



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:14 PM UTC

PDB ID : 6X3Z / pdb_00006x3z
EMDB ID : EMD-22037
Title : Human GABAA receptor alpha1-beta2-gamma2 subtype in complex with GABA
Authors : Kim, J.J.; Gharpure, A.; Teng, J.; Zhuang, Y.; Howard, R.J.; Zhu, S.; Novello, C.M.; Walsh, R.M.; Lindahl, E.; Hibbs, R.E.
Deposited on : 2020-05-21
Resolution : 3.23 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

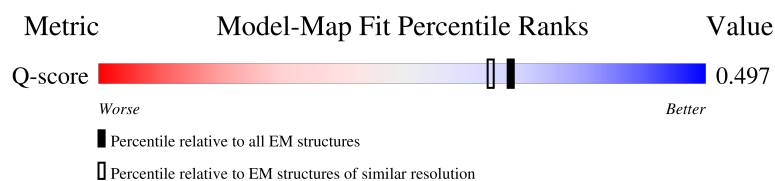
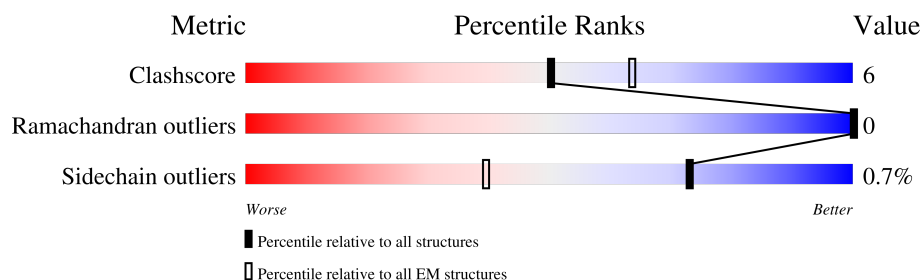
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.23 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.73 - 3.73)

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	364	10% 81% 10% 8%
1	C	364	10% 75% 16% 8%
2	B	358	9% 80% 15% 6%
2	D	358	8% 77% 16% 6%

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Mol	Chain	Length	Quality of chain
3	E	417	
4	I	213	
4	L	213	
5	J	454	
5	K	454	
6	F	3	
6	H	3	
7	G	10	
8	M	2	

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
6	NAG	F	1	X	-	-	-
6	NAG	H	1	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17365 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 Gamma-aminobutyric acid receptor subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2732	1791	440	485	16		
1	C	334	Total	C	N	O	S	0	0
			2732	1791	440	485	16		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	SER	-	linker	UNP P47870
A	309	GLN	-	linker	UNP P47870
A	310	PRO	-	linker	UNP P47870
A	311	ALA	-	linker	UNP P47870
A	312	ARG	-	linker	UNP P47870
A	313	ALA	-	linker	UNP P47870
A	314	ALA	-	linker	UNP P47870
A	315	ALA	-	linker	UNP P47870
C	308	SER	-	linker	UNP P47870
C	309	GLN	-	linker	UNP P47870
C	310	PRO	-	linker	UNP P47870
C	311	ALA	-	linker	UNP P47870
C	312	ARG	-	linker	UNP P47870
C	313	ALA	-	linker	UNP P47870
C	314	ALA	-	linker	UNP P47870
C	315	ALA	-	linker	UNP P47870

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2730	1763	461	490	16		
2	D	338	Total	C	N	O	S	0	0
			2730	1763	461	490	16		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	313	SER	-	linker	UNP P14867
B	314	GLN	-	linker	UNP P14867
B	315	PRO	-	linker	UNP P14867
B	316	ALA	-	linker	UNP P14867
B	317	ARG	-	linker	UNP P14867
B	318	ALA	-	linker	UNP P14867
B	319	ALA	-	linker	UNP P14867
D	313	SER	-	linker	UNP P14867
D	314	GLN	-	linker	UNP P14867
D	315	PRO	-	linker	UNP P14867
D	316	ALA	-	linker	UNP P14867
D	317	ARG	-	linker	UNP P14867
D	318	ALA	-	linker	UNP P14867
D	319	ALA	-	linker	UNP P14867

- Molecule 3 is a protein called Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	333	Total	C	N	O	S	0	0
			2729	1781	448	485	15		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	323	SER	-	linker	UNP P18507
E	324	GLN	-	linker	UNP P18507
E	325	PRO	-	linker	UNP P18507
E	326	ALA	-	linker	UNP P18507
E	327	ARG	-	linker	UNP P18507
E	328	ALA	-	linker	UNP P18507
E	329	ALA	-	linker	UNP P18507

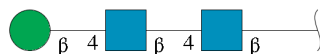
- Molecule 4 is a protein called Kappa Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	105	Total	C	N	O	S	0	0
			802	504	130	163	5		
4	L	106	Total	C	N	O	S	0	0
			811	510	132	164	5		

- Molecule 5 is a protein called IgG2b Fab Heavy Chain.

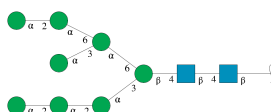
Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	116	Total	C	N	O	S	0	0
			907	574	151	178	4		
5	K	117	Total	C	N	O	S	0	0
			914	578	152	180	4		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	3	Total	C	N	O	0	0
			39	22	2	15		
6	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



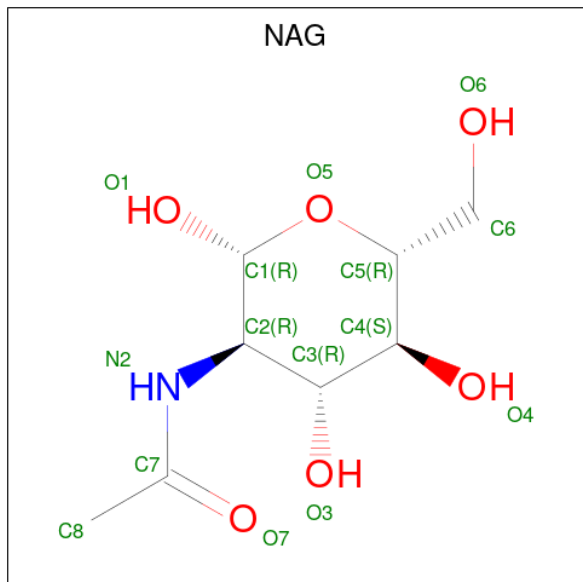
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



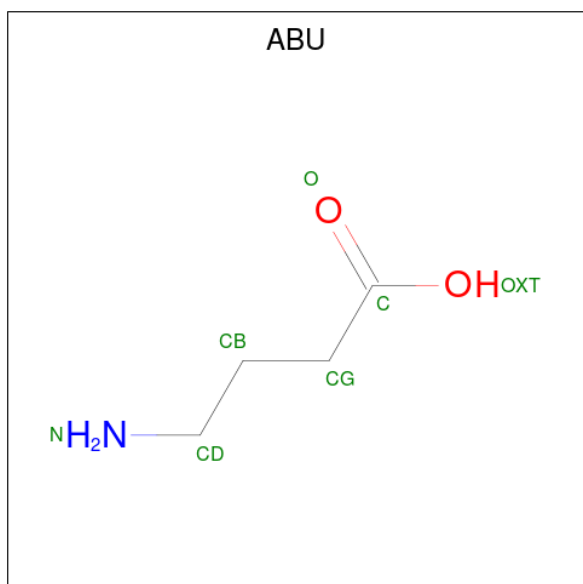
Mol	Chain	Residues	Atoms				AltConf	Trace
8	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).

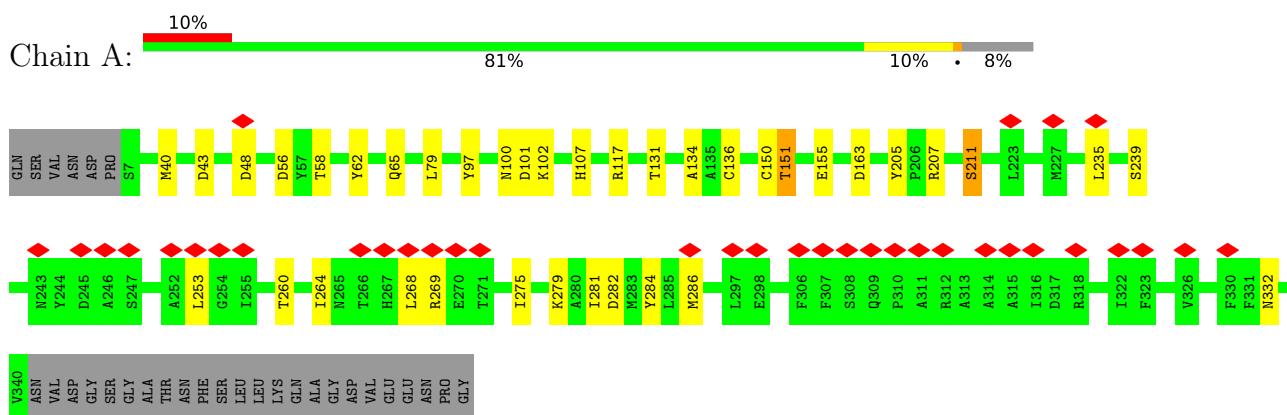


Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			7	4	1	2	
10	C	1	Total	C	N	O	0
			7	4	1	2	

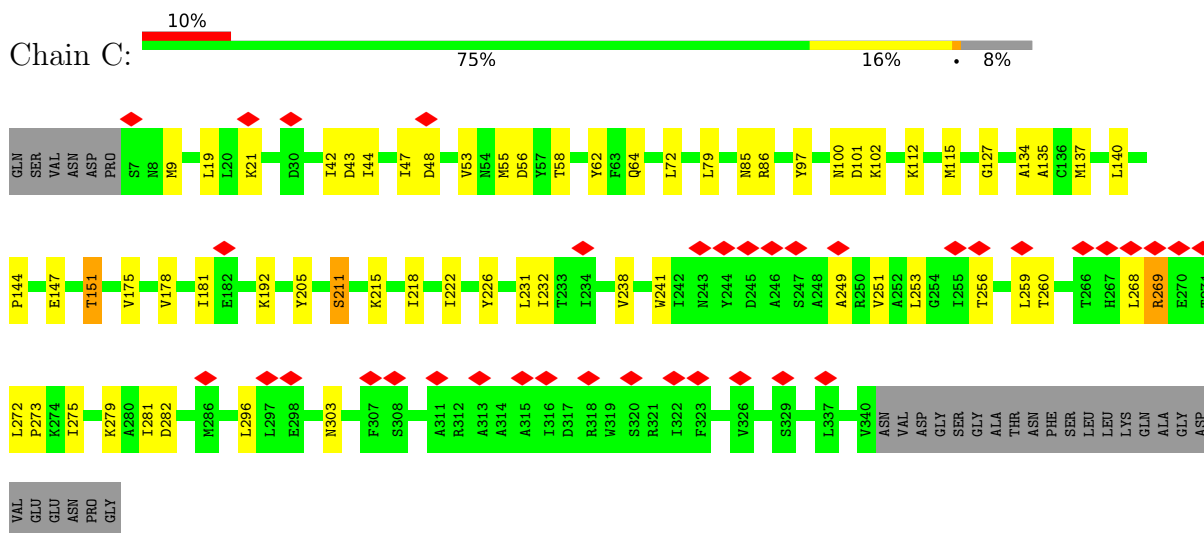
3 Residue-property plots

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.

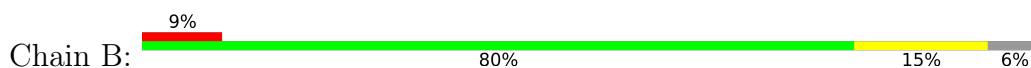
- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2

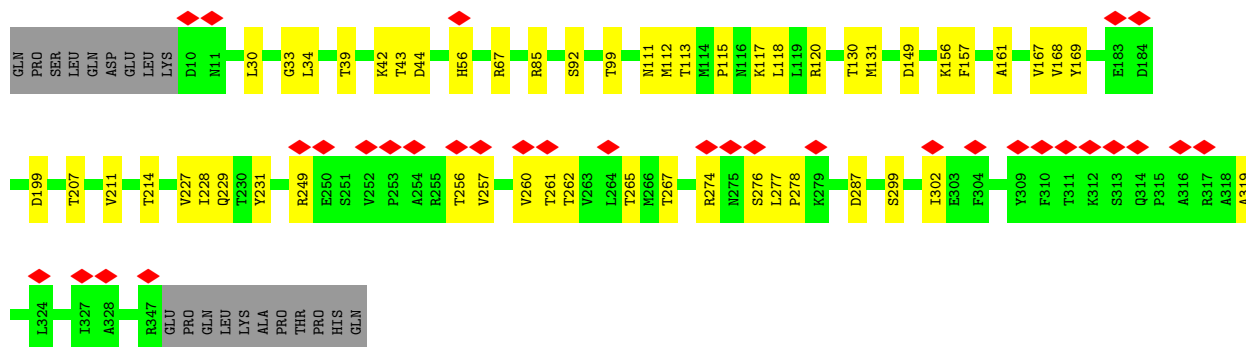


- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2

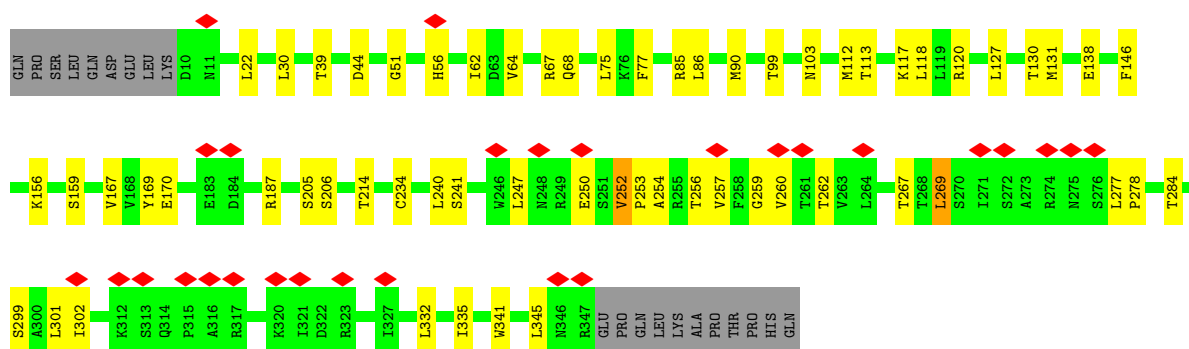
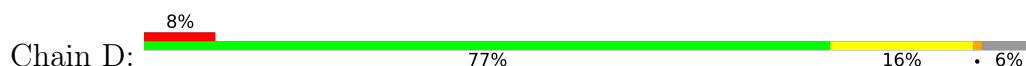


- Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

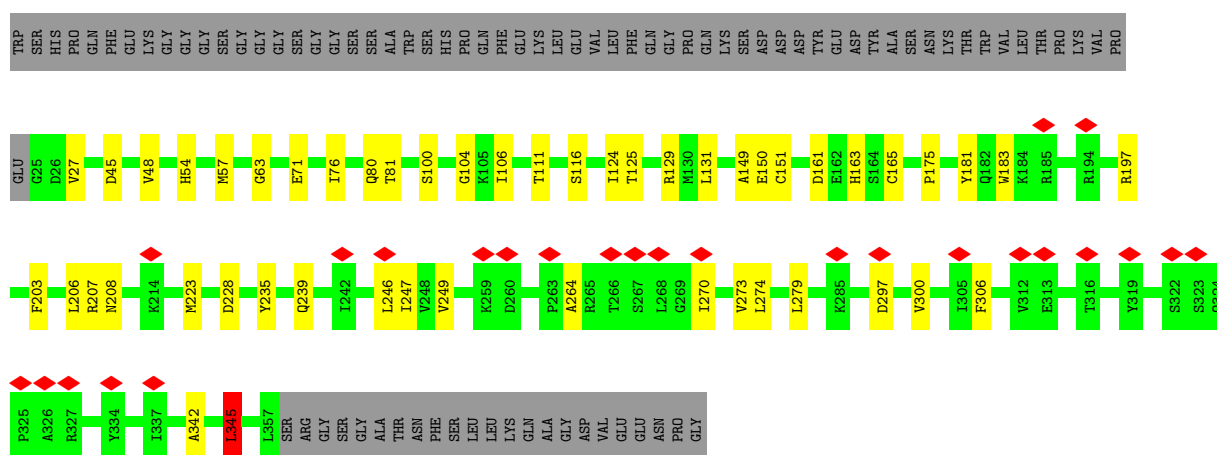




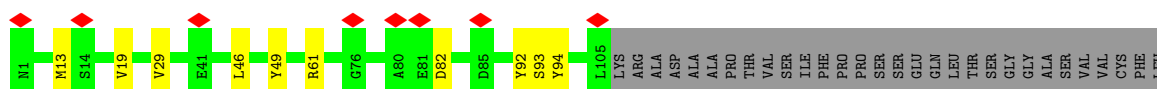
• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

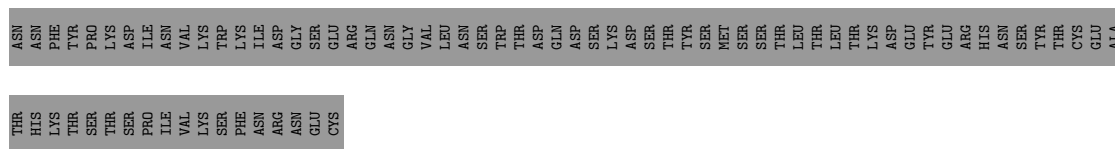


• Molecule 3: Gamma-aminobutyric acid receptor subunit gamma-2

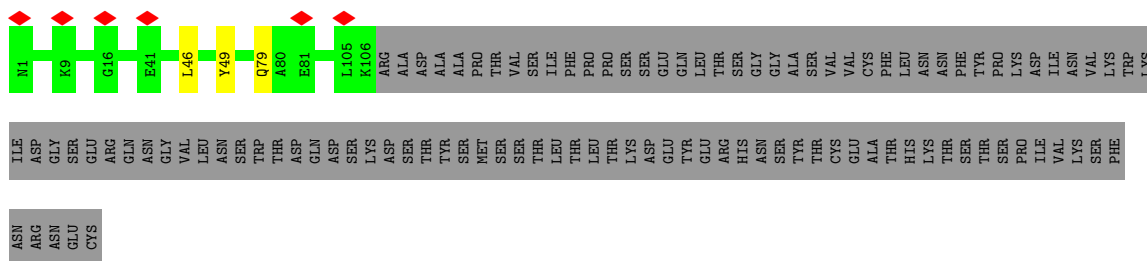


• Molecule 4: Kappa Fab Light Chain

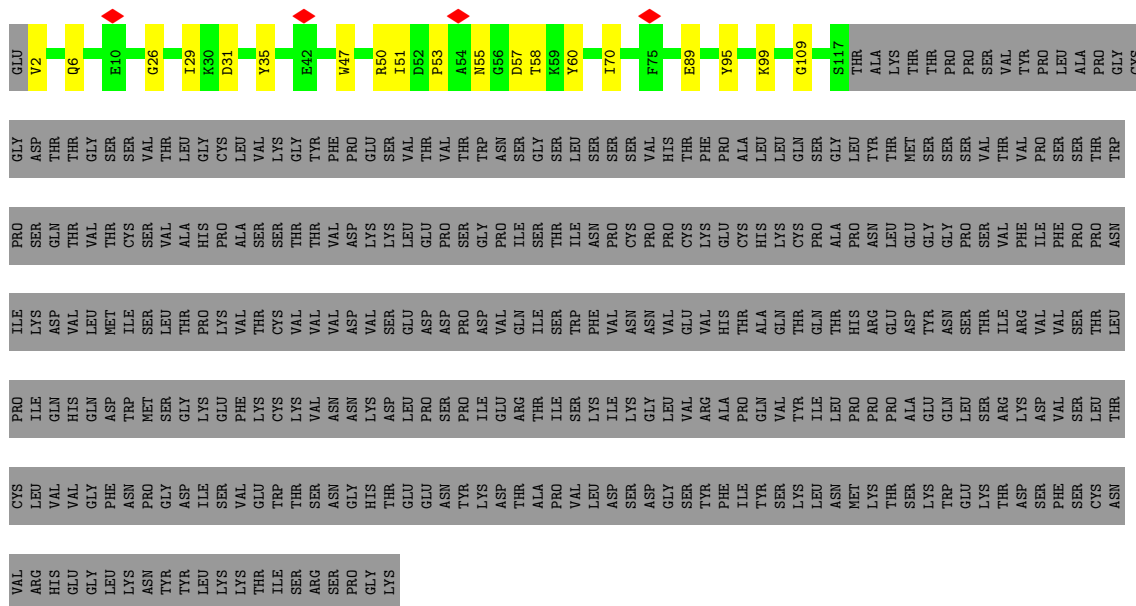




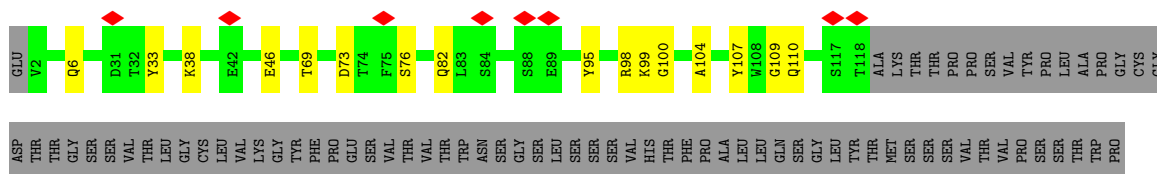
- Molecule 4: Kappa Fab Light Chain



- Molecule 5: IgG2b Fab Heavy Chain



- Molecule 5: IgG2b Fab Heavy Chain



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

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%

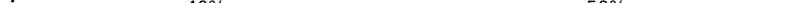


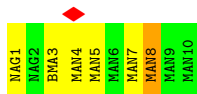
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 33% 33% 33%



- Molecule 7: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain G: 



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	171838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.79	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	237.59999, 237.59999, 237.59999	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, ABU, NAG, MAN

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	0.35	0/2804	0.63	0/3818
1	C	0.36	0/2804	0.65	1/3818 (0.0%)
2	B	0.36	0/2799	0.60	0/3805
2	D	0.34	0/2799	0.58	0/3805
3	E	0.33	0/2805	0.61	1/3822 (0.0%)
4	I	0.28	0/820	0.59	0/1112
4	L	0.26	0/829	0.56	0/1123
5	J	0.25	0/928	0.52	0/1260
5	K	0.24	0/935	0.52	0/1270
All	All	0.33	0/17523	0.60	2/23833 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	ARG	CA-CB-CG	6.14	126.39	114.10
3	E	345	LEU	CA-CB-CG	5.63	135.99	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2732	0	2741	26	0
1	C	2732	0	2741	44	0
2	B	2730	0	2723	38	0
2	D	2730	0	2724	39	0
3	E	2729	0	2714	30	0
4	I	802	0	771	5	0
4	L	811	0	784	1	0
5	J	907	0	877	10	0
5	K	914	0	884	10	0
6	F	39	0	34	1	0
6	H	39	0	34	7	0
7	G	116	0	97	5	0
8	M	28	0	25	2	0
9	A	14	0	13	1	0
9	C	14	0	13	1	0
9	D	14	0	13	2	0
10	A	7	0	0	2	0
10	C	7	0	0	2	0
All	All	17365	0	17188	194	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 6.

The worst 5 of 194 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)
6:H:2:NAG:H83	6:H:2:NAG:H3	1.48	0.93
9:D:401:NAG:H83	7:G:7:MAN:H62	1.60	0.83
1:C:97:TYR:HH	10:C:405:ABU:N	1.81	0.79
9:D:401:NAG:C8	7:G:7:MAN:H62	2.14	0.77
1:A:97:TYR:HH	10:A:405:ABU:N	1.83	0.77

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	332/364 (91%)	320 (96%)	12 (4%)	0	100	100
1	C	332/364 (91%)	322 (97%)	10 (3%)	0	100	100
2	B	336/358 (94%)	327 (97%)	9 (3%)	0	100	100
2	D	336/358 (94%)	328 (98%)	8 (2%)	0	100	100
3	E	331/417 (79%)	313 (95%)	18 (5%)	0	100	100
4	I	103/213 (48%)	96 (93%)	7 (7%)	0	100	100
4	L	104/213 (49%)	94 (90%)	10 (10%)	0	100	100
5	J	114/454 (25%)	107 (94%)	7 (6%)	0	100	100
5	K	115/454 (25%)	107 (93%)	8 (7%)	0	100	100
All	All	2103/3195 (66%)	2014 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/326 (93%)	299 (99%)	3 (1%)	68	78
1	C	302/326 (93%)	298 (99%)	4 (1%)	61	75
2	B	300/319 (94%)	300 (100%)	0	100	100
2	D	300/319 (94%)	298 (99%)	2 (1%)	76	81
3	E	305/372 (82%)	303 (99%)	2 (1%)	76	81
4	I	89/188 (47%)	89 (100%)	0	100	100
4	L	90/188 (48%)	89 (99%)	1 (1%)	65	77
5	J	97/407 (24%)	96 (99%)	1 (1%)	68	78
5	K	98/407 (24%)	98 (100%)	0	100	100
All	All	1883/2852 (66%)	1870 (99%)	13 (1%)	73	81

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	252	VAL
2	D	269	LEU
4	L	79	GLN
3	E	345	LEU
5	J	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	1	ASN
4	I	53	ASN
4	L	79	GLN
1	C	309	GLN
1	C	303	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 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	$\# Z > 2$
6	NAG	F	1	1,6	14,14,15	0.50	0	17,19,21	1.20	2 (11%)
6	NAG	F	2	6	14,14,15	0.31	0	17,19,21	0.60	0
6	BMA	F	3	6	11,11,12	0.24	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	1	7,2	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
7	MAN	G	10	7	11,11,12	0.26	0	15,15,17	0.78	0
7	NAG	G	2	7	14,14,15	0.36	0	17,19,21	0.72	0
7	BMA	G	3	7	11,11,12	0.27	0	15,15,17	0.64	0
7	MAN	G	4	7	11,11,12	0.22	0	15,15,17	0.64	0
7	MAN	G	5	7	11,11,12	0.30	0	15,15,17	0.58	0
7	MAN	G	6	7	11,11,12	0.25	0	15,15,17	0.57	0
7	MAN	G	7	7	11,11,12	0.34	0	15,15,17	1.02	0
7	MAN	G	8	7	11,11,12	0.25	0	15,15,17	0.89	1 (6%)
7	MAN	G	9	7	11,11,12	0.24	0	15,15,17	0.54	0
6	NAG	H	1	1,6	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
6	NAG	H	2	6	14,14,15	0.28	0	17,19,21	0.75	0
6	BMA	H	3	6	11,11,12	0.24	0	15,15,17	0.75	0
8	NAG	M	1	8,3	14,14,15	0.28	0	17,19,21	0.61	0
8	NAG	M	2	8	14,14,15	0.28	0	17,19,21	0.68	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1	1,6	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1
7	NAG	G	1	7,2	-	2/6/23/26	0/1/1/1
7	MAN	G	10	7	-	1/2/19/22	0/1/1/1
7	NAG	G	2	7	-	4/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	0/2/19/22	0/1/1/1
7	MAN	G	5	7	-	1/2/19/22	0/1/1/1
7	MAN	G	6	7	-	0/2/19/22	0/1/1/1
7	MAN	G	7	7	-	0/2/19/22	0/1/1/1
7	MAN	G	8	7	-	2/2/19/22	0/1/1/1
7	MAN	G	9	7	-	0/2/19/22	0/1/1/1
6	NAG	H	1	1,6	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1
8	NAG	M	1	8,3	-	2/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1	NAG	O5-C1-C2	-3.02	106.62	111.29
6	H	1	NAG	O5-C1-C2	-2.94	106.74	111.29
7	G	1	NAG	C1-O5-C5	-2.60	108.71	112.19
7	G	8	MAN	O2-C2-C3	-2.27	105.46	110.15
6	F	1	NAG	C1-O5-C5	2.23	115.17	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	F	1	NAG	C1
6	H	1	NAG	C1

5 of 28 torsion outliers are listed below:

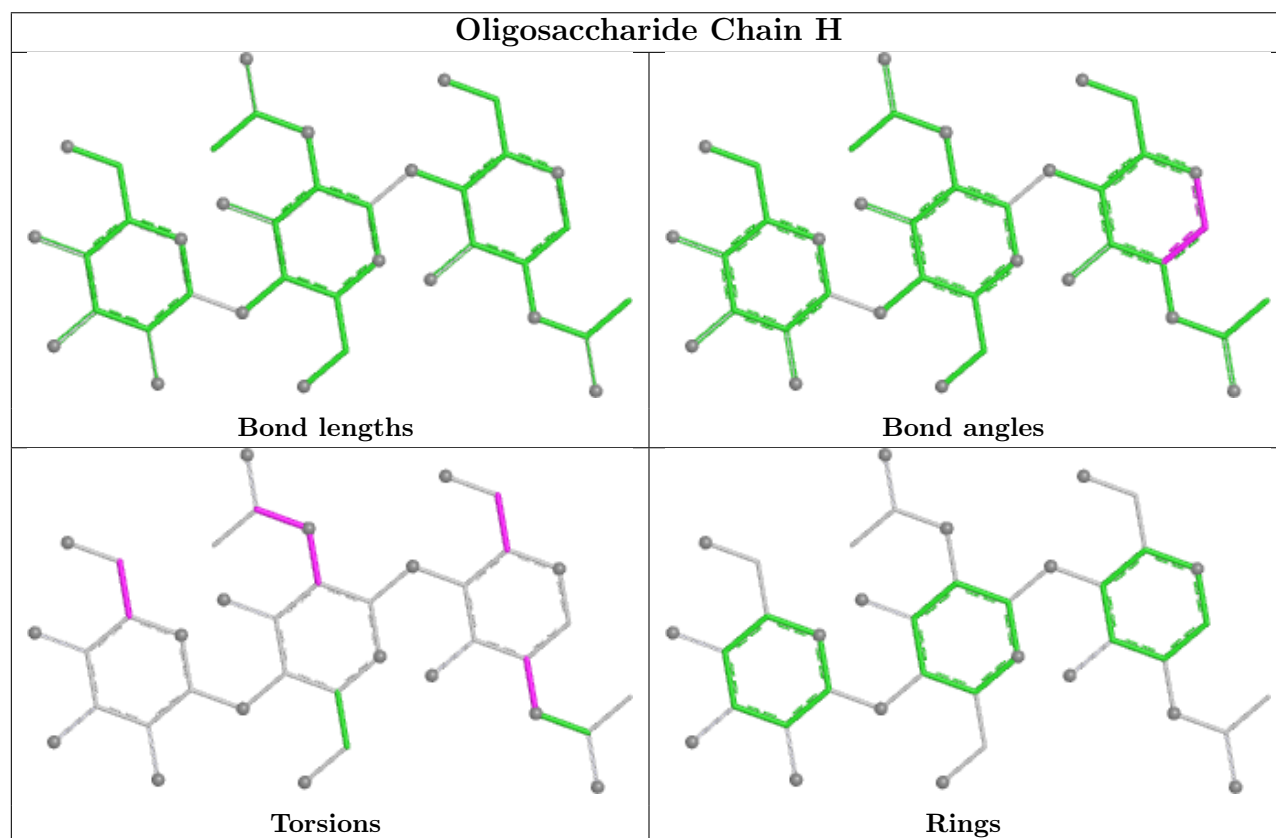
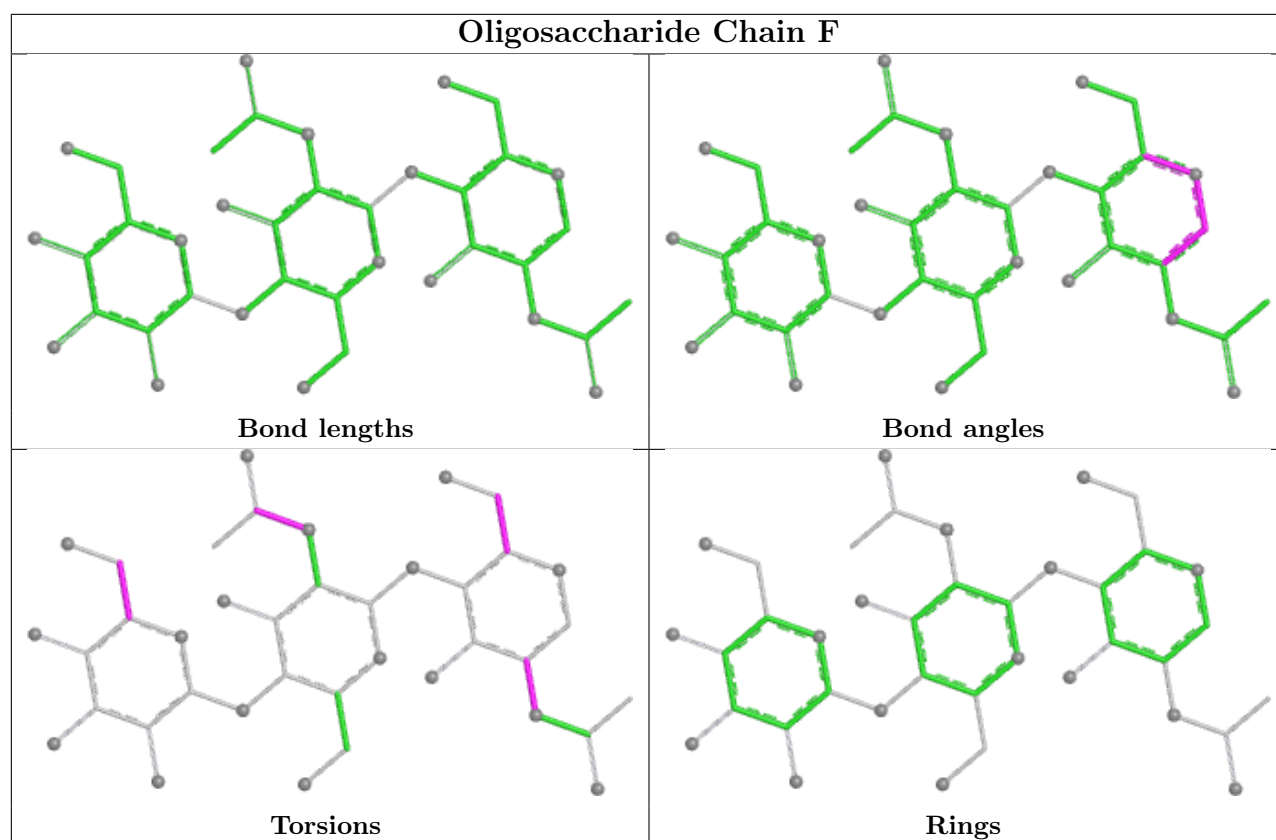
Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C3-C2-N2-C7
6	H	1	NAG	C3-C2-N2-C7
8	M	1	NAG	C8-C7-N2-C2
8	M	1	NAG	O7-C7-N2-C2
8	M	2	NAG	C8-C7-N2-C2

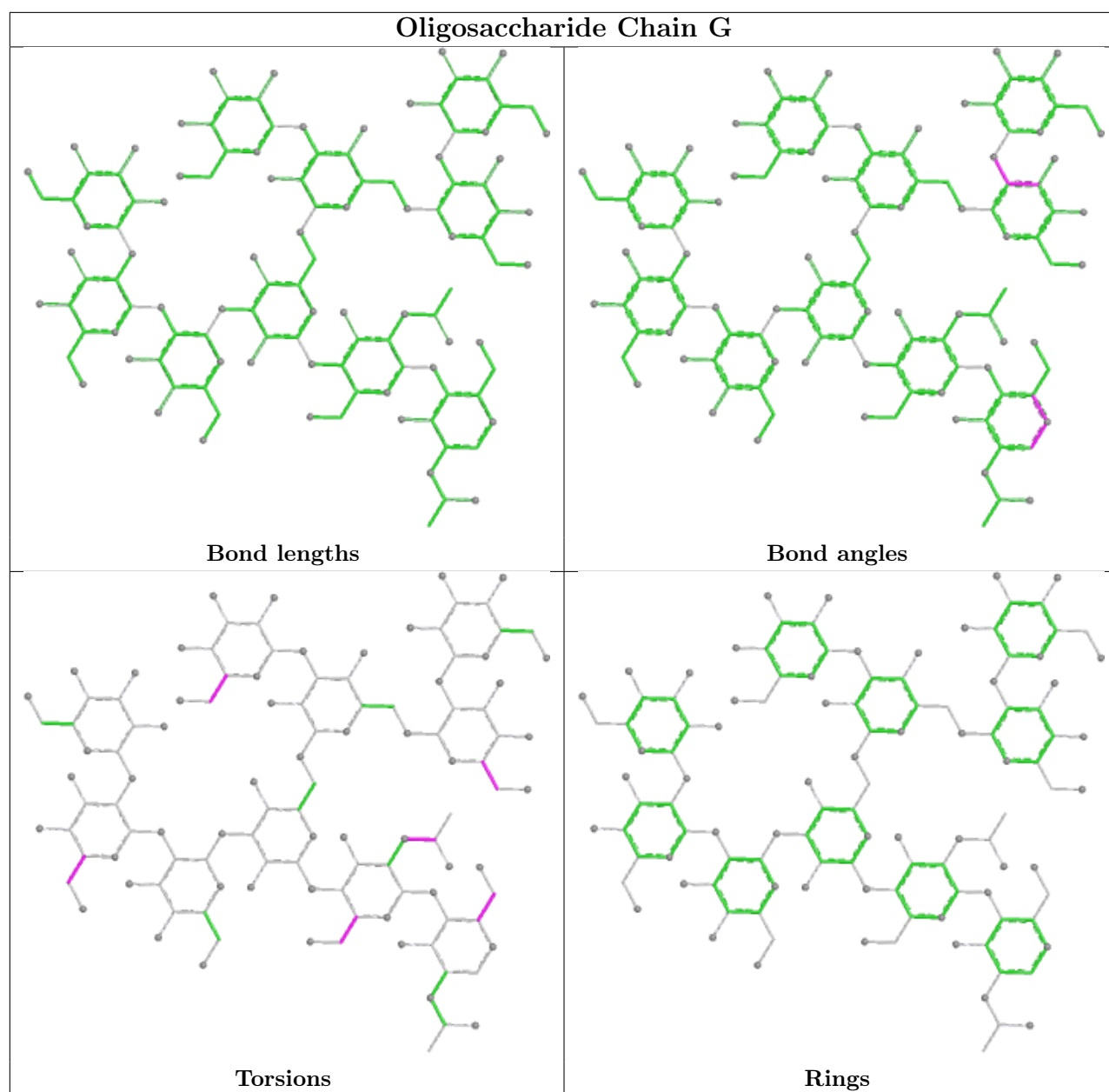
There are no ring outliers.

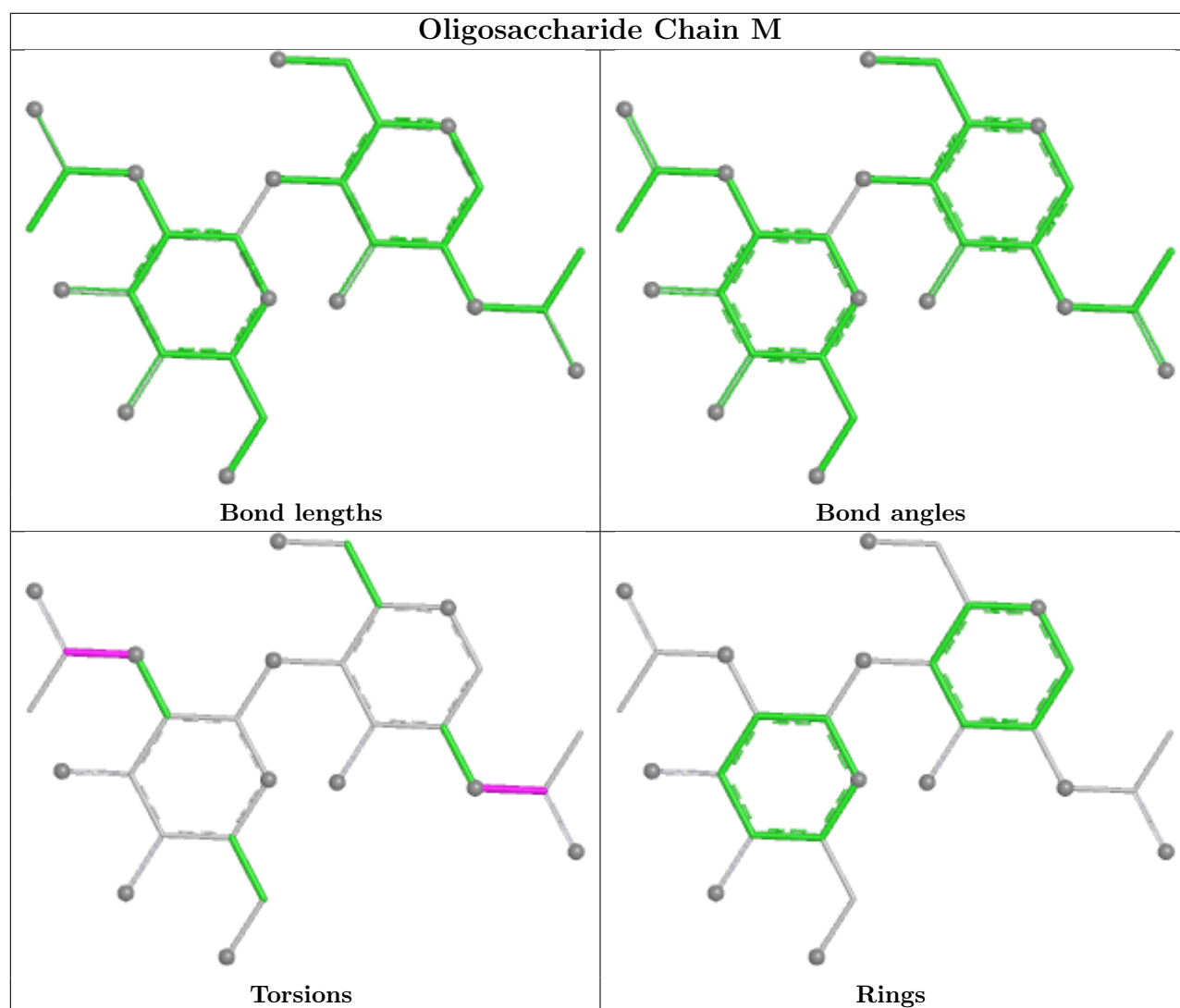
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	7	MAN	2	0
8	M	1	NAG	2	0
7	G	4	MAN	1	0
7	G	5	MAN	1	0
6	H	2	NAG	6	0
6	H	1	NAG	2	0
6	F	1	NAG	1	0
7	G	8	MAN	1	0
7	G	3	BMA	2	0
8	M	2	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 oligosaccharide.







5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
10	ABU	A	405	-	6,6,6	1.93	2 (33%)	6,6,6	1.55	1 (16%)
9	NAG	D	401	2	14,14,15	0.21	0	17,19,21	0.51	0
9	NAG	A	404	1	14,14,15	0.30	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ABU	C	405	-	6,6,6	0.47	0	6,6,6	1.59	2 (33%)
9	NAG	C	404	1	14,14,15	0.37	0	17,19,21	0.48	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
10	ABU	A	405	-	-	1/4/4/4	-
9	NAG	D	401	2	-	2/6/23/26	0/1/1/1
9	NAG	A	404	1	-	0/6/23/26	0/1/1/1
10	ABU	C	405	-	-	0/4/4/4	-
9	NAG	C	404	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	405	ABU	O-C	3.66	1.34	1.22
10	A	405	ABU	OXT-C	-2.99	1.20	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	405	ABU	CB-CG-C	-2.52	107.93	114.51
10	C	405	ABU	CB-CG-C	-2.42	108.19	114.51
10	C	405	ABU	OXT-C-CG	2.15	120.81	114.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

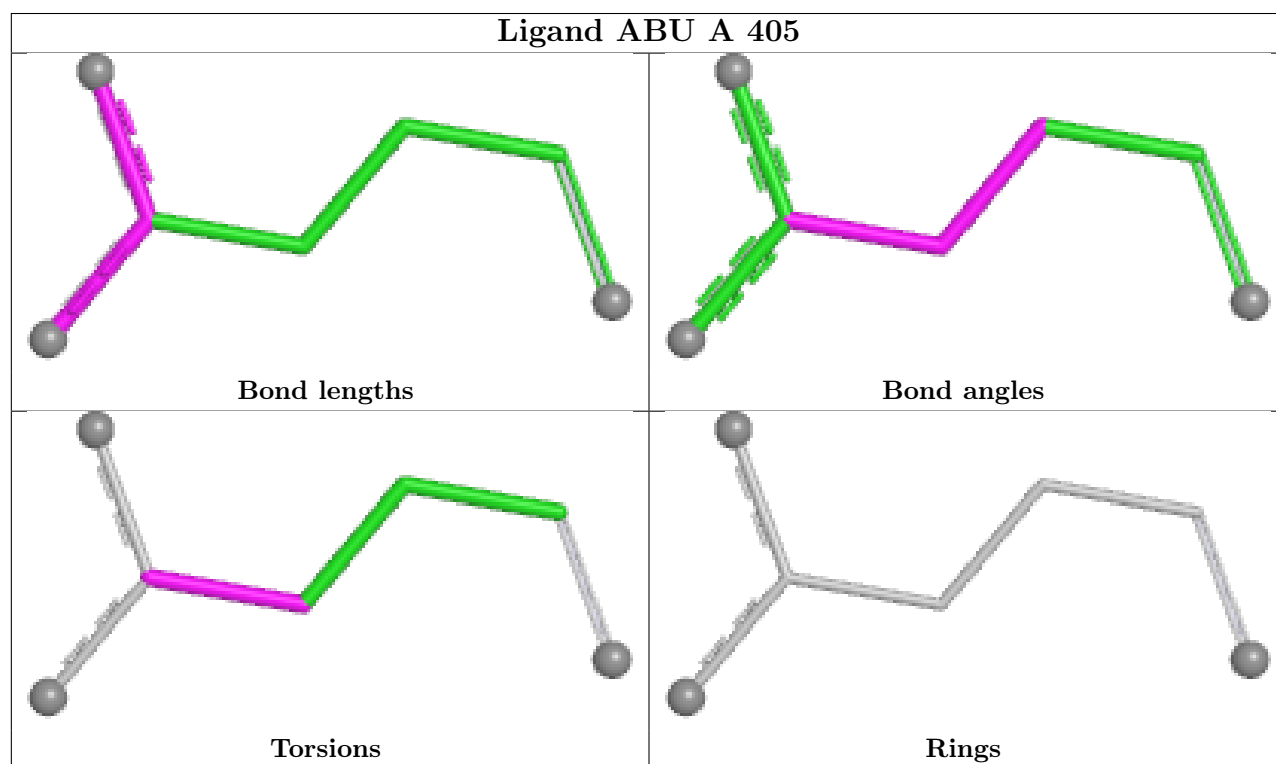
Mol	Chain	Res	Type	Atoms
9	D	401	NAG	O5-C5-C6-O6
9	D	401	NAG	C4-C5-C6-O6
9	C	404	NAG	O5-C5-C6-O6
9	C	404	NAG	C4-C5-C6-O6
10	A	405	ABU	O-C-CG-CB

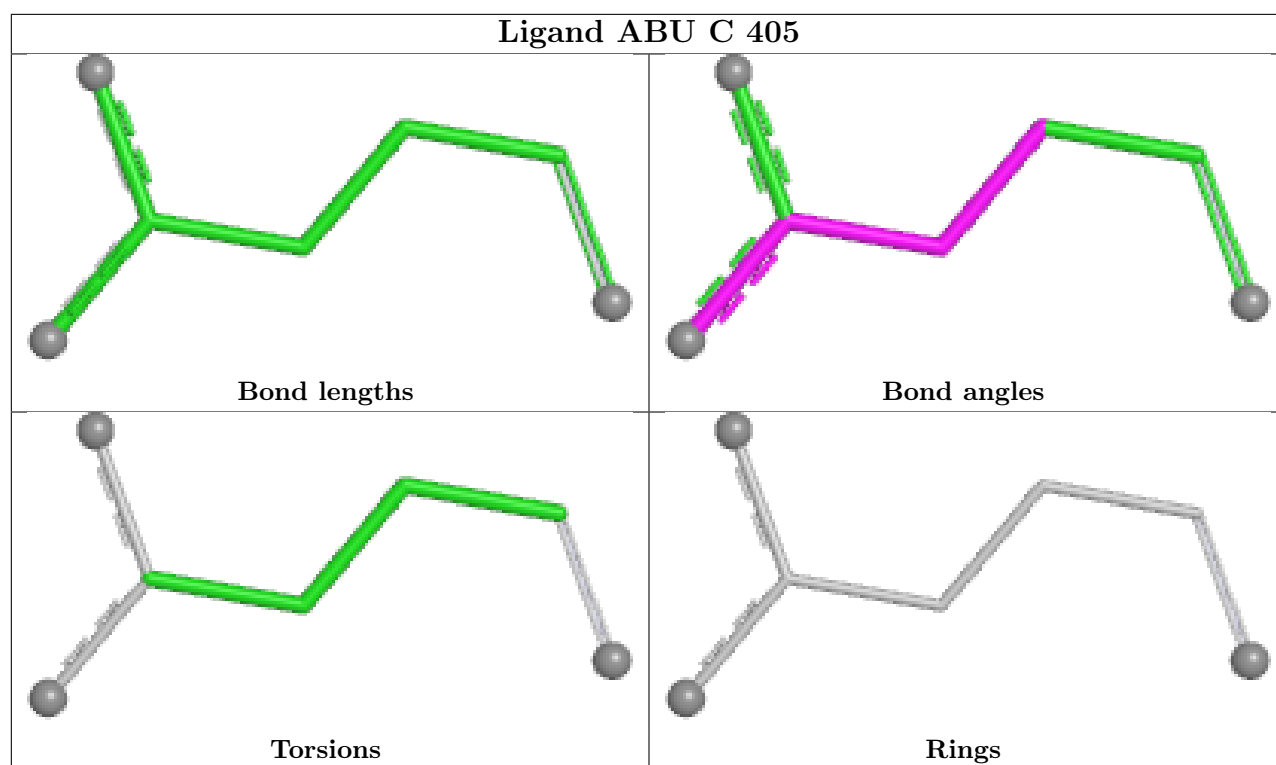
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	405	ABU	2	0
9	D	401	NAG	2	0
9	A	404	NAG	1	0
10	C	405	ABU	2	0
9	C	404	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.

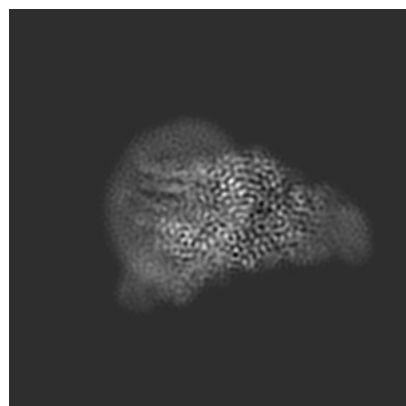
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22037. These allow visual inspection of the internal detail of the map and identification of artifacts.

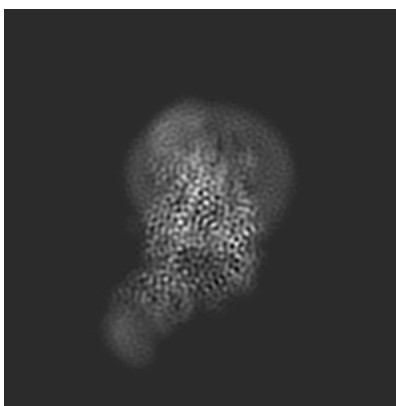
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

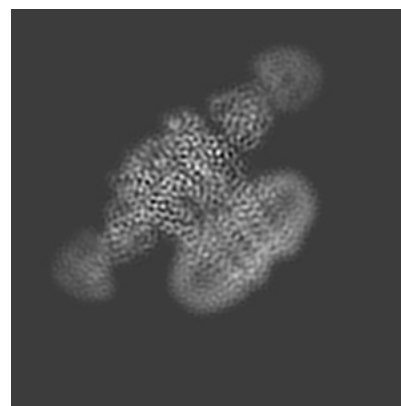
6.1.1 Primary map



X

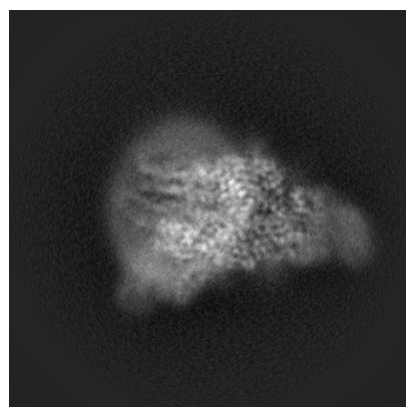


Y

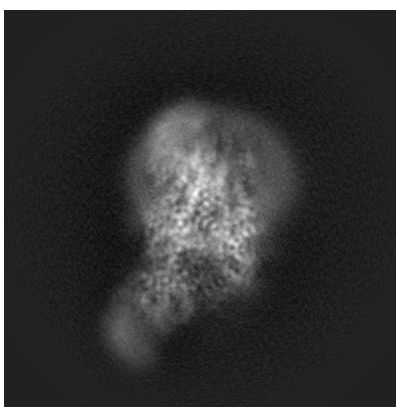


Z

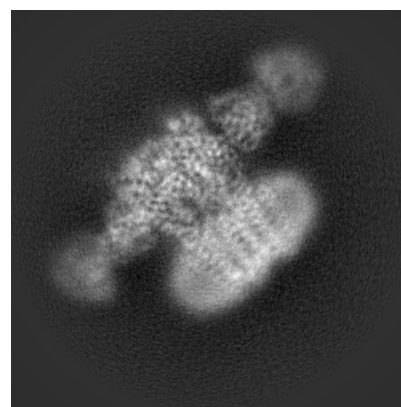
6.1.2 Raw map



X



Y

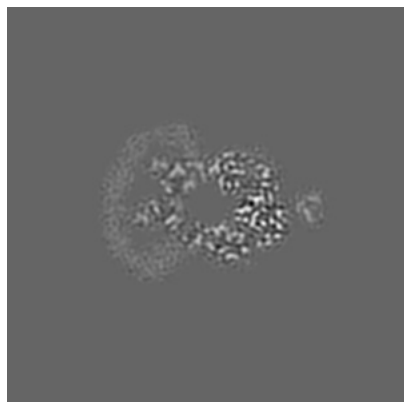


Z

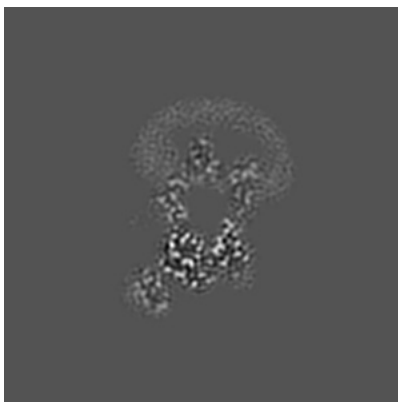
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

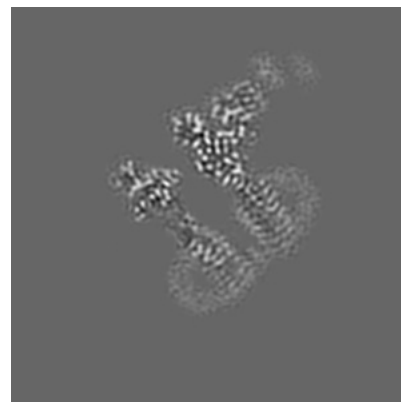
6.2.1 Primary map



X Index: 144

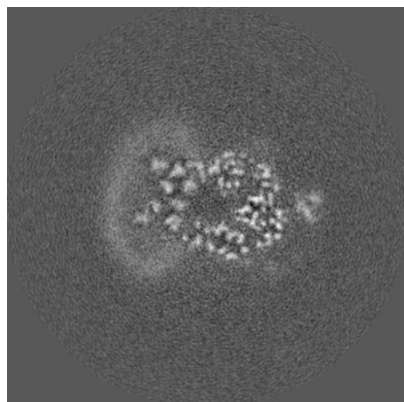


Y Index: 144

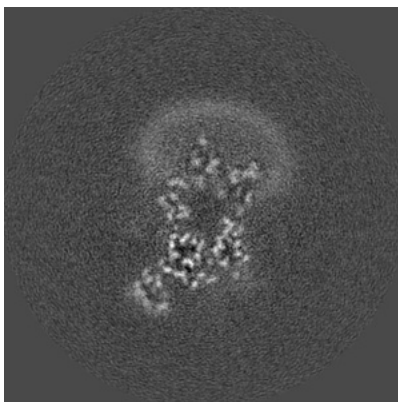


Z Index: 144

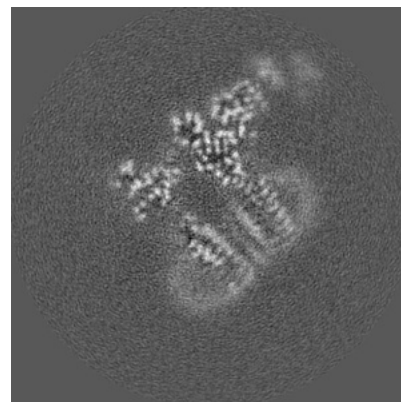
6.2.2 Raw map



X Index: 144



Y Index: 144

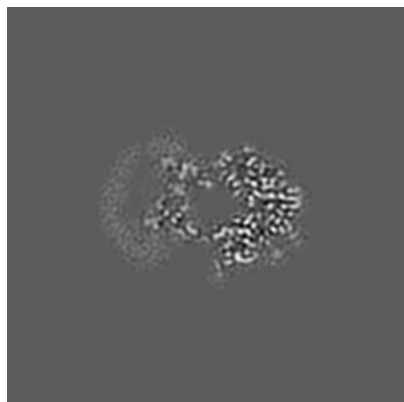


Z Index: 144

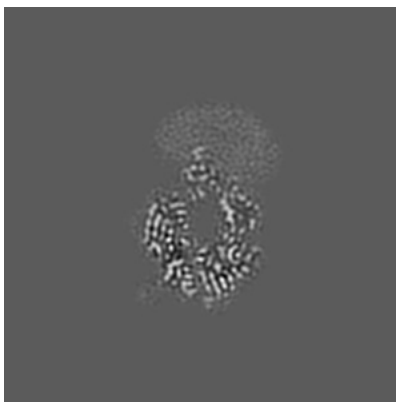
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

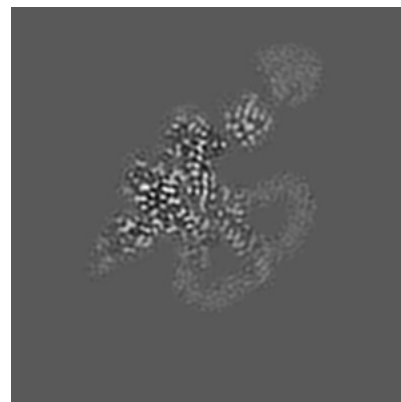
6.3.1 Primary map



X Index: 133

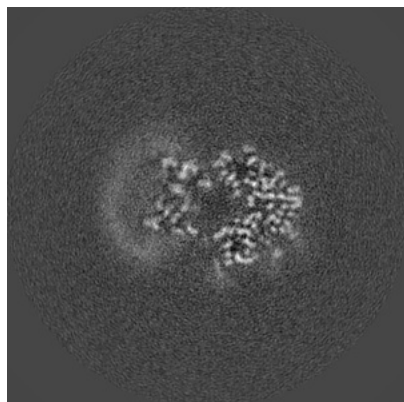


Y Index: 159

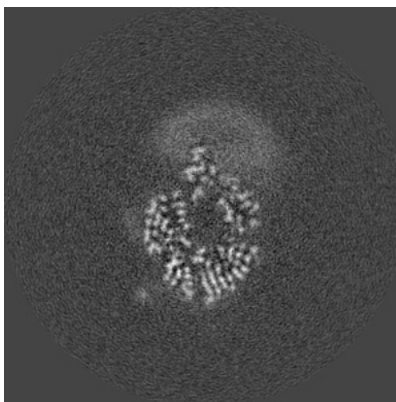


Z Index: 125

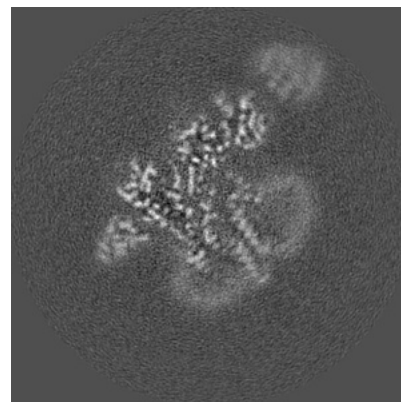
6.3.2 Raw map



X Index: 133



Y Index: 158

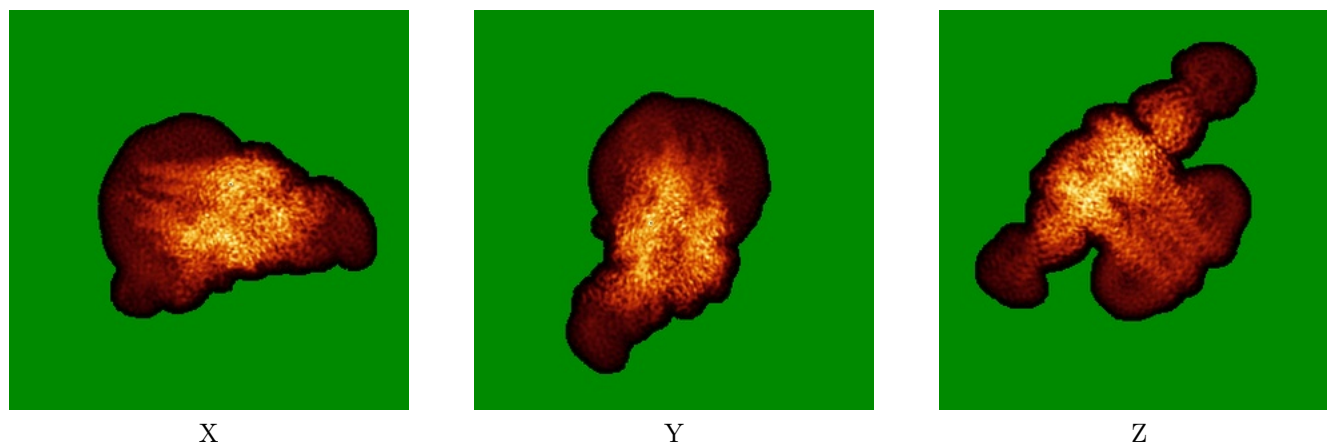


Z Index: 130

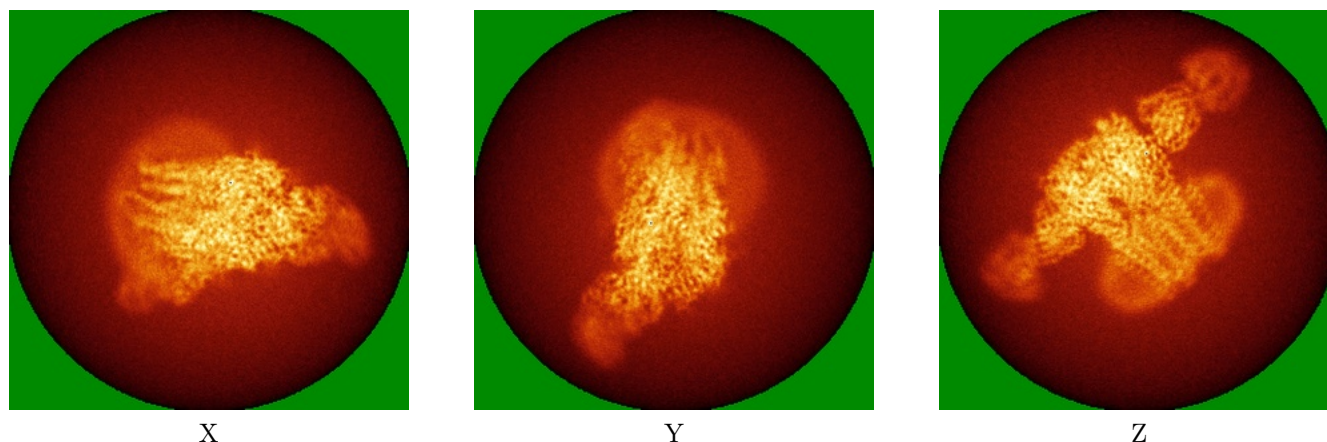
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

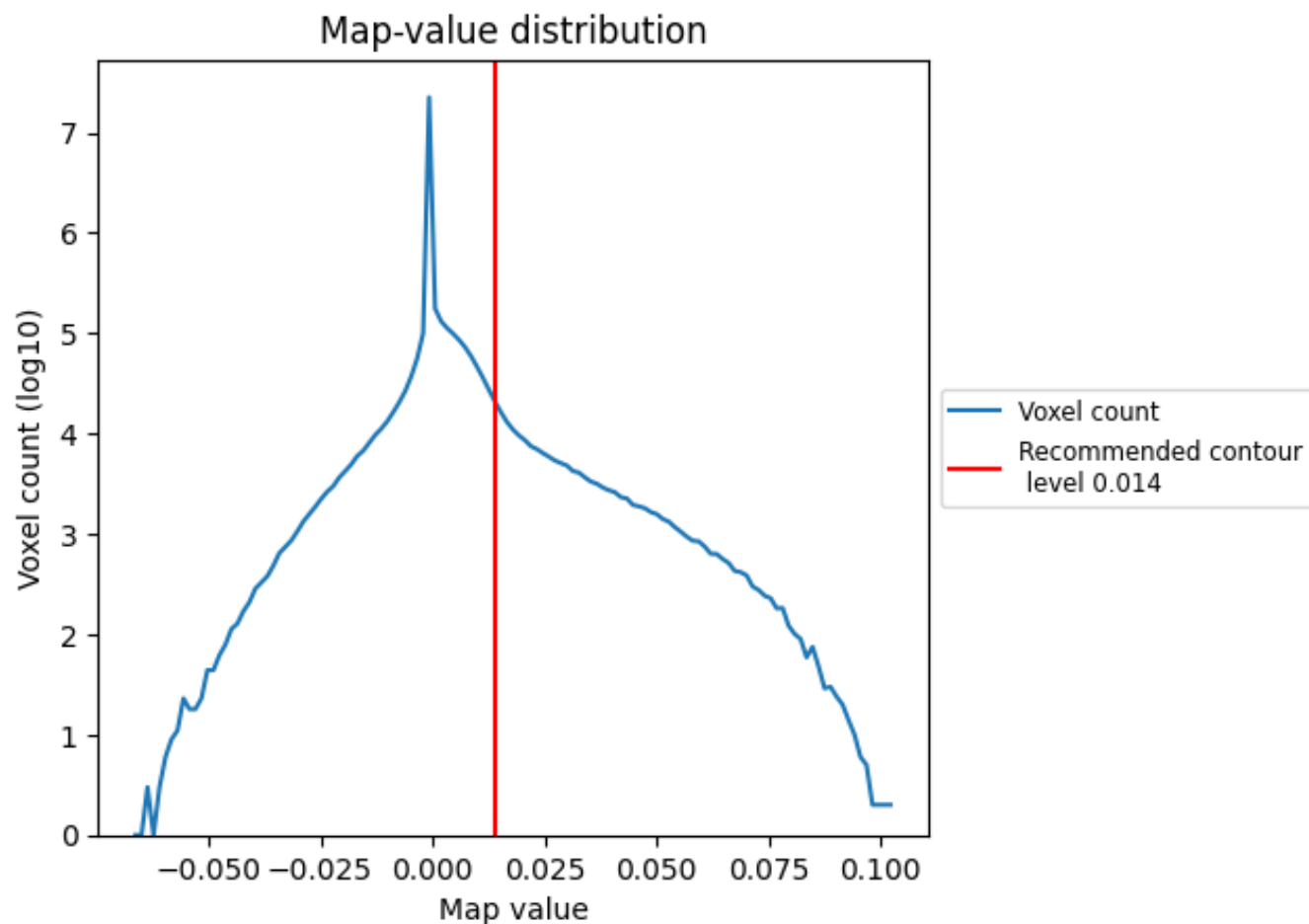
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

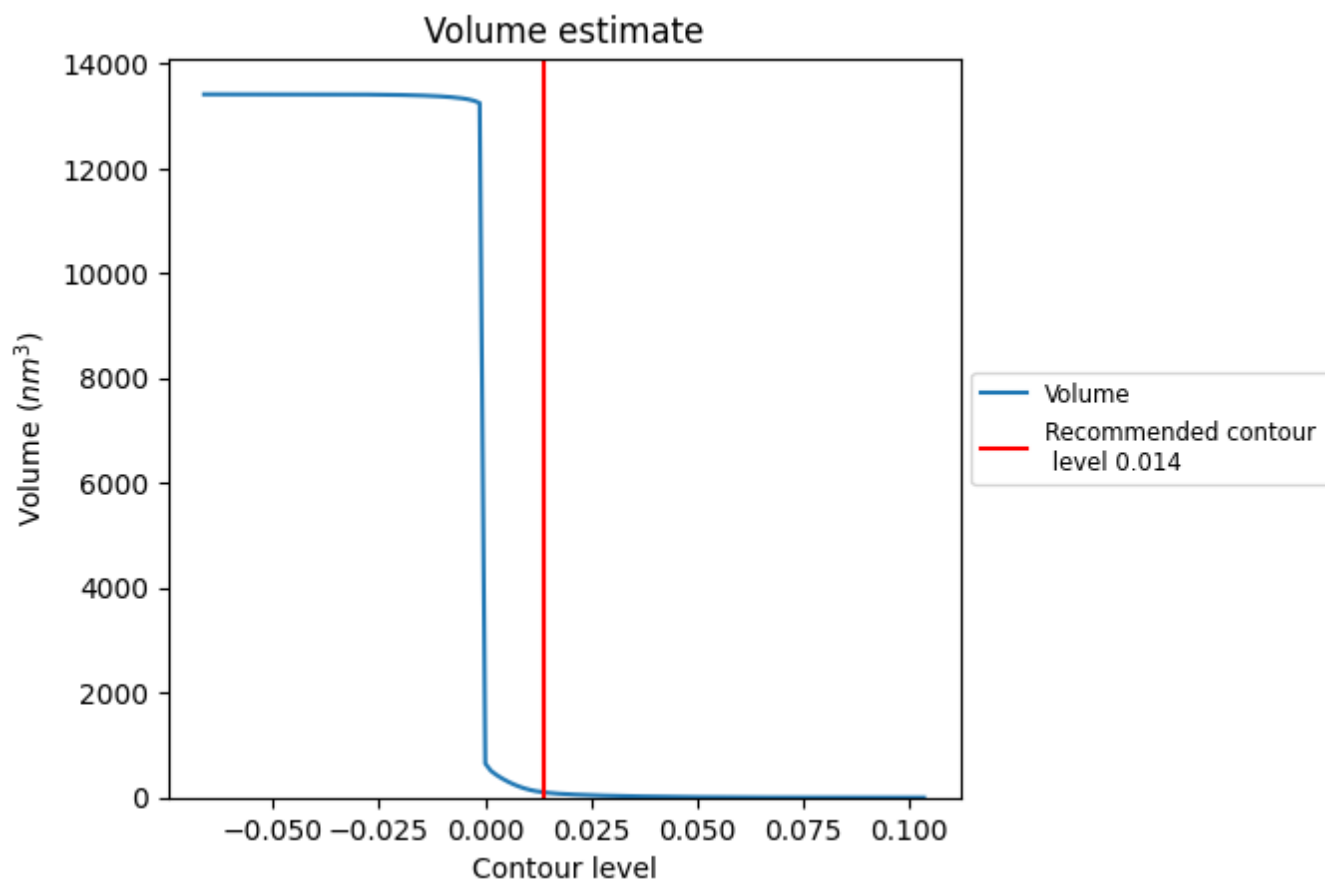
This section contains the results of statistical analysis of the map.

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.

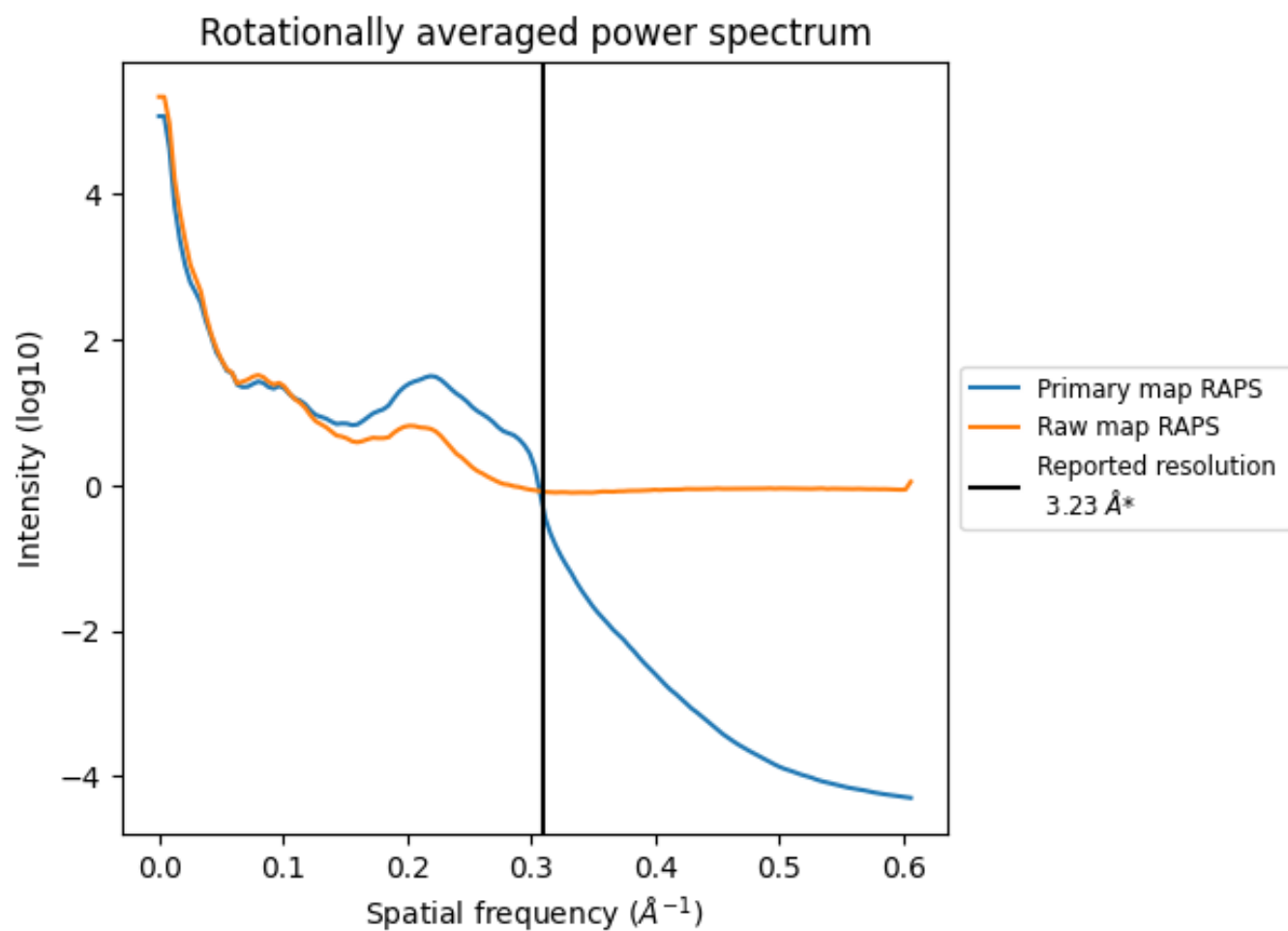
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm³; this corresponds to an approximate mass of 89 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 ⓘ

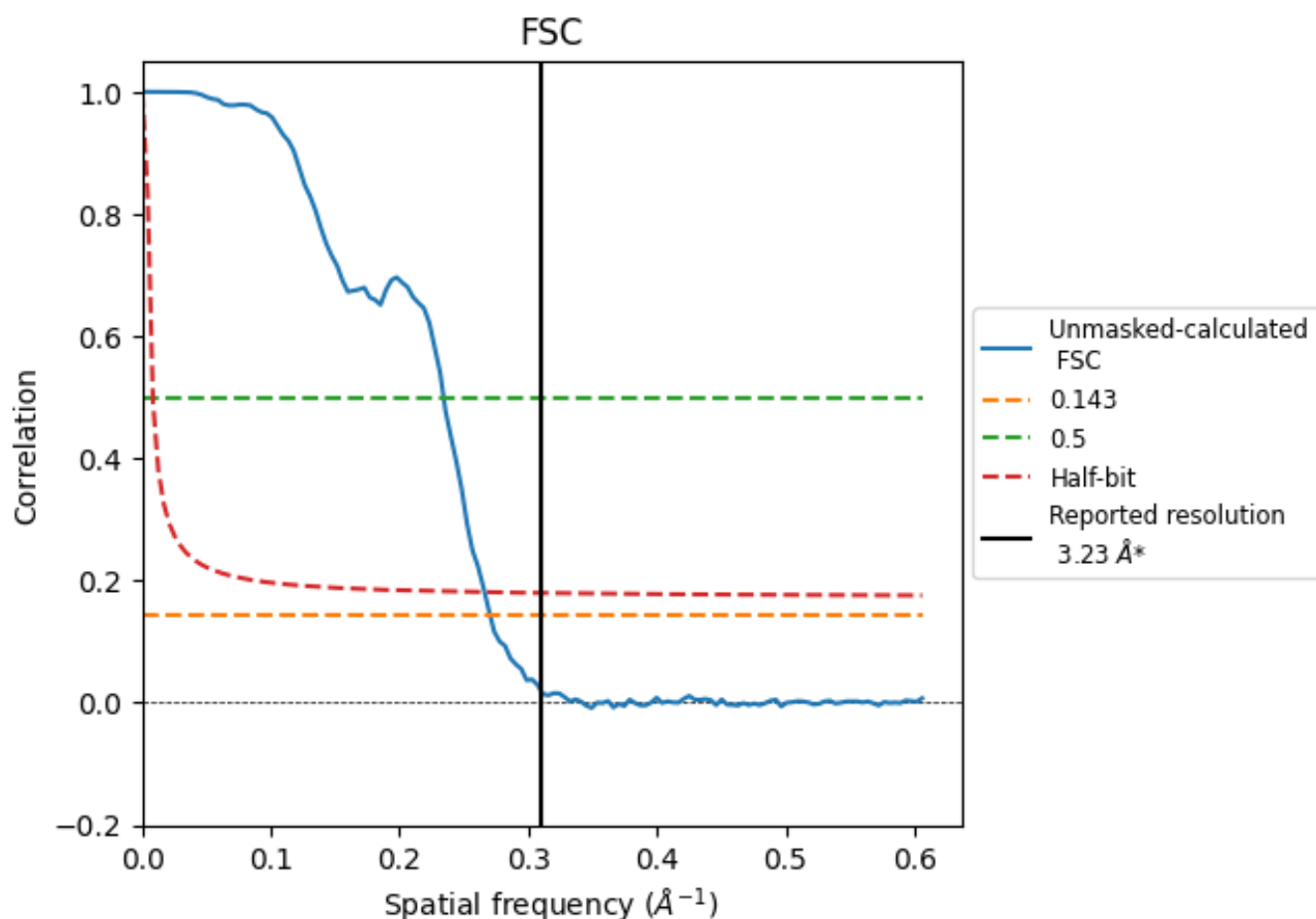


*Reported resolution corresponds to spatial frequency of $0.310 \text{ \AA}^{-1}$

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 0.310 Å⁻¹

8.2 Resolution estimates [i](#)

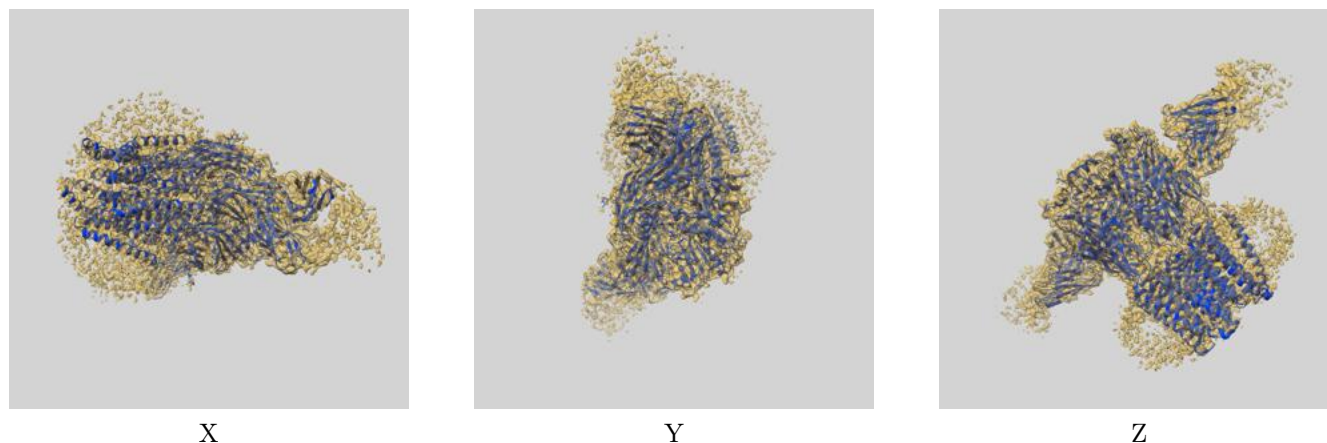
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	4.27	3.76

*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 3.70 differs from the reported value 3.23 by more than 10 %

9 Map-model fit [i](#)

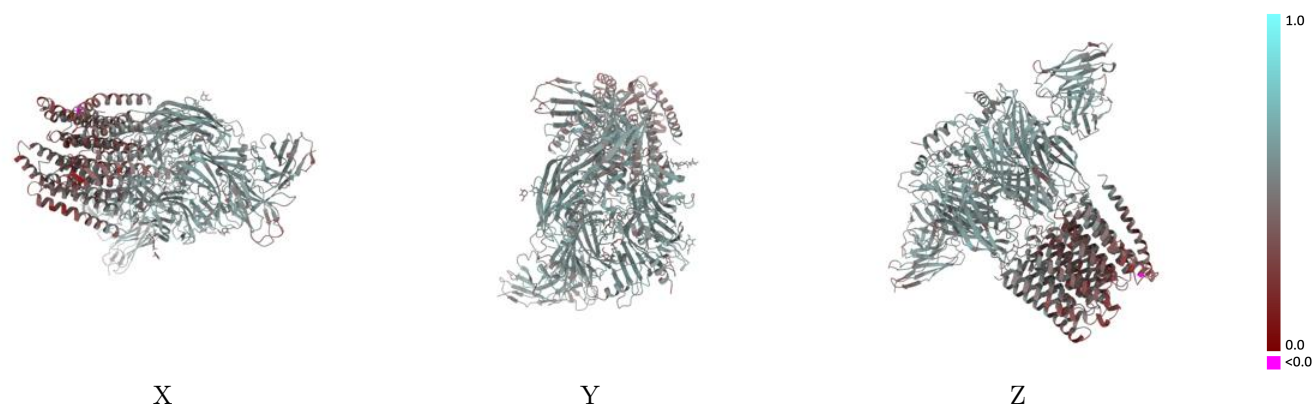
This section contains information regarding the fit between EMDB map EMD-22037 and PDB model 6X3Z. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



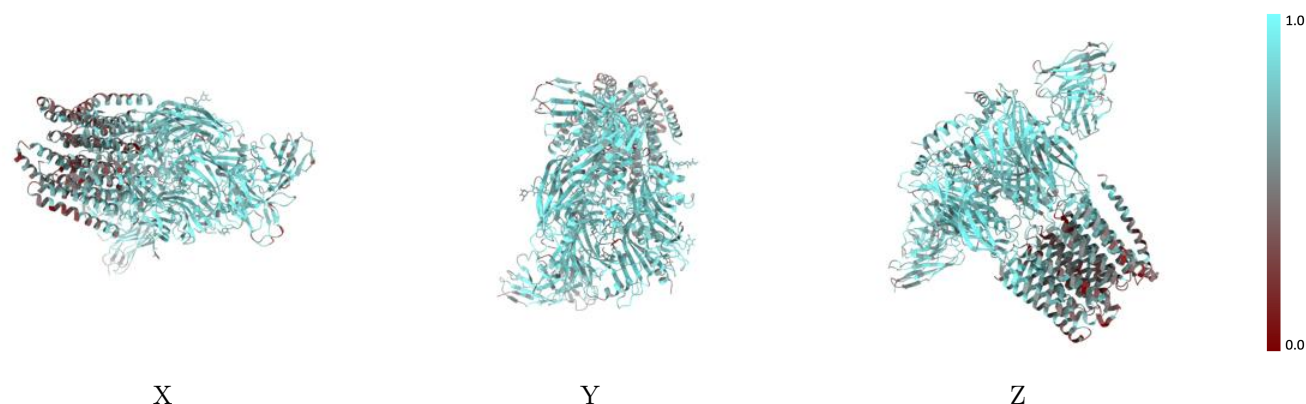
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



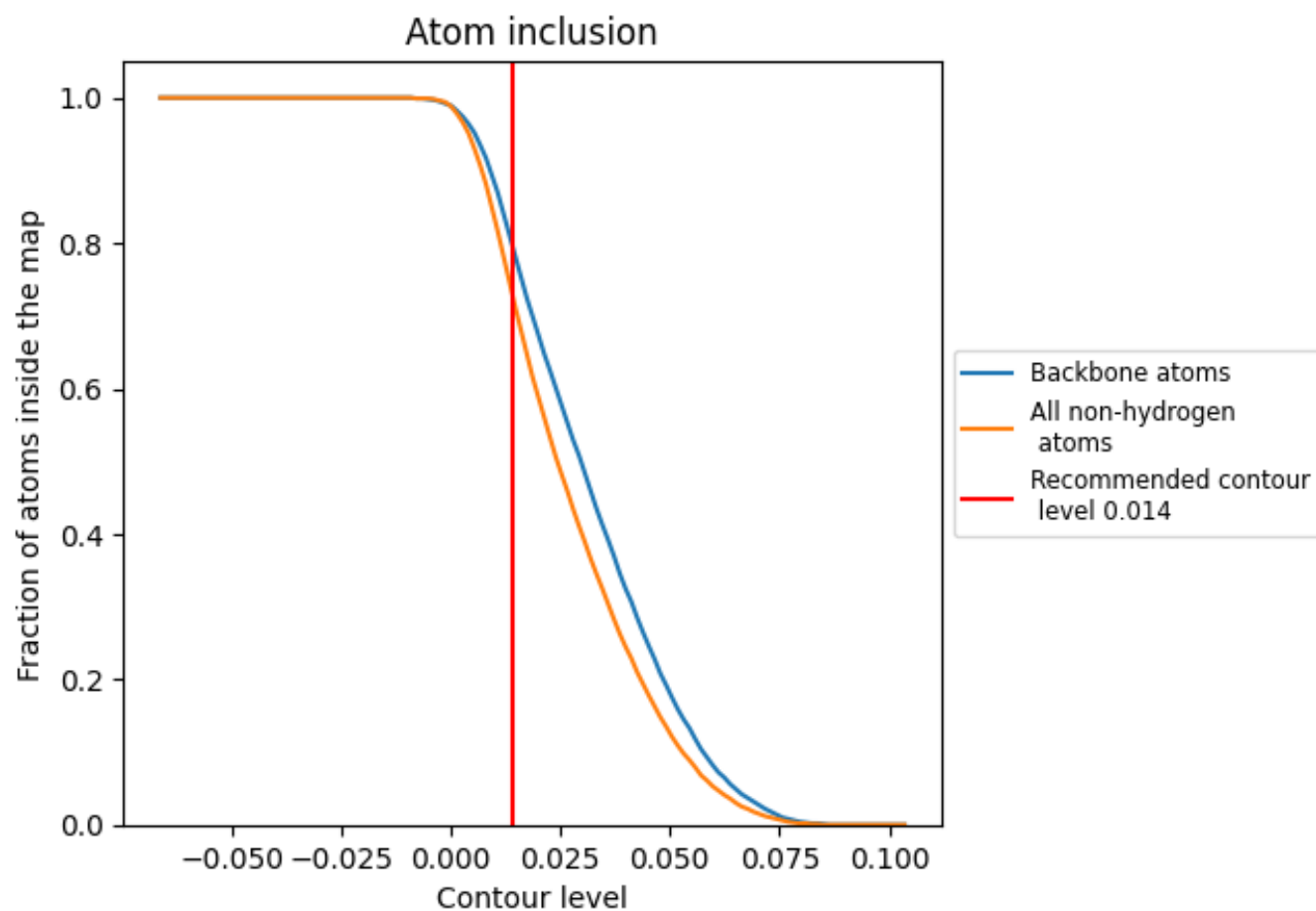
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 0.4970
A	 0.7100	 0.4830
B	 0.7260	 0.4960
C	 0.7260	 0.4990
D	 0.7510	 0.5070
E	 0.7320	 0.4880
F	 0.7440	 0.4790
G	 0.6120	 0.4640
H	 0.6410	 0.3970
I	 0.7400	 0.5070
J	 0.7350	 0.5050
K	 0.7550	 0.5140
L	 0.7360	 0.5080
M	 0.4640	 0.3850

