



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 06:28 PM EDT

PDB ID : 12BN / pdb_000012bn
EMDB ID : EMD-76288
Title : Structural insights into the exosite-mediated activation of Factor IX by Factor XIa using cryoEM
Authors : Mohammed, B.M.
Deposited on : 2026-03-25
Resolution : 3.40 Å (reported)
Based on initial models : ., 1NL0, 6I58, 9ZQY

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:

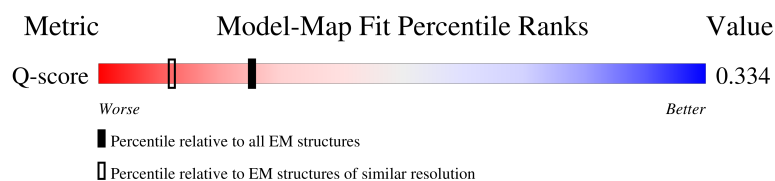
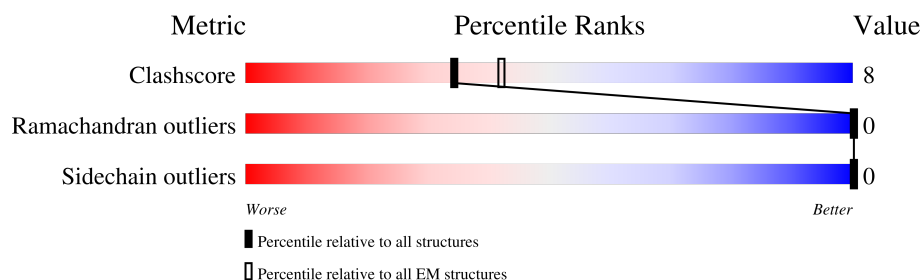
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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	14717 (2.90 - 3.90)

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	E	415	 9% 68% 25% 7%
1	F	415	 7% 88%
2	A	369	 79% 21%
2	C	369	 82% 18%

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Mol	Chain	Length	Quality of chain
3	B	236	 81%18%
3	D	236	 86%14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CGU	F	33	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13151 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 Coagulation factor IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	386	Total	C	N	O	S	0	0
			3074	1914	524	611	25		
1	F	48	Total	C	N	O	S	0	0
			443	264	66	110	3		

- Molecule 2 is a protein called Coagulation factor XIa heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	369	Total	C	N	O	S	0	0
			2879	1805	500	544	30		
2	C	369	Total	C	N	O	S	0	0
			2879	1805	500	544	30		

- Molecule 3 is a protein called Coagulation factor XIa light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	236	Total	C	N	O	S	0	0
			1874	1184	332	347	11		
3	D	236	Total	C	N	O	S	0	0
			1874	1184	332	347	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	557	ALA	SER	engineered mutation	UNP P03951
D	557	ALA	SER	engineered mutation	UNP P03951

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

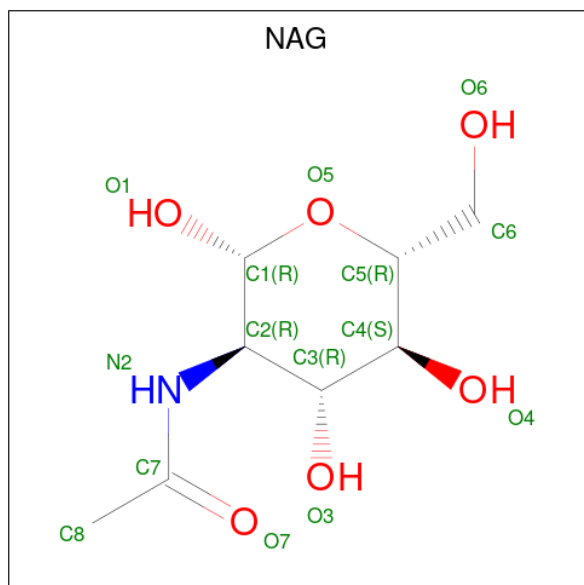
Mol	Chain	Residues	Atoms		AltConf
4	E	8	Total	Ca	0
			8	8	

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Mol	Chain	Residues	Atoms		AltConf
4	F	8	Total	Ca	0
			8	8	

- Molecule 5 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
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	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	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	

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

• Molecule 2: Coagulation factor XIa heavy chain

Chain A:  79% 21%

C328	E1	T22	Y27	C28	Q29	V30	V31	C32	T33	Y34	C38	F43	F56	L60	T65	L68	F82	H87	Q88	A91	C92	M102	K103	G104	T105	N106	V111	T123	D124	D125	C128	I146	L149	K150	H151	T152	Q153	T154	G155	T156	P157	T158	R159
D164	K165	F170	S171	L172	K173	S174	T190	S199	V207	T211	C212	T213	C218	F221	W228	P229	K230	C237	L238	L239	K240	R250	T251	K252	K253	H267	P270	T281	L284	G285	E286	E287	L288	A292	Q300	F312	T313	Y314	G326	K327			
L332	K340	H343	K357	N360	T363	T364	K367	P368	R369																																		

• Molecule 2: Coagulation factor XIa heavy chain

Chain C:  82% 18%

E1	L7	T22	Y27	C28	V31	C32	T33	C38	F43	F56	L60	T65	L68	P69	R70	F82	K83	Q84	H87	Q88	C92	M102	K103	V111	T123	C128	Y133	A134	T135	R136	Q137	I146	C147	L148	L149	P157	T158	R159		
D164	K165	L172	K173	S174	T190	V207	T211	C212	F221	W228	P229	K230	R234	R250	H267	V271	T281	L284	G285	E286	A292	Q300	V307	F312	T313	Y314	K327	C328	K340	H343	C356	K357	K358	D359	K360	E361	C362	T363	T364	
K367	P368	R369																																						

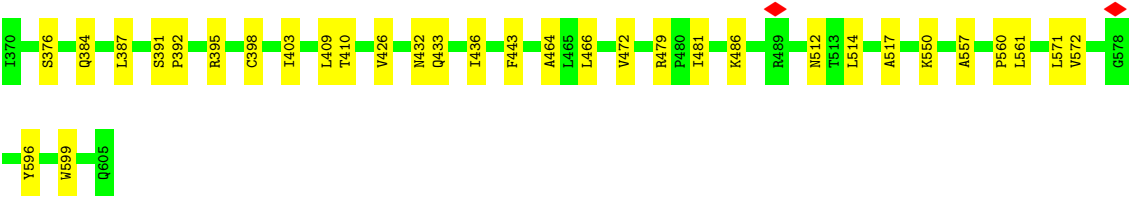
• Molecule 3: Coagulation factor XIa light chain

Chain B:  81% 18%

L370	V371	W381	Q384	L387	S391	P392	R395	C398	N405	T410	H413	V426	N432	Q433	I436	F443	A464	L465	L466	V472	I481	K486	R489	N490	V491	T499	R504	R507	N512	A517	M540	K550	D551
A557	P560	K564	E567	L571	V572	G573	W577	G578	E579	V589	V593	Y596	W599	Q605																			

• Molecule 3: Coagulation factor XIa light chain

Chain D:  86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	87309, 87309	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56, 57.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON IV (4k x 4k), FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.523	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.0398	Depositor
Map size ($\text{\AA}$)	386.04797, 386.04797, 386.04797	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.9279999, 0.9279999, 0.9279999	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, CGU

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	E	0.11	0/2986	0.36	1/4021 (0.0%)
1	F	0.12	0/297	0.35	0/382
2	A	0.12	0/2944	0.34	0/3982
2	C	0.12	0/2944	0.34	0/3982
3	B	0.14	0/1919	0.38	2/2601 (0.1%)
3	D	0.12	0/1919	0.30	0/2601
All	All	0.12	0/13009	0.35	3/17569 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	491	VAL	N-CA-C	6.77	117.76	109.30
1	E	100	LYS	N-CA-C	5.36	118.45	110.14
3	B	489	ARG	N-CA-C	-5.27	106.98	113.41

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	E	3074	0	2875	66	0
1	F	443	0	341	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2879	0	2802	48	0
2	C	2879	0	2802	49	0
3	B	1874	0	1833	32	0
3	D	1874	0	1833	21	0
4	E	8	0	0	0	0
4	F	8	0	0	0	0
5	A	28	0	26	1	0
5	B	28	0	26	0	0
5	C	28	0	26	0	0
5	D	28	0	26	0	0
All	All	13151	0	12590	209	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 209 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:E:100:LYS:HB2	1:E:108:VAL:HG23	1.31	1.08
1:F:33:CGU:OE12	2:C:267:HIS:NE2	1.86	1.07
1:E:100:LYS:HB2	1:E:108:VAL:CG2	1.91	1.00
1:F:33:CGU:OE12	2:C:267:HIS:CD2	2.33	0.80
1:E:91:LYS:HE3	1:E:94:ARG:NH1	1.99	0.78

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	E	370/415 (89%)	350 (95%)	20 (5%)	0	100	100
1	F	34/415 (8%)	31 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	367/369 (100%)	353 (96%)	14 (4%)	0	100	100
2	C	367/369 (100%)	353 (96%)	14 (4%)	0	100	100
3	B	234/236 (99%)	220 (94%)	14 (6%)	0	100	100
3	D	234/236 (99%)	222 (95%)	12 (5%)	0	100	100
All	All	1606/2040 (79%)	1529 (95%)	77 (5%)	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	E	322/350 (92%)	322 (100%)	0	100	100
1	F	32/350 (9%)	32 (100%)	0	100	100
2	A	331/331 (100%)	331 (100%)	0	100	100
2	C	331/331 (100%)	331 (100%)	0	100	100
3	B	202/202 (100%)	202 (100%)	0	100	100
3	D	202/202 (100%)	202 (100%)	0	100	100
All	All	1420/1766 (80%)	1420 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
3	B	478	GLN
2	C	267	HIS
3	D	524	ASN
1	E	264	ASN
1	F	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CGU	F	15	1,4	9,11,12	1.51	2 (22%)	10,14,16	0.79	0
1	CGU	E	30	1,4	9,11,12	1.49	2 (22%)	10,14,16	0.82	0
1	CGU	E	21	1,4	9,11,12	1.52	2 (22%)	10,14,16	0.77	0
1	CGU	E	36	1	9,11,12	1.55	2 (22%)	10,14,16	0.76	0
1	CGU	F	33	1	9,11,12	1.57	2 (22%)	10,14,16	0.84	0
1	CGU	E	27	1,4	9,11,12	1.54	2 (22%)	10,14,16	0.76	0
1	CGU	E	26	1,4	9,11,12	1.51	2 (22%)	10,14,16	0.78	0
1	CGU	F	20	1,4	9,11,12	1.51	2 (22%)	10,14,16	0.81	0
1	CGU	F	40	1,4	9,11,12	1.55	2 (22%)	10,14,16	0.71	0
1	CGU	F	27	1,4	9,11,12	1.54	2 (22%)	10,14,16	0.75	0
1	CGU	E	8	1,4	9,11,12	1.49	1 (11%)	10,14,16	0.77	0
1	CGU	E	7	1,4	9,11,12	1.54	2 (22%)	10,14,16	0.76	0
1	CGU	E	15	1,4	9,11,12	1.49	1 (11%)	10,14,16	0.84	0
1	CGU	E	17	1,4	9,11,12	1.57	2 (22%)	10,14,16	0.80	0
1	CGU	E	20	1,4	9,11,12	1.50	2 (22%)	10,14,16	0.83	0
1	CGU	F	8	1,4	9,11,12	1.50	2 (22%)	10,14,16	0.80	0
1	CGU	E	40	1,4	9,11,12	1.53	2 (22%)	10,14,16	0.78	0
1	CGU	F	7	1,4	9,11,12	1.51	2 (22%)	10,14,16	0.80	0
1	CGU	E	33	1	9,11,12	1.55	2 (22%)	10,14,16	0.83	0
1	CGU	F	26	1,4	9,11,12	1.53	2 (22%)	10,14,16	0.76	0
1	CGU	F	30	1,4	9,11,12	1.53	2 (22%)	10,14,16	0.78	0
1	CGU	F	17	1,4	9,11,12	1.54	2 (22%)	10,14,16	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CGU	F	36	1,4	9,11,12	1.56	2 (22%)	10,14,16	0.74	0
1	CGU	F	21	1,4	9,11,12	1.53	2 (22%)	10,14,16	0.77	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
1	CGU	F	15	1,4	-	1/13/14/16	-
1	CGU	E	30	1,4	-	1/13/14/16	-
1	CGU	E	21	1,4	-	1/13/14/16	-
1	CGU	E	36	1	-	1/13/14/16	-
1	CGU	F	33	1	-	4/13/14/16	-
1	CGU	E	27	1,4	-	4/13/14/16	-
1	CGU	E	26	1,4	-	2/13/14/16	-
1	CGU	F	20	1,4	-	2/13/14/16	-
1	CGU	F	40	1,4	-	0/13/14/16	-
1	CGU	F	27	1,4	-	4/13/14/16	-
1	CGU	E	8	1,4	-	3/13/14/16	-
1	CGU	E	7	1,4	-	4/13/14/16	-
1	CGU	E	15	1,4	-	0/13/14/16	-
1	CGU	E	17	1,4	-	3/13/14/16	-
1	CGU	E	20	1,4	-	0/13/14/16	-
1	CGU	F	8	1,4	-	4/13/14/16	-
1	CGU	E	40	1,4	-	0/13/14/16	-
1	CGU	F	7	1,4	-	1/13/14/16	-
1	CGU	E	33	1	-	7/13/14/16	-
1	CGU	F	26	1,4	-	2/13/14/16	-
1	CGU	F	30	1,4	-	0/13/14/16	-
1	CGU	F	17	1,4	-	2/13/14/16	-
1	CGU	F	36	1,4	-	1/13/14/16	-
1	CGU	F	21	1,4	-	3/13/14/16	-

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	17	CGU	CG-CD1	2.63	1.55	1.52
1	F	33	CGU	CG-CD1	2.61	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	17	CGU	CG-CD1	2.56	1.55	1.52
1	E	36	CGU	CG-CD1	2.55	1.55	1.52
1	E	33	CGU	CG-CD1	2.53	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	7	CGU	N-CA-CB-CG
1	E	7	CGU	C-CA-CB-CG
1	E	7	CGU	CA-CB-CG-CD1
1	E	7	CGU	CA-CB-CG-CD2
1	E	8	CGU	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	15	CGU	1	0
1	F	33	CGU	6	0
1	E	15	CGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	402	2	14,14,15	0.72	0	17,19,21	0.82	0
5	NAG	A	402	2	14,14,15	0.74	0	17,19,21	1.10	1 (5%)
5	NAG	B	701	3	14,14,15	0.81	1 (7%)	17,19,21	1.98	3 (17%)
5	NAG	D	702	3	14,14,15	0.76	0	17,19,21	0.84	0
5	NAG	C	401	2	14,14,15	0.75	0	17,19,21	0.73	0
5	NAG	A	401	2	14,14,15	0.73	0	17,19,21	0.76	0
5	NAG	B	702	3	14,14,15	0.77	0	17,19,21	0.82	0
5	NAG	D	701	3	14,14,15	0.75	0	17,19,21	1.45	1 (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	402	2	-	1/6/23/26	0/1/1/1
5	NAG	A	402	2	-	0/6/23/26	0/1/1/1
5	NAG	B	701	3	-	0/6/23/26	0/1/1/1
5	NAG	D	702	3	-	2/6/23/26	0/1/1/1
5	NAG	C	401	2	-	1/6/23/26	0/1/1/1
5	NAG	A	401	2	-	1/6/23/26	0/1/1/1
5	NAG	B	702	3	-	2/6/23/26	0/1/1/1
5	NAG	D	701	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	NAG	C1-C2	2.06	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	701	NAG	C1-O5-C5	5.73	119.86	112.19
5	D	701	NAG	C1-O5-C5	4.54	118.27	112.19
5	B	701	NAG	O5-C1-C2	4.14	117.70	111.29
5	B	701	NAG	C3-C4-C5	-2.77	105.21	110.23
5	A	402	NAG	C1-O5-C5	-2.21	109.22	112.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

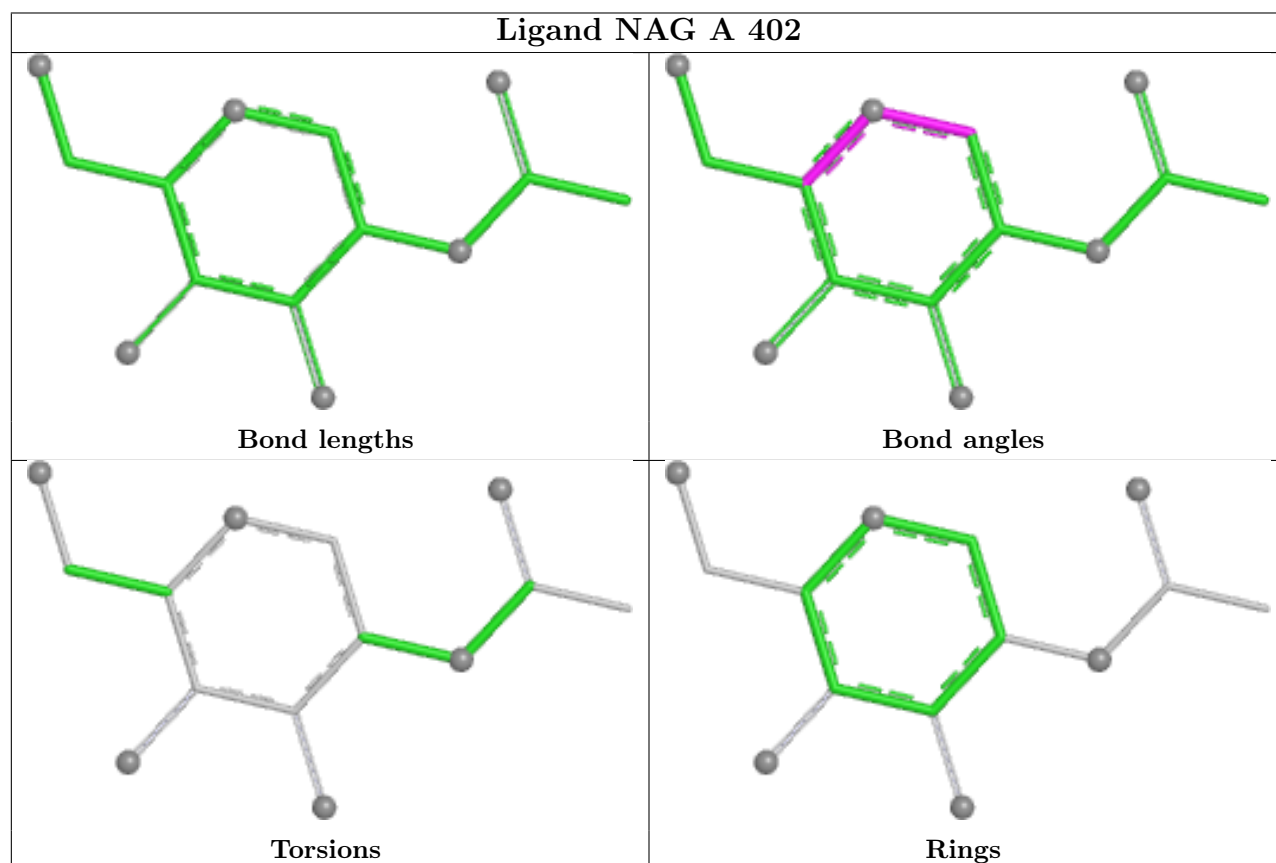
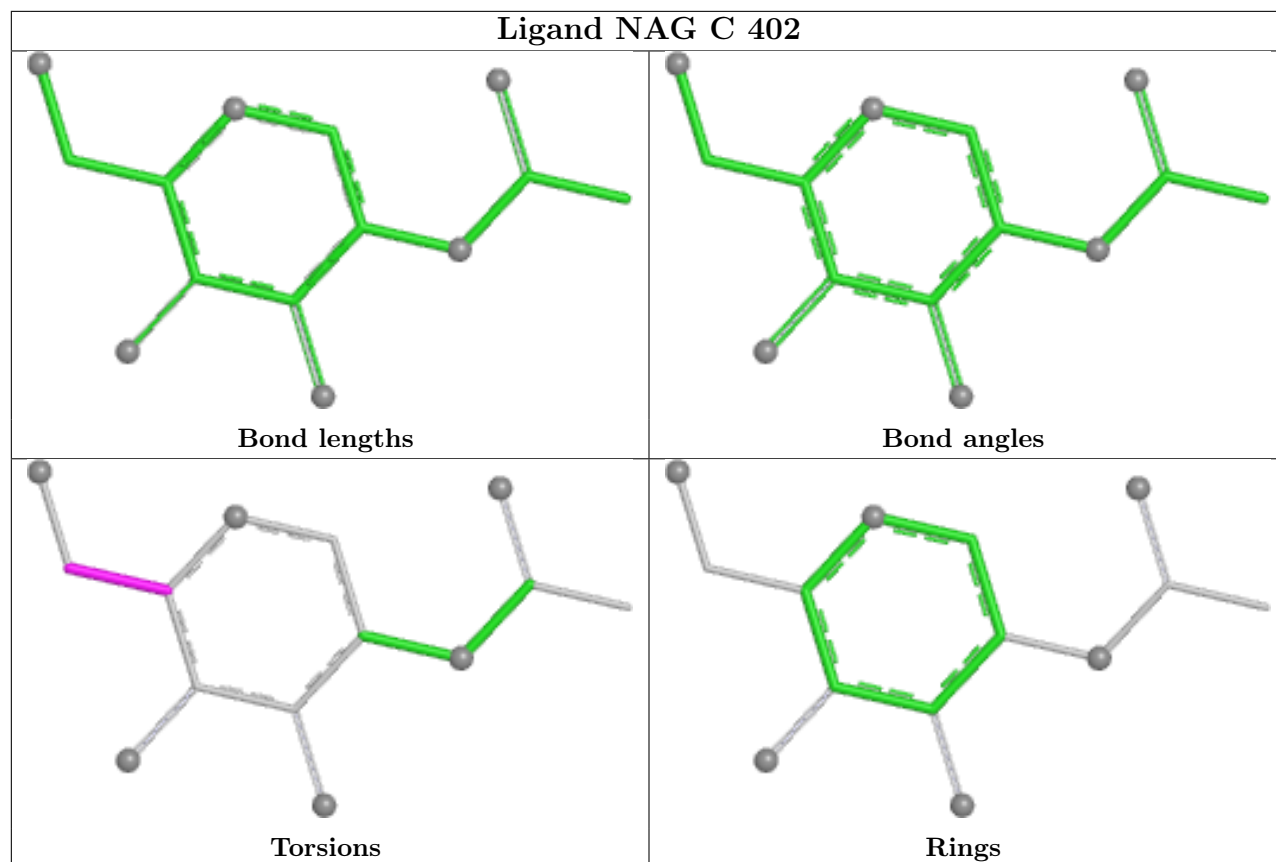
Mol	Chain	Res	Type	Atoms
5	B	702	NAG	C8-C7-N2-C2
5	B	702	NAG	O7-C7-N2-C2
5	D	702	NAG	C8-C7-N2-C2
5	D	702	NAG	O7-C7-N2-C2
5	C	401	NAG	O5-C5-C6-O6

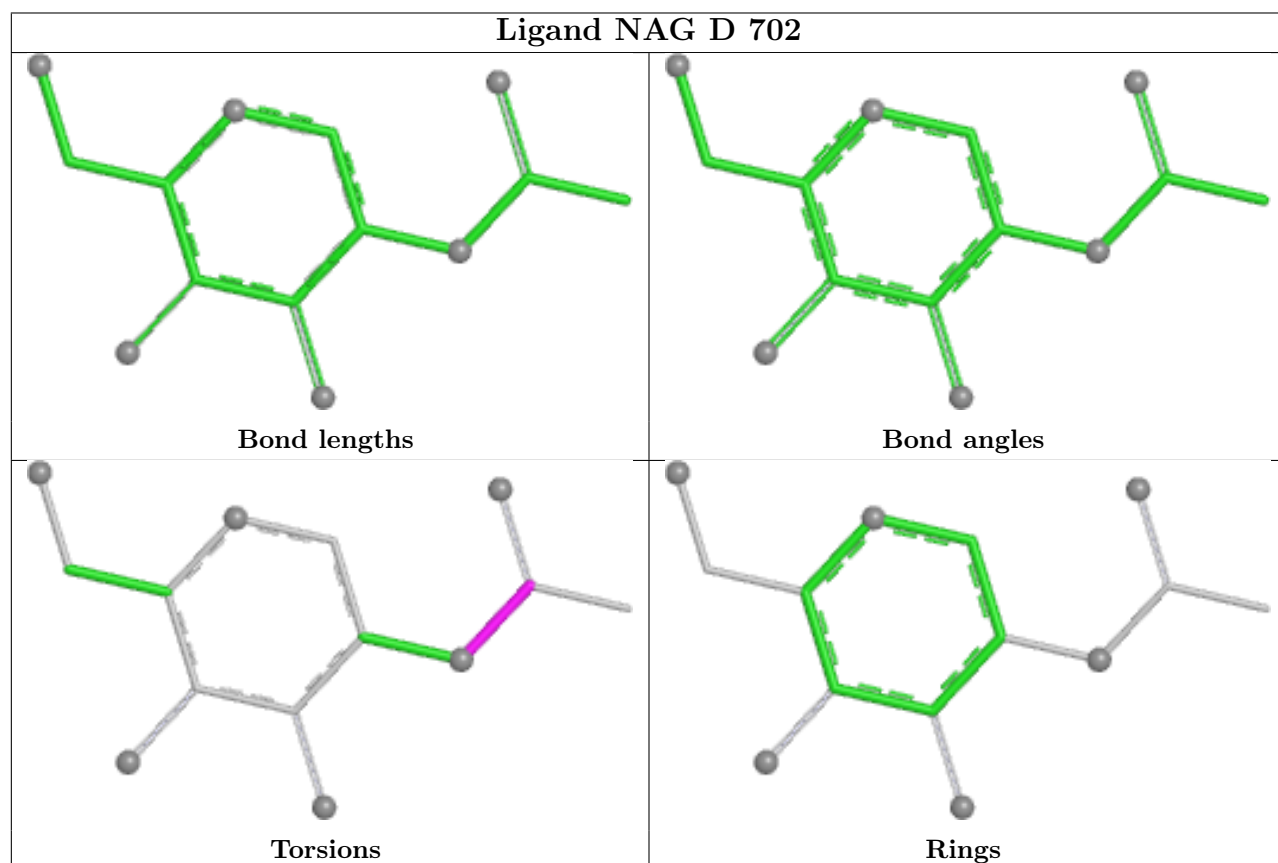
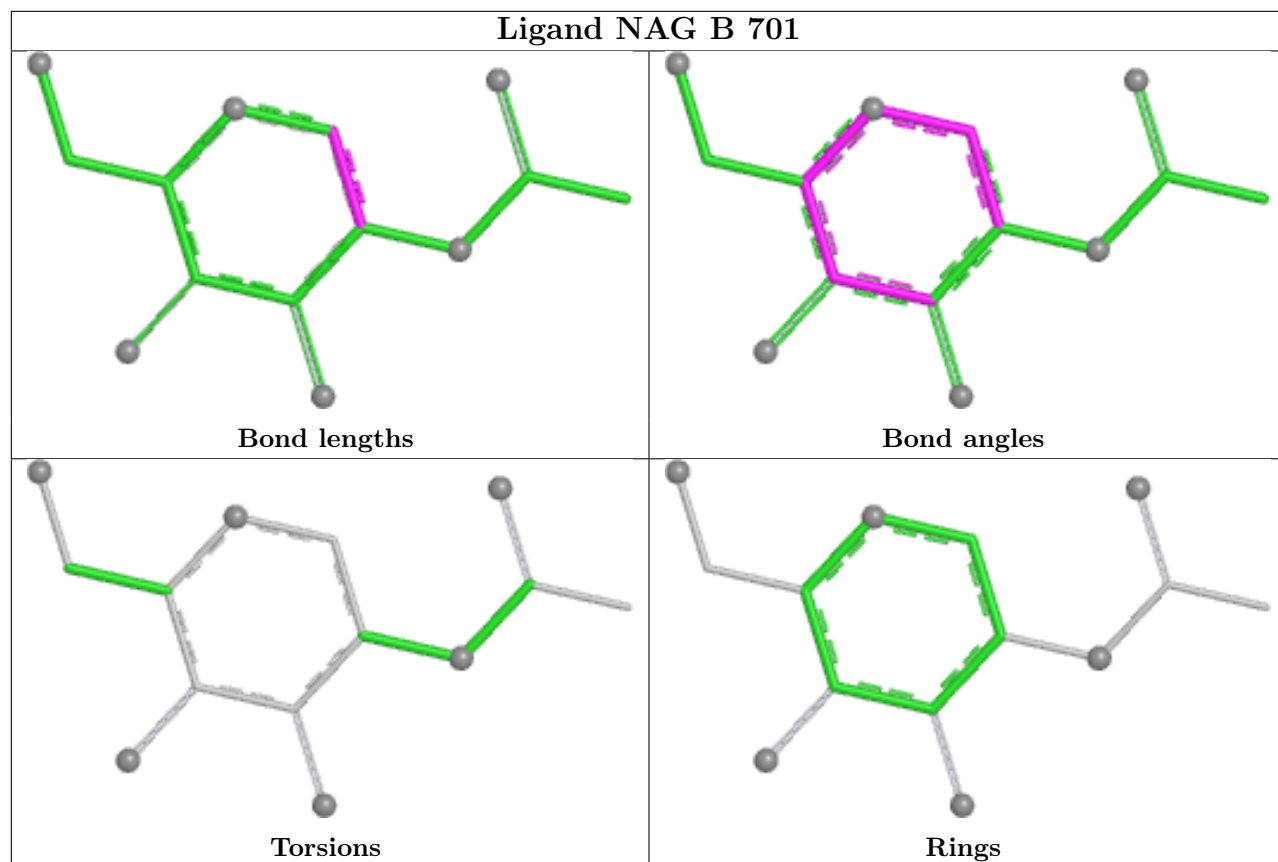
There are no ring outliers.

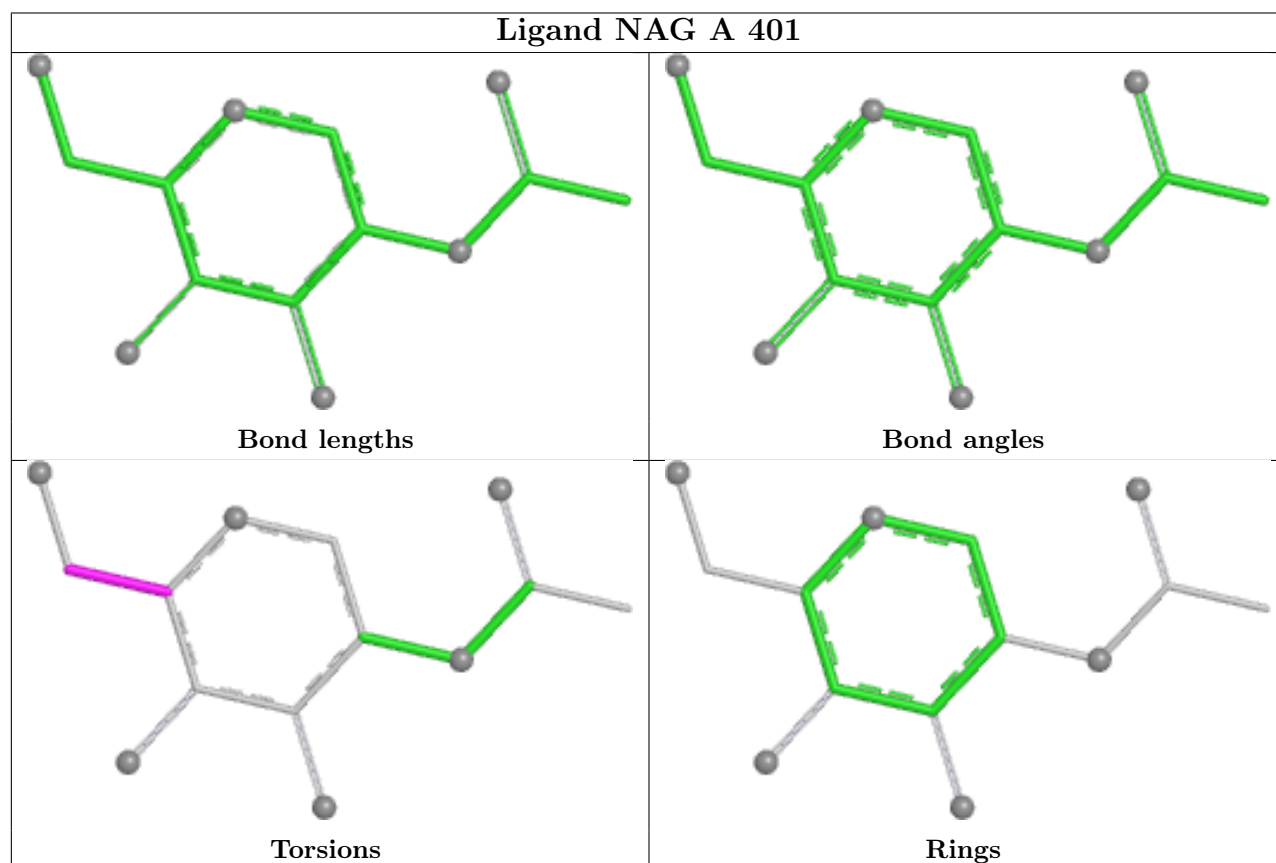
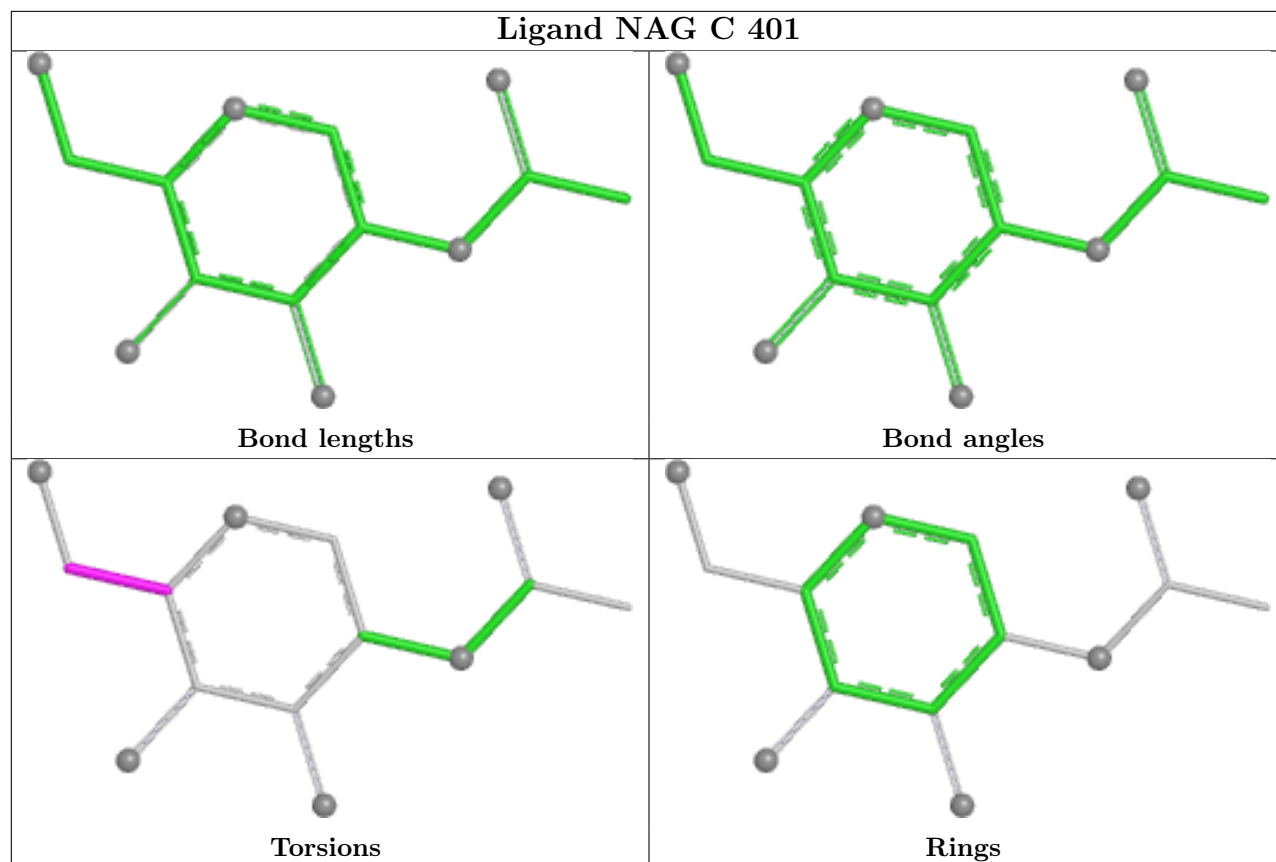
1 monomer is involved in 1 short contact:

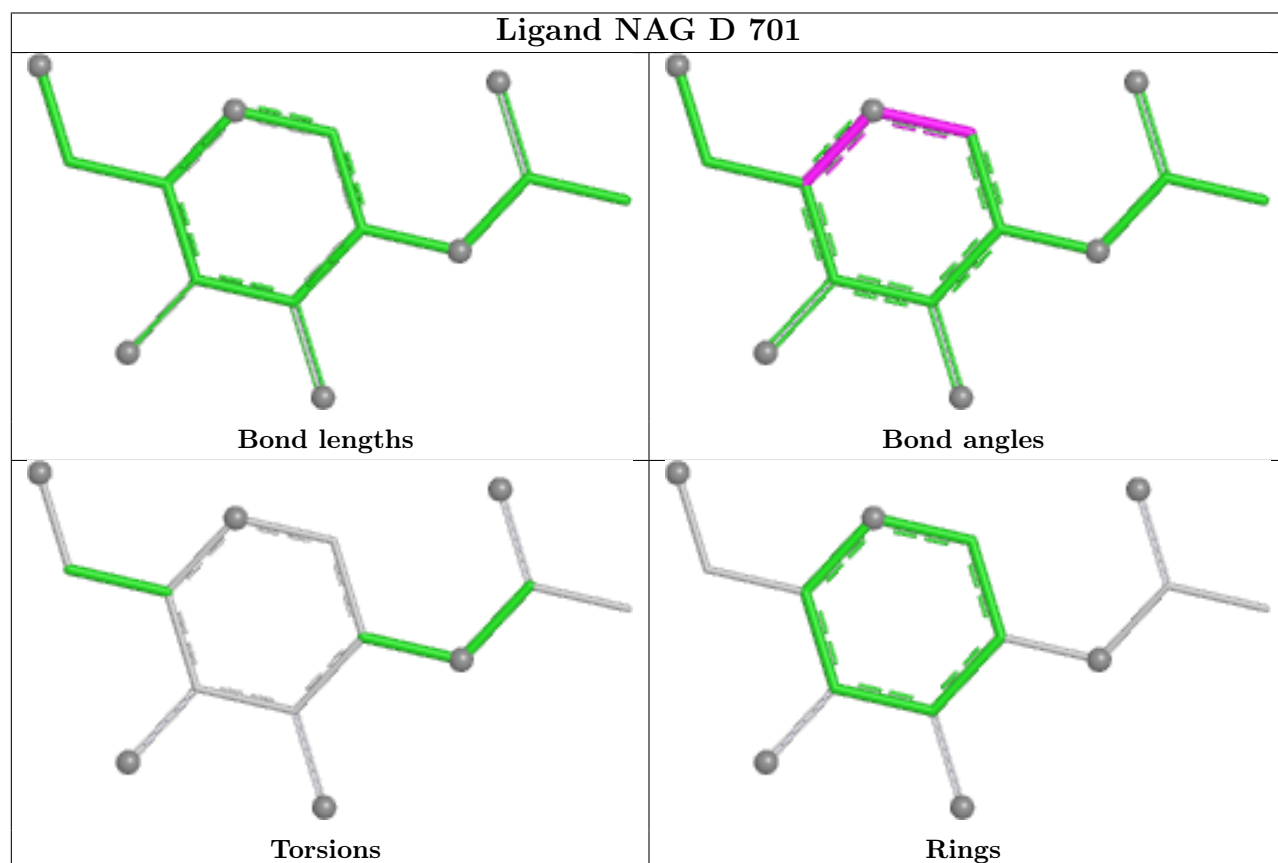
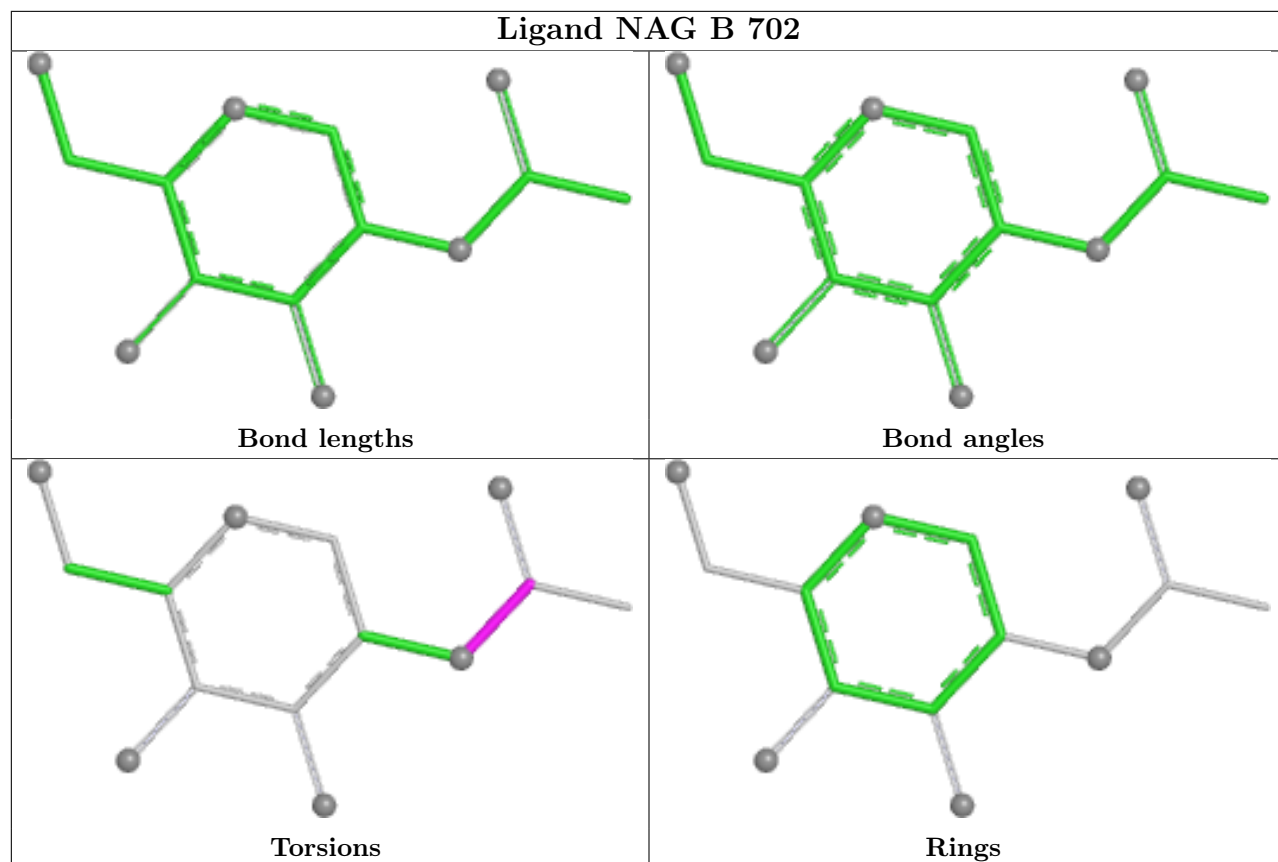
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	NAG	1	0

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.









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.

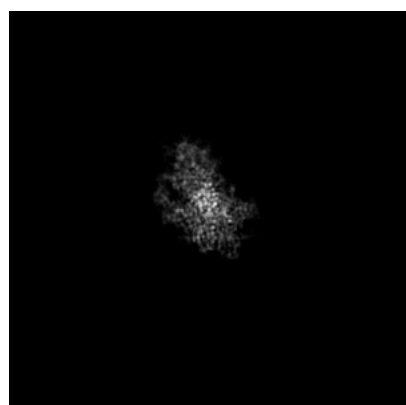
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76288. These allow visual inspection of the internal detail of the map and identification of artifacts.

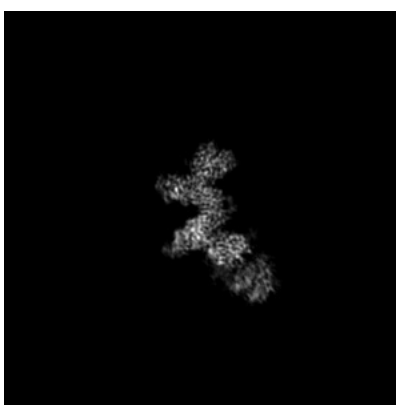
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

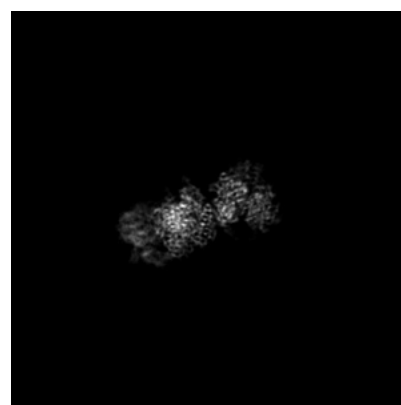
6.1.1 Primary map



X



Y



Z

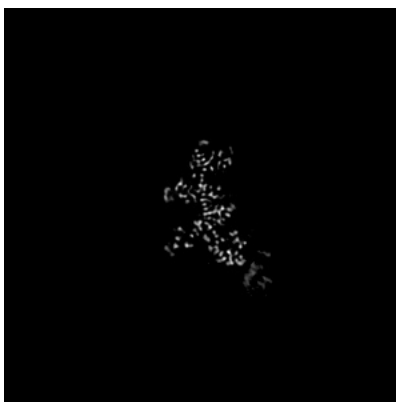
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

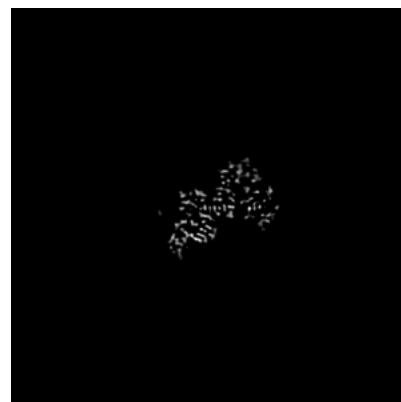
6.2.1 Primary map



X Index: 208



Y Index: 208



Z Index: 208

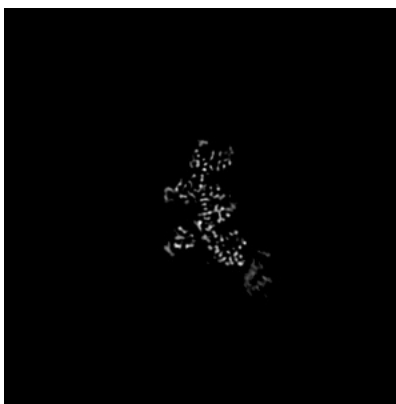
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 168



Y Index: 207

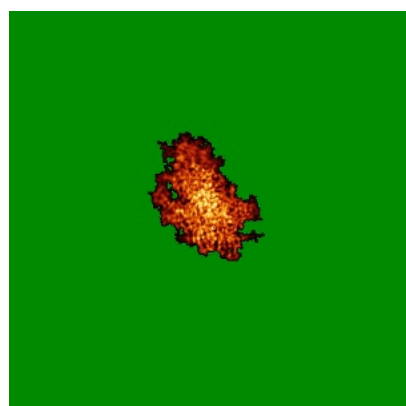


Z Index: 215

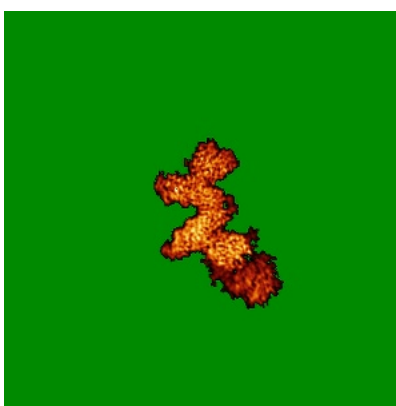
The images above show the largest variance slices of the map in three orthogonal directions.

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

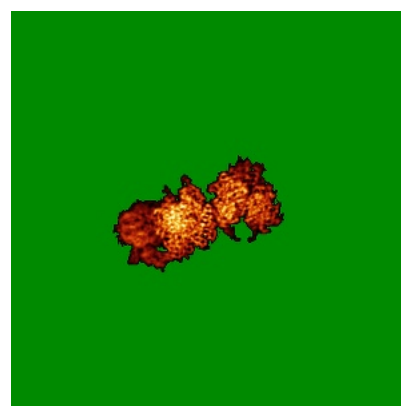
6.4.1 Primary map



X



Y

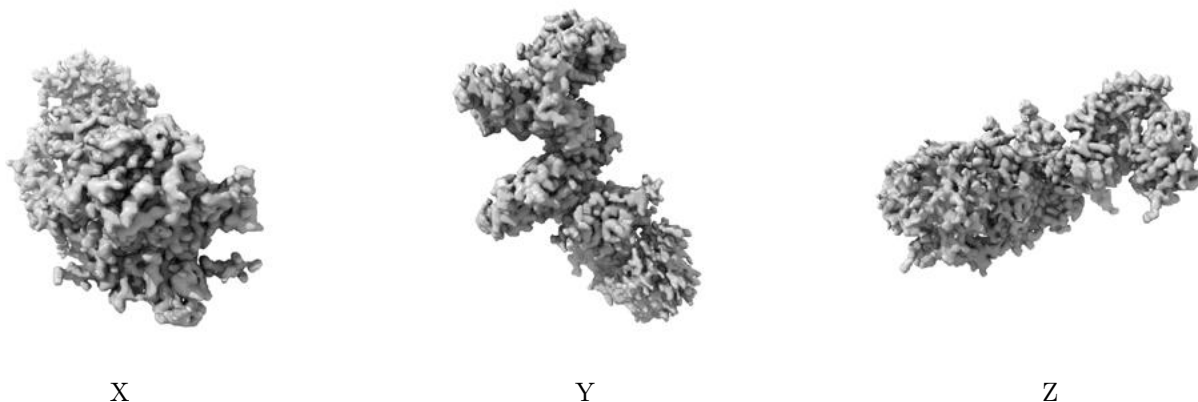


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0398. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

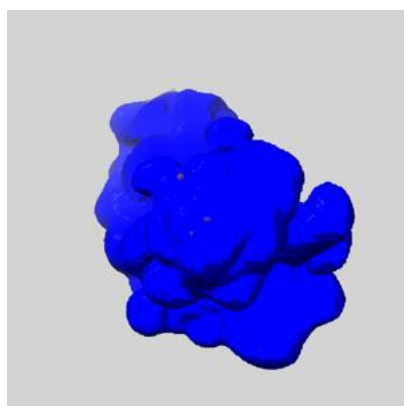
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

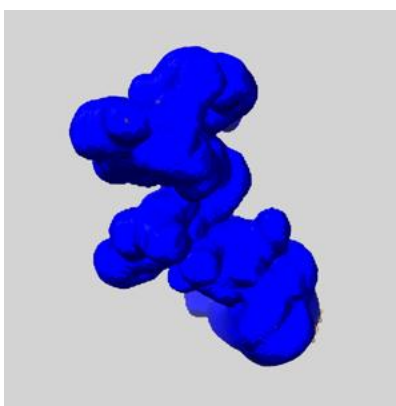
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

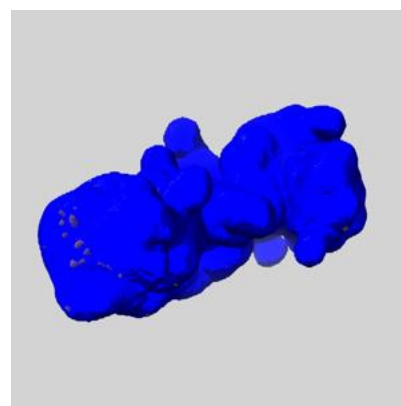
6.6.1 emd_76288_msk_1.map [i](#)



X



Y

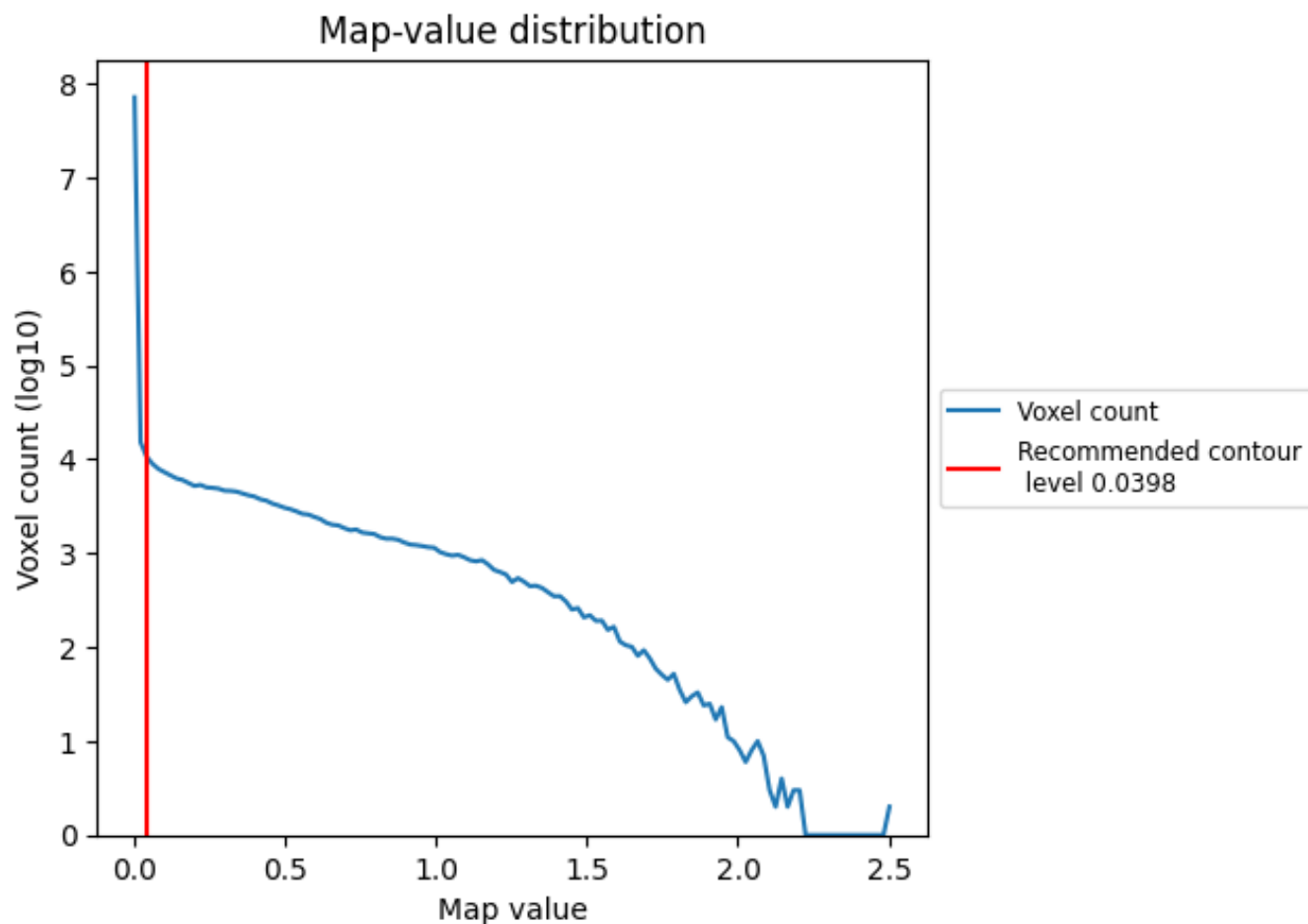


Z

7 Map analysis [i](#)

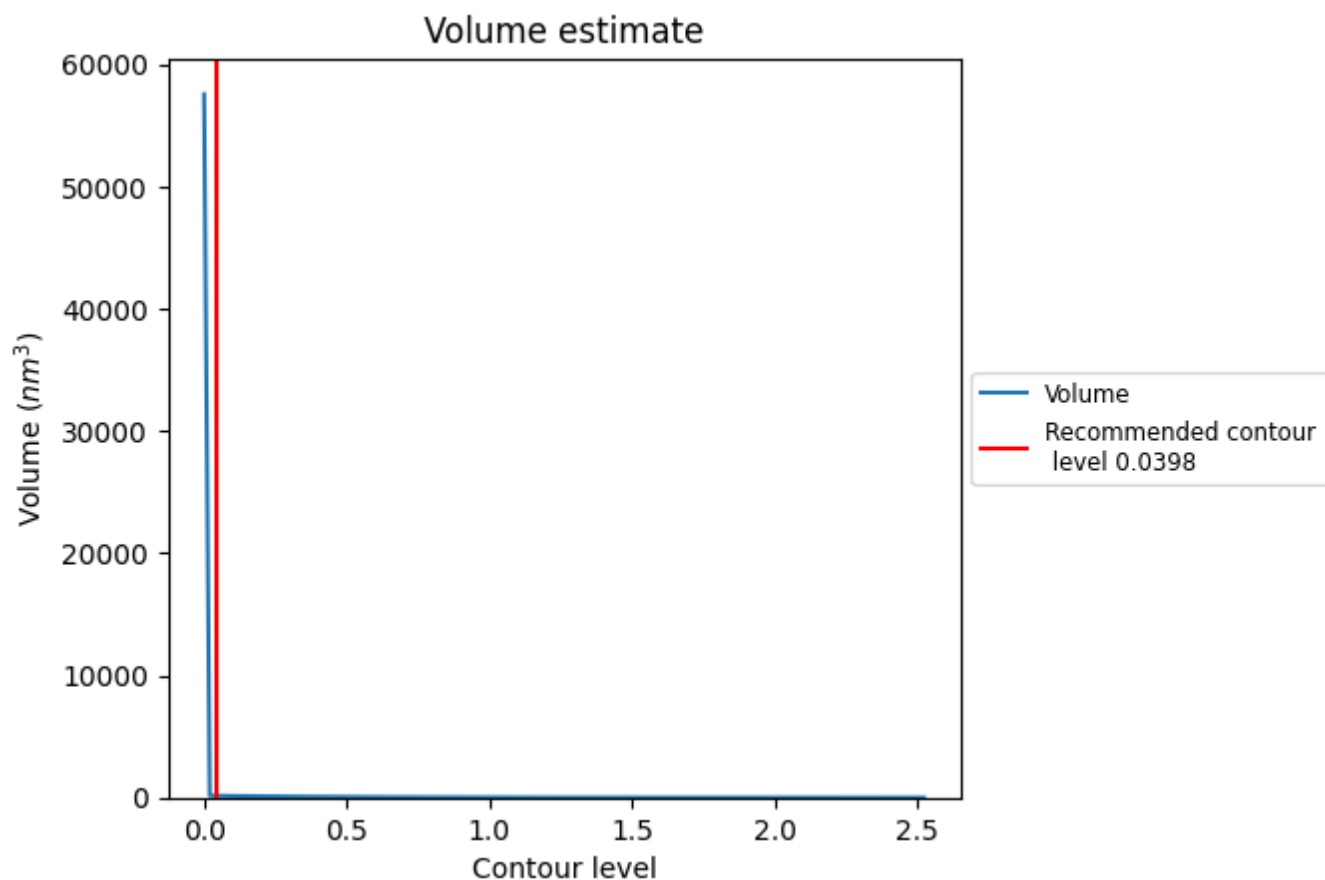
This section contains the results of statistical analysis of the map.

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.

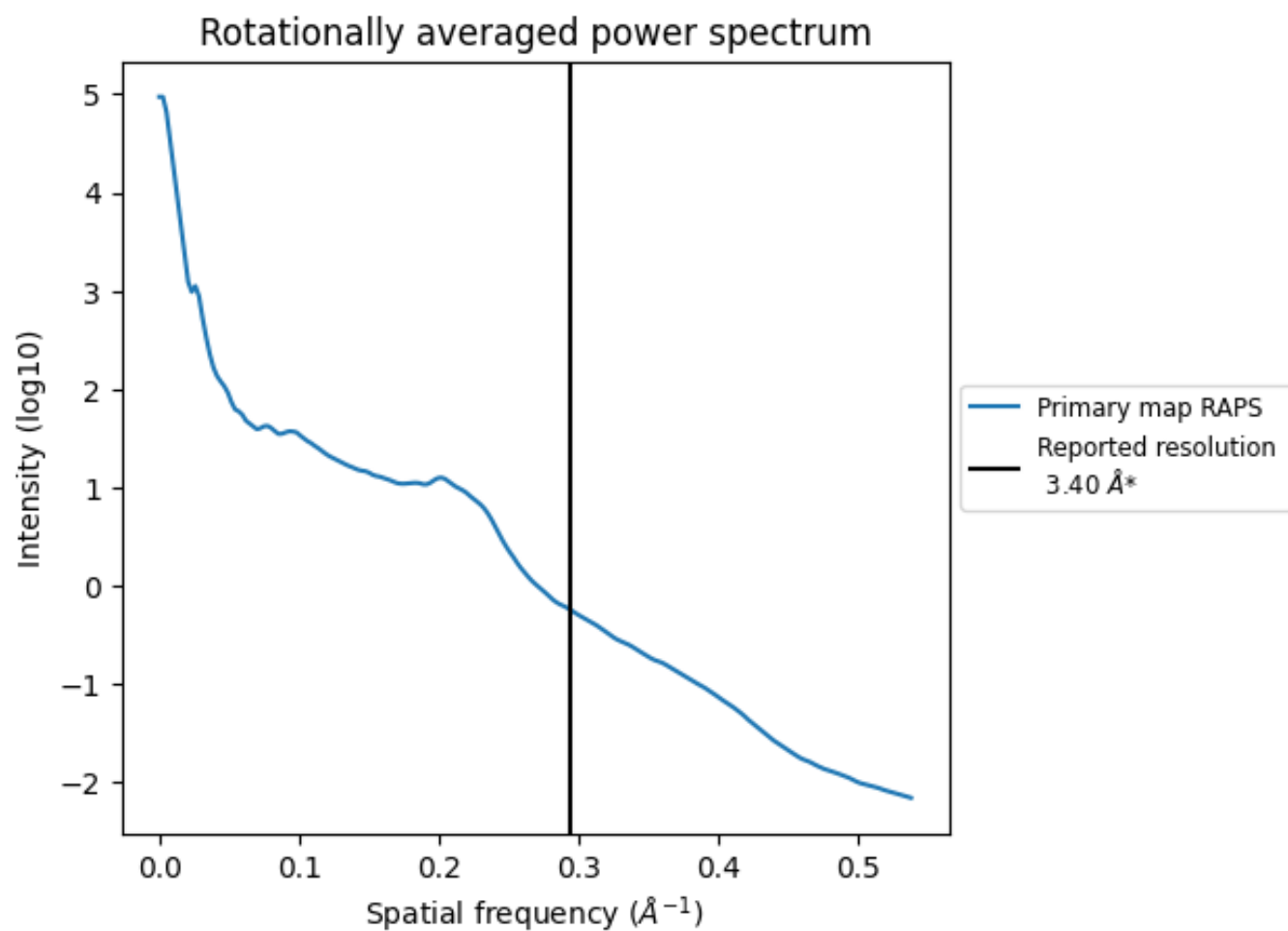
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 137 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 0.294 Å⁻¹

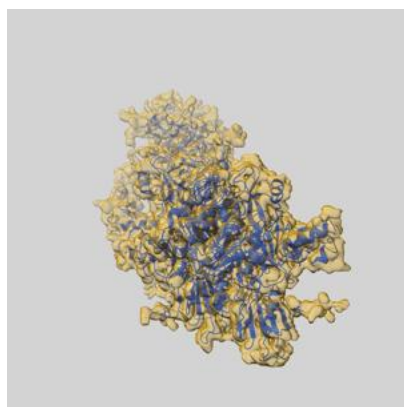
8 Fourier-Shell correlation

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

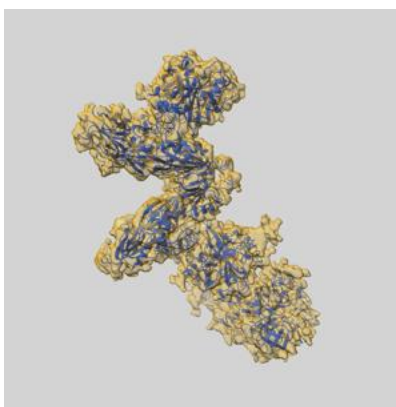
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-76288 and PDB model 12BN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

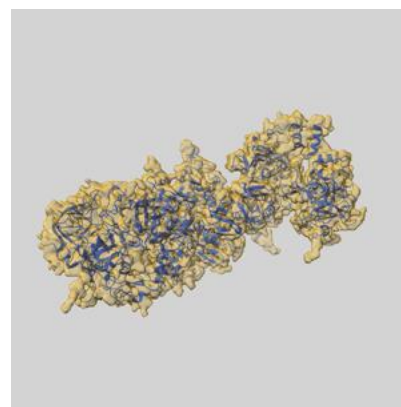
9.1 Map-model overlay [i](#)



X



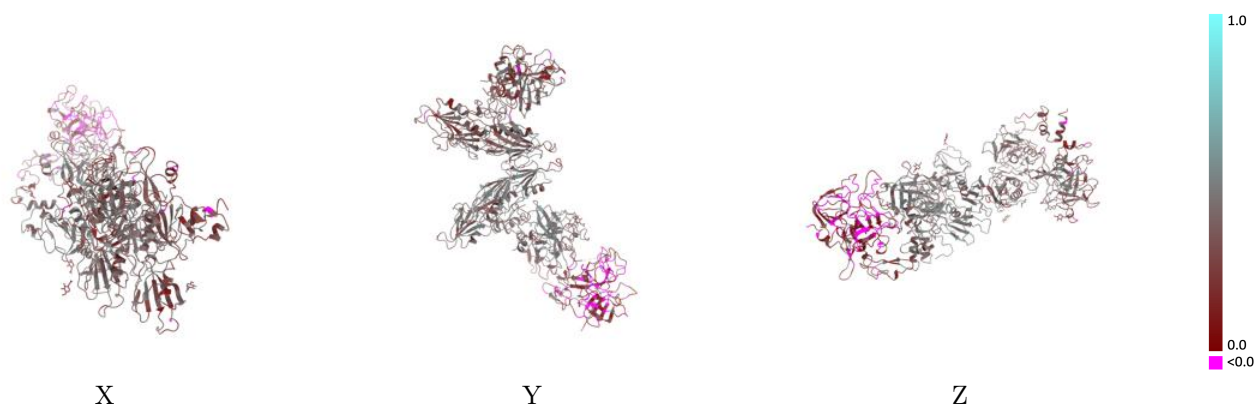
Y



Z

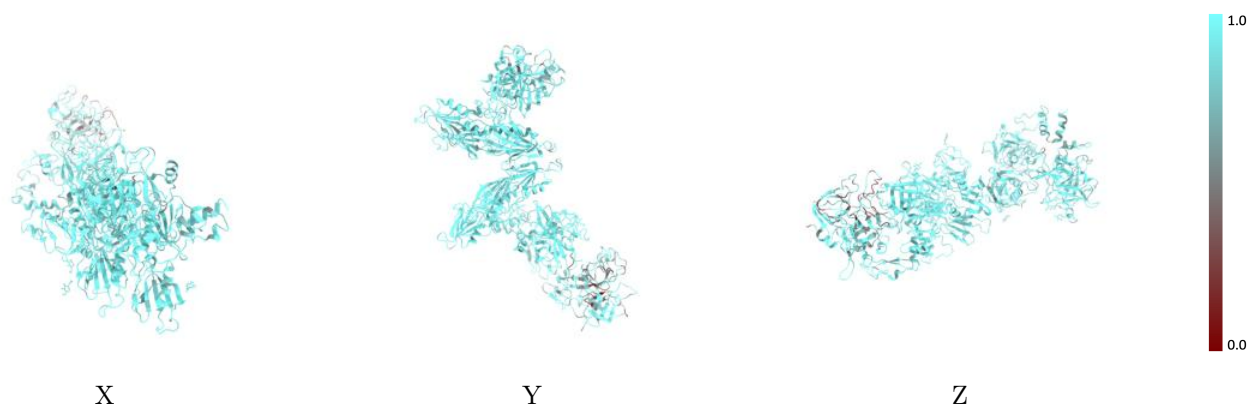
The images above show the 3D surface view of the map at the recommended contour level 0.0398 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



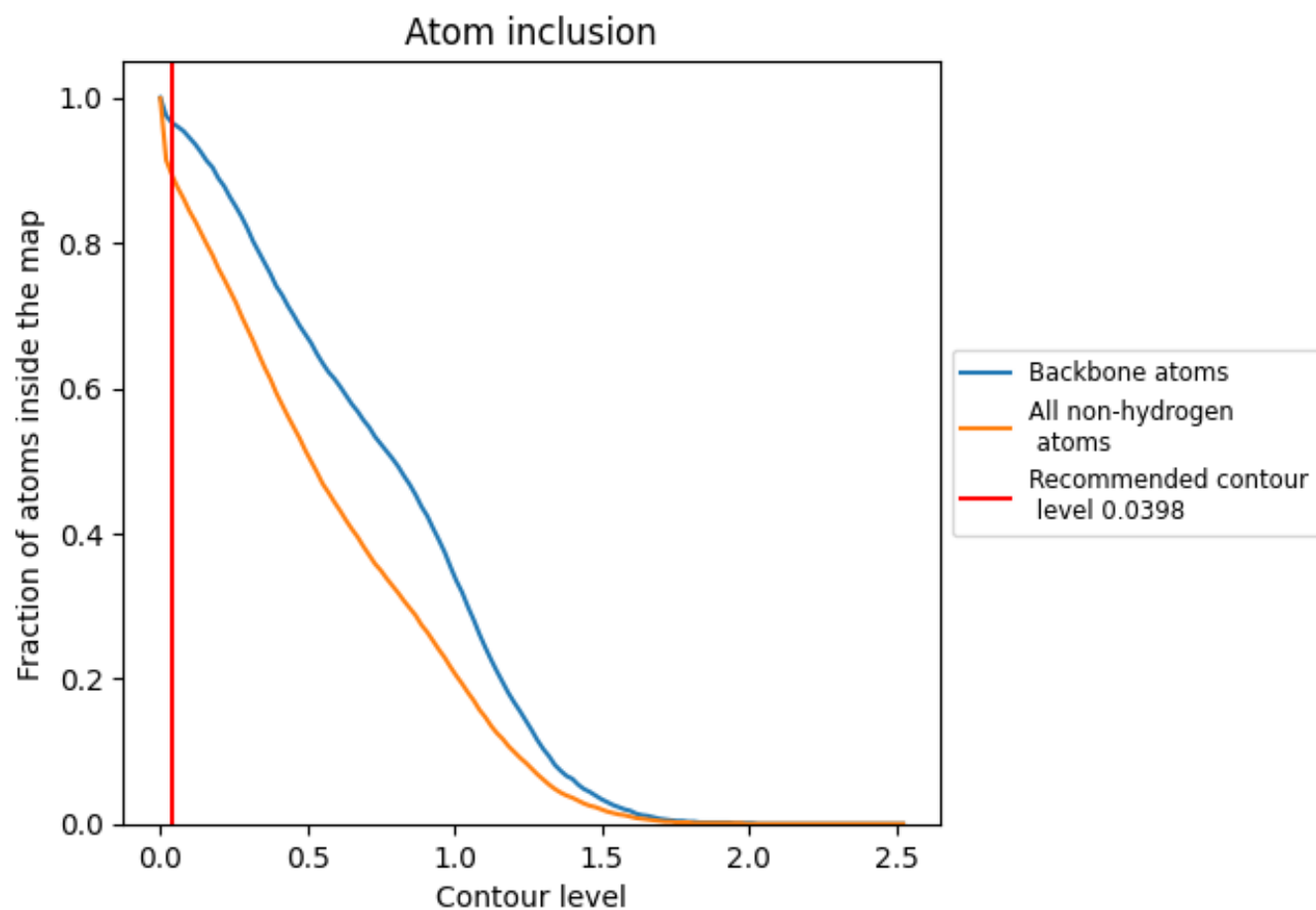
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0398).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.0398) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8920	0.3340
A	0.9580	0.4280
B	0.9520	0.4310
C	0.9130	0.3750
D	0.8680	0.3400
E	0.7910	0.1520
F	0.8530	0.2890

1.0

0.0

<0.0