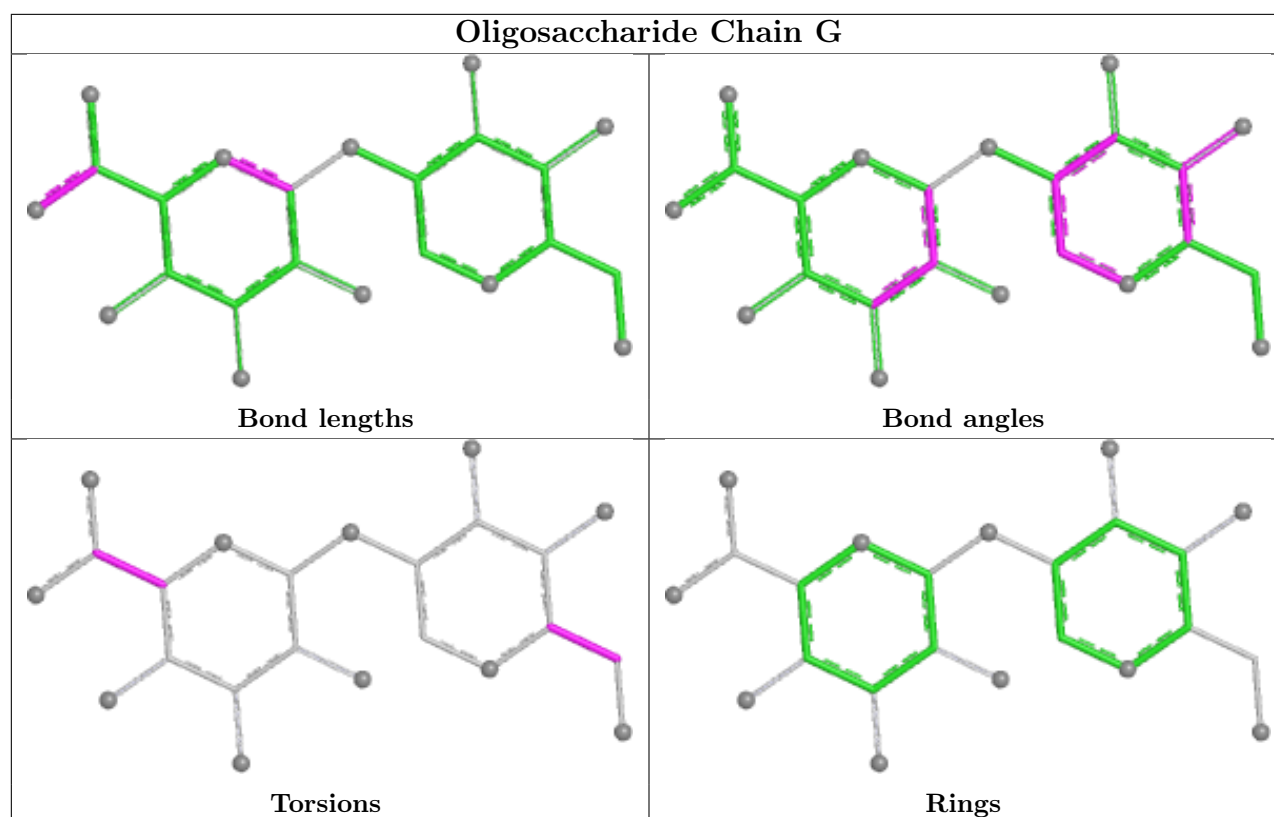
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	1	GAL	3	0
7	J	1	GAL	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 oligosaccharide.





## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	$\# Z  > 2$
11	PTY	A	1004	-	49,49,49	0.46	0	52,54,54	0.39	0
9	DGA	A	1001	3	43,43,43	0.34	0	45,45,45	0.40	0
11	PTY	A	1003	-	49,49,49	0.46	0	52,54,54	0.45	0
10	JSG	A	1002	-	204,206,206	0.71	2 (0%)	264,278,278	1.67	40 (15%)
12	MAN	C	601	-	11,11,12	1.02	1 (9%)	15,15,17	0.96	1 (6%)
13	PLM	C	602	3	15,16,17	0.31	0	14,15,17	0.37	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
11	PTY	A	1004	-	-	25/53/53/53	-
9	DGA	A	1001	3	-	18/45/45/45	-
11	PTY	A	1003	-	-	21/53/53/53	-
10	JSG	A	1002	-	-	65/195/333/333	0/7/7/7
12	MAN	C	601	-	-	2/2/19/22	0/1/1/1
13	PLM	C	602	3	-	5/14/14/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	601	MAN	O5-C1	-2.67	1.39	1.43
10	A	1002	JSG	ODA-CDB	2.49	1.44	1.40
10	A	1002	JSG	CAN-NAO	2.02	1.49	1.45

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1002	JSG	CDP-CDO-NAO	7.39	126.35	116.25
10	A	1002	JSG	CAN-NAO-CDO	7.14	133.41	122.90
10	A	1002	JSG	CCB-OCL-CCF	7.08	124.41	113.07
10	A	1002	JSG	OFJ-CGB-CGC	5.22	122.77	111.48
10	A	1002	JSG	O3-CFK-CFL	4.98	120.35	111.43

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1001	DGA	OG2-CG2-CG3-OXT
10	A	1002	JSG	C5-C4-O4-PHC
10	A	1002	JSG	C2-C1-O1-CAV
10	A	1002	JSG	OAU-CAL-OAM-PHG
10	A	1002	JSG	CAL-CAN-NAO-CDO

There are no ring outliers.

5 monomers are involved in 12 short contacts:

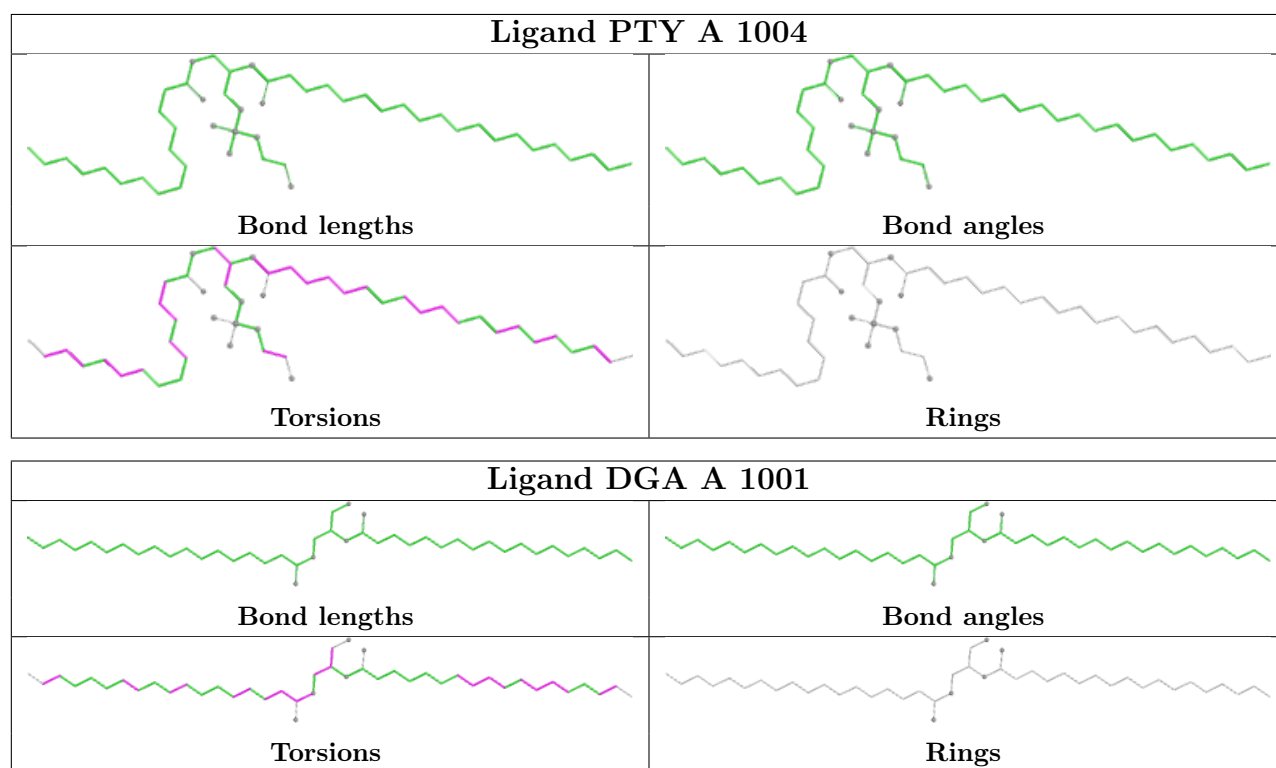
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1001	DGA	3	0

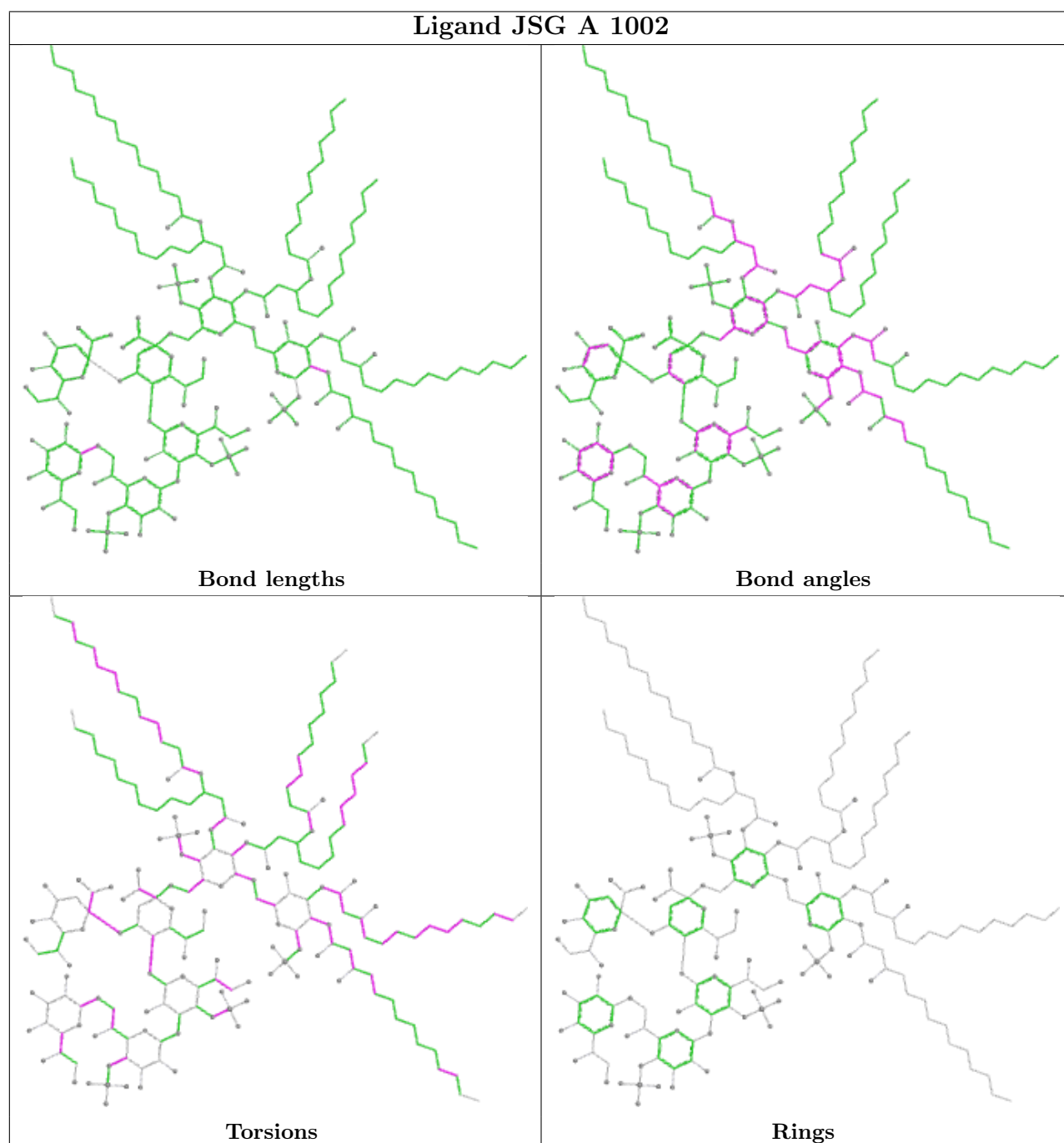
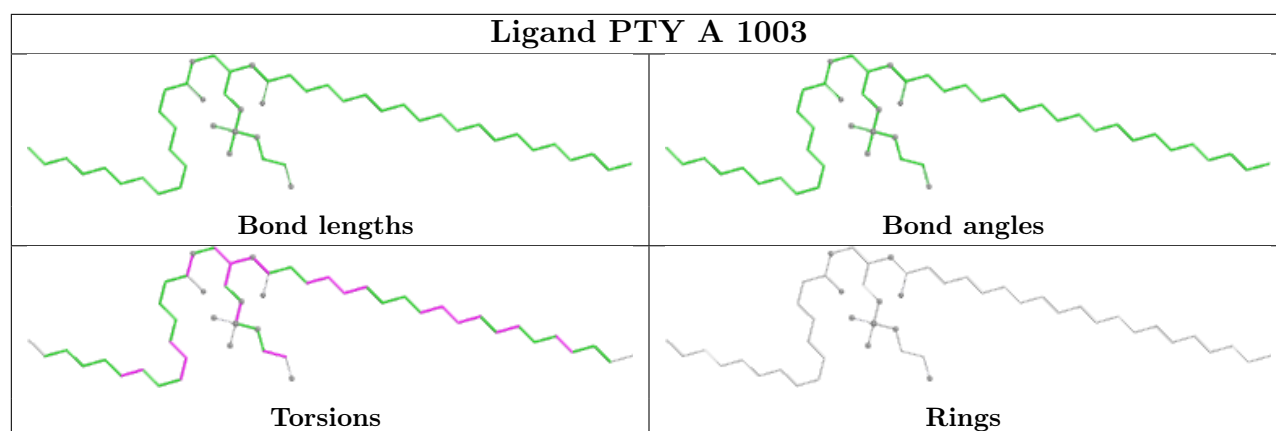
*Continued on next page...*

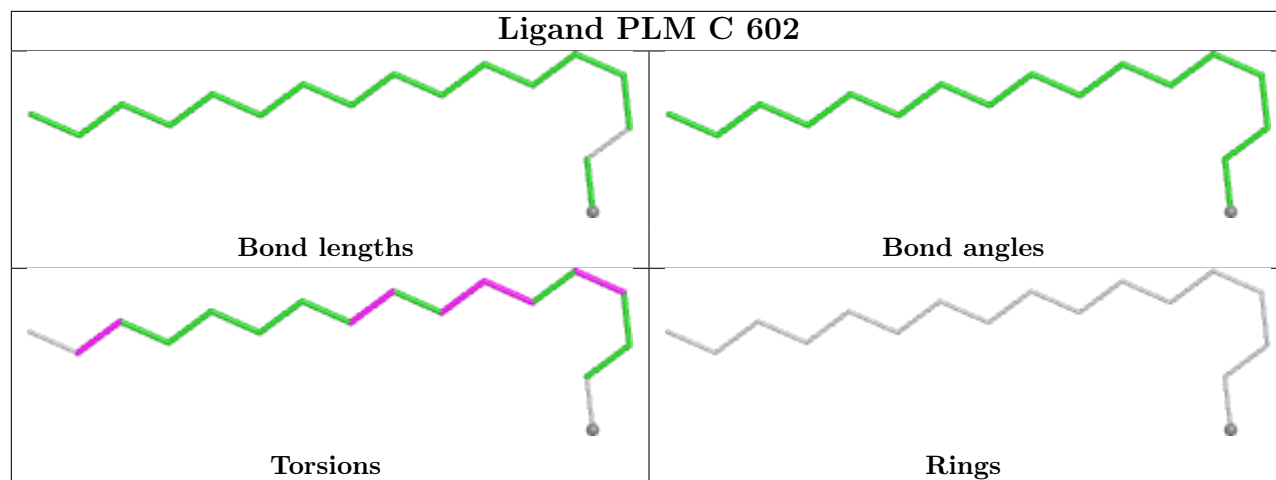
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1003	PTY	1	0
10	A	1002	JSG	2	0
12	C	601	MAN	3	0
13	C	602	PLM	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 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.

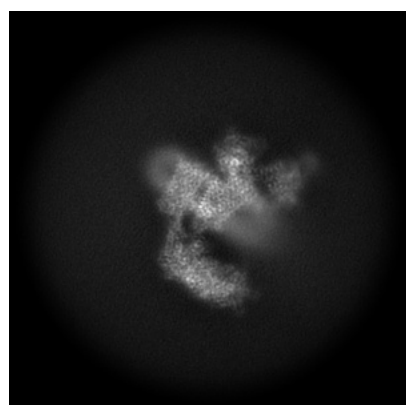
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48835. These allow visual inspection of the internal detail of the map and identification of artifacts.

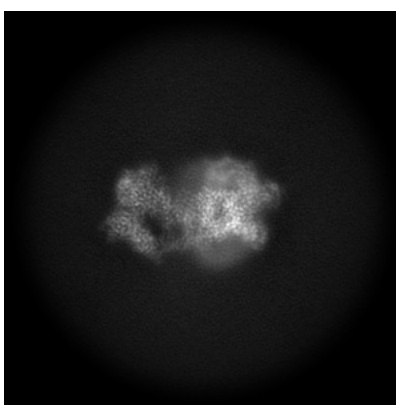
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

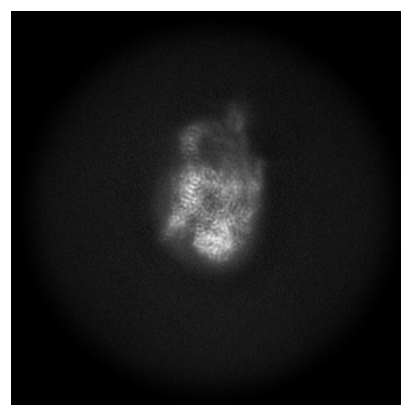
#### 6.1.1 Primary map



X



Y

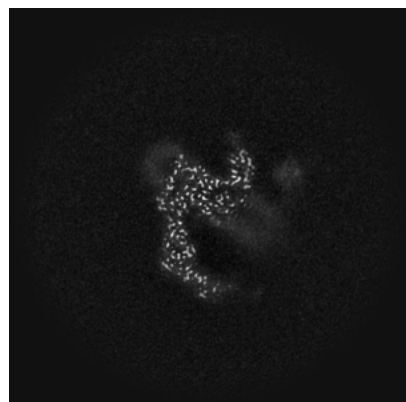


Z

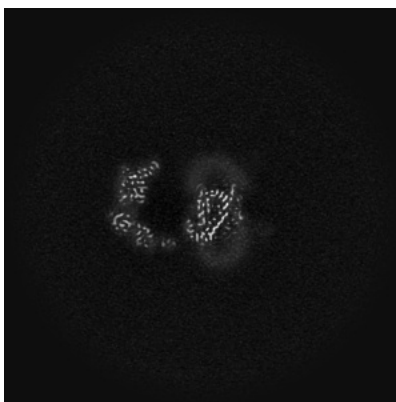
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

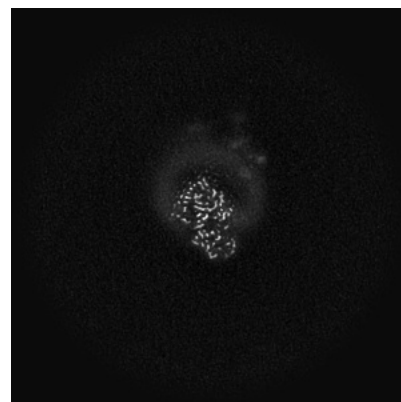
#### 6.2.1 Primary map



X Index: 256



Y Index: 256



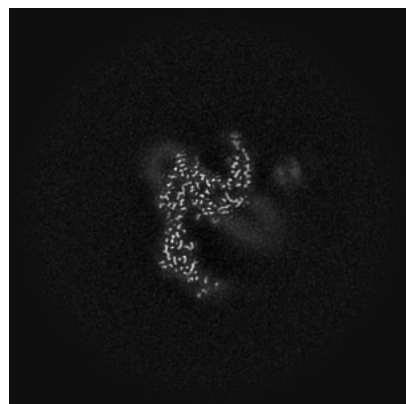
Z Index: 256



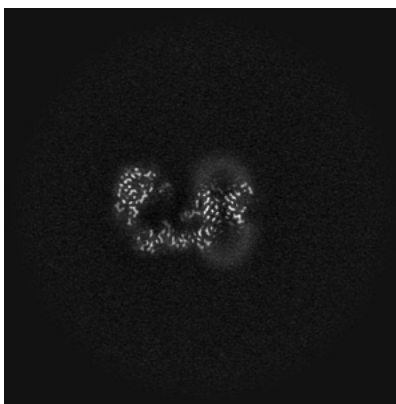
The images above show central slices of the map in three orthogonal directions.

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

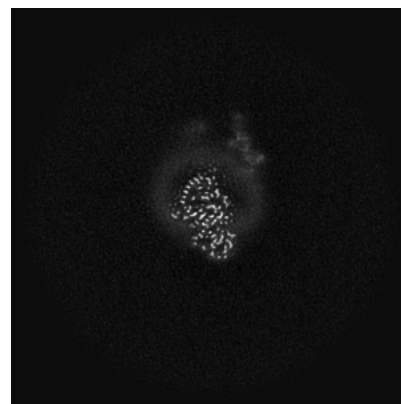
### 6.3.1 Primary map



X Index: 259



Y Index: 244

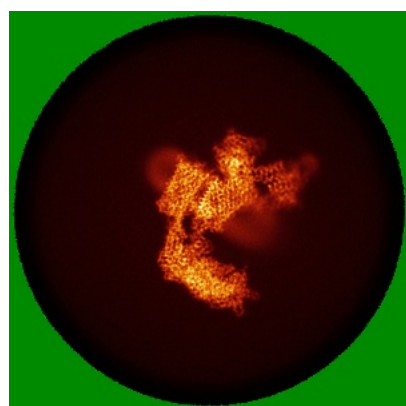


Z Index: 261

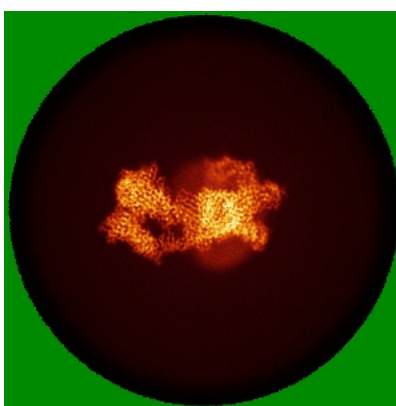
The images above show the largest variance slices of the map in three orthogonal directions.

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

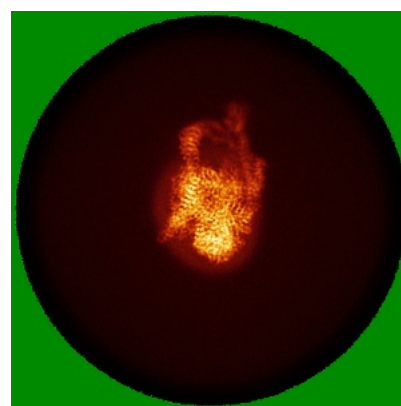
### 6.4.1 Primary map



X



Y

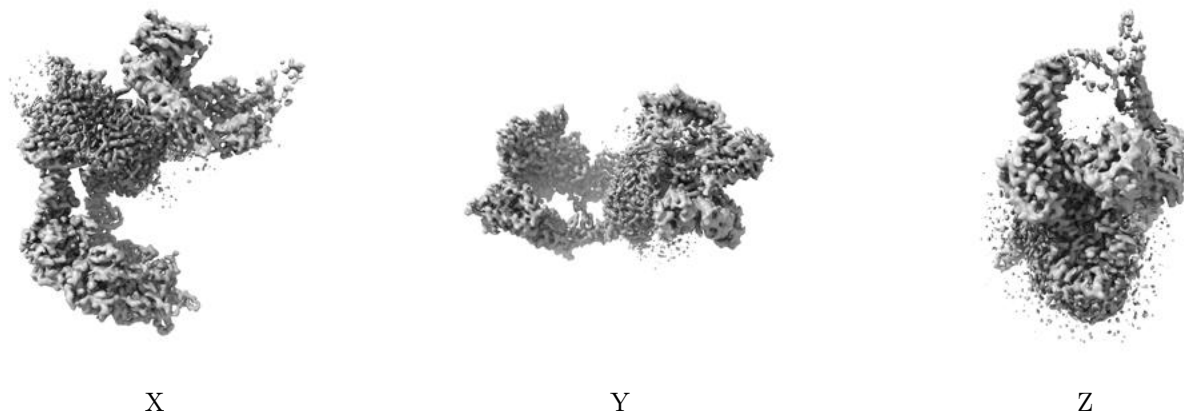


Z

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 2.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

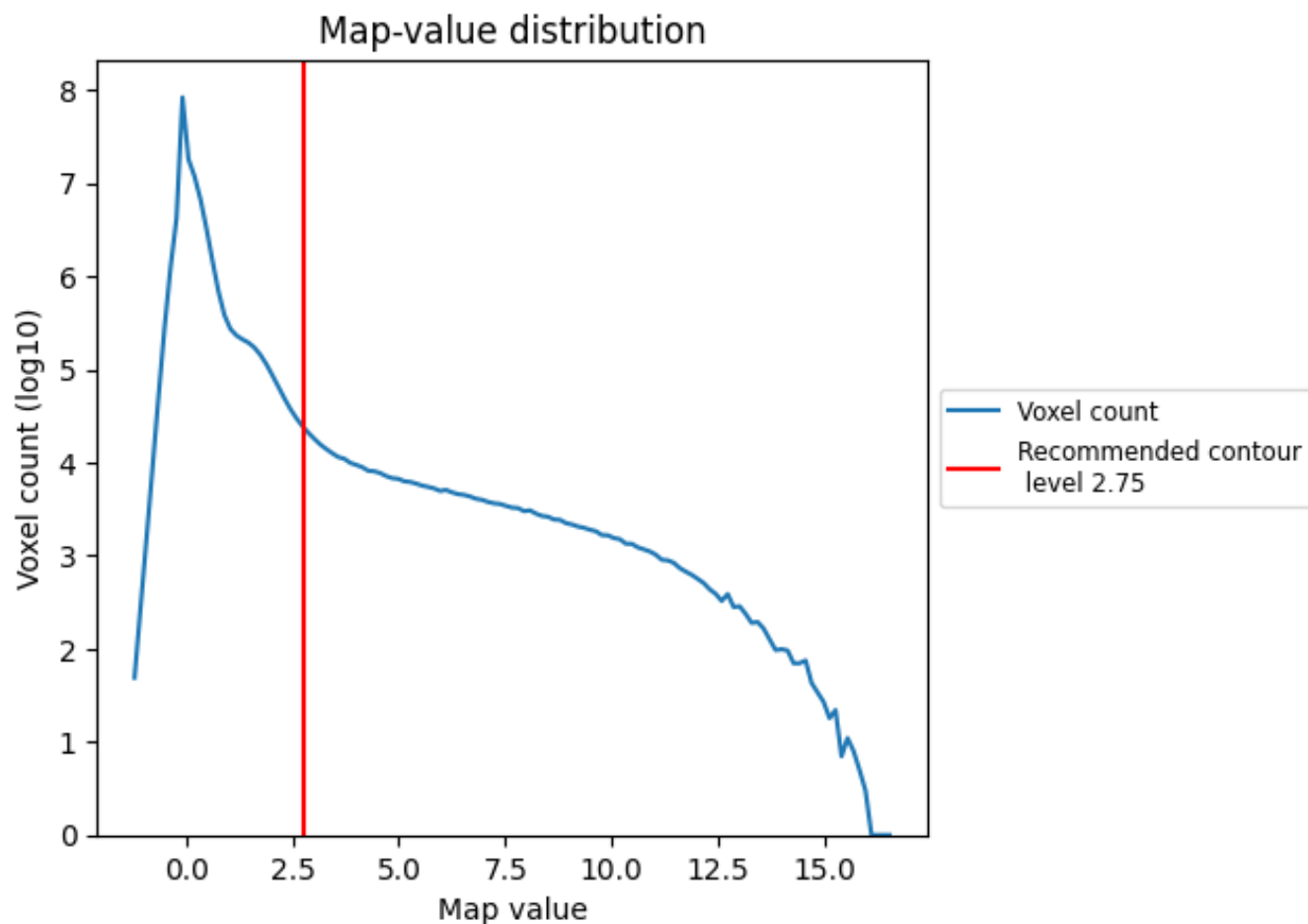
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

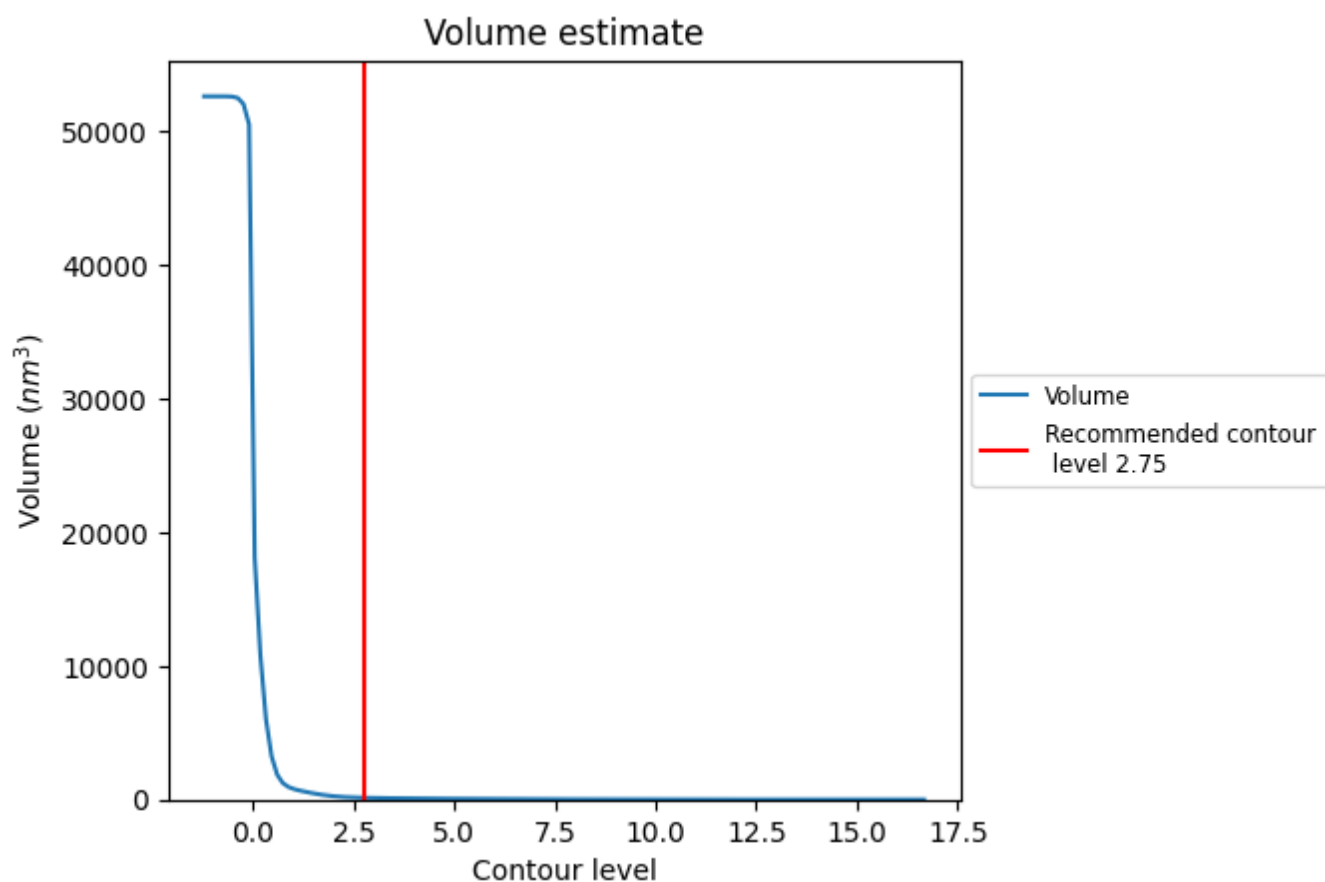
This section contains the results of statistical analysis of the map.

### 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.

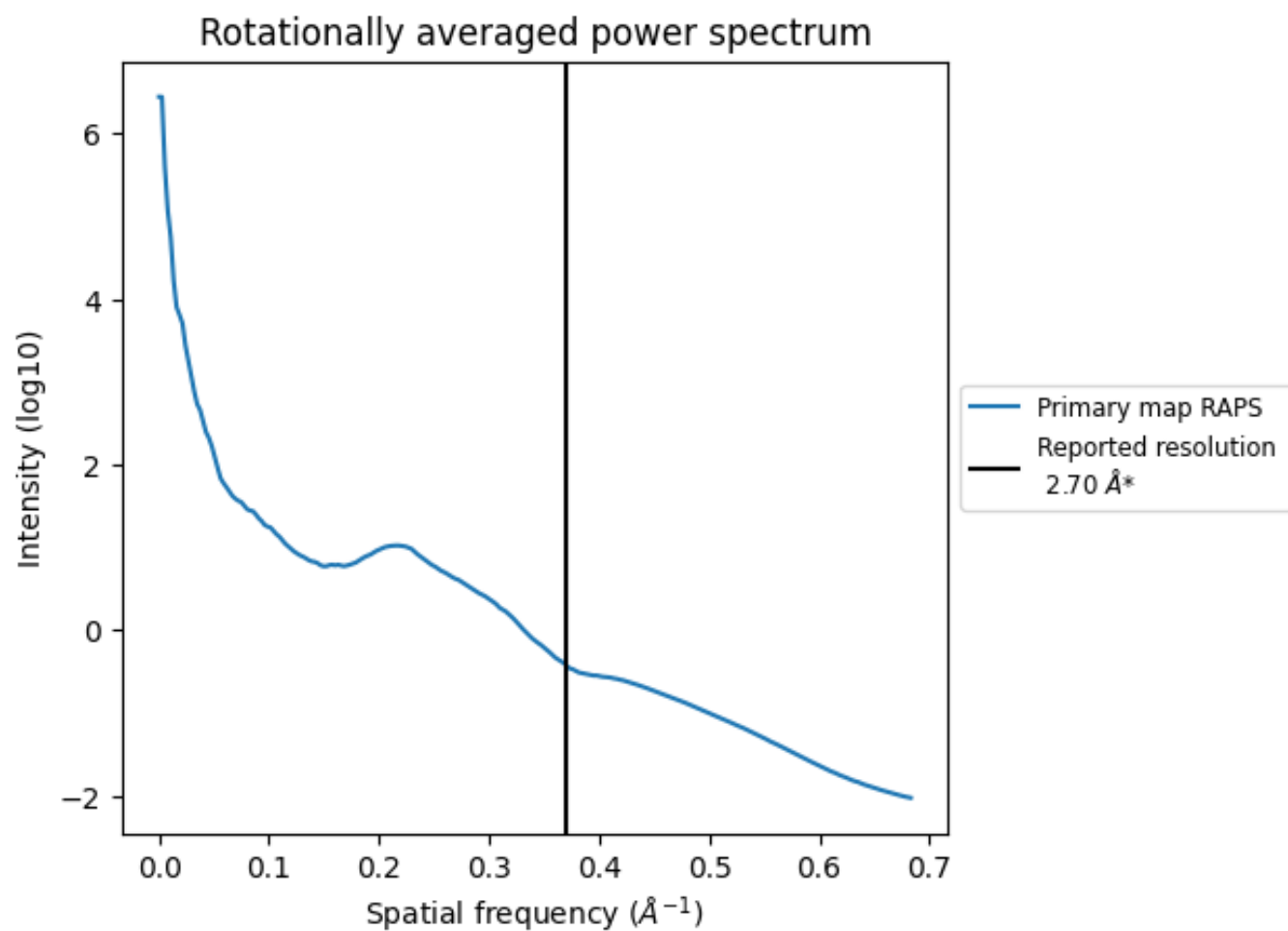
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135  $\text{nm}^3$ ; this corresponds to an approximate mass of 122 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 0.370 Å<sup>-1</sup>

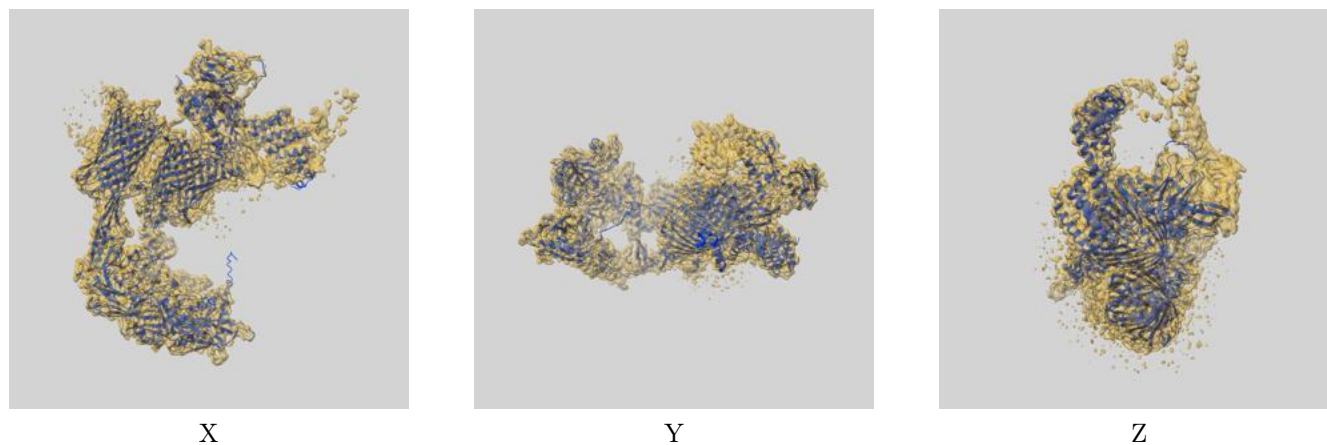
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

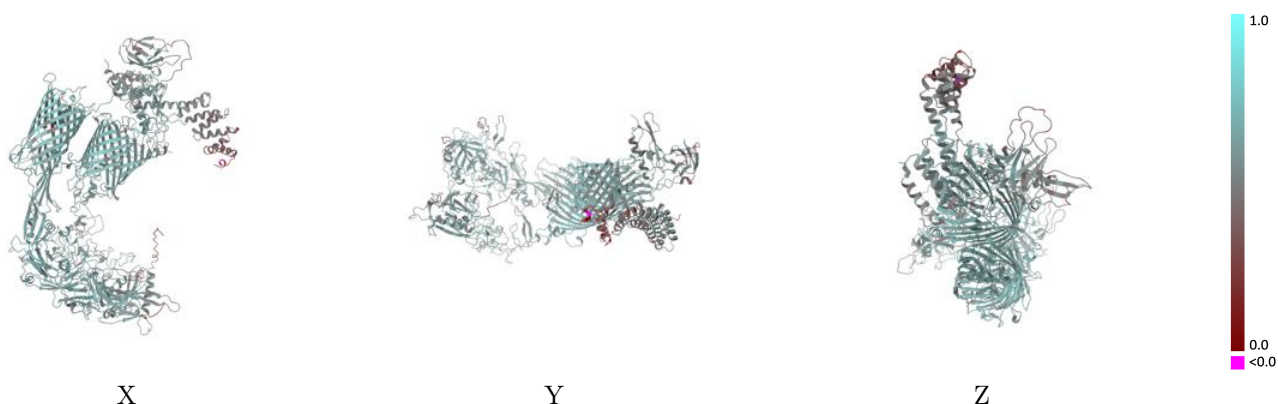
This section contains information regarding the fit between EMDB map EMD-48835 and PDB model 9N2D. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



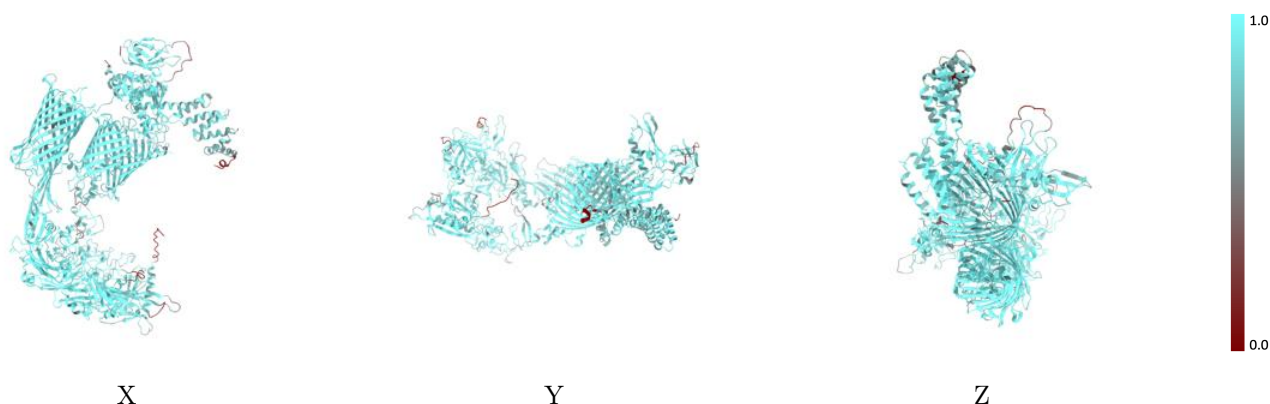
The images above show the 3D surface view of the map at the recommended contour level 2.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

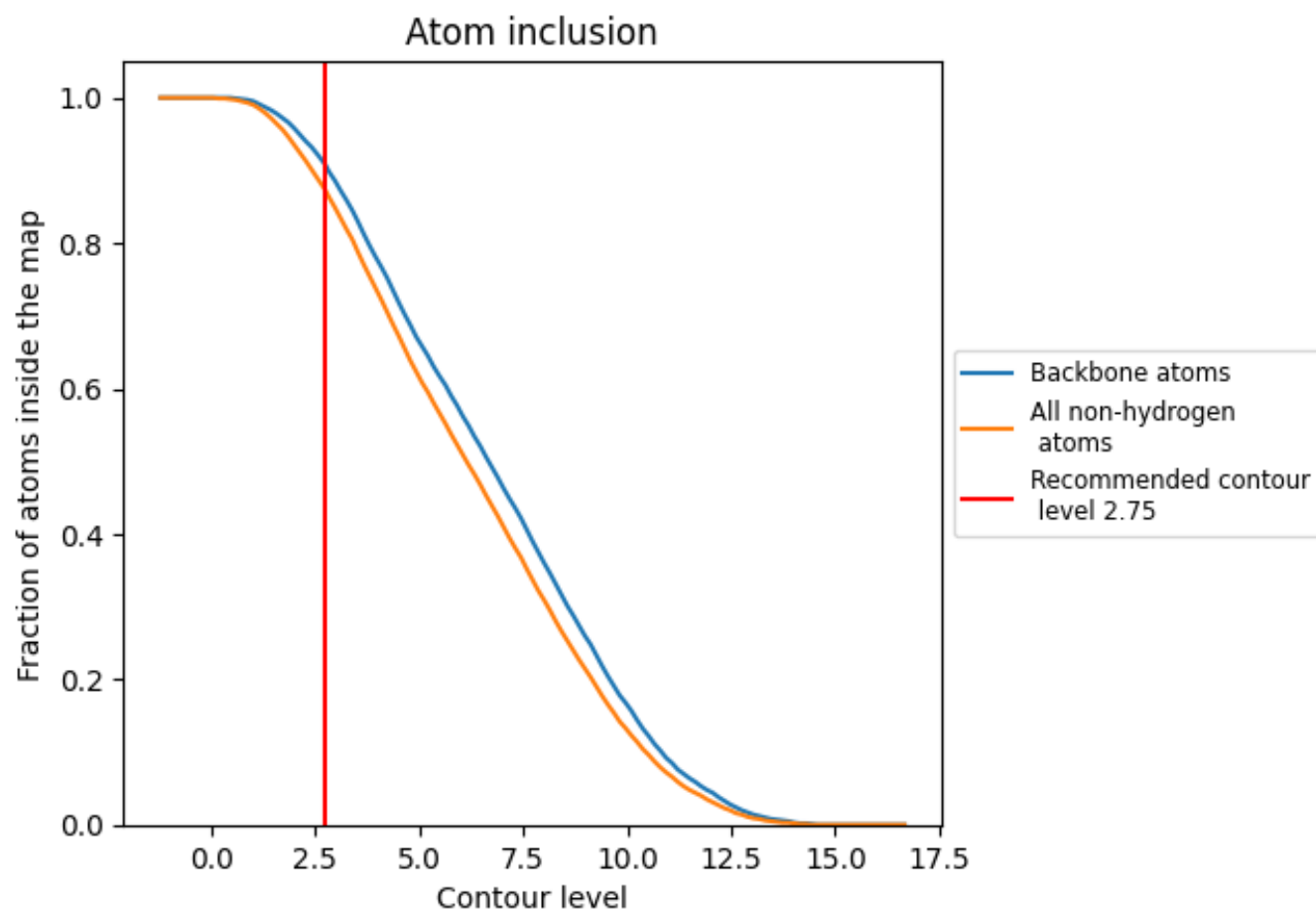
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (2.75).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (2.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8730	<div><div></div></div> 0.5560
A	<div><div></div></div> 0.8780	<div><div></div></div> 0.5680
B	<div><div></div></div> 0.9330	<div><div></div></div> 0.5990
C	<div><div></div></div> 0.9060	<div><div></div></div> 0.5770
D	<div><div></div></div> 0.8360	<div><div></div></div> 0.5460
E	<div><div></div></div> 0.7960	<div><div></div></div> 0.5070
F	<div><div></div></div> 0.8070	<div><div></div></div> 0.4600
G	<div><div></div></div> 0.7830	<div><div></div></div> 0.5080
J	<div><div></div></div> 0.9710	<div><div></div></div> 0.5880

1.0

0.0

<0.0