



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:25 PM UTC

PDB ID : 7K18 / pdb_00007k18
EMDB ID : EMD-22621
Title : Cardiac Sodium channel with toxin bound
Authors : Jiang, D.; Catterall, W.A.
Deposited on : 2020-09-07
Resolution : 3.30 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 EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

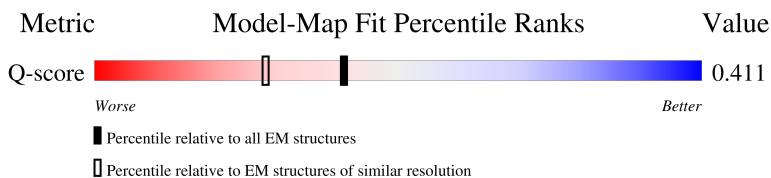
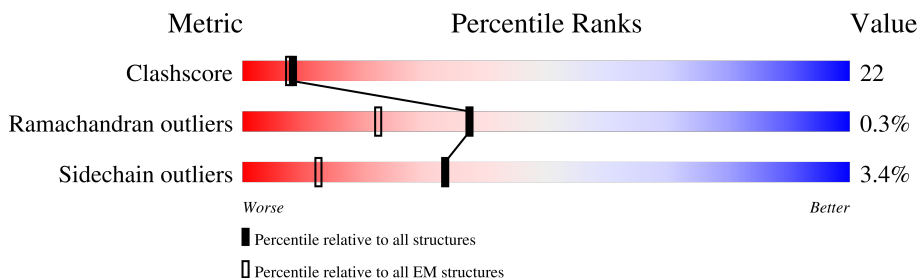
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1838	7% 37% 23% • 39%
2	B	67	63% 58% 39% •
3	C	2	100%
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	D	3	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9749 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 Sodium channel protein type 5 subunit alpha, Enhanced Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1128	Total	C	N	O	S	0	0
			8861	5858	1413	1522	68		

There are 341 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ILE	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	TRP	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	TYR	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	TYR	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	TYR	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	TRP	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	TRP	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	TYR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ILE	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	1899	GLU	-	linker	UNP P15389
A	1900	VAL	-	linker	UNP P15389
A	1901	LEU	-	linker	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1902	PHE	-	linker	UNP P15389
A	1903	GLN	-	linker	UNP P15389
A	1904	GLY	-	linker	UNP P15389
A	1905	PRO	-	linker	UNP P15389
A	1906	GLY	-	linker	UNP P15389
A	1907	SER	-	linker	UNP P15389
A	1909	VAL	-	insertion	UNP P42212
A	1972	LEU	PHE	conflict	UNP P42212
A	1973	THR	SER	conflict	UNP P42212
A	2139	LEU	HIS	conflict	UNP P42212
A	2147	GLY	-	expression tag	UNP P42212
A	2148	SER	-	expression tag	UNP P42212
A	2149	ASP	-	expression tag	UNP P42212
A	2150	TYR	-	expression tag	UNP P42212
A	2151	LYS	-	expression tag	UNP P42212
A	2152	ASP	-	expression tag	UNP P42212
A	2153	ASP	-	expression tag	UNP P42212
A	2154	ASP	-	expression tag	UNP P42212
A	2155	ASP	-	expression tag	UNP P42212
A	2156	LYS	-	expression tag	UNP P42212

- Molecule 2 is a protein called Alpha-like toxin Lqh3.

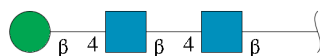
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	67	Total	C	N	O	S	0	0
			489	301	87	93	8		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



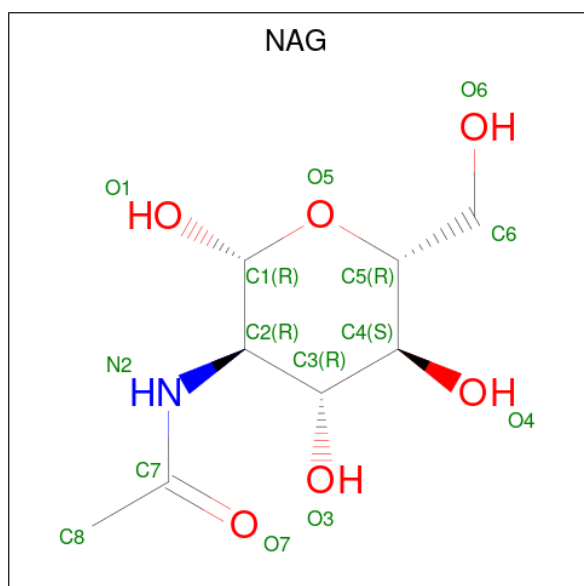
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	2	Total	C	N	O		0	0
			28	16	2	10			
3	E	2	Total	C	N	O		0	0
			28	16	2	10			

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



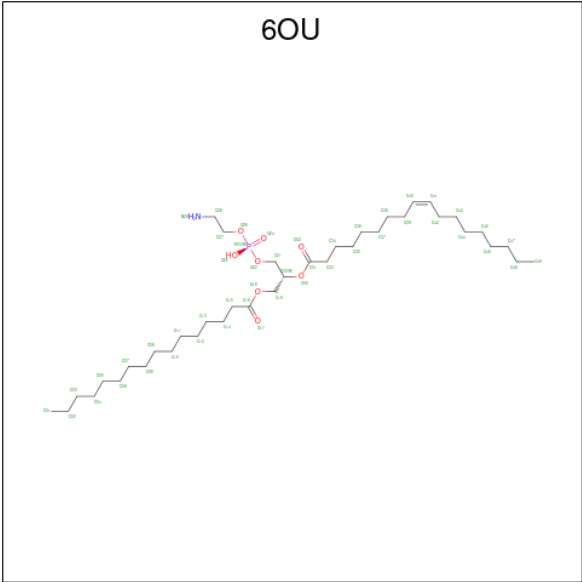
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: $C_{39}H_{76}NO_8P$).

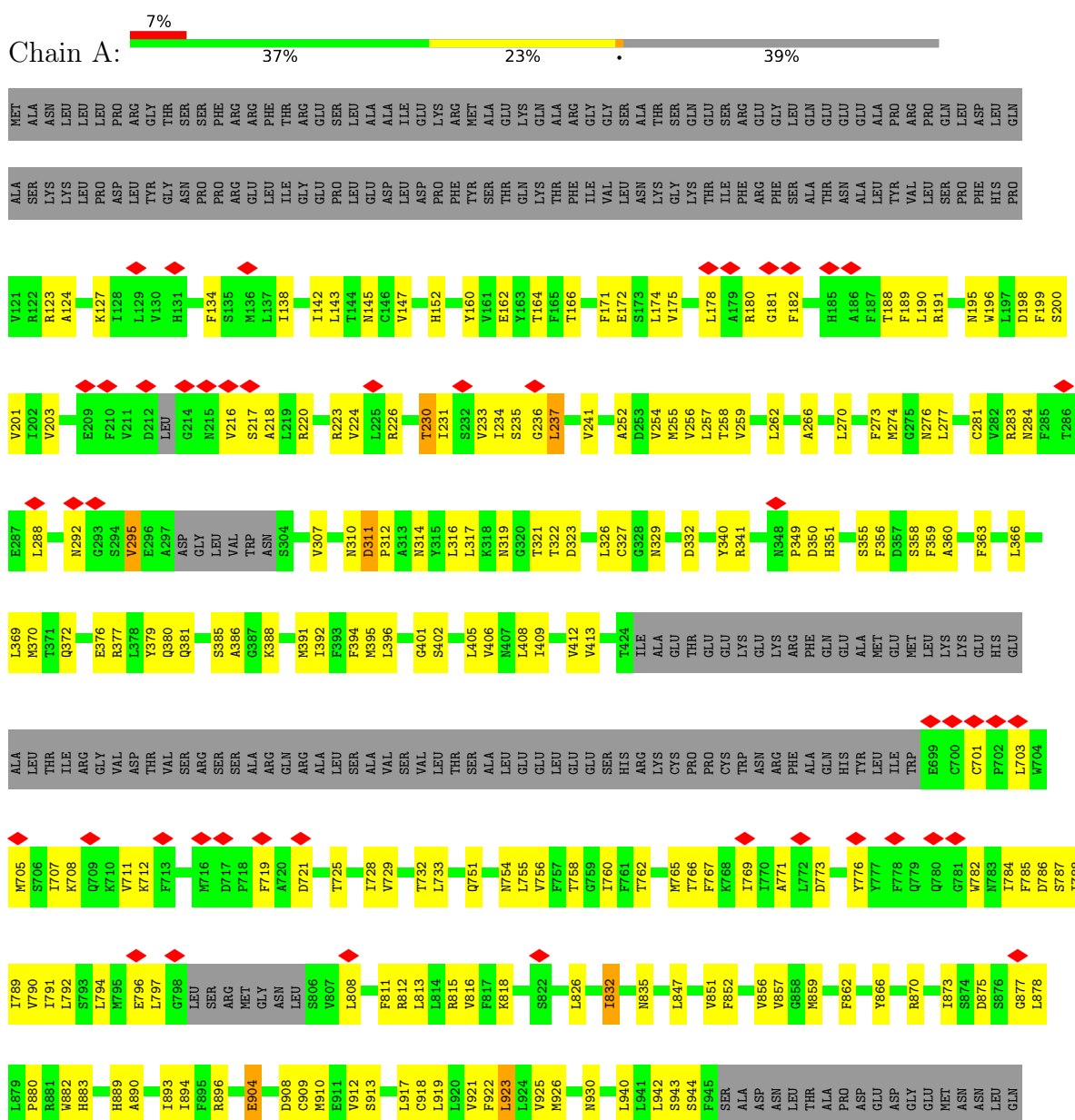


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
6	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
6	A	1	Total	C	O			0
			15	12	3			
6	A	1	Total	C	O			0
			26	21	5			
6	A	1	Total	C	O			0
			29	25	4			
6	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	A	1	Total	C	N	O	P	0
			26	16	1	8	1	
6	A	1	Total	C	O			0
			27	23	4			
6	A	1	Total	C	O	P		0
			25	16	8	1		
6	A	1	Total	C	O			0
			17	15	2			
6	A	1	Total	C	O			0
			15	13	2			

3 Residue-property plots

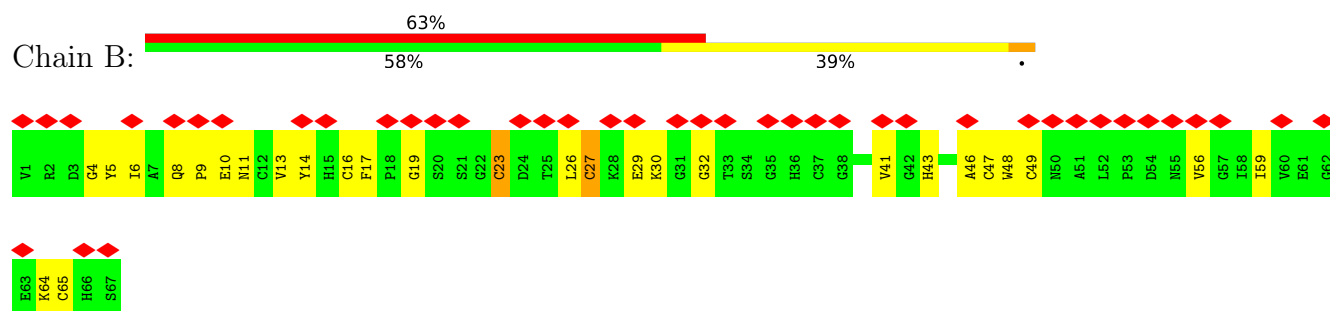
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sodium channel protein type 5 subunit alpha, Enhanced Green fluorescent protein

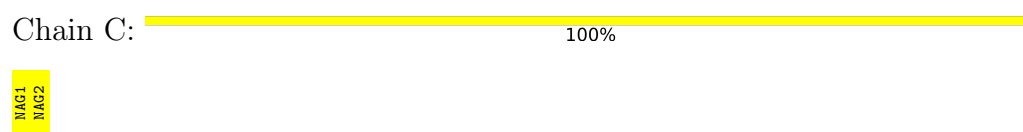




- Molecule 2: Alpha-like toxin Lqh3



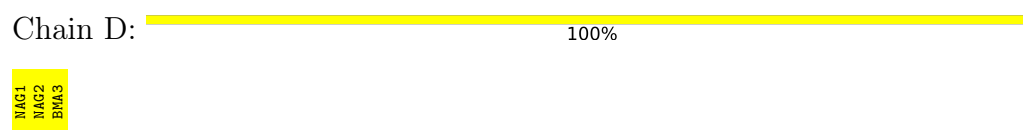
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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	267595	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.084	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	270.336, 270.336, 270.336	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 6OU, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	1/9072 (0.0%)	0.49	9/12328 (0.1%)
2	B	0.26	0/501	0.64	2/676 (0.3%)
All	All	0.22	1/9573 (0.0%)	0.50	11/13004 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1374	PRO	N-CD	7.97	1.58	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1302	LYS	N-CA-C	-8.86	102.04	113.12
1	A	1366	ILE	N-CA-C	8.15	120.32	108.58
1	A	1365	CYS	N-CA-C	7.82	122.39	108.24
1	A	1365	CYS	CB-CA-C	-6.90	101.56	112.05
1	A	1366	ILE	N-CA-CB	-6.48	103.66	110.72
1	A	1375	LEU	N-CA-C	6.36	119.70	110.42
2	B	23	CYS	N-CA-C	6.26	121.05	113.17
1	A	311	ASP	CA-C-N	-6.21	112.44	119.28
1	A	311	ASP	C-N-CA	-6.21	112.44	119.28
1	A	1377	TYR	N-CA-C	5.58	117.44	111.36
2	B	27	CYS	N-CA-CB	5.35	117.98	110.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8861	0	8880	389	0
2	B	489	0	450	26	0
3	C	28	0	25	1	0
3	E	28	0	25	1	0
4	D	39	0	34	2	0
5	A	14	0	13	4	0
6	A	290	0	0	2	0
All	All	9749	0	9427	413	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 22.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASN:ND2	5:A:2201:NAG:C1	1.69	1.55
1:A:273:PHE:HA	1:A:276:ASN:ND2	1.39	1.37
1:A:1365:CYS:SG	1:A:1397:TRP:HD1	1.54	1.31
1:A:1420:PHE:HA	1:A:1423:TRP:CD1	1.65	1.30
1:A:270:LEU:O	1:A:274:MET:HG3	1.19	1.29
1:A:1365:CYS:HG	1:A:1397:TRP:CD1	1.51	1.28
1:A:391:MET:SD	1:A:1704:LEU:HD23	1.82	1.18
1:A:1365:CYS:SG	1:A:1397:TRP:CD1	2.36	1.14
1:A:1420:PHE:CA	1:A:1423:TRP:CD1	2.37	1.06
2:B:27:CYS:O	2:B:32:GLY:N	1.94	1.01
1:A:270:LEU:O	1:A:274:MET:CG	2.09	1.00
2:B:27:CYS:HB3	2:B:32:GLY:HA3	1.46	0.96
1:A:273:PHE:HA	1:A:276:ASN:HD22	1.20	0.95
1:A:1683:TYR:CE1	1:A:1736:ASN:HB3	2.02	0.94
2:B:14:TYR:CE2	2:B:26:LEU:HD22	2.03	0.93
1:A:1423:TRP:HE3	1:A:1427:MET:SD	1.90	0.93
1:A:1365:CYS:HB2	1:A:1439:GLN:NE2	1.86	0.91
1:A:1417:VAL:HA	1:A:1423:TRP:HB3	1.49	0.91
2:B:14:TYR:CD2	2:B:26:LEU:HD22	2.05	0.90
1:A:391:MET:SD	1:A:1704:LEU:CD2	2.62	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PHE:CA	1:A:276:ASN:ND2	2.32	0.88
1:A:1300:PRO:HB2	1:A:1304:LEU:HB2	1.54	0.88
1:A:1380:VAL:O	1:A:1439:GLN:HG3	1.73	0.88
1:A:1374:PRO:HG2	1:A:1439:GLN:NE2	1.90	0.87
1:A:1423:TRP:CE3	1:A:1427:MET:SD	2.67	0.87
1:A:1358:PHE:HB3	1:A:1362:PHE:CE1	2.11	0.85
1:A:329:ASN:OD1	4:D:1:NAG:O7	1.95	0.84
1:A:1374:PRO:CG	1:A:1439:GLN:NE2	2.41	0.84
1:A:1420:PHE:HA	1:A:1423:TRP:HD1	1.42	0.84
1:A:1523:ILE:O	1:A:1527:VAL:HG23	1.77	0.83
1:A:1357:LEU:HD22	1:A:1448:MET:HE1	1.63	0.80
1:A:134:PHE:HE2	1:A:172:GLU:HG2	1.46	0.80
1:A:1420:PHE:C	1:A:1423:TRP:CD1	2.59	0.80
1:A:270:LEU:HD12	1:A:274:MET:HG2	1.64	0.80
1:A:1443:GLU:O	1:A:1443:GLU:HG2	1.80	0.80
1:A:1364:ARG:NH2	1:A:1400:VAL:CG1	2.45	0.80
1:A:319:ASN:CG	5:A:2201:NAG:C1	2.54	0.79
1:A:307:VAL:HG12	1:A:311:ASP:OD2	1.83	0.79
1:A:1367:ASN:HB3	1:A:1395:LEU:CD2	2.13	0.78
2:B:14:TYR:CD2	2:B:26:LEU:CD2	2.67	0.77
1:A:1543:ASN:ND2	1:A:1628:ARG:HH21	1.82	0.77
1:A:1365:CYS:O	1:A:1374:PRO:HG3	1.83	0.77
1:A:1543:ASN:HD21	1:A:1628:ARG:HH21	1.32	0.77
2:B:23:CYS:CB	2:B:47:CYS:SG	2.73	0.76
1:A:1490:THR:HG22	1:A:1491:GLU:N	2.00	0.76
1:A:832:ILE:HD11	1:A:944:SER:HB2	1.67	0.76
1:A:273:PHE:CA	1:A:276:ASN:HD22	1.96	0.75
1:A:273:PHE:HB2	1:A:356:PHE:HD2	1.50	0.75
1:A:1653:MET:HA	1:A:1656:LEU:HD12	1.67	0.75
1:A:1420:PHE:HB3	1:A:1423:TRP:HE1	1.50	0.74
1:A:1752:LEU:O	1:A:1756:THR:OG1	2.05	0.74
1:A:1358:PHE:HB3	1:A:1362:PHE:HE1	1.51	0.73
1:A:1420:PHE:CA	1:A:1423:TRP:NE1	2.51	0.73
1:A:1374:PRO:CG	1:A:1439:GLN:HE22	2.01	0.73
1:A:145:ASN:HD21	1:A:226:ARG:HD2	1.54	0.72
1:A:201:VAL:HG21	1:A:226:ARG:HG2	1.71	0.72
1:A:1687:GLU:HB2	1:A:1721:PRO:HB3	1.70	0.72
1:A:1458:PHE:HA	1:A:1462:PHE:HD2	1.53	0.72
1:A:152:HIS:CE1	6:A:2210:6OU:O25	2.44	0.71
1:A:1365:CYS:HB2	1:A:1439:GLN:HE21	1.55	0.71
1:A:1554:GLN:HB2	1:A:1558:LYS:HD3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1514:ARG:HH21	1:A:1515:PRO:HD2	1.57	0.70
1:A:919:LEU:HD12	1:A:923:LEU:HD23	1.72	0.70
1:A:231:ILE:HD13	1:A:241:VAL:HG21	1.73	0.70
1:A:1344:LEU:O	1:A:1411:TYR:OH	2.07	0.70
1:A:1357:LEU:HD22	1:A:1448:MET:CE	2.22	0.70
1:A:1367:ASN:HB3	1:A:1395:LEU:HD23	1.73	0.70
1:A:1597:ASP:HB2	1:A:1631:ARG:HE	1.55	0.69
1:A:270:LEU:C	1:A:274:MET:HG3	2.12	0.69
1:A:1363:GLY:HA3	1:A:1397:TRP:CZ2	2.28	0.69
1:A:307:VAL:CG1	1:A:311:ASP:OD2	2.41	0.69
1:A:1367:ASN:HA	1:A:1395:LEU:HD23	1.74	0.69
1:A:1490:THR:HG22	1:A:1491:GLU:H	1.58	0.69
1:A:1619:PHE:CD1	1:A:1623:LEU:HD13	2.29	0.68
1:A:1368:GLN:H	1:A:1394:GLU:HG3	1.59	0.68
1:A:1420:PHE:CA	1:A:1423:TRP:HD1	1.96	0.67
1:A:152:HIS:ND1	6:A:2210:6OU:O25	2.28	0.67
1:A:719:PHE:CD2	1:A:719:PHE:O	2.49	0.66
1:A:254:VAL:HG11	1:A:412:VAL:HG11	1.76	0.66
1:A:350:ASP:OD1	1:A:351:HIS:N	2.24	0.66
1:A:266:ALA:HA	1:A:366:LEU:HD12	1.78	0.66
1:A:785:PHE:HA	1:A:788:ILE:HD12	1.77	0.66
1:A:134:PHE:CZ	1:A:138:ILE:HD11	2.32	0.65
1:A:1423:TRP:CZ2	1:A:1424:MET:HE2	2.32	0.65
1:A:188:THR:HA	1:A:191:ARG:HE	1.62	0.64
1:A:1367:ASN:CA	1:A:1395:LEU:HD23	2.28	0.64
1:A:1382:ASN:HA	1:A:1438:GLU:HA	1.79	0.64
1:A:145:ASN:ND2	1:A:226:ARG:HD2	2.12	0.64
1:A:1612:ASP:OD1	2:B:43:HIS:ND1	2.31	0.64
1:A:372:GLN:NE2	1:A:402:SER:OG	2.31	0.63
1:A:909:CYS:HB3	1:A:918:CYS:SG	2.39	0.63
1:A:180:ARG:HG3	1:A:189:PHE:CB	2.29	0.62
1:A:1367:ASN:HB3	1:A:1395:LEU:HD21	1.80	0.62
1:A:1475:PHE:HD2	1:A:1770:ILE:HG21	1.64	0.62
1:A:856:VAL:HA	1:A:859:MET:HG2	1.80	0.62
1:A:1220:SER:HB2	1:A:1311:ARG:HH21	1.65	0.62
1:A:896:ARG:HE	1:A:1424:MET:HE1	1.65	0.61
1:A:1420:PHE:HA	1:A:1423:TRP:NE1	2.07	0.61
1:A:311:ASP:HB3	1:A:314:ASN:HB2	1.83	0.61
1:A:1586:HIS:O	1:A:1590:THR:OG1	2.13	0.61
1:A:307:VAL:O	1:A:311:ASP:HB2	2.00	0.61
1:A:794:LEU:HD13	1:A:797:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:PHE:C	1:A:1423:TRP:HD1	2.06	0.61
1:A:1435:GLY:HA3	1:A:1438:GLU:HG2	1.82	0.61
1:A:1380:VAL:O	1:A:1380:VAL:HG23	2.00	0.61
1:A:1380:VAL:HG23	1:A:1439:GLN:HG3	1.83	0.61
1:A:145:ASN:HD21	1:A:226:ARG:CD	2.13	0.60
1:A:323:ASP:OD2	1:A:377:ARG:NH2	2.33	0.60
1:A:1543:ASN:HD21	1:A:1628:ARG:NH2	1.98	0.60
1:A:873:ILE:HD11	1:A:908:ASP:HB3	1.83	0.60
1:A:1464:LEU:O	1:A:1468:ILE:HG12	2.02	0.60
1:A:1569:PHE:HA	1:A:1572:ILE:HD12	1.83	0.60
2:B:5:TYR:HD2	2:B:59:ILE:HG21	1.66	0.60
1:A:796:GLU:OE1	1:A:812:ARG:NH2	2.35	0.60
1:A:401:GLY:O	1:A:405:LEU:HB2	2.02	0.60
1:A:266:ALA:HA	1:A:366:LEU:CD1	2.32	0.59
1:A:1420:PHE:HB3	1:A:1423:TRP:NE1	2.16	0.59
1:A:1351:SER:O	1:A:1355:VAL:HG23	2.02	0.59
1:A:1573:PHE:HA	1:A:1576:GLU:HG2	1.85	0.59
1:A:134:PHE:CE2	1:A:172:GLU:HG2	2.34	0.58
1:A:1544:MET:HB2	1:A:1629:LEU:HD11	1.84	0.58
1:A:277:LEU:HD11	1:A:356:PHE:CE2	2.38	0.58
1:A:1364:ARG:CZ	1:A:1364:ARG:HB3	2.33	0.58
1:A:1615:GLN:HA	1:A:1621:PRO:HD3	1.85	0.58
2:B:23:CYS:HB3	2:B:47:CYS:SG	2.42	0.58
1:A:1273:TRP:HB3	1:A:1317:SER:HB3	1.86	0.58
1:A:1443:GLU:O	1:A:1443:GLU:CG	2.51	0.57
1:A:1490:THR:CG2	1:A:1491:GLU:N	2.66	0.57
1:A:1535:THR:O	1:A:1539:LEU:HG	2.04	0.57
1:A:270:LEU:CD1	1:A:274:MET:HG2	2.35	0.57
1:A:751:GLN:HE21	1:A:755:LEU:HD13	1.70	0.57
1:A:1367:ASN:CB	1:A:1395:LEU:HD23	2.33	0.57
1:A:224:VAL:HG11	1:A:857:VAL:HG23	1.86	0.57
1:A:162:GLU:O	1:A:166:THR:HG23	2.03	0.57
1:A:1347:TRP:HB3	1:A:1414:LEU:HD12	1.87	0.57
1:A:1490:THR:CG2	1:A:1491:GLU:H	2.18	0.57
1:A:1677:GLY:O	1:A:1681:PHE:N	2.37	0.57
1:A:1423:TRP:CH2	1:A:1424:MET:CE	2.87	0.57
2:B:27:CYS:HB3	2:B:32:GLY:CA	2.30	0.57
1:A:835:ASN:ND2	1:A:943:SER:OG	2.38	0.57
1:A:1374:PRO:HG2	1:A:1439:GLN:CD	2.30	0.57
1:A:1762:PHE:O	1:A:1766:VAL:HG23	2.05	0.57
2:B:11:ASN:O	2:B:65:CYS:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASN:HA	1:A:341:ARG:CD	2.34	0.56
1:A:1364:ARG:HH21	1:A:1400:VAL:CG1	2.18	0.56
1:A:319:ASN:ND2	5:A:2201:NAG:C2	2.65	0.56
1:A:719:PHE:O	1:A:719:PHE:CG	2.57	0.56
1:A:1279:LEU:O	1:A:1283:VAL:HG23	2.06	0.56
1:A:1614:ILE:HG13	1:A:1621:PRO:HB3	1.86	0.56
1:A:195:ASN:HA	1:A:198:ASP:OD2	2.06	0.56
1:A:379:TYR:HE2	1:A:1694:PHE:HE2	1.53	0.56
1:A:1734:LEU:HD12	1:A:1735:PRO:HD2	1.87	0.56
1:A:1276:LEU:O	1:A:1280:ILE:HG13	2.05	0.55
1:A:171:PHE:O	1:A:175:VAL:HG23	2.06	0.55
1:A:181:GLY:O	1:A:182:PHE:CG	2.59	0.55
1:A:728:ILE:O	1:A:732:THR:HG23	2.05	0.55
1:A:1475:PHE:CD2	1:A:1770:ILE:HG21	2.40	0.55
1:A:785:PHE:O	1:A:789:ILE:HG12	2.05	0.55
1:A:1497:TYR:OH	1:A:1775:GLU:OE2	2.24	0.55
1:A:138:ILE:O	1:A:142:ILE:HG13	2.07	0.55
1:A:266:ALA:CA	1:A:366:LEU:HD12	2.36	0.55
1:A:1282:ASP:O	1:A:1286:VAL:HG23	2.07	0.55
1:A:1537:MET:SD	1:A:1635:ILE:HG12	2.46	0.54
1:A:1420:PHE:CB	1:A:1423:TRP:HE1	2.17	0.54
1:A:1459:GLY:O	1:A:1463:THR:OG1	2.20	0.54
1:A:255:MET:HA	1:A:258:THR:HG22	1.90	0.54
1:A:1619:PHE:HZ	1:A:1624:PHE:CE1	2.25	0.54
1:A:1236:THR:O	1:A:1240:LEU:HG	2.08	0.54
1:A:216:VAL:HG23	1:A:218:ALA:H	1.72	0.54
1:A:786:ASP:O	1:A:790:VAL:HG23	2.08	0.54
1:A:1555:SER:O	1:A:1559:VAL:HG23	2.08	0.54
1:A:754:ASN:O	1:A:758:THR:HG23	2.07	0.54
1:A:1561:ILE:O	1:A:1565:ILE:HG13	2.08	0.54
1:A:919:LEU:CD1	1:A:923:LEU:HD23	2.38	0.53
1:A:880:PRO:HD2	1:A:883:HIS:ND1	2.23	0.53
1:A:1585:ARG:NH2	1:A:1588:TYR:OH	2.41	0.53
1:A:1598:PHE:O	1:A:1602:ILE:HG12	2.08	0.53
1:A:1335:SER:OG	1:A:1474:ASN:OD1	2.25	0.53
1:A:1374:PRO:HG3	1:A:1439:GLN:NE2	2.19	0.53
1:A:782:TRP:HZ2	1:A:818:LYS:HA	1.74	0.53
1:A:909:CYS:CB	1:A:918:CYS:SG	2.97	0.53
1:A:1602:ILE:O	1:A:1606:VAL:HG23	2.09	0.52
1:A:160:TYR:O	1:A:164:THR:HG23	2.09	0.52
1:A:1619:PHE:CZ	1:A:1624:PHE:CZ	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ALA:O	1:A:256:VAL:HG23	2.08	0.52
1:A:273:PHE:HA	1:A:276:ASN:HD21	1.62	0.52
1:A:123:ARG:H	1:A:123:ARG:HD2	1.74	0.52
2:B:6:ILE:HD11	2:B:49:CYS:HB2	1.92	0.52
1:A:217:SER:HA	1:A:220:ARG:HD2	1.92	0.52
1:A:392:ILE:O	1:A:396:LEU:HG	2.09	0.52
1:A:1423:TRP:CH2	1:A:1424:MET:HE1	2.45	0.52
1:A:1361:LYS:HB3	1:A:1433:SER:HB2	1.92	0.51
1:A:321:THR:HG22	1:A:322:THR:H	1.75	0.51
1:A:835:ASN:ND2	1:A:943:SER:CB	2.72	0.51
1:A:1363:GLY:HA3	1:A:1397:TRP:CH2	2.45	0.51
1:A:1722:ILE:HG21	1:A:1750:GLY:HA3	1.93	0.51
1:A:143:LEU:O	1:A:147:VAL:HG23	2.10	0.51
1:A:1544:MET:HG2	1:A:1548:MET:HE3	1.92	0.51
2:B:27:CYS:O	2:B:32:GLY:CA	2.58	0.51
1:A:1550:GLU:OE1	1:A:1550:GLU:N	2.39	0.51
1:A:1420:PHE:CB	1:A:1423:TRP:NE1	2.74	0.51
1:A:773:ASP:OD2	1:A:776:TYR:N	2.44	0.51
1:A:786:ASP:OD1	1:A:818:LYS:HD3	2.11	0.51
1:A:792:LEU:HD23	1:A:811:PHE:CG	2.46	0.50
1:A:1445:ASN:ND2	1:A:1448:MET:HG3	2.26	0.50
1:A:1199:THR:O	1:A:1203:ILE:HG13	2.11	0.50
1:A:273:PHE:HB3	1:A:276:ASN:HB2	1.93	0.50
1:A:234:ILE:HB	1:A:237:LEU:HB2	1.93	0.50
1:A:1300:PRO:HB2	1:A:1304:LEU:CB	2.36	0.50
1:A:1253:VAL:O	1:A:1257:LEU:HG	2.12	0.50
1:A:1420:PHE:C	1:A:1423:TRP:NE1	2.70	0.50
1:A:1612:ASP:HB2	2:B:43:HIS:HA	1.93	0.50
1:A:145:ASN:ND2	1:A:226:ARG:CD	2.73	0.50
1:A:284:ASN:HA	1:A:341:ARG:HD2	1.94	0.50
1:A:786:ASP:CG	1:A:818:LYS:HD3	2.36	0.50
1:A:1307:LEU:HB3	1:A:1310:LEU:HD12	1.94	0.49
1:A:1456:ILE:O	1:A:1460:SER:HB2	2.11	0.49
1:A:1314:ARG:O	1:A:1317:SER:OG	2.30	0.49
1:A:319:ASN:CB	5:A:2201:NAG:C1	2.89	0.49
1:A:349:PRO:HG2	1:A:355:SER:HB3	1.94	0.49
1:A:896:ARG:HH11	1:A:1424:MET:HE3	1.78	0.49
1:A:134:PHE:CE1	1:A:171:PHE:HE2	2.30	0.49
1:A:1686:TRP:NE1	1:A:1695:ASN:OD1	2.42	0.49
1:A:1420:PHE:CA	1:A:1423:TRP:HE1	2.26	0.49
1:A:1364:ARG:NH2	1:A:1400:VAL:HG13	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:PRO:HA	2:B:10:GLU:HA	1.55	0.49
1:A:835:ASN:HD21	1:A:943:SER:CB	2.26	0.48
1:A:1555:SER:HB2	1:A:1558:LYS:HB2	1.95	0.48
1:A:1666:LEU:O	1:A:1670:MET:HG3	2.14	0.48
2:B:23:CYS:SG	2:B:47:CYS:CB	3.00	0.48
1:A:762:THR:O	1:A:766:THR:HG23	2.13	0.48
1:A:926:MET:SD	1:A:930:ASN:ND2	2.86	0.48
1:A:134:PHE:CE1	1:A:171:PHE:CE2	3.02	0.48
1:A:1368:GLN:N	1:A:1394:GLU:HG3	2.28	0.48
1:A:1706:LEU:HD13	1:A:1757:TYR:CE2	2.49	0.48
1:A:409:ILE:O	1:A:413:VAL:HG23	2.13	0.48
1:A:124:ALA:HA	1:A:127:LYS:HG2	1.95	0.48
1:A:402:SER:O	1:A:406:VAL:HB	2.14	0.48
1:A:1431:VAL:HG11	1:A:1449:TYR:CD2	2.48	0.48
1:A:1338:ASN:O	1:A:1342:VAL:HG23	2.12	0.48
1:A:1619:PHE:CZ	1:A:1624:PHE:CE1	3.02	0.48
1:A:292:ASN:OD1	1:A:292:ASN:N	2.44	0.48
1:A:1200:CYS:HA	1:A:1203:ILE:HD12	1.95	0.48
1:A:1619:PHE:CE1	1:A:1623:LEU:HD13	2.49	0.48
1:A:1300:PRO:O	1:A:1304:LEU:HB3	2.14	0.48
1:A:223:ARG:HG2	1:A:226:ARG:HH21	1.78	0.48
1:A:262:LEU:HD11	1:A:370:MET:HE2	1.96	0.47
1:A:784:ILE:O	1:A:788:ILE:HG13	2.14	0.47
1:A:1247:MET:O	1:A:1251:VAL:HG12	2.14	0.47
1:A:917:LEU:O	1:A:921:VAL:HG12	2.14	0.47
1:A:1338:ASN:OD1	1:A:1338:ASN:N	2.46	0.47
1:A:1374:PRO:HG3	1:A:1439:GLN:HE22	1.75	0.47
1:A:787:SER:O	1:A:791:ILE:HG13	2.14	0.47
1:A:1537:MET:HA	1:A:1540:ILE:HG22	1.96	0.47
1:A:329:ASN:ND2	4:D:1:NAG:C7	2.77	0.47
1:A:1468:ILE:O	1:A:1472:ILE:HG12	2.14	0.47
1:A:1305:ARG:O	1:A:1308:ARG:HB2	2.15	0.47
1:A:1361:LYS:NZ	1:A:1434:ARG:O	2.48	0.47
1:A:1486:ASP:O	1:A:1494:LYS:NZ	2.40	0.47
1:A:1523:ILE:O	1:A:1527:VAL:CG2	2.58	0.47
1:A:873:ILE:HG23	1:A:880:PRO:HG3	1.95	0.47
1:A:1316:LEU:HD22	1:A:1326:VAL:HG21	1.96	0.47
1:A:910:MET:HG2	1:A:918:CYS:HB3	1.97	0.47
1:A:1460:SER:O	1:A:1464:LEU:HB2	2.15	0.47
1:A:1487:ILE:HG13	1:A:1488:PHE:N	2.30	0.47
1:A:862:PHE:CZ	1:A:921:VAL:HG11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1294:GLY:C	1:A:1296:ALA:H	2.23	0.47
1:A:1662:ILE:HG21	1:A:1768:MET:HG3	1.97	0.47
1:A:181:GLY:O	1:A:182:PHE:CD2	2.68	0.46
2:B:26:LEU:HD12	2:B:29:GLU:OE2	2.16	0.46
1:A:408:LEU:HD12	1:A:1648:LEU:HG	1.96	0.46
1:A:1591:ASN:HB2	1:A:1594:ASN:OD1	2.16	0.46
2:B:16:CYS:HB2	2:B:46:ALA:O	2.15	0.46
1:A:789:ILE:HG21	1:A:815:ARG:HG3	1.97	0.46
1:A:866:TYR:O	1:A:870:ARG:HG3	2.16	0.46
1:A:1380:VAL:O	1:A:1439:GLN:CG	2.55	0.46
1:A:1414:LEU:HD22	1:A:1455:PHE:CE2	2.51	0.46
1:A:1610:LEU:O	1:A:1614:ILE:HG12	2.16	0.46
1:A:277:LEU:CD1	1:A:356:PHE:CE2	2.98	0.46
1:A:1361:LYS:HE2	1:A:1436:TYR:HA	1.97	0.46
1:A:1435:GLY:CA	1:A:1438:GLU:HG2	2.46	0.46
1:A:1601:VAL:O	1:A:1605:ILE:HG12	2.16	0.46
1:A:1619:PHE:HE1	1:A:1623:LEU:HB3	1.80	0.46
1:A:721:ASP:OD1	1:A:721:ASP:N	2.48	0.46
1:A:1423:TRP:CZ3	1:A:1427:MET:SD	3.09	0.46
1:A:1666:LEU:HD21	1:A:1710:THR:HG21	1.97	0.46
1:A:319:ASN:O	1:A:319:ASN:OD1	2.34	0.46
1:A:882:TRP:NE1	1:A:1428:TYR:OH	2.46	0.46
2:B:30:LYS:HB3	2:B:56:VAL:HG21	1.98	0.46
1:A:1534:VAL:HG13	1:A:1537:MET:HE2	1.98	0.46
1:A:1567:LEU:HD11	2:B:41:VAL:HG23	1.98	0.46
2:B:13:VAL:HG12	2:B:59:ILE:HD13	1.98	0.46
1:A:273:PHE:CB	1:A:276:ASN:HD22	2.29	0.45
1:A:922:PHE:HA	1:A:925:VAL:HG12	1.98	0.45
1:A:1347:TRP:HE1	1:A:1463:THR:HG21	1.80	0.45
1:A:756:VAL:O	1:A:760:ILE:HG13	2.15	0.45
1:A:283:ARG:HA	1:A:340:TYR:HA	1.99	0.45
1:A:174:LEU:O	1:A:178:LEU:HG	2.17	0.45
1:A:199:PHE:O	1:A:203:VAL:HG13	2.17	0.45
1:A:281:CYS:SG	1:A:327:CYS:HB3	2.57	0.45
1:A:332:ASP:HB3	1:A:388:LYS:H	1.80	0.45
1:A:1294:GLY:C	1:A:1296:ALA:N	2.74	0.45
1:A:1308:ARG:O	1:A:1311:ARG:HB2	2.17	0.45
1:A:1514:ARG:HD2	1:A:1514:ARG:HA	1.84	0.45
1:A:1536:ILE:HD12	1:A:1576:GLU:OE1	2.16	0.45
1:A:1649:LEU:O	1:A:1653:MET:HG2	2.15	0.45
1:A:904:GLU:H	1:A:904:GLU:HG2	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1593:TRP:CD1	1:A:1634:ARG:HG3	2.51	0.45
1:A:1736:ASN:C	1:A:1738:ASN:N	2.74	0.45
1:A:847:LEU:O	1:A:851:VAL:HG23	2.16	0.45
1:A:1766:VAL:O	1:A:1770:ILE:HG12	2.17	0.45
1:A:1373:LEU:H	1:A:1373:LEU:HD12	1.82	0.45
2:B:4:GLY:HA2	2:B:48:TRP:CZ3	2.52	0.45
1:A:231:ILE:HA	1:A:237:LEU:HB3	1.99	0.45
1:A:877:GLY:O	1:A:878:LEU:HD12	2.17	0.45
1:A:1723:LEU:O	1:A:1725:THR:HG23	2.17	0.44
1:A:385:SER:OG	1:A:386:ALA:N	2.50	0.44
1:A:767:PHE:O	1:A:771:ALA:CB	2.65	0.44
1:A:277:LEU:HD13	1:A:356:PHE:CD2	2.52	0.44
1:A:326:LEU:HD12	1:A:381:GLN:O	2.17	0.44
1:A:1636:LEU:HD11	1:A:1645:ILE:HD11	1.98	0.44
2:B:17:PHE:O	2:B:19:GLY:N	2.49	0.44
1:A:856:VAL:O	1:A:859:MET:HG2	2.18	0.44
1:A:1217:ILE:HD12	1:A:1220:SER:OG	2.18	0.44
1:A:1544:MET:O	1:A:1548:MET:HG3	2.18	0.44
1:A:1726:GLY:H	1:A:1730:CYS:HB2	1.83	0.44
1:A:1231:LEU:HD23	1:A:1231:LEU:HA	1.82	0.44
1:A:1487:ILE:HG23	1:A:1488:PHE:CD2	2.53	0.44
1:A:1574:THR:CG2	1:A:1605:ILE:HD11	2.48	0.44
1:A:1709:ILE:O	1:A:1712:SER:N	2.46	0.44
1:A:273:PHE:HB2	1:A:356:PHE:CD2	2.40	0.44
1:A:259:VAL:HG23	1:A:363:PHE:CZ	2.53	0.43
1:A:1531:ALA:O	1:A:1535:THR:HG23	2.18	0.43
1:A:288:LEU:H	1:A:295:VAL:HG11	1.83	0.43
1:A:358:SER:O	1:A:360:ALA:N	2.51	0.43
1:A:890:ALA:O	1:A:894:ILE:HG12	2.18	0.43
1:A:388:LYS:HE2	1:A:1693:MET:HG3	1.99	0.43
1:A:1420:PHE:O	1:A:1423:TRP:NE1	2.51	0.43
1:A:725:THR:O	1:A:729:VAL:HG23	2.18	0.43
2:B:16:CYS:SG	2:B:17:PHE:N	2.90	0.43
1:A:701:CYS:O	1:A:705:MET:HG2	2.18	0.43
1:A:765:MET:O	1:A:769:ILE:HG12	2.19	0.43
1:A:1297:GLU:OE2	1:A:1297:GLU:HA	2.17	0.43
1:A:1364:ARG:NH2	1:A:1400:VAL:HG12	2.31	0.43
1:A:1256:MET:HE2	1:A:1256:MET:HB3	1.87	0.43
1:A:1333:ILE:N	1:A:1334:PRO:HD2	2.34	0.43
1:A:1574:THR:HG21	1:A:1605:ILE:HD11	2.01	0.43
1:A:310:ASN:C	1:A:312:PRO:HD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1705:CYS:HB3	1:A:1718:LEU:HD21	2.01	0.43
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.87	0.42
1:A:883:HIS:HE2	1:A:889:HIS:CD2	2.37	0.42
1:A:1595:ILE:O	1:A:1599:VAL:HG12	2.19	0.42
1:A:1770:ILE:O	1:A:1773:ILE:HG13	2.19	0.42
1:A:707:ILE:O	1:A:711:VAL:HG13	2.19	0.42
1:A:762:THR:CG2	1:A:794:LEU:HD21	2.50	0.42
1:A:1217:ILE:HG21	1:A:1318:ARG:HH21	1.84	0.42
1:A:1313:LEU:O	1:A:1316:LEU:HD12	2.19	0.42
1:A:732:THR:HG21	1:A:816:VAL:HG22	2.01	0.42
1:A:1344:LEU:HD23	1:A:1411:TYR:CE1	2.53	0.42
1:A:1736:ASN:C	1:A:1738:ASN:H	2.26	0.42
1:A:1567:LEU:HA	1:A:1570:VAL:HG12	2.00	0.42
1:A:1686:TRP:HD1	1:A:1690:ILE:HG22	1.84	0.42
2:B:64:LYS:HA	2:B:64:LYS:HD3	1.60	0.42
3:C:1:NAG:H4	3:C:2:NAG:H2	1.73	0.42
1:A:1592:SER:HA	1:A:1595:ILE:HG12	2.01	0.42
1:A:230:THR:HA	1:A:233:VAL:HG12	2.01	0.42
1:A:1365:CYS:O	1:A:1374:PRO:CG	2.62	0.42
1:A:1499:ALA:O	1:A:1503:LEU:HG	2.20	0.42
1:A:1761:SER:O	1:A:1765:VAL:HG13	2.19	0.42
1:A:875:ASP:OD1	1:A:875:ASP:N	2.52	0.42
1:A:1237:ILE:HA	1:A:1240:LEU:HD12	2.01	0.42
1:A:1241:LEU:HD13	1:A:1241:LEU:HA	1.93	0.42
1:A:1421:LYS:O	1:A:1716:ASP:HB3	2.19	0.42
1:A:1607:GLY:O	1:A:1610:LEU:HD23	2.19	0.42
1:A:369:LEU:HD11	1:A:394:PHE:HE1	1.85	0.42
1:A:379:TYR:CE2	1:A:1694:PHE:HE2	2.36	0.42
1:A:1350:PHE:HD1	1:A:1451:TYR:HE1	1.68	0.42
1:A:1455:PHE:O	1:A:1456:ILE:C	2.62	0.42
1:A:852:PHE:O	1:A:856:VAL:HG22	2.20	0.42
1:A:190:LEU:O	1:A:196:TRP:NE1	2.50	0.41
1:A:882:TRP:HB3	1:A:893:ILE:HD11	2.01	0.41
1:A:729:VAL:O	1:A:733:LEU:HG	2.20	0.41
1:A:1192:VAL:HA	1:A:1195:ARG:HB3	2.02	0.41
1:A:1532:PHE:O	1:A:1536:ILE:HG12	2.21	0.41
1:A:1662:ILE:CG2	1:A:1768:MET:HG3	2.51	0.41
1:A:1534:VAL:HA	1:A:1537:MET:HG2	2.02	0.41
1:A:826:LEU:HD13	1:A:1342:VAL:HG13	2.03	0.41
1:A:1673:TYR:HD2	1:A:1753:PHE:CE2	2.39	0.41
1:A:376:GLU:O	1:A:380:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ILE:HD13	1:A:832:ILE:HA	1.70	0.41
2:B:8:GLN:HG3	2:B:14:TYR:HD1	1.85	0.41
1:A:235:SER:OG	1:A:236:GLY:N	2.53	0.41
1:A:254:VAL:O	1:A:258:THR:HG22	2.21	0.41
1:A:1618:PHE:HE2	1:A:1624:PHE:HZ	1.68	0.41
1:A:921:VAL:O	1:A:925:VAL:HG12	2.21	0.41
1:A:1458:PHE:O	1:A:1462:PHE:HB2	2.20	0.41
1:A:1540:ILE:HD12	1:A:1540:ILE:HA	1.90	0.41
1:A:1738:ASN:OD1	1:A:1739:GLY:N	2.53	0.41
1:A:790:VAL:O	1:A:794:LEU:HD23	2.20	0.41
1:A:1725:THR:HG21	1:A:1747:PRO:HD3	2.03	0.41
1:A:1514:ARG:NH2	1:A:1515:PRO:HD2	2.31	0.40
1:A:257:LEU:HD12	1:A:1645:ILE:HG13	2.03	0.40
1:A:273:PHE:CB	1:A:356:PHE:HD2	2.25	0.40
1:A:1397:TRP:H	3:E:1:NAG:H83	1.85	0.40
1:A:1455:PHE:CE1	1:A:1459:GLY:HA3	2.57	0.40
1:A:1519:TYR:O	1:A:1523:ILE:HG13	2.21	0.40
1:A:284:ASN:OD1	1:A:284:ASN:N	2.54	0.40
1:A:708:LYS:O	1:A:712:LYS:HG2	2.22	0.40
1:A:1364:ARG:HH21	1:A:1400:VAL:HG12	1.85	0.40
1:A:1361:LYS:HG2	1:A:1436:TYR:HA	2.04	0.40
1:A:813:LEU:HD21	1:A:1352:ILE:HG21	2.04	0.40
1:A:1423:TRP:CH2	1:A:1424:MET:HE2	2.55	0.40
1:A:1649:LEU:HD23	1:A:1649:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1116/1838 (61%)	1028 (92%)	84 (8%)	4 (0%)	30 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
All	All	1181/1905 (62%)	1084 (92%)	93 (8%)	4 (0%)	37	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	PHE
1	A	1732	PRO
1	A	1298	MET
1	A	1371	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	943/1612 (58%)	909 (96%)	34 (4%)	31	58
2	B	53/53 (100%)	53 (100%)	0	100	100
All	All	996/1665 (60%)	962 (97%)	34 (3%)	33	59

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	SER
1	A	230	THR
1	A	237	LEU
1	A	295	VAL
1	A	317	LEU
1	A	395	MET
1	A	703	LEU
1	A	808	LEU
1	A	832	ILE
1	A	904	GLU
1	A	912	VAL
1	A	913	SER

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Mol	Chain	Res	Type
1	A	923	LEU
1	A	940	LEU
1	A	942	LEU
1	A	1214	ILE
1	A	1298	MET
1	A	1316	LEU
1	A	1326	VAL
1	A	1333	ILE
1	A	1376	ASN
1	A	1456	ILE
1	A	1494	LYS
1	A	1546	THR
1	A	1551	THR
1	A	1608	THR
1	A	1612	ASP
1	A	1613	ILE
1	A	1636	LEU
1	A	1645	ILE
1	A	1662	ILE
1	A	1690	ILE
1	A	1708	GLN
1	A	1709	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	276	ASN
1	A	779	GLN
1	A	835	ASN
1	A	889	HIS
1	A	1206	HIS
1	A	1439	GLN
1	A	1498	ASN
1	A	1520	GLN
1	A	1543	ASN
1	A	1591	ASN
1	A	1680	ASN
2	B	15	HIS
2	B	66	HIS

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 ⓘ

7 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$
3	NAG	C	1	1,3	14,14,15	0.50	0	17,19,21	0.40	0
3	NAG	C	2	3	14,14,15	0.42	0	17,19,21	0.44	0
4	NAG	D	1	1,4	14,14,15	0.22	0	17,19,21	0.52	0
4	NAG	D	2	4	14,14,15	0.39	0	17,19,21	0.94	1 (5%)
4	BMA	D	3	4	11,11,12	0.57	0	15,15,17	0.99	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.49	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	3	BMA	C1-O5-C5	3.00	116.21	112.19
4	D	2	NAG	C1-O5-C5	2.76	115.88	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

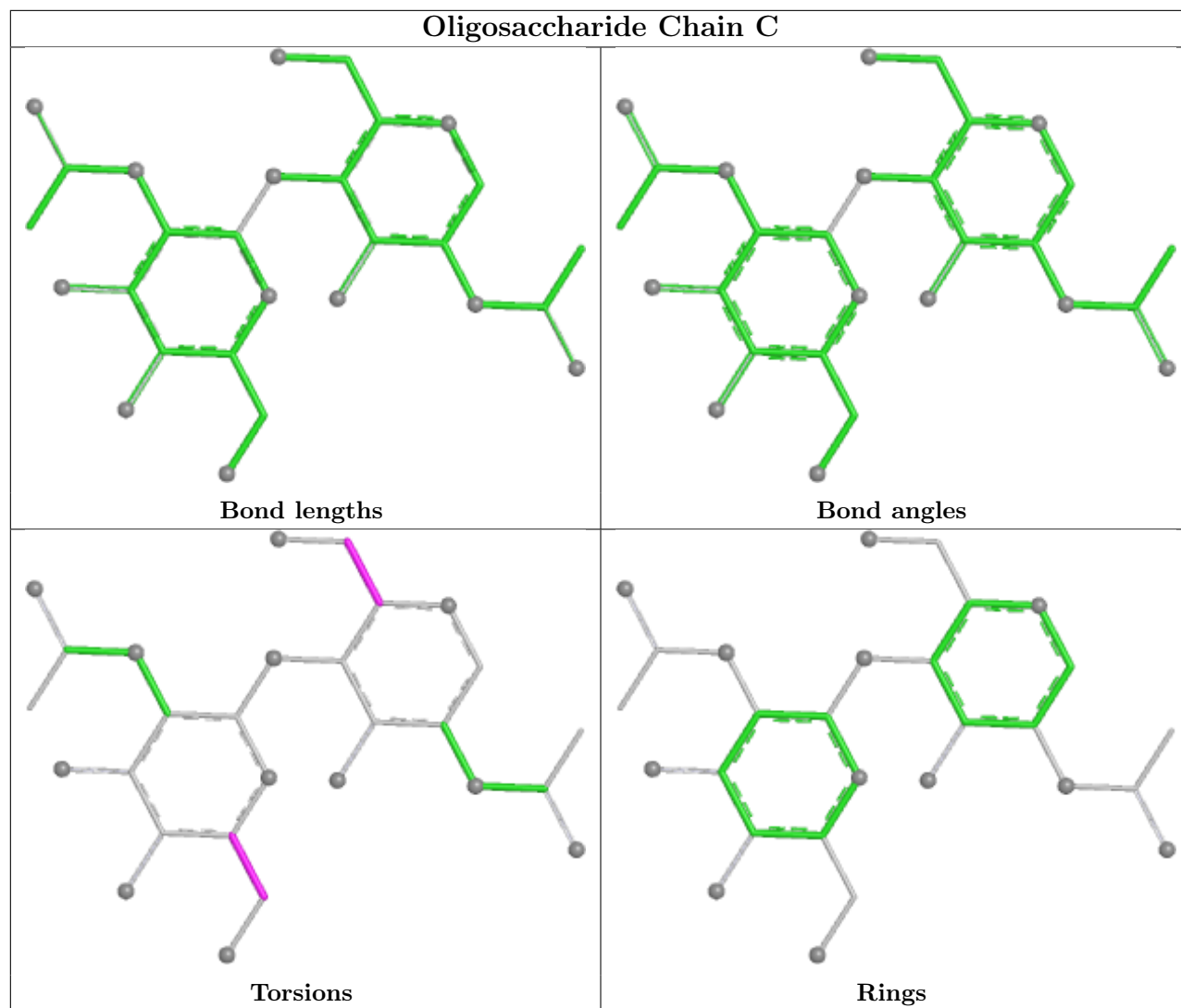
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6

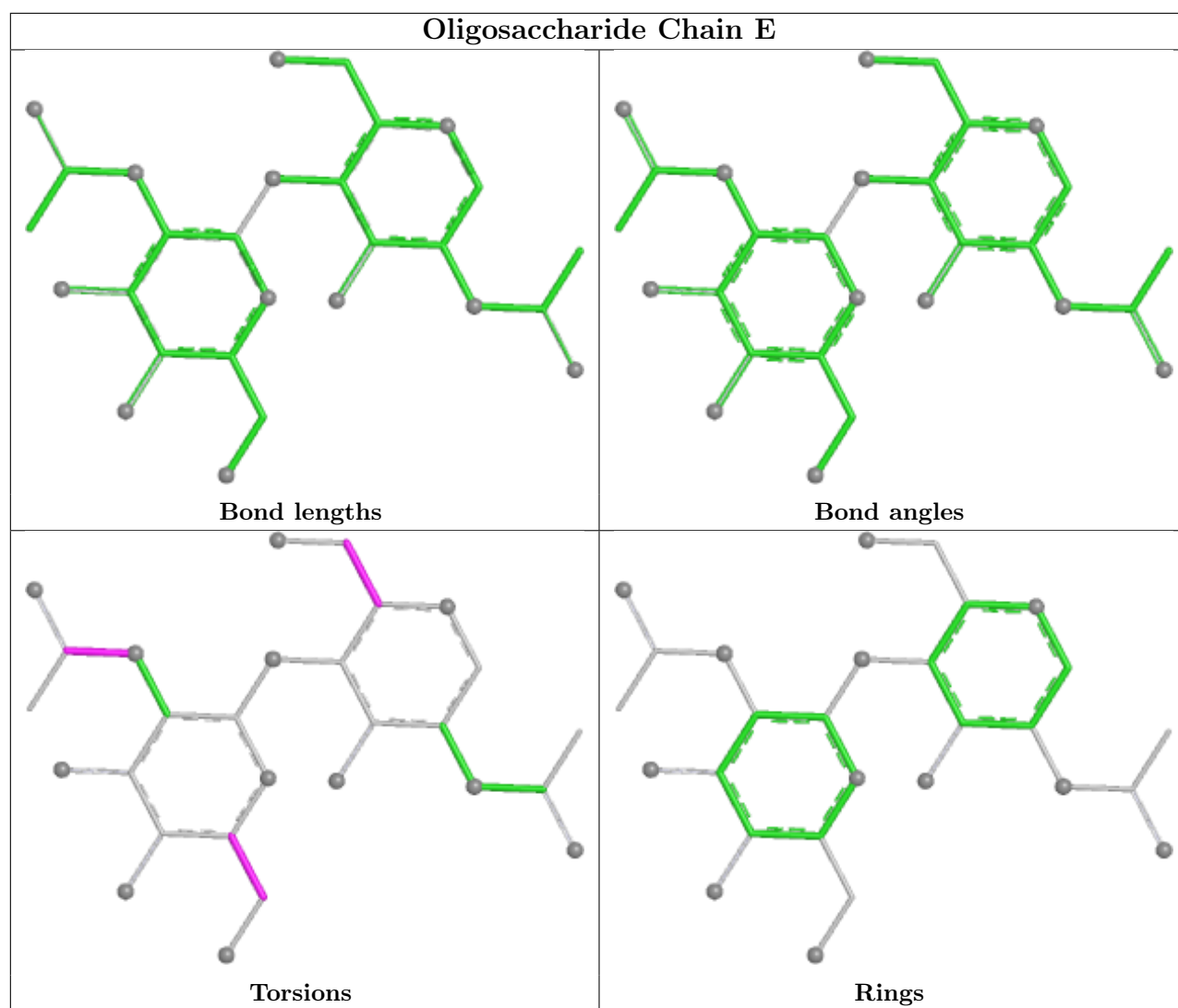
There are no ring outliers.

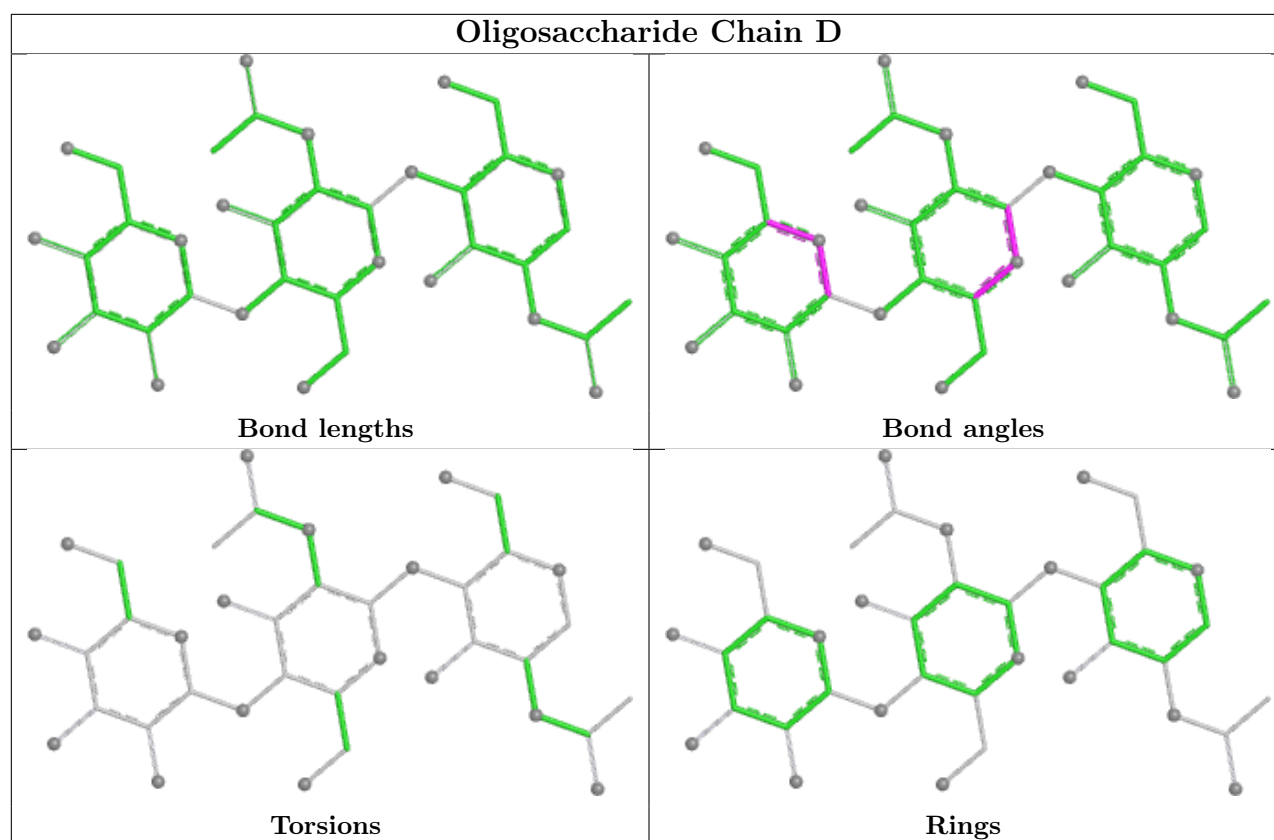
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	2	NAG	1	0
3	E	1	NAG	1	0
4	D	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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	6OU	A	2211	-	16,16,48	1.35	3 (18%)	16,16,53	1.09	1 (6%)
5	NAG	A	2201	-	14,14,15	0.30	0	17,19,21	0.40	0
6	6OU	A	2203	-	34,34,48	1.06	4 (11%)	37,39,53	1.16	2 (5%)
6	6OU	A	2205	-	25,25,48	1.09	4 (16%)	27,27,53	1.37	2 (7%)
6	6OU	A	2202	-	34,34,48	1.04	4 (11%)	37,39,53	1.19	2 (5%)
6	6OU	A	2212	-	14,14,48	1.45	3 (21%)	14,14,53	1.10	1 (7%)
6	6OU	A	2206	-	28,28,48	1.16	4 (14%)	30,30,53	1.33	2 (6%)
6	6OU	A	2208	-	25,25,48	1.21	4 (16%)	28,30,53	1.20	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	6OU	A	2210	-	24,24,48	1.30	5 (20%)	27,29,53	1.28	2 (7%)
6	6OU	A	2204	-	14,14,48	0.96	1 (7%)	14,14,53	1.17	1 (7%)
6	6OU	A	2207	-	39,39,48	0.98	4 (10%)	42,44,53	1.12	2 (4%)
6	6OU	A	2209	-	26,26,48	0.97	2 (7%)	27,27,53	1.14	2 (7%)

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	6OU	A	2211	-	-	9/15/15/52	-
5	NAG	A	2201	-	-	2/6/23/26	0/1/1/1
6	6OU	A	2203	-	-	17/38/38/52	-
6	6OU	A	2205	-	-	13/27/27/52	-
6	6OU	A	2202	-	-	17/38/38/52	-
6	6OU	A	2212	-	-	5/13/13/52	-
6	6OU	A	2206	-	-	14/29/29/52	-
6	6OU	A	2208	-	-	12/29/29/52	-
6	6OU	A	2210	-	-	8/26/26/52	-
6	6OU	A	2204	-	-	4/13/13/52	-
6	6OU	A	2207	-	-	22/43/43/52	-
6	6OU	A	2209	-	-	12/26/26/52	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2212	6OU	C08-C07	-4.02	1.31	1.51
6	A	2211	6OU	C08-C07	-3.93	1.32	1.51
6	A	2206	6OU	O30-C20	-3.83	1.40	1.47
6	A	2210	6OU	P23-O26	2.81	1.65	1.54
6	A	2208	6OU	O30-C20	-2.74	1.40	1.46
6	A	2207	6OU	O30-C20	-2.63	1.40	1.46
6	A	2205	6OU	O30-C20	-2.61	1.40	1.46
6	A	2203	6OU	O30-C20	-2.61	1.40	1.46
6	A	2202	6OU	O30-C20	-2.57	1.40	1.46
6	A	2210	6OU	O30-C20	-2.53	1.40	1.46
6	A	2202	6OU	O18-C16	2.47	1.40	1.33
6	A	2207	6OU	O18-C16	2.47	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2208	6OU	O18-C16	2.44	1.40	1.33
6	A	2206	6OU	O18-C16	2.44	1.40	1.33
6	A	2203	6OU	O18-C16	2.42	1.40	1.33
6	A	2209	6OU	O30-C31	2.42	1.40	1.33
6	A	2209	6OU	O18-C16	2.41	1.40	1.33
6	A	2204	6OU	O30-C31	2.41	1.40	1.33
6	A	2212	6OU	O18-C16	2.39	1.40	1.33
6	A	2210	6OU	O18-C16	2.39	1.40	1.33
6	A	2211	6OU	O18-C16	2.37	1.40	1.33
6	A	2205	6OU	O18-C16	2.31	1.40	1.33
6	A	2202	6OU	O30-C31	2.26	1.40	1.34
6	A	2206	6OU	O30-C31	2.25	1.40	1.34
6	A	2205	6OU	O18-C19	-2.25	1.40	1.45
6	A	2211	6OU	O18-C19	-2.24	1.40	1.45
6	A	2205	6OU	O30-C31	2.24	1.40	1.34
6	A	2212	6OU	O18-C19	-2.19	1.40	1.45
6	A	2203	6OU	O30-C31	2.19	1.40	1.34
6	A	2206	6OU	O18-C19	-2.18	1.40	1.45
6	A	2210	6OU	O18-C19	-2.17	1.40	1.45
6	A	2210	6OU	O30-C31	2.17	1.40	1.34
6	A	2207	6OU	O30-C31	2.14	1.40	1.34
6	A	2207	6OU	O18-C19	-2.12	1.40	1.45
6	A	2208	6OU	O30-C31	2.11	1.40	1.34
6	A	2203	6OU	O18-C19	-2.11	1.40	1.45
6	A	2208	6OU	O18-C19	-2.07	1.40	1.45
6	A	2202	6OU	O18-C19	-2.04	1.40	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2205	6OU	O30-C31-C33	4.11	120.38	111.48
6	A	2203	6OU	O30-C31-C33	4.10	120.36	111.48
6	A	2206	6OU	O30-C31-C33	4.10	120.35	111.48
6	A	2207	6OU	O30-C31-C33	3.92	119.96	111.48
6	A	2208	6OU	O30-C31-C33	3.90	119.92	111.48
6	A	2210	6OU	O30-C31-C33	3.86	119.83	111.48
6	A	2202	6OU	O30-C31-C33	3.80	119.70	111.48
6	A	2202	6OU	O18-C16-C15	3.05	121.13	111.83
6	A	2207	6OU	O18-C16-C15	2.91	120.71	111.83
6	A	2209	6OU	O30-C31-C33	2.87	120.59	111.83
6	A	2205	6OU	O18-C16-C15	2.81	120.39	111.83
6	A	2208	6OU	O18-C16-C15	2.78	120.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2210	6OU	O18-C16-C15	2.78	120.30	111.83
6	A	2204	6OU	O30-C31-C33	2.67	119.98	111.83
6	A	2203	6OU	O18-C16-C15	2.66	119.94	111.83
6	A	2209	6OU	O18-C16-C15	2.51	119.48	111.83
6	A	2206	6OU	O18-C16-C15	2.42	119.21	111.83
6	A	2211	6OU	O18-C16-C15	2.16	120.29	112.14
6	A	2212	6OU	O18-C16-C15	2.07	119.97	112.14

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2202	6OU	C21-O22-P23-O25
6	A	2202	6OU	C21-O22-P23-O26
6	A	2203	6OU	C21-O22-P23-O24
6	A	2203	6OU	C21-O22-P23-O26
6	A	2203	6OU	O26-C27-C28-N29
6	A	2205	6OU	O30-C20-C21-O22
6	A	2206	6OU	C19-C20-O30-C31
6	A	2206	6OU	C33-C31-O30-C20
6	A	2207	6OU	C15-C16-O18-C19
6	A	2207	6OU	O17-C16-O18-C19
6	A	2207	6OU	C27-O26-P23-O22
6	A	2207	6OU	C27-O26-P23-O25
6	A	2207	6OU	O26-C27-C28-N29
6	A	2208	6OU	O18-C19-C20-O30
6	A	2208	6OU	C27-O26-P23-O22
6	A	2208	6OU	C27-O26-P23-O25
6	A	2208	6OU	O26-C27-C28-N29
6	A	2210	6OU	C21-O22-P23-O25
6	A	2210	6OU	C21-O22-P23-O26
6	A	2206	6OU	O32-C31-O30-C20
6	A	2211	6OU	C06-C07-C08-C09
6	A	2206	6OU	C21-C20-O30-C31
6	A	2210	6OU	C33-C31-O30-C20
6	A	2205	6OU	C33-C31-O30-C20
6	A	2208	6OU	C13-C14-C15-C16
6	A	2210	6OU	O32-C31-O30-C20
6	A	2206	6OU	C15-C16-O18-C19
6	A	2208	6OU	C15-C16-O18-C19
6	A	2207	6OU	C33-C31-O30-C20
6	A	2203	6OU	O18-C19-C20-O30

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Mol	Chain	Res	Type	Atoms
6	A	2203	6OU	C15-C16-O18-C19
6	A	2209	6OU	C15-C16-O18-C19
6	A	2204	6OU	O30-C20-C21-O22
6	A	2207	6OU	C31-C33-C34-C35
6	A	2206	6OU	O17-C16-O18-C19
6	A	2208	6OU	O17-C16-O18-C19
6	A	2205	6OU	O32-C31-O30-C20
6	A	2203	6OU	O17-C16-O18-C19
6	A	2207	6OU	O32-C31-O30-C20
6	A	2206	6OU	C31-C33-C34-C35
6	A	2208	6OU	C33-C31-O30-C20
5	A	2201	NAG	O5-C5-C6-O6
6	A	2208	6OU	O32-C31-O30-C20
6	A	2209	6OU	O17-C16-O18-C19
6	A	2202	6OU	C10-C11-C12-C13
6	A	2209	6OU	C35-C36-C37-C38
6	A	2211	6OU	C13-C14-C15-C16
6	A	2205	6OU	C31-C33-C34-C35
6	A	2203	6OU	C08-C09-C10-C11
6	A	2205	6OU	C34-C35-C36-C37
6	A	2202	6OU	C34-C35-C36-C37
6	A	2202	6OU	C33-C31-O30-C20
6	A	2202	6OU	C15-C16-O18-C19
6	A	2211	6OU	C12-C13-C14-C15
6	A	2202	6OU	C12-C13-C14-C15
6	A	2209	6OU	C11-C12-C13-C14
6	A	2212	6OU	C07-C08-C09-C10
6	A	2209	6OU	C31-C33-C34-C35
6	A	2202	6OU	O32-C31-O30-C20
6	A	2205	6OU	C10-C11-C12-C13
6	A	2209	6OU	C37-C38-C39-C40
6	A	2210	6OU	C35-C36-C37-C38
6	A	2207	6OU	C10-C11-C12-C13
6	A	2202	6OU	O17-C16-O18-C19
6	A	2202	6OU	C31-C33-C34-C35
6	A	2212	6OU	C08-C09-C10-C11
6	A	2206	6OU	C06-C07-C08-C09
6	A	2203	6OU	O18-C19-C20-C21
6	A	2207	6OU	C08-C09-C10-C11
6	A	2209	6OU	C41-C42-C43-C44
6	A	2207	6OU	C12-C13-C14-C15
6	A	2205	6OU	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
6	A	2207	6OU	C13-C14-C15-C16
6	A	2205	6OU	O18-C19-C20-O30
6	A	2212	6OU	C11-C12-C13-C14
6	A	2202	6OU	C08-C09-C10-C11
6	A	2211	6OU	C11-C12-C13-C14
6	A	2211	6OU	C08-C09-C10-C11
6	A	2207	6OU	C06-C07-C08-C09
6	A	2205	6OU	O18-C19-C20-C21
6	A	2205	6OU	C19-C20-C21-O22
6	A	2206	6OU	O18-C19-C20-O30
6	A	2206	6OU	C34-C35-C36-C37
6	A	2202	6OU	C38-C39-C40-C41
6	A	2209	6OU	C12-C13-C14-C15
6	A	2205	6OU	C11-C12-C13-C14
6	A	2209	6OU	C34-C35-C36-C37
6	A	2207	6OU	C19-C20-C21-O22
6	A	2203	6OU	C10-C11-C12-C13
6	A	2203	6OU	C07-C08-C09-C10
6	A	2207	6OU	C09-C10-C11-C12
6	A	2203	6OU	C38-C39-C40-C41
6	A	2207	6OU	O30-C20-C21-O22
6	A	2210	6OU	O18-C19-C20-C21
6	A	2205	6OU	C33-C34-C35-C36
6	A	2211	6OU	C10-C11-C12-C13
6	A	2210	6OU	O18-C19-C20-O30
6	A	2208	6OU	O18-C19-C20-C21
6	A	2207	6OU	C33-C34-C35-C36
6	A	2202	6OU	C21-O22-P23-O24
6	A	2202	6OU	O26-C27-C28-N29
6	A	2203	6OU	C27-O26-P23-O24
6	A	2207	6OU	C21-O22-P23-O24
6	A	2207	6OU	C27-O26-P23-O24
6	A	2207	6OU	C11-C12-C13-C14
6	A	2211	6OU	C09-C10-C11-C12
6	A	2202	6OU	C11-C12-C13-C14
6	A	2202	6OU	C14-C15-C16-O18
6	A	2209	6OU	C14-C15-C16-O18
6	A	2206	6OU	C13-C14-C15-C16
6	A	2202	6OU	O30-C31-C33-C34
6	A	2211	6OU	C07-C08-C09-C10
6	A	2212	6OU	C05-C06-C07-C08
6	A	2203	6OU	O30-C20-C21-O22

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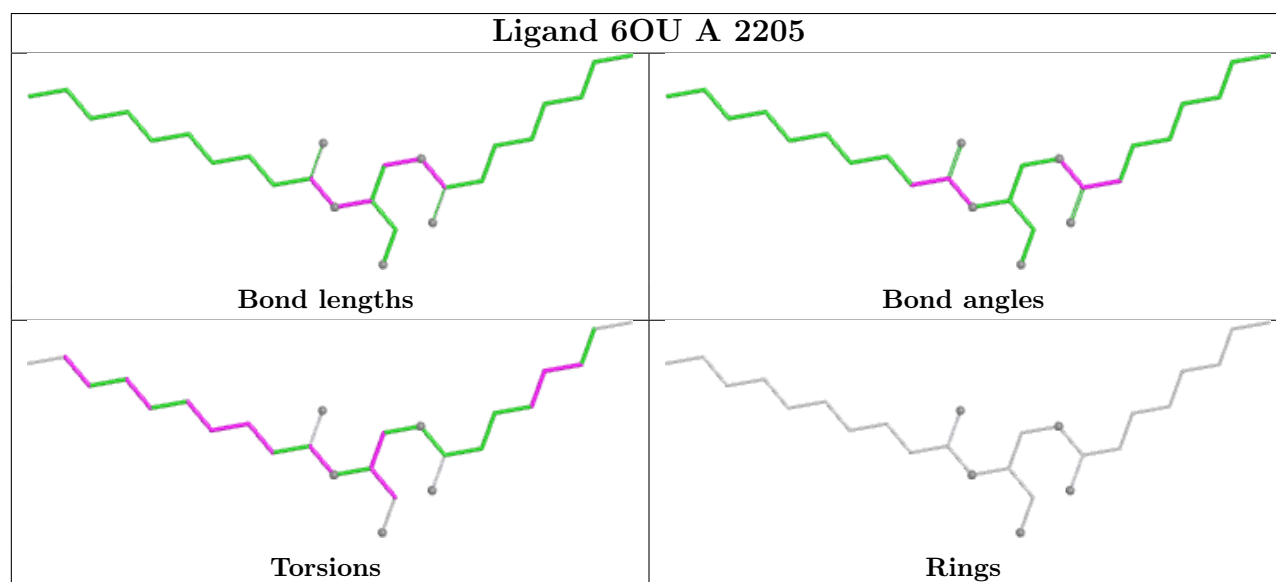
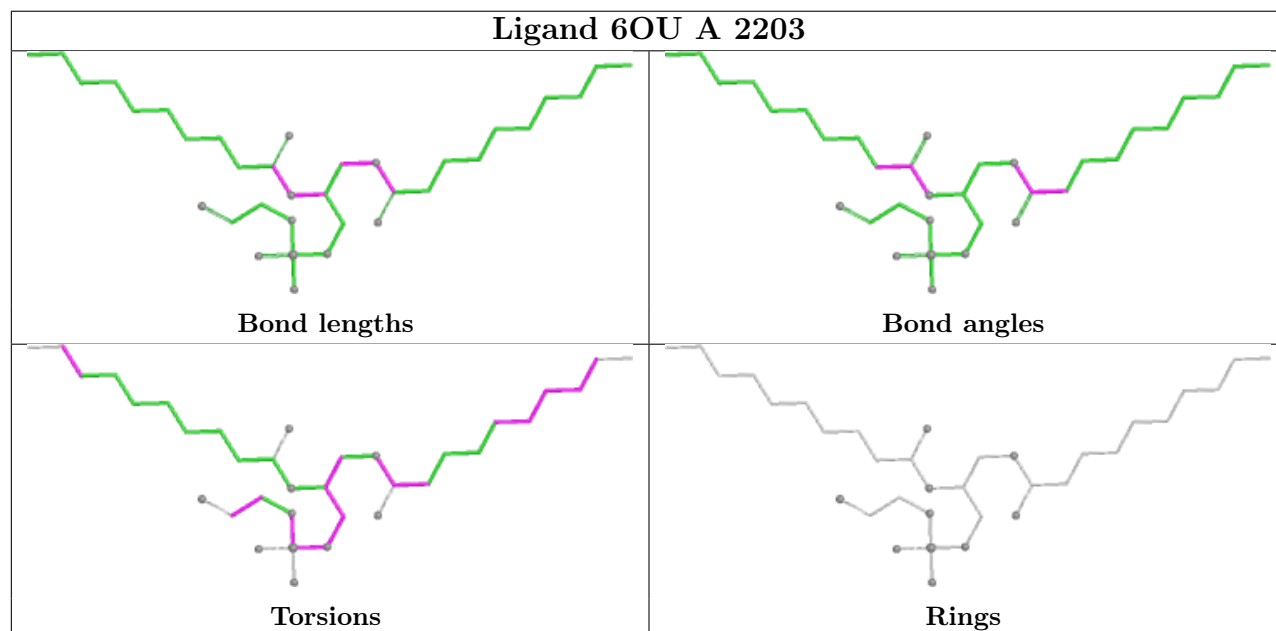
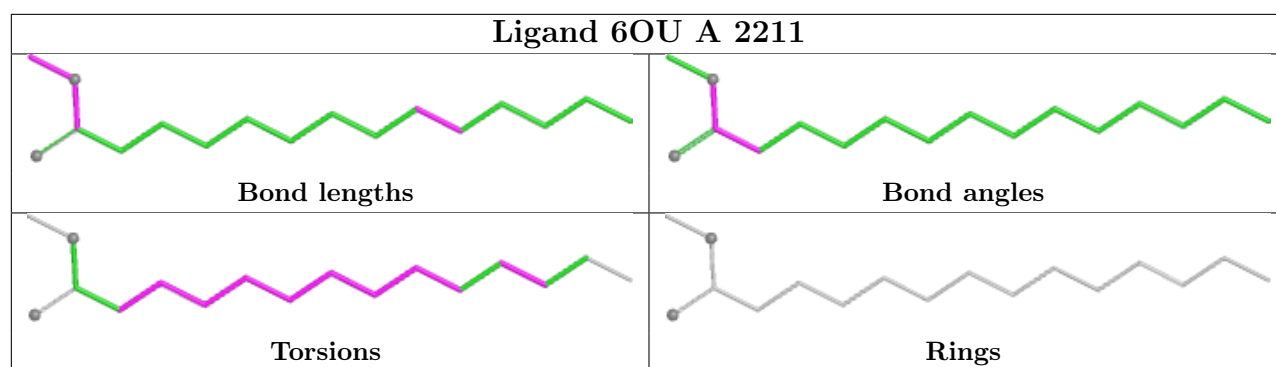
Mol	Chain	Res	Type	Atoms
6	A	2209	6OU	C40-C41-C42-C43
6	A	2206	6OU	C14-C15-C16-O18
6	A	2207	6OU	C38-C39-C40-C41
6	A	2206	6OU	C08-C09-C10-C11
6	A	2210	6OU	C33-C34-C35-C36
6	A	2211	6OU	C04-C05-C06-C07
6	A	2204	6OU	C38-C39-C40-C41
6	A	2204	6OU	O32-C31-O30-C20
6	A	2203	6OU	C20-C21-O22-P23
6	A	2212	6OU	C12-C13-C14-C15
6	A	2204	6OU	C33-C31-O30-C20
6	A	2207	6OU	C40-C41-C42-C43
6	A	2209	6OU	C38-C39-C40-C41
6	A	2205	6OU	C38-C39-C40-C41
6	A	2203	6OU	C09-C10-C11-C12
6	A	2203	6OU	C14-C15-C16-O18
6	A	2208	6OU	C14-C15-C16-O18
6	A	2206	6OU	C38-C39-C40-C41
5	A	2201	NAG	C4-C5-C6-O6
6	A	2203	6OU	C14-C15-C16-O17
6	A	2208	6OU	C14-C15-C16-O17

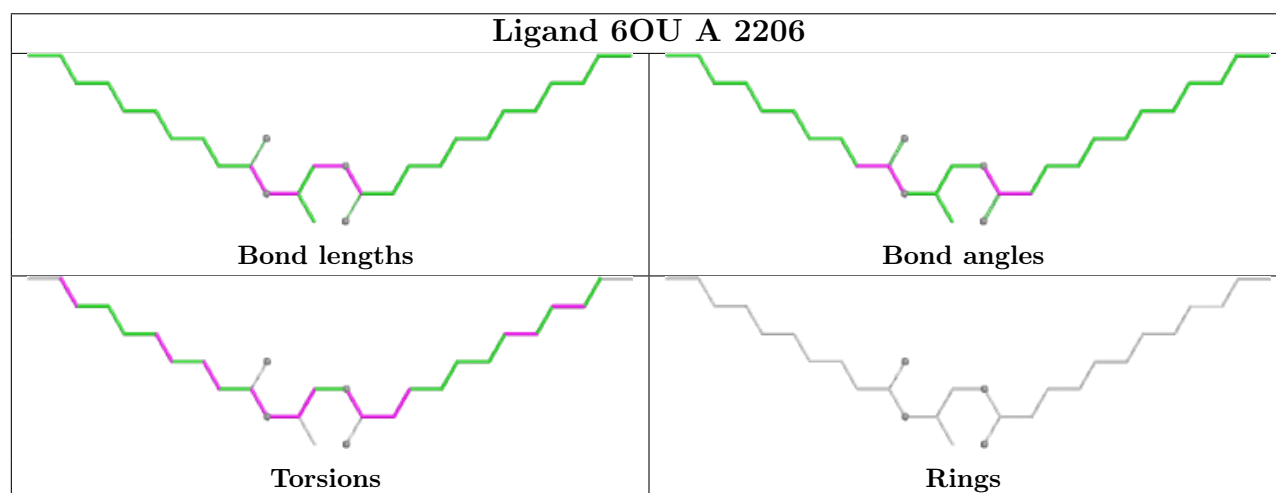
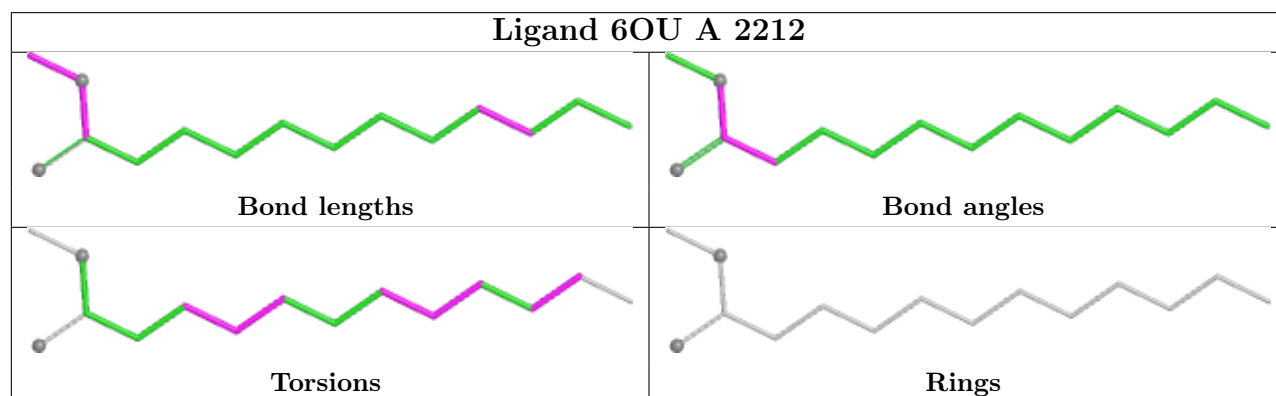
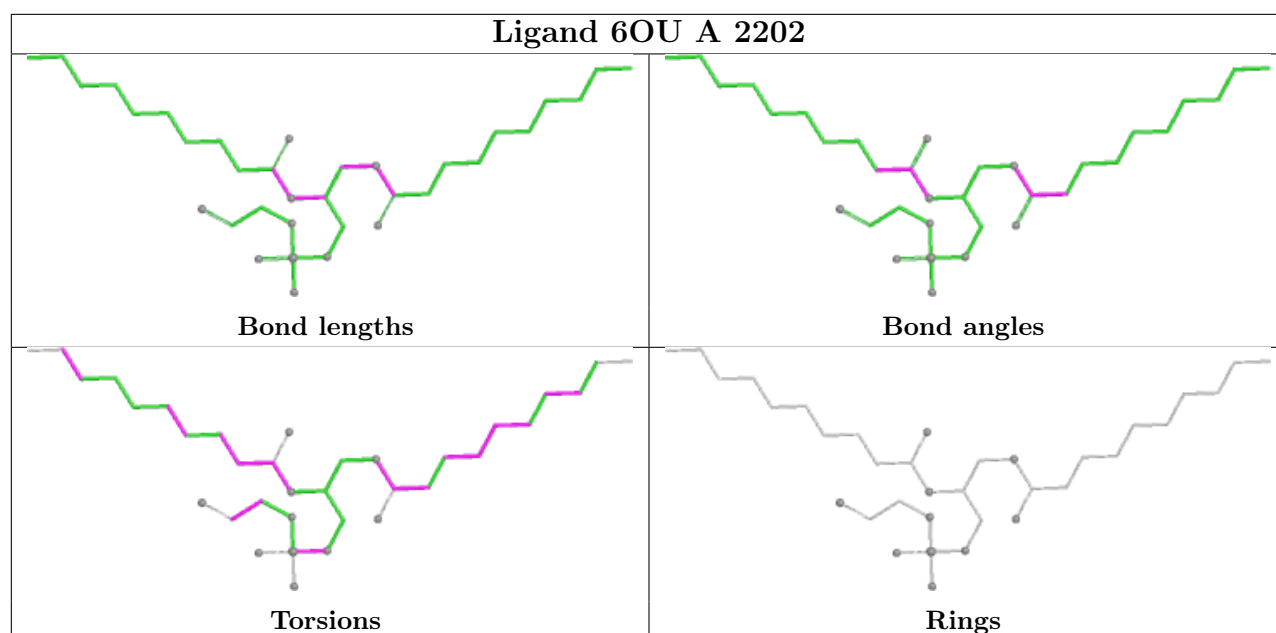
There are no ring outliers.

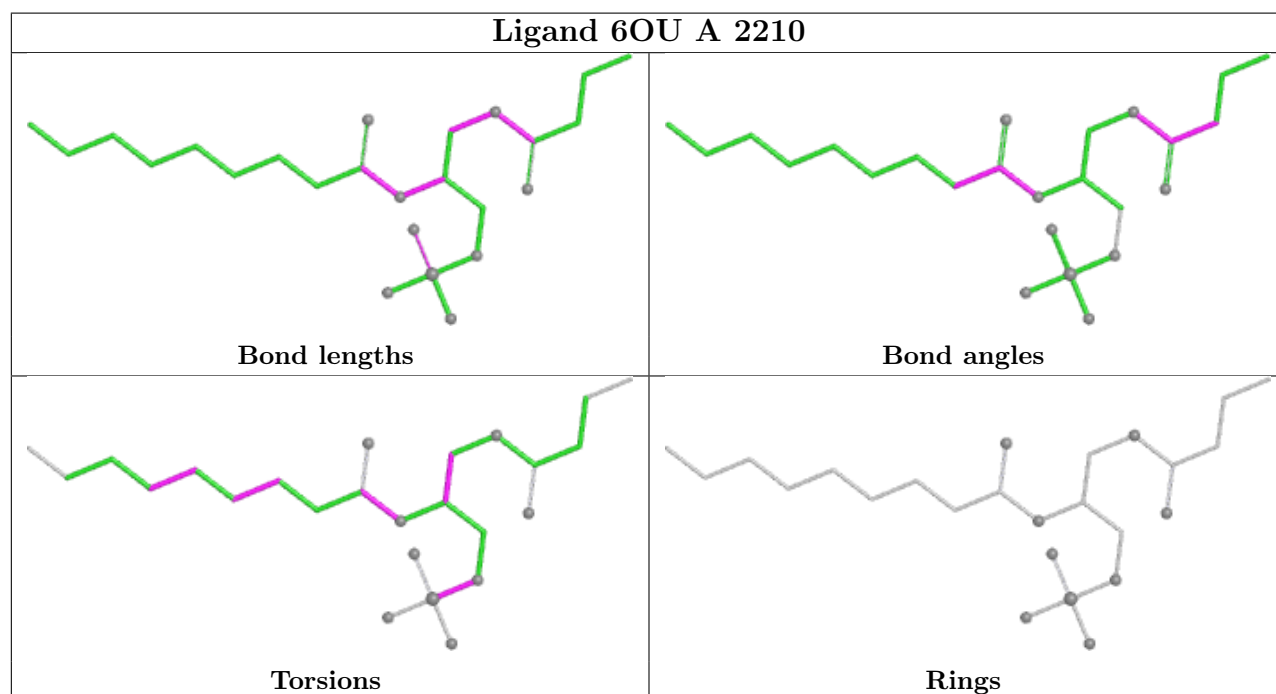
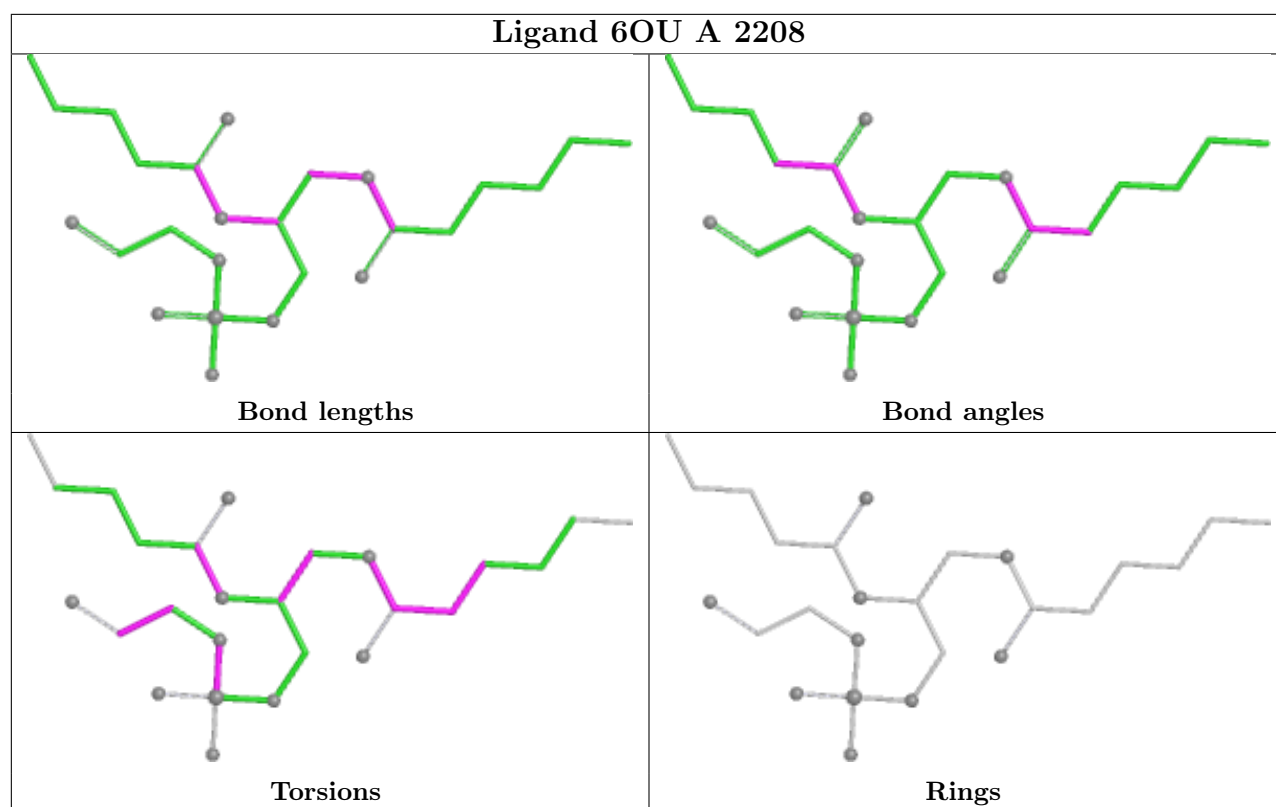
2 monomers are involved in 6 short contacts:

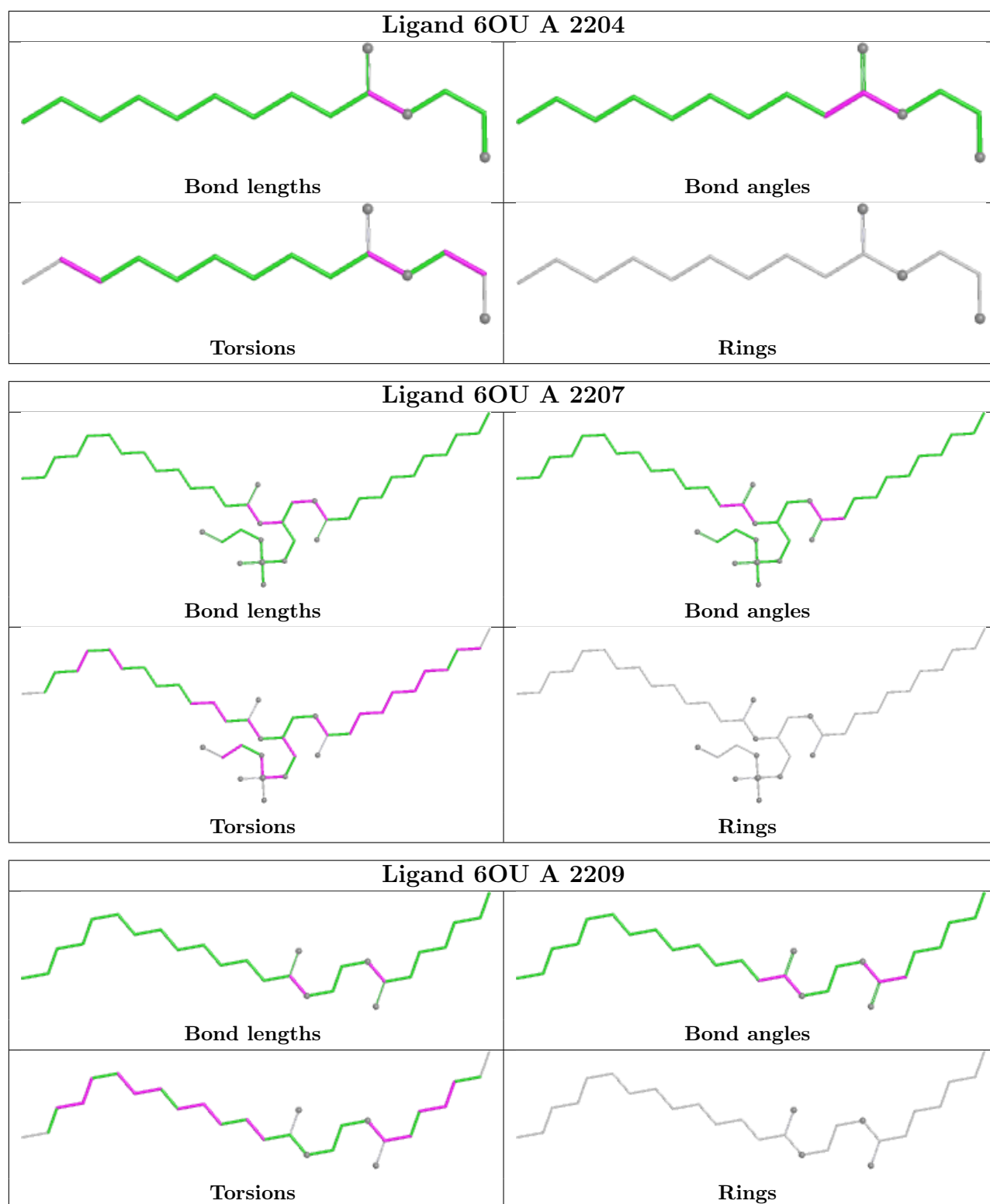
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2201	NAG	4	0
6	A	2210	6OU	2	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

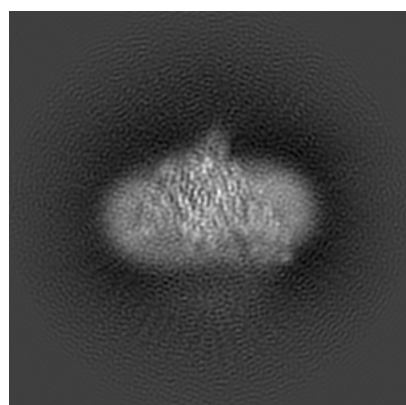
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22621. These allow visual inspection of the internal detail of the map and identification of artifacts.

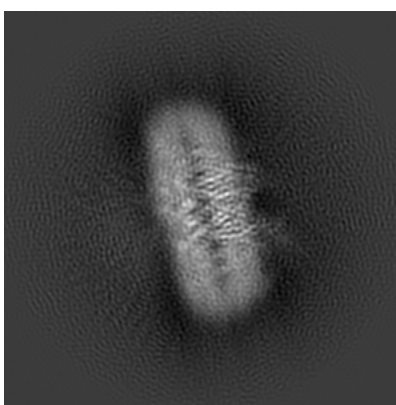
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

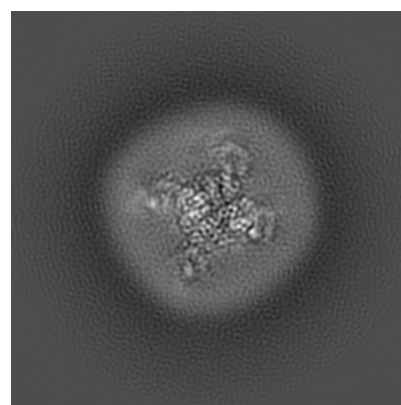
6.1.1 Primary map



X



Y

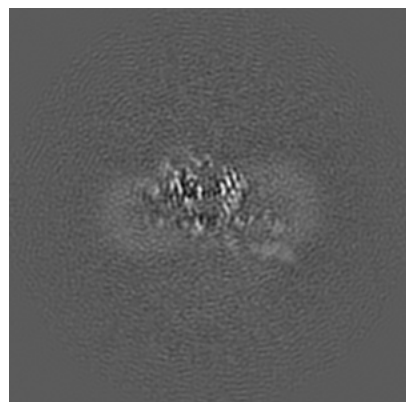


Z

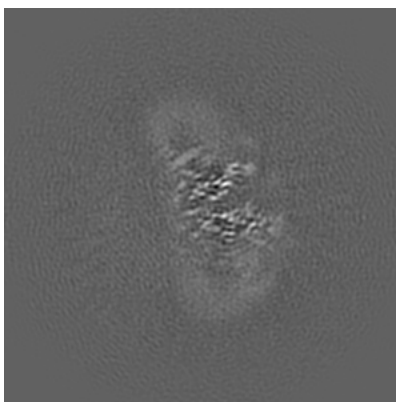
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

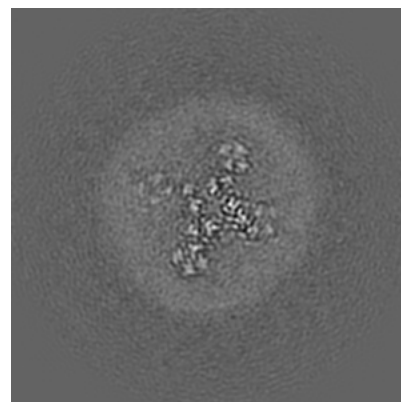
6.2.1 Primary map



X Index: 128



Y Index: 128

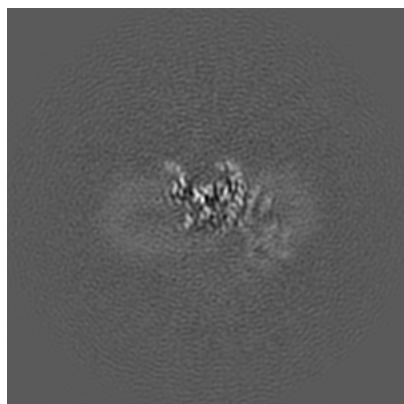


Z Index: 128

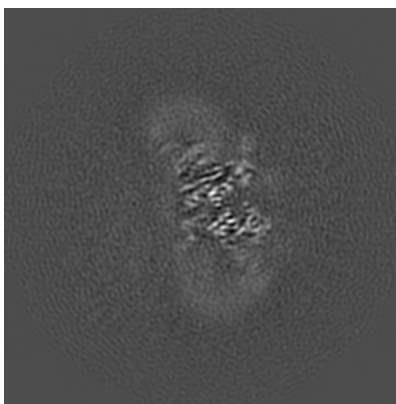
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

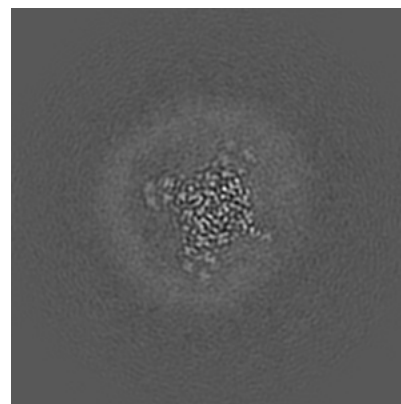
6.3.1 Primary map



X Index: 137



Y Index: 125

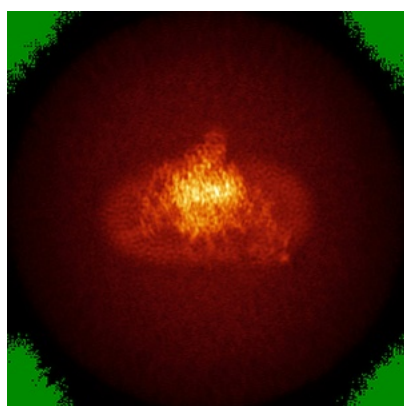


Z Index: 138

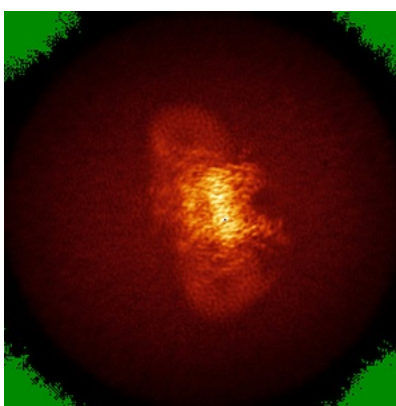
The images above show the largest variance slices of the map in three orthogonal directions.

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

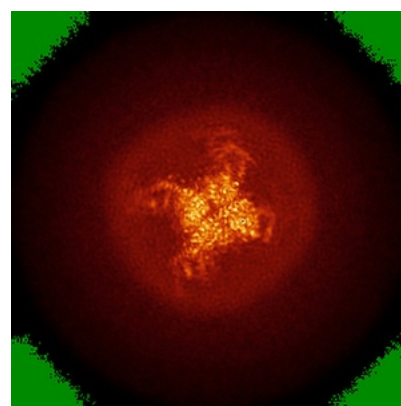
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

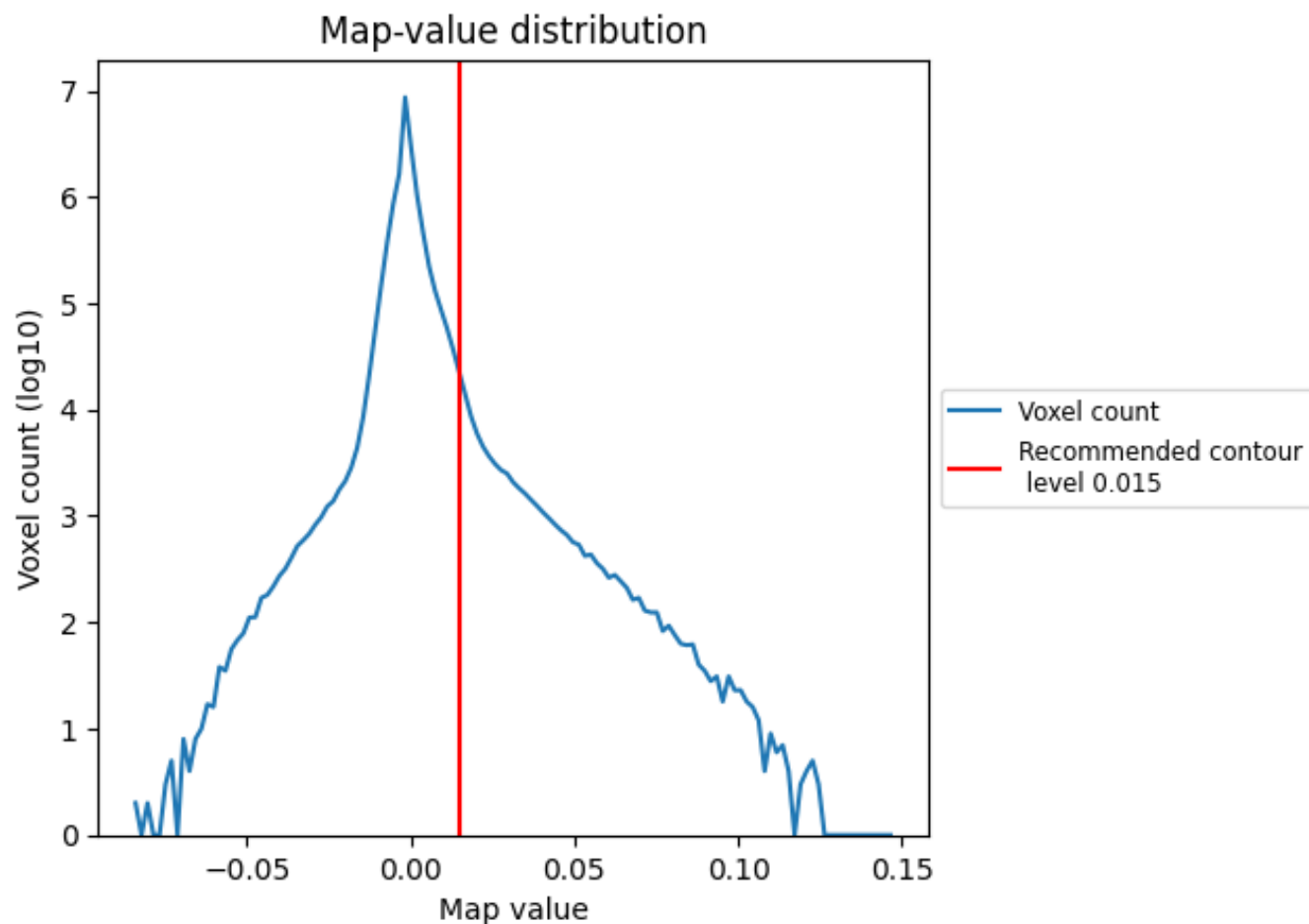
6.6 Mask visualisation

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

7 Map analysis [i](#)

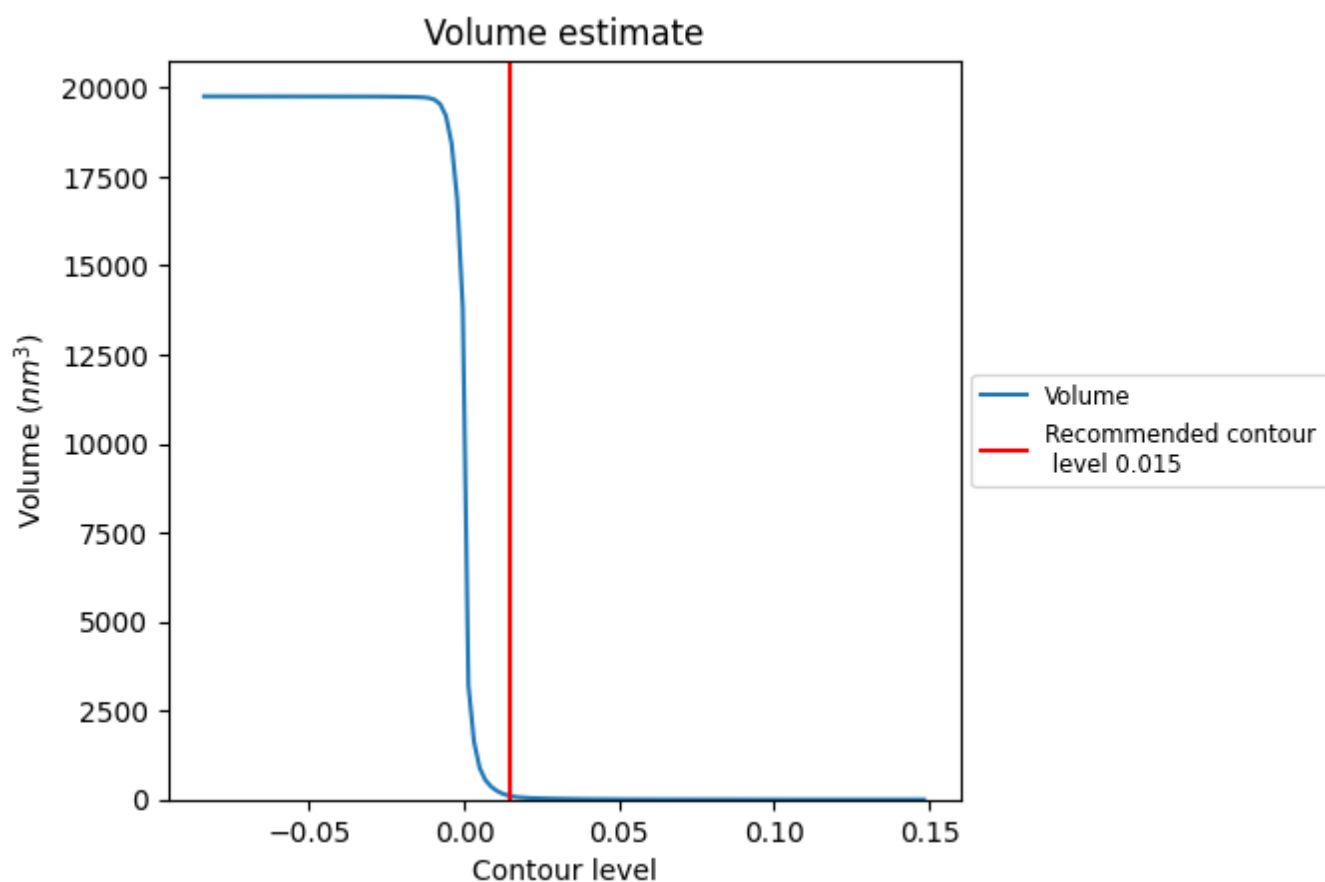
This section contains the results of statistical analysis of the map.

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.

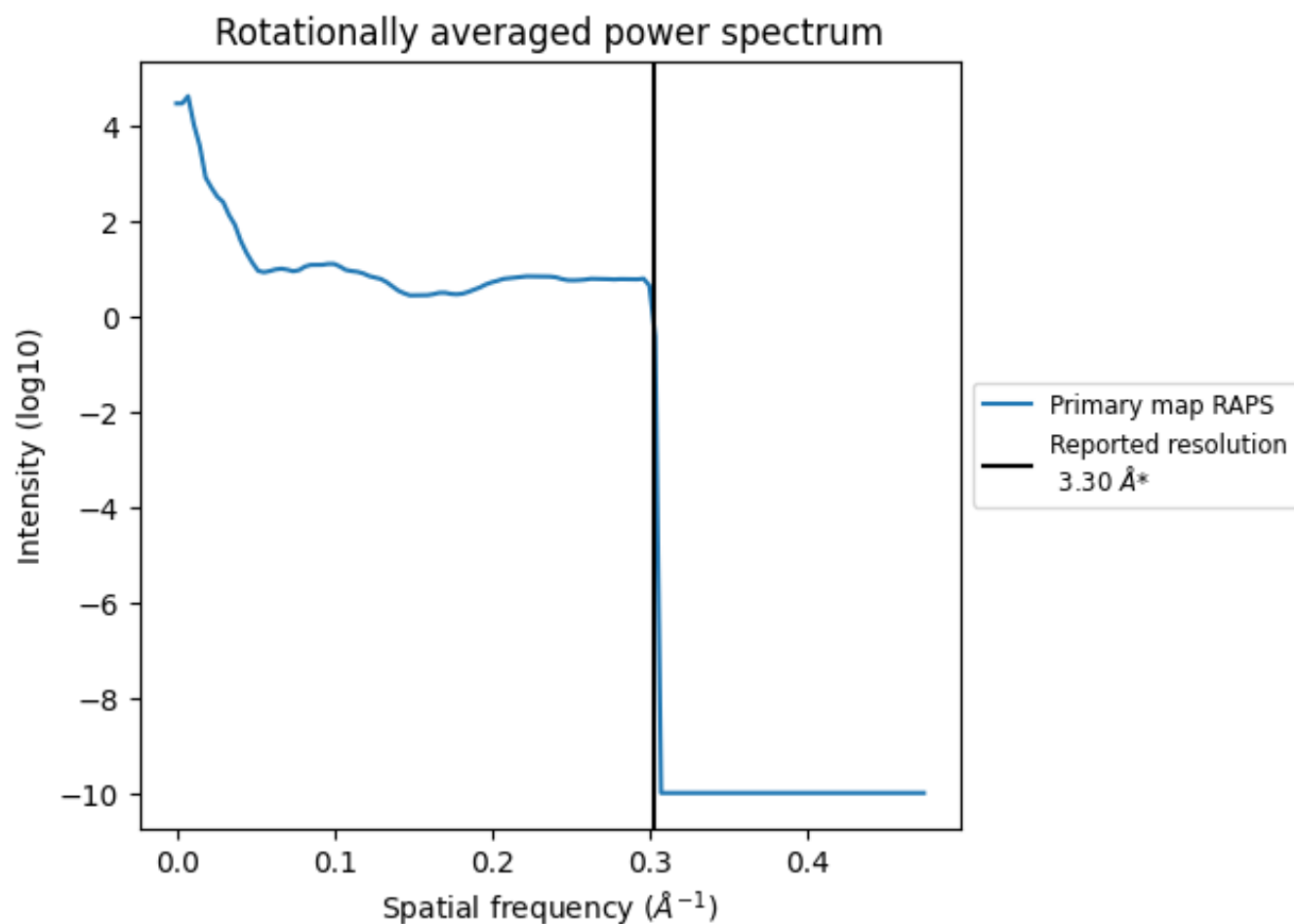
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 ⓘ

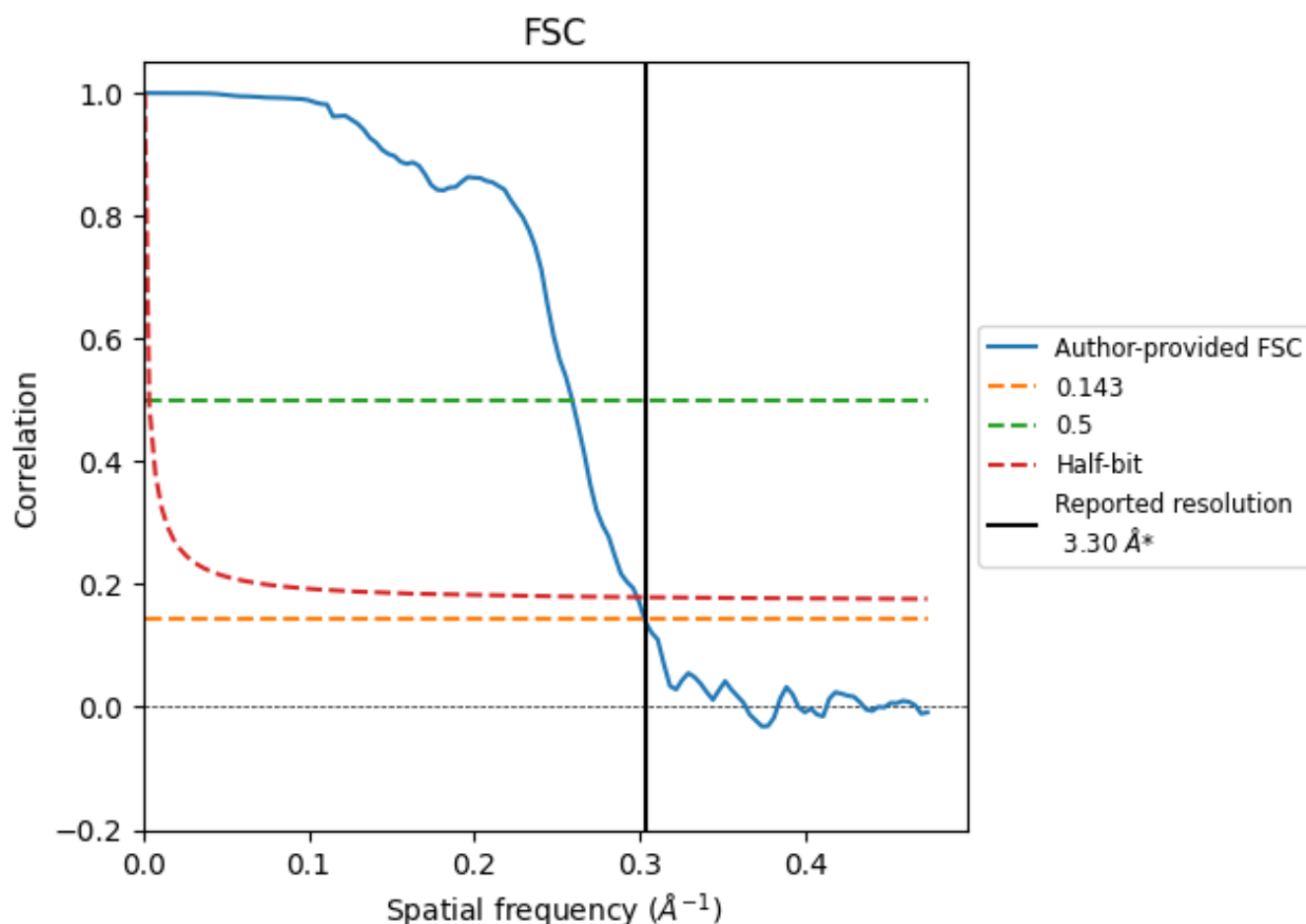


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.86	3.35
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

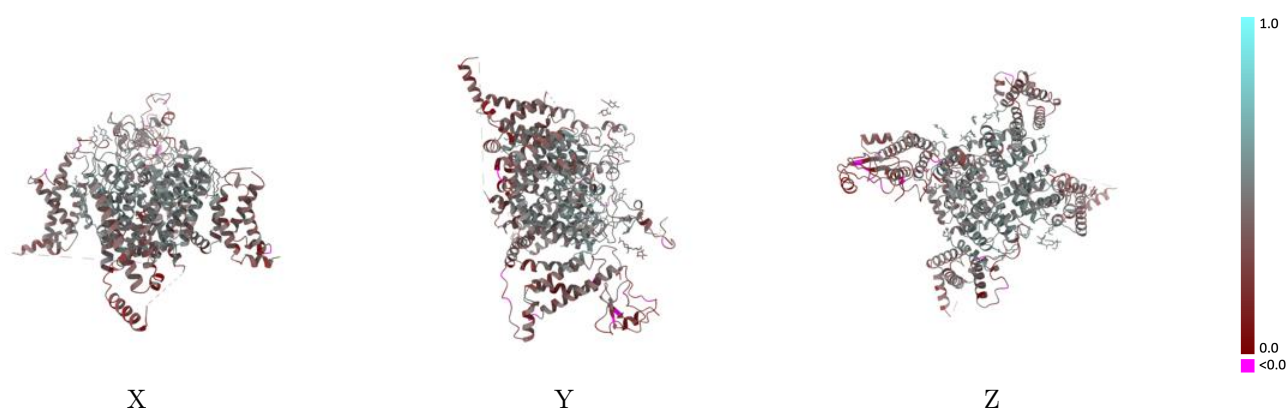
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-22621 and PDB model 7K18. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)

This section was not generated.

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

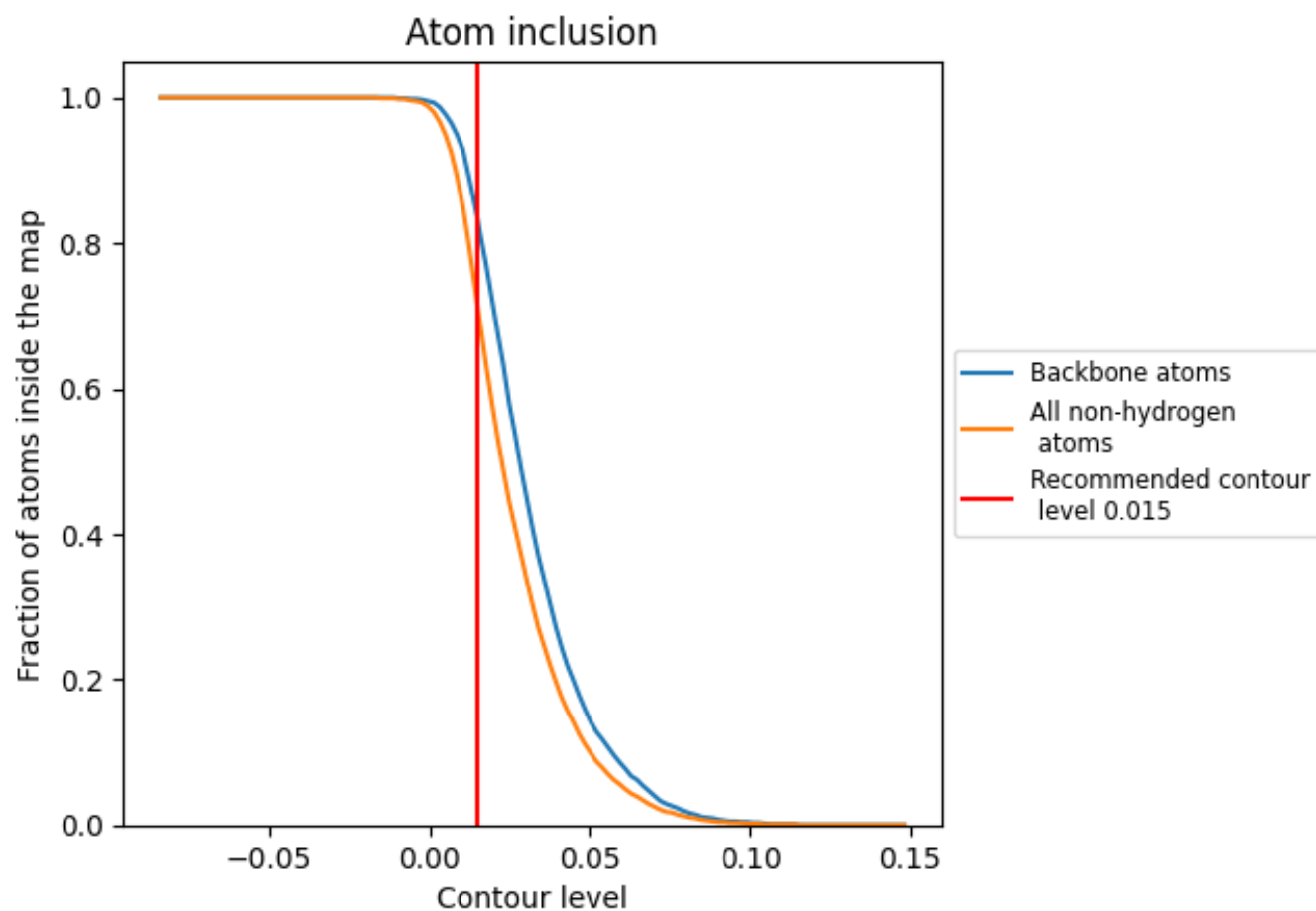


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 72% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.4110
A	0.7330	0.4210
B	0.3700	0.2220
C	0.7860	0.4070
D	0.7690	0.3920
E	0.9290	0.5090

