Full wwPDB EM Validation Report ⓘ

Feb 21, 2022 – 11:00 am GMT

PDB ID	:	7PC0
EMDB ID	:	EMD-13315
Title	:	GABA-A receptor bound by a-Cobratoxin
Authors	:	Kasaragod, V.B.; Miller, P.S.
Deposited on	:	2021-08-03
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

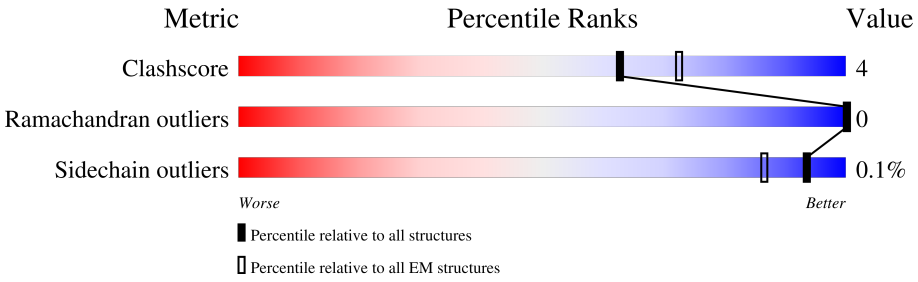
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 3.00 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 <=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	5% 18% 78%
2	A	368	82% 8% 9%
3	B	451	64% 9% 27%
3	C	451	61% 12% 27%
3	E	451	65% 8% 27%
4	D	411	73% 9% 18%
5	K	71	59% 85% 15%
5	L	71	66% 75% 18% 6%

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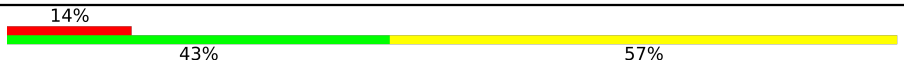
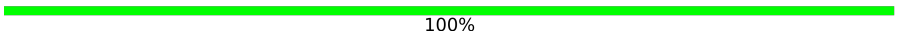
Mol	Chain	Length	Quality of chain
6	G	7	
7	H	2	
8	I	6	
9	J	4	

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
10	NAG	C	501	X	-	-	-
10	NAG	E	501	X	-	-	-
6	NAG	G	1	X	-	-	-
6	BMA	G	3	X	-	-	-
6	MAN	G	4	X	-	-	-
6	MAN	G	5	X	-	-	-
6	MAN	G	6	X	-	-	-
8	MAN	I	5	X	-	-	-
9	NAG	J	1	X	-	-	-
9	NAG	J	2	X	-	-	-
9	BMA	J	3	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 15748 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
			2709	1775	442	476	16		
3	C	330	Total	C	N	O	S	0	0
			2709	1775	442	476	16		
3	E	330	Total	C	N	O	S	0	0
			2709	1775	442	476	16		

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLN	-	expression tag	UNP P28472
B	2	SER	-	expression tag	UNP P28472
B	3	VAL	-	expression tag	UNP P28472
B	4	ASN	-	expression tag	UNP P28472
B	5	ASP	-	expression tag	UNP P28472
B	6	PRO	-	expression tag	UNP P28472
B	7	GLY	-	expression tag	UNP P28472
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	421	ALA	-	linker	UNP P28472
C	1	GLN	-	expression tag	UNP P28472
C	2	SER	-	expression tag	UNP P28472
C	3	VAL	-	expression tag	UNP P28472
C	4	ASN	-	expression tag	UNP P28472
C	5	ASP	-	expression tag	UNP P28472
C	6	PRO	-	expression tag	UNP P28472
C	7	GLY	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1	GLN	-	expression tag	UNP P28472
E	2	SER	-	expression tag	UNP P28472
E	3	VAL	-	expression tag	UNP P28472
E	4	ASN	-	expression tag	UNP P28472
E	5	ASP	-	expression tag	UNP P28472
E	6	PRO	-	expression tag	UNP P28472
E	7	GLY	-	expression tag	UNP P28472
E	308	SER	-	linker	UNP P28472
E	308A	GLN	-	linker	UNP P28472
E	308B	PRO	-	linker	UNP P28472
E	308C	ALA	-	linker	UNP P28472
E	308D	GLY	-	linker	UNP P28472
E	308E	THR	-	linker	UNP P28472
E	308F	ALA	-	linker	UNP P28472
E	308G	ASP	-	linker	UNP P28472
E	308H	LEU	-	linker	UNP P28472
E	308I	GLU	-	linker	UNP P28472
E	308J	ASP	-	linker	UNP P28472
E	308K	ASN	-	linker	UNP P28472
E	308L	TRP	-	linker	UNP P28472
E	308M	GLU	-	linker	UNP P28472
E	308N	THR	-	linker	UNP P28472
E	308O	LEU	-	linker	UNP P28472
E	308P	ASN	-	linker	UNP P28472
E	308Q	ASP	-	linker	UNP P28472
E	308R	ASN	-	linker	UNP P28472
E	308S	LEU	-	linker	UNP P28472
E	308T	LYS	-	linker	UNP P28472
E	308U	VAL	-	linker	UNP P28472
E	308V	ILE	-	linker	UNP P28472
E	308W	GLU	-	linker	UNP P28472
E	308X	LYS	-	linker	UNP P28472
E	308Y	ALA	-	linker	UNP P28472
E	308Z	ASP	-	linker	UNP P28472
E	309A	ASN	-	linker	UNP P28472
E	309B	ALA	-	linker	UNP P28472

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	312I	GLY	-	linker	UNP P28472
E	419	ARG	-	linker	UNP P28472
E	420	ALA	-	linker	UNP P28472
E	421	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 a protein called Alpha-cobratoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	71	Total	C	N	O	S	0	0
			518	316	91	101	10		

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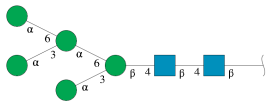
Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	67	Total	C	N	O	S	0	0
			497	304	87	96	10		

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

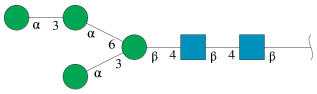


Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 7 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
7	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



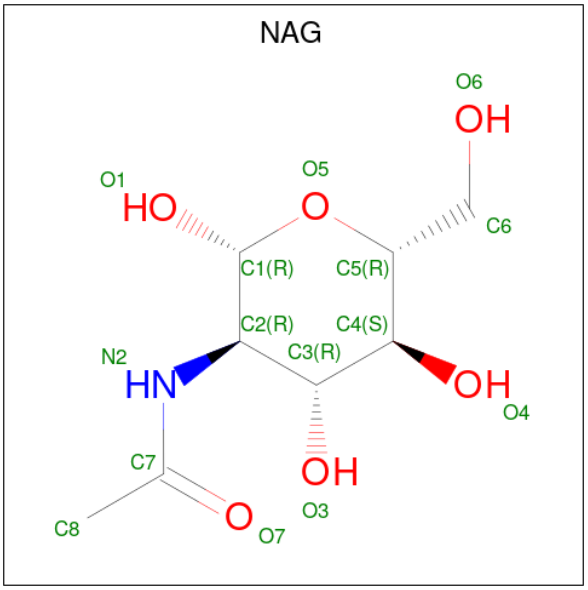
Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 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-gluco

pyranose.

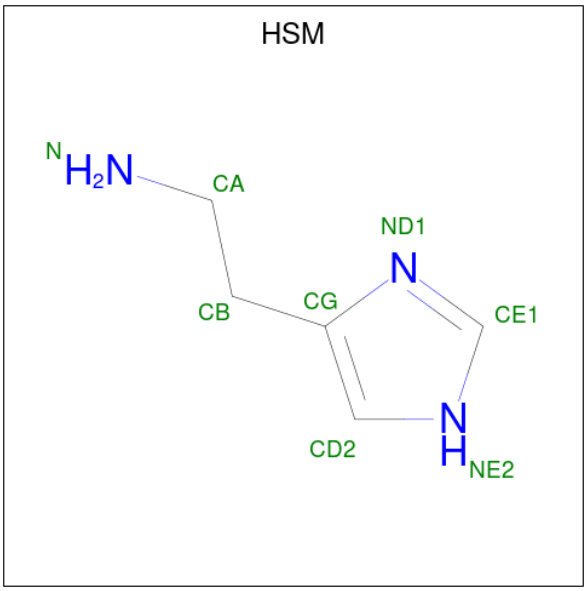
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is HISTAMINE (three-letter code: HSM) (formula: $C_5H_9N_3$) (labeled as "Ligand of Interest" by depositor).

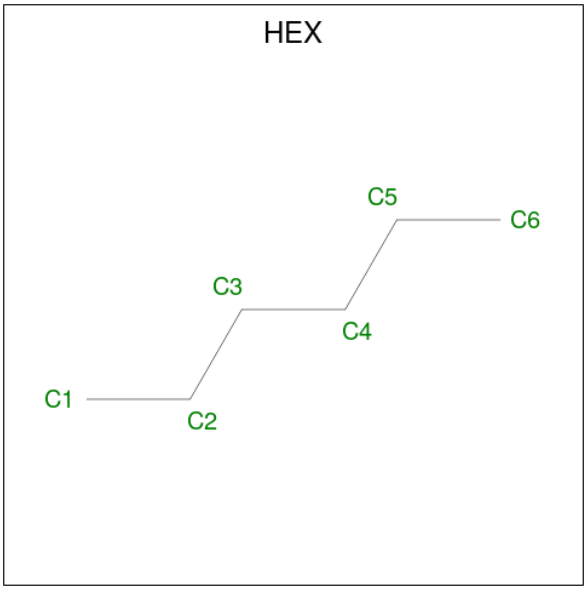


Mol	Chain	Residues	Atoms	AltConf
11	B	1	Total C N 8 5 3	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 13 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).

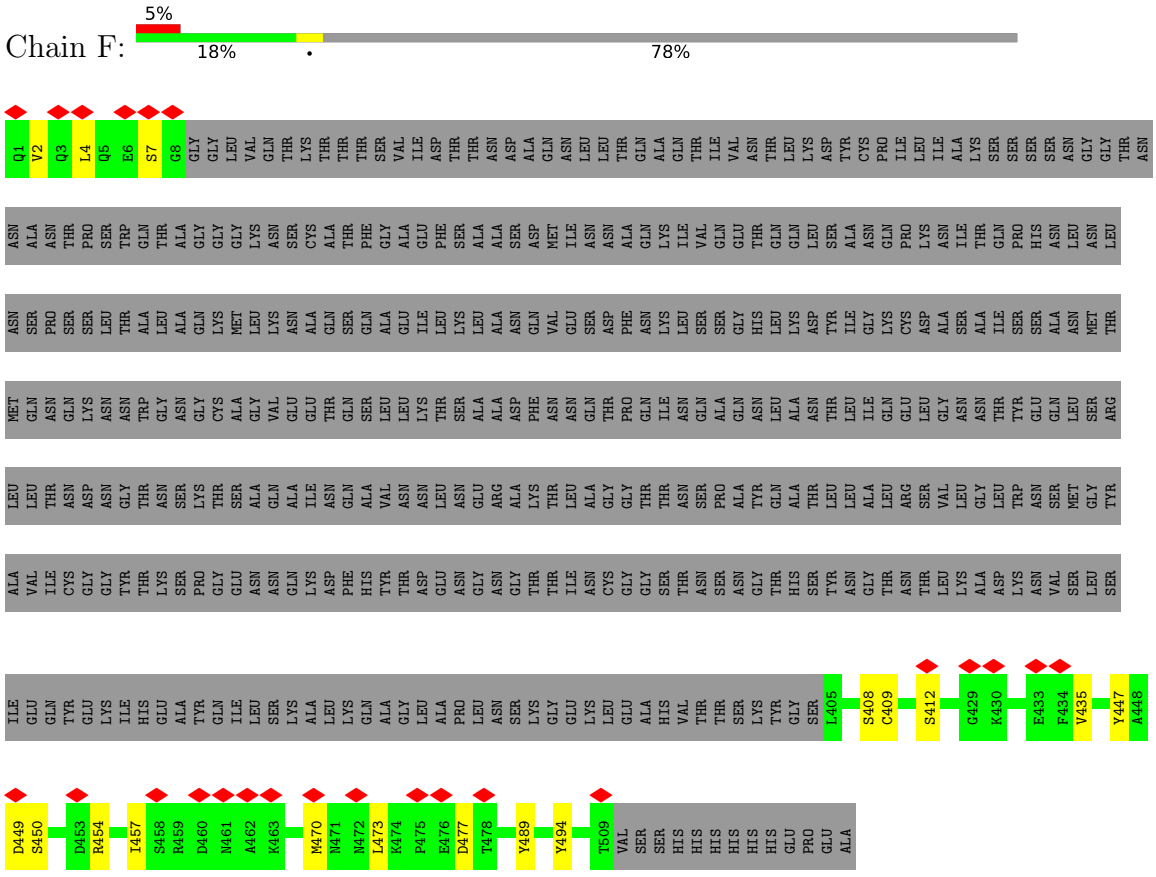


Mol	Chain	Residues	Atoms		AltConf
13	D	1	Total	C	0
			6	6	

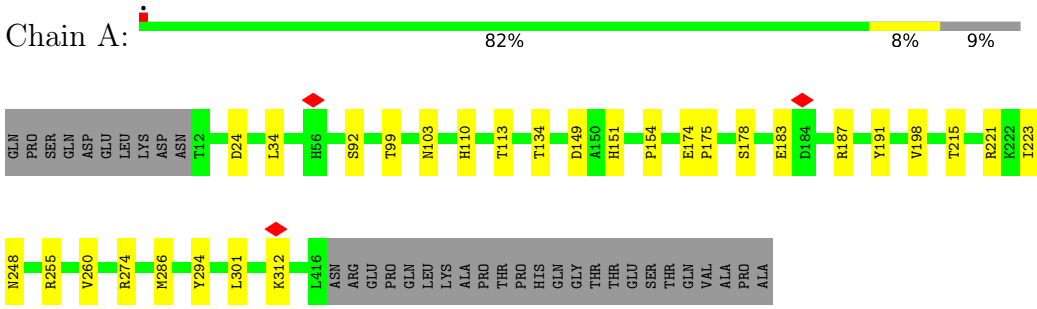
3 Residue-property plots

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

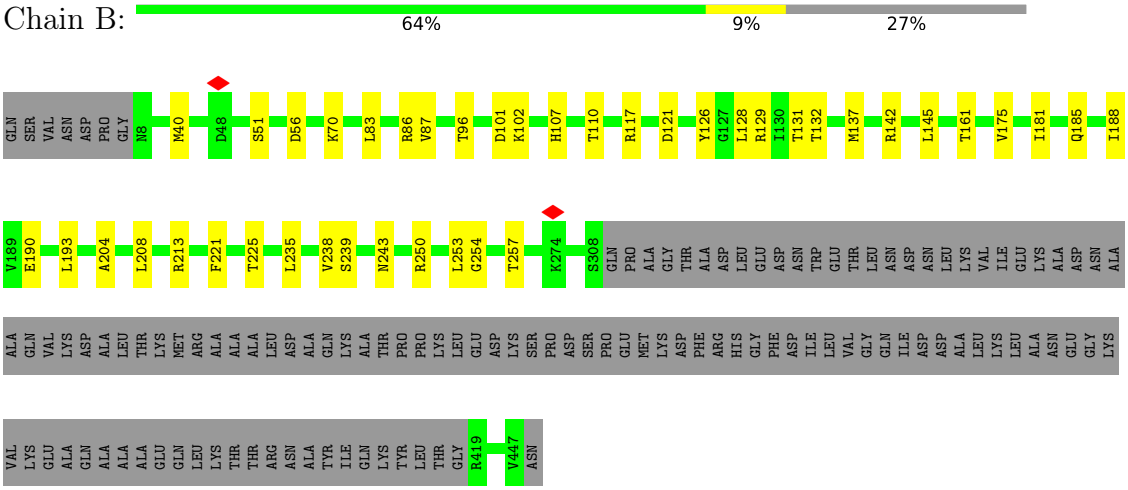


• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1



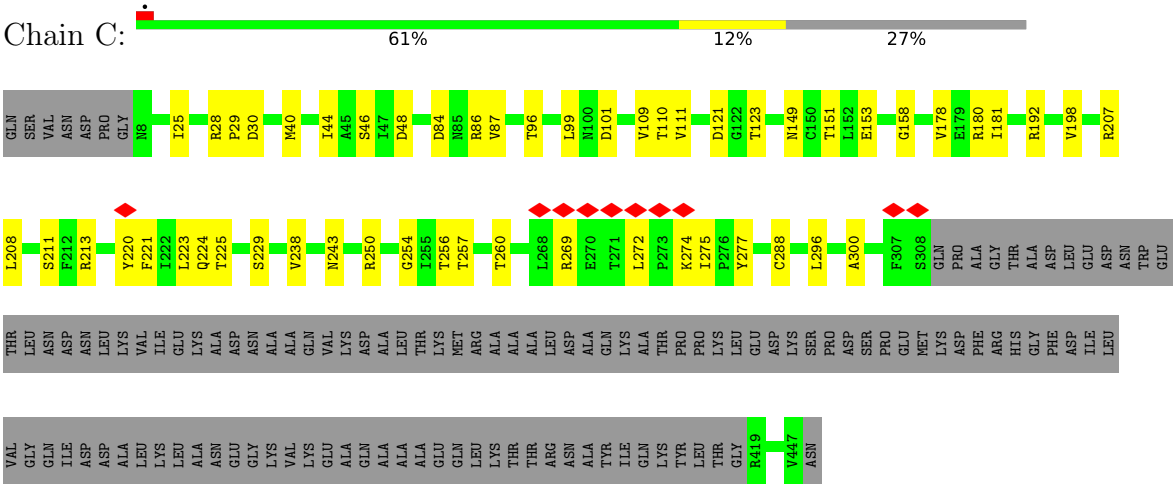
• Molecule 3: Gamma-aminobutyric acid receptor subunit beta-3

Chain B:



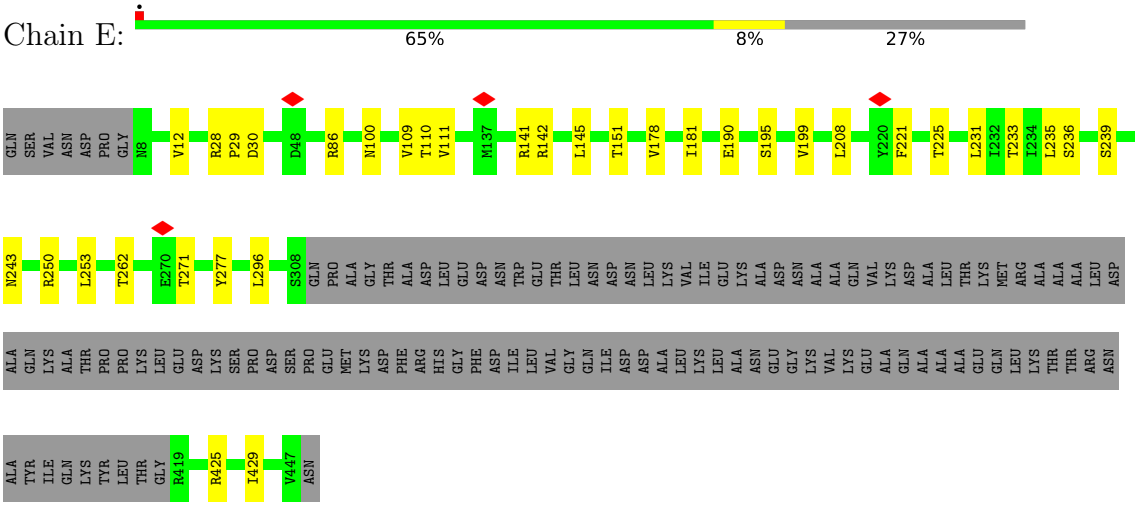
• Molecule 3: Gamma-aminobutyric acid receptor subunit beta-3

Chain C:



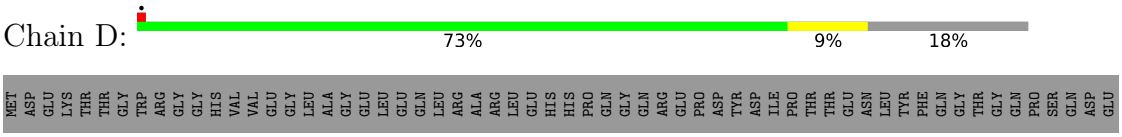
• Molecule 3: Gamma-aminobutyric acid receptor subunit beta-3

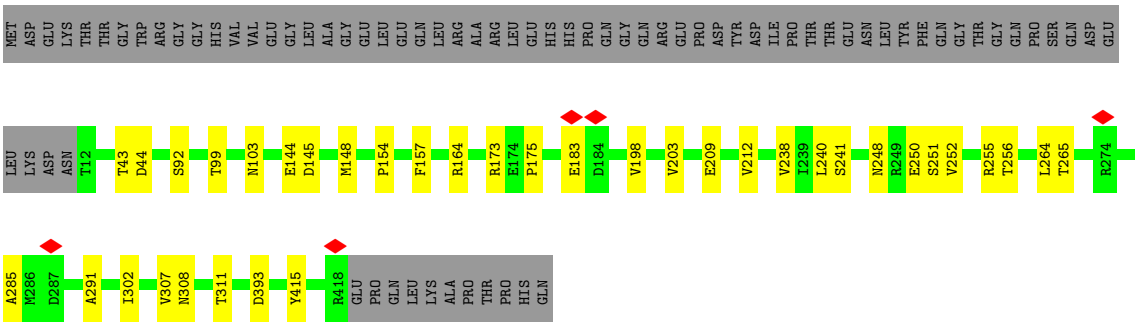
Chain E:



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

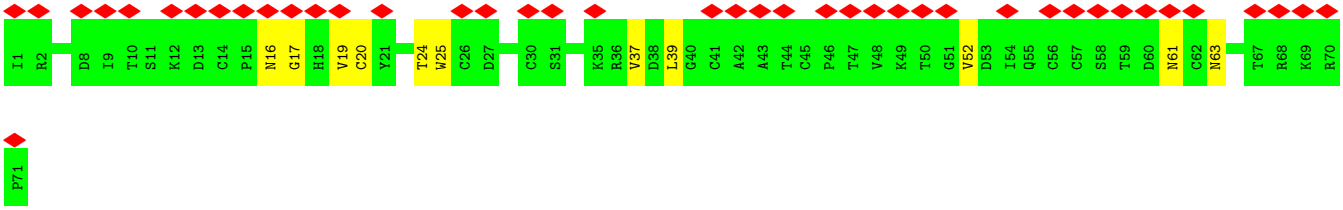
Chain D:





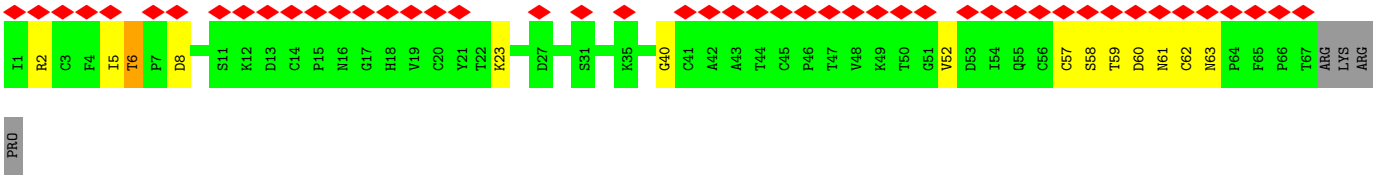
• Molecule 5: Alpha-cobratoxin

Chain K:



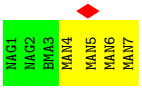
• Molecule 5: Alpha-cobratoxin

Chain L:



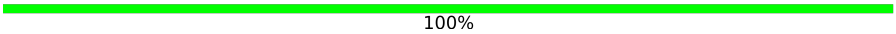
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



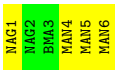
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 8: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 9: 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

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78662	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 ($e^-/Å^2$)	50.69	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.506	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.108	Depositor
Map size (Å)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/916	0.60	0/1240
2	A	0.29	0/2764	0.57	0/3758
3	B	0.28	0/2781	0.57	0/3783
3	C	0.27	0/2781	0.56	0/3783
3	E	0.28	0/2781	0.57	0/3783
4	D	0.27	0/2783	0.58	0/3783
5	K	0.34	0/530	0.66	0/720
5	L	0.27	0/508	0.65	1/691 (0.1%)
All	All	0.28	0/15844	0.58	1/21541 (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
5	K	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	6	THR	CA-CB-CG2	5.15	119.61	112.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	K	19	VAL	Peptide

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Mol	Chain	Res	Type	Group
5	K	61	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	893	0	835	9	0
2	A	2695	0	2696	21	0
3	B	2709	0	2704	28	0
3	C	2709	0	2703	42	0
3	E	2709	0	2703	26	0
4	D	2714	0	2715	24	0
5	K	518	0	475	5	0
5	L	497	0	464	8	0
6	G	83	0	70	0	0
7	H	28	0	25	0	0
8	I	72	0	61	2	0
9	J	50	0	43	2	0
10	A	14	0	13	0	0
10	C	14	0	13	0	0
10	D	14	0	13	0	0
10	E	14	0	13	0	0
11	B	8	0	9	0	0
12	B	1	0	0	0	0
13	D	6	0	14	0	0
All	All	15748	0	15569	139	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 (139) 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:B:221:PHE:O	3:B:225:THR:OG1	2.00	0.77
3:E:221:PHE:O	3:E:225:THR:OG1	2.02	0.74
5:L:8:ASP:OD2	9:J:4:MAN:O3	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:243:ASN:O	3:B:250:ARG:NH1	2.23	0.71
3:B:129:ARG:NH2	3:C:101:ASP:OD1	2.24	0.71
2:A:110:HIS:HE2	2:A:134:THR:HG1	1.37	0.71
3:B:51:SER:OG	3:B:56:ASP:OD1	2.09	0.70
1:F:7:SER:OG	1:F:408:SER:OG	2.09	0.69
3:B:101:ASP:OD2	3:B:132:THR:OG1	2.10	0.69
3:C:110:THR:OG1	4:D:99:THR:O	2.11	0.69
3:C:46:SER:OG	3:C:48:ASP:OD1	2.11	0.67
2:A:191:TYR:OH	2:A:221:ARG:NH2	2.28	0.66
2:A:248:ASN:O	2:A:255:ARG:NH1	2.29	0.66
3:B:235:LEU:HD22	3:C:296:LEU:HD23	1.76	0.66
2:A:92:SER:O	3:E:86:ARG:NH1	2.29	0.65
3:C:229:SER:OG	3:C:288:CYS:SG	2.55	0.64
3:B:107:HIS:NE2	3:B:131:THR:OG1	2.27	0.64
3:B:238:VAL:HG13	3:C:300:ALA:HB2	1.78	0.64
3:C:243:ASN:O	3:C:250:ARG:NH1	2.31	0.63
2:A:34:LEU:HD23	3:E:12:VAL:HG11	1.81	0.63
3:C:198:VAL:HG21	3:C:207:ARG:HE	1.65	0.62
5:K:20:CYS:SG	5:K:63:ASN:ND2	2.73	0.62
2:A:187:ARG:NH1	3:B:137:MET:SD	2.74	0.61
4:D:164:ARG:NH1	4:D:209:GLU:OE1	2.33	0.61
5:K:16:ASN:OD1	5:K:17:GLY:N	2.34	0.61
3:E:141:ARG:NE	3:E:277:TYR:OH	2.34	0.60
3:C:223:LEU:HD21	4:D:291:ALA:HB2	1.84	0.59
3:E:243:ASN:O	3:E:250:ARG:NH1	2.34	0.59
4:D:183:GLU:N	4:D:183:GLU:OE1	2.37	0.58
2:A:260:VAL:HG11	3:E:253:LEU:HA	1.86	0.57
2:A:175:PRO:O	2:A:198:VAL:HG21	2.05	0.57
3:C:256:THR:O	3:C:260:THR:HG23	2.05	0.57
1:F:2:VAL:HG13	1:F:412:SER:O	2.06	0.56
2:A:113:THR:OG1	3:B:96:THR:O	2.22	0.55
5:L:57:CYS:SG	5:L:58:SER:N	2.78	0.55
4:D:44:ASP:OD2	4:D:173:ARG:NH1	2.40	0.55
1:F:4:LEU:HD12	1:F:409:CYS:SG	2.47	0.54
3:E:296:LEU:HD23	4:D:240:LEU:HD22	1.89	0.54
3:C:224:GLN:N	3:C:224:GLN:OE1	2.41	0.54
3:E:100:ASN:ND2	3:E:151:THR:O	2.41	0.53
1:F:454:ARG:NH2	1:F:477:ASP:OD2	2.41	0.53
3:B:126:TYR:CE2	3:B:128:LEU:HD11	2.43	0.52
5:L:62:CYS:SG	5:L:63:ASN:ND2	2.82	0.52
3:B:175:VAL:HG21	3:B:193:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:175:VAL:CG2	3:B:193:LEU:HD21	2.40	0.52
3:C:269:ARG:HE	3:C:272:LEU:HD12	1.75	0.51
2:A:230:THR:HG21	2:A:286:MET:SD	2.51	0.51
3:B:101:ASP:OD1	3:B:102:LYS:N	2.44	0.51
3:B:117:ARG:NH2	3:C:158:GLY:O	2.43	0.51
3:B:181:ILE:HG21	3:B:188:ILE:HD11	1.93	0.51
5:K:39:LEU:HD22	5:K:63:ASN:HB3	1.92	0.51
4:D:308:ASN:O	4:D:311:THR:HG22	2.11	0.51
2:A:301:LEU:HD23	3:E:235:LEU:HD22	1.93	0.51
1:F:435:VAL:HG21	1:F:494:TYR:HA	1.93	0.50
3:E:178:VAL:HA	3:E:181:ILE:HD12	1.93	0.50
2:A:183:GLU:N	2:A:183:GLU:OE1	2.45	0.50
4:D:145:ASP:O	4:D:148:MET:N	2.44	0.50
4:D:103:ASN:ND2	4:D:154:PRO:O	2.45	0.50
3:C:86:ARG:NH1	4:D:92:SER:O	2.43	0.49
3:C:109:VAL:O	3:C:110:THR:OG1	2.30	0.49
4:D:175:PRO:O	4:D:198:VAL:HG21	2.12	0.49
4:D:238:VAL:O	4:D:241:SER:OG	2.17	0.49
3:B:185:GLN:OE1	3:B:185:GLN:N	2.42	0.48
2:A:103:ASN:ND2	2:A:154:PRO:O	2.46	0.48
2:A:174:GLU:O	2:A:178:SER:OG	2.15	0.48
3:B:110:THR:OG1	3:C:96:THR:O	2.31	0.48
3:C:110:THR:O	3:C:111:VAL:HG13	2.13	0.48
3:E:190:GLU:OE1	9:J:1:NAG:H81	2.13	0.48
5:L:5:ILE:HG23	5:L:40:GLY:HA2	1.95	0.48
3:B:126:TYR:CZ	3:B:128:LEU:HD11	2.49	0.48
3:E:262:THR:HG21	4:D:265:THR:CG2	2.44	0.47
4:D:252:VAL:O	4:D:256:THR:OG1	2.22	0.47
3:B:83:LEU:HB3	3:B:87:VAL:HG21	1.95	0.47
3:C:84:ASP:OD1	3:C:87:VAL:HG23	2.15	0.47
3:B:190:GLU:OE2	3:B:213:ARG:NH2	2.47	0.47
3:C:221:PHE:O	3:C:225:THR:OG1	2.32	0.47
2:A:99:THR:O	3:E:110:THR:OG1	2.33	0.47
2:A:24:ASP:OD1	2:A:24:ASP:N	2.47	0.47
1:F:447:TYR:OH	1:F:457:ILE:N	2.45	0.47
3:B:254:GLY:O	3:B:257:THR:OG1	2.29	0.47
3:C:44:ILE:HG21	3:C:181:ILE:HD11	1.97	0.47
3:C:149:ASN:OD1	3:C:211:SER:OG	2.32	0.47
3:E:109:VAL:O	3:E:110:THR:OG1	2.29	0.46
3:C:192:ARG:NH1	8:I:1:NAG:O7	2.48	0.46
3:E:425:ARG:O	3:E:429:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:285:ALA:HB2	4:D:415:TYR:CE2	2.51	0.45
1:F:449:ASP:OD1	1:F:450:SER:N	2.48	0.45
3:E:110:THR:O	3:E:111:VAL:HG13	2.16	0.45
5:L:60:ASP:OD1	5:L:61:ASN:N	2.49	0.45
3:C:254:GLY:O	3:C:257:THR:OG1	2.33	0.45
3:E:239:SER:HA	3:E:253:LEU:HD23	1.99	0.45
4:D:250:GLU:N	4:D:250:GLU:OE1	2.49	0.45
3:C:121:ASP:OD1	3:C:123:THR:OG1	2.25	0.45
3:E:109:VAL:O	3:E:109:VAL:HG13	2.17	0.45
4:D:248:ASN:ND2	4:D:251:SER:OG	2.50	0.45
4:D:248:ASN:O	4:D:255:ARG:NH1	2.46	0.45
2:A:149:ASP:OD2	2:A:151:HIS:NE2	2.50	0.44
3:C:238:VAL:HG21	4:D:302:ILE:HD13	1.98	0.44
2:A:274:ARG:NH1	3:E:271:THR:HG21	2.31	0.44
3:C:40:MET:HG3	3:C:208:LEU:HD12	2.00	0.44
3:C:28:ARG:NH1	3:C:30:ASP:O	2.51	0.44
3:C:153:GLU:OE1	3:C:207:ARG:NH1	2.51	0.44
4:D:144:GLU:N	4:D:144:GLU:OE1	2.50	0.44
3:B:70:LYS:NZ	3:B:121:ASP:O	2.45	0.44
3:E:195:SER:HA	3:E:208:LEU:HD23	1.99	0.44
3:C:28:ARG:NH1	3:C:29:PRO:O	2.50	0.44
3:E:28:ARG:NH1	3:E:29:PRO:O	2.50	0.44
1:F:489:TYR:O	3:C:207:ARG:NH2	2.51	0.43
3:B:40:MET:HG3	3:B:208:LEU:HD12	2.00	0.43
3:C:178:VAL:HA	3:C:181:ILE:HD12	2.00	0.43
2:A:294:TYR:HE2	3:E:231:LEU:HD12	1.81	0.43
3:B:142:ARG:O	3:B:145:LEU:N	2.51	0.43
3:C:220:TYR:O	3:C:224:GLN:NE2	2.48	0.43
3:C:213:ARG:HB2	8:I:1:NAG:H82	2.00	0.43
3:C:269:ARG:O	3:C:274:LYS:NZ	2.48	0.43
3:C:260:THR:HG22	4:D:264:LEU:HD13	2.01	0.43
4:D:307:VAL:HG21	4:D:393:ASP:OD1	2.18	0.42
5:K:24:THR:HG23	5:K:37:VAL:HG12	2.02	0.42
3:B:161:THR:CG2	3:B:204:ALA:HB3	2.49	0.42
3:C:151:THR:HG22	3:C:211:SER:CB	2.50	0.42
3:C:99:LEU:HD22	3:C:207:ARG:HH12	1.85	0.42
3:E:142:ARG:O	3:E:145:LEU:N	2.52	0.42
5:L:23:LYS:HG2	5:L:52:VAL:HG21	2.01	0.42
3:C:109:VAL:O	3:C:109:VAL:HG13	2.19	0.42
2:A:198:VAL:HG12	2:A:215:THR:HG23	2.00	0.42
2:A:223:ILE:HG12	2:A:227:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:199:VAL:HG21	5:L:6:THR:CG2	2.51	0.41
4:D:43:THR:HG21	4:D:157:PHE:CE2	2.56	0.41
3:B:86:ARG:HE	3:C:25:ILE:HD12	1.85	0.41
5:L:2:ARG:N	5:L:59:THR:O	2.53	0.41
3:E:28:ARG:NH1	3:E:30:ASP:O	2.54	0.41
3:C:149:ASN:O	3:C:151:THR:HG23	2.21	0.41
1:F:470:MET:HB3	1:F:473:LEU:HD21	2.02	0.41
3:E:233:THR:O	3:E:236:SER:OG	2.28	0.41
3:B:239:SER:HA	3:B:253:LEU:HD23	2.03	0.40
3:C:198:VAL:HG21	3:C:207:ARG:NE	2.33	0.40
4:D:203:VAL:HG21	4:D:212:VAL:HG21	2.03	0.40
3:C:275:ILE:O	3:C:277:TYR:N	2.52	0.40
5:K:25:TRP:HB3	5:K:52:VAL:HG23	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%)	102 (94%)	7 (6%)	0	100	100
2	A	332/368 (90%)	317 (96%)	15 (4%)	0	100	100
3	B	326/451 (72%)	315 (97%)	11 (3%)	0	100	100
3	C	326/451 (72%)	312 (96%)	14 (4%)	0	100	100
3	E	326/451 (72%)	308 (94%)	18 (6%)	0	100	100
4	D	334/411 (81%)	317 (95%)	17 (5%)	0	100	100
5	K	69/71 (97%)	54 (78%)	15 (22%)	0	100	100
5	L	65/71 (92%)	56 (86%)	9 (14%)	0	100	100
All	All	1887/2796 (68%)	1781 (94%)	106 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	92/430 (21%)	92 (100%)	0	100	100
2	A	296/326 (91%)	295 (100%)	1 (0%)	92	97
3	B	296/393 (75%)	296 (100%)	0	100	100
3	C	296/393 (75%)	295 (100%)	1 (0%)	92	97
3	E	296/393 (75%)	296 (100%)	0	100	100
4	D	298/362 (82%)	298 (100%)	0	100	100
5	K	60/64 (94%)	60 (100%)	0	100	100
5	L	59/64 (92%)	59 (100%)	0	100	100
All	All	1693/2425 (70%)	1691 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	312	LYS
3	C	180	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

19 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	G	1	6,3	14,14,15	0.27	0	17,19,21	0.49	0
6	NAG	G	2	6	14,14,15	0.21	0	17,19,21	0.41	0
6	BMA	G	3	6	11,11,12	0.56	0	15,15,17	0.80	0
6	MAN	G	4	6	11,11,12	0.69	0	15,15,17	1.13	1 (6%)
6	MAN	G	5	6	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
6	MAN	G	6	6	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
6	MAN	G	7	6	11,11,12	0.67	0	15,15,17	1.08	2 (13%)
7	NAG	H	1	7,3	14,14,15	0.31	0	17,19,21	0.47	0
7	NAG	H	2	7	14,14,15	0.21	0	17,19,21	0.46	0
8	NAG	I	1	8,3	14,14,15	0.52	0	17,19,21	0.46	0
8	NAG	I	2	8	14,14,15	0.21	0	17,19,21	0.48	0
8	BMA	I	3	8	11,11,12	0.59	0	15,15,17	0.77	0
8	MAN	I	4	8	11,11,12	0.70	0	15,15,17	1.00	2 (13%)
8	MAN	I	5	8	11,11,12	0.67	0	15,15,17	1.10	2 (13%)
8	MAN	I	6	8	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
9	NAG	J	1	3,9	14,14,15	0.43	0	17,19,21	0.73	1 (5%)
9	NAG	J	2	9	14,14,15	0.41	0	17,19,21	0.98	1 (5%)
9	BMA	J	3	9	11,11,12	0.62	0	15,15,17	0.77	0
9	MAN	J	4	9	11,11,12	0.64	0	15,15,17	0.99	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
6	NAG	G	1	6,3	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	1/1/4/5	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	2	NAG	C1-O5-C5	3.65	117.13	112.19
9	J	1	NAG	C1-O5-C5	2.64	115.77	112.19
6	G	4	MAN	O2-C2-C3	-2.50	105.13	110.14
6	G	6	MAN	C1-O5-C5	2.47	115.54	112.19
8	I	5	MAN	C1-O5-C5	2.43	115.48	112.19
9	J	4	MAN	C1-O5-C5	2.42	115.47	112.19
8	I	6	MAN	C1-O5-C5	2.41	115.46	112.19
6	G	7	MAN	C1-O5-C5	2.40	115.44	112.19
6	G	5	MAN	C1-O5-C5	2.35	115.38	112.19
8	I	4	MAN	O2-C2-C3	-2.33	105.47	110.14
8	I	6	MAN	O2-C2-C3	-2.29	105.55	110.14
8	I	5	MAN	O2-C2-C3	-2.29	105.55	110.14
6	G	7	MAN	O2-C2-C3	-2.26	105.62	110.14
9	J	4	MAN	O2-C2-C3	-2.23	105.66	110.14
6	G	6	MAN	O2-C2-C3	-2.22	105.69	110.14
6	G	5	MAN	O2-C2-C3	-2.21	105.71	110.14
8	I	4	MAN	C1-O5-C5	2.09	115.02	112.19

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	G	1	NAG	C1
6	G	3	BMA	C1
6	G	4	MAN	C1
6	G	5	MAN	C1
6	G	6	MAN	C1
8	I	5	MAN	C1
9	J	1	NAG	C1
9	J	2	NAG	C1
9	J	3	BMA	C1

All (18) torsion outliers are listed below:

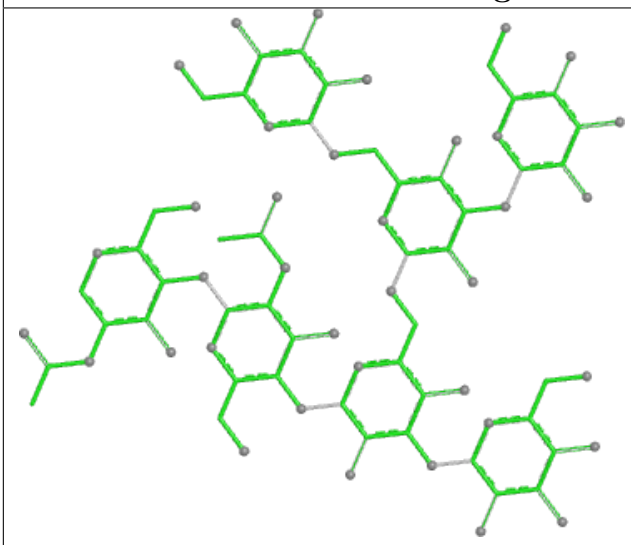
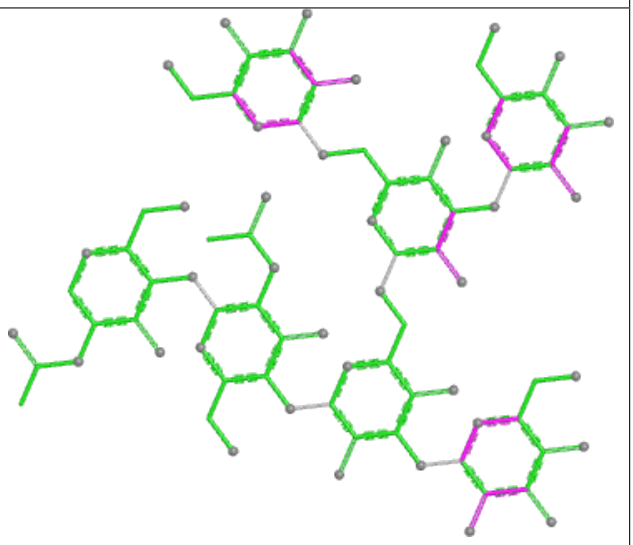
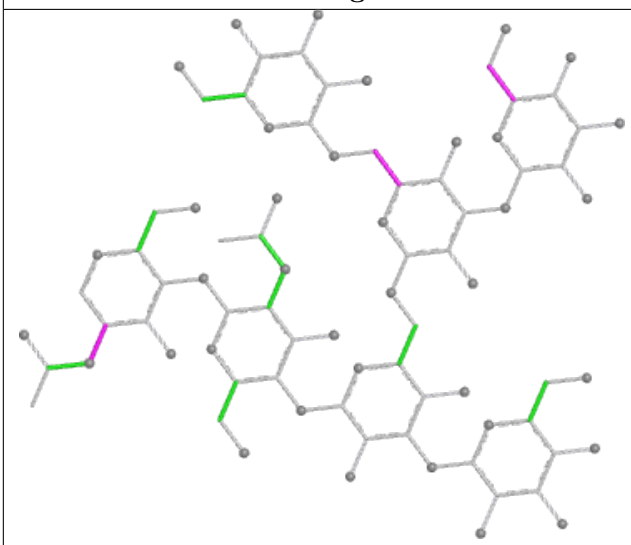
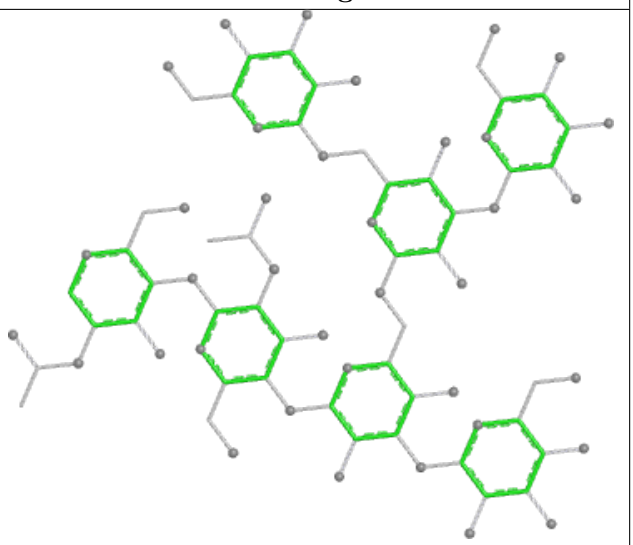
Mol	Chain	Res	Type	Atoms
7	H	1	NAG	C4-C5-C6-O6
6	G	4	MAN	O5-C5-C6-O6
7	H	1	NAG	O5-C5-C6-O6
9	J	4	MAN	O5-C5-C6-O6
8	I	1	NAG	O5-C5-C6-O6
8	I	5	MAN	O5-C5-C6-O6
6	G	5	MAN	O5-C5-C6-O6
6	G	4	MAN	C4-C5-C6-O6
8	I	1	NAG	C4-C5-C6-O6
6	G	1	NAG	C1-C2-N2-C7
7	H	2	NAG	C3-C2-N2-C7
9	J	3	BMA	C4-C5-C6-O6
7	H	2	NAG	C1-C2-N2-C7
8	I	2	NAG	C1-C2-N2-C7
9	J	2	NAG	C1-C2-N2-C7
6	G	1	NAG	C3-C2-N2-C7
8	I	2	NAG	C3-C2-N2-C7
9	J	2	NAG	C3-C2-N2-C7

There are no ring outliers.

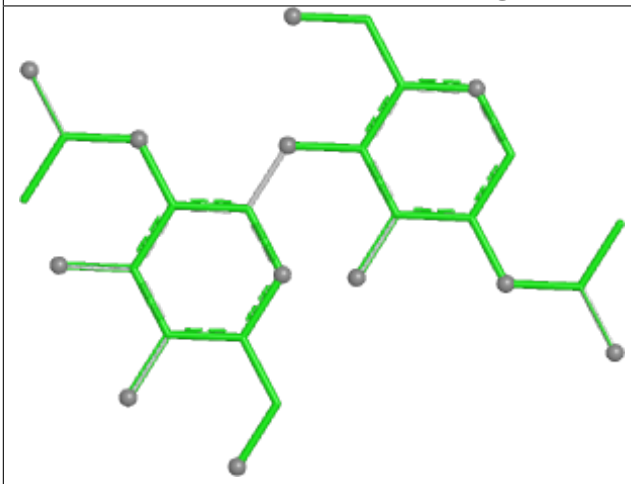
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1	NAG	1	0
8	I	1	NAG	2	0
9	J	4	MAN	1	0

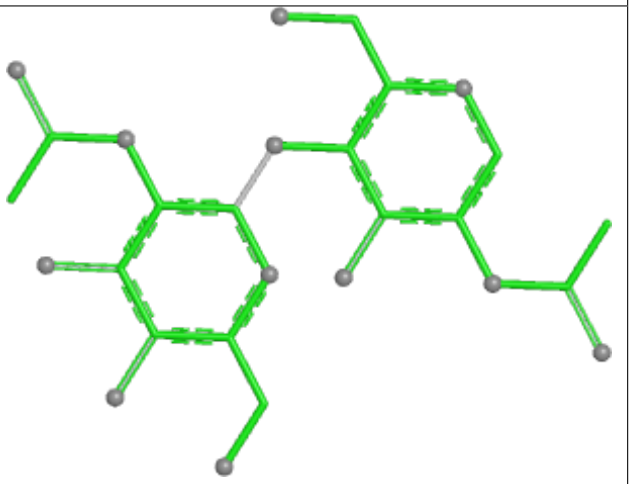
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

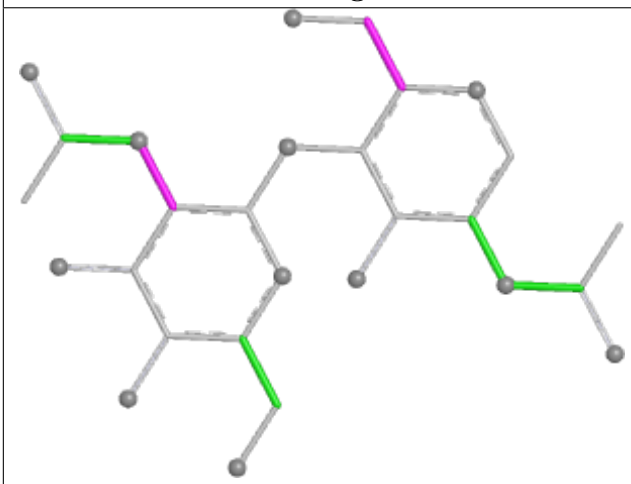
Oligosaccharide Chain H



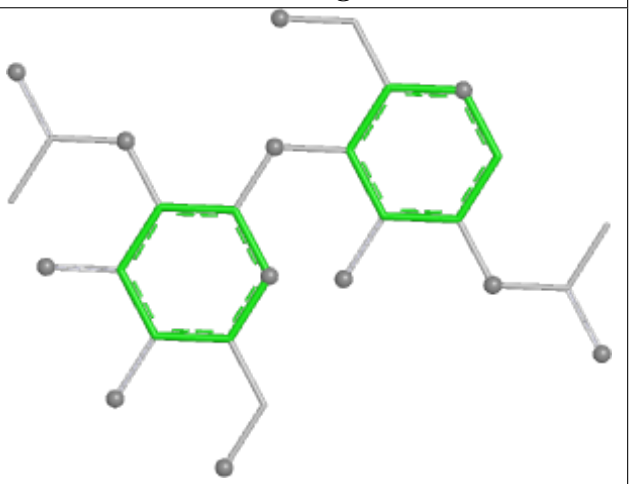
Bond lengths



Bond angles

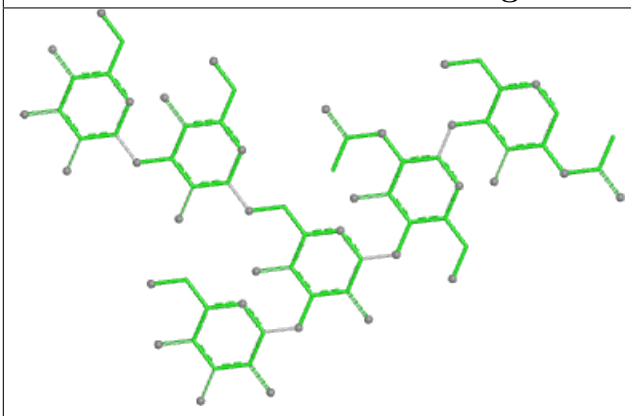


Torsions

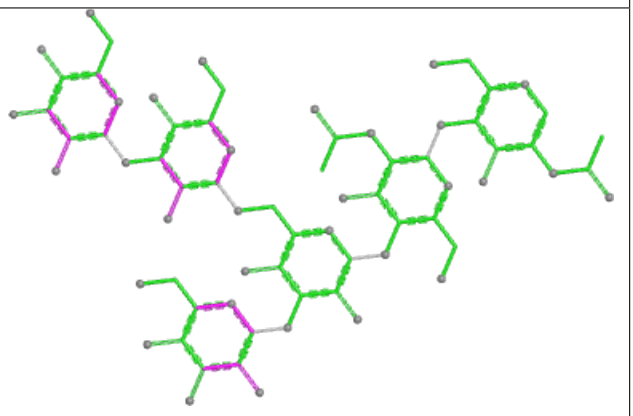


Rings

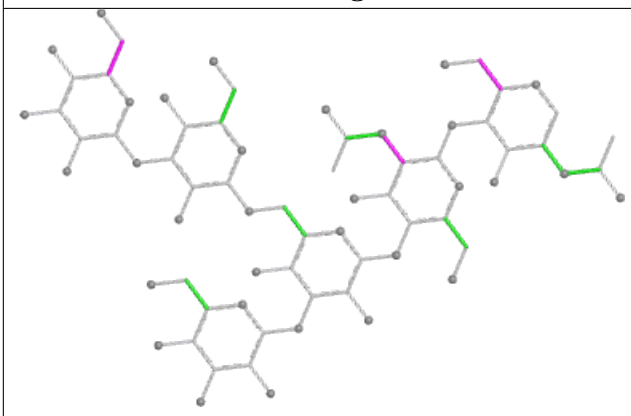
Oligosaccharide Chain I



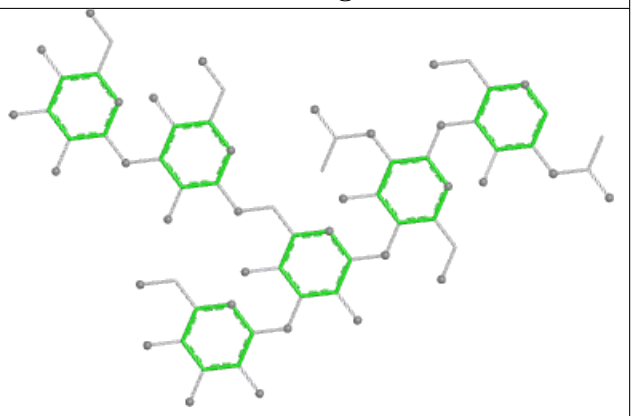
Bond lengths



Bond angles

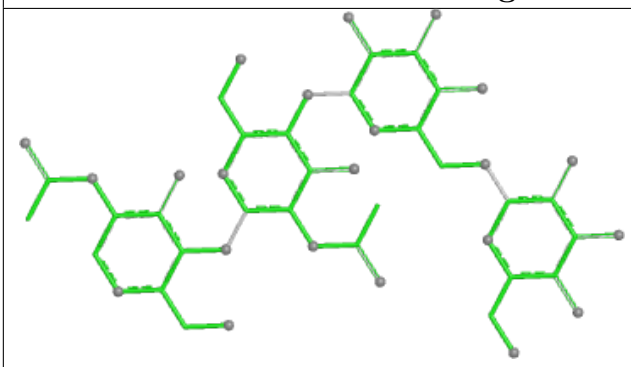


Torsions

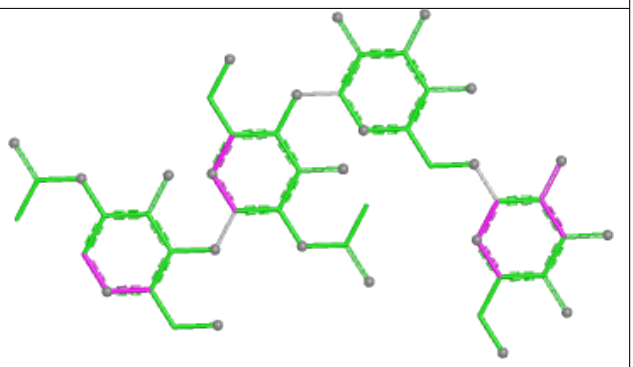


Rings

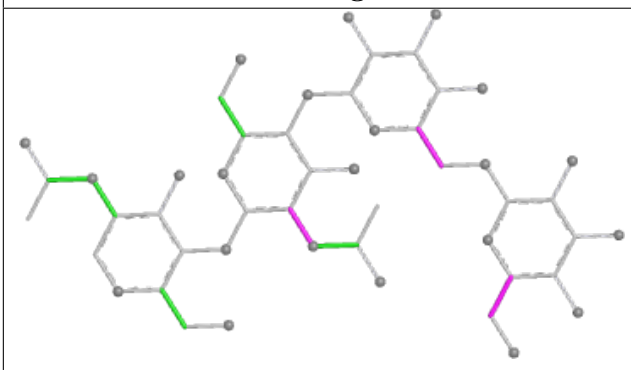
Oligosaccharide Chain J



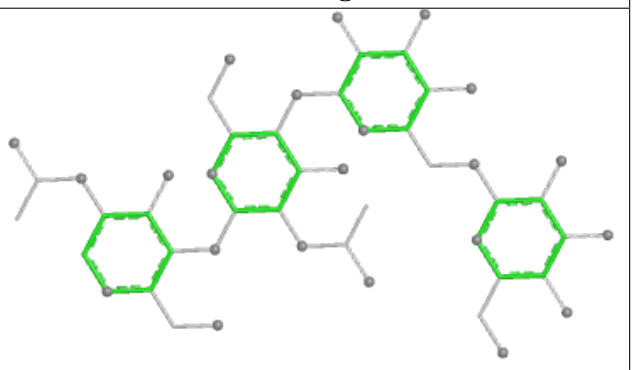
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\#\|Z\| > 2$
11	HSM	B	601	-	3,8,8	0.93	0	3,9,9	0.94	0
10	NAG	A	501	-	14,14,15	0.37	0	17,19,21	0.71	1 (5%)
10	NAG	E	501	3	14,14,15	0.23	0	17,19,21	0.45	0
10	NAG	C	501	3	14,14,15	0.21	0	17,19,21	0.39	0
13	HEX	D	502	-	5,5,5	0.30	0	4,4,4	0.57	0
10	NAG	D	501	-	14,14,15	0.21	0	17,19,21	0.41	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
11	HSM	B	601	-	-	1/2/3/3	0/1/1/1
10	NAG	A	501	-	-	0/6/23/26	0/1/1/1
10	NAG	E	501	3	1/1/5/7	2/6/23/26	0/1/1/1
10	NAG	C	501	3	1/1/5/7	2/6/23/26	0/1/1/1
13	HEX	D	502	-	-	0/3/3/3	-
10	NAG	D	501	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	501	NAG	C1-O5-C5	2.64	115.76	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	C	501	NAG	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	E	501	NAG	C1

All (7) torsion outliers are listed below:

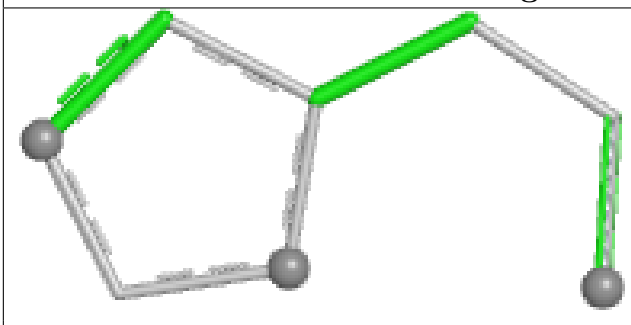
Mol	Chain	Res	Type	Atoms
11	B	601	HSM	CA-CB-CG-CD2
10	D	501	NAG	O5-C5-C6-O6
10	C	501	NAG	O5-C5-C6-O6
10	D	501	NAG	C4-C5-C6-O6
10	C	501	NAG	C4-C5-C6-O6
10	E	501	NAG	C3-C2-N2-C7
10	E	501	NAG	C1-C2-N2-C7

There are no ring outliers.

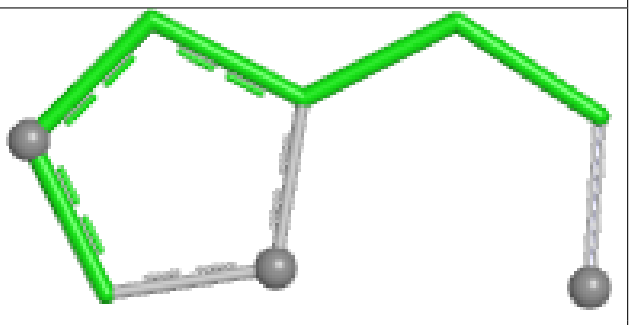
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

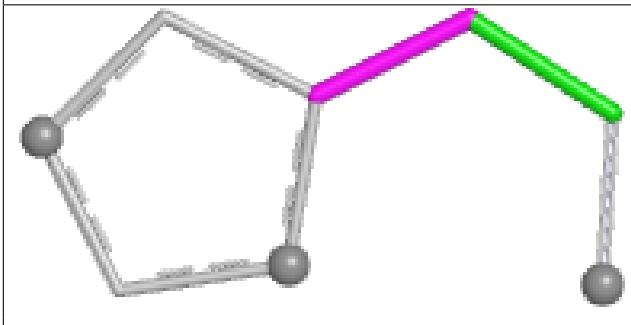
Ligand HSM B 601



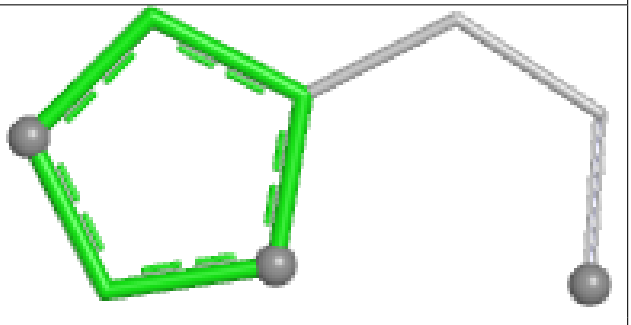
Bond lengths



Bond angles



Torsions



Rings

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.

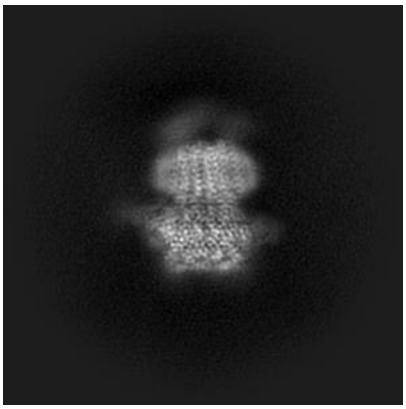
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13315. These allow visual inspection of the internal detail of the map and identification of artifacts.

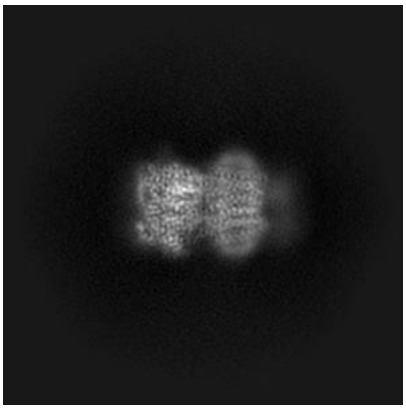
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

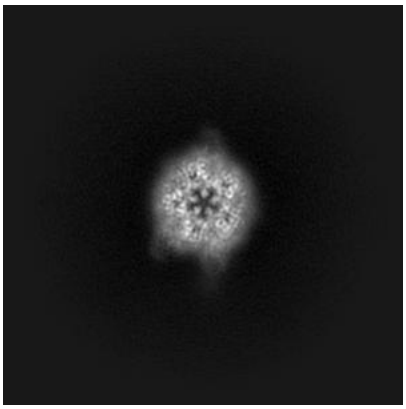
6.1.1 Primary map



X

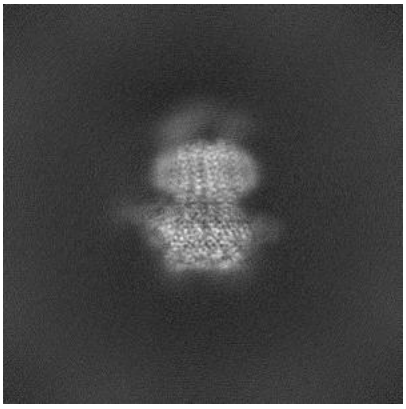


Y

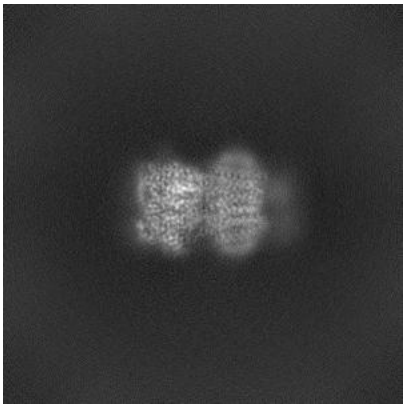


Z

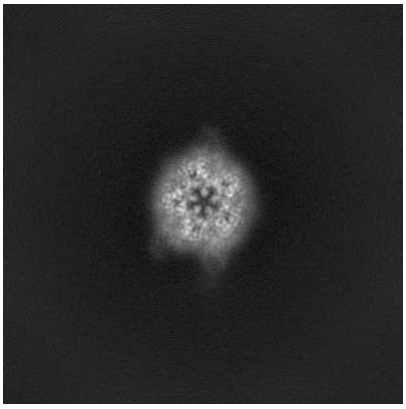
6.1.2 Raw map



X



Y

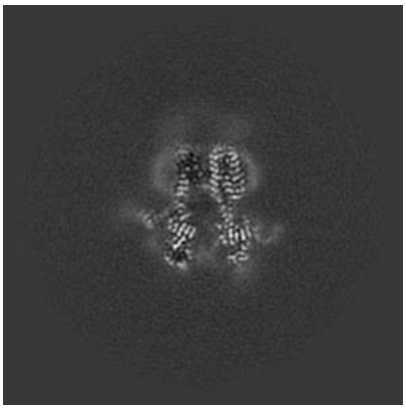


Z

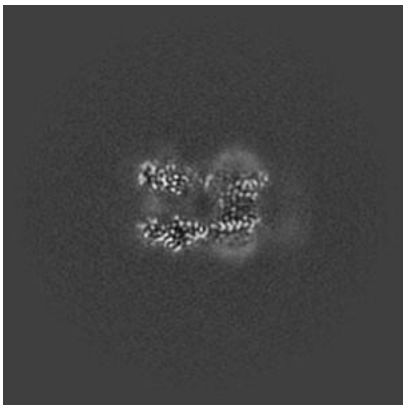
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

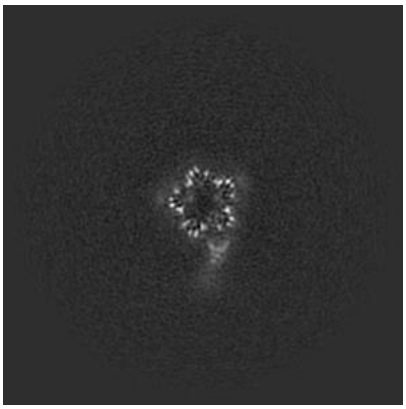
6.2.1 Primary map



X Index: 200

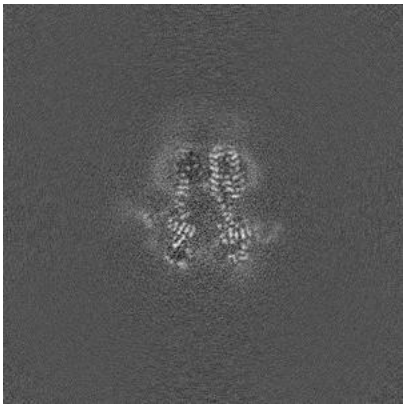


Y Index: 200

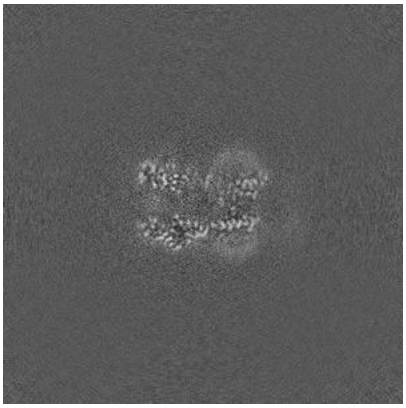


Z Index: 200

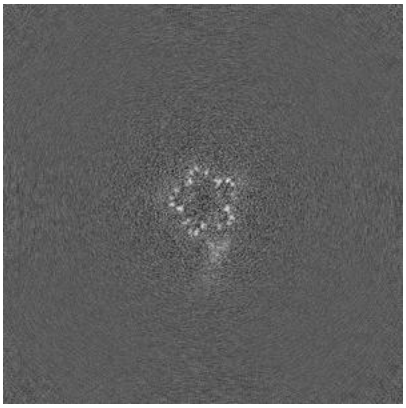
6.2.2 Raw map



X Index: 200



Y Index: 200

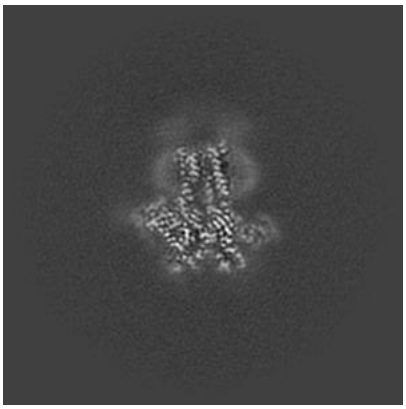


Z Index: 200

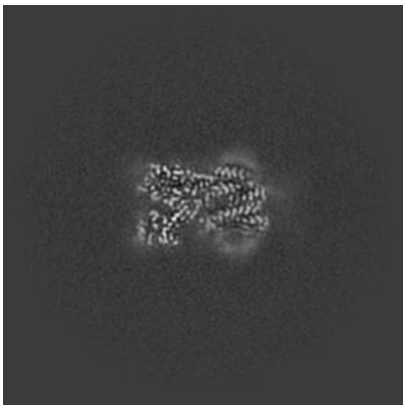
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

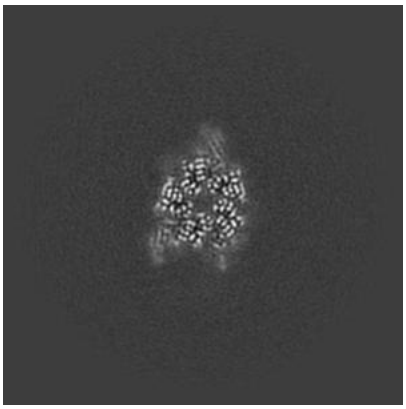
6.3.1 Primary map



X Index: 215

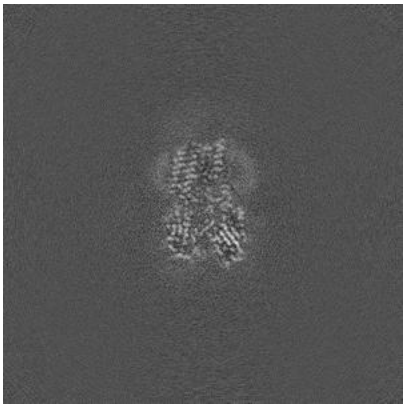


Y Index: 218

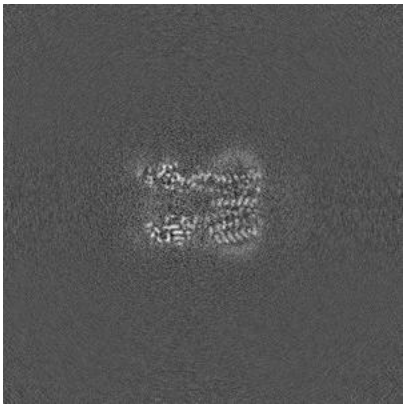


Z Index: 173

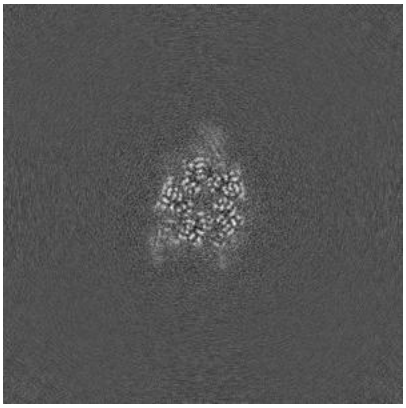
6.3.2 Raw map



X Index: 185



Y Index: 209

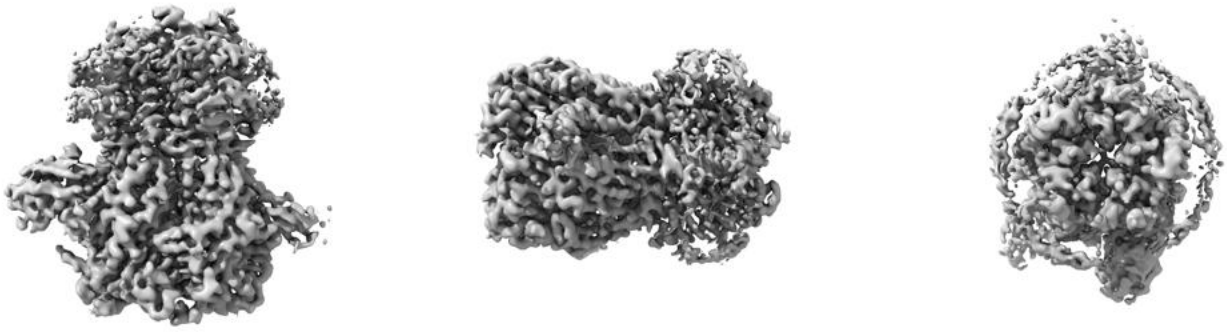


Z Index: 173

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.108. 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

X Y Z

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

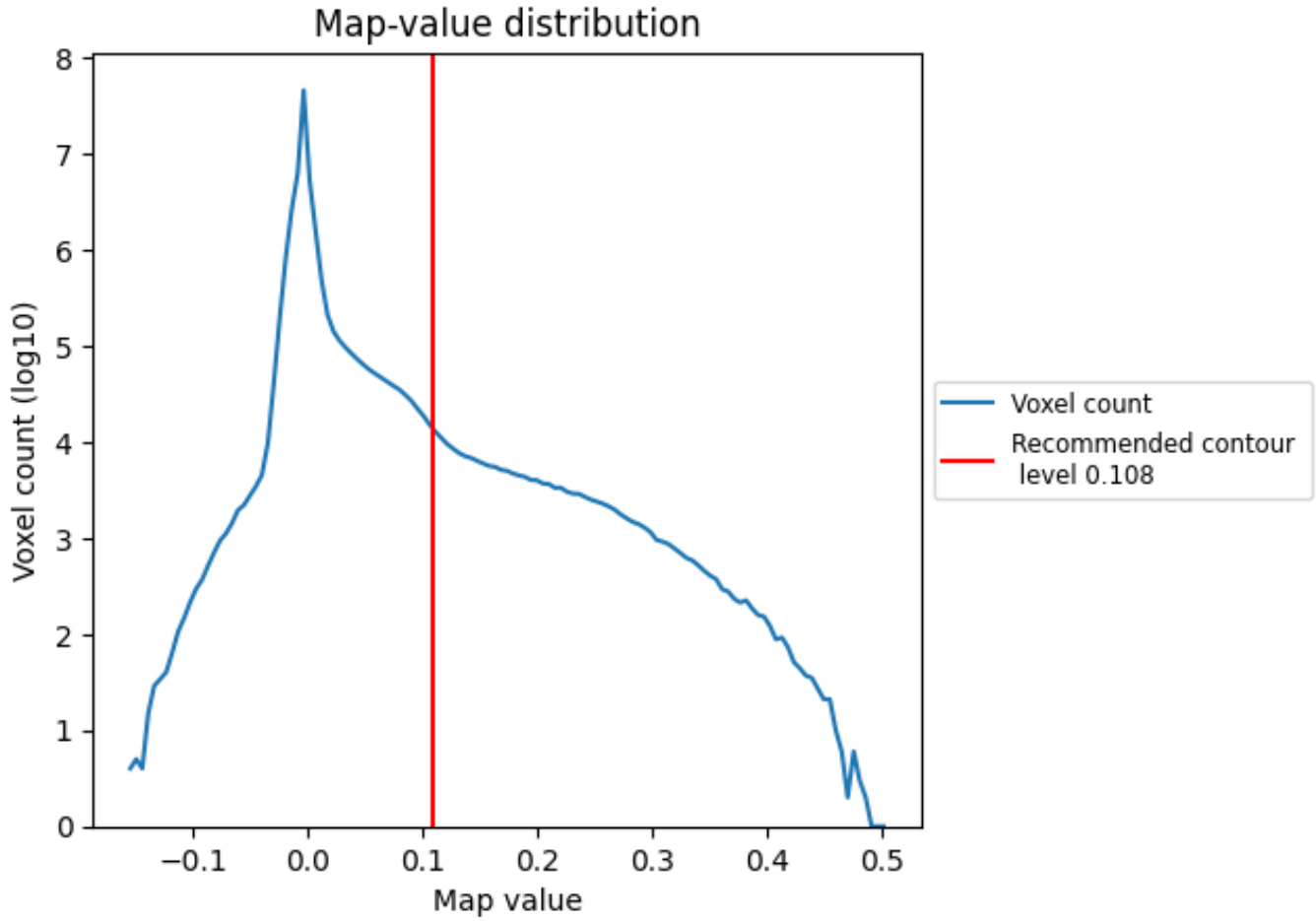
6.5 Mask visualisation (i)

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

7 Map analysis

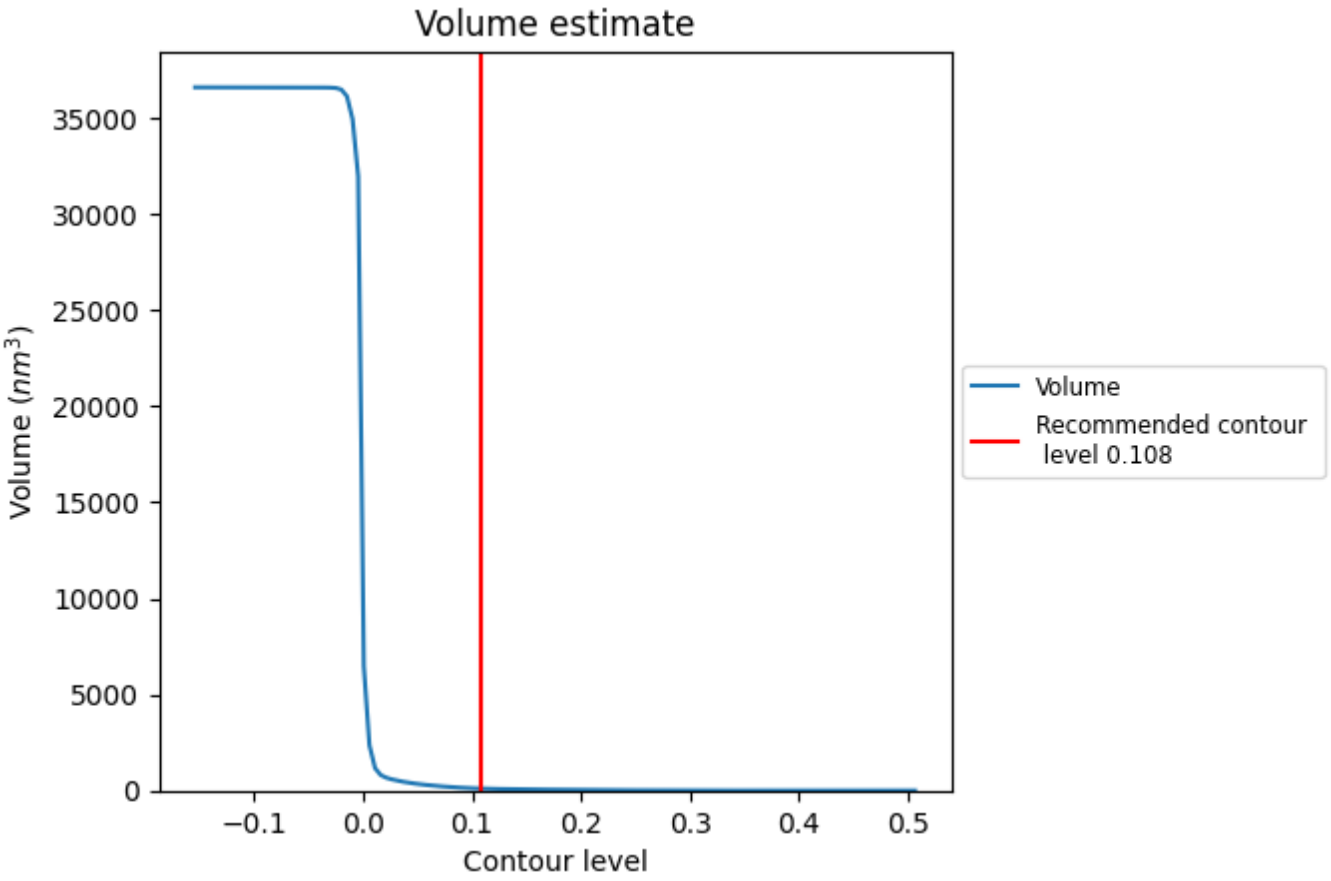
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

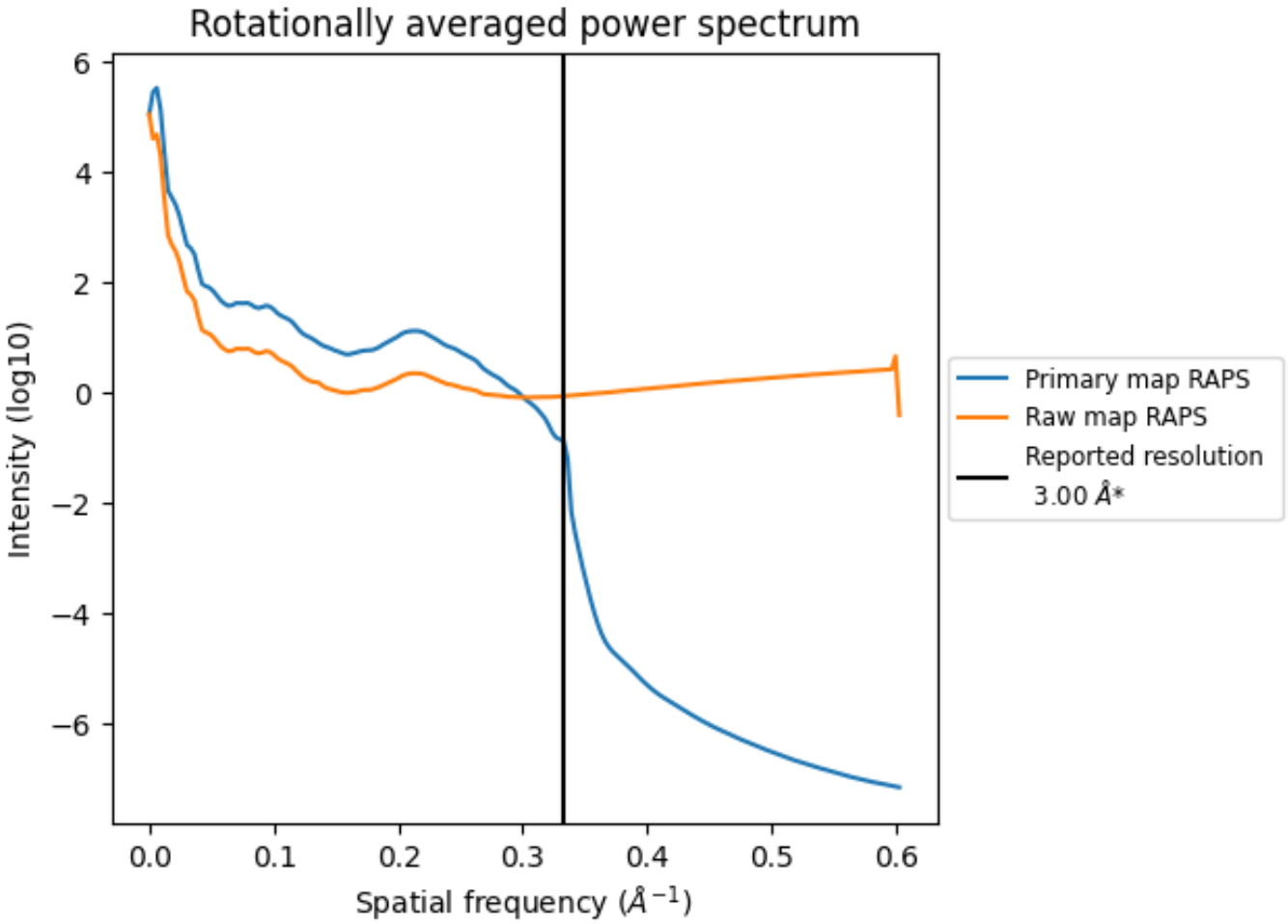
7.2 Volume estimate



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

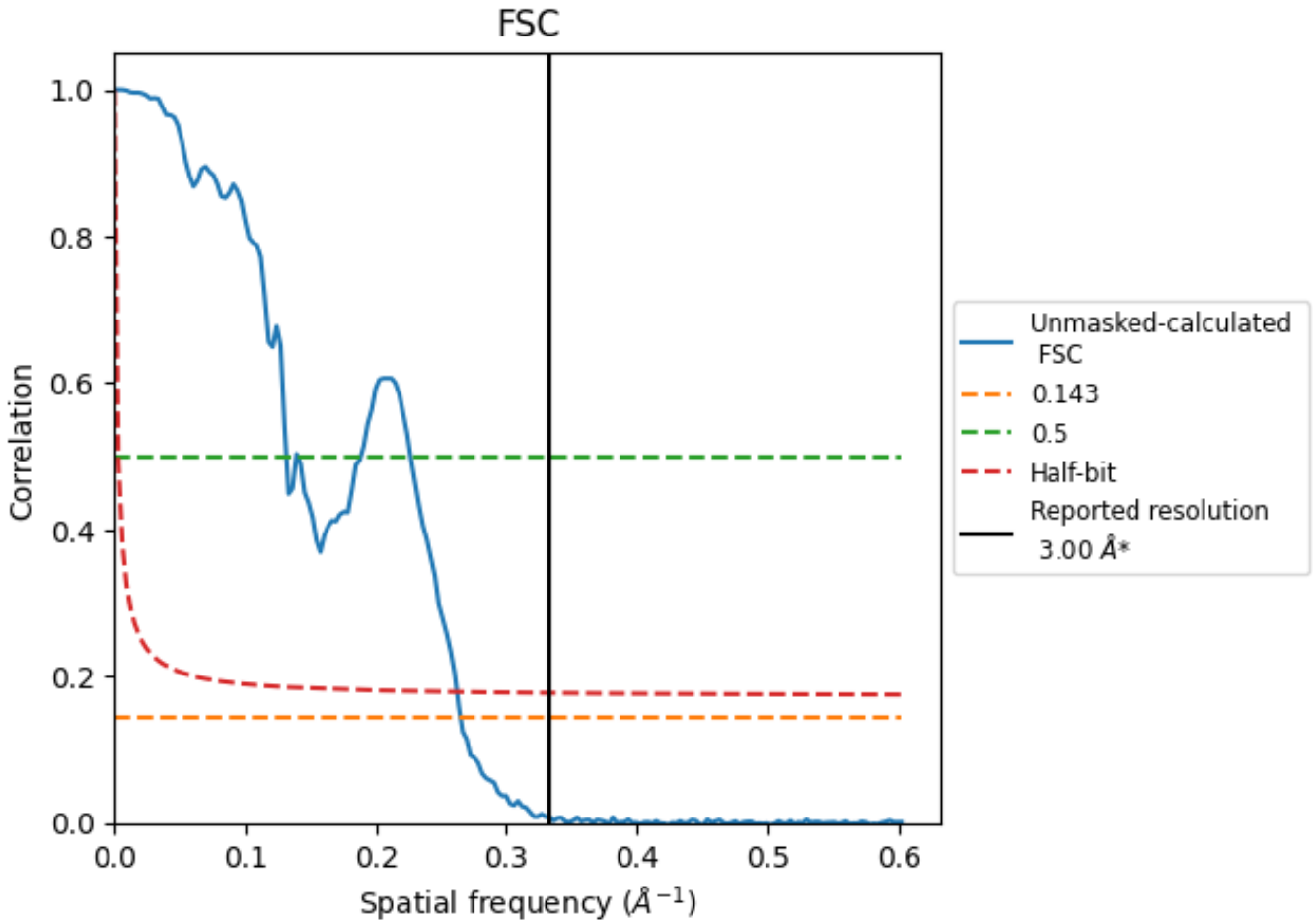


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

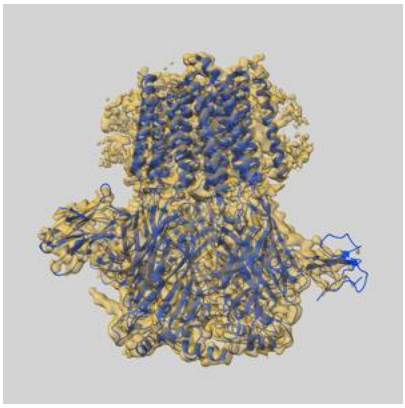
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	7.61	3.82

*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 3.78 differs from the reported value 3.0 by more than 10 %

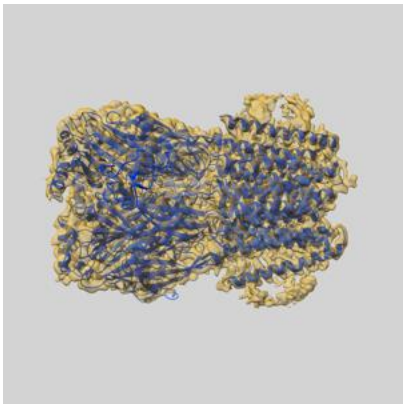
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13315 and PDB model 7PC0. Per-residue inclusion information can be found in section 3 on page 20.

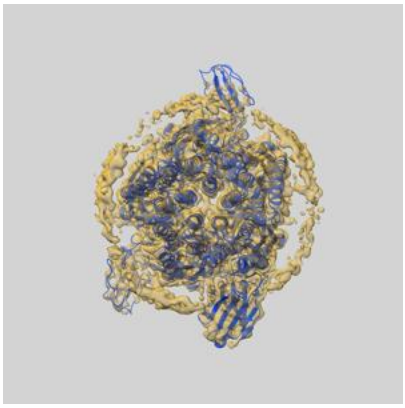
9.1 Map-model overlay



X



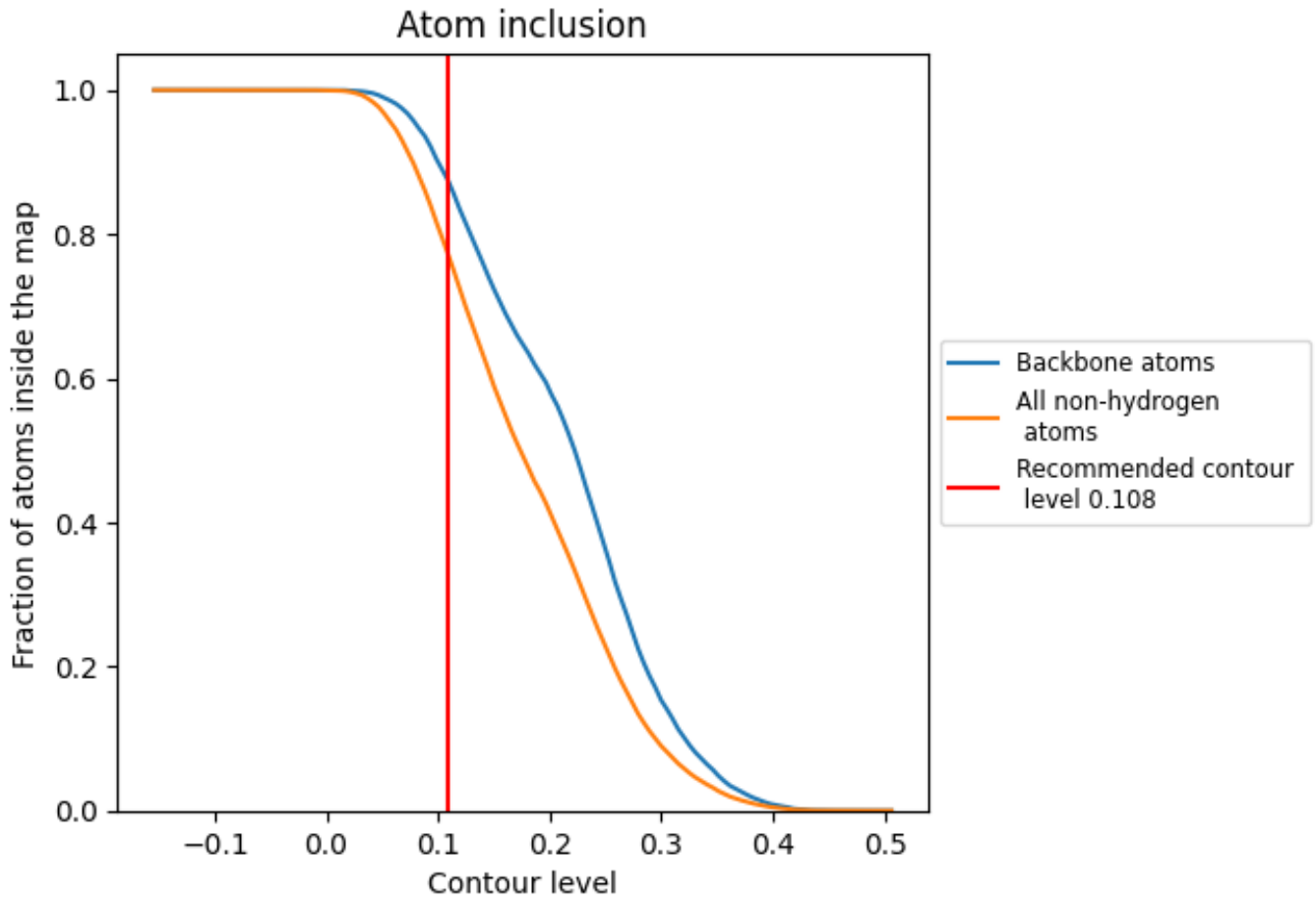
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.108 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, 88% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.