



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 05:28 PM UTC

PDB ID : 7FBJ / pdb_00007fbj
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing nanobody 17F6
Authors : Zhu, J.; Xu, T.; Feng, B.; Liu, J.
Deposited on : 2021-07-11
Resolution : 2.85 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

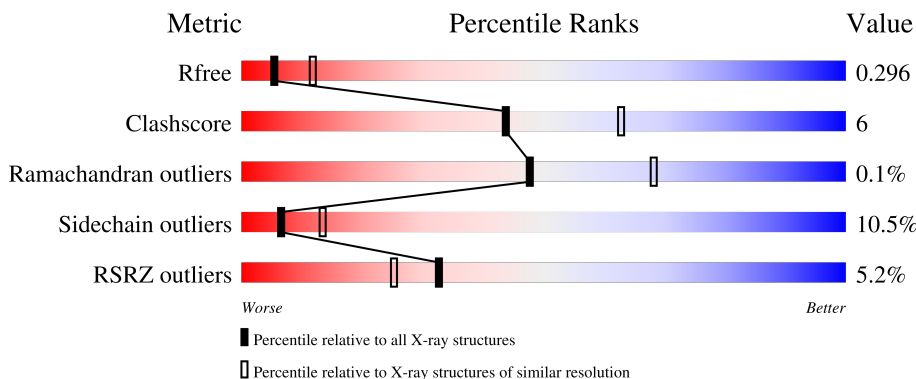
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	230	 2% 70% 13% 13%
1	C	230	 5% 73% 11% 14%
1	E	230	 3% 71% 10% 15%
1	G	230	 8% 72% 11% 14%
1	I	230	 7% 73% 11% 14%

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Mol	Chain	Length	Quality of chain
1	K	230	 4% 73% 10% 14%
1	M	230	 % 72% 13% 14%
1	O	230	 3% 73% 10% 14%
2	B	127	 3% 61% 17% 9% 13%
2	D	127	 16% 62% 19% 6% 12%
2	F	127	 12% 63% 20% 6% 11%
2	H	127	 3% 61% 23% 5% 10%
2	J	127	 2% 66% 18% 10%
2	L	127	 2% 61% 20% 5% 12%
2	N	127	 2% 62% 17% 8% 11%
2	P	127	 2% 61% 20% 6% 13%
3	Q	2	 50% 50%
3	R	2	 50% 50%
3	T	2	 100%
3	U	2	 50% 50%
4	S	3	 33% 67%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 19487 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	Total 1566	C 1004	N 261	O 293	S 8	0	0	0
1	C	197	Total 1553	C 995	N 259	O 291	S 8	0	0	0
1	E	195	Total 1543	C 989	N 257	O 289	S 8	0	0	0
1	G	198	Total 1558	C 998	N 260	O 292	S 8	0	0	0
1	I	198	Total 1558	C 998	N 260	O 292	S 8	0	0	0
1	K	198	Total 1558	C 998	N 260	O 292	S 8	0	0	0
1	M	198	Total 1558	C 998	N 260	O 292	S 8	0	0	0
1	O	197	Total 1553	C 995	N 259	O 291	S 8	0	0	0

There are 272 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	ASP	-	expression tag	UNP P0DTC2
A	327	ALA	-	expression tag	UNP P0DTC2
A	328	ALA	-	expression tag	UNP P0DTC2
A	329	GLN	-	expression tag	UNP P0DTC2
A	330	PRO	-	expression tag	UNP P0DTC2
A	331	ALA	-	expression tag	UNP P0DTC2
A	528	ALA	-	expression tag	UNP P0DTC2
A	529	ALA	-	expression tag	UNP P0DTC2
A	530	ALA	-	expression tag	UNP P0DTC2
A	531	ARG	-	expression tag	UNP P0DTC2
A	532	GLY	-	expression tag	UNP P0DTC2
A	533	GLY	-	expression tag	UNP P0DTC2
A	534	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	535	GLU	-	expression tag	UNP P0DTC2
A	536	GLN	-	expression tag	UNP P0DTC2
A	537	LYS	-	expression tag	UNP P0DTC2
A	538	LEU	-	expression tag	UNP P0DTC2
A	539	ILE	-	expression tag	UNP P0DTC2
A	540	SER	-	expression tag	UNP P0DTC2
A	541	GLU	-	expression tag	UNP P0DTC2
A	542	GLU	-	expression tag	UNP P0DTC2
A	543	ASP	-	expression tag	UNP P0DTC2
A	544	LEU	-	expression tag	UNP P0DTC2
A	545	ASN	-	expression tag	UNP P0DTC2
A	546	SER	-	expression tag	UNP P0DTC2
A	547	ALA	-	expression tag	UNP P0DTC2
A	548	VAL	-	expression tag	UNP P0DTC2
A	549	ASP	-	expression tag	UNP P0DTC2
A	550	HIS	-	expression tag	UNP P0DTC2
A	551	HIS	-	expression tag	UNP P0DTC2
A	552	HIS	-	expression tag	UNP P0DTC2
A	553	HIS	-	expression tag	UNP P0DTC2
A	554	HIS	-	expression tag	UNP P0DTC2
A	555	HIS	-	expression tag	UNP P0DTC2
C	326	ASP	-	expression tag	UNP P0DTC2
C	327	ALA	-	expression tag	UNP P0DTC2
C	328	ALA	-	expression tag	UNP P0DTC2
C	329	GLN	-	expression tag	UNP P0DTC2
C	330	PRO	-	expression tag	UNP P0DTC2
C	331	ALA	-	expression tag	UNP P0DTC2
C	528	ALA	-	expression tag	UNP P0DTC2
C	529	ALA	-	expression tag	UNP P0DTC2
C	530	ALA	-	expression tag	UNP P0DTC2
C	531	ARG	-	expression tag	UNP P0DTC2
C	532	GLY	-	expression tag	UNP P0DTC2
C	533	GLY	-	expression tag	UNP P0DTC2
C	534	PRO	-	expression tag	UNP P0DTC2
C	535	GLU	-	expression tag	UNP P0DTC2
C	536	GLN	-	expression tag	UNP P0DTC2
C	537	LYS	-	expression tag	UNP P0DTC2
C	538	LEU	-	expression tag	UNP P0DTC2
C	539	ILE	-	expression tag	UNP P0DTC2
C	540	SER	-	expression tag	UNP P0DTC2
C	541	GLU	-	expression tag	UNP P0DTC2
C	542	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	543	ASP	-	expression tag	UNP P0DTC2
C	544	LEU	-	expression tag	UNP P0DTC2
C	545	ASN	-	expression tag	UNP P0DTC2
C	546	SER	-	expression tag	UNP P0DTC2
C	547	ALA	-	expression tag	UNP P0DTC2
C	548	VAL	-	expression tag	UNP P0DTC2
C	549	ASP	-	expression tag	UNP P0DTC2
C	550	HIS	-	expression tag	UNP P0DTC2
C	551	HIS	-	expression tag	UNP P0DTC2
C	552	HIS	-	expression tag	UNP P0DTC2
C	553	HIS	-	expression tag	UNP P0DTC2
C	554	HIS	-	expression tag	UNP P0DTC2
C	555	HIS	-	expression tag	UNP P0DTC2
E	326	ASP	-	expression tag	UNP P0DTC2
E	327	ALA	-	expression tag	UNP P0DTC2
E	328	ALA	-	expression tag	UNP P0DTC2
E	329	GLN	-	expression tag	UNP P0DTC2
E	330	PRO	-	expression tag	UNP P0DTC2
E	331	ALA	-	expression tag	UNP P0DTC2
E	528	ALA	-	expression tag	UNP P0DTC2
E	529	ALA	-	expression tag	UNP P0DTC2
E	530	ALA	-	expression tag	UNP P0DTC2
E	531	ARG	-	expression tag	UNP P0DTC2
E	532	GLY	-	expression tag	UNP P0DTC2
E	533	GLY	-	expression tag	UNP P0DTC2
E	534	PRO	-	expression tag	UNP P0DTC2
E	535	GLU	-	expression tag	UNP P0DTC2
E	536	GLN	-	expression tag	UNP P0DTC2
E	537	LYS	-	expression tag	UNP P0DTC2
E	538	LEU	-	expression tag	UNP P0DTC2
E	539	ILE	-	expression tag	UNP P0DTC2
E	540	SER	-	expression tag	UNP P0DTC2
E	541	GLU	-	expression tag	UNP P0DTC2
E	542	GLU	-	expression tag	UNP P0DTC2
E	543	ASP	-	expression tag	UNP P0DTC2
E	544	LEU	-	expression tag	UNP P0DTC2
E	545	ASN	-	expression tag	UNP P0DTC2
E	546	SER	-	expression tag	UNP P0DTC2
E	547	ALA	-	expression tag	UNP P0DTC2
E	548	VAL	-	expression tag	UNP P0DTC2
E	549	ASP	-	expression tag	UNP P0DTC2
E	550	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	551	HIS	-	expression tag	UNP P0DTC2
E	552	HIS	-	expression tag	UNP P0DTC2
E	553	HIS	-	expression tag	UNP P0DTC2
E	554	HIS	-	expression tag	UNP P0DTC2
E	555	HIS	-	expression tag	UNP P0DTC2
G	326	ASP	-	expression tag	UNP P0DTC2
G	327	ALA	-	expression tag	UNP P0DTC2
G	328	ALA	-	expression tag	UNP P0DTC2
G	329	GLN	-	expression tag	UNP P0DTC2
G	330	PRO	-	expression tag	UNP P0DTC2
G	331	ALA	-	expression tag	UNP P0DTC2
G	528	ALA	-	expression tag	UNP P0DTC2
G	529	ALA	-	expression tag	UNP P0DTC2
G	530	ALA	-	expression tag	UNP P0DTC2
G	531	ARG	-	expression tag	UNP P0DTC2
G	532	GLY	-	expression tag	UNP P0DTC2
G	533	GLY	-	expression tag	UNP P0DTC2
G	534	PRO	-	expression tag	UNP P0DTC2
G	535	GLU	-	expression tag	UNP P0DTC2
G	536	GLN	-	expression tag	UNP P0DTC2
G	537	LYS	-	expression tag	UNP P0DTC2
G	538	LEU	-	expression tag	UNP P0DTC2
G	539	ILE	-	expression tag	UNP P0DTC2
G	540	SER	-	expression tag	UNP P0DTC2
G	541	GLU	-	expression tag	UNP P0DTC2
G	542	GLU	-	expression tag	UNP P0DTC2
G	543	ASP	-	expression tag	UNP P0DTC2
G	544	LEU	-	expression tag	UNP P0DTC2
G	545	ASN	-	expression tag	UNP P0DTC2
G	546	SER	-	expression tag	UNP P0DTC2
G	547	ALA	-	expression tag	UNP P0DTC2
G	548	VAL	-	expression tag	UNP P0DTC2
G	549	ASP	-	expression tag	UNP P0DTC2
G	550	HIS	-	expression tag	UNP P0DTC2
G	551	HIS	-	expression tag	UNP P0DTC2
G	552	HIS	-	expression tag	UNP P0DTC2
G	553	HIS	-	expression tag	UNP P0DTC2
G	554	HIS	-	expression tag	UNP P0DTC2
G	555	HIS	-	expression tag	UNP P0DTC2
I	326	ASP	-	expression tag	UNP P0DTC2
I	327	ALA	-	expression tag	UNP P0DTC2
I	328	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	329	GLN	-	expression tag	UNP P0DTC2
I	330	PRO	-	expression tag	UNP P0DTC2
I	331	ALA	-	expression tag	UNP P0DTC2
I	528	ALA	-	expression tag	UNP P0DTC2
I	529	ALA	-	expression tag	UNP P0DTC2
I	530	ALA	-	expression tag	UNP P0DTC2
I	531	ARG	-	expression tag	UNP P0DTC2
I	532	GLY	-	expression tag	UNP P0DTC2
I	533	GLY	-	expression tag	UNP P0DTC2
I	534	PRO	-	expression tag	UNP P0DTC2
I	535	GLU	-	expression tag	UNP P0DTC2
I	536	GLN	-	expression tag	UNP P0DTC2
I	537	LYS	-	expression tag	UNP P0DTC2
I	538	LEU	-	expression tag	UNP P0DTC2
I	539	ILE	-	expression tag	UNP P0DTC2
I	540	SER	-	expression tag	UNP P0DTC2
I	541	GLU	-	expression tag	UNP P0DTC2
I	542	GLU	-	expression tag	UNP P0DTC2
I	543	ASP	-	expression tag	UNP P0DTC2
I	544	LEU	-	expression tag	UNP P0DTC2
I	545	ASN	-	expression tag	UNP P0DTC2
I	546	SER	-	expression tag	UNP P0DTC2
I	547	ALA	-	expression tag	UNP P0DTC2
I	548	VAL	-	expression tag	UNP P0DTC2
I	549	ASP	-	expression tag	UNP P0DTC2
I	550	HIS	-	expression tag	UNP P0DTC2
I	551	HIS	-	expression tag	UNP P0DTC2
I	552	HIS	-	expression tag	UNP P0DTC2
I	553	HIS	-	expression tag	UNP P0DTC2
I	554	HIS	-	expression tag	UNP P0DTC2
I	555	HIS	-	expression tag	UNP P0DTC2
K	326	ASP	-	expression tag	UNP P0DTC2
K	327	ALA	-	expression tag	UNP P0DTC2
K	328	ALA	-	expression tag	UNP P0DTC2
K	329	GLN	-	expression tag	UNP P0DTC2
K	330	PRO	-	expression tag	UNP P0DTC2
K	331	ALA	-	expression tag	UNP P0DTC2
K	528	ALA	-	expression tag	UNP P0DTC2
K	529	ALA	-	expression tag	UNP P0DTC2
K	530	ALA	-	expression tag	UNP P0DTC2
K	531	ARG	-	expression tag	UNP P0DTC2
K	532	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	533	GLY	-	expression tag	UNP P0DTC2
K	534	PRO	-	expression tag	UNP P0DTC2
K	535	GLU	-	expression tag	UNP P0DTC2
K	536	GLN	-	expression tag	UNP P0DTC2
K	537	LYS	-	expression tag	UNP P0DTC2
K	538	LEU	-	expression tag	UNP P0DTC2
K	539	ILE	-	expression tag	UNP P0DTC2
K	540	SER	-	expression tag	UNP P0DTC2
K	541	GLU	-	expression tag	UNP P0DTC2
K	542	GLU	-	expression tag	UNP P0DTC2
K	543	ASP	-	expression tag	UNP P0DTC2
K	544	LEU	-	expression tag	UNP P0DTC2
K	545	ASN	-	expression tag	UNP P0DTC2
K	546	SER	-	expression tag	UNP P0DTC2
K	547	ALA	-	expression tag	UNP P0DTC2
K	548	VAL	-	expression tag	UNP P0DTC2
K	549	ASP	-	expression tag	UNP P0DTC2
K	550	HIS	-	expression tag	UNP P0DTC2
K	551	HIS	-	expression tag	UNP P0DTC2
K	552	HIS	-	expression tag	UNP P0DTC2
K	553	HIS	-	expression tag	UNP P0DTC2
K	554	HIS	-	expression tag	UNP P0DTC2
K	555	HIS	-	expression tag	UNP P0DTC2
M	326	ASP	-	expression tag	UNP P0DTC2
M	327	ALA	-	expression tag	UNP P0DTC2
M	328	ALA	-	expression tag	UNP P0DTC2
M	329	GLN	-	expression tag	UNP P0DTC2
M	330	PRO	-	expression tag	UNP P0DTC2
M	331	ALA	-	expression tag	UNP P0DTC2
M	528	ALA	-	expression tag	UNP P0DTC2
M	529	ALA	-	expression tag	UNP P0DTC2
M	530	ALA	-	expression tag	UNP P0DTC2
M	531	ARG	-	expression tag	UNP P0DTC2
M	532	GLY	-	expression tag	UNP P0DTC2
M	533	GLY	-	expression tag	UNP P0DTC2
M	534	PRO	-	expression tag	UNP P0DTC2
M	535	GLU	-	expression tag	UNP P0DTC2
M	536	GLN	-	expression tag	UNP P0DTC2
M	537	LYS	-	expression tag	UNP P0DTC2
M	538	LEU	-	expression tag	UNP P0DTC2
M	539	ILE	-	expression tag	UNP P0DTC2
M	540	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	541	GLU	-	expression tag	UNP P0DTC2
M	542	GLU	-	expression tag	UNP P0DTC2
M	543	ASP	-	expression tag	UNP P0DTC2
M	544	LEU	-	expression tag	UNP P0DTC2
M	545	ASN	-	expression tag	UNP P0DTC2
M	546	SER	-	expression tag	UNP P0DTC2
M	547	ALA	-	expression tag	UNP P0DTC2
M	548	VAL	-	expression tag	UNP P0DTC2
M	549	ASP	-	expression tag	UNP P0DTC2
M	550	HIS	-	expression tag	UNP P0DTC2
M	551	HIS	-	expression tag	UNP P0DTC2
M	552	HIS	-	expression tag	UNP P0DTC2
M	553	HIS	-	expression tag	UNP P0DTC2
M	554	HIS	-	expression tag	UNP P0DTC2
M	555	HIS	-	expression tag	UNP P0DTC2
O	326	ASP	-	expression tag	UNP P0DTC2
O	327	ALA	-	expression tag	UNP P0DTC2
O	328	ALA	-	expression tag	UNP P0DTC2
O	329	GLN	-	expression tag	UNP P0DTC2
O	330	PRO	-	expression tag	UNP P0DTC2
O	331	ALA	-	expression tag	UNP P0DTC2
O	528	ALA	-	expression tag	UNP P0DTC2
O	529	ALA	-	expression tag	UNP P0DTC2
O	530	ALA	-	expression tag	UNP P0DTC2
O	531	ARG	-	expression tag	UNP P0DTC2
O	532	GLY	-	expression tag	UNP P0DTC2
O	533	GLY	-	expression tag	UNP P0DTC2
O	534	PRO	-	expression tag	UNP P0DTC2
O	535	GLU	-	expression tag	UNP P0DTC2
O	536	GLN	-	expression tag	UNP P0DTC2
O	537	LYS	-	expression tag	UNP P0DTC2
O	538	LEU	-	expression tag	UNP P0DTC2
O	539	ILE	-	expression tag	UNP P0DTC2
O	540	SER	-	expression tag	UNP P0DTC2
O	541	GLU	-	expression tag	UNP P0DTC2
O	542	GLU	-	expression tag	UNP P0DTC2
O	543	ASP	-	expression tag	UNP P0DTC2
O	544	LEU	-	expression tag	UNP P0DTC2
O	545	ASN	-	expression tag	UNP P0DTC2
O	546	SER	-	expression tag	UNP P0DTC2
O	547	ALA	-	expression tag	UNP P0DTC2
O	548	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
O	549	ASP	-	expression tag	UNP P0DTC2
O	550	HIS	-	expression tag	UNP P0DTC2
O	551	HIS	-	expression tag	UNP P0DTC2
O	552	HIS	-	expression tag	UNP P0DTC2
O	553	HIS	-	expression tag	UNP P0DTC2
O	554	HIS	-	expression tag	UNP P0DTC2
O	555	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called New antigen receptor variable domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	111	Total 845	C 520	N 145	O 174	S 6	0	0	0
2	D	112	Total 851	C 523	N 146	O 176	S 6	0	0	0
2	F	113	Total 855	C 525	N 147	O 177	S 6	0	0	0
2	H	114	Total 864	C 531	N 148	O 178	S 7	0	0	0
2	J	114	Total 864	C 531	N 148	O 178	S 7	0	0	0
2	L	112	Total 851	C 523	N 146	O 176	S 6	0	0	0
2	N	113	Total 859	C 528	N 147	O 177	S 7	0	0	0
2	P	111	Total 846	C 520	N 145	O 175	S 6	0	0	0

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



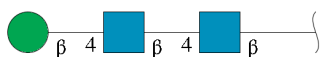
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	Q	2	Total 28	C 16	N 2	O 10	0	0	0
3	R	2	Total 28	C 16	N 2	O 10	0	0	0
3	T	2	Total 28	C 16	N 2	O 10	0	0	0

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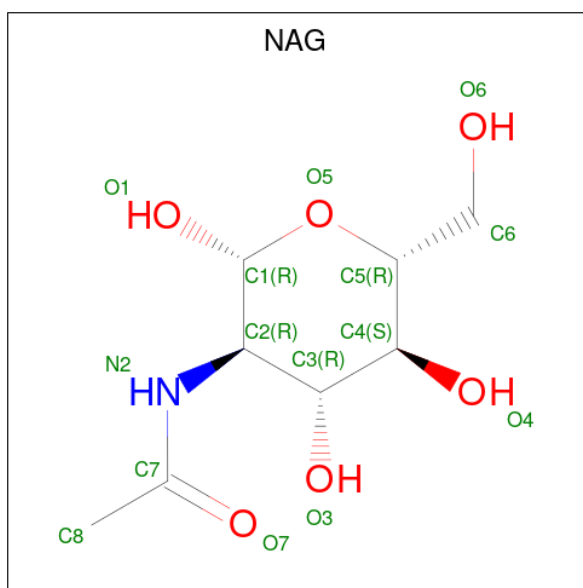
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	U	2	28	16	2	10	0	0	0

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

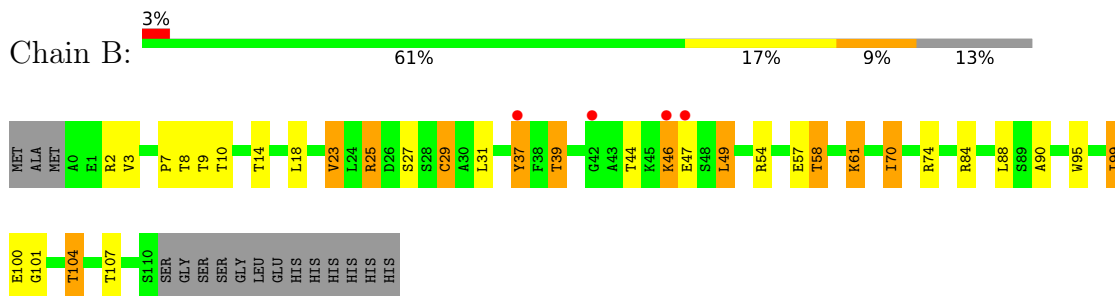


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0

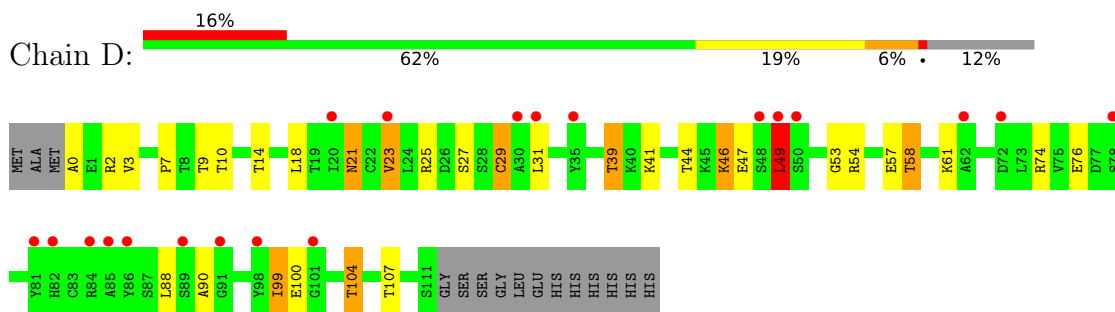
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0
6	H	1	Total O 1 1	0	0
6	J	2	Total O 2 2	0	0
6	L	1	Total O 1 1	0	0
6	M	3	Total O 3 3	0	0
6	P	1	Total O 1 1	0	0

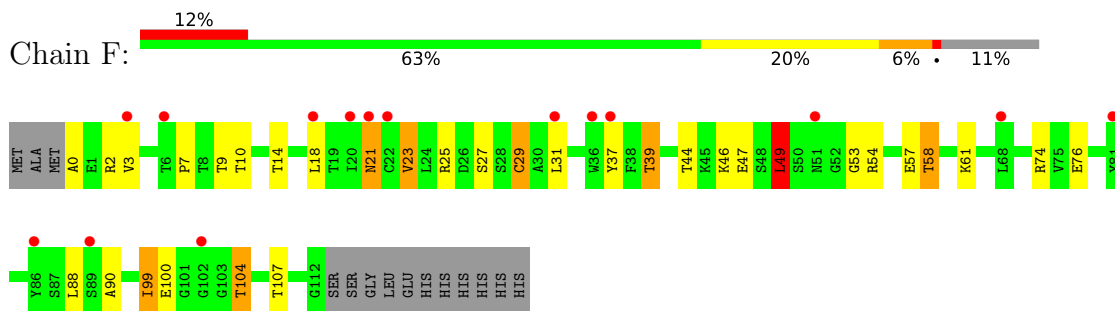
• Molecule 2: New antigen receptor variable domain



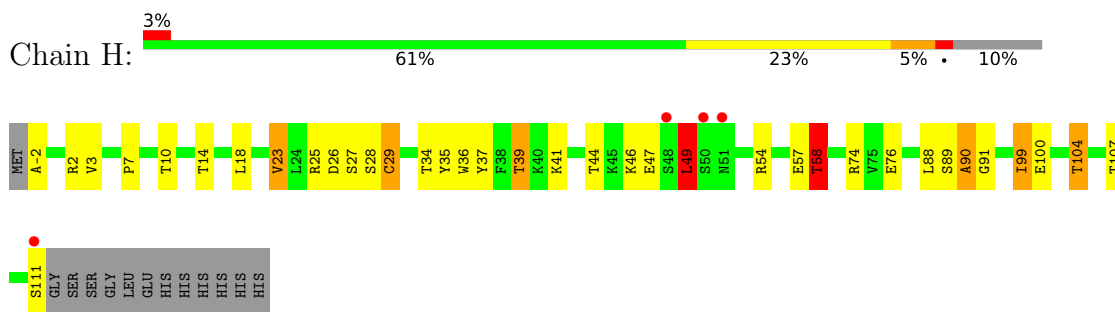
• Molecule 2: New antigen receptor variable domain



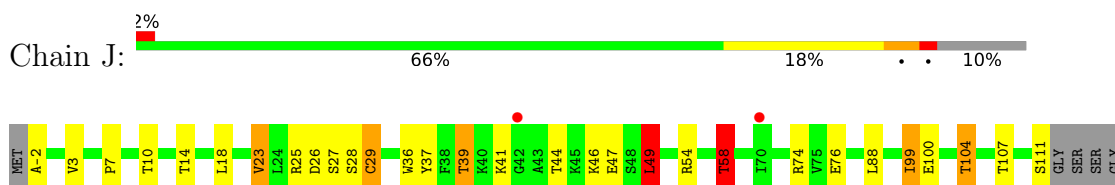
• Molecule 2: New antigen receptor variable domain

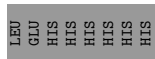


• Molecule 2: New antigen receptor variable domain

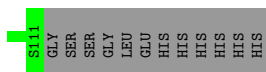


• Molecule 2: New antigen receptor variable domain

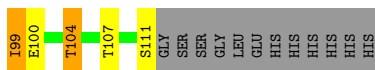
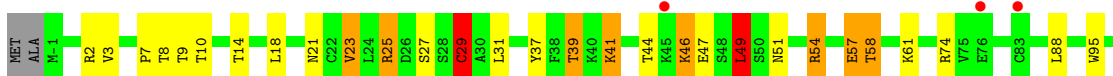




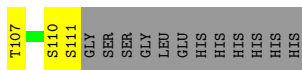
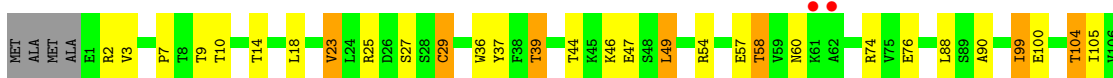
• Molecule 2: New antigen receptor variable domain



• Molecule 2: New antigen receptor variable domain



• Molecule 2: New antigen receptor variable domain



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



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




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

Chain T:  100%

MAG1
MAG2

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

Chain U:  50%

MAG1
MAG2

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

Chain S:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 73.75Å 270.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.40 – 2.85 90.40 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (90.40-2.85) 99.8 (90.40-2.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.254 , 0.300 0.253 , 0.296	Depositor DCC
R_{free} test set	3648 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtrriage
Anisotropy	0.463	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	19487	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: 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	1.15	3/1610 (0.2%)	1.35	6/2193 (0.3%)
1	C	1.17	1/1597 (0.1%)	1.31	2/2175 (0.1%)
1	E	1.13	4/1587 (0.3%)	1.32	3/2161 (0.1%)
1	G	1.10	1/1602 (0.1%)	1.32	6/2182 (0.3%)
1	I	1.10	1/1602 (0.1%)	1.32	6/2182 (0.3%)
1	K	1.10	3/1602 (0.2%)	1.32	1/2182 (0.0%)
1	M	1.19	2/1602 (0.1%)	1.30	3/2182 (0.1%)
1	O	1.11	3/1597 (0.2%)	1.33	2/2175 (0.1%)
2	B	1.20	3/858 (0.3%)	1.48	6/1158 (0.5%)
2	D	1.16	2/864 (0.2%)	1.46	5/1166 (0.4%)
2	F	1.16	2/868 (0.2%)	1.45	6/1171 (0.5%)
2	H	1.17	3/877 (0.3%)	1.48	6/1183 (0.5%)
2	J	1.12	1/877 (0.1%)	1.47	6/1183 (0.5%)
2	L	1.21	3/864 (0.3%)	1.47	8/1166 (0.7%)
2	N	1.14	1/872 (0.1%)	1.49	7/1176 (0.6%)
2	P	1.19	3/859 (0.3%)	1.48	7/1159 (0.6%)
All	All	1.15	36/19738 (0.2%)	1.38	80/26794 (0.3%)

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	90	ALA	C-O	9.82	1.34	1.24
2	P	90	ALA	C-O	9.74	1.34	1.24
1	C	341	VAL	C-O	8.04	1.31	1.24
2	D	104	THR	C-O	7.35	1.32	1.24
2	F	104	THR	C-O	7.30	1.32	1.24

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	21	ASN	CA-CB-CG	7.91	120.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	21	ASN	CA-CB-CG	7.90	120.50	112.60
1	G	466	ARG	CB-CG-CD	7.28	128.05	111.30
2	N	54	ARG	N-CA-CB	7.20	122.66	110.49
2	L	58	THR	CA-C-O	-6.67	113.30	121.11

There are no chirality outliers.

There are no planarity outliers.

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	1566	0	1485	31	0
1	C	1553	0	1469	15	1
1	E	1543	0	1459	23	0
1	G	1558	0	1474	17	0
1	I	1558	0	1474	14	0
1	K	1558	0	1474	14	0
1	M	1558	0	1474	22	0
1	O	1553	0	1469	13	0
2	B	845	0	820	19	0
2	D	851	0	825	15	0
2	F	855	0	828	12	0
2	H	864	0	839	24	0
2	J	864	0	839	17	0
2	L	851	0	825	16	0
2	N	859	0	834	17	0
2	P	846	0	820	8	1
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	1	0
4	S	39	0	34	0	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	14	0	13	0	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	H	1	0	0	3	0
6	J	2	0	0	0	0
6	L	1	0	0	1	0
6	M	3	0	0	0	0
6	P	1	0	0	0	0
All	All	19487	0	18581	232	1

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.

The worst 5 of 232 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)
2:J:25:ARG:NH2	1:M:484:GLU:OE1	1.79	1.15
1:A:484:GLU:OE1	2:H:25:ARG:NH2	1.91	1.03
2:H:91:GLY:N	6:H:201:HOH:O	2.02	0.92
1:A:372:ALA:HA	2:B:84:ARG:NH2	1.94	0.82
1:A:372:ALA:HA	2:B:84:ARG:HH2	1.47	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:GLU:OE2	2:P:25:ARG:NH2[1_565]	2.19	0.01

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 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	197/230 (86%)	189 (96%)	7 (4%)	1 (0%)	24	42
1	C	195/230 (85%)	188 (96%)	7 (4%)	0	100	100
1	E	193/230 (84%)	188 (97%)	5 (3%)	0	100	100
1	G	196/230 (85%)	189 (96%)	7 (4%)	0	100	100
1	I	196/230 (85%)	189 (96%)	7 (4%)	0	100	100
1	K	196/230 (85%)	191 (97%)	5 (3%)	0	100	100
1	M	196/230 (85%)	188 (96%)	8 (4%)	0	100	100
1	O	195/230 (85%)	191 (98%)	4 (2%)	0	100	100
2	B	109/127 (86%)	105 (96%)	4 (4%)	0	100	100
2	D	110/127 (87%)	104 (94%)	5 (4%)	1 (1%)	14	28
2	F	111/127 (87%)	105 (95%)	5 (4%)	1 (1%)	14	28
2	H	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
2	J	112/127 (88%)	106 (95%)	6 (5%)	0	100	100
2	L	110/127 (87%)	105 (96%)	5 (4%)	0	100	100
2	N	111/127 (87%)	106 (96%)	5 (4%)	0	100	100
2	P	109/127 (86%)	106 (97%)	3 (3%)	0	100	100
All	All	2448/2856 (86%)	2357 (96%)	88 (4%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	53	GLY
1	A	372	ALA
2	D	53	GLY

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 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	169/194 (87%)	159 (94%)	10 (6%)	18	37
1	C	168/194 (87%)	159 (95%)	9 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	168/194 (87%)	158 (94%)	10 (6%)	17	36
1	G	168/194 (87%)	156 (93%)	12 (7%)	13	28
1	I	168/194 (87%)	156 (93%)	12 (7%)	13	28
1	K	168/194 (87%)	157 (94%)	11 (6%)	15	32
1	M	168/194 (87%)	158 (94%)	10 (6%)	17	36
1	O	168/194 (87%)	158 (94%)	10 (6%)	17	36
2	B	93/106 (88%)	75 (81%)	18 (19%)	1	2
2	D	94/106 (89%)	76 (81%)	18 (19%)	1	2
2	F	94/106 (89%)	78 (83%)	16 (17%)	2	3
2	H	95/106 (90%)	78 (82%)	17 (18%)	2	3
2	J	95/106 (90%)	80 (84%)	15 (16%)	2	4
2	L	94/106 (89%)	76 (81%)	18 (19%)	1	2
2	N	95/106 (90%)	76 (80%)	19 (20%)	1	2
2	P	94/106 (89%)	78 (83%)	16 (17%)	2	3
All	All	2099/2400 (88%)	1878 (90%)	221 (10%)	6	13

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	468	ILE
1	K	472	ILE
2	P	105	ILE
1	O	403	ARG
1	I	498	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	493	GLN
1	K	460	ASN
1	O	493	GLN
1	I	498	GLN
2	J	82	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

11 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	Q	1	3,1	14,14,15	0.69	0	17,19,21	2.31	5 (29%)
3	NAG	Q	2	3	14,14,15	0.45	0	17,19,21	0.93	0
3	NAG	R	1	3,1	14,14,15	0.66	0	17,19,21	1.67	1 (5%)
3	NAG	R	2	3	14,14,15	0.55	0	17,19,21	0.95	0
4	NAG	S	1	4,1	14,14,15	0.60	0	17,19,21	1.42	1 (5%)
4	NAG	S	2	4	14,14,15	0.52	0	17,19,21	1.13	1 (5%)
4	BMA	S	3	4	11,11,12	0.49	0	15,15,17	0.77	0
3	NAG	T	1	3,1	14,14,15	0.59	0	17,19,21	1.29	2 (11%)
3	NAG	T	2	3	14,14,15	0.36	0	17,19,21	1.31	3 (17%)
3	NAG	U	1	3,1	14,14,15	0.71	0	17,19,21	2.31	7 (41%)
3	NAG	U	2	3	14,14,15	0.57	0	17,19,21	1.42	3 (17%)

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	Q	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	R	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1
3	NAG	T	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	1	NAG	C1-C2-N2	5.99	119.87	110.43
3	R	1	NAG	C1-O5-C5	5.73	119.87	112.19
3	U	1	NAG	O5-C1-C2	-4.97	103.60	111.29
3	U	1	NAG	C2-N2-C7	4.60	129.07	122.90
3	Q	1	NAG	C1-O5-C5	4.39	118.07	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

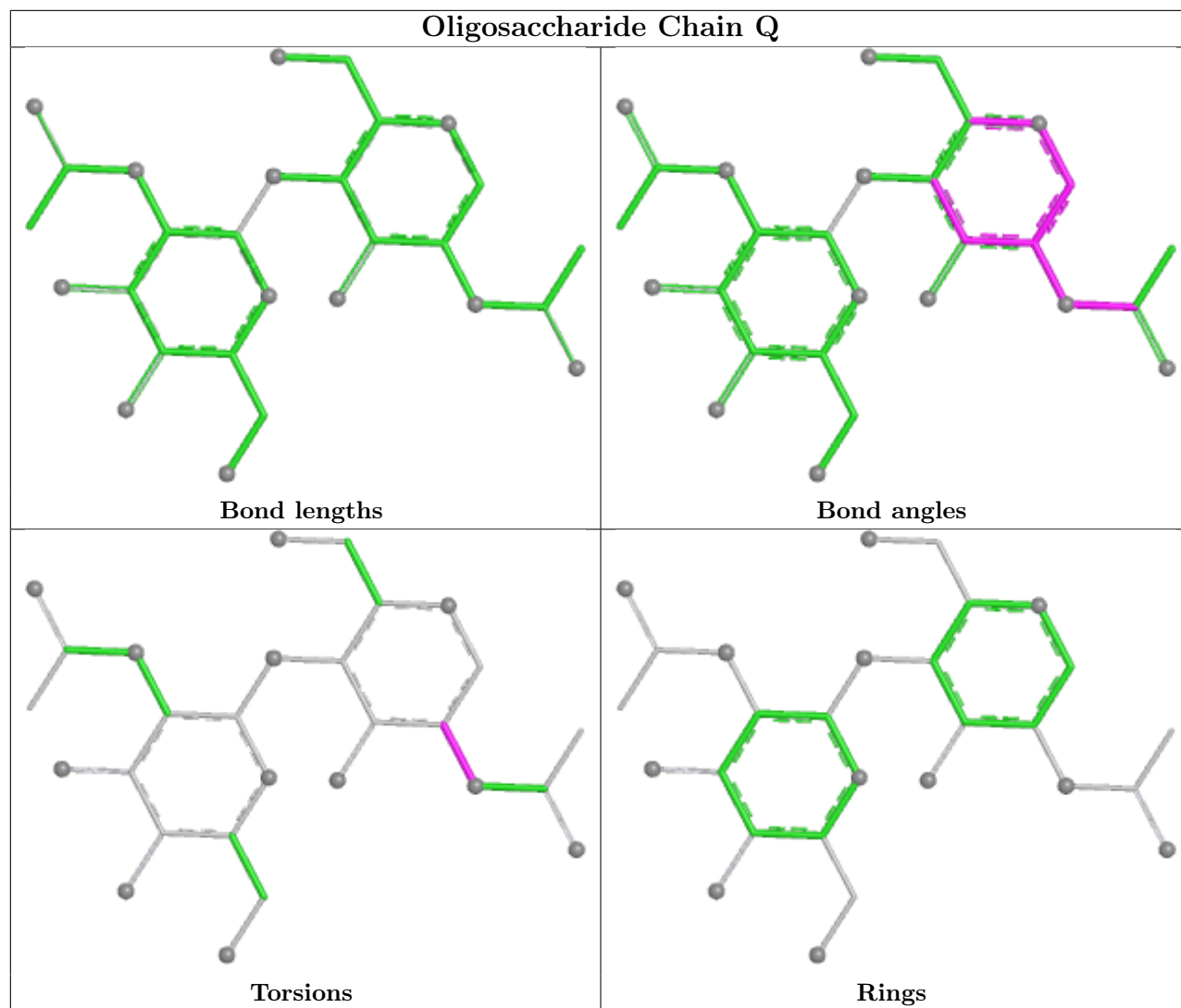
Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	C1-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
4	S	3	BMA	O5-C5-C6-O6
4	S	3	BMA	C4-C5-C6-O6
3	T	2	NAG	C8-C7-N2-C2

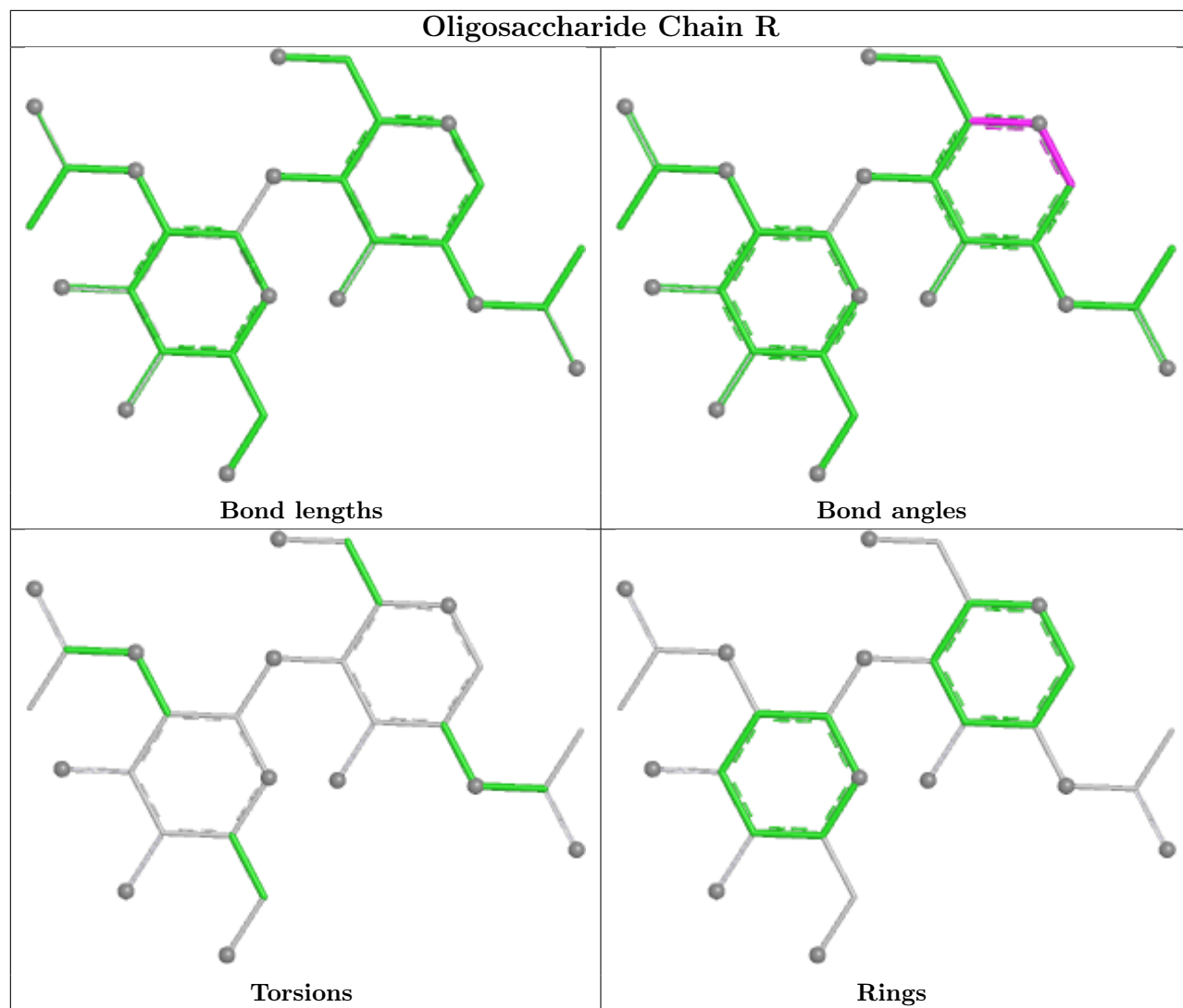
There are no ring outliers.

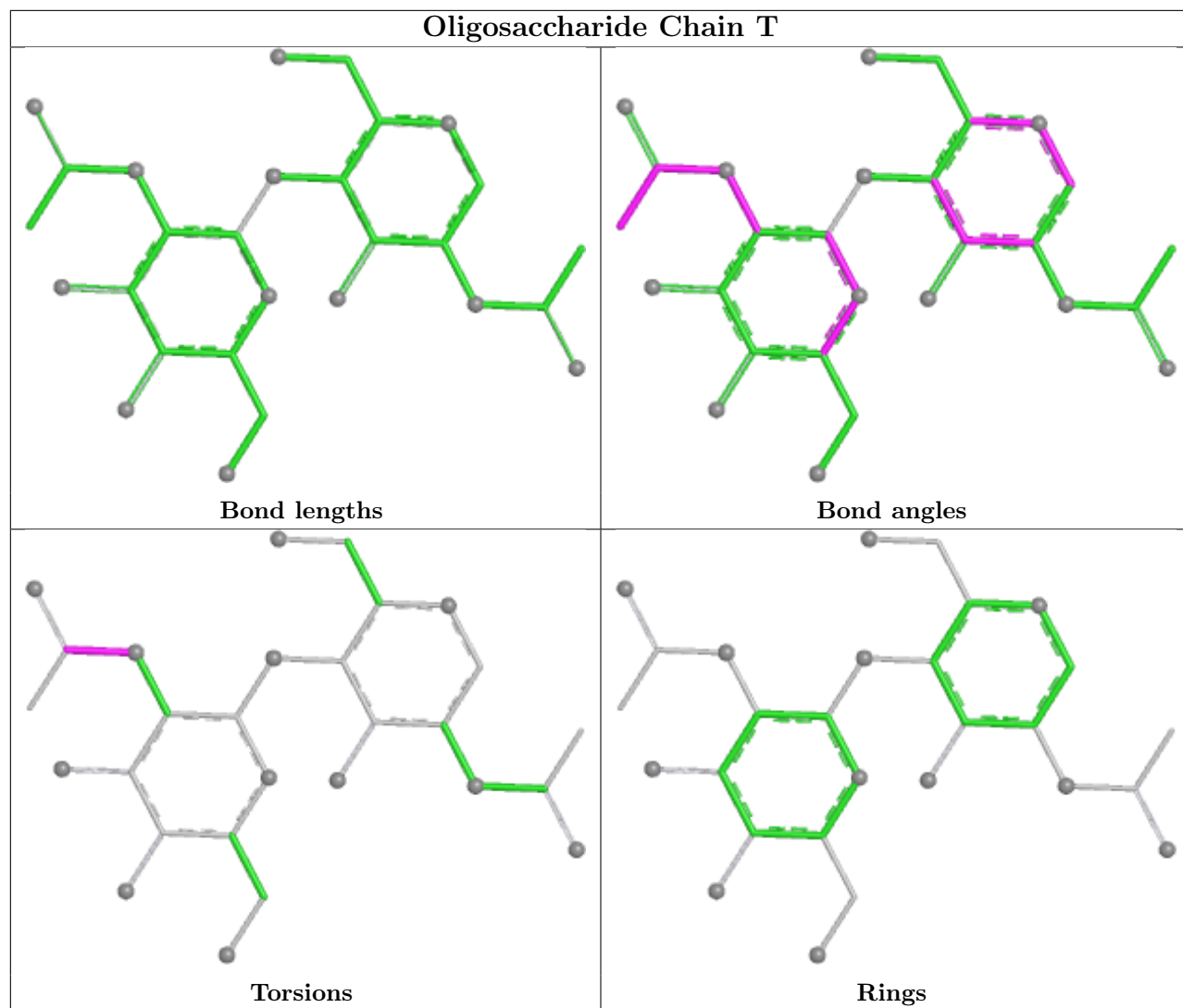
1 monomer is involved in 1 short contact:

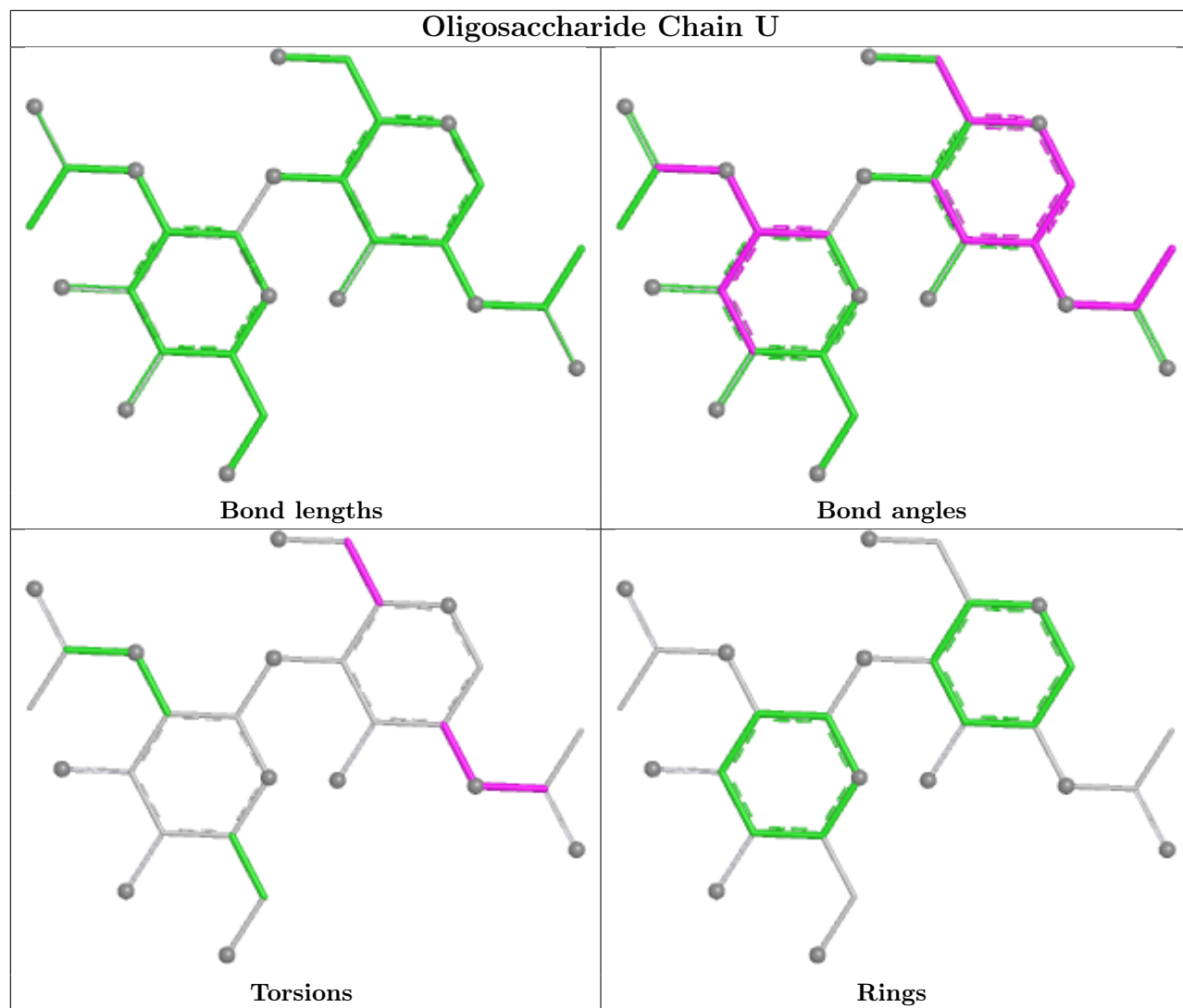
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	1	NAG	1	0

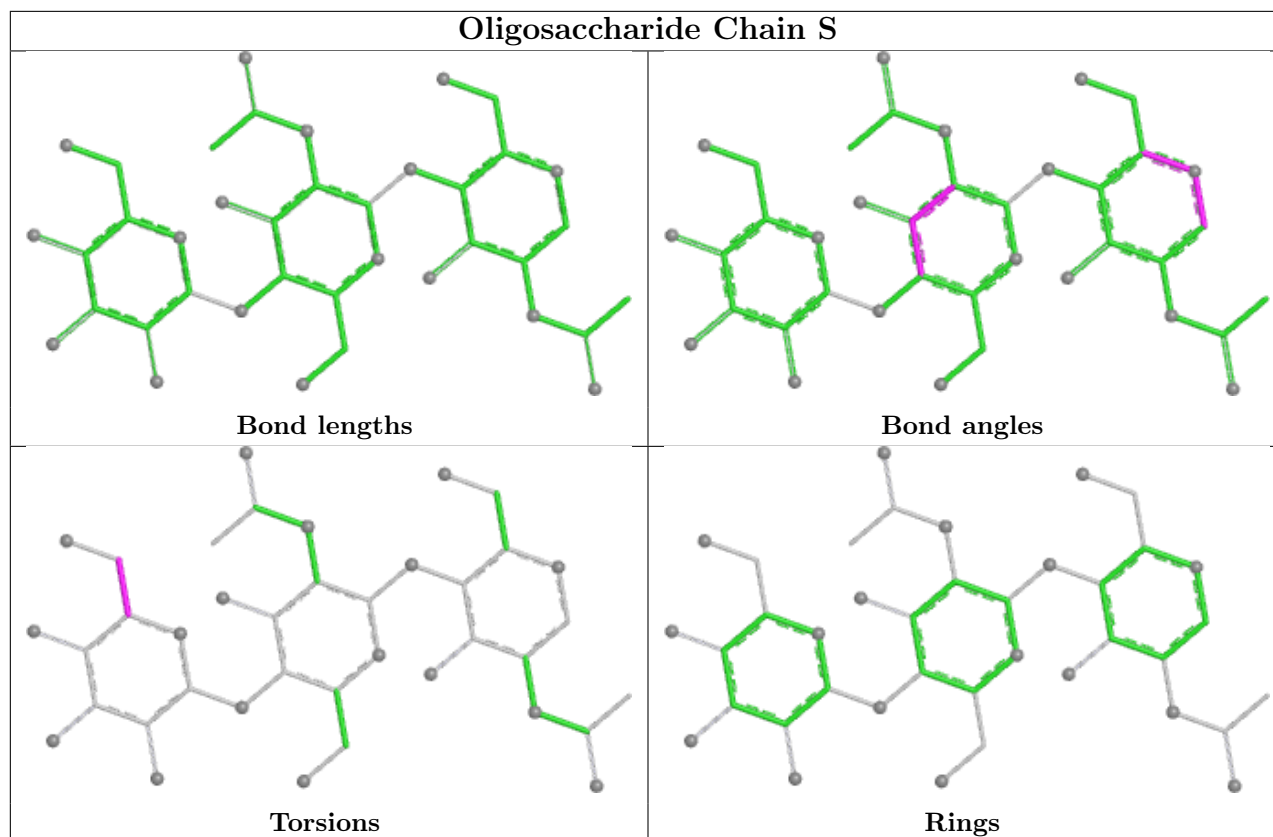
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

3 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$
5	NAG	A	701	1	14,14,15	1.16	0	17,19,21	2.32	4 (23%)
5	NAG	C	701	1	14,14,15	1.35	2 (14%)	17,19,21	2.38	3 (17%)
5	NAG	E	701	1	14,14,15	1.28	1 (7%)	17,19,21	1.88	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	701	1	-	4/6/23/26	0/1/1/1
5	NAG	C	701	1	-	1/6/23/26	0/1/1/1
5	NAG	E	701	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	701	NAG	C1-C2	3.02	1.56	1.52
5	E	701	NAG	C1-C2	2.46	1.55	1.52
5	C	701	NAG	O5-C1	2.38	1.47	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	701	NAG	C1-O5-C5	7.67	122.47	112.19
5	A	701	NAG	C1-O5-C5	7.44	122.15	112.19
5	E	701	NAG	C1-O5-C5	5.21	119.17	112.19
5	C	701	NAG	C1-C2-N2	4.03	116.78	110.43
5	E	701	NAG	O5-C5-C6	2.65	112.81	107.66

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	NAG	O5-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6
5	A	701	NAG	C8-C7-N2-C2
5	A	701	NAG	O7-C7-N2-C2
5	E	701	NAG	C4-C5-C6-O6

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](#)

There are no chain breaks in this entry.

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	199/230 (86%)	0.26	4 (2%) 65 57	46, 66, 107, 140	0
1	C	197/230 (85%)	0.60	11 (5%) 30 22	57, 82, 132, 162	0
1	E	195/230 (84%)	0.65	8 (4%) 41 32	57, 82, 127, 165	0
1	G	198/230 (86%)	0.78	18 (9%) 15 11	58, 87, 132, 155	0
1	I	198/230 (86%)	0.70	17 (8%) 16 12	62, 88, 130, 149	0
1	K	198/230 (86%)	0.51	9 (4%) 38 29	57, 83, 127, 147	0
1	M	198/230 (86%)	0.24	2 (1%) 79 74	49, 65, 108, 140	0
1	O	197/230 (85%)	0.51	7 (3%) 46 36	57, 83, 130, 148	0
2	B	111/127 (87%)	0.38	4 (3%) 46 36	52, 78, 127, 143	0
2	D	112/127 (88%)	1.08	20 (17%) 3 3	78, 109, 150, 173	0
2	F	113/127 (88%)	0.99	15 (13%) 7 5	77, 109, 150, 166	0
2	H	114/127 (89%)	0.31	4 (3%) 47 37	54, 72, 102, 144	0
2	J	114/127 (89%)	0.33	2 (1%) 67 61	53, 72, 102, 144	0
2	L	112/127 (88%)	0.31	3 (2%) 56 47	51, 71, 96, 129	0
2	N	113/127 (88%)	0.39	3 (2%) 56 47	52, 80, 128, 149	0
2	P	111/127 (87%)	0.35	2 (1%) 67 61	52, 70, 96, 131	0
All	All	2480/2856 (86%)	0.52	129 (5%) 33 25	46, 80, 134, 173	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	351	TYR	5.0
1	M	363	ALA	4.6
1	G	523	THR	4.3
2	D	49	LEU	4.2
2	F	102	GLY	3.9

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](#)

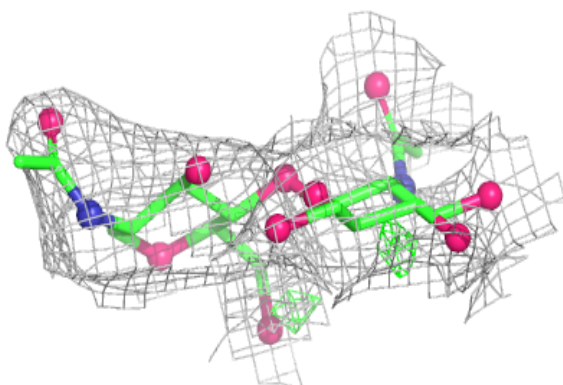
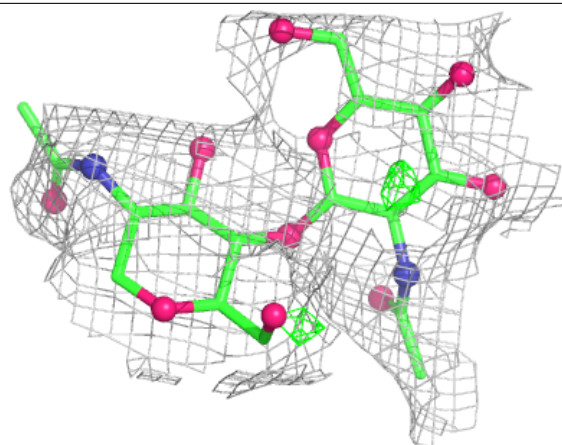
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	U	1	14/15	0.90	0.14	100,114,122,136	0
3	NAG	T	2	14/15	0.92	0.13	91,130,141,145	0
3	NAG	R	2	14/15	0.92	0.11	106,132,143,144	0
3	NAG	R	1	14/15	0.94	0.10	79,92,94,106	0
3	NAG	Q	2	14/15	0.94	0.11	113,124,134,134	0
3	NAG	U	2	14/15	0.94	0.14	136,141,153,154	0
4	NAG	S	1	14/15	0.94	0.10	89,106,111,128	0
4	NAG	S	2	14/15	0.95	0.13	130,151,162,163	0
4	BMA	S	3	11/12	0.95	0.10	143,158,168,170	0
3	NAG	Q	1	14/15	0.96	0.12	83,96,102,115	0
3	NAG	T	1	14/15	0.96	0.12	92,103,115,126	0

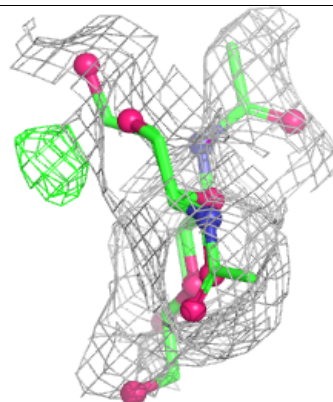
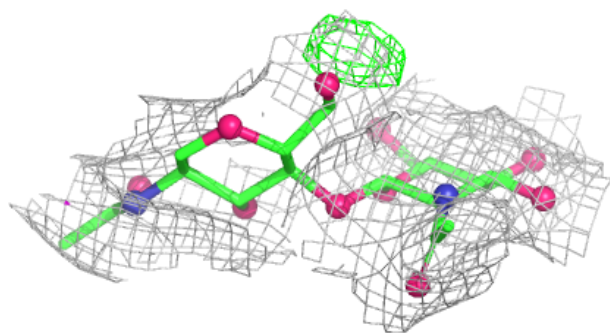
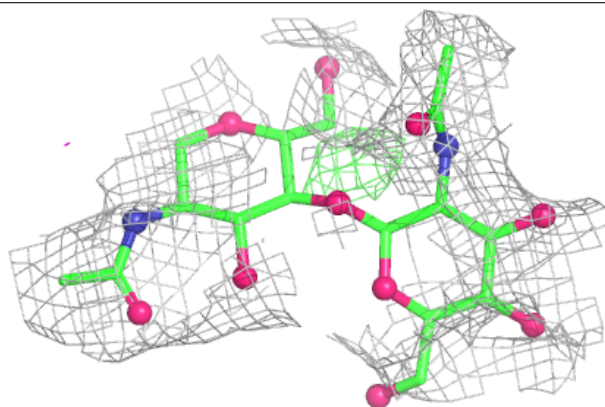
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

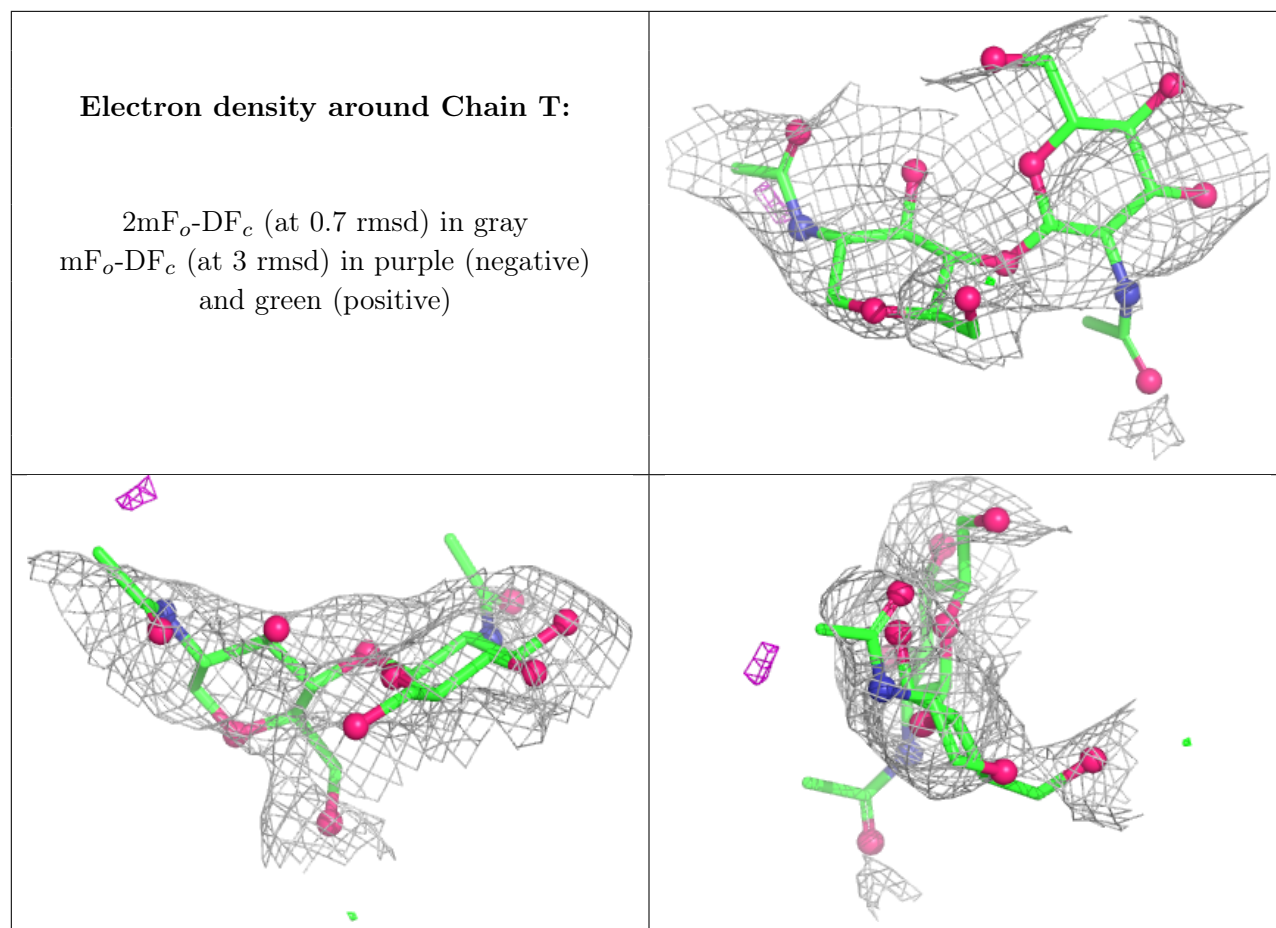
Electron density around Chain Q:

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

**Electron density around Chain R:**

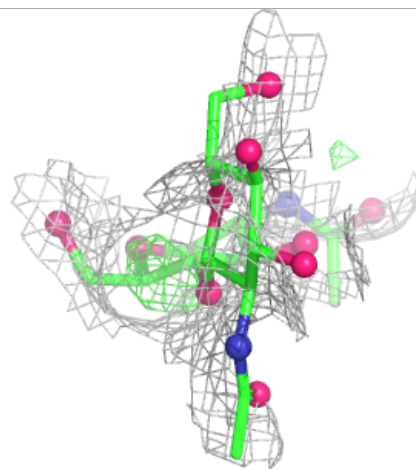
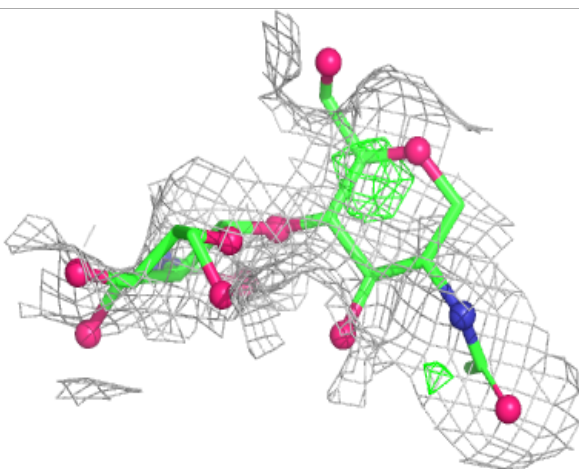
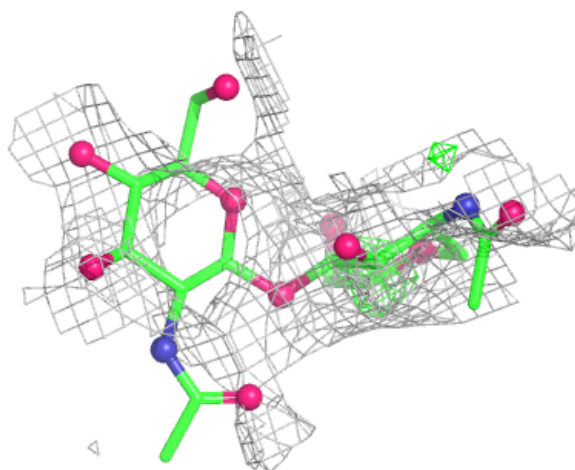
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

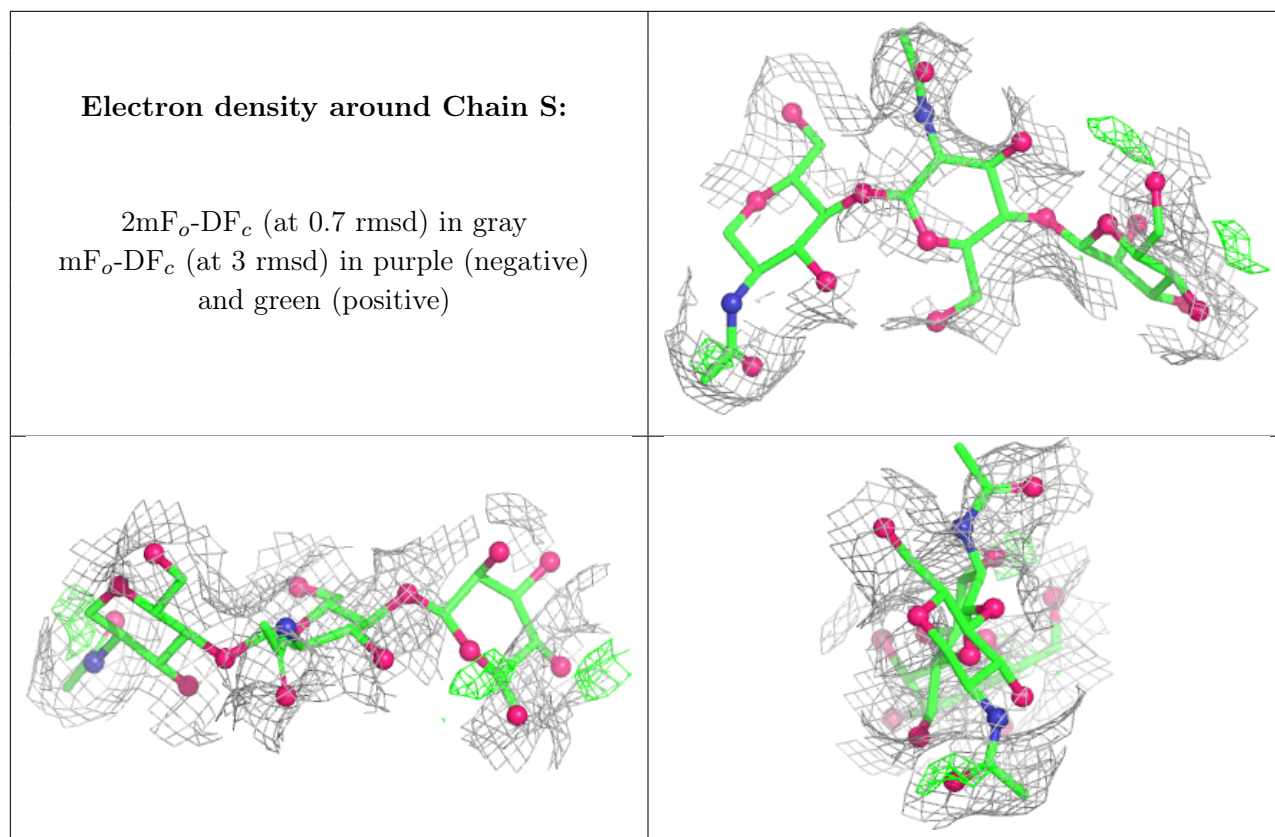




Electron density around Chain U:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
5	NAG	C	701	14/15	0.95	0.10	106,119,124,125	0
5	NAG	E	701	14/15	0.95	0.12	104,116,120,122	0
5	NAG	A	701	14/15	0.96	0.12	89,95,99,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.