



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:03 AM UTC

PDB ID : 6UZ3 / pdb_00006uz3
EMDB ID : EMD-20951
Title : Cardiac sodium channel
Authors : Jiang, D.; Shi, H.; Tonggu, L.; Lenaeus, M.J.; Zheng, N.; Catterall, W.A.
Deposited on : 2019-11-14
Resolution : 3.50 Å(reported)
Based on initial model : 6AGF

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

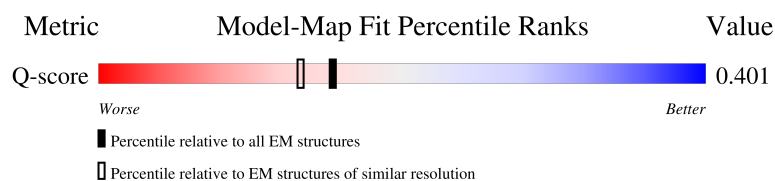
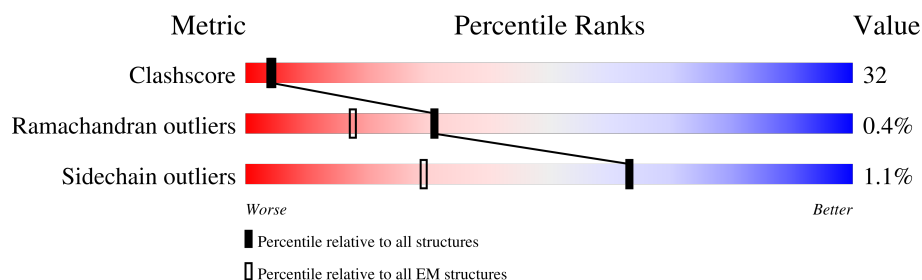
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	19% 31% 29% 39%
2	B	2	50% 100%
2	D	2	100%
3	C	3	33% 67% 33%

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
3	NAG	C	1	-	-	X	-
4	NAG	A	3009	X	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9446 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, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1126	8887	5885	1412	1523	67	0	0

There are 342 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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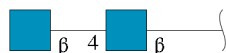
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ILE	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	LEU	deletion	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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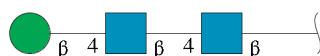
Chain	Residue	Modelled	Actual	Comment	Reference
A	1902	PHE	-	linker	UNP P15389
A	1903	GLN	-	linker	UNP P15389
A	1904	GLY	-	linker	UNP P15389
A	1905	PRO	-	linker	UNP P15389
A	1906	GLY	-	linker	UNP P15389
A	1907	SER	-	linker	UNP P15389
A	1908	MET	-	linker	UNP P15389
A	1909	VAL	-	linker	UNP P15389
A	1972	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 an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



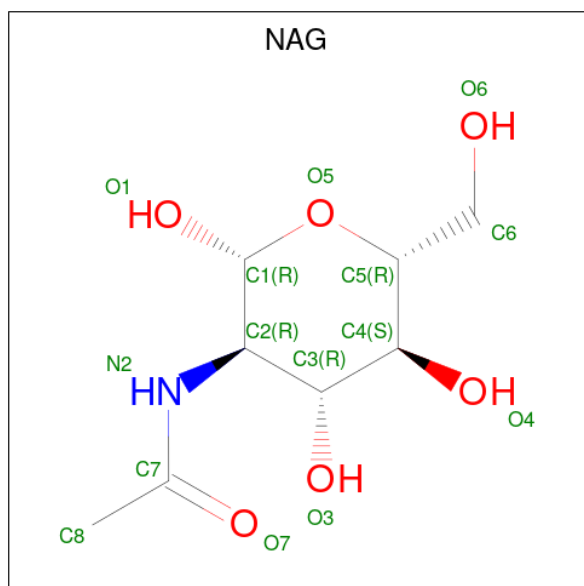
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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.



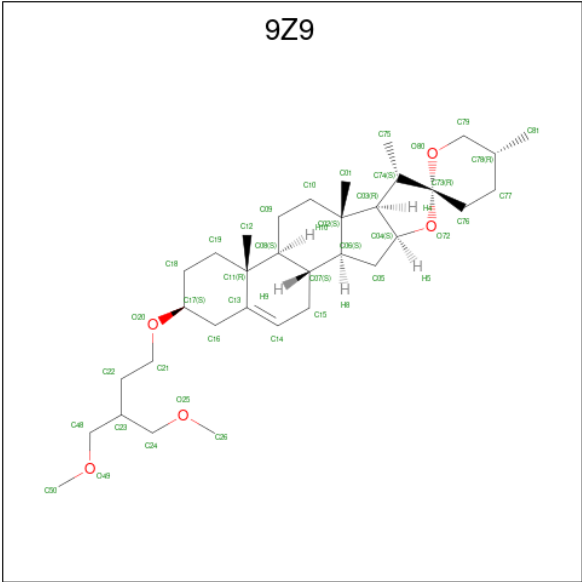
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



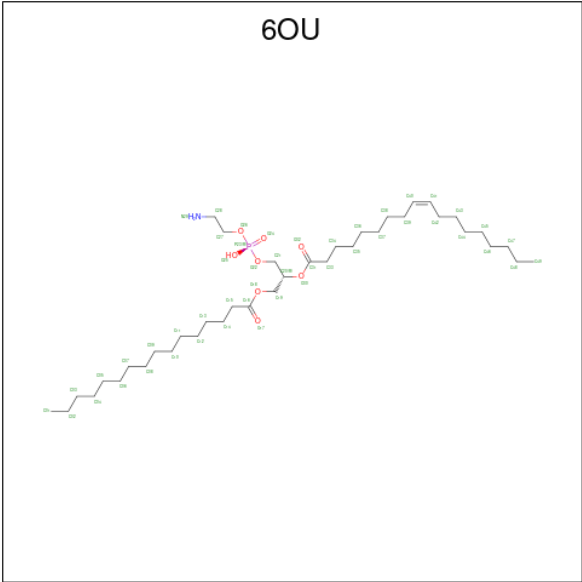
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: $C_{34}H_{56}O_5$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			31	28	3	
5	A	1	Total	C	O	0
			20	18	2	
5	A	1	Total	C	O	0
			37	33	4	
5	A	1	Total	C	O	0
			29	27	2	
5	A	1	Total	C	O	0
			29	27	2	

- 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: C₃₉H₇₆NO₈P).



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			

ARG ILE CYS MET ASP ILE LEU PHE PHE PHE PHE THR GLY LYS ARG VAL LEU GLY GLY MET	SER GLU ASP PHE ASP MET PHE TYR GLU GLU ILE THR GLY LYS PHE ASP GLY THR PRO LEU ASP	G1717 L1718 P1721 I1722 L1723 P1727 P1728 Y1729 D1730 D1731 P1732 L1733 L1734 P1735 P1736 S1737 M1738 G1739 S1740 R1741 G1742 M1743 S1746 V1749 G1750 I1751 I1758 F1762 L1763 I1764 V1765 V1766 M1767 M1768 Y1769 I1770 A1771 I1772 I1773 L1774 E1775 N1776 F1777 S1778 V1779 A1780 THR GLU GLU SER THR PRO LEU	L1638 I1639 R1640 G1641 L1642 G1644 I1645 R1646 T1647 L1648 L1649 F1650 A1651 L1652 M1653 M1654 S1655 L1656 P1657 A1658 L1659 T1662 L1665 V1669 M1670 F1671 I1675 F1676 G1677 M1678 F1681 E1687 A1688 G1689 I1690 D1691 M1692 F1694 N1695 F1696 Q1697 S1702 Q1708 I1709 T1710 T1711 S1712 W1715 D1716	I1572 F1573 T1574 G1575 E1576 C1577 I1578 V1579 K1580 M1581 A1582 A1583 L1584 R1585 H1586 Y1587 Y1588 F1589 M1591 S1592 W1593 M1594 I1595 F1596 D1597 F1598 V1599 V1600 V1601 I1602 V1606 L1610 S1611 I1612 I1613 Q1615 K1616 Y1617 F1618 F1619 S1620 P1621 T1622 L1623 F1624 R1625 V1626 I1627 R1628 I1632 G1633 R1634 I1635 L1636 R1637	S1505 K1506 K1507 P1508 Q1509 K1510 P1511 I1512 P1515 L1516 M1517 K1518 Y1519 Q1520 G1521 F1522 F1523 F1524 D1525 I1526 V1527 T1528 K1529 Q1530 F1532 D1533 T1535 I1536 M1537 F1538 L1539 I1540 M1544 V1545 V1549 E1550 T1551 D1552 D1553 Q1554 S1555 K1558 V1559 L1562 A1563 K1564 I1565 M1566 L1567 L1568 F1569 V1570 A1571	Y1436 E1437 Q1441 E1442 E1443 D1444 N1445 L1446 Y1447 Y1448 Y1449 T1450 Y1451 F1452 F1455 I1456 F1457 F1458 G1459 S1460 F1461 F1461 F1462 T1463 L1464 L1466 I1468 F1467 I1470 I1471 I1472 D1473 N1474 F1475 N1476 K1480 K1481 L1482 G1483 G1484 Q1485 D1486 I1487 F1488 M1489 T1490 E1491 Y1497 M1498 A1499 M1500 K1501 K1502 L1503 G1504	R1364 C1365 I1366 N1367 Q1368 G1371 D1372 L1373 N1376 Y1377 T1378 I1379 V1380 M1381 N1382 K1383 C1386 E1387 S1388 F1389 N1390 V1391 L1392 G1393 E1394 L1395 K1399 V1400 M1403 F1404 D1405 N1406 V1407 G1408 A1409 G1410 Y1411 L1412 A1413 L1414 T1419 F1420 K1421 G1422 M1424 M1427 A1430 V1431 R1434 G1435	F1295 A1296 E1297 M1298 D1299 I1301 K1302 L1304 T1306 L1307 R1308 A1309 L1310 R1311 R1314 A1315 L1316 S1317 R1318 G1321 M1322 R1323 V1324 V1326 M1327 A1332 I1333 F1334 S1335 I1336 M1337 N1338 V1339 L1340 L1341 G1343 L1344 I1345 F1350 S1351 I1352 M1353 G1354 L1357 F1358 A1359 G1360 F1362 G1363	R1234 K1235 T1236 K1237 K1238 V1239 L1240 L1241 E1242 Y1243 A1244 D1245 K1246 M1247 F1248 T1249 Y1250 V1251 F1252 V1253 L1254 E1255 M1256 L1257 L1258 K1259 W1260 K1198 A1262 Y1263 G1264 F1265 L1266 K1267 Y1268 F1269 T1270 M1271 C1274 W1275 L1276 D1277 F1278 L1279 I1280 V1281 D1282 V1283 S1284 L1285 V1286 S1287 L1288 V1289 A1290 M1291 T1292 L1293 G1294	VAL CYS VAL PRO ILE ALA VAL GLU SER THR GLU ASP GLN GLU ASP GLU GLU ASN G1190 W1194 R1195 L1196 R1197 K1198 T1199 C1200 Y1201 G1202 I1203 V1204 E1205 H1206 S1207 W1208 F1209 E1210 I1213 I1214 F1215 M1216 I1217 L1218 L1219 S1220 S1221 L1224 A1225 F1226 I1229 Y1230 L1231 E1232 E1233	LEU ARG ARG ARG PRO LYS LYS PRO ALA SER LEU ALA THR HIS SER GLN LEU PRO SER CYS ILE THR ALA PRO PRO PRO GLU VAL LYS PRO ALA ARG LYS THR ARG PHE GLU ASP LYS ARG VAL PHE LVS ARG THR THR GLY GLN PRO GLY ASP PHE CYS GLY ILE	F922 L924 V925 M926 V927 I928 G929 N930 L934 L938 L942 S943 S944 F945 I830 K831 I832 I833 G834 M835 S836 V837 G838 A839 L840 G841 N842 L843 T844 L845 I853 V857 G858 M859 Q860 L861 F862 G863 Y866 S867 I873 S874 D875 S876 G877 L878 W882 H883 H889 L892 I893 C899 G900 E901 W902 I903 E904 T905 M906 V907 D908 C909 M910 L920 V921
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ASP	HIS	ASN	VAL	VAL	VAL
TYR	GLN	ILE	THR	THR	LYS
LYS	ASN	LEU	LEU	GLY	GLU
ASP	THR	LYS	TYR	GLY	GLU
ASP	PRO	GLY	GLY	GLY	LEU
LYS	ILE	ILE	VAL	VAL	PHE
	GLY	ASP	GLN	CYS	THR
	GLY	PHE	PHE	VAL	GLY
	PRO	GLU	SER	VAL	VAL
	VAL	ASP	ARG	PRO	PRO
	LEU	GLY	TYR	ILE	ILE
	LEU	ASN	PRO	LEU	VAL
	PRO	ILE	ASP	VAL	GLY
	ASP	LEU	HIS	GLU	LEU
	ASN	GLY	MET	LEU	ASP
	HIS	HIS	LYS	GLY	GLY
	TYR	LYS	GLN	ASP	GLY
	LEU	LEU	HIS	ASP	VAL
	SER	GLU	ASP	VAL	ASP
	THR	TYR	PHE	ASN	ASN
	GLN	ASN	PHE	GLY	GLY
	SER	TYR	LYS	HIS	HIS
	ALA	ASN	SER	ALA	PHE
	LEU	SER	ALA	SER	PHE
	SER	HIS	MET	SER	SER
	LYS	ASN	PRO	VAL	VAL
	ASP	VAL	GLU	SER	SER
	PRO	TYR	GLY	GLY	GLY
	ASN	ILE	TYR	GLU	GLY
	GLU	MET	VAL	GLN	GLU
	LYS	ALA	GLN	GLY	GLY
	ARG	ASP	GLU	GLY	ASP
	ASP	LYS	ARG	ASP	ASP
	HIS	GLN	THR	ALA	ALA
	MET	LYS	ILE	THR	THR
	VAL	ASN	PHE	TYR	LYS
	LEU	GLY	PHE	GLY	GLY
	LEU	ILE	LYS	LEU	LEU
	GLU	LYS	ASP	THR	THR
	PHE	VAL	ASP	THR	CYS
	VAL	ASN	GLY	LEU	LYS
	THR	PHE	ASN	LYS	THR
	ALA	ILE	LYS	ILE	GLY
	GLY	ARG	THR	THR	GLY
	ILE	HIS	ARG	THR	GLY
	THR	ASN	ALA	GLY	LYS
	LEU	ILE	VAL	VAL	LEU
	MET	GLU	VAL	LEU	LEU
	GLY	ASP	PHE	PRO	PRO
	ASP	GLY	THR	VAL	THR
	GLU	SER	GLU	VAL	THR
	LEU	VAL	GLY	PRO	THR
	TYR	GLN	ASP	TRP	THR
	LYS	LYS	THR	PRO	THR
	GLY	ALA	LEU	THR	THR
	SER	ASN	VAL	THR	THR

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



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



- Molecule 3: 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, C1	Depositor
Number of particles used	106104	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)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.122	Depositor
Minimum map value	-10.434	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.849	Depositor
Recommended contour level	3	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6OU, 9Z9, NAG, BMA

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	0.37	1/9099 (0.0%)	0.58	14/12358 (0.1%)

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
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1621	PRO	N-CD	9.03	1.60	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1616	LYS	N-CA-C	10.46	122.77	111.36
1	A	1302	LYS	N-CA-C	-8.54	102.85	113.18
1	A	1621	PRO	N-CA-CB	7.94	111.59	103.25
1	A	1622	THR	N-CA-CB	-6.99	100.46	110.81
1	A	1622	THR	N-CA-C	-6.61	105.84	114.04
1	A	1305	ARG	N-CA-C	6.47	118.33	111.28
1	A	1621	PRO	N-CA-C	6.02	124.88	112.47
1	A	1366	ILE	N-CA-C	5.95	114.95	107.70
1	A	1301	ILE	CB-CA-C	-5.91	99.77	111.60
1	A	1623	LEU	N-CA-C	-5.87	104.88	111.28
1	A	1293	LEU	N-CA-C	5.50	117.87	109.62
1	A	1621	PRO	CA-N-CD	-5.41	104.42	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1365	CYS	CA-C-N	-5.08	116.89	121.97
1	A	1365	CYS	C-N-CA	-5.08	116.89	121.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1364	ARG	Peptide
1	A	1406	ASN	Peptide
1	A	1732	PRO	Peptide

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	8887	0	8925	562	0
2	B	28	0	25	2	0
2	D	28	0	25	10	0
3	C	39	0	33	11	0
4	A	28	0	26	18	0
5	A	146	0	0	27	0
6	A	290	0	0	0	0
All	All	9446	0	9034	584	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 32.

All (584) 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:1256:MET:CE	1:A:1281:VAL:HG21	1.16	1.63
5:A:3012:9Z9:C08	5:A:3012:9Z9:C11	1.75	1.61
5:A:3014:9Z9:C08	5:A:3014:9Z9:C11	1.75	1.60
5:A:3013:9Z9:C04	5:A:3013:9Z9:C05	1.77	1.56
1:A:1256:MET:HE1	1:A:1281:VAL:CG2	1.25	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3014:9Z9:C05	5:A:3014:9Z9:C04	1.77	1.50
1:A:1610:LEU:HD23	1:A:1627:ILE:CG2	1.42	1.49
1:A:1235:LYS:HA	1:A:1238:LYS:CD	1.45	1.46
5:A:3011:9Z9:C04	5:A:3011:9Z9:C05	1.77	1.45
1:A:342:CYS:SG	3:C:1:NAG:C8	2.05	1.44
1:A:1488:PHE:CE1	1:A:1662:ILE:HD11	1.51	1.44
5:A:3010:9Z9:C04	5:A:3010:9Z9:C05	1.77	1.43
1:A:138:ILE:CD1	1:A:172:GLU:OE1	1.66	1.41
5:A:3012:9Z9:C81	5:A:3013:9Z9:C81	1.98	1.39
5:A:3012:9Z9:C04	5:A:3012:9Z9:C05	1.77	1.37
1:A:1235:LYS:CA	1:A:1238:LYS:HD2	1.58	1.31
1:A:1610:LEU:HD21	1:A:1627:ILE:CG1	1.71	1.20
1:A:1354:GLY:O	1:A:1358:PHE:HB2	1.41	1.17
1:A:1488:PHE:CD1	1:A:1662:ILE:HD11	1.79	1.17
1:A:1727:PRO:HG2	2:D:2:NAG:O3	1.45	1.16
1:A:1610:LEU:CD2	1:A:1627:ILE:HG12	1.75	1.15
1:A:1610:LEU:HD21	1:A:1627:ILE:CD1	1.75	1.15
1:A:342:CYS:O	3:C:1:NAG:C7	1.95	1.14
1:A:1256:MET:CE	1:A:1281:VAL:CG2	1.98	1.13
1:A:1610:LEU:HD21	1:A:1627:ILE:HG12	1.26	1.10
1:A:138:ILE:HD11	1:A:172:GLU:OE1	0.94	1.09
1:A:131:HIS:O	1:A:134:PHE:CD2	2.07	1.08
1:A:1610:LEU:CD2	1:A:1627:ILE:CG1	2.32	1.05
1:A:1256:MET:HE1	1:A:1281:VAL:HG23	1.39	1.04
1:A:1239:VAL:HG22	1:A:1243:TYR:CE2	1.93	1.03
1:A:1610:LEU:CD2	1:A:1627:ILE:CG2	2.36	1.03
1:A:1256:MET:HE3	1:A:1281:VAL:HG21	1.07	1.02
1:A:1488:PHE:CE1	1:A:1662:ILE:CD1	2.42	1.01
1:A:342:CYS:SG	3:C:1:NAG:H83	1.98	1.01
1:A:343:LEU:HA	3:C:1:NAG:O7	1.61	1.00
1:A:340:TYR:H	4:A:3009:NAG:H81	1.24	0.99
1:A:1610:LEU:HD23	1:A:1627:ILE:HG23	1.01	0.97
1:A:1488:PHE:HE1	1:A:1662:ILE:CD1	1.78	0.96
1:A:340:TYR:H	4:A:3009:NAG:C8	1.77	0.96
1:A:342:CYS:O	3:C:1:NAG:C8	2.13	0.96
1:A:339:GLY:N	4:A:3009:NAG:H81	1.79	0.96
1:A:1610:LEU:CD2	1:A:1627:ILE:HG23	1.94	0.96
1:A:340:TYR:N	4:A:3009:NAG:H81	1.84	0.93
1:A:340:TYR:N	4:A:3009:NAG:C8	2.32	0.92
1:A:780:GLN:HE21	1:A:782:TRP:H	1.17	0.92
1:A:1610:LEU:HD23	1:A:1627:ILE:HG21	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:VAL:HG22	1:A:1243:TYR:HE2	1.30	0.91
1:A:134:PHE:O	1:A:138:ILE:HG12	1.72	0.89
1:A:1602:ILE:O	1:A:1606:VAL:HG23	1.74	0.88
1:A:1488:PHE:HE1	1:A:1662:ILE:HD11	1.09	0.88
1:A:1339:VAL:HG21	1:A:1470:VAL:HG11	1.57	0.86
1:A:1367:ASN:HA	1:A:1395:LEU:HA	1.56	0.86
1:A:1297:GLU:N	1:A:1297:GLU:OE2	2.08	0.86
1:A:138:ILE:CG1	1:A:172:GLU:OE1	2.24	0.85
1:A:278:ARG:NH2	1:A:346:GLY:O	2.09	0.85
1:A:342:CYS:O	3:C:1:NAG:O7	1.94	0.85
1:A:1610:LEU:HD21	1:A:1627:ILE:HD13	1.58	0.84
1:A:327:CYS:SG	1:A:328:GLY:N	2.46	0.84
1:A:342:CYS:SG	3:C:1:NAG:H82	2.18	0.83
1:A:369:LEU:HD23	1:A:375:TRP:HB2	1.60	0.82
1:A:1746:SER:HB3	1:A:1749:VAL:HG12	1.60	0.82
5:A:3012:9Z9:C78	5:A:3013:9Z9:C81	2.57	0.82
1:A:720:ALA:O	1:A:724:ILE:HG23	1.78	0.82
1:A:1610:LEU:CD2	1:A:1627:ILE:CD1	2.54	0.81
1:A:1610:LEU:CD2	1:A:1627:ILE:HD13	2.11	0.81
1:A:171:PHE:O	1:A:174:LEU:HB3	1.81	0.80
1:A:311:ASP:O	1:A:314:ASN:N	2.14	0.80
1:A:1614:ILE:HD11	1:A:1627:ILE:CD1	2.11	0.80
1:A:1727:PRO:CG	2:D:2:NAG:O3	2.27	0.80
1:A:721:ASP:HA	1:A:724:ILE:HG12	1.62	0.80
1:A:1377:TYR:N	1:A:1378:THR:HA	1.97	0.80
1:A:1458:PHE:HA	1:A:1462:PHE:HD2	1.47	0.80
1:A:271:GLN:O	1:A:1625:ARG:HD2	1.83	0.79
1:A:926:MET:SD	1:A:930:ASN:ND2	2.55	0.79
1:A:138:ILE:HD11	1:A:172:GLU:CD	2.04	0.79
1:A:1296:ALA:HB1	1:A:1297:GLU:OE2	1.81	0.78
1:A:1677:GLY:O	1:A:1681:PHE:N	2.15	0.78
1:A:1555:SER:HB2	1:A:1558:LYS:HD3	1.66	0.77
1:A:397:VAL:O	1:A:401:GLY:N	2.18	0.77
1:A:1614:ILE:HA	1:A:1618:PHE:O	1.84	0.77
1:A:170:THR:O	1:A:173:SER:HB3	1.84	0.77
1:A:1419:THR:HG21	1:A:1715:TRP:HE1	1.49	0.77
1:A:788:ILE:HA	1:A:791:ILE:HD12	1.67	0.77
1:A:1691:ASP:O	1:A:1695:ASN:ND2	2.17	0.76
1:A:725:THR:HA	1:A:728:ILE:HD12	1.67	0.76
1:A:823:TRP:CZ3	5:A:3013:9Z9:C19	2.69	0.76
5:A:3014:9Z9:C08	5:A:3014:9Z9:C12	2.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:VAL:CG2	1:A:1243:TYR:HE2	1.99	0.75
1:A:1614:ILE:HD11	1:A:1627:ILE:HD13	1.67	0.74
1:A:773:ASP:HB3	1:A:776:TYR:HB3	1.69	0.74
1:A:1610:LEU:HD23	1:A:1627:ILE:CB	2.15	0.74
5:A:3012:9Z9:C08	5:A:3012:9Z9:C12	2.65	0.74
1:A:339:GLY:H	4:A:3009:NAG:H81	1.53	0.73
1:A:1235:LYS:HA	1:A:1238:LYS:CG	2.17	0.73
1:A:342:CYS:C	3:C:1:NAG:C8	2.61	0.73
1:A:1235:LYS:CA	1:A:1238:LYS:CD	2.37	0.73
1:A:832:ILE:HD11	1:A:944:SER:HB2	1.71	0.72
1:A:165:PHE:HA	1:A:168:ILE:HD12	1.73	0.71
1:A:1614:ILE:HG23	1:A:1619:PHE:HA	1.73	0.71
1:A:859:MET:O	1:A:863:GLY:N	2.24	0.71
1:A:391:MET:HE1	1:A:395:MET:HE3	1.72	0.71
1:A:1376:ASN:HD22	1:A:1442:TRP:H	1.39	0.70
1:A:131:HIS:O	1:A:134:PHE:CE2	2.44	0.70
1:A:340:TYR:N	4:A:3009:NAG:H83	2.07	0.70
1:A:121:VAL:O	1:A:125:ALA:N	2.26	0.69
1:A:1224:LEU:HB3	1:A:1675:ILE:HD13	1.72	0.69
1:A:1296:ALA:CB	1:A:1297:GLU:OE2	2.40	0.69
1:A:1400:VAL:O	1:A:1403:ASN:ND2	2.25	0.69
1:A:1517:ASN:O	1:A:1521:GLY:N	2.24	0.69
1:A:1344:LEU:O	1:A:1411:TYR:OH	2.09	0.69
1:A:1345:ILE:HD11	5:A:3013:9Z9:C79	2.22	0.68
1:A:339:GLY:CA	4:A:3009:NAG:H81	2.24	0.68
1:A:1623:LEU:HD12	1:A:1626:VAL:HG13	1.75	0.68
1:A:234:ILE:HG21	1:A:237:LEU:HD23	1.75	0.67
1:A:1285:LEU:HD23	1:A:1288:LEU:HD21	1.75	0.67
1:A:341:ARG:HH21	4:A:3009:NAG:H3	1.57	0.67
1:A:1239:VAL:CG2	1:A:1243:TYR:CE2	2.74	0.67
1:A:1488:PHE:CD1	1:A:1662:ILE:CD1	2.71	0.67
1:A:1727:PRO:HG2	2:D:2:NAG:C3	2.25	0.66
1:A:1419:THR:HG23	1:A:1421:LYS:H	1.60	0.66
1:A:310:ASN:C	1:A:312:PRO:HD2	2.21	0.66
1:A:721:ASP:CA	1:A:724:ILE:HG12	2.26	0.65
1:A:1487:ILE:O	1:A:1488:PHE:HB2	1.96	0.65
1:A:1622:THR:HG23	1:A:1625:ARG:NH2	2.12	0.65
1:A:905:THR:HG23	1:A:922:PHE:HE2	1.62	0.65
1:A:1266:LYS:O	1:A:1270:THR:OG1	2.07	0.65
1:A:1235:LYS:O	1:A:1238:LYS:HG3	1.96	0.65
1:A:1238:LYS:O	1:A:1242:GLU:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1635:ILE:O	1:A:1638:LEU:HG	1.97	0.64
1:A:188:THR:HA	1:A:191:ARG:HE	1.62	0.64
1:A:1427:MET:HG2	1:A:1452:PHE:CD2	2.32	0.64
1:A:1235:LYS:C	1:A:1238:LYS:HG3	2.23	0.64
1:A:124:ALA:HA	1:A:127:LYS:HG2	1.78	0.64
1:A:1217:ILE:HG12	1:A:1318:ARG:HH22	1.63	0.64
1:A:317:LEU:HD11	1:A:322:THR:HA	1.79	0.64
1:A:1256:MET:HE1	1:A:1281:VAL:HG22	1.62	0.64
1:A:790:VAL:O	1:A:794:LEU:HG	1.98	0.63
1:A:1431:VAL:HG11	1:A:1449:TYR:CD1	2.33	0.63
1:A:1443:GLU:HB3	1:A:1446:LEU:HD12	1.80	0.63
1:A:318:LYS:N	1:A:323:ASP:O	2.20	0.63
1:A:350:ASP:OD1	1:A:351:HIS:N	2.30	0.63
1:A:251:LEU:HD12	1:A:254:VAL:HB	1.80	0.63
1:A:316:LEU:HD11	1:A:337:PRO:HD2	1.80	0.63
1:A:1333:ILE:HA	1:A:1336:ILE:HG22	1.79	0.63
1:A:785:PHE:HA	1:A:788:ILE:HD12	1.80	0.63
1:A:873:ILE:HD11	1:A:908:ASP:HB3	1.81	0.63
1:A:1570:VAL:O	1:A:1574:THR:HG23	1.99	0.63
1:A:156:PRO:O	1:A:159:LYS:HB3	1.99	0.62
1:A:273:PHE:HA	1:A:276:ASN:HB2	1.81	0.62
1:A:721:ASP:HA	1:A:724:ILE:CG1	2.28	0.62
1:A:721:ASP:O	1:A:724:ILE:HG12	1.98	0.62
5:A:3014:9Z9:C08	5:A:3014:9Z9:C19	2.77	0.62
1:A:1363:GLY:HA2	1:A:1399:LYS:HA	1.80	0.62
1:A:740:TYR:O	1:A:1436:TYR:OH	2.17	0.62
1:A:789:ILE:HA	1:A:792:LEU:HD12	1.80	0.62
1:A:1597:ASP:OD1	1:A:1637:ARG:HD3	1.99	0.62
1:A:1734:LEU:HD13	1:A:1743:ASN:HB3	1.81	0.62
1:A:342:CYS:CB	3:C:1:NAG:H83	2.28	0.61
1:A:1255:GLU:O	1:A:1259:LYS:HG2	1.99	0.61
1:A:1395:LEU:O	2:D:1:NAG:N2	2.32	0.61
5:A:3012:9Z9:C11	5:A:3012:9Z9:C09	2.75	0.61
1:A:743:THR:HB	1:A:746:PHE:HB2	1.82	0.61
1:A:1245:ASP:O	1:A:1249:THR:HG23	2.00	0.61
1:A:1723:LEU:HD21	1:A:1751:ILE:HD11	1.83	0.61
1:A:1619:PHE:HD1	1:A:1619:PHE:H	1.48	0.60
1:A:1366:ILE:HG13	1:A:1367:ASN:O	2.00	0.60
1:A:1239:VAL:O	1:A:1243:TYR:HD2	1.84	0.60
1:A:192:ASP:HB3	1:A:195:ASN:HD22	1.66	0.60
1:A:1235:LYS:HA	1:A:1238:LYS:HD2	0.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1610:LEU:CD2	1:A:1627:ILE:HG21	2.22	0.60
1:A:1727:PRO:HG2	2:D:2:NAG:C4	2.31	0.60
1:A:125:ALA:HB2	1:A:178:LEU:HG	1.84	0.60
1:A:1597:ASP:O	1:A:1601:VAL:HG23	2.01	0.60
1:A:721:ASP:O	1:A:724:ILE:CG1	2.49	0.60
1:A:826:LEU:HD13	1:A:1342:VAL:HG13	1.84	0.60
1:A:1637:ARG:O	1:A:1640:ARG:N	2.30	0.60
1:A:138:ILE:CD1	1:A:172:GLU:CD	2.67	0.59
1:A:1368:GLN:N	1:A:1394:GLU:O	2.28	0.59
1:A:1390:ASN:ND2	2:D:1:NAG:H82	2.16	0.59
1:A:1475:PHE:HD2	1:A:1770:ILE:HG21	1.66	0.59
1:A:1597:ASP:OD1	1:A:1637:ARG:NE	2.35	0.59
1:A:131:HIS:O	1:A:134:PHE:HD2	1.79	0.59
1:A:1373:LEU:H	1:A:1373:LEU:HD12	1.67	0.59
1:A:1390:ASN:CG	2:D:1:NAG:H82	2.27	0.59
1:A:1421:LYS:HE3	1:A:1712:SER:O	2.02	0.59
1:A:1633:GLY:HA2	1:A:1636:LEU:HD13	1.85	0.59
1:A:1458:PHE:HA	1:A:1462:PHE:CD2	2.35	0.59
5:A:3014:9Z9:C11	5:A:3014:9Z9:C09	2.73	0.59
1:A:1623:LEU:HD12	1:A:1626:VAL:CG1	2.32	0.58
1:A:752:VAL:O	1:A:756:VAL:HG23	2.04	0.58
1:A:863:GLY:HA2	1:A:866:TYR:HB2	1.85	0.58
1:A:279:HIS:HA	1:A:344:LYS:HA	1.84	0.58
1:A:395:MET:O	1:A:399:PHE:N	2.30	0.58
1:A:780:GLN:O	1:A:784:ILE:HG13	2.03	0.58
1:A:1653:MET:HA	1:A:1656:LEU:HD12	1.85	0.58
5:A:3014:9Z9:C12	5:A:3014:9Z9:C09	2.81	0.58
1:A:257:LEU:HD13	1:A:1645:ILE:HG23	1.85	0.58
1:A:172:GLU:O	1:A:175:VAL:N	2.37	0.58
1:A:784:ILE:O	1:A:788:ILE:HG13	2.03	0.58
1:A:721:ASP:HA	1:A:724:ILE:CD1	2.33	0.58
1:A:1196:LEU:O	1:A:1199:THR:OG1	2.19	0.58
1:A:1307:LEU:HD12	1:A:1310:LEU:HD13	1.86	0.58
1:A:1434:ARG:NH1	1:A:1444:ASP:OD1	2.37	0.58
5:A:3012:9Z9:C12	5:A:3012:9Z9:C09	2.82	0.58
1:A:1708:GLN:O	1:A:1711:THR:OG1	2.22	0.58
1:A:1577:CYS:HB2	1:A:1601:VAL:HG21	1.85	0.57
1:A:1610:LEU:HD23	1:A:1627:ILE:CG1	2.20	0.57
1:A:735:MET:HE1	1:A:812:ARG:HB2	1.85	0.57
1:A:1302:LYS:HA	1:A:1305:ARG:HB2	1.86	0.57
1:A:721:ASP:C	1:A:724:ILE:HG12	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:TRP:CE3	1:A:824:PRO:HD2	2.38	0.57
1:A:1376:ASN:HB2	1:A:1441:GLN:HG3	1.87	0.57
1:A:1624:PHE:HA	1:A:1627:ILE:HD12	1.86	0.57
1:A:201:VAL:HG21	1:A:226:ARG:HG2	1.85	0.57
1:A:796:GLU:HG2	1:A:808:LEU:HD22	1.86	0.57
1:A:1619:PHE:N	1:A:1619:PHE:CD1	2.73	0.57
1:A:1736:ASN:HD22	1:A:1741:ARG:HA	1.69	0.57
1:A:254:VAL:HG21	1:A:412:VAL:HG11	1.86	0.57
1:A:853:ILE:O	1:A:857:VAL:HG23	2.05	0.57
1:A:124:ALA:O	1:A:128:ILE:HG12	2.05	0.57
1:A:1517:ASN:HB3	1:A:1520:GLN:HB3	1.86	0.57
1:A:1364:ARG:HG2	1:A:1365:CYS:HA	1.87	0.57
1:A:358:SER:O	1:A:360:ALA:N	2.37	0.56
1:A:407:ASN:HD21	1:A:1769:TYR:HA	1.71	0.56
1:A:883:HIS:O	1:A:889:HIS:HB3	2.04	0.56
1:A:311:ASP:O	1:A:313:ALA:N	2.38	0.56
1:A:274:MET:HB2	1:A:1552:ASP:HB3	1.87	0.56
1:A:365:ALA:O	1:A:368:ARG:HG2	2.06	0.56
1:A:858:GLY:O	1:A:862:PHE:N	2.37	0.56
1:A:123:ARG:H	1:A:123:ARG:HD2	1.71	0.56
1:A:276:ASN:HA	1:A:279:HIS:HE1	1.69	0.56
1:A:762:THR:HG22	1:A:790:VAL:HG13	1.88	0.56
1:A:1475:PHE:CD2	1:A:1770:ILE:HG21	2.40	0.56
1:A:1210:GLU:O	1:A:1214:ILE:HG12	2.06	0.56
5:A:3012:9Z9:C08	5:A:3012:9Z9:C19	2.81	0.56
1:A:195:ASN:HA	1:A:198:ASP:OD2	2.06	0.56
1:A:1423:TRP:CD1	1:A:1423:TRP:C	2.84	0.56
1:A:1769:TYR:O	1:A:1773:ILE:HG12	2.06	0.56
1:A:319:ASN:ND2	4:A:3003:NAG:O7	2.38	0.55
1:A:128:ILE:O	1:A:134:PHE:CD2	2.59	0.55
1:A:234:ILE:HG22	1:A:236:GLY:H	1.71	0.55
1:A:251:LEU:HG	1:A:255:MET:HG2	1.88	0.55
1:A:340:TYR:O	4:A:3009:NAG:C7	2.55	0.55
1:A:339:GLY:H	4:A:3009:NAG:C8	2.17	0.55
1:A:368:ARG:O	1:A:372:GLN:N	2.40	0.55
1:A:926:MET:O	1:A:930:ASN:ND2	2.39	0.55
1:A:1533:ASP:OD1	1:A:1640:ARG:NH2	2.40	0.55
5:A:3012:9Z9:C08	5:A:3012:9Z9:C13	2.48	0.55
1:A:814:LEU:HA	1:A:817:PHE:HE1	1.72	0.55
1:A:1457:ILE:O	1:A:1461:PHE:N	2.32	0.55
1:A:339:GLY:C	4:A:3009:NAG:H81	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASN:O	1:A:279:HIS:ND1	2.39	0.54
1:A:899:CYS:SG	1:A:1420:PHE:HE2	2.30	0.54
1:A:389:ILE:HD12	1:A:389:ILE:H	1.73	0.54
1:A:1592:SER:HA	1:A:1595:ILE:HG12	1.90	0.54
1:A:1254:LEU:O	1:A:1258:LEU:HG	2.07	0.54
1:A:1366:ILE:HG21	1:A:1371:GLY:HA2	1.89	0.54
1:A:155:PRO:O	1:A:158:THR:OG1	2.25	0.54
5:A:3013:9Z9:C79	5:A:3013:9Z9:C75	2.85	0.54
1:A:902:TRP:HZ3	1:A:903:ILE:HD13	1.73	0.54
1:A:1622:THR:HG23	1:A:1625:ARG:HH22	1.71	0.54
1:A:1625:ARG:O	1:A:1628:ARG:HG2	2.08	0.54
1:A:921:VAL:HG13	1:A:922:PHE:HD1	1.73	0.54
1:A:339:GLY:N	4:A:3009:NAG:C8	2.65	0.53
1:A:1614:ILE:HD11	1:A:1627:ILE:HD12	1.90	0.53
1:A:183:CYS:SG	1:A:184:LEU:N	2.81	0.53
1:A:203:VAL:O	1:A:207:THR:HG23	2.08	0.53
1:A:1357:LEU:HD13	1:A:1448:MET:HE1	1.91	0.53
1:A:1452:PHE:O	1:A:1456:ILE:N	2.26	0.53
1:A:342:CYS:CB	3:C:1:NAG:C8	2.85	0.53
1:A:1727:PRO:HG2	2:D:2:NAG:H4	1.90	0.53
1:A:1210:GLU:O	1:A:1213:ILE:HG22	2.08	0.53
1:A:1323:ARG:O	1:A:1327:ASN:ND2	2.41	0.53
1:A:1594:ASN:HA	1:A:1597:ASP:OD2	2.08	0.53
1:A:246:GLN:O	1:A:250:LYS:HD3	2.09	0.53
1:A:740:TYR:OH	1:A:1383:LYS:NZ	2.41	0.53
1:A:1597:ASP:OD1	1:A:1637:ARG:CD	2.56	0.53
1:A:786:ASP:O	1:A:790:VAL:HG23	2.08	0.53
1:A:231:ILE:HG23	1:A:237:LEU:HB3	1.90	0.53
1:A:1568:LEU:O	1:A:1572:ILE:HG13	2.08	0.53
1:A:785:PHE:O	1:A:789:ILE:HG12	2.10	0.52
1:A:841:GLY:O	1:A:844:THR:OG1	2.18	0.52
1:A:922:PHE:HA	1:A:925:VAL:HG12	1.90	0.52
1:A:1338:ASN:OD1	1:A:1338:ASN:N	2.41	0.52
1:A:1376:ASN:C	1:A:1378:THR:HG22	2.34	0.52
1:A:1377:TYR:H	1:A:1378:THR:HA	1.71	0.52
1:A:1545:VAL:O	1:A:1549:VAL:HG13	2.10	0.52
1:A:728:ILE:O	1:A:732:THR:HG23	2.09	0.52
1:A:1644:GLY:O	1:A:1647:THR:OG1	2.21	0.52
1:A:380:GLN:HA	1:A:1694:PHE:HE2	1.75	0.52
1:A:772:LEU:HB2	1:A:777:TYR:HE2	1.74	0.52
1:A:1350:PHE:HD1	1:A:1451:TYR:HE1	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:O	1:A:404:TYR:HB3	2.09	0.52
1:A:1235:LYS:CB	1:A:1238:LYS:HD2	2.36	0.52
1:A:1531:ALA:O	1:A:1535:THR:HG23	2.10	0.52
1:A:1358:PHE:HB3	1:A:1362:PHE:HE1	1.74	0.52
1:A:1420:PHE:CD2	1:A:1423:TRP:HZ3	2.28	0.52
5:A:3014:9Z9:C11	5:A:3014:9Z9:C07	2.55	0.52
1:A:834:GLY:O	1:A:838:GLY:N	2.41	0.52
1:A:1253:VAL:O	1:A:1257:LEU:HG	2.10	0.52
1:A:1544:MET:HG3	1:A:1635:ILE:HG12	1.92	0.52
1:A:819:LEU:O	1:A:823:TRP:N	2.43	0.51
1:A:1337:MET:O	1:A:1341:LEU:HG	2.10	0.51
1:A:1462:PHE:HA	1:A:1465:ASN:HB3	1.92	0.51
1:A:1586:HIS:O	1:A:1590:THR:HG23	2.10	0.51
1:A:170:THR:HG22	1:A:202:ILE:HG23	1.90	0.51
1:A:902:TRP:O	1:A:904:GLU:N	2.43	0.51
1:A:1637:ARG:O	1:A:1638:LEU:C	2.52	0.51
1:A:812:ARG:O	1:A:815:ARG:NH2	2.32	0.51
1:A:1610:LEU:CG	1:A:1627:ILE:HD13	2.41	0.51
1:A:707:ILE:O	1:A:711:VAL:HG22	2.11	0.51
1:A:842:ASN:HA	1:A:845:LEU:HG	1.91	0.51
1:A:1324:VAL:HA	1:A:1327:ASN:HD22	1.74	0.51
1:A:703:LEU:O	1:A:707:ILE:HG12	2.10	0.51
1:A:312:PRO:HA	1:A:315:TYR:CD1	2.46	0.51
1:A:813:LEU:O	1:A:816:VAL:HG23	2.10	0.51
1:A:1220:SER:HB2	1:A:1311:ARG:HH21	1.76	0.51
1:A:1340:LEU:O	1:A:1344:LEU:HG	2.11	0.51
1:A:159:LYS:HE3	1:A:163:TYR:CE2	2.46	0.51
1:A:903:ILE:HD12	1:A:906:MET:HB3	1.93	0.51
1:A:1235:LYS:O	1:A:1238:LYS:CG	2.57	0.51
1:A:1716:ASP:OD1	1:A:1717:GLY:N	2.43	0.51
1:A:392:ILE:O	1:A:395:MET:HG3	2.11	0.51
1:A:728:ILE:HD13	1:A:818:LYS:HD2	1.93	0.51
1:A:1237:ILE:HG23	1:A:1241:LEU:HD23	1.91	0.50
1:A:1382:ASN:HB2	2:B:1:NAG:O5	2.11	0.50
1:A:1575:GLY:O	1:A:1578:ILE:HG12	2.12	0.50
1:A:840:LEU:O	1:A:843:LEU:HB3	2.12	0.50
1:A:1366:ILE:HD13	1:A:1372:ASP:O	2.11	0.50
1:A:172:GLU:O	1:A:173:SER:C	2.54	0.50
1:A:823:TRP:CE3	5:A:3013:9Z9:C19	2.95	0.50
1:A:1275:TRP:O	1:A:1279:LEU:HG	2.11	0.50
1:A:1354:GLY:O	1:A:1358:PHE:CB	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1675:ILE:HA	1:A:1678:MET:HE2	1.94	0.50
1:A:1709:ILE:HD11	1:A:1718:LEU:HD22	1.94	0.50
1:A:393:PHE:O	1:A:396:LEU:HB3	2.12	0.50
1:A:905:THR:HA	1:A:908:ASP:OD2	2.12	0.50
1:A:788:ILE:O	1:A:792:LEU:HG	2.11	0.50
1:A:877:GLY:O	1:A:878:LEU:HG	2.12	0.50
1:A:1487:ILE:HG22	1:A:1488:PHE:H	1.77	0.50
1:A:237:LEU:O	1:A:241:VAL:HG22	2.12	0.50
1:A:1217:ILE:HD12	1:A:1220:SER:OG	2.12	0.49
1:A:1551:THR:OG1	1:A:1552:ASP:N	2.43	0.49
1:A:1640:ARG:O	1:A:1646:ARG:NH1	2.45	0.49
1:A:369:LEU:HD21	1:A:378:LEU:HD23	1.95	0.49
1:A:1361:LYS:HG2	1:A:1436:TYR:HA	1.93	0.49
1:A:1736:ASN:ND2	1:A:1740:SER:O	2.45	0.49
1:A:138:ILE:HG13	1:A:172:GLU:OE1	2.11	0.49
1:A:733:LEU:O	1:A:737:LEU:HD12	2.12	0.49
1:A:906:MET:HE2	1:A:922:PHE:HB3	1.93	0.49
1:A:1341:LEU:O	1:A:1345:ILE:HG12	2.12	0.49
1:A:1376:ASN:ND2	1:A:1442:TRP:H	2.07	0.49
1:A:751:GLN:O	1:A:755:LEU:HG	2.12	0.49
1:A:1217:ILE:HD13	1:A:1314:ARG:HD2	1.95	0.49
1:A:769:ILE:HA	1:A:777:TYR:CD2	2.48	0.49
1:A:1204:VAL:HA	1:A:1209:PHE:HD2	1.76	0.48
1:A:1301:ILE:O	1:A:1301:ILE:HG13	2.12	0.48
1:A:294:SER:OG	1:A:294:SER:O	2.31	0.48
1:A:1619:PHE:HD1	1:A:1619:PHE:N	2.11	0.48
1:A:311:ASP:HB3	1:A:314:ASN:HB2	1.95	0.48
1:A:1555:SER:O	1:A:1559:VAL:HG23	2.13	0.48
1:A:1256:MET:HE3	1:A:1281:VAL:CG2	2.03	0.48
1:A:1239:VAL:HG22	1:A:1243:TYR:CD2	2.44	0.48
1:A:1247:MET:O	1:A:1251:VAL:HG12	2.13	0.48
1:A:1764:ILE:HA	1:A:1767:ASN:HD22	1.79	0.48
1:A:143:LEU:O	1:A:147:VAL:HG23	2.14	0.48
1:A:221:THR:O	1:A:224:VAL:HG22	2.14	0.48
1:A:1345:ILE:HD11	5:A:3013:9Z9:O80	2.14	0.48
1:A:305:LEU:HD12	1:A:308:TYR:HB2	1.95	0.48
1:A:164:THR:O	1:A:167:ALA:HB3	2.13	0.48
1:A:859:MET:HG3	1:A:860:GLN:H	1.78	0.48
1:A:902:TRP:CZ3	1:A:903:ILE:HD13	2.48	0.48
1:A:134:PHE:CD1	1:A:134:PHE:C	2.92	0.48
1:A:180:ARG:HG3	1:A:186:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:TRP:HE1	1:A:926:MET:HE2	1.79	0.48
1:A:1217:ILE:HG21	1:A:1318:ARG:NH2	2.29	0.48
1:A:1427:MET:HE3	1:A:1452:PHE:HB2	1.96	0.48
1:A:371:THR:C	1:A:373:ASP:H	2.21	0.47
1:A:1458:PHE:O	1:A:1460:SER:N	2.47	0.47
1:A:1762:PHE:O	1:A:1766:VAL:HG23	2.15	0.47
1:A:1278:PHE:HA	1:A:1281:VAL:HG22	1.96	0.47
1:A:1564:LYS:HA	1:A:1567:LEU:HD12	1.96	0.47
1:A:796:GLU:HG2	1:A:808:LEU:HB3	1.96	0.47
1:A:1351:SER:OG	1:A:1410:GLY:HA3	2.14	0.47
1:A:1410:GLY:O	1:A:1414:LEU:HG	2.14	0.47
5:A:3012:9Z9:C11	5:A:3012:9Z9:C07	2.54	0.47
1:A:1221:SER:HB3	1:A:1671:PHE:HE2	1.79	0.47
1:A:236:GLY:O	1:A:239:THR:OG1	2.17	0.47
1:A:407:ASN:OD1	1:A:1773:ILE:HD11	2.13	0.47
1:A:1390:ASN:OD1	1:A:1393:GLY:HA2	2.14	0.47
1:A:347:GLU:HG2	1:A:348:ASN:ND2	2.29	0.47
1:A:734:PHE:CE2	1:A:753:GLY:HA3	2.49	0.47
1:A:1376:ASN:HD22	1:A:1442:TRP:N	2.10	0.47
1:A:356:PHE:O	1:A:362:ALA:HB2	2.15	0.47
1:A:1488:PHE:HD1	1:A:1662:ILE:HD11	1.66	0.47
1:A:1345:ILE:CD1	5:A:3013:9Z9:C79	2.93	0.47
1:A:1421:LYS:HB2	1:A:1421:LYS:HE2	1.41	0.47
1:A:149:MET:HE3	1:A:149:MET:O	2.14	0.46
1:A:1554:GLN:HG3	1:A:1555:SER:H	1.80	0.46
1:A:710:LYS:O	1:A:714:VAL:HG23	2.15	0.46
1:A:307:VAL:HG13	1:A:308:TYR:CD1	2.50	0.46
1:A:349:PRO:CG	1:A:355:SER:HB2	2.45	0.46
1:A:882:TRP:HB3	1:A:893:ILE:HD11	1.97	0.46
1:A:902:TRP:NE1	1:A:926:MET:HE2	2.31	0.46
1:A:1298:MET:O	1:A:1299:GLY:C	2.59	0.46
1:A:282:VAL:O	1:A:340:TYR:HA	2.16	0.46
1:A:1239:VAL:O	1:A:1243:TYR:CD2	2.66	0.46
1:A:1469:GLY:HA2	1:A:1472:ILE:HD12	1.97	0.46
1:A:1574:THR:O	1:A:1578:ILE:HG23	2.15	0.46
1:A:280:LYS:HD3	1:A:324:VAL:HG11	1.98	0.46
1:A:1364:ARG:HG3	1:A:1373:LEU:HD23	1.98	0.46
1:A:199:PHE:O	1:A:203:VAL:HG22	2.16	0.46
1:A:906:MET:SD	1:A:910:MET:HE2	2.56	0.46
1:A:1290:ALA:HB3	1:A:1301:ILE:HD13	1.97	0.46
1:A:1731:ASP:HB3	1:A:1732:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASN:O	1:A:424:THR:OG1	2.34	0.46
1:A:736:ALA:O	1:A:738:GLU:N	2.40	0.46
1:A:1462:PHE:O	1:A:1466:LEU:N	2.30	0.46
1:A:1276:LEU:O	1:A:1280:ILE:HG13	2.16	0.46
1:A:1395:LEU:O	2:D:1:NAG:C7	2.64	0.46
1:A:1598:PHE:CZ	1:A:1602:ILE:HD11	2.51	0.46
1:A:862:PHE:CE2	1:A:921:VAL:HG11	2.51	0.46
1:A:138:ILE:O	1:A:142:ILE:HG13	2.16	0.45
1:A:271:GLN:OE1	1:A:1632:ILE:HD11	2.16	0.45
1:A:276:ASN:HA	1:A:279:HIS:CE1	2.50	0.45
1:A:390:TYR:O	1:A:393:PHE:HB3	2.17	0.45
1:A:900:GLY:HA2	1:A:926:MET:HE1	1.97	0.45
1:A:1238:LYS:NZ	1:A:1238:LYS:HB3	2.31	0.45
1:A:1220:SER:HB2	1:A:1311:ARG:HD3	1.98	0.45
1:A:1460:SER:O	1:A:1464:LEU:HB2	2.17	0.45
1:A:264:VAL:O	1:A:268:ILE:HG13	2.16	0.45
1:A:383:LEU:HB2	1:A:1694:PHE:HZ	1.82	0.45
1:A:252:ALA:O	1:A:256:VAL:HG23	2.16	0.45
1:A:709:GLN:HA	1:A:712:LYS:HB3	1.99	0.45
1:A:721:ASP:O	1:A:724:ILE:HG13	2.17	0.45
1:A:873:ILE:CD1	1:A:908:ASP:HB3	2.45	0.45
1:A:339:GLY:CA	4:A:3009:NAG:C8	2.95	0.45
1:A:725:THR:O	1:A:729:VAL:HG23	2.17	0.45
1:A:1456:ILE:O	1:A:1460:SER:N	2.46	0.45
1:A:223:ARG:HG2	1:A:226:ARG:HH21	1.82	0.45
1:A:273:PHE:HE2	1:A:393:PHE:CE2	2.35	0.45
1:A:312:PRO:HA	1:A:315:TYR:CG	2.52	0.45
1:A:1238:LYS:HG3	1:A:1238:LYS:H	1.53	0.45
1:A:1256:MET:HE2	1:A:1278:PHE:HA	1.99	0.45
1:A:1537:MET:O	1:A:1540:ILE:HG22	2.16	0.45
1:A:280:LYS:HE2	1:A:346:GLY:HA3	1.98	0.44
1:A:282:VAL:HG12	1:A:315:TYR:HD1	1.82	0.44
1:A:380:GLN:HG2	1:A:1694:PHE:CD2	2.52	0.44
1:A:833:ILE:HD12	1:A:836:SER:HB3	1.99	0.44
1:A:1278:PHE:CD2	1:A:1279:LEU:HD23	2.53	0.44
1:A:1610:LEU:HG	1:A:1627:ILE:HD13	1.99	0.44
1:A:253:ASP:OD1	1:A:253:ASP:N	2.47	0.44
1:A:883:HIS:NE2	1:A:889:HIS:CD2	2.85	0.44
1:A:713:PHE:HA	1:A:716:MET:HG3	2.00	0.44
1:A:762:THR:O	1:A:766:THR:OG1	2.28	0.44
1:A:892:LEU:HD13	1:A:1449:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:ILE:N	1:A:1334:PRO:HD2	2.33	0.44
1:A:1353:MET:HE3	1:A:1353:MET:HB2	1.79	0.44
1:A:1431:VAL:HG21	1:A:1449:TYR:HE1	1.82	0.44
1:A:1350:PHE:HB3	1:A:1451:TYR:OH	2.18	0.43
1:A:1623:LEU:HA	1:A:1626:VAL:CG1	2.48	0.43
1:A:1734:LEU:HD12	1:A:1735:PRO:HD2	2.00	0.43
1:A:327:CYS:O	1:A:385:SER:HA	2.18	0.43
1:A:731:ASN:ND2	1:A:757:PHE:HB3	2.32	0.43
1:A:1464:LEU:O	1:A:1468:ILE:HG12	2.16	0.43
1:A:1656:LEU:N	1:A:1657:PRO:HD2	2.33	0.43
1:A:882:TRP:CZ3	1:A:892:LEU:HB3	2.54	0.43
1:A:1282:ASP:O	1:A:1286:VAL:HG23	2.18	0.43
1:A:1731:ASP:O	1:A:1732:PRO:C	2.62	0.43
1:A:857:VAL:HA	1:A:860:GLN:HE21	1.83	0.43
1:A:920:LEU:HD13	1:A:920:LEU:HA	1.83	0.43
1:A:1390:ASN:CG	2:D:1:NAG:C8	2.90	0.43
1:A:1592:SER:O	1:A:1595:ILE:HG12	2.19	0.43
1:A:1733:ASN:C	1:A:1742:GLY:HA2	2.44	0.43
1:A:863:GLY:O	1:A:867:SER:N	2.51	0.43
1:A:1279:LEU:O	1:A:1283:VAL:HG23	2.18	0.43
1:A:1643:LYS:HG3	1:A:1644:GLY:N	2.33	0.43
1:A:391:MET:C	1:A:391:MET:SD	3.01	0.43
1:A:409:ILE:O	1:A:413:VAL:HG23	2.18	0.43
1:A:1500:MET:SD	1:A:1653:MET:HG2	2.58	0.43
1:A:1665:LEU:O	1:A:1669:VAL:HG23	2.19	0.43
1:A:1758:ILE:O	1:A:1762:PHE:HB3	2.19	0.43
1:A:411:ALA:HB2	1:A:1773:ILE:HD12	2.00	0.43
1:A:1317:SER:OG	1:A:1318:ARG:HG3	2.18	0.43
1:A:1646:ARG:O	1:A:1650:PHE:HB2	2.18	0.43
1:A:1638:LEU:O	1:A:1642:ALA:N	2.43	0.43
1:A:276:ASN:O	1:A:385:SER:OG	2.19	0.43
1:A:1214:ILE:HA	1:A:1217:ILE:HG22	2.01	0.43
1:A:193:PRO:O	1:A:196:TRP:HB2	2.18	0.42
1:A:733:LEU:O	1:A:736:ALA:N	2.52	0.42
1:A:751:GLN:O	1:A:754:ASN:HB3	2.18	0.42
1:A:780:GLN:HE21	1:A:782:TRP:N	2.00	0.42
1:A:705:MET:O	1:A:709:GLN:HG2	2.19	0.42
1:A:924:LEU:HD23	1:A:924:LEU:HA	1.78	0.42
1:A:177:ILE:HG23	1:A:186:ALA:HB1	2.00	0.42
1:A:1229:ILE:HG23	1:A:1697:GLN:O	2.20	0.42
1:A:170:THR:HA	1:A:173:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1383:LYS:HE2	1:A:1437:GLU:OE1	2.19	0.42
1:A:1596:PHE:O	1:A:1600:VAL:HG13	2.19	0.42
1:A:278:ARG:HB2	1:A:344:LYS:HE2	2.01	0.42
1:A:1372:ASP:OD1	1:A:1373:LEU:N	2.53	0.42
1:A:1436:TYR:CD1	1:A:1437:GLU:HG3	2.54	0.42
1:A:217:SER:O	1:A:217:SER:OG	2.35	0.42
1:A:1431:VAL:HG21	1:A:1449:TYR:CE1	2.54	0.42
1:A:1733:ASN:O	1:A:1734:LEU:HB2	2.18	0.42
1:A:397:VAL:HG12	1:A:398:ILE:HD13	2.01	0.42
1:A:1316:LEU:HD23	1:A:1326:VAL:HG21	2.02	0.42
1:A:1427:MET:HG2	1:A:1452:PHE:CE2	2.54	0.42
1:A:305:LEU:HA	1:A:308:TYR:CD2	2.55	0.42
1:A:384:ARG:HA	1:A:384:ARG:NE	2.35	0.42
1:A:1455:PHE:O	1:A:1456:ILE:C	2.63	0.42
1:A:1655:SER:HB2	1:A:1775:GLU:HG2	2.01	0.42
1:A:172:GLU:C	1:A:174:LEU:N	2.77	0.42
1:A:729:VAL:O	1:A:733:LEU:HD23	2.20	0.42
1:A:902:TRP:CD1	1:A:926:MET:HE2	2.55	0.42
1:A:159:LYS:HA	1:A:159:LYS:HD2	1.93	0.41
1:A:341:ARG:HH21	4:A:3009:NAG:C3	2.29	0.41
1:A:410:LEU:HD13	1:A:934:LEU:HD11	2.02	0.41
1:A:773:ASP:HB3	1:A:776:TYR:CB	2.45	0.41
1:A:782:TRP:CD1	1:A:785:PHE:HE2	2.38	0.41
1:A:819:LEU:HD11	5:A:3013:9Z9:C15	2.49	0.41
1:A:1687:GLU:CB	1:A:1721:PRO:HB3	2.50	0.41
1:A:413:VAL:HG21	1:A:934:LEU:HD23	2.02	0.41
1:A:903:ILE:HD12	1:A:903:ILE:HA	1.86	0.41
1:A:923:LEU:O	1:A:927:VAL:HG23	2.19	0.41
1:A:1359:ALA:HA	1:A:1404:PHE:O	2.20	0.41
1:A:1427:MET:O	1:A:1431:VAL:HG22	2.20	0.41
1:A:1456:ILE:O	1:A:1457:ILE:C	2.63	0.41
1:A:1650:PHE:O	1:A:1654:MET:HG2	2.20	0.41
1:A:280:LYS:HD3	1:A:324:VAL:HG21	2.02	0.41
1:A:1231:LEU:HA	1:A:1231:LEU:HD23	1.80	0.41
1:A:319:ASN:ND2	4:A:3003:NAG:C7	2.84	0.41
1:A:342:CYS:HB3	3:C:1:NAG:H83	2.02	0.41
1:A:742:MET:HE3	1:A:746:PHE:HD2	1.84	0.41
1:A:1380:VAL:HG11	1:A:1386:CYS:HB3	2.02	0.41
1:A:369:LEU:O	1:A:402:SER:HB3	2.21	0.41
1:A:404:TYR:OH	1:A:408:LEU:HD11	2.20	0.41
1:A:934:LEU:HD12	1:A:934:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1500:MET:HB3	1:A:1654:MET:HE1	2.02	0.41
1:A:1551:THR:HG23	1:A:1554:GLN:HB3	2.03	0.41
1:A:1718:LEU:C	1:A:1721:PRO:HD2	2.46	0.41
1:A:1758:ILE:HD13	1:A:1758:ILE:HA	1.81	0.41
1:A:1768:MET:HE3	1:A:1768:MET:HB2	1.79	0.41
1:A:396:LEU:HD12	1:A:400:LEU:HD23	2.01	0.41
1:A:159:LYS:HD2	1:A:159:LYS:O	2.21	0.41
1:A:339:GLY:C	4:A:3009:NAG:C8	2.91	0.41
1:A:1285:LEU:O	1:A:1289:VAL:HG22	2.20	0.41
1:A:1427:MET:HA	1:A:1452:PHE:CE2	2.55	0.41
1:A:1563:ALA:O	1:A:1567:LEU:HG	2.20	0.41
1:A:210:PHE:CD2	1:A:211:VAL:HG23	2.56	0.41
1:A:316:LEU:HD12	1:A:340:TYR:CG	2.56	0.41
1:A:1235:LYS:CA	1:A:1238:LYS:CG	2.93	0.41
1:A:121:VAL:HG22	1:A:178:LEU:HD21	2.03	0.41
1:A:254:VAL:O	1:A:258:THR:HG22	2.21	0.41
1:A:308:TYR:O	1:A:311:ASP:HB2	2.21	0.41
1:A:349:PRO:HG2	1:A:355:SER:HB2	2.03	0.41
1:A:403:PHE:CZ	1:A:1772:ILE:HG13	2.56	0.41
1:A:776:TYR:O	1:A:779:GLN:N	2.53	0.41
1:A:902:TRP:CD1	1:A:902:TRP:H	2.37	0.41
1:A:1285:LEU:O	1:A:1288:LEU:HG	2.21	0.41
1:A:1690:ILE:CG1	1:A:1718:LEU:HG	2.50	0.41
1:A:775:TYR:O	1:A:778:PHE:HB3	2.20	0.41
1:A:1696:PHE:HA	1:A:1702:SER:OG	2.21	0.41
1:A:372:GLN:HA	1:A:375:TRP:HB3	2.02	0.40
1:A:754:ASN:O	1:A:758:THR:HG23	2.21	0.40
1:A:813:LEU:O	1:A:815:ARG:N	2.54	0.40
1:A:1242:GLU:O	1:A:1246:LYS:HG3	2.21	0.40
1:A:1376:ASN:HB3	1:A:1441:GLN:HA	2.03	0.40
1:A:140:CYS:O	1:A:144:THR:HG23	2.22	0.40
1:A:829:LEU:HD12	1:A:1466:LEU:HD23	2.02	0.40
1:A:1271:ASN:ND2	1:A:1274:CYS:SG	2.91	0.40
1:A:1614:ILE:CA	1:A:1618:PHE:O	2.61	0.40
1:A:1649:LEU:HD23	1:A:1649:LEU:HA	1.88	0.40
1:A:1767:ASN:O	1:A:1770:ILE:HG22	2.21	0.40
1:A:863:GLY:O	1:A:867:SER:OG	2.32	0.40
1:A:1296:ALA:C	1:A:1297:GLU:OE2	2.61	0.40
1:A:1412:LEU:HD12	1:A:1412:LEU:HA	1.85	0.40
2:B:1:NAG:H83	2:B:2:NAG:H82	2.03	0.40
1:A:399:PHE:O	1:A:403:PHE:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:ILE:O	1:A:1305:ARG:N	2.55	0.40
1:A:1536:ILE:HD13	1:A:1539:LEU:HD12	2.02	0.40
1:A:380:GLN:HG2	1:A:1694:PHE:CE2	2.57	0.40
1:A:384:ARG:NH2	1:A:388:LYS:HG2	2.37	0.40
1:A:1226:PHE:O	1:A:1231:LEU:HD21	2.21	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	1110/1838 (60%)	982 (88%)	124 (11%)	4 (0%)	30 62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	PHE
1	A	1621	PRO
1	A	1365	CYS
1	A	312	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	949/1612 (59%)	939 (99%)	10 (1%)	65 74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1215	PHE
1	A	1238	LYS
1	A	1293	LEU
1	A	1297	GLU
1	A	1419	THR
1	A	1421	LYS
1	A	1618	PHE
1	A	1619	PHE
1	A	1626	VAL
1	A	1711	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	195	ASN
1	A	314	ASN
1	A	731	ASN
1	A	780	GLN
1	A	783	ASN
1	A	827	ASN
1	A	842	ASN
1	A	860	GLN
1	A	865	ASN
1	A	871	HIS
1	A	889	HIS
1	A	1327	ASN
1	A	1406	ASN
1	A	1441	GLN
1	A	1498	ASN
1	A	1543	ASN
1	A	1615	GLN
1	A	1767	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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$
2	NAG	B	1	1,2	14,14,15	0.48	0	17,19,21	0.51	0
2	NAG	B	2	2	14,14,15	0.19	0	17,19,21	0.56	0
3	NAG	C	1	3,1	14,14,15	0.30	0	17,19,21	0.83	1 (5%)
3	NAG	C	2	3	14,14,15	0.32	0	17,19,21	1.12	2 (11%)
3	BMA	C	3	3	11,11,12	0.41	0	15,15,17	1.09	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.29	0	17,19,21	0.93	0
2	NAG	D	2	2	14,14,15	0.28	0	17,19,21	0.65	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C4-C3-C2	-2.35	107.57	111.02
3	C	1	NAG	O5-C1-C2	-2.10	108.05	111.29
3	C	2	NAG	C2-N2-C7	-2.05	120.16	122.90
3	C	3	BMA	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

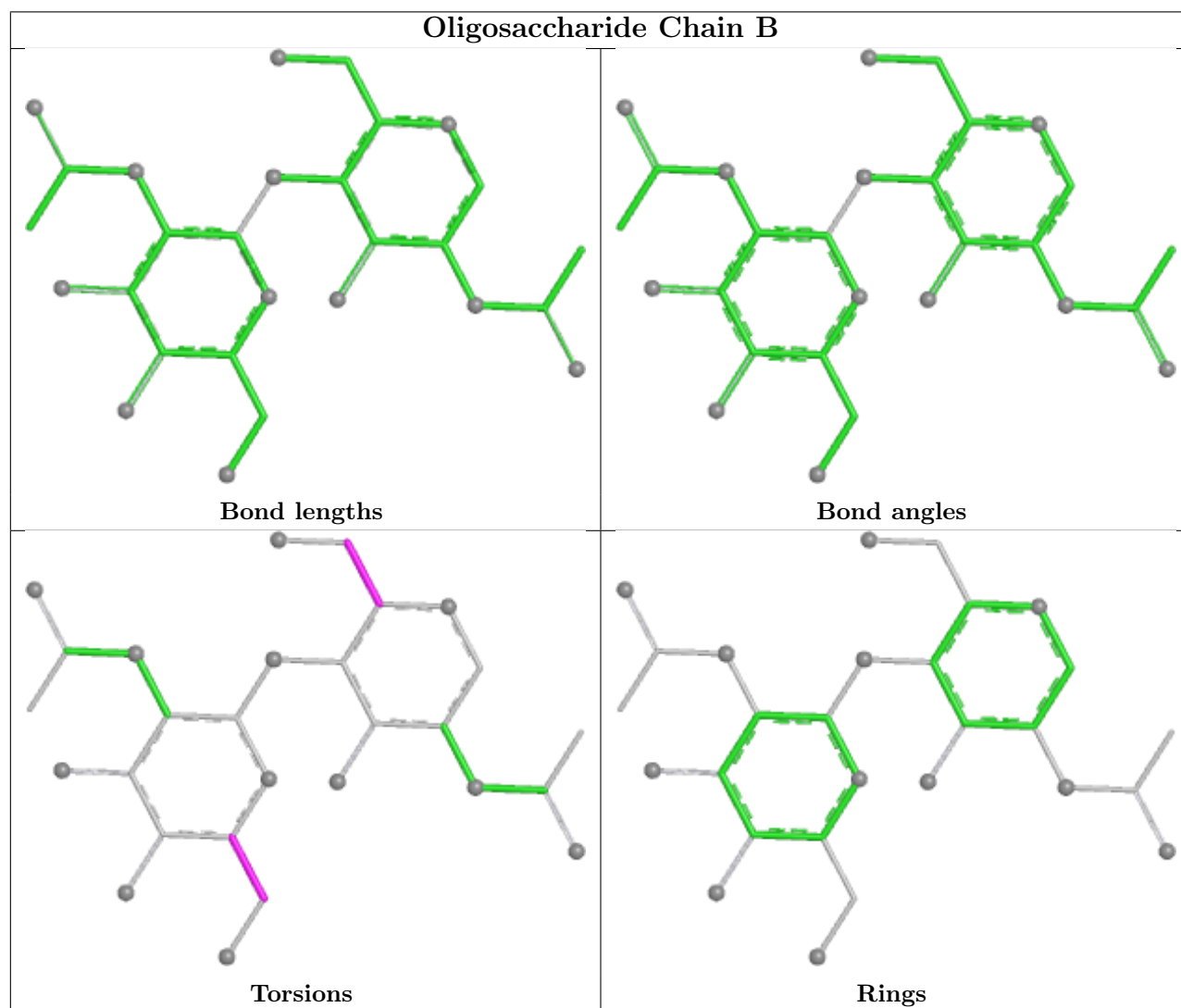
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6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

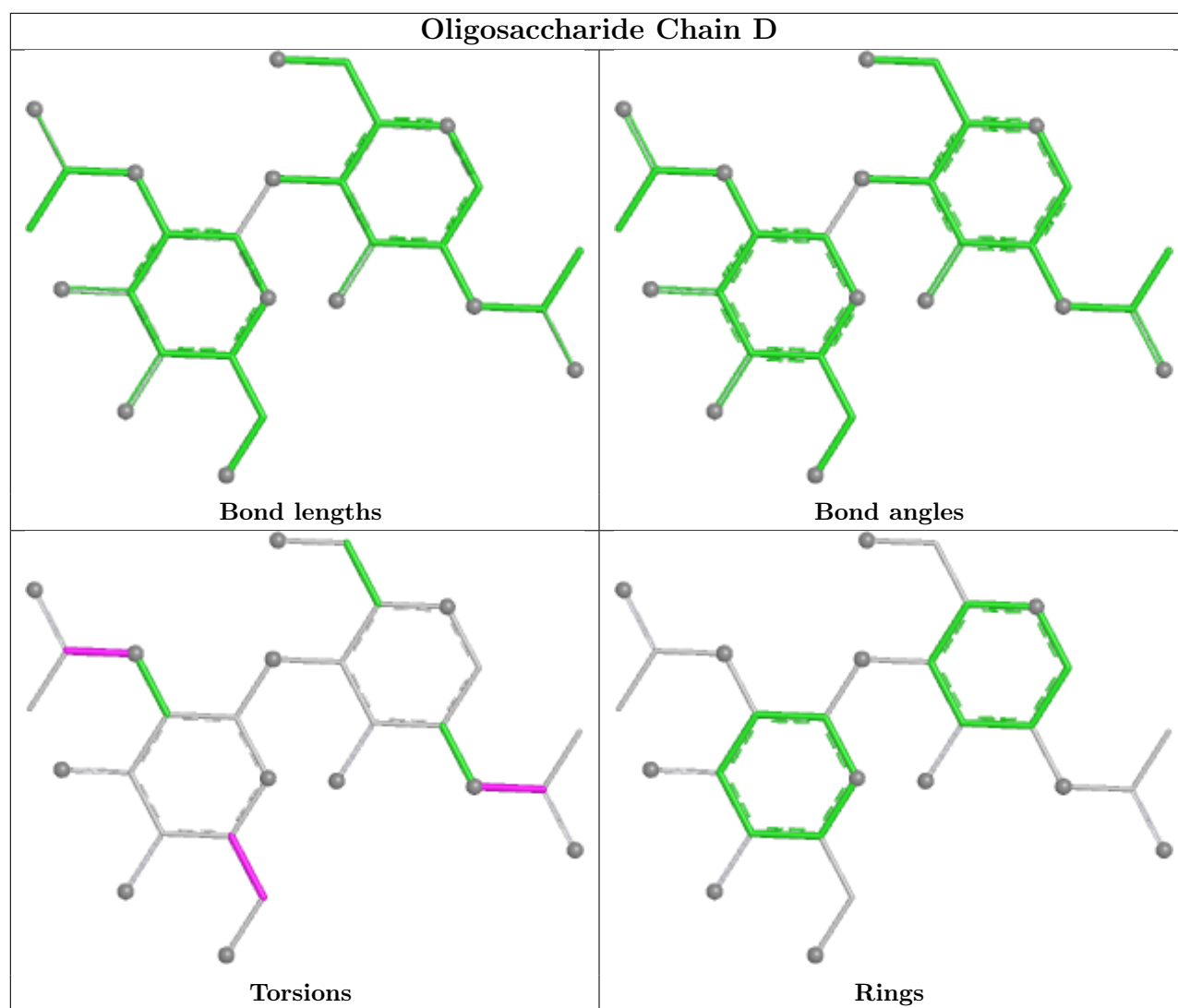
There are no ring outliers.

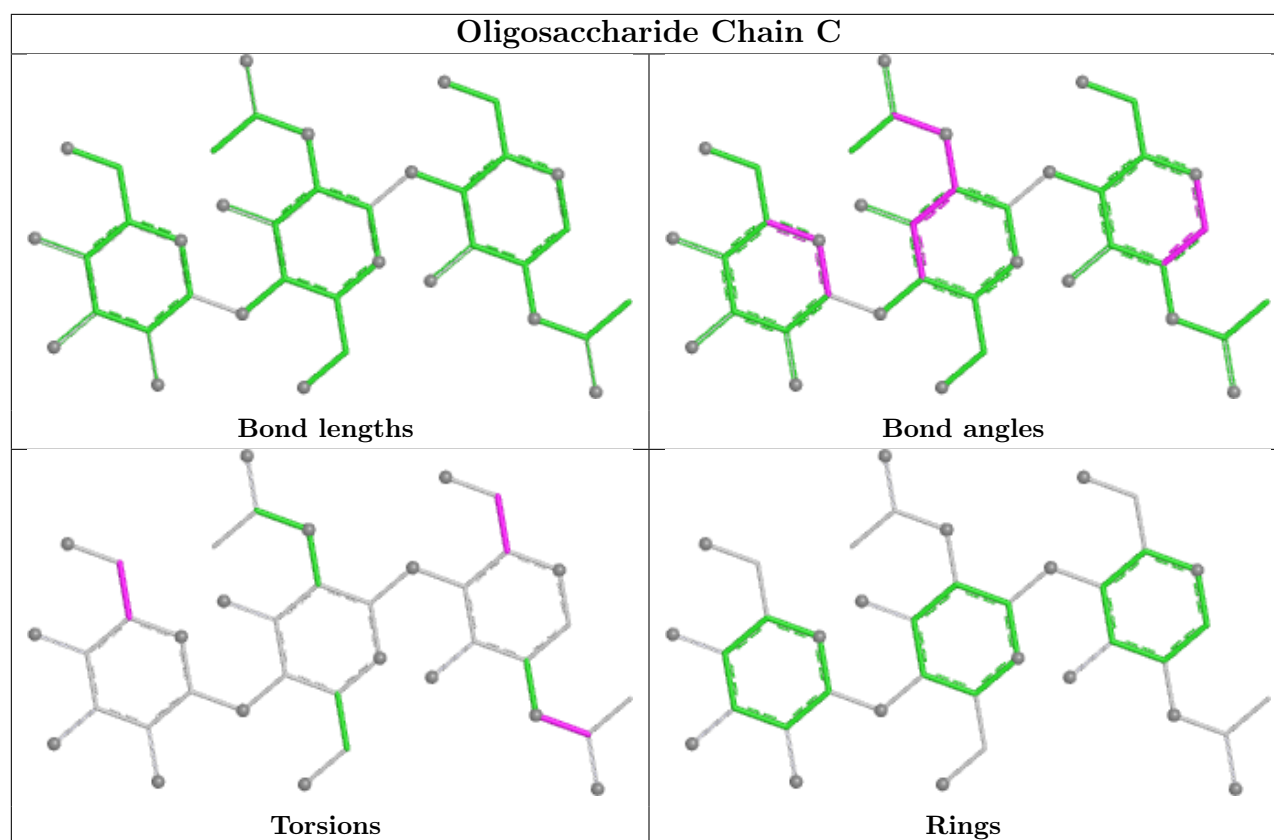
5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	2	0
2	B	2	NAG	1	0
2	D	1	NAG	5	0
2	D	2	NAG	5	0
3	C	1	NAG	11	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](#)

18 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	3019	-	28,28,48	1.15	4 (14%)	30,30,53	1.40	2 (6%)
6	6OU	A	3025	-	14,14,48	1.44	3 (21%)	14,14,53	1.06	1 (7%)
4	NAG	A	3003	1	14,14,15	0.38	0	17,19,21	0.42	0
6	6OU	A	3021	-	25,25,48	1.21	4 (16%)	28,30,53	1.25	2 (7%)
5	9Z9	A	3012	-	42,42,44	7.55	26 (61%)	63,66,68	2.28	24 (38%)
5	9Z9	A	3010	-	36,36,44	8.41	25 (69%)	59,59,68	2.46	24 (40%)
5	9Z9	A	3013	-	34,34,44	8.27	24 (70%)	56,56,68	2.40	22 (39%)
4	NAG	A	3009	1	14,14,15	0.29	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	9Z9	A	3014	-	34,34,44	8.59	21 (61%)	56,56,68	2.40	23 (41%)
6	6OU	A	3015	-	34,34,48	1.03	4 (11%)	37,39,53	1.24	2 (5%)
6	6OU	A	3024	-	16,16,48	1.36	3 (18%)	16,16,53	1.08	1 (6%)
6	6OU	A	3017	-	14,14,48	0.97	1 (7%)	14,14,53	1.14	1 (7%)
6	6OU	A	3016	-	34,34,48	1.03	4 (11%)	37,39,53	1.21	2 (5%)
6	6OU	A	3022	-	26,26,48	0.98	2 (7%)	27,27,53	1.13	2 (7%)
6	6OU	A	3020	-	39,39,48	0.99	3 (7%)	42,44,53	1.04	2 (4%)
6	6OU	A	3018	-	25,25,48	1.10	4 (16%)	27,27,53	1.43	2 (7%)
5	9Z9	A	3011	-	23,23,44	6.76	13 (56%)	35,37,68	2.04	14 (40%)
6	6OU	A	3023	-	24,24,48	1.28	5 (20%)	27,29,53	1.41	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	3019	-	-	11/29/29/52	-
6	6OU	A	3025	-	-	3/13/13/52	-
4	NAG	A	3003	1	-	2/6/23/26	0/1/1/1
6	6OU	A	3021	-	-	15/29/29/52	-
5	9Z9	A	3012	-	-	2/9/97/100	0/6/6/6
5	9Z9	A	3010	-	-	1/2/90/100	0/6/6/6
6	6OU	A	3024	-	-	7/15/15/52	-
4	NAG	A	3009	1	1/1/5/7	2/6/23/26	0/1/1/1
5	9Z9	A	3013	-	-	-	0/6/6/6
6	6OU	A	3015	-	-	13/38/38/52	-
5	9Z9	A	3014	-	-	-	0/6/6/6
6	6OU	A	3017	-	-	5/13/13/52	-
6	6OU	A	3016	-	-	19/38/38/52	-
6	6OU	A	3022	-	-	11/26/26/52	-
6	6OU	A	3020	-	-	24/43/43/52	-
6	6OU	A	3018	-	-	16/27/27/52	-
5	9Z9	A	3011	-	-	-	0/4/4/6
6	6OU	A	3023	-	-	7/26/26/52	-

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3010	9Z9	C15-C07	-22.05	1.17	1.53
5	A	3012	9Z9	C15-C07	-21.96	1.17	1.53
5	A	3014	9Z9	C15-C07	-21.72	1.18	1.53
5	A	3014	9Z9	C07-C06	-21.33	1.13	1.53
5	A	3013	9Z9	C15-C07	-21.25	1.18	1.53
5	A	3010	9Z9	C07-C06	-21.02	1.14	1.53
5	A	3012	9Z9	C07-C06	-19.97	1.16	1.53
5	A	3013	9Z9	C07-C06	-19.77	1.16	1.53
5	A	3010	9Z9	C11-C13	-18.56	1.17	1.52
5	A	3013	9Z9	C11-C13	-18.44	1.17	1.52
5	A	3014	9Z9	C11-C13	-18.34	1.17	1.52
5	A	3012	9Z9	C11-C13	-18.26	1.18	1.52
5	A	3010	9Z9	C10-C02	-18.14	1.22	1.54
5	A	3014	9Z9	C10-C02	-18.06	1.22	1.54
5	A	3011	9Z9	C10-C02	-18.06	1.22	1.54
5	A	3012	9Z9	C10-C02	-16.64	1.25	1.54
5	A	3013	9Z9	C10-C02	-16.64	1.25	1.54
5	A	3011	9Z9	C07-C06	-16.22	1.14	1.53
5	A	3010	9Z9	C10-C09	-12.32	1.28	1.53
5	A	3012	9Z9	C11-C08	12.17	1.75	1.56
5	A	3014	9Z9	C10-C09	-12.11	1.29	1.53
5	A	3014	9Z9	C11-C08	12.05	1.75	1.56
5	A	3013	9Z9	C05-C04	11.85	1.77	1.52
5	A	3011	9Z9	C05-C04	11.72	1.77	1.52
5	A	3010	9Z9	C05-C04	11.62	1.77	1.52
5	A	3012	9Z9	C05-C04	11.61	1.77	1.52
5	A	3014	9Z9	C05-C04	11.58	1.77	1.52
5	A	3010	9Z9	C11-C08	11.42	1.74	1.56
5	A	3013	9Z9	C11-C08	11.39	1.74	1.56
5	A	3010	9Z9	C07-C08	-11.13	1.32	1.53
5	A	3013	9Z9	C10-C09	-11.03	1.31	1.53
5	A	3014	9Z9	C07-C08	-10.94	1.33	1.53
5	A	3012	9Z9	C10-C09	-10.76	1.32	1.53
5	A	3011	9Z9	C10-C09	-10.04	1.28	1.52
5	A	3012	9Z9	C07-C08	-9.55	1.35	1.53
5	A	3013	9Z9	C19-C11	9.44	1.71	1.54
5	A	3013	9Z9	C07-C08	-9.43	1.35	1.53
5	A	3012	9Z9	C19-C11	9.25	1.71	1.54
5	A	3014	9Z9	C19-C11	9.08	1.70	1.54
5	A	3010	9Z9	C19-C11	9.08	1.70	1.54
5	A	3011	9Z9	C08-C07	-7.98	1.33	1.53
5	A	3010	9Z9	C18-C17	-7.82	1.30	1.51
5	A	3012	9Z9	C18-C17	-7.76	1.30	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3012	9Z9	C02-C03	7.12	1.69	1.56
5	A	3013	9Z9	C02-C03	6.68	1.68	1.56
5	A	3014	9Z9	C02-C03	6.49	1.67	1.56
5	A	3010	9Z9	C02-C03	6.47	1.67	1.56
5	A	3011	9Z9	C02-C03	6.29	1.67	1.56
5	A	3013	9Z9	C15-C14	6.20	1.62	1.50
5	A	3012	9Z9	C15-C14	6.08	1.62	1.50
5	A	3013	9Z9	C16-C13	6.08	1.60	1.50
5	A	3014	9Z9	C16-C13	6.07	1.60	1.50
5	A	3014	9Z9	C15-C14	5.82	1.62	1.50
5	A	3013	9Z9	C18-C17	-5.80	1.30	1.51
5	A	3014	9Z9	C18-C17	-5.76	1.30	1.51
5	A	3014	9Z9	C03-C04	-5.71	1.43	1.54
5	A	3010	9Z9	C15-C14	5.64	1.61	1.50
5	A	3012	9Z9	C03-C04	-5.59	1.44	1.54
5	A	3010	9Z9	C03-C04	-5.40	1.44	1.54
5	A	3011	9Z9	C03-C04	-5.35	1.44	1.54
5	A	3013	9Z9	C03-C04	-5.18	1.44	1.54
5	A	3014	9Z9	C03-C74	-5.15	1.39	1.54
5	A	3011	9Z9	C03-C74	-4.92	1.40	1.54
5	A	3010	9Z9	C03-C74	-4.88	1.40	1.54
5	A	3014	9Z9	O72-C73	-4.85	1.32	1.42
5	A	3012	9Z9	C03-C74	-4.78	1.40	1.54
5	A	3013	9Z9	C03-C74	-4.70	1.41	1.54
5	A	3011	9Z9	O72-C73	-4.54	1.32	1.42
5	A	3012	9Z9	O72-C73	-4.41	1.33	1.42
5	A	3013	9Z9	O72-C73	-4.39	1.33	1.42
5	A	3010	9Z9	O72-C73	-4.34	1.33	1.42
5	A	3012	9Z9	C16-C13	4.22	1.60	1.51
5	A	3010	9Z9	C16-C13	4.20	1.60	1.51
5	A	3010	9Z9	O80-C73	4.16	1.48	1.42
6	A	3024	6OU	C08-C07	-4.04	1.31	1.51
6	A	3025	6OU	C08-C07	-4.01	1.31	1.51
5	A	3012	9Z9	O80-C73	3.87	1.48	1.42
5	A	3014	9Z9	C76-C77	-3.78	1.45	1.53
6	A	3019	6OU	O30-C20	-3.73	1.40	1.47
5	A	3013	9Z9	O80-C73	3.69	1.47	1.42
5	A	3010	9Z9	C76-C77	-3.46	1.46	1.53
5	A	3013	9Z9	C76-C77	-3.35	1.46	1.53
5	A	3012	9Z9	C76-C77	-3.35	1.46	1.53
5	A	3011	9Z9	O80-C73	3.22	1.47	1.42
5	A	3010	9Z9	O20-C17	3.22	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3011	9Z9	C76-C77	-3.17	1.47	1.53
6	A	3020	6OU	O30-C20	-2.89	1.39	1.46
5	A	3014	9Z9	O80-C73	2.80	1.46	1.42
5	A	3012	9Z9	C16-C17	2.76	1.58	1.52
5	A	3010	9Z9	C16-C17	2.76	1.58	1.52
5	A	3010	9Z9	C76-C73	2.75	1.56	1.51
5	A	3011	9Z9	C05-C06	2.73	1.59	1.53
5	A	3012	9Z9	O20-C17	2.73	1.51	1.43
6	A	3018	6OU	O30-C20	-2.72	1.40	1.46
6	A	3021	6OU	O30-C20	-2.71	1.40	1.46
6	A	3023	6OU	P23-O26	2.67	1.64	1.54
5	A	3013	9Z9	C05-C06	2.66	1.59	1.54
6	A	3015	6OU	O30-C20	-2.66	1.40	1.46
6	A	3023	6OU	O30-C20	-2.62	1.40	1.46
5	A	3012	9Z9	C76-C73	2.61	1.55	1.51
5	A	3013	9Z9	C76-C73	2.58	1.55	1.51
5	A	3014	9Z9	C05-C06	2.57	1.59	1.54
5	A	3010	9Z9	C05-C06	2.56	1.59	1.54
6	A	3016	6OU	O30-C20	-2.47	1.40	1.46
6	A	3020	6OU	O18-C16	2.45	1.40	1.33
6	A	3018	6OU	O18-C19	-2.45	1.39	1.45
5	A	3012	9Z9	C05-C06	2.43	1.59	1.54
6	A	3016	6OU	O18-C16	2.41	1.40	1.33
6	A	3017	6OU	O30-C31	2.40	1.40	1.33
5	A	3011	9Z9	C76-C73	2.39	1.55	1.51
6	A	3022	6OU	O18-C16	2.35	1.40	1.33
6	A	3024	6OU	O18-C16	2.34	1.40	1.33
5	A	3010	9Z9	C19-C18	-2.34	1.48	1.53
6	A	3025	6OU	O18-C16	2.33	1.40	1.33
6	A	3019	6OU	O18-C16	2.33	1.40	1.33
6	A	3021	6OU	O18-C16	2.32	1.40	1.33
6	A	3022	6OU	O30-C31	2.30	1.40	1.33
6	A	3015	6OU	O18-C16	2.29	1.40	1.33
6	A	3019	6OU	O30-C31	2.28	1.40	1.34
6	A	3019	6OU	O18-C19	-2.27	1.40	1.45
6	A	3024	6OU	O18-C19	-2.27	1.40	1.45
6	A	3025	6OU	O18-C19	-2.25	1.40	1.45
6	A	3015	6OU	O18-C19	-2.24	1.40	1.45
5	A	3012	9Z9	C19-C18	-2.23	1.49	1.53
6	A	3021	6OU	O18-C19	-2.22	1.40	1.45
6	A	3023	6OU	O18-C19	-2.21	1.40	1.45
6	A	3015	6OU	O30-C31	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3023	6OU	O18-C16	2.19	1.39	1.33
5	A	3012	9Z9	O80-C79	2.18	1.46	1.43
6	A	3016	6OU	O30-C31	2.16	1.40	1.34
5	A	3013	9Z9	C79-C78	2.16	1.55	1.51
6	A	3023	6OU	O30-C31	2.16	1.40	1.34
6	A	3018	6OU	O30-C31	2.14	1.40	1.34
5	A	3014	9Z9	C79-C78	2.13	1.55	1.51
5	A	3012	9Z9	C79-C78	2.11	1.55	1.51
6	A	3020	6OU	O18-C19	-2.11	1.40	1.45
5	A	3013	9Z9	O80-C79	2.10	1.46	1.43
5	A	3013	9Z9	C02-C06	2.08	1.58	1.55
6	A	3018	6OU	O18-C16	2.08	1.39	1.33
6	A	3021	6OU	O30-C31	2.07	1.40	1.34
5	A	3010	9Z9	C77-C78	-2.07	1.46	1.52
5	A	3014	9Z9	C17-C16	2.06	1.58	1.52
5	A	3010	9Z9	C14-C13	-2.06	1.28	1.33
6	A	3016	6OU	O18-C19	-2.05	1.40	1.45
5	A	3012	9Z9	C02-C06	2.03	1.58	1.55
5	A	3013	9Z9	C17-C16	2.02	1.58	1.52

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3010	9Z9	O80-C73-C76	7.99	117.72	110.76
5	A	3014	9Z9	C10-C02-C06	5.80	115.92	107.25
5	A	3012	9Z9	C10-C02-C03	5.68	123.44	115.36
5	A	3013	9Z9	C15-C14-C13	-5.59	115.58	125.02
5	A	3010	9Z9	C10-C02-C06	5.35	115.25	107.25
5	A	3010	9Z9	C15-C14-C13	-5.06	116.48	125.02
5	A	3013	9Z9	C10-C02-C03	4.95	122.40	115.36
5	A	3012	9Z9	C08-C07-C06	4.85	115.42	109.09
5	A	3014	9Z9	C08-C11-C13	4.76	116.62	109.65
5	A	3010	9Z9	C01-C02-C03	-4.62	101.53	111.58
5	A	3012	9Z9	C01-C02-C06	-4.62	103.30	111.68
5	A	3010	9Z9	C10-C02-C03	4.61	121.92	115.36
5	A	3012	9Z9	C01-C02-C10	-4.54	103.92	110.61
5	A	3013	9Z9	C10-C02-C06	4.51	114.00	107.25
5	A	3013	9Z9	C15-C07-C08	4.46	114.88	109.72
5	A	3013	9Z9	C08-C07-C06	4.31	114.71	109.09
5	A	3012	9Z9	C15-C14-C13	-4.28	117.80	125.02
6	A	3018	6OU	O30-C31-C33	4.27	120.72	111.48
6	A	3019	6OU	O30-C31-C33	4.27	120.72	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3014	9Z9	C75-C74-C03	-4.18	106.14	114.50
6	A	3021	6OU	O30-C31-C33	4.17	120.50	111.48
5	A	3010	9Z9	C05-C06-C02	-4.15	98.92	103.85
5	A	3014	9Z9	C75-C74-C73	-4.15	108.24	114.94
5	A	3011	9Z9	C10-C02-C03	4.03	121.10	115.36
5	A	3012	9Z9	C05-C06-C02	-4.03	99.07	103.85
5	A	3012	9Z9	C03-C02-C06	4.01	105.43	100.18
5	A	3014	9Z9	C10-C02-C03	4.00	121.05	115.36
6	A	3015	6OU	O30-C31-C33	4.00	120.13	111.48
6	A	3023	6OU	O30-C31-C33	4.00	120.13	111.48
5	A	3013	9Z9	C11-C13-C14	-3.99	117.11	122.93
6	A	3016	6OU	O30-C31-C33	3.96	120.04	111.48
5	A	3012	9Z9	C10-C02-C06	3.96	113.16	107.25
5	A	3014	9Z9	C06-C05-C04	-3.93	95.56	102.40
5	A	3014	9Z9	C12-C11-C08	-3.92	107.27	111.66
5	A	3014	9Z9	C01-C02-C03	-3.86	103.19	111.58
5	A	3013	9Z9	C01-C02-C10	-3.79	105.01	110.61
5	A	3012	9Z9	C16-C13-C11	-3.79	111.58	116.42
5	A	3013	9Z9	C09-C10-C02	3.73	119.04	112.74
5	A	3014	9Z9	C15-C14-C13	-3.71	118.76	125.02
5	A	3014	9Z9	C77-C78-C79	3.71	113.09	108.59
5	A	3013	9Z9	C01-C02-C06	-3.65	105.06	111.68
5	A	3011	9Z9	C01-C02-C03	-3.64	103.68	111.58
5	A	3010	9Z9	C12-C11-C08	-3.58	107.64	111.66
5	A	3012	9Z9	C12-C11-C08	-3.57	107.65	111.66
5	A	3014	9Z9	C05-C06-C07	3.56	126.43	119.53
5	A	3011	9Z9	C75-C74-C73	-3.55	109.22	114.94
5	A	3010	9Z9	C01-C02-C10	-3.53	105.39	110.61
5	A	3013	9Z9	C12-C11-C08	-3.53	107.70	111.66
5	A	3010	9Z9	C08-C11-C13	3.43	114.67	109.65
5	A	3012	9Z9	C08-C11-C13	3.41	114.65	109.65
6	A	3020	6OU	O30-C31-C33	3.36	118.75	111.48
5	A	3012	9Z9	C11-C13-C14	-3.31	118.09	122.93
5	A	3014	9Z9	C01-C02-C06	-3.30	105.70	111.68
5	A	3013	9Z9	O80-C73-C76	3.29	113.63	110.76
5	A	3010	9Z9	C03-C02-C06	3.21	104.39	100.18
6	A	3023	6OU	O18-C16-C15	3.21	121.62	111.83
5	A	3010	9Z9	C15-C07-C08	3.20	113.42	109.72
5	A	3014	9Z9	C01-C02-C10	-3.20	105.89	110.61
5	A	3013	9Z9	C01-C02-C03	-3.15	104.74	111.58
5	A	3011	9Z9	C01-C02-C10	-3.14	105.98	110.61
5	A	3013	9Z9	C05-C06-C02	-3.12	100.15	103.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3014	9Z9	C05-C06-C02	-3.10	100.17	103.85
5	A	3010	9Z9	C02-C03-C74	-3.08	111.39	120.50
5	A	3014	9Z9	C15-C07-C08	3.08	113.28	109.72
5	A	3013	9Z9	C19-C11-C13	3.07	114.04	108.74
5	A	3013	9Z9	C11-C08-C07	-3.06	108.25	112.71
5	A	3013	9Z9	C75-C74-C73	-3.03	110.06	114.94
5	A	3013	9Z9	C03-C02-C06	2.98	104.08	100.18
5	A	3013	9Z9	C05-C06-C07	2.98	125.30	119.53
6	A	3018	6OU	O18-C16-C15	2.97	120.90	111.83
6	A	3020	6OU	O18-C16-C15	2.97	120.90	111.83
5	A	3011	9Z9	C02-C03-C74	-2.96	111.74	120.50
5	A	3010	9Z9	C05-C06-C07	2.94	125.23	119.53
5	A	3012	9Z9	C75-C74-C73	-2.94	110.20	114.94
5	A	3012	9Z9	C05-C06-C07	2.93	125.21	119.53
5	A	3010	9Z9	C77-C76-C73	2.92	116.51	111.93
6	A	3022	6OU	O30-C31-C33	2.92	120.75	111.83
5	A	3014	9Z9	C02-C03-C74	-2.92	111.87	120.50
6	A	3016	6OU	O18-C16-C15	2.92	120.72	111.83
5	A	3010	9Z9	C09-C08-C07	-2.89	107.75	111.78
5	A	3012	9Z9	C09-C10-C02	2.88	117.60	112.74
5	A	3011	9Z9	C02-C03-C04	2.88	107.31	104.20
5	A	3011	9Z9	C75-C74-C03	-2.85	108.80	114.50
5	A	3012	9Z9	C06-C05-C04	-2.84	97.45	102.40
5	A	3011	9Z9	C01-C02-C06	-2.83	107.79	112.07
5	A	3013	9Z9	C02-C03-C74	-2.82	112.17	120.50
5	A	3012	9Z9	O80-C73-C76	2.80	113.20	110.76
6	A	3021	6OU	O18-C16-C15	2.77	120.30	111.83
5	A	3010	9Z9	C76-C73-C74	-2.77	110.64	115.66
5	A	3012	9Z9	C01-C02-C03	-2.77	105.56	111.58
5	A	3010	9Z9	C01-C02-C06	-2.76	106.66	111.68
5	A	3013	9Z9	C02-C03-C04	2.71	107.13	104.20
5	A	3012	9Z9	C15-C07-C08	2.69	112.83	109.72
5	A	3014	9Z9	C02-C03-C04	2.68	107.10	104.20
5	A	3011	9Z9	C73-O72-C04	-2.68	100.73	108.14
6	A	3017	6OU	O30-C31-C33	2.64	119.89	111.83
5	A	3012	9Z9	O72-C04-C03	2.62	108.68	105.12
6	A	3022	6OU	O18-C16-C15	2.56	119.63	111.83
6	A	3015	6OU	O18-C16-C15	2.55	119.62	111.83
5	A	3010	9Z9	C09-C08-C11	-2.55	109.94	113.08
5	A	3014	9Z9	C03-C02-C06	2.52	103.48	100.18
5	A	3014	9Z9	C77-C76-C73	-2.52	107.99	111.93
5	A	3010	9Z9	C75-C74-C73	-2.51	110.89	114.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3014	9Z9	C81-C78-C79	-2.51	107.17	111.03
5	A	3010	9Z9	C79-O80-C73	2.50	118.00	113.69
5	A	3012	9Z9	C75-C74-C03	-2.49	109.52	114.50
5	A	3010	9Z9	C12-C11-C19	-2.47	105.68	109.43
5	A	3011	9Z9	O72-C73-C74	-2.44	101.32	104.56
5	A	3012	9Z9	C76-C73-C74	-2.42	111.28	115.66
5	A	3013	9Z9	C77-C78-C79	2.42	111.53	108.59
6	A	3019	6OU	O18-C16-C15	2.40	119.14	111.83
5	A	3010	9Z9	C02-C03-C04	2.38	106.77	104.20
5	A	3010	9Z9	C75-C74-C03	-2.36	109.79	114.50
5	A	3012	9Z9	C11-C08-C07	-2.29	109.37	112.71
5	A	3014	9Z9	C08-C07-C06	-2.26	106.14	109.09
5	A	3014	9Z9	O72-C73-C74	2.24	107.53	104.56
5	A	3010	9Z9	O72-C73-C74	-2.24	101.59	104.56
5	A	3012	9Z9	C02-C03-C74	-2.21	113.95	120.50
5	A	3011	9Z9	O72-C73-C76	2.21	113.02	108.54
5	A	3011	9Z9	C05-C06-C07	2.14	124.08	114.87
5	A	3011	9Z9	C76-C73-C74	-2.10	111.86	115.66
5	A	3014	9Z9	C79-O80-C73	-2.07	110.11	113.69
6	A	3025	6OU	O18-C16-C15	2.05	119.87	112.14
5	A	3011	9Z9	O80-C73-C76	2.03	112.53	110.76
5	A	3013	9Z9	O72-C73-C74	-2.03	101.86	104.56
6	A	3024	6OU	O18-C16-C15	2.03	119.79	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3009	NAG	C1

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3009	NAG	C8-C7-N2-C2
4	A	3009	NAG	O7-C7-N2-C2
5	A	3012	9Z9	C16-C17-O20-C21
6	A	3015	6OU	C27-O26-P23-O22
6	A	3015	6OU	C27-O26-P23-O24
6	A	3015	6OU	C27-O26-P23-O25
6	A	3015	6OU	O26-C27-C28-N29
6	A	3016	6OU	C21-O22-P23-O24
6	A	3016	6OU	C27-O26-P23-O22
6	A	3016	6OU	C27-O26-P23-O24

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Mol	Chain	Res	Type	Atoms
6	A	3016	6OU	O26-C27-C28-N29
6	A	3018	6OU	C19-C20-C21-O22
6	A	3018	6OU	O30-C20-C21-O22
6	A	3019	6OU	O18-C19-C20-O30
6	A	3020	6OU	C15-C16-O18-C19
6	A	3020	6OU	O17-C16-O18-C19
6	A	3020	6OU	C27-O26-P23-O22
6	A	3020	6OU	C27-O26-P23-O25
6	A	3020	6OU	O26-C27-C28-N29
6	A	3021	6OU	C21-O22-P23-O24
6	A	3021	6OU	C21-O22-P23-O26
6	A	3021	6OU	O26-C27-C28-N29
6	A	3023	6OU	C33-C31-O30-C20
6	A	3023	6OU	O32-C31-O30-C20
6	A	3024	6OU	C06-C07-C08-C09
6	A	3019	6OU	O17-C16-O18-C19
4	A	3003	NAG	O5-C5-C6-O6
6	A	3019	6OU	C15-C16-O18-C19
6	A	3021	6OU	C15-C16-O18-C19
6	A	3021	6OU	O17-C16-O18-C19
4	A	3003	NAG	C4-C5-C6-O6
6	A	3019	6OU	C33-C31-O30-C20
6	A	3015	6OU	C31-C33-C34-C35
6	A	3017	6OU	C31-C33-C34-C35
6	A	3022	6OU	C13-C14-C15-C16
6	A	3019	6OU	O32-C31-O30-C20
6	A	3024	6OU	C13-C14-C15-C16
6	A	3019	6OU	C36-C37-C38-C39
6	A	3016	6OU	C11-C12-C13-C14
6	A	3022	6OU	C35-C36-C37-C38
6	A	3020	6OU	C12-C13-C14-C15
6	A	3024	6OU	C10-C11-C12-C13
6	A	3020	6OU	C33-C31-O30-C20
6	A	3019	6OU	C13-C14-C15-C16
6	A	3019	6OU	C35-C36-C37-C38
6	A	3024	6OU	C04-C05-C06-C07
6	A	3018	6OU	C10-C11-C12-C13
6	A	3021	6OU	C31-C33-C34-C35
6	A	3016	6OU	C09-C10-C11-C12
5	A	3010	9Z9	C18-C17-O20-C21
6	A	3020	6OU	C07-C08-C09-C10
6	A	3018	6OU	C33-C31-O30-C20

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Mol	Chain	Res	Type	Atoms
6	A	3021	6OU	C33-C31-O30-C20
6	A	3020	6OU	O32-C31-O30-C20
6	A	3020	6OU	C10-C11-C12-C13
6	A	3015	6OU	C34-C35-C36-C37
6	A	3022	6OU	C34-C35-C36-C37
6	A	3018	6OU	C34-C35-C36-C37
6	A	3017	6OU	C37-C38-C39-C40
6	A	3021	6OU	O18-C19-C20-O30
6	A	3016	6OU	C35-C36-C37-C38
6	A	3024	6OU	C11-C12-C13-C14
6	A	3022	6OU	C33-C34-C35-C36
6	A	3020	6OU	C19-C20-C21-O22
6	A	3020	6OU	C34-C35-C36-C37
6	A	3025	6OU	C13-C14-C15-C16
6	A	3016	6OU	O18-C19-C20-C21
6	A	3018	6OU	O18-C19-C20-C21
6	A	3018	6OU	O32-C31-O30-C20
6	A	3019	6OU	C06-C07-C08-C09
6	A	3016	6OU	O18-C19-C20-O30
6	A	3018	6OU	O18-C19-C20-O30
6	A	3015	6OU	C36-C37-C38-C39
6	A	3020	6OU	C08-C09-C10-C11
6	A	3021	6OU	O32-C31-O30-C20
6	A	3023	6OU	C19-C20-C21-O22
6	A	3019	6OU	O18-C19-C20-C21
6	A	3021	6OU	O18-C19-C20-C21
6	A	3020	6OU	C06-C07-C08-C09
6	A	3024	6OU	C09-C10-C11-C12
6	A	3023	6OU	O30-C20-C21-O22
6	A	3020	6OU	C37-C38-C39-C40
6	A	3020	6OU	C11-C12-C13-C14
6	A	3017	6OU	C36-C37-C38-C39
6	A	3018	6OU	C38-C39-C40-C41
5	A	3012	9Z9	C22-C21-O20-C17
6	A	3022	6OU	C37-C38-C39-C40
6	A	3021	6OU	C19-C20-C21-O22
6	A	3020	6OU	C35-C36-C37-C38
6	A	3018	6OU	C09-C10-C11-C12
6	A	3017	6OU	C34-C35-C36-C37
6	A	3020	6OU	O30-C20-C21-O22
6	A	3016	6OU	C34-C35-C36-C37
6	A	3022	6OU	O18-C19-C20-O30

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Mol	Chain	Res	Type	Atoms
6	A	3021	6OU	O30-C20-C21-O22
6	A	3025	6OU	C15-C16-O18-C19
6	A	3016	6OU	C21-O22-P23-O26
6	A	3020	6OU	C21-O22-P23-O24
6	A	3020	6OU	C27-O26-P23-O24
6	A	3018	6OU	C31-C33-C34-C35
6	A	3016	6OU	C20-C21-O22-P23
6	A	3016	6OU	C10-C11-C12-C13
6	A	3015	6OU	O17-C16-O18-C19
6	A	3015	6OU	C07-C08-C09-C10
6	A	3015	6OU	C15-C16-O18-C19
6	A	3016	6OU	C37-C38-C39-C40
6	A	3022	6OU	C40-C41-C42-C43
6	A	3015	6OU	C20-C21-O22-P23
6	A	3023	6OU	C35-C36-C37-C38
6	A	3015	6OU	C35-C36-C37-C38
6	A	3016	6OU	C08-C09-C10-C11
6	A	3016	6OU	C38-C39-C40-C41
6	A	3020	6OU	C33-C34-C35-C36
6	A	3018	6OU	C15-C16-O18-C19
6	A	3020	6OU	C40-C41-C42-C43
6	A	3015	6OU	C38-C39-C40-C41
6	A	3018	6OU	O17-C16-O18-C19
6	A	3023	6OU	C21-O22-P23-O26
6	A	3018	6OU	C13-C14-C15-C16
6	A	3016	6OU	C12-C13-C14-C15
6	A	3022	6OU	C41-C42-C43-C44
6	A	3018	6OU	C12-C13-C14-C15
6	A	3020	6OU	O18-C19-C20-O30
6	A	3022	6OU	C38-C39-C40-C41
6	A	3025	6OU	O17-C16-O18-C19
6	A	3016	6OU	O30-C31-C33-C34
6	A	3020	6OU	C09-C10-C11-C12
6	A	3023	6OU	O18-C19-C20-O30
6	A	3021	6OU	C13-C14-C15-C16
6	A	3021	6OU	C14-C15-C16-O18
6	A	3019	6OU	C14-C15-C16-O18
6	A	3017	6OU	C38-C39-C40-C41
6	A	3024	6OU	C12-C13-C14-C15
6	A	3022	6OU	O17-C16-O18-C19
6	A	3021	6OU	C14-C15-C16-O17
6	A	3022	6OU	C14-C15-C16-O18

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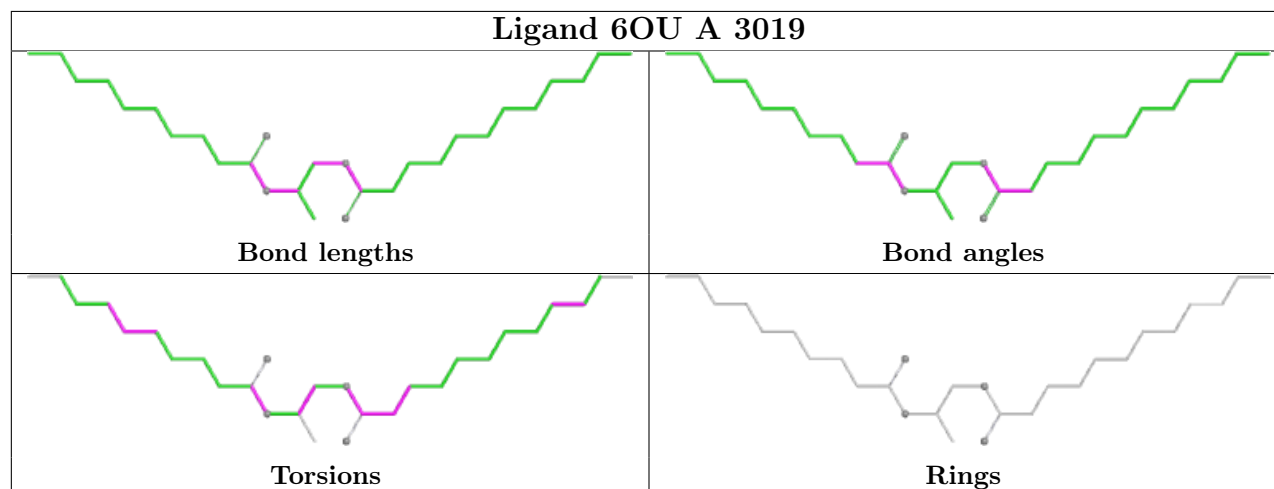
Mol	Chain	Res	Type	Atoms
6	A	3016	6OU	C14-C15-C16-O18
6	A	3018	6OU	O30-C31-C33-C34

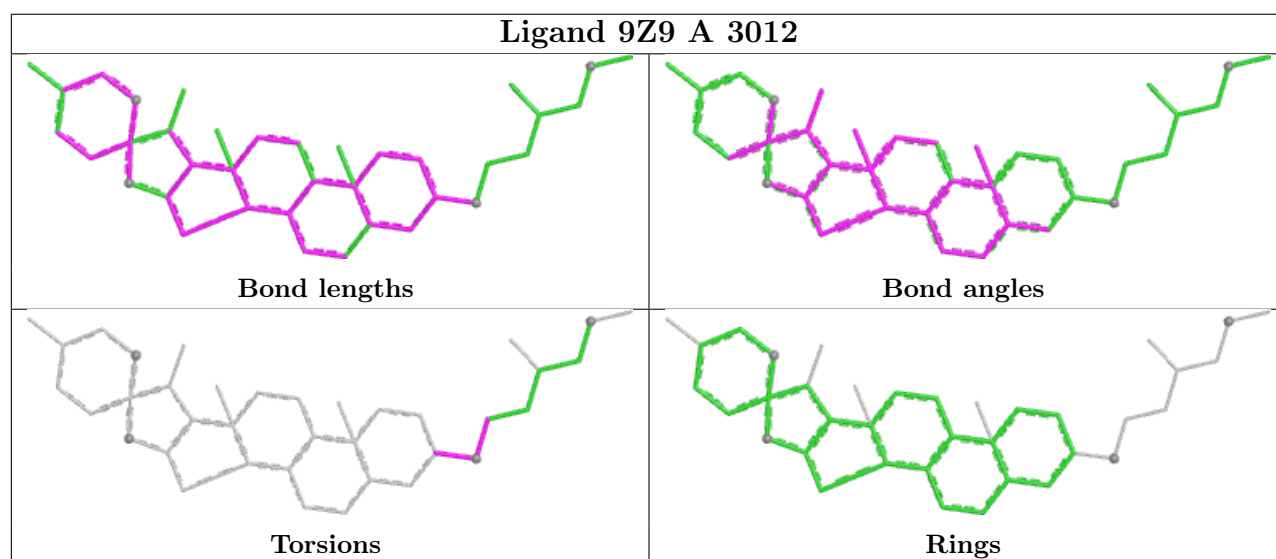
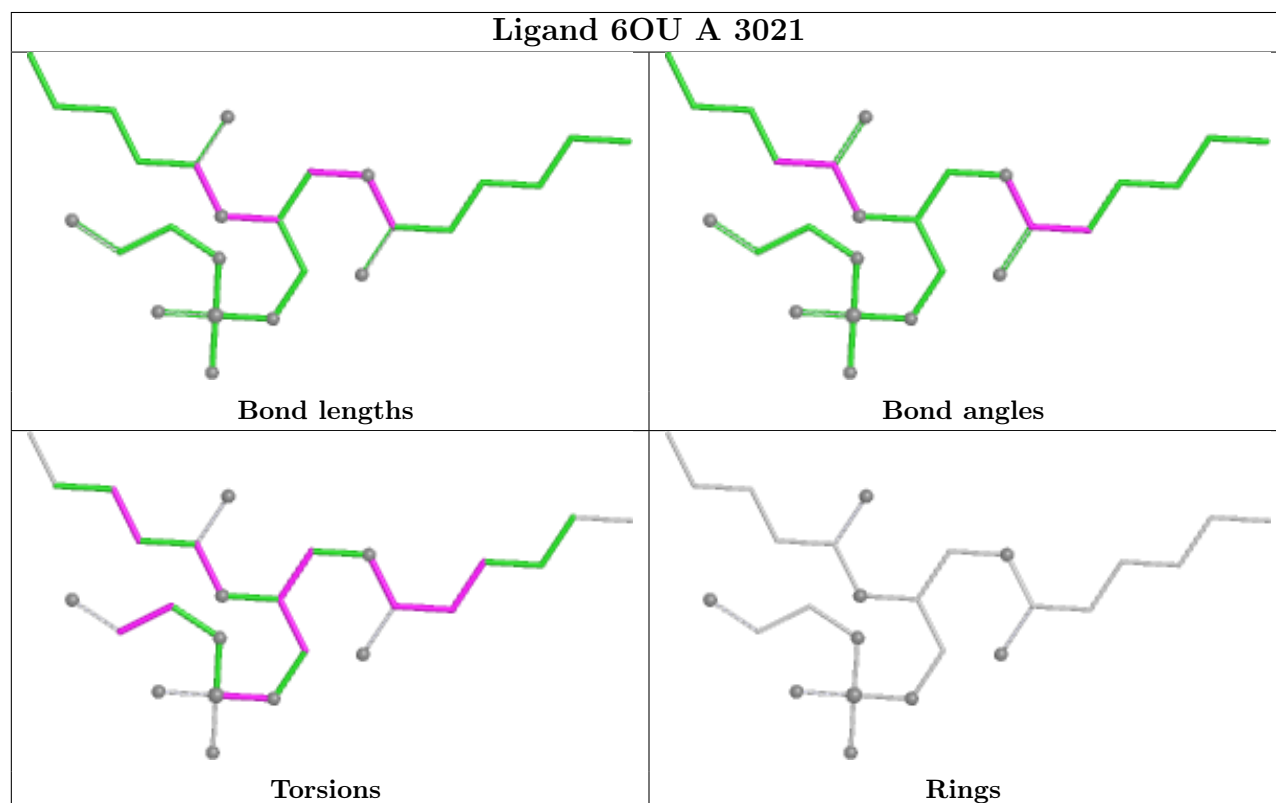
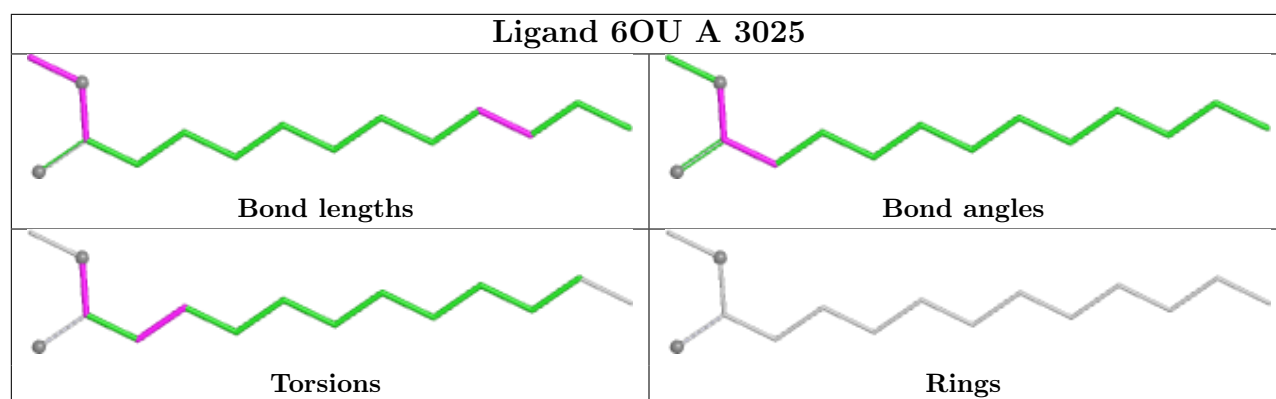
There are no ring outliers.

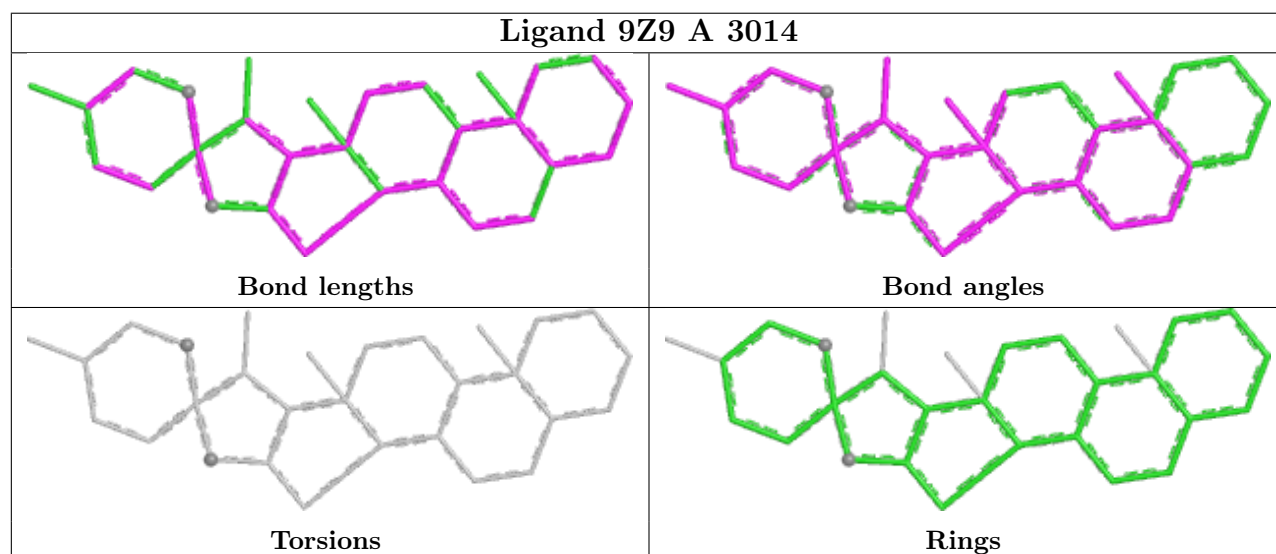
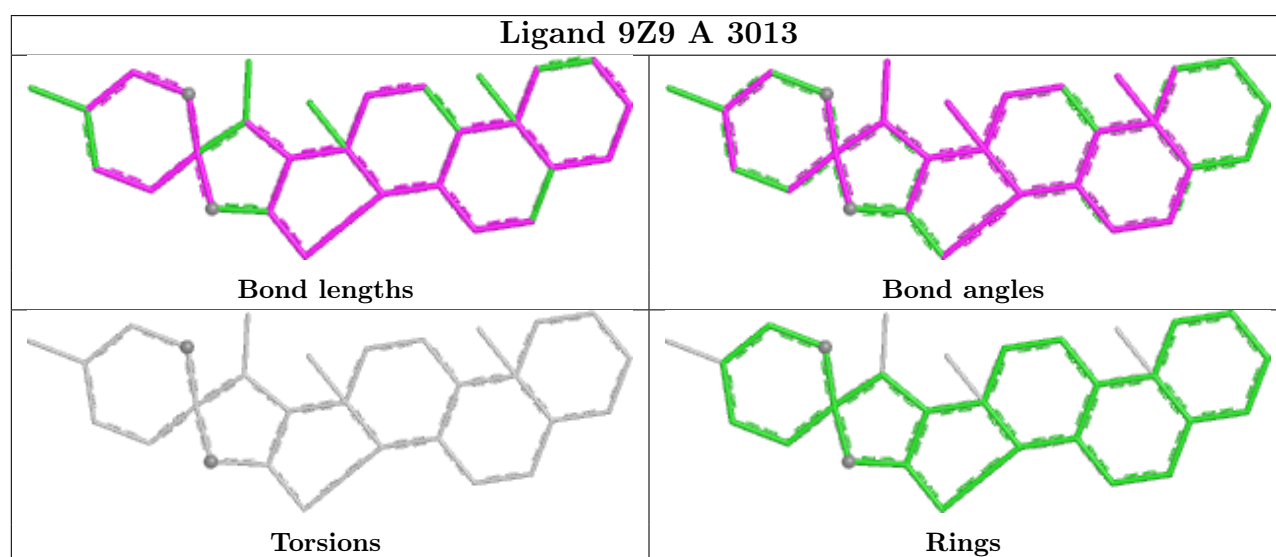
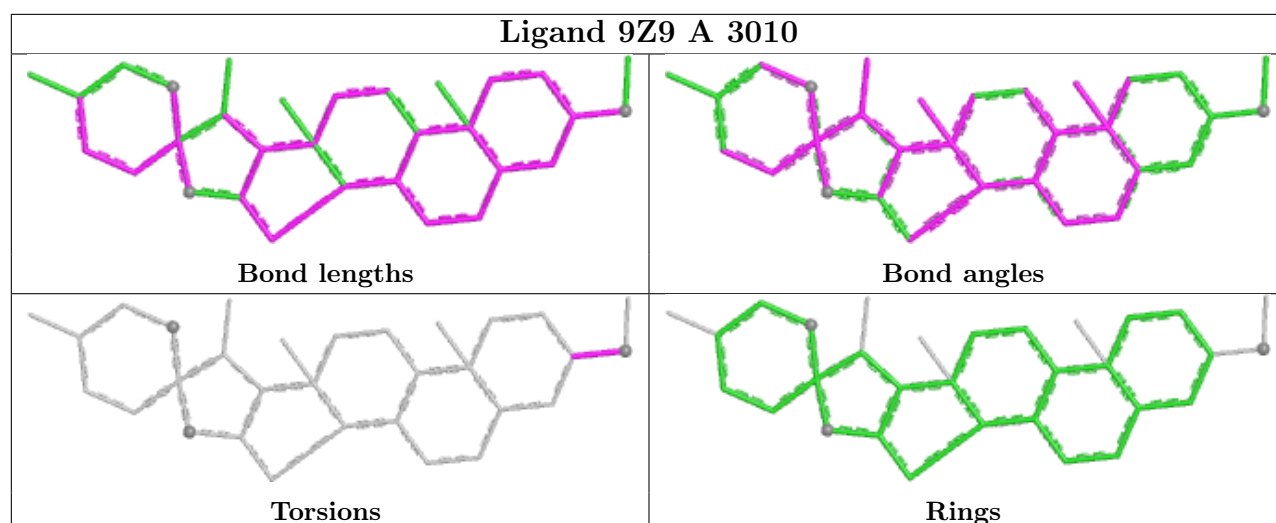
7 monomers are involved in 45 short contacts:

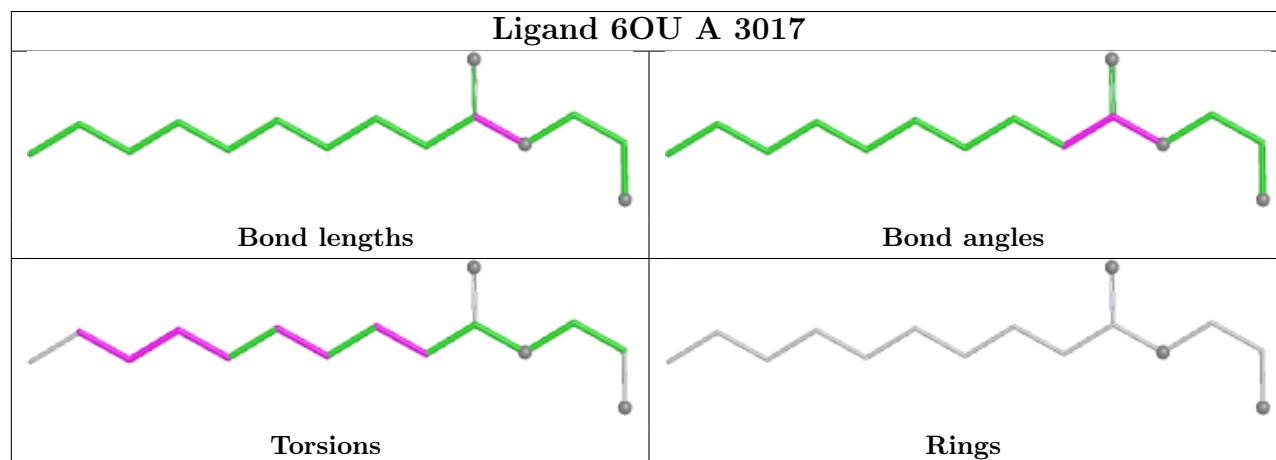
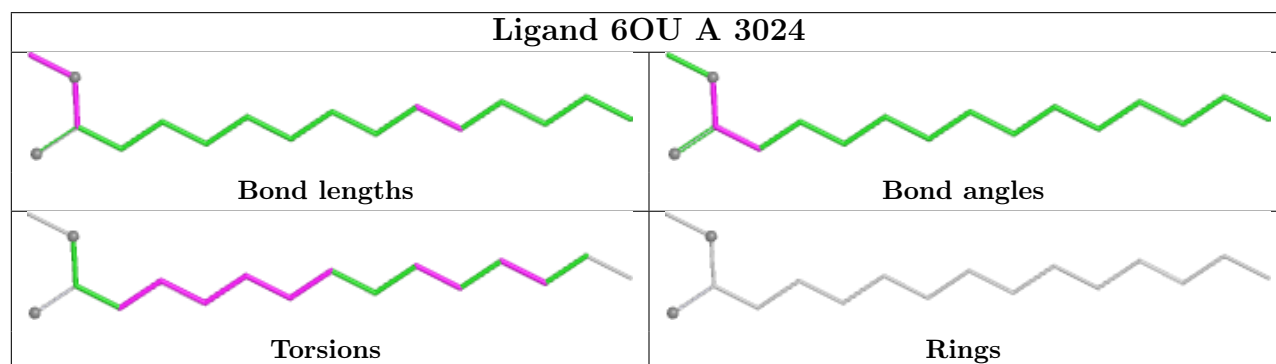
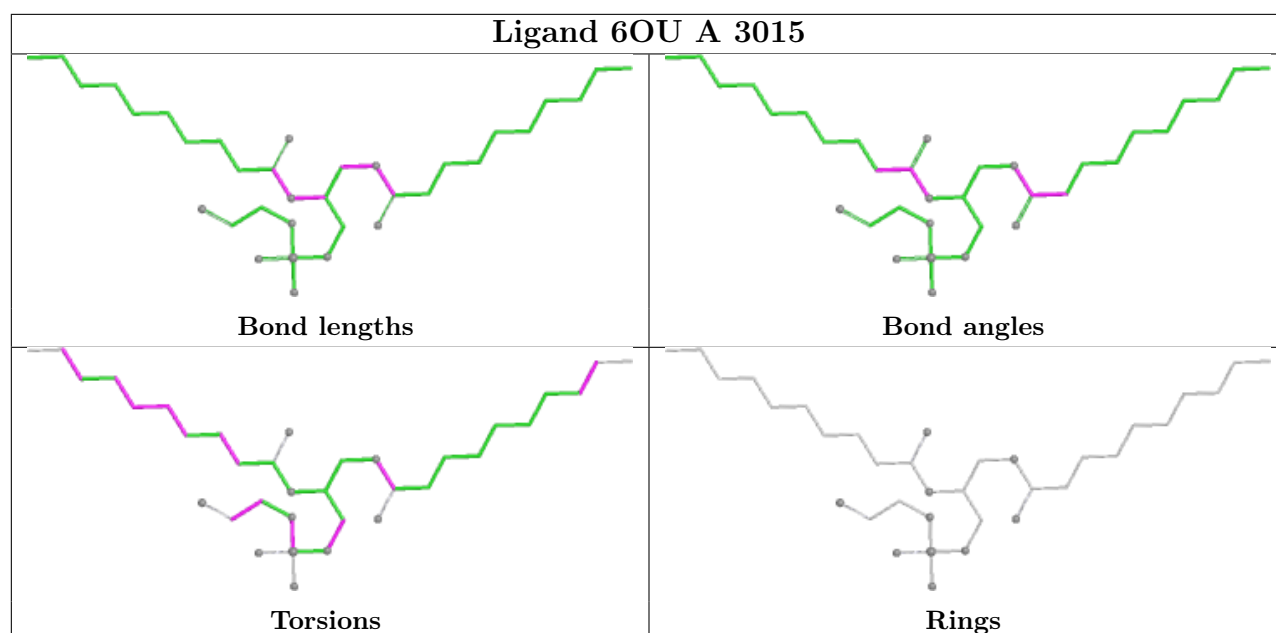
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3003	NAG	2	0
5	A	3012	9Z9	10	0
5	A	3010	9Z9	1	0
5	A	3013	9Z9	10	0
4	A	3009	NAG	16	0
5	A	3014	9Z9	7	0
5	A	3011	9Z9	1	0

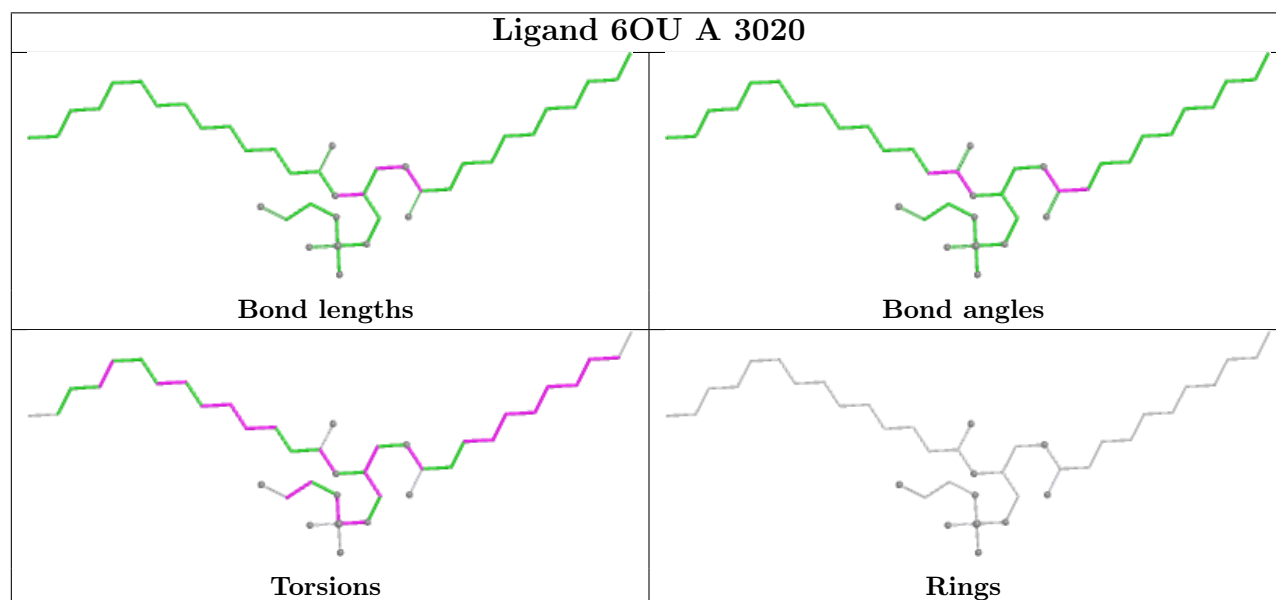
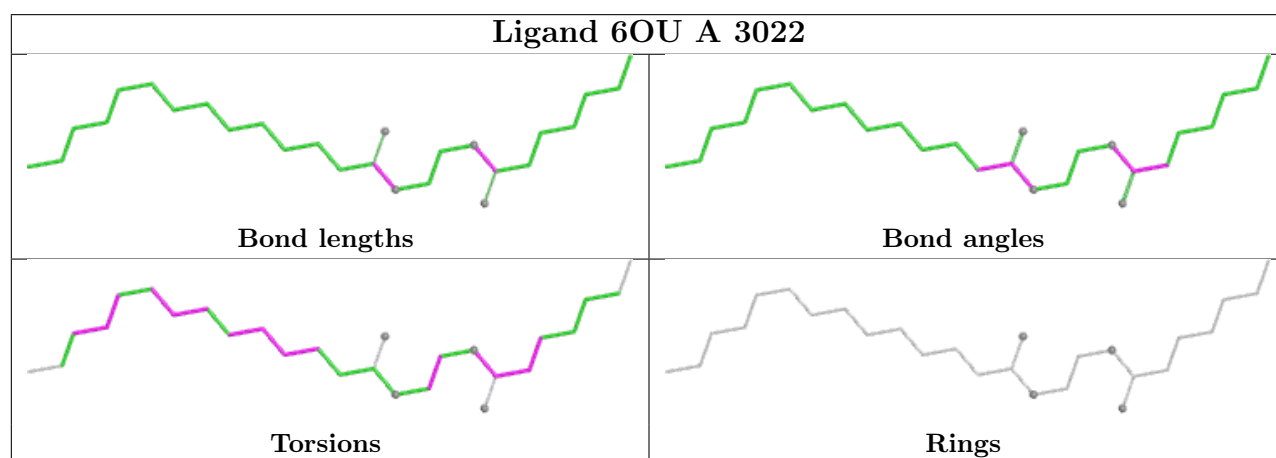
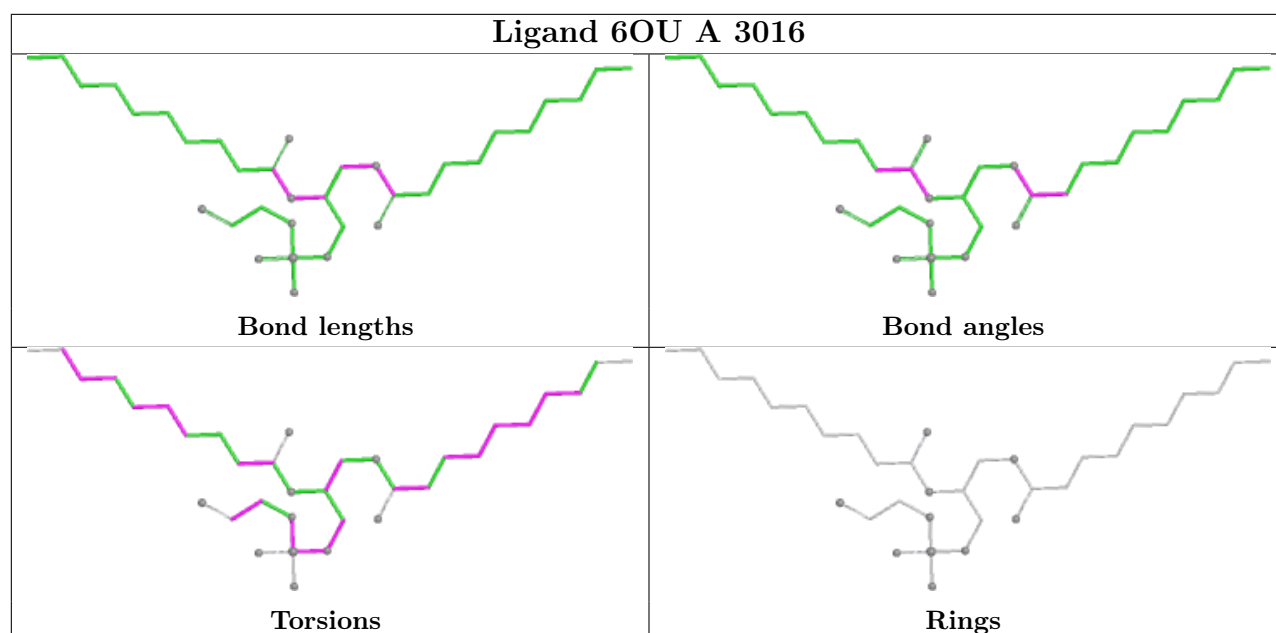
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

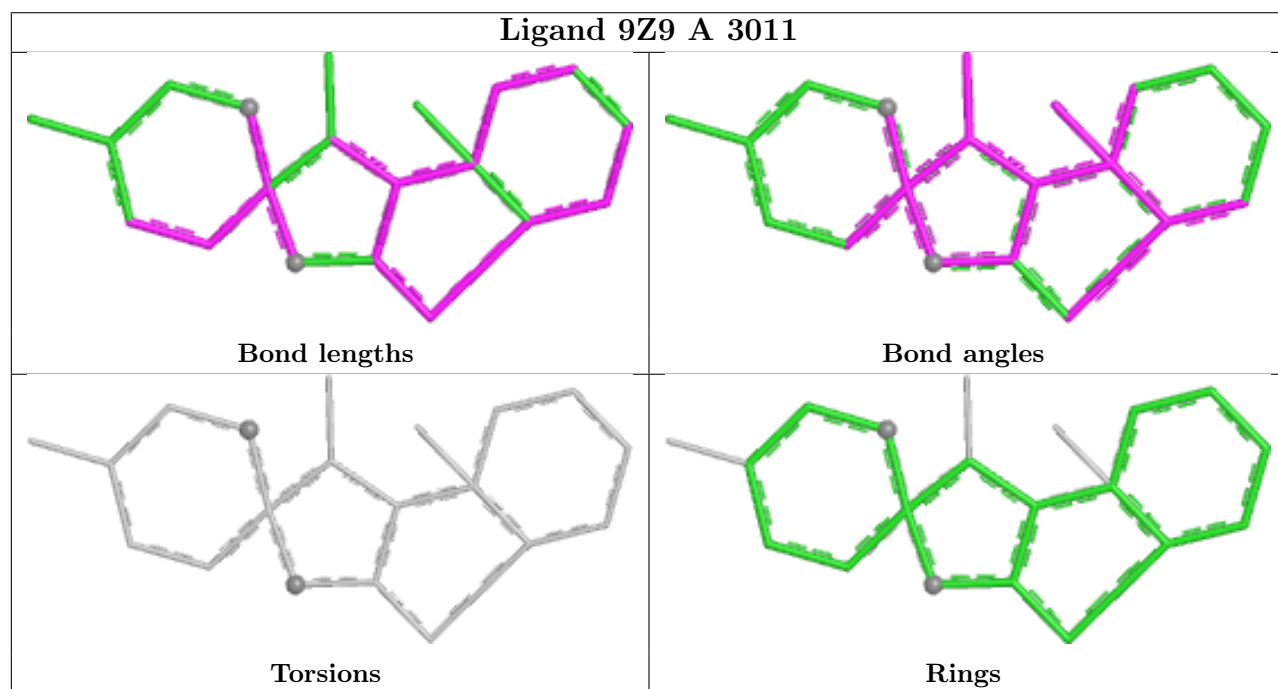
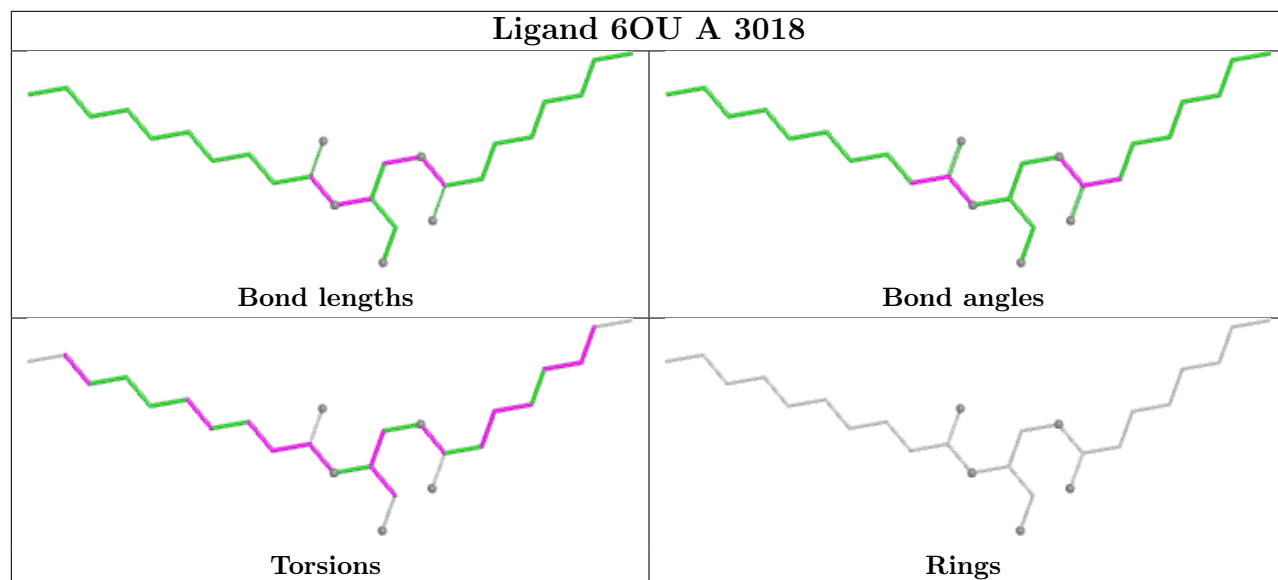


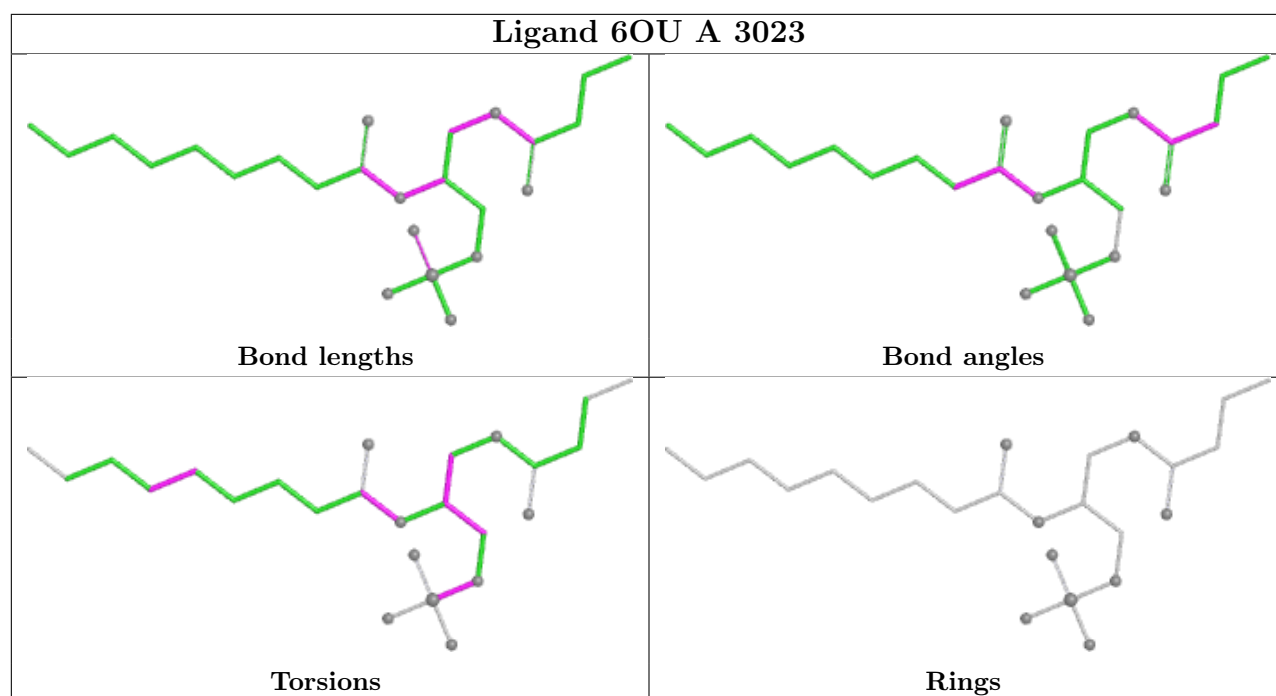












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

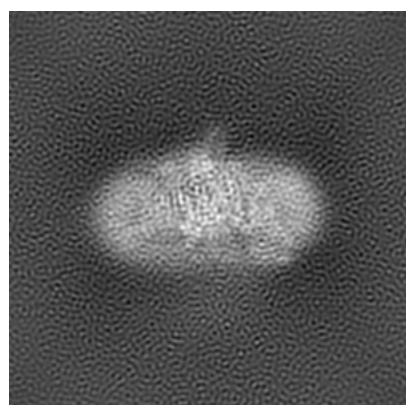
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20951. These allow visual inspection of the internal detail of the map and identification of artifacts.

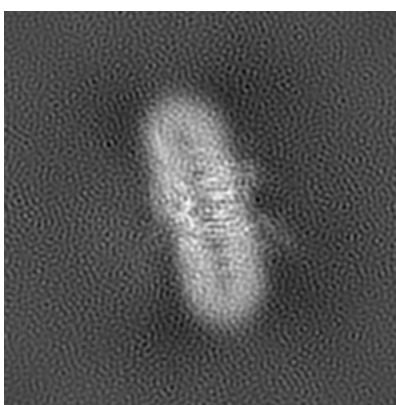
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

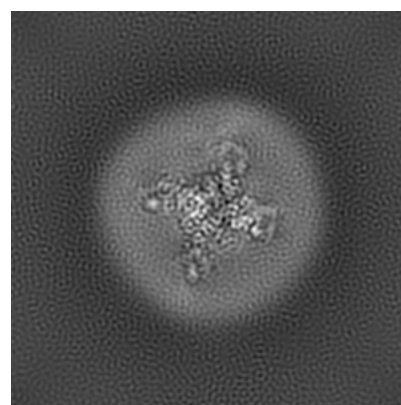
6.1.1 Primary map



X



Y

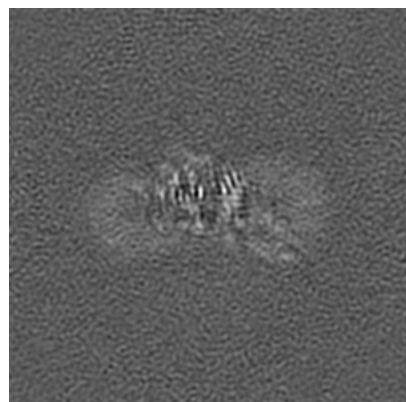


Z

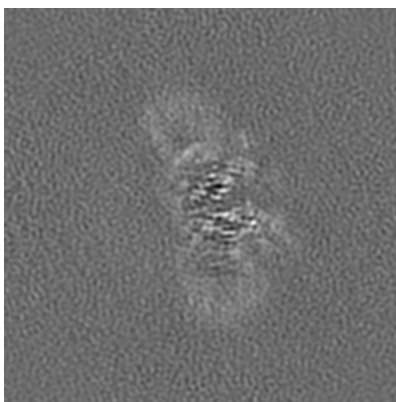
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

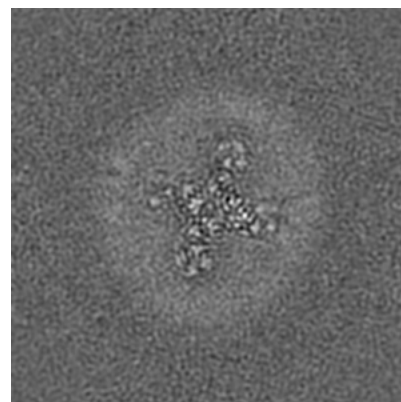
6.2.1 Primary map



X Index: 128



Y Index: 128

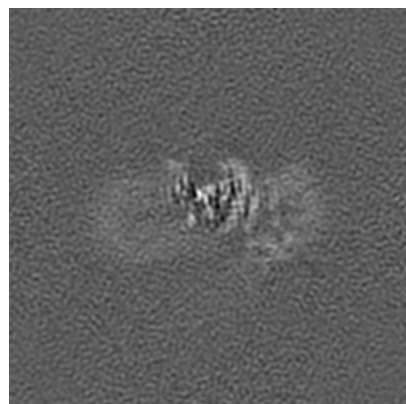


Z Index: 128

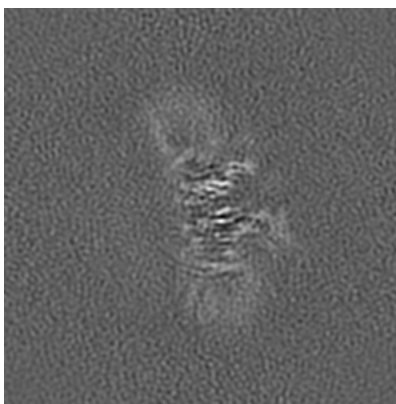
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

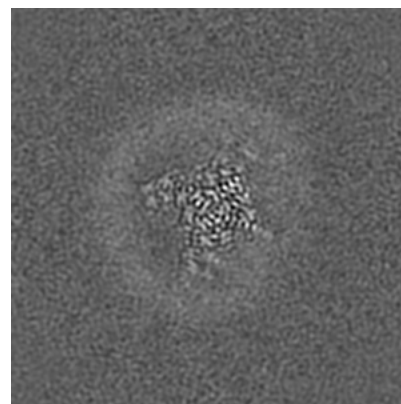
6.3.1 Primary map



X Index: 138



Y Index: 130

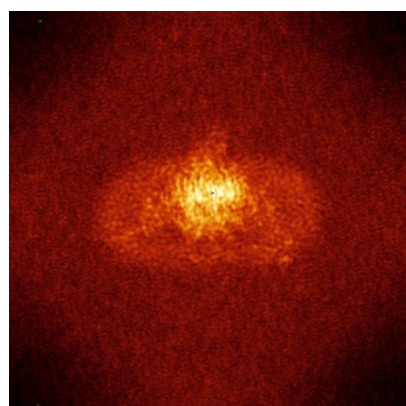


Z Index: 138

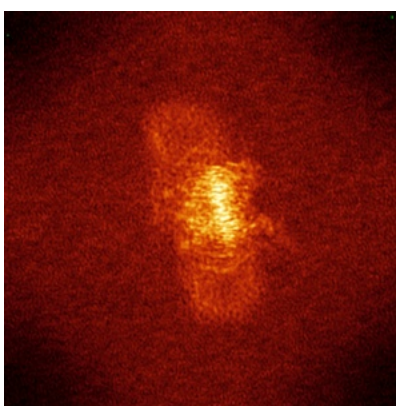
The images above show the largest variance slices of the map in three orthogonal directions.

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

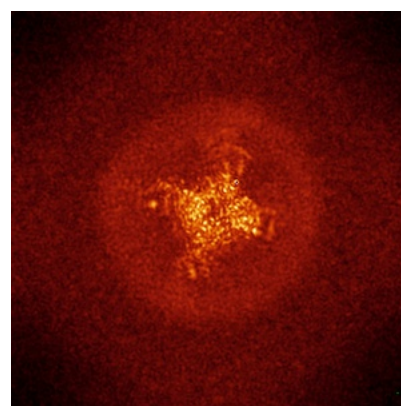
6.4.1 Primary map



X



Y

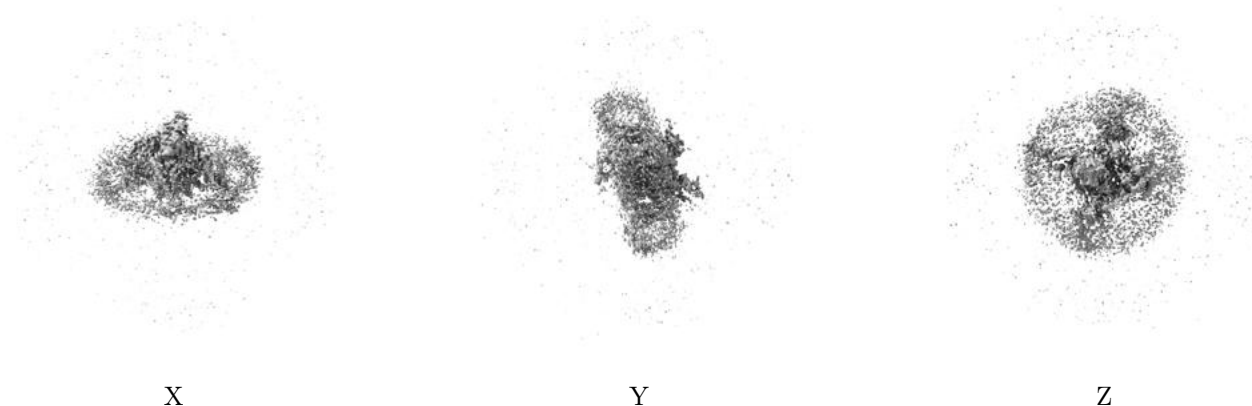


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

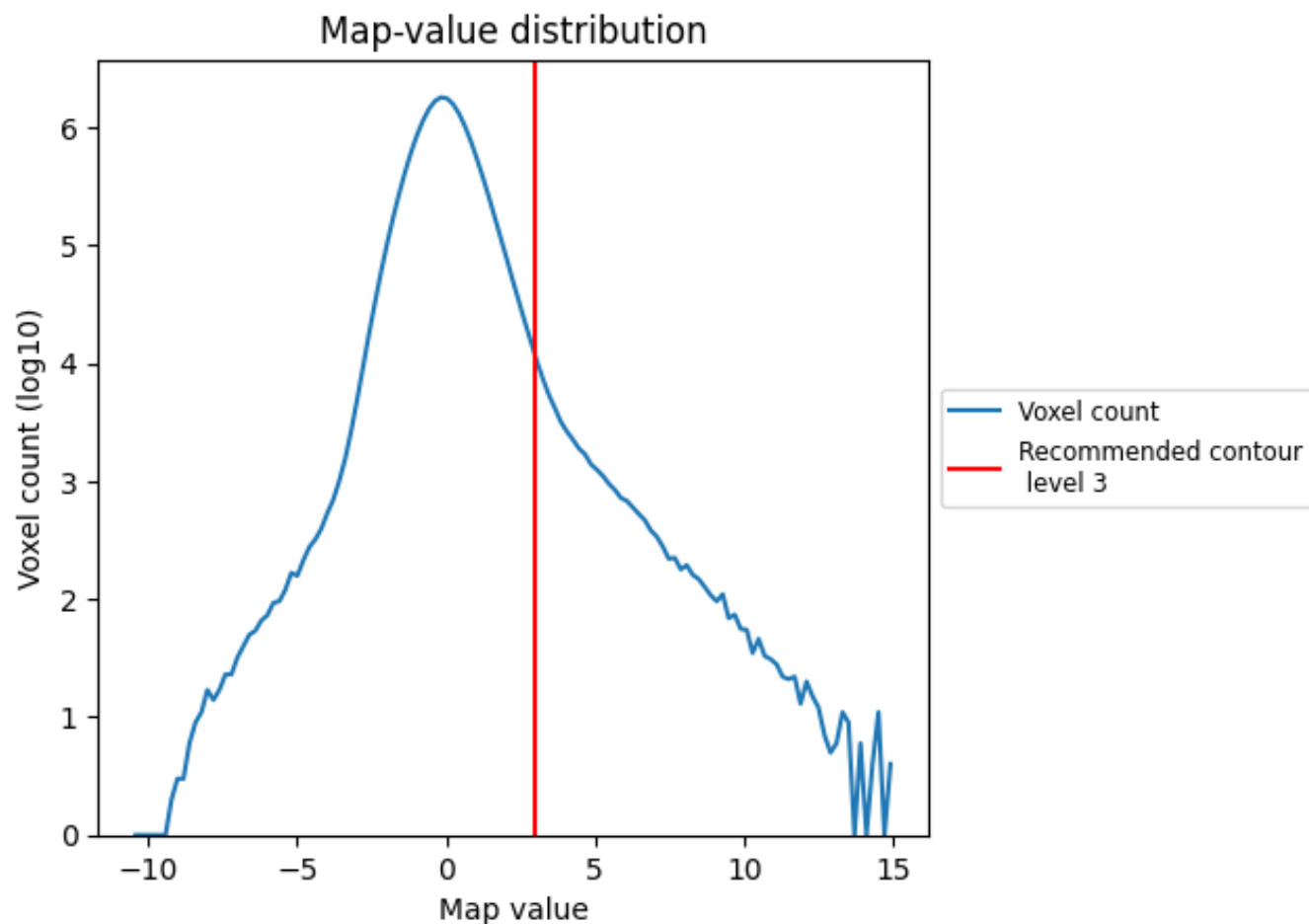
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

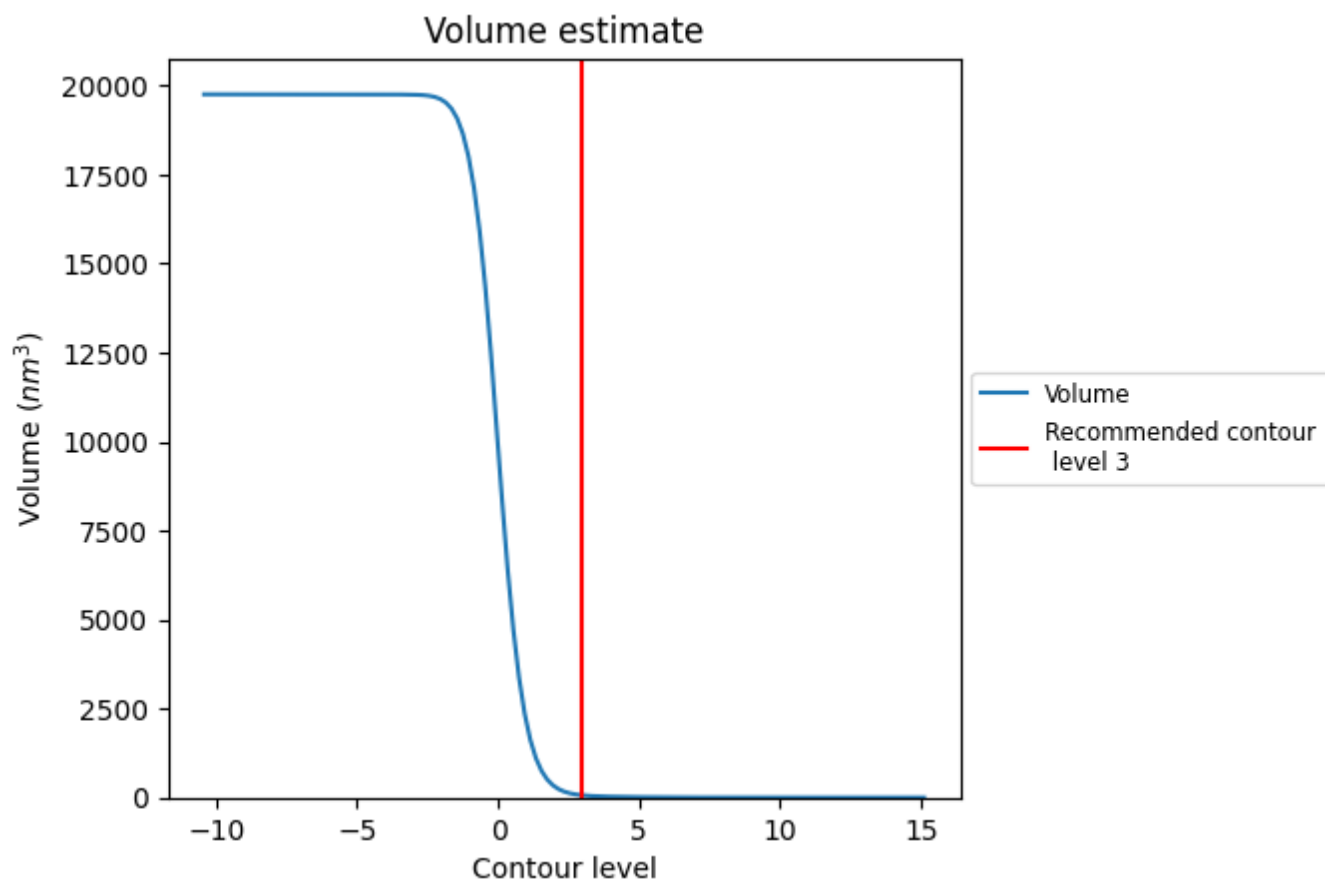
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

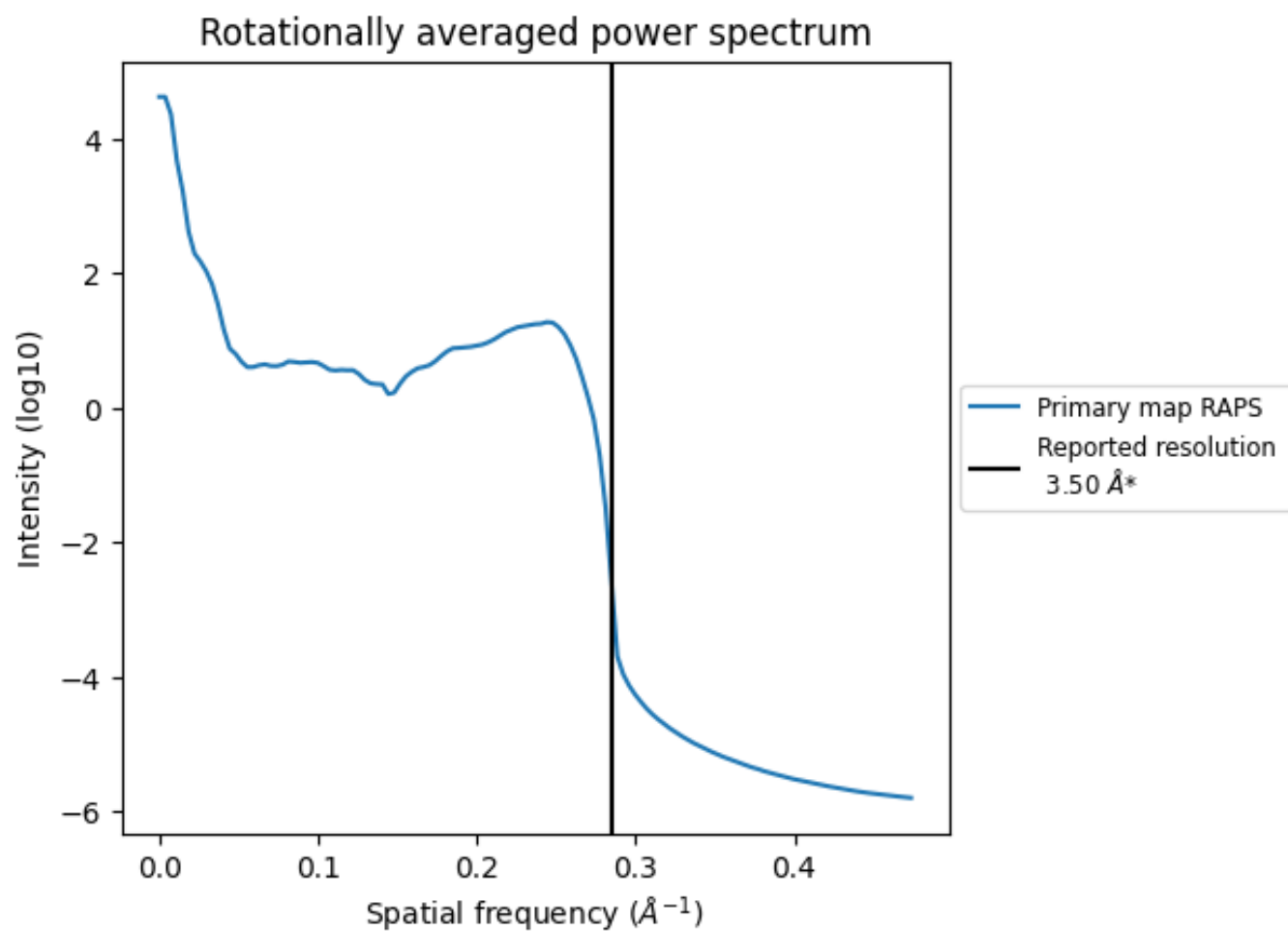
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 58 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 ⓘ

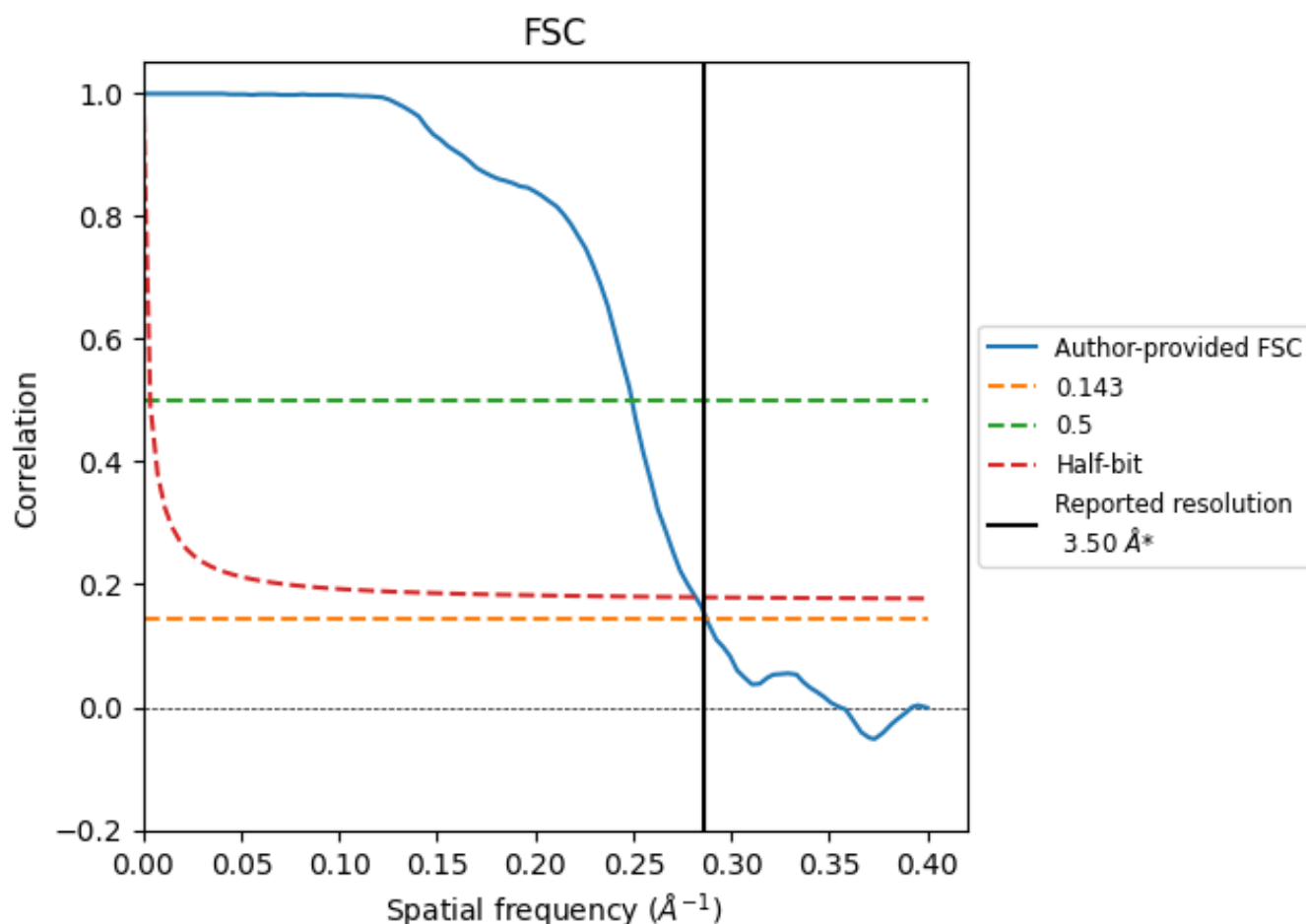


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

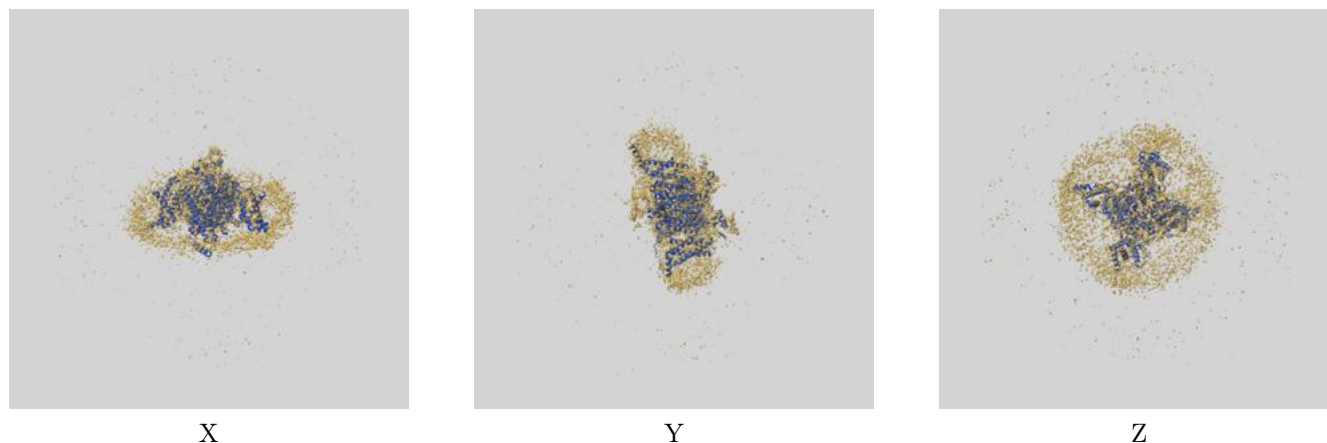
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	4.01	3.55
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

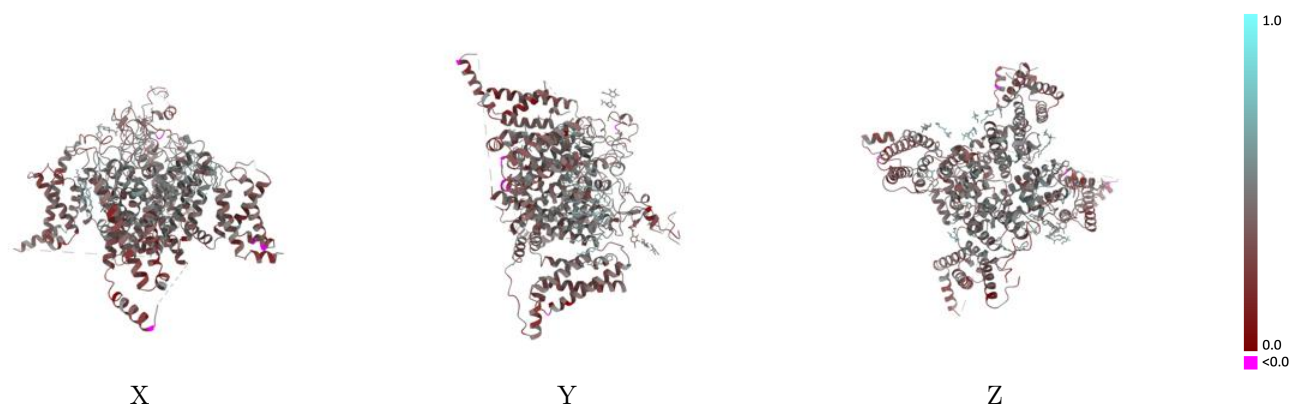
This section contains information regarding the fit between EMDB map EMD-20951 and PDB model 6UZ3. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



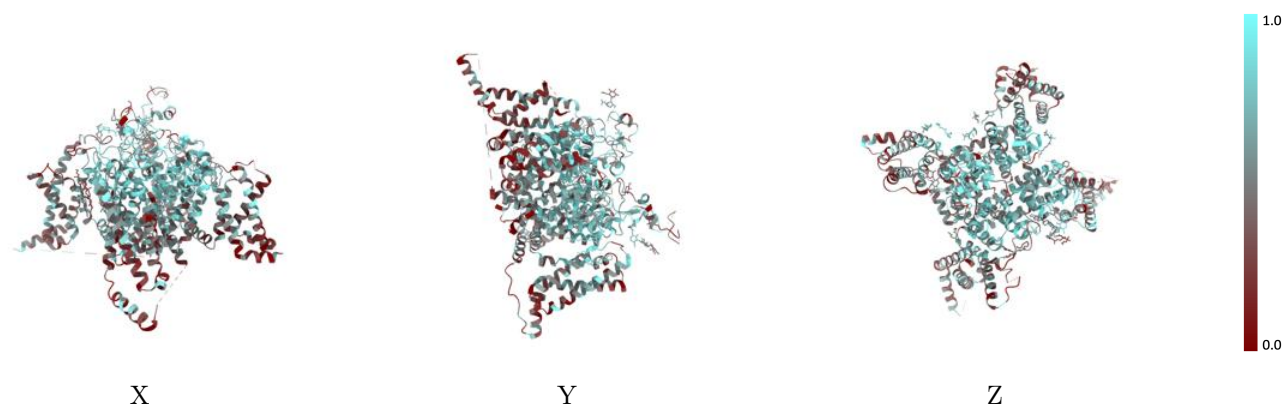
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



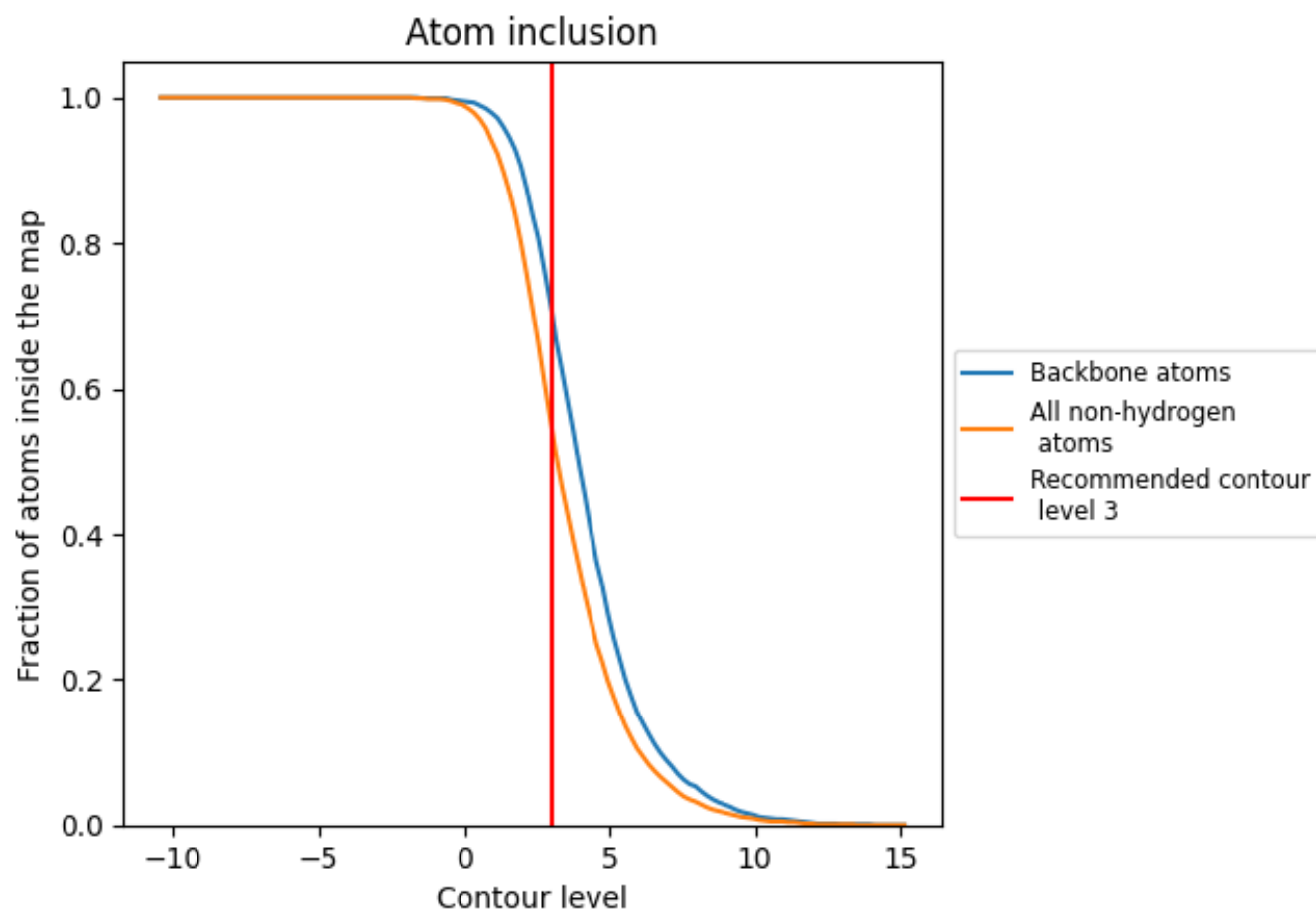
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 55% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5470	0.4010
A	0.5470	0.4000
B	0.4640	0.4580
C	0.5380	0.4360
D	0.6430	0.4840

