



wwPDB EM Validation Summary Report ⓘ

May 19, 2026 – 10:39 AM EDT

PDB ID : 8G81 / pdb_00008g81
EMDB ID : EMD-29831
Title : Cryo-EM structure of full length Neuroligin-2 from Mouse bound to two
Neurexin-1 Beta conformation three
Authors : Boyd, R.; Wang, W.
Deposited on : 2023-02-17
Resolution : 3.22 Å(reported)
Based on initial model : 3BL8

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

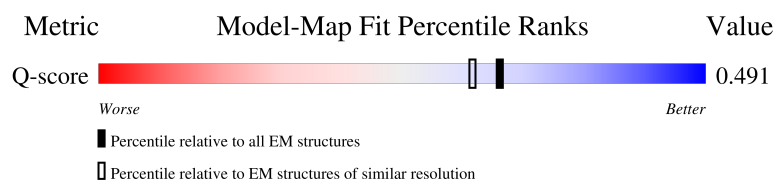
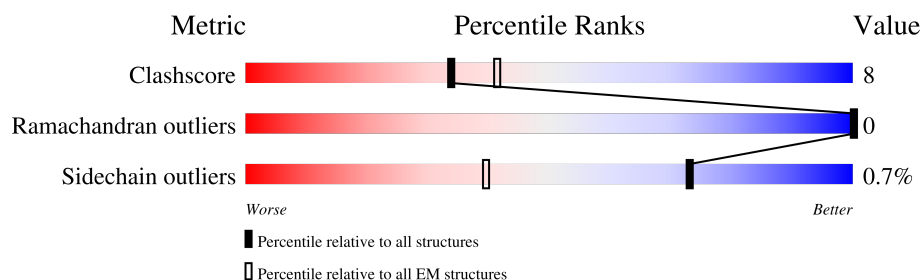
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.72 - 3.72)

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	870	 51% 11% 38%
1	B	870	 50% 11% 38%
2	C	470	 8% 28% 9% 62%
2	D	470	 8% 29% 9% 62%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11148 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 Neuroligin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	539	Total	C	N	O	S	0	0
			4180	2676	716	770	18		
1	B	539	Total	C	N	O	S	0	0
			4176	2674	716	768	18		

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-41	MET	-	initiating methionine	UNP Q62888
A	-40	ALA	-	expression tag	UNP Q62888
A	-39	LEU	-	expression tag	UNP Q62888
A	-38	PRO	-	expression tag	UNP Q62888
A	-37	ARG	-	expression tag	UNP Q62888
A	-36	CYS	-	expression tag	UNP Q62888
A	-35	MET	-	expression tag	UNP Q62888
A	-34	TRP	-	expression tag	UNP Q62888
A	-33	PRO	-	expression tag	UNP Q62888
A	-32	ASN	-	expression tag	UNP Q62888
A	-31	TYR	-	expression tag	UNP Q62888
A	-30	VAL	-	expression tag	UNP Q62888
A	-29	TRP	-	expression tag	UNP Q62888
A	-28	ARG	-	expression tag	UNP Q62888
A	-27	ALA	-	expression tag	UNP Q62888
A	-26	MET	-	expression tag	UNP Q62888
A	-25	MET	-	expression tag	UNP Q62888
A	-24	ALA	-	expression tag	UNP Q62888
A	-23	CYS	-	expression tag	UNP Q62888
A	-22	VAL	-	expression tag	UNP Q62888
A	-21	VAL	-	expression tag	UNP Q62888
A	-20	HIS	-	expression tag	UNP Q62888
A	-19	ARG	-	expression tag	UNP Q62888
A	-18	GLY	-	expression tag	UNP Q62888
A	-17	SER	-	expression tag	UNP Q62888
A	-16	GLY	-	expression tag	UNP Q62888

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	ALA	-	expression tag	UNP Q62888
A	-14	PRO	-	expression tag	UNP Q62888
A	-13	LEU	-	expression tag	UNP Q62888
A	-12	THR	-	expression tag	UNP Q62888
A	-11	LEU	-	expression tag	UNP Q62888
A	-10	CYS	-	expression tag	UNP Q62888
A	-9	LEU	-	expression tag	UNP Q62888
A	-8	LEU	-	expression tag	UNP Q62888
A	-7	GLY	-	expression tag	UNP Q62888
A	-6	CYS	-	expression tag	UNP Q62888
A	-5	LEU	-	expression tag	UNP Q62888
A	-4	LEU	-	expression tag	UNP Q62888
A	-3	GLN	-	expression tag	UNP Q62888
A	-2	THR	-	expression tag	UNP Q62888
A	-1	PHE	-	expression tag	UNP Q62888
A	0	HIS	-	expression tag	UNP Q62888
A	1	VAL	-	expression tag	UNP Q62888
A	2	LEU	-	expression tag	UNP Q62888
A	3	SER	-	expression tag	UNP Q62888
A	4	GLN	-	expression tag	UNP Q62888
A	5	LYS	-	expression tag	UNP Q62888
A	6	TYR	-	expression tag	UNP Q62888
A	7	PRO	-	expression tag	UNP Q62888
A	8	TYR	-	expression tag	UNP Q62888
A	9	ASP	-	expression tag	UNP Q62888
A	10	VAL	-	expression tag	UNP Q62888
A	11	PRO	-	expression tag	UNP Q62888
A	12	ASP	-	expression tag	UNP Q62888
A	13	TYR	-	expression tag	UNP Q62888
A	210	VAL	ALA	conflict	UNP Q62888
A	837	SER	-	expression tag	UNP Q62888
A	838	ASN	-	expression tag	UNP Q62888
A	839	SER	-	expression tag	UNP Q62888
A	840	LEU	-	expression tag	UNP Q62888
A	841	GLU	-	expression tag	UNP Q62888
A	842	VAL	-	expression tag	UNP Q62888
A	843	LEU	-	expression tag	UNP Q62888
A	844	PHE	-	expression tag	UNP Q62888
A	845	GLN	-	expression tag	UNP Q62888
B	-41	MET	-	initiating methionine	UNP Q62888
B	-40	ALA	-	expression tag	UNP Q62888
B	-39	LEU	-	expression tag	UNP Q62888

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	PRO	-	expression tag	UNP Q62888
B	-37	ARG	-	expression tag	UNP Q62888
B	-36	CYS	-	expression tag	UNP Q62888
B	-35	MET	-	expression tag	UNP Q62888
B	-34	TRP	-	expression tag	UNP Q62888
B	-33	PRO	-	expression tag	UNP Q62888
B	-32	ASN	-	expression tag	UNP Q62888
B	-31	TYR	-	expression tag	UNP Q62888
B	-30	VAL	-	expression tag	UNP Q62888
B	-29	TRP	-	expression tag	UNP Q62888
B	-28	ARG	-	expression tag	UNP Q62888
B	-27	ALA	-	expression tag	UNP Q62888
B	-26	MET	-	expression tag	UNP Q62888
B	-25	MET	-	expression tag	UNP Q62888
B	-24	ALA	-	expression tag	UNP Q62888
B	-23	CYS	-	expression tag	UNP Q62888
B	-22	VAL	-	expression tag	UNP Q62888
B	-21	VAL	-	expression tag	UNP Q62888
B	-20	HIS	-	expression tag	UNP Q62888
B	-19	ARG	-	expression tag	UNP Q62888
B	-18	GLY	-	expression tag	UNP Q62888
B	-17	SER	-	expression tag	UNP Q62888
B	-16	GLY	-	expression tag	UNP Q62888
B	-15	ALA	-	expression tag	UNP Q62888
B	-14	PRO	-	expression tag	UNP Q62888
B	-13	LEU	-	expression tag	UNP Q62888
B	-12	THR	-	expression tag	UNP Q62888
B	-11	LEU	-	expression tag	UNP Q62888
B	-10	CYS	-	expression tag	UNP Q62888
B	-9	LEU	-	expression tag	UNP Q62888
B	-8	LEU	-	expression tag	UNP Q62888
B	-7	GLY	-	expression tag	UNP Q62888
B	-6	CYS	-	expression tag	UNP Q62888
B	-5	LEU	-	expression tag	UNP Q62888
B	-4	LEU	-	expression tag	UNP Q62888
B	-3	GLN	-	expression tag	UNP Q62888
B	-2	THR	-	expression tag	UNP Q62888
B	-1	PHE	-	expression tag	UNP Q62888
B	0	HIS	-	expression tag	UNP Q62888
B	1	VAL	-	expression tag	UNP Q62888
B	2	LEU	-	expression tag	UNP Q62888
B	3	SER	-	expression tag	UNP Q62888

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	-	expression tag	UNP Q62888
B	5	LYS	-	expression tag	UNP Q62888
B	6	TYR	-	expression tag	UNP Q62888
B	7	PRO	-	expression tag	UNP Q62888
B	8	TYR	-	expression tag	UNP Q62888
B	9	ASP	-	expression tag	UNP Q62888
B	10	VAL	-	expression tag	UNP Q62888
B	11	PRO	-	expression tag	UNP Q62888
B	12	ASP	-	expression tag	UNP Q62888
B	13	TYR	-	expression tag	UNP Q62888
B	210	VAL	ALA	conflict	UNP Q62888
B	837	SER	-	expression tag	UNP Q62888
B	838	ASN	-	expression tag	UNP Q62888
B	839	SER	-	expression tag	UNP Q62888
B	840	LEU	-	expression tag	UNP Q62888
B	841	GLU	-	expression tag	UNP Q62888
B	842	VAL	-	expression tag	UNP Q62888
B	843	LEU	-	expression tag	UNP Q62888
B	844	PHE	-	expression tag	UNP Q62888
B	845	GLN	-	expression tag	UNP Q62888

- Molecule 2 is a protein called Neurexin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	177	Total	C	N	O	S	0	0
			1353	853	241	258	1		
2	D	177	Total	C	N	O	S	0	0
			1353	853	241	258	1		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	15	GLY	SER	conflict	UNP E0CZA5
C	40	LYS	-	insertion	UNP E0CZA5
C	41	GLU	-	insertion	UNP E0CZA5
C	42	PHE	-	insertion	UNP E0CZA5
C	43	GLU	-	insertion	UNP E0CZA5
C	44	GLN	-	insertion	UNP E0CZA5
C	45	LYS	-	insertion	UNP E0CZA5
C	46	LEU	-	insertion	UNP E0CZA5
C	47	ILE	-	insertion	UNP E0CZA5
C	48	SER	-	insertion	UNP E0CZA5

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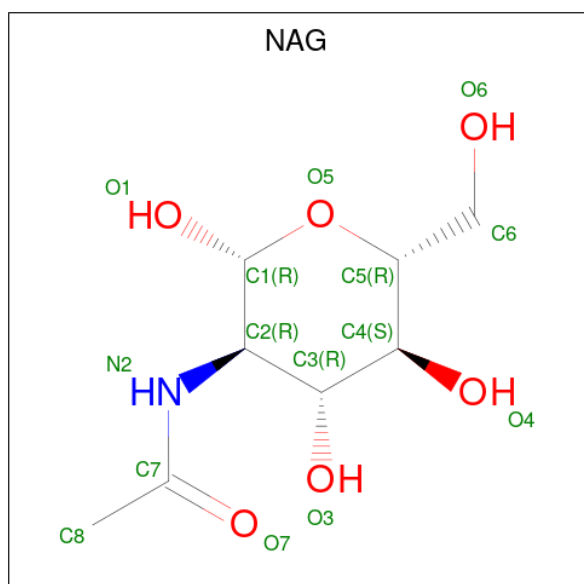
Chain	Residue	Modelled	Actual	Comment	Reference
C	49	GLU	-	insertion	UNP E0CZA5
C	50	GLU	-	insertion	UNP E0CZA5
C	51	ASP	-	insertion	UNP E0CZA5
C	52	LEU	-	insertion	UNP E0CZA5
C	53	GLY	-	insertion	UNP E0CZA5
C	54	PHE	-	insertion	UNP E0CZA5
C	55	GLU	-	insertion	UNP E0CZA5
C	56	ILE	-	insertion	UNP E0CZA5
C	57	ASP	-	insertion	UNP E0CZA5
C	58	LYS	-	insertion	UNP E0CZA5
C	59	VAL	-	insertion	UNP E0CZA5
C	60	TRP	-	insertion	UNP E0CZA5
C	61	HIS	-	insertion	UNP E0CZA5
C	62	ASP	-	insertion	UNP E0CZA5
C	63	PHE	-	insertion	UNP E0CZA5
C	64	PRO	-	insertion	UNP E0CZA5
C	65	ALA	-	insertion	UNP E0CZA5
C	66	THR	-	insertion	UNP E0CZA5
C	67	SER	-	insertion	UNP E0CZA5
C	469	SER	-	expression tag	UNP E0CZA5
C	470	ASN	-	expression tag	UNP E0CZA5
C	471	SER	-	expression tag	UNP E0CZA5
C	472	LEU	-	expression tag	UNP E0CZA5
C	473	GLU	-	expression tag	UNP E0CZA5
C	474	VAL	-	expression tag	UNP E0CZA5
C	475	LEU	-	expression tag	UNP E0CZA5
C	476	PHE	-	expression tag	UNP E0CZA5
C	477	GLN	-	expression tag	UNP E0CZA5
D	15	GLY	SER	conflict	UNP E0CZA5
D	40	LYS	-	insertion	UNP E0CZA5
D	41	GLU	-	insertion	UNP E0CZA5
D	42	PHE	-	insertion	UNP E0CZA5
D	43	GLU	-	insertion	UNP E0CZA5
D	44	GLN	-	insertion	UNP E0CZA5
D	45	LYS	-	insertion	UNP E0CZA5
D	46	LEU	-	insertion	UNP E0CZA5
D	47	ILE	-	insertion	UNP E0CZA5
D	48	SER	-	insertion	UNP E0CZA5
D	49	GLU	-	insertion	UNP E0CZA5
D	50	GLU	-	insertion	UNP E0CZA5
D	51	ASP	-	insertion	UNP E0CZA5
D	52	LEU	-	insertion	UNP E0CZA5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	53	GLY	-	insertion	UNP E0CZA5
D	54	PHE	-	insertion	UNP E0CZA5
D	55	GLU	-	insertion	UNP E0CZA5
D	56	ILE	-	insertion	UNP E0CZA5
D	57	ASP	-	insertion	UNP E0CZA5
D	58	LYS	-	insertion	UNP E0CZA5
D	59	VAL	-	insertion	UNP E0CZA5
D	60	TRP	-	insertion	UNP E0CZA5
D	61	HIS	-	insertion	UNP E0CZA5
D	62	ASP	-	insertion	UNP E0CZA5
D	63	PHE	-	insertion	UNP E0CZA5
D	64	PRO	-	insertion	UNP E0CZA5
D	65	ALA	-	insertion	UNP E0CZA5
D	66	THR	-	insertion	UNP E0CZA5
D	67	SER	-	insertion	UNP E0CZA5
D	469	SER	-	expression tag	UNP E0CZA5
D	470	ASN	-	expression tag	UNP E0CZA5
D	471	SER	-	expression tag	UNP E0CZA5
D	472	LEU	-	expression tag	UNP E0CZA5
D	473	GLU	-	expression tag	UNP E0CZA5
D	474	VAL	-	expression tag	UNP E0CZA5
D	475	LEU	-	expression tag	UNP E0CZA5
D	476	PHE	-	expression tag	UNP E0CZA5
D	477	GLN	-	expression tag	UNP E0CZA5

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

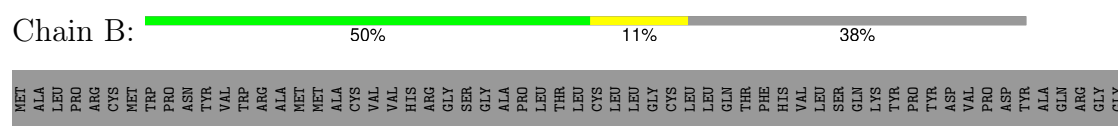
3 Residue-property plots

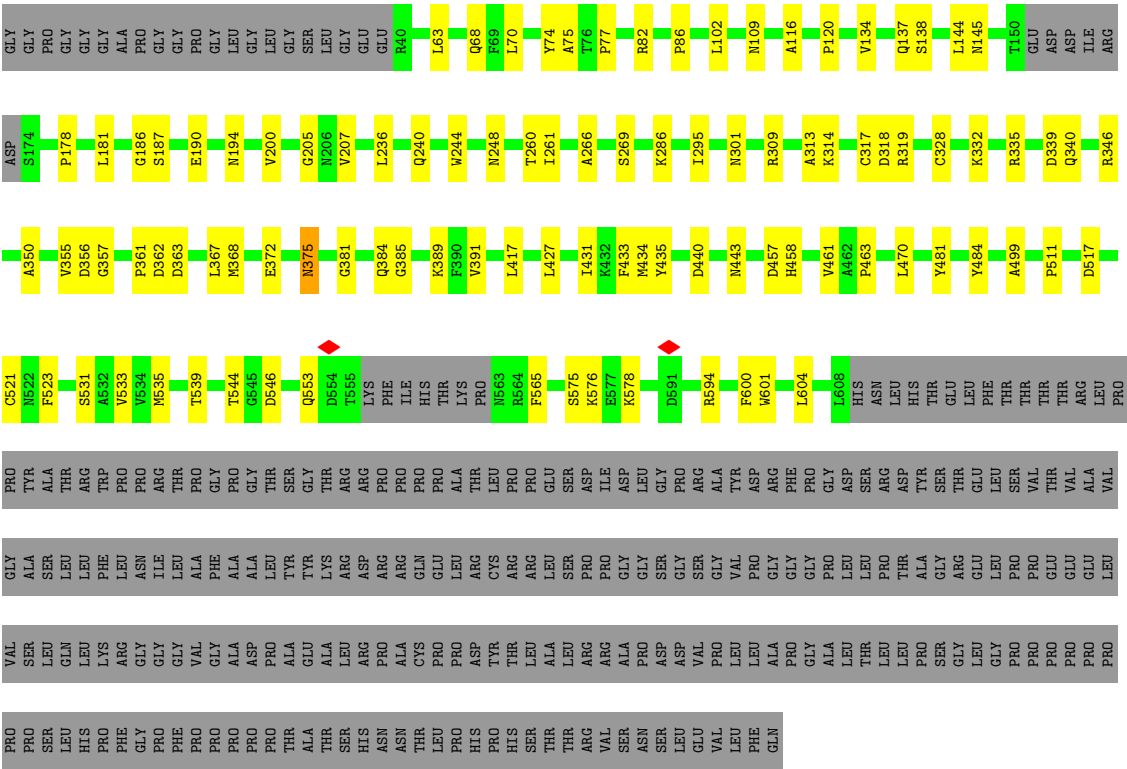
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Neuroligin-2

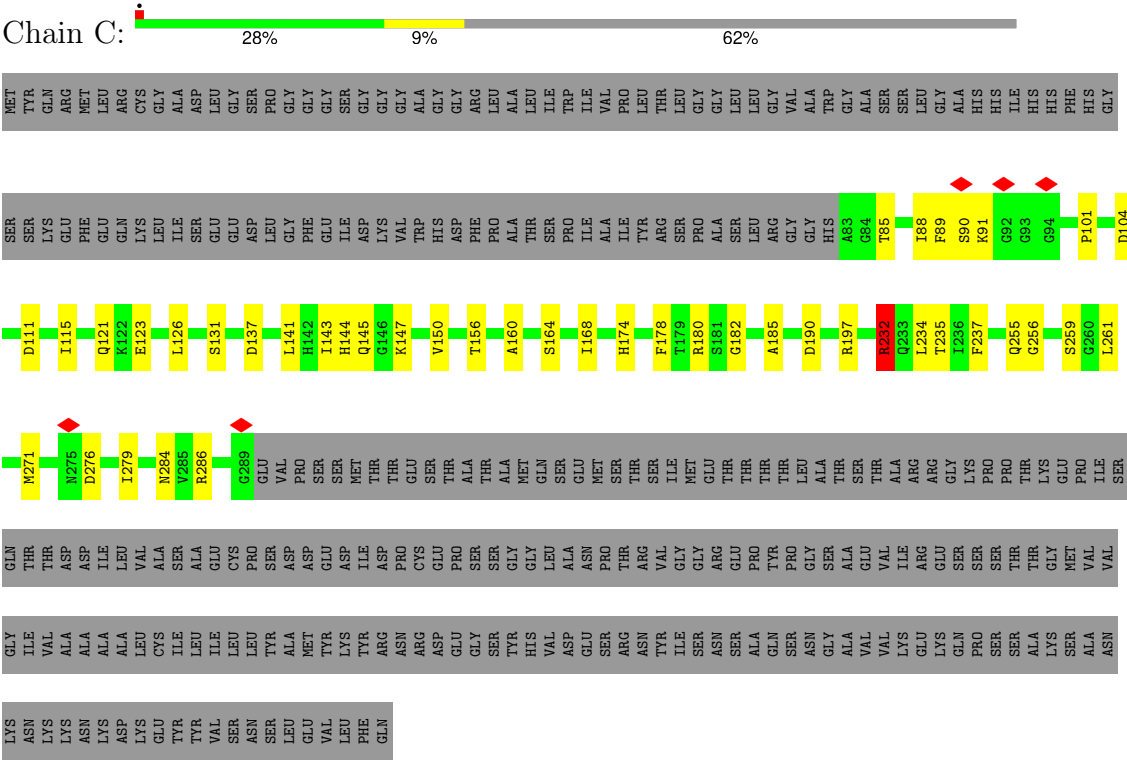


• Molecule 1: Neuroligin-2





● Molecule 2: Neurexin-1



● Molecule 2: Neurexin-1

GLU	ASN	MET	I195	K99	SER	MET
SER	PRO	THR	Y198	W100	SER	TYR
ARG	THR	THR	F199	P101	LYS	PRO
ASN	ARG	SER	F199	D104	PHE	ARG
TYR	VAL	ILE	A200	R109	GLU	MET
ILE	GLY	MET	G201	I115	GLN	LEU
SER	GLY	THR	R232	I119	LYS	ARG
ASN	ARG	THR	T236	T119	LEU	GLY
SER	GLU	THR	T242	V120	ILE	ALA
PRO	TYR	THR	T242	Q121	SER	ASP
GLN	PRO	LEU	I245	K122	GLU	ASP
SER	GLY	ALA	I245	E123	GLU	GLY
GLY	ALA	THR	I245	A124	PHE	GLY
ALA	ALA	SER	K248	E123	GLY	GLY
VAL	GLU	THR	R249	A124	ILE	SER
VAL	VAL	ALA	Q250	V125	GLU	GLY
ILE	ILE	ARG	Q250	L126	ILE	GLY
ARG	ARG	ARG	G251	D137	ASP	SER
GLU	GLU	GLY	Q252	L137	GLY	GLY
GLY	SER	PRO	Q252	L137	LYS	GLY
PRO	SER	PRO	Q255	I143	VAL	GLY
SER	SER	THR	Q256	I143	THR	GLY
SER	THR	THR	Q257	H144	HIS	GLY
ALA	THR	LYS	Q257	Q145	HIS	GLY
LYS	LYS	GLU	L258	G146	PHE	ARG
SER	MET	GLU	Q259	G146	PRO	LEU
LYS	GLY	ILE	S259	K147	ALA	ALA
ALA	VAL	ILE	G260	K147	THR	LEU
VAL	VAL	SER	L261	M153	THR	ALA
GLY	GLY	GLN	L261	M153	SER	LEU
LYS	GLY	THR	M271	I156	ILE	ILE
ASN	ILE	THR	M271	T156	PRO	TRP
LYS	VAL	THR	E274	D157	ILE	ILE
LYS	ALA	ASP	E274	D158	ALA	VAL
ASN	ALA	ASP	M275	I159	ILE	PRO
LYS	ALA	ILE	M275	I159	TYR	LEU
ASP	ALA	LEU	I281	E162	ARG	THR
LYS	LEU	VAL	I281	E162	SER	LEU
ASP	LEU	VAL	I281	E162	SER	LEU
GLU	CYS	ALA	G282	E163	PRO	GLY
TYR	ILE	SER	G283	E163	GLY	GLY
TYR	LEU	ALA	M284	S164	ALA	LEU
VAL	ILE	GLU	G285	M165	SER	LEU
SER	LEU	CYS	G286	A166	LEU	LEU
ASN	LEU	PRO	L287	I167	ARG	GLY
SER	TYR	SER	L287	I168	GLY	VAL
LEU	ALA	ASP	G288	I168	ALA	GLY
GLU	MET	ASP	G288	M169	THR	TRP
VAL	TYR	GLU	GLU	D170	HIS	GLY
LEU	LYS	ASP	VAL	D170	ALA	GLY
PHE	TYR	ILE	PRO	G171	SER	ALA
GLN	ARG	ASP	SER	K172	SER	SER
	ASN	PRO	SER	Y173	T86	LEU
	ARG	CYS	MET	H174	T87	GLY
	ASP	GLU	THR	R177	T88	ALA
	GLU	PRO	THR	F178	F89	HIS
	GLY	SER	GLU	F178	S90	HIS
	SER	SER	SER	A185	K91	ILE
	TYR	GLY	THR	A185	G92	HIS
	HIS	GLY	ALA	Q188	G93	HIS
	VAL	LEU	THR	V189	G94	PHE
	ASP	ALA	ALA	D190	G95	HIS
		MET	MET	S191	T96	GLY
		GLN	GLN	V192		
		SER	SER	P193		
		GLU	GLU	V194		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.795	Depositor
Minimum map value	-3.284	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	239.04, 239.04, 239.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: CA, NAG

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	0.13	0/4295	0.31	1/5859 (0.0%)
1	B	0.12	0/4291	0.30	0/5854
2	C	0.14	0/1378	0.35	1/1867 (0.1%)
2	D	0.13	0/1378	0.33	0/1867
All	All	0.12	0/11342	0.31	2/15447 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	PRO	CA-N-CD	-6.48	102.93	112.00
2	C	232	ARG	CA-C-O	-5.15	114.89	120.81

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	4180	0	4002	65	0
1	B	4176	0	3998	61	0
2	C	1353	0	1342	34	0
2	D	1353	0	1342	28	0
3	A	28	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	26	2	0
3	C	14	0	13	1	0
3	D	14	0	13	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	11148	0	10762	179	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 179 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:232:ARG:HH11	2:D:232:ARG:HB2	1.18	1.06
1:A:370:GLN:OE1	2:C:232:ARG:NH2	2.06	0.89
2:D:137:ASP:HA	2:D:153:ASN:O	1.76	0.85
2:D:232:ARG:HH11	2:D:232:ARG:CB	1.96	0.76
2:D:89:PHE:HB2	2:D:256:GLY:H	1.51	0.74

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	533/870 (61%)	509 (96%)	24 (4%)	0	100	100
1	B	533/870 (61%)	509 (96%)	24 (4%)	0	100	100
2	C	175/470 (37%)	166 (95%)	9 (5%)	0	100	100
2	D	175/470 (37%)	169 (97%)	6 (3%)	0	100	100
All	All	1416/2680 (53%)	1353 (96%)	63 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	435/718 (61%)	435 (100%)	0	100	100
1	B	434/718 (60%)	429 (99%)	5 (1%)	63	77
2	C	142/380 (37%)	140 (99%)	2 (1%)	59	75
2	D	142/380 (37%)	141 (99%)	1 (1%)	76	81
All	All	1153/2196 (52%)	1145 (99%)	8 (1%)	73	81

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	232	ARG
2	C	232	ARG
1	B	553	GLN
1	B	375	ASN
2	C	85	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	553	GLN
1	B	548	ASN
1	B	126	ASN
1	B	109	ASN
1	B	194	ASN

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 2 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	$\# Z > 2$
3	NAG	C	1008	2	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	A	1017	1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	B	1017	1	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
3	NAG	A	1018	1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	B	1018	1	14,14,15	0.38	0	17,19,21	1.36	2 (11%)
3	NAG	D	1008	2	14,14,15	0.32	0	17,19,21	0.49	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
3	NAG	C	1008	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1017	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1017	1	-	6/6/23/26	0/1/1/1
3	NAG	A	1018	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1018	1	-	6/6/23/26	0/1/1/1
3	NAG	D	1008	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1018	NAG	C2-N2-C7	4.65	129.14	122.90
3	B	1017	NAG	C2-N2-C7	4.65	129.13	122.90
3	B	1018	NAG	C1-C2-N2	2.34	114.12	110.43
3	B	1017	NAG	C1-C2-N2	2.31	114.07	110.43

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1017	NAG	C4-C5-C6-O6
3	D	1008	NAG	C4-C5-C6-O6
3	B	1017	NAG	O5-C5-C6-O6
3	D	1008	NAG	O5-C5-C6-O6
3	B	1017	NAG	C8-C7-N2-C2

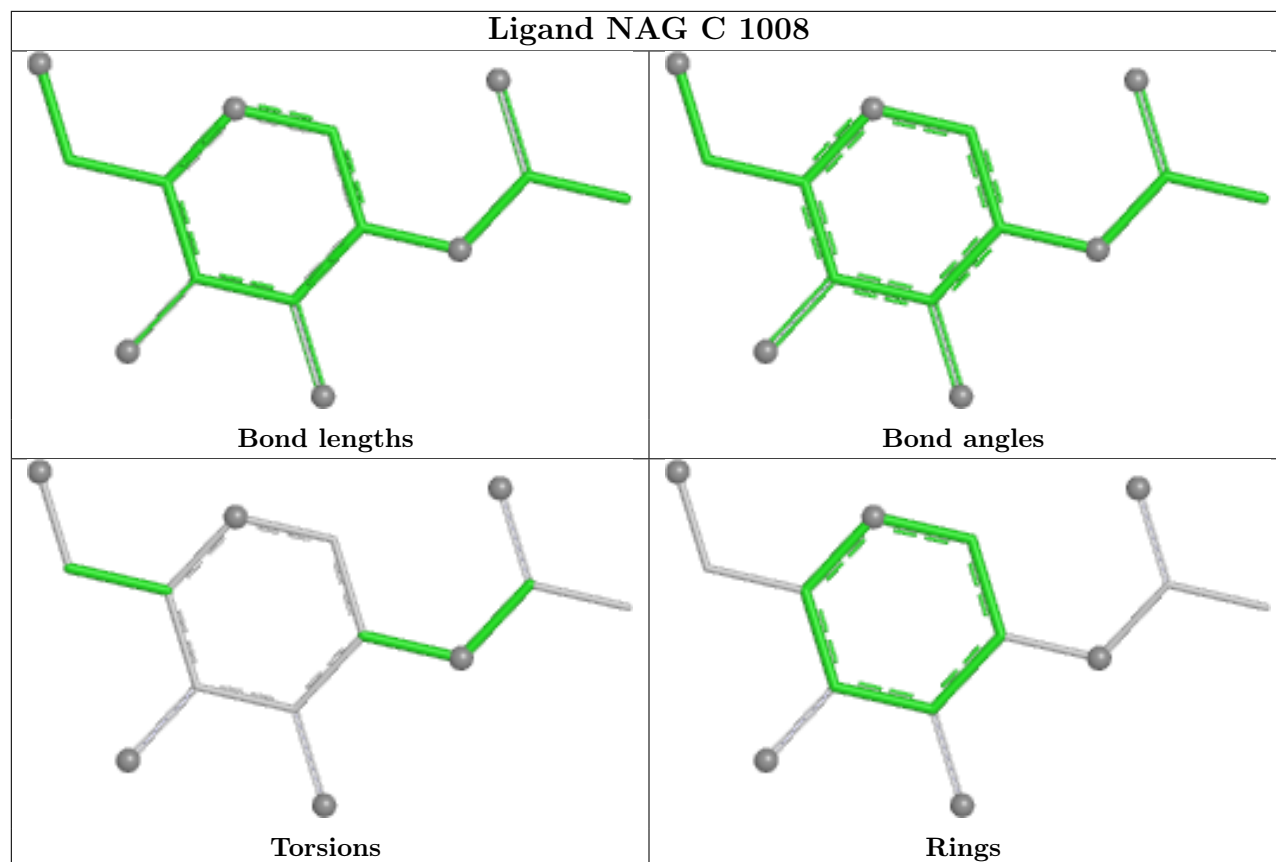
There are no ring outliers.

4 monomers are involved in 4 short contacts:

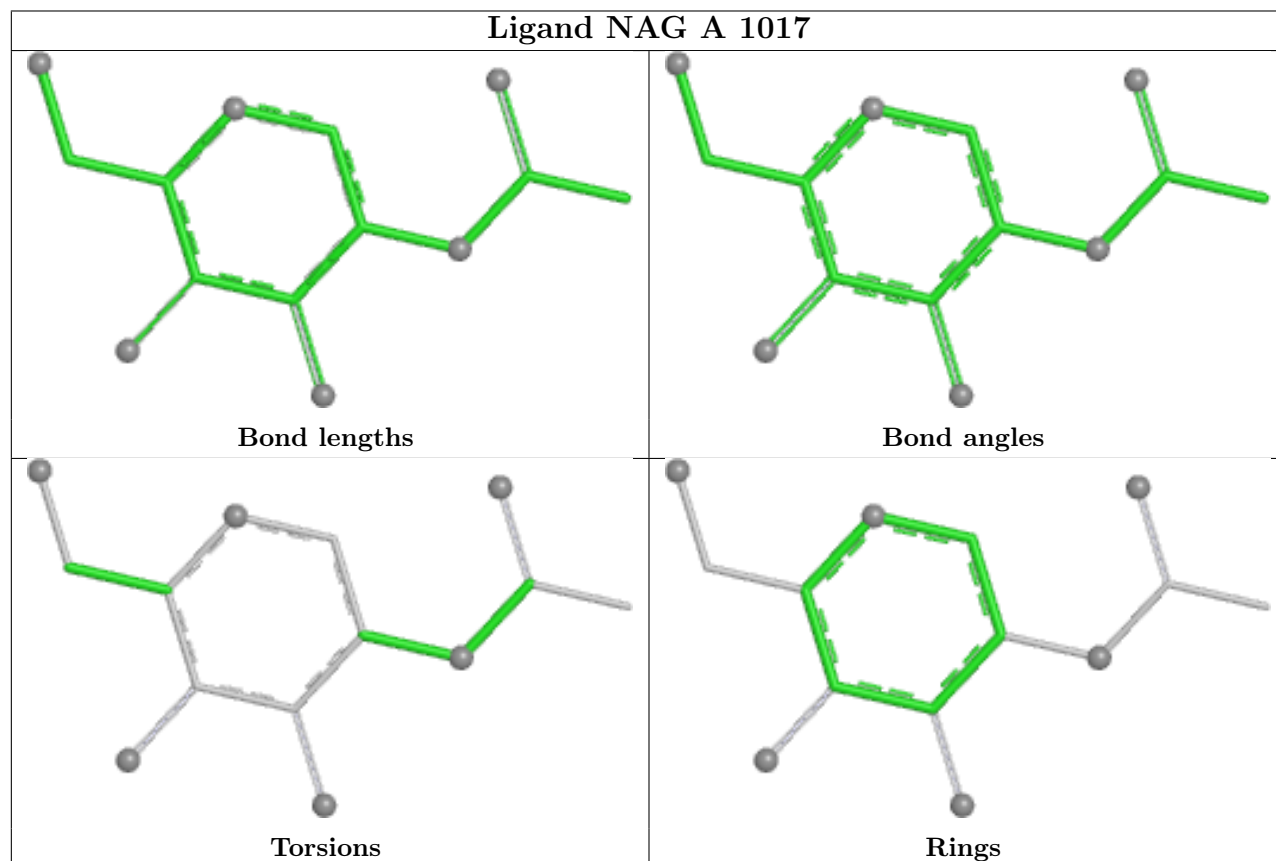
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1008	NAG	1	0
3	B	1017	NAG	1	0
3	B	1018	NAG	1	0
3	D	1008	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

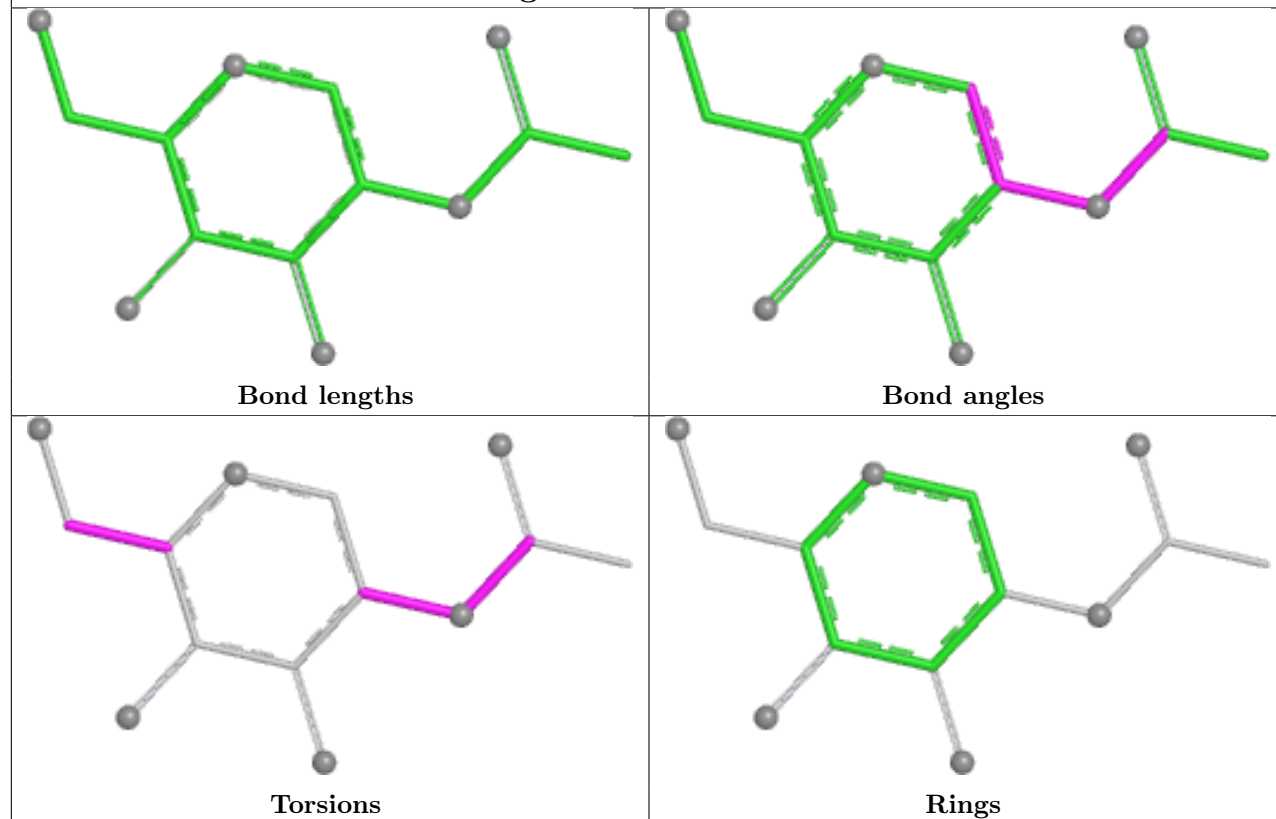
Ligand NAG C 1008



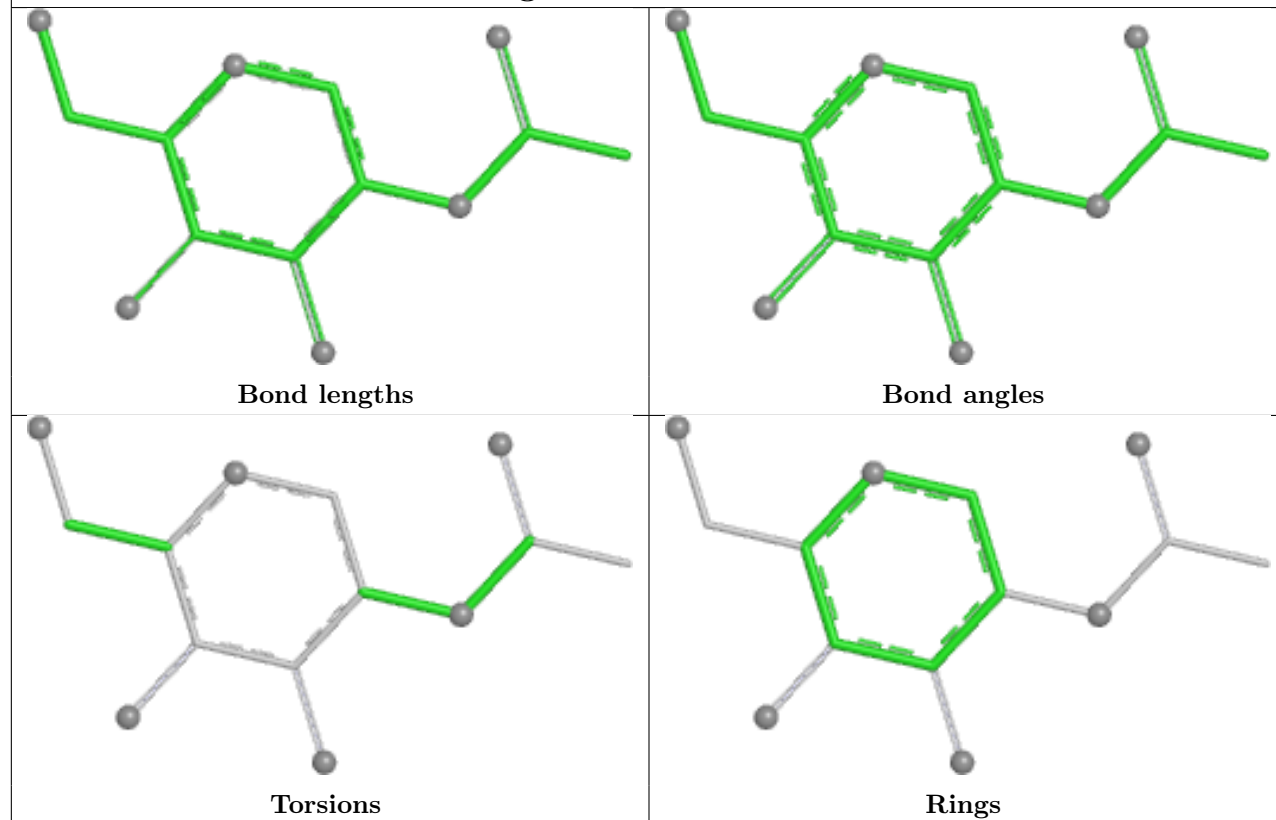
Ligand NAG A 1017



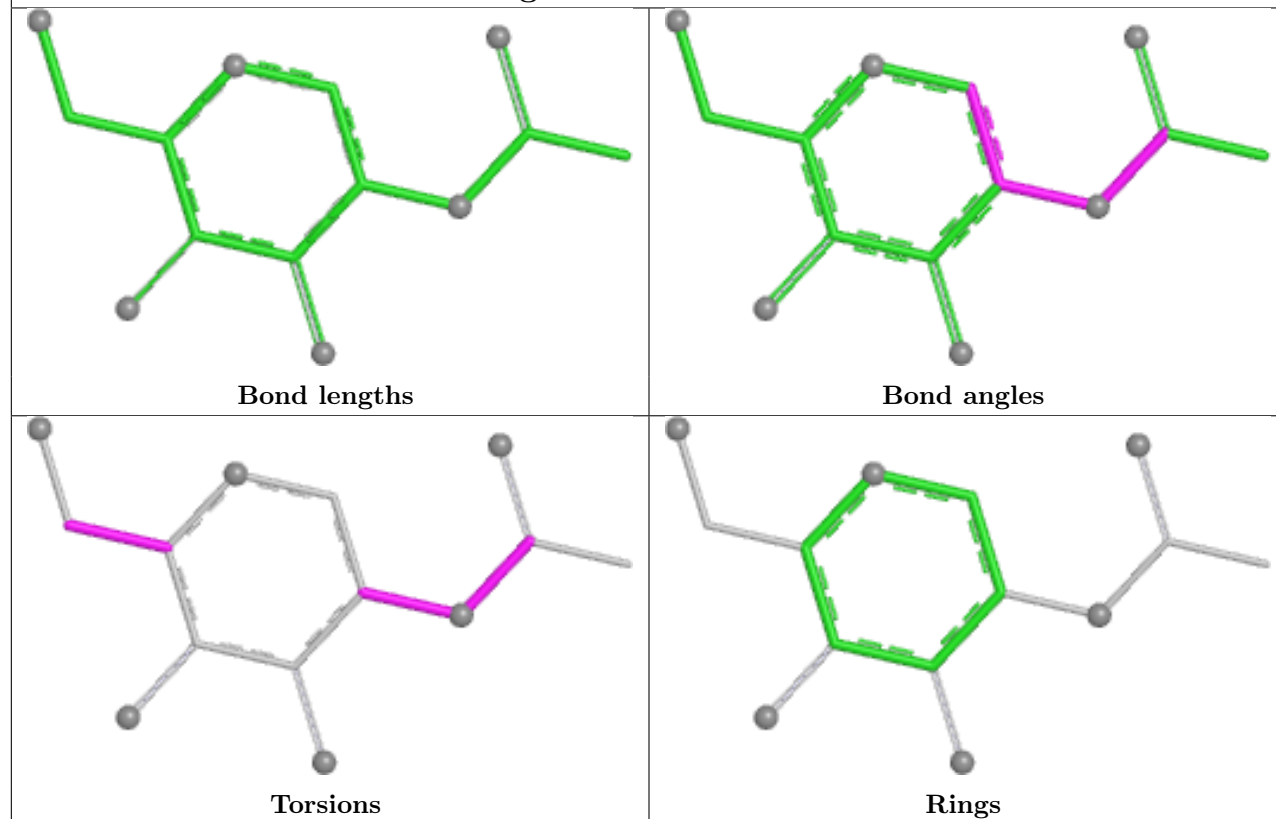
Ligand NAG B 1017



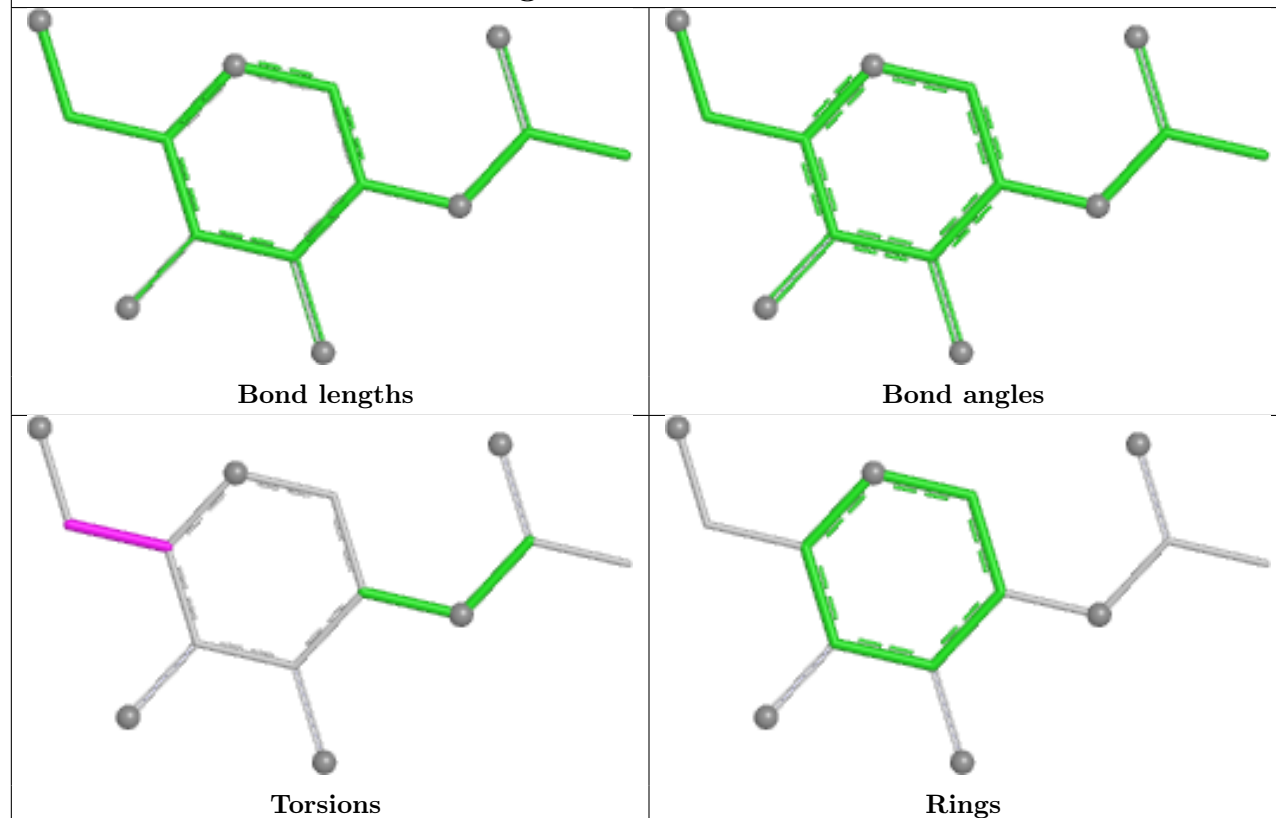
Ligand NAG A 1018



Ligand NAG B 1018



Ligand NAG D 1008



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.

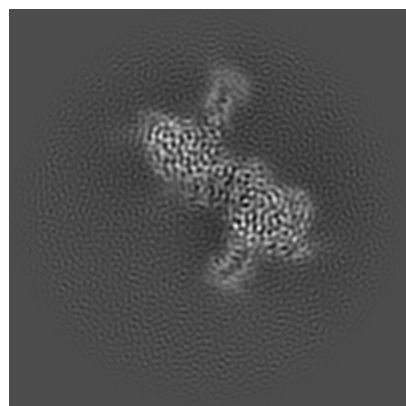
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29831. These allow visual inspection of the internal detail of the map and identification of artifacts.

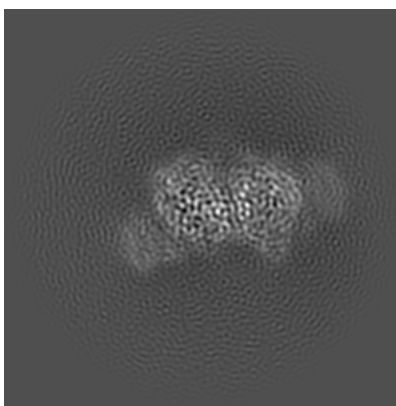
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

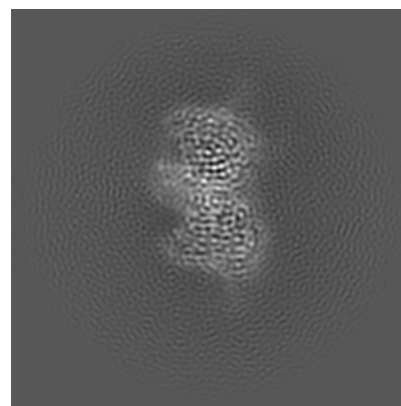
6.1.1 Primary map



X

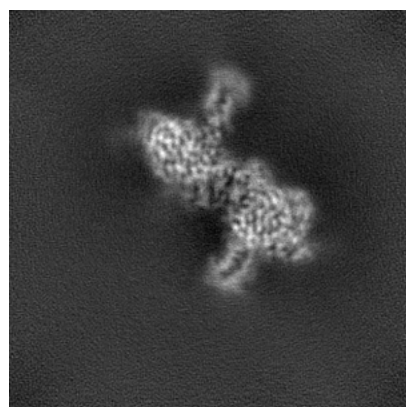


Y

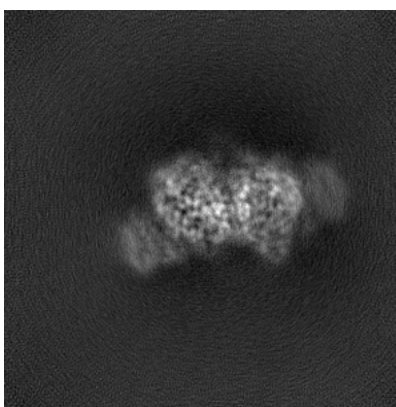


Z

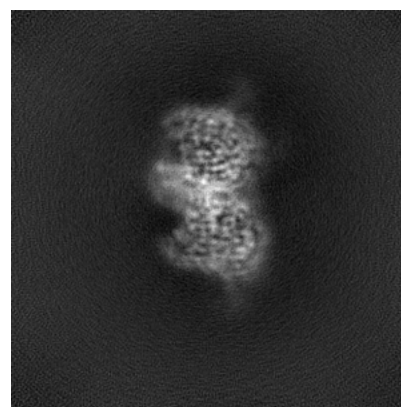
6.1.2 Raw map



X



Y

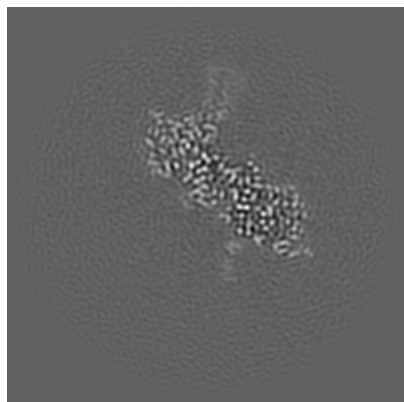


Z

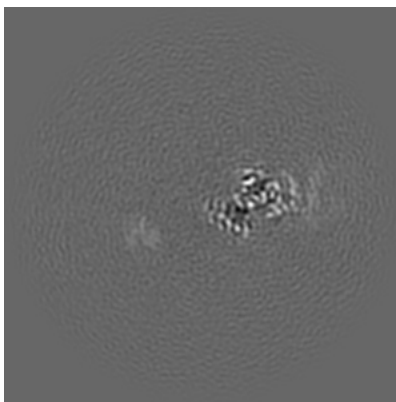
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

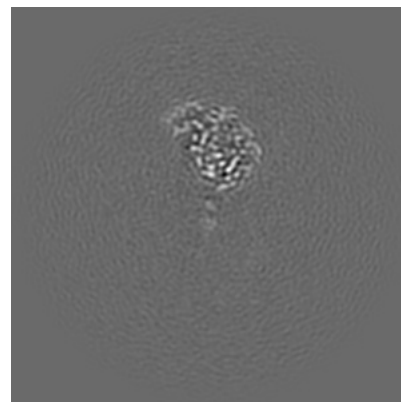
6.2.1 Primary map



X Index: 144

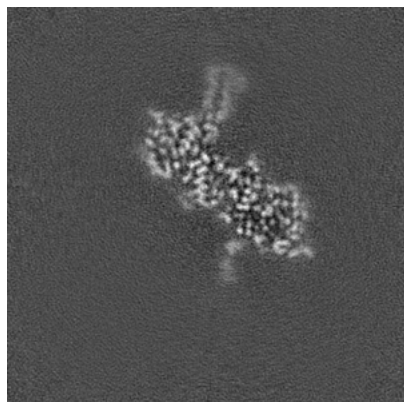


Y Index: 144

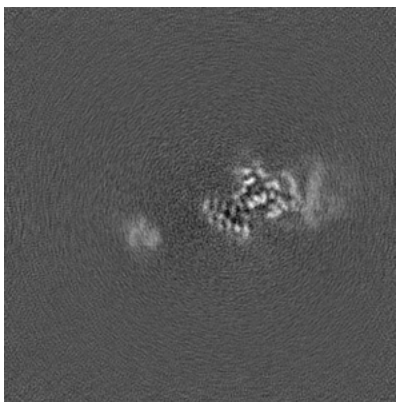


Z Index: 144

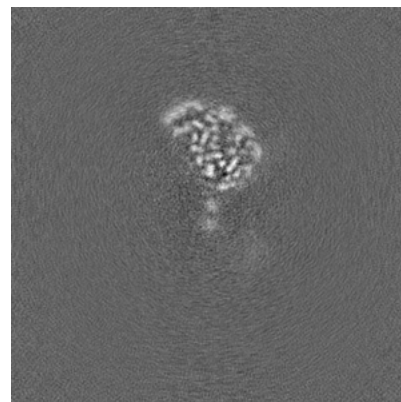
6.2.2 Raw map



X Index: 144



Y Index: 144

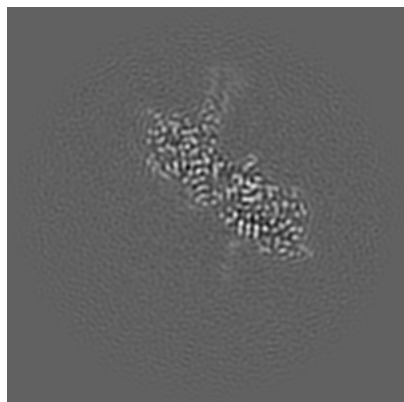


Z Index: 144

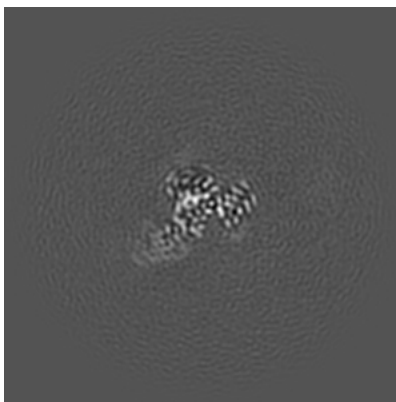
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

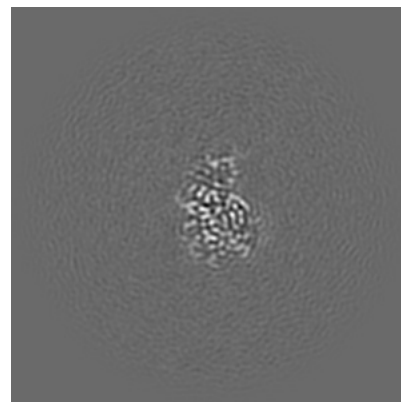
6.3.1 Primary map



X Index: 146

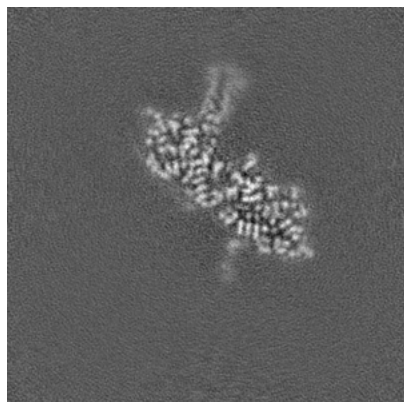


Y Index: 174

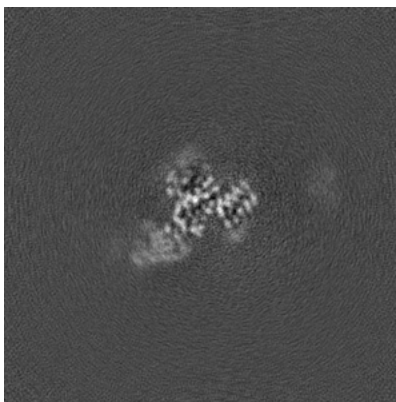


Z Index: 174

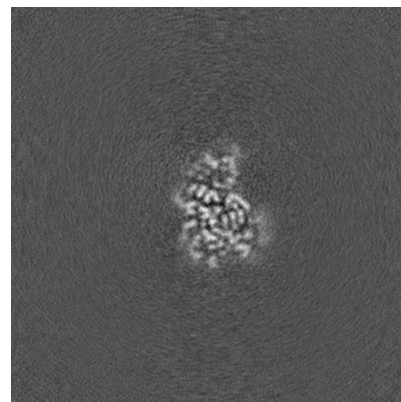
6.3.2 Raw map



X Index: 146



Y Index: 174

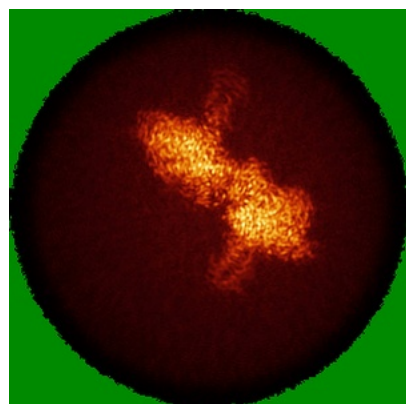


Z Index: 174

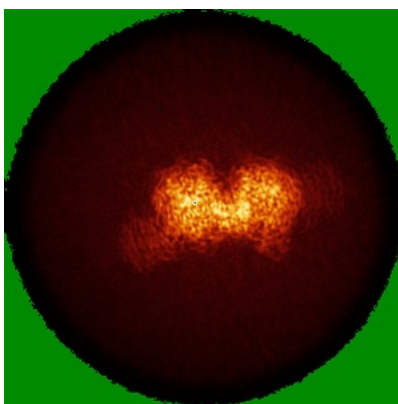
The images above show the largest variance slices of the map in three orthogonal directions.

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

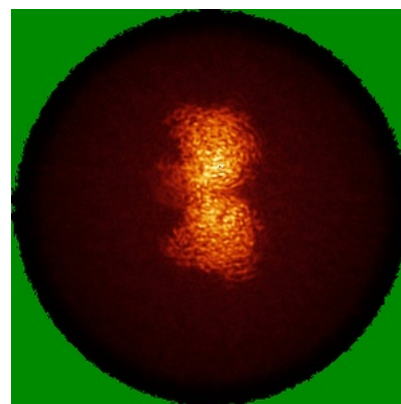
6.4.1 Primary map



X

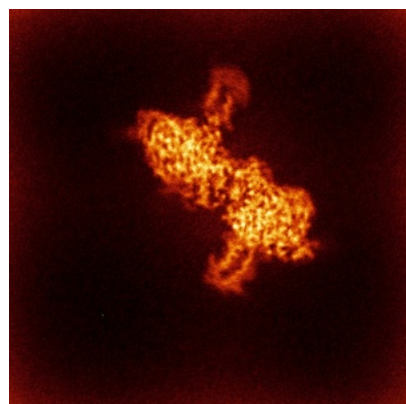


Y

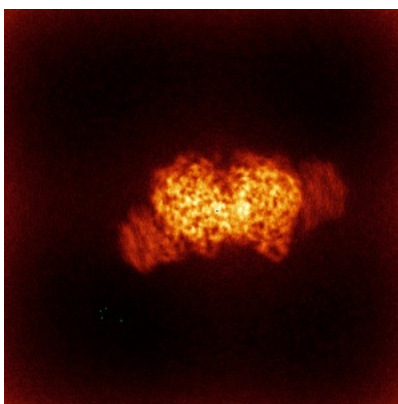


Z

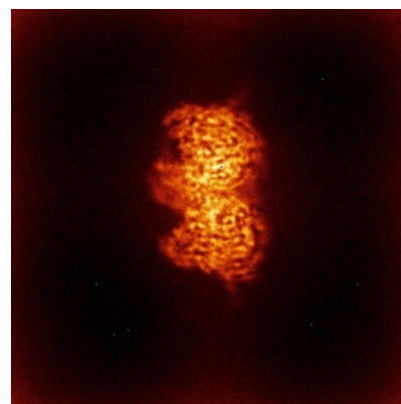
6.4.2 Raw map



X



Y

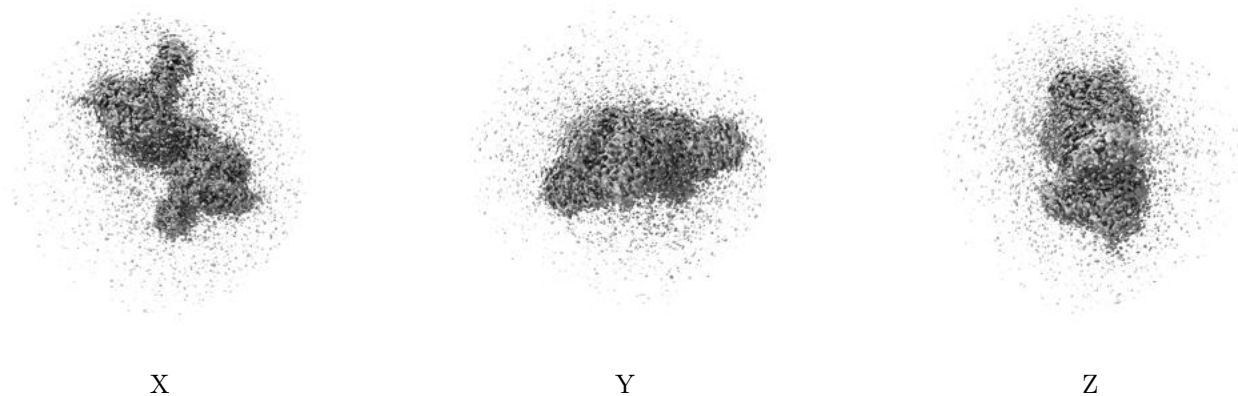


Z

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.

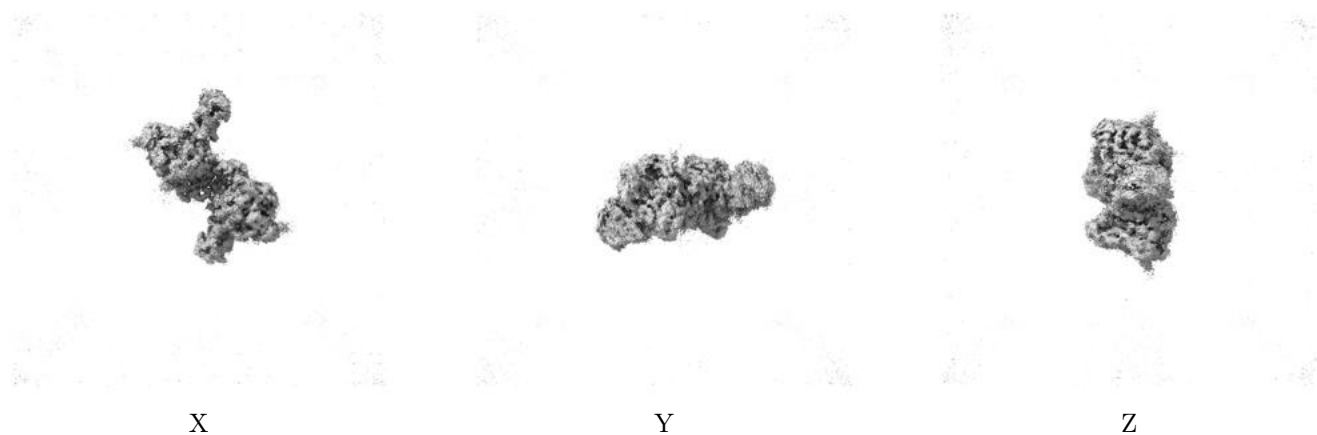
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

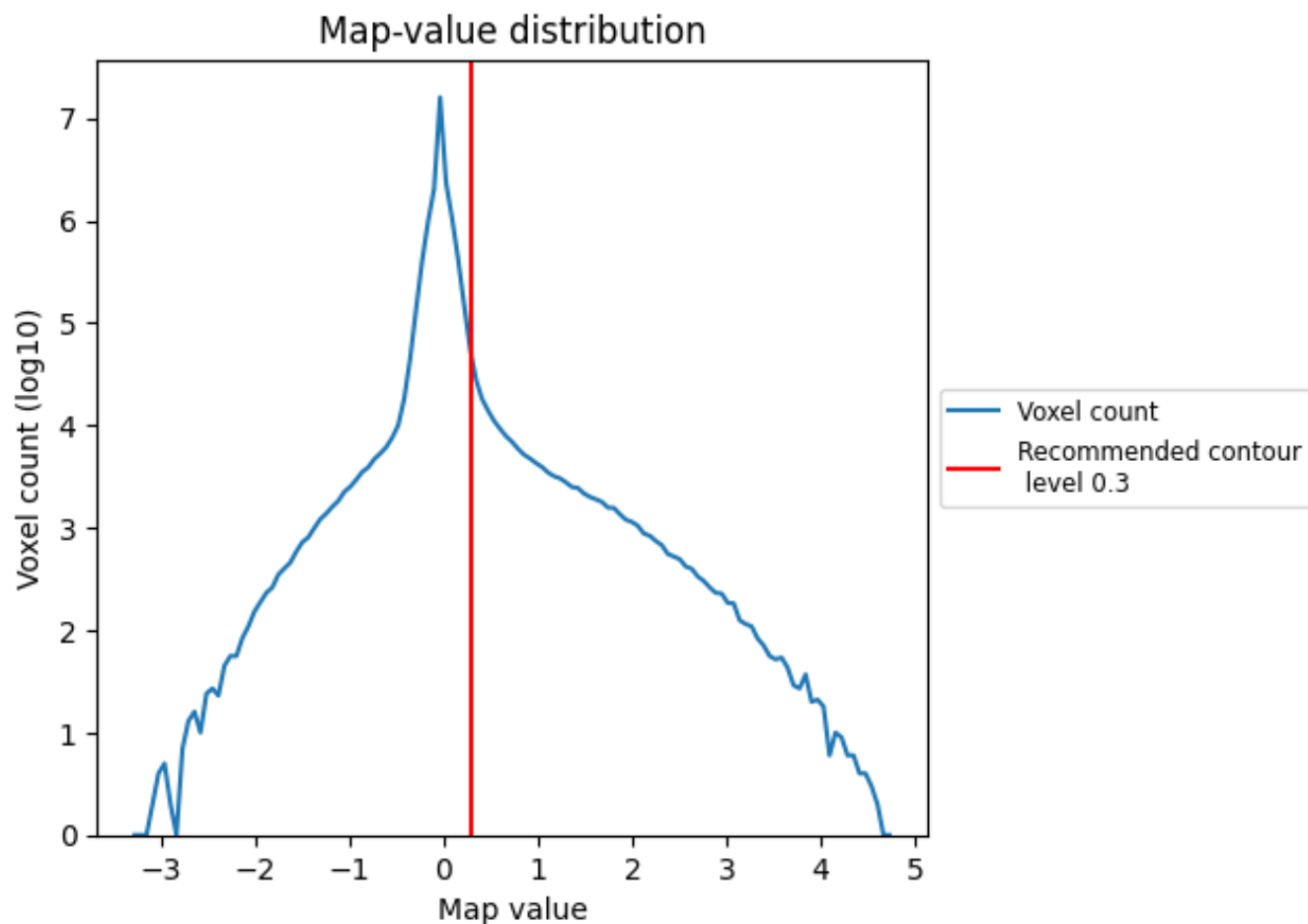
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

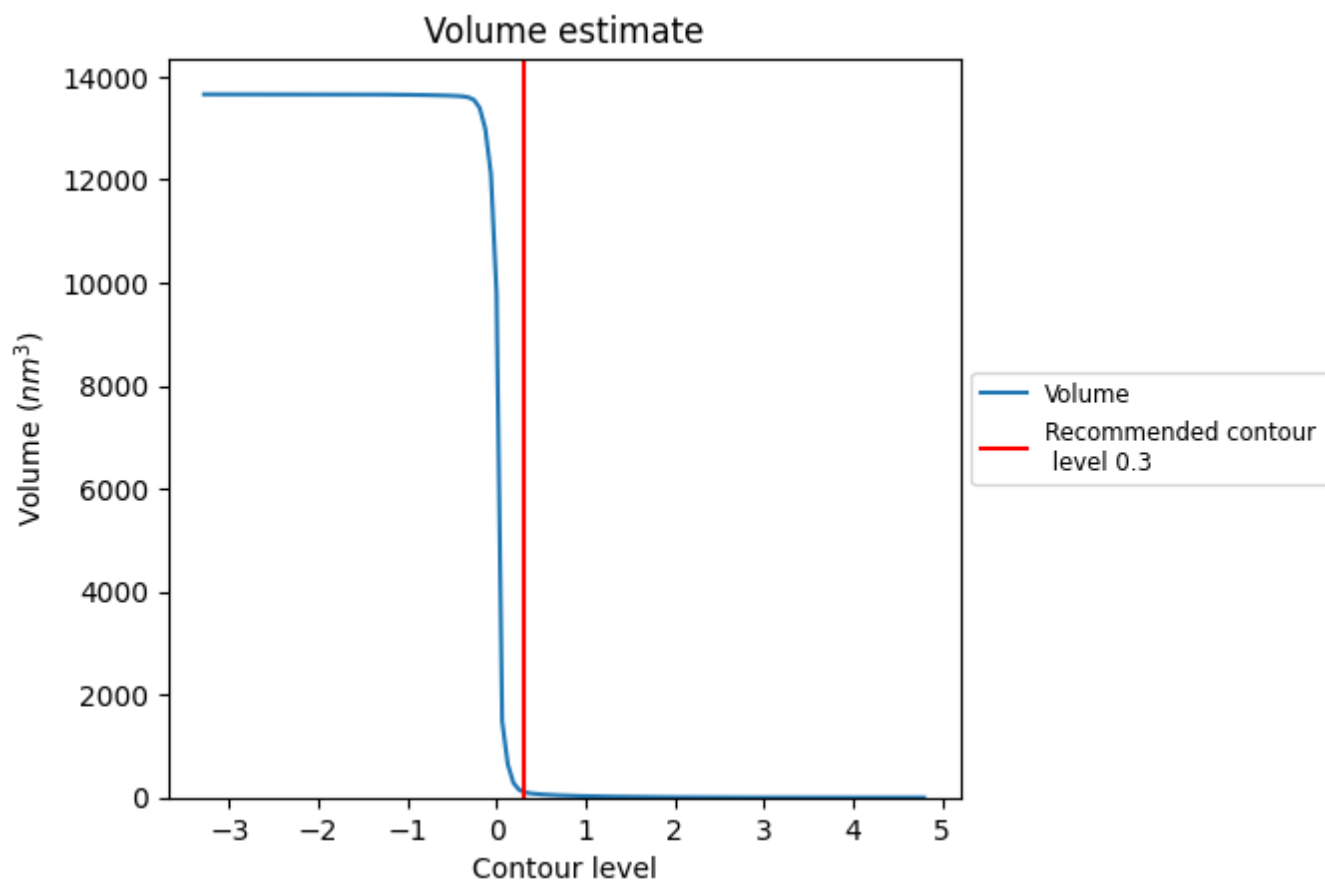
This section contains the results of statistical analysis of the map.

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.

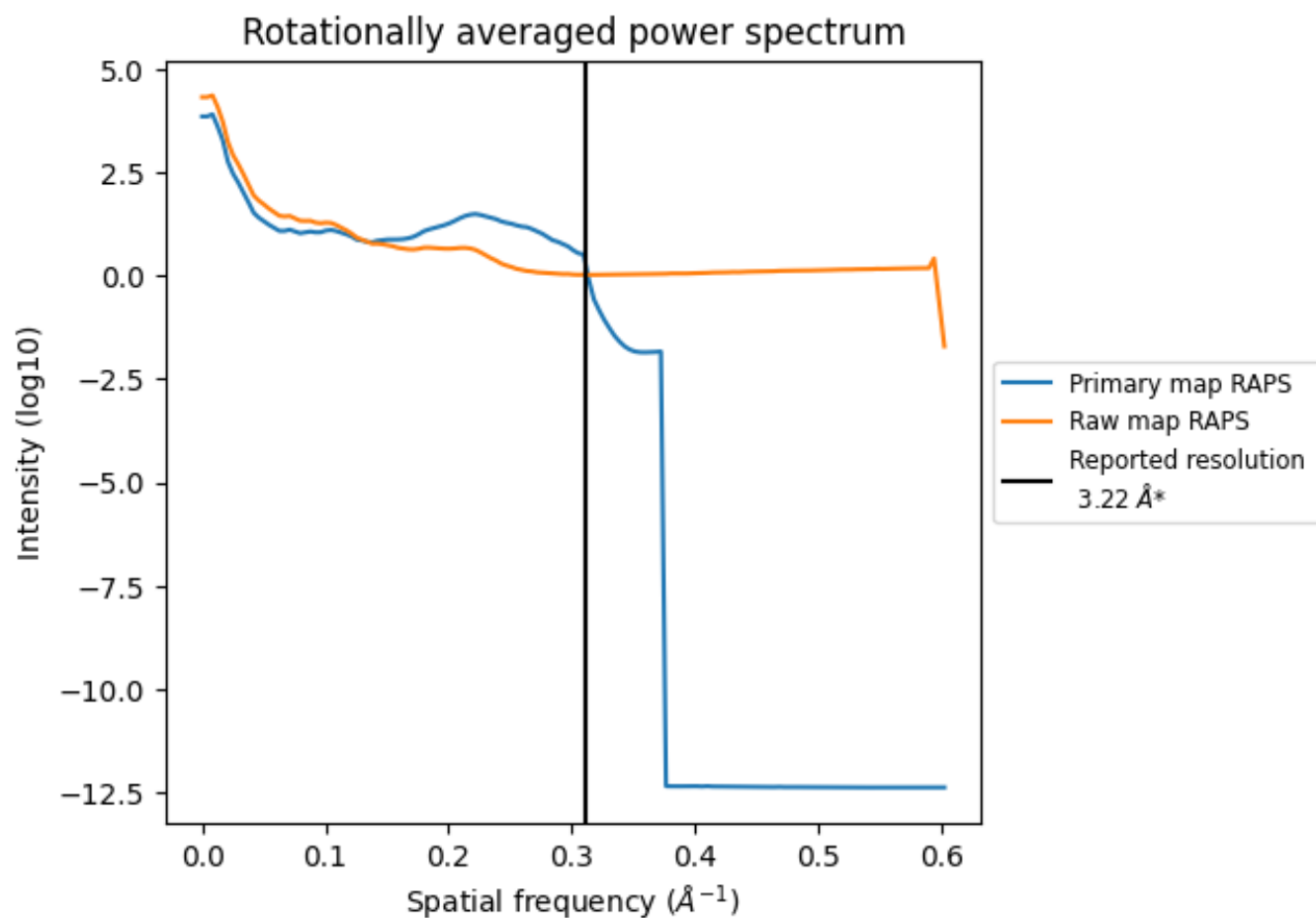
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

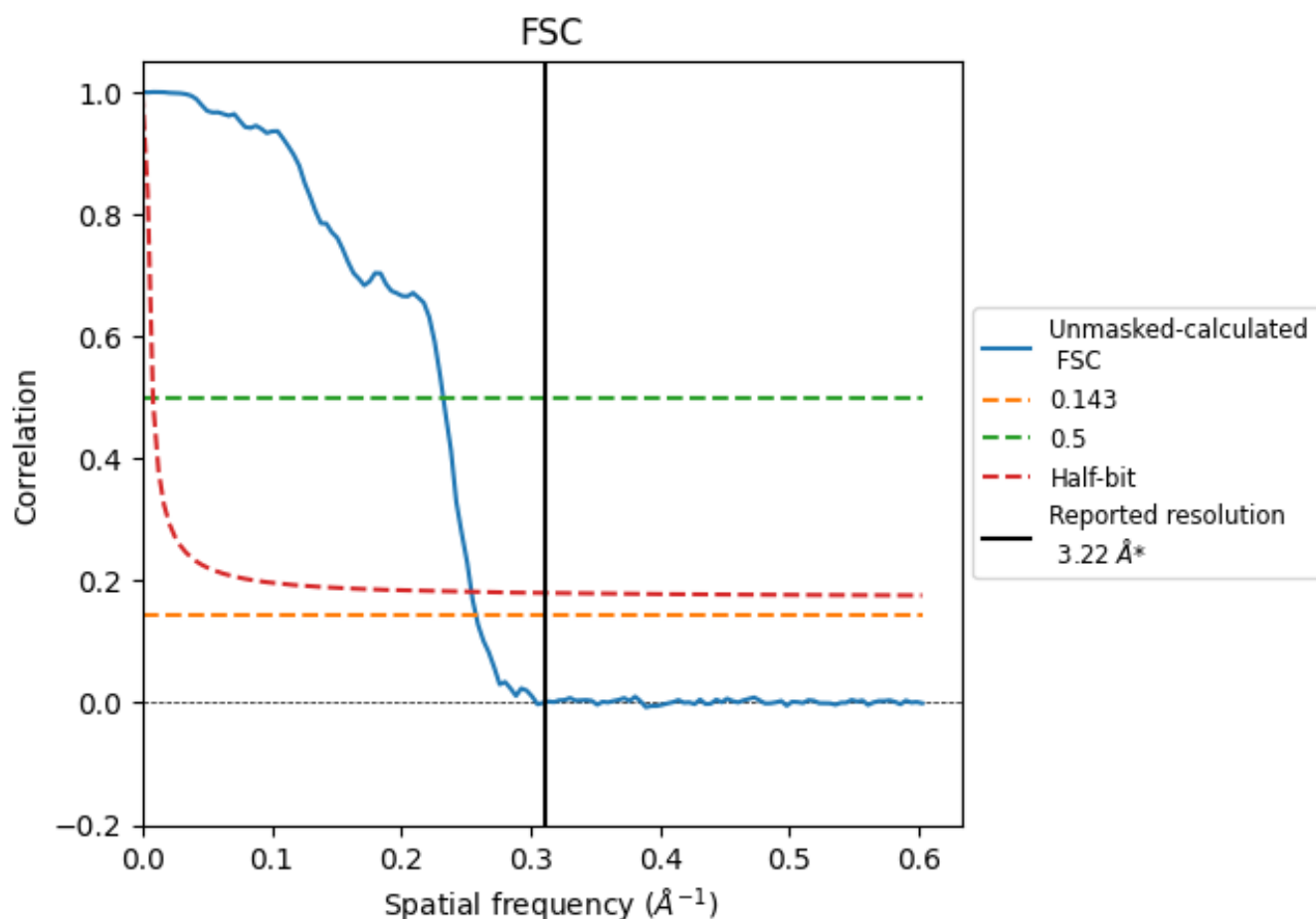


*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

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 0.311 Å⁻¹

8.2 Resolution estimates [i](#)

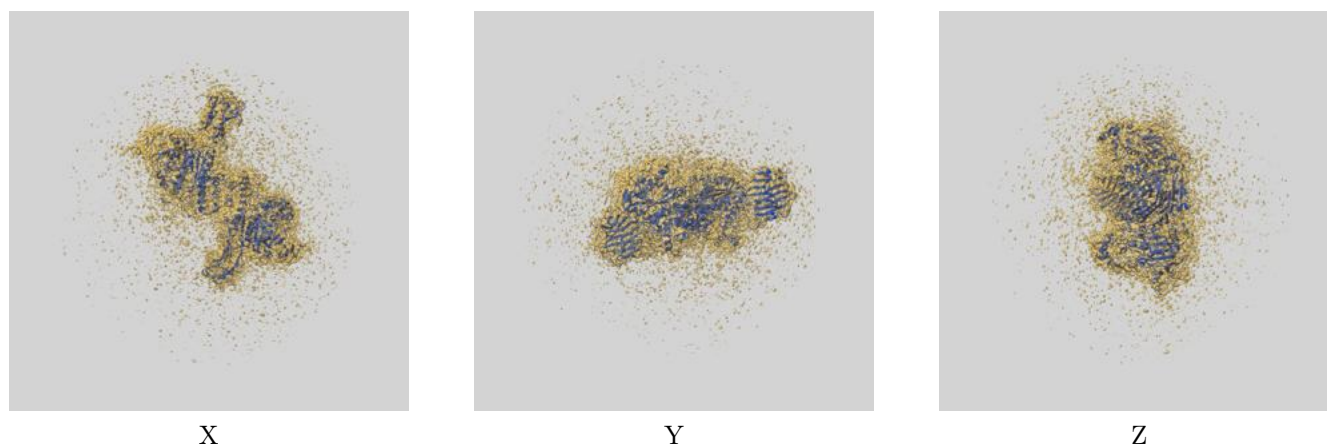
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	4.30	3.93

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

9 Map-model fit [i](#)

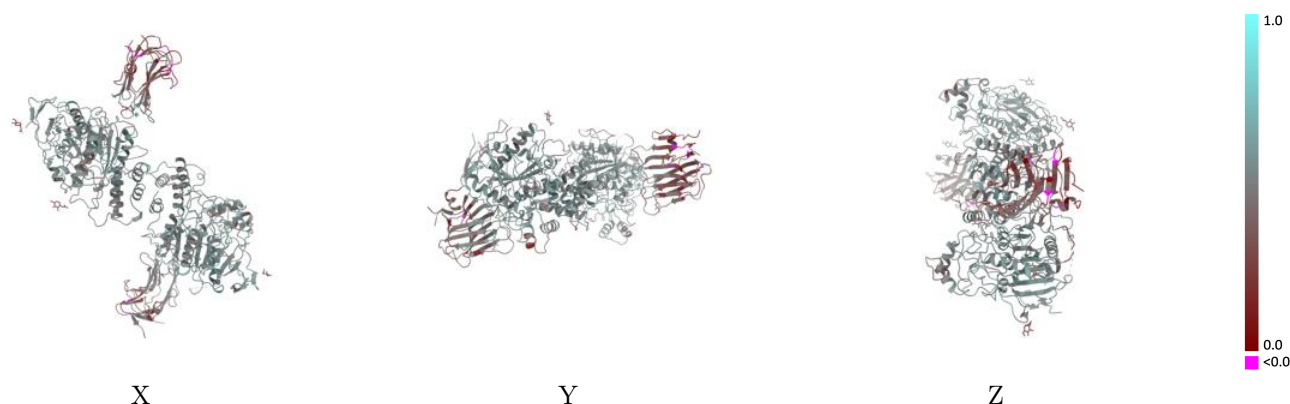
This section contains information regarding the fit between EMDB map EMD-29831 and PDB model 8G81. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



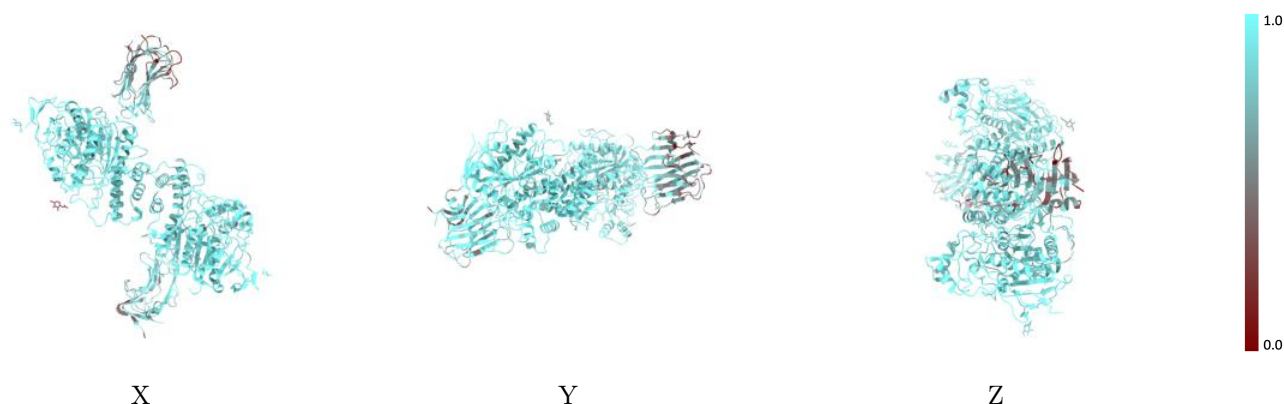
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



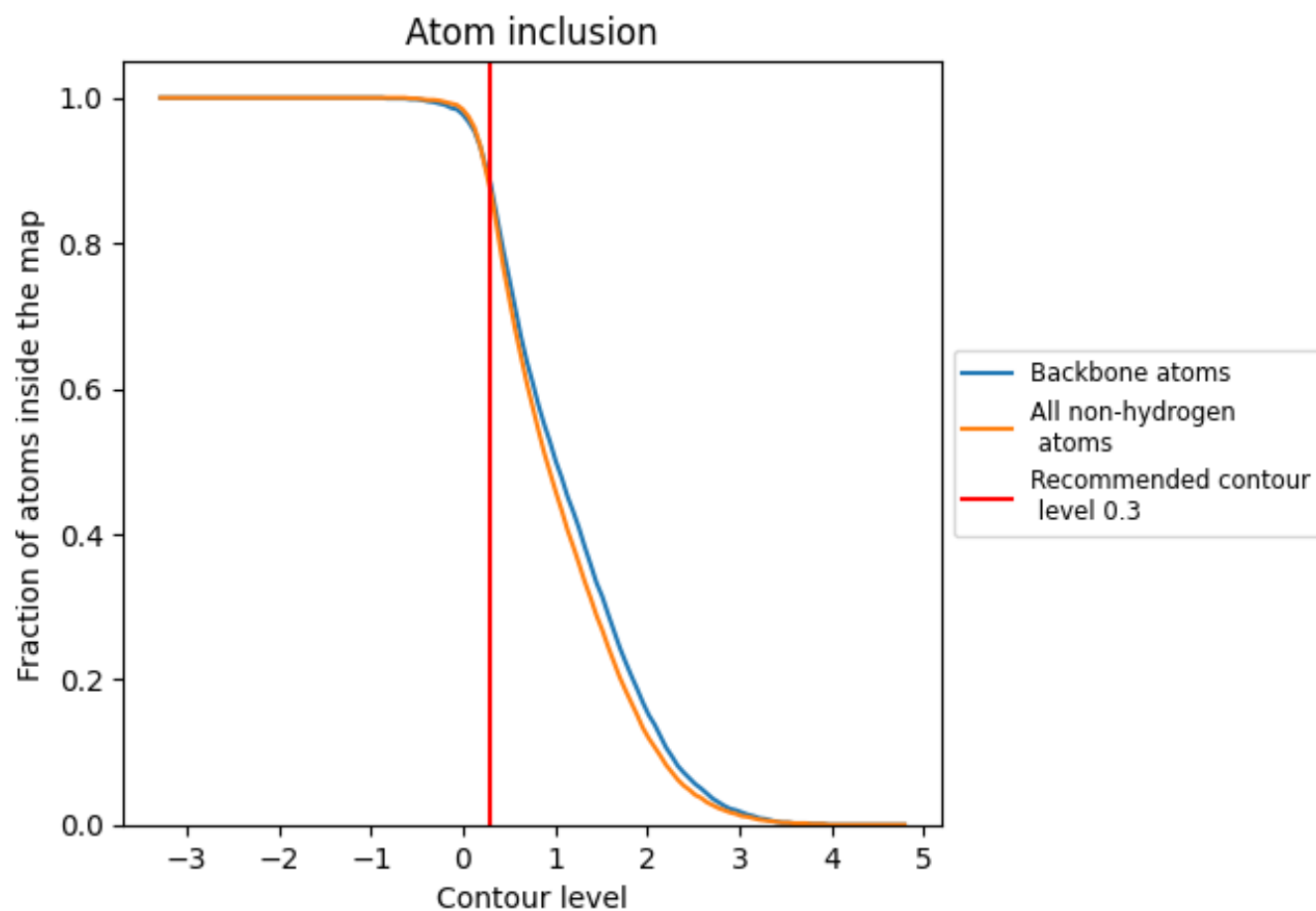
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.4910
A	0.9280	0.5350
B	0.9190	0.5250
C	0.8110	0.4100
D	0.6120	0.3350

