



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:41 PM UTC

PDB ID : 7PBZ / pdb_00007pbz
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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:

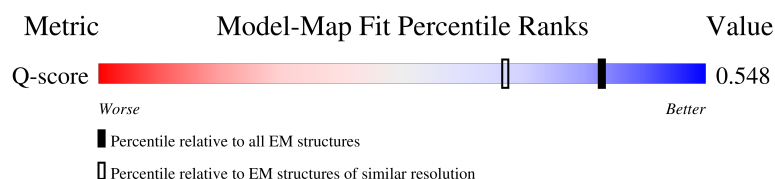
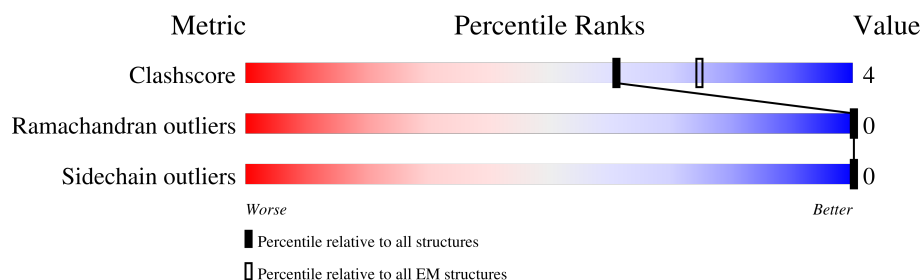
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

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	

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Mol	Chain	Length	Quality of chain
3	E	451	
4	D	411	
5	G	2	
5	I	2	
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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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.



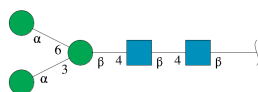
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.



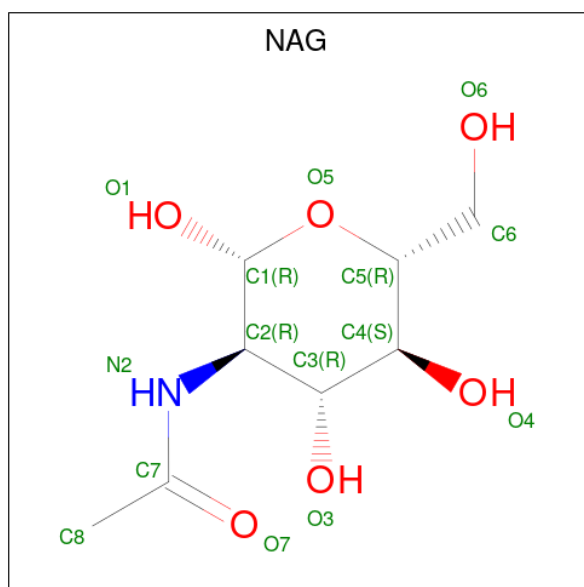
Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	4	Total	C	N	O	0	0
			50	28	2	20		

- 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.



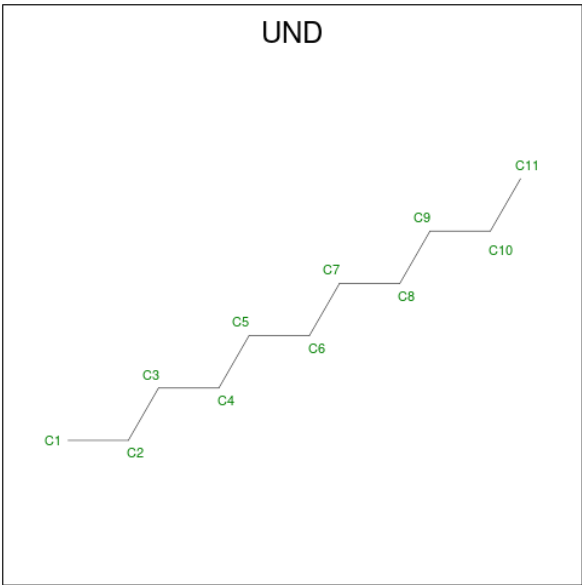
Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	5	Total	C	N	O	0	0
			61	34	2	25		
7	L	5	Total	C	N	O	0	0
			61	34	2	25		

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



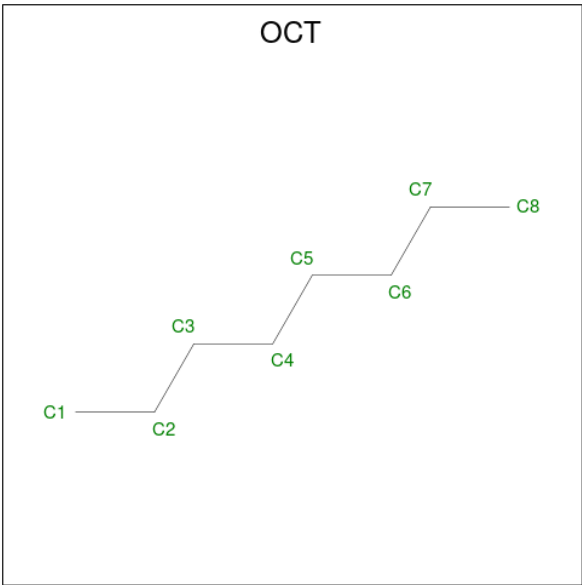
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is UNDECANE (CCD ID: UND) (formula: $C_{11}H_{24}$).



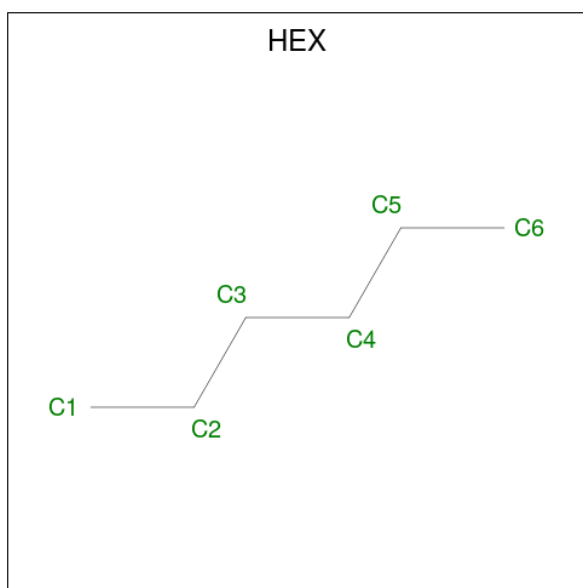
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	C	0
			11	11	
9	A	1	Total	C	0
			11	11	

- Molecule 10 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



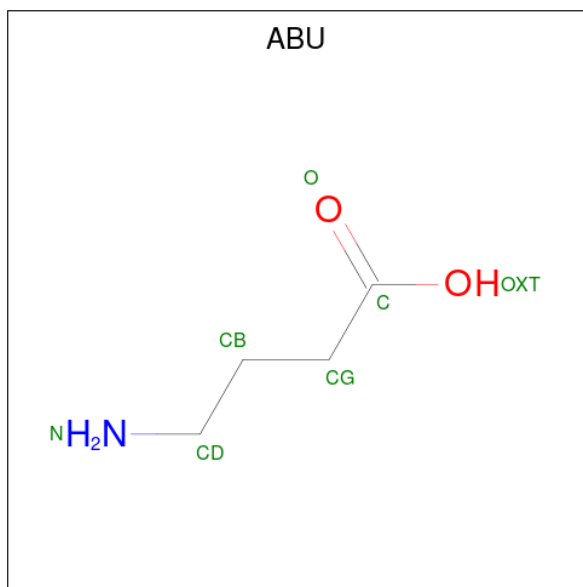
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	C	0
			8	8	
10	A	1	Total	C	0
			8	8	

- Molecule 11 is HEXANE (CCD ID: 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
			6	6	
11	D	1	Total	C	0
			6	6	

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

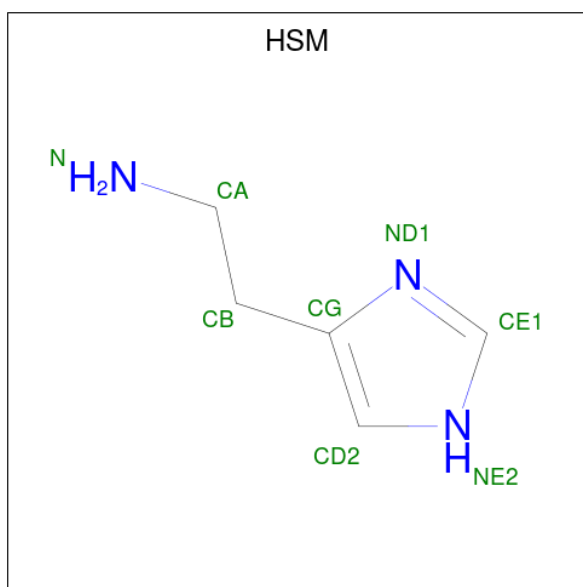


Mol	Chain	Residues	Atoms				AltConf
12	B	1	Total	C	N	O	0
			7	4	1	2	
12	E	1	Total	C	N	O	0
			7	4	1	2	

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

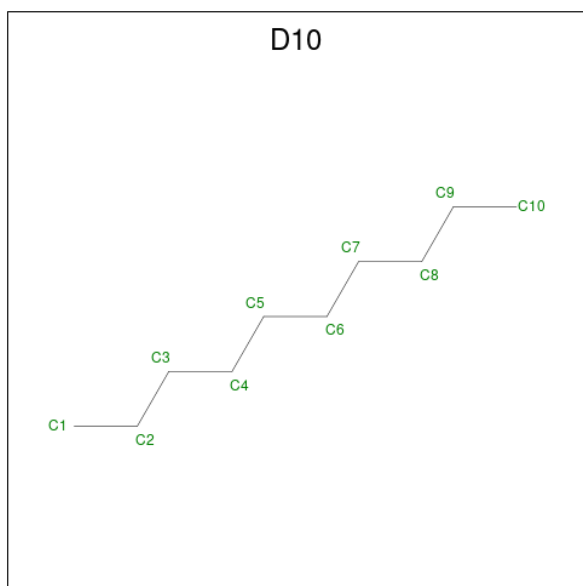
Mol	Chain	Residues	Atoms		AltConf
13	B	1	Total	Zn	0
			1	1	

- Molecule 14 is HISTAMINE (CCD ID: HSM) (formula: C₅H₉N₃).



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

- Molecule 15 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



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

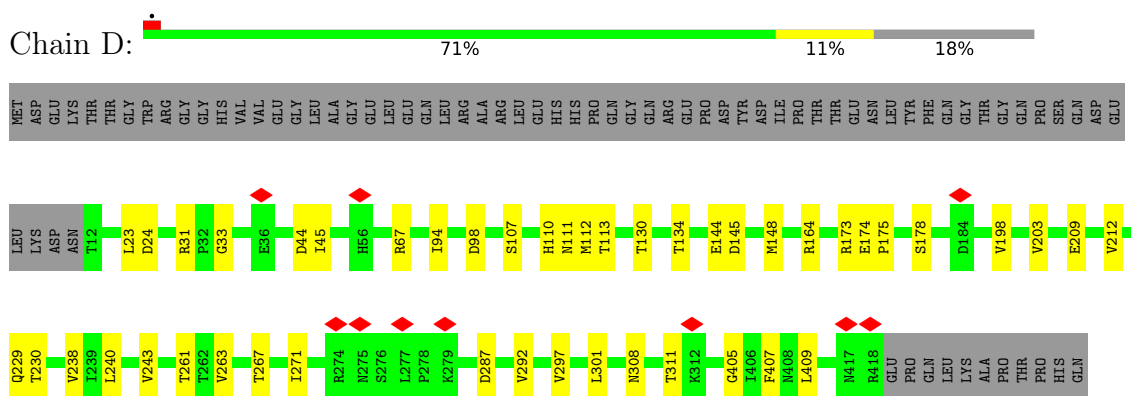
Chain B:

Sequence logo for Chain B. The y-axis represents information content in bits. The x-axis shows 28 positions. The top bar indicates the overall conservation: 66% (green), 7% (yellow), and 27% (grey). A red diamond indicates a position with a mutation.

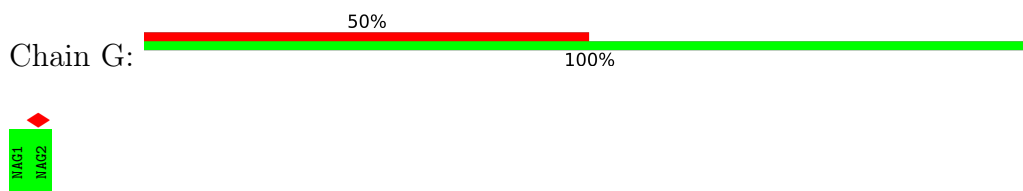
Position	Amino Acid	Information Content (bits)
1	GLN	1.8
2	SER	1.8
3	VAL	1.8
4	ASN	1.8
5	ASP	1.8
6	PRO	1.8
7	GLY	1.8
8	N8	1.8
9	M9	1.8
10	S10	1.8
11	K13	1.8
12	E14	1.8
13	K21	1.8
14	R86	1.8
15	T96	1.8
16	Y97	1.8
17	N100	1.8
18	D101	1.8
19	K102	1.8
20	K103	1.8
21	S104	1.8
22	H107	1.8
23	T131	1.8
24	T151	1.8
25	L152	1.8
26	E153	1.8
27	I154	1.8
28	E155	1.8
29	T160	1.8
30	T161	1.8
31	D162	1.8
32	D163	1.8
33	D172	1.8
34	I181	1.8
35	T188	1.8
36	V189	1.8
37	E190	1.8
38	H191	1.8
39	R192	1.8
40	R207	1.8
41	R213	1.8
42	L235	1.8
43	V238	1.8

[illegible][illegible]

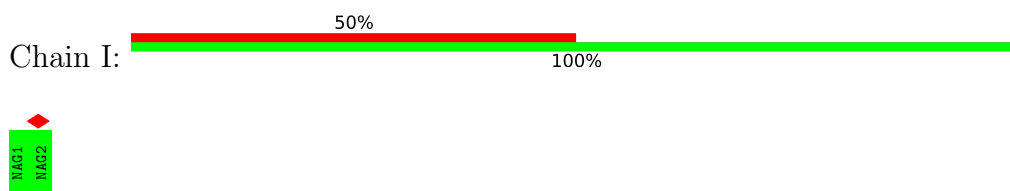
- Molecule 4: Gamma-aminobutyric acid receptor subunit alpha-1



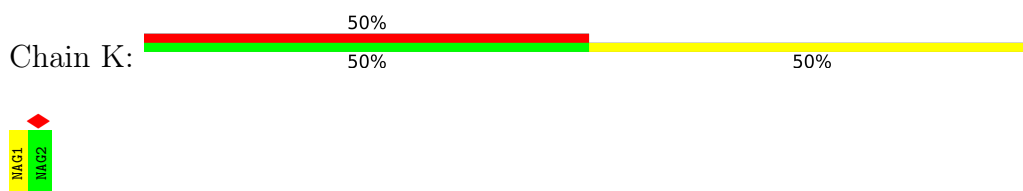
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



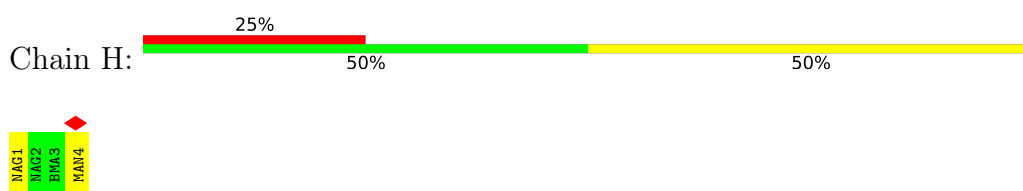
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

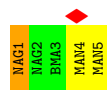


- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

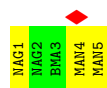


- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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 ($\text{\AA}$)	339.04, 339.04, 339.04	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.652, 0.652, 0.652	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ABU, MAN, UND, D10, HEX, NAG, ZN, BMA, HSM, OCT

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	0.16	0/916	0.35	0/1240
2	A	0.16	0/2764	0.41	2/3758 (0.1%)
3	B	0.16	0/2779	0.38	0/3780
3	C	0.15	0/2779	0.39	2/3780 (0.1%)
3	E	0.17	0/2779	0.41	1/3780 (0.0%)
4	D	0.16	0/2783	0.37	0/3783
All	All	0.16	0/14800	0.39	5/20121 (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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	316	ALA	CA-C-N	8.50	131.67	120.28
2	A	316	ALA	C-N-CA	8.50	131.67	120.28
3	E	150	CYS	CA-CB-SG	6.27	128.82	114.40
3	C	110	THR	CA-C-N	5.50	128.27	122.11
3	C	110	THR	C-N-CA	5.50	128.27	122.11

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	5	0
2	A	2695	0	2695	24	0
3	B	2707	0	2700	23	0
3	C	2707	0	2700	27	0
3	E	2707	0	2700	31	0
4	D	2714	0	2714	32	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	0	4	0
12	E	7	0	0	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	14807	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (126) 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	1.01
2:A:111:ASN:CG	8:A:501:NAG:C1	2.45	0.89
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
3:B:97:TYR:HH	12:B:501:ABU:N	1.87	0.72
3:E:155:GLU:OE2	12:E:501:ABU:N	2.22	0.72
3:C:109:VAL:HG21	4:D:107:SER:HB2	1.75	0.67
3:E:80:ASN:OD1	5:K:1:NAG:C1	2.42	0.67
3:C:198:VAL:HG21	3:C:207:ARG:HE	1.60	0.67
3:E:198:VAL:HG21	3:E:207:ARG:HE	1.60	0.67
4:D:111:ASN:CG	8:D:501:NAG:C1	2.63	0.66
3:B:160:THR:OG1	3:B:162:ASP:OD1	2.14	0.65
2:A:99:THR:O	3:E:110:THR:OG1	2.15	0.64
3:B:243:ASN:O	3:B:250:ARG:NH1	2.33	0.61
2:A:113:THR:OG1	3:B:96:THR:O	2.18	0.60
1:F:440:TRP:O	1:F:459:ARG:NH1	2.34	0.60
3:E:233:THR:O	3:E:236:SER:OG	2.17	0.59
3:C:235:LEU:HD22	4:D:301:LEU:HD23	1.85	0.58
3:C:239:SER:HB2	3:C:253:LEU:HD22	1.85	0.58
2:A:119:LEU:HD11	2:A:127:LEU:HD21	1.86	0.58
3:B:181:ILE:HG21	3:B:188:ILE:HD11	1.85	0.57
3:C:175:VAL:HG21	3:C:210:LEU:HD13	1.88	0.55
2:A:240:LEU:O	2:A:243:VAL:HG22	2.06	0.55
4:D:175:PRO:O	4:D:198:VAL:HG21	2.06	0.55
3:B:153:GLU:OE1	3:B:207:ARG:NH1	2.40	0.54
3:E:255:ILE:HG21	4:D:261:THR:OG1	2.06	0.54
3:B:235:LEU:O	3:B:253:LEU:HD21	2.08	0.53
3:E:96:THR:O	4:D:113:THR:OG1	2.26	0.53
4:D:112:MET:O	4:D:113:THR:OG1	2.26	0.53
4:D:229:GLN:OE1	4:D:230:THR:HG23	2.08	0.53
4:D:31:ARG:NH2	4:D:33:GLY:O	2.42	0.53
3:B:155:GLU:OE2	12:B:501:ABU:N	2.42	0.52
3:B:238:VAL:HG13	3:C:300:ALA:HB2	1.92	0.52
3:C:153:GLU:OE1	3:C:209:SER:OG	2.24	0.52
3:E:192:ARG:HG3	7:L:1:NAG:H83	1.92	0.52
3:B:192:ARG:NH1	6:H:1:NAG:O7	2.44	0.51
3:C:84:ASP:OD2	3:C:86:ARG:NE	2.43	0.51
2:A:112:MET:O	2:A:113:THR:OG1	2.29	0.51
2:A:223:ILE:HG12	2:A:227:VAL:HG23	1.94	0.50
3:E:297:LEU:CD2	4:D:243:VAL:HG21	2.41	0.50
1:F:405:LEU:HD23	1:F:470:MET:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:119:LEU:CD1	2:A:127:LEU:HD21	2.41	0.49
2:A:85:ARG:NH2	3:B:163:ASP:OD1	2.46	0.49
4:D:145:ASP:O	4:D:148:MET:N	2.46	0.49
2:A:256:THR:O	2:A:260:VAL:HG22	2.12	0.48
3:C:192:ARG:NH1	7:J:1:NAG:O3	2.46	0.48
3:E:293:PHE:CE2	3:E:297:LEU:HD11	2.48	0.48
3:B:101:ASP:OD1	3:B:102:LYS:N	2.46	0.48
3:E:44:ILE:HG21	3:E:181:ILE:HD11	1.94	0.48
4:D:238:VAL:HG12	4:D:297:VAL:HG23	1.94	0.48
3:C:111:VAL:HG21	4:D:98:ASP:HB2	1.94	0.48
4:D:144:GLU:N	4:D:144:GLU:OE1	2.47	0.48
2:A:88:ASN:ND2	2:A:115:PRO:O	2.44	0.48
4:D:203:VAL:CG2	4:D:212:VAL:HG21	2.44	0.48
4:D:263:VAL:HG22	4:D:297:VAL:HG12	1.95	0.48
2:A:263:VAL:HG22	2:A:297:VAL:HG12	1.96	0.47
2:A:241:SER:HB3	2:A:262:THR:HG21	1.97	0.47
3:C:47:ILE:HG12	3:C:59:LEU:HD13	1.96	0.47
3:C:221:PHE:O	3:C:225:THR:OG1	2.33	0.47
4:D:174:GLU:O	4:D:178:SER:OG	2.22	0.47
2:A:191:TYR:OH	2:A:221:ARG:NH1	2.48	0.47
3:B:172:ASP:N	3:B:172:ASP:OD1	2.48	0.47
3:B:10:SER:O	3:B:13:LYS:N	2.47	0.47
4:D:405:GLY:O	4:D:409:LEU:HD23	2.15	0.47
3:E:100:ASN:ND2	3:E:151:THR:O	2.48	0.46
3:E:126:TYR:CE2	3:E:128:LEU:HD11	2.50	0.46
3:E:110:THR:O	3:E:111:VAL:HG13	2.15	0.46
3:E:190:GLU:OE1	3:E:213:ARG:NH2	2.46	0.46
3:C:230:ILE:O	3:C:233:THR:OG1	2.30	0.46
3:B:235:LEU:HD22	3:C:296:LEU:HD23	1.97	0.45
3:C:95:ASP:OD2	3:C:158:GLY:N	2.46	0.45
1:F:421:MET:SD	1:F:440:TRP:NE1	2.89	0.45
3:C:224:GLN:NE2	4:D:287:ASP:OD1	2.49	0.45
1:F:449:ASP:OD1	1:F:450:SER:N	2.49	0.45
3:C:80:ASN:OD1	3:C:119:HIS:ND1	2.49	0.45
2:A:229:GLN:O	3:B:269:ARG:NH2	2.46	0.45
2:A:239:ILE:O	2:A:243:VAL:HG13	2.16	0.45
4:D:292:VAL:HG21	4:D:407:PHE:CE1	2.52	0.45
4:D:24:ASP:N	4:D:24:ASP:OD1	2.50	0.45
3:B:86:ARG:NH1	3:C:89:ASP:O	2.49	0.45
3:B:107:HIS:NE2	3:B:131:THR:OG1	2.43	0.44
3:C:99:LEU:HD22	3:C:207:ARG:HH12	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:111:ASN:OD1	8:A:501:NAG:C1	2.65	0.44
3:B:100:ASN:ND2	3:B:151:THR:O	2.50	0.44
3:B:97:TYR:OH	12:B:501:ABU:N	2.48	0.44
3:E:178:VAL:HA	3:E:181:ILE:HD12	1.98	0.44
3:C:84:ASP:O	3:C:87:VAL:HG12	2.18	0.44
3:E:44:ILE:CG2	3:E:181:ILE:HD11	2.46	0.44
4:D:267:THR:HG22	4:D:271:ILE:HD12	1.99	0.44
3:C:272:LEU:HD21	3:C:281:ILE:HD13	2.00	0.44
3:E:47:ILE:HD12	3:E:181:ILE:HD13	2.00	0.44
3:E:83:LEU:HB3	3:E:87:VAL:HG21	1.99	0.44
4:D:44:ASP:OD1	4:D:45:ILE:N	2.51	0.44
4:D:110:HIS:NE2	4:D:134:THR:OG1	2.39	0.44
3:C:66:TYR:CZ	3:C:125:LEU:HD13	2.53	0.43
3:E:126:TYR:CZ	3:E:128:LEU:HD11	2.53	0.43
3:C:66:TYR:CE2	3:C:125:LEU:HD13	2.53	0.43
3:E:109:VAL:O	3:E:110:THR:OG1	2.31	0.43
4:D:23:LEU:HD21	4:D:94:ILE:HD11	2.00	0.43
4:D:44:ASP:OD2	4:D:173:ARG:NH2	2.48	0.42
3:E:109:VAL:O	3:E:109:VAL:HG13	2.20	0.42
3:E:61:MET:HE2	3:E:63:PHE:HB2	2.00	0.42
2:A:112:MET:HE1	3:B:104:SER:CB	2.50	0.42
2:A:130:THR:HG21	12:B:501:ABU:OXT	2.19	0.42
3:E:196:ARG:NH1	3:E:198:VAL:HG22	2.35	0.42
2:A:145:ASP:O	2:A:148:MET:N	2.53	0.42
3:E:179:GLU:OE2	3:E:180:ARG:NH1	2.52	0.41
3:B:254:GLY:O	3:B:257:THR:OG1	2.33	0.41
3:C:44:ILE:HG12	3:C:59:LEU:HD11	2.01	0.41
2:A:55:ASP:OD1	2:A:56:HIS:N	2.53	0.41
3:C:110:THR:O	3:C:111:VAL:HG13	2.21	0.41
4:D:175:PRO:C	4:D:198:VAL:HG21	2.46	0.41
4:D:67:ARG:HG3	4:D:130:THR:HG23	2.02	0.41
7:J:1:NAG:H3	7:J:1:NAG:H83	2.02	0.41
2:A:67:ARG:HG3	2:A:130:THR:HG23	2.03	0.41
4:D:164:ARG:NH2	4:D:209:GLU:OE1	2.54	0.41
3:E:127:GLY:C	3:E:128:LEU:HD12	2.44	0.41
1:F:447:TYR:HE1	1:F:457:ILE:HD12	1.85	0.41
4:D:308:ASN:O	4:D:311:THR:HG22	2.20	0.41
3:C:40:MET:HG3	3:C:208:LEU:HD12	2.02	0.41
3:E:198:VAL:HG21	3:E:207:ARG:NE	2.32	0.41
2:A:111:ASN:ND2	8:A:501:NAG:O5	2.42	0.40
3:B:190:GLU:OE1	3:B:213:ARG:NH2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:404:PHE:O	2:A:408:ASN:ND2	2.54	0.40
3:E:255:ILE:HD13	4:D:240:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	296/326 (91%)	296 (100%)	0	100	100
3	B	295/393 (75%)	295 (100%)	0	100	100
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%)	1571 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	464	ASN
1	F	507	GLN
3	B	197	ASN
3	C	217	ASN
3	C	439	ASN
3	E	85	ASN
3	E	267	HIS
4	D	68	GLN
4	D	408	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	3,5	14,14,15	0.32	0	17,19,21	0.43	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.45	0
6	NAG	H	1	3,6	14,14,15	0.25	0	17,19,21	0.41	0
6	NAG	H	2	6	14,14,15	0.22	0	17,19,21	0.41	0
6	BMA	H	3	6	11,11,12	0.58	0	15,15,17	0.70	0
6	MAN	H	4	6	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
5	NAG	I	1	3,5	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	I	2	5	14,14,15	0.21	0	17,19,21	0.47	0
7	NAG	J	1	3,7	14,14,15	0.30	0	17,19,21	1.51	2 (11%)
7	NAG	J	2	7	14,14,15	0.19	0	17,19,21	0.73	0
7	BMA	J	3	7	11,11,12	0.47	0	15,15,17	0.75	0
7	MAN	J	4	7	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
7	MAN	J	5	7	11,11,12	0.96	1 (9%)	15,15,17	1.22	2 (13%)
5	NAG	K	1	3,5	14,14,15	0.31	0	17,19,21	0.56	0
5	NAG	K	2	5	14,14,15	0.20	0	17,19,21	0.48	0
7	NAG	L	1	3,7	14,14,15	0.25	0	17,19,21	0.43	0
7	NAG	L	2	7	14,14,15	0.20	0	17,19,21	0.44	0
7	BMA	L	3	7	11,11,12	0.54	0	15,15,17	0.72	0
7	MAN	L	4	7	11,11,12	0.66	0	15,15,17	1.00	2 (13%)
7	MAN	L	5	7	11,11,12	0.64	0	15,15,17	1.00	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	3,5	-	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	3,6	-	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	3,5	-	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	3,7	-	4/6/23/26	0/1/1/1
7	NAG	J	2	7	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
5	NAG	K	1	3,5	-	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	3,7	-	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	-2.26	1.39	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	1	NAG	C2-N2-C7	4.77	129.30	122.90
7	J	5	MAN	C1-O5-C5	3.24	116.53	112.19
7	J	1	NAG	C1-C2-N2	2.59	114.51	110.43
7	L	4	MAN	C1-O5-C5	2.33	115.31	112.19
7	L	5	MAN	C1-O5-C5	2.32	115.30	112.19
7	J	4	MAN	C1-O5-C5	2.31	115.29	112.19
6	H	4	MAN	C1-O5-C5	2.23	115.18	112.19
7	J	4	MAN	O2-C2-C3	-2.22	105.54	110.15
7	L	4	MAN	O2-C2-C3	-2.19	105.61	110.15
7	L	5	MAN	O2-C2-C3	-2.18	105.63	110.15
7	J	5	MAN	O2-C2-C3	-2.17	105.65	110.15
6	H	4	MAN	O2-C2-C3	-2.17	105.65	110.15

There are no chirality outliers.

All (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

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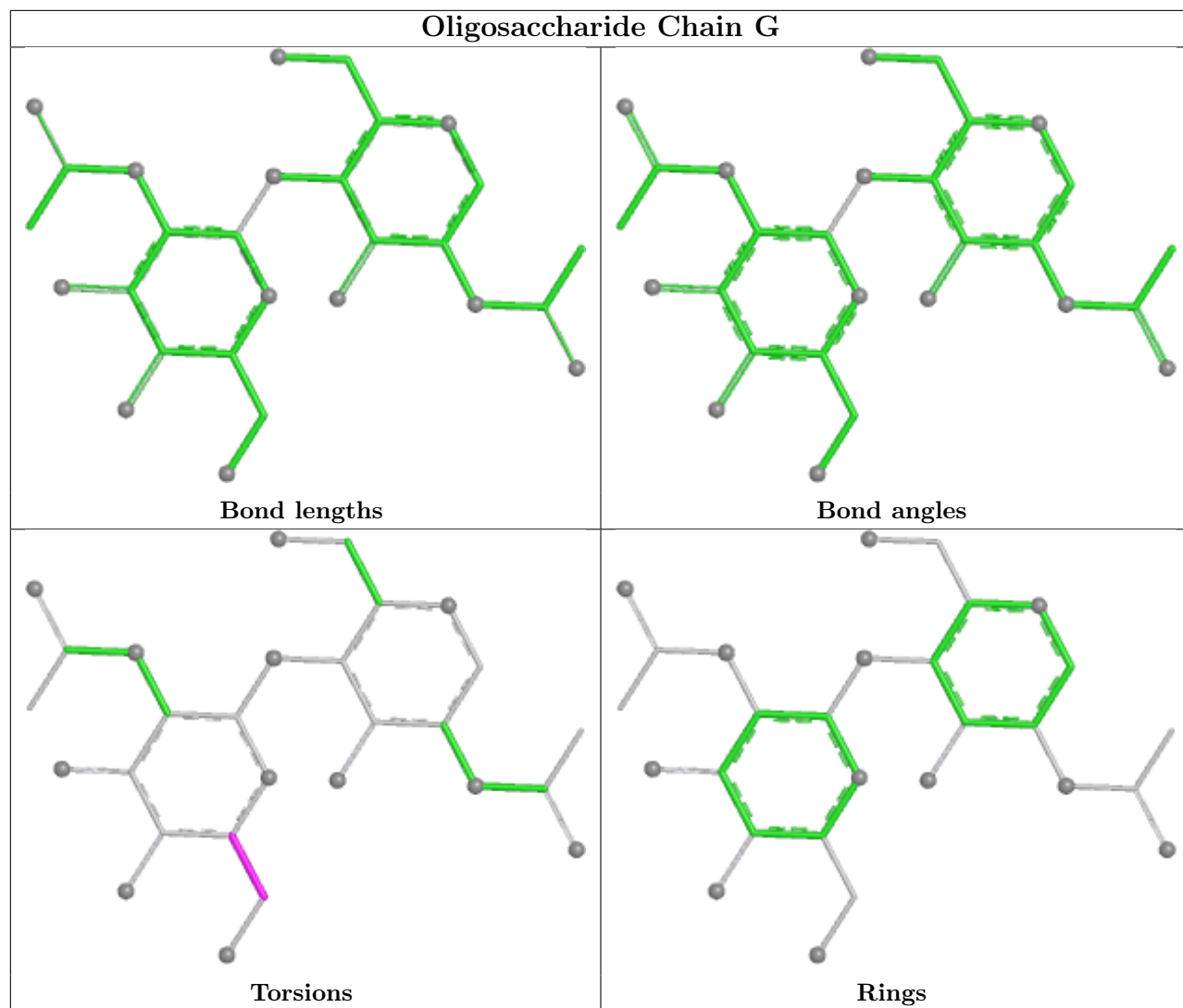
Mol	Chain	Res	Type	Atoms
7	J	2	NAG	O7-C7-N2-C2
6	H	4	MAN	O5-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
7	J	5	MAN	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C1-C2-N2-C7
5	I	2	NAG	C1-C2-N2-C7
5	K	1	NAG	C1-C2-N2-C7
5	K	2	NAG	C1-C2-N2-C7
7	J	1	NAG	C1-C2-N2-C7
5	K	2	NAG	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C3-C2-N2-C7
6	H	1	NAG	O5-C5-C6-O6
5	I	2	NAG	C3-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
7	J	1	NAG	C3-C2-N2-C7

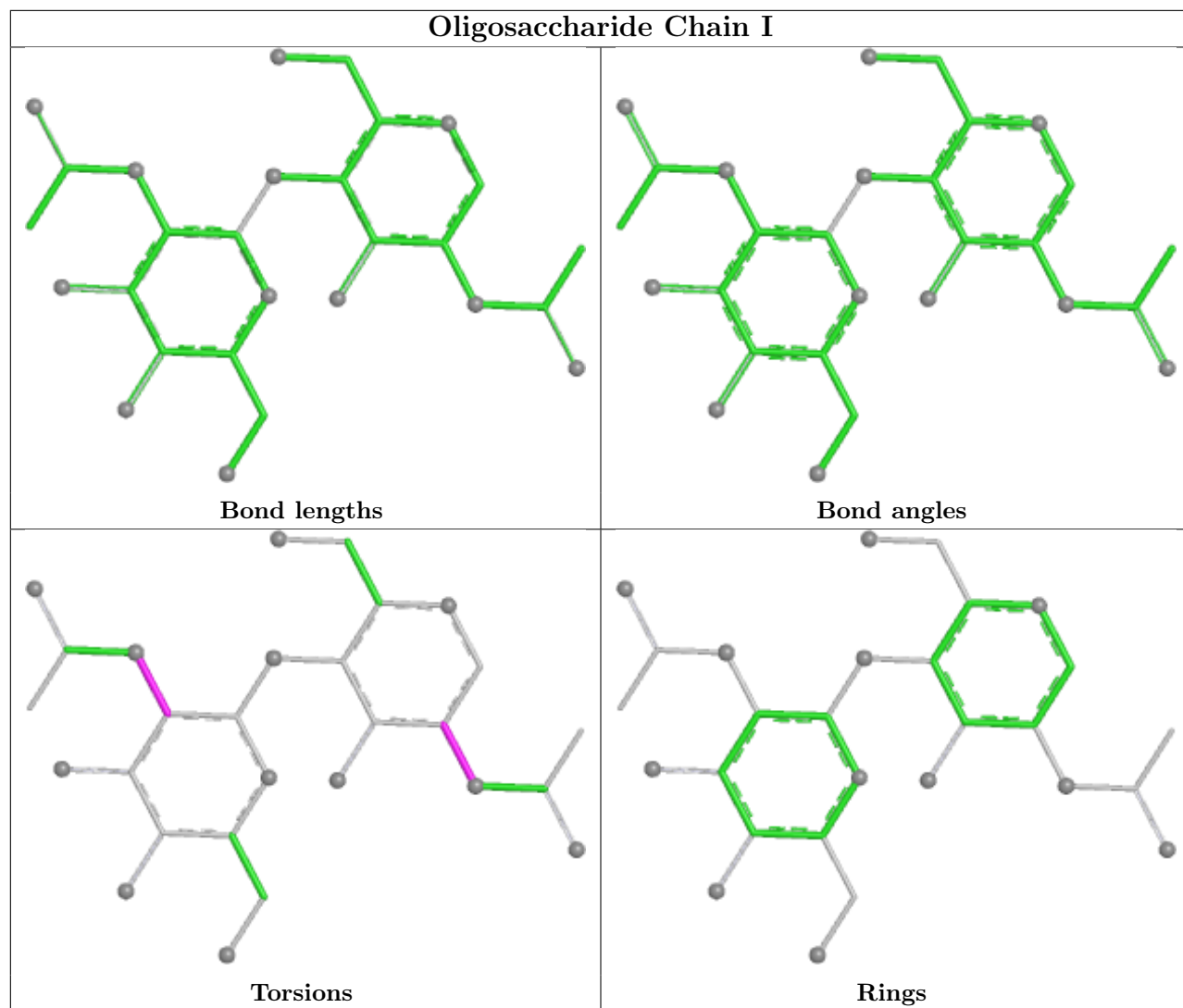
There are no ring outliers.

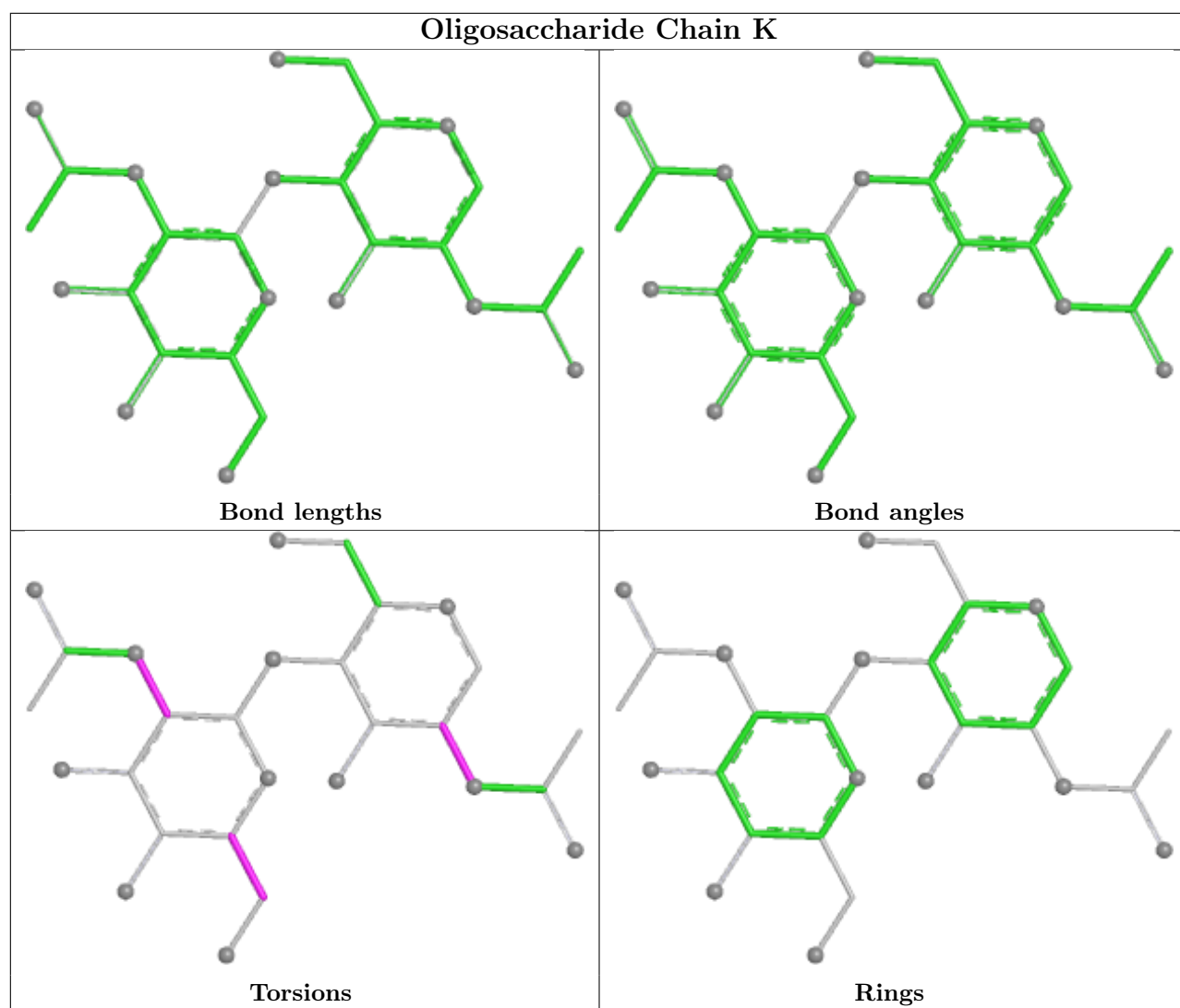
4 monomers are involved in 6 short contacts:

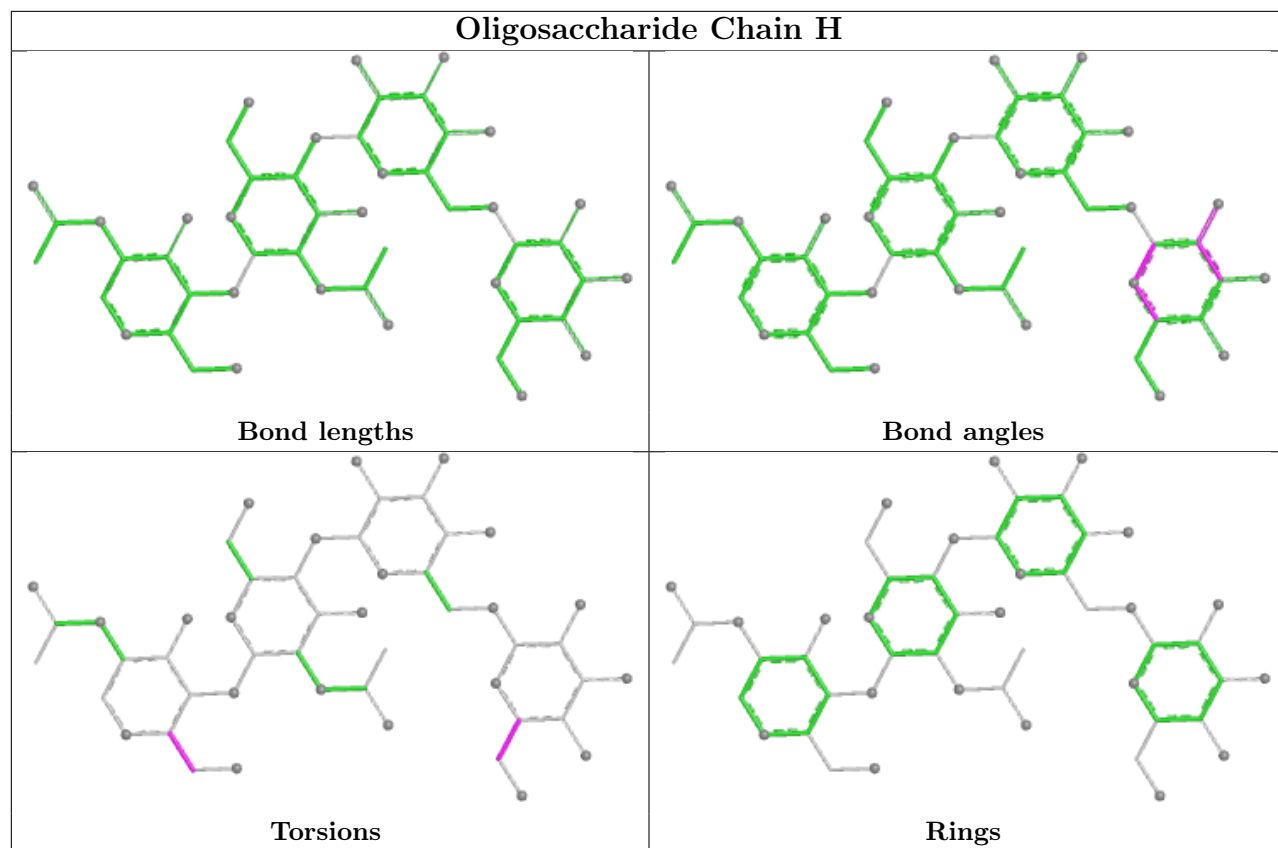
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1	NAG	1	0
7	L	1	NAG	1	0
5	K	1	NAG	2	0
7	J	1	NAG	2	0

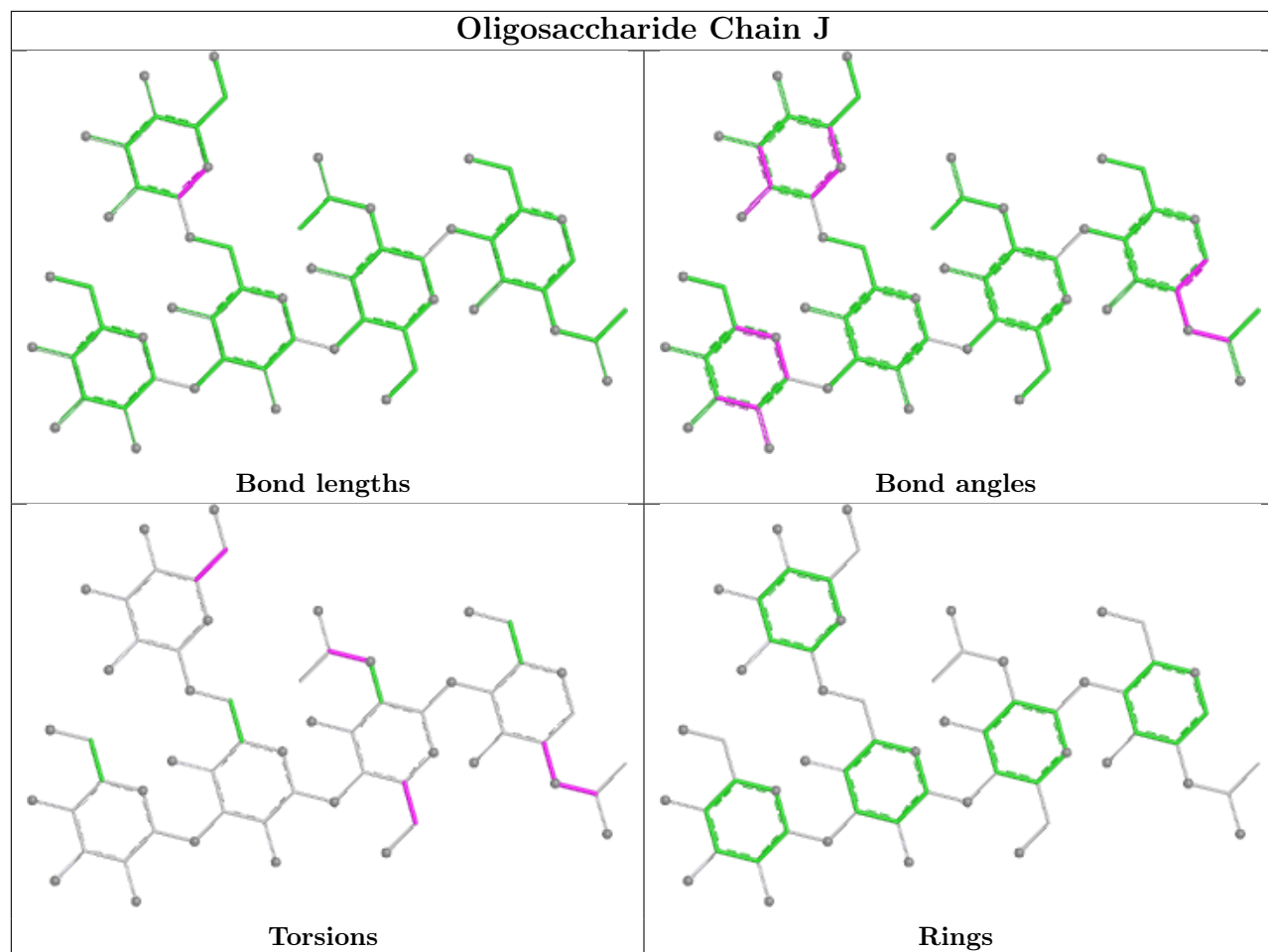
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

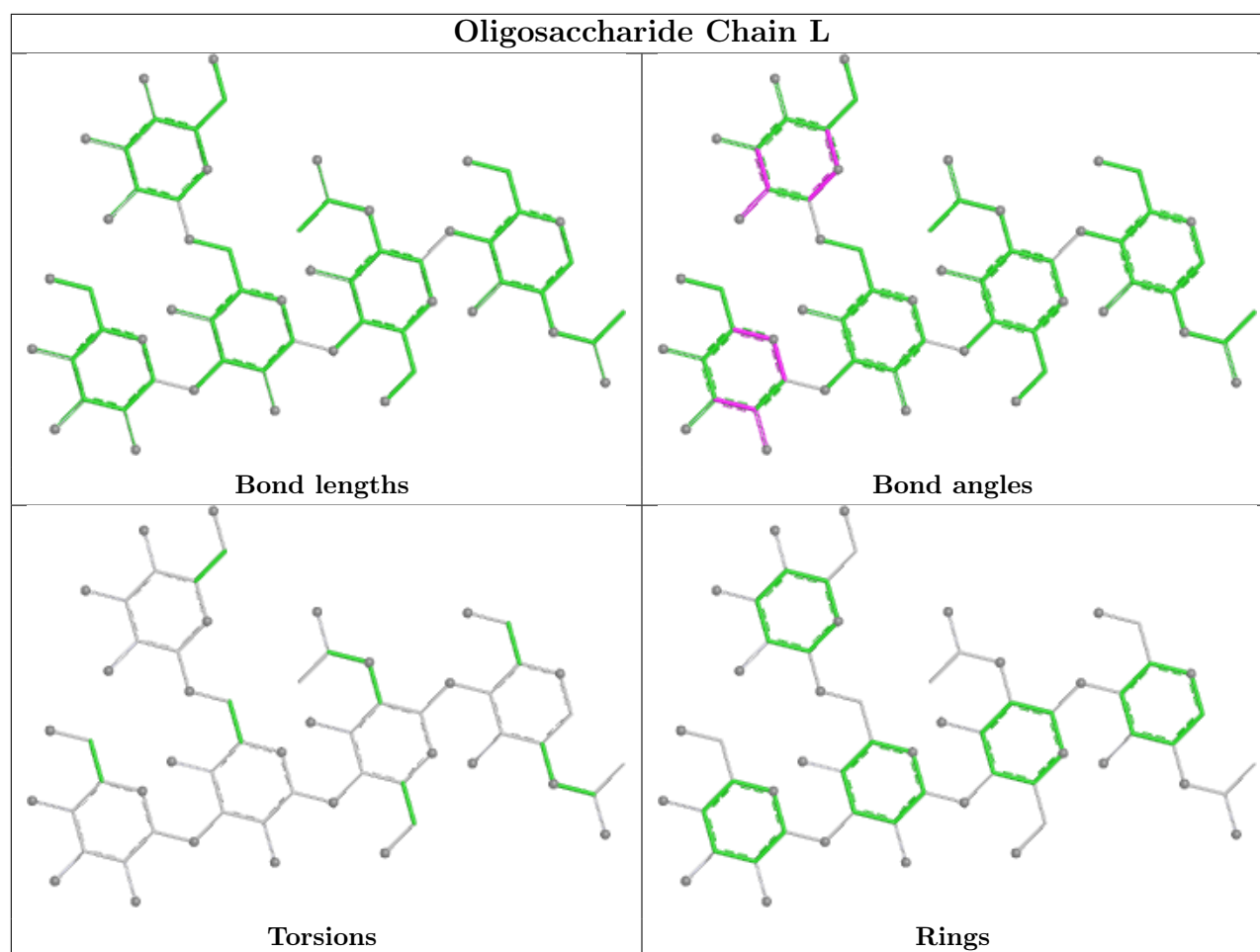












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
8	NAG	D	501	4	14,14,15	0.21	0	17,19,21	0.43	0
15	D10	C	602	-	9,9,9	0.30	0	8,8,8	0.77	0
12	ABU	E	501	-	6,6,6	0.87	0	6,6,6	1.42	1 (16%)
11	HEX	D	503	-	5,5,5	0.31	0	4,4,4	0.62	0
15	D10	D	504	-	9,9,9	0.31	0	8,8,8	0.73	0
9	UND	A	504	-	10,10,10	0.31	0	9,9,9	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HEX	B	502	-	5,5,5	0.31	0	4,4,4	0.60	0
15	D10	D	505	-	9,9,9	0.29	0	8,8,8	0.80	0
14	HSM	C	601	-	8,8,8	1.30	1 (12%)	9,9,9	0.93	0
12	ABU	B	501	-	6,6,6	0.90	0	6,6,6	1.36	1 (16%)
11	HEX	D	502	-	5,5,5	0.31	0	4,4,4	0.61	0
10	OCT	A	505	-	7,7,7	0.31	0	6,6,6	0.73	0
11	HEX	A	506	-	5,5,5	0.32	0	4,4,4	0.60	0
8	NAG	A	501	2	14,14,15	0.22	0	17,19,21	0.48	0
9	UND	A	502	-	10,10,10	0.30	0	9,9,9	0.79	0
10	OCT	A	503	-	7,7,7	0.31	0	6,6,6	0.72	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
8	NAG	D	501	4	-	1/6/23/26	0/1/1/1
15	D10	C	602	-	-	1/7/7/7	-
12	ABU	E	501	-	-	2/4/4/4	-
11	HEX	D	503	-	-	0/3/3/3	-
15	D10	D	504	-	-	0/7/7/7	-
9	UND	A	504	-	-	1/8/8/8	-
11	HEX	B	502	-	-	0/3/3/3	-
15	D10	D	505	-	-	0/7/7/7	-
14	HSM	C	601	-	-	0/3/3/3	0/1/1/1
12	ABU	B	501	-	-	2/4/4/4	-
11	HEX	D	502	-	-	0/3/3/3	-
10	OCT	A	505	-	-	1/5/5/5	-
11	HEX	A	506	-	-	0/3/3/3	-
8	NAG	A	501	2	-	3/6/23/26	0/1/1/1
9	UND	A	502	-	-	0/8/8/8	-
10	OCT	A	503	-	-	1/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	601	HSM	CG-ND1	-2.63	1.31	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	501	ABU	CB-CG-C	-2.21	108.73	114.51
12	B	501	ABU	CB-CG-C	-2.02	109.24	114.51

There are no chirality outliers.

All (12) torsion outliers are listed below:

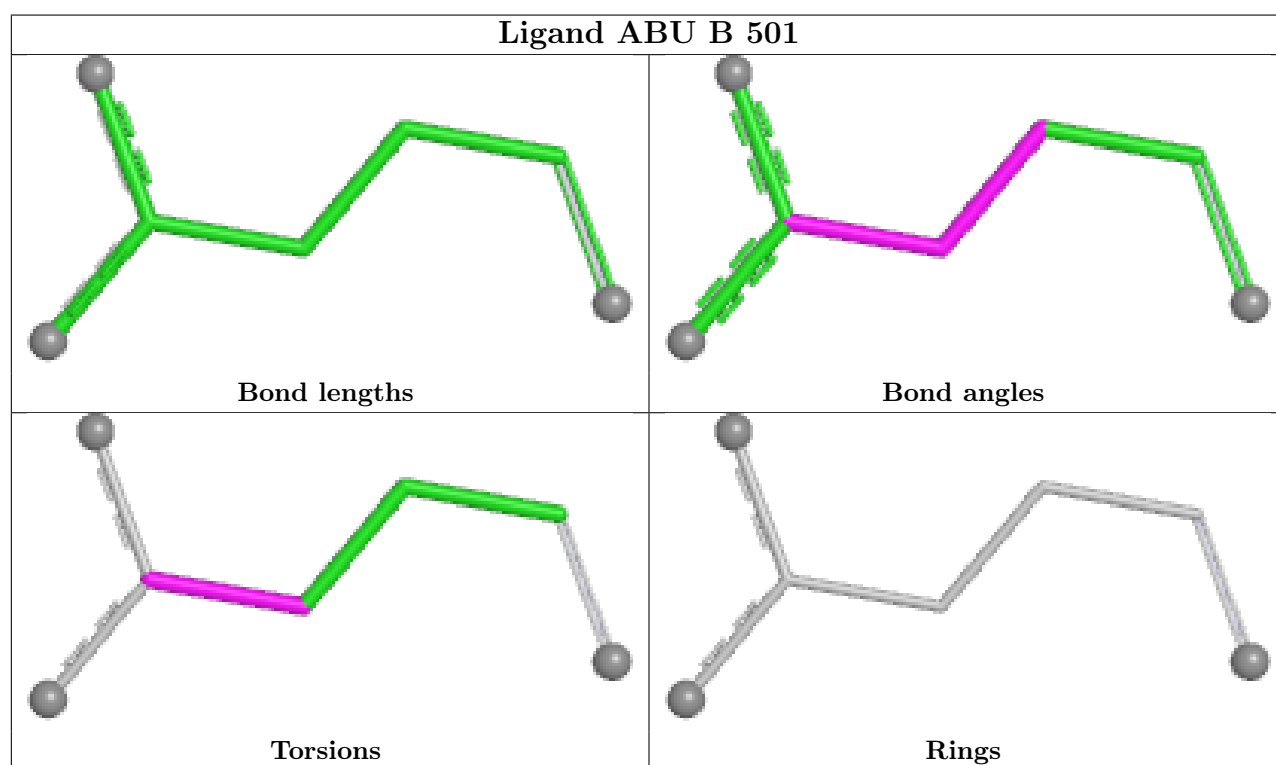
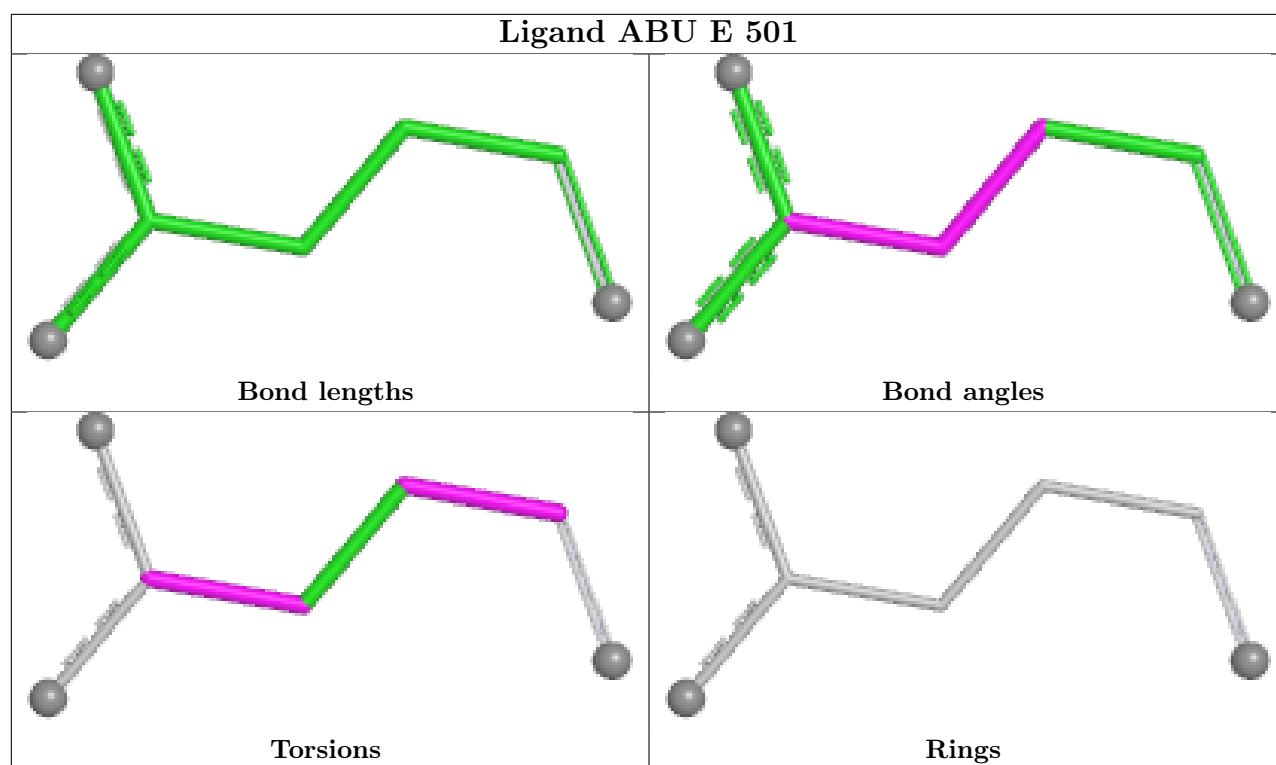
Mol	Chain	Res	Type	Atoms
9	A	504	UND	C5-C6-C7-C8
15	C	602	D10	C4-C5-C6-C7
8	D	501	NAG	O5-C5-C6-O6
8	A	501	NAG	C1-C2-N2-C7
10	A	503	OCT	C2-C3-C4-C5
8	A	501	NAG	C3-C2-N2-C7
12	E	501	ABU	CG-CB-CD-N
12	B	501	ABU	O-C-CG-CB
12	B	501	ABU	OXT-C-CG-CB
10	A	505	OCT	C2-C3-C4-C5
8	A	501	NAG	C4-C5-C6-O6
12	E	501	ABU	OXT-C-CG-CB

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	NAG	1	0
12	E	501	ABU	1	0
12	B	501	ABU	4	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

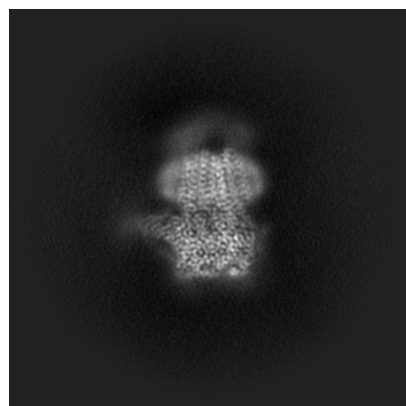
6 Map visualisation [i](#)

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.

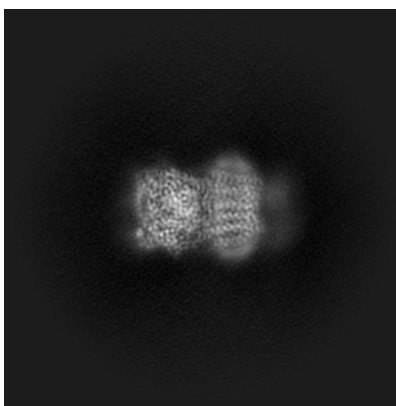
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

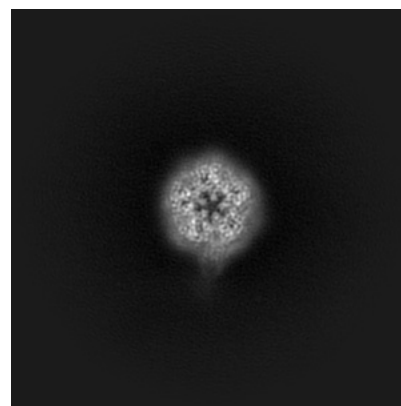
6.1.1 Primary map



X

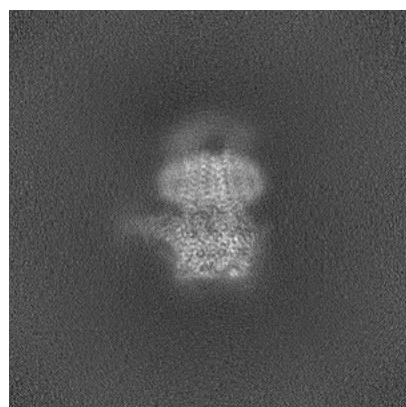


Y

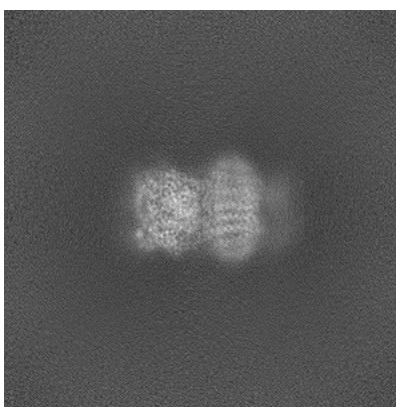


Z

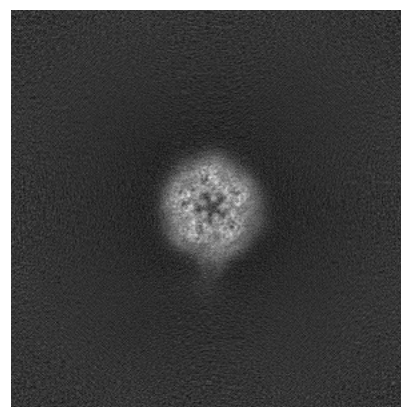
6.1.2 Raw map



X



Y

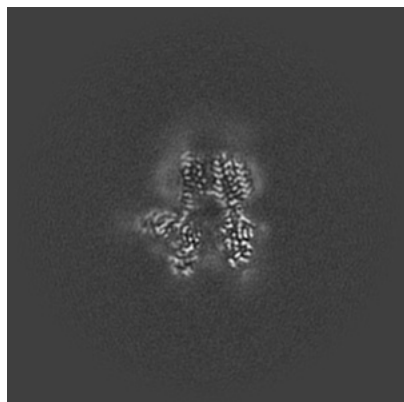


Z

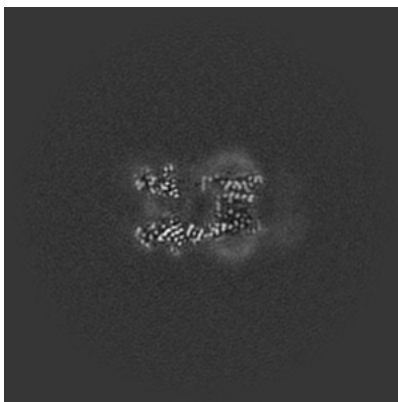
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

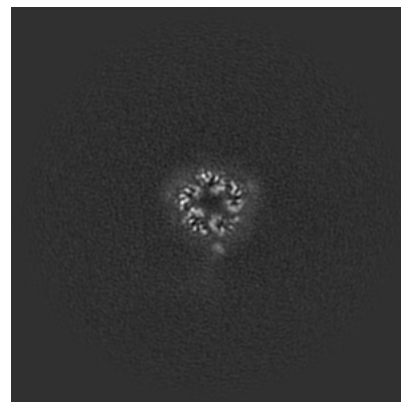
6.2.1 Primary map



X Index: 260

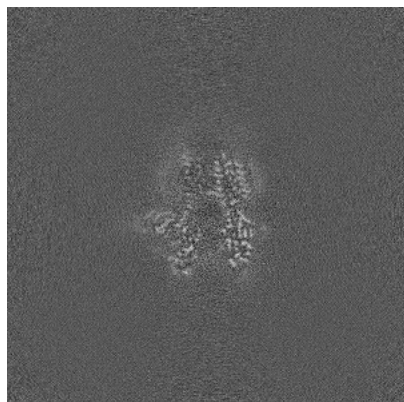


Y Index: 260

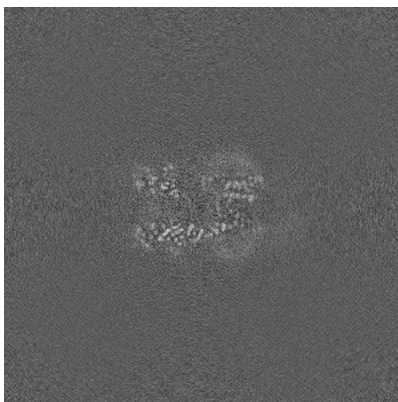


Z Index: 260

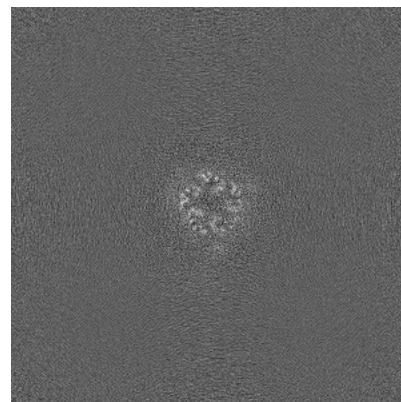
6.2.2 Raw map



X Index: 260



Y Index: 260

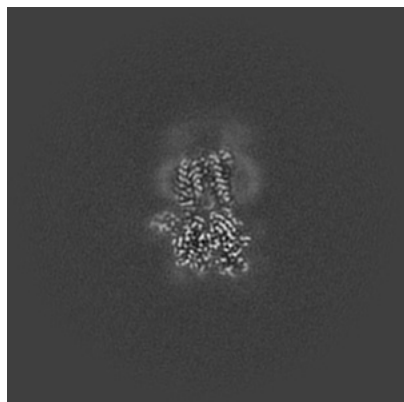


Z Index: 260

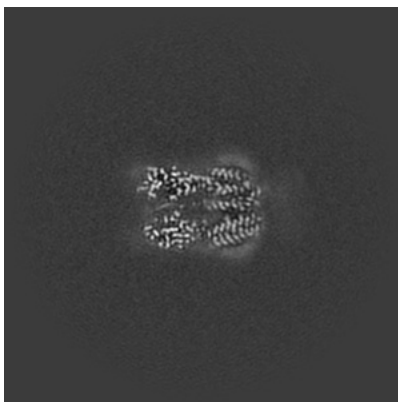
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

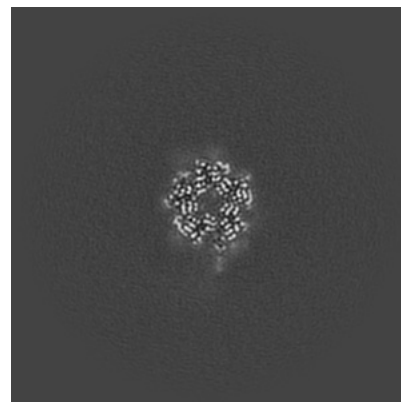
6.3.1 Primary map



X Index: 281

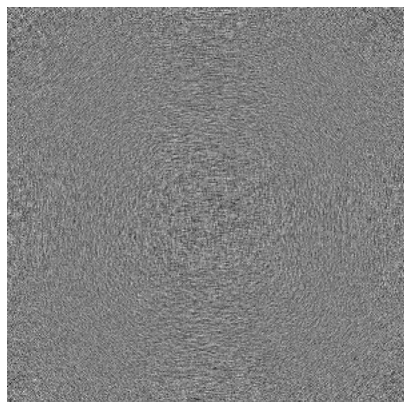


Y Index: 278

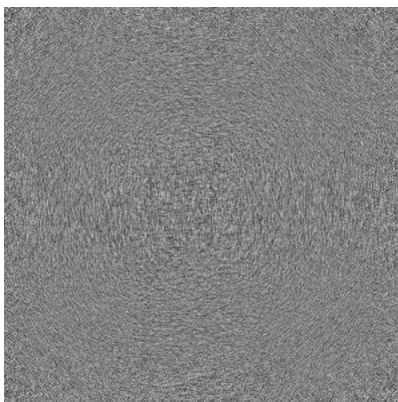


Z Index: 219

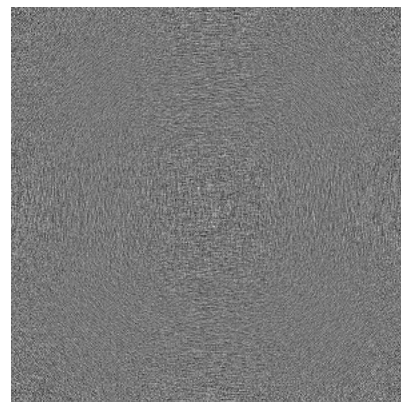
6.3.2 Raw map



X Index: 0



Y Index: 0

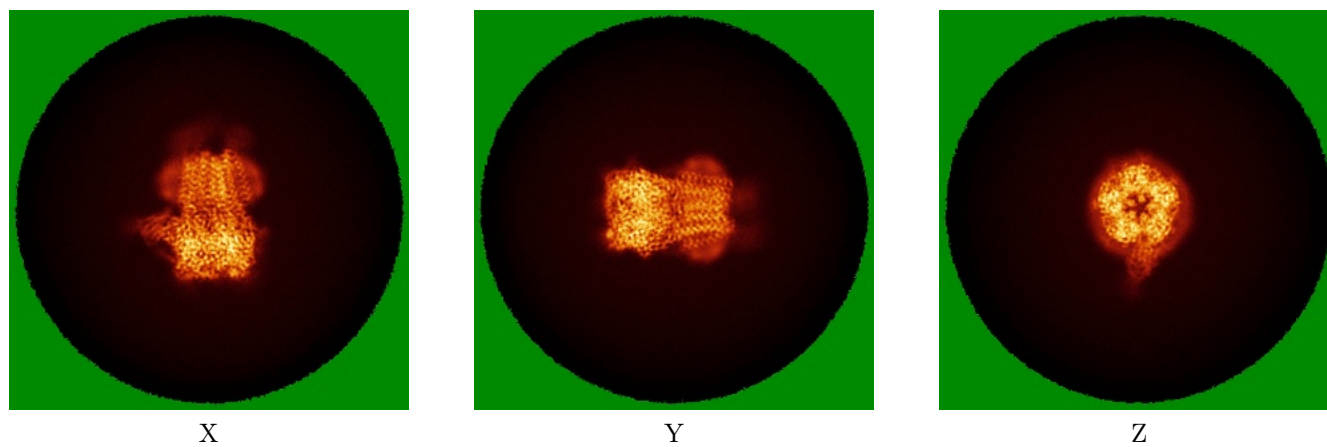


Z Index: 0

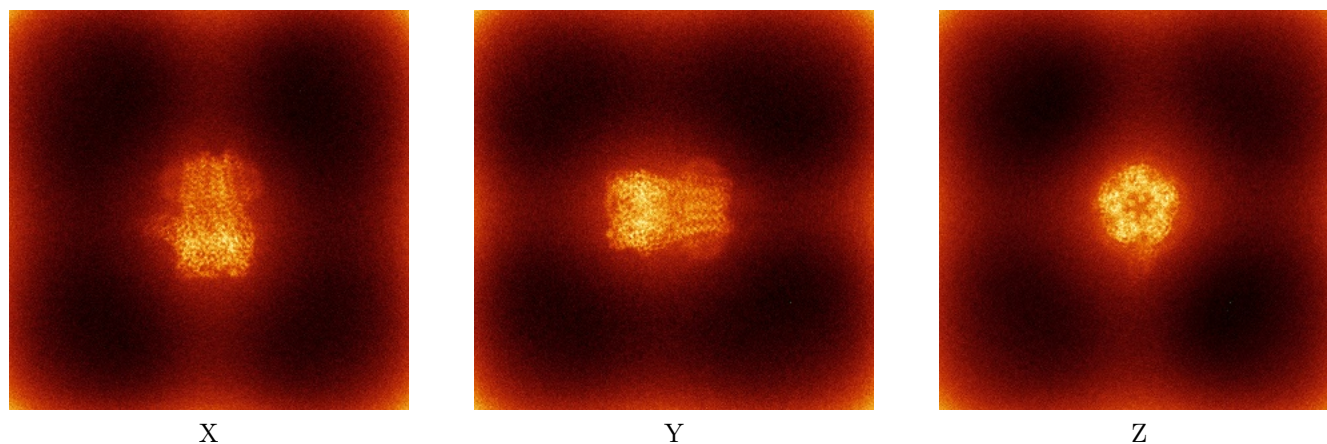
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal 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.

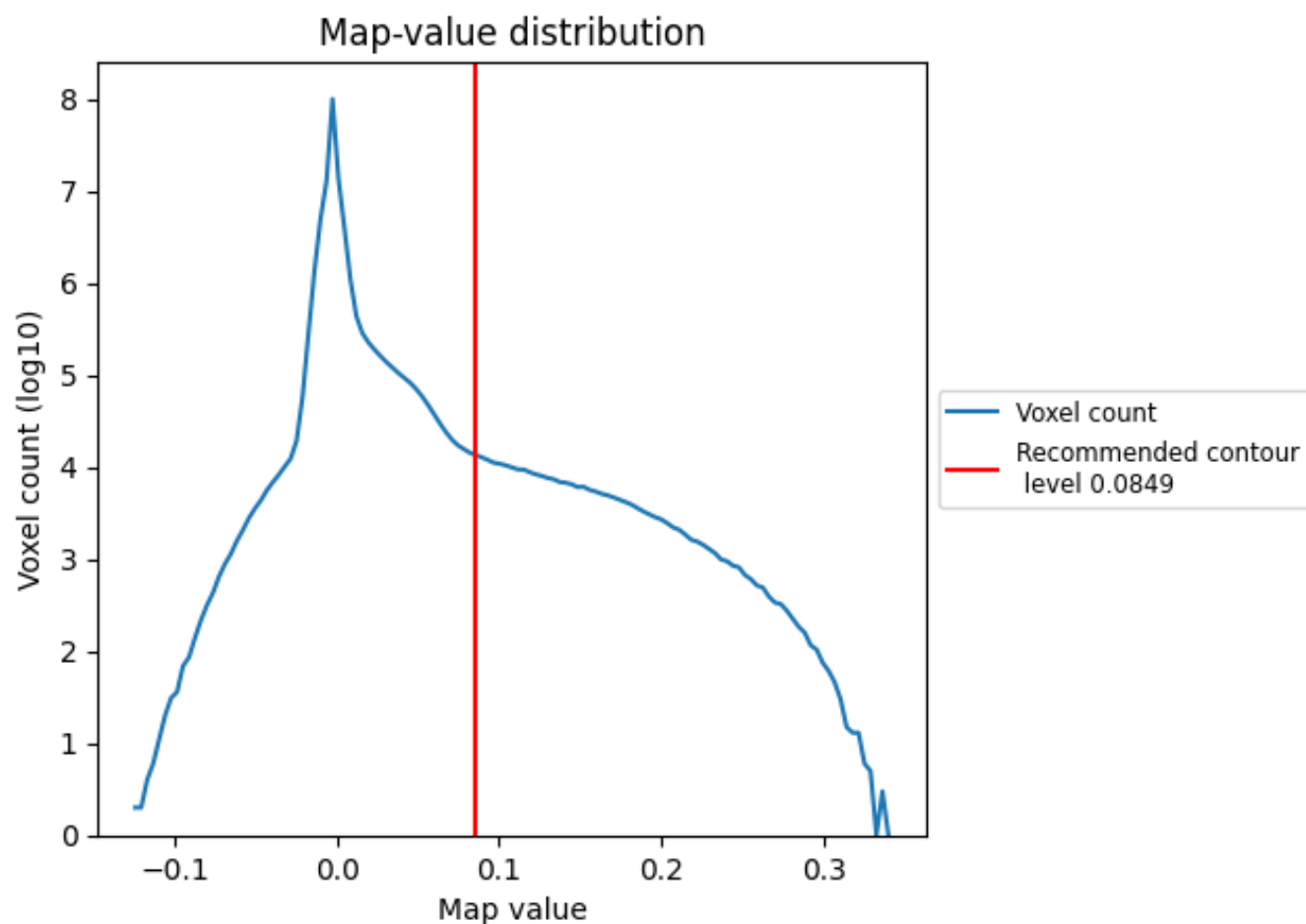
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

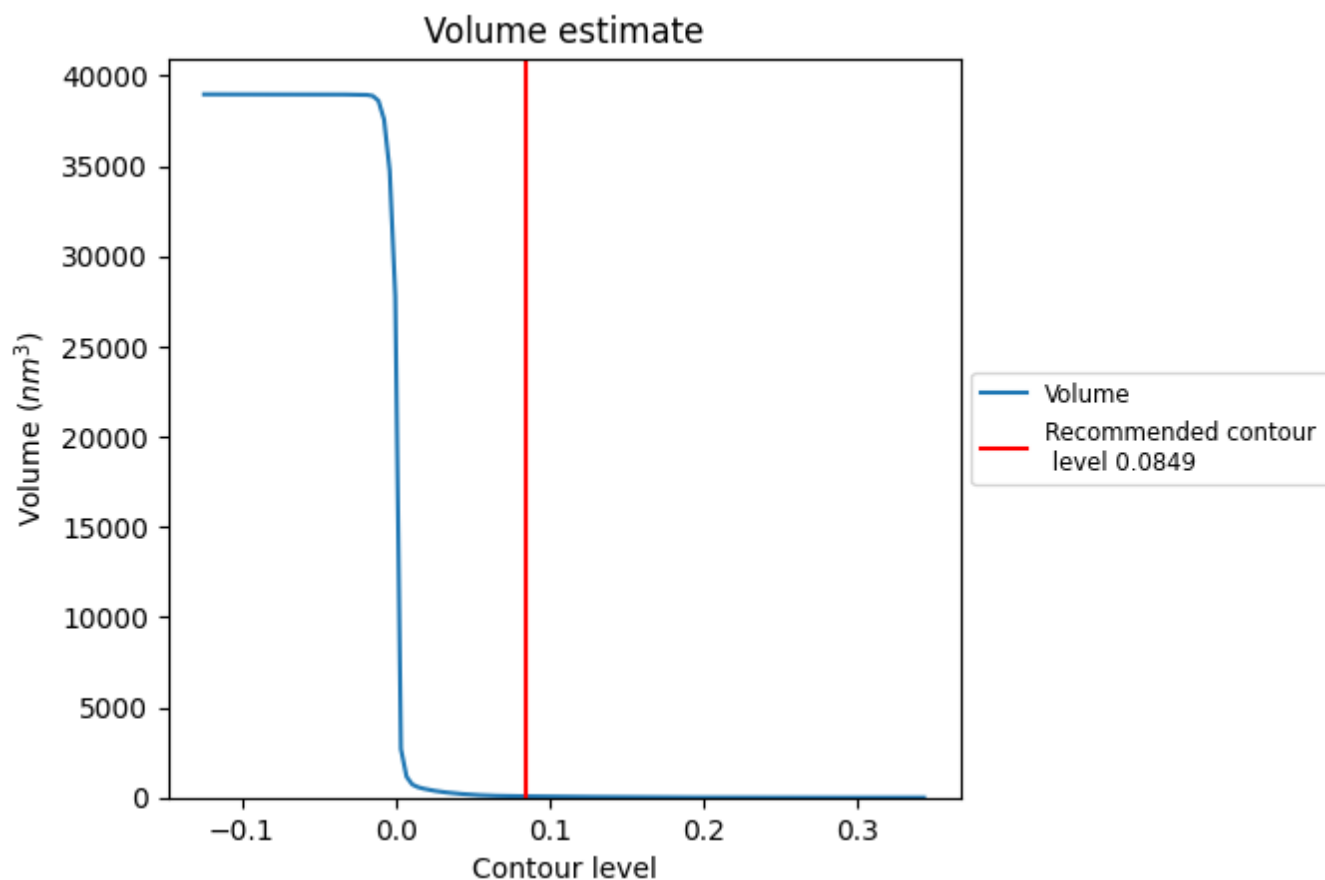
This section contains the results of statistical analysis of the map.

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.

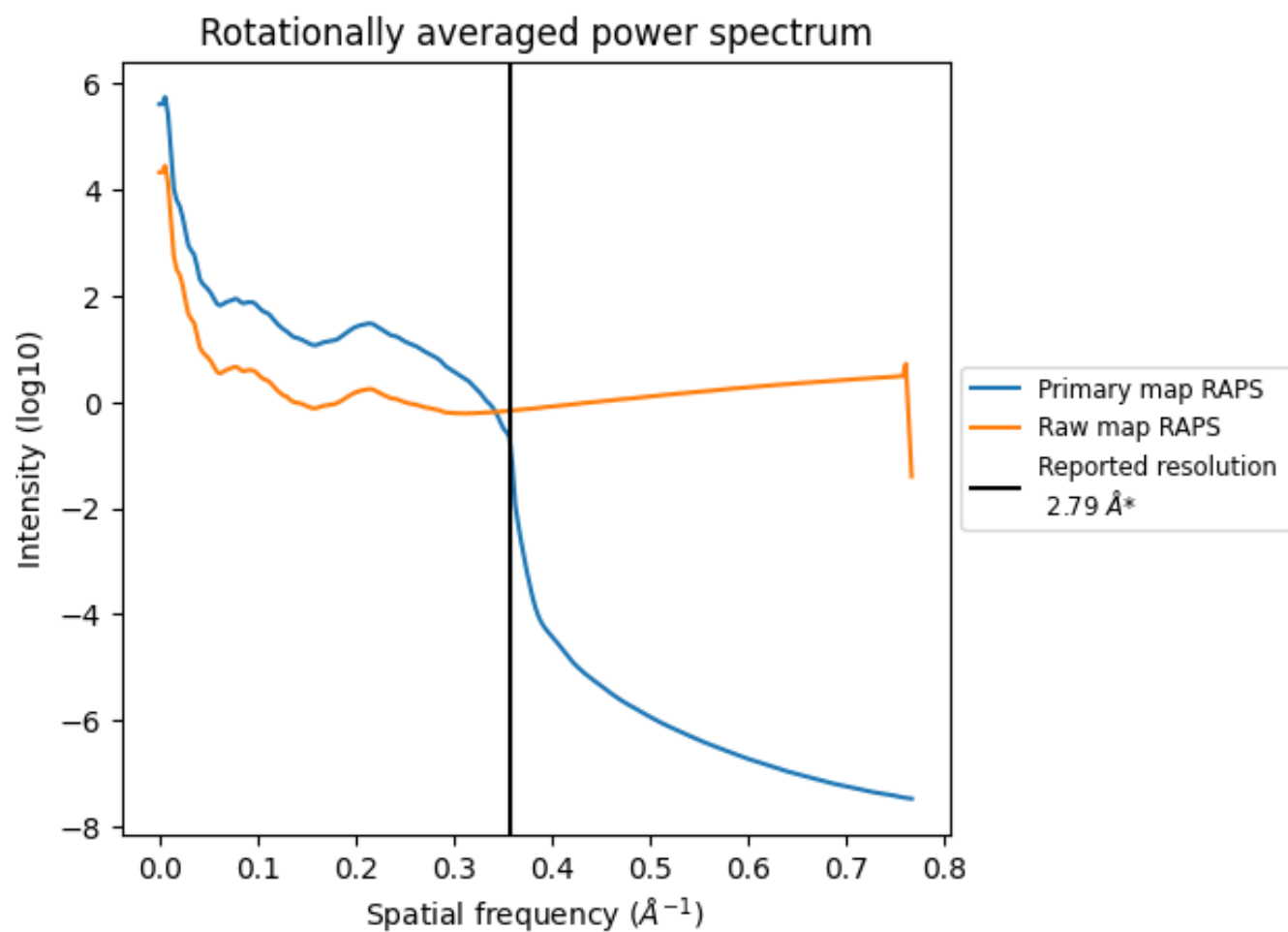
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm³; 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 ⓘ

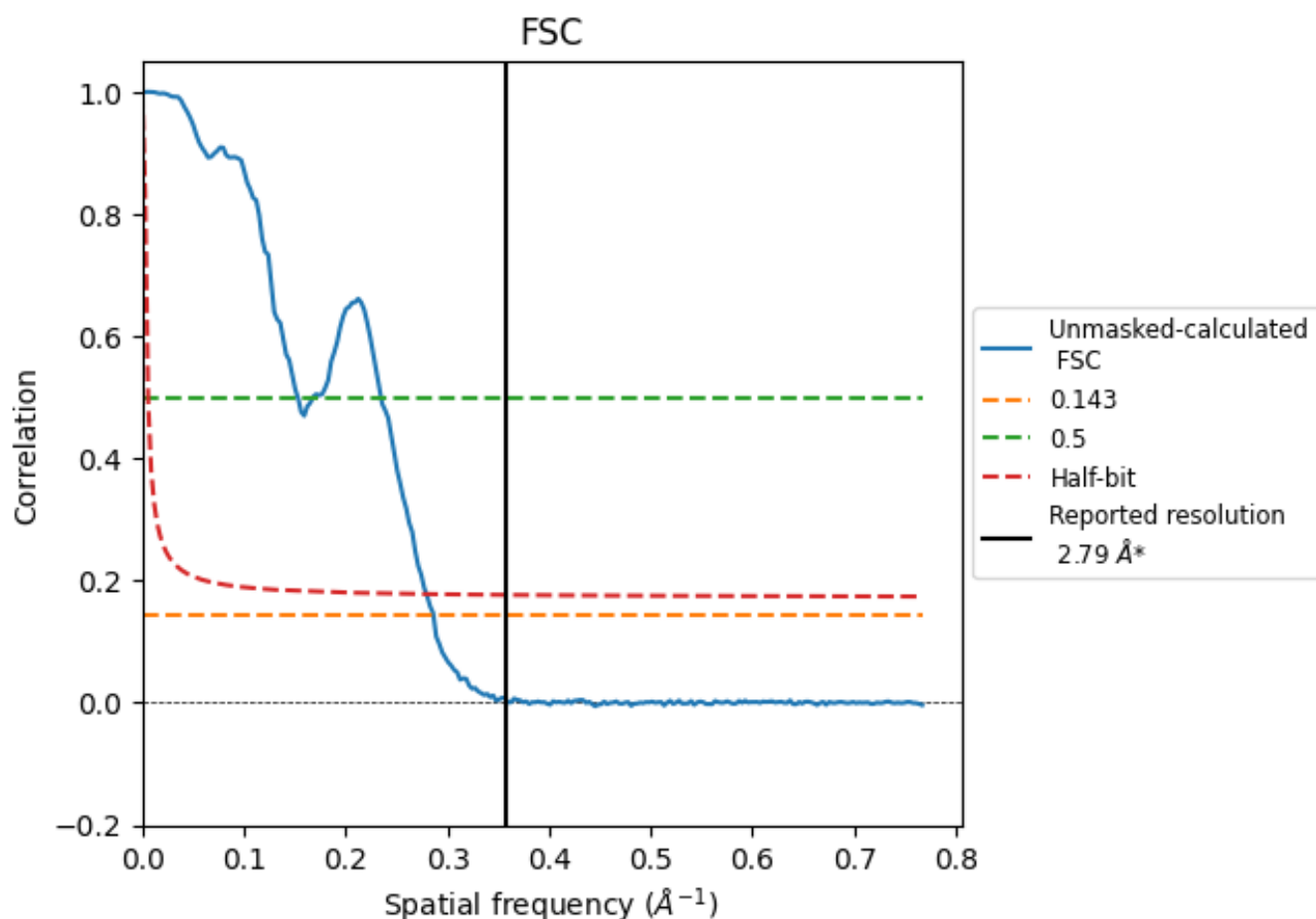


*Reported resolution corresponds to spatial frequency of 0.358 $\text{\AA}^{-1}$

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 $0.358 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

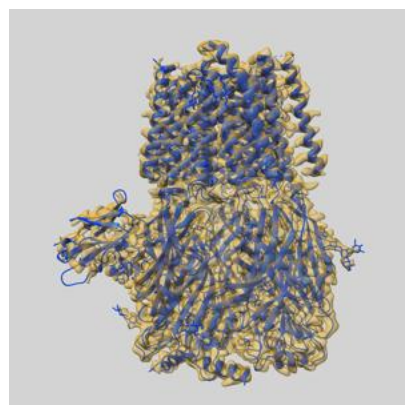
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	6.54	3.58

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

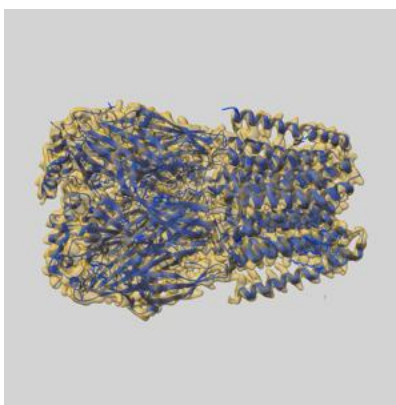
9 Map-model fit [i](#)

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.

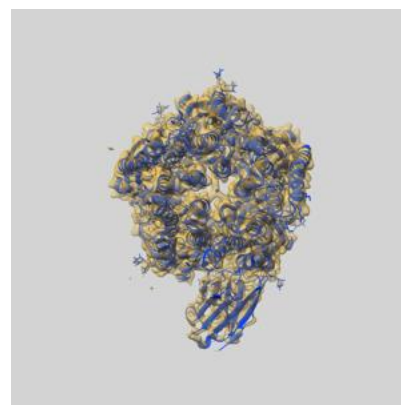
9.1 Map-model overlay [i](#)



X



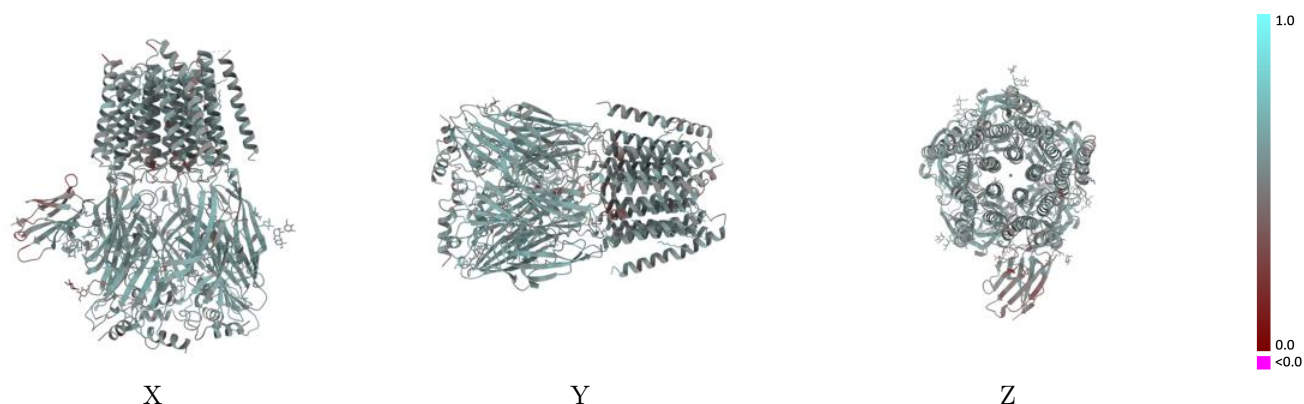
Y



Z

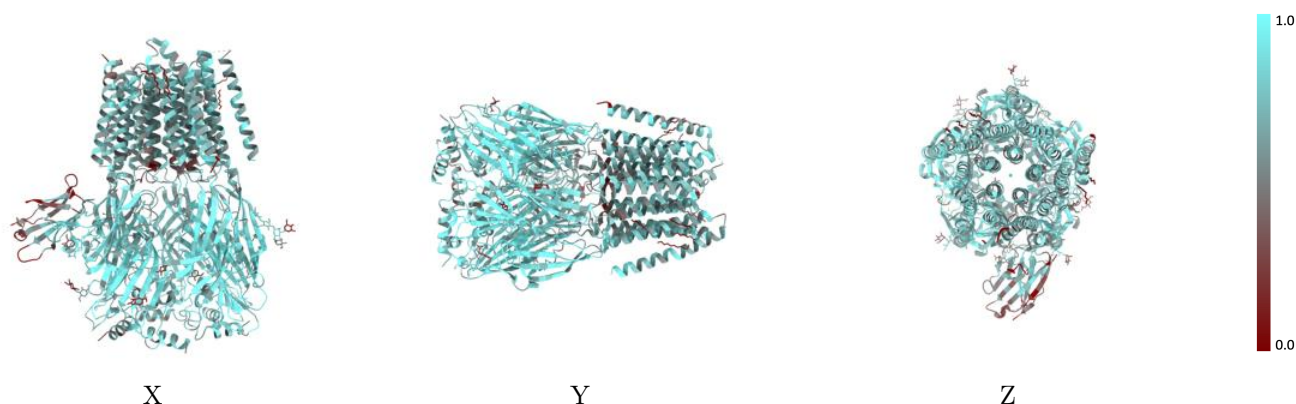
The images above show the 3D surface view of the map at the recommended contour level 0.0849 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



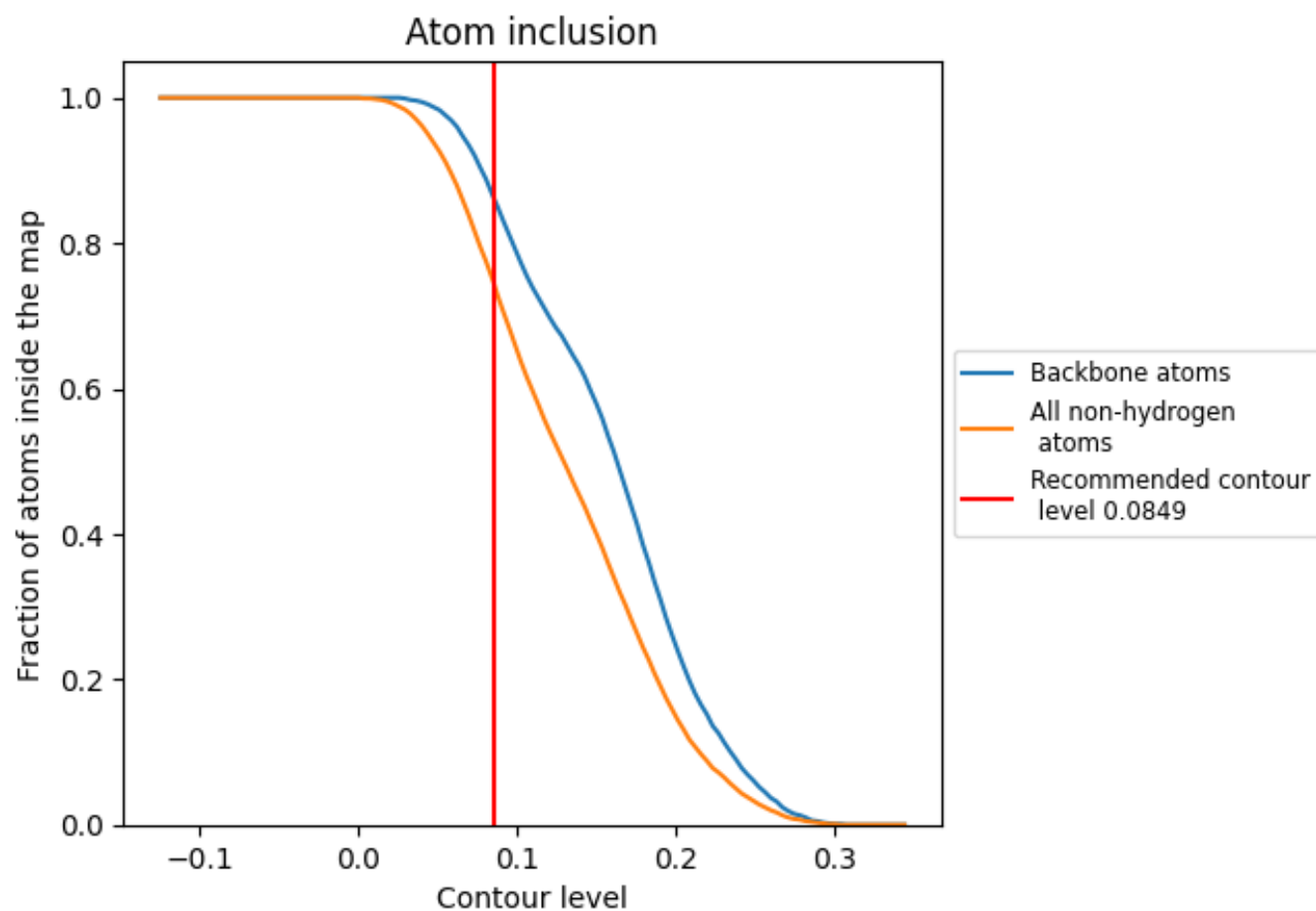
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0849).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.0849) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7480	0.5480
A	0.7740	0.5590
B	0.7640	0.5560
C	0.7300	0.5430
D	0.7710	0.5520
E	0.7800	0.5560
F	0.5480	0.4810
G	0.3570	0.3490
H	0.6800	0.5630
I	0.3930	0.4680
J	0.7210	0.5280
K	0.4290	0.4730
L	0.5900	0.5520

1.0

0.0

<0.0