



wwPDB EM Validation Summary Report ⓘ

Aug 19, 2026 – 12:57 PM EDT

PDB ID : 9OEO / pdb_00009oeo
EMDB ID : EMD-70405
Title : GluN1/GluN3A in complex with glycine, LBD-TMD focused, in desensitized conformation
Authors : Kim, J.; Gouaux, E.
Deposited on : 2025-04-29
Resolution : 4.21 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

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.dev133
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) : 2.50

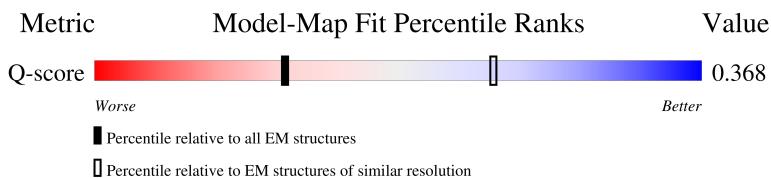
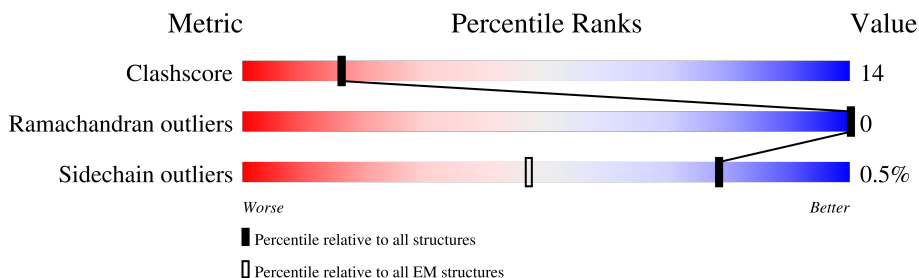
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.21 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	4806 (3.71 - 4.71)

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	
1	C	870	
2	B	993	
2	D	993	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10884 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 Isoform E of Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	385	Total	C	N	O	S	0	0
			2618	1679	451	473	15		
1	C	385	Total	C	N	O	S	0	0
			2642	1695	455	477	15		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	848	LEU	-	expression tag	UNP P35439
A	849	VAL	-	expression tag	UNP P35439
A	850	PRO	-	expression tag	UNP P35439
A	851	ARG	-	expression tag	UNP P35439
A	852	GLY	-	expression tag	UNP P35439
A	853	SER	-	expression tag	UNP P35439
A	854	ALA	-	expression tag	UNP P35439
A	855	ALA	-	expression tag	UNP P35439
A	856	ALA	-	expression tag	UNP P35439
A	857	ALA	-	expression tag	UNP P35439
A	858	SER	-	expression tag	UNP P35439
A	859	GLY	-	expression tag	UNP P35439
A	860	LEU	-	expression tag	UNP P35439
A	861	ARG	-	expression tag	UNP P35439
A	862	SER	-	expression tag	UNP P35439
A	863	HIS	-	expression tag	UNP P35439
A	864	HIS	-	expression tag	UNP P35439
A	865	HIS	-	expression tag	UNP P35439
A	866	HIS	-	expression tag	UNP P35439
A	867	HIS	-	expression tag	UNP P35439
A	868	HIS	-	expression tag	UNP P35439
A	869	HIS	-	expression tag	UNP P35439
A	870	HIS	-	expression tag	UNP P35439
C	848	LEU	-	expression tag	UNP P35439
C	849	VAL	-	expression tag	UNP P35439
C	850	PRO	-	expression tag	UNP P35439

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Chain	Residue	Modelled	Actual	Comment	Reference
C	851	ARG	-	expression tag	UNP P35439
C	852	GLY	-	expression tag	UNP P35439
C	853	SER	-	expression tag	UNP P35439
C	854	ALA	-	expression tag	UNP P35439
C	855	ALA	-	expression tag	UNP P35439
C	856	ALA	-	expression tag	UNP P35439
C	857	ALA	-	expression tag	UNP P35439
C	858	SER	-	expression tag	UNP P35439
C	859	GLY	-	expression tag	UNP P35439
C	860	LEU	-	expression tag	UNP P35439
C	861	ARG	-	expression tag	UNP P35439
C	862	SER	-	expression tag	UNP P35439
C	863	HIS	-	expression tag	UNP P35439
C	864	HIS	-	expression tag	UNP P35439
C	865	HIS	-	expression tag	UNP P35439
C	866	HIS	-	expression tag	UNP P35439
C	867	HIS	-	expression tag	UNP P35439
C	868	HIS	-	expression tag	UNP P35439
C	869	HIS	-	expression tag	UNP P35439
C	870	HIS	-	expression tag	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	397	Total	C	N	O	S	0	0
			2755	1762	470	506	17		
2	D	396	Total	C	N	O	S	0	0
			2729	1748	468	498	15		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	971	LEU	-	expression tag	UNP Q9R1M7
B	972	VAL	-	expression tag	UNP Q9R1M7
B	973	PRO	-	expression tag	UNP Q9R1M7
B	974	ARG	-	expression tag	UNP Q9R1M7
B	975	GLY	-	expression tag	UNP Q9R1M7
B	976	SER	-	expression tag	UNP Q9R1M7
B	977	ALA	-	expression tag	UNP Q9R1M7
B	978	ALA	-	expression tag	UNP Q9R1M7
B	979	ALA	-	expression tag	UNP Q9R1M7
B	980	ALA	-	expression tag	UNP Q9R1M7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	981	SER	-	expression tag	UNP Q9R1M7
B	982	GLY	-	expression tag	UNP Q9R1M7
B	983	LEU	-	expression tag	UNP Q9R1M7
B	984	ARG	-	expression tag	UNP Q9R1M7
B	985	SER	-	expression tag	UNP Q9R1M7
B	986	TRP	-	expression tag	UNP Q9R1M7
B	987	SER	-	expression tag	UNP Q9R1M7
B	988	HIS	-	expression tag	UNP Q9R1M7
B	989	PRO	-	expression tag	UNP Q9R1M7
B	990	GLN	-	expression tag	UNP Q9R1M7
B	991	PHE	-	expression tag	UNP Q9R1M7
B	992	GLU	-	expression tag	UNP Q9R1M7
B	993	LYS	-	expression tag	UNP Q9R1M7
D	971	LEU	-	expression tag	UNP Q9R1M7
D	972	VAL	-	expression tag	UNP Q9R1M7
D	973	PRO	-	expression tag	UNP Q9R1M7
D	974	ARG	-	expression tag	UNP Q9R1M7
D	975	GLY	-	expression tag	UNP Q9R1M7
D	976	SER	-	expression tag	UNP Q9R1M7
D	977	ALA	-	expression tag	UNP Q9R1M7
D	978	ALA	-	expression tag	UNP Q9R1M7
D	979	ALA	-	expression tag	UNP Q9R1M7
D	980	ALA	-	expression tag	UNP Q9R1M7
D	981	SER	-	expression tag	UNP Q9R1M7
D	982	GLY	-	expression tag	UNP Q9R1M7
D	983	LEU	-	expression tag	UNP Q9R1M7
D	984	ARG	-	expression tag	UNP Q9R1M7
D	985	SER	-	expression tag	UNP Q9R1M7
D	986	TRP	-	expression tag	UNP Q9R1M7
D	987	SER	-	expression tag	UNP Q9R1M7
D	988	HIS	-	expression tag	UNP Q9R1M7
D	989	PRO	-	expression tag	UNP Q9R1M7
D	990	GLN	-	expression tag	UNP Q9R1M7
D	991	PHE	-	expression tag	UNP Q9R1M7
D	992	GLU	-	expression tag	UNP Q9R1M7
D	993	LYS	-	expression tag	UNP Q9R1M7

- 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).

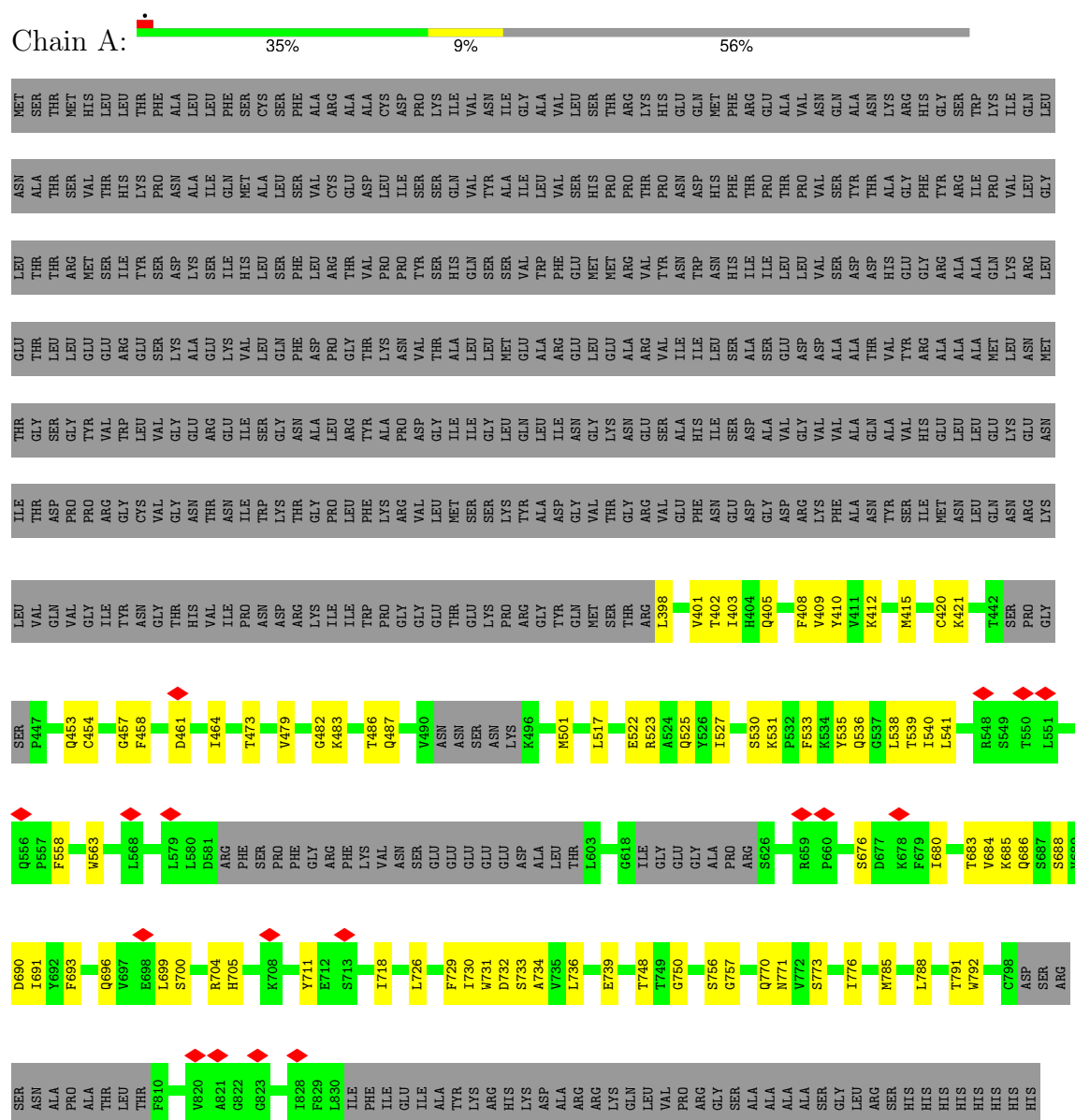


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3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

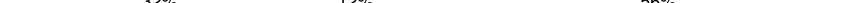
3 Residue-property plots

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: Isoform E of Glutamate receptor ionotropic, NMDA 1

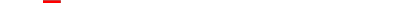


- Molecule 1: Isoform E of Glutamate receptor ionotropic, NMDA 1

Chain C: 

HIS	Q742	A640	R523	PRO	LEU	ILE	THR	GLU	LEU	ASN	MET
	K743	I643	A524	GLY	VAL	THR	GLY	THR	THR	ALA	SER
	T749	I643	O526	S446	GLN	ASP	SER	THR	ALA	THR	SER
	G750	Y647	Y526	P447	VAL	PRO	GLY	GLU	ARG	SER	MET
	F753	D658	I527	R448	ILE	ARG	VAL	GLU	MET	VAL	HIS
		D658	E528	H449	ASN	GLY	THR	GLU	SER	THR	LEU
	S756	I664	F529	Q453	THR	VAL	GLY	SER	PRO	ASN	PHE
	G757	I664	K534	Y456	THR	GLY	GLY	LYS	ALA	ALA	LEU
	F758	I667	Y536	G457	HIS	THR	GLU	ALA	LYS	ALA	LEU
		I667	Q537	L463	VAL	THR	ARG	GLU	SER	ILE	LEU
HIS	W762	P675	L538	L463	ILE	ASN	GLU	LYS	ILE	GLM	PHE
	R763	S676	L541	T473	PRO	TRP	ILE	VAL	HIS	MET	SER
		D677			ASN	LYS	GLY	GLN	LEU	ALA	CYS
	H760	K678	V476		THR	THR	ASN	PHE	SER	SER	PHE
		K678	R548		ARG	GLY	ALA	ASP	LEU	VAL	ALA
	D789	T683	L551	V479	LYS	PRO	LEU	PRO	ARG	CYS	ARG
	K790	V684		A480	ILE	THR	ARG	GLY	THR	GLU	ALA
	T791	K685	F558	D481	TRP	PHE	TYR	VAL	VAL	ASP	ALA
	W792	K686	O559	C482	PRO	LYS	LYS	PRO	LYS	LEU	CYS
	F793	K687	S560	K483	GLY	ARG	VAL	PRO	ASN	ILE	ASP
HIS	R794	S687		F484	GLY	VAL	ASP	ASN	TYR	SER	PRO
	Y795	S687		C485	GLU	LEU	GLY	THR	SER	SER	LYS
	Q796	R694		T486	THR	THR	ILE	ALA	HIS	ILE	ALA
	E797	R695		Q487	GLU	SER	ILE	LEU	GLN	VAL	ASN
	F798	D696		E488	LYS	SER	GLY	MET	SER	ALA	ILE
	ASP	E697	R681	R489	PRO	LYS	LEU	GLU	VAL	ILE	GLY
	SER	E698			ARG	TYR	GLN	GLU	TRP	ALA	VAL
	ARG	L699		VAL	GLY	ALA	LEU	ALA	TRP	LEU	VAL
	SER	S700		ASN	THR	ASP	ILE	ARG	PHE	VAL	VAL
	ASN	T701		ASN	GLN	GLY	ASN	GLU	SER	SER	SER
HIS	ALA	W702	GLY	SER	MET	VAL	GLY	LEU	MET	HIS	SER
	PRO	Y703	ARG	ASN	SER	THR	THR	LYS	MET	PRO	THR
	ALA	R704	PHE	LYS	THR	GLY	ASN	ALA	ARG	PRO	LYS
	THR	W705	LYS	K496	ARG	ARG	GLU	VAL	VAL	THR	ARG
	LEU	W706	VAL	E497	L398	VAL	SER	VAL	THR	THR	HIS
	THR	E707	ASN	W498	K398	GLU	ALA	ILE	TYR	PRO	ASN
	F810	E707	SER	N499	1400	PHE	HIS	ILE	TRP	ASP	GLN
	E811	W709	GLU	M501	V401	ASN	ILE	LEU	TRP	MET	HIS
	K812	H709	GLU	M502		GLU	SER	SER	ASP	PHE	PHE
		W710	GLU	G503	H404	ASP	ILE	ALA	THR	THR	ARG
HIS	W816	Y711	GLU	E504		GLY	ALA	SER	ILE	PRO	ASN
	F817	E712	GLU	L506	P407	ASP	VAL	GLU	LEU	THR	VAL
	N818	E716	ALA	L506		ARG	GLY	ASP	LEU	PRO	ASN
		E716	ALA	S507	F412	LYS	VAL	ASP	VAL	VAL	GLN
	K821	Q719	THR	A510	F413	PHE	VAL	ALA	SER	SER	GLN
		Q719			T414	ALA	ALA	THR	ASP	TYR	GLN
		R722	L603		M415	TYR	ALA	ASP	ASP	THR	ALA
	R828	F729	ILE	I513	C420	ILE	VAL	VAL	GLY	GLY	HIS
	F829	W731	GLY	V514		MET	THR	ARG	ARG	TYR	ARG
	L830	D732	GLU	A515	C436	GLU	LEU	ALA	ALA	SER	GLY
HIS	ILE	W731	GLU	P516	T437	ASN	LEU	ALA	ALA	ILE	TRP
	PHE	D732	GLY	L517		LEU	GLU	MET	ALA	ILE	LYS
	ILE	S733	ALA	F518		GLN	GLU	LYS	GLN	VAL	PRO
	GLU	S733	ALA	I440		ASN	LEU	LEU	LYS	PRO	ALA
	ILE	A734	ALA	I519	D441	ASN	LEU	LEU	LYS	VAL	ILE
	ALA	W735	PRO	I519	T442	ASN	GLU	ASN	GLN	GLY	THR
		W735	ARG	N520		YS	ASN	GLY	LYS	THR	LEU
		L736		N521			THR	THR	THR	THR	LEU

- Molecule 2: Glutamate receptor ionotropic, NMDA 3A

Chain B:  30% 10% 60%

LEU	GLN	LEU	THR	ALA	MET
GLN	ARG	TRP	PRO	ARG	ARG
SER	VAL	PRO	ALA	LEU	SER
CYS	HIS	ASP	ARG	SER	LEU
THR	THR	LEU	ALA	ARG	TRP
VAL	VAL	LEU	LEU	GLN	LEU
GLN	VAL	PHE	GLU	GLY	SER
GLY	GLY	VAL	ALA	GLY	ARG
VAL	VAL	GLU	VAL	ARG	VAL
SER	SER	ASN	ASN	ALA	CYS
LEU	ALA	LEU	ASN	ALA	LEU
LEU	LEU	VAL	VAL	ARG	LEU
ALA	PHE	GLU	GLU	ASP	PRO
PRO	PRO	GLN	LEU	ASP	PRO
GLN	SER	LEU	LEU	PRO	CYS
SER	GLN	PRO	PRO	GLU	ALA
GLY	GLY	TYR	GLY	SER	LEU
GLU	GLU	ASN	THR	GLY	VAL
MET	MET	LEU	TRP	ARG	LEU
LEU	GLY	LEU	LEU	PRO	VAL
LEU	ASP	GLU	VAL	ALA	PRO
VAL	VAL	VAL	VAL	PRO	SER
SER	SER	ILE	GLN	GLY	SER
VAL	VAL	GLU	GLU	ALA	HIS
LEU	LEU	ALA	ALA	ARG	PRO
HIS	HIS	GLY	GLY	TRP	GLN
ILE	ILE	LEU	GLY	LEU	CYS
SER	SER	VAL	ASP	SER	ILE
LEU	LEU	LEU	LEU	ALA	LEU
SER	SER	PRO	PRO	LEU	LYS
ILE	ILE	LEU	HIS	HIS	ARG
VAL	VAL	MET	GLY	ILE	GLY
ARG	ARG	PRO	ARG	GLY	HIS
HIS	HIS	PHE	GLY	GLY	ALA
GLU	GLU	SER	SER	PRO	VAL
PHE	PHE	SER	PRO	GLY	ARG
VAL	VAL	ASN	TRP	LEU	VAL
LEU	LEU	ASN	SER	GLY	HIS
PRO	PRO	LEU	SER	GLY	VAL
LEU	LEU	ASP	GLU	GLY	ALA
HIS	HIS	PRO	PRO	ALA	THR
THR	THR	PHE	PHE	GLY	THR
LEU	LEU	THR	THR	ALA	THR





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	173386	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.910	Depositor
Minimum map value	-0.590	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.11	Depositor
Map size ($\text{\AA}$)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 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	0.15	0/2677	0.30	0/3669
1	C	0.20	0/2699	0.35	0/3693
2	B	0.14	0/2823	0.27	0/3862
2	D	0.14	0/2795	0.26	0/3823
All	All	0.16	0/10994	0.30	0/15047

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2618	0	2143	72	0
1	C	2642	0	2182	88	0
2	B	2755	0	2275	64	0
2	D	2729	0	2250	64	0
3	A	28	0	24	1	0
3	B	42	0	39	1	0
3	C	28	0	26	0	0
3	D	42	0	39	1	0
All	All	10884	0	8978	282	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 14.

The worst 5 of 282 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:LEU:HG	1:A:748:THR:HG22	1.26	1.17
1:A:736:LEU:HG	1:A:748:THR:CG2	1.80	1.11
1:C:400:ILE:CD1	1:C:463:LEU:HD11	2.04	0.88
1:A:736:LEU:CG	1:A:748:THR:HG22	2.05	0.86
1:A:517:LEU:HD12	1:A:517:LEU:O	1.76	0.85

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	373/870 (43%)	348 (93%)	25 (7%)	0	100	100
1	C	373/870 (43%)	343 (92%)	30 (8%)	0	100	100
2	B	387/993 (39%)	372 (96%)	15 (4%)	0	100	100
2	D	386/993 (39%)	367 (95%)	19 (5%)	0	100	100
All	All	1519/3726 (41%)	1430 (94%)	89 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/747 (27%)	201 (100%)	0	100	100
1	C	204/747 (27%)	202 (99%)	2 (1%)	68	75
2	B	226/861 (26%)	226 (100%)	0	100	100
2	D	219/861 (25%)	217 (99%)	2 (1%)	70	76
All	All	850/3216 (26%)	846 (100%)	4 (0%)	78	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	499	ASN
1	C	780	HIS
2	D	543	CYS
2	D	799	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	635	ASN
2	D	781	HIS
2	D	821	ASN
1	C	686	GLN
1	A	771	ASN

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](#)

10 ligands 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
3	NAG	B	1002	-	14,14,15	0.27	0	17,19,21	0.53	0
3	NAG	C	901	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	1001	2	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	A	902	-	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	D	1001	2	14,14,15	0.25	0	17,19,21	0.36	0
3	NAG	D	1002	-	14,14,15	0.24	0	17,19,21	0.56	0
3	NAG	B	1003	2	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	A	901	1	14,14,15	0.96	2 (14%)	17,19,21	0.90	1 (5%)
3	NAG	D	1003	2	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	C	902	1	14,14,15	0.21	0	17,19,21	0.55	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	B	1002	-	-	4/6/23/26	0/1/1/1
3	NAG	C	901	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
3	NAG	A	902	-	-	2/6/23/26	0/1/1/1
3	NAG	D	1001	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1002	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	A	901	1	-	4/6/23/26	0/1/1/1
3	NAG	D	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	C	902	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAG	O5-C1	2.60	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAG	C1-C2	2.28	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	NAG	C1-O5-C5	3.34	116.66	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1003	NAG	C4-C5-C6-O6
3	A	902	NAG	C4-C5-C6-O6
3	B	1003	NAG	C4-C5-C6-O6
3	B	1001	NAG	O5-C5-C6-O6
3	A	902	NAG	O5-C5-C6-O6

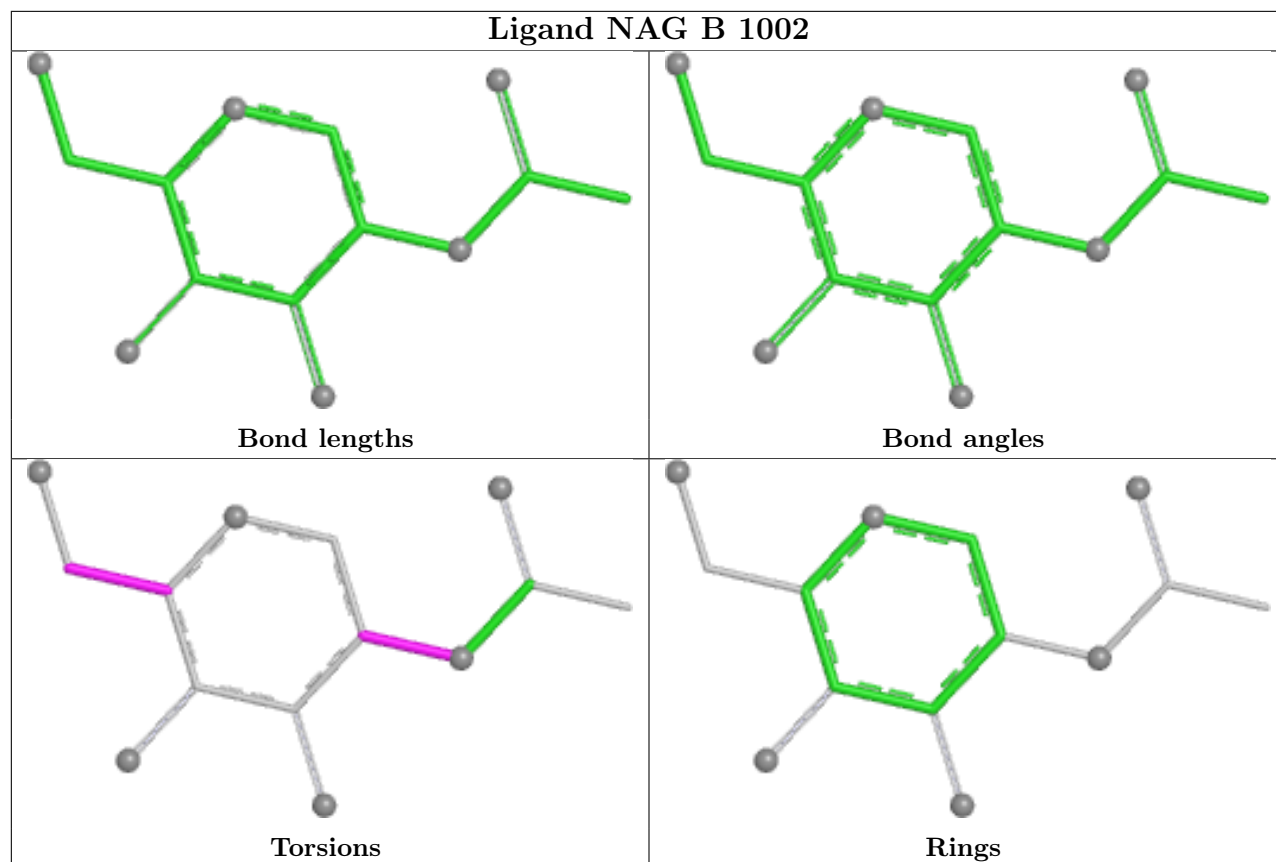
There are no ring outliers.

3 monomers are involved in 3 short contacts:

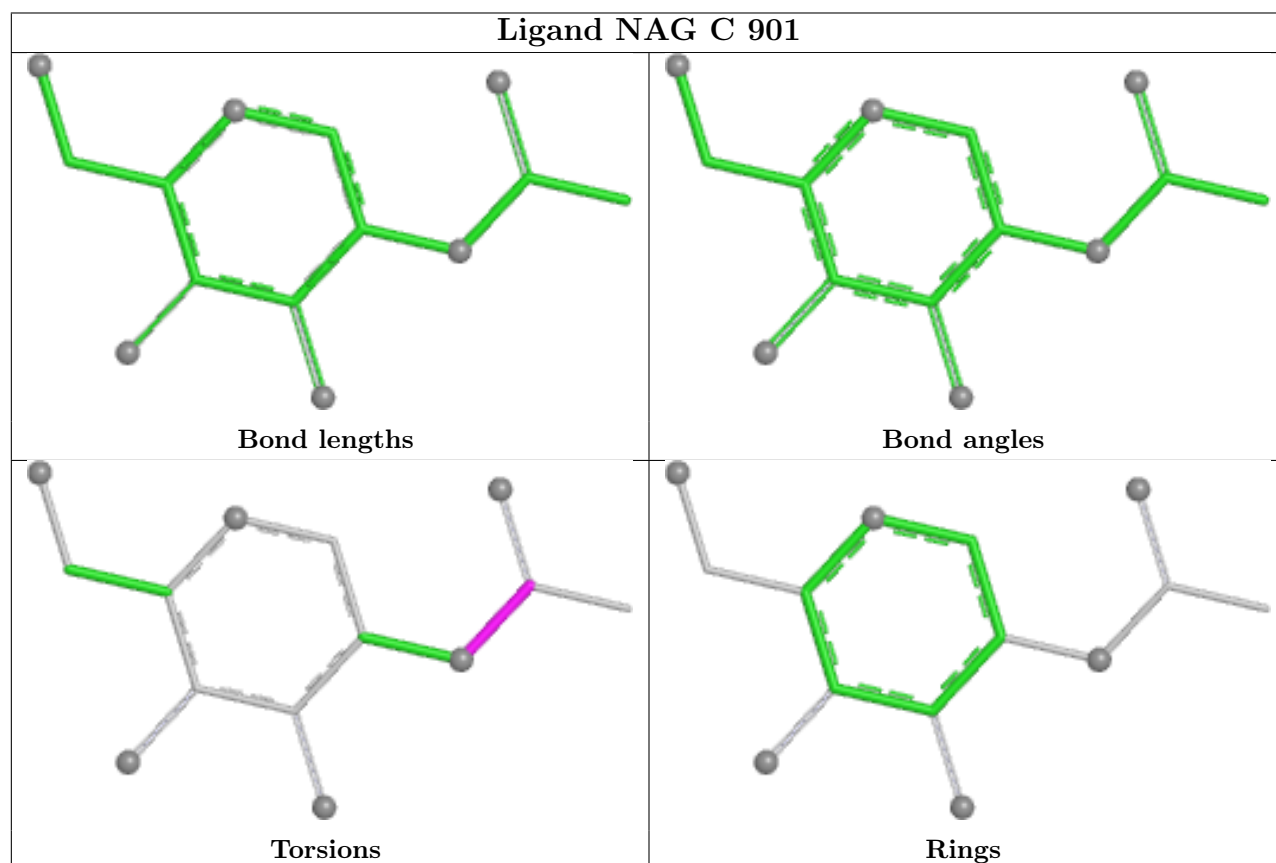
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	NAG	1	0
3	A	902	NAG	1	0
3	D	1001	NAG	1	0

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.

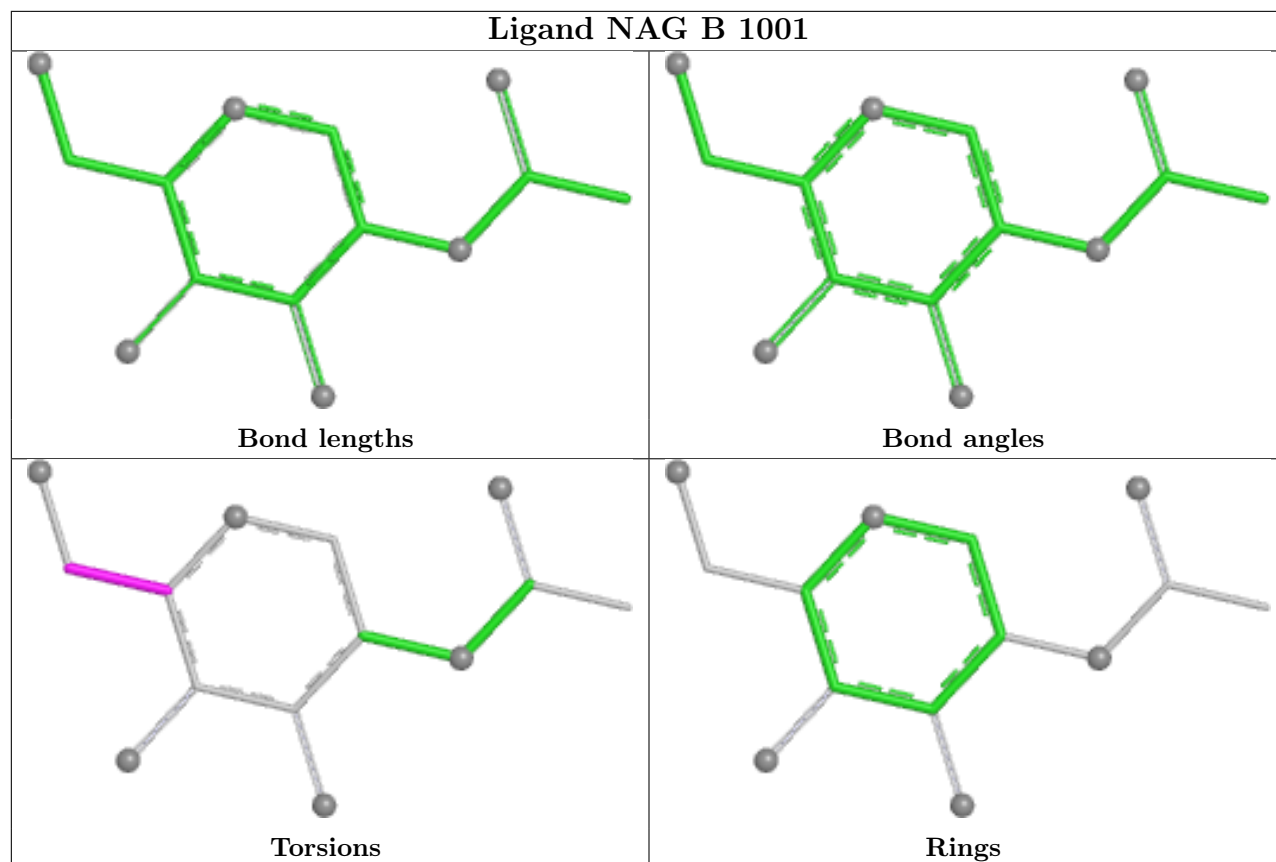
Ligand NAG B 1002



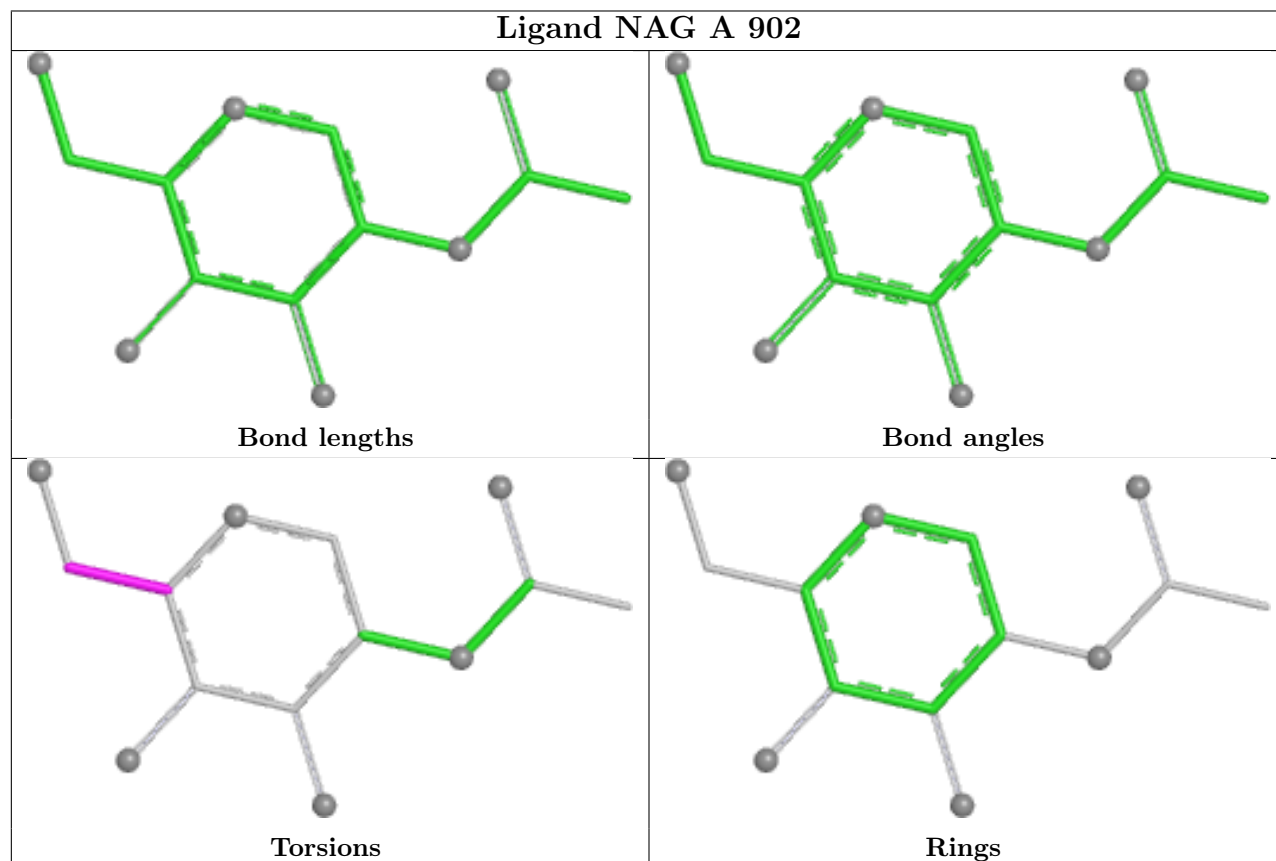
Ligand NAG C 901



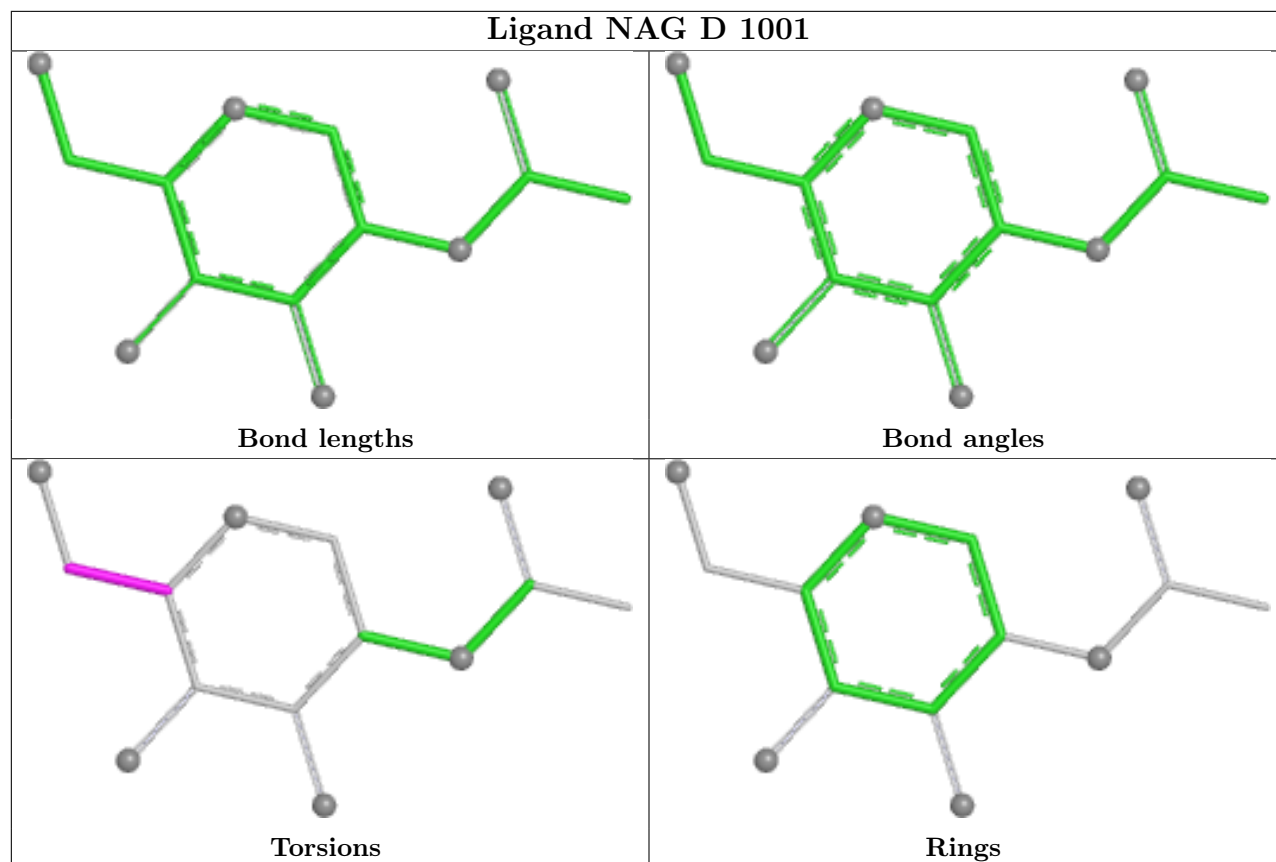
Ligand NAG B 1001



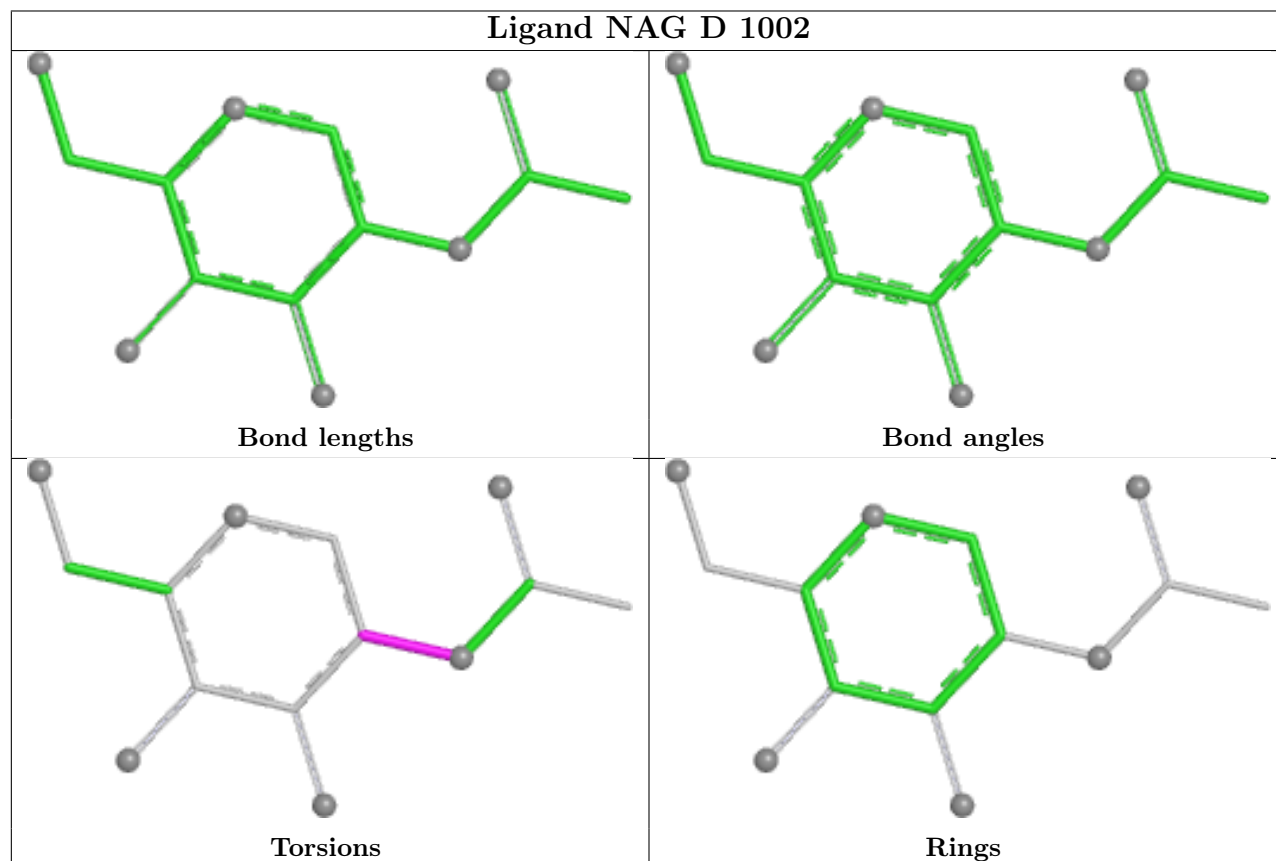
Ligand NAG A 902



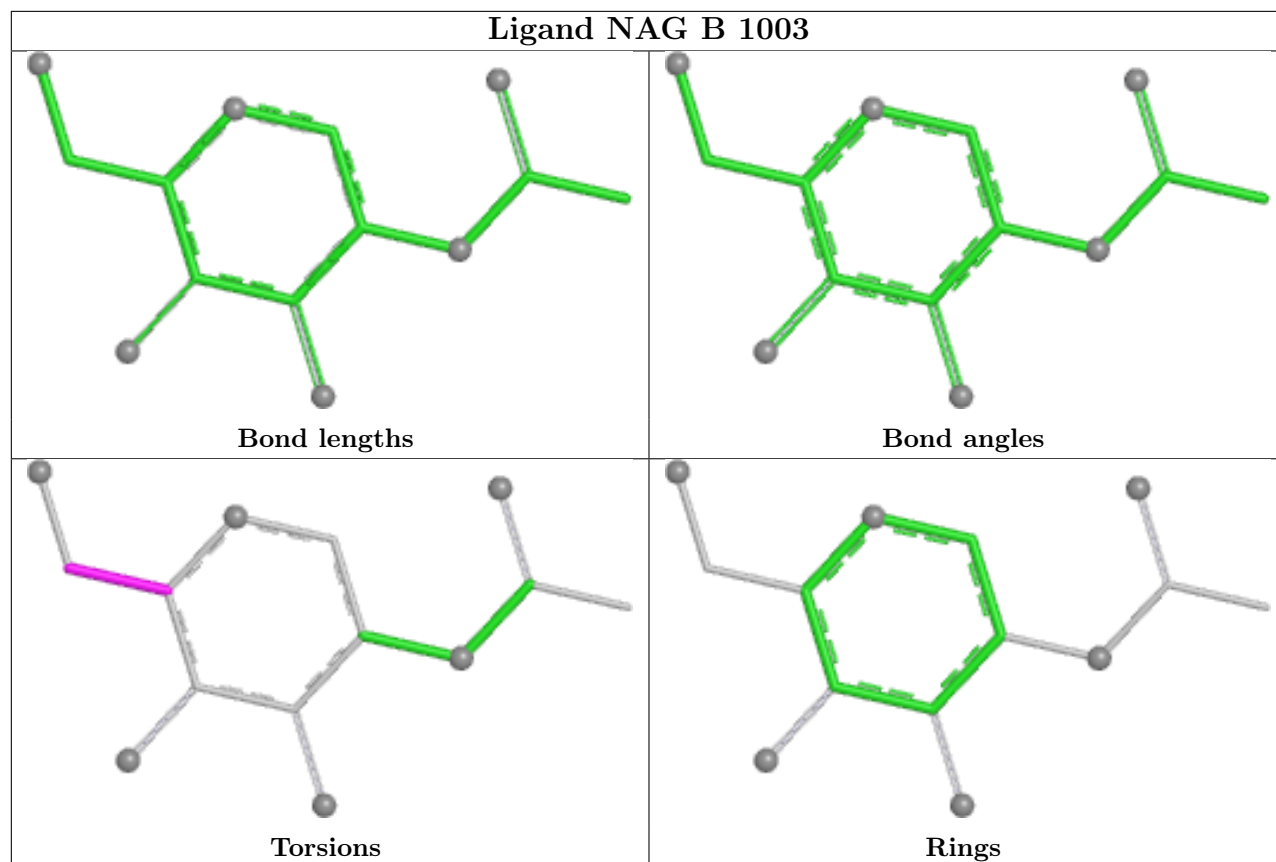
Ligand NAG D 1001



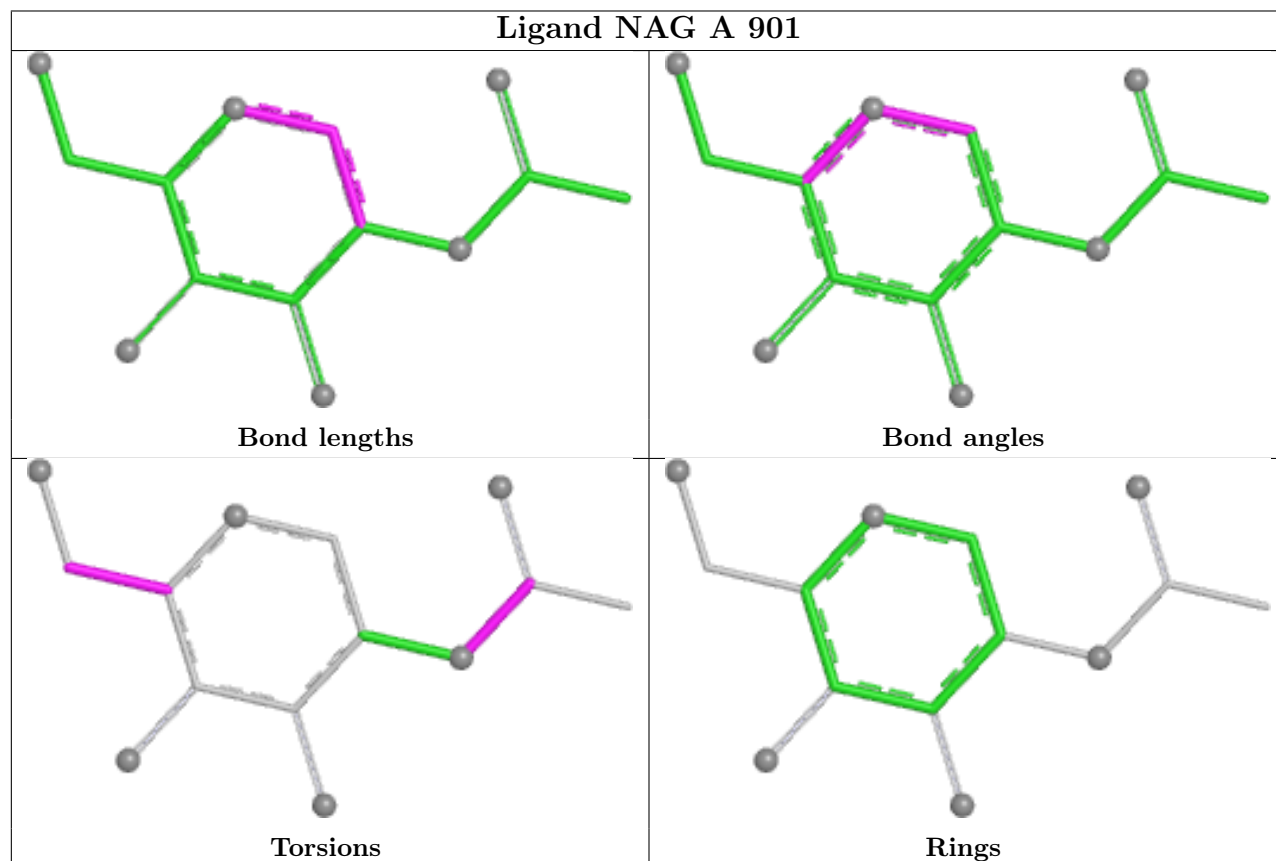
Ligand NAG D 1002



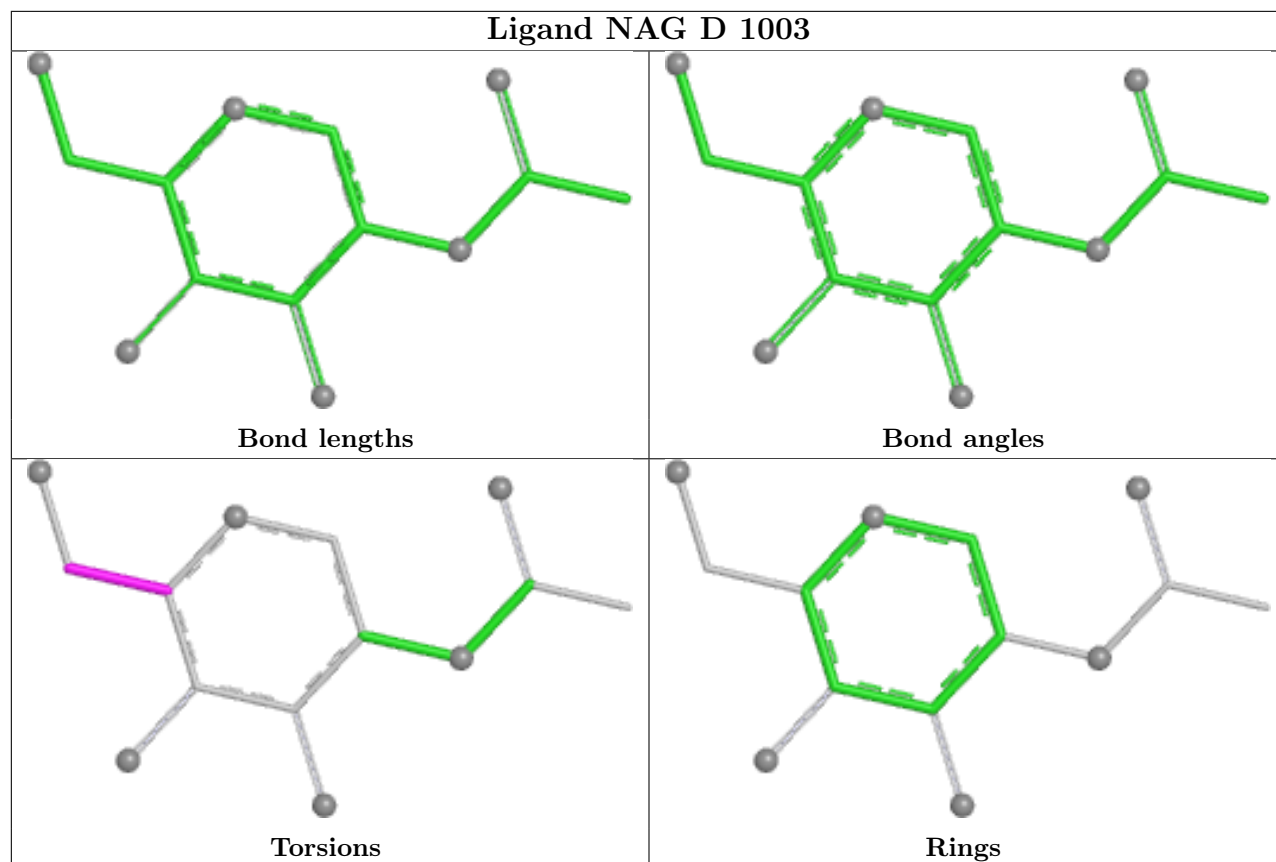
Ligand NAG B 1003



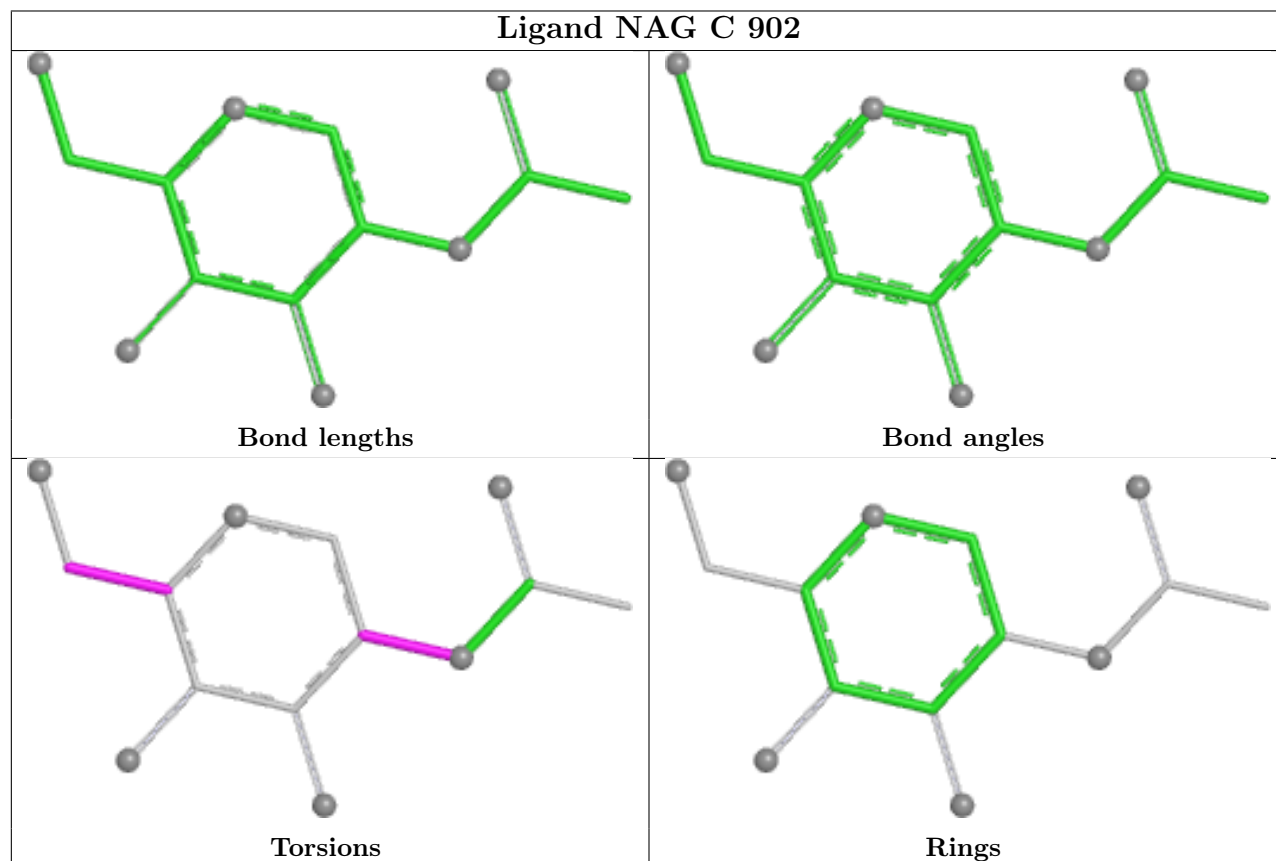
Ligand NAG A 901



Ligand NAG D 1003



Ligand NAG C 902



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.

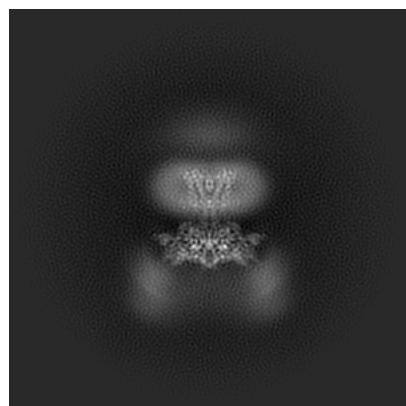
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70405. These allow visual inspection of the internal detail of the map and identification of artifacts.

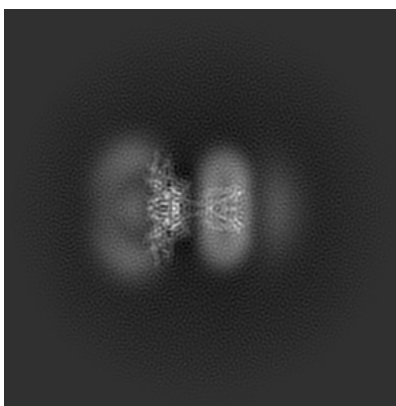
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

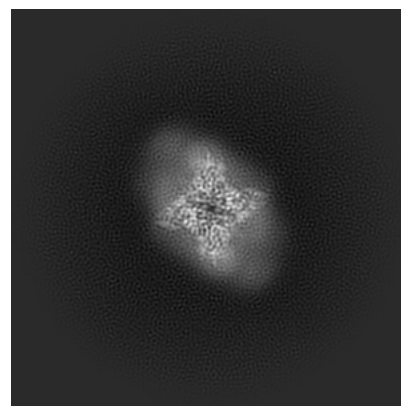
6.1.1 Primary map



X

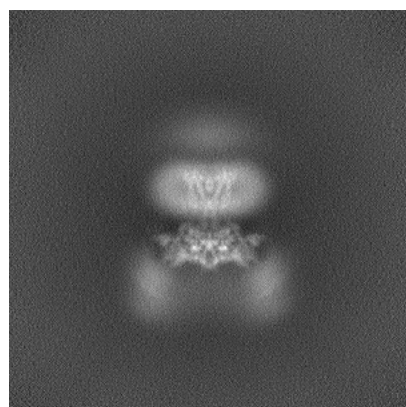


Y

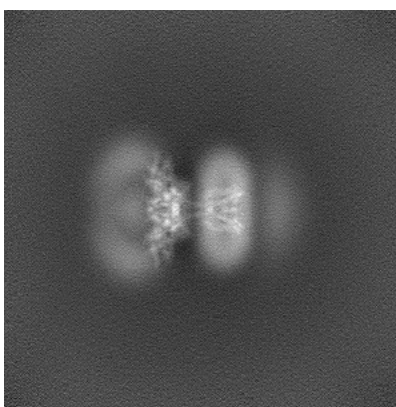


Z

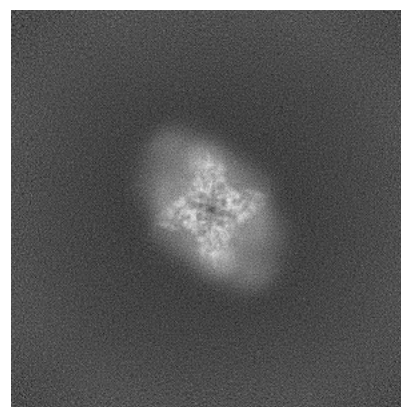
6.1.2 Raw map



X



Y

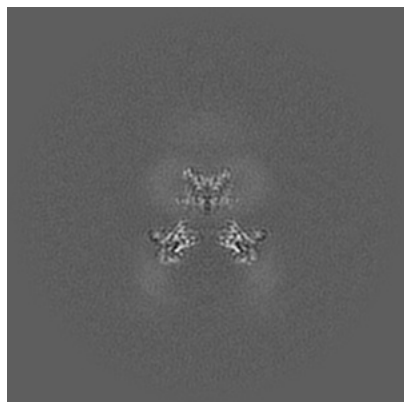


Z

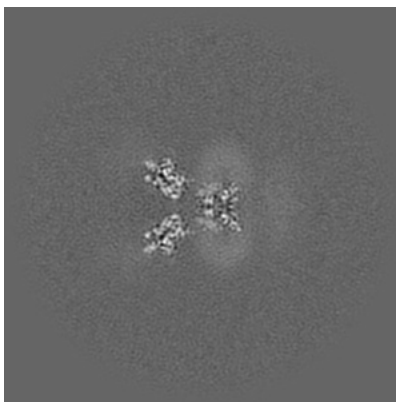
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

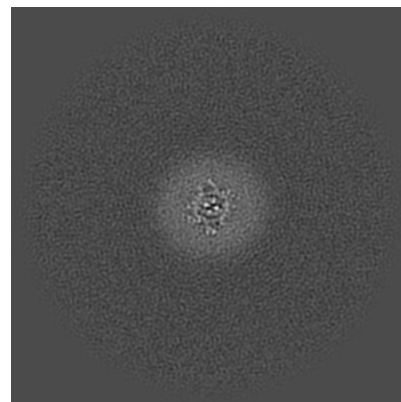
6.2.1 Primary map



X Index: 256

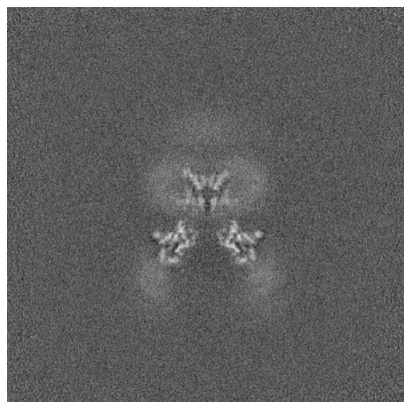


Y Index: 256

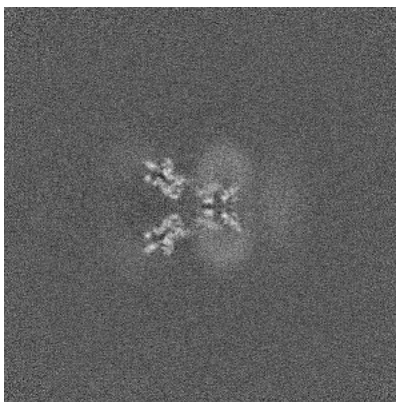


Z Index: 256

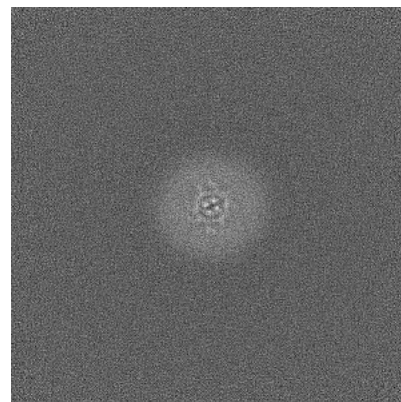
6.2.2 Raw map



X Index: 256



Y Index: 256

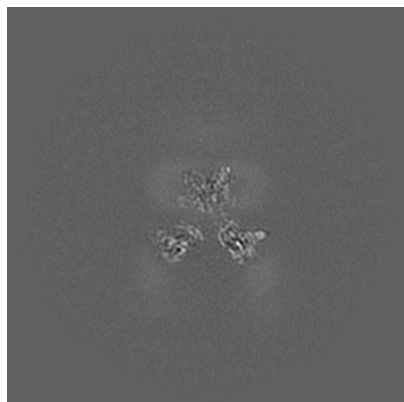


Z Index: 256

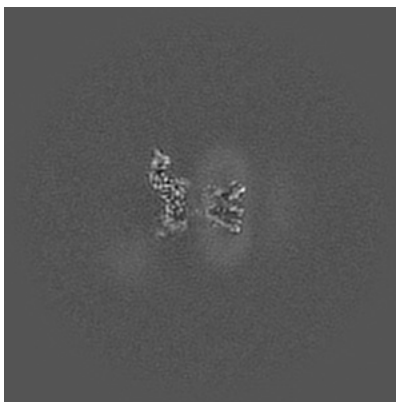
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

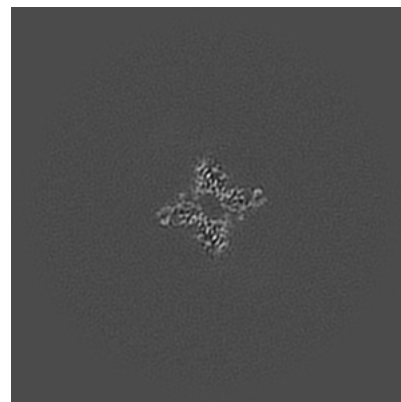
6.3.1 Primary map



X Index: 252

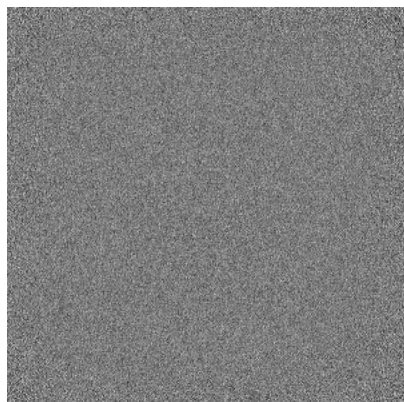


Y Index: 275

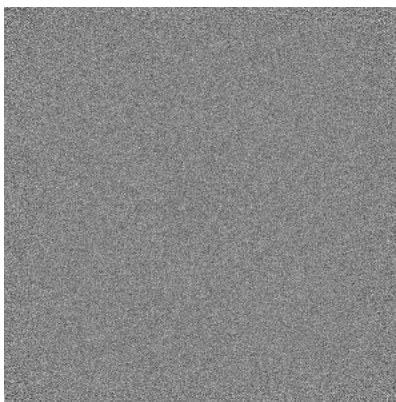


Z Index: 208

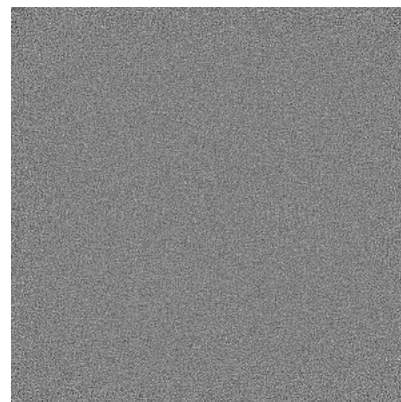
6.3.2 Raw map



X Index: 0



Y Index: 0

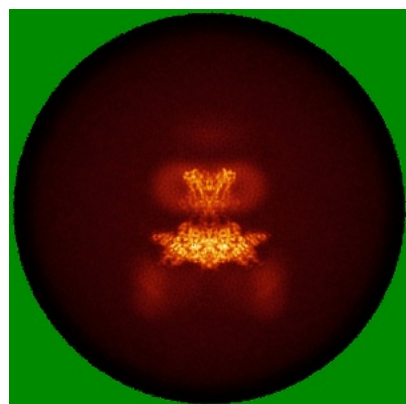


Z Index: 0

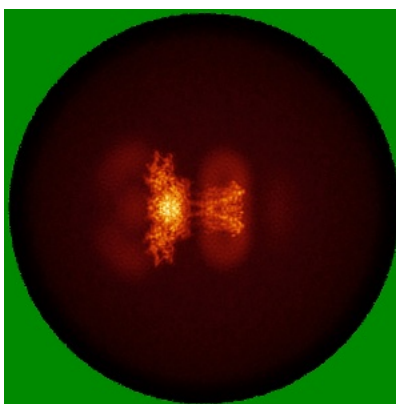
The images above show the largest variance slices of the map in three orthogonal directions.

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

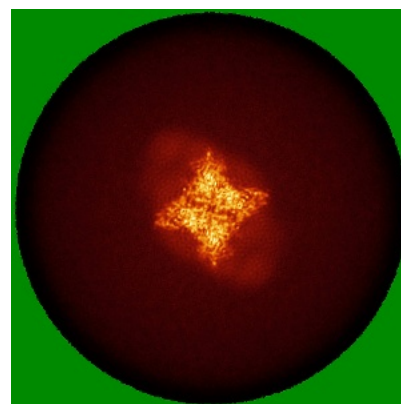
6.4.1 Primary map



X

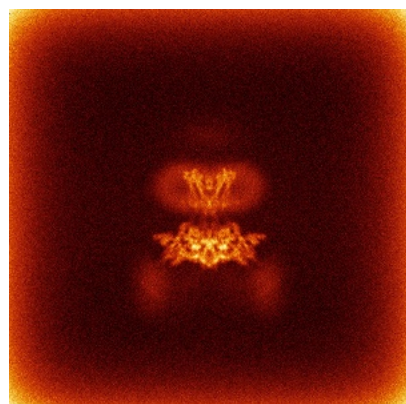


Y

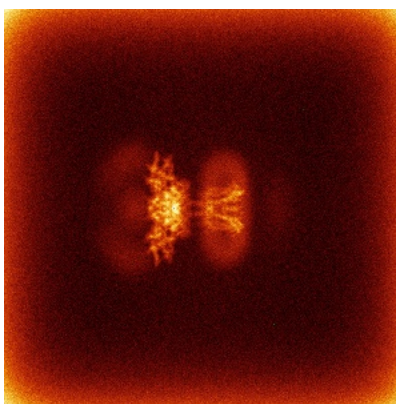


Z

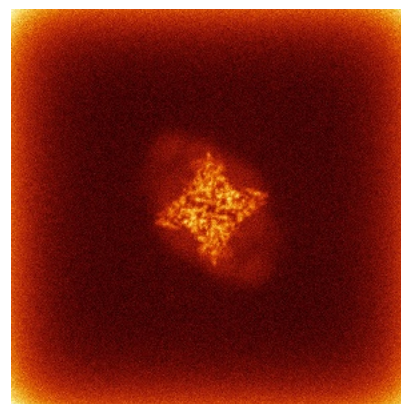
6.4.2 Raw map



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.

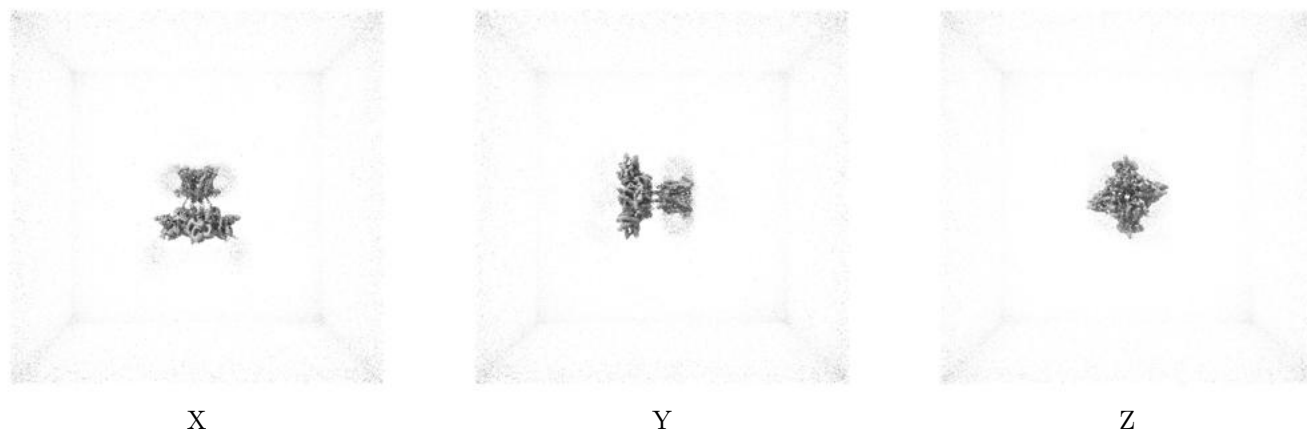
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

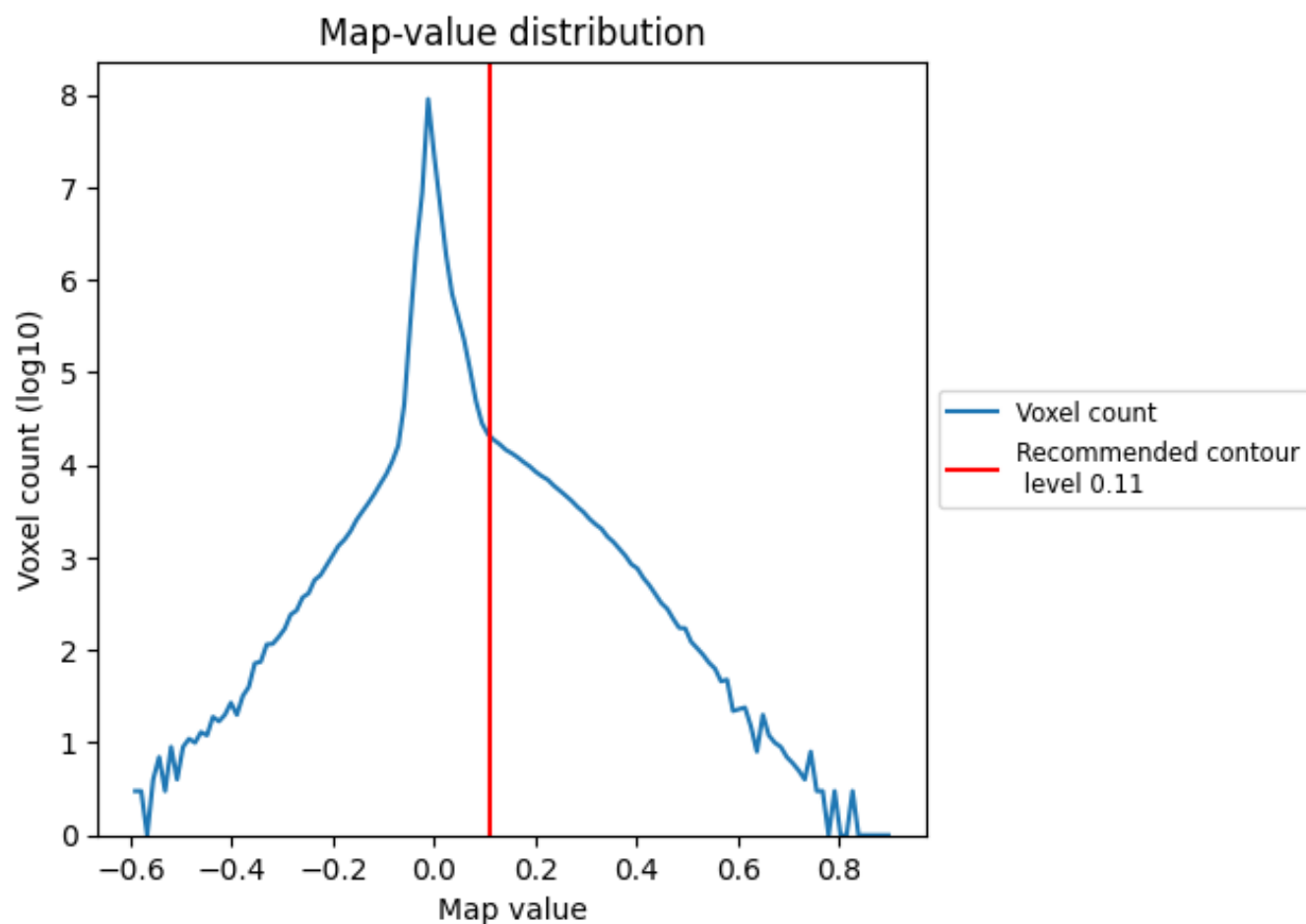
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

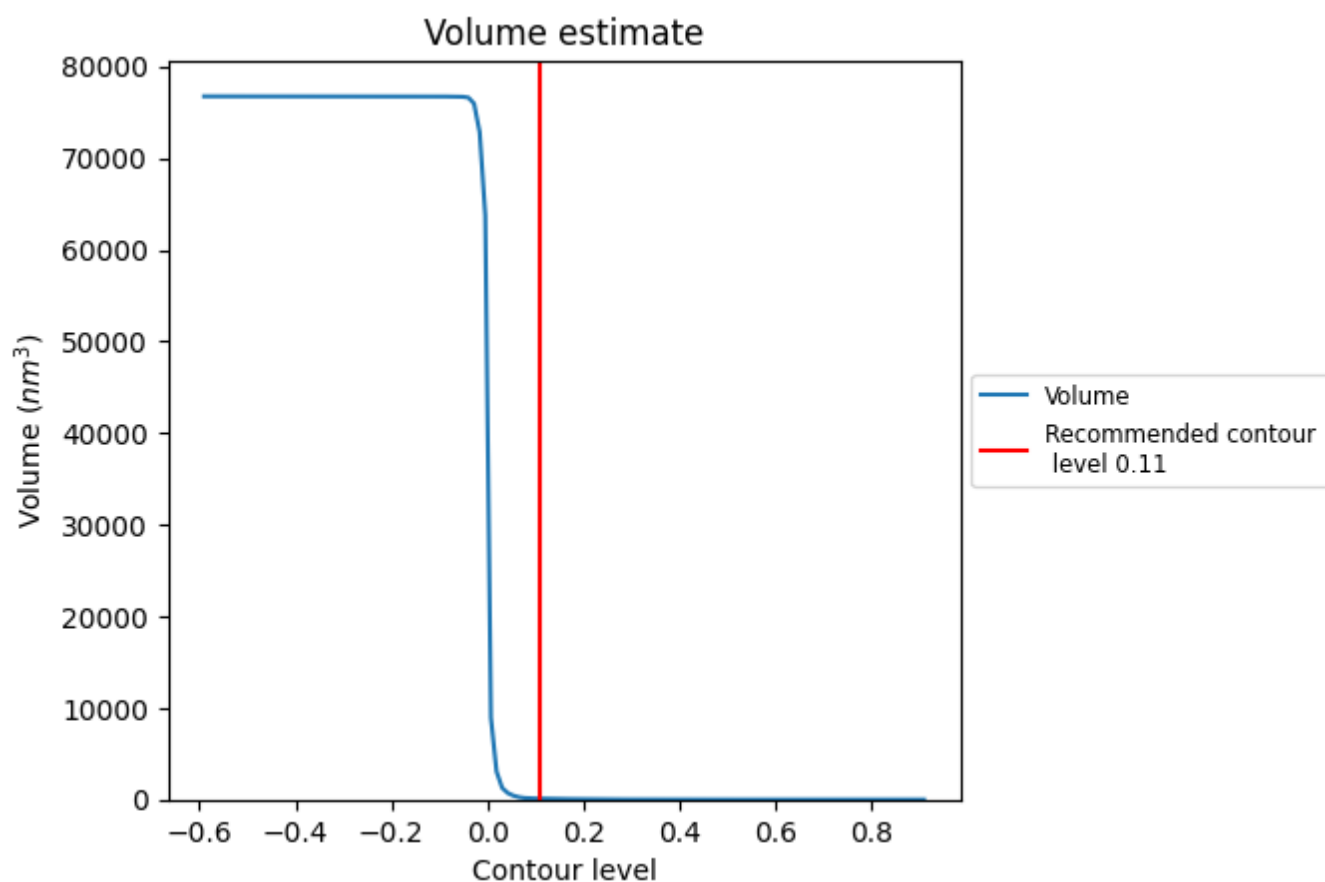
This section contains the results of statistical analysis of the map.

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.

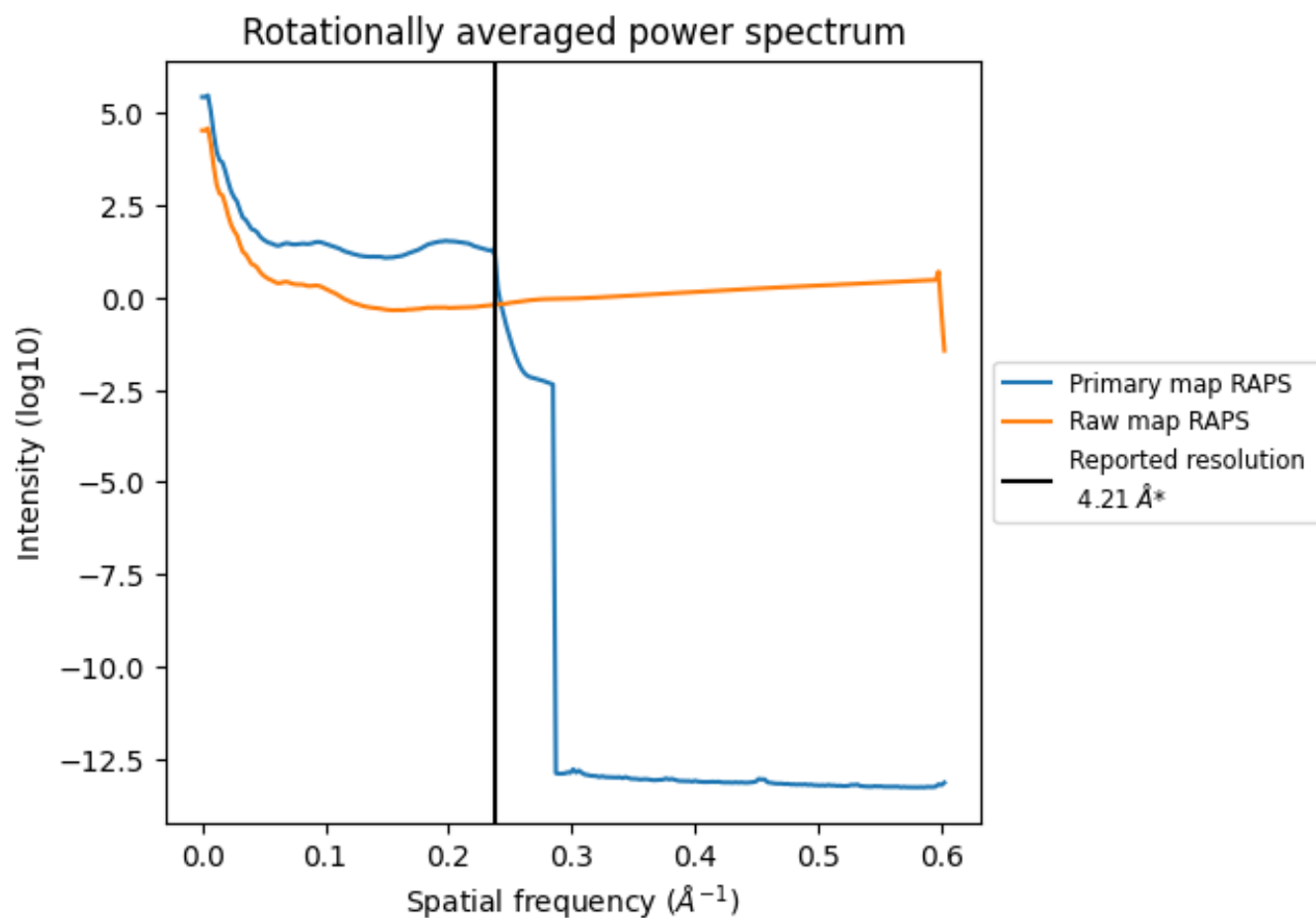
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm^3 ; this corresponds to an approximate mass of 92 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 ⓘ

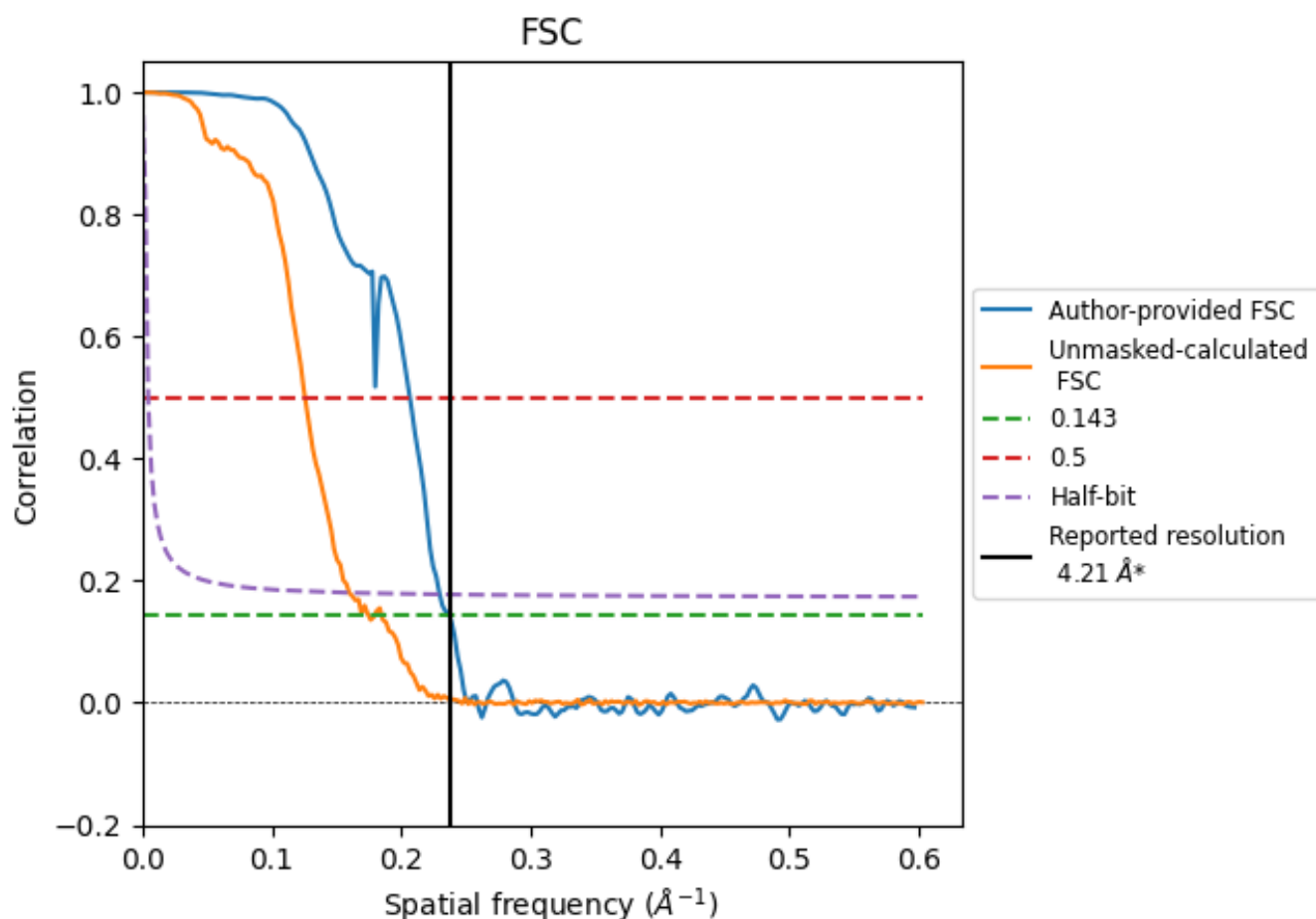


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

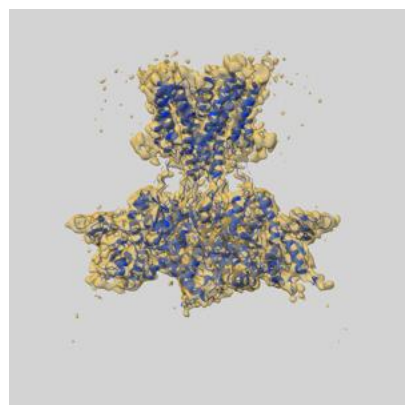
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.21	-	-
Author-provided FSC curve	4.21	4.84	4.35
Unmasked-calculated*	5.72	7.96	6.25

*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 5.72 differs from the reported value 4.21 by more than 10 %

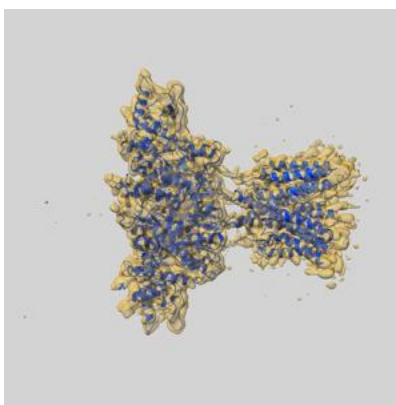
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70405 and PDB model 9OEO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

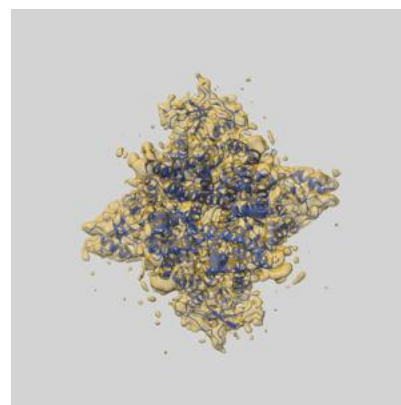
9.1 Map-model overlay [i](#)



X



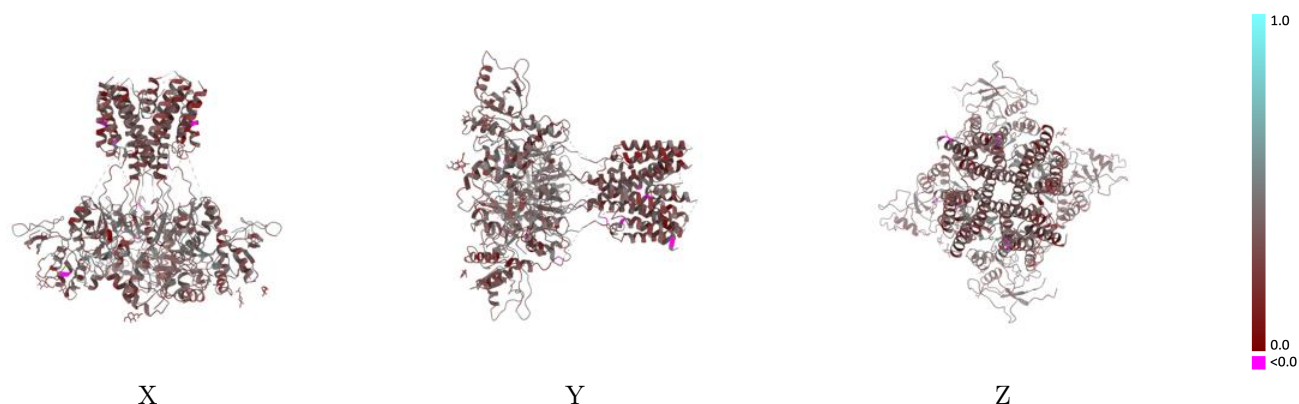
Y



Z

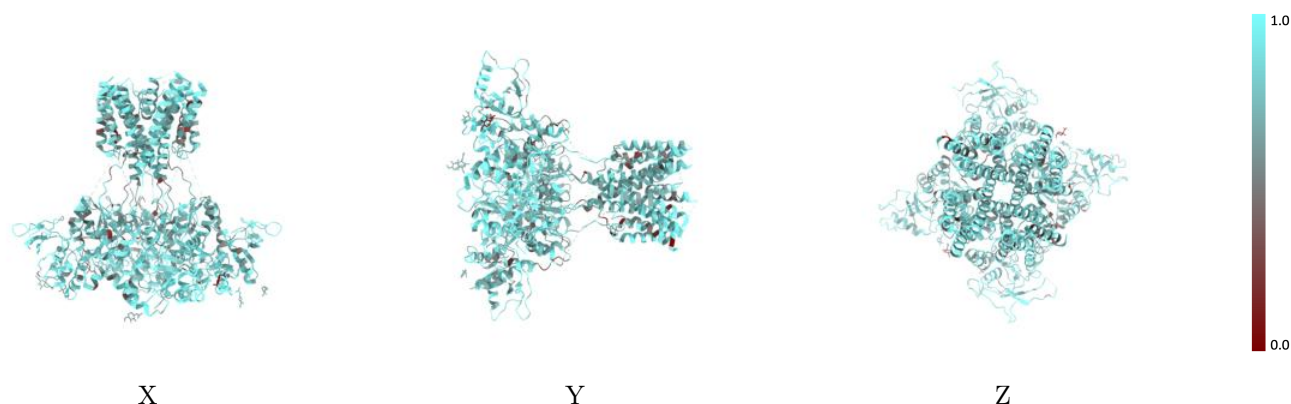
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



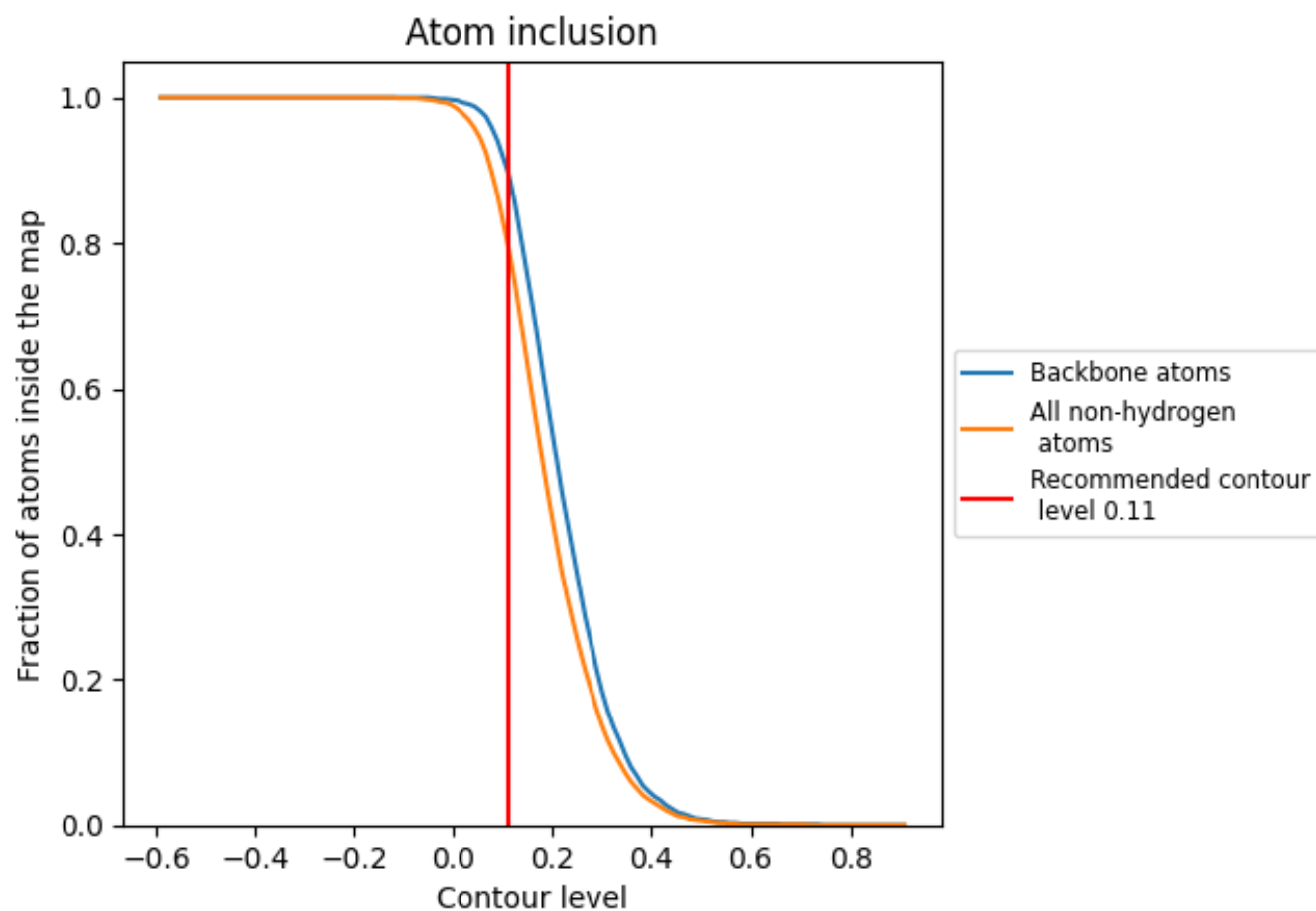
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.3680
A	0.7960	0.3650
B	0.8010	0.3690
C	0.7860	0.3640
D	0.8130	0.3740

