Full wwPDB EM Validation Report (i)

Sep 22, 2026 – 06:12 PM EDT

PDB ID	:	13BD / pdb_000013bd
EMDB ID	:	EMD-76936
Title	:	Local refinement of the RBD and NTD in the closed BA.3.2.1 spike with N529Q mutant
Authors	:	Wang, Y.; Hu, Y.; Xie, X.
Deposited on	:	2026-04-27
Resolution	:	2.65 Å(reported)

This is a Full wwPDB EM Validation 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 (i) 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 (i)) were used in the production of this report:

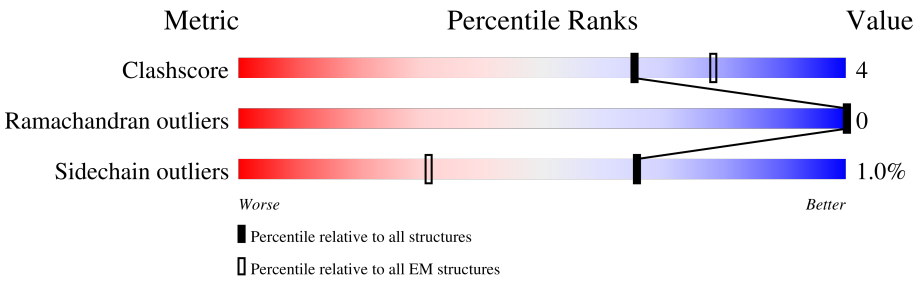
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

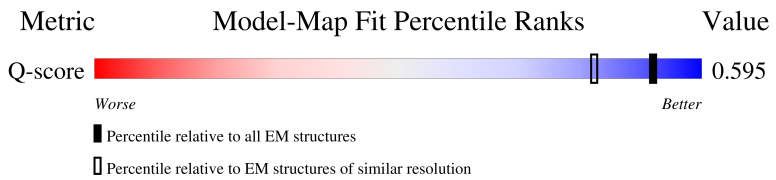
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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	9050 (2.15 - 3.15)

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 <=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	1271	16% • 82%
1	C	1271	16% • 82%
2	B	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3825 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.

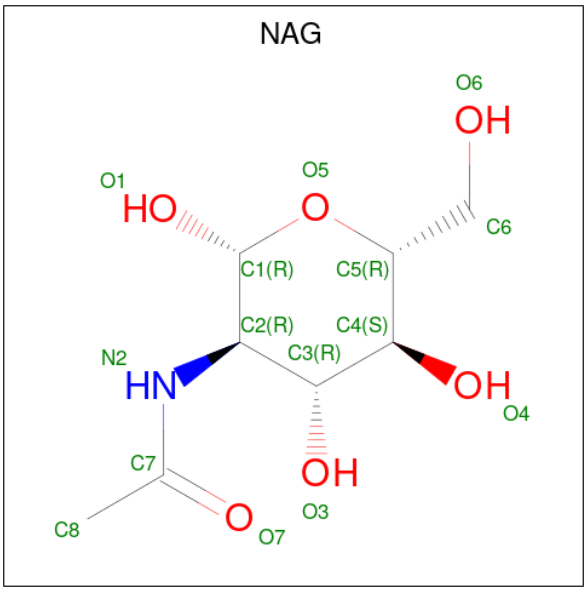
- Molecule 1 is a protein called BA.3.2.2 Spike with N529Q mutation.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	232	1873	1226	302	341	4	0	0
1	A	229	1840	1188	307	336	9	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0

- 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).



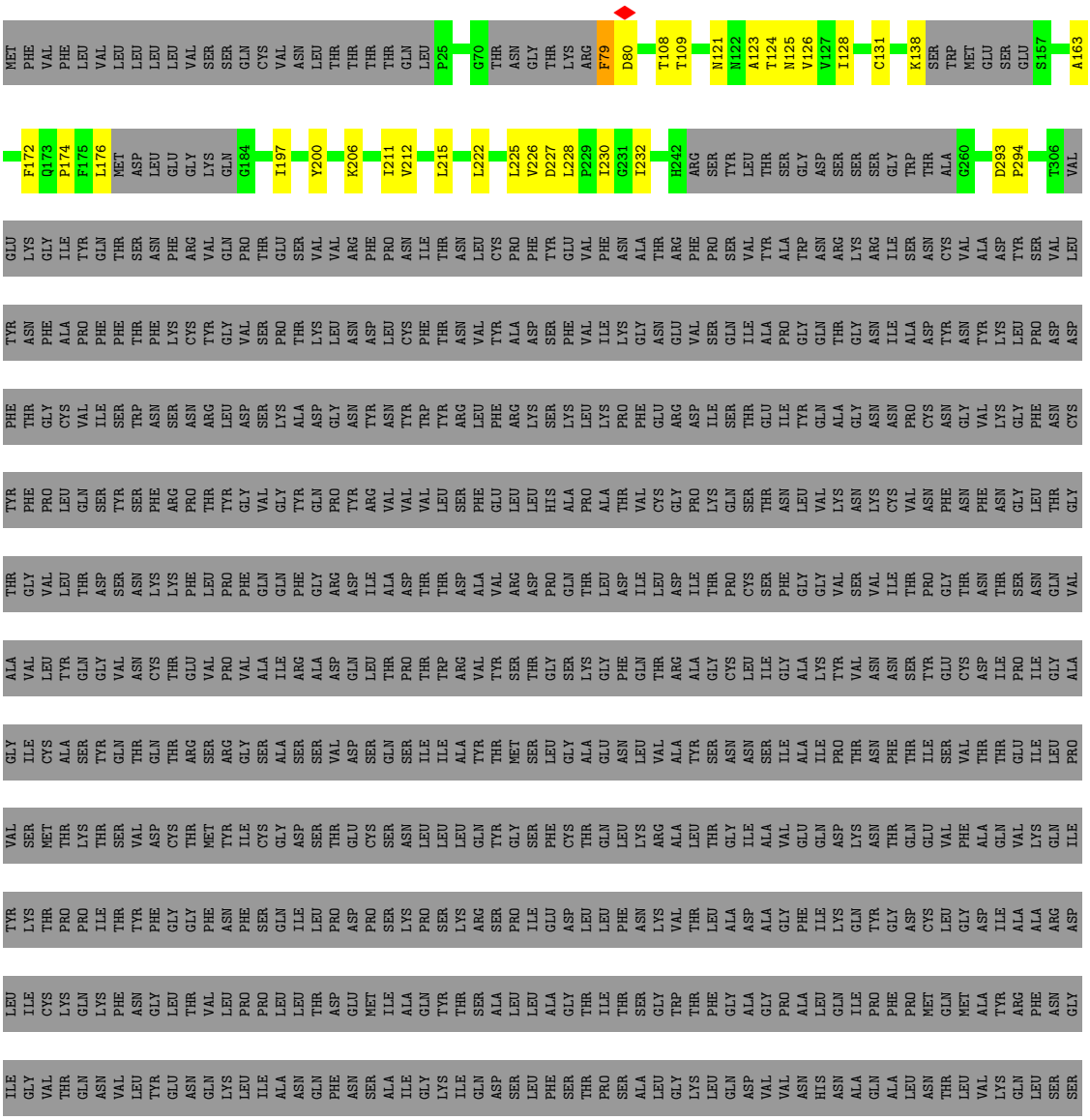
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	A	1	14	8	1	5	0

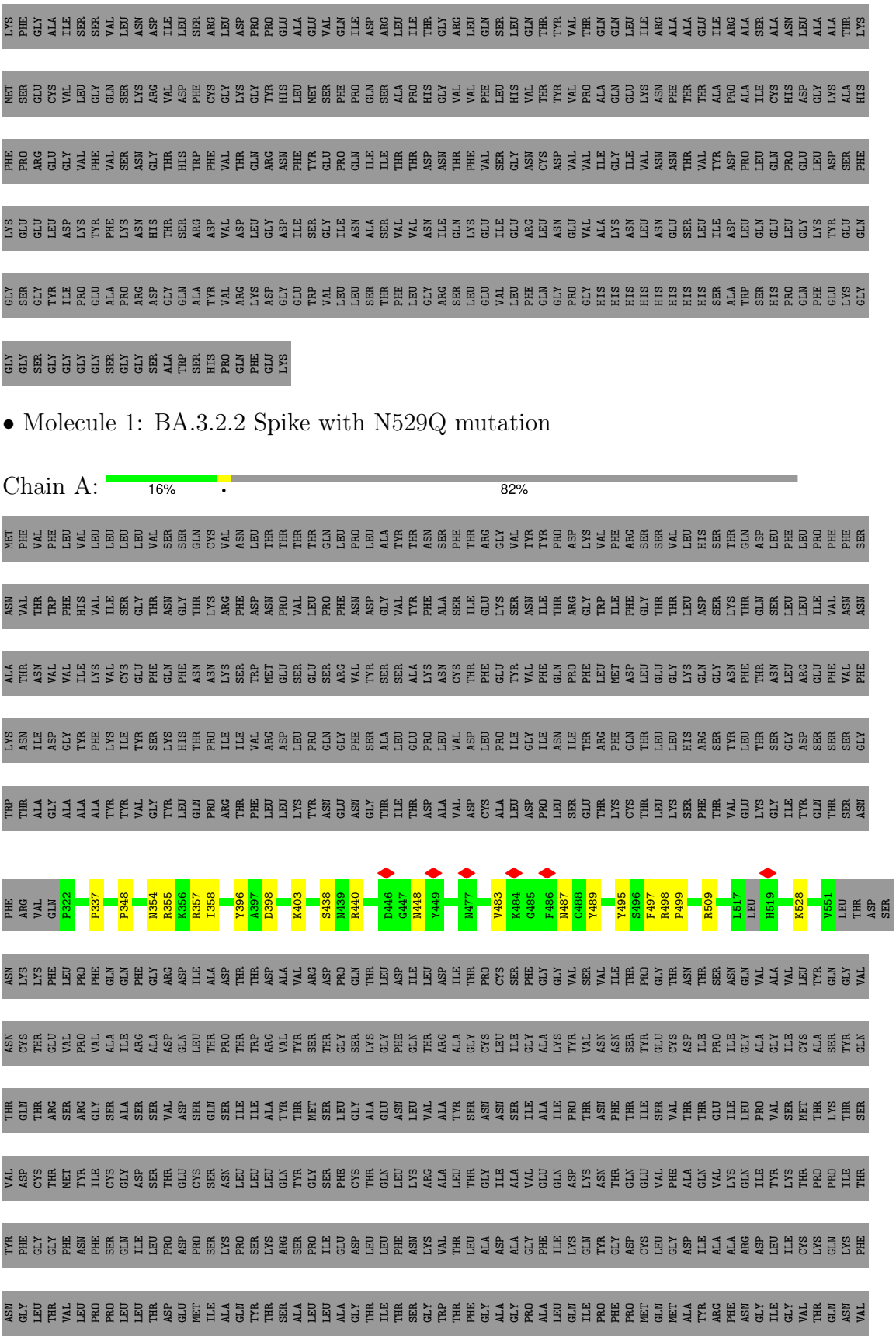
3 Residue-property plots (i)

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: BA.3.2.2 Spike with N529Q mutation

Chain C:




LYS PHE GLY ALA ILE SER SER VAL LEU ASN ASP ILE LEU SER ARG LEU ASP PRO PRO GLU ALA GLU VAL GLN ILE ASP ARG LEU ILE THR GLY ARG LEU GLN SER LEU GLN THR TYR VAL THR GLN GLN LEU ILE ARG ALA ALA GLU ILE ARG ALA SER ALA ASN LEU ALA ALA THR LYS
MET SER GLU CYS VAL LEU GLY GLN SER LYS ARG VAL ASP PHE CYS GLY LYS GLY TYR HIS LEU MET SER PHE PRO GLN SER ALA PRO HIS GLY VAL VAL PHE LEU HIS VAL THR TYR VAL PRO ALA GLN GLU LYS ASN PHE THR THR ALA PRO ALA ILE CYS HIS ASP GLY LYS ALA HIS
PHE PRO ARG GLU GLY VAL PHE VAL SER ASN GLY THR HIS TRP PHE VAL THR GLN ARG ASN PHE TYR GLU PRO GLN ILE ILE THR THR ASP ASN THR PHE VAL SER GLY ASN CYS ASP VAL VAL ILE GLY ILE VAL ASN ASN THR VAL TYR ASP PRO LEU GLN PRO GLU LEU ASP SER PHE
LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER ARG ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE GLU ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN
GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY
GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS
• Molecule 1: BA.3.2.2 Spike with N529Q mutation
Chain A:
16%
82%
MET PHE VAL PHE LEU VAL LEU LEU LEU LEU VAL SER SER GLN CYS VAL ASN LEU THR THR THR THR GLN LEU PRO LEU ALA TYR THR ASN SER PHE THR ARG GLY VAL TYR TYR PRO ASP LYS VAL PHE ARG SER SER VAL LEU HIS SER THR GLN ASP LEU PHE LEU PRO PHE PHE SER
ASN VAL THR TRP PHE HIS VAL ILE SER GLY THR ASN GLY THR LYS ARG PHE ASP ASN PRO VAL LEU PRO PHE ASN ASP GLY VAL TYR PHE ALA SER ILE GLU LYS SER ASN ILE THR ARG GLY TRP ILE PHE GLY THR THR LEU ASP SER LYS THR GLN SER LEU LEU ILE VAL ASN ASN
ALA THR ASN VAL VAL ILE LYS VAL CYS GLU PHE GLN PHE ASN ASN LYS SER TRP MET GLU SER GLU SER ARG VAL TYR SER SER ALA LYS ASN CYS THR PHE GLU TYR VAL PHE GLN PRO PHE LEU MET ASP LEU GLU GLY LYS GLN GLY ASN PHE THR ASN LEU ARG GLU PHE VAL PHE
LYS ASN ILE ASP GLY TYR PHE LYS ILE TYR SER LYS HIS THR PRO ILE ILE VAL ARG ASP LEU PRO GLN GLY PHE SER ALA LEU GLU PRO LEU VAL ASP LEU PRO ILE GLY ILE ASN ILE THR THR ARG PHE GLN THR LEU LEU HIS ARG SER TYR LEU THR SER GLY ASP SER SER GLY
TRP THR ALA GLY ALA ALA ALA TYR TYR VAL GLY TYR LEU GLN PRO ARG THR PHE LEU LEU LYS TYR ASN GLU ASN GLY THR ILE THR ASP ALA VAL ASP CYS ALA LEU ASP PRO LEU SER GLU THR LYS CYS THR LEU LEU LYS SER PHE THR VAL GLU LYS GLY ILE TYR GLN THR SER ASN
PHE ARG VAL GLN P322 P337 P348 N354 R355 K356 R357 I358 Y396 A397 D398 K403 S438 N439 R440 D446 G447 N448 Y449 N477 V483 K484 G485 F486 N487 C488 Y489 Y495 S496 F497 R498 P499 R509 L517 LEU H519 K528 V551 LEU THR ASP SER
ASN LYS LYS PHE LEU PRO PHE GLN GLN PHE GLY ARG ASP ILE ALA ASP THR THR ASP ALA VAL ARG ASP PRO GLN THR LEU ASP ILE LEU ASP ILE THR PRO CYS SER PHE GLY GLY VAL SER VAL ILE THR PRO GLY THR ASN THR SER ASN GLN VAL ALA VAL LEU TYR GLN GLY VAL
ASN CYS THR GLU VAL PRO VAL ALA ILE ARG ALA ASP GLN LEU THR PRO THR THR TRP ARG VAL TYR SER THR GLY SER LYS GLY PHE GLN THR ARG ALA GLY CYS LEU ILE GLY ALA LYS TYR VAL ASN ASN SER TYR GLU CYS ASP ILE PRO ILE GLY ALA GLY ILE CYS ALA SER TYR GLN
THR GLN THR ARG SER ARG GLY SER SER ALA SER SER VAL ASP SER GLN SER ILE ILE ALA TYR THR MET SER LEU GLY ALA GLU ASN LEU VAL ALA TYR SER ASN SER ILE ALA ILE PRO THR ASN PHE THR ILE SER VAL THR THR GLU ILE LEU PRO VAL SER MET THR LYS THR SER
VAL ASP CYS THR MET TYR ILE CYS GLY ASP SER THR GLU CYS SER ASN LEU LEU LEU GLN TYR GLY SER PHE CYS THR GLN LEU LYS ARG ALA LEU THR GLY ILE ALA ASP VAL GLU GLN ASP LYS ASN THR GLN GLU VAL PHE ALA GLN VAL LYS GLN ILE TYR LYS THR PRO PRO ILE THR
TYR PHE GLY GLY PHE ASN PHE SER GLN ILE ILE LEU PRO ASP PRO SER LYS PRO SER LYS ARG SER PRO ILE GLU ASP LEU LEU PHE ASN LYS VAL THR LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS LYS GLN LYS PHE
ASN GLY LEU THR VAL LEU PRO PRO LEU LEU THR ASP GLU MET ILE ALA GLN TYR THR SER ALA LEU LEU ILE ALA GLY THR ILE THR SER GLY TRP THR PHE GLY ALA GLY PRO ALA LEU GLN ILE PRO PHE PRO MET GLN MET ALA TYR ARG PHE ASN GLY ILE GLY VAL THR VAL ASN

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

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

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

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

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

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

SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	516314	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.880	Depositor
Minimum map value	-0.405	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	346.112, 346.112, 346.112	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	0.16	0/1896	0.39	0/2580
1	C	0.20	0/1923	0.41	0/2612
All	All	0.18	0/3819	0.40	0/5192

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	1840	0	1753	12	0
1	C	1873	0	1828	18	0
2	B	28	0	25	0	0
3	A	14	0	13	0	0
3	C	70	0	65	2	0
All	All	3825	0	3684	30	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 4.

All (30) 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:C:126:VAL:HG23	1:C:174:PRO:HA	1.71	0.72
1:C:125:ASN:HD22	3:C:1304:NAG:H5	1.59	0.68
1:A:498:ARG:HG3	1:A:499:PRO:HD2	1.78	0.65
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.35	0.62
1:C:124:THR:HA	1:C:174:PRO:HG3	1.80	0.61
1:C:230:ILE:HD12	1:C:232:ILE:HG12	1.83	0.58
1:A:487:ASN:HA	1:A:489:TYR:CE1	2.45	0.51
1:C:121:ASN:ND2	1:C:176:LEU:HB2	2.27	0.50
1:C:225:LEU:HG	1:C:226:VAL:HG23	1.92	0.50
1:A:440:ARG:HH11	1:A:440:ARG:HG3	1.76	0.50
1:C:108:THR:HG22	1:C:109:THR:HG23	1.93	0.49
1:C:197:ILE:O	1:C:200:TYR:HB2	2.11	0.49
1:A:403:LYS:HG2	1:A:497:PHE:HE1	1.78	0.48
1:A:337:PRO:HD2	1:A:358:ILE:HG23	1.94	0.48
1:C:128:ILE:HG21	1:C:228:LEU:HD13	1.95	0.47
1:A:483:VAL:HG23	1:A:483:VAL:O	2.14	0.47
1:A:355:ARG:HD2	1:A:396:TYR:CD1	2.50	0.46
1:C:206:LYS:HB3	1:C:222:LEU:HD22	1.97	0.46
1:A:354:ASN:O	1:A:398:ASP:HA	2.16	0.46
1:C:123:ALA:HB3	3:C:1304:NAG:H82	1.98	0.46
1:C:211:ILE:HD12	1:C:212:VAL:HG23	1.99	0.45
1:C:79:PHE:HB3	1:C:80:ASP:H	1.51	0.44
1:A:403:LYS:HG3	1:A:495:TYR:CE1	2.52	0.44
1:A:348:PRO:HG3	1:A:354:ASN:HB2	1.99	0.43
1:C:293:ASP:HB2	1:C:294:PRO:HD2	1.99	0.43
1:C:131:CYS:SG	1:C:163:ALA:HB1	2.60	0.42
1:C:138:LYS:HA	1:C:138:LYS:HD2	1.85	0.41
1:C:200:TYR:HD2	1:C:227:ASP:OD1	2.03	0.41
1:C:215:LEU:HD23	1:C:215:LEU:HA	1.88	0.41
1:A:438:SER:OG	1:A:509:ARG:HG3	2.20	0.40

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	225/1271 (18%)	212 (94%)	13 (6%)	0	100	100
1	C	222/1271 (18%)	213 (96%)	9 (4%)	0	100	100
All	All	447/2542 (18%)	425 (95%)	22 (5%)	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	203/1106 (18%)	201 (99%)	2 (1%)	68	81
1	C	210/1106 (19%)	208 (99%)	2 (1%)	68	81
All	All	413/2212 (19%)	409 (99%)	4 (1%)	65	81

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

Mol	Chain	Res	Type
1	C	79	PHE
1	C	172	PHE
1	A	448	ASN
1	A	528	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	121	ASN
1	C	125	ASN
1	C	196	ASN
1	A	439	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)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1	2,1	14,14,15	0.77	0	17,19,21	0.88	0
2	NAG	B	2	2	14,14,15	0.70	0	17,19,21	0.83	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
2	NAG	B	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

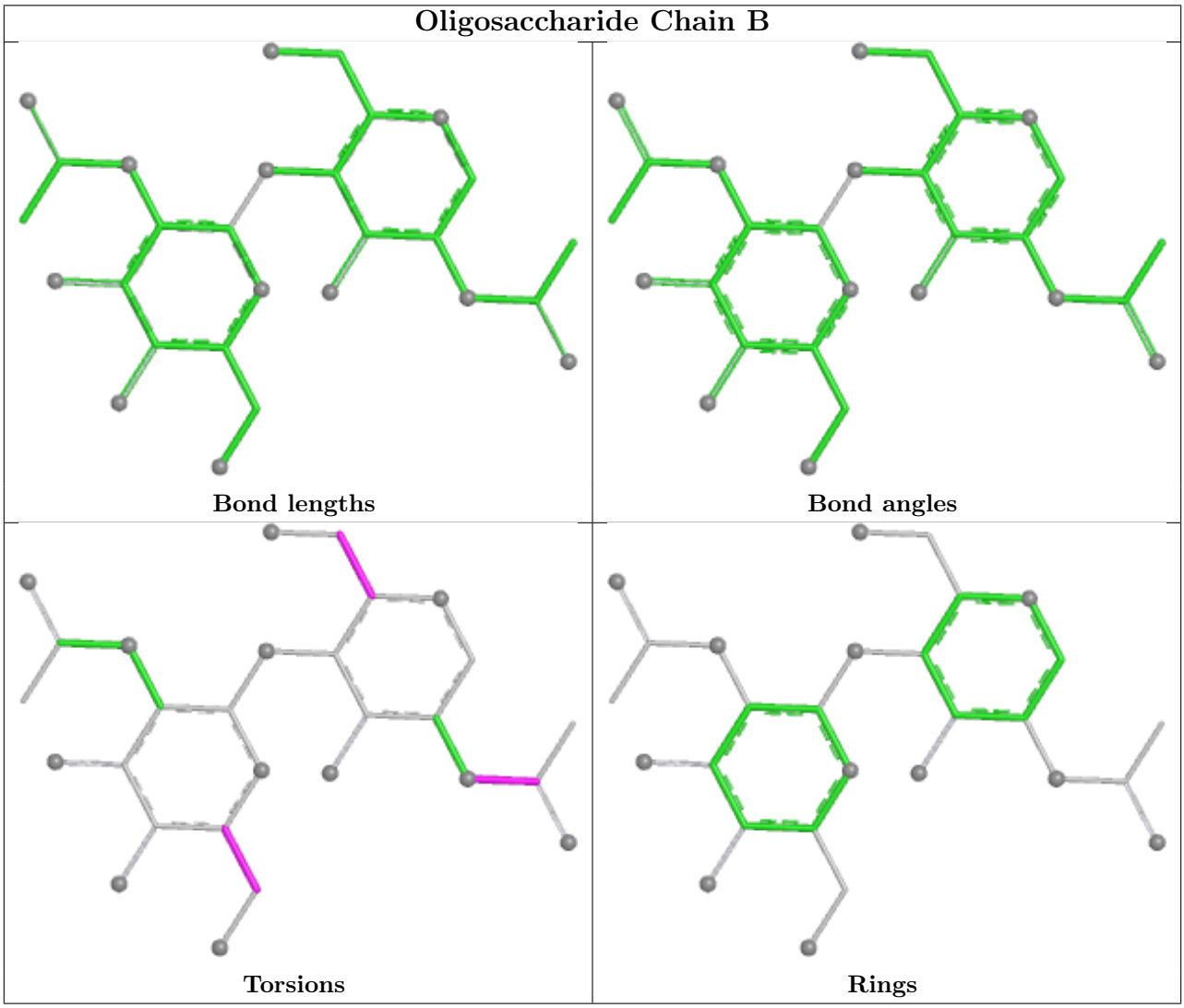
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

6 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	C	1304	1	14,14,15	0.72	0	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1303	1	14,14,15	0.73	0	17,19,21	0.70	0
3	NAG	C	1301	1	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	A	1301	1	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	C	1305	1	14,14,15	0.78	0	17,19,21	1.55	2 (11%)
3	NAG	C	1302	1	14,14,15	0.81	0	17,19,21	1.41	2 (11%)

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	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	3/6/23/26	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(^{o})	Ideal(^{o})
3	C	1305	NAG	C1-O5-C5	4.66	118.43	112.19
3	C	1302	NAG	C2-N2-C7	3.18	127.16	122.90
3	C	1302	NAG	C1-O5-C5	2.82	115.97	112.19
3	C	1305	NAG	C3-C4-C5	-2.04	106.53	110.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	A	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1302	NAG	C1-C2-N2-C7
3	C	1302	NAG	C3-C2-N2-C7

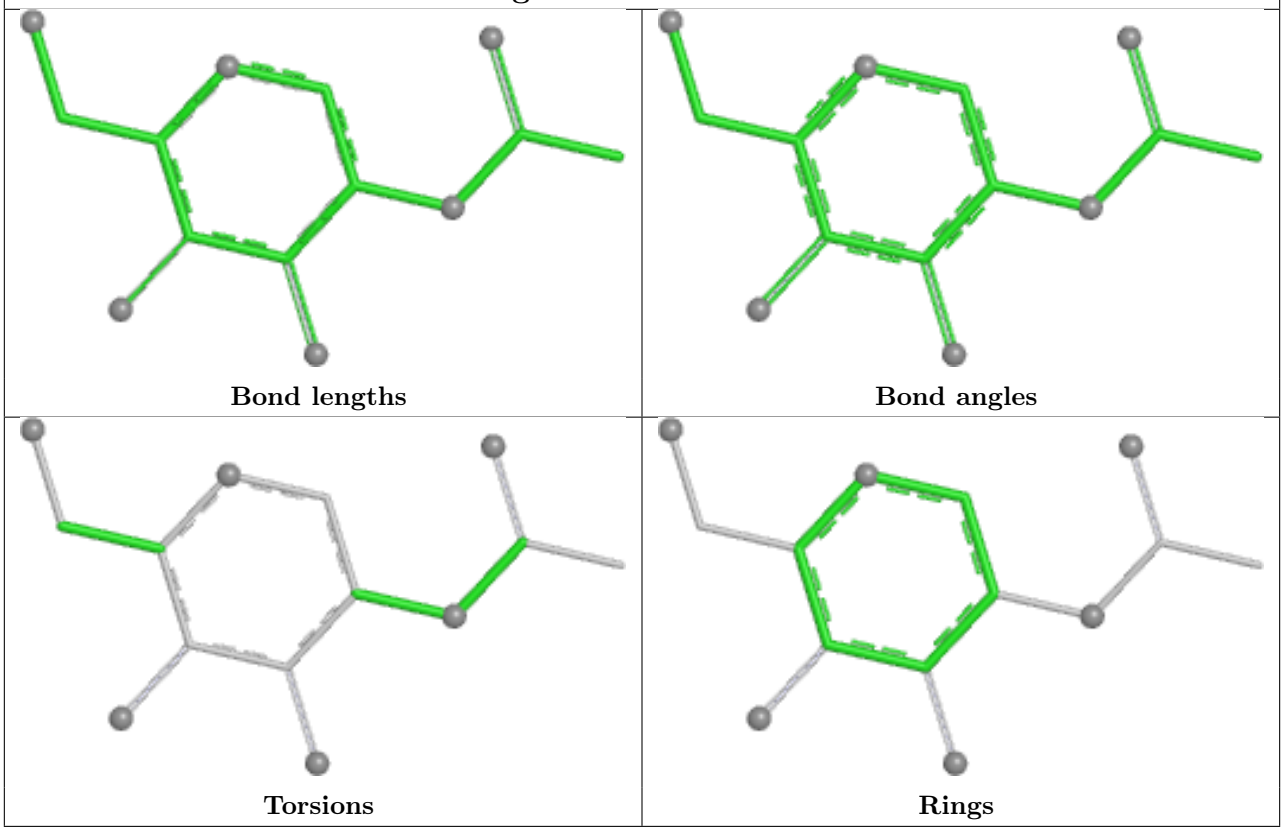
There are no ring outliers.

1 monomer is involved in 2 short contacts:

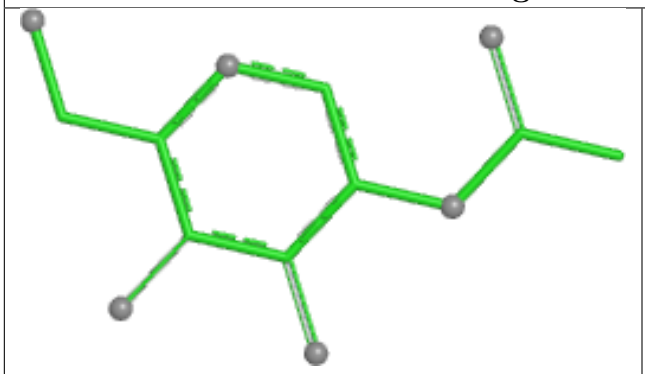
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1304	NAG	2	0

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 then 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.

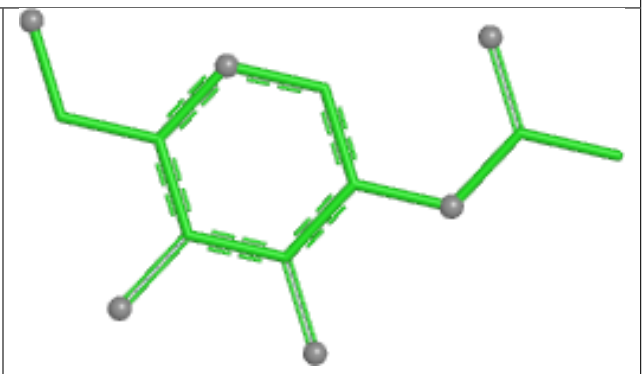
Ligand NAG C 1304



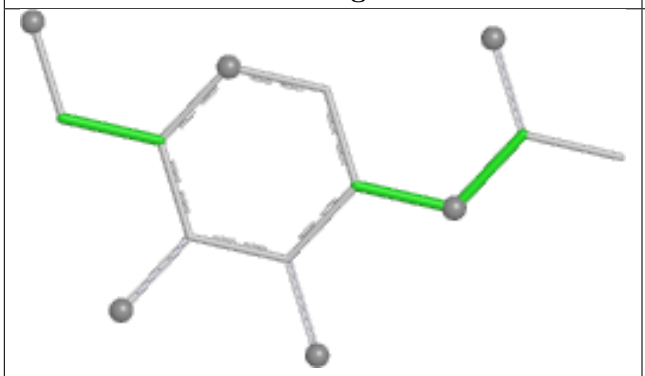
Ligand NAG C 1303



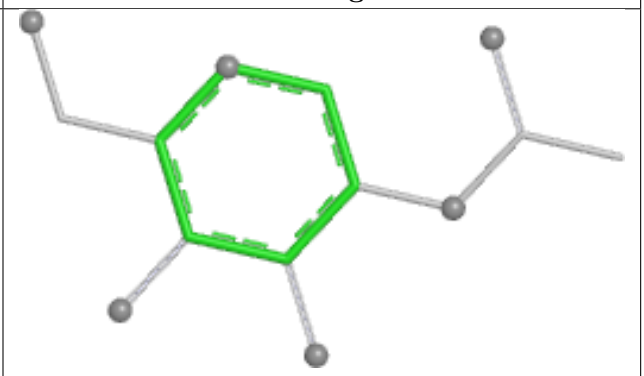
Bond lengths



Bond angles

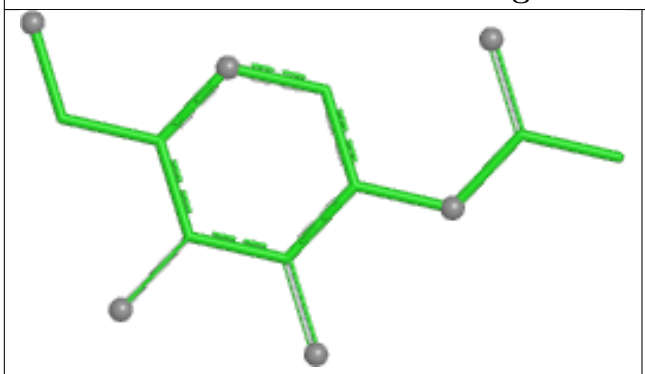


Torsions

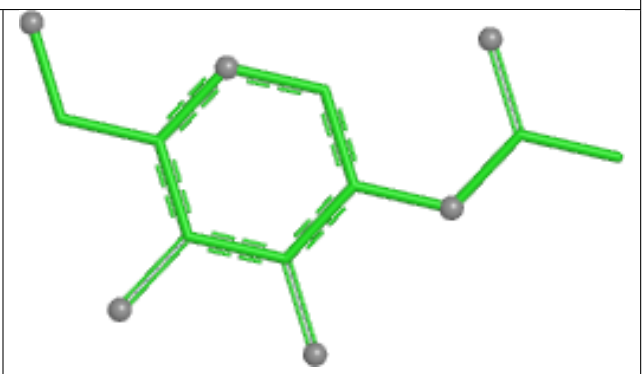


Rings

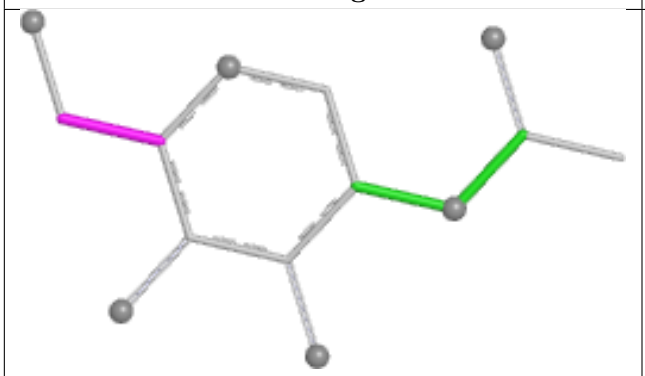
Ligand NAG C 1301



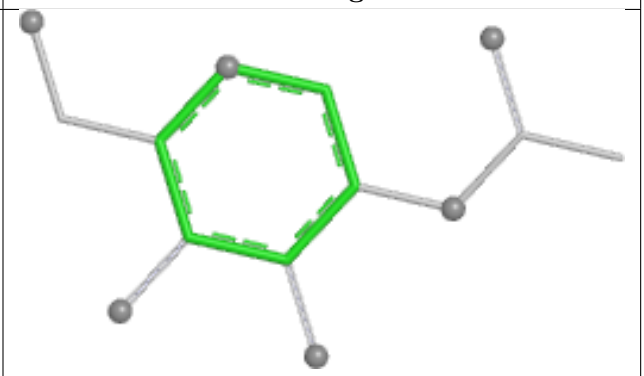
Bond lengths



Bond angles

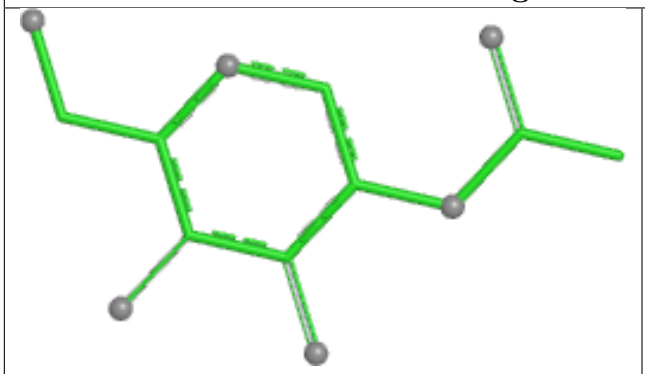


Torsions

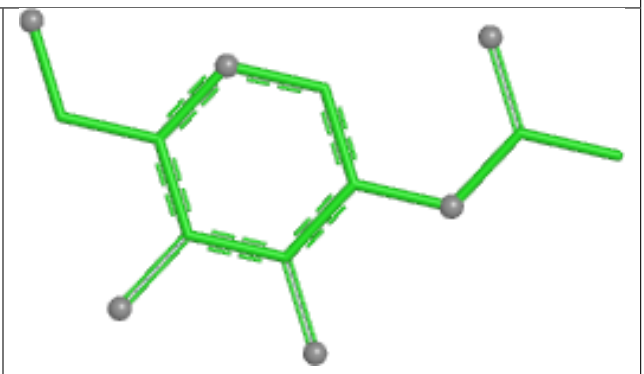


Rings

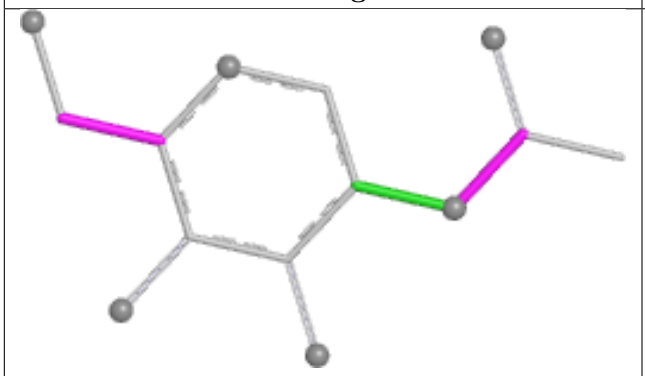
Ligand NAG A 1301



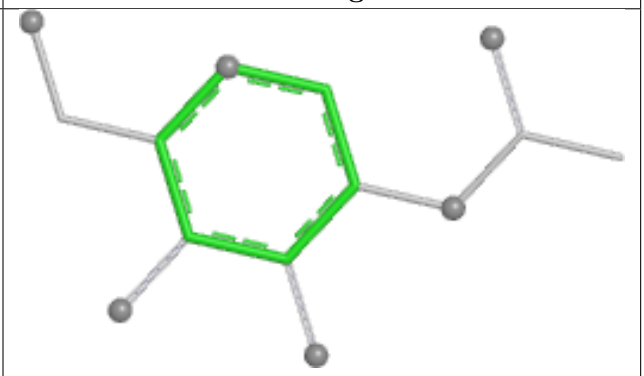
Bond lengths



Bond angles

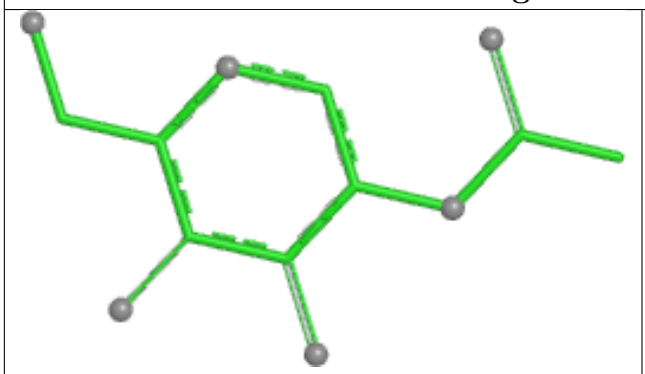


Torsions

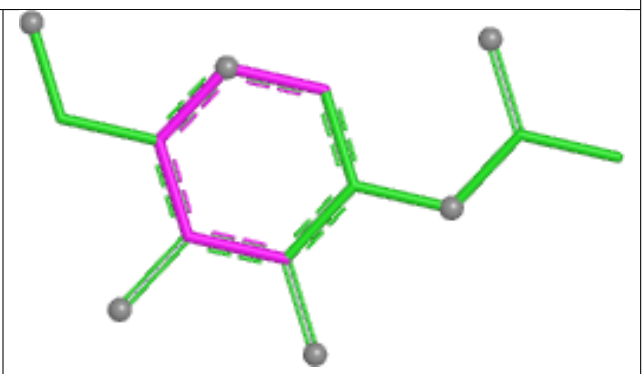


Rings

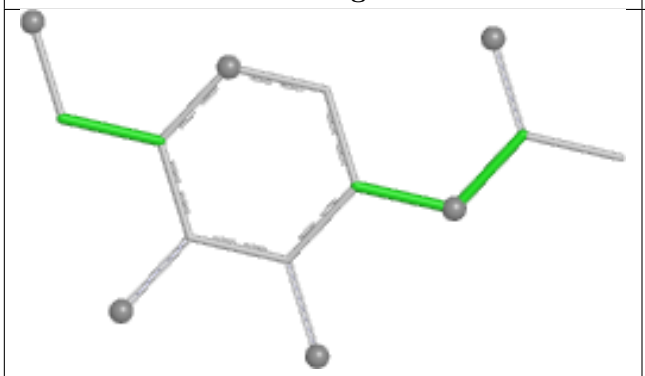
Ligand NAG C 1305



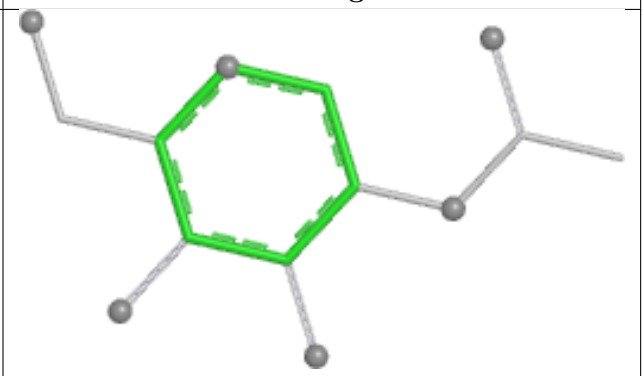
Bond lengths



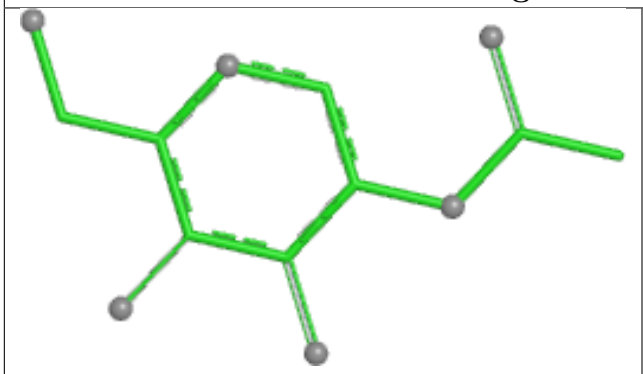
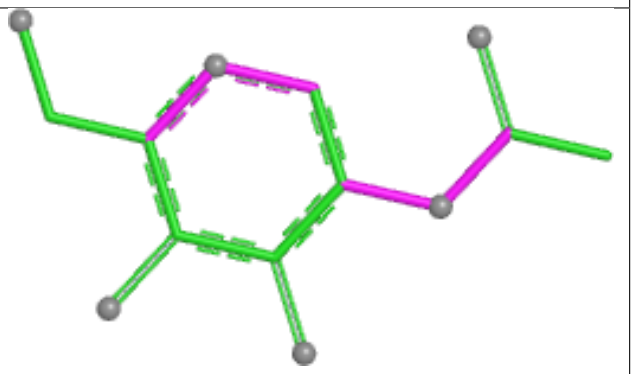
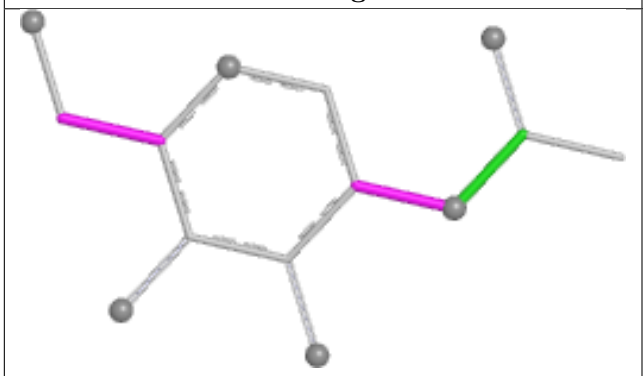
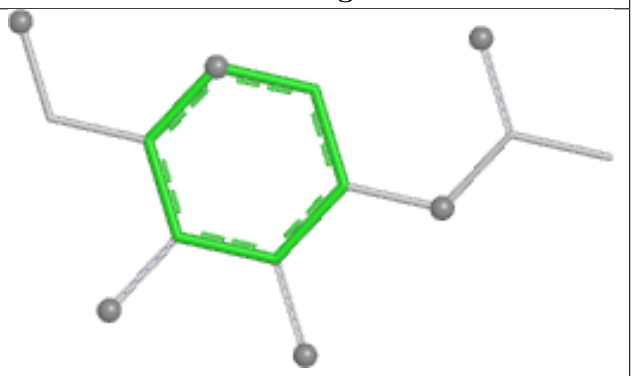
Bond angles



Torsions



Rings

Ligand NAG C 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

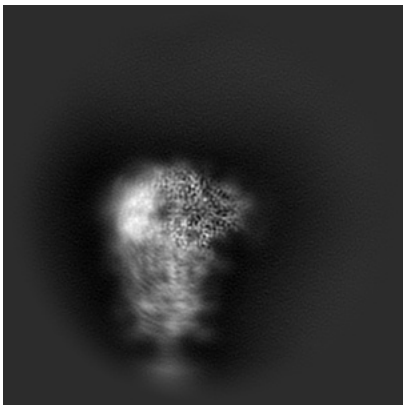
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-76936. These allow visual inspection of the internal detail of the map and identification of artifacts.

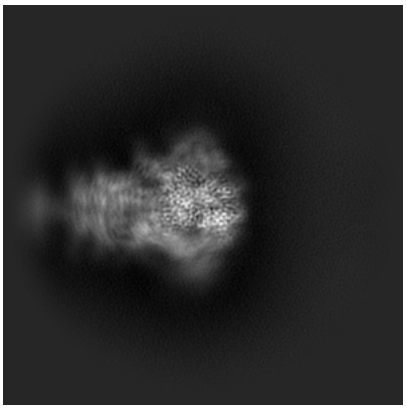
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

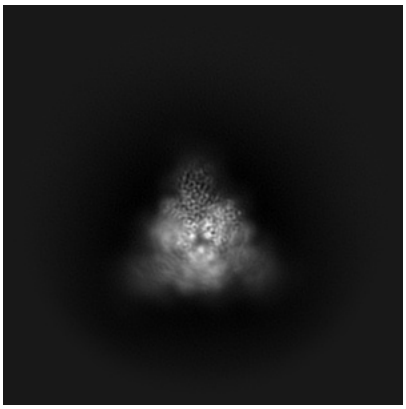
6.1.1 Primary map



X

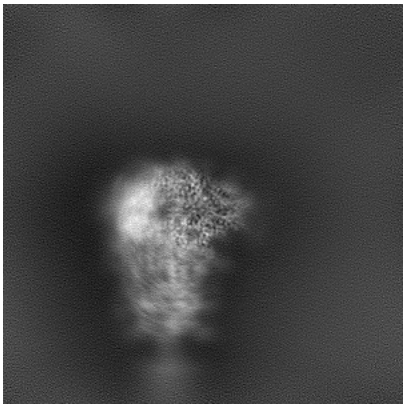


Y

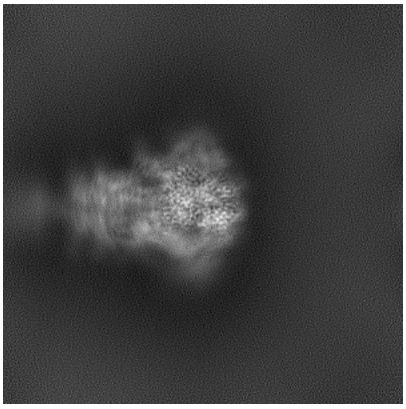


Z

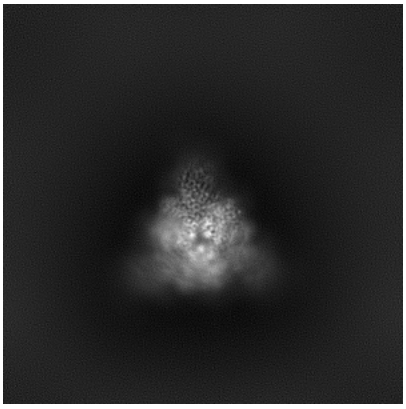
6.1.2 Raw map



X



Y

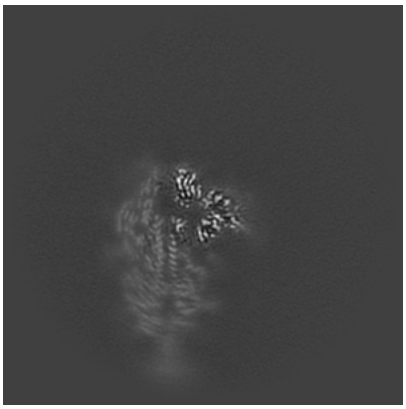


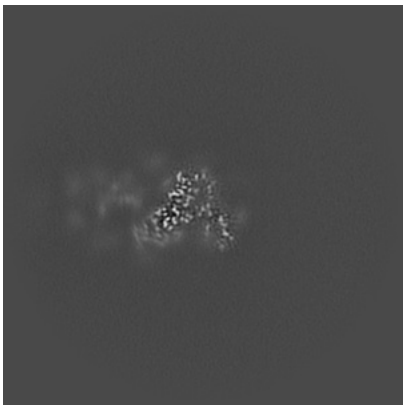
Z

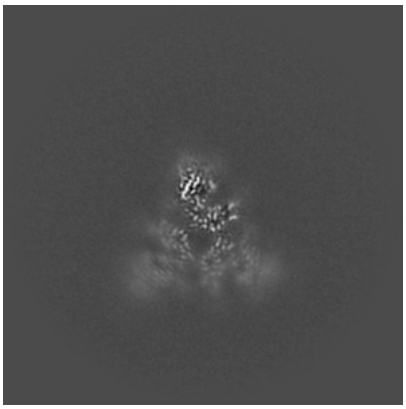
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

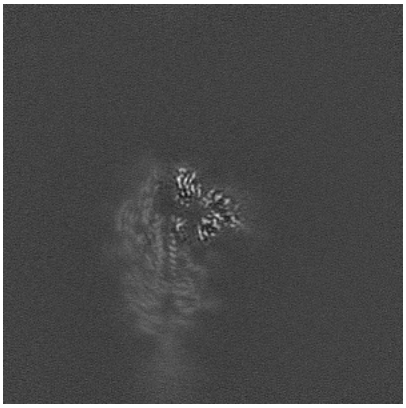
6.2.1 Primary map

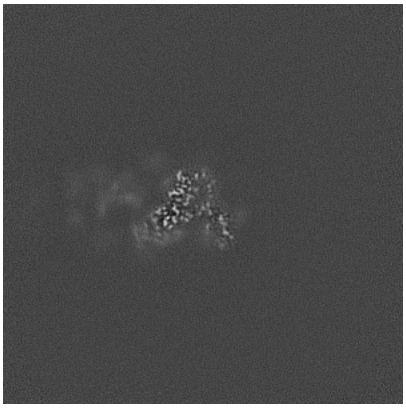

X Index: 208

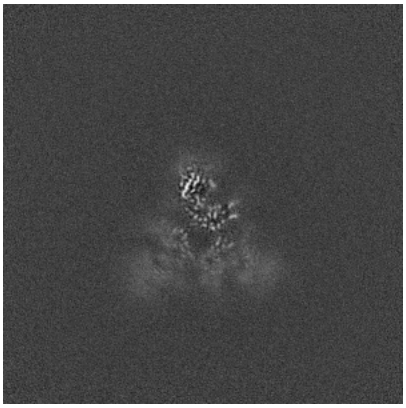

Y Index: 208


Z Index: 208

6.2.2 Raw map


X Index: 208

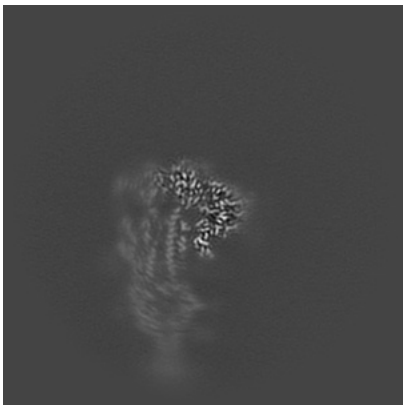

Y Index: 208

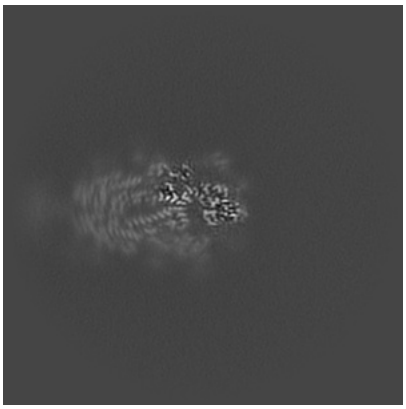

Z Index: 208

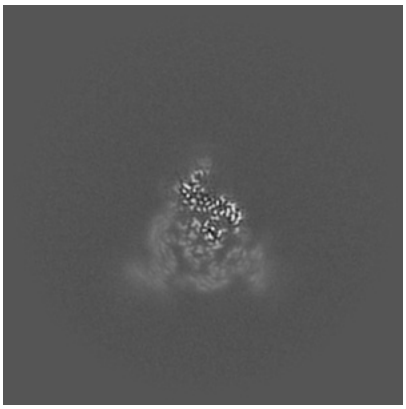
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

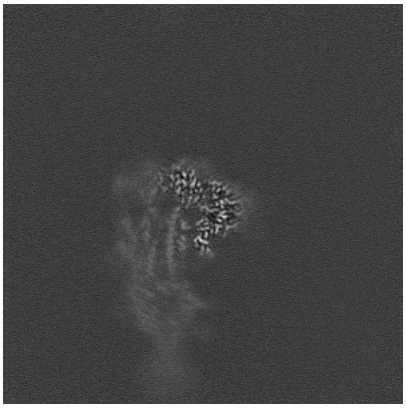
6.3.1 Primary map

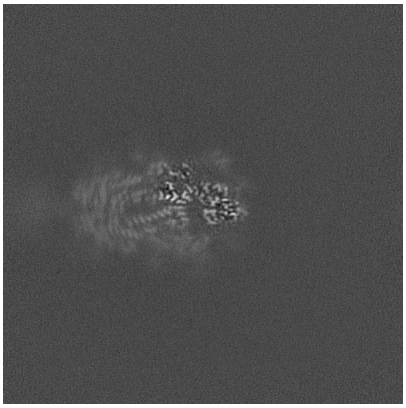

X Index: 198

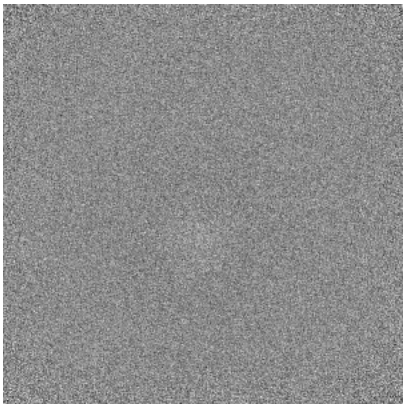

Y Index: 187


Z Index: 183

6.3.2 Raw map


X Index: 198

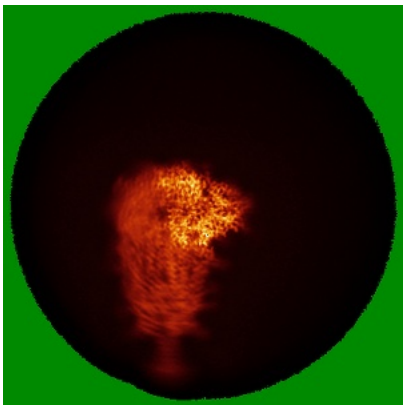

Y Index: 187


Z Index: 415

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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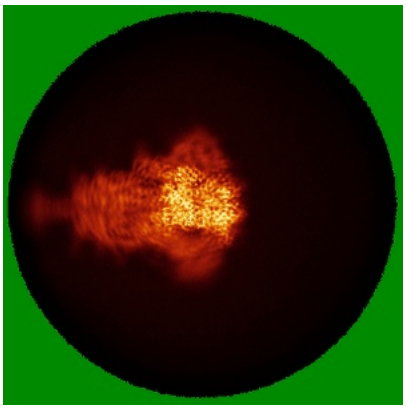
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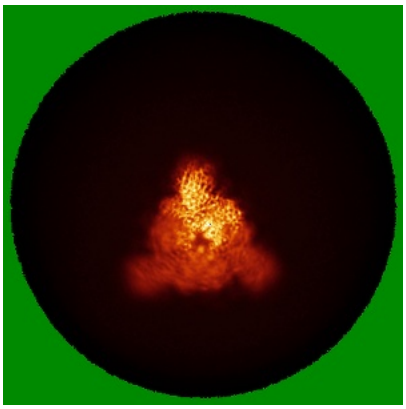
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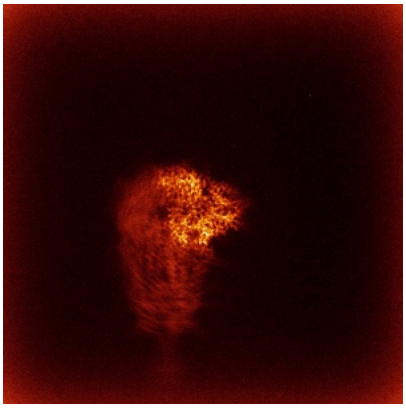
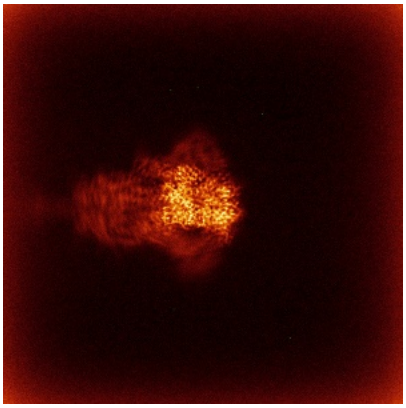
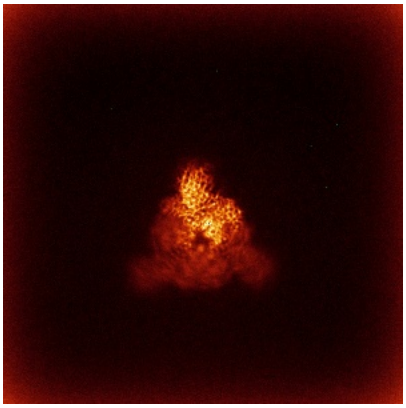
6.4.2 Raw map


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. 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

X Y Z

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.

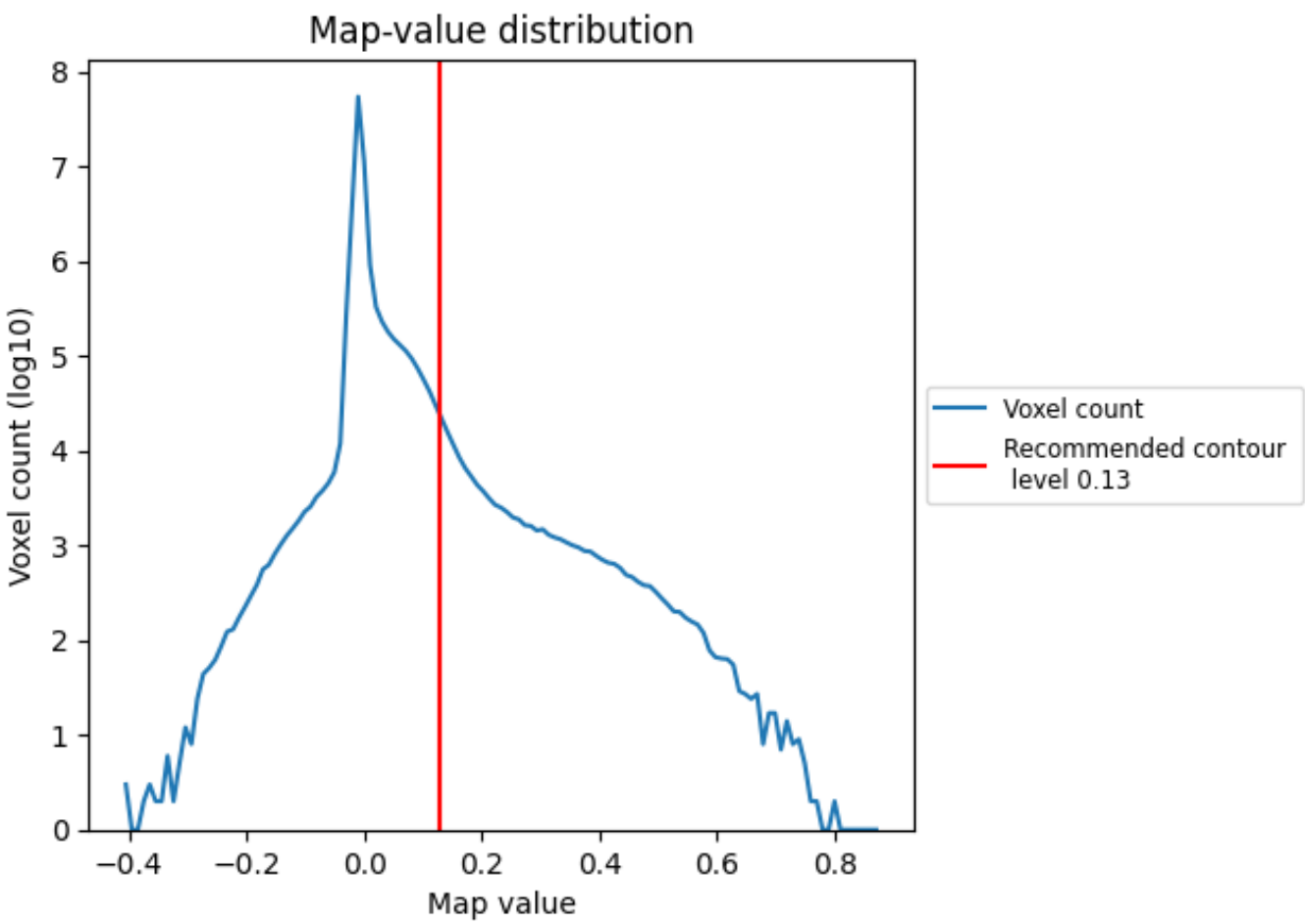
6.6 Mask visualisation (i)

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

7 Map analysis (i)

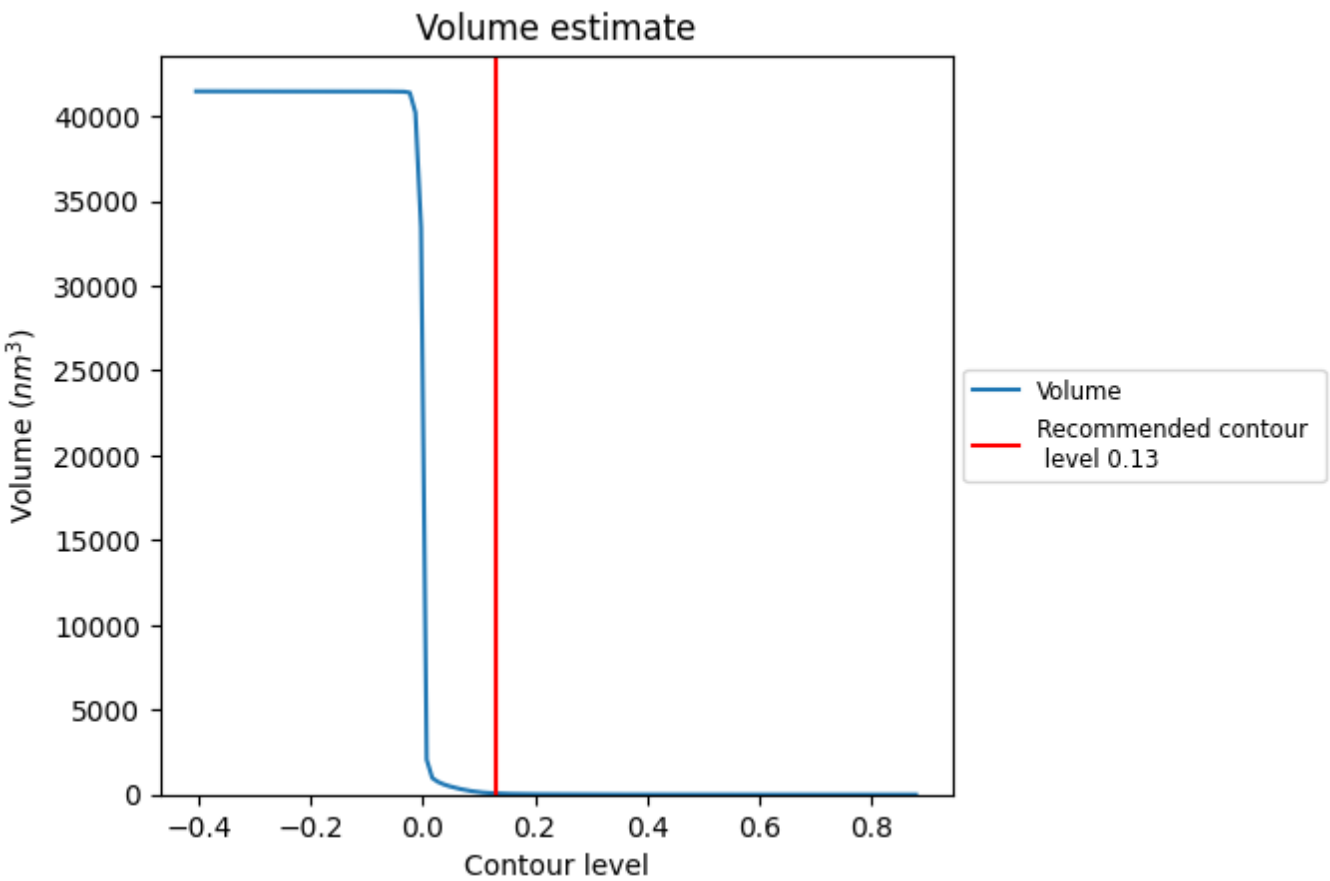
This section contains the results of statistical analysis of the map.

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.

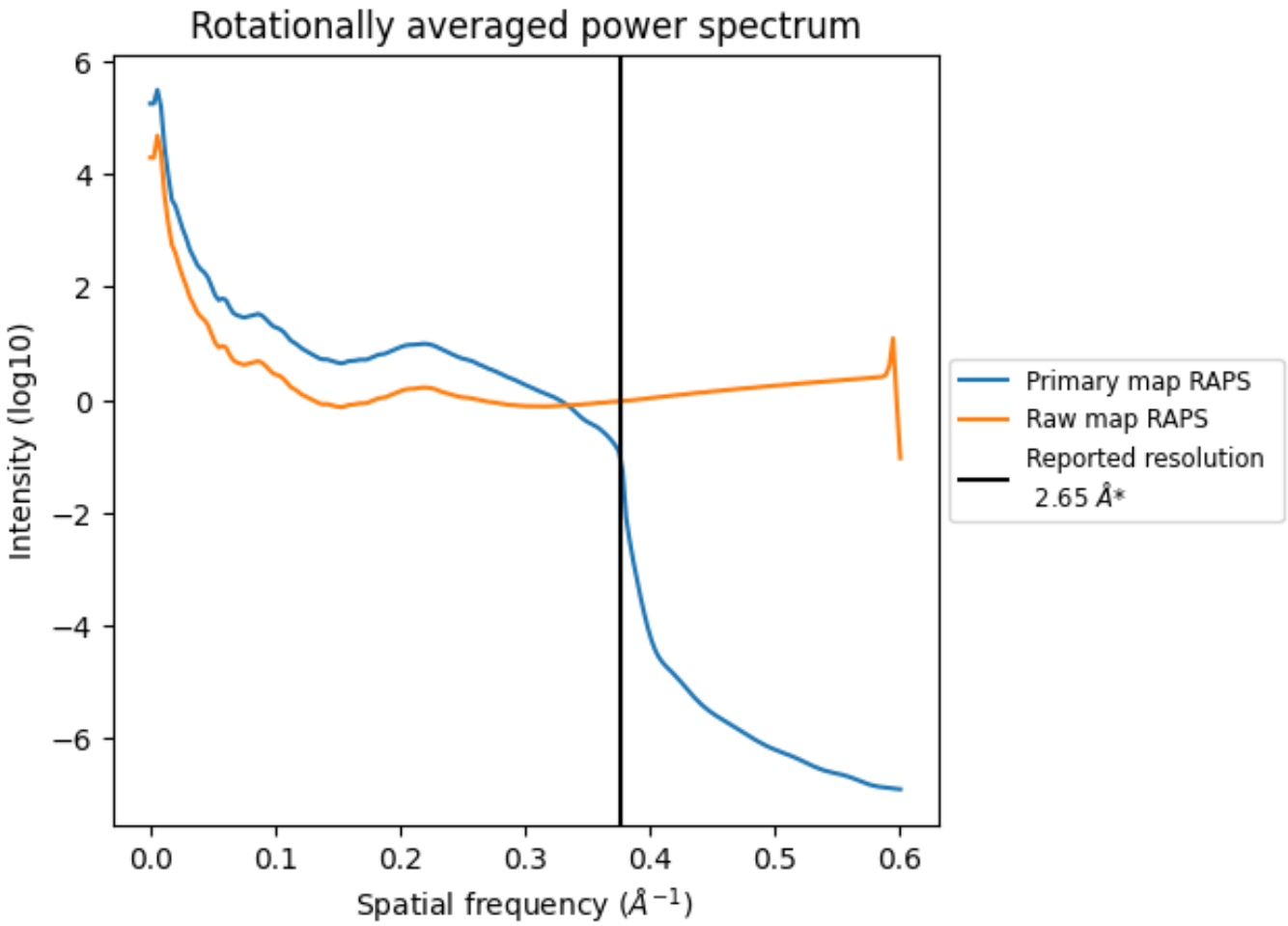
7.2 Volume estimate (i)



The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 62 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 (i)

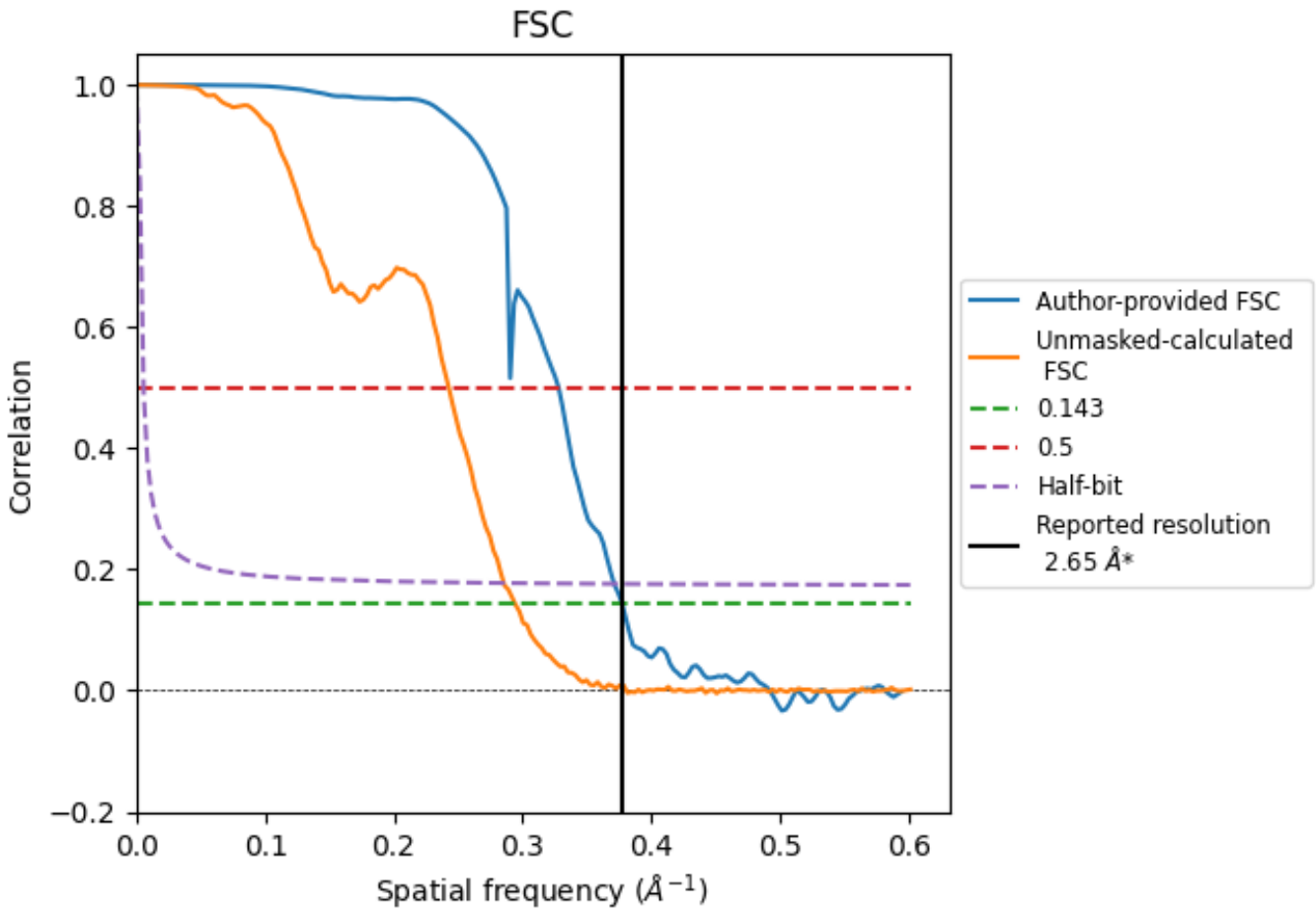


*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

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 0.377 Å^{-1}

8.2 Resolution estimates (i)

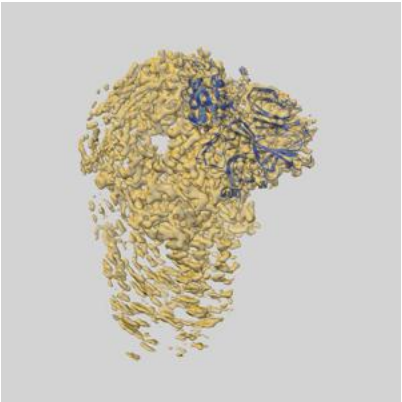
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	3.05	2.70
Unmasked-calculated*	3.40	4.12	3.50

*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 3.40 differs from the reported value 2.65 by more than 10 %

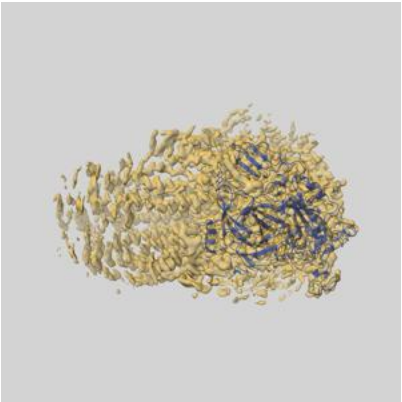
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-76936 and PDB model 13BD. Per-residue inclusion information can be found in section 3 on page 5.

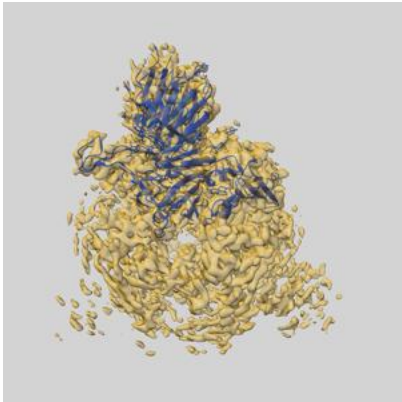
9.1 Map-model overlay (i)



X



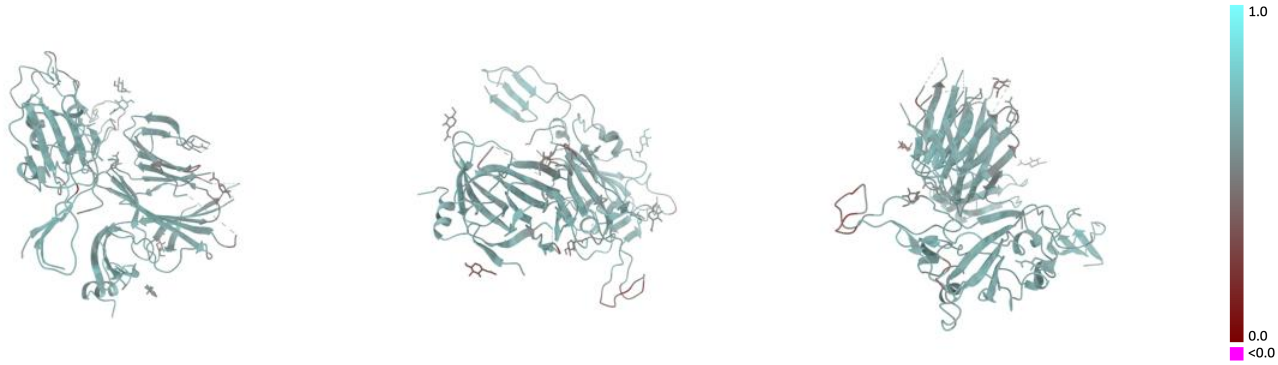
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

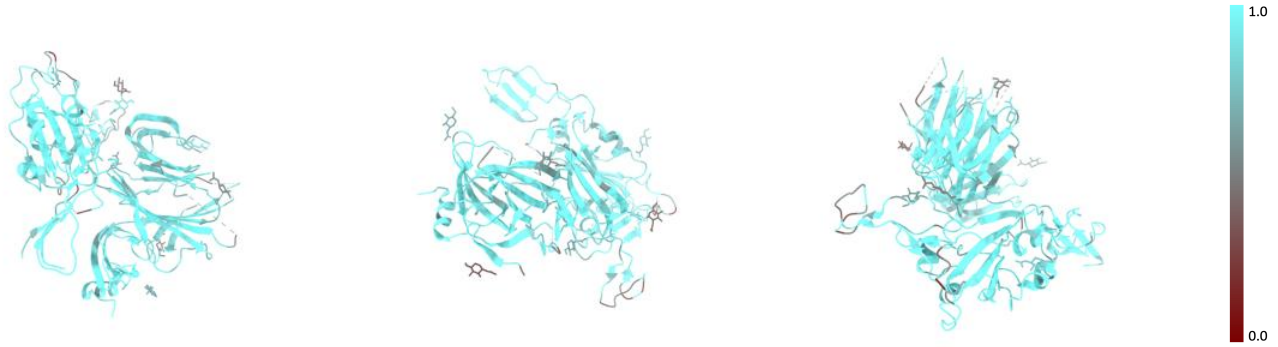
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

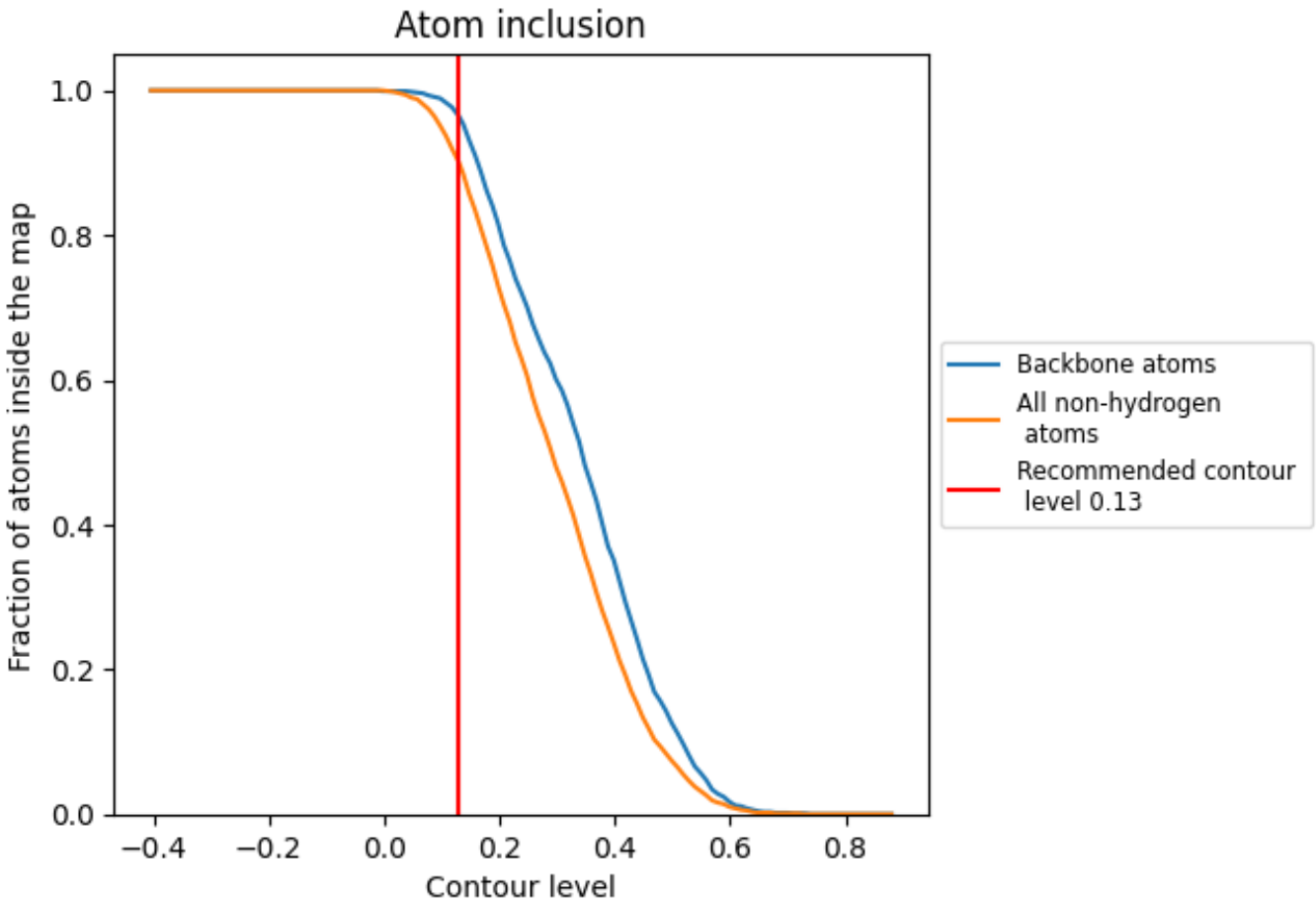
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.5950
A	0.8940	0.5920
B	0.6430	0.5560
C	0.9090	0.6000