



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2022 – 06:11 AM JST

PDB ID : 7FBJ
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 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:

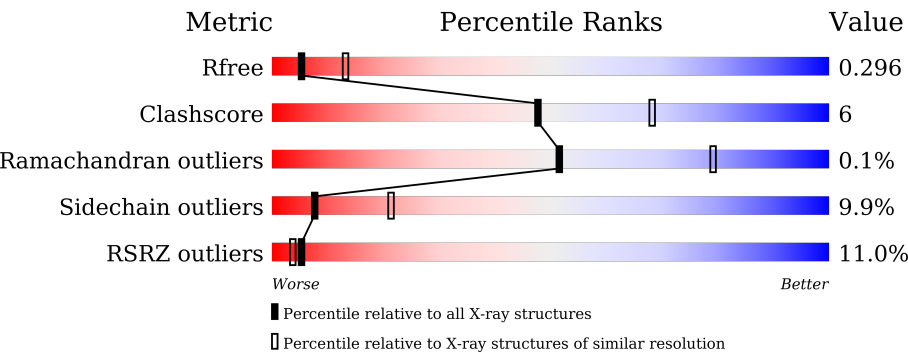
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance i

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	<div><div>4%</div><div><div></div><div>73%</div><div>12%</div><div>•</div><div>13%</div></div></div>
1	C	230	<div><div>8%</div><div><div></div><div>74%</div><div>10%</div><div>•</div><div>14%</div></div></div>
1	E	230	<div><div>13%</div><div><div></div><div>73%</div><div>9%</div><div>•</div><div>15%</div></div></div>
1	G	230	<div><div>17%</div><div><div></div><div>74%</div><div>8%</div><div>•</div><div>14%</div></div></div>
1	I	230	<div><div>19%</div><div><div></div><div>76%</div><div>7%</div><div>•</div><div>14%</div></div></div>
1	K	230	<div><div>6%</div><div><div></div><div>76%</div><div>8%</div><div>•</div><div>14%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	M	230	
1	O	230	
2	B	127	
2	D	127	
2	F	127	
2	H	127	
2	J	127	
2	L	127	
2	N	127	
2	P	127	
3	Q	2	
3	R	2	
3	T	2	
3	U	2	
4	S	3	

2 Entry composition

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

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

- 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
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

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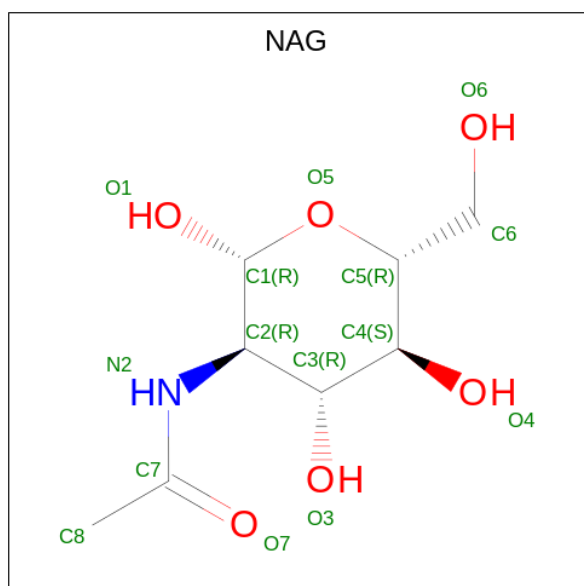
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

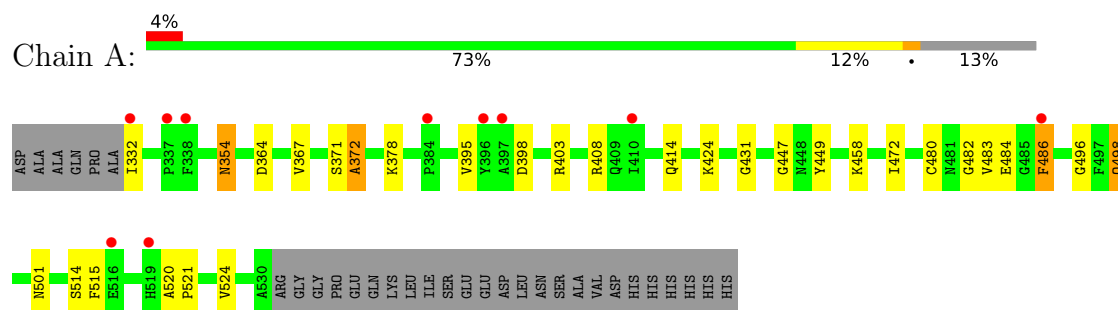
- Molecule 6 is water.

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

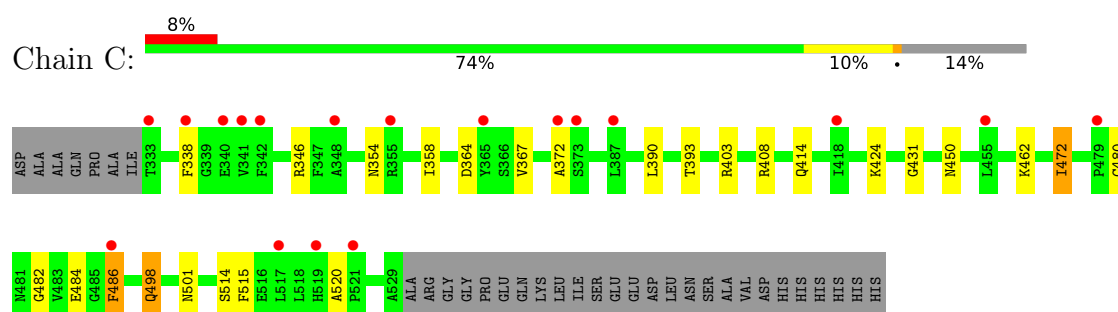
3 Residue-property plots [i](#)

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.

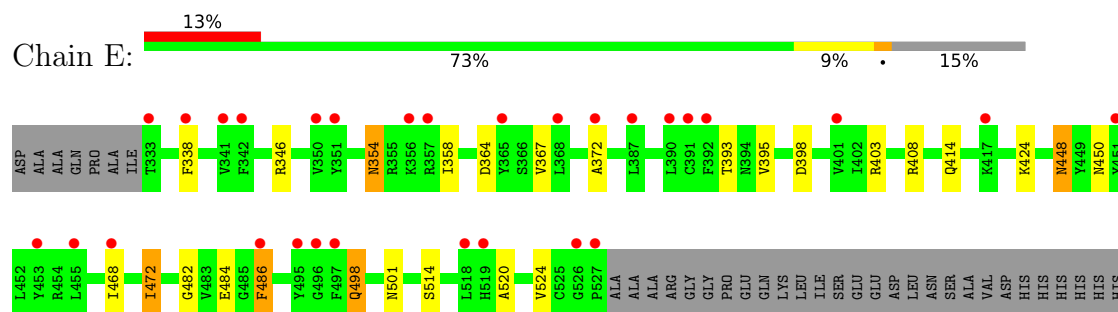
• Molecule 1: Spike protein S1



• Molecule 1: Spike protein S1

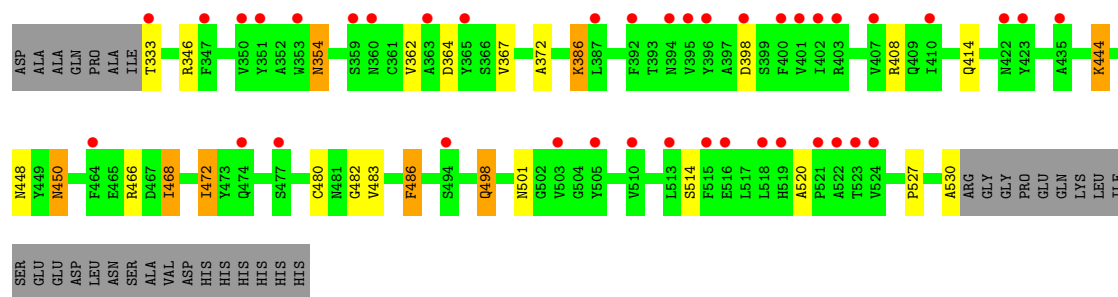


• Molecule 1: Spike protein S1

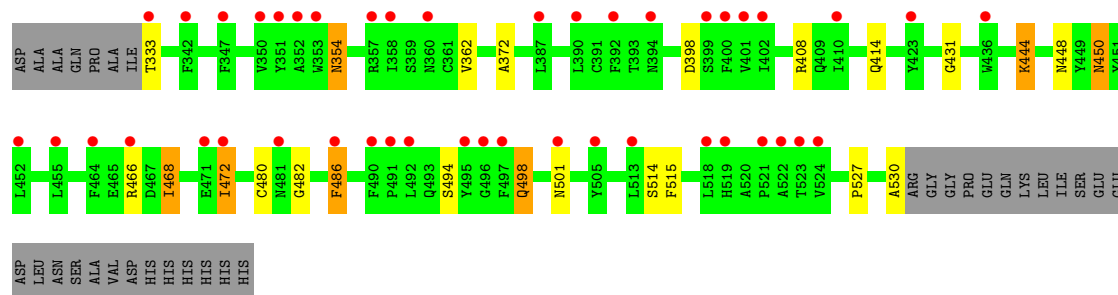
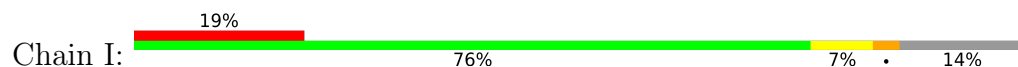


• Molecule 1: Spike protein S1

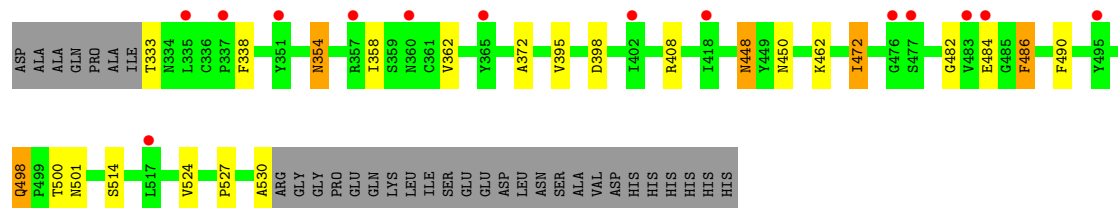
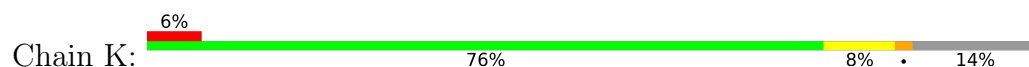




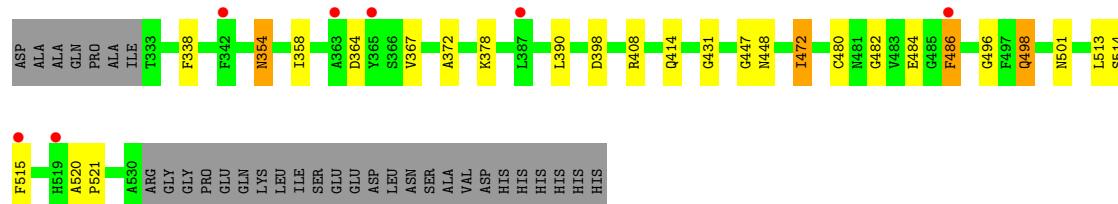
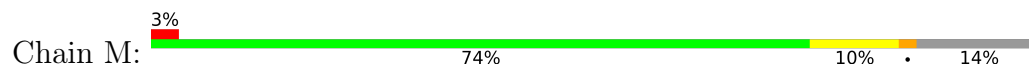
• Molecule 1: Spike protein S1



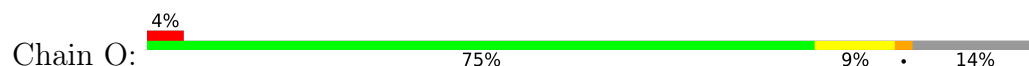
• Molecule 1: Spike protein S1



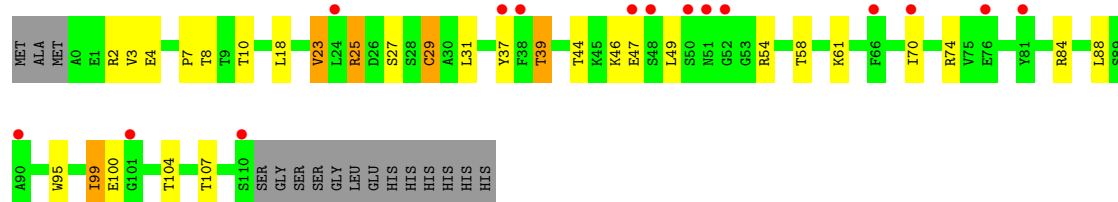
• Molecule 1: Spike protein S1



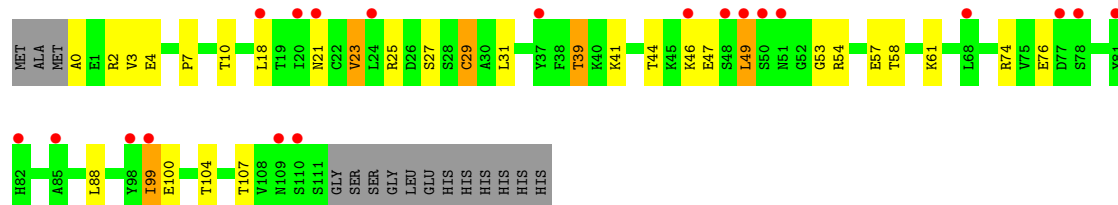
• Molecule 1: Spike protein S1



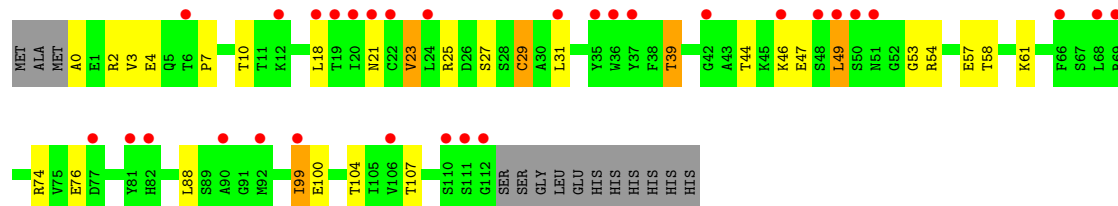
- Molecule 2: New antigen receptor variable domain



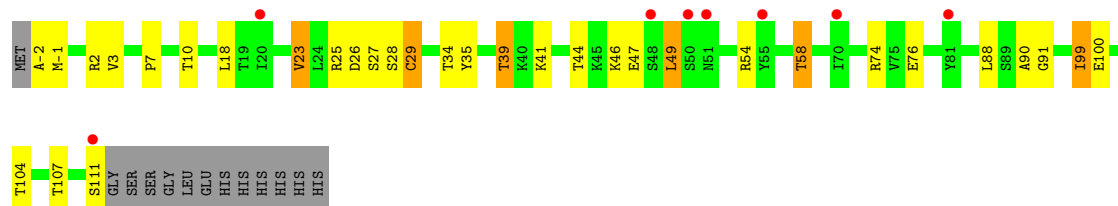
- Molecule 2: New antigen receptor variable domain



- Molecule 2: New antigen receptor variable domain




- Molecule 2: New antigen receptor variable domain



Chain R:  50% 50%


MAG1
MAG2

- 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% 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:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

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 90.24 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (90.40-2.85) 99.8 (90.24-2.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.254 , 0.300 0.253 , 0.296	Depositor DCC
R_{free} test set	3645 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	19487	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 3.20% 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

5.1 Standard geometry

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	0.78	0/1610	0.92	0/2193
1	C	0.78	0/1597	0.87	0/2175
1	E	0.75	0/1587	0.88	0/2161
1	G	0.73	0/1602	0.87	1/2182 (0.0%)
1	I	0.73	0/1602	0.88	1/2182 (0.0%)
1	K	0.73	0/1602	0.88	0/2182
1	M	0.79	0/1602	0.88	0/2182
1	O	0.74	0/1597	0.90	1/2175 (0.0%)
2	B	0.84	0/858	1.00	0/1158
2	D	0.81	0/864	0.98	0/1166
2	F	0.80	0/868	0.98	0/1171
2	H	0.82	0/877	1.00	0/1183
2	J	0.78	0/877	1.02	0/1183
2	L	0.85	1/864 (0.1%)	1.02	0/1166
2	N	0.79	0/872	1.04	1/1176 (0.1%)
2	P	0.84	1/859 (0.1%)	1.02	0/1159
All	All	0.78	2/19738 (0.0%)	0.93	4/26794 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	90	ALA	C-O	6.13	1.34	1.23
2	P	90	ALA	C-O	6.08	1.34	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	403	ARG	CG-CD-NE	6.88	126.24	111.80
2	N	54	ARG	N-CA-CB	6.70	122.66	110.60
1	G	466	ARG	CB-CG-CD	6.33	128.05	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	466	ARG	CB-CG-CD	5.30	125.38	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	13	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	16	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
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	H	1	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	231	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.

All (231) 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:HH22	1.47	0.80
2:L:89:SER:O	6:L:201:HOH:O	2.04	0.74
1:I:372:ALA:O	2:J:46:LYS:HE3	1.87	0.74
1:E:484:GLU:OE2	2:L:25:ARG:NH2	2.22	0.73
1:G:372:ALA:O	2:H:46:LYS:HE3	1.89	0.71
1:A:472:ILE:HD12	1:A:472:ILE:H	1.56	0.70
1:M:372:ALA:O	2:N:46:LYS:CE	2.40	0.70
2:B:70:ILE:N	2:B:70:ILE:HD12	2.07	0.69
1:A:372:ALA:O	2:B:46:LYS:CE	2.42	0.68
1:O:333:THR:HG21	1:O:529:ALA:HB1	1.76	0.67
1:A:371:SER:O	1:A:372:ALA:HB3	1.95	0.66
1:C:372:ALA:O	2:D:46:LYS:CE	2.44	0.66
1:M:372:ALA:O	2:N:46:LYS:HE3	1.96	0.65
1:E:468:ILE:HD12	1:G:520:ALA:HB2	1.79	0.65
1:E:486:PHE:O	1:E:486:PHE:CD2	2.51	0.64
1:M:486:PHE:CD2	1:M:486:PHE:O	2.51	0.64
1:I:444:LYS:HD3	1:I:448:ASN:HA	1.79	0.64
1:E:372:ALA:O	2:F:46:LYS:HE3	1.96	0.64
1:C:486:PHE:O	1:C:486:PHE:CD2	2.51	0.63
1:A:486:PHE:CD2	1:A:486:PHE:O	2.52	0.63
2:L:23:VAL:HG22	2:L:25:ARG:HG2	1.79	0.62
2:P:23:VAL:HG22	2:P:25:ARG:HG2	1.79	0.62
1:C:372:ALA:O	2:D:46:LYS:HE3	1.99	0.62
1:K:486:PHE:CD2	1:K:486:PHE:O	2.53	0.61
2:F:23:VAL:HG22	2:F:25:ARG:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:SER:O	1:A:372:ALA:CB	2.48	0.61
2:J:58:THR:CG2	1:M:486:PHE:CD2	2.84	0.60
2:J:23:VAL:HG22	2:J:25:ARG:HG2	1.82	0.60
2:D:23:VAL:HG22	2:D:25:ARG:HG2	1.84	0.60
1:G:486:PHE:O	1:G:486:PHE:CD2	2.54	0.60
1:G:444:LYS:HD3	1:G:448:ASN:HA	1.81	0.60
1:E:372:ALA:O	2:F:46:LYS:CE	2.48	0.60
1:I:486:PHE:O	1:I:486:PHE:CD2	2.54	0.60
2:H:23:VAL:HG22	2:H:25:ARG:HG2	1.82	0.60
2:J:27:SER:OG	2:J:29:CYS:HB2	2.01	0.59
1:C:408:ARG:NH2	1:C:414:GLN:OE1	2.36	0.59
2:D:27:SER:OG	2:D:29:CYS:HB2	2.02	0.59
1:E:468:ILE:CD1	1:G:520:ALA:HB2	2.33	0.59
1:O:333:THR:CG2	1:O:529:ALA:HB1	2.32	0.59
2:F:27:SER:OG	2:F:29:CYS:HB2	2.03	0.59
1:M:408:ARG:NH2	1:M:414:GLN:OE1	2.36	0.59
1:I:333:THR:HG21	1:I:530:ALA:HB2	1.83	0.59
1:A:372:ALA:O	2:B:46:LYS:HE2	2.03	0.59
1:A:408:ARG:NH2	1:A:414:GLN:OE1	2.36	0.58
1:E:486:PHE:CD2	2:L:58:THR:CG2	2.86	0.58
2:J:58:THR:HG23	1:M:486:PHE:CD2	2.38	0.58
2:H:27:SER:OG	2:H:29:CYS:HB2	2.03	0.58
1:E:408:ARG:NH2	1:E:414:GLN:OE1	2.37	0.58
2:L:27:SER:OG	2:L:29:CYS:HB2	2.03	0.58
2:P:27:SER:OG	2:P:29:CYS:HB2	2.03	0.58
1:E:484:GLU:CD	2:L:25:ARG:NH2	2.57	0.58
1:G:333:THR:HG21	1:G:530:ALA:HB2	1.85	0.57
2:N:27:SER:OG	2:N:29:CYS:HB2	2.04	0.57
1:A:372:ALA:O	2:B:46:LYS:HE3	2.04	0.57
1:M:498:GLN:HB2	1:M:501:ASN:ND2	2.19	0.57
2:P:3:VAL:HG23	2:P:99:ILE:HG13	1.85	0.56
2:B:27:SER:OG	2:B:29:CYS:HB2	2.05	0.56
1:A:498:GLN:HB2	1:A:501:ASN:ND2	2.20	0.56
1:E:498:GLN:HB2	1:E:501:ASN:ND2	2.20	0.56
2:L:3:VAL:HG23	2:L:99:ILE:HG13	1.86	0.56
2:N:51:ASN:ND2	2:N:57:GLU:OE2	2.38	0.56
1:I:408:ARG:NH2	1:I:414:GLN:OE1	2.39	0.56
1:C:498:GLN:HB2	1:C:501:ASN:ND2	2.20	0.56
1:E:393:THR:HG23	1:E:520:ALA:HB3	1.88	0.56
1:E:486:PHE:CD2	2:L:58:THR:HG21	2.41	0.56
1:G:408:ARG:NH2	1:G:414:GLN:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:498:GLN:HB2	1:G:501:ASN:ND2	2.21	0.55
2:N:3:VAL:HG23	2:N:99:ILE:HG13	1.88	0.55
1:G:468:ILE:HD13	1:G:468:ILE:H	1.71	0.55
1:I:498:GLN:HB2	1:I:501:ASN:ND2	2.21	0.55
2:H:3:VAL:HG23	2:H:99:ILE:HG13	1.88	0.55
1:A:486:PHE:CD2	2:H:58:THR:CG2	2.89	0.55
1:O:498:GLN:HB2	1:O:501:ASN:ND2	2.22	0.55
1:I:468:ILE:HD13	1:I:468:ILE:H	1.72	0.54
2:J:3:VAL:HG23	2:J:99:ILE:HG13	1.89	0.54
1:K:498:GLN:HB2	1:K:501:ASN:ND2	2.22	0.54
2:B:3:VAL:HG23	2:B:99:ILE:HG13	1.89	0.54
2:J:58:THR:HG21	1:M:486:PHE:HB2	1.87	0.54
2:H:34:THR:O	2:H:35:TYR:CD2	2.61	0.53
2:F:3:VAL:HG23	2:F:99:ILE:HG13	1.89	0.53
2:D:3:VAL:HG23	2:D:99:ILE:HG13	1.89	0.53
1:M:372:ALA:O	2:N:46:LYS:HE2	2.07	0.53
1:A:480:CYS:O	1:A:483:VAL:HG22	2.07	0.53
1:A:472:ILE:HD13	1:A:482:GLY:HA2	1.92	0.51
1:O:364:ASP:O	1:O:367:VAL:HG12	2.11	0.51
1:E:364:ASP:O	1:E:367:VAL:HG12	2.11	0.51
1:A:486:PHE:CD2	2:H:58:THR:HG23	2.46	0.50
1:A:364:ASP:O	1:A:367:VAL:HG12	2.12	0.50
2:J:58:THR:HG21	1:M:486:PHE:CD2	2.47	0.50
1:A:372:ALA:HB1	2:B:37:TYR:CE2	2.47	0.49
1:E:486:PHE:CD2	2:L:58:THR:HG23	2.47	0.49
1:K:408:ARG:HD2	2:L:0:ALA:N	2.28	0.49
2:N:39:THR:HG22	2:N:46:LYS:HG2	1.94	0.49
1:G:364:ASP:O	1:G:367:VAL:HG12	2.12	0.49
2:L:7:PRO:O	2:L:104:THR:HG23	2.12	0.49
1:A:449:TYR:HB3	2:H:-2:ALA:CB	2.43	0.49
2:P:7:PRO:O	2:P:104:THR:HG23	2.12	0.49
1:A:378:LYS:HD2	2:B:95:TRP:CE2	2.48	0.49
1:A:486:PHE:CD2	2:H:58:THR:HG21	2.48	0.49
2:J:28:SER:HB2	1:M:496:GLY:N	2.28	0.48
1:O:362:VAL:CG1	1:O:527:PRO:HA	2.43	0.48
1:E:393:THR:CG2	1:E:520:ALA:HB3	2.44	0.48
1:O:362:VAL:HG13	1:O:527:PRO:HA	1.96	0.48
1:C:364:ASP:O	1:C:367:VAL:HG12	2.14	0.47
1:C:472:ILE:CG1	1:C:482:GLY:HA2	2.45	0.47
1:O:472:ILE:CG1	1:O:482:GLY:HA2	2.45	0.47
1:M:364:ASP:O	1:M:367:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:ILE:CG1	1:E:482:GLY:HA2	2.45	0.47
2:J:46:LYS:NZ	2:J:100:GLU:OE1	2.48	0.47
1:G:472:ILE:CG1	1:G:482:GLY:HA2	2.45	0.47
2:D:39:THR:HG22	2:D:46:LYS:HG2	1.96	0.47
2:H:46:LYS:NZ	2:H:100:GLU:OE1	2.48	0.47
2:H:90:ALA:CA	6:H:201:HOH:O	2.63	0.47
2:B:39:THR:HG22	2:B:46:LYS:HG2	1.97	0.46
1:K:362:VAL:CG1	1:K:527:PRO:HA	2.45	0.46
1:A:486:PHE:HB2	2:H:58:THR:HG21	1.96	0.46
1:A:496:GLY:N	2:H:28:SER:HB2	2.31	0.46
1:O:354:ASN:O	1:O:398:ASP:HA	2.15	0.46
1:C:372:ALA:O	2:D:46:LYS:HE2	2.13	0.46
2:J:7:PRO:O	2:J:104:THR:HG23	2.15	0.46
1:K:354:ASN:O	1:K:398:ASP:HA	2.15	0.46
1:C:393:THR:HG23	1:C:520:ALA:HB3	1.96	0.46
1:G:386:LYS:HB3	1:G:386:LYS:HE2	1.65	0.46
2:H:7:PRO:O	2:H:104:THR:HG23	2.15	0.46
1:I:333:THR:CG2	1:I:530:ALA:HB2	2.45	0.45
1:K:362:VAL:HG13	1:K:527:PRO:HA	1.97	0.45
2:F:7:PRO:O	2:F:104:THR:HG23	2.15	0.45
2:H:-2:ALA:HA	2:H:26:ASP:HB3	1.97	0.45
1:I:354:ASN:O	1:I:398:ASP:HA	2.16	0.45
1:K:372:ALA:O	2:L:46:LYS:HE2	2.17	0.45
2:D:49:LEU:HD23	2:D:49:LEU:HA	1.86	0.45
1:E:354:ASN:O	1:E:398:ASP:HA	2.16	0.45
1:E:408:ARG:HD2	2:F:0:ALA:HA	1.98	0.45
1:G:354:ASN:O	1:G:398:ASP:HA	2.16	0.45
2:D:7:PRO:O	2:D:104:THR:HG23	2.16	0.45
1:G:333:THR:CG2	1:G:530:ALA:HB2	2.46	0.45
2:N:7:PRO:O	2:N:104:THR:HG23	2.16	0.45
2:F:39:THR:HG22	2:F:46:LYS:HG2	1.98	0.45
2:F:49:LEU:HD23	2:F:49:LEU:HA	1.85	0.44
1:M:472:ILE:CG1	1:M:482:GLY:HA2	2.48	0.44
1:I:472:ILE:CG1	1:I:482:GLY:HA2	2.47	0.44
1:K:472:ILE:CG1	1:K:482:GLY:HA2	2.48	0.44
2:N:46:LYS:NZ	2:N:100:GLU:OE1	2.50	0.44
1:A:354:ASN:O	1:A:398:ASP:HA	2.17	0.44
2:B:7:PRO:O	2:B:104:THR:HG23	2.17	0.44
1:A:480:CYS:O	1:A:483:VAL:CG2	2.66	0.44
2:J:-2:ALA:HA	2:J:26:ASP:HB3	1.98	0.44
2:N:31:LEU:O	2:N:61:LYS:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:LYS:NZ	2:B:100:GLU:OE1	2.51	0.43
2:L:49:LEU:HD23	2:L:49:LEU:HA	1.91	0.43
1:M:338:PHE:HE1	1:M:358:ILE:HD13	1.83	0.43
1:E:450:ASN:N	1:E:450:ASN:HD22	2.16	0.43
2:B:31:LEU:O	2:B:61:LYS:HD3	2.19	0.43
1:G:362:VAL:HG13	1:G:527:PRO:HA	2.01	0.43
1:G:362:VAL:CG1	1:G:527:PRO:HA	2.48	0.43
2:P:54:ARG:HD3	2:P:74:ARG:NH2	2.33	0.43
1:K:333:THR:CG2	1:K:530:ALA:HB2	2.49	0.43
1:M:431:GLY:HA2	1:M:515:PHE:CD2	2.53	0.43
2:N:49:LEU:HD12	2:N:49:LEU:HA	1.72	0.43
1:A:372:ALA:CA	2:B:84:ARG:HH22	2.24	0.43
1:C:338:PHE:HE1	1:C:358:ILE:HD13	1.84	0.43
1:E:395:VAL:HG21	1:E:524:VAL:HG11	2.01	0.43
2:N:54:ARG:HD3	2:N:74:ARG:NH2	2.34	0.43
2:D:31:LEU:O	2:D:61:LYS:HD3	2.19	0.42
1:G:450:ASN:N	1:G:450:ASN:HD22	2.16	0.42
1:A:449:TYR:HB3	2:H:-2:ALA:HB1	2.02	0.42
2:D:54:ARG:HD3	2:D:74:ARG:NH2	2.34	0.42
1:I:450:ASN:N	1:I:450:ASN:HD22	2.17	0.42
1:E:448:ASN:ND2	1:E:450:ASN:H	2.17	0.42
2:N:39:THR:CG2	2:N:46:LYS:HG2	2.49	0.42
1:C:408:ARG:HD2	2:D:0:ALA:HA	2.01	0.42
2:N:41:LYS:HE2	2:N:41:LYS:HB3	1.93	0.42
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.50	0.42
2:F:54:ARG:HD3	2:F:74:ARG:NH2	2.35	0.42
2:B:54:ARG:HD3	2:B:74:ARG:NH2	2.34	0.42
1:M:520:ALA:HB1	1:M:521:PRO:CD	2.50	0.42
1:A:447:GLY:HA3	1:A:498:GLN:HE22	1.85	0.42
1:C:393:THR:CG2	1:C:520:ALA:HB3	2.50	0.42
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.54	0.42
2:H:54:ARG:HD3	2:H:74:ARG:NH2	2.34	0.42
2:H:90:ALA:C	6:H:201:HOH:O	2.48	0.42
2:N:23:VAL:HG22	2:N:25:ARG:HG2	2.01	0.42
2:F:31:LEU:O	2:F:61:LYS:HD3	2.19	0.41
2:H:39:THR:HG22	2:H:46:LYS:HA	2.02	0.41
1:I:362:VAL:CG1	1:I:527:PRO:HA	2.49	0.41
3:U:1:NAG:H83	3:U:1:NAG:H3	2.02	0.41
2:B:23:VAL:HG22	2:B:25:ARG:HG2	2.01	0.41
2:J:39:THR:HG22	2:J:46:LYS:HG2	2.02	0.41
1:A:395:VAL:HG21	1:A:524:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:THR:CG2	2:D:46:LYS:HG2	2.51	0.41
1:K:484:GLU:OE2	1:K:490:PHE:HB2	2.20	0.41
2:J:39:THR:HG22	2:J:46:LYS:HA	2.03	0.41
1:O:448:ASN:ND2	1:O:450:ASN:H	2.18	0.41
1:O:484:GLU:OE2	1:O:490:PHE:HB2	2.21	0.41
1:E:338:PHE:CE1	1:E:358:ILE:HD13	2.55	0.41
1:I:362:VAL:HG13	1:I:527:PRO:HA	2.03	0.41
2:P:46:LYS:NZ	2:P:100:GLU:OE1	2.54	0.41
2:D:46:LYS:NZ	2:D:100:GLU:OE1	2.53	0.41
2:H:39:THR:HG22	2:H:46:LYS:HG2	2.02	0.41
1:K:448:ASN:ND2	1:K:450:ASN:H	2.19	0.41
2:D:39:THR:HG22	2:D:46:LYS:HA	2.02	0.41
1:E:486:PHE:HB2	2:L:58:THR:HG21	2.02	0.41
1:K:338:PHE:HE1	1:K:358:ILE:HD13	1.86	0.41
2:B:39:THR:HG22	2:B:46:LYS:HA	2.02	0.41
2:J:54:ARG:HD3	2:J:74:ARG:NH2	2.35	0.41
1:M:447:GLY:HA3	1:M:498:GLN:HE22	1.85	0.41
1:O:395:VAL:HG21	1:O:524:VAL:HG11	2.02	0.41
2:B:39:THR:CG2	2:B:46:LYS:HG2	2.50	0.41
1:C:338:PHE:CE1	1:C:358:ILE:HD13	2.56	0.41
2:H:49:LEU:HD23	2:H:49:LEU:HA	1.93	0.41
2:P:39:THR:HG22	2:P:46:LYS:HA	2.03	0.41
1:I:431:GLY:HA2	1:I:515:PHE:CD2	2.56	0.40
2:J:49:LEU:HD23	2:J:49:LEU:HA	1.90	0.40
1:K:395:VAL:HG21	1:K:524:VAL:HG11	2.02	0.40
1:M:338:PHE:CE1	1:M:358:ILE:HD13	2.55	0.40
1:O:338:PHE:HE1	1:O:358:ILE:HD13	1.86	0.40
1:O:338:PHE:CE1	1:O:358:ILE:HD13	2.56	0.40
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.55	0.40
1:C:450:ASN:HD22	1:C:450:ASN:N	2.19	0.40
1:M:431:GLY:HA3	1:M:513:LEU:O	2.21	0.40
2:P:110:SER:O	2:P:111:SER:CB	2.69	0.40
2:L:54:ARG:HD3	2:L:74:ARG:NH2	2.36	0.40
1:M:378:LYS:HE3	2:N:95:TRP:CE2	2.56	0.40
2:F:46:LYS:NZ	2:F:100:GLU:OE1	2.54	0.40
2:H:-2:ALA:HA	2:H:26:ASP:CB	2.51	0.40
2:L:39:THR:HG22	2:L:46:LYS:HA	2.04	0.40
1:M:354:ASN:O	1:M:398:ASP:HA	2.21	0.40

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

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	197/230 (86%)	189 (96%)	7 (4%)	1 (0%)	29	57
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%)	17	43
2	F	111/127 (87%)	105 (95%)	5 (4%)	1 (1%)	17	43
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%)	51	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	53	GLY

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	161 (95%)	8 (5%)	26	56
1	C	168/194 (87%)	157 (94%)	11 (6%)	17	41
1	E	168/194 (87%)	159 (95%)	9 (5%)	22	49
1	G	168/194 (87%)	156 (93%)	12 (7%)	14	36
1	I	168/194 (87%)	158 (94%)	10 (6%)	19	45
1	K	168/194 (87%)	160 (95%)	8 (5%)	25	55
1	M	168/194 (87%)	160 (95%)	8 (5%)	25	55
1	O	168/194 (87%)	159 (95%)	9 (5%)	22	49
2	B	93/106 (88%)	77 (83%)	16 (17%)	2	5
2	D	94/106 (89%)	76 (81%)	18 (19%)	1	3
2	F	94/106 (89%)	77 (82%)	17 (18%)	1	4
2	H	95/106 (90%)	78 (82%)	17 (18%)	2	4
2	J	95/106 (90%)	79 (83%)	16 (17%)	2	5
2	L	94/106 (89%)	78 (83%)	16 (17%)	2	5
2	N	95/106 (90%)	78 (82%)	17 (18%)	2	4
2	P	94/106 (89%)	79 (84%)	15 (16%)	2	6
All	All	2099/2400 (88%)	1892 (90%)	207 (10%)	8	21

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ILE
1	A	354	ASN

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Mol	Chain	Res	Type
1	A	403	ARG
1	A	424	LYS
1	A	458	LYS
1	A	486	PHE
1	A	498	GLN
1	A	514	SER
2	B	2	ARG
2	B	4	GLU
2	B	8	THR
2	B	10	THR
2	B	18	LEU
2	B	23	VAL
2	B	25	ARG
2	B	29	CYS
2	B	39	THR
2	B	44	THR
2	B	47	GLU
2	B	49	LEU
2	B	58	THR
2	B	88	LEU
2	B	99	ILE
2	B	107	THR
1	C	346	ARG
1	C	354	ASN
1	C	390	LEU
1	C	403	ARG
1	C	424	LYS
1	C	462	LYS
1	C	472	ILE
1	C	480	CYS
1	C	486	PHE
1	C	498	GLN
1	C	514	SER
2	D	2	ARG
2	D	4	GLU
2	D	10	THR
2	D	18	LEU
2	D	21	ASN
2	D	23	VAL
2	D	29	CYS
2	D	39	THR
2	D	41	LYS

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Mol	Chain	Res	Type
2	D	44	THR
2	D	47	GLU
2	D	49	LEU
2	D	57	GLU
2	D	58	THR
2	D	76	GLU
2	D	88	LEU
2	D	99	ILE
2	D	107	THR
1	E	346	ARG
1	E	354	ASN
1	E	403	ARG
1	E	424	LYS
1	E	448	ASN
1	E	472	ILE
1	E	486	PHE
1	E	498	GLN
1	E	514	SER
2	F	2	ARG
2	F	4	GLU
2	F	10	THR
2	F	18	LEU
2	F	21	ASN
2	F	23	VAL
2	F	29	CYS
2	F	39	THR
2	F	44	THR
2	F	47	GLU
2	F	49	LEU
2	F	57	GLU
2	F	58	THR
2	F	76	GLU
2	F	88	LEU
2	F	99	ILE
2	F	107	THR
1	G	346	ARG
1	G	354	ASN
1	G	386	LYS
1	G	444	LYS
1	G	450	ASN
1	G	468	ILE
1	G	472	ILE

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Mol	Chain	Res	Type
1	G	480	CYS
1	G	483	VAL
1	G	486	PHE
1	G	498	GLN
1	G	514	SER
2	H	-1	MET
2	H	2	ARG
2	H	10	THR
2	H	18	LEU
2	H	23	VAL
2	H	29	CYS
2	H	39	THR
2	H	41	LYS
2	H	44	THR
2	H	47	GLU
2	H	49	LEU
2	H	58	THR
2	H	76	GLU
2	H	88	LEU
2	H	99	ILE
2	H	107	THR
2	H	111	SER
1	I	354	ASN
1	I	444	LYS
1	I	450	ASN
1	I	468	ILE
1	I	472	ILE
1	I	480	CYS
1	I	486	PHE
1	I	494	SER
1	I	498	GLN
1	I	514	SER
2	J	-1	MET
2	J	10	THR
2	J	18	LEU
2	J	23	VAL
2	J	29	CYS
2	J	39	THR
2	J	41	LYS
2	J	44	THR
2	J	47	GLU
2	J	49	LEU

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Mol	Chain	Res	Type
2	J	58	THR
2	J	76	GLU
2	J	88	LEU
2	J	99	ILE
2	J	107	THR
2	J	111	SER
1	K	354	ASN
1	K	448	ASN
1	K	462	LYS
1	K	472	ILE
1	K	486	PHE
1	K	498	GLN
1	K	500	THR
1	K	514	SER
2	L	1	GLU
2	L	2	ARG
2	L	10	THR
2	L	18	LEU
2	L	23	VAL
2	L	29	CYS
2	L	39	THR
2	L	44	THR
2	L	45	LYS
2	L	47	GLU
2	L	49	LEU
2	L	58	THR
2	L	76	GLU
2	L	88	LEU
2	L	99	ILE
2	L	107	THR
1	M	354	ASN
1	M	390	LEU
1	M	448	ASN
1	M	472	ILE
1	M	480	CYS
1	M	486	PHE
1	M	498	GLN
1	M	514	SER
2	N	2	ARG
2	N	4	GLU
2	N	10	THR
2	N	18	LEU

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Mol	Chain	Res	Type
2	N	23	VAL
2	N	25	ARG
2	N	29	CYS
2	N	39	THR
2	N	41	LYS
2	N	44	THR
2	N	47	GLU
2	N	57	GLU
2	N	58	THR
2	N	88	LEU
2	N	99	ILE
2	N	107	THR
2	N	111	SER
1	O	354	ASN
1	O	386	LYS
1	O	403	ARG
1	O	448	ASN
1	O	472	ILE
1	O	480	CYS
1	O	486	PHE
1	O	498	GLN
1	O	514	SER
2	P	2	ARG
2	P	10	THR
2	P	18	LEU
2	P	23	VAL
2	P	29	CYS
2	P	39	THR
2	P	44	THR
2	P	45	LYS
2	P	47	GLU
2	P	49	LEU
2	P	58	THR
2	P	76	GLU
2	P	88	LEU
2	P	99	ILE
2	P	107	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN

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Mol	Chain	Res	Type
1	A	460	ASN
1	A	498	GLN
1	C	450	ASN
1	C	498	GLN
2	D	21	ASN
2	D	60	ASN
1	E	448	ASN
1	E	450	ASN
1	E	498	GLN
2	F	21	ASN
2	F	51	ASN
1	G	450	ASN
1	G	493	GLN
1	G	498	GLN
2	H	60	ASN
1	I	450	ASN
1	I	493	GLN
1	I	498	GLN
2	J	51	ASN
2	J	60	ASN
1	K	448	ASN
1	K	450	ASN
1	K	460	ASN
1	K	493	GLN
1	K	498	GLN
2	L	60	ASN
1	M	448	ASN
1	M	450	ASN
1	M	460	ASN
1	M	498	GLN
1	O	448	ASN
1	O	450	ASN
1	O	493	GLN
2	P	60	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 ⓘ

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	1,3	14,14,15	0.66	0	17,19,21	2.21	5 (29%)
3	NAG	Q	2	3	14,14,15	0.44	0	17,19,21	0.91	0
3	NAG	R	1	1,3	14,14,15	0.64	0	17,19,21	1.68	1 (5%)
3	NAG	R	2	3	14,14,15	0.52	0	17,19,21	0.94	0
4	NAG	S	1	4,1	14,14,15	0.60	0	17,19,21	1.47	2 (11%)
4	NAG	S	2	4	14,14,15	0.51	0	17,19,21	1.14	1 (5%)
4	BMA	S	3	4	11,11,12	0.50	0	15,15,17	0.94	1 (6%)
3	NAG	T	1	1,3	14,14,15	0.58	0	17,19,21	1.35	3 (17%)
3	NAG	T	2	3	14,14,15	0.35	0	17,19,21	1.30	3 (17%)
3	NAG	U	1	1,3	14,14,15	0.70	0	17,19,21	2.31	7 (41%)
3	NAG	U	2	3	14,14,15	0.54	0	17,19,21	1.41	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	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	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	1,3	-	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	1,3	-	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.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	1	NAG	C1-O5-C5	5.67	119.87	112.19
3	Q	1	NAG	C1-C2-N2	5.49	119.87	110.49
3	U	1	NAG	O5-C1-C2	-4.87	103.60	111.29
3	Q	1	NAG	C1-O5-C5	4.34	118.07	112.19
3	U	1	NAG	C2-N2-C7	4.33	129.07	122.90
4	S	1	NAG	C1-O5-C5	4.23	117.93	112.19
3	U	1	NAG	O5-C5-C6	3.46	112.62	107.20
3	Q	1	NAG	C2-N2-C7	3.33	127.64	122.90
4	S	2	NAG	C4-C3-C2	3.15	115.63	111.02
3	U	1	NAG	C1-O5-C5	3.02	116.29	112.19
3	Q	1	NAG	C4-C3-C2	-2.96	106.69	111.02
3	Q	1	NAG	O5-C1-C2	-2.83	106.83	111.29
3	T	2	NAG	C1-O5-C5	2.82	116.01	112.19
3	U	1	NAG	C1-C2-N2	2.79	115.26	110.49
3	T	2	NAG	C2-N2-C7	2.74	126.81	122.90
3	U	2	NAG	C1-C2-N2	2.68	115.06	110.49
4	S	1	NAG	O5-C5-C6	2.62	111.30	107.20
3	T	1	NAG	O5-C5-C6	2.56	111.22	107.20
4	S	3	BMA	O5-C5-C6	2.54	111.18	107.20
3	U	2	NAG	C2-N2-C7	2.51	126.48	122.90
3	T	1	NAG	C1-O5-C5	2.50	115.58	112.19
3	U	2	NAG	C4-C3-C2	2.38	114.50	111.02
3	U	1	NAG	C8-C7-N2	2.32	120.03	116.10
3	U	1	NAG	C4-C3-C2	-2.19	107.80	111.02
3	T	2	NAG	C8-C7-N2	2.10	119.65	116.10
3	T	1	NAG	C4-C3-C2	2.02	113.98	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	1	NAG	C3-C2-N2-C7
4	S	3	BMA	O5-C5-C6-O6
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
4	S	3	BMA	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6

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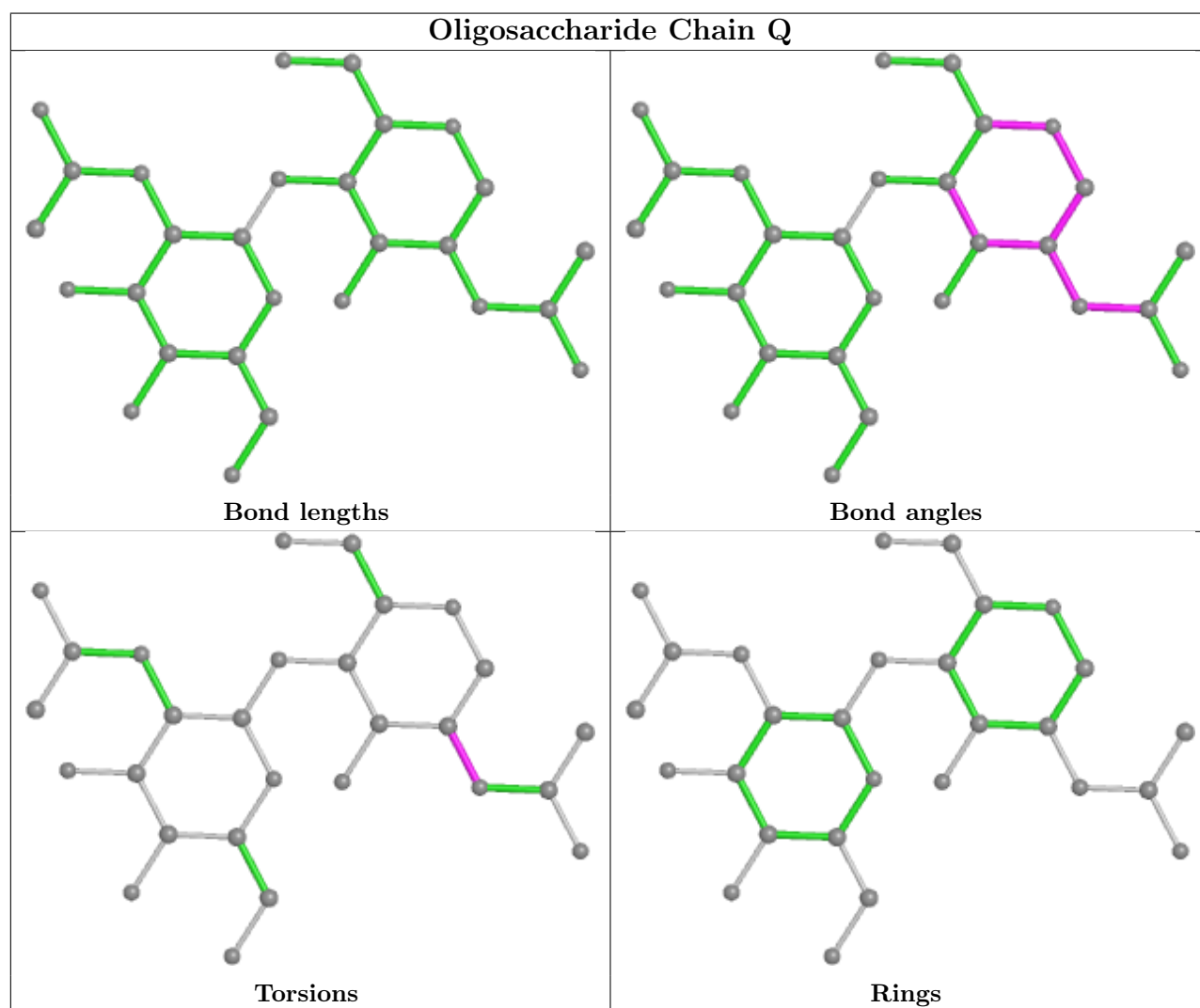
Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	C1-C2-N2-C7

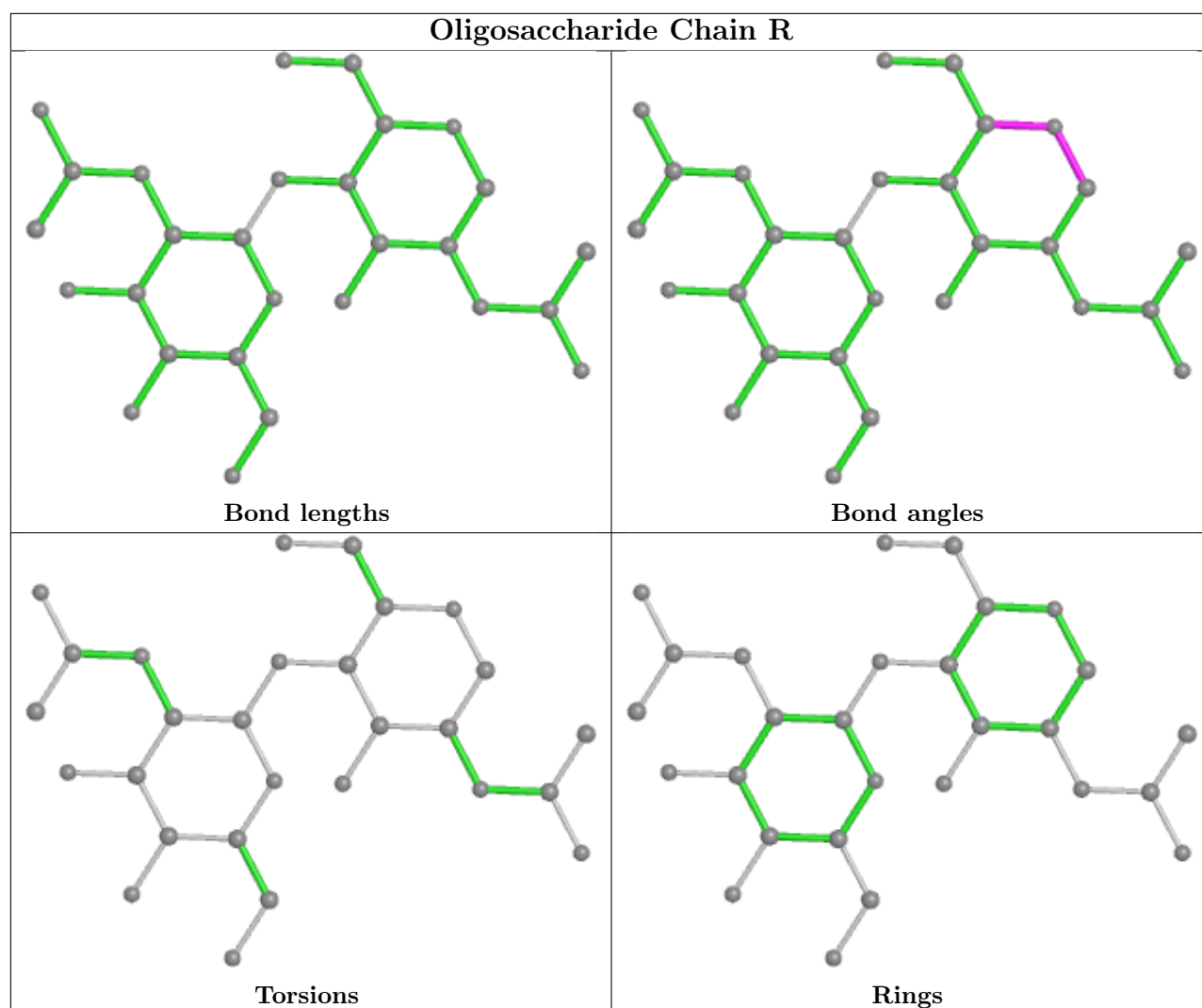
There are no ring outliers.

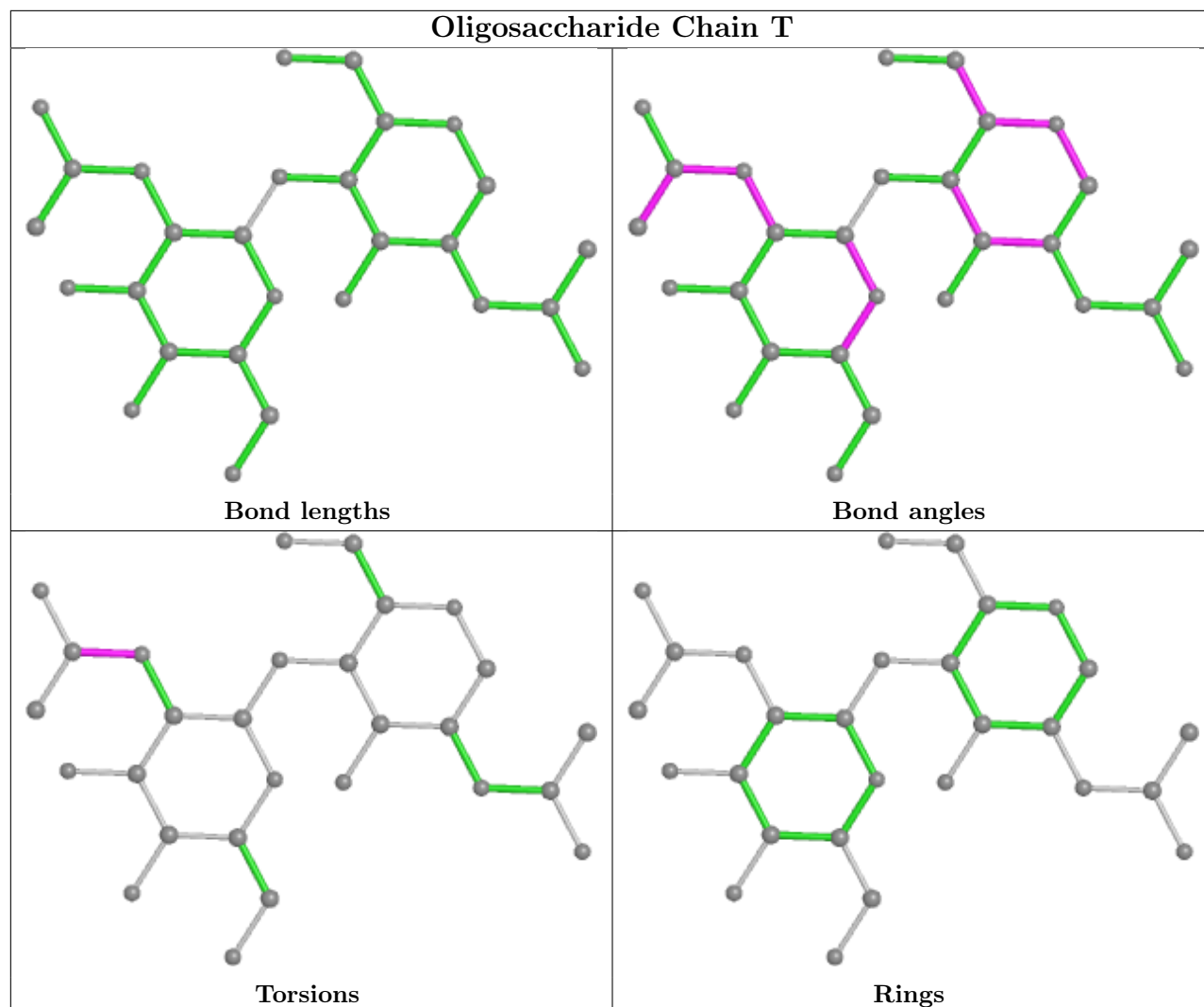
1 monomer is involved in 1 short contact:

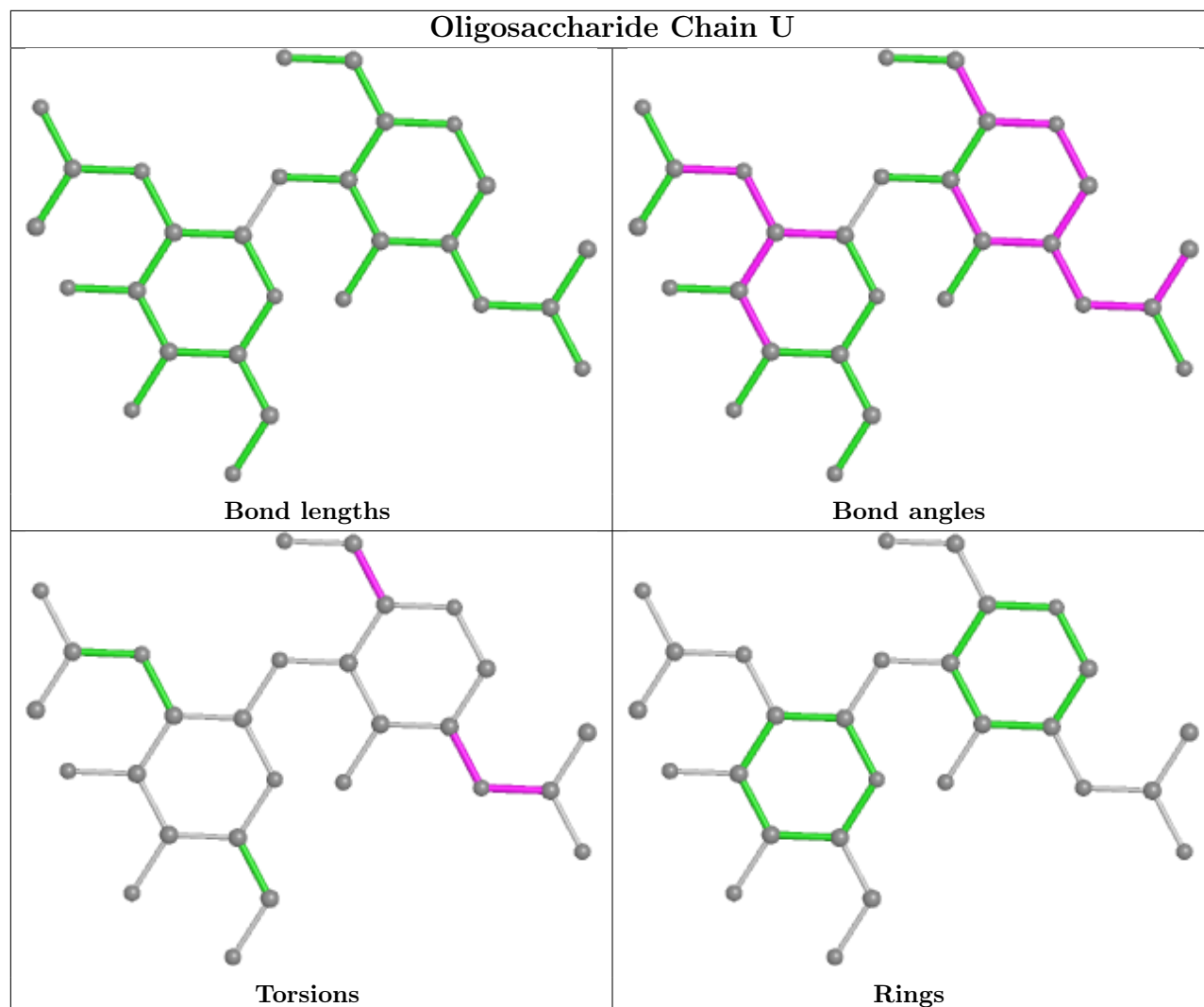
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	1	NAG	1	0

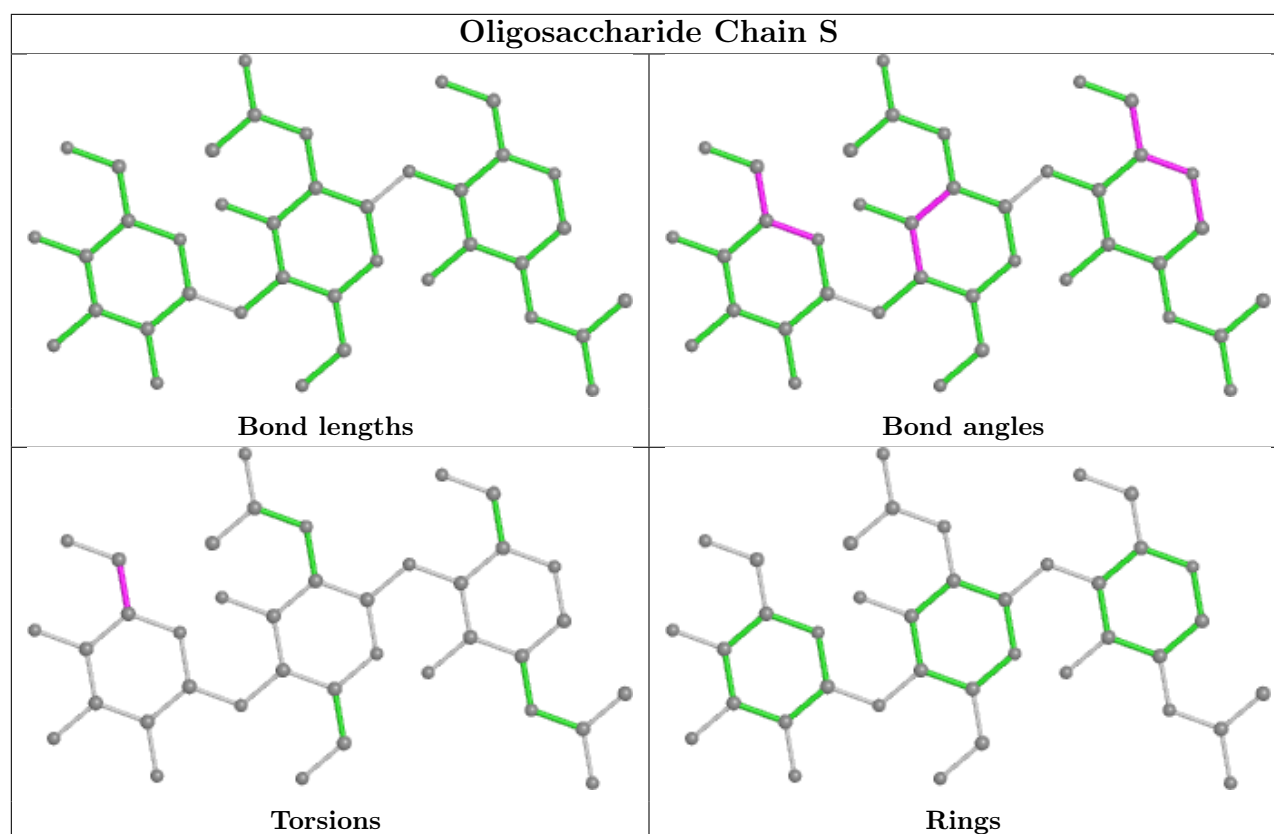
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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	E	701	1	14,14,15	1.25	1 (7%)	17,19,21	1.94	3 (17%)
5	NAG	A	701	1	14,14,15	1.17	0	17,19,21	2.33	4 (23%)
5	NAG	C	701	1	14,14,15	1.32	2 (14%)	17,19,21	2.39	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	E	701	1	-	2/6/23/26	0/1/1/1
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	701	NAG	C1-C2	2.76	1.56	1.52
5	C	701	NAG	O5-C1	2.49	1.47	1.43
5	E	701	NAG	C1-C2	2.25	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	701	NAG	C1-O5-C5	7.59	122.47	112.19
5	A	701	NAG	C1-O5-C5	7.35	122.15	112.19
5	E	701	NAG	C1-O5-C5	5.15	119.17	112.19
5	C	701	NAG	C1-C2-N2	3.68	116.78	110.49
5	E	701	NAG	O5-C5-C6	3.58	112.81	107.20
5	C	701	NAG	O5-C5-C6	3.17	112.17	107.20
5	A	701	NAG	C8-C7-N2	2.57	120.45	116.10
5	A	701	NAG	O3-C3-C2	-2.51	104.26	109.47
5	E	701	NAG	C4-C3-C2	2.44	114.60	111.02
5	A	701	NAG	C4-C3-C2	2.15	114.16	111.02

There are no chirality outliers.

All (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
5	E	701	NAG	O5-C5-C6-O6
5	C	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.45	10 (5%) 28 24	46, 66, 107, 140	0
1	C	197/230 (85%)	0.70	18 (9%) 9 6	57, 82, 132, 162	0
1	E	195/230 (84%)	0.84	29 (14%) 2 1	57, 82, 127, 165	0
1	G	198/230 (86%)	1.06	40 (20%) 1 0	58, 87, 132, 155	0
1	I	198/230 (86%)	1.03	44 (22%) 0 0	62, 88, 130, 149	0
1	K	198/230 (86%)	0.56	14 (7%) 16 12	57, 83, 127, 147	0
1	M	198/230 (86%)	0.41	7 (3%) 44 38	49, 65, 108, 140	0
1	O	197/230 (85%)	0.58	10 (5%) 28 23	57, 83, 130, 148	0
2	B	111/127 (87%)	0.79	15 (13%) 3 2	52, 78, 127, 143	0
2	D	112/127 (88%)	1.11	20 (17%) 1 1	78, 109, 150, 173	0
2	F	113/127 (88%)	1.38	31 (27%) 0 0	77, 109, 150, 166	0
2	H	114/127 (89%)	0.52	8 (7%) 16 12	54, 72, 102, 144	0
2	J	114/127 (89%)	0.41	4 (3%) 44 38	53, 72, 102, 144	0
2	L	112/127 (88%)	0.55	8 (7%) 16 12	51, 71, 96, 129	0
2	N	113/127 (88%)	0.70	11 (9%) 7 5	52, 80, 128, 149	0
2	P	111/127 (87%)	0.56	4 (3%) 42 37	52, 70, 96, 131	0
All	All	2480/2856 (86%)	0.72	273 (11%) 5 4	46, 80, 134, 173	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	333	THR	8.3
2	D	49	LEU	7.7
2	F	50	SER	7.7
1	G	333	THR	6.8
2	D	48	SER	6.2

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Mol	Chain	Res	Type	RSRZ
2	F	68	LEU	6.1
2	D	24	LEU	6.0
2	F	18	LEU	5.6
1	I	351	TYR	5.3
1	G	521	PRO	5.3
2	F	51	ASN	5.2
1	G	423	TYR	5.1
1	G	523	THR	4.9
2	B	47	GLU	4.8
1	G	402	ILE	4.8
2	H	111	SER	4.8
1	M	519	HIS	4.7
2	D	50	SER	4.6
1	I	452	LEU	4.6
2	F	77	ASP	4.6
1	E	527	PRO	4.6
2	D	81	TYR	4.6
2	B	50	SER	4.5
2	N	35	TYR	4.4
1	K	483	VAL	4.4
1	G	400	PHE	4.4
1	C	372	ALA	4.4
1	E	351	TYR	4.4
2	L	24	LEU	4.3
1	C	341	VAL	4.3
1	C	338	PHE	4.1
1	C	519	HIS	4.1
2	F	31	LEU	4.1
2	F	112	GLY	4.0
2	J	70	ILE	3.9
1	I	505	TYR	3.9
2	F	24	LEU	3.9
2	F	21	ASN	3.9
1	K	477	SER	3.9
1	E	519	HIS	3.8
2	B	110	SER	3.8
2	F	20	ILE	3.8
2	B	38	PHE	3.8
2	H	51	ASN	3.7
2	B	52	GLY	3.7
1	E	468	ILE	3.7
2	F	49	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	N	50	SER	3.6
2	D	20	ILE	3.6
1	G	360	ASN	3.5
1	E	455	LEU	3.5
1	I	402	ILE	3.5
2	D	98	TYR	3.5
2	F	6	THR	3.5
1	E	338	PHE	3.5
1	K	476	GLY	3.4
1	I	521	PRO	3.4
1	I	491	PRO	3.4
1	G	410	ILE	3.4
1	I	523	THR	3.4
2	F	37	TYR	3.4
1	G	510	VAL	3.4
2	F	106	VAL	3.4
1	G	464	PHE	3.4
1	G	351	TYR	3.3
2	B	81	TYR	3.3
1	I	387	LEU	3.3
1	M	486	PHE	3.3
1	G	518	LEU	3.3
2	F	81	TYR	3.2
2	F	46	LYS	3.2
1	C	486	PHE	3.2
1	G	515	PHE	3.2
1	G	522	ALA	3.2
2	F	36	TRP	3.2
2	F	35	TYR	3.2
1	I	392	PHE	3.2
1	I	471	GLU	3.2
1	C	348	ALA	3.2
1	G	494	SER	3.2
1	I	524	VAL	3.1
2	L	85	ALA	3.1
2	N	40	LYS	3.1
1	G	387	LEU	3.1
1	I	464	PHE	3.1
1	C	517	LEU	3.1
2	D	46	LYS	3.1
1	G	394	ASN	3.1
1	I	423	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	337	PRO	3.1
1	E	401	VAL	3.1
1	I	350	VAL	3.1
2	D	82	HIS	3.1
2	D	18	LEU	3.1
1	I	472	ILE	3.0
2	L	69	ARG	3.0
1	M	342	PHE	3.0
1	I	495	TYR	3.0
1	I	496	GLY	3.0
2	B	70	ILE	3.0
2	F	92	MET	3.0
1	K	517	LEU	3.0
1	O	357	ARG	3.0
1	I	358	ILE	3.0
1	I	522	ALA	2.9
1	E	495	TYR	2.9
2	J	51	ASN	2.9
2	P	69	ARG	2.9
1	O	340	GLU	2.9
1	C	479	PRO	2.9
1	E	341	VAL	2.9
1	G	477	SER	2.9
2	F	110	SER	2.9
1	C	455	LEU	2.9
1	M	365	TYR	2.9
1	I	410	ILE	2.9
1	E	342	PHE	2.8
2	L	1	GLU	2.8
2	F	48	SER	2.8
1	I	342	PHE	2.8
2	F	66	PHE	2.8
1	O	495	TYR	2.8
2	B	76	GLU	2.8
2	P	111	SER	2.8
1	G	350	VAL	2.8
1	G	407	VAL	2.8
1	I	518	LEU	2.8
2	F	90	ALA	2.8
1	A	486	PHE	2.8
1	C	342	PHE	2.7
2	F	69	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	99	ILE	2.7
2	D	21	ASN	2.7
1	O	470	THR	2.7
1	E	356	LYS	2.7
2	F	12	LYS	2.7
2	N	83	CYS	2.7
1	C	365	TYR	2.7
1	E	417	LYS	2.7
1	I	352	ALA	2.7
1	I	519	HIS	2.7
2	F	111	SER	2.6
1	A	396	TYR	2.6
1	A	519	HIS	2.6
1	O	483	VAL	2.6
1	A	338	PHE	2.6
1	G	474	GLN	2.6
2	N	81	TYR	2.6
1	C	521	PRO	2.6
1	K	335	LEU	2.6
1	E	451	TYR	2.6
2	B	37	TYR	2.6
1	M	515	PHE	2.6
2	J	38	PHE	2.6
1	G	524	VAL	2.6
1	I	353	TRP	2.6
2	H	48	SER	2.5
1	C	387	LEU	2.5
1	G	401	VAL	2.5
1	G	359	SER	2.5
1	E	387	LEU	2.5
1	O	492	LEU	2.5
2	D	37	TYR	2.5
1	M	363	ALA	2.5
2	B	90	ALA	2.5
2	F	19	THR	2.5
1	G	516	GLU	2.4
1	G	422	ASN	2.4
1	E	497	PHE	2.4
2	N	44	THR	2.4
1	E	357	ARG	2.4
2	H	50	SER	2.4
1	I	360	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	401	VAL	2.4
1	I	486	PHE	2.4
1	I	455	LEU	2.4
2	D	110	SER	2.4
1	K	365	TYR	2.4
1	I	390	LEU	2.4
1	C	355	ARG	2.4
1	C	333	THR	2.4
2	D	51	ASN	2.4
1	A	397	ALA	2.3
1	E	496	GLY	2.3
2	N	108	VAL	2.3
1	E	372	ALA	2.3
1	I	513	LEU	2.3
2	F	22	CYS	2.3
1	G	519	HIS	2.3
1	M	387	LEU	2.3
2	P	24	LEU	2.3
1	G	513	LEU	2.3
1	I	357	ARG	2.3
1	G	395	VAL	2.3
2	D	68	LEU	2.3
1	O	468	ILE	2.3
2	D	99	ILE	2.3
2	B	101	GLY	2.2
2	L	30	ALA	2.2
2	H	20	ILE	2.2
1	E	390	LEU	2.2
1	A	410	ILE	2.2
1	I	490	PHE	2.2
2	N	70	ILE	2.2
1	K	360	ASN	2.2
1	A	337	PRO	2.2
2	B	24	LEU	2.2
2	D	85	ALA	2.2
1	G	396	TYR	2.2
1	O	511	VAL	2.2
1	G	398	ASP	2.2
1	K	351	TYR	2.2
2	F	42	GLY	2.2
1	E	518	LEU	2.2
1	I	399	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	-2	ALA	2.2
1	I	436	TRP	2.2
1	I	492	LEU	2.2
1	E	486	PHE	2.2
1	O	486	PHE	2.2
1	K	495	TYR	2.2
2	D	109	ASN	2.2
1	E	453	TYR	2.2
1	G	505	TYR	2.2
1	G	353	TRP	2.1
2	B	48	SER	2.1
1	I	497	PHE	2.1
1	G	363	ALA	2.1
2	H	55	TYR	2.1
1	E	391	CYS	2.1
1	G	435	ALA	2.1
1	K	418	ILE	2.1
1	K	484	GLU	2.1
1	I	501	ASN	2.1
2	N	111	SER	2.1
1	E	333	THR	2.1
2	L	10	THR	2.1
1	G	347	PHE	2.1
1	I	347	PHE	2.1
1	C	373	SER	2.1
1	G	392	PHE	2.1
1	G	403	ARG	2.1
2	H	81	TYR	2.1
2	H	70	ILE	2.1
1	G	365	TYR	2.1
1	A	332	ILE	2.1
2	N	29	CYS	2.1
1	C	418	ILE	2.1
1	E	526	GLY	2.1
1	A	516	GLU	2.1
1	G	503	VAL	2.1
2	N	49	LEU	2.0
2	B	51	ASN	2.0
2	F	82	HIS	2.0
1	K	357	ARG	2.0
2	L	27	SER	2.0
1	E	365	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	384	PRO	2.0
1	E	392	PHE	2.0
2	B	66	PHE	2.0
1	K	402	ILE	2.0
2	L	20	ILE	2.0
1	C	340	GLU	2.0
1	I	394	ASN	2.0
1	I	466	ARG	2.0
1	I	481	ASN	2.0
1	O	354	ASN	2.0
2	D	77	ASP	2.0
2	D	78	SER	2.0
1	E	350	VAL	2.0
2	P	44	THR	2.0
1	I	400	PHE	2.0
1	E	368	LEU	2.0

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

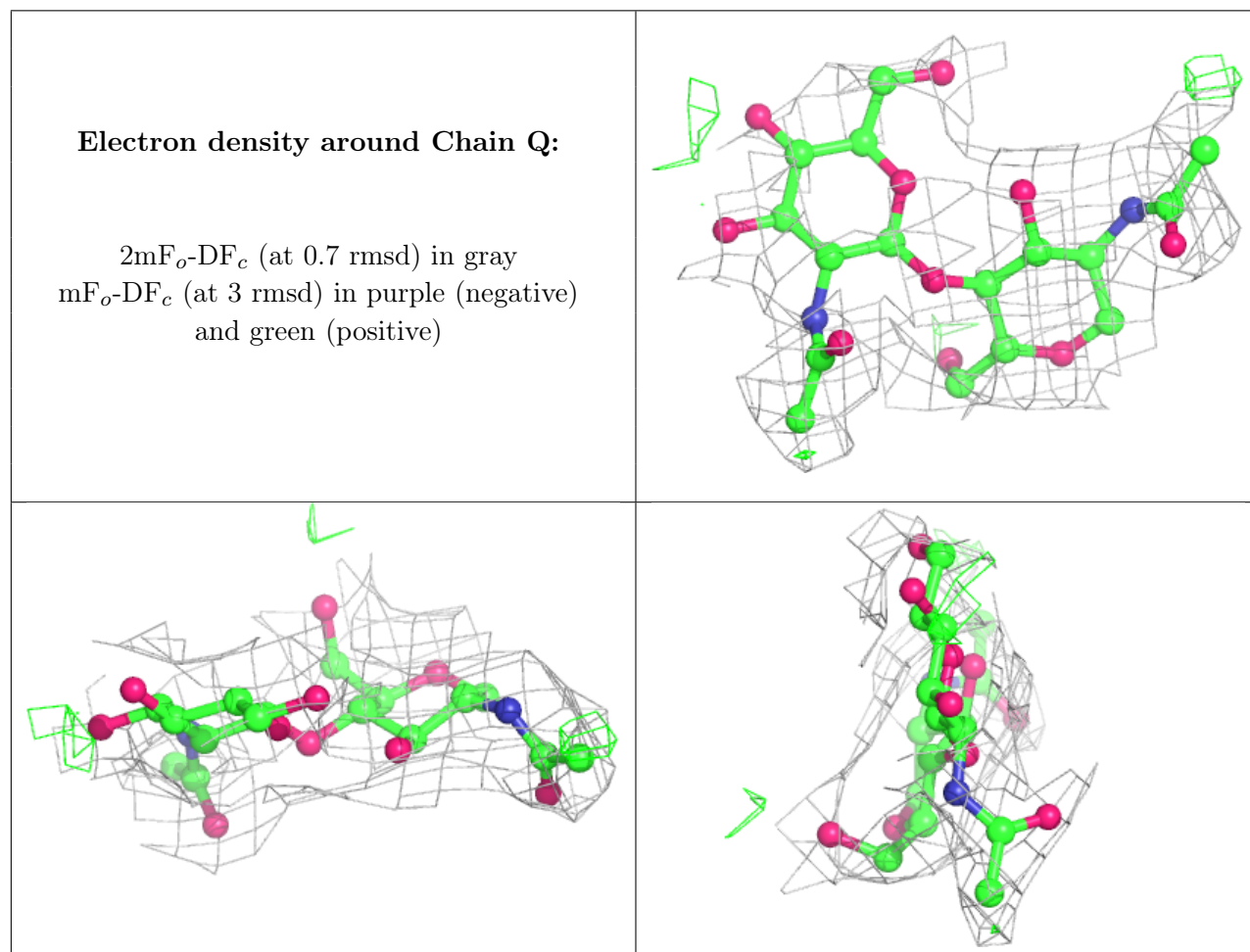
There are no non-standard protein/DNA/RNA residues in this entry.

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.

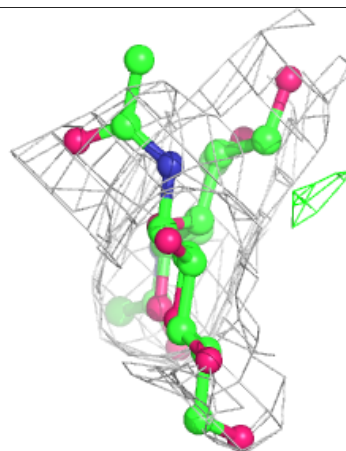
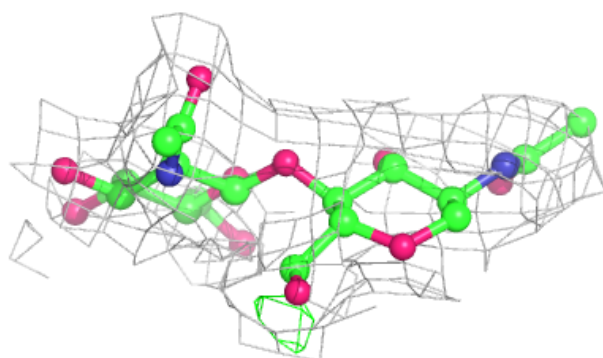
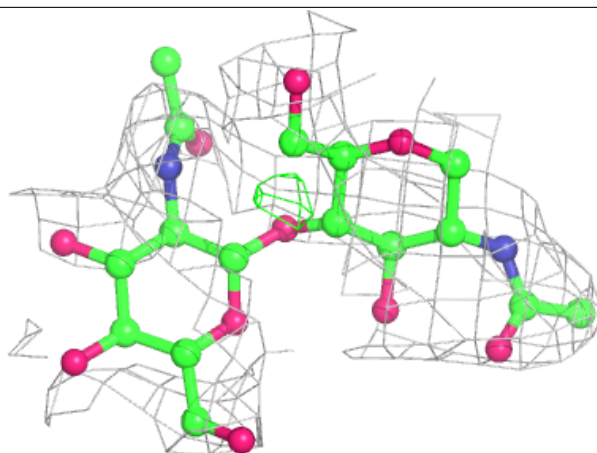
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	S	3	11/12	0.33	0.33	143,158,168,170	0
3	NAG	U	2	14/15	0.61	0.34	136,141,153,154	0
3	NAG	U	1	14/15	0.67	0.23	100,114,122,136	0
3	NAG	T	2	14/15	0.69	0.22	91,130,141,145	0
3	NAG	Q	2	14/15	0.73	0.20	113,124,134,134	0
3	NAG	T	1	14/15	0.76	0.24	92,103,115,126	0
3	NAG	R	2	14/15	0.78	0.20	106,132,143,144	0
4	NAG	S	2	14/15	0.82	0.21	130,151,162,163	0
4	NAG	S	1	14/15	0.85	0.17	89,106,111,128	0
3	NAG	Q	1	14/15	0.88	0.16	83,96,102,115	0
3	NAG	R	1	14/15	0.88	0.14	79,92,94,106	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.



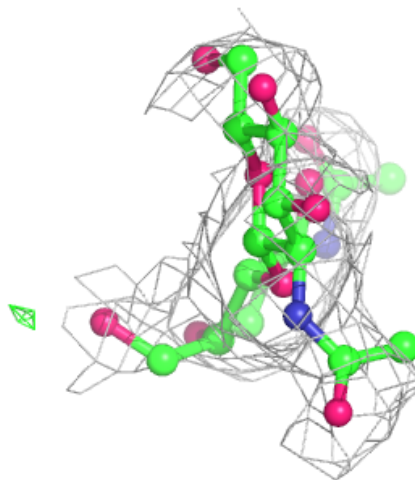
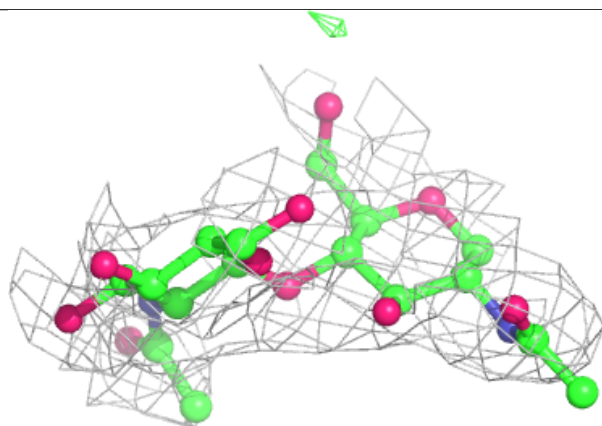
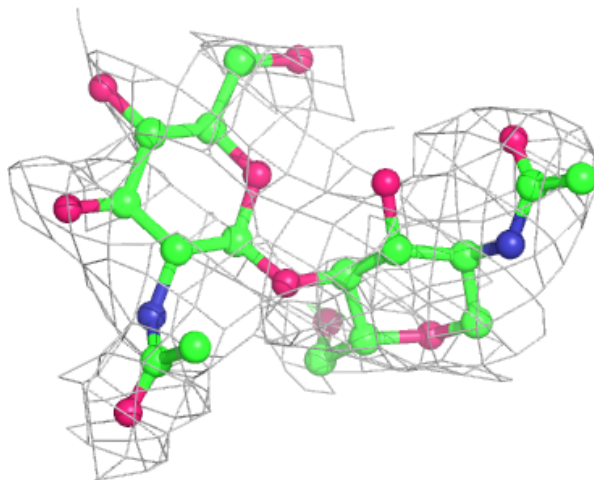
Electron density around Chain R:

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



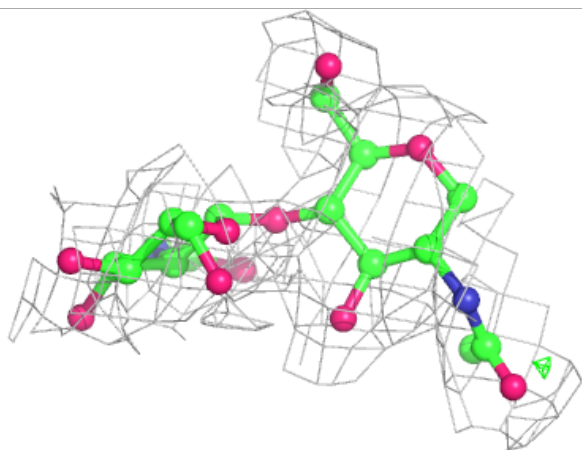
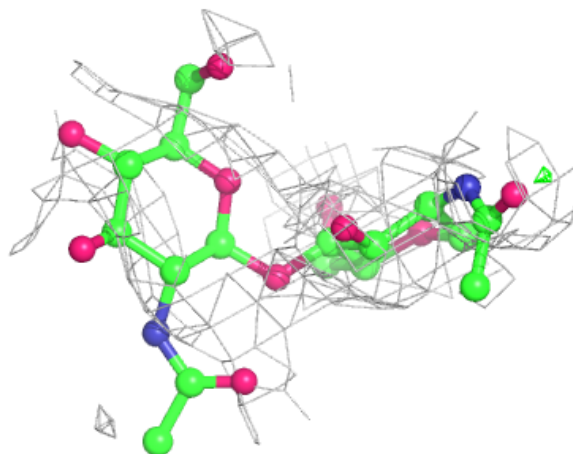
Electron density around Chain T:

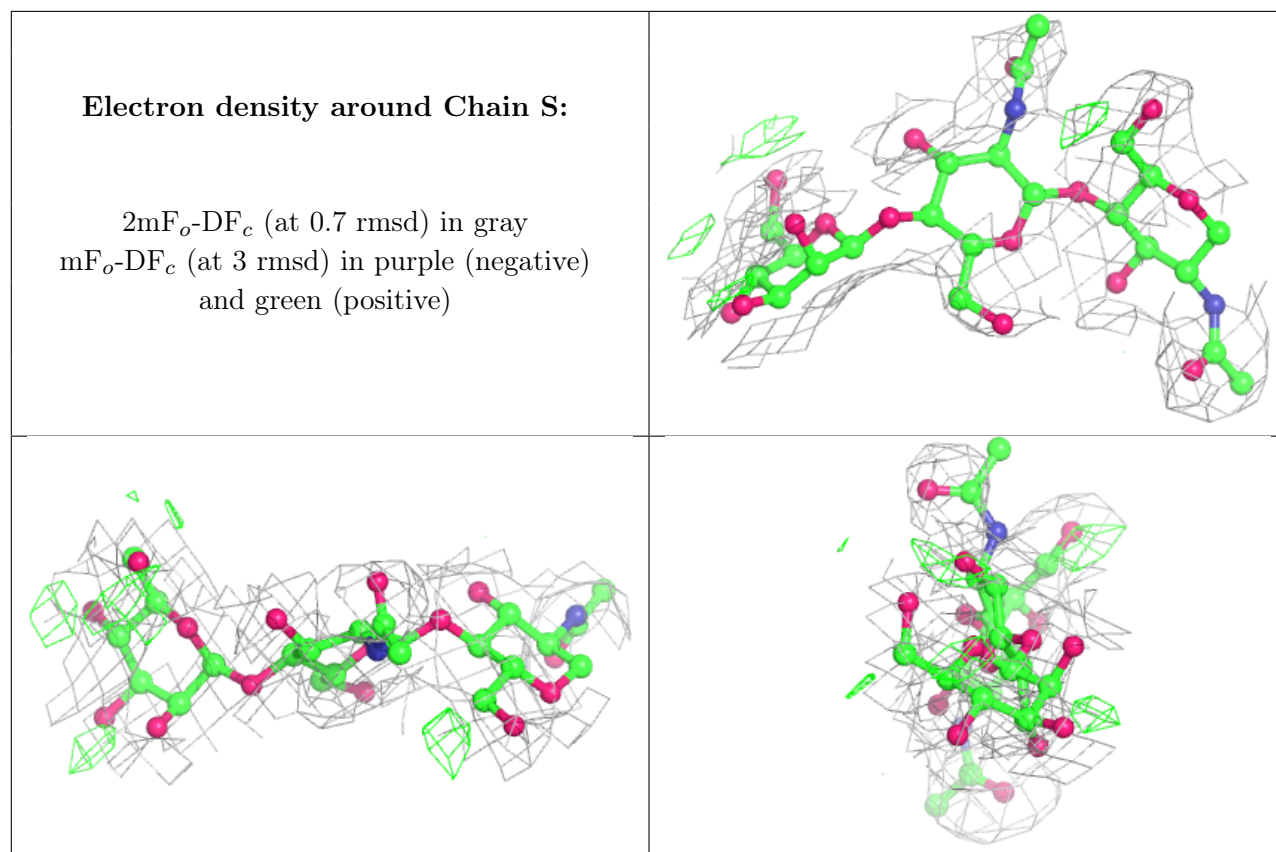
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(Å ²)	Q<0.9
5	NAG	E	701	14/15	0.58	0.30	104,116,120,122	0
5	NAG	C	701	14/15	0.60	0.25	106,119,124,125	0
5	NAG	A	701	14/15	0.81	0.20	89,95,99,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.