



wwPDB EM Validation Summary Report ⓘ

Feb 21, 2022 – 07:14 pm GMT

PDB ID : 7PBZ
EMDB ID : EMD-13314
Title : a1b3 GABA-A receptor + GABA + Zn2+
Authors : Miller, P.S.; Kasaragod, V.B.
Deposited on : 2021-08-03
Resolution : 2.79 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

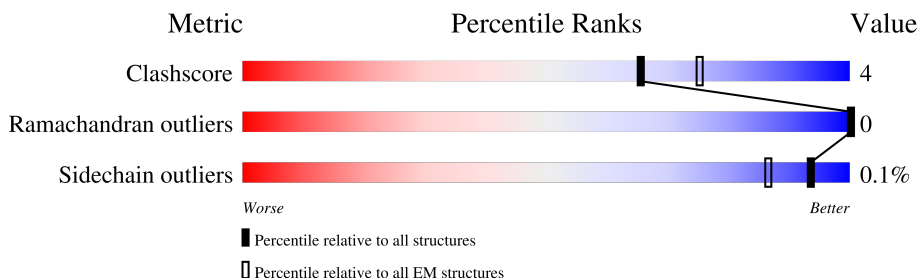
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	F	522	
2	A	368	
3	B	451	
3	C	451	
3	E	451	
4	D	411	
5	G	2	
5	I	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	K	2	
6	H	4	
7	J	5	
7	L	5	

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
12	ABU	B	501	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 14822 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 Megabody 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	113	Total	C	N	O	S	0	0
			893	563	153	173	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	334	Total	C	N	O	S	0	0
			2695	1745	452	482	16		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLN	-	expression tag	UNP P14867
A	3	PRO	-	expression tag	UNP P14867
A	4	SER	-	expression tag	UNP P14867
A	313	SER	-	linker	UNP P14867
A	314	GLN	-	linker	UNP P14867
A	315	PRO	-	linker	UNP P14867
A	316	ALA	-	linker	UNP P14867
A	317	ARG	-	linker	UNP P14867
A	318	ALA	-	linker	UNP P14867
A	319	ALA	-	linker	UNP P14867
A	430	GLY	-	expression tag	UNP P14867
A	431	THR	-	expression tag	UNP P14867
A	432	THR	-	expression tag	UNP P14867
A	433	GLU	-	expression tag	UNP P14867
A	434	SER	-	expression tag	UNP P14867
A	435	THR	-	expression tag	UNP P14867
A	436	GLN	-	expression tag	UNP P14867
A	437	VAL	-	expression tag	UNP P14867
A	438	ALA	-	expression tag	UNP P14867
A	439	PRO	-	expression tag	UNP P14867
A	440	ALA	-	expression tag	UNP P14867

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	330	Total	C	N	O	S	0	0
			2707	1774	442	475	16		
3	C	330	Total	C	N	O	S	0	0
			2707	1774	442	475	16		
3	E	330	Total	C	N	O	S	0	0
			2707	1774	442	475	16		

There are 351 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	308	SER	-	linker	UNP P28472
B	308A	GLN	-	linker	UNP P28472
B	308B	PRO	-	linker	UNP P28472
B	308C	ALA	-	linker	UNP P28472
B	308D	GLY	-	linker	UNP P28472
B	308E	THR	-	linker	UNP P28472
B	308F	ALA	-	linker	UNP P28472
B	308G	ASP	-	linker	UNP P28472
B	308H	LEU	-	linker	UNP P28472
B	308I	GLU	-	linker	UNP P28472
B	308J	ASP	-	linker	UNP P28472
B	308K	ASN	-	linker	UNP P28472
B	308L	TRP	-	linker	UNP P28472
B	308M	GLU	-	linker	UNP P28472
B	308N	THR	-	linker	UNP P28472
B	308O	LEU	-	linker	UNP P28472
B	308P	ASN	-	linker	UNP P28472
B	308Q	ASP	-	linker	UNP P28472
B	308R	ASN	-	linker	UNP P28472
B	308S	LEU	-	linker	UNP P28472
B	308T	LYS	-	linker	UNP P28472
B	308U	VAL	-	linker	UNP P28472
B	308V	ILE	-	linker	UNP P28472
B	308W	GLU	-	linker	UNP P28472
B	308X	LYS	-	linker	UNP P28472
B	308Y	ALA	-	linker	UNP P28472
B	308Z	ASP	-	linker	UNP P28472
B	309A	ASN	-	linker	UNP P28472
B	309B	ALA	-	linker	UNP P28472
B	309C	ALA	-	linker	UNP P28472
B	309D	GLN	-	linker	UNP P28472
B	309E	VAL	-	linker	UNP P28472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	309F	LYS	-	linker	UNP P28472
B	309G	ASP	-	linker	UNP P28472
B	309H	ALA	-	linker	UNP P28472
B	309I	LEU	-	linker	UNP P28472
B	309J	THR	-	linker	UNP P28472
B	309K	LYS	-	linker	UNP P28472
B	309L	MET	-	linker	UNP P28472
B	309M	ARG	-	linker	UNP P28472
B	309N	ALA	-	linker	UNP P28472
B	309O	ALA	-	linker	UNP P28472
B	309P	ALA	-	linker	UNP P28472
B	309Q	LEU	-	linker	UNP P28472
B	309R	ASP	-	linker	UNP P28472
B	309S	ALA	-	linker	UNP P28472
B	309T	GLN	-	linker	UNP P28472
B	309U	LYS	-	linker	UNP P28472
B	309V	ALA	-	linker	UNP P28472
B	309W	THR	-	linker	UNP P28472
B	309X	PRO	-	linker	UNP P28472
B	309Y	PRO	-	linker	UNP P28472
B	309Z	LYS	-	linker	UNP P28472
B	310A	LEU	-	linker	UNP P28472
B	310B	GLU	-	linker	UNP P28472
B	310C	ASP	-	linker	UNP P28472
B	310D	LYS	-	linker	UNP P28472
B	310E	SER	-	linker	UNP P28472
B	310F	PRO	-	linker	UNP P28472
B	310G	ASP	-	linker	UNP P28472
B	310H	SER	-	linker	UNP P28472
B	310I	PRO	-	linker	UNP P28472
B	310J	GLU	-	linker	UNP P28472
B	310K	MET	-	linker	UNP P28472
B	310L	LYS	-	linker	UNP P28472
B	310M	ASP	-	linker	UNP P28472
B	310N	PHE	-	linker	UNP P28472
B	310O	ARG	-	linker	UNP P28472
B	310P	HIS	-	linker	UNP P28472
B	310Q	GLY	-	linker	UNP P28472
B	310R	PHE	-	linker	UNP P28472
B	310S	ASP	-	linker	UNP P28472
B	310T	ILE	-	linker	UNP P28472
B	310U	LEU	-	linker	UNP P28472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	310V	VAL	-	linker	UNP P28472
B	310W	GLY	-	linker	UNP P28472
B	310X	GLN	-	linker	UNP P28472
B	310Y	ILE	-	linker	UNP P28472
B	310Z	ASP	-	linker	UNP P28472
B	311A	ASP	-	linker	UNP P28472
B	311B	ALA	-	linker	UNP P28472
B	311C	LEU	-	linker	UNP P28472
B	311D	LYS	-	linker	UNP P28472
B	311E	LEU	-	linker	UNP P28472
B	311F	ALA	-	linker	UNP P28472
B	311G	ASN	-	linker	UNP P28472
B	311H	GLU	-	linker	UNP P28472
B	311I	GLY	-	linker	UNP P28472
B	311J	LYS	-	linker	UNP P28472
B	311K	VAL	-	linker	UNP P28472
B	311L	LYS	-	linker	UNP P28472
B	311M	GLU	-	linker	UNP P28472
B	311N	ALA	-	linker	UNP P28472
B	311O	GLN	-	linker	UNP P28472
B	311P	ALA	-	linker	UNP P28472
B	311Q	ALA	-	linker	UNP P28472
B	311R	ALA	-	linker	UNP P28472
B	311S	GLU	-	linker	UNP P28472
B	311T	GLN	-	linker	UNP P28472
B	311U	LEU	-	linker	UNP P28472
B	311V	LYS	-	linker	UNP P28472
B	311W	THR	-	linker	UNP P28472
B	311X	THR	-	linker	UNP P28472
B	311Y	ARG	-	linker	UNP P28472
B	311Z	ASN	-	linker	UNP P28472
B	312A	ALA	-	linker	UNP P28472
B	312B	TYR	-	linker	UNP P28472
B	312C	ILE	-	linker	UNP P28472
B	312D	GLN	-	linker	UNP P28472
B	312E	LYS	-	linker	UNP P28472
B	312F	TYR	-	linker	UNP P28472
B	312G	LEU	-	linker	UNP P28472
B	312H	THR	-	linker	UNP P28472
B	312I	GLY	-	linker	UNP P28472
B	419	ARG	-	linker	UNP P28472
B	420	ALA	-	linker	UNP P28472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	421	ALA	-	linker	UNP P28472
C	308	SER	-	linker	UNP P28472
C	308A	GLN	-	linker	UNP P28472
C	308B	PRO	-	linker	UNP P28472
C	308C	ALA	-	linker	UNP P28472
C	308D	GLY	-	linker	UNP P28472
C	308E	THR	-	linker	UNP P28472
C	308F	ALA	-	linker	UNP P28472
C	308G	ASP	-	linker	UNP P28472
C	308H	LEU	-	linker	UNP P28472
C	308I	GLU	-	linker	UNP P28472
C	308J	ASP	-	linker	UNP P28472
C	308K	ASN	-	linker	UNP P28472
C	308L	TRP	-	linker	UNP P28472
C	308M	GLU	-	linker	UNP P28472
C	308N	THR	-	linker	UNP P28472
C	308O	LEU	-	linker	UNP P28472
C	308P	ASN	-	linker	UNP P28472
C	308Q	ASP	-	linker	UNP P28472
C	308R	ASN	-	linker	UNP P28472
C	308S	LEU	-	linker	UNP P28472
C	308T	LYS	-	linker	UNP P28472
C	308U	VAL	-	linker	UNP P28472
C	308V	ILE	-	linker	UNP P28472
C	308W	GLU	-	linker	UNP P28472
C	308X	LYS	-	linker	UNP P28472
C	308Y	ALA	-	linker	UNP P28472
C	308Z	ASP	-	linker	UNP P28472
C	309A	ASN	-	linker	UNP P28472
C	309B	ALA	-	linker	UNP P28472
C	309C	ALA	-	linker	UNP P28472
C	309D	GLN	-	linker	UNP P28472
C	309E	VAL	-	linker	UNP P28472
C	309F	LYS	-	linker	UNP P28472
C	309G	ASP	-	linker	UNP P28472
C	309H	ALA	-	linker	UNP P28472
C	309I	LEU	-	linker	UNP P28472
C	309J	THR	-	linker	UNP P28472
C	309K	LYS	-	linker	UNP P28472
C	309L	MET	-	linker	UNP P28472
C	309M	ARG	-	linker	UNP P28472
C	309N	ALA	-	linker	UNP P28472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	309O	ALA	-	linker	UNP P28472
C	309P	ALA	-	linker	UNP P28472
C	309Q	LEU	-	linker	UNP P28472
C	309R	ASP	-	linker	UNP P28472
C	309S	ALA	-	linker	UNP P28472
C	309T	GLN	-	linker	UNP P28472
C	309U	LYS	-	linker	UNP P28472
C	309V	ALA	-	linker	UNP P28472
C	309W	THR	-	linker	UNP P28472
C	309X	PRO	-	linker	UNP P28472
C	309Y	PRO	-	linker	UNP P28472
C	309Z	LYS	-	linker	UNP P28472
C	310A	LEU	-	linker	UNP P28472
C	310B	GLU	-	linker	UNP P28472
C	310C	ASP	-	linker	UNP P28472
C	310D	LYS	-	linker	UNP P28472
C	310E	SER	-	linker	UNP P28472
C	310F	PRO	-	linker	UNP P28472
C	310G	ASP	-	linker	UNP P28472
C	310H	SER	-	linker	UNP P28472
C	310I	PRO	-	linker	UNP P28472
C	310J	GLU	-	linker	UNP P28472
C	310K	MET	-	linker	UNP P28472
C	310L	LYS	-	linker	UNP P28472
C	310M	ASP	-	linker	UNP P28472
C	310N	PHE	-	linker	UNP P28472
C	310O	ARG	-	linker	UNP P28472
C	310P	HIS	-	linker	UNP P28472
C	310Q	GLY	-	linker	UNP P28472
C	310R	PHE	-	linker	UNP P28472
C	310S	ASP	-	linker	UNP P28472
C	310T	ILE	-	linker	UNP P28472
C	310U	LEU	-	linker	UNP P28472
C	310V	VAL	-	linker	UNP P28472
C	310W	GLY	-	linker	UNP P28472
C	310X	GLN	-	linker	UNP P28472
C	310Y	ILE	-	linker	UNP P28472
C	310Z	ASP	-	linker	UNP P28472
C	311A	ASP	-	linker	UNP P28472
C	311B	ALA	-	linker	UNP P28472
C	311C	LEU	-	linker	UNP P28472
C	311D	LYS	-	linker	UNP P28472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	311E	LEU	-	linker	UNP P28472
C	311F	ALA	-	linker	UNP P28472
C	311G	ASN	-	linker	UNP P28472
C	311H	GLU	-	linker	UNP P28472
C	311I	GLY	-	linker	UNP P28472
C	311J	LYS	-	linker	UNP P28472
C	311K	VAL	-	linker	UNP P28472
C	311L	LYS	-	linker	UNP P28472
C	311M	GLU	-	linker	UNP P28472
C	311N	ALA	-	linker	UNP P28472
C	311O	GLN	-	linker	UNP P28472
C	311P	ALA	-	linker	UNP P28472
C	311Q	ALA	-	linker	UNP P28472
C	311R	ALA	-	linker	UNP P28472
C	311S	GLU	-	linker	UNP P28472
C	311T	GLN	-	linker	UNP P28472
C	311U	LEU	-	linker	UNP P28472
C	311V	LYS	-	linker	UNP P28472
C	311W	THR	-	linker	UNP P28472
C	311X	THR	-	linker	UNP P28472
C	311Y	ARG	-	linker	UNP P28472
C	311Z	ASN	-	linker	UNP P28472
C	312A	ALA	-	linker	UNP P28472
C	312B	TYR	-	linker	UNP P28472
C	312C	ILE	-	linker	UNP P28472
C	312D	GLN	-	linker	UNP P28472
C	312E	LYS	-	linker	UNP P28472
C	312F	TYR	-	linker	UNP P28472
C	312G	LEU	-	linker	UNP P28472
C	312H	THR	-	linker	UNP P28472
C	312I	GLY	-	linker	UNP P28472
C	419	ARG	-	linker	UNP P28472
C	420	ALA	-	linker	UNP P28472
C	421	ALA	-	linker	UNP P28472
E	308	SER	-	linker	UNP P28472
E	309	GLN	-	linker	UNP P28472
E	310	PRO	-	linker	UNP P28472
E	311	ALA	-	linker	UNP P28472
E	312	GLY	-	linker	UNP P28472
E	313	THR	-	linker	UNP P28472
E	314	ALA	-	linker	UNP P28472
E	315	ASP	-	linker	UNP P28472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	316	LEU	-	linker	UNP P28472
E	317	GLU	-	linker	UNP P28472
E	318	ASP	-	linker	UNP P28472
E	319	ASN	-	linker	UNP P28472
E	320	TRP	-	linker	UNP P28472
E	321	GLU	-	linker	UNP P28472
E	322	THR	-	linker	UNP P28472
E	323	LEU	-	linker	UNP P28472
E	324	ASN	-	linker	UNP P28472
E	325	ASP	-	linker	UNP P28472
E	326	ASN	-	linker	UNP P28472
E	327	LEU	-	linker	UNP P28472
E	328	LYS	-	linker	UNP P28472
E	329	VAL	-	linker	UNP P28472
E	330	ILE	-	linker	UNP P28472
E	331	GLU	-	linker	UNP P28472
E	332	LYS	-	linker	UNP P28472
E	333	ALA	-	linker	UNP P28472
E	334	ASP	-	linker	UNP P28472
E	335	ASN	-	linker	UNP P28472
E	336	ALA	-	linker	UNP P28472
E	337	ALA	-	linker	UNP P28472
E	338	GLN	-	linker	UNP P28472
E	339	VAL	-	linker	UNP P28472
E	340	LYS	-	linker	UNP P28472
E	341	ASP	-	linker	UNP P28472
E	342	ALA	-	linker	UNP P28472
E	343	LEU	-	linker	UNP P28472
E	344	THR	-	linker	UNP P28472
E	345	LYS	-	linker	UNP P28472
E	346	MET	-	linker	UNP P28472
E	347	ARG	-	linker	UNP P28472
E	348	ALA	-	linker	UNP P28472
E	349	ALA	-	linker	UNP P28472
E	350	ALA	-	linker	UNP P28472
E	351	LEU	-	linker	UNP P28472
E	352	ASP	-	linker	UNP P28472
E	353	ALA	-	linker	UNP P28472
E	354	GLN	-	linker	UNP P28472
E	355	LYS	-	linker	UNP P28472
E	356	ALA	-	linker	UNP P28472
E	357	THR	-	linker	UNP P28472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	358	PRO	-	linker	UNP P28472
E	359	PRO	-	linker	UNP P28472
E	360	LYS	-	linker	UNP P28472
E	361	LEU	-	linker	UNP P28472
E	362	GLU	-	linker	UNP P28472
E	363	ASP	-	linker	UNP P28472
E	364	LYS	-	linker	UNP P28472
E	365	SER	-	linker	UNP P28472
E	366	PRO	-	linker	UNP P28472
E	367	ASP	-	linker	UNP P28472
E	368	SER	-	linker	UNP P28472
E	369	PRO	-	linker	UNP P28472
E	370	GLU	-	linker	UNP P28472
E	371	MET	-	linker	UNP P28472
E	372	LYS	-	linker	UNP P28472
E	373	ASP	-	linker	UNP P28472
E	374	PHE	-	linker	UNP P28472
E	375	ARG	-	linker	UNP P28472
E	376	HIS	-	linker	UNP P28472
E	377	GLY	-	linker	UNP P28472
E	378	PHE	-	linker	UNP P28472
E	379	ASP	-	linker	UNP P28472
E	380	ILE	-	linker	UNP P28472
E	381	LEU	-	linker	UNP P28472
E	382	VAL	-	linker	UNP P28472
E	383	GLY	-	linker	UNP P28472
E	384	GLN	-	linker	UNP P28472
E	385	ILE	-	linker	UNP P28472
E	386	ASP	-	linker	UNP P28472
E	387	ASP	-	linker	UNP P28472
E	388	ALA	-	linker	UNP P28472
E	389	LEU	-	linker	UNP P28472
E	390	LYS	-	linker	UNP P28472
E	391	LEU	-	linker	UNP P28472
E	392	ALA	-	linker	UNP P28472
E	393	ASN	-	linker	UNP P28472
E	394	GLU	-	linker	UNP P28472
E	395	GLY	-	linker	UNP P28472
E	396	LYS	-	linker	UNP P28472
E	397	VAL	-	linker	UNP P28472
E	398	LYS	-	linker	UNP P28472
E	399	GLU	-	linker	UNP P28472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	400	ALA	-	linker	UNP P28472
E	401	GLN	-	linker	UNP P28472
E	402	ALA	-	linker	UNP P28472
E	403	ALA	-	linker	UNP P28472
E	404	ALA	-	linker	UNP P28472
E	405	GLU	-	linker	UNP P28472
E	406	GLN	-	linker	UNP P28472
E	407	LEU	-	linker	UNP P28472
E	408	LYS	-	linker	UNP P28472
E	409	THR	-	linker	UNP P28472
E	410	THR	-	linker	UNP P28472
E	411	ARG	-	linker	UNP P28472
E	412	ASN	-	linker	UNP P28472
E	413	ALA	-	linker	UNP P28472
E	414	TYR	-	linker	UNP P28472
E	415	ILE	-	linker	UNP P28472
E	416	GLN	-	linker	UNP P28472
E	417	LYS	-	linker	UNP P28472
E	418	TYR	-	linker	UNP P28472
E	419	LEU	-	linker	UNP P28472
E	420	THR	-	linker	UNP P28472
E	421	GLY	-	linker	UNP P28472
E	422	ARG	-	linker	UNP P28472
E	423	ALA	-	linker	UNP P28472
E	424	ALA	-	linker	UNP P28472

- Molecule 4 is a protein called Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	336	Total	C	N	O	S	0	0
			2714	1755	458	485	16		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	MET	-	initiating methionine	UNP P14867
D	-51	ASP	-	expression tag	UNP P14867
D	-50	GLU	-	expression tag	UNP P14867
D	-49	LYS	-	expression tag	UNP P14867
D	-48	THR	-	expression tag	UNP P14867
D	-47	THR	-	expression tag	UNP P14867
D	-46	GLY	-	expression tag	UNP P14867

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-45	TRP	-	expression tag	UNP P14867
D	-44	ARG	-	expression tag	UNP P14867
D	-43	GLY	-	expression tag	UNP P14867
D	-42	GLY	-	expression tag	UNP P14867
D	-41	HIS	-	expression tag	UNP P14867
D	-40	VAL	-	expression tag	UNP P14867
D	-39	VAL	-	expression tag	UNP P14867
D	-38	GLU	-	expression tag	UNP P14867
D	-37	GLY	-	expression tag	UNP P14867
D	-36	LEU	-	expression tag	UNP P14867
D	-35	ALA	-	expression tag	UNP P14867
D	-34	GLY	-	expression tag	UNP P14867
D	-33	GLU	-	expression tag	UNP P14867
D	-32	LEU	-	expression tag	UNP P14867
D	-31	GLU	-	expression tag	UNP P14867
D	-30	GLN	-	expression tag	UNP P14867
D	-29	LEU	-	expression tag	UNP P14867
D	-28	ARG	-	expression tag	UNP P14867
D	-27	ALA	-	expression tag	UNP P14867
D	-26	ARG	-	expression tag	UNP P14867
D	-25	LEU	-	expression tag	UNP P14867
D	-24	GLU	-	expression tag	UNP P14867
D	-23	HIS	-	expression tag	UNP P14867
D	-22	HIS	-	expression tag	UNP P14867
D	-21	PRO	-	expression tag	UNP P14867
D	-20	GLN	-	expression tag	UNP P14867
D	-19	GLY	-	expression tag	UNP P14867
D	-18	GLN	-	expression tag	UNP P14867
D	-17	ARG	-	expression tag	UNP P14867
D	-16	GLU	-	expression tag	UNP P14867
D	-15	PRO	-	expression tag	UNP P14867
D	-14	ASP	-	expression tag	UNP P14867
D	-13	TYR	-	expression tag	UNP P14867
D	-12	ASP	-	expression tag	UNP P14867
D	-11	ILE	-	expression tag	UNP P14867
D	-10	PRO	-	expression tag	UNP P14867
D	-9	THR	-	expression tag	UNP P14867
D	-8	THR	-	expression tag	UNP P14867
D	-7	GLU	-	expression tag	UNP P14867
D	-6	ASN	-	expression tag	UNP P14867
D	-5	LEU	-	expression tag	UNP P14867
D	-4	TYR	-	expression tag	UNP P14867

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	PHE	-	expression tag	UNP P14867
D	-2	GLN	-	expression tag	UNP P14867
D	-1	GLY	-	expression tag	UNP P14867
D	0	THR	-	expression tag	UNP P14867
D	1	GLY	-	expression tag	UNP P14867
D	2	GLN	-	expression tag	UNP P14867
D	3	PRO	-	expression tag	UNP P14867
D	4	SER	-	expression tag	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 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



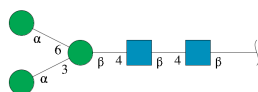
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called 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.



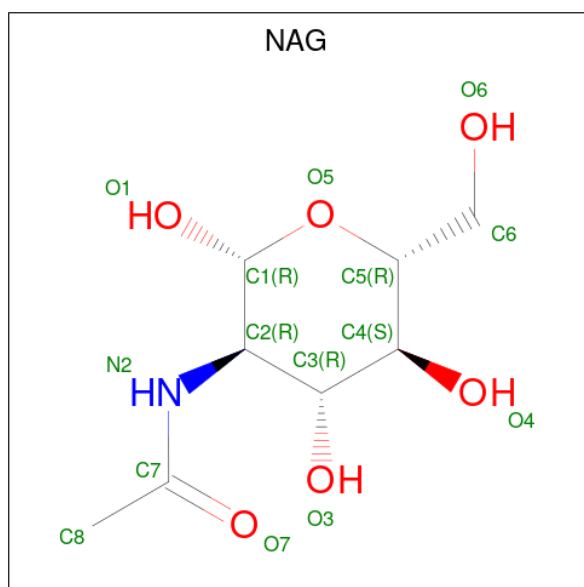
Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is an oligosaccharide called 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.



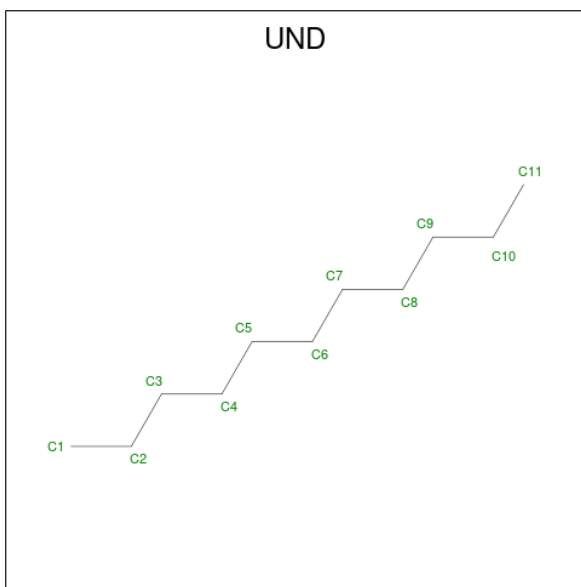
Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	5	Total	C	N	O	0	0
			61	34	2	25		
7	L	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



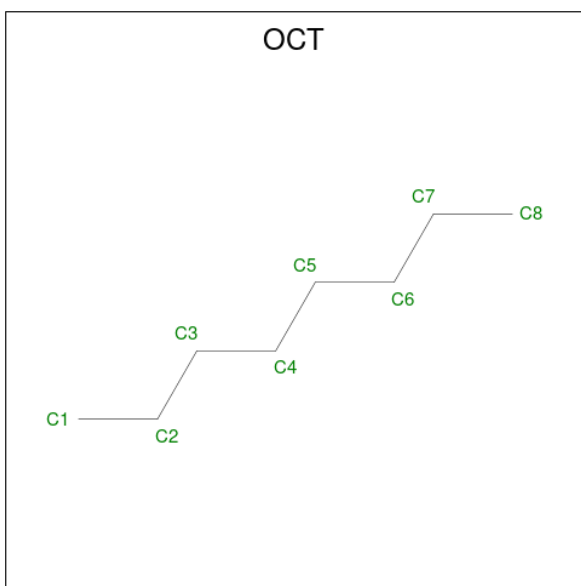
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).



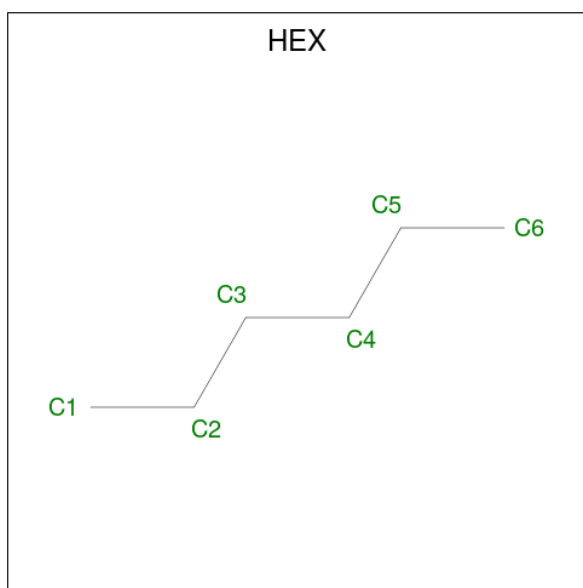
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	C	0
			22	22	
9	A	1	Total	C	0
			22	22	

- Molecule 10 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



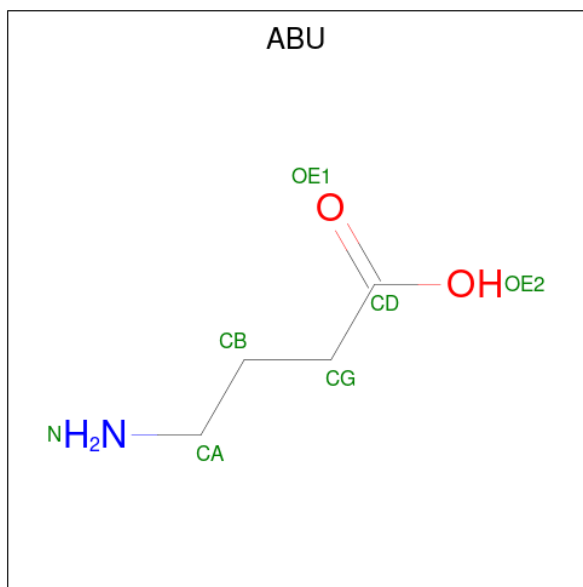
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	C	0
			16	16	
10	A	1	Total	C	0
			16	16	

- Molecule 11 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	C	0
			6	6	
11	B	1	Total	C	0
			6	6	
11	D	1	Total	C	0
			12	12	
11	D	1	Total	C	0
			12	12	

- Molecule 12 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).

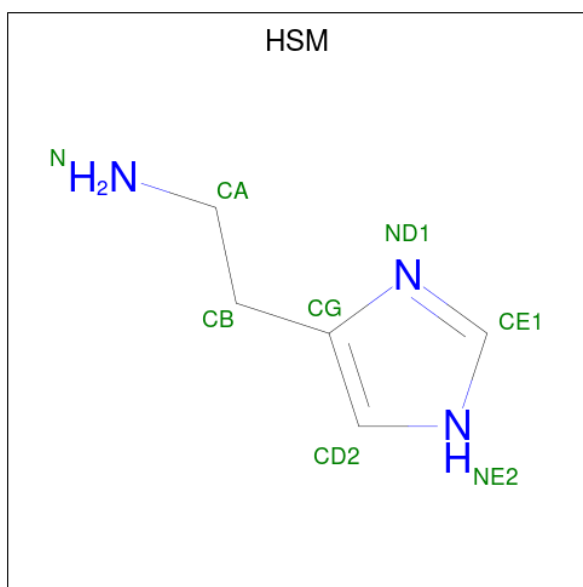


Mol	Chain	Residues	Atoms				AltConf
12	B	1	Total	C	N	O	0
			7	4	1	2	
12	E	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

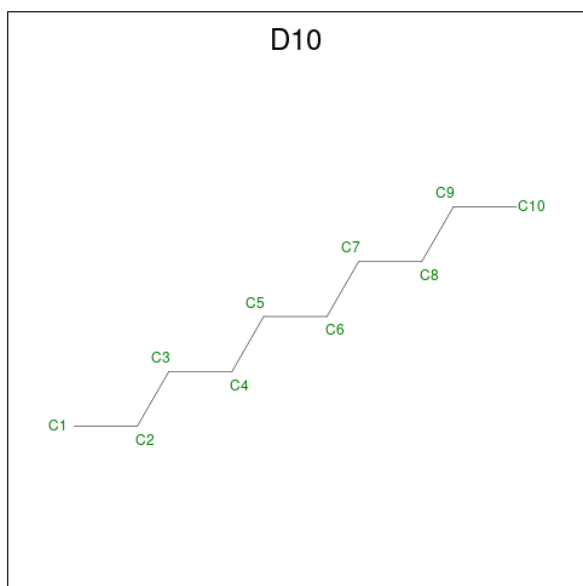
Mol	Chain	Residues	Atoms		AltConf
13	B	1	Total	Zn	0
			1	1	

- Molecule 14 is HISTAMINE (three-letter code: HSM) (formula: C₅H₉N₃).



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

- Molecule 15 is DECANE (three-letter code: D10) (formula: C₁₀H₂₂).

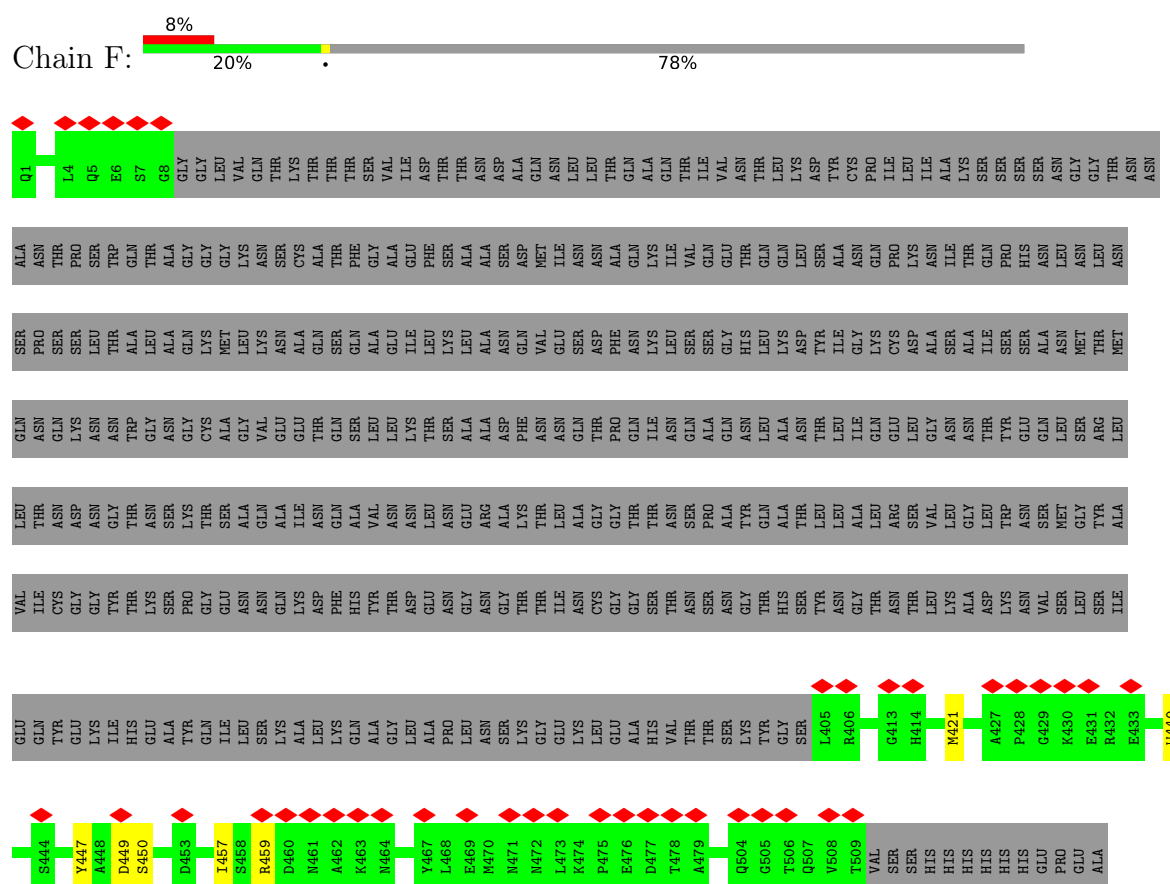


Mol	Chain	Residues	Atoms		AltConf
15	C	1	Total	C	0
			10	10	
15	D	1	Total	C	0
			20	20	
15	D	1	Total	C	0
			20	20	

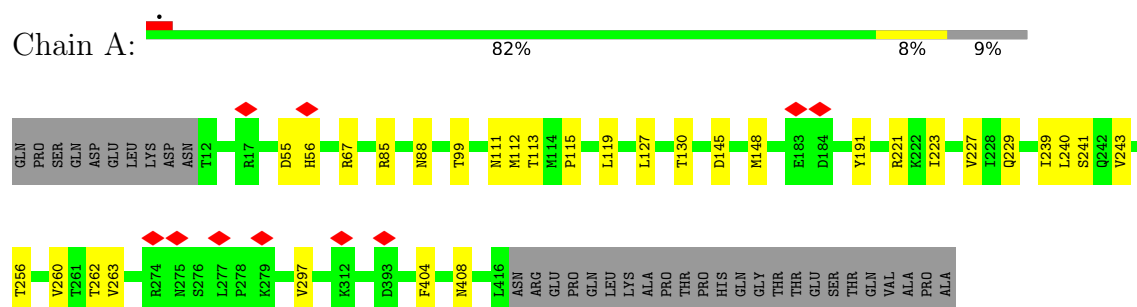
3 Residue-property plots

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: Megabody 25



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



Chain B:

Chain C:

Sequence logo for Chain C. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 300. A green bar at the top indicates the overall conservation level: 5% (red), 65% (green), 8% (yellow), and 27% (grey).

Key residues (positions and amino acids) are highlighted with red diamonds above the sequence:

- Position 1: Y220 (TYR)
- Position 2: L223 (LEU)
- Position 3: Q224 (GLN)
- Position 4: T230 (THR)
- Position 5: T233 (THR)
- Position 6: T234 (THR)
- Position 7: L235 (LEU)
- Position 8: S239 (SER)
- Position 9: N243 (ASN)
- Position 10: Y244 (TYR)
- Position 11: D245 (ASP)
- Position 12: L253 (LEU)
- Position 13: R269 (ARG)
- Position 14: E270 (GLU)
- Position 15: T271 (THR)
- Position 16: L272 (LEU)
- Position 17: P273 (PRO)
- Position 18: K274 (LYS)
- Position 19: I275 (ILE)
- Position 20: I281 (ILE)
- Position 21: M286 (MET)
- Position 22: L296 (LEU)
- Position 23: A300 (ALA)
- Position 24: F307 (PHE)
- Position 25: S308 (SER)
- Position 26: G139 (GLY)
- Position 27: E153 (GLU)
- Position 28: G158 (GLY)
- Position 29: V175 (VAL)
- Position 30: E179 (GLU)
- Position 31: R192 (ARG)
- Position 32: V198 (VAL)
- Position 33: R207 (ARG)
- Position 34: L208 (LEU)
- Position 35: S209 (SER)
- Position 36: L210 (LEU)
- Position 37: L210 (LEU)
- Position 38: L210 (LEU)
- Position 39: L210 (LEU)
- Position 40: L210 (LEU)
- Position 41: L210 (LEU)
- Position 42: L210 (LEU)
- Position 43: L210 (LEU)
- Position 44: L210 (LEU)
- Position 45: L210 (LEU)
- Position 46: L210 (LEU)
- Position 47: L210 (LEU)
- Position 48: L210 (LEU)
- Position 49: L210 (LEU)
- Position 50: L210 (LEU)
- Position 51: L210 (LEU)
- Position 52: L210 (LEU)
- Position 53: L210 (LEU)
- Position 54: L210 (LEU)
- Position 55: L210 (LEU)
- Position 56: L210 (LEU)
- Position 57: L210 (LEU)
- Position 58: L210 (LEU)
- Position 59: L210 (LEU)
- Position 60: L210 (LEU)
- Position 61: L210 (LEU)
- Position 62: L210 (LEU)
- Position 63: L210 (LEU)
- Position 64: L210 (LEU)
- Position 65: L210 (LEU)
- Position 66: L210 (LEU)
- Position 67: L210 (LEU)
- Position 68: L210 (LEU)
- Position 69: L210 (LEU)
- Position 70: L210 (LEU)
- Position 71: L210 (LEU)
- Position 72: L210 (LEU)
- Position 73: L210 (LEU)
- Position 74: L210 (LEU)
- Position 75: L210 (LEU)
- Position 76: L210 (LEU)
- Position 77: L210 (LEU)
- Position 78: L210 (LEU)
- Position 79: L210 (LEU)
- Position 80: L210 (LEU)
- Position 81: L210 (LEU)
- Position 82: L210 (LEU)
- Position 83: L210 (LEU)
- Position 84: L210 (LEU)
- Position 85: L210 (LEU)
- Position 86: L210 (LEU)
- Position 87: L210 (LEU)
- Position 88: L210 (LEU)
- Position 89: L210 (LEU)
- Position 90: L210 (LEU)
- Position 91: L210 (LEU)
- Position 92: L210 (LEU)
- Position 93: L210 (LEU)
- Position 94: L210 (LEU)
- Position 95: L210 (LEU)
- Position 96: L210 (LEU)
- Position 97: L210 (LEU)
- Position 98: L210 (LEU)
- Position 99: L210 (LEU)
- Position 100: L210 (LEU)
- Position 101: L210 (LEU)
- Position 102: L210 (LEU)
- Position 103: L210 (LEU)
- Position 104: L210 (LEU)
- Position 105: L210 (LEU)
- Position 106: L210 (LEU)
- Position 107: L210 (LEU)
- Position 108: L210 (LEU)
- Position 109: L210 (LEU)
- Position 110: L210 (LEU)
- Position 111: L210 (LEU)
- Position 112: L210 (LEU)
- Position 113: L210 (LEU)
- Position 114: L210 (LEU)
- Position 115: L210 (LEU)
- Position 116: L210 (LEU)
- Position 117: L210 (LEU)
- Position 118: L210 (LEU)
- Position 119: L210 (LEU)
- Position 120: L210 (LEU)
- Position 121: L210 (LEU)
- Position 122: L210 (LEU)
- Position 123: L210 (LEU)
- Position 124: L210 (LEU)
- Position 125: L210 (LEU)
- Position 126: L210 (LEU)
- Position 127: L210 (LEU)
- Position 128: L210 (LEU)
- Position 129: L210 (LEU)
- Position 130: L210 (LEU)
- Position 131: L210 (LEU)
- Position 132: L210 (LEU)
- Position 133: L210 (LEU)
- Position 134: L210 (LEU)
- Position 135: L210 (LEU)
- Position 136: L210 (LEU)
- Position 137: L210 (LEU)
- Position 138: L210 (LEU)
- Position 139: L210 (LEU)
- Position 140: L210 (LEU)
- Position 141: L210 (LEU)
- Position 142: L210 (LEU)
- Position 143: L210 (LEU)
- Position 144: L210 (LEU)
- Position 145: L210 (LEU)
- Position 146: L210 (LEU)
- Position 147: L210 (LEU)
- Position 148: L210 (LEU)
- Position 149: L210 (LEU)
- Position 150: L210 (LEU)
- Position 151: L210 (LEU)
- Position 152: L210 (LEU)
- Position 153: L210 (LEU)
- Position 154: L210 (LEU)
- Position 155: L210 (LEU)
- Position 156: L210 (LEU)
- Position 157: L210 (LEU)
- Position 158: L210 (LEU)
- Position 159: L210 (LEU)
- Position 160: L210 (LEU)
- Position 161: L210 (LEU)
- Position 162: L210 (LEU)
- Position 163: L210 (LEU)
- Position 164: L210 (LEU)
- Position 165: L210 (LEU)
- Position 166: L210 (LEU)
- Position 167: L210 (LEU)
- Position 168: L210 (LEU)
- Position 169: L210 (LEU)
- Position 170: L210 (LEU)
- Position 171: L210 (LEU)
- Position 172: L210 (LEU)
- Position 173: L210 (LEU)
- Position 174: L210 (LEU)
- Position 175: L210 (LEU)
- Position 176: L210 (LEU)
- Position 177: L210 (LEU)
- Position 178: L210 (LEU)
- Position 179: L210 (LEU)
- Position 180: L210 (LEU)
- Position 181: L210 (LEU)
- Position 182: L210 (LEU)
- Position 183: L210 (LEU)
- Position 184: L210 (LEU)
- Position 185: L210 (LEU)
- Position 186: L210 (LEU)
- Position 187: L210 (LEU)
- Position 188: L210 (LEU)
- Position 189: L210 (LEU)
- Position 190: L210 (LEU)
- Position 191: L210 (LEU)
- Position 192: L210 (LEU)
- Position 193: L210 (LEU)
- Position 194: L210 (LEU)
- Position 195: L210 (LEU)
- Position 196: L210 (LEU)
- Position 197: L210 (LEU)
- Position 198: L210 (LEU)
- Position 199: L210 (LEU)
- Position 200: L210 (LEU)
- Position 201: L210 (LEU)
- Position 202: L210 (LEU)
- Position 203: L210 (LEU)
- Position 204: L210 (LEU)
- Position 205: L210 (LEU)
- Position 206: L210 (LEU)
- Position 207: L210 (LEU)
- Position 208: L210 (LEU)
- Position 209: L210 (LEU)
- Position 210: L210 (LEU)
- Position 211: L210 (LEU)
- Position 212: L210 (LEU)
- Position 213: L210 (LEU)
- Position 214: L210 (LEU)
- Position 215: L210 (LEU)
- Position 216: L210 (LEU)
- Position 217: L210 (LEU)
- Position 218: L210 (LEU)
- Position 219: L210 (LEU)
- Position 220: L210 (LEU)
- Position 221: L210 (LEU)
- Position 222: L210 (LEU)
- Position 223: L210 (LEU)
- Position 2

Chain E:

66% 7% 27%

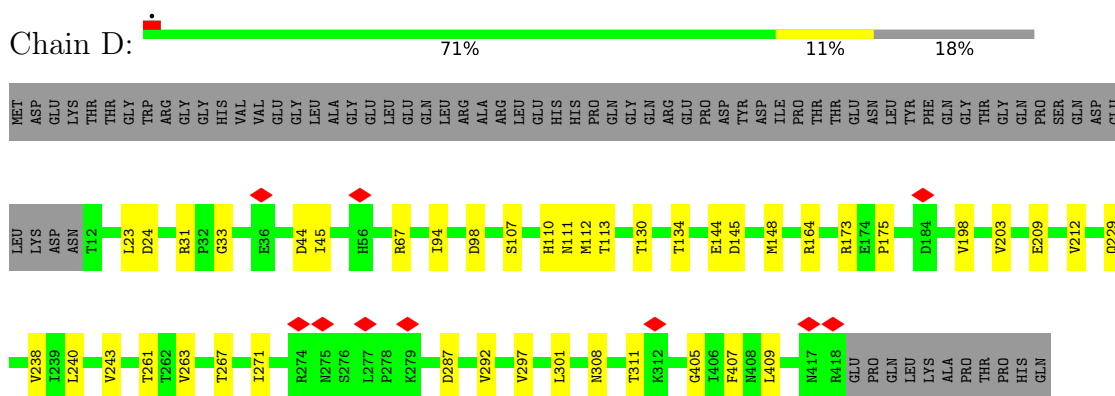
GLN SER VAL ASN ASP PRO GLY N8 I44 I47 D48 N80 L83 V87 A88 D89 T96 N100 H107 G108 V109 T110 V111 Y126 G127 L128 T131 C150 T151 E155 V178 E179 R180 I181 E190 H191 R192 R196 H197 V198 R207 R213

I222 I223 I255 R269 E270 T271 K274 F293 L296 L297 S308

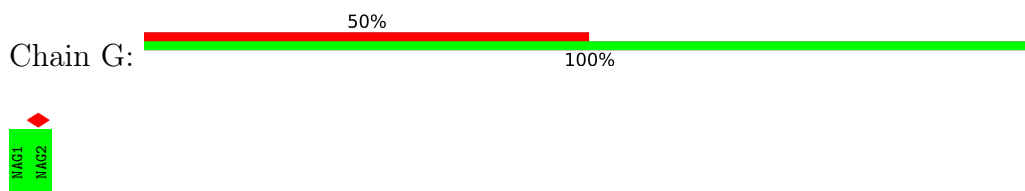
ASP ALA GLN LYS ALA THR PRO PRO PRO LYS LEU GLU ASP LYS SER PRO ASP SER PRO GLU MET LYS ASP PHE ARG HIS GLY PHE ILE LEU VAL GLY GLN ILE ASP ASP ALA LEU LYS LEU ALA ASN GLU GLY LYS VAL LYS GLU ALA GLN ALA ALA GLU GLN LEU LYS THR THR ARG

ASN ALA TYR ILE GLN LYS TYR LEU THR GLY R422 V450 ASN

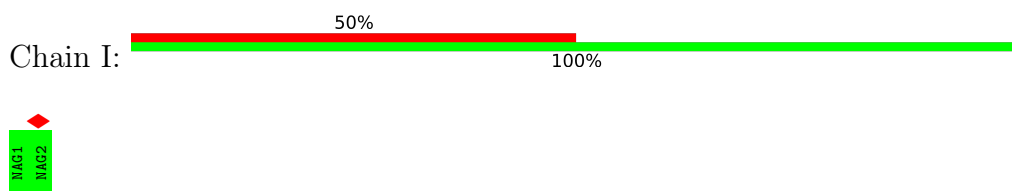
- Molecule 4: Gamma-aminobutyric acid receptor subunit alpha-1



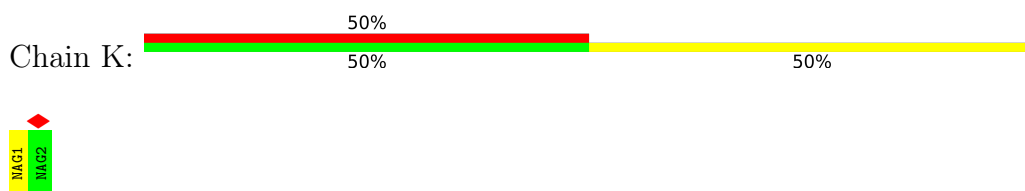
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



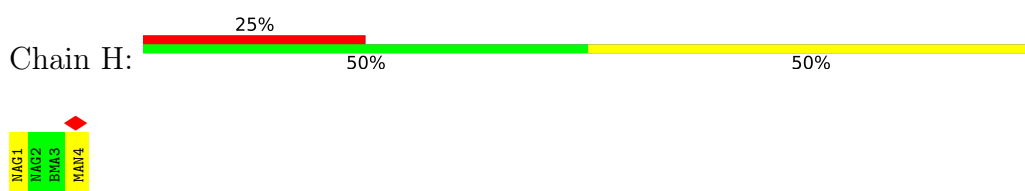
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

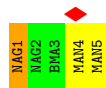


- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

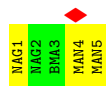


- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

nose



● Molecule 7: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92749	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 ($e^-/\text{\AA}^2$)	46.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.344	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0849	Depositor
Map size (Å)	339.04, 339.04, 339.04	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.652, 0.652, 0.652	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: ABU, UND, HSM, D10, BMA, NAG, HEX, OCT, MAN, ZN

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	F	0.29	0/916	0.59	0/1240
2	A	0.28	0/2764	0.57	0/3758
3	B	0.28	0/2779	0.58	0/3780
3	C	0.27	0/2779	0.57	0/3780
3	E	0.28	0/2779	0.59	1/3780 (0.0%)
4	D	0.27	0/2783	0.58	0/3783
All	All	0.28	0/14800	0.58	1/20121 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	150	CYS	CA-CB-SG	8.23	128.82	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	269	ARG	Sidechain

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	F	893	0	835	4	0
2	A	2695	0	2695	23	0
3	B	2707	0	2700	22	0
3	C	2707	0	2700	26	0
3	E	2707	0	2700	28	0
4	D	2714	0	2714	30	0
5	G	28	0	25	0	0
5	I	28	0	25	0	0
5	K	28	0	25	2	0
6	H	50	0	43	1	0
7	J	61	0	52	2	0
7	L	61	0	52	1	0
8	A	14	0	13	3	0
8	D	14	0	13	1	0
9	A	22	0	48	0	0
10	A	16	0	36	0	0
11	A	6	0	14	0	0
11	B	6	0	14	0	0
11	D	12	0	28	0	0
12	B	7	0	5	4	0
12	E	7	0	5	1	0
13	B	1	0	0	0	0
14	C	8	0	9	0	0
15	C	10	0	22	0	0
15	D	20	0	44	0	0
All	All	14822	0	14817	118	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.

The worst 5 of 118 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)
3:E:80:ASN:CG	5:K:1:NAG:C1	2.34	0.96
2:A:111:ASN:CG	8:A:501:NAG:C1	2.45	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:296:LEU:HD23	4:D:240:LEU:HD11	1.60	0.83
3:E:107:HIS:HE2	3:E:131:THR:HG1	1.32	0.77
3:C:243:ASN:ND2	3:C:245:ASP:OD2	2.21	0.74

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	109/522 (21%)	104 (95%)	5 (5%)	0	100	100
2	A	332/368 (90%)	326 (98%)	6 (2%)	0	100	100
3	B	326/451 (72%)	314 (96%)	12 (4%)	0	100	100
3	C	326/451 (72%)	315 (97%)	11 (3%)	0	100	100
3	E	326/451 (72%)	314 (96%)	12 (4%)	0	100	100
4	D	334/411 (81%)	329 (98%)	5 (2%)	0	100	100
All	All	1753/2654 (66%)	1702 (97%)	51 (3%)	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	F	92/430 (21%)	92 (100%)	0	100	100
2	A	296/326 (91%)	296 (100%)	0	100	100
3	B	295/393 (75%)	294 (100%)	1 (0%)	92	98
3	C	295/393 (75%)	295 (100%)	0	100	100
3	E	295/393 (75%)	295 (100%)	0	100	100
4	D	298/362 (82%)	298 (100%)	0	100	100
All	All	1571/2297 (68%)	1570 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	18	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	243	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 ⓘ

20 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
5	NAG	G	1	5,3	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	H	1	6,3	14,14,15	0.25	0	17,19,21	0.39	0
6	NAG	H	2	6	14,14,15	0.23	0	17,19,21	0.39	0
6	BMA	H	3	6	11,11,12	0.61	0	15,15,17	0.75	0
6	MAN	H	4	6	11,11,12	0.68	0	15,15,17	1.07	2 (13%)
5	NAG	I	1	5,3	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	I	2	5	14,14,15	0.21	0	17,19,21	0.45	0
7	NAG	J	1	7,3	14,14,15	0.28	0	17,19,21	1.42	2 (11%)
7	NAG	J	2	7	14,14,15	0.18	0	17,19,21	0.70	0
7	BMA	J	3	7	11,11,12	0.49	0	15,15,17	0.81	0
7	MAN	J	4	7	11,11,12	0.66	0	15,15,17	1.07	2 (13%)
7	MAN	J	5	7	11,11,12	0.99	1 (9%)	15,15,17	1.27	2 (13%)
5	NAG	K	1	5,3	14,14,15	0.30	0	17,19,21	0.53	0
5	NAG	K	2	5	14,14,15	0.21	0	17,19,21	0.46	0
7	NAG	L	1	7,3	14,14,15	0.25	0	17,19,21	0.41	0
7	NAG	L	2	7	14,14,15	0.19	0	17,19,21	0.42	0
7	BMA	L	3	7	11,11,12	0.57	0	15,15,17	0.77	0
7	MAN	L	4	7	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
7	MAN	L	5	7	11,11,12	0.67	0	15,15,17	1.06	2 (13%)

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	G	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
6	NAG	H	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	1/2/19/22	0/1/1/1
5	NAG	I	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
7	NAG	J	1	7,3	-	4/6/23/26	0/1/1/1
7	NAG	J	2	7	-	4/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
7	MAN	J	5	7	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	K	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
7	NAG	L	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	0/2/19/22	0/1/1/1
7	MAN	L	4	7	-	0/2/19/22	0/1/1/1
7	MAN	L	5	7	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	5	MAN	O5-C1	-2.39	1.39	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	1	NAG	C2-N2-C7	4.49	129.30	122.90
7	J	5	MAN	C1-O5-C5	3.20	116.53	112.19
7	J	1	NAG	C1-C2-N2	2.36	114.51	110.49
7	L	4	MAN	C1-O5-C5	2.30	115.31	112.19
7	L	5	MAN	C1-O5-C5	2.30	115.30	112.19

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

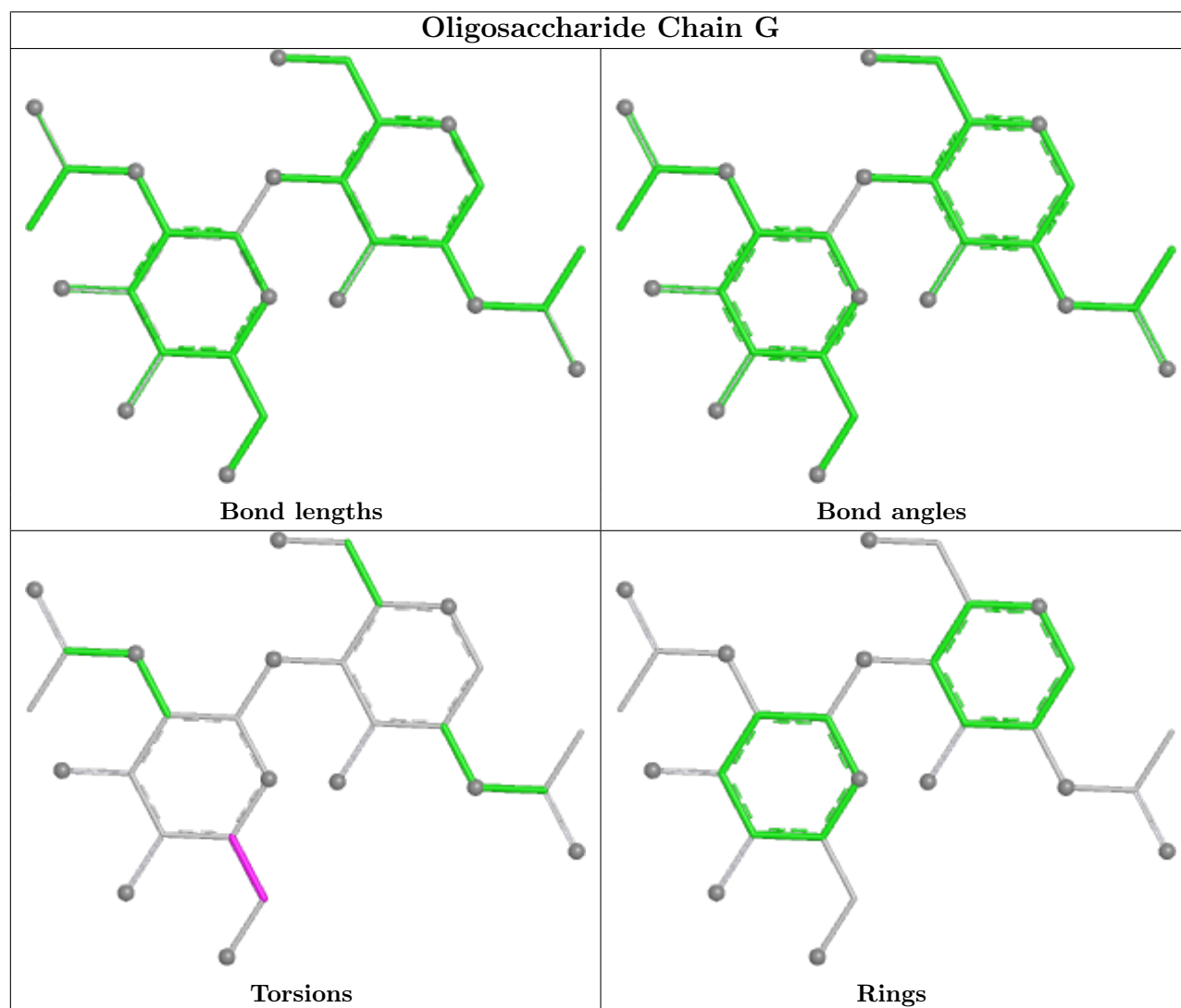
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2
7	J	2	NAG	C8-C7-N2-C2

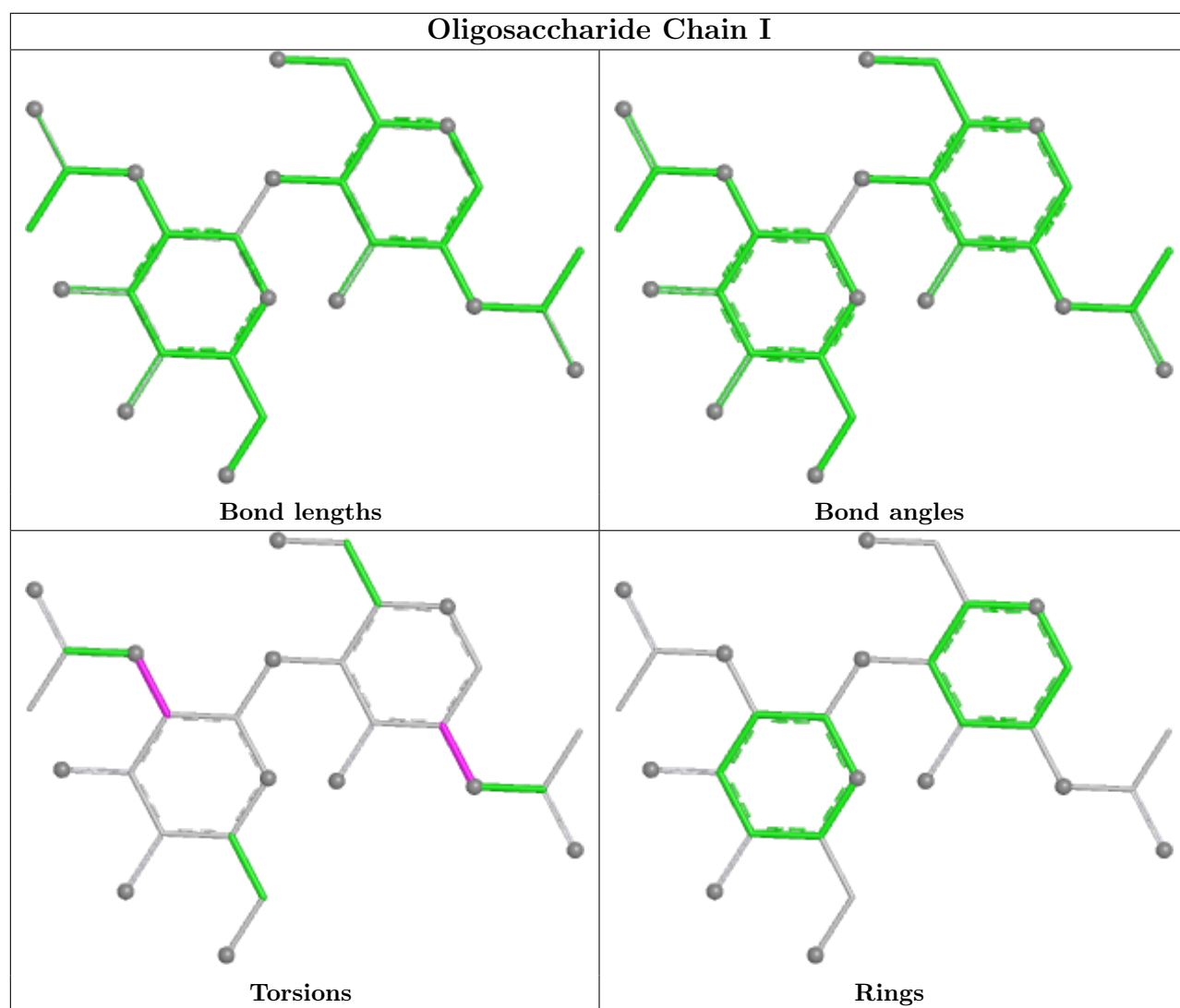
There are no ring outliers.

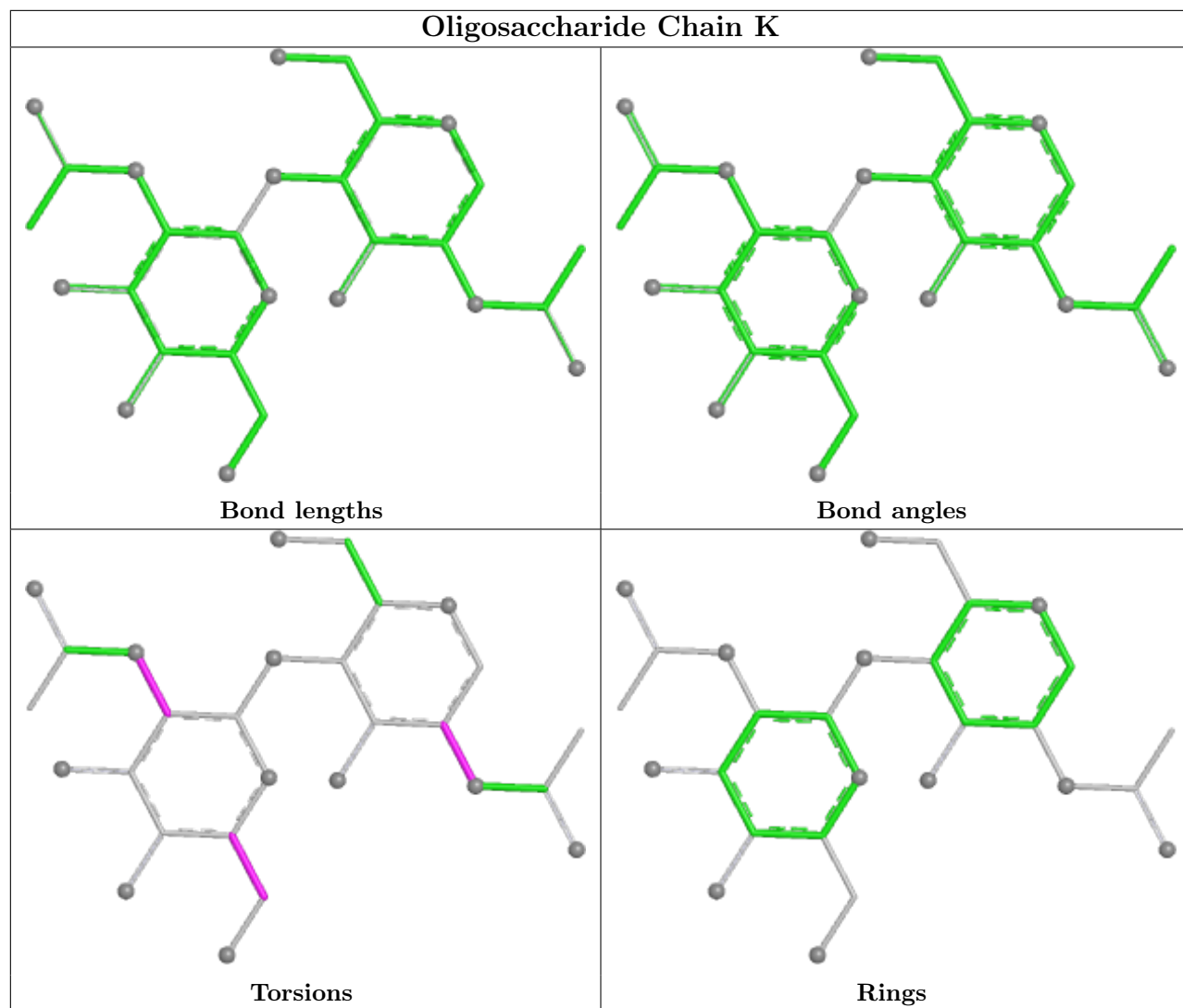
4 monomers are involved in 6 short contacts:

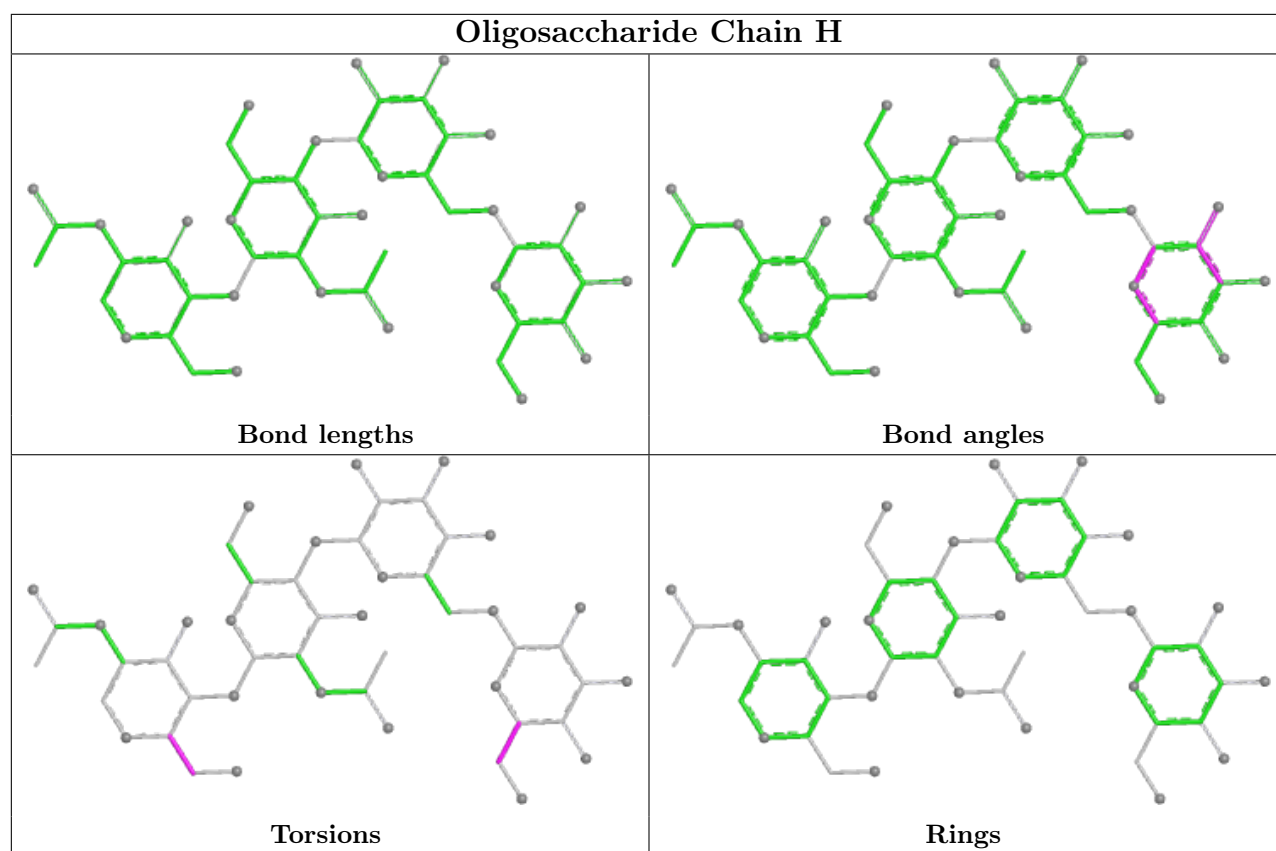
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	1	NAG	2	0
6	H	1	NAG	1	0
7	L	1	NAG	1	0
5	K	1	NAG	2	0

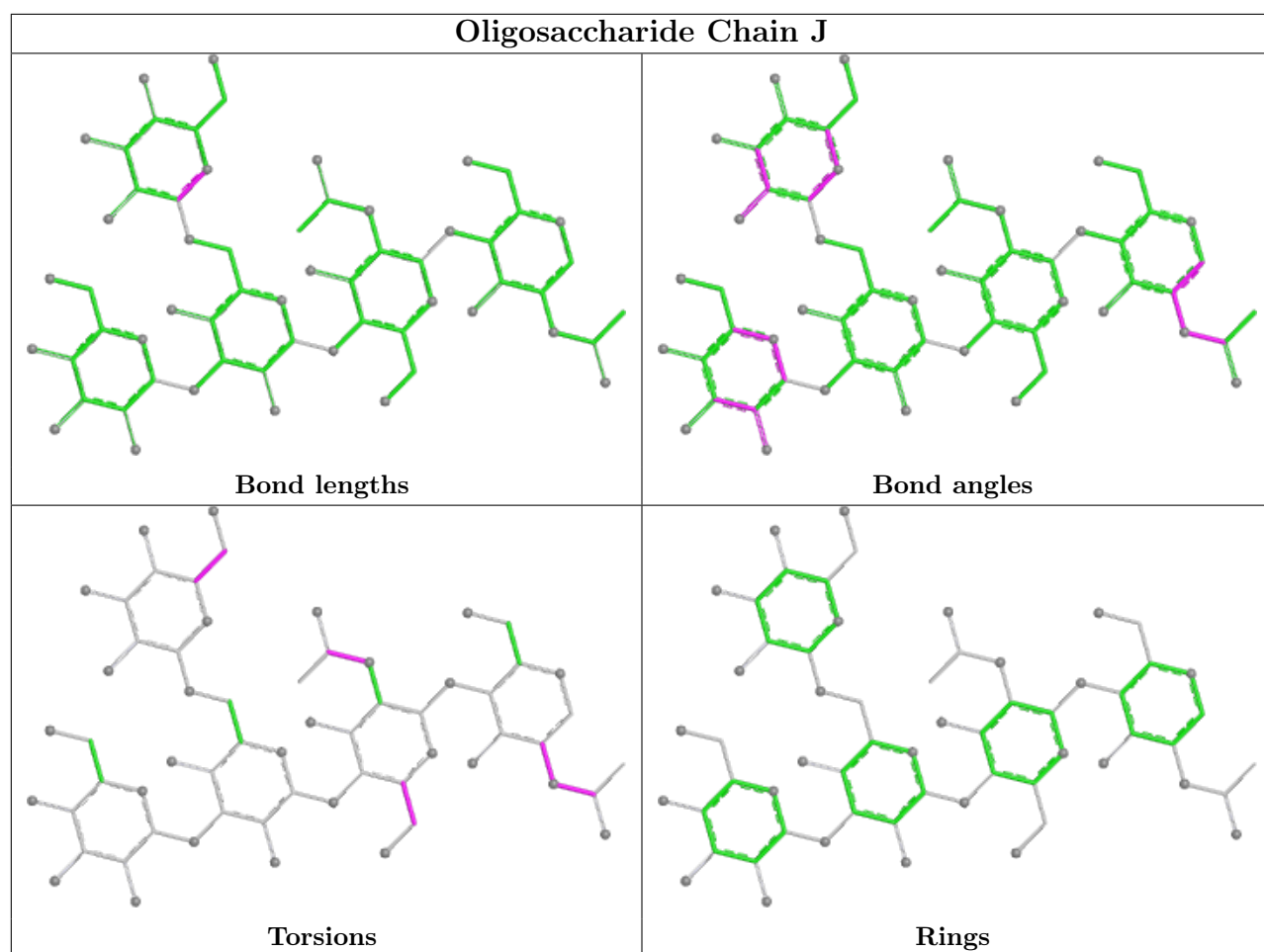
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

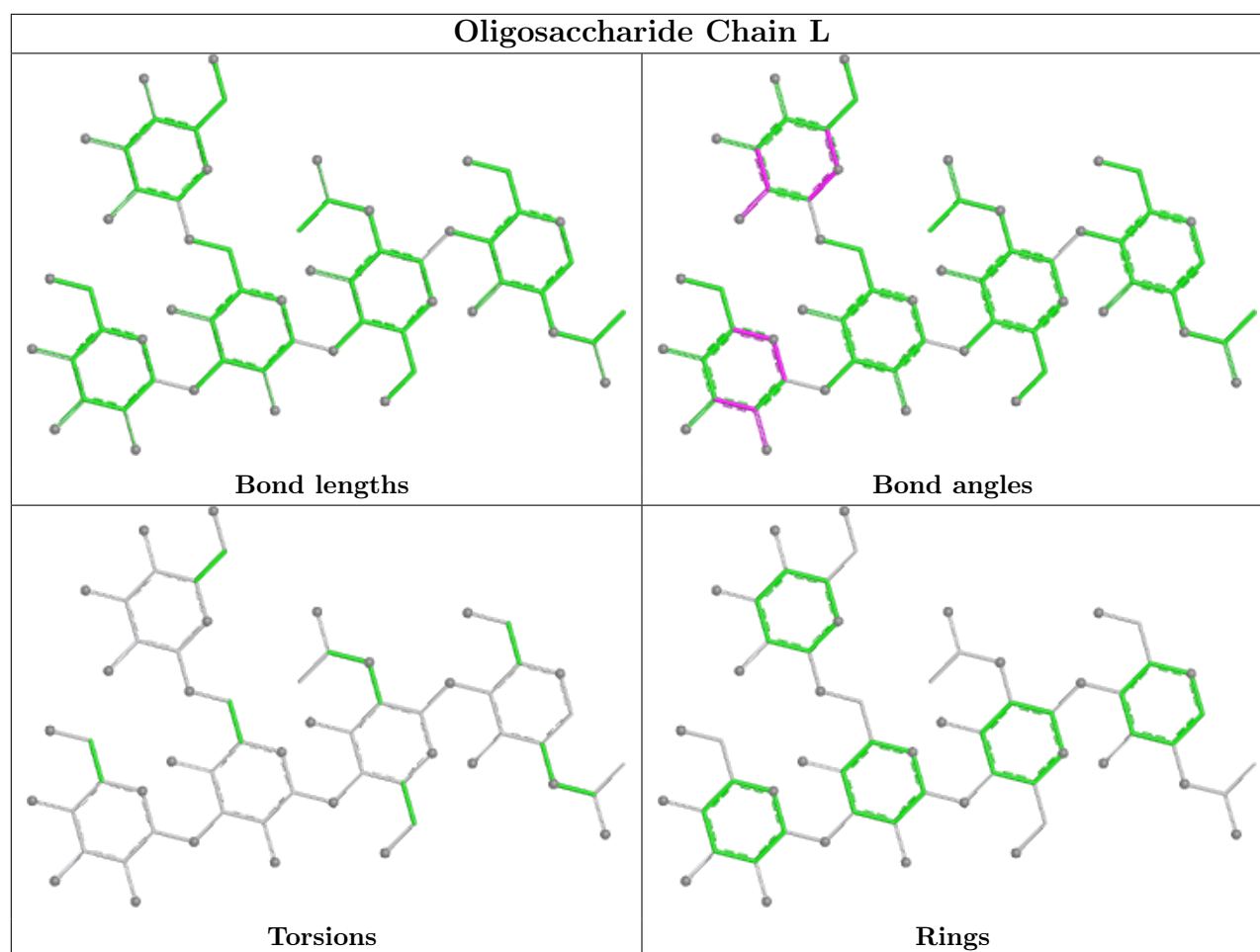












5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\# Z > 2$
10	OCT	A	503	-	7,7,7	0.31	0	6,6,6	0.70	0
10	OCT	A	505	-	7,7,7	0.30	0	6,6,6	0.71	0
12	ABU	B	501	-	3,6,6	0.21	0	2,6,6	0.89	0
11	HEX	D	502	-	5,5,5	0.31	0	4,4,4	0.57	0
8	NAG	D	501	4	14,14,15	0.21	0	17,19,21	0.42	0
11	HEX	A	506	-	5,5,5	0.31	0	4,4,4	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	D10	C	602	-	9,9,9	0.30	0	8,8,8	0.76	0
11	HEX	B	502	-	5,5,5	0.31	0	4,4,4	0.56	0
15	D10	D	505	-	9,9,9	0.29	0	8,8,8	0.79	0
14	HSM	C	601	-	3,8,8	0.92	0	3,9,9	0.91	0
15	D10	D	504	-	9,9,9	0.31	0	8,8,8	0.72	0
12	ABU	E	501	-	3,6,6	0.19	0	2,6,6	0.90	0
9	UND	A	502	-	10,10,10	0.30	0	9,9,9	0.78	0
8	NAG	A	501	2	14,14,15	0.22	0	17,19,21	0.46	0
9	UND	A	504	-	10,10,10	0.30	0	9,9,9	0.76	0
11	HEX	D	503	-	5,5,5	0.30	0	4,4,4	0.57	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	OCT	A	503	-	-	1/5/5/5	-
10	OCT	A	505	-	-	1/5/5/5	-
12	ABU	B	501	-	-	0/2/4/4	-
11	HEX	D	502	-	-	0/3/3/3	-
8	NAG	D	501	4	-	1/6/23/26	0/1/1/1
11	HEX	A	506	-	-	0/3/3/3	-
15	D10	C	602	-	-	1/7/7/7	-
11	HEX	B	502	-	-	0/3/3/3	-
15	D10	D	505	-	-	0/7/7/7	-
14	HSM	C	601	-	-	1/2/3/3	0/1/1/1
15	D10	D	504	-	-	0/7/7/7	-
12	ABU	E	501	-	-	1/2/4/4	-
9	UND	A	502	-	-	0/8/8/8	-
8	NAG	A	501	2	-	3/6/23/26	0/1/1/1
9	UND	A	504	-	-	1/8/8/8	-
11	HEX	D	503	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	504	UND	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

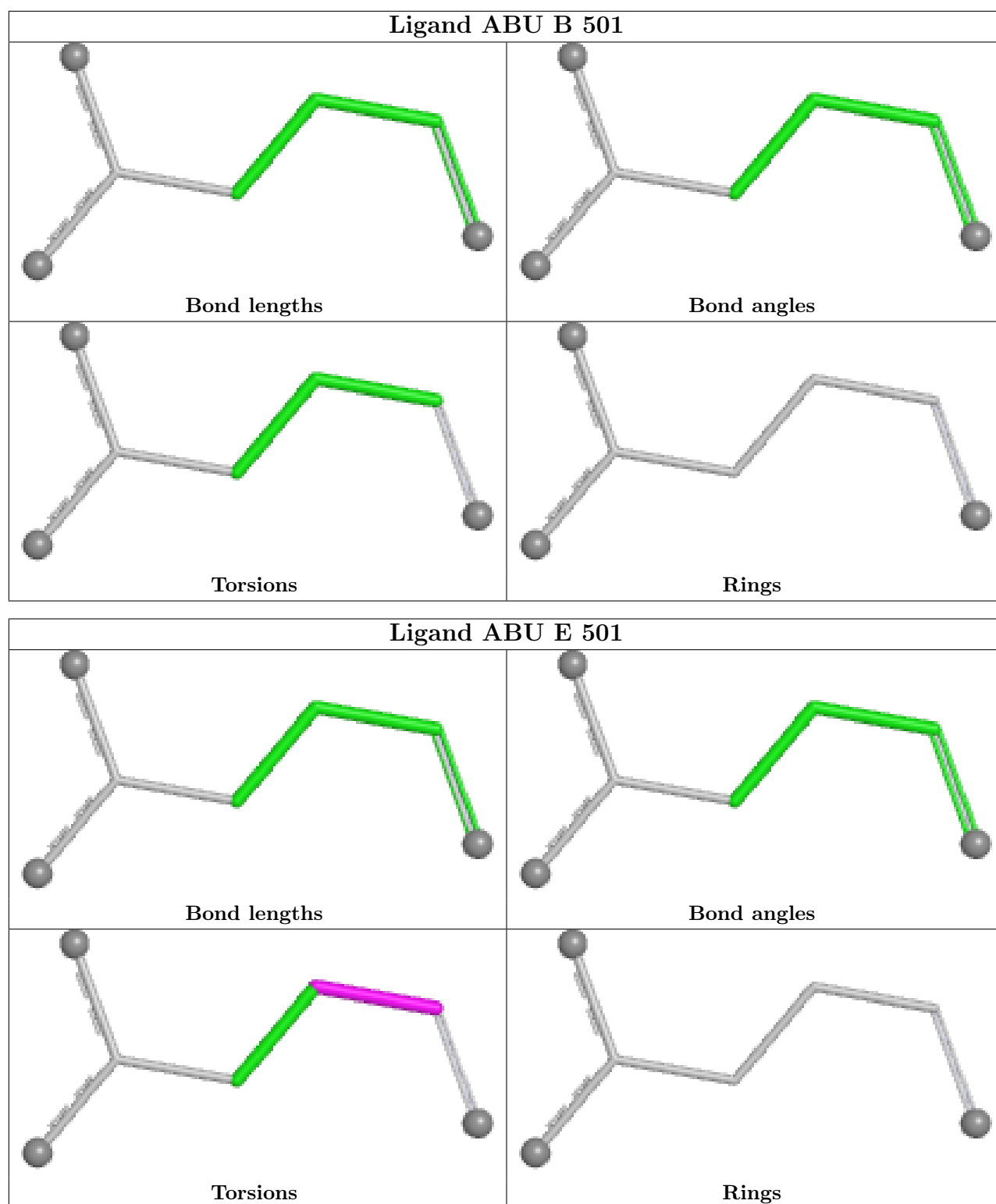
Mol	Chain	Res	Type	Atoms
15	C	602	D10	C4-C5-C6-C7
8	D	501	NAG	O5-C5-C6-O6
10	A	503	OCT	C2-C3-C4-C5
8	A	501	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	501	ABU	4	0
8	D	501	NAG	1	0
12	E	501	ABU	1	0
8	A	501	NAG	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

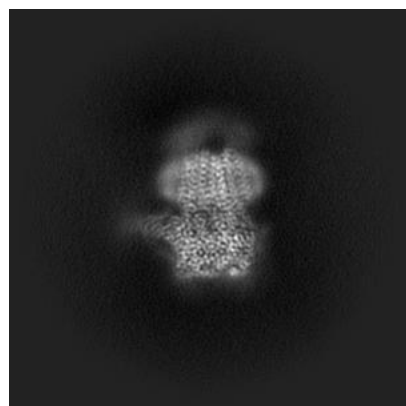
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13314. These allow visual inspection of the internal detail of the map and identification of artifacts.

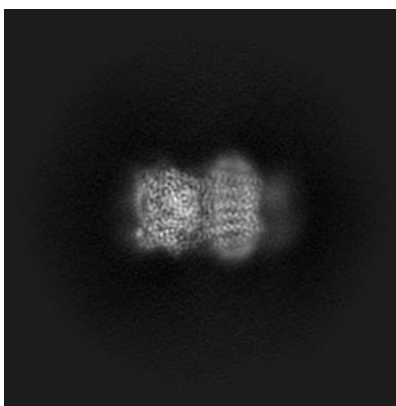
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

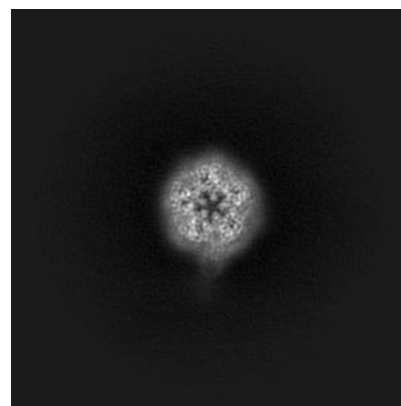
6.1.1 Primary map



X

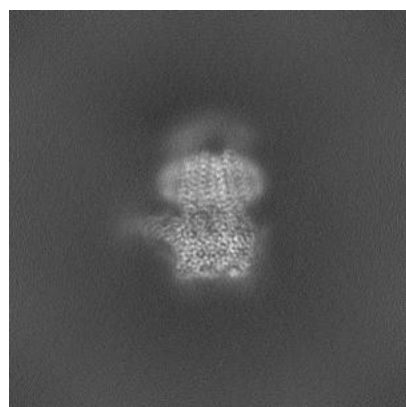


Y

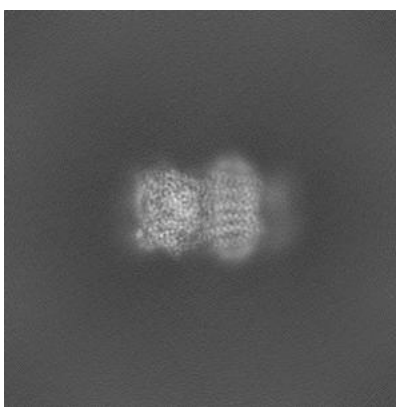


Z

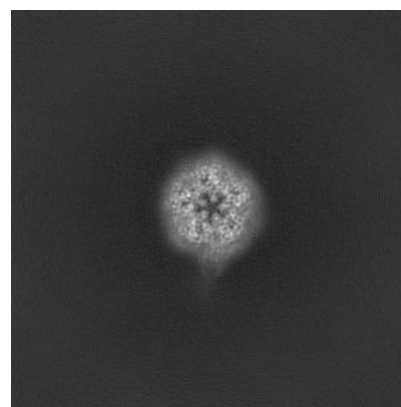
6.1.2 Raw map



X



Y

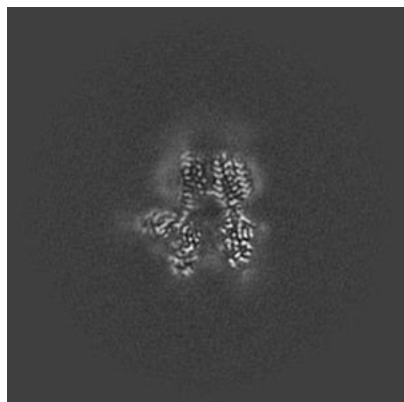


Z

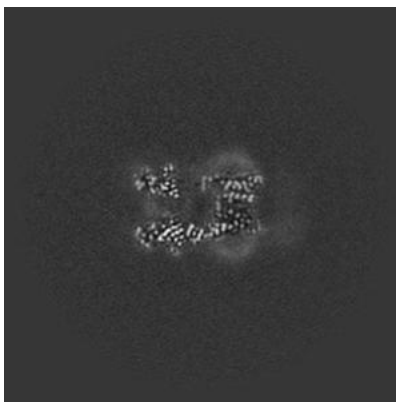
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

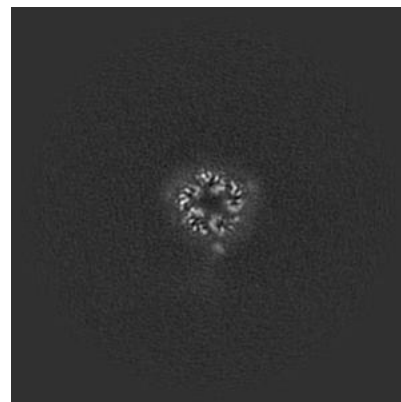
6.2.1 Primary map



X Index: 260

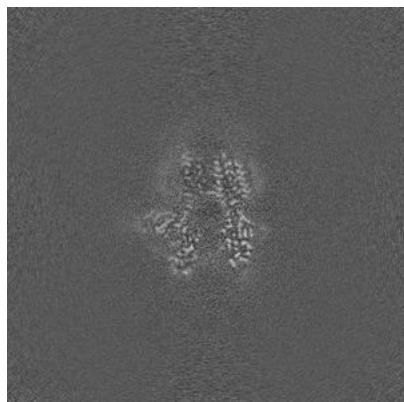


Y Index: 260

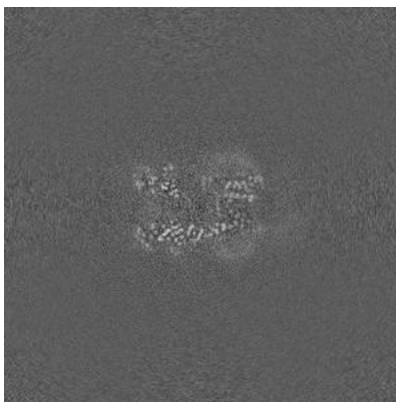


Z Index: 260

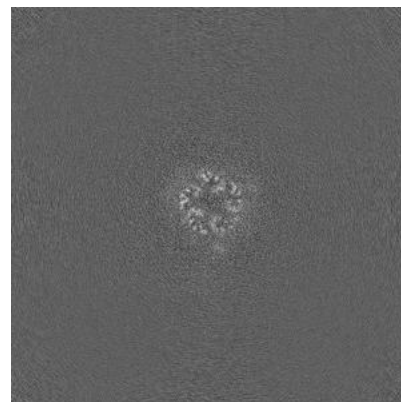
6.2.2 Raw map



X Index: 260



Y Index: 260

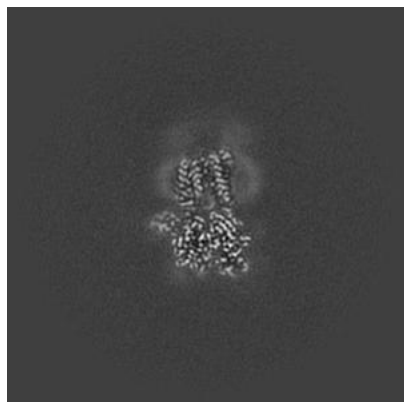


Z Index: 260

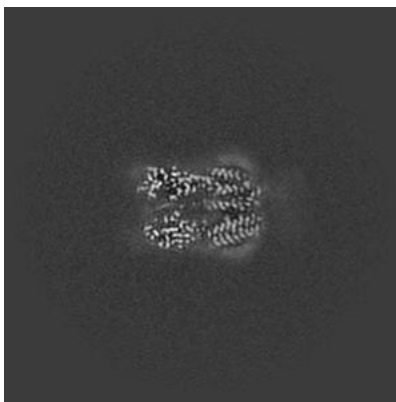
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

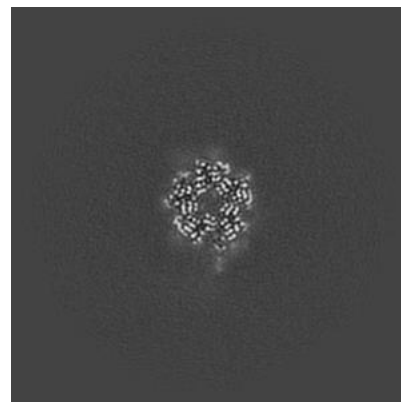
6.3.1 Primary map



X Index: 281

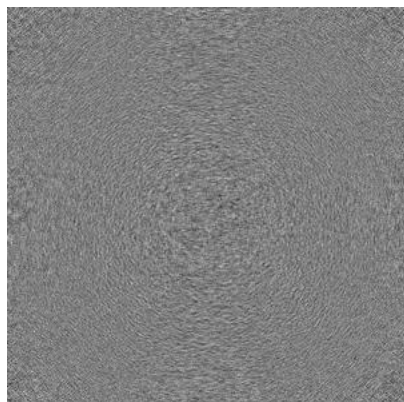


Y Index: 278

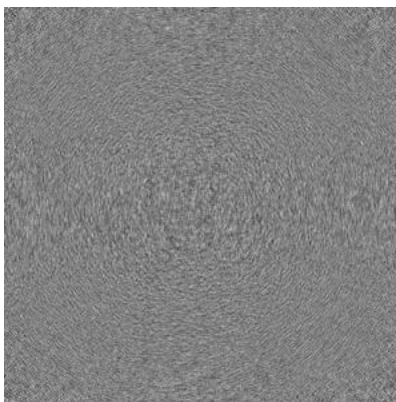


Z Index: 219

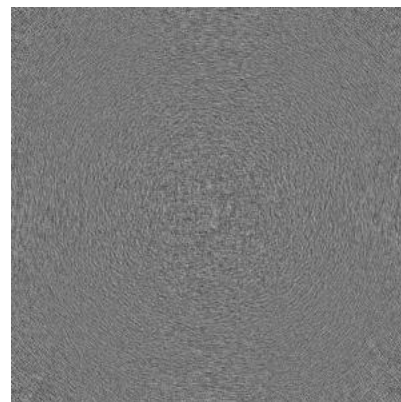
6.3.2 Raw map



X Index: 0



Y Index: 0

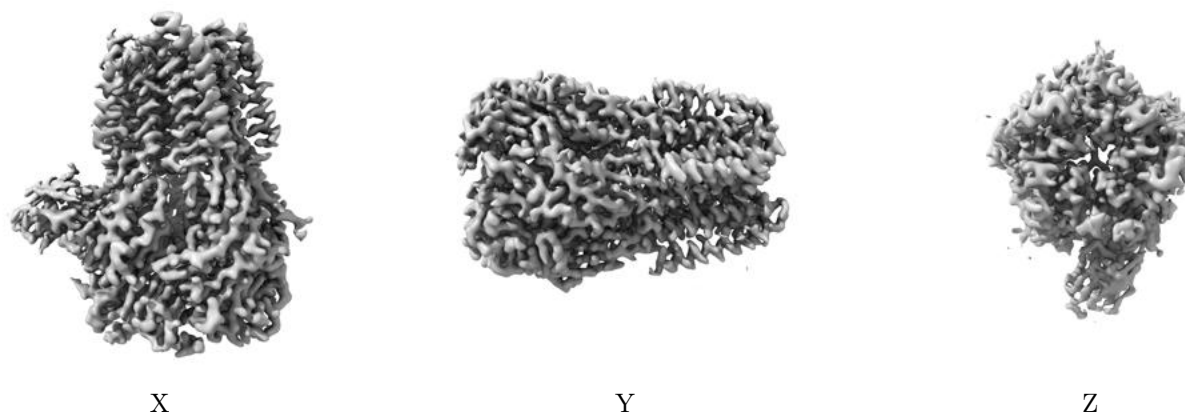


Z Index: 0

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

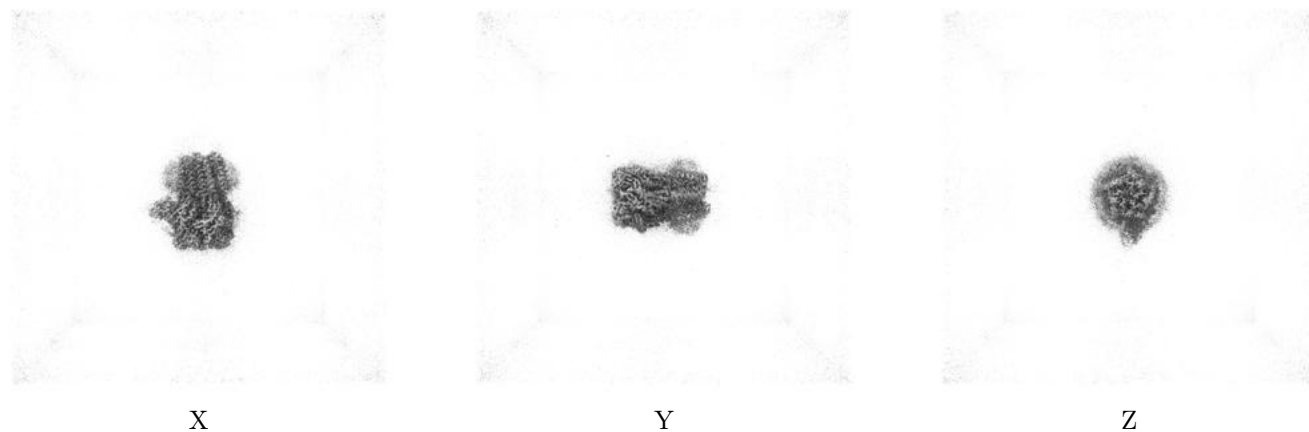
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0849. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

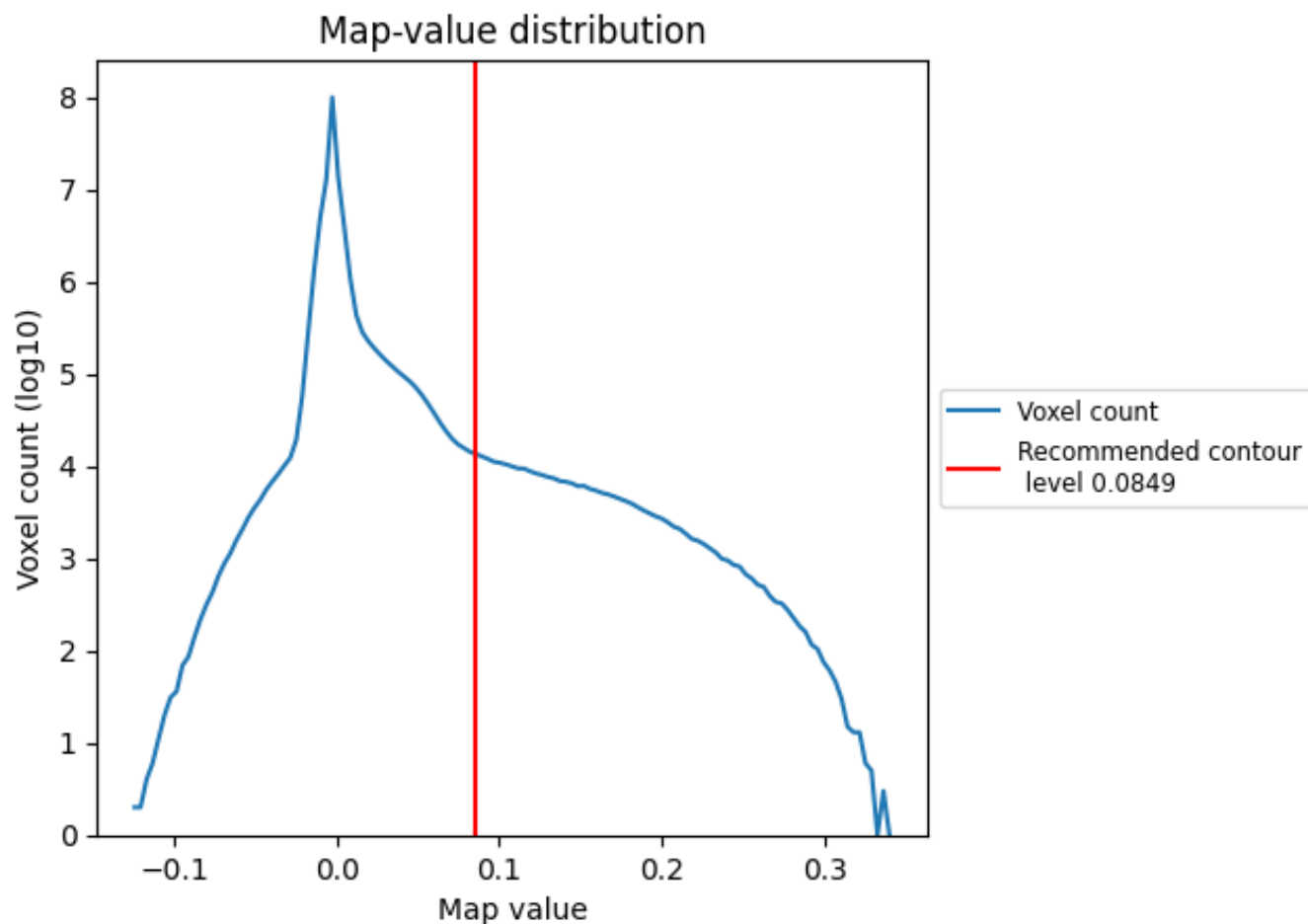
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

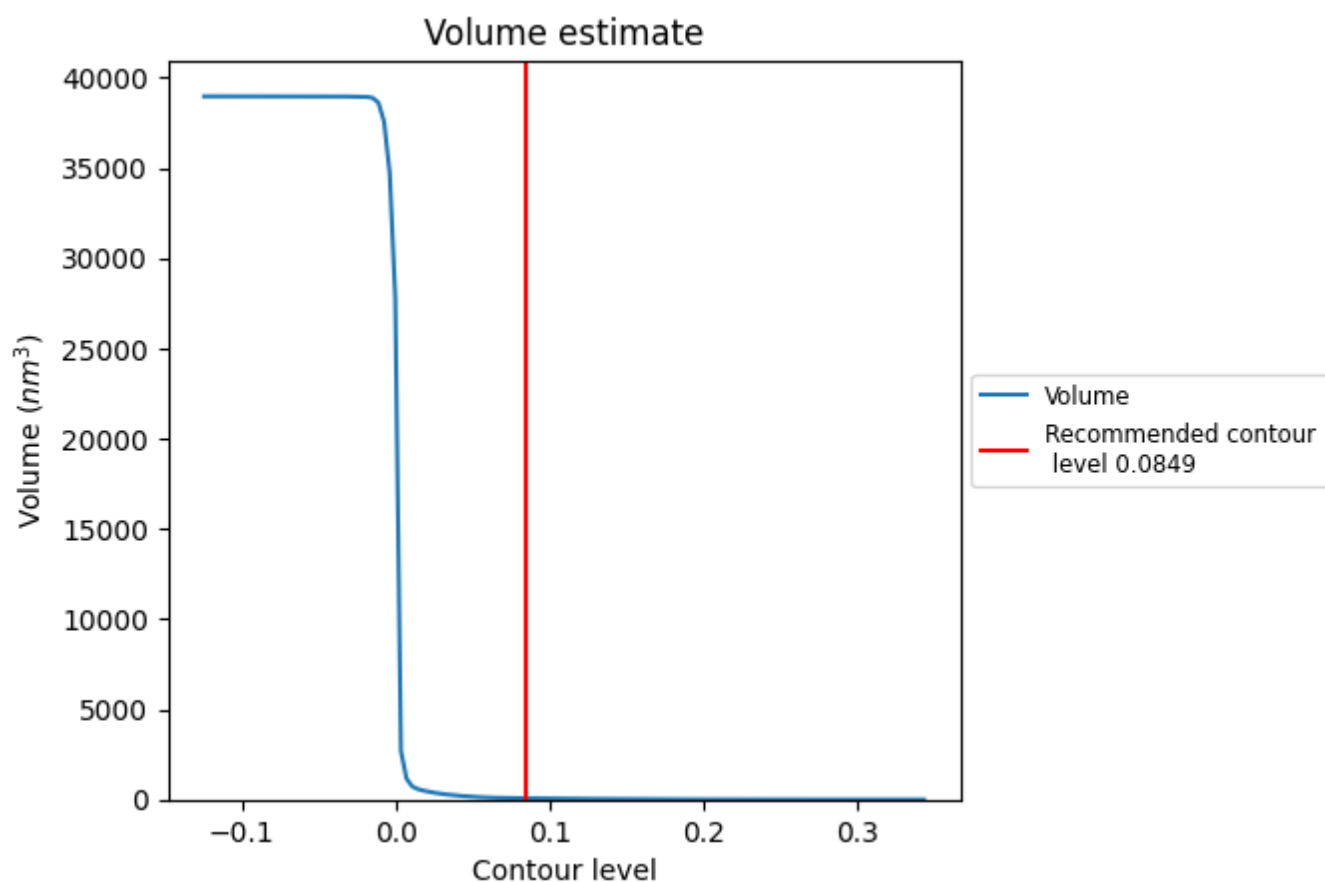
This section contains the results of statistical analysis of the map.

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.

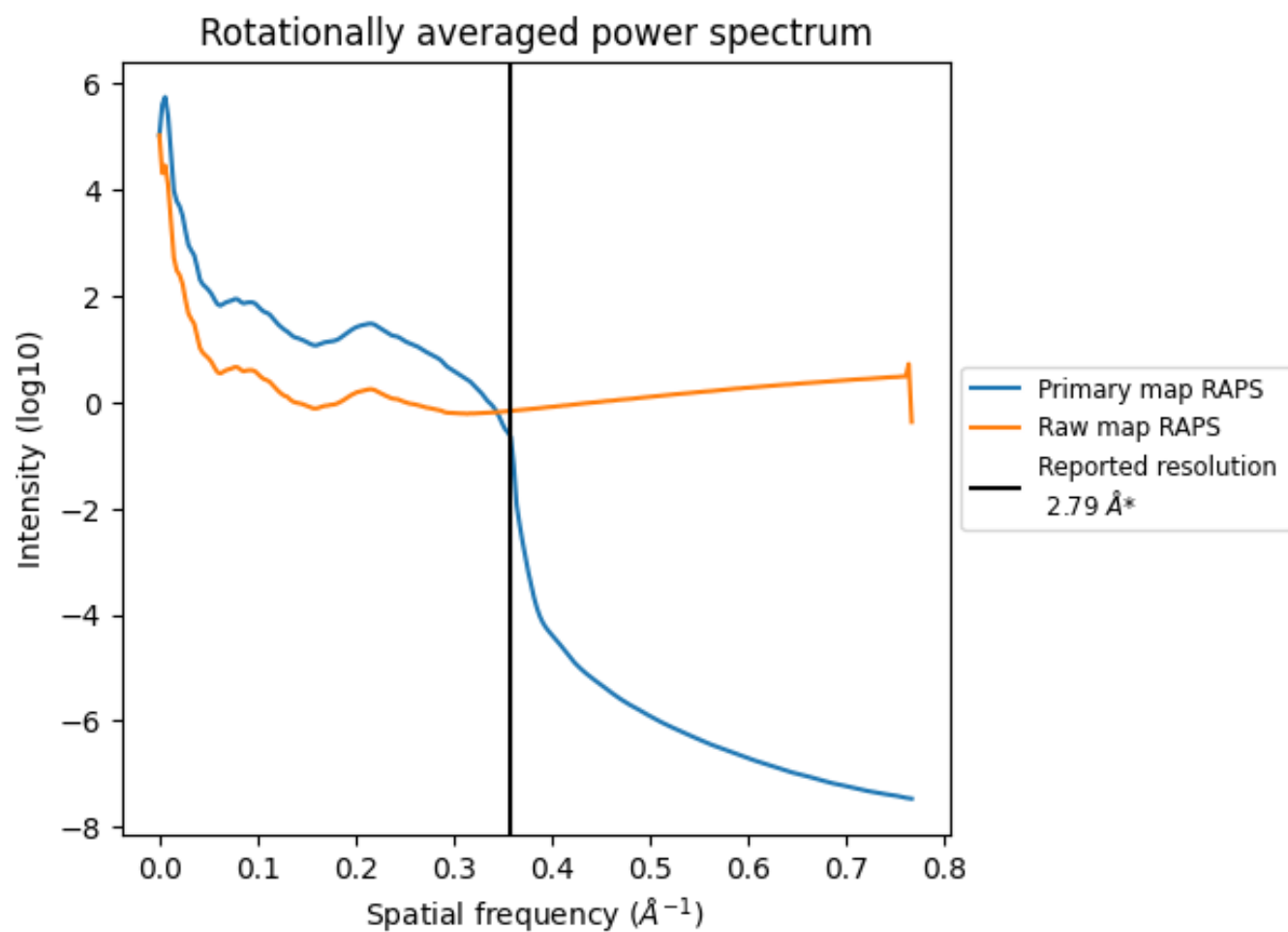
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 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 ⓘ

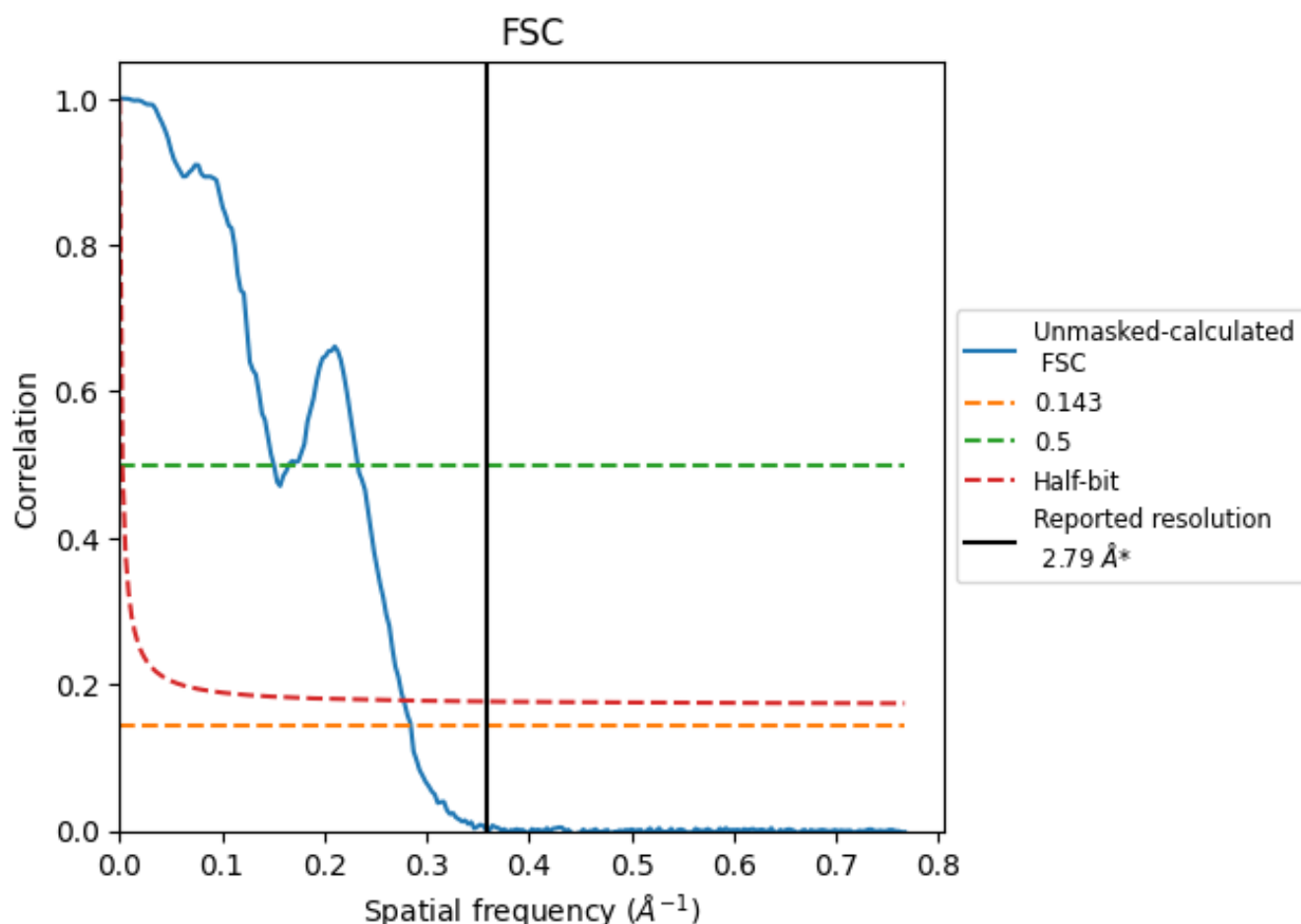


*Reported resolution corresponds to spatial frequency of 0.358 \AA^{-1}

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 0.358 \AA^{-1}

8.2 Resolution estimates [i](#)

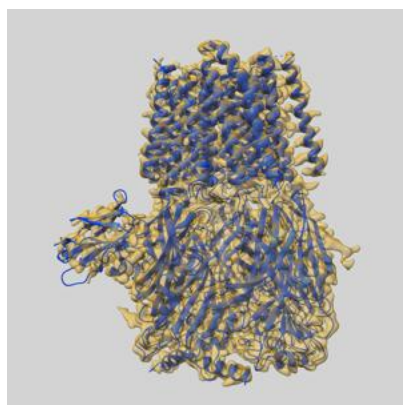
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	6.64	3.60

*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 3.51 differs from the reported value 2.79 by more than 10 %

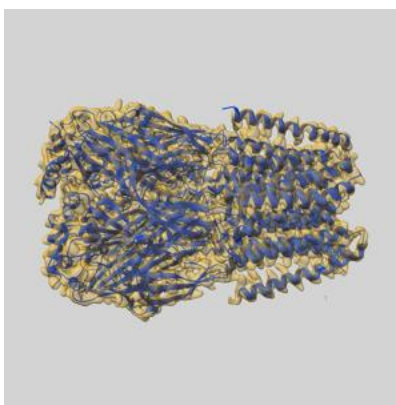
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13314 and PDB model 7PBZ. Per-residue inclusion information can be found in section [3](#) on page [21](#).

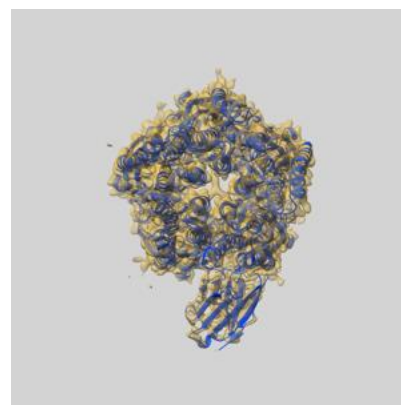
9.1 Map-model overlay [i](#)



X



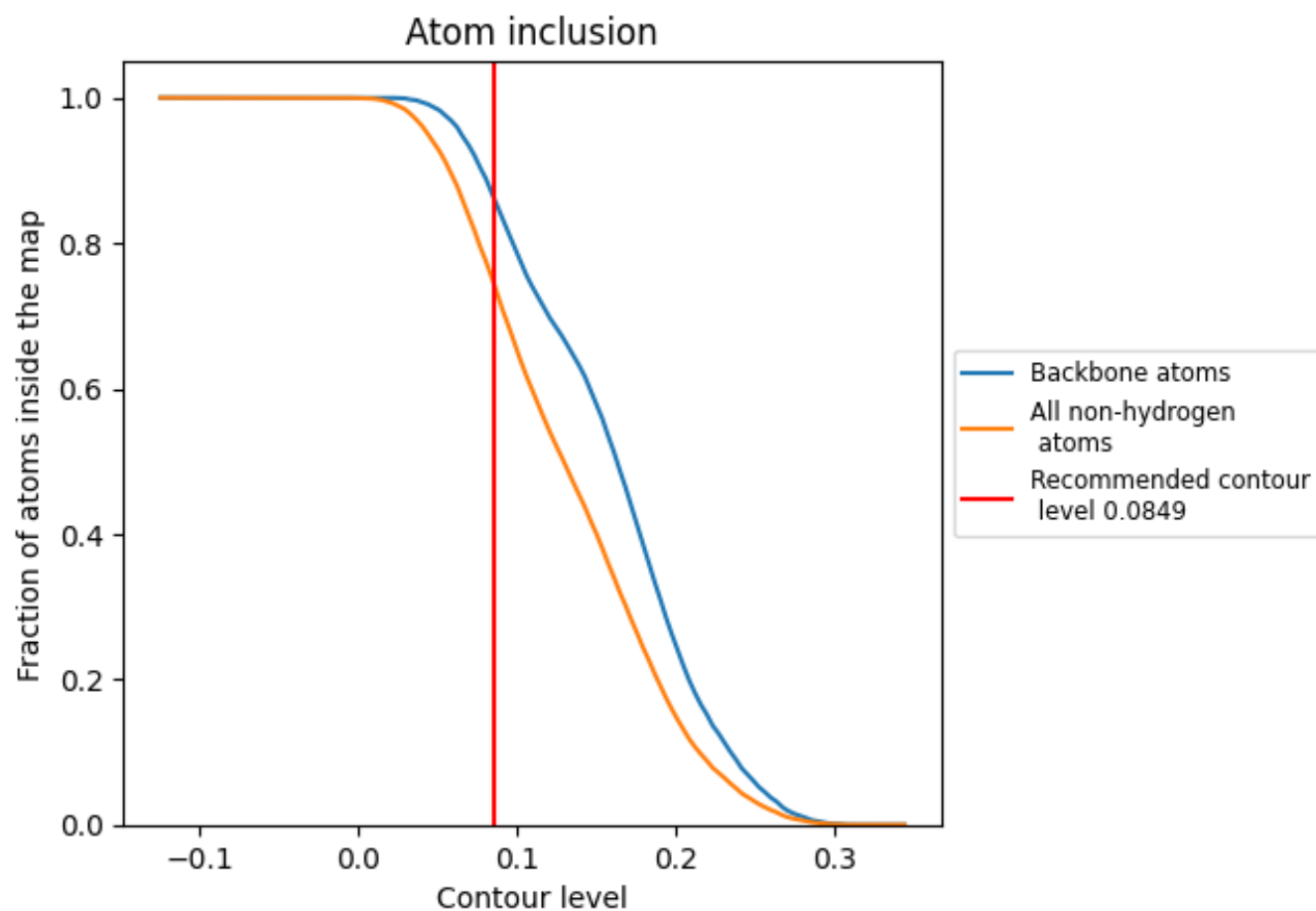
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0849 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 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.