



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:02 AM UTC

PDB ID : 7QQB / pdb_00007qqb
Title : Crystal structure of the envelope glycoprotein complex of Puumala virus in complex with the scFv fragment of the broadly neutralizing human antibody ADI-42898
Authors : Serris, A.; Rey, F.A.; Guardado-Calvo, P.
Deposited on : 2022-01-07
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

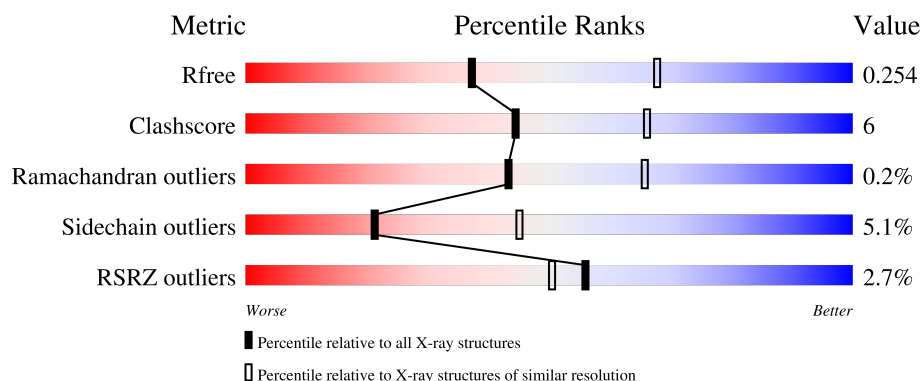
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	889	0% 34% 6% 60%
1	B	889	0% 38% 9% 52%
2	H	298	2% 34% 7% 59%
2	L	298	0% 26% 9% 63%
3	C	6	50% 50%

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Mol	Chain	Length	Quality of chain
4	D	2	 100%
4	E	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Envelope polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2689	1698	441	528	22			
1	B	423	Total	C	N	O	S	0	0	0
			3211	2009	539	632	31			

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ARG	-	expression tag	UNP A0A0B4U5I0
A	19	SER	-	expression tag	UNP A0A0B4U5I0
A	362	ASP	GLU	conflict	UNP A0A0B4U5I0
A	382	GLY	-	linker	UNP A0A0B4U5I0
A	383	GLY	-	linker	UNP A0A0B4U5I0
A	384	SER	-	linker	UNP A0A0B4U5I0
A	385	GLY	-	linker	UNP A0A0B4U5I0
A	386	LEU	-	linker	UNP A0A0B4U5I0
A	387	VAL	-	linker	UNP A0A0B4U5I0
A	388	PRO	-	linker	UNP A0A0B4U5I0
A	389	ARG	-	linker	UNP A0A0B4U5I0
A	390	GLY	-	linker	UNP A0A0B4U5I0
A	391	SER	-	linker	UNP A0A0B4U5I0
A	392	GLY	-	linker	UNP A0A0B4U5I0
A	393	GLY	-	linker	UNP A0A0B4U5I0
A	394	GLY	-	linker	UNP A0A0B4U5I0
A	395	SER	-	linker	UNP A0A0B4U5I0
A	396	GLY	-	linker	UNP A0A0B4U5I0
A	397	GLY	-	linker	UNP A0A0B4U5I0
A	398	GLY	-	linker	UNP A0A0B4U5I0
A	399	SER	-	linker	UNP A0A0B4U5I0
A	400	TRP	-	linker	UNP A0A0B4U5I0
A	401	SER	-	linker	UNP A0A0B4U5I0
A	402	HIS	-	linker	UNP A0A0B4U5I0
A	403	PRO	-	linker	UNP A0A0B4U5I0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	404	GLN	-	linker	UNP A0A0B4U5I0
A	405	PHE	-	linker	UNP A0A0B4U5I0
A	406	GLU	-	linker	UNP A0A0B4U5I0
A	407	LYS	-	linker	UNP A0A0B4U5I0
A	408	GLY	-	linker	UNP A0A0B4U5I0
A	409	GLY	-	linker	UNP A0A0B4U5I0
A	410	GLY	-	linker	UNP A0A0B4U5I0
A	411	THR	-	linker	UNP A0A0B4U5I0
A	412	GLY	-	linker	UNP A0A0B4U5I0
A	413	GLY	-	linker	UNP A0A0B4U5I0
A	414	GLY	-	linker	UNP A0A0B4U5I0
A	415	THR	-	linker	UNP A0A0B4U5I0
A	416	LEU	-	linker	UNP A0A0B4U5I0
A	417	VAL	-	linker	UNP A0A0B4U5I0
A	418	PRO	-	linker	UNP A0A0B4U5I0
A	419	ARG	-	linker	UNP A0A0B4U5I0
A	420	GLY	-	linker	UNP A0A0B4U5I0
A	421	SER	-	linker	UNP A0A0B4U5I0
A	422	GLY	-	linker	UNP A0A0B4U5I0
A	423	THR	-	linker	UNP A0A0B4U5I0
A	424	GLY	-	linker	UNP A0A0B4U5I0
A	425	GLY	-	linker	UNP A0A0B4U5I0
A	861	GLY	-	expression tag	UNP A0A6M3W7M6
A	862	LEU	-	expression tag	UNP A0A6M3W7M6
A	863	VAL	-	expression tag	UNP A0A6M3W7M6
A	864	PRO	-	expression tag	UNP A0A6M3W7M6
A	865	ARG	-	expression tag	UNP A0A6M3W7M6
A	866	GLY	-	expression tag	UNP A0A6M3W7M6
A	867	SER	-	expression tag	UNP A0A6M3W7M6
A	868	GLY	-	expression tag	UNP A0A6M3W7M6
A	869	PRO	-	expression tag	UNP A0A6M3W7M6
A	870	PHE	-	expression tag	UNP A0A6M3W7M6
A	871	GLU	-	expression tag	UNP A0A6M3W7M6
A	872	ASP	-	expression tag	UNP A0A6M3W7M6
A	873	ASP	-	expression tag	UNP A0A6M3W7M6
A	874	ASP	-	expression tag	UNP A0A6M3W7M6
A	875	ASP	-	expression tag	UNP A0A6M3W7M6
A	876	LYS	-	expression tag	UNP A0A6M3W7M6
A	877	ALA	-	expression tag	UNP A0A6M3W7M6
A	878	GLY	-	expression tag	UNP A0A6M3W7M6
A	879	TRP	-	expression tag	UNP A0A6M3W7M6
A	880	SER	-	expression tag	UNP A0A6M3W7M6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	881	HIS	-	expression tag	UNP A0A6M3W7M6
A	882	PRO	-	expression tag	UNP A0A6M3W7M6
A	883	GLN	-	expression tag	UNP A0A6M3W7M6
A	884	PHE	-	expression tag	UNP A0A6M3W7M6
A	885	GLU	-	expression tag	UNP A0A6M3W7M6
A	886	LYS	-	expression tag	UNP A0A6M3W7M6
A	887	GLY	-	expression tag	UNP A0A6M3W7M6
A	888	GLY	-	expression tag	UNP A0A6M3W7M6
A	889	GLY	-	expression tag	UNP A0A6M3W7M6
A	890	SER	-	expression tag	UNP A0A6M3W7M6
A	891	GLY	-	expression tag	UNP A0A6M3W7M6
A	892	GLY	-	expression tag	UNP A0A6M3W7M6
A	893	GLY	-	expression tag	UNP A0A6M3W7M6
A	894	SER	-	expression tag	UNP A0A6M3W7M6
A	895	GLY	-	expression tag	UNP A0A6M3W7M6
A	896	GLY	-	expression tag	UNP A0A6M3W7M6
A	897	GLY	-	expression tag	UNP A0A6M3W7M6
A	898	SER	-	expression tag	UNP A0A6M3W7M6
A	899	TRP	-	expression tag	UNP A0A6M3W7M6
A	900	SER	-	expression tag	UNP A0A6M3W7M6
A	901	HIS	-	expression tag	UNP A0A6M3W7M6
A	902	PRO	-	expression tag	UNP A0A6M3W7M6
A	903	GLN	-	expression tag	UNP A0A6M3W7M6
A	904	PHE	-	expression tag	UNP A0A6M3W7M6
A	905	GLU	-	expression tag	UNP A0A6M3W7M6
A	906	LYS	-	expression tag	UNP A0A6M3W7M6
B	251	ARG	-	expression tag	UNP A0A0B4U5I0
B	252	SER	-	expression tag	UNP A0A0B4U5I0
B	595	ASP	GLU	conflict	UNP A0A0B4U5I0
B	615	GLY	-	linker	UNP A0A0B4U5I0
B	616	GLY	-	linker	UNP A0A0B4U5I0
B	617	SER	-	linker	UNP A0A0B4U5I0
B	618	GLY	-	linker	UNP A0A0B4U5I0
B	619	LEU	-	linker	UNP A0A0B4U5I0
B	620	VAL	-	linker	UNP A0A0B4U5I0
B	621	PRO	-	linker	UNP A0A0B4U5I0
B	622	ARG	-	linker	UNP A0A0B4U5I0
B	623	GLY	-	linker	UNP A0A0B4U5I0
B	624	SER	-	linker	UNP A0A0B4U5I0
B	625	GLY	-	linker	UNP A0A0B4U5I0
B	626	GLY	-	linker	UNP A0A0B4U5I0
B	627	GLY	-	linker	UNP A0A0B4U5I0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	628	SER	-	linker	UNP A0A0B4U5I0
B	629	GLY	-	linker	UNP A0A0B4U5I0
B	630	GLY	-	linker	UNP A0A0B4U5I0
B	631	GLY	-	linker	UNP A0A0B4U5I0
B	632	SER	-	linker	UNP A0A0B4U5I0
B	633	TRP	-	linker	UNP A0A0B4U5I0
B	634	SER	-	linker	UNP A0A0B4U5I0
B	635	HIS	-	linker	UNP A0A0B4U5I0
B	636	PRO	-	linker	UNP A0A0B4U5I0
B	637	GLN	-	linker	UNP A0A0B4U5I0
B	638	PHE	-	linker	UNP A0A0B4U5I0
B	639	GLU	-	linker	UNP A0A0B4U5I0
B	640	LYS	-	linker	UNP A0A0B4U5I0
B	641	GLY	-	linker	UNP A0A0B4U5I0
B	642	GLY	-	linker	UNP A0A0B4U5I0
B	643	GLY	-	linker	UNP A0A0B4U5I0
B	644	THR	-	linker	UNP A0A0B4U5I0
B	645	GLY	-	linker	UNP A0A0B4U5I0
B	646	GLY	-	linker	UNP A0A0B4U5I0
B	647	GLY	-	linker	UNP A0A0B4U5I0
B	648	THR	-	linker	UNP A0A0B4U5I0
B	649	LEU	-	linker	UNP A0A0B4U5I0
B	650	VAL	-	linker	UNP A0A0B4U5I0
B	651	PRO	-	linker	UNP A0A0B4U5I0
B	652	ARG	-	linker	UNP A0A0B4U5I0
B	653	GLY	-	linker	UNP A0A0B4U5I0
B	654	SER	-	linker	UNP A0A0B4U5I0
B	655	GLY	-	linker	UNP A0A0B4U5I0
B	656	THR	-	linker	UNP A0A0B4U5I0
B	657	GLY	-	linker	UNP A0A0B4U5I0
B	658	GLY	-	linker	UNP A0A0B4U5I0
B	1094	GLY	-	expression tag	UNP A0A6M3W7M6
B	1095	LEU	-	expression tag	UNP A0A6M3W7M6
B	1096	VAL	-	expression tag	UNP A0A6M3W7M6
B	1097	PRO	-	expression tag	UNP A0A6M3W7M6
B	1098	ARG	-	expression tag	UNP A0A6M3W7M6
B	1099	GLY	-	expression tag	UNP A0A6M3W7M6
B	1100	SER	-	expression tag	UNP A0A6M3W7M6
B	1101	GLY	-	expression tag	UNP A0A6M3W7M6
B	1102	PRO	-	expression tag	UNP A0A6M3W7M6
B	1103	PHE	-	expression tag	UNP A0A6M3W7M6
B	1104	GLU	-	expression tag	UNP A0A6M3W7M6

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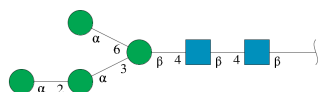
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1105	ASP	-	expression tag	UNP A0A6M3W7M6
B	1106	ASP	-	expression tag	UNP A0A6M3W7M6
B	1107	ASP	-	expression tag	UNP A0A6M3W7M6
B	1108	ASP	-	expression tag	UNP A0A6M3W7M6
B	1109	LYS	-	expression tag	UNP A0A6M3W7M6
B	1110	ALA	-	expression tag	UNP A0A6M3W7M6
B	1111	GLY	-	expression tag	UNP A0A6M3W7M6
B	1112	TRP	-	expression tag	UNP A0A6M3W7M6
B	1113	SER	-	expression tag	UNP A0A6M3W7M6
B	1114	HIS	-	expression tag	UNP A0A6M3W7M6
B	1115	PRO	-	expression tag	UNP A0A6M3W7M6
B	1116	GLN	-	expression tag	UNP A0A6M3W7M6
B	1117	PHE	-	expression tag	UNP A0A6M3W7M6
B	1118	GLU	-	expression tag	UNP A0A6M3W7M6
B	1119	LYS	-	expression tag	UNP A0A6M3W7M6
B	1120	GLY	-	expression tag	UNP A0A6M3W7M6
B	1121	GLY	-	expression tag	UNP A0A6M3W7M6
B	1122	GLY	-	expression tag	UNP A0A6M3W7M6
B	1123	SER	-	expression tag	UNP A0A6M3W7M6
B	1124	GLY	-	expression tag	UNP A0A6M3W7M6
B	1125	GLY	-	expression tag	UNP A0A6M3W7M6
B	1126	GLY	-	expression tag	UNP A0A6M3W7M6
B	1127	SER	-	expression tag	UNP A0A6M3W7M6
B	1128	GLY	-	expression tag	UNP A0A6M3W7M6
B	1129	GLY	-	expression tag	UNP A0A6M3W7M6
B	1130	GLY	-	expression tag	UNP A0A6M3W7M6
B	1131	SER	-	expression tag	UNP A0A6M3W7M6
B	1132	TRP	-	expression tag	UNP A0A6M3W7M6
B	1133	SER	-	expression tag	UNP A0A6M3W7M6
B	1134	HIS	-	expression tag	UNP A0A6M3W7M6
B	1135	PRO	-	expression tag	UNP A0A6M3W7M6
B	1136	GLN	-	expression tag	UNP A0A6M3W7M6
B	1137	PHE	-	expression tag	UNP A0A6M3W7M6
B	1138	GLU	-	expression tag	UNP A0A6M3W7M6
B	1139	LYS	-	expression tag	UNP A0A6M3W7M6

- Molecule 2 is a protein called Single Chain Variable Fragment (scFv) of ADI-42898.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	122	Total	C	N	O	S	0	0	0
			950	604	165	176	5			
2	L	109	Total	C	N	O	S	0	0	0
			824	521	138	160	5			

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



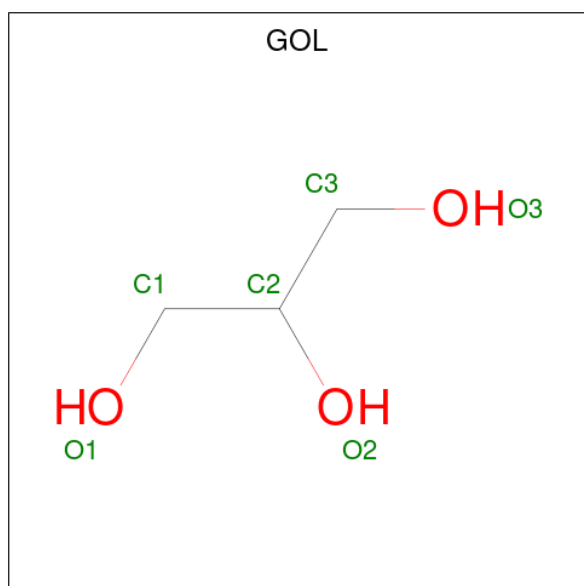
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

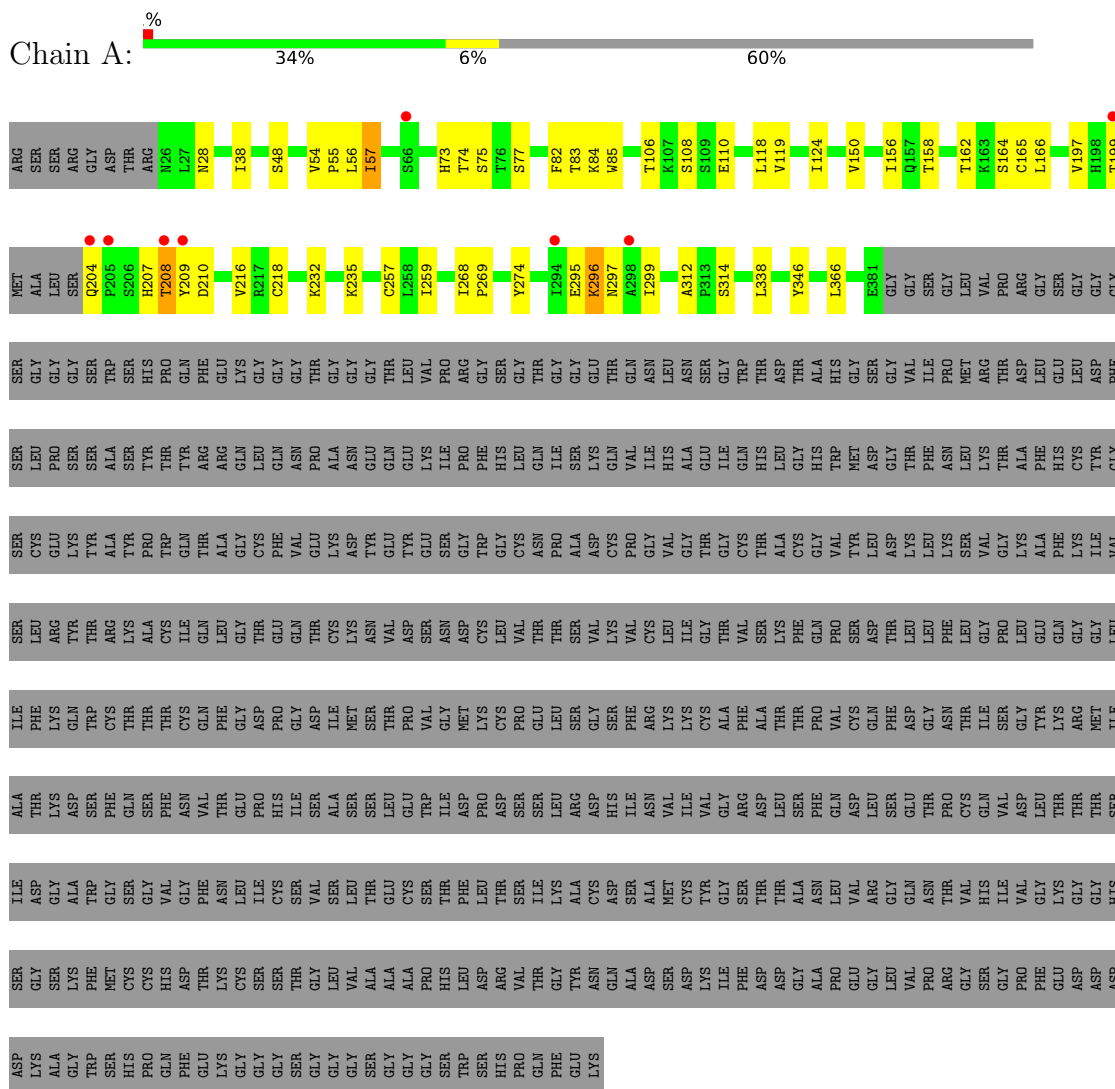
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	13	Total	O	0	0
			13	13		
6	H	1	Total	O	0	0
			1	1		
6	L	1	Total	O	0	0
			1	1		

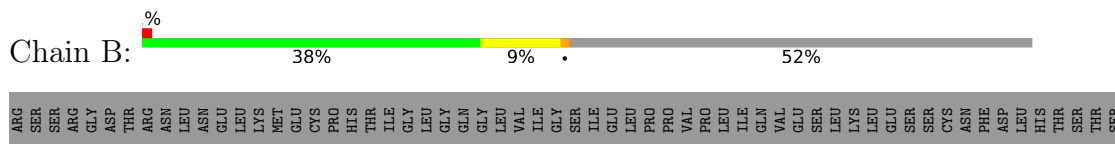
3 Residue-property plots

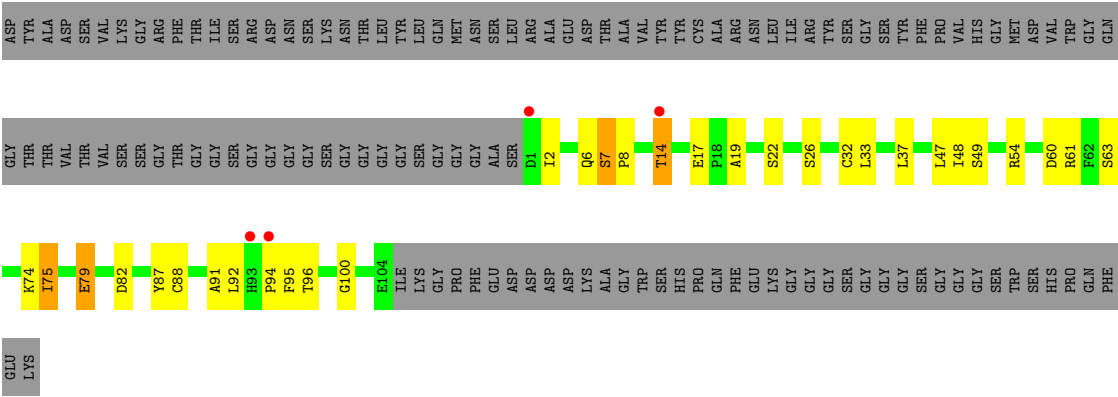
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Envelope polypeptide



- Molecule 1: Envelope polypeptide

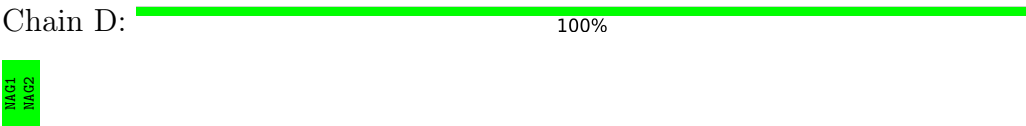




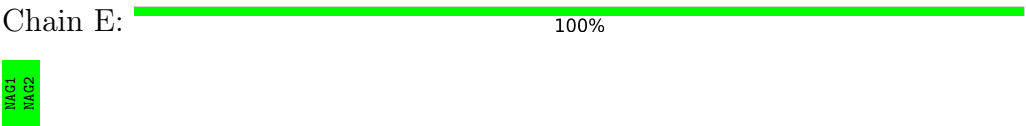
• Molecule 3: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	83.88Å 109.30Å 149.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 2.60 39.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.00-2.60) 99.9 (39.00-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.212 , 0.249 0.217 , 0.254	Depositor DCC
R_{free} test set	2130 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7834	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MAN, NAG, GOL, 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	0.10	0/2743	0.31	0/3731
1	B	0.09	0/3283	0.26	0/4452
2	H	0.10	0/973	0.32	0/1318
2	L	0.11	0/844	0.34	0/1146
All	All	0.10	0/7843	0.30	0/10647

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
2	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	7	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2689	0	2664	24	0
1	B	3211	0	3069	44	0
2	H	950	0	922	8	0
2	L	824	0	797	17	0
3	C	72	0	61	0	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
5	A	6	0	8	0	0
6	A	11	0	0	0	0
6	B	13	0	0	0	0
6	H	1	0	0	0	0
6	L	1	0	0	0	0
All	All	7834	0	7571	92	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 6.

All (92) 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:165:CYS:SG	1:A:166:LEU:N	2.54	0.76
2:L:92:LEU:O	2:L:95:PHE:N	2.22	0.71
1:B:992:TRP:HE1	1:B:1070:PRO:HD3	1.58	0.67
1:B:813:ARG:HD2	1:B:959:ASP:OD2	1.95	0.65
1:B:1019:CYS:HA	1:B:1024:CYS:HA	1.78	0.65
1:B:714:HIS:HB3	1:B:818:GLN:HB3	1.79	0.65
1:B:991:ALA:HB3	1:B:996:VAL:HG21	1.81	0.63
1:B:702:GLN:NE2	1:B:707:GLU:O	2.29	0.62
1:B:683:LEU:HB3	1:B:965:VAL:HB	1.84	0.58
1:B:812:THR:HG22	1:B:829:ASP:HB3	1.86	0.58
1:B:902:ARG:HD3	1:B:916:ASP:OD2	2.03	0.58
1:B:769:TYR:HE2	2:H:98:ARG:HH21	1.51	0.57
1:A:119:VAL:HG11	1:A:124:ILE:HG13	1.87	0.57
1:B:726:ILE:HD13	1:B:948:LEU:HB2	1.87	0.56
1:A:110:GLU:OE1	1:A:314:SER:OG	2.23	0.56
1:B:988:ILE:HG22	1:B:1065:LEU:HD23	1.88	0.56
1:A:232:LYS:HD3	1:A:235:LYS:HD2	1.88	0.56
1:B:712:PRO:HD2	1:B:820:GLY:HA2	1.87	0.55
1:B:1083:SER:HB2	1:B:1085:LYS:HZ3	1.72	0.55
1:B:733:MET:HG3	1:B:892:MET:HE1	1.90	0.54
1:A:197:VAL:O	1:A:274:TYR:OH	2.23	0.54
2:L:14:THR:OG1	2:L:17:GLU:OE1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:VAL:HG12	1:B:951:ILE:HG12	1.91	0.53
1:B:885:ILE:HG22	1:B:892:MET:HE2	1.92	0.51
2:H:7:SER:OG	2:H:21:SER:OG	2.29	0.51
1:B:685:LEU:HB2	1:B:963:VAL:HB	1.93	0.51
1:B:992:TRP:HB3	1:B:1067:ALA:HB3	1.93	0.51
1:A:38:ILE:HG23	1:A:156:ILE:HG22	1.92	0.51
1:B:877:CYS:SG	1:B:884:ASP:HA	2.51	0.50
2:L:6:GLN:NE2	2:L:88:CYS:H	2.10	0.50
1:A:296:LYS:HD2	1:A:297:ASN:H	1.76	0.50
1:A:296:LYS:HD2	1:A:297:ASN:N	2.26	0.50
1:B:692:SER:HB3	1:B:952:ASP:O	2.11	0.50
2:L:63:SER:HB3	2:L:74:LYS:HE3	1.92	0.50
1:B:849:LYS:HD2	1:B:956:SER:HB3	1.94	0.49
2:L:6:GLN:HE22	2:L:87:TYR:HA	1.76	0.49
2:L:75:ILE:HD11	2:L:82:ASP:OD2	2.12	0.49
2:L:19:ALA:HB3	2:L:75:ILE:HG23	1.94	0.48
2:L:32:CYS:HB3	2:L:91:ALA:HB3	1.94	0.48
1:B:823:GLN:NE2	1:B:1031:ASN:OD1	2.38	0.48
2:L:48:ILE:HD13	2:L:54:ARG:HA	1.95	0.48
1:B:681:THR:OG1	1:B:682:ASP:N	2.47	0.47
1:B:985:THR:HG23	1:B:1000:LEU:HD21	1.96	0.47
2:L:6:GLN:OE1	2:L:100:GLY:N	2.46	0.47
2:L:61:ARG:CZ	2:L:79:GLU:HG3	2.43	0.47
1:A:162:THR:O	1:A:164:SER:N	2.45	0.47
1:B:992:TRP:NE1	1:B:1070:PRO:HD3	2.28	0.47
2:H:22:CYS:N	2:H:78:LEU:O	2.46	0.46
1:B:698:ARG:NH2	1:B:1057:ASP:OD1	2.37	0.46
2:H:10:GLY:O	2:H:109:VAL:HA	2.15	0.46
1:B:884:ASP:HB2	1:B:895:PRO:HG3	1.98	0.45
1:B:682:ASP:OD1	1:B:967:ARG:N	2.49	0.45
1:A:118:LEU:HD21	1:A:346:TYR:CE1	2.51	0.45
2:L:33:LEU:HD11	2:L:88:CYS:HB2	1.99	0.45
1:A:74:THR:O	1:A:77:SER:OG	2.32	0.45
1:B:848:SER:HA	1:B:957:LEU:HD13	1.99	0.45
1:A:209:TYR:HB3	1:A:210:ASP:H	1.58	0.45
1:A:199:THR:HG21	1:A:204:GLN:N	2.32	0.44
1:B:884:ASP:N	1:B:884:ASP:OD1	2.51	0.44
1:B:718:SER:HB2	1:B:814:LYS:HB3	2.00	0.44
1:B:938:VAL:HG13	1:B:950:TRP:HB2	1.99	0.44
1:B:1052:PHE:N	1:B:1065:LEU:O	2.42	0.43
1:B:1017:LYS:HE3	1:B:1024:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:TYR:CE2	2:H:69:ILE:HG22	2.53	0.43
1:A:84:LYS:O	1:A:108:SER:HA	2.18	0.43
1:A:82:PHE:CE1	1:A:346:TYR:HB3	2.54	0.43
1:A:207:HIS:HB3	1:A:208:THR:H	1.66	0.43
1:A:73:HIS:HD2	1:A:75:SER:H	1.66	0.43
1:B:987:SER:HB2	1:B:1001:ILE:HB	2.01	0.42
2:L:14:THR:O	2:L:17:GLU:OE2	2.37	0.42
1:A:85:TRP:NE1	1:A:106:THR:OG1	2.52	0.42
1:B:659:GLU:OE1	1:B:660:THR:N	2.52	0.42
1:A:55:PRO:HB2	1:A:57:ILE:HD12	2.01	0.42
1:B:805:LYS:HE3	1:B:805:LYS:HB2	1.83	0.42
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.76	0.42
1:A:268:ILE:HA	1:A:269:PRO:HA	1.84	0.42
1:A:216:VAL:HG12	1:A:259:ILE:HG12	2.02	0.42
1:B:1006:LEU:HD21	1:B:1034:ARG:HA	2.01	0.41
2:L:6:GLN:HE21	2:L:88:CYS:H	1.67	0.41
1:B:690:PRO:HG3	1:B:958:ARG:NH1	2.34	0.41
1:B:777:PRO:HA	1:B:909:THR:HG22	2.02	0.41
2:H:52:TRP:HB2	2:H:97:ILE:HD13	2.02	0.41
2:L:94:PRO:C	2:L:96:THR:HG23	2.45	0.41
1:B:733:MET:HE3	1:B:797:LEU:HB3	2.03	0.41
2:L:37:LEU:HB2	2:L:47:LEU:HD11	2.03	0.41
1:A:48:SER:HA	1:A:150:VAL:O	2.21	0.40
2:L:7:SER:OG	2:L:22:SER:HB2	2.21	0.40
1:B:725:GLU:HB3	1:B:807:VAL:HB	2.01	0.40
1:B:955:SER:O	1:B:955:SER:OG	2.38	0.40
1:A:83:THR:HG21	1:A:312:ALA:HA	2.02	0.40
2:H:6:GLU:OE1	2:H:92:CYS:N	2.52	0.40
2:H:39:GLN:HG3	2:H:44:GLY:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	348/889 (39%)	329 (94%)	19 (6%)	0	100	100
1	B	419/889 (47%)	398 (95%)	20 (5%)	1 (0%)	43	66
2	H	118/298 (40%)	112 (95%)	6 (5%)	0	100	100
2	L	105/298 (35%)	97 (92%)	7 (7%)	1 (1%)	12	28
All	All	990/2374 (42%)	936 (94%)	52 (5%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	8	PRO
1	B	1057	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	312/750 (42%)	299 (96%)	13 (4%)	26	52
1	B	362/750 (48%)	346 (96%)	16 (4%)	25	50
2	H	101/234 (43%)	93 (92%)	8 (8%)	11	26
2	L	92/234 (39%)	85 (92%)	7 (8%)	12	27
All	All	867/1968 (44%)	823 (95%)	44 (5%)	21	45

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	54	VAL
1	A	56	LEU
1	A	57	ILE
1	A	158	THR
1	A	208	THR
1	A	218	CYS
1	A	257	CYS
1	A	295	GLU

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Mol	Chain	Res	Type
1	A	296	LYS
1	A	299	ILE
1	A	338	LEU
1	A	366	LEU
1	B	681	THR
1	B	711	ILE
1	B	722	ILE
1	B	749	CYS
1	B	821	THR
1	B	842	CYS
1	B	873	CYS
1	B	890	VAL
1	B	910	THR
1	B	913	CYS
1	B	1000	LEU
1	B	1002	CYS
1	B	1017	LYS
1	B	1024	CYS
1	B	1029	THR
1	B	1059	LYS
2	H	18	LEU
2	H	45	LEU
2	H	58	ASP
2	H	63	VAL
2	H	85	GLU
2	H	89	VAL
2	H	102	VAL
2	H	109	VAL
2	L	2	ILE
2	L	14	THR
2	L	26	SER
2	L	49	SER
2	L	60	ASP
2	L	75	ILE
2	L	79	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	198	HIS
2	H	1	GLN

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Mol	Chain	Res	Type
2	H	76	ASN
2	L	42	GLN

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 ⓘ

10 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	0.27	0	17,19,21	0.47	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	BMA	C	3	3	11,11,12	0.58	0	15,15,17	0.94	0
3	MAN	C	4	3	11,11,12	0.69	0	15,15,17	1.07	1 (6%)
3	MAN	C	5	3	11,11,12	0.70	0	15,15,17	1.09	2 (13%)
3	MAN	C	6	3	11,11,12	0.66	0	15,15,17	1.17	2 (13%)
4	NAG	D	1	1,4	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	D	2	4	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	E	1	1,4	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.53	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	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	1/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	MAN	C1-O5-C5	3.53	116.92	112.19
3	C	5	MAN	C1-O5-C5	3.20	116.47	112.19
3	C	4	MAN	C1-O5-C5	2.69	115.79	112.19
3	C	5	MAN	O2-C2-C3	-2.28	105.44	110.15
3	C	6	MAN	O2-C2-C3	-2.05	105.90	110.15

There are no chirality outliers.

All (11) torsion outliers are listed below:

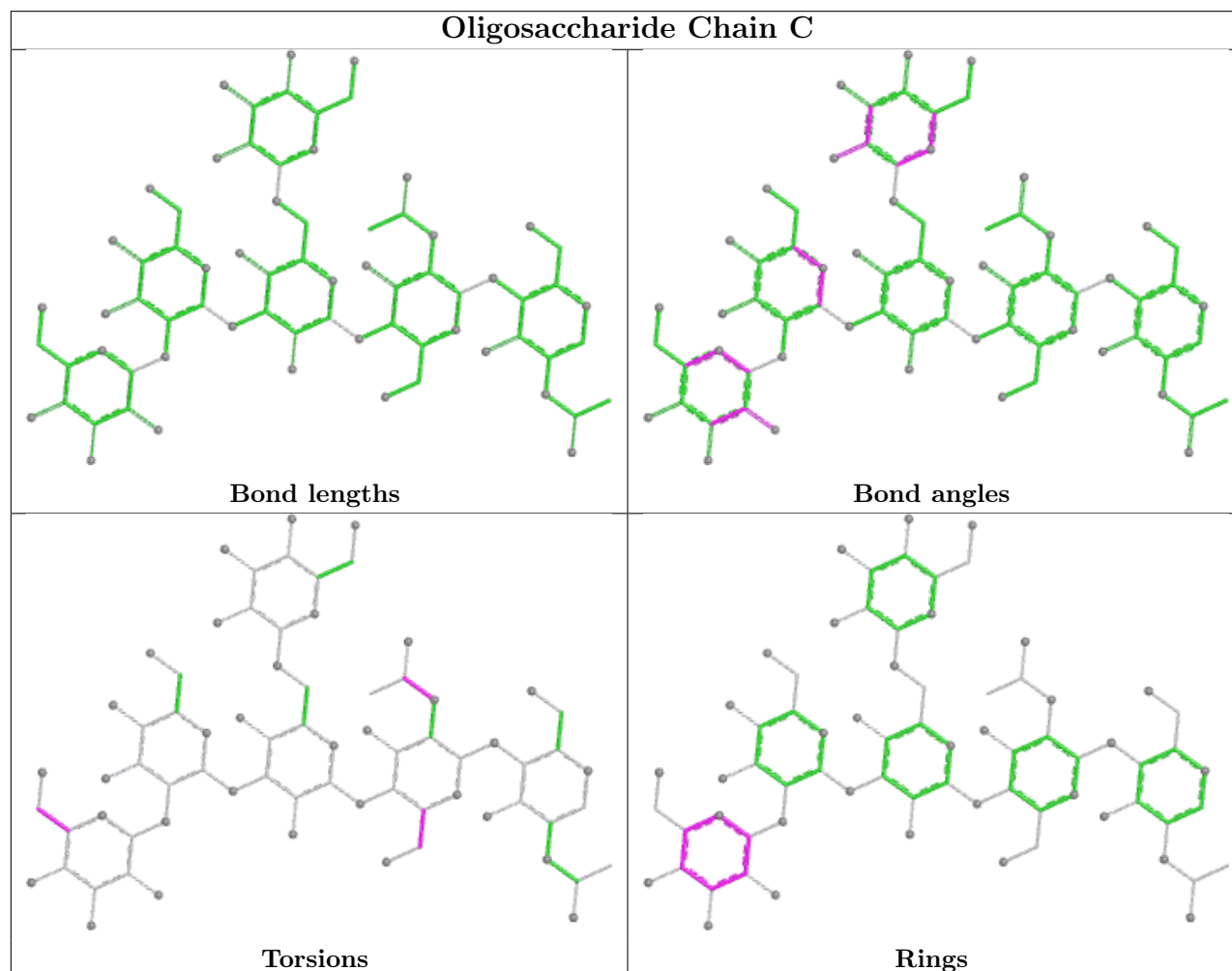
Mol	Chain	Res	Type	Atoms
3	C	5	MAN	O5-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7

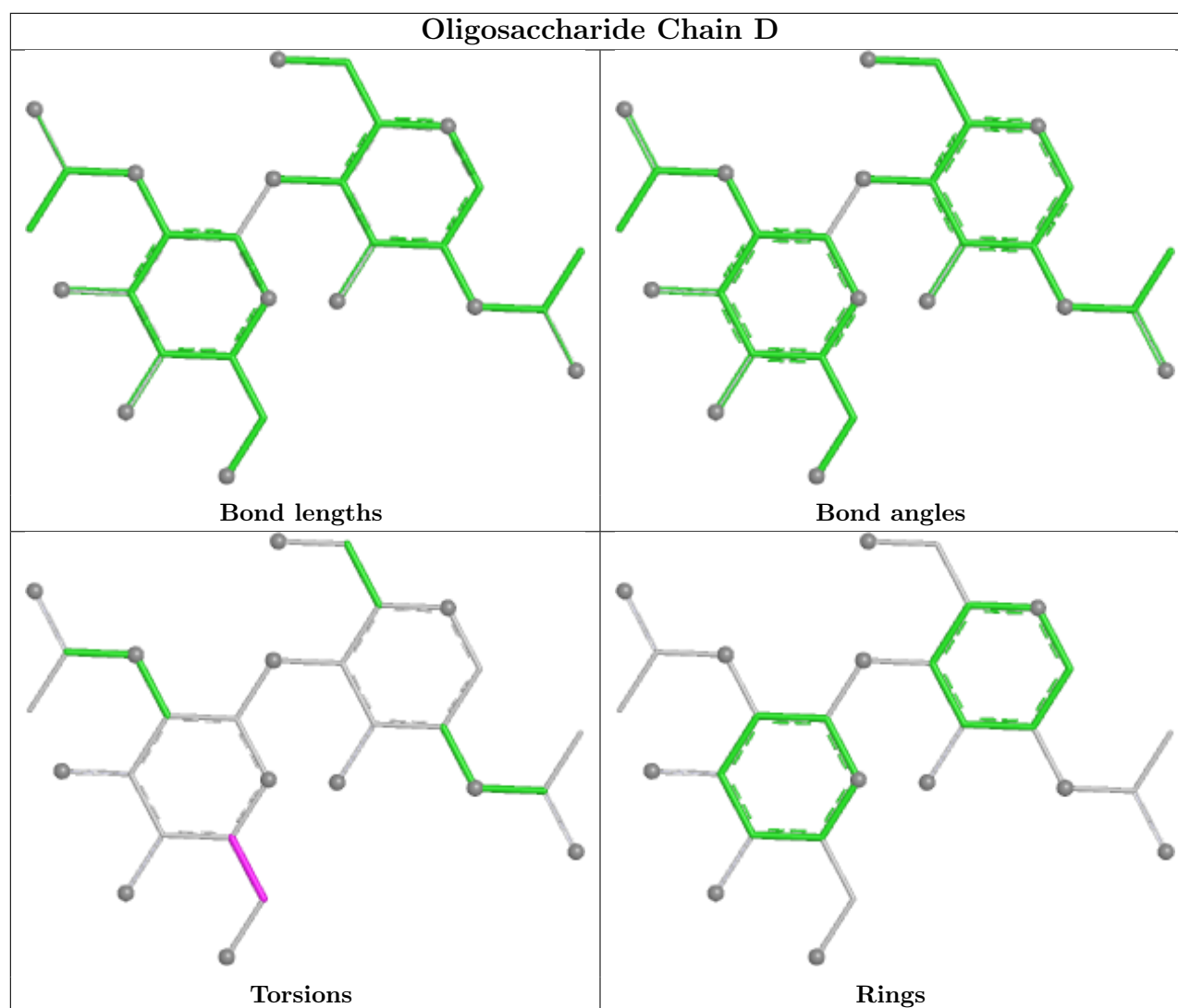
All (1) ring outliers are listed below:

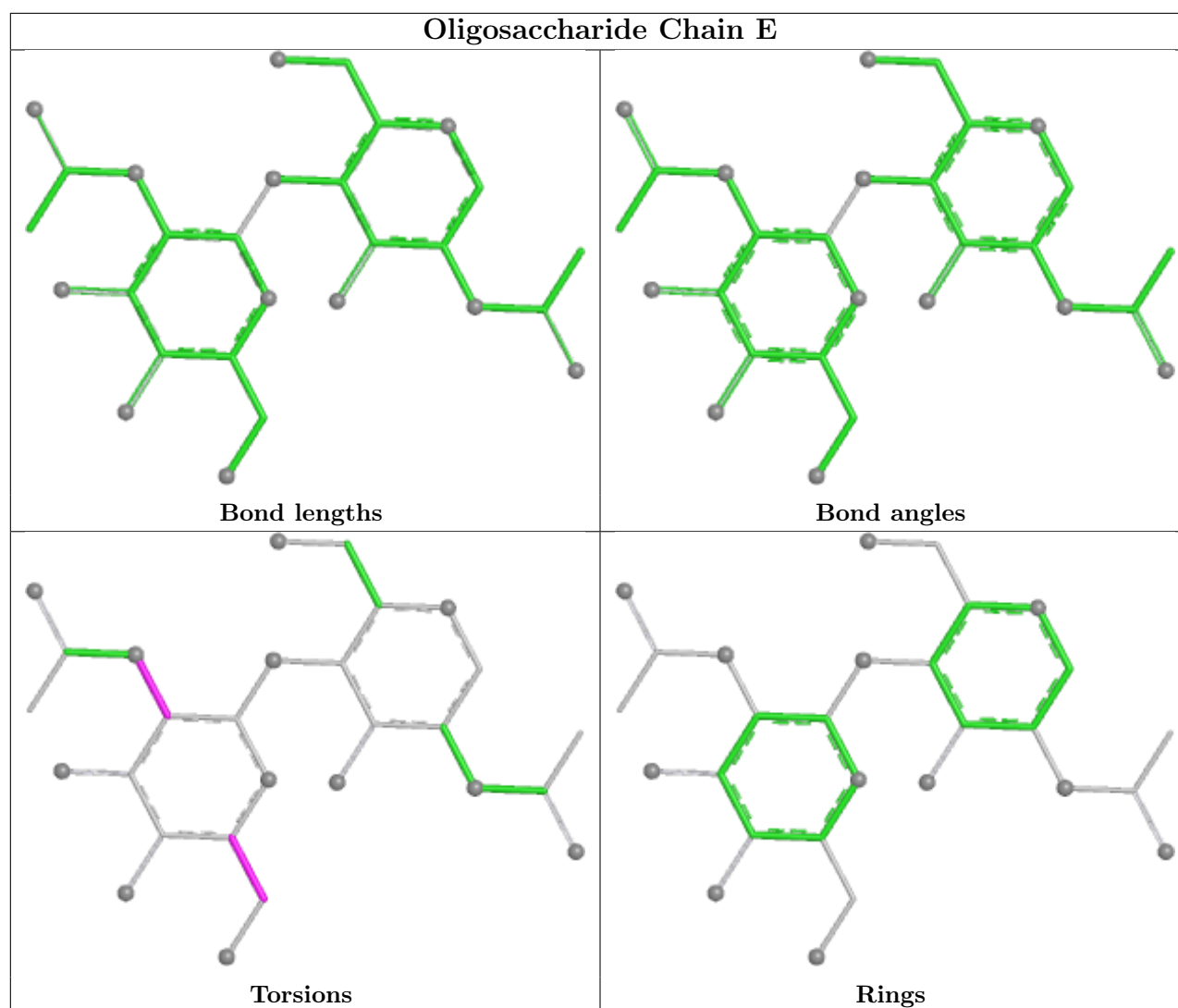
Mol	Chain	Res	Type	Atoms
3	C	5	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	A	1001	-	5,5,5	0.93	0	5,5,5	1.10	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
5	GOL	A	1001	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	94:PRO	C	95:PHE	N	3.01

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/889 (39%)	0.12	8 (2%) 61 55	52, 72, 111, 205	0
1	B	423/889 (47%)	0.17	8 (1%) 66 61	50, 81, 129, 189	0
2	H	122/298 (40%)	0.41	7 (5%) 29 24	58, 94, 126, 157	0
2	L	109/298 (36%)	0.47	4 (3%) 45 39	77, 108, 134, 174	0
All	All	1006/2374 (42%)	0.22	27 (2%) 56 50	50, 81, 128, 205	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	1	ASP	4.5
1	A	199	THR	4.3
1	A	294	ILE	3.6
2	H	12	VAL	3.0
1	A	204	GLN	2.7
1	A	209	TYR	2.5
1	B	1046	GLY	2.5
1	A	205	PRO	2.5
1	B	1048	SER	2.5
2	L	94	PRO	2.5
2	H	112	SER	2.4
1	B	1069	ALA	2.4
2	H	54	VAL	2.4
1	A	208	THR	2.3
1	A	298	ALA	2.3
2	L	93	HIS	2.3
2	H	111	VAL	2.3
2	H	11	VAL	2.2
2	H	110	THR	2.2
2	L	14	THR	2.1
2	H	70	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1085	LYS	2.1
1	B	957	LEU	2.1
1	B	761	CYS	2.1
1	B	894	CYS	2.1
1	B	1070	PRO	2.0
1	A	66	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

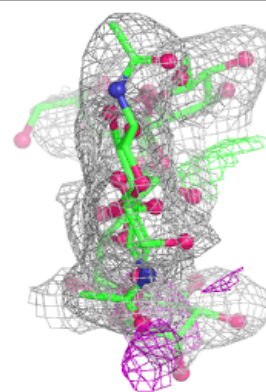
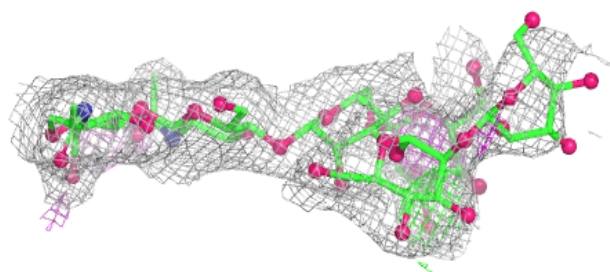
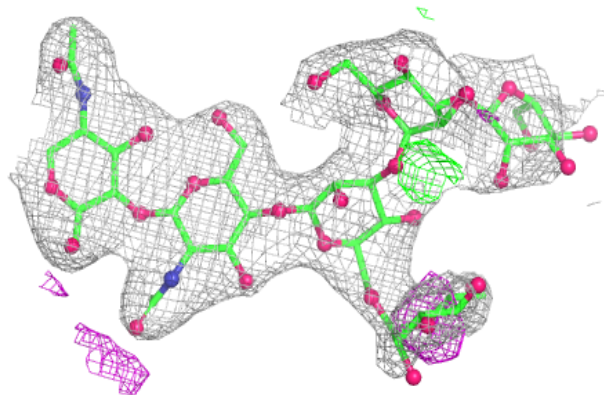
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	-	-	48,53,67,73	0
3	NAG	C	2	14/15	-	-	55,66,84,84	0
3	BMA	C	3	11/12	-	-	76,96,115,115	0
3	MAN	C	4	11/12	-	-	74,104,118,121	0
3	MAN	C	5	11/12	-	-	121,126,132,134	0
3	MAN	C	6	11/12	-	-	102,121,126,129	0
4	NAG	D	1	14/15	-	-	71,81,93,93	0
4	NAG	D	2	14/15	-	-	84,100,115,115	0
4	NAG	E	2	14/15	0.88	0.10	104,121,128,128	0
4	NAG	E	1	14/15	0.95	0.08	81,107,113,119	0

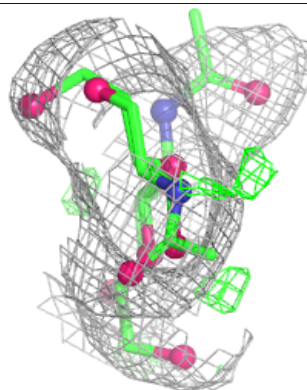
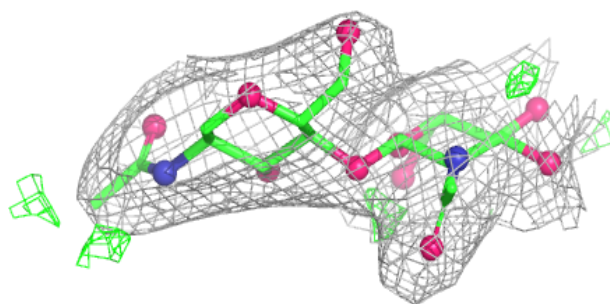
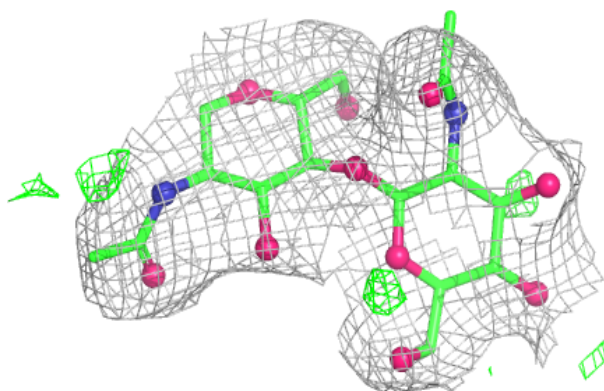
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

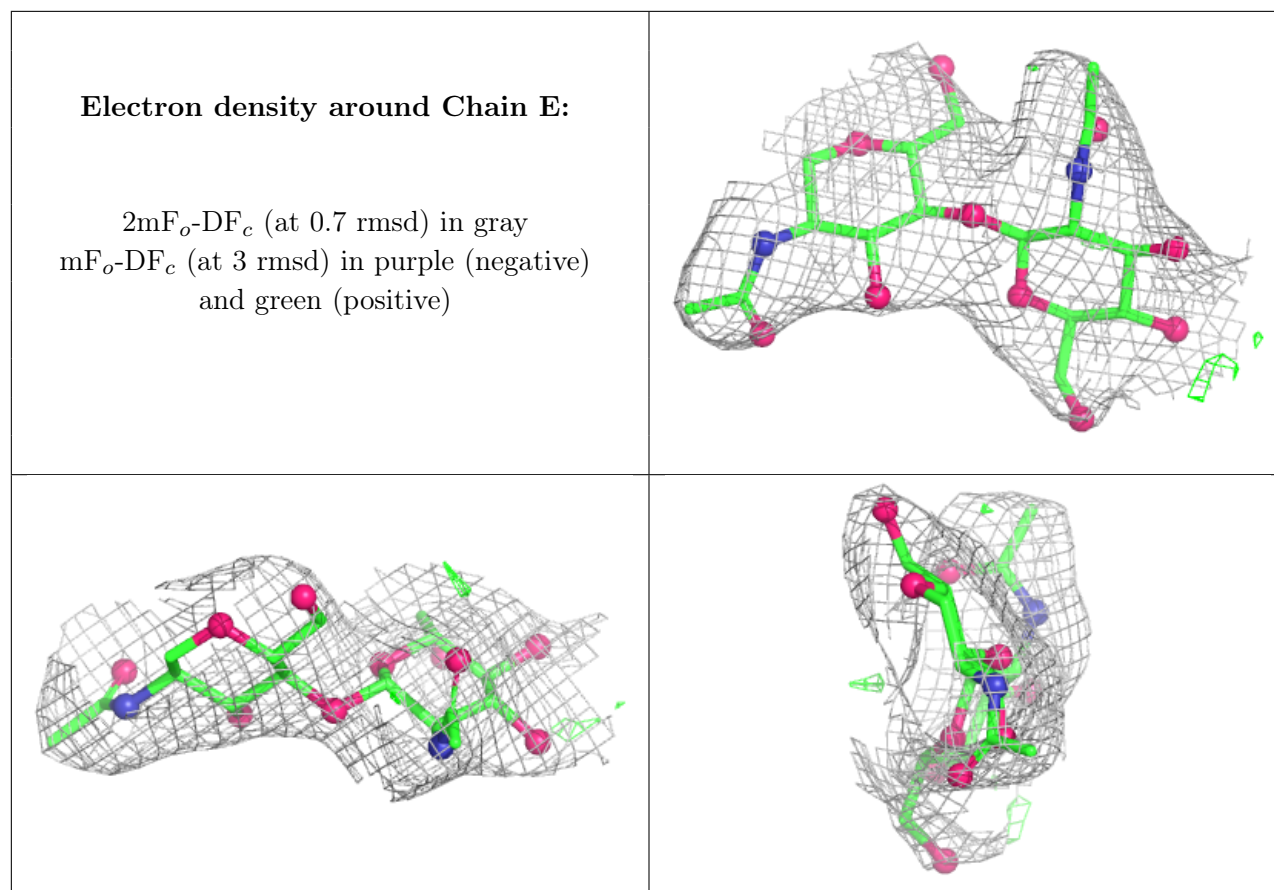
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	1001	6/6	0.91	0.15	59,68,79,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.