



## wwPDB EM Validation Summary Report ⓘ

May 12, 2025 – 12:15 PM JST

PDB ID : 8ZKH / pdb\_00008zkh  
EMDB ID : EMD-60196  
Title : Structure of Polycystin-1/Polycystin-2 complex with phosphatidylglycerol-bo  
und  
Authors : Chen, M.Y.; Su, Q.; Shi, Y.G.  
Deposited on : 2024-05-16  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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) : 2.43.1

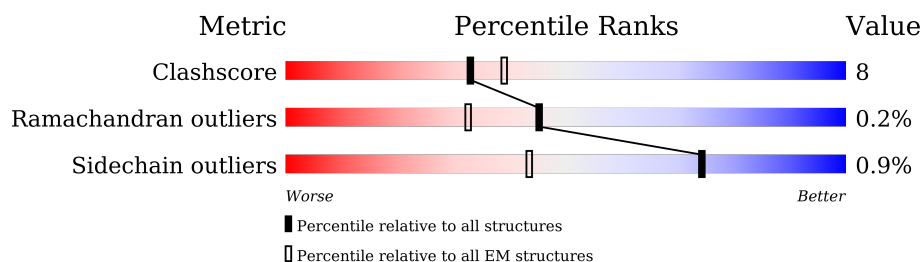
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1261	
2	B	1007	
2	C	1007	
2	D	1007	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17200 atoms, of which 76 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 Polycystin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	776	Total	C	N	O	S	0	0
			5347	3427	982	920	18		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3043	MET	-	initiating methionine	UNP P98161
A	3044	ASP	-	expression tag	UNP P98161
A	3045	TYR	-	expression tag	UNP P98161
A	3046	LYS	-	expression tag	UNP P98161
A	3047	ASP	-	expression tag	UNP P98161
A	3048	ASP	-	expression tag	UNP P98161
A	3049	ASP	-	expression tag	UNP P98161
A	3050	ASP	-	expression tag	UNP P98161
A	3051	LYS	-	expression tag	UNP P98161

- Molecule 2 is a protein called Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	472	Total	C	N	O	S	0	0
			3896	2571	615	690	20		
2	C	471	Total	C	N	O	S	0	0
			3891	2568	614	689	20		
2	D	462	Total	C	N	O	S	0	0
			3811	2516	600	676	19		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	MET	-	initiating methionine	UNP Q13563
B	-37	GLY	-	expression tag	UNP Q13563
B	-36	ALA	-	expression tag	UNP Q13563
B	-35	SER	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	SER	-	expression tag	UNP Q13563
B	-33	ALA	-	expression tag	UNP Q13563
B	-32	TRP	-	expression tag	UNP Q13563
B	-31	SER	-	expression tag	UNP Q13563
B	-30	HIS	-	expression tag	UNP Q13563
B	-29	PRO	-	expression tag	UNP Q13563
B	-28	GLN	-	expression tag	UNP Q13563
B	-27	PHE	-	expression tag	UNP Q13563
B	-26	GLU	-	expression tag	UNP Q13563
B	-25	LYS	-	expression tag	UNP Q13563
B	-24	GLY	-	expression tag	UNP Q13563
B	-23	GLY	-	expression tag	UNP Q13563
B	-22	GLY	-	expression tag	UNP Q13563
B	-21	SER	-	expression tag	UNP Q13563
B	-20	GLY	-	expression tag	UNP Q13563
B	-19	GLY	-	expression tag	UNP Q13563
B	-18	GLY	-	expression tag	UNP Q13563
B	-17	SER	-	expression tag	UNP Q13563
B	-16	GLY	-	expression tag	UNP Q13563
B	-15	GLY	-	expression tag	UNP Q13563
B	-14	SER	-	expression tag	UNP Q13563
B	-13	ALA	-	expression tag	UNP Q13563
B	-12	TRP	-	expression tag	UNP Q13563
B	-11	SER	-	expression tag	UNP Q13563
B	-10	HIS	-	expression tag	UNP Q13563
B	-9	PRO	-	expression tag	UNP Q13563
B	-8	GLN	-	expression tag	UNP Q13563
B	-7	PHE	-	expression tag	UNP Q13563
B	-6	GLU	-	expression tag	UNP Q13563
B	-5	LYS	-	expression tag	UNP Q13563
B	-4	GLY	-	expression tag	UNP Q13563
B	-3	SER	-	linker	UNP Q13563
B	-2	ALA	-	linker	UNP Q13563
B	-1	ALA	-	linker	UNP Q13563
B	0	ALA	-	linker	UNP Q13563
C	-38	MET	-	initiating methionine	UNP Q13563
C	-37	GLY	-	expression tag	UNP Q13563
C	-36	ALA	-	expression tag	UNP Q13563
C	-35	SER	-	expression tag	UNP Q13563
C	-34	SER	-	expression tag	UNP Q13563
C	-33	ALA	-	expression tag	UNP Q13563
C	-32	TRP	-	expression tag	UNP Q13563

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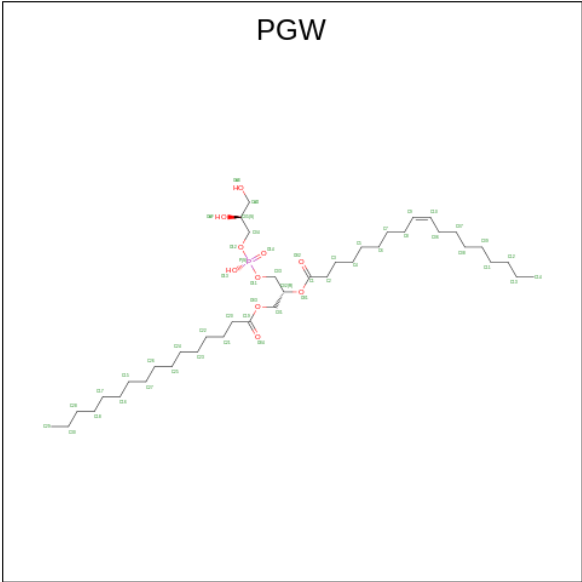
Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	SER	-	expression tag	UNP Q13563
C	-30	HIS	-	expression tag	UNP Q13563
C	-29	PRO	-	expression tag	UNP Q13563
C	-28	GLN	-	expression tag	UNP Q13563
C	-27	PHE	-	expression tag	UNP Q13563
C	-26	GLU	-	expression tag	UNP Q13563
C	-25	LYS	-	expression tag	UNP Q13563
C	-24	GLY	-	expression tag	UNP Q13563
C	-23	GLY	-	expression tag	UNP Q13563
C	-22	GLY	-	expression tag	UNP Q13563
C	-21	SER	-	expression tag	UNP Q13563
C	-20	GLY	-	expression tag	UNP Q13563
C	-19	GLY	-	expression tag	UNP Q13563
C	-18	GLY	-	expression tag	UNP Q13563
C	-17	SER	-	expression tag	UNP Q13563
C	-16	GLY	-	expression tag	UNP Q13563
C	-15	GLY	-	expression tag	UNP Q13563
C	-14	SER	-	expression tag	UNP Q13563
C	-13	ALA	-	expression tag	UNP Q13563
C	-12	TRP	-	expression tag	UNP Q13563
C	-11	SER	-	expression tag	UNP Q13563
C	-10	HIS	-	expression tag	UNP Q13563
C	-9	PRO	-	expression tag	UNP Q13563
C	-8	GLN	-	expression tag	UNP Q13563
C	-7	PHE	-	expression tag	UNP Q13563
C	-6	GLU	-	expression tag	UNP Q13563
C	-5	LYS	-	expression tag	UNP Q13563
C	-4	GLY	-	expression tag	UNP Q13563
C	-3	SER	-	linker	UNP Q13563
C	-2	ALA	-	linker	UNP Q13563
C	-1	ALA	-	linker	UNP Q13563
C	0	ALA	-	linker	UNP Q13563
D	-38	MET	-	initiating methionine	UNP Q13563
D	-37	GLY	-	expression tag	UNP Q13563
D	-36	ALA	-	expression tag	UNP Q13563
D	-35	SER	-	expression tag	UNP Q13563
D	-34	SER	-	expression tag	UNP Q13563
D	-33	ALA	-	expression tag	UNP Q13563
D	-32	TRP	-	expression tag	UNP Q13563
D	-31	SER	-	expression tag	UNP Q13563
D	-30	HIS	-	expression tag	UNP Q13563
D	-29	PRO	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-28	GLN	-	expression tag	UNP Q13563
D	-27	PHE	-	expression tag	UNP Q13563
D	-26	GLU	-	expression tag	UNP Q13563
D	-25	LYS	-	expression tag	UNP Q13563
D	-24	GLY	-	expression tag	UNP Q13563
D	-23	GLY	-	expression tag	UNP Q13563
D	-22	GLY	-	expression tag	UNP Q13563
D	-21	SER	-	expression tag	UNP Q13563
D	-20	GLY	-	expression tag	UNP Q13563
D	-19	GLY	-	expression tag	UNP Q13563
D	-18	GLY	-	expression tag	UNP Q13563
D	-17	SER	-	expression tag	UNP Q13563
D	-16	GLY	-	expression tag	UNP Q13563
D	-15	GLY	-	expression tag	UNP Q13563
D	-14	SER	-	expression tag	UNP Q13563
D	-13	ALA	-	expression tag	UNP Q13563
D	-12	TRP	-	expression tag	UNP Q13563
D	-11	SER	-	expression tag	UNP Q13563
D	-10	HIS	-	expression tag	UNP Q13563
D	-9	PRO	-	expression tag	UNP Q13563
D	-8	GLN	-	expression tag	UNP Q13563
D	-7	PHE	-	expression tag	UNP Q13563
D	-6	GLU	-	expression tag	UNP Q13563
D	-5	LYS	-	expression tag	UNP Q13563
D	-4	GLY	-	expression tag	UNP Q13563
D	-3	SER	-	linker	UNP Q13563
D	-2	ALA	-	linker	UNP Q13563
D	-1	ALA	-	linker	UNP Q13563
D	0	ALA	-	linker	UNP Q13563

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).

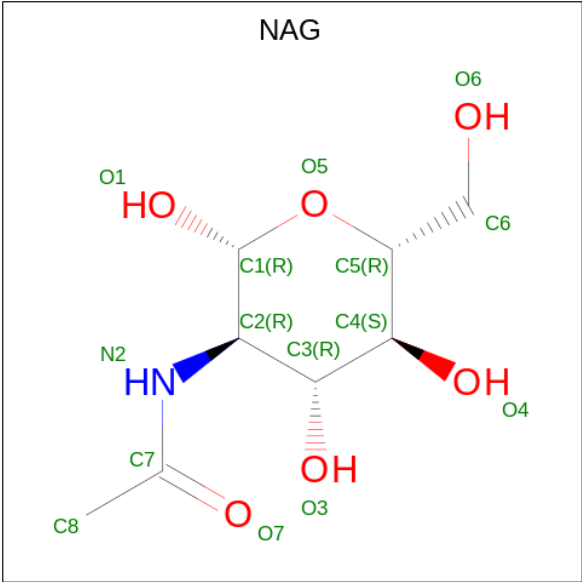


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
3	A	1	127	40	76	10	1	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

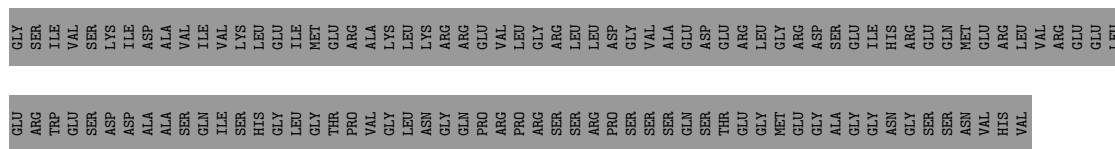


Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5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

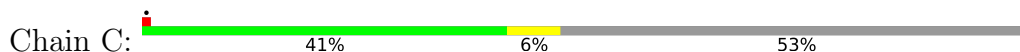








- Molecule 2: Polycystin-2



MET	GLY	ALA	SER	SER	TRP	SER	HIS	GLN	PHE	GLU	LYS	GLY	GLY	GLY	SER	GLY	GLY	SER	TRP	ALA	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	SER	VAL	ASN	SER	SER	ARG	VAL	GLN	PRO	GLN	PRO	PRO	ASP	ALA	LYS	ARG	PRO	PRO	ALA	PRO
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ARG	ALA	PRO	PRO	ASP	PRO	GLY	ARG	GLY	LEU	MET	ALA	ALA	GLY	CYS	ALA	ALA	VAL	GLY	ALA	SER	LEU	ALA	ALA	ALA	GLY	GLY	LEU	CYS	GLU	GLN	ARG	GLY	LEU	GLU	ILE	GLU	GLU	MET	GLN	ARG	GLN	ILE	ARG	ASP	PRO	PRO	PRO	ALA	ALA	GLY	ALA	ALA	SER	PRO	SER	PRO	PRO	LEU	SER	SER
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GLY	GLY	TYR	HIS	GLY	ALA	GLY	HIS	PRO	SER	GLY	ARG	ARG	ARG	ARG	ASP	GLN	GLY	PRO	PRO	CYS	PRO	SER	SER	VAL	GLY	GLY	ASP	PRO	PRO	LEU	LEU	GLY	GLN	PRO	PRO	ARG	VAL	ALA	TRP	ALA	GLU	ARG	VAL	LEU	VAL	ARG	GLY	GLY	GLY	LEU	PER
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Amino Acid	Number of Mutations
GLY	1
THR	1
ARG	1
LEU	1
MET	1
GIU	1
GLU	1
SER	1
THR	1
ASN	1
ARG	1
GLU	1
TYR	1
LEU	1
LYS	1
S219	1
E223	1
Y227	1
L234	1
T238	1
Y247	1
M252	1
M253	1
S254	1
L258	1
K264	1
T265	1
T266	1
K271	1
M295	1
GLN	1
PRO	1
SER	1
ASN	1
GLN	1
THR	1
ALA	1
D304	1
I309	1
E312	1
N313	1
L314	1

Amino Acid	Count
L597	10
L614	15
V623	25
D624	25
I639	20
I644	25
T683	30
V687	35
K688	40
S689	45
D690	50
L691	55
K695	60
A696	65
E697	70

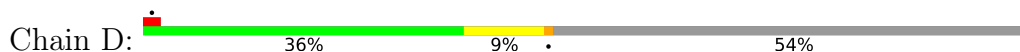
[illegible]

SER	LEU	PRO	ARG	MET	SER	SER	ARG	SER	PHE	PRO	ARG	SER	LEU	ASP	ASP	SER	GLU	GLU	ASP	ASP	GLU	ASP	SER	GLY	HIS	SER	SER	ARG	ARG	ARG	GLY	SER	ILE	SER	GLY	GLY	PHE	GLN	VAL	VAL	LEU	VAL	ARG	ARG	MET	GLU	HIS	SER	HIS	ILE	TYR
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SER	ILE	VAL	SER	LYS	ILE	ASP	ALA	VAL	VAL	VAL	VAL	LYS	LEU	GLU	MET	GLU	ARG	ALA	LYS	LEU	LYS	ARG	ARG	GLU	VAL	LEU	GLY	GLY	ASP	VAL	ALA	GLU	ASP	GLU	GLU	ARG	ARG	LEU	GLY	ARG	SER	ASP	GLU	ILE	HIS	ARG	GLU	GLN	GLU	ARG	LEU	VAL	GLU	GLU	LEU	LEU
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ARG	TRP	GLU	SER	ASP	ASP	ALA	ALA	SER	GLN	ILE	SER	HIS	GLY	GLY	THR	PRO	VAL	GLY	LEU	ASN	GLY	GLN	PRO	ARG	PRO	ARG	SER	SER	ARG	PRO	SER	SER	SER	GLN	SER	THR	GLU	GLY	GLY	ALA	GLY	GLY	ASN	GLY	SER	SER	ASN	VAL	HIS	VAL
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- Molecule 2: Polycystin-2



MET	GLY	ALA	SER	SER	ALA	TRP	SER	HIS	PRO	PRO	GLN	PHE	GLU	GLY	GLY	GLY	SER	GLY	GLY	GLY	SER	ALA	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	GLY	GLY	GLY	SER	VAL	ASN	SER	SER	ARG	VAL	VAL	GLN	PRO	PRO	GLN	PRO	PRO	ASP	ALA	ALA	LYS	ARG	PRO	PRO	ALA	PRO
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[illegible][illegible]



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162204	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.401	Depositor
Minimum map value	-1.560	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.34	Depositor
Map size ( $\text{\AA}$ )	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.087, 1.087, 1.087	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: NAG, PGW, 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	A	0.21	0/5451	0.46	8/7458 (0.1%)
2	B	0.13	0/3999	0.32	0/5426
2	C	0.13	0/3994	0.30	0/5419
2	D	0.19	0/3912	0.39	2/5311 (0.0%)
All	All	0.17	0/17356	0.38	10/23614 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3753	ARG	N-CA-C	-7.46	104.69	114.31
1	A	3751	GLN	N-CA-C	7.38	118.93	108.74
2	D	570	TRP	N-CA-C	-7.03	105.24	113.88
2	D	576	PHE	N-CA-C	-6.92	104.84	113.55
1	A	3334	TYR	CA-C-N	6.54	126.31	119.05

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	5347	0	4889	101	0
2	B	3896	0	3844	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3891	0	3840	62	0
2	D	3811	0	3760	90	0
3	A	51	76	76	5	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	42	0	39	2	0
5	C	42	0	39	3	0
5	D	42	0	39	4	0
All	All	17124	76	16526	275	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 8.

The worst 5 of 275 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)
2:D:375:ASN:HD21	5:D:1001:NAG:C1	1.51	1.21
2:D:572:LYS:HE3	2:D:575:LYS:CE	1.75	1.15
1:A:3331:VAL:CG2	1:A:3603:TRP:CZ2	2.32	1.12
2:D:572:LYS:HE3	2:D:575:LYS:HE2	1.35	1.04
2:D:608:PHE:CE2	2:D:637:PHE:CE1	2.46	1.03

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	766/1261 (61%)	693 (90%)	69 (9%)	4 (0%)	25	32
2	B	468/1007 (46%)	437 (93%)	31 (7%)	0	100	100
2	C	467/1007 (46%)	440 (94%)	27 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	458/1007 (46%)	430 (94%)	27 (6%)	1 (0%)	44	55
All	All	2159/4282 (50%)	2000 (93%)	154 (7%)	5 (0%)	45	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3754	LEU
1	A	3774	GLY
2	D	578	ASN
1	A	3773	ALA
1	A	3332	VAL

### 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	434/1041 (42%)	427 (98%)	7 (2%)	58	74
2	B	426/860 (50%)	424 (100%)	2 (0%)	86	93
2	C	426/860 (50%)	425 (100%)	1 (0%)	92	96
2	D	417/860 (48%)	412 (99%)	5 (1%)	67	81
All	All	1703/3621 (47%)	1688 (99%)	15 (1%)	74	87

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

Mol	Chain	Res	Type
2	B	237	LEU
2	D	572	LYS
2	B	596	ASP
2	D	633	ILE
2	D	313	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:



Mol	Chain	Res	Type
2	D	313	ASN
2	D	375	ASN
2	D	430	ASN
2	B	375	ASN
2	C	379	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	NAG	C	1002	2	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	D	1003	2	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	D	1002	2	14,14,15	1.09	2 (14%)	17,19,21	1.70	3 (17%)
5	NAG	B	1002	-	14,14,15	0.39	0	17,19,21	0.75	1 (5%)
5	NAG	C	1003	2	14,14,15	0.99	1 (7%)	17,19,21	1.22	1 (5%)
5	NAG	C	1004	2	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	B	1003	2	14,14,15	0.51	0	17,19,21	1.29	1 (5%)
5	NAG	D	1001	2	14,14,15	0.30	0	17,19,21	0.62	0
5	NAG	B	1004	2	14,14,15	0.20	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PGW	A	4401	-	50,50,50	0.93	4 (8%)	53,56,56	0.93	3 (5%)

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	NAG	C	1002	2	-	2/6/23/26	0/1/1/1
5	NAG	D	1003	2	-	1/6/23/26	0/1/1/1
5	NAG	D	1002	2	-	5/6/23/26	0/1/1/1
5	NAG	B	1002	-	-	1/6/23/26	0/1/1/1
5	NAG	C	1003	2	-	3/6/23/26	0/1/1/1
5	NAG	C	1004	2	-	2/6/23/26	0/1/1/1
5	NAG	B	1003	2	-	5/6/23/26	0/1/1/1
5	NAG	D	1001	2	-	5/6/23/26	0/1/1/1
5	NAG	B	1004	2	-	2/6/23/26	0/1/1/1
3	PGW	A	4401	-	-	25/55/55/55	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	NAG	O5-C1	3.49	1.49	1.43
5	D	1002	NAG	O5-C1	3.36	1.49	1.43
3	A	4401	PGW	O01-C02	-2.47	1.40	1.46
3	A	4401	PGW	O03-C19	2.31	1.40	1.33
3	A	4401	PGW	O03-C01	-2.15	1.40	1.45

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1003	NAG	C1-O5-C5	4.80	118.69	112.19
5	D	1002	NAG	C1-O5-C5	4.73	118.60	112.19
5	D	1002	NAG	C2-N2-C7	4.33	129.07	122.90
3	A	4401	PGW	O01-C1-C2	4.30	120.76	111.50
5	B	1003	NAG	C2-N2-C7	4.24	128.95	122.90

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4401	PGW	C03-O11-P-O14
3	A	4401	PGW	C04-O12-P-O11
3	A	4401	PGW	C04-O12-P-O13
3	A	4401	PGW	C04-O12-P-O14
5	D	1001	NAG	C3-C2-N2-C7

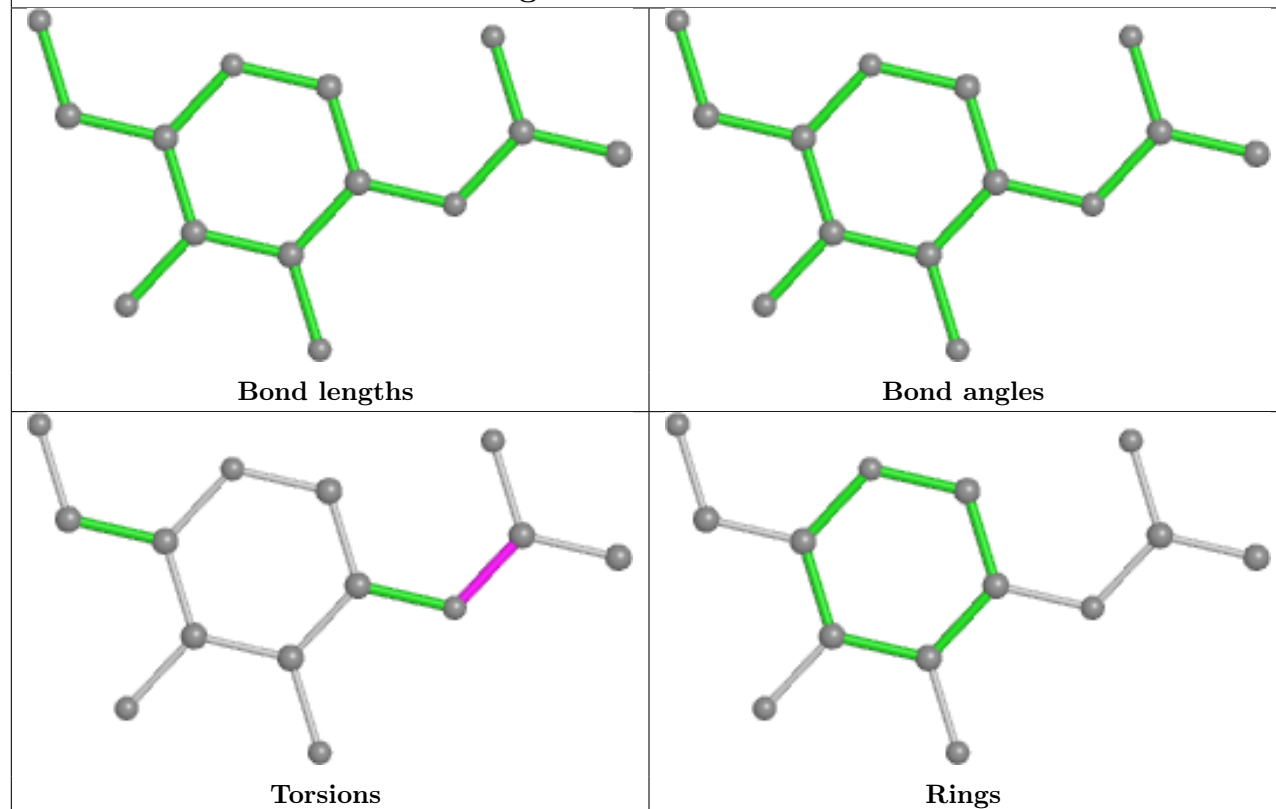
There are no ring outliers.

8 monomers are involved in 14 short contacts:

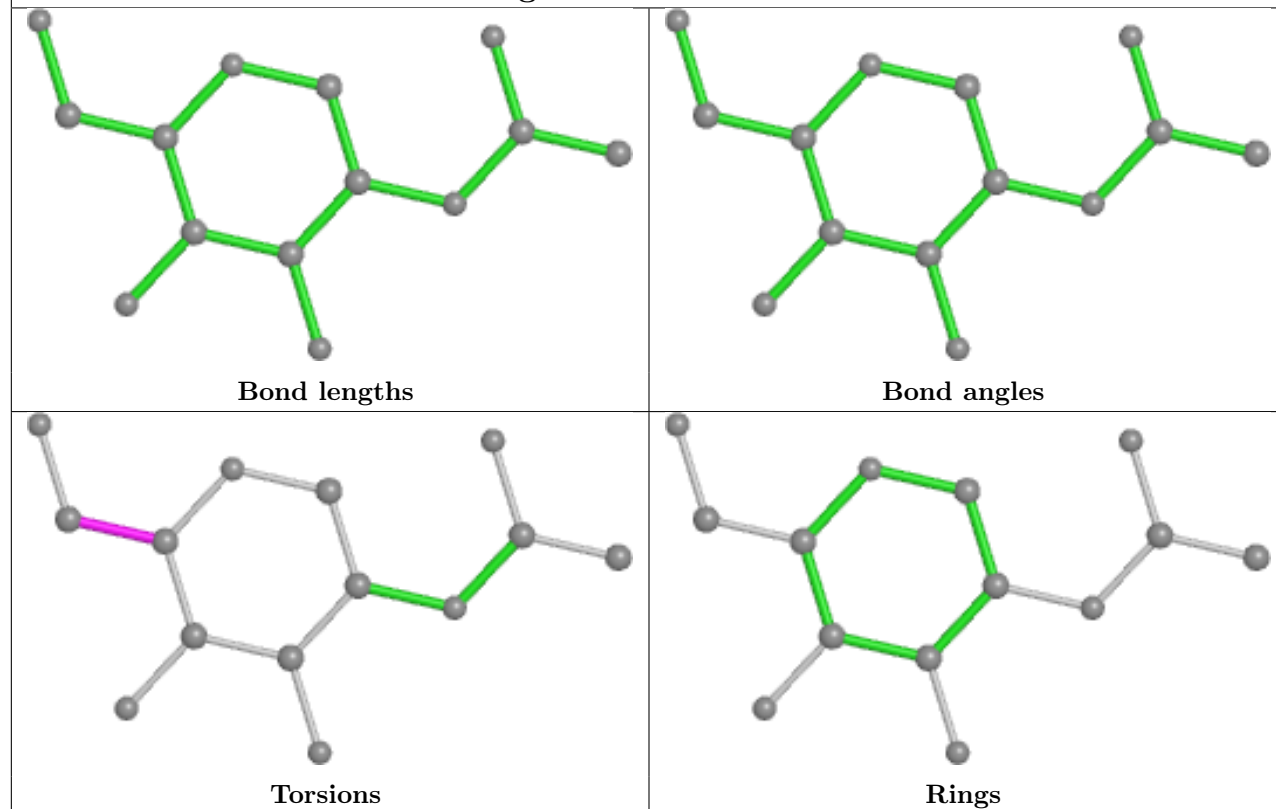
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1002	NAG	1	0
5	D	1002	NAG	1	0
5	B	1002	NAG	1	0
5	C	1003	NAG	1	0
5	C	1004	NAG	1	0
5	B	1003	NAG	1	0
5	D	1001	NAG	3	0
3	A	4401	PGW	5	0

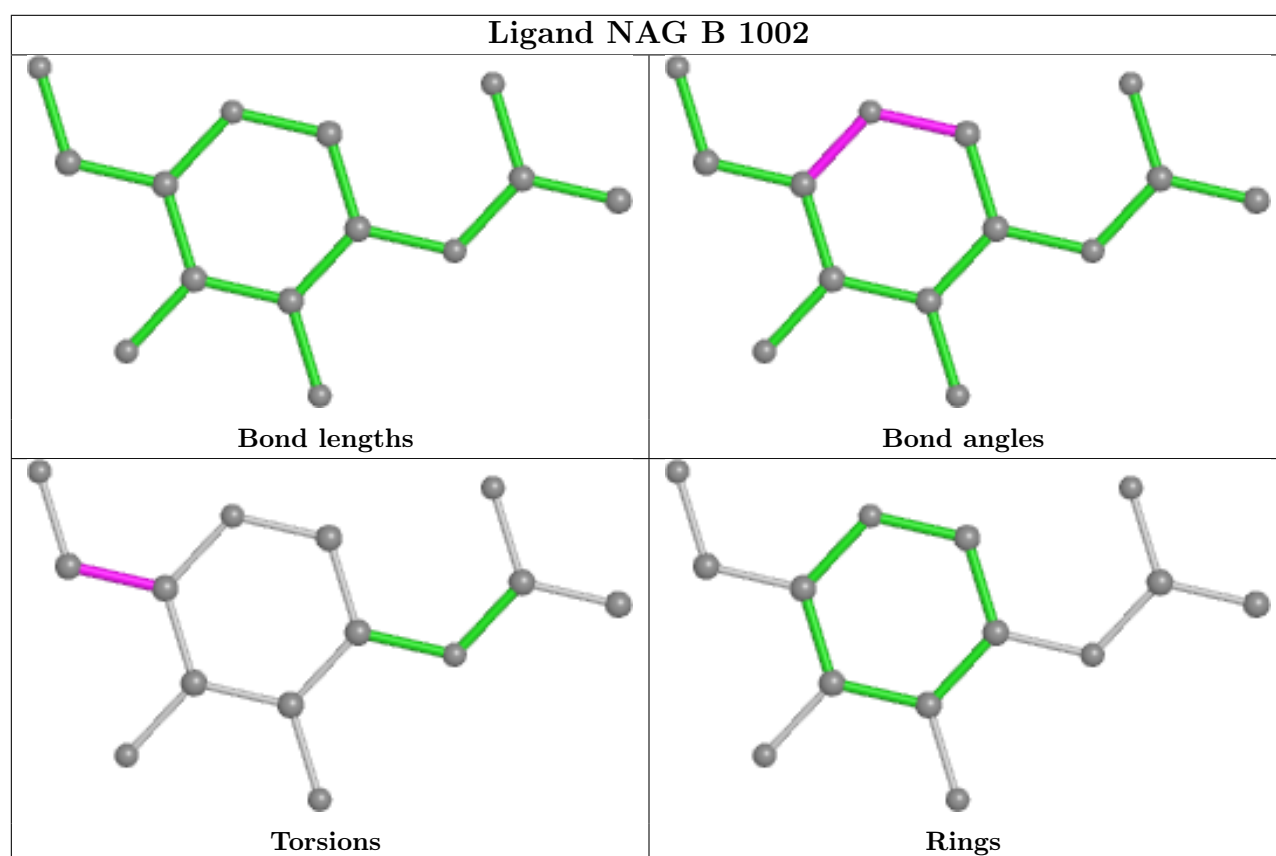
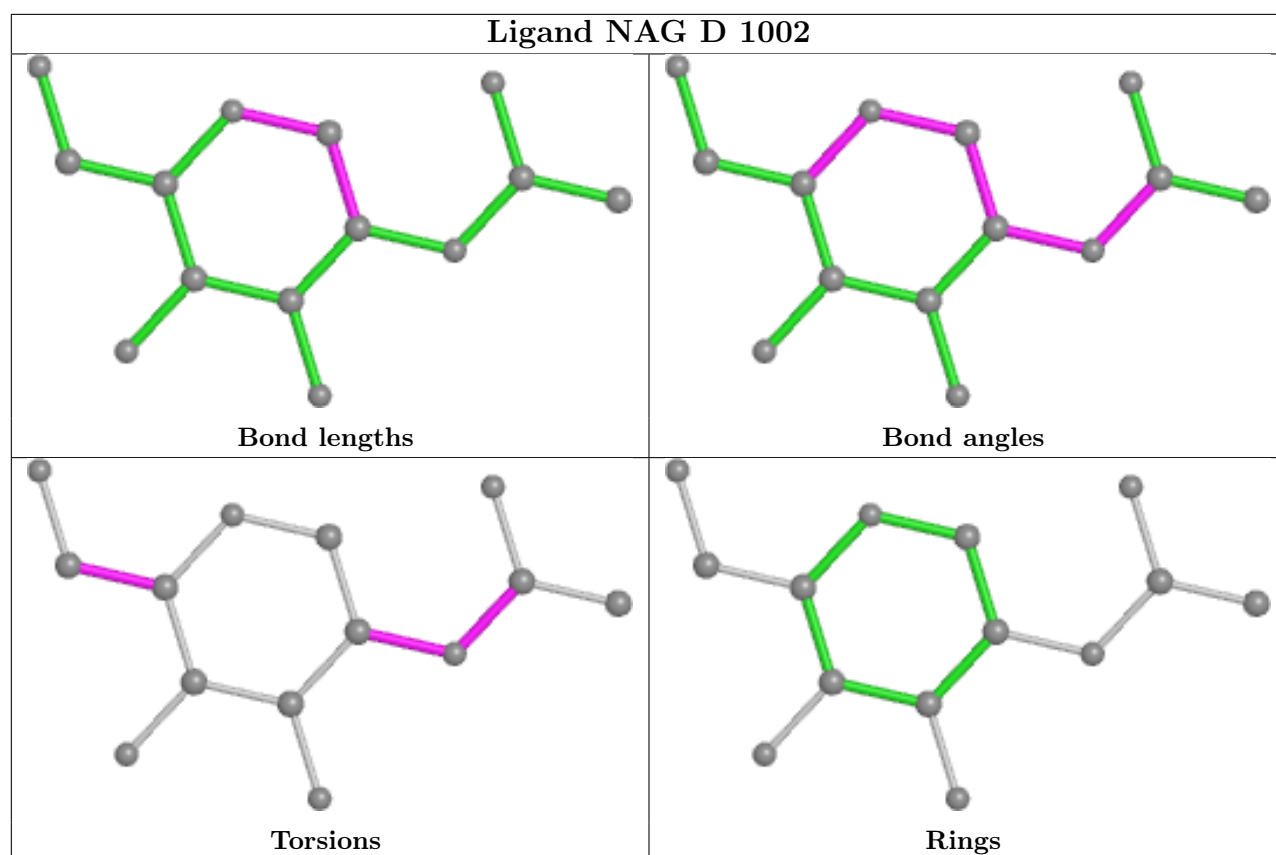
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

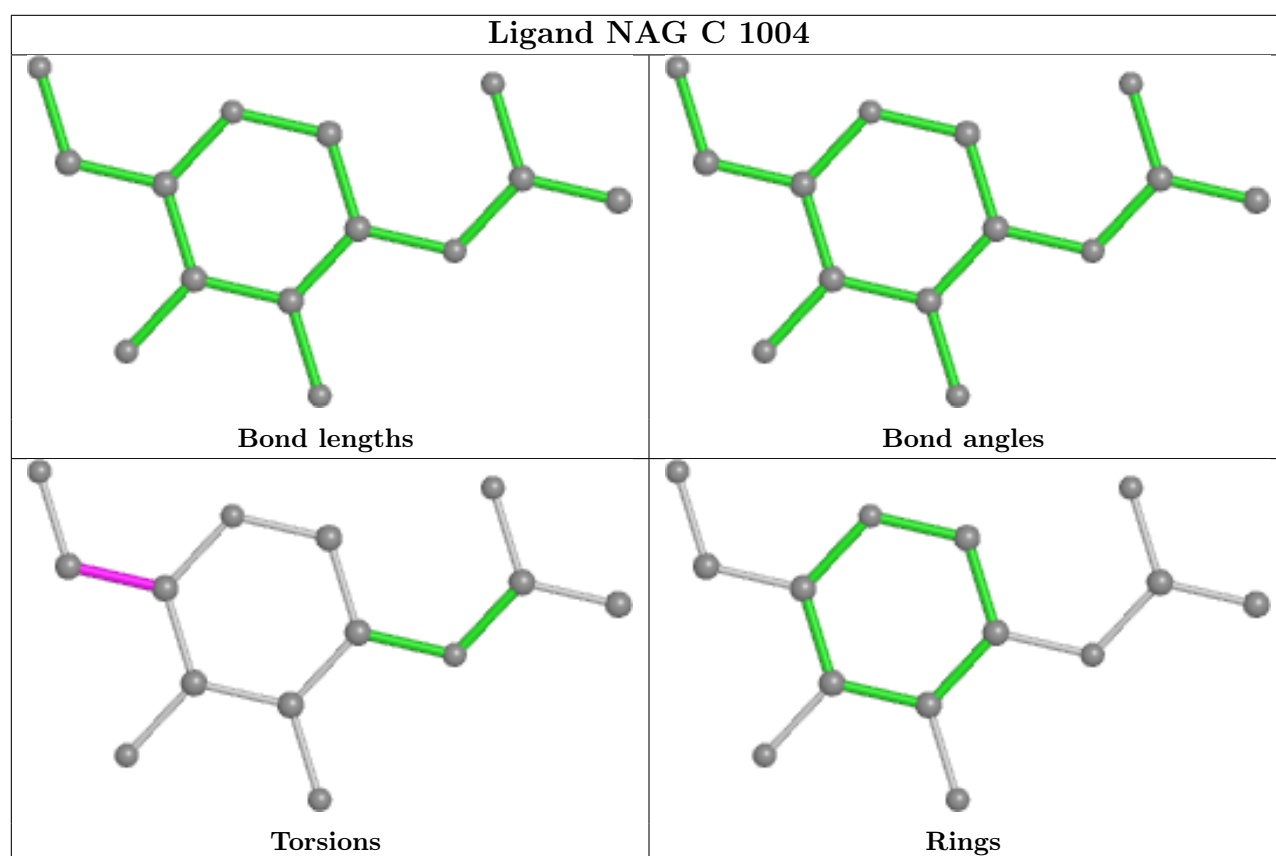
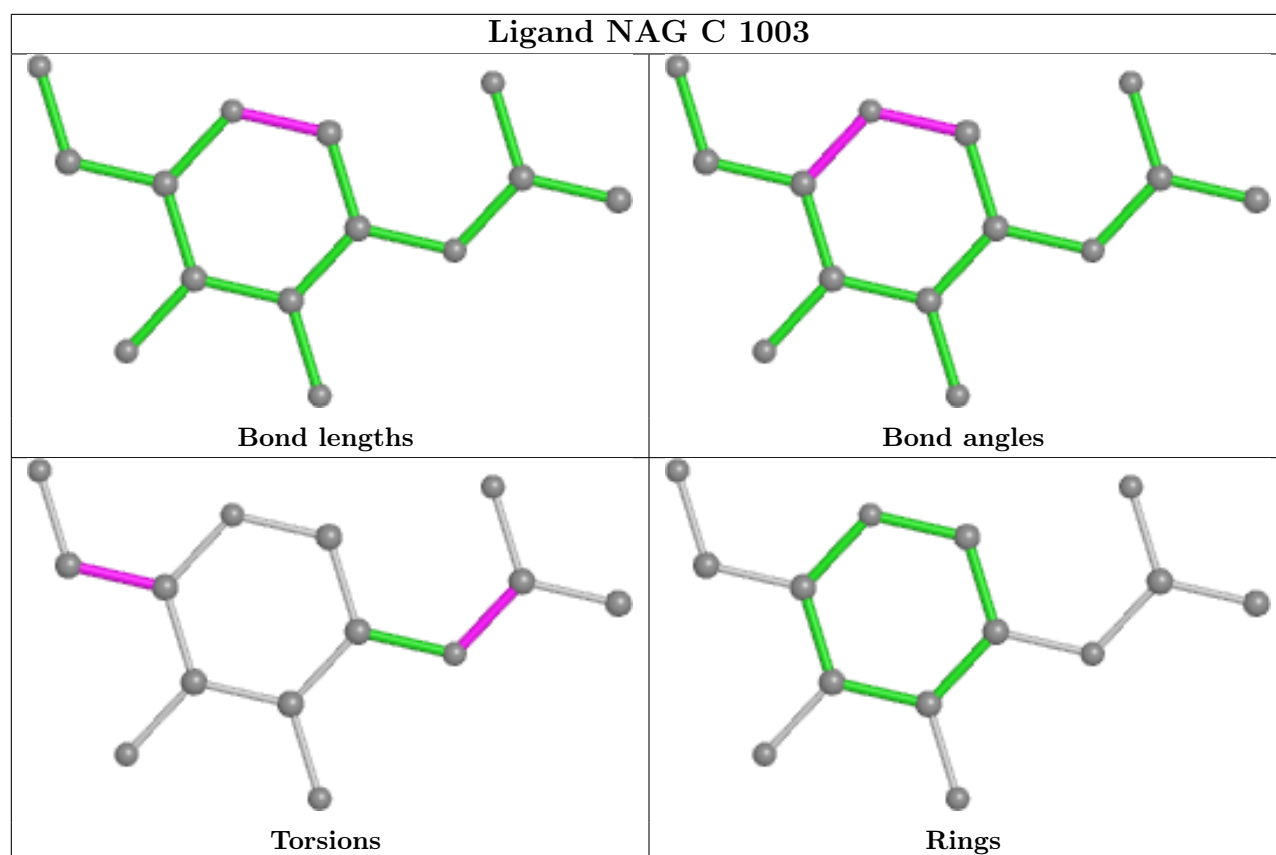
## Ligand NAG C 1002

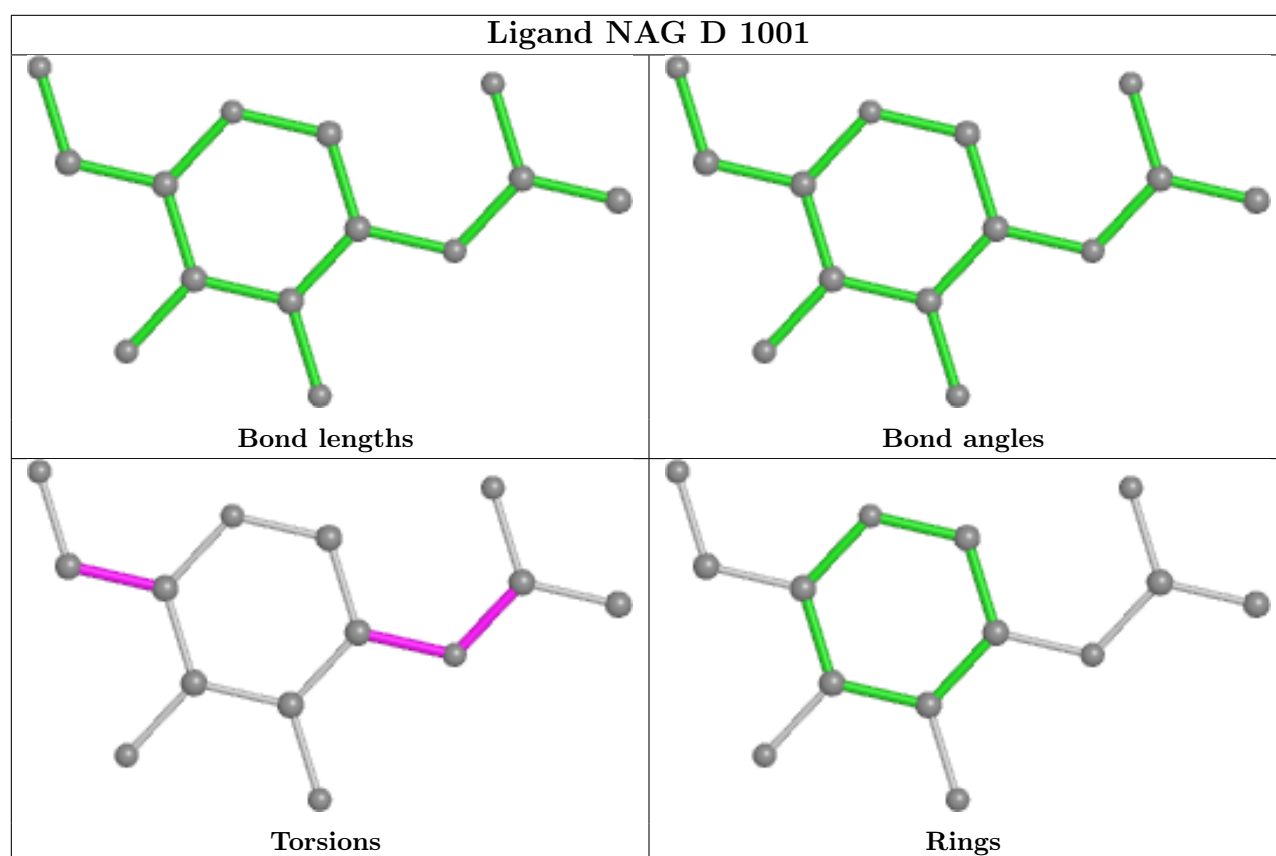
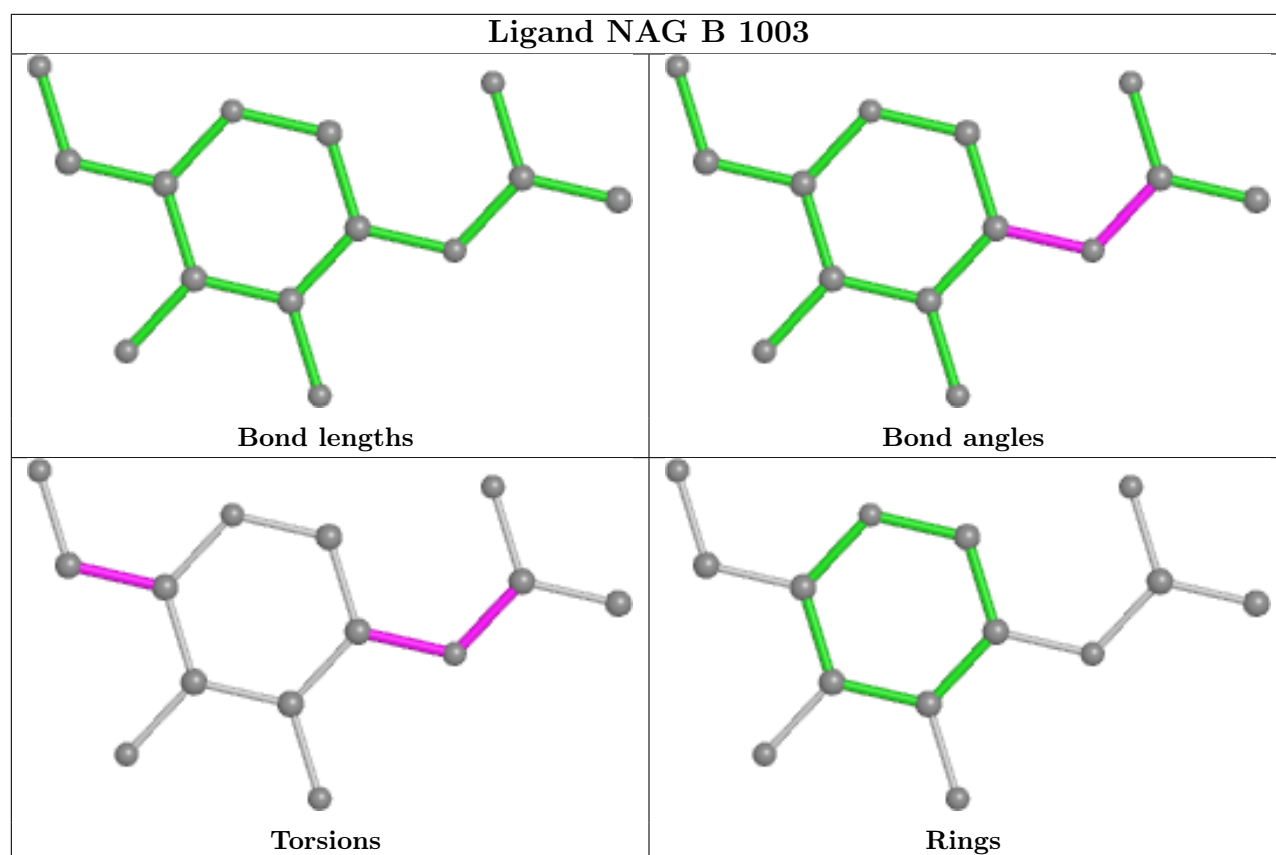


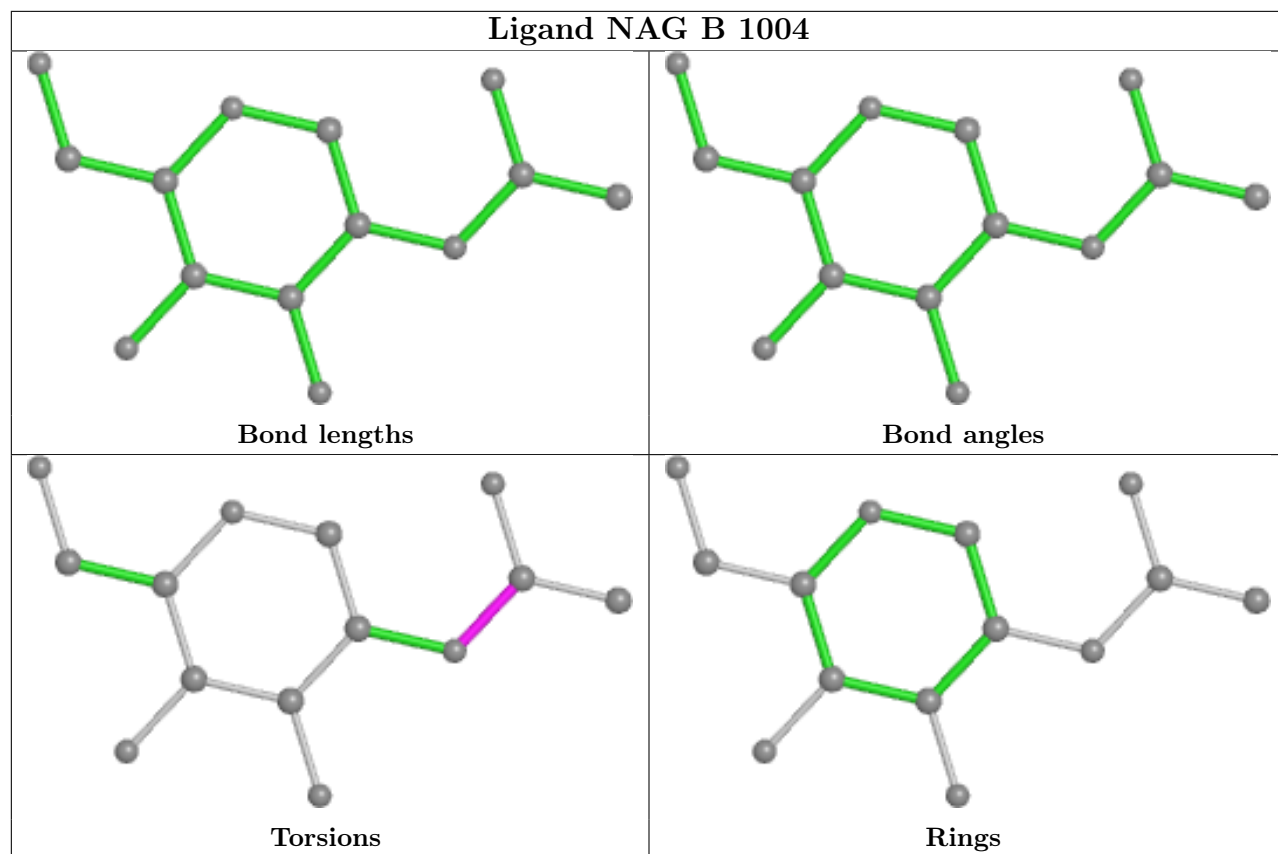
## Ligand NAG D 1003



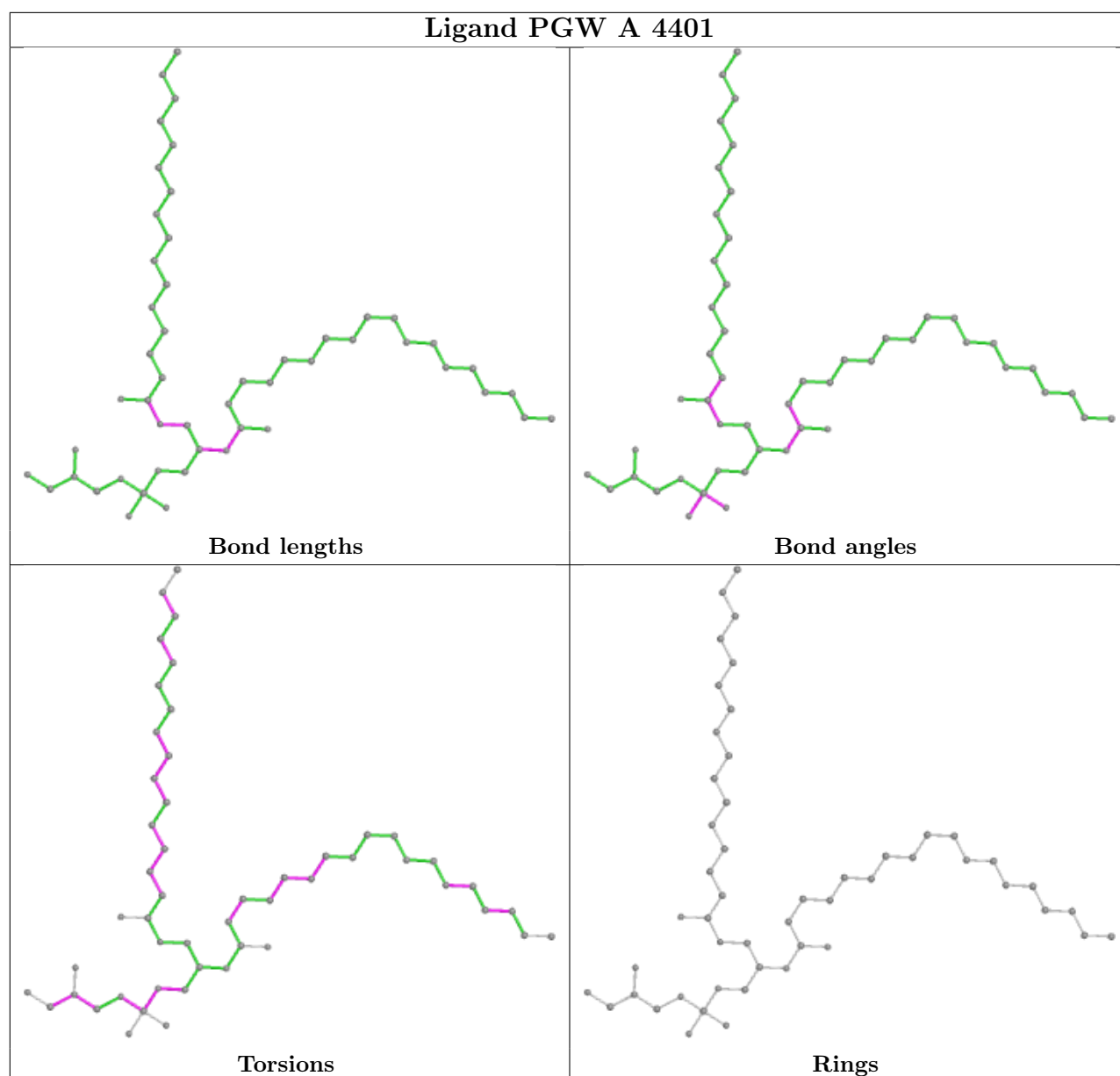












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

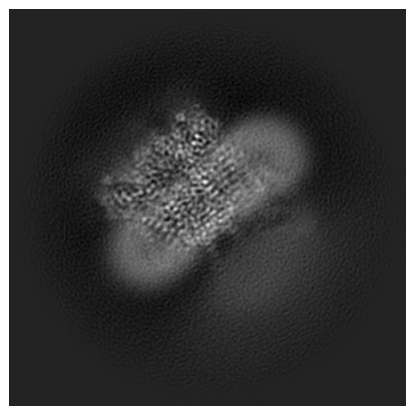
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60196. These allow visual inspection of the internal detail of the map and identification of artifacts.

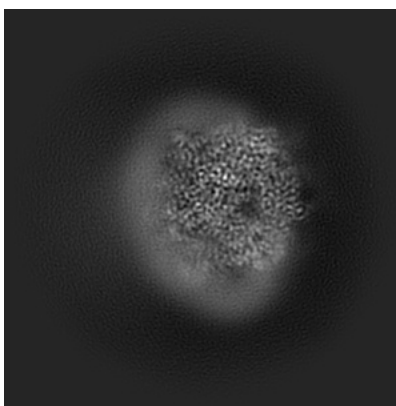
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

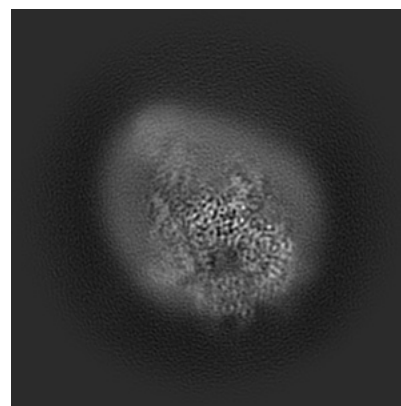
#### 6.1.1 Primary map



X

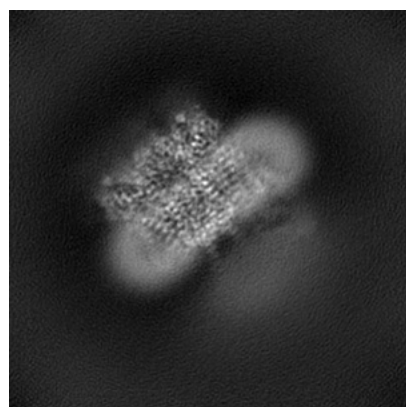


Y

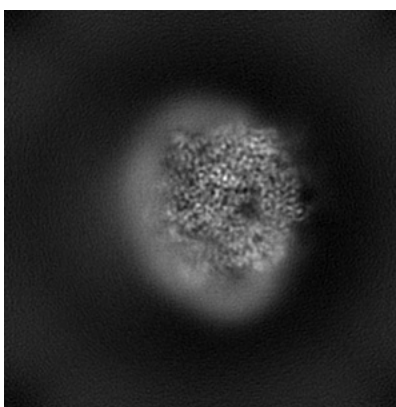


Z

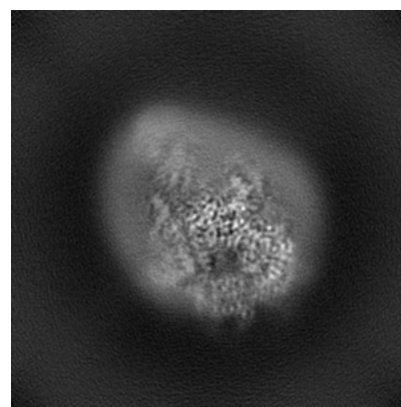
#### 6.1.2 Raw map



X



Y

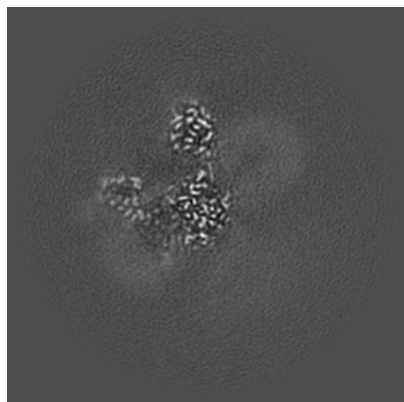


Z

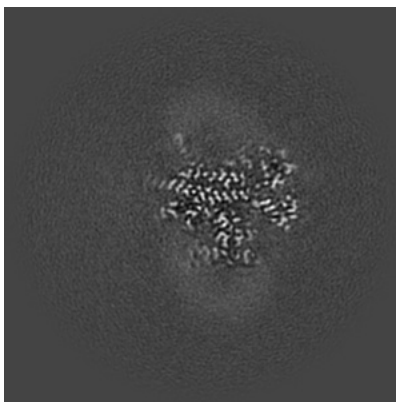
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

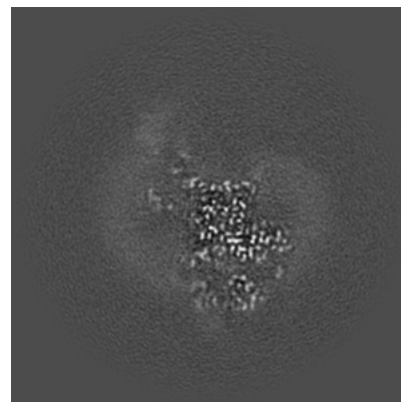
### 6.2.1 Primary map



X Index: 120

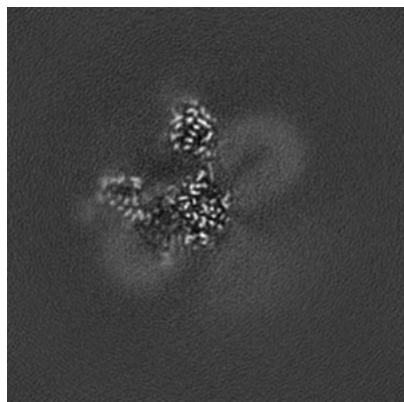


Y Index: 120

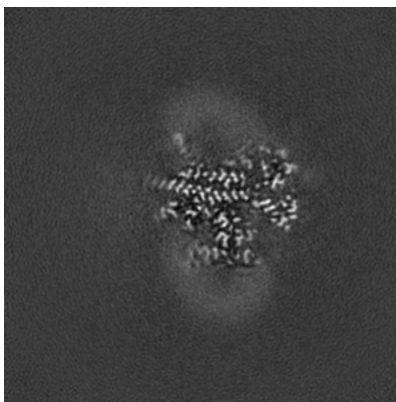


Z Index: 120

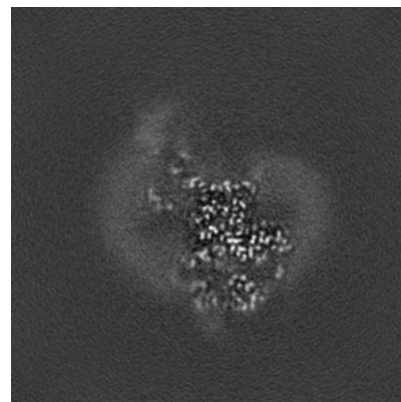
### 6.2.2 Raw map



X Index: 120



Y Index: 120

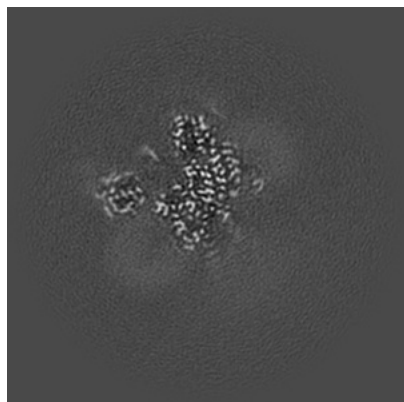


Z Index: 120

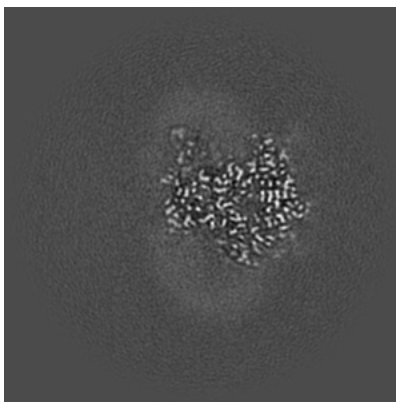
The images above show central slices of the map in three orthogonal directions.

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

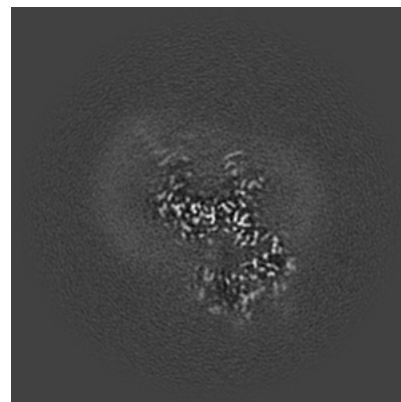
### 6.3.1 Primary map



X Index: 136

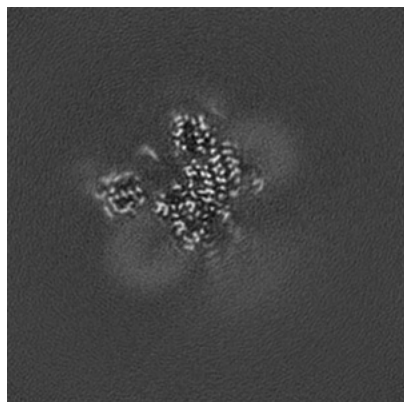


Y Index: 111

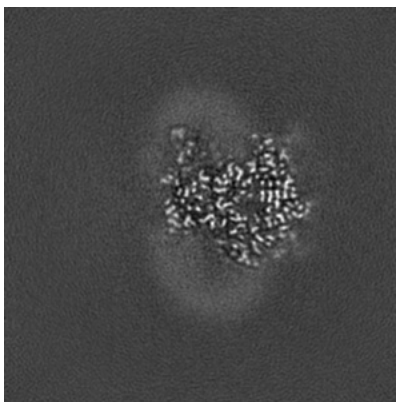


Z Index: 132

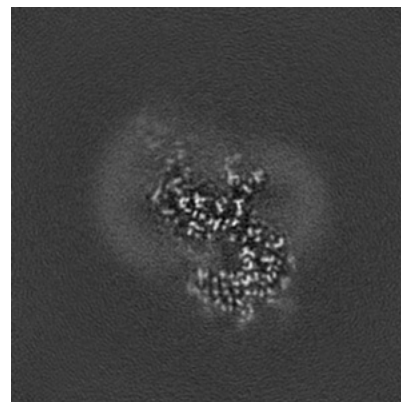
### 6.3.2 Raw map



X Index: 136



Y Index: 111

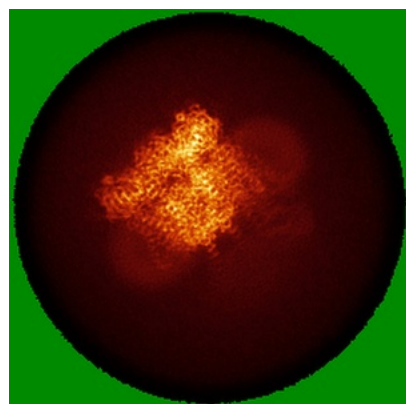


Z Index: 129

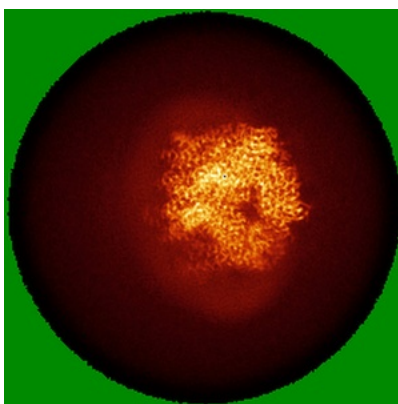
The images above show the largest variance slices of the map in three orthogonal directions.

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

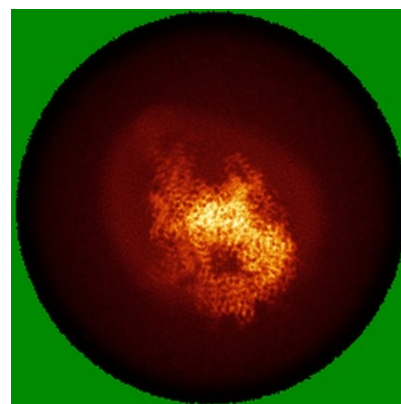
### 6.4.1 Primary map



X

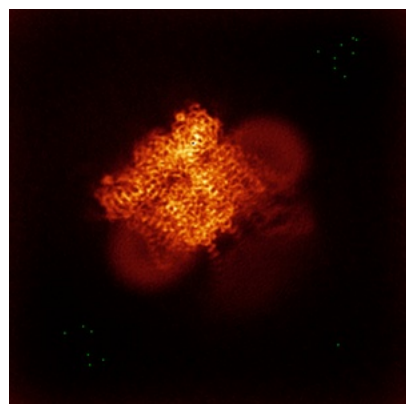


Y

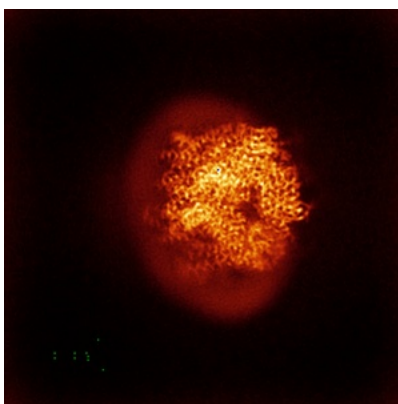


Z

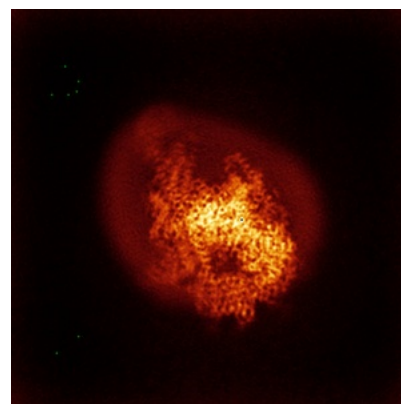
### 6.4.2 Raw map



X



Y



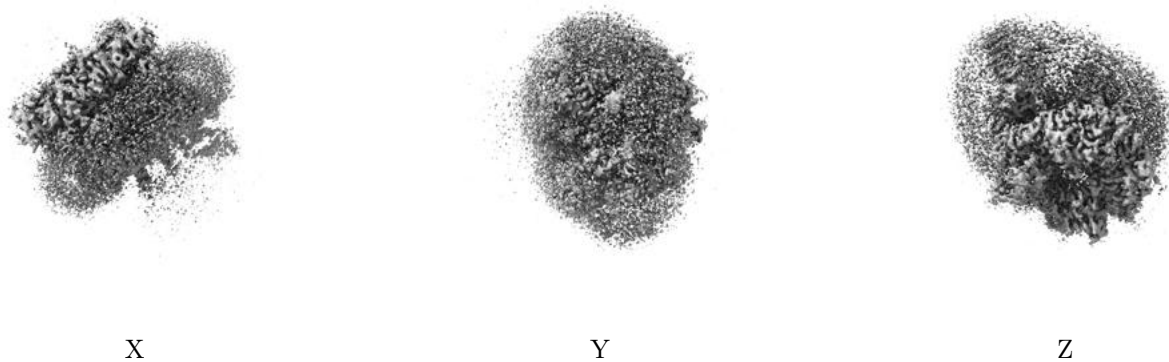
Z

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.



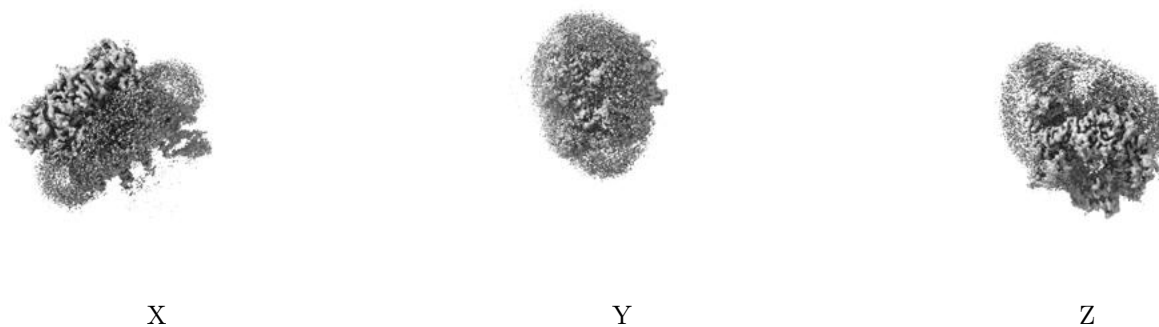
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.34. 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.

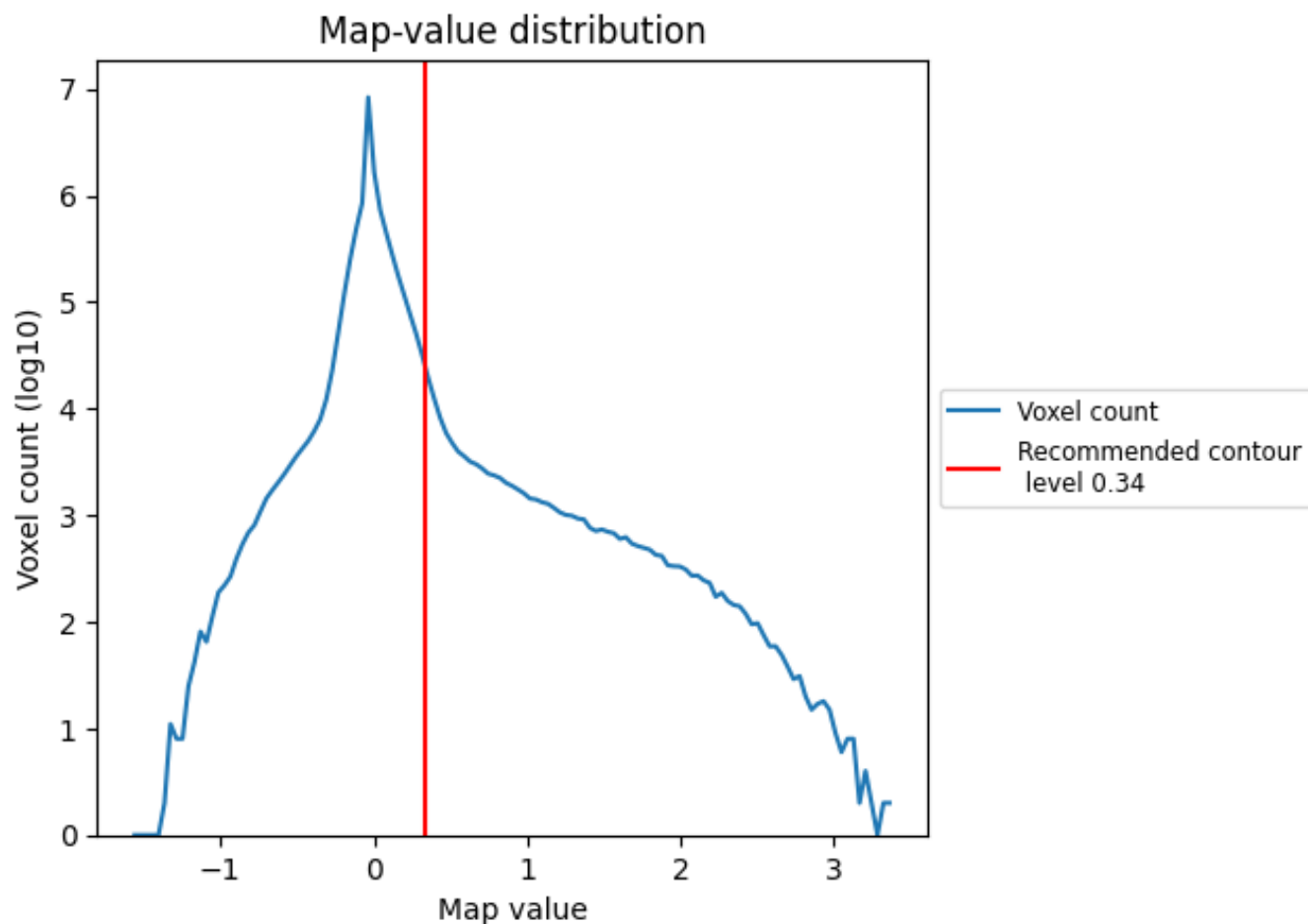
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

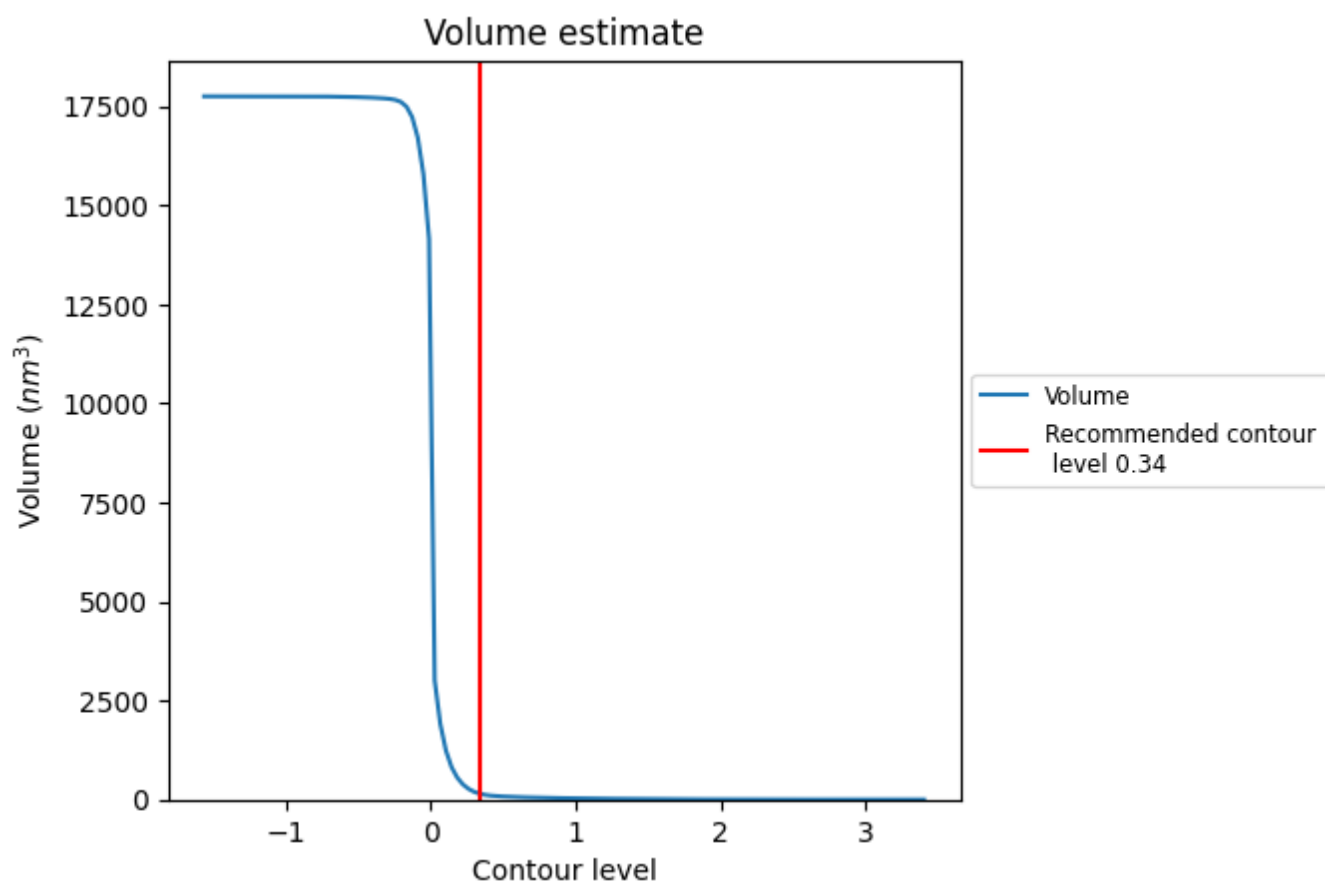
This section contains the results of statistical analysis of the map.

### 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](#)

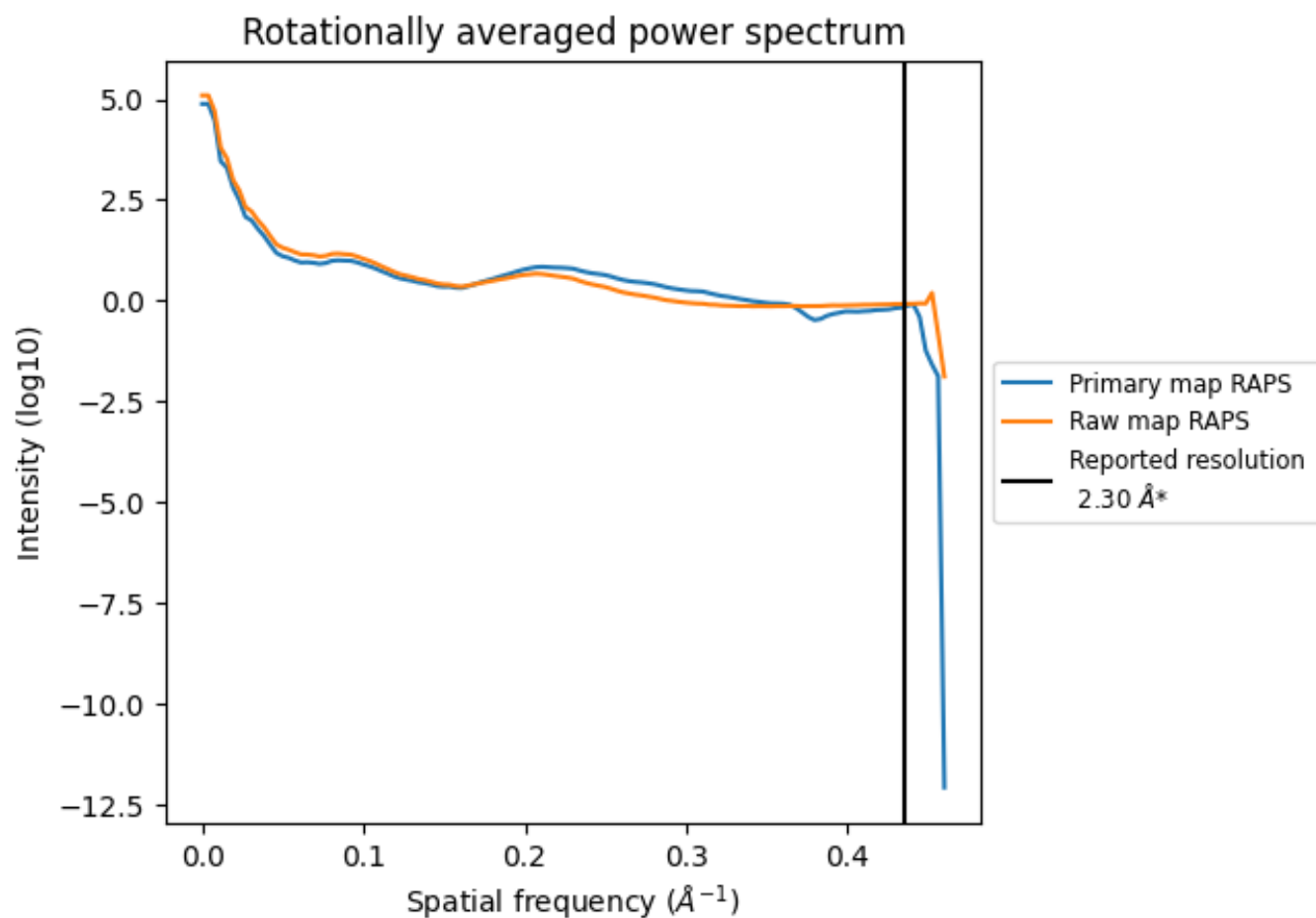


The volume at the recommended contour level is 147 nm<sup>3</sup>; this corresponds to an approximate mass of 133 kDa.

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 ⓘ

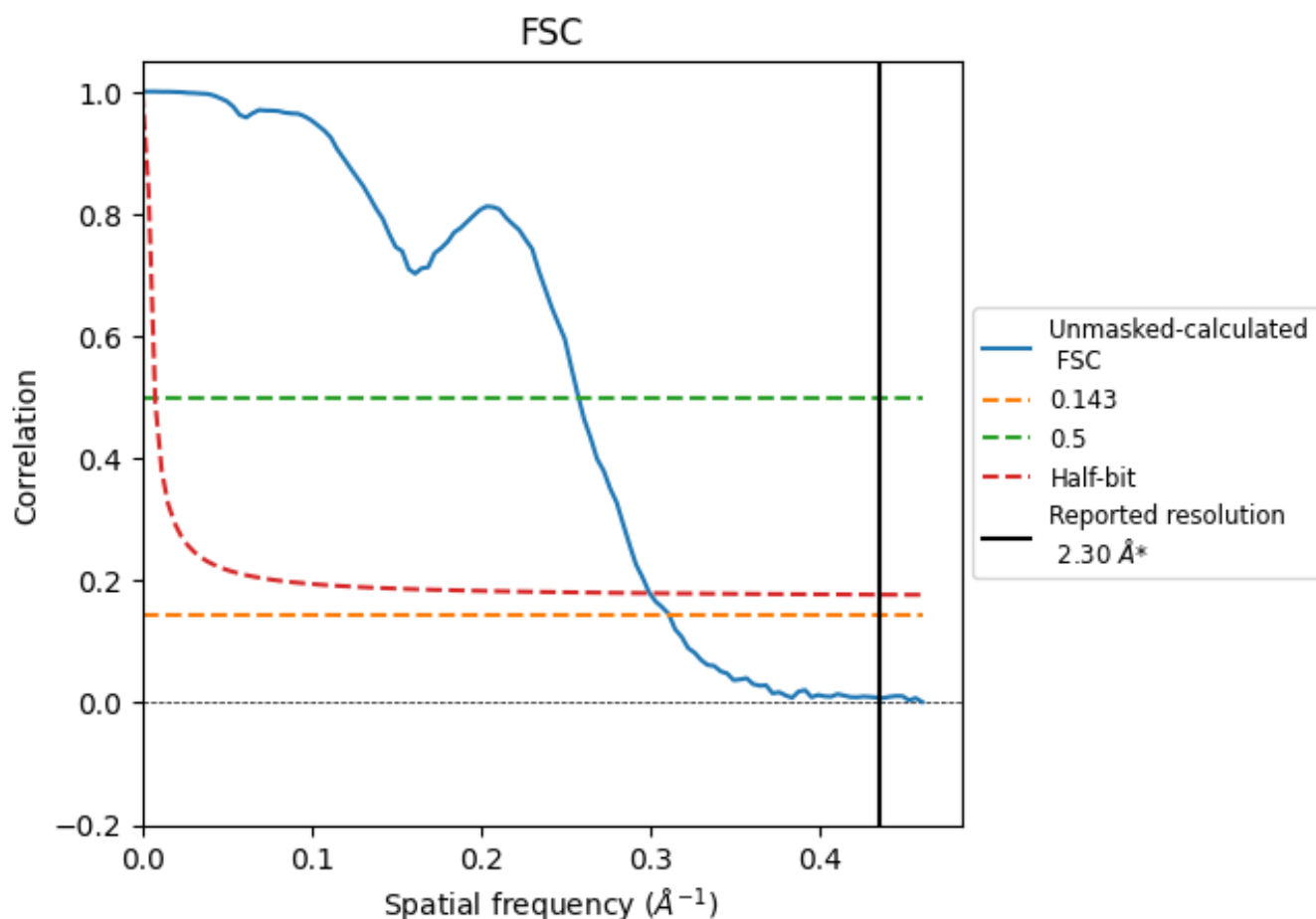


\*Reported resolution corresponds to spatial frequency of 0.435 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.435 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

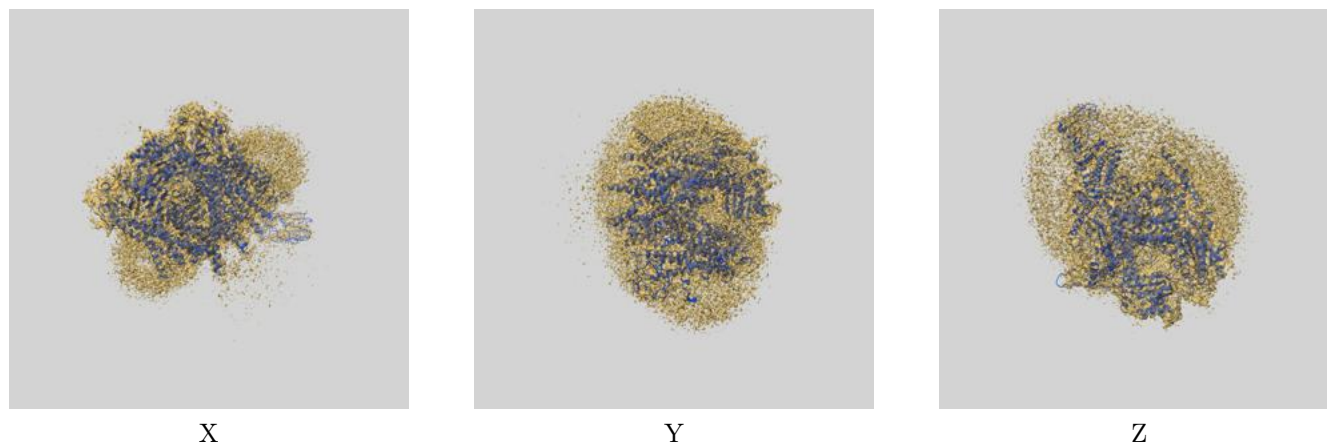
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	3.89	3.34

\*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 3.22 differs from the reported value 2.3 by more than 10 %

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

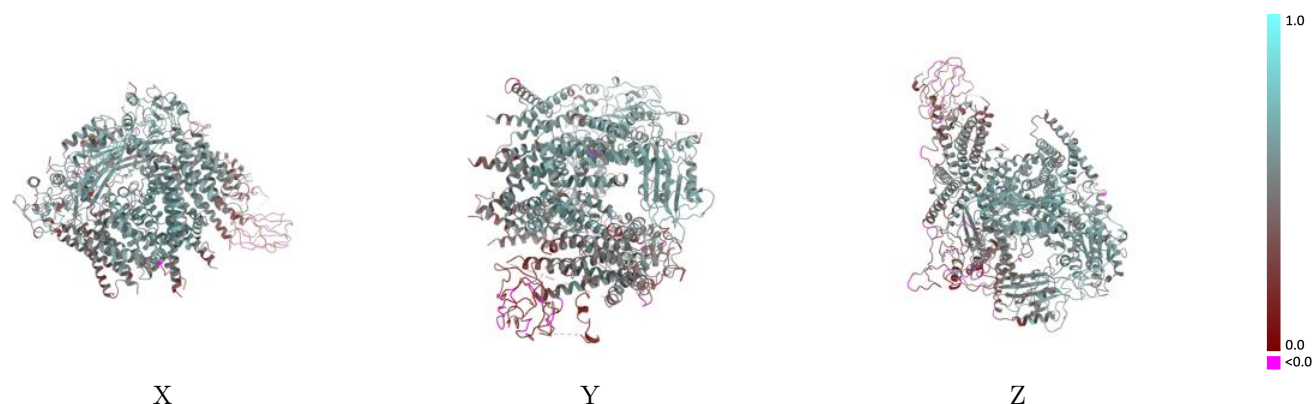
This section contains information regarding the fit between EMDB map EMD-60196 and PDB model 8ZKH. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



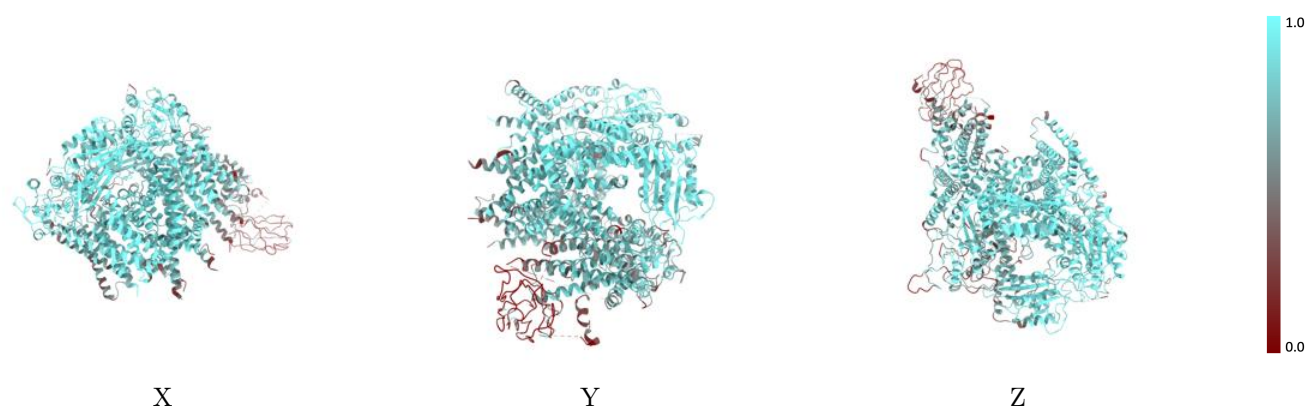
The images above show the 3D surface view of the map at the recommended contour level 0.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



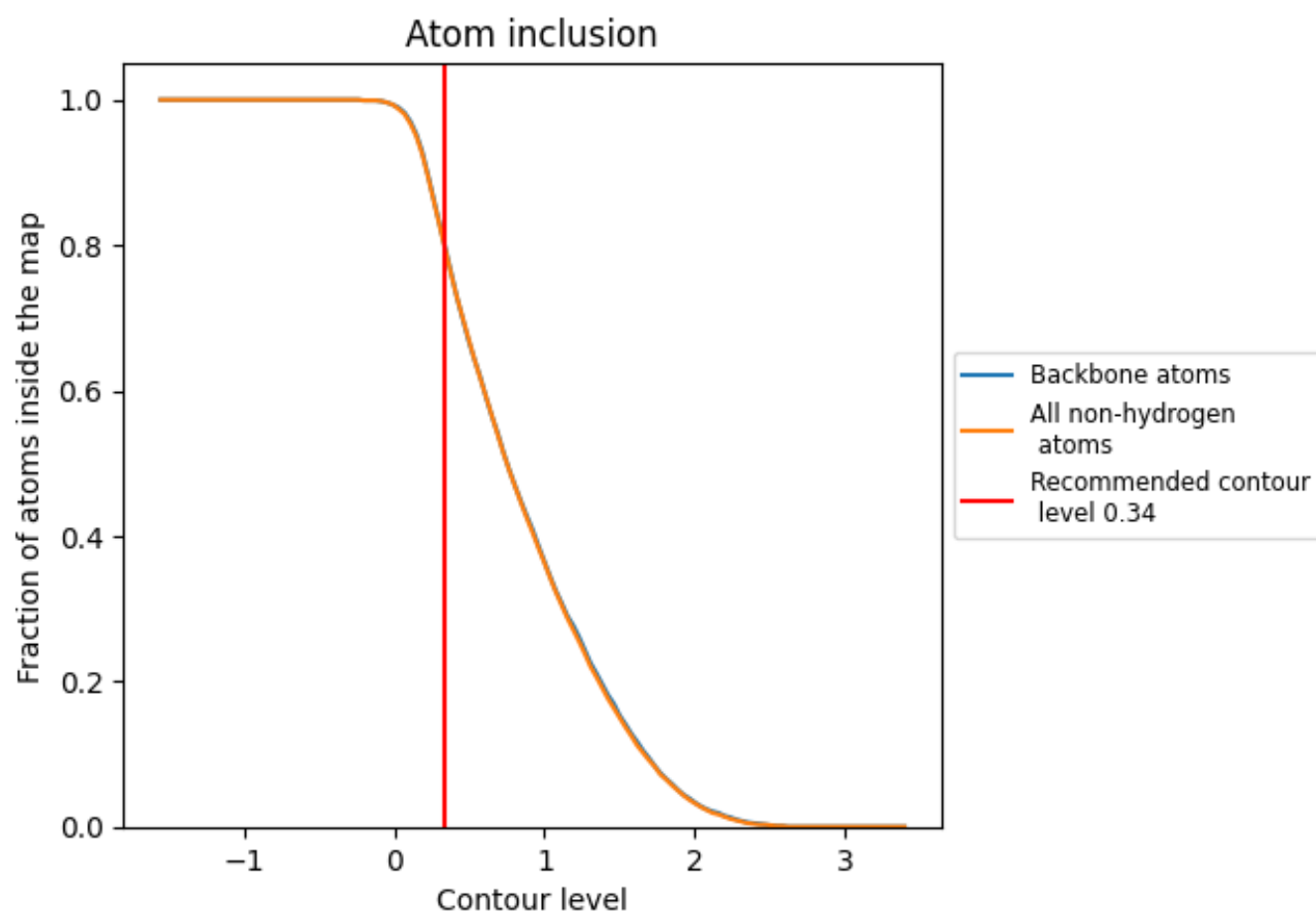
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.34).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7910	<div></div> 0.4930
A	<div></div> 0.6400	<div></div> 0.3930
B	<div></div> 0.8940	<div></div> 0.5650
C	<div></div> 0.8960	<div></div> 0.5670
D	<div></div> 0.7990	<div></div> 0.4840

