



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:29 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

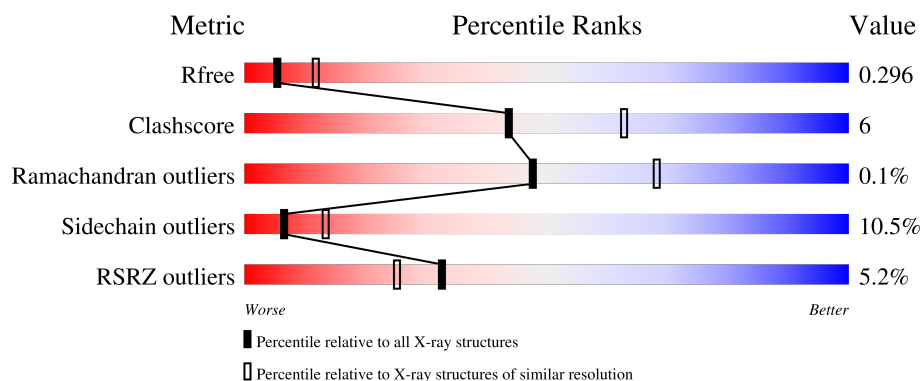
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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

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.



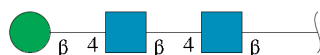
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

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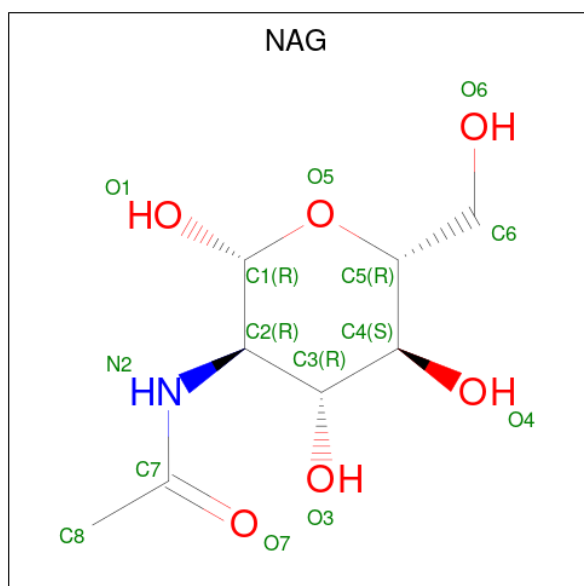
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 (CCD ID: 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		

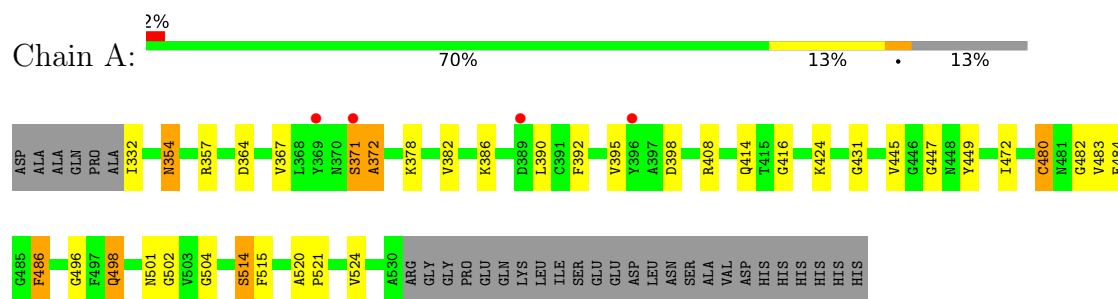
- Molecule 6 is water.

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

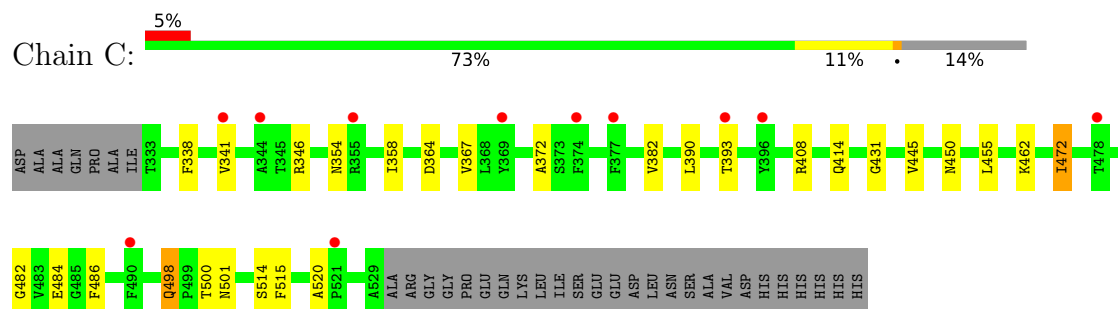
3 Residue-property plots

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.

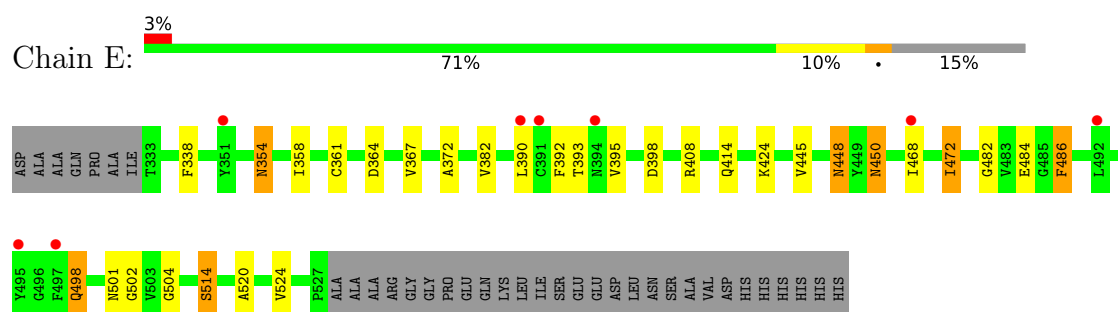
• Molecule 1: Spike protein S1



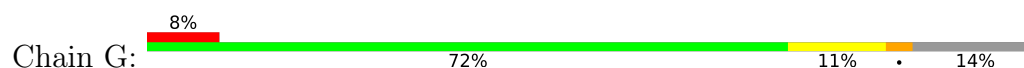
• Molecule 1: Spike protein S1

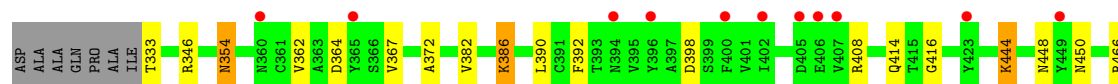


• Molecule 1: Spike protein S1

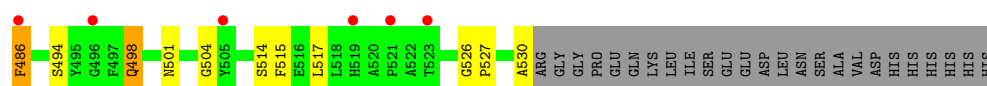
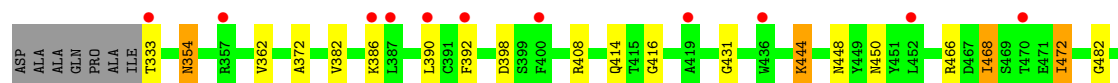


• Molecule 1: Spike protein S1

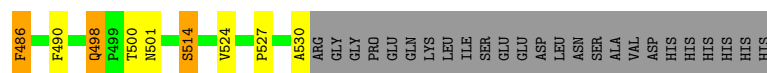
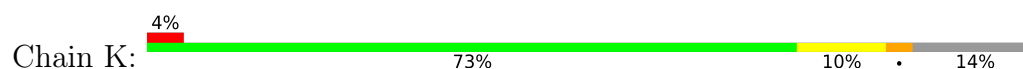




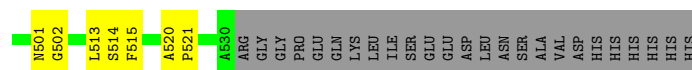
• Molecule 1: Spike protein S1



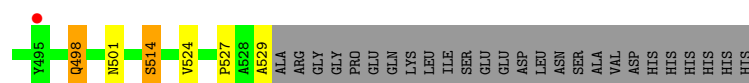
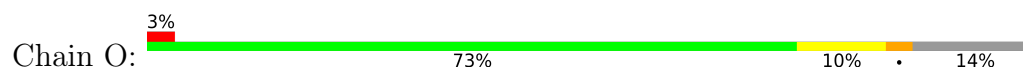
• Molecule 1: Spike protein S1



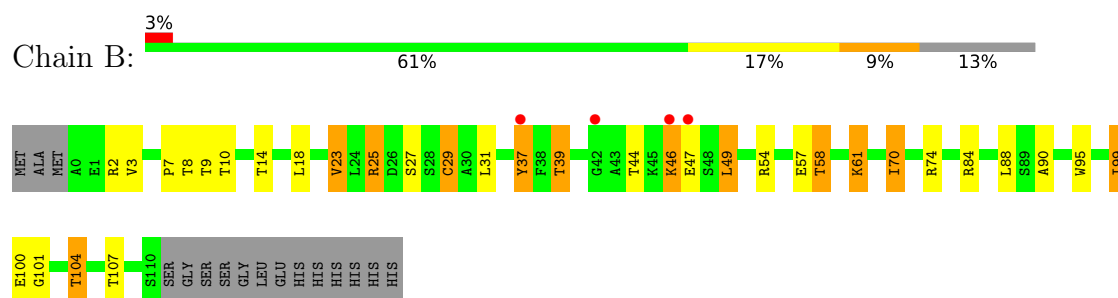
• Molecule 1: Spike protein S1



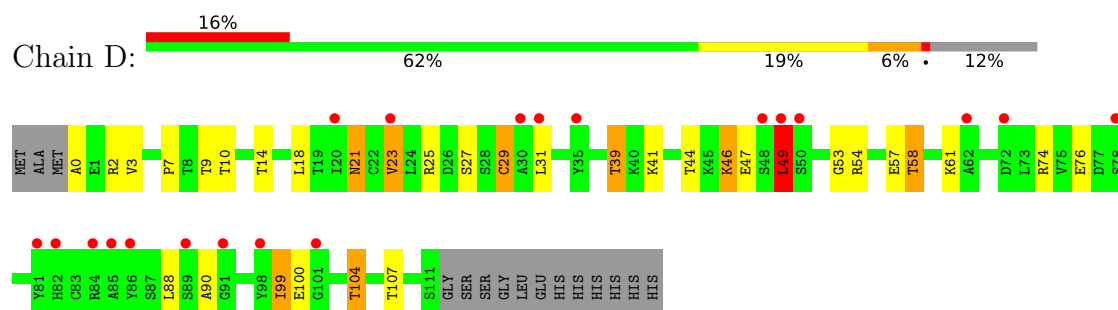
• Molecule 1: Spike protein S1



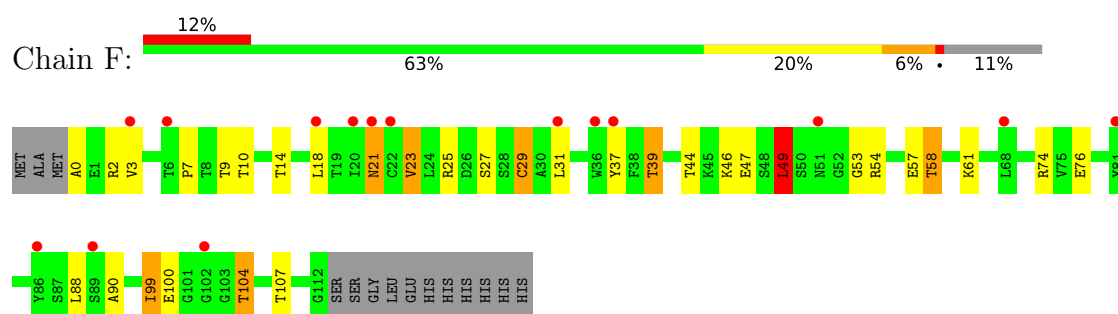
- Molecule 2: New antigen receptor variable domain



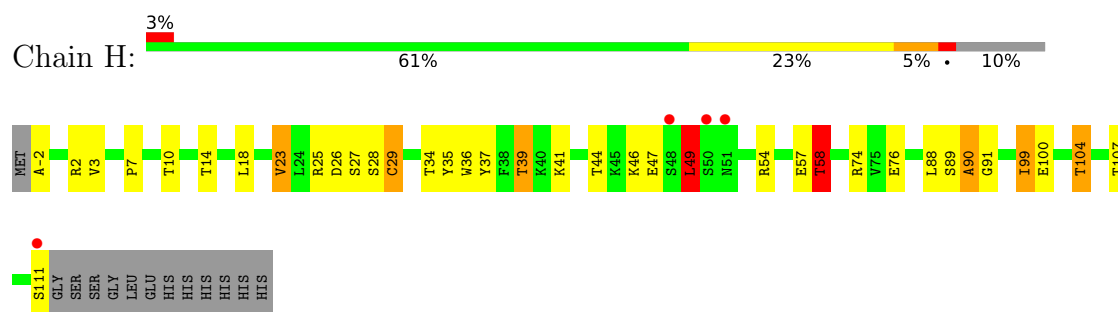
- Molecule 2: New antigen receptor variable domain



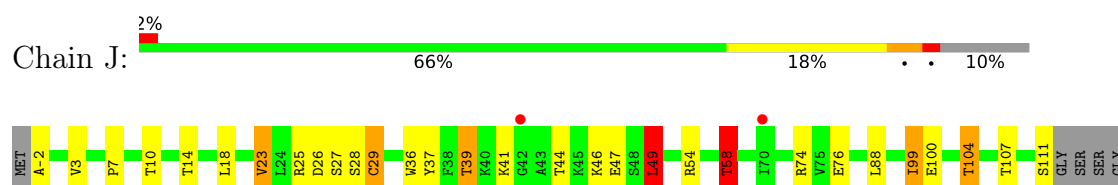
- Molecule 2: New antigen receptor variable domain



- Molecule 2: New antigen receptor variable domain



- Molecule 2: New antigen receptor variable domain



LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 2: New antigen receptor variable domain

Chain L: 2% 61% 20% 5% 12%

MET ALA MET AO E1 R2 V3 P7 T8 T9 T10 T14 L18 V23 L24 R25 D26 S27 S28 C29 V36 Y37 F38 T39 T44 K45 K46 E47 S48 L49 R54 E57 T58 V59 N60 R74 V75 E76 Y81 L88 S89 A90 I99 T104 I105 V106 T107

S111
GLY
SER
SER
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 2: New antigen receptor variable domain

Chain N: 2% 62% 17% 8% 11%

MET ALA M-1 R2 V3 P7 T8 T9 T10 T14 L18 N21 C22 V23 L24 R25 D26 S27 S28 C29 A30 L31 Y37 F38 T39 K40 K41 T44 K45 K46 E47 S48 L49 S50 N51 R54 E57 T58 K61 R74 V75 E76 C83 L88 W95

I99 E100 T104 T107 S111
GLY
SER
SER
GLY
LEU
GLU
HIS
HIS
HIS
HIS

- Molecule 2: New antigen receptor variable domain

Chain P: 2% 61% 20% 6% 13%

MET ALA MET MET E1 R2 V3 P7 T8 T9 T10 T14 L18 V23 L24 R25 D26 S27 S28 C29 V36 Y37 F38 T39 T44 K45 K46 E47 S48 L49 R54 E57 T58 V59 N60 K61 A62 R74 V75 E76 L88 S89 A90 I99 E100 T104 I105 V106

T107 S110 S111
GLY
SER
SER
GLY
LEU
GLU
HIS
HIS
HIS
HIS

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

Chain Q: 50% 50%

MAG1
MAG2

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

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:  33%  67%

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 90.40 – 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)	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	3648 reflections (4.79%)	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)	0.31 , 75.0	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	0.80	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 [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%)

All (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
2	B	90	ALA	C-O	7.18	1.32	1.24
2	H	90	ALA	C-O	7.11	1.31	1.24
2	H	104	THR	C-O	7.07	1.32	1.24
2	L	104	THR	C-O	7.03	1.32	1.24
2	P	104	THR	C-O	6.95	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	104	THR	C-O	6.89	1.31	1.24
2	B	104	THR	C-O	6.51	1.31	1.24
1	M	341	VAL	C-O	6.51	1.31	1.24
2	F	90	ALA	C-O	6.42	1.31	1.24
2	D	90	ALA	C-O	6.36	1.31	1.24
2	N	104	THR	C-O	6.33	1.31	1.24
1	K	514	SER	C-O	6.00	1.30	1.23
1	E	514	SER	C-O	5.98	1.30	1.23
1	O	361	CYS	C-O	5.91	1.30	1.23
1	A	504	GLY	C-O	5.84	1.31	1.23
1	O	514	SER	C-O	5.79	1.30	1.23
2	H	89	SER	C-O	5.70	1.31	1.23
1	M	502	GLY	C-O	5.61	1.31	1.23
1	K	361	CYS	C-O	5.61	1.30	1.23
1	O	430	THR	C-O	5.46	1.30	1.24
1	A	502	GLY	C-O	5.38	1.31	1.23
1	E	502	GLY	C-O	5.37	1.31	1.23
1	A	514	SER	C-O	5.33	1.30	1.24
1	K	430	THR	C-O	5.32	1.30	1.24
1	I	504	GLY	C-O	5.30	1.30	1.23
1	E	361	CYS	C-O	5.28	1.30	1.23
1	G	504	GLY	C-O	5.28	1.30	1.23
1	E	504	GLY	C-O	5.24	1.30	1.23
2	L	60	ASN	C-O	5.19	1.29	1.24
2	P	60	ASN	C-O	5.16	1.29	1.24
2	B	101	GLY	C-O	5.15	1.30	1.23

All (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
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
2	P	58	THR	CA-C-O	-6.50	113.50	121.11
1	A	480	CYS	CA-C-O	-6.48	112.09	119.41
1	O	403	ARG	CG-CD-NE	6.47	126.24	112.00
1	A	371	SER	CA-C-O	-6.39	111.37	120.51
2	H	58	THR	CA-C-O	-6.38	113.65	121.11
2	J	58	THR	CA-C-O	-6.15	113.91	121.11
1	I	466	ARG	CB-CG-CD	6.12	125.38	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	14	THR	CA-C-O	-5.97	114.97	120.95
2	D	58	THR	CA-C-O	-5.95	114.15	121.11
2	F	58	THR	CA-C-O	-5.88	114.23	121.11
2	L	37	TYR	CA-C-O	-5.83	114.28	121.11
2	N	14	THR	CA-C-O	-5.82	115.13	120.95
2	B	14	THR	CA-C-O	-5.82	115.13	120.95
1	A	445	VAL	N-CA-C	-5.81	101.31	109.21
1	E	445	VAL	N-CA-C	-5.75	101.40	109.21
2	B	58	THR	CA-C-O	-5.74	114.40	121.11
2	H	14	THR	CA-C-O	-5.72	115.22	120.95
2	H	37	TYR	CA-C-O	-5.71	114.43	121.11
2	D	14	THR	CA-C-O	-5.70	115.25	120.95
1	G	526	GLY	CA-C-N	5.66	125.33	119.56
1	G	526	GLY	C-N-CA	5.66	125.33	119.56
1	I	526	GLY	CA-C-N	5.66	125.33	119.56
1	I	526	GLY	C-N-CA	5.66	125.33	119.56
2	P	36	TRP	CA-C-N	5.65	131.43	122.62
2	P	36	TRP	C-N-CA	5.65	131.43	122.62
2	L	36	TRP	CA-C-N	5.64	131.41	122.62
2	L	36	TRP	C-N-CA	5.64	131.41	122.62
1	G	392	PHE	CA-C-N	5.62	128.07	120.65
1	G	392	PHE	C-N-CA	5.62	128.07	120.65
2	P	37	TYR	CA-C-O	-5.61	114.55	121.11
2	J	37	TYR	CA-C-O	-5.60	114.56	121.11
2	P	49	LEU	CA-C-O	-5.60	115.03	121.19
2	F	14	THR	CA-C-O	-5.59	115.36	120.95
1	C	445	VAL	N-CA-C	-5.58	101.62	109.21
1	A	416	GLY	CA-C-O	-5.56	117.83	122.33
2	L	14	THR	CA-C-O	-5.54	115.08	121.07
1	O	416	GLY	CA-C-O	-5.54	117.84	122.33
1	K	416	GLY	CA-C-O	-5.51	117.87	122.33
1	A	392	PHE	CA-C-N	5.45	127.85	120.65
1	A	392	PHE	C-N-CA	5.45	127.85	120.65
2	F	49	LEU	CA-C-O	-5.45	115.20	121.47
2	N	9	THR	CA-C-O	-5.45	114.74	121.06
2	D	49	LEU	CA-C-O	-5.45	115.21	121.47
2	J	14	THR	CA-C-O	-5.45	115.19	121.07
2	H	36	TRP	CA-C-N	5.41	131.06	122.62
2	H	36	TRP	C-N-CA	5.41	131.06	122.62
2	N	37	TYR	CA-C-O	-5.38	114.81	121.11
1	I	392	PHE	CA-C-N	5.37	127.74	120.65
1	I	392	PHE	C-N-CA	5.37	127.74	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	THR	CA-C-O	-5.37	114.84	121.06
1	M	392	PHE	CA-C-N	5.36	127.73	120.65
1	M	392	PHE	C-N-CA	5.36	127.73	120.65
2	N	58	THR	CA-C-O	-5.35	114.85	121.11
2	H	49	LEU	CA-C-O	-5.34	115.31	121.19
2	J	36	TRP	CA-C-N	5.33	130.94	122.62
2	J	36	TRP	C-N-CA	5.33	130.94	122.62
2	L	49	LEU	CA-C-O	-5.31	115.35	121.19
2	B	37	TYR	CA-C-O	-5.29	114.92	121.11
2	L	1	GLU	CB-CG-CD	5.29	121.59	112.60
2	J	49	LEU	CA-C-O	-5.26	115.40	121.19
1	I	416	GLY	CA-C-O	-5.26	118.07	122.33
2	D	9	THR	CA-C-O	-5.18	115.05	121.06
2	L	9	THR	CA-C-O	-5.17	115.06	121.06
2	B	61	LYS	CA-C-O	-5.17	114.94	120.42
2	P	9	THR	CA-C-O	-5.15	115.09	121.06
2	N	29	CYS	N-CA-CB	-5.14	102.30	110.06
2	B	49	LEU	CA-C-O	-5.13	115.57	121.47
1	G	416	GLY	CA-C-O	-5.11	118.19	122.33
1	C	455	LEU	N-CA-CB	-5.08	103.06	110.53
2	F	9	THR	CA-C-O	-5.06	115.19	121.06
2	N	49	LEU	CA-C-O	-5.06	115.28	121.05
1	E	392	PHE	CA-C-N	5.02	127.28	120.65
1	E	392	PHE	C-N-CA	5.02	127.28	120.65
2	F	37	TYR	CA-C-O	-5.01	115.25	121.11
1	M	455	LEU	N-CA-CB	-5.00	103.17	110.53

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

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

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:484:GLU:CD	2:L:25:ARG:NH2	2.57	0.62
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:90:ALA:C	6:H:201:HOH:O	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:K:486:PHE:CG	2:N:21:ASN:CG	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	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 ⓘ

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

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ILE
1	A	354	ASN
1	A	357	ARG
1	A	382	VAL
1	A	386	LYS
1	A	390	LEU
1	A	424	LYS
1	A	486	PHE
1	A	498	GLN
1	A	514	SER
2	B	2	ARG
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

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Mol	Chain	Res	Type
2	B	44	THR
2	B	46	LYS
2	B	47	GLU
2	B	49	LEU
2	B	57	GLU
2	B	58	THR
2	B	70	ILE
2	B	88	LEU
2	B	99	ILE
2	B	107	THR
1	C	346	ARG
1	C	354	ASN
1	C	382	VAL
1	C	390	LEU
1	C	462	LYS
1	C	472	ILE
1	C	498	GLN
1	C	500	THR
1	C	514	SER
2	D	2	ARG
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
2	D	44	THR
2	D	46	LYS
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	354	ASN
1	E	382	VAL
1	E	390	LEU
1	E	424	LYS
1	E	448	ASN

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Mol	Chain	Res	Type
1	E	450	ASN
1	E	472	ILE
1	E	486	PHE
1	E	498	GLN
1	E	514	SER
2	F	2	ARG
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	382	VAL
1	G	386	LYS
1	G	390	LEU
1	G	444	LYS
1	G	468	ILE
1	G	472	ILE
1	G	483	VAL
1	G	486	PHE
1	G	498	GLN
1	G	514	SER
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

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Mol	Chain	Res	Type
2	H	49	LEU
2	H	57	GLU
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	382	VAL
1	I	386	LYS
1	I	390	LEU
1	I	444	LYS
1	I	468	ILE
1	I	472	ILE
1	I	486	PHE
1	I	494	SER
1	I	498	GLN
1	I	514	SER
1	I	517	LEU
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
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	382	VAL
1	K	390	LEU
1	K	448	ASN
1	K	458	LYS
1	K	462	LYS
1	K	472	ILE

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Mol	Chain	Res	Type
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	57	GLU
2	L	58	THR
2	L	76	GLU
2	L	88	LEU
2	L	99	ILE
2	L	105	ILE
2	L	107	THR
1	M	354	ASN
1	M	357	ARG
1	M	382	VAL
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	8	THR
2	N	10	THR
2	N	18	LEU
2	N	23	VAL
2	N	25	ARG
2	N	29	CYS
2	N	39	THR
2	N	41	LYS
2	N	44	THR

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Mol	Chain	Res	Type
2	N	46	LYS
2	N	47	GLU
2	N	49	LEU
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	382	VAL
1	O	386	LYS
1	O	390	LEU
1	O	403	ARG
1	O	448	ASN
1	O	472	ILE
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	47	GLU
2	P	49	LEU
2	P	57	GLU
2	P	58	THR
2	P	76	GLU
2	P	88	LEU
2	P	99	ILE
2	P	105	ILE
2	P	107	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	460	ASN
1	A	487	ASN

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Mol	Chain	Res	Type
1	A	498	GLN
2	B	60	ASN
2	B	82	HIS
1	C	450	ASN
1	C	487	ASN
1	C	498	GLN
2	D	51	ASN
2	D	60	ASN
2	D	82	HIS
1	E	448	ASN
1	E	450	ASN
1	E	487	ASN
1	E	498	GLN
2	F	51	ASN
2	F	82	HIS
1	G	354	ASN
1	G	450	ASN
1	G	487	ASN
1	G	493	GLN
1	G	498	GLN
2	H	60	ASN
2	H	82	HIS
1	I	354	ASN
1	I	450	ASN
1	I	487	ASN
1	I	493	GLN
1	I	498	GLN
2	J	51	ASN
2	J	60	ASN
2	J	82	HIS
1	K	448	ASN
1	K	450	ASN
1	K	460	ASN
1	K	487	ASN
1	K	493	GLN
1	K	498	GLN
2	L	60	ASN
2	L	82	HIS
1	M	448	ASN
1	M	450	ASN
1	M	460	ASN
1	M	487	ASN

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Mol	Chain	Res	Type
1	M	498	GLN
2	N	82	HIS
1	O	448	ASN
1	O	450	ASN
1	O	493	GLN
2	P	60	ASN
2	P	82	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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.

All (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
4	S	1	NAG	C1-O5-C5	4.28	117.93	112.19
3	Q	1	NAG	C2-N2-C7	3.54	127.64	122.90
4	S	2	NAG	C4-C3-C2	3.15	115.63	111.02
3	U	1	NAG	C1-O5-C5	3.06	116.29	112.19
3	U	1	NAG	C1-C2-N2	3.06	115.26	110.43
3	Q	1	NAG	C4-C3-C2	-2.96	106.69	111.02
3	U	2	NAG	C1-C2-N2	2.94	115.06	110.43
3	T	2	NAG	C2-N2-C7	2.91	126.81	122.90
3	Q	1	NAG	O5-C1-C2	-2.89	106.83	111.29
3	T	2	NAG	C1-O5-C5	2.86	116.01	112.19
3	U	2	NAG	C2-N2-C7	2.67	126.48	122.90
3	U	1	NAG	O5-C5-C6	2.55	112.62	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C1-O5-C5	2.54	115.58	112.19
3	U	2	NAG	C4-C3-C2	2.38	114.50	111.02
3	U	1	NAG	C8-C7-N2	2.36	120.03	116.12
3	U	1	NAG	C4-C3-C2	-2.19	107.80	111.02
3	T	2	NAG	C8-C7-N2	2.13	119.65	116.12
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:

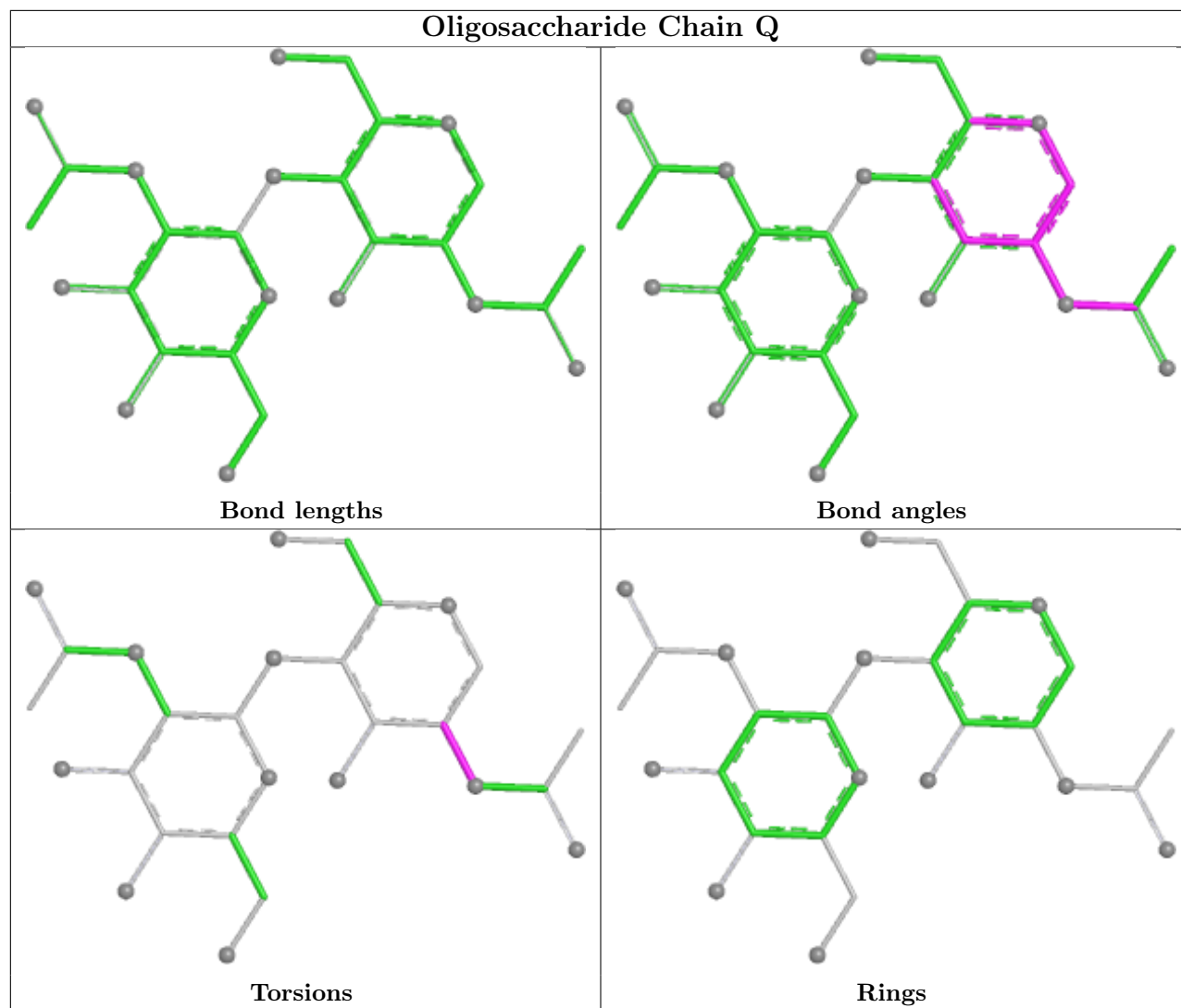
Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	C1-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
4	S	3	BMA	O5-C5-C6-O6
4	S	3	BMA	C4-C5-C6-O6
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6

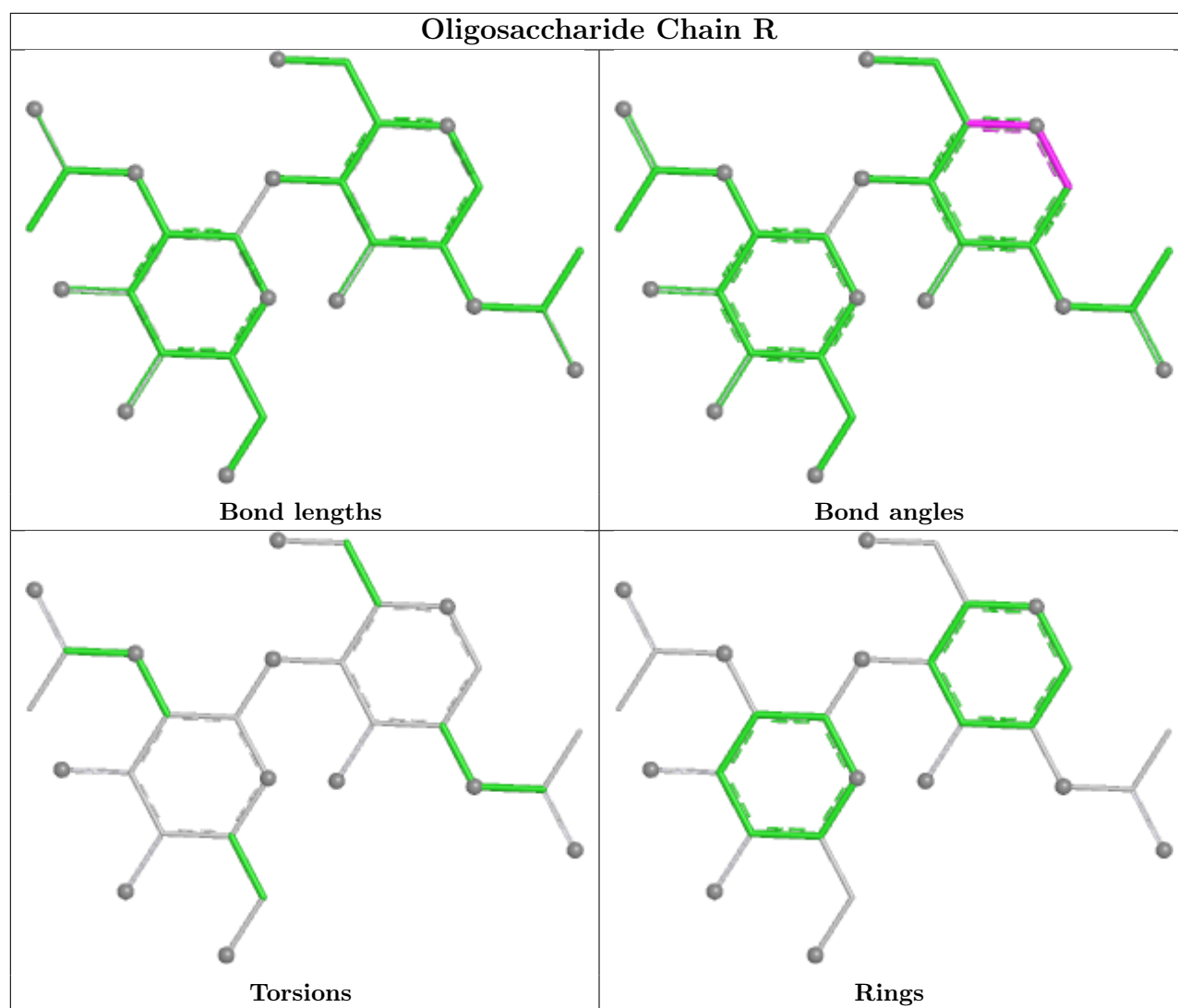
There are no ring outliers.

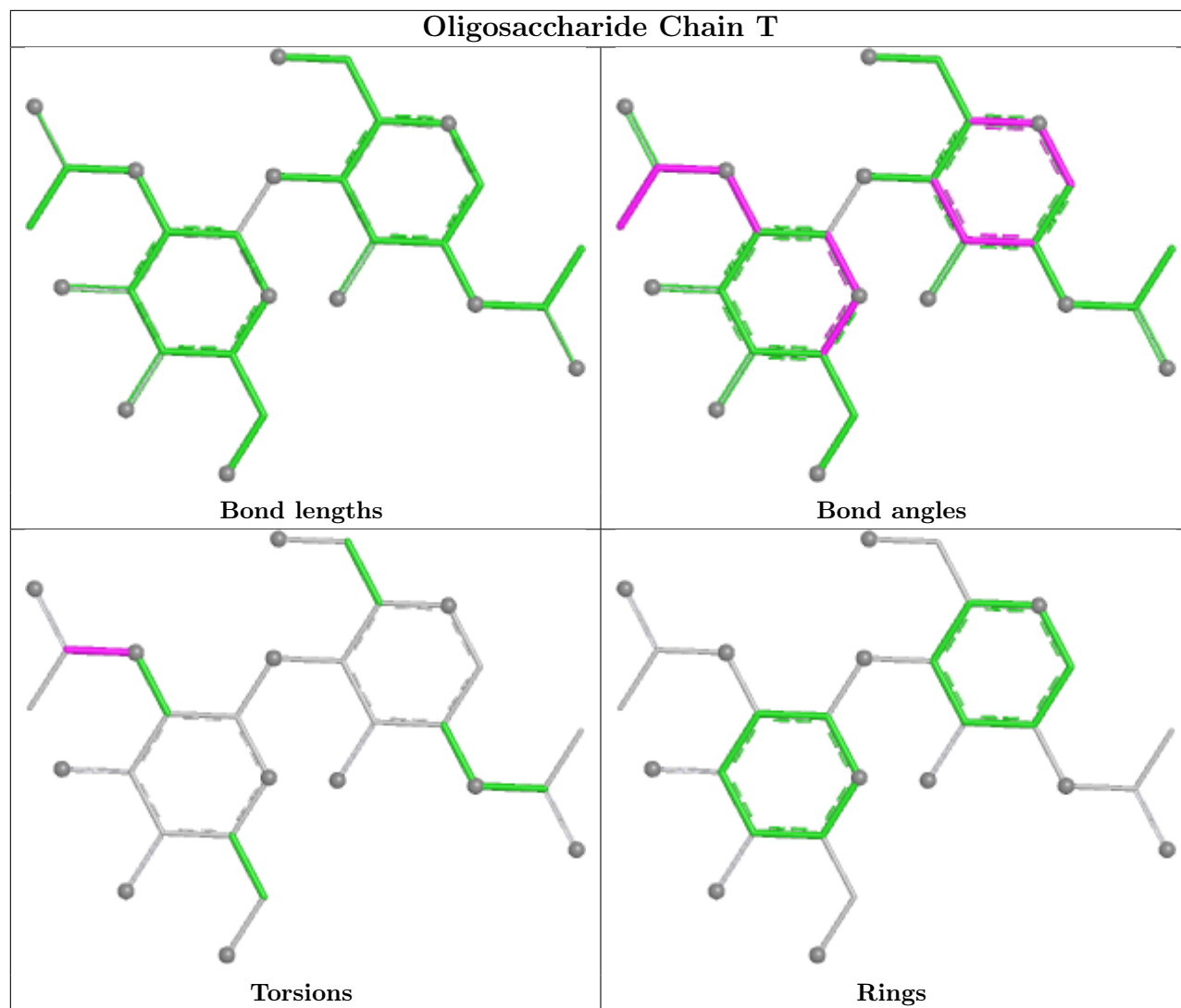
1 monomer is involved in 1 short contact:

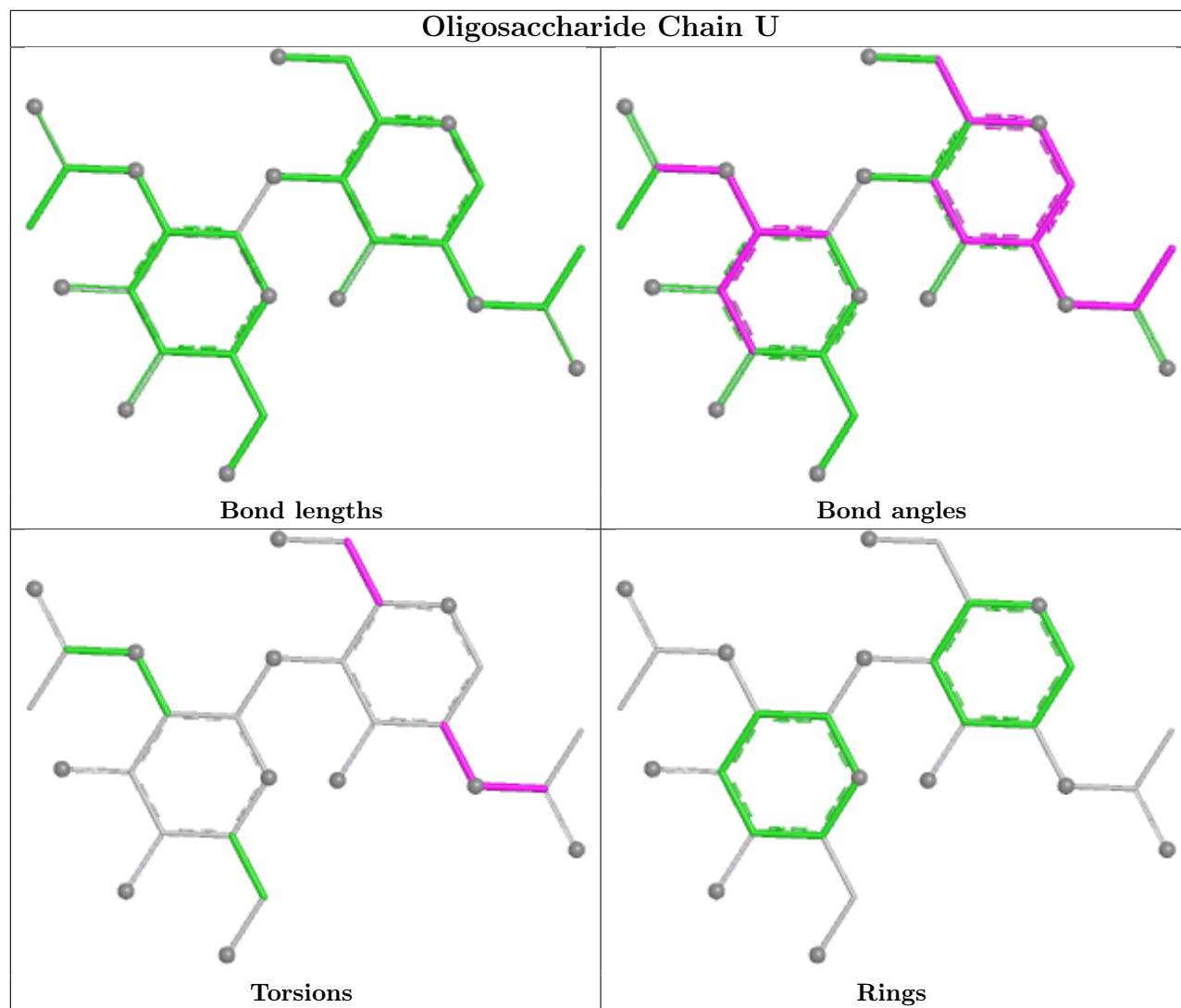
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	1	NAG	1	0

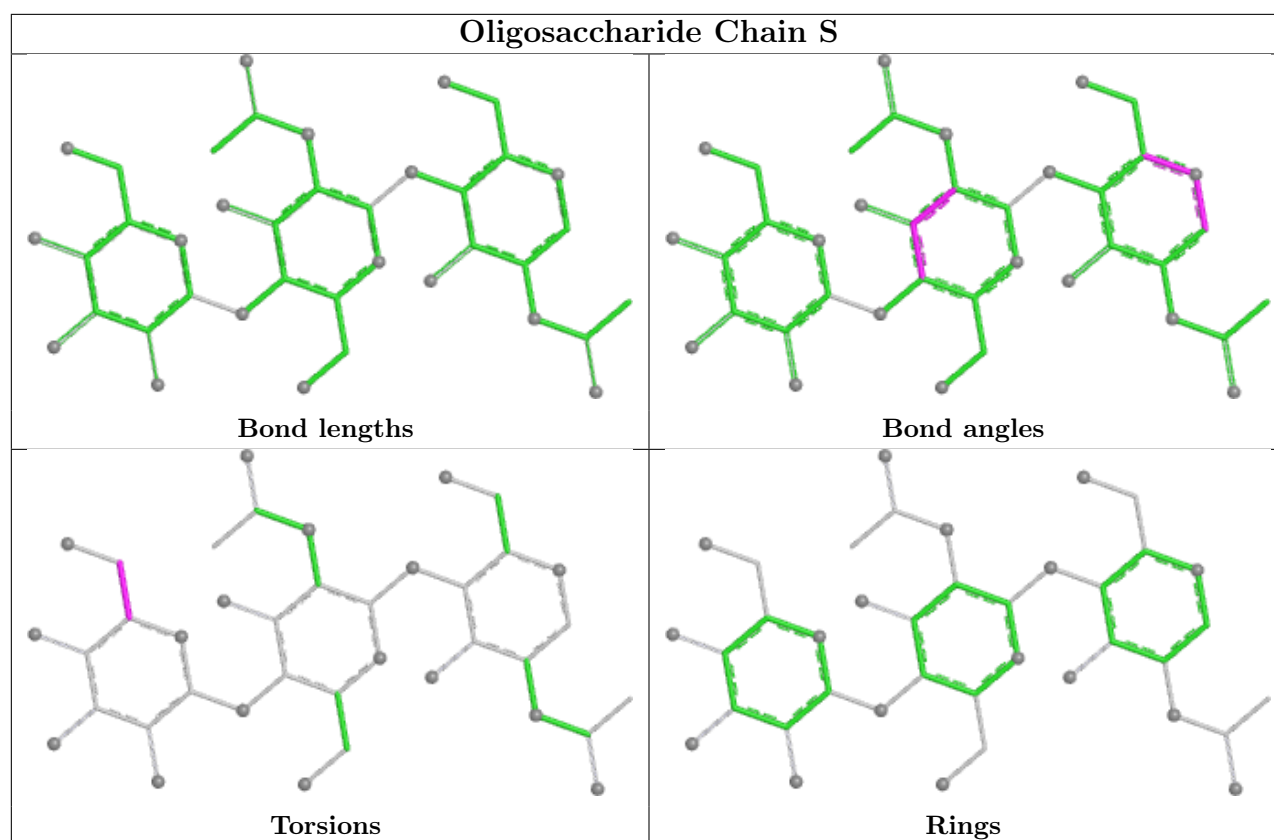
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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

All (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
5	A	701	NAG	C8-C7-N2	2.61	120.45	116.12
5	A	701	NAG	O3-C3-C2	-2.47	104.26	109.40
5	E	701	NAG	C4-C3-C2	2.44	114.60	111.02
5	C	701	NAG	O5-C5-C6	2.32	112.17	107.66
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	C	701	NAG	C4-C5-C6-O6
5	E	701	NAG	O5-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%)	0.26	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

All (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

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Mol	Chain	Res	Type	RSRZ
2	D	81	TYR	3.9
2	H	51	ASN	3.8
1	K	482	GLY	3.8
1	G	521	PRO	3.7
2	F	68	LEU	3.7
1	G	504	GLY	3.7
2	D	98	TYR	3.6
2	D	62	ALA	3.4
2	B	47	GLU	3.4
1	C	521	PRO	3.3
2	L	1	GLU	3.3
1	G	400	PHE	3.3
1	G	407	VAL	3.2
1	A	371	SER	3.2
1	G	405	ASP	3.1
1	K	484	GLU	3.1
1	G	503	VAL	3.1
1	I	392	PHE	3.1
1	I	452	LEU	3.1
1	I	436	TRP	3.0
1	K	378	LYS	3.0
2	D	30	ALA	3.0
1	I	521	PRO	3.0
1	E	495	TYR	2.9
1	K	441	LEU	2.9
2	D	89	SER	2.9
1	C	478	THR	2.9
2	F	89	SER	2.8
2	D	84	ARG	2.8
1	G	394	ASN	2.8
1	I	505	TYR	2.8
1	C	396	TYR	2.7
1	K	418	ILE	2.7
2	D	23	VAL	2.7
2	J	42	GLY	2.7
2	F	21	ASN	2.7
2	F	20	ILE	2.7
1	C	341	VAL	2.7
1	M	373	SER	2.6
1	G	514	SER	2.6
2	B	42	GLY	2.6
1	I	390	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	497	PHE	2.6
2	F	51	ASN	2.6
1	G	402	ILE	2.5
1	K	347	PHE	2.5
2	H	48	SER	2.5
2	H	50	SER	2.5
1	C	344	ALA	2.5
1	I	357	ARG	2.5
1	G	360	ASN	2.5
1	E	492	LEU	2.4
1	K	443	SER	2.4
2	F	36	TRP	2.4
1	C	377	PHE	2.4
1	G	423	TYR	2.4
2	F	81	TYR	2.4
1	A	396	TYR	2.4
2	F	6	THR	2.4
1	K	483	VAL	2.4
1	O	483	VAL	2.4
1	A	369	TYR	2.4
1	O	495	TYR	2.4
1	I	333	THR	2.4
1	E	391	CYS	2.4
2	N	76	GLU	2.4
1	C	355	ARG	2.3
2	D	85	ALA	2.3
2	B	37	TYR	2.3
2	P	61	LYS	2.3
2	F	3	VAL	2.3
2	F	22	CYS	2.3
2	D	78	SER	2.3
2	N	45	LYS	2.3
1	I	386	LYS	2.3
1	I	470	THR	2.3
1	C	374	PHE	2.3
1	E	394	ASN	2.3
2	P	62	ALA	2.3
1	K	335	LEU	2.3
1	C	490	PHE	2.2
2	L	81	TYR	2.2
2	L	0	ALA	2.2
1	O	408	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	369	TYR	2.2
1	G	396	TYR	2.2
1	E	468	ILE	2.2
1	O	457	ARG	2.2
2	D	35	TYR	2.2
2	F	86	TYR	2.2
1	O	458	LYS	2.2
2	D	101	GLY	2.2
1	I	400	PHE	2.2
2	D	86	TYR	2.2
2	H	111	SER	2.2
1	C	393	THR	2.1
1	I	496	GLY	2.1
1	I	523	THR	2.1
2	D	91	GLY	2.1
2	F	31	LEU	2.1
1	G	494	SER	2.1
2	D	82	HIS	2.1
1	G	406	GLU	2.1
2	D	50	SER	2.1
1	E	390	LEU	2.1
2	D	20	ILE	2.1
2	D	31	LEU	2.1
1	I	486	PHE	2.1
2	D	72	ASP	2.1
1	O	435	ALA	2.1
2	J	70	ILE	2.1
2	F	37	TYR	2.1
1	I	519	HIS	2.0
1	O	492	LEU	2.0
2	F	18	LEU	2.0
1	G	522	ALA	2.0
1	G	365	TYR	2.0
1	G	449	TYR	2.0
2	B	46	LYS	2.0
2	D	48	SER	2.0
2	N	83	CYS	2.0
1	I	387	LEU	2.0
1	I	419	ALA	2.0
1	A	389	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

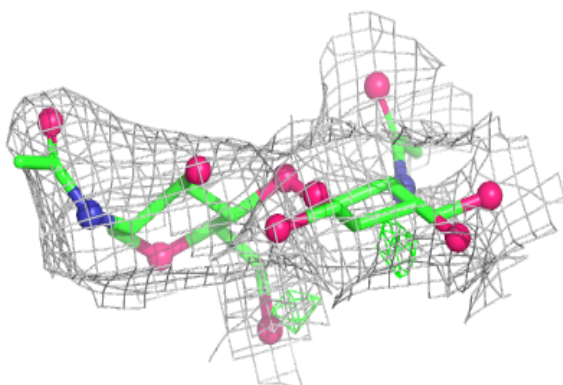
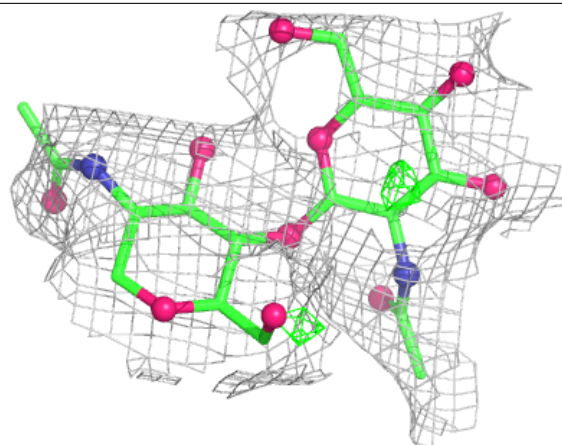
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	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

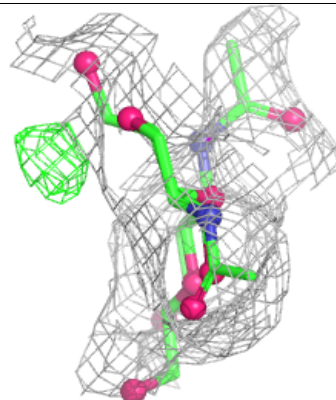
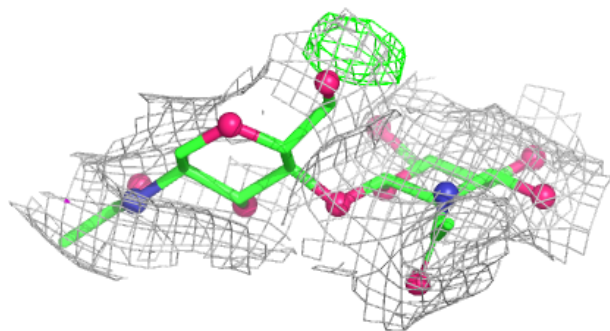
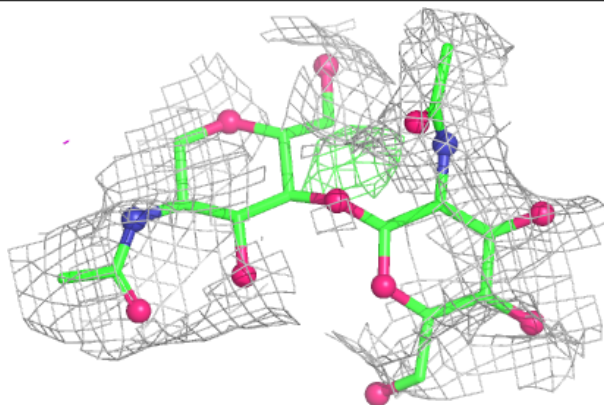
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

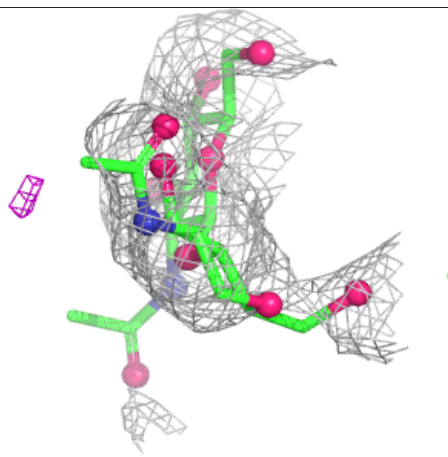
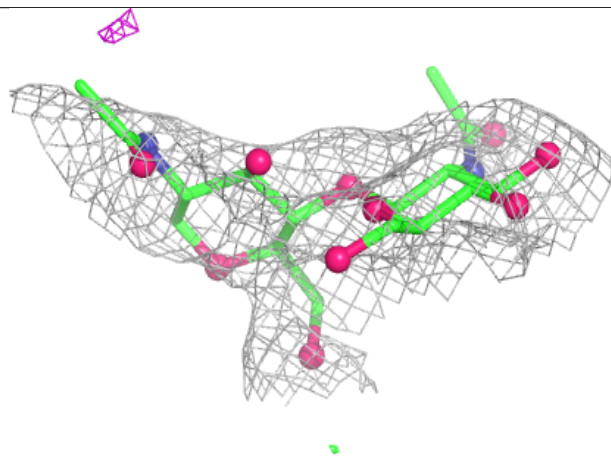
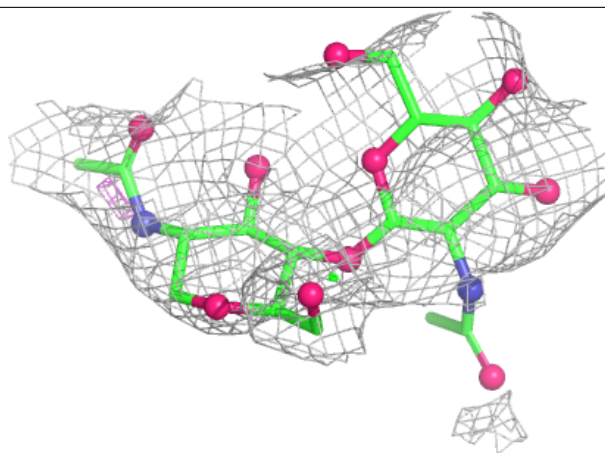
**Electron density around Chain R:**

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



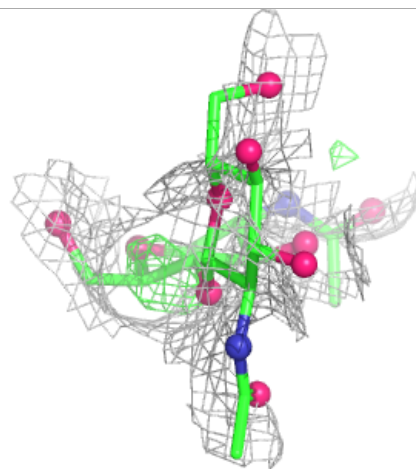
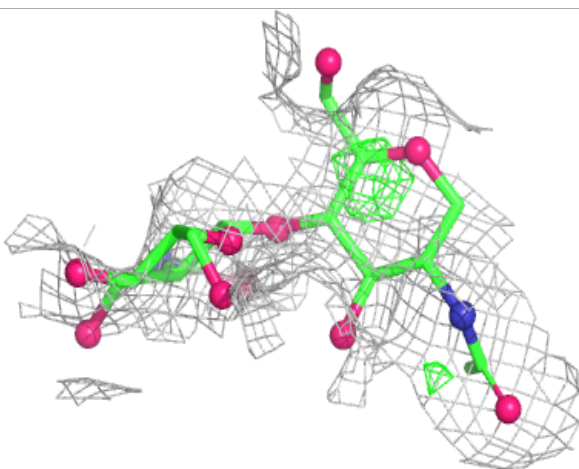
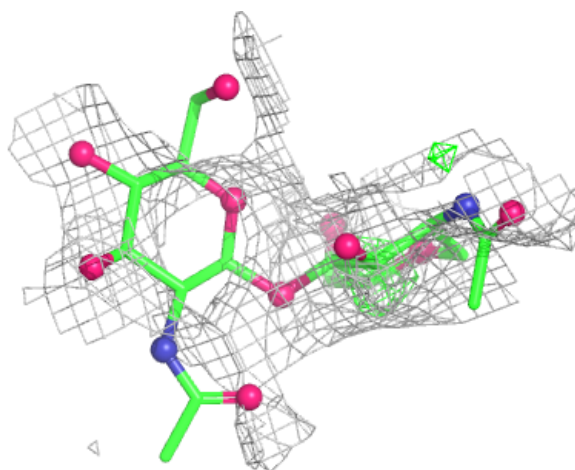
Electron density around Chain T:

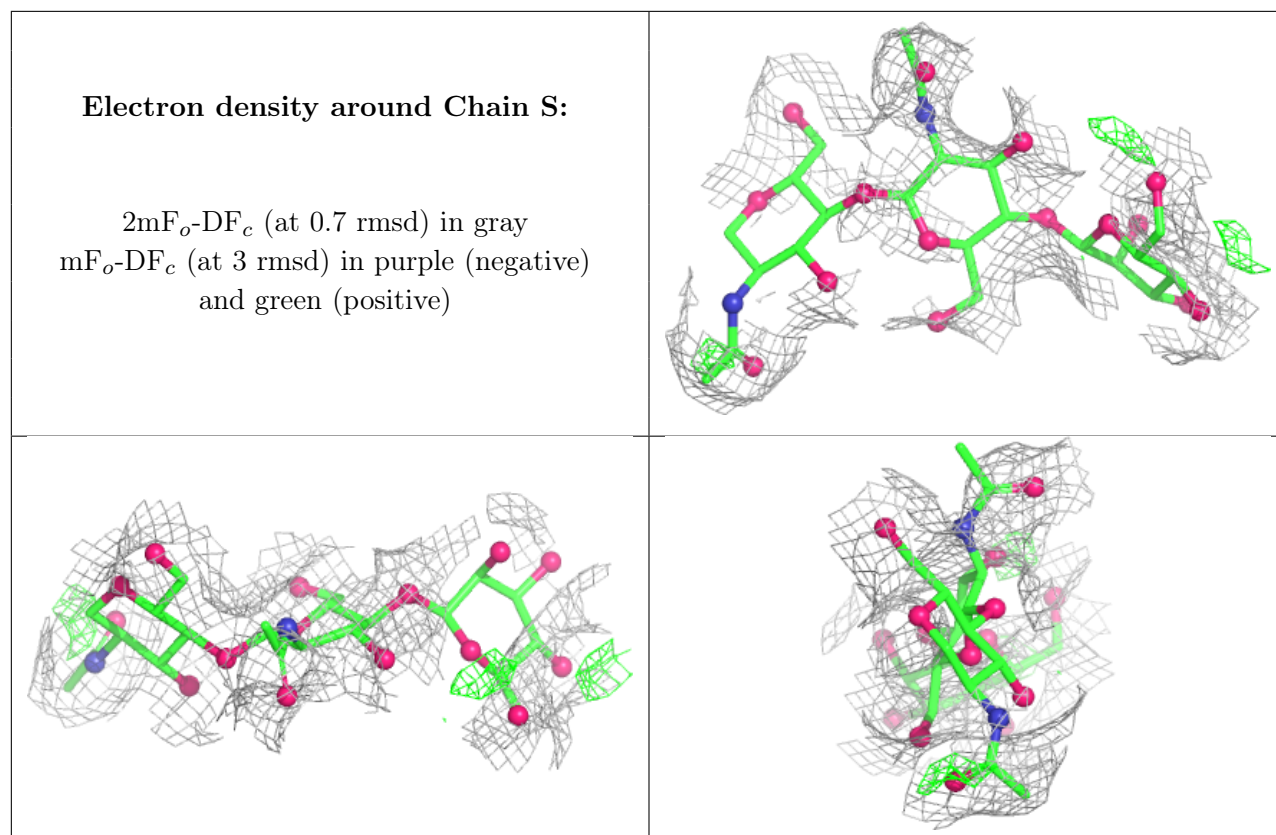
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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($\text{\AA}^2$)	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.