Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 06:18 PM JST

PDB ID	:	7WQV
Title	:	Crystal structure of a neutralizing monoclonal antibody (Ab08) in complex with SARS-CoV-2 receptor-binding domain (RBD)
Authors	:	Zha, J.; Meng, L.; Zhang, X.; Li, D.
Deposited on	:	2022-01-26
Resolution	:	2.80 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:

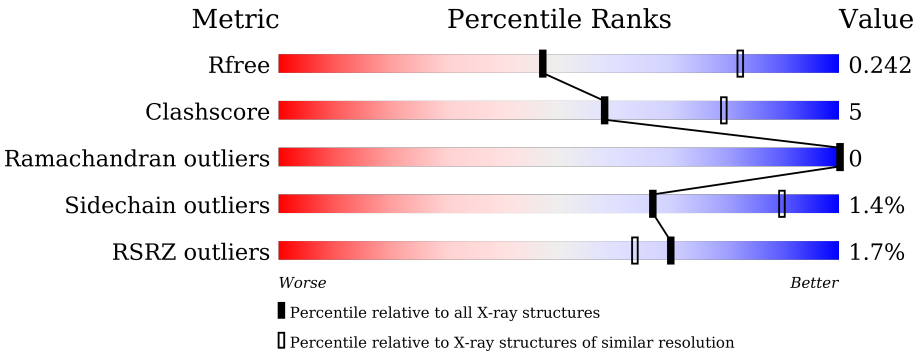
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	234	78% 8% 15%
1	C	234	5% 66% 18% 16%
1	E	234	2% 75% 8% 16%
1	G	234	% 72% 12% 16%
1	I	234	75% 8% 16%
1	K	234	2% 72% 11% 17%

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Mol	Chain	Length	Quality of chain
1	M	234	3% 76% 9% 15%
1	O	234	% 72% 12% 16%
2	B	303	% 72% 6% 22%
2	D	303	% 70% 7% 22%
2	F	303	66% 12% 22%
2	H	303	% 68% 11% 21%
2	J	303	% 64% 15% 21%
2	L	303	% 70% 8% 21%
2	N	303	66% 11% 23%
2	P	303	3% 65% 13% 22%
3	Q	2	100%
3	S	2	50% 50%
4	R	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	R	2	-	-	-	X
5	MPD	I	601	-	-	-	X
5	MPD	O	602	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 26586 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	200	Total	C	N	O	S	0	0	0
			1566	1001	261	296	8			
1	C	196	Total	C	N	O	S	0	0	0
			1552	996	260	288	8			
1	E	196	Total	C	N	O	S	0	0	0
			1546	992	259	287	8			
1	G	197	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			
1	I	196	Total	C	N	O	S	0	0	0
			1535	983	254	290	8			
1	K	194	Total	C	N	O	S	0	0	0
			1526	978	255	285	8			
1	M	198	Total	C	N	O	S	0	0	0
			1538	987	255	288	8			
1	O	196	Total	C	N	O	S	0	0	0
			1552	996	260	288	8			

There are 256 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	MET	-	initiating methionine	UNP P0DTC2
A	307	LYS	-	expression tag	UNP P0DTC2
A	308	PHE	-	expression tag	UNP P0DTC2
A	309	LEU	-	expression tag	UNP P0DTC2
A	310	VAL	-	expression tag	UNP P0DTC2
A	311	ASN	-	expression tag	UNP P0DTC2
A	312	VAL	-	expression tag	UNP P0DTC2
A	313	ALA	-	expression tag	UNP P0DTC2
A	314	LEU	-	expression tag	UNP P0DTC2
A	315	VAL	-	expression tag	UNP P0DTC2
A	316	PHE	-	expression tag	UNP P0DTC2
A	317	MET	-	expression tag	UNP P0DTC2
A	318	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	319	VAL	-	expression tag	UNP P0DTC2
A	320	TYR	-	expression tag	UNP P0DTC2
A	321	ILE	-	expression tag	UNP P0DTC2
A	322	SER	-	expression tag	UNP P0DTC2
A	323	TYR	-	expression tag	UNP P0DTC2
A	324	ILE	-	expression tag	UNP P0DTC2
A	325	TYR	-	expression tag	UNP P0DTC2
A	326	ALA	-	expression tag	UNP P0DTC2
A	327	ALA	-	expression tag	UNP P0DTC2
A	328	GLY	-	expression tag	UNP P0DTC2
A	329	SER	-	expression tag	UNP P0DTC2
A	532	GLY	-	expression tag	UNP P0DTC2
A	533	THR	-	expression tag	UNP P0DTC2
A	534	LEU	-	expression tag	UNP P0DTC2
A	535	GLU	-	expression tag	UNP P0DTC2
A	536	VAL	-	expression tag	UNP P0DTC2
A	537	LEU	-	expression tag	UNP P0DTC2
A	538	PHE	-	expression tag	UNP P0DTC2
A	539	GLN	-	expression tag	UNP P0DTC2
C	306	MET	-	initiating methionine	UNP P0DTC2
C	307	LYS	-	expression tag	UNP P0DTC2
C	308	PHE	-	expression tag	UNP P0DTC2
C	309	LEU	-	expression tag	UNP P0DTC2
C	310	VAL	-	expression tag	UNP P0DTC2
C	311	ASN	-	expression tag	UNP P0DTC2
C	312	VAL	-	expression tag	UNP P0DTC2
C	313	ALA	-	expression tag	UNP P0DTC2
C	314	LEU	-	expression tag	UNP P0DTC2
C	315	VAL	-	expression tag	UNP P0DTC2
C	316	PHE	-	expression tag	UNP P0DTC2
C	317	MET	-	expression tag	UNP P0DTC2
C	318	VAL	-	expression tag	UNP P0DTC2
C	319	VAL	-	expression tag	UNP P0DTC2
C	320	TYR	-	expression tag	UNP P0DTC2
C	321	ILE	-	expression tag	UNP P0DTC2
C	322	SER	-	expression tag	UNP P0DTC2
C	323	TYR	-	expression tag	UNP P0DTC2
C	324	ILE	-	expression tag	UNP P0DTC2
C	325	TYR	-	expression tag	UNP P0DTC2
C	326	ALA	-	expression tag	UNP P0DTC2
C	327	ALA	-	expression tag	UNP P0DTC2
C	328	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	329	SER	-	expression tag	UNP P0DTC2
C	532	GLY	-	expression tag	UNP P0DTC2
C	533	THR	-	expression tag	UNP P0DTC2
C	534	LEU	-	expression tag	UNP P0DTC2
C	535	GLU	-	expression tag	UNP P0DTC2
C	536	VAL	-	expression tag	UNP P0DTC2
C	537	LEU	-	expression tag	UNP P0DTC2
C	538	PHE	-	expression tag	UNP P0DTC2
C	539	GLN	-	expression tag	UNP P0DTC2
E	306	MET	-	initiating methionine	UNP P0DTC2
E	307	LYS	-	expression tag	UNP P0DTC2
E	308	PHE	-	expression tag	UNP P0DTC2
E	309	LEU	-	expression tag	UNP P0DTC2
E	310	VAL	-	expression tag	UNP P0DTC2
E	311	ASN	-	expression tag	UNP P0DTC2
E	312	VAL	-	expression tag	UNP P0DTC2
E	313	ALA	-	expression tag	UNP P0DTC2
E	314	LEU	-	expression tag	UNP P0DTC2
E	315	VAL	-	expression tag	UNP P0DTC2
E	316	PHE	-	expression tag	UNP P0DTC2
E	317	MET	-	expression tag	UNP P0DTC2
E	318	VAL	-	expression tag	UNP P0DTC2
E	319	VAL	-	expression tag	UNP P0DTC2
E	320	TYR	-	expression tag	UNP P0DTC2
E	321	ILE	-	expression tag	UNP P0DTC2
E	322	SER	-	expression tag	UNP P0DTC2
E	323	TYR	-	expression tag	UNP P0DTC2
E	324	ILE	-	expression tag	UNP P0DTC2
E	325	TYR	-	expression tag	UNP P0DTC2
E	326	ALA	-	expression tag	UNP P0DTC2
E	327	ALA	-	expression tag	UNP P0DTC2
E	328	GLY	-	expression tag	UNP P0DTC2
E	329	SER	-	expression tag	UNP P0DTC2
E	532	GLY	-	expression tag	UNP P0DTC2
E	533	THR	-	expression tag	UNP P0DTC2
E	534	LEU	-	expression tag	UNP P0DTC2
E	535	GLU	-	expression tag	UNP P0DTC2
E	536	VAL	-	expression tag	UNP P0DTC2
E	537	LEU	-	expression tag	UNP P0DTC2
E	538	PHE	-	expression tag	UNP P0DTC2
E	539	GLN	-	expression tag	UNP P0DTC2
G	306	MET	-	initiating methionine	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	307	LYS	-	expression tag	UNP P0DTC2
G	308	PHE	-	expression tag	UNP P0DTC2
G	309	LEU	-	expression tag	UNP P0DTC2
G	310	VAL	-	expression tag	UNP P0DTC2
G	311	ASN	-	expression tag	UNP P0DTC2
G	312	VAL	-	expression tag	UNP P0DTC2
G	313	ALA	-	expression tag	UNP P0DTC2
G	314	LEU	-	expression tag	UNP P0DTC2
G	315	VAL	-	expression tag	UNP P0DTC2
G	316	PHE	-	expression tag	UNP P0DTC2
G	317	MET	-	expression tag	UNP P0DTC2
G	318	VAL	-	expression tag	UNP P0DTC2
G	319	VAL	-	expression tag	UNP P0DTC2
G	320	TYR	-	expression tag	UNP P0DTC2
G	321	ILE	-	expression tag	UNP P0DTC2
G	322	SER	-	expression tag	UNP P0DTC2
G	323	TYR	-	expression tag	UNP P0DTC2
G	324	ILE	-	expression tag	UNP P0DTC2
G	325	TYR	-	expression tag	UNP P0DTC2
G	326	ALA	-	expression tag	UNP P0DTC2
G	327	ALA	-	expression tag	UNP P0DTC2
G	328	GLY	-	expression tag	UNP P0DTC2
G	329	SER	-	expression tag	UNP P0DTC2
G	532	GLY	-	expression tag	UNP P0DTC2
G	533	THR	-	expression tag	UNP P0DTC2
G	534	LEU	-	expression tag	UNP P0DTC2
G	535	GLU	-	expression tag	UNP P0DTC2
G	536	VAL	-	expression tag	UNP P0DTC2
G	537	LEU	-	expression tag	UNP P0DTC2
G	538	PHE	-	expression tag	UNP P0DTC2
G	539	GLN	-	expression tag	UNP P0DTC2
I	306	MET	-	initiating methionine	UNP P0DTC2
I	307	LYS	-	expression tag	UNP P0DTC2
I	308	PHE	-	expression tag	UNP P0DTC2
I	309	LEU	-	expression tag	UNP P0DTC2
I	310	VAL	-	expression tag	UNP P0DTC2
I	311	ASN	-	expression tag	UNP P0DTC2
I	312	VAL	-	expression tag	UNP P0DTC2
I	313	ALA	-	expression tag	UNP P0DTC2
I	314	LEU	-	expression tag	UNP P0DTC2
I	315	VAL	-	expression tag	UNP P0DTC2
I	316	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	317	MET	-	expression tag	UNP P0DTC2
I	318	VAL	-	expression tag	UNP P0DTC2
I	319	VAL	-	expression tag	UNP P0DTC2
I	320	TYR	-	expression tag	UNP P0DTC2
I	321	ILE	-	expression tag	UNP P0DTC2
I	322	SER	-	expression tag	UNP P0DTC2
I	323	TYR	-	expression tag	UNP P0DTC2
I	324	ILE	-	expression tag	UNP P0DTC2
I	325	TYR	-	expression tag	UNP P0DTC2
I	326	ALA	-	expression tag	UNP P0DTC2
I	327	ALA	-	expression tag	UNP P0DTC2
I	328	GLY	-	expression tag	UNP P0DTC2
I	329	SER	-	expression tag	UNP P0DTC2
I	532	GLY	-	expression tag	UNP P0DTC2
I	533	THR	-	expression tag	UNP P0DTC2
I	534	LEU	-	expression tag	UNP P0DTC2
I	535	GLU	-	expression tag	UNP P0DTC2
I	536	VAL	-	expression tag	UNP P0DTC2
I	537	LEU	-	expression tag	UNP P0DTC2
I	538	PHE	-	expression tag	UNP P0DTC2
I	539	GLN	-	expression tag	UNP P0DTC2
K	306	MET	-	initiating methionine	UNP P0DTC2
K	307	LYS	-	expression tag	UNP P0DTC2
K	308	PHE	-	expression tag	UNP P0DTC2
K	309	LEU	-	expression tag	UNP P0DTC2
K	310	VAL	-	expression tag	UNP P0DTC2
K	311	ASN	-	expression tag	UNP P0DTC2
K	312	VAL	-	expression tag	UNP P0DTC2
K	313	ALA	-	expression tag	UNP P0DTC2
K	314	LEU	-	expression tag	UNP P0DTC2
K	315	VAL	-	expression tag	UNP P0DTC2
K	316	PHE	-	expression tag	UNP P0DTC2
K	317	MET	-	expression tag	UNP P0DTC2
K	318	VAL	-	expression tag	UNP P0DTC2
K	319	VAL	-	expression tag	UNP P0DTC2
K	320	TYR	-	expression tag	UNP P0DTC2
K	321	ILE	-	expression tag	UNP P0DTC2
K	322	SER	-	expression tag	UNP P0DTC2
K	323	TYR	-	expression tag	UNP P0DTC2
K	324	ILE	-	expression tag	UNP P0DTC2
K	325	TYR	-	expression tag	UNP P0DTC2
K	326	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	327	ALA	-	expression tag	UNP P0DTC2
K	328	GLY	-	expression tag	UNP P0DTC2
K	329	SER	-	expression tag	UNP P0DTC2
K	532	GLY	-	expression tag	UNP P0DTC2
K	533	THR	-	expression tag	UNP P0DTC2
K	534	LEU	-	expression tag	UNP P0DTC2
K	535	GLU	-	expression tag	UNP P0DTC2
K	536	VAL	-	expression tag	UNP P0DTC2
K	537	LEU	-	expression tag	UNP P0DTC2
K	538	PHE	-	expression tag	UNP P0DTC2
K	539	GLN	-	expression tag	UNP P0DTC2
M	306	MET	-	initiating methionine	UNP P0DTC2
M	307	LYS	-	expression tag	UNP P0DTC2
M	308	PHE	-	expression tag	UNP P0DTC2
M	309	LEU	-	expression tag	UNP P0DTC2
M	310	VAL	-	expression tag	UNP P0DTC2
M	311	ASN	-	expression tag	UNP P0DTC2
M	312	VAL	-	expression tag	UNP P0DTC2
M	313	ALA	-	expression tag	UNP P0DTC2
M	314	LEU	-	expression tag	UNP P0DTC2
M	315	VAL	-	expression tag	UNP P0DTC2
M	316	PHE	-	expression tag	UNP P0DTC2
M	317	MET	-	expression tag	UNP P0DTC2
M	318	VAL	-	expression tag	UNP P0DTC2
M	319	VAL	-	expression tag	UNP P0DTC2
M	320	TYR	-	expression tag	UNP P0DTC2
M	321	ILE	-	expression tag	UNP P0DTC2
M	322	SER	-	expression tag	UNP P0DTC2
M	323	TYR	-	expression tag	UNP P0DTC2
M	324	ILE	-	expression tag	UNP P0DTC2
M	325	TYR	-	expression tag	UNP P0DTC2
M	326	ALA	-	expression tag	UNP P0DTC2
M	327	ALA	-	expression tag	UNP P0DTC2
M	328	GLY	-	expression tag	UNP P0DTC2
M	329	SER	-	expression tag	UNP P0DTC2
M	532	GLY	-	expression tag	UNP P0DTC2
M	533	THR	-	expression tag	UNP P0DTC2
M	534	LEU	-	expression tag	UNP P0DTC2
M	535	GLU	-	expression tag	UNP P0DTC2
M	536	VAL	-	expression tag	UNP P0DTC2
M	537	LEU	-	expression tag	UNP P0DTC2
M	538	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	539	GLN	-	expression tag	UNP P0DTC2
O	306	MET	-	initiating methionine	UNP P0DTC2
O	307	LYS	-	expression tag	UNP P0DTC2
O	308	PHE	-	expression tag	UNP P0DTC2
O	309	LEU	-	expression tag	UNP P0DTC2
O	310	VAL	-	expression tag	UNP P0DTC2
O	311	ASN	-	expression tag	UNP P0DTC2
O	312	VAL	-	expression tag	UNP P0DTC2
O	313	ALA	-	expression tag	UNP P0DTC2
O	314	LEU	-	expression tag	UNP P0DTC2
O	315	VAL	-	expression tag	UNP P0DTC2
O	316	PHE	-	expression tag	UNP P0DTC2
O	317	MET	-	expression tag	UNP P0DTC2
O	318	VAL	-	expression tag	UNP P0DTC2
O	319	VAL	-	expression tag	UNP P0DTC2
O	320	TYR	-	expression tag	UNP P0DTC2
O	321	ILE	-	expression tag	UNP P0DTC2
O	322	SER	-	expression tag	UNP P0DTC2
O	323	TYR	-	expression tag	UNP P0DTC2
O	324	ILE	-	expression tag	UNP P0DTC2
O	325	TYR	-	expression tag	UNP P0DTC2
O	326	ALA	-	expression tag	UNP P0DTC2
O	327	ALA	-	expression tag	UNP P0DTC2
O	328	GLY	-	expression tag	UNP P0DTC2
O	329	SER	-	expression tag	UNP P0DTC2
O	532	GLY	-	expression tag	UNP P0DTC2
O	533	THR	-	expression tag	UNP P0DTC2
O	534	LEU	-	expression tag	UNP P0DTC2
O	535	GLU	-	expression tag	UNP P0DTC2
O	536	VAL	-	expression tag	UNP P0DTC2
O	537	LEU	-	expression tag	UNP P0DTC2
O	538	PHE	-	expression tag	UNP P0DTC2
O	539	GLN	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Ab08.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1747	1096	291	354	6			
2	D	235	Total	C	N	O	S	0	0	0
			1744	1096	292	350	6			
2	F	236	Total	C	N	O	S	0	0	0
			1751	1100	292	353	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	240	Total	C	N	O	S	0	0	0
			1772	1111	300	355	6			
2	J	238	Total	C	N	O	S	0	0	0
			1762	1104	296	356	6			
2	L	238	Total	C	N	O	S	0	0	0
			1753	1100	292	355	6			
2	N	234	Total	C	N	O	S	0	0	0
			1738	1092	291	349	6			
2	P	235	Total	C	N	O	S	0	0	0
			1739	1093	292	348	6			

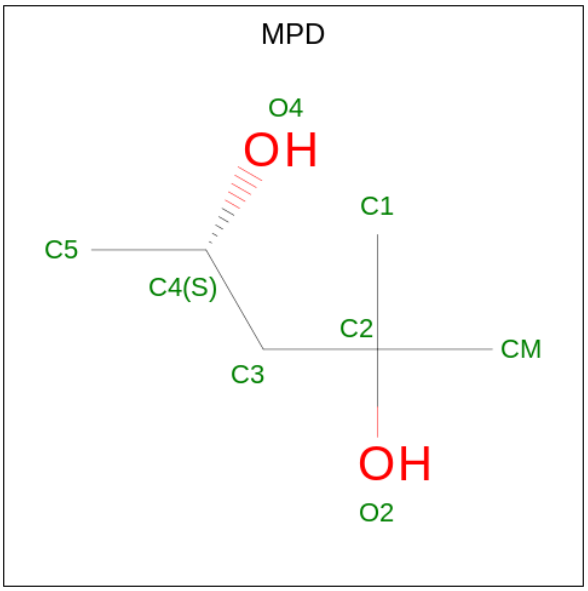
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	S	2	Total	C	N	O	0	0	0
			24	14	1	9			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	H	1	Total C O 8 6 2	0	0
5	I	1	Total C O 8 6 2	0	0
5	I	1	Total C O 8 6 2	0	0
5	J	1	Total C O 8 6 2	0	0
5	J	1	Total C O 8 6 2	0	0
5	O	1	Total C O 8 6 2	0	0
5	P	1	Total C O 8 6 2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0

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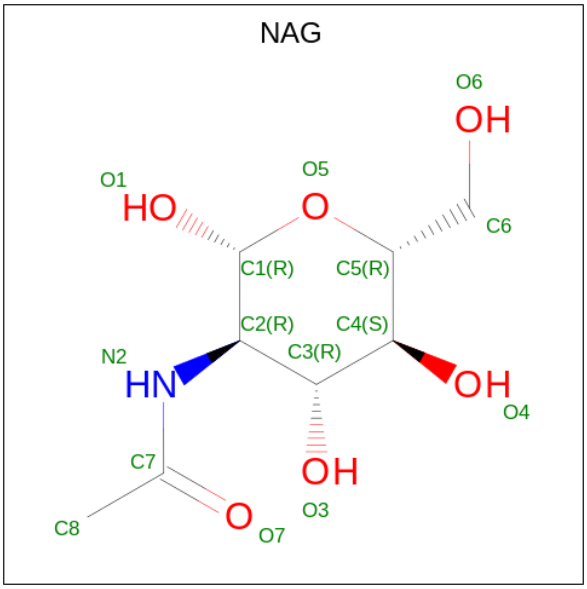
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0
6	L	1	Total Ca 1 1	0	0
6	N	1	Total Ca 1 1	0	0
6	P	1	Total Ca 1 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cl 1 1	0	0
7	G	1	Total Cl 1 1	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is water.

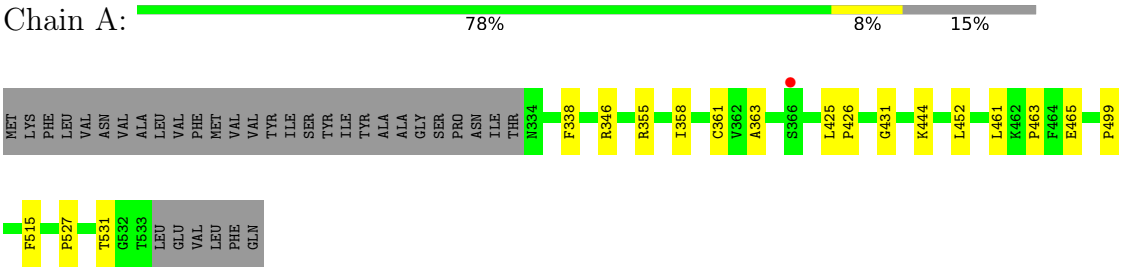
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O 2 2	0	0
9	B	6	Total O 6 6	0	0
9	C	1	Total O 1 1	0	0
9	F	2	Total O 2 2	0	0
9	L	3	Total O 3 3	0	0
9	N	4	Total O 4 4	0	0
9	O	1	Total O 1 1	0	0
9	P	2	Total O 2 2	0	0

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.

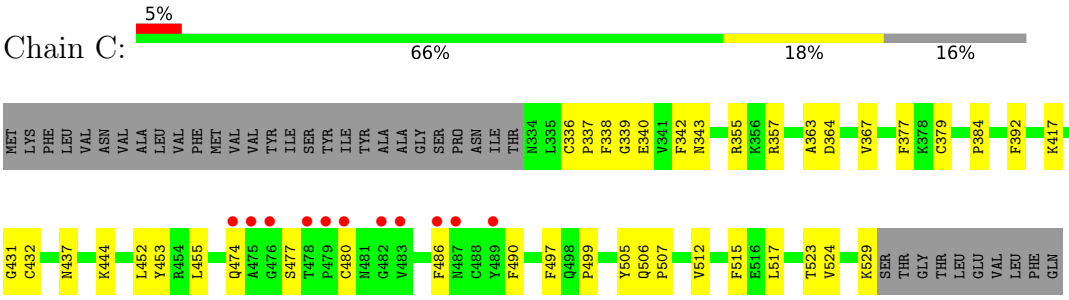
• Molecule 1: Spike protein S1

Chain A:



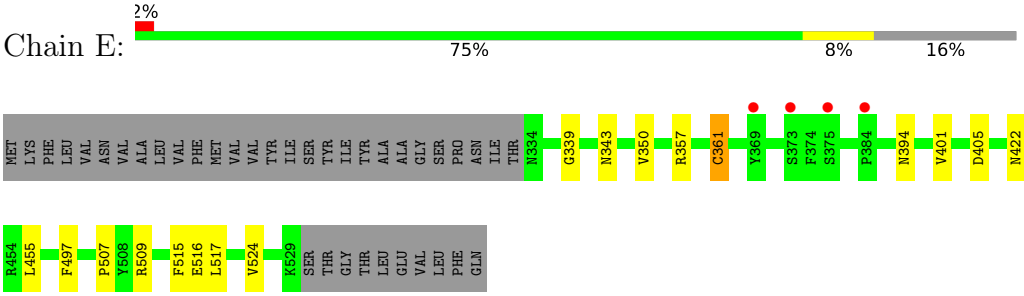
• Molecule 1: Spike protein S1

Chain C:



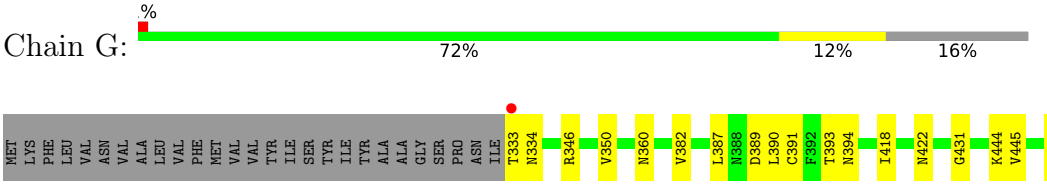
• Molecule 1: Spike protein S1

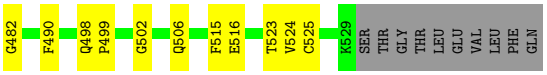
Chain E:



• Molecule 1: Spike protein S1

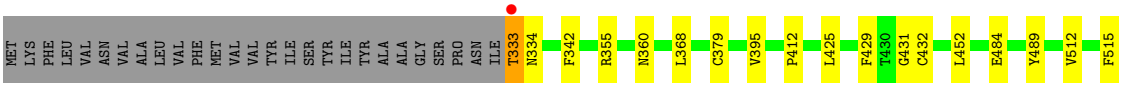
Chain G:





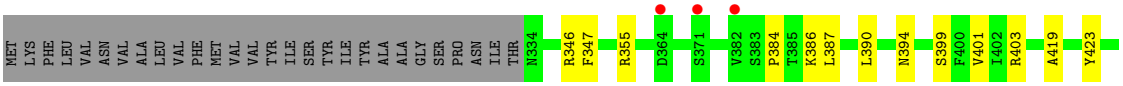
• Molecule 1: Spike protein S1

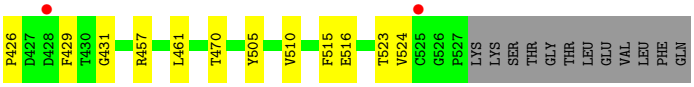
Chain I:



• Molecule 1: Spike protein S1

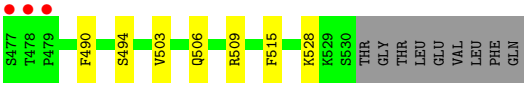
Chain K:





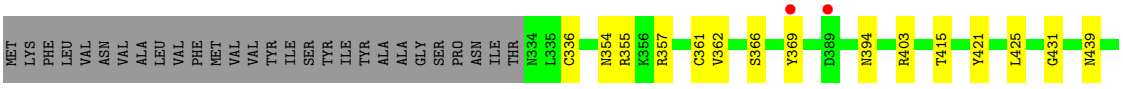
• Molecule 1: Spike protein S1

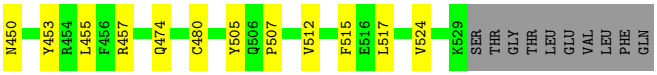
Chain M:



• Molecule 1: Spike protein S1

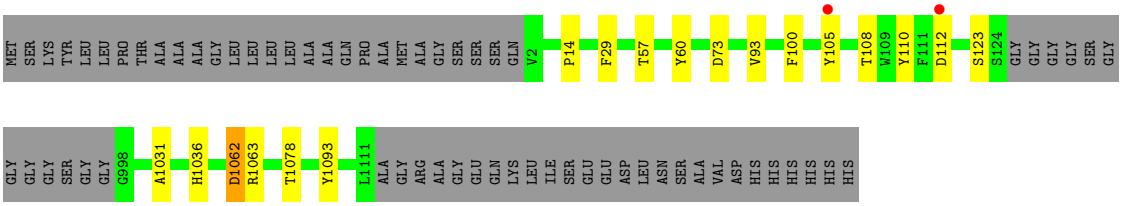
Chain O:





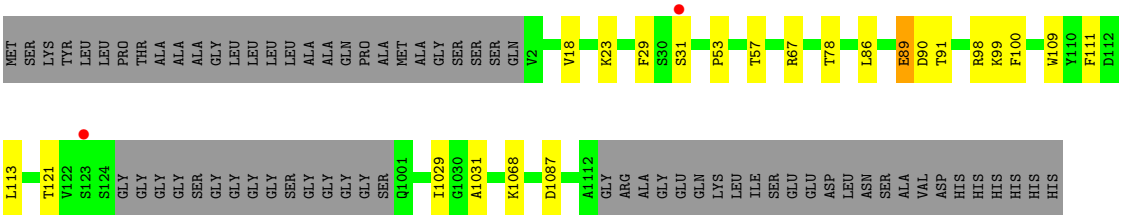
• Molecule 2: Ab08

Chain B:



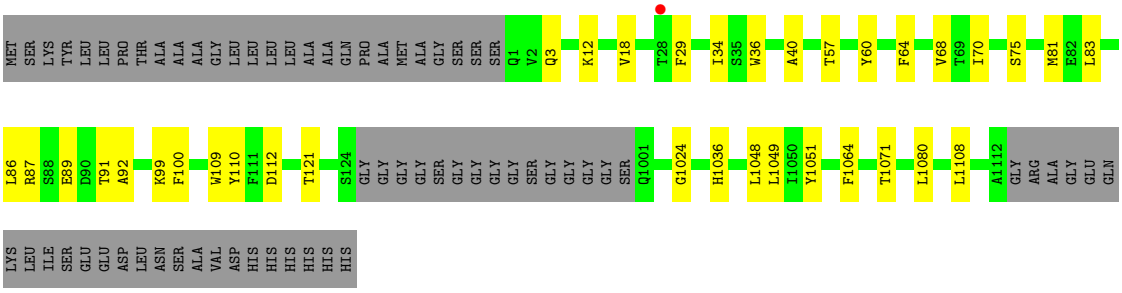
• Molecule 2: Ab08

Chain D:



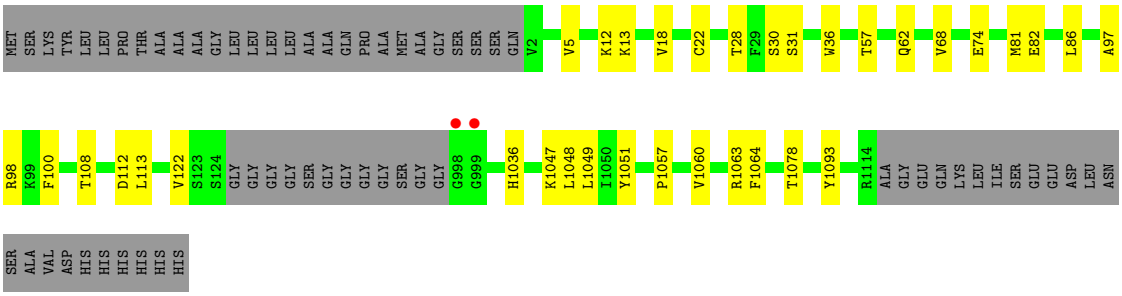
• Molecule 2: Ab08

Chain F:



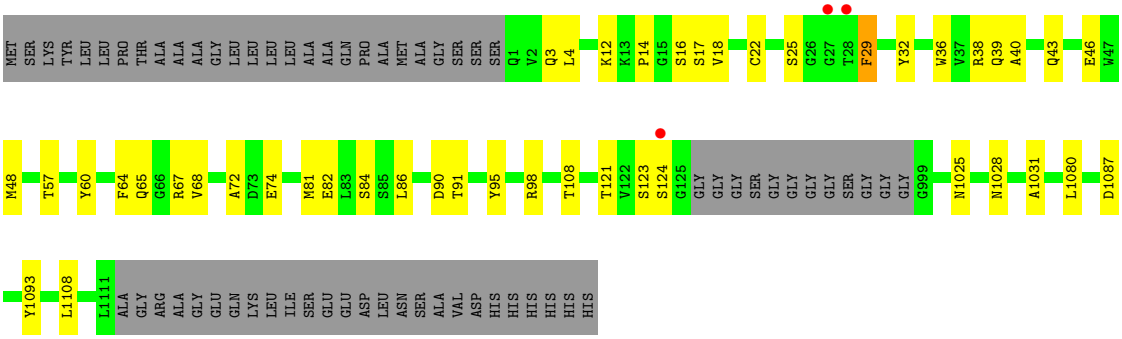
• Molecule 2: Ab08

Chain H:



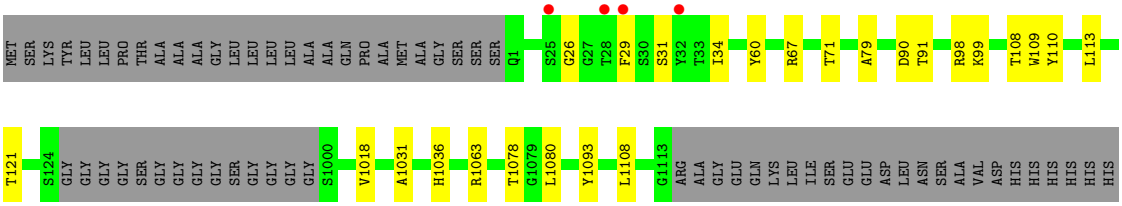
• Molecule 2: Ab08

Chain J:



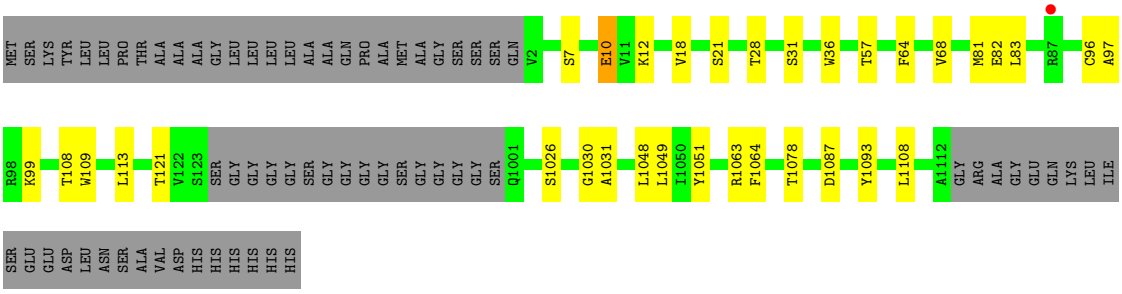
• Molecule 2: Ab08

Chain L:



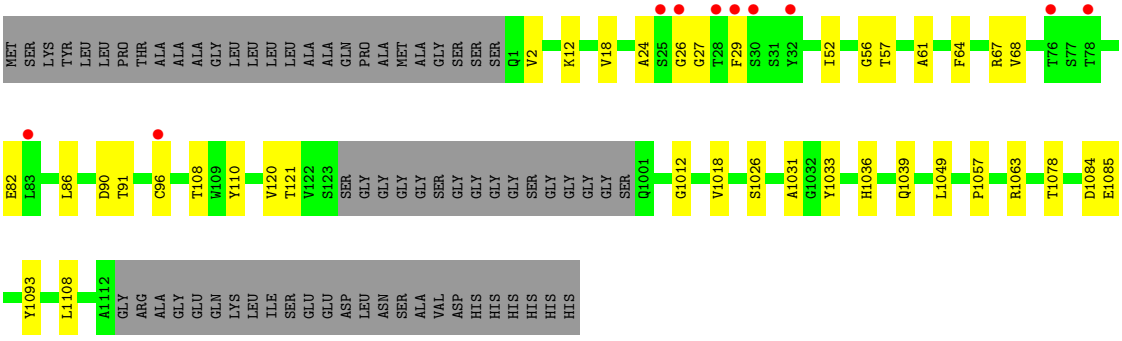
• Molecule 2: Ab08

Chain N:



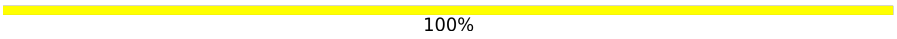
• Molecule 2: Ab08

Chain P:



• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.64Å 116.74Å 180.72Å 90.00° 90.31° 90.00°	Depositor
Resolution (Å)	44.93 – 2.80 49.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.93-2.80) 99.2 (49.39-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.220 , 0.251 0.219 , 0.242	Depositor DCC
R_{free} test set	4719 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	26586	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MPD, NAG, CA, CL, FUC

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	0.26	0/1610	0.45	0/2194
1	C	0.27	0/1596	0.45	0/2170
1	E	0.26	0/1590	0.45	0/2164
1	G	0.26	0/1592	0.44	0/2170
1	I	0.27	0/1579	0.46	0/2153
1	K	0.26	0/1570	0.45	0/2139
1	M	0.26	0/1582	0.44	0/2157
1	O	0.26	0/1596	0.46	0/2170
2	B	0.27	0/1787	0.47	0/2429
2	D	0.26	0/1784	0.47	0/2424
2	F	0.27	0/1791	0.48	0/2434
2	H	0.27	0/1812	0.49	0/2460
2	J	0.26	0/1802	0.48	0/2448
2	L	0.26	0/1793	0.48	0/2438
2	N	0.27	0/1778	0.48	0/2417
2	P	0.26	0/1779	0.49	0/2419
All	All	0.26	0/27041	0.47	0/36786

There are no bond length outliers.

There are no bond angle outliers.

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	1467	13	0
1	C	1552	0	1473	25	0
1	E	1546	0	1463	11	0
1	G	1548	0	1449	16	0
1	I	1535	0	1431	11	0
1	K	1526	0	1431	14	0
1	M	1538	0	1432	12	0
1	O	1552	0	1473	15	0
2	B	1747	0	1663	10	0
2	D	1744	0	1673	13	0
2	F	1751	0	1679	21	0
2	H	1772	0	1697	23	0
2	J	1762	0	1685	29	0
2	L	1753	0	1670	16	0
2	N	1738	0	1663	18	0
2	P	1739	0	1664	25	0
3	Q	24	0	22	0	0
3	S	24	0	22	0	0
4	R	24	0	22	0	0
5	A	16	0	28	2	0
5	B	8	0	14	0	0
5	D	8	0	14	0	0
5	H	8	0	14	0	0
5	I	16	0	28	0	0
5	J	16	0	28	0	0
5	O	8	0	14	0	0
5	P	8	0	14	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	L	1	0	0	0	0
6	N	1	0	0	0	0
6	P	1	0	0	0	0
7	B	1	0	0	0	0
7	G	1	0	0	0	0
8	C	14	0	13	0	0
8	O	14	0	13	0	0
9	A	2	0	0	0	0
9	B	6	0	0	0	0
9	C	1	0	0	0	0
9	F	2	0	0	0	0
9	L	3	0	0	0	0
9	N	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	O	1	0	0	0	0
9	P	2	0	0	0	0
All	All	26586	0	25259	246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (246) 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:F:18:VAL:HG23	2:F:86:LEU:HD11	1.63	0.79
2:H:12:LYS:HG3	2:H:18:VAL:HG22	1.68	0.76
1:M:452:LEU:HD21	2:N:57:THR:HG21	1.70	0.74
2:F:12:LYS:HG3	2:F:18:VAL:HG22	1.73	0.70
2:N:10:GLU:HG2	2:N:12:LYS:HE2	1.74	0.70
2:H:1048:LEU:HD21	2:H:1051:TYR:HB3	1.76	0.68
1:K:384:PRO:HA	1:K:387:LEU:HD13	1.76	0.68
2:F:99:LYS:HG2	2:F:109:TRP:HB3	1.76	0.67
1:E:452:LEU:HD21	2:F:57:THR:HG21	1.75	0.67
2:F:89:GLU:OE1	2:F:89:GLU:N	2.22	0.66
2:P:12:LYS:HG3	2:P:18:VAL:HG22	1.75	0.66
2:L:99:LYS:HG2	2:L:109:TRP:HB3	1.78	0.65
1:M:461:LEU:HG	1:M:465:GLU:HB3	1.82	0.62
2:F:29:PHE:CZ	2:F:34:ILE:HG13	2.35	0.61
1:K:523:THR:HG23	1:K:524:VAL:HG23	1.82	0.61
2:D:91:THR:HG23	2:D:121:THR:HA	1.83	0.61
2:J:12:LYS:HG3	2:J:18:VAL:HG22	1.83	0.61
1:G:452:LEU:HD21	2:H:57:THR:HG21	1.82	0.60
2:N:1048:LEU:HD21	2:N:1051:TYR:HB3	1.82	0.60
2:P:1039:GLN:HB2	2:P:1049:LEU:HG	1.84	0.59
2:F:91:THR:HG23	2:F:121:THR:HA	1.83	0.59
1:C:523:THR:HG23	1:C:524:VAL:HG23	1.86	0.58
1:C:379:CYS:SG	1:C:384:PRO:HG3	2.44	0.58
1:O:355:ARG:HG2	2:P:1031:ALA:HB1	1.85	0.58
1:O:361:CYS:SG	1:O:362:VAL:N	2.77	0.57
2:N:68:VAL:HG22	2:N:83:LEU:HD13	1.87	0.57
1:O:474:GLN:HG2	1:O:480:CYS:SG	2.45	0.57
2:P:18:VAL:HG23	2:P:86:LEU:HD11	1.87	0.57
1:C:474:GLN:HG2	1:C:480:CYS:SG	2.45	0.56
1:I:452:LEU:HD21	2:J:57:THR:HG21	1.88	0.56
1:M:355:ARG:HG2	2:N:1031:ALA:HB1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:PHE:CE1	2:B:112:ASP:HB3	2.41	0.55
1:G:523:THR:HG23	1:G:524:VAL:HG23	1.88	0.55
2:P:2:VAL:HG13	2:P:26:GLY:H	1.70	0.55
1:A:465:GLU:HA	2:B:105:TYR:HA	1.87	0.55
1:C:340:GLU:OE2	1:C:340:GLU:N	2.36	0.55
1:G:482:GLY:O	2:H:30:SER:OG	2.25	0.55
2:N:1026:SER:HA	2:N:1030:GLY:HA3	1.89	0.55
1:O:357:ARG:HH21	1:O:394:ASN:HB3	1.71	0.55
2:F:87:ARG:HB3	2:F:89:GLU:OE1	2.07	0.54
2:L:91:THR:HG23	2:L:121:THR:HA	1.88	0.54
2:N:7:SER:HB3	2:N:21:SER:HB3	1.89	0.54
2:J:60:TYR:HB2	2:J:65:GLN:HG3	1.90	0.54
2:J:38:ARG:NH1	2:J:46:GLU:OE2	2.39	0.54
2:P:52:ILE:O	2:P:56:GLY:N	2.40	0.54
2:H:18:VAL:HG23	2:H:86:LEU:HD11	1.90	0.54
1:K:470:THR:O	2:L:31:SER:OG	2.26	0.54
2:L:1063:ARG:HA	2:L:1078:THR:HG22	1.90	0.54
1:C:497:PHE:CG	1:C:507:PRO:HG3	2.43	0.54
1:E:453:TYR:HE2	1:E:455:LEU:HD13	1.73	0.54
1:K:394:ASN:HB2	1:K:516:GLU:HB2	1.88	0.54
1:O:453:TYR:HE1	1:O:455:LEU:HD13	1.73	0.54
2:N:99:LYS:HG2	2:N:109:TRP:HB3	1.90	0.53
1:I:360:ASN:H	1:I:523:THR:HB	1.74	0.53
1:C:355:ARG:HG2	2:D:1031:ALA:HB1	1.90	0.53
1:E:401:VAL:HG22	1:E:509:ARG:HG2	1.91	0.52
2:P:1063:ARG:HD2	2:P:1078:THR:O	2.09	0.52
1:E:357:ARG:HH12	1:E:394:ASN:HB3	1.74	0.52
1:C:486:PHE:CD2	2:L:26:GLY:HA2	2.44	0.52
1:O:336:CYS:N	1:O:361:CYS:SG	2.82	0.51
1:K:355:ARG:HG2	2:L:1031:ALA:HB1	1.91	0.51
1:E:361:CYS:HB3	1:E:524:VAL:HG13	1.92	0.51
1:G:418:ILE:HA	1:G:422:ASN:HD22	1.74	0.51
1:A:531:THR:O	5:A:702:MPD:HM1	2.11	0.51
2:L:98:ARG:HH21	2:L:113:LEU:HD21	1.76	0.51
1:M:350:VAL:HG22	1:M:422:ASN:HB3	1.93	0.51
2:J:3:GLN:H	2:J:25:SER:HB3	1.76	0.50
2:P:24:ALA:HB2	2:P:29:PHE:CE1	2.46	0.50
2:J:38:ARG:NH2	2:J:90:ASP:HA	2.27	0.50
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.93	0.50
2:B:1062:ASP:OD1	2:B:1062:ASP:N	2.43	0.50
2:J:91:THR:HG23	2:J:121:THR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1049:LEU:HD21	2:N:1064:PHE:CD2	2.47	0.50
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.46	0.50
2:F:68:VAL:HG22	2:F:83:LEU:HD13	1.94	0.50
1:O:403:ARG:HG2	1:O:505:TYR:HA	1.94	0.50
1:C:453:TYR:HE1	1:C:455:LEU:HG	1.77	0.50
1:C:339:GLY:O	1:C:343:ASN:HB2	2.12	0.49
1:G:431:GLY:HA2	1:G:515:PHE:CD2	2.47	0.49
1:O:366:SER:HA	1:O:369:TYR:CZ	2.47	0.49
2:H:100:PHE:CE1	2:H:112:ASP:HB3	2.46	0.49
2:P:1063:ARG:HH21	2:P:1084:ASP:CG	2.16	0.49
2:H:68:VAL:HA	2:H:82:GLU:O	2.13	0.49
1:I:425:LEU:HD21	1:I:512:VAL:HG11	1.94	0.49
1:C:336:CYS:SG	1:C:363:ALA:HB2	2.52	0.49
1:C:452:LEU:HD21	2:D:57:THR:HG21	1.95	0.49
1:I:484:GLU:HG3	1:I:489:TYR:HA	1.95	0.49
1:A:431:GLY:HA2	1:A:515:PHE:HD2	1.78	0.49
1:K:426:PRO:HG2	1:K:429:PHE:HB2	1.94	0.48
2:L:110:TYR:HB3	2:L:1036:HIS:CG	2.47	0.48
2:H:1057:PRO:HD2	2:H:1060:VAL:HG21	1.93	0.48
2:J:18:VAL:O	2:J:82:GLU:HA	2.13	0.48
2:H:28:THR:HG23	2:H:30:SER:HB2	1.95	0.48
2:N:97:ALA:HA	2:N:113:LEU:O	2.13	0.48
1:A:358:ILE:HG22	1:A:361:CYS:SG	2.53	0.48
1:G:333:THR:HG22	1:G:334:ASN:H	1.79	0.48
1:I:333:THR:HG23	1:I:334:ASN:H	1.77	0.48
1:I:395:VAL:HG23	1:I:524:VAL:HG11	1.94	0.48
2:P:1049:LEU:O	2:P:1057:PRO:HD2	2.13	0.48
1:I:412:PRO:HG3	1:I:429:PHE:HB3	1.96	0.48
1:K:346:ARG:NH2	2:L:60:TYR:O	2.47	0.48
1:K:431:GLY:HA2	1:K:515:PHE:CD2	2.49	0.48
1:M:503:VAL:HA	1:M:506:GLN:HE21	1.78	0.48
2:P:1012:GLY:HA3	2:P:1018:VAL:HG11	1.95	0.48
1:C:490:PHE:CE1	2:D:31:SER:HB3	2.49	0.48
1:A:461:LEU:HD22	1:A:465:GLU:HB3	1.96	0.47
1:A:463:PRO:HG2	5:A:701:MPD:H4	1.96	0.47
1:G:346:ARG:HD2	2:H:62:GLN:HG3	1.97	0.47
2:P:2:VAL:HG22	2:P:27:GLY:H	1.78	0.47
2:D:99:LYS:HG2	2:D:109:TRP:HB3	1.97	0.47
2:H:5:VAL:O	2:H:22:CYS:HA	2.14	0.47
2:L:108:THR:OG1	2:L:1093:TYR:HB2	2.14	0.47
1:M:401:VAL:HG22	1:M:509:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:394:ASN:OD1	1:G:516:GLU:HB2	2.14	0.47
1:I:379:CYS:HA	1:I:432:CYS:HA	1.96	0.47
1:K:399:SER:HA	1:K:510:VAL:O	2.15	0.47
2:L:29:PHE:CZ	2:L:34:ILE:HG13	2.49	0.47
1:O:421:TYR:CD1	1:O:457:ARG:HB3	2.50	0.47
2:P:67:ARG:NH2	2:P:90:ASP:OD2	2.47	0.47
1:E:431:GLY:HA2	1:E:515:PHE:HD2	1.80	0.47
2:F:110:TYR:HB3	2:F:1036:HIS:CD2	2.50	0.47
1:G:393:THR:O	1:G:523:THR:HG22	2.14	0.47
1:G:360:ASN:N	1:G:523:THR:OG1	2.46	0.47
2:H:108:THR:HG23	2:H:1036:HIS:HE2	1.79	0.46
2:N:64:PHE:HB3	2:N:68:VAL:HG21	1.96	0.46
2:F:1048:LEU:HD21	2:F:1051:TYR:HB3	1.96	0.46
2:D:89:GLU:H	2:D:89:GLU:HG3	1.53	0.46
2:B:14:PRO:HD3	2:B:123:SER:O	2.15	0.46
2:J:39:GLN:HB2	2:J:95:TYR:HE2	1.81	0.46
2:L:67:ARG:NH2	2:L:90:ASP:OD2	2.48	0.46
1:O:450:ASN:HA	2:P:57:THR:HG23	1.97	0.46
1:A:363:ALA:O	1:A:527:PRO:HD3	2.16	0.46
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.51	0.46
2:J:16:SER:OG	2:J:17:SER:N	2.49	0.46
2:P:1063:ARG:NH2	2:P:1084:ASP:OD1	2.48	0.46
2:J:1025:ASN:OD1	2:J:1028:ASN:ND2	2.49	0.46
1:K:457:ARG:NH1	1:K:461:LEU:HB3	2.31	0.46
2:L:1018:VAL:HG21	2:L:1080:LEU:HD22	1.96	0.46
2:J:18:VAL:CG2	2:J:86:LEU:HD11	2.47	0.45
1:G:382:VAL:HG11	1:G:387:LEU:HD21	1.98	0.45
1:C:417:LYS:HB2	1:C:417:LYS:HE2	1.87	0.45
1:C:437:ASN:ND2	1:C:506:GLN:OE1	2.40	0.45
2:H:98:ARG:HD3	2:H:113:LEU:HD12	1.98	0.45
1:O:357:ARG:HB3	2:P:1026:SER:HB2	1.99	0.45
1:E:339:GLY:O	1:E:343:ASN:HB2	2.17	0.45
2:F:1080:LEU:HD11	2:F:1108:LEU:HD21	1.98	0.45
2:J:29:PHE:HE1	2:J:74:GLU:HA	1.81	0.45
2:J:1080:LEU:HD11	2:J:1108:LEU:HD21	1.98	0.45
1:M:456:PHE:HB3	1:M:473:TYR:CG	2.51	0.45
2:J:14:PRO:HG3	2:J:124:SER:HA	1.98	0.45
2:P:108:THR:OG1	2:P:1093:TYR:HB2	2.16	0.45
2:P:1085:GLU:HG3	2:P:1108:LEU:O	2.17	0.45
2:H:1047:LYS:HD3	2:H:1048:LEU:H	1.80	0.45
1:O:431:GLY:HA2	1:O:515:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:68:VAL:HA	2:J:82:GLU:O	2.17	0.45
2:B:1063:ARG:HB3	2:B:1078:THR:O	2.16	0.45
1:I:431:GLY:HA2	1:I:515:PHE:CD2	2.52	0.45
2:J:38:ARG:HH21	2:J:90:ASP:HA	1.82	0.45
2:J:29:PHE:CZ	2:J:72:ALA:HB1	2.52	0.44
2:D:98:ARG:HD3	2:D:113:LEU:HD12	1.99	0.44
2:H:1049:LEU:HD21	2:H:1064:PHE:CD1	2.52	0.44
2:P:64:PHE:O	2:P:68:VAL:HG12	2.17	0.44
2:L:29:PHE:HZ	2:L:79:ALA:HB2	1.83	0.44
1:M:490:PHE:HE1	2:N:31:SER:HB2	1.83	0.44
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.51	0.44
1:K:347:PHE:HB3	1:K:401:VAL:HG23	1.99	0.44
2:P:18:VAL:O	2:P:82:GLU:HA	2.18	0.44
2:L:1080:LEU:HD11	2:L:1108:LEU:HD21	1.99	0.44
1:C:529:LYS:HB2	1:C:529:LYS:HE3	1.85	0.44
2:J:38:ARG:HD2	2:J:48:MET:SD	2.57	0.44
2:B:110:TYR:HB3	2:B:1036:HIS:CD2	2.53	0.44
2:H:108:THR:OG1	2:H:1093:TYR:HB2	2.18	0.44
1:K:419:ALA:HA	1:K:423:TYR:O	2.17	0.44
1:C:364:ASP:OD2	1:C:367:VAL:HG13	2.18	0.43
2:D:18:VAL:HB	2:D:86:LEU:HD11	1.99	0.43
2:J:64:PHE:O	2:J:68:VAL:HG12	2.19	0.43
1:G:350:VAL:HG22	1:G:422:ASN:HB3	1.99	0.43
2:J:4:LEU:HB3	2:J:22:CYS:SG	2.58	0.43
2:J:32:TYR:HB3	2:J:98:ARG:HD3	2.01	0.43
2:B:108:THR:OG1	2:B:1093:TYR:HB2	2.18	0.43
1:I:355:ARG:HG2	2:J:1031:ALA:HB1	2.00	0.43
1:C:505:TYR:CD1	1:M:528:LYS:HA	2.53	0.43
1:A:444:LYS:O	1:A:499:PRO:HD3	2.18	0.43
2:F:36:TRP:CE2	2:F:81:MET:HB2	2.54	0.43
2:H:12:LYS:O	2:H:122:VAL:HA	2.19	0.43
2:J:14:PRO:CG	2:J:124:SER:HA	2.49	0.43
1:M:455:LEU:HD23	1:M:455:LEU:H	1.83	0.43
2:J:108:THR:OG1	2:J:1093:TYR:HB2	2.19	0.43
2:D:29:PHE:HB3	2:D:53:PRO:HG2	2.01	0.42
1:C:425:LEU:HD21	1:C:512:VAL:HG11	2.01	0.42
1:C:444:LYS:O	1:C:499:PRO:HD3	2.19	0.42
1:I:342:PHE:CZ	1:I:368:LEU:HD21	2.54	0.42
2:N:99:LYS:HD3	2:N:109:TRP:CG	2.54	0.42
1:O:354:ASN:HA	2:P:1033:TYR:OH	2.20	0.42
1:C:338:PHE:O	1:C:342:PHE:HD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:CYS:HA	1:C:432:CYS:HA	2.01	0.42
2:H:74:GLU:H	2:H:74:GLU:CD	2.22	0.42
2:F:64:PHE:HB3	2:F:68:VAL:CG2	2.49	0.42
1:E:431:GLY:HA2	1:E:515:PHE:CD2	2.55	0.42
2:F:40:ALA:HB2	2:F:92:ALA:HB2	2.02	0.42
1:K:403:ARG:HG2	1:K:505:TYR:HA	2.01	0.42
2:J:67:ARG:HD2	2:J:84:SER:O	2.19	0.42
1:M:421:TYR:CD1	1:M:457:ARG:HB3	2.54	0.42
1:K:386:LYS:HG3	1:K:390:LEU:HD11	2.01	0.42
2:N:18:VAL:O	2:N:82:GLU:HA	2.20	0.42
2:P:91:THR:HG23	2:P:121:THR:HA	2.02	0.42
1:A:425:LEU:HD22	1:A:426:PRO:HD2	2.02	0.42
2:D:23:LYS:HG2	2:D:78:THR:HG23	2.02	0.42
1:E:497:PHE:CD2	1:E:507:PRO:HB3	2.54	0.42
2:H:13:LYS:HA	2:H:13:LYS:HD3	1.89	0.42
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.55	0.41
1:C:392:PHE:CD1	1:C:515:PHE:HB3	2.55	0.41
2:P:61:ALA:HB3	2:P:64:PHE:HD2	1.85	0.41
2:P:110:TYR:HB3	2:P:1036:HIS:CE1	2.55	0.41
1:A:355:ARG:HG2	2:B:1031:ALA:HB1	2.02	0.41
2:D:99:LYS:HG3	2:D:111:PHE:CE1	2.55	0.41
2:D:1029:ILE:HG23	2:D:1068:LYS:HD2	2.01	0.41
1:G:490:PHE:HE1	2:H:31:SER:HB2	1.85	0.41
2:F:64:PHE:HB3	2:F:68:VAL:HG23	2.03	0.41
2:F:100:PHE:CE1	2:F:112:ASP:HB3	2.55	0.41
1:O:439:ASN:HA	1:O:507:PRO:HG2	2.03	0.41
1:G:445:VAL:O	1:G:498:GLN:NE2	2.53	0.41
2:J:40:ALA:HB3	2:J:43:GLN:HB2	2.02	0.41
2:H:97:ALA:HA	2:H:113:LEU:O	2.21	0.41
2:N:64:PHE:HB3	2:N:68:VAL:CG2	2.51	0.41
2:F:60:TYR:HE1	2:F:70:ILE:HG13	1.86	0.41
1:G:444:LYS:O	1:G:499:PRO:HD3	2.21	0.41
1:A:346:ARG:NH1	2:B:60:TYR:O	2.54	0.41
1:C:444:LYS:HB3	1:C:444:LYS:HE2	1.80	0.41
2:F:12:LYS:HG3	2:F:18:VAL:CG2	2.47	0.41
2:F:1024:GLY:O	2:F:1071:THR:HB	2.20	0.41
2:F:1049:LEU:HD21	2:F:1064:PHE:CD1	2.56	0.41
2:J:36:TRP:CE2	2:J:81:MET:HB2	2.55	0.41
2:N:1063:ARG:HB3	2:N:1078:THR:O	2.20	0.41
2:J:123:SER:O	2:J:124:SER:OG	2.32	0.41
2:P:91:THR:HA	2:P:120:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:CYS:HA	1:C:337:PRO:HD3	1.82	0.40
2:H:1063:ARG:HB2	2:H:1078:THR:O	2.22	0.40
2:L:108:THR:HG23	2:L:1036:HIS:HE2	1.86	0.40
2:N:108:THR:OG1	2:N:1093:TYR:HB2	2.21	0.40
1:E:394:ASN:OD1	1:E:516:GLU:HB2	2.21	0.40
2:N:36:TRP:CE2	2:N:81:MET:HB2	2.56	0.40
1:O:425:LEU:HD21	1:O:512:VAL:HG11	2.03	0.40
1:A:452:LEU:HD21	2:B:57:THR:HG21	2.04	0.40
1:G:502:GLY:O	1:G:506:GLN:HG3	2.21	0.40
1:M:431:GLY:HA2	1:M:515:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	198/234 (85%)	194 (98%)	4 (2%)	0	100	100
1	C	194/234 (83%)	185 (95%)	9 (5%)	0	100	100
1	E	194/234 (83%)	188 (97%)	6 (3%)	0	100	100
1	G	195/234 (83%)	187 (96%)	8 (4%)	0	100	100
1	I	194/234 (83%)	187 (96%)	7 (4%)	0	100	100
1	K	192/234 (82%)	185 (96%)	7 (4%)	0	100	100
1	M	196/234 (84%)	190 (97%)	6 (3%)	0	100	100
1	O	194/234 (83%)	191 (98%)	3 (2%)	0	100	100
2	B	233/303 (77%)	231 (99%)	2 (1%)	0	100	100
2	D	231/303 (76%)	229 (99%)	2 (1%)	0	100	100
2	F	232/303 (77%)	231 (100%)	1 (0%)	0	100	100
2	H	236/303 (78%)	228 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	234/303 (77%)	232 (99%)	2 (1%)	0	100	100
2	L	234/303 (77%)	231 (99%)	3 (1%)	0	100	100
2	N	230/303 (76%)	226 (98%)	4 (2%)	0	100	100
2	P	231/303 (76%)	226 (98%)	5 (2%)	0	100	100
All	All	3418/4296 (80%)	3341 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/202 (84%)	168 (99%)	1 (1%)	86	96
1	C	168/202 (83%)	164 (98%)	4 (2%)	49	81
1	E	167/202 (83%)	164 (98%)	3 (2%)	59	86
1	G	166/202 (82%)	162 (98%)	4 (2%)	49	81
1	I	165/202 (82%)	162 (98%)	3 (2%)	59	86
1	K	164/202 (81%)	164 (100%)	0	100	100
1	M	163/202 (81%)	161 (99%)	2 (1%)	71	92
1	O	168/202 (83%)	165 (98%)	3 (2%)	59	86
2	B	187/231 (81%)	183 (98%)	4 (2%)	53	84
2	D	187/231 (81%)	184 (98%)	3 (2%)	62	88
2	F	188/231 (81%)	186 (99%)	2 (1%)	73	92
2	H	188/231 (81%)	188 (100%)	0	100	100
2	J	189/231 (82%)	187 (99%)	2 (1%)	73	92
2	L	187/231 (81%)	186 (100%)	1 (0%)	88	96
2	N	186/231 (80%)	180 (97%)	6 (3%)	39	73
2	P	185/231 (80%)	184 (100%)	1 (0%)	88	96
All	All	2827/3464 (82%)	2788 (99%)	39 (1%)	67	90

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	PHE
2	B	29	PHE
2	B	73	ASP
2	B	93	VAL
2	B	1062	ASP
1	C	357	ARG
1	C	377	PHE
1	C	477	SER
1	C	517	LEU
2	D	89	GLU
2	D	100	PHE
2	D	1087	ASP
1	E	361	CYS
1	E	405	ASP
1	E	517	LEU
2	F	3	GLN
2	F	75	SER
1	G	389	ASP
1	G	390	LEU
1	G	391	CYS
1	G	525	CYS
1	I	333	THR
1	I	517	LEU
1	I	524	VAL
2	J	29	PHE
2	J	1087	ASP
2	L	71	THR
1	M	471	GLU
1	M	494	SER
2	N	10	GLU
2	N	28	THR
2	N	96	CYS
2	N	121	THR
2	N	1087	ASP
2	N	1108	LEU
1	O	415	THR
1	O	517	LEU
1	O	524	VAL
2	P	96	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

6 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	0.43	0	17,19,21	0.91	1 (5%)
3	FUC	Q	2	3	10,10,11	0.80	0	14,14,16	1.08	1 (7%)
4	NAG	R	1	1,4	14,14,15	0.30	0	17,19,21	0.68	0
4	FUC	R	2	4	10,10,11	1.09	1 (10%)	14,14,16	0.75	0
3	NAG	S	1	1,3	14,14,15	0.40	0	17,19,21	0.57	0
3	FUC	S	2	3	10,10,11	0.82	0	14,14,16	1.05	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	1,3	-	1/6/23/26	0/1/1/1
3	FUC	Q	2	3	-	-	0/1/1/1
4	NAG	R	1	1,4	-	3/6/23/26	0/1/1/1
4	FUC	R	2	4	-	-	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	S	2	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	2	FUC	O5-C1	-2.53	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	1	NAG	C1-O5-C5	2.59	115.70	112.19
3	Q	2	FUC	C1-O5-C5	2.49	118.43	112.78
3	S	2	FUC	O5-C5-C4	2.19	113.45	109.52

There are no chirality outliers.

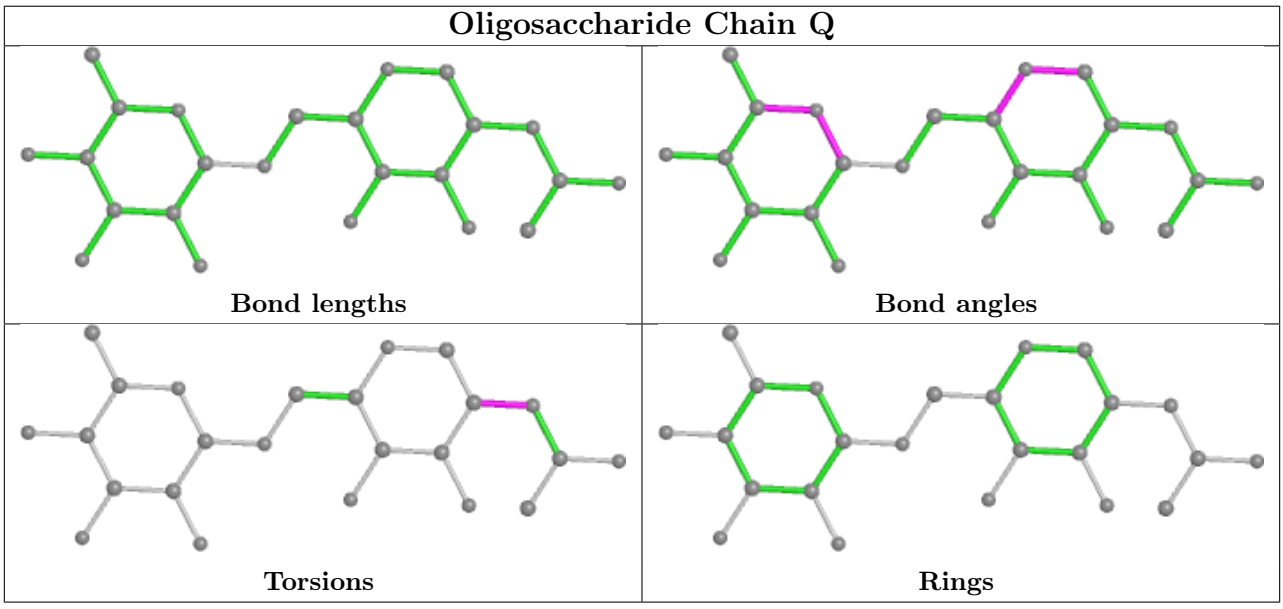
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7

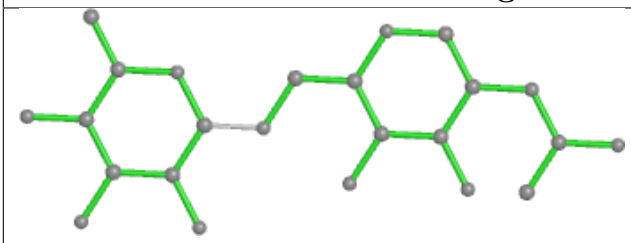
There are no ring outliers.

No monomer is involved in short contacts.

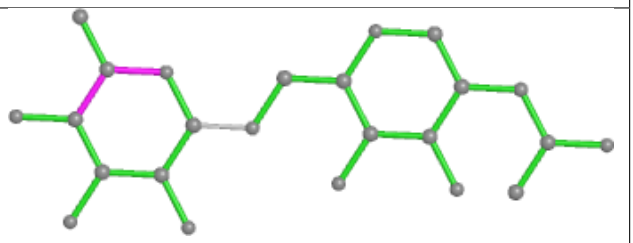
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



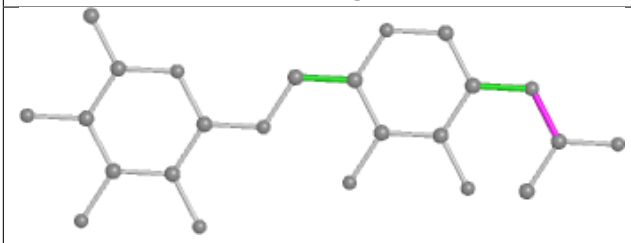
Oligosaccharide Chain S



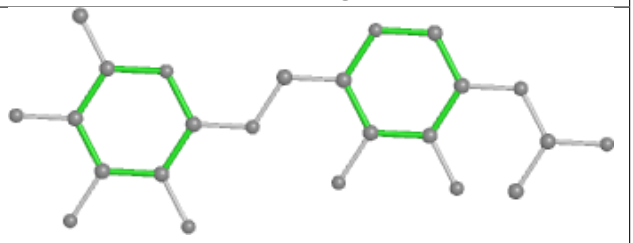
Bond lengths



Bond angles

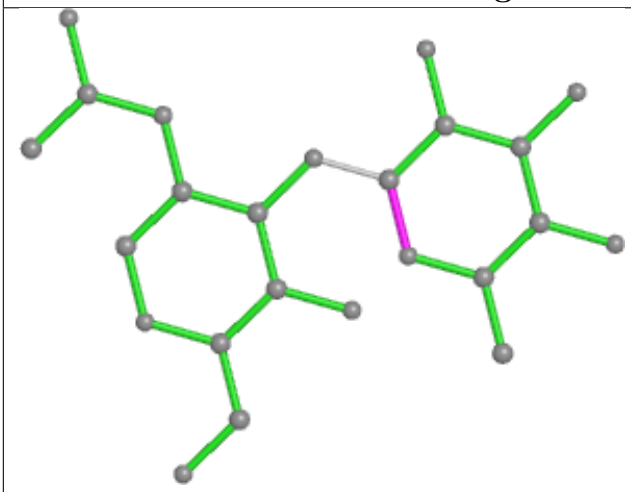


Torsions

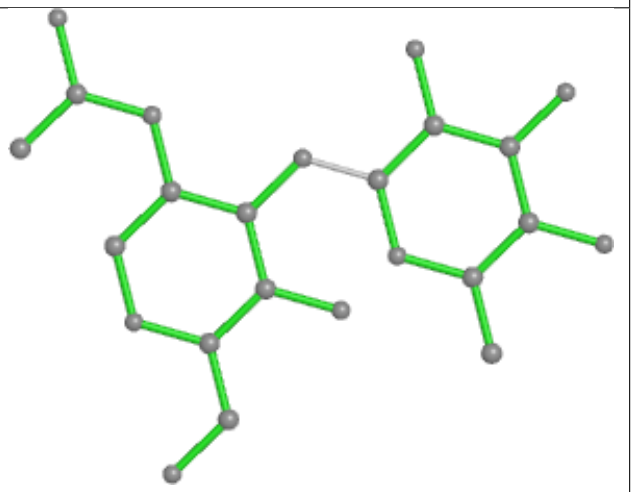


Rings

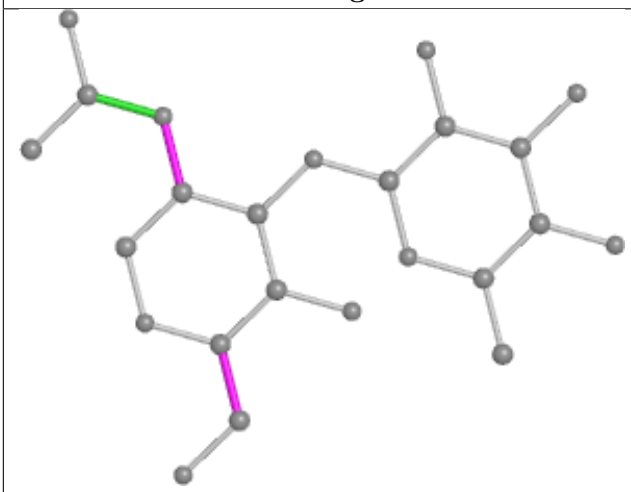
Oligosaccharide Chain R



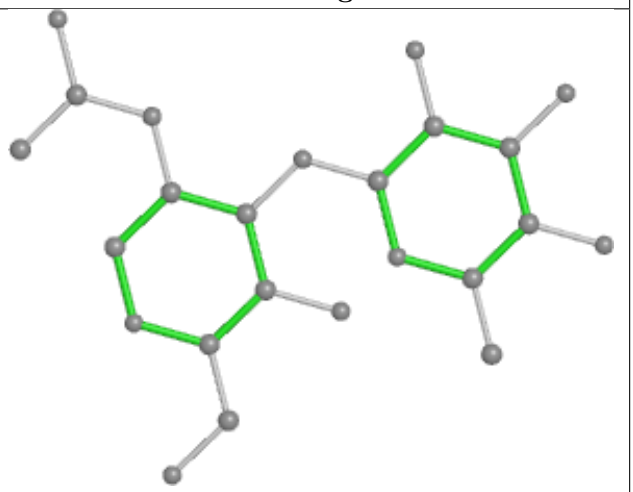
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 for Mogul analysis.

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	MPD	D	1201	-	7,7,7	0.68	0	9,10,10	0.34	0
5	MPD	J	1202	-	7,7,7	0.69	0	9,10,10	0.31	0
5	MPD	O	602	-	7,7,7	0.68	0	9,10,10	0.33	0
8	NAG	C	601	1	14,14,15	0.25	0	17,19,21	0.47	0
5	MPD	A	702	-	7,7,7	0.63	0	9,10,10	0.70	0
5	MPD	J	1201	-	7,7,7	0.69	0	9,10,10	0.33	0
8	NAG	O	601	1	14,14,15	0.33	0	17,19,21	0.42	0
5	MPD	B	1201	-	7,7,7	0.67	0	9,10,10	0.43	0
5	MPD	P	1201	-	7,7,7	0.65	0	9,10,10	0.43	0
5	MPD	A	701	-	7,7,7	0.68	0	9,10,10	0.38	0
5	MPD	I	601	-	7,7,7	0.69	0	9,10,10	0.34	0
5	MPD	H	1201	-	7,7,7	0.70	0	9,10,10	0.34	0
5	MPD	I	602	-	7,7,7	0.68	0	9,10,10	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	D	1201	-	-	0/5/5/5	-
5	MPD	J	1202	-	-	2/5/5/5	-
5	MPD	O	602	-	-	0/5/5/5	-
8	NAG	C	601	1	-	3/6/23/26	0/1/1/1
5	MPD	A	702	-	-	0/5/5/5	-
5	MPD	J	1201	-	-	3/5/5/5	-
8	NAG	O	601	1	-	0/6/23/26	0/1/1/1
5	MPD	B	1201	-	-	0/5/5/5	-
5	MPD	P	1201	-	-	0/5/5/5	-
5	MPD	A	701	-	-	0/5/5/5	-
5	MPD	I	601	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	H	1201	-	-	2/5/5/5	-
5	MPD	I	602	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	601	NAG	C8-C7-N2-C2
8	C	601	NAG	O7-C7-N2-C2
8	C	601	NAG	O5-C5-C6-O6
5	I	602	MPD	O2-C2-C3-C4
5	J	1201	MPD	O2-C2-C3-C4
5	J	1202	MPD	C2-C3-C4-O4
5	I	602	MPD	C1-C2-C3-C4
5	I	602	MPD	CM-C2-C3-C4
5	J	1201	MPD	C1-C2-C3-C4
5	J	1201	MPD	CM-C2-C3-C4
5	H	1201	MPD	C2-C3-C4-C5
5	I	601	MPD	C2-C3-C4-C5
5	J	1202	MPD	C2-C3-C4-C5
5	H	1201	MPD	C2-C3-C4-O4
5	I	601	MPD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	MPD	1	0
5	A	701	MPD	1	0

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, 95^{th} 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	200/234 (85%)	0.07	1 (0%)	91	88	31, 48, 81, 110	0
1	C	196/234 (83%)	0.35	11 (5%)	24	16	39, 63, 113, 132	0
1	E	196/234 (83%)	0.16	4 (2%)	65	56	36, 52, 94, 126	0
1	G	197/234 (84%)	0.07	2 (1%)	82	77	38, 65, 101, 129	0
1	I	196/234 (83%)	0.00	1 (0%)	91	88	34, 54, 94, 136	0
1	K	194/234 (82%)	0.23	5 (2%)	56	46	42, 62, 106, 138	0
1	M	198/234 (84%)	0.30	8 (4%)	38	28	39, 63, 109, 126	0
1	O	196/234 (83%)	0.19	2 (1%)	82	77	43, 64, 102, 117	0
2	B	237/303 (78%)	-0.00	2 (0%)	86	81	31, 44, 81, 105	0
2	D	235/303 (77%)	0.03	2 (0%)	84	80	33, 49, 89, 126	0
2	F	236/303 (77%)	-0.06	1 (0%)	92	91	32, 47, 85, 130	0
2	H	240/303 (79%)	-0.02	2 (0%)	86	81	32, 45, 79, 126	0
2	J	238/303 (78%)	-0.04	3 (1%)	77	72	31, 44, 80, 138	0
2	L	238/303 (78%)	0.05	4 (1%)	70	63	33, 46, 85, 147	0
2	N	234/303 (77%)	-0.01	1 (0%)	92	91	30, 46, 87, 107	0
2	P	235/303 (77%)	0.20	10 (4%)	35	25	33, 51, 91, 136	0
All	All	3466/4296 (80%)	0.09	59 (1%)	70	63	30, 52, 95, 147	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	479	PRO	4.4
2	D	123	SER	4.0
2	L	28	THR	3.8
1	C	487	ASN	3.8
2	H	999	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	J	27	GLY	3.5
2	P	25	SER	3.5
2	P	28	THR	3.5
2	L	25	SER	3.5
1	K	371	SER	3.4
2	L	29	PHE	3.4
1	C	483	VAL	3.3
2	B	105	TYR	3.2
2	H	998	GLY	3.2
1	K	364	ASP	3.2
1	M	333	THR	3.1
1	C	478	THR	3.1
2	B	112	ASP	3.0
2	P	26	GLY	3.0
2	P	30	SER	2.9
1	I	333	THR	2.9
2	L	32	TYR	2.8
1	M	479	PRO	2.8
1	M	475	ALA	2.8
1	C	476	GLY	2.8
1	E	373	SER	2.7
1	G	472	ILE	2.7
2	P	29	PHE	2.7
1	C	486	PHE	2.6
2	J	124	SER	2.6
1	C	482	GLY	2.6
1	C	480	CYS	2.6
1	M	477	SER	2.5
1	E	384	PRO	2.5
1	C	475	ALA	2.5
1	O	369	TYR	2.4
2	P	96	CYS	2.4
2	P	78	THR	2.4
1	K	382	VAL	2.3
1	K	525	CYS	2.3
1	E	369	TYR	2.3
2	N	87	ARG	2.3
2	F	28	THR	2.3
1	M	473	TYR	2.3
1	C	489	TYR	2.3
1	M	478	THR	2.2
2	D	31	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	389	ASP	2.1
1	G	333	THR	2.1
1	A	366	SER	2.1
2	J	28	THR	2.1
1	C	474	GLN	2.1
1	K	428	ASP	2.1
1	M	441	LEU	2.1
2	P	83	LEU	2.1
1	M	371	SER	2.1
2	P	32	TYR	2.1
1	E	375	SER	2.0
2	P	76	THR	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)

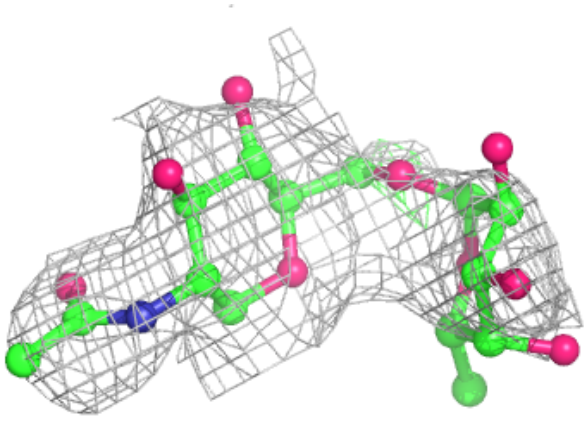
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

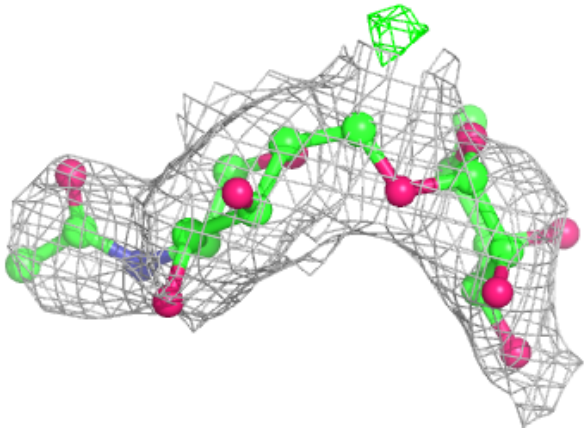
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	S	1	14/15	0.54	0.25	101,119,126,131	0
4	FUC	R	2	10/11	0.65	0.42	116,119,125,126	0
3	FUC	S	2	10/11	0.76	0.34	130,137,139,141	0
4	NAG	R	1	14/15	0.77	0.19	82,95,103,111	0
3	NAG	Q	1	14/15	0.82	0.20	73,100,114,121	0
3	FUC	Q	2	10/11	0.85	0.29	122,132,134,137	0

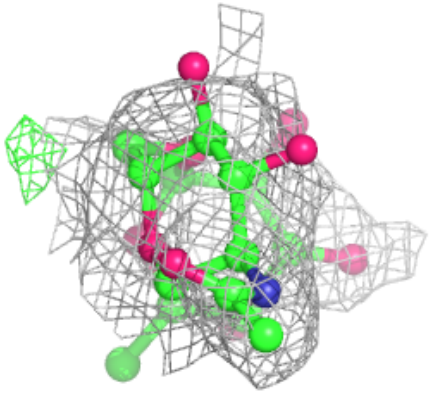
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

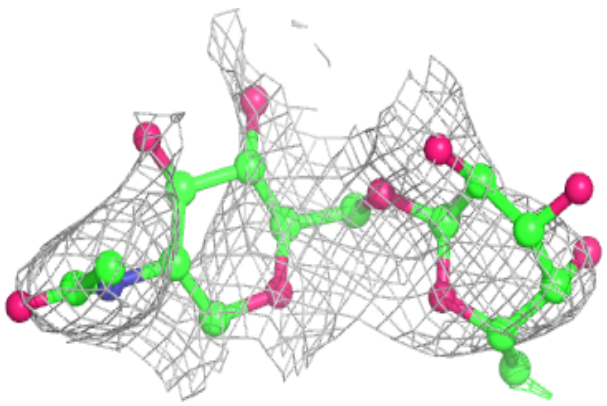


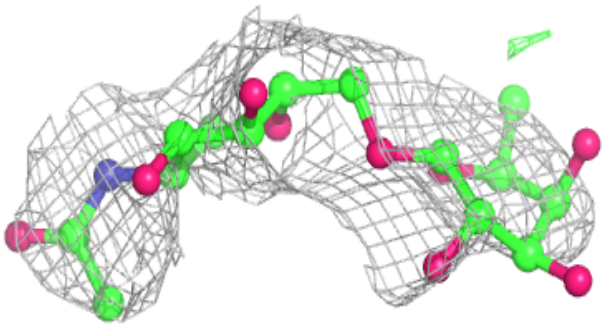


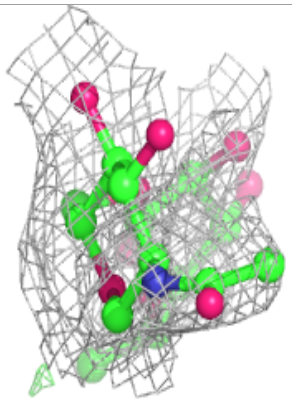


Electron density around Chain S:

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

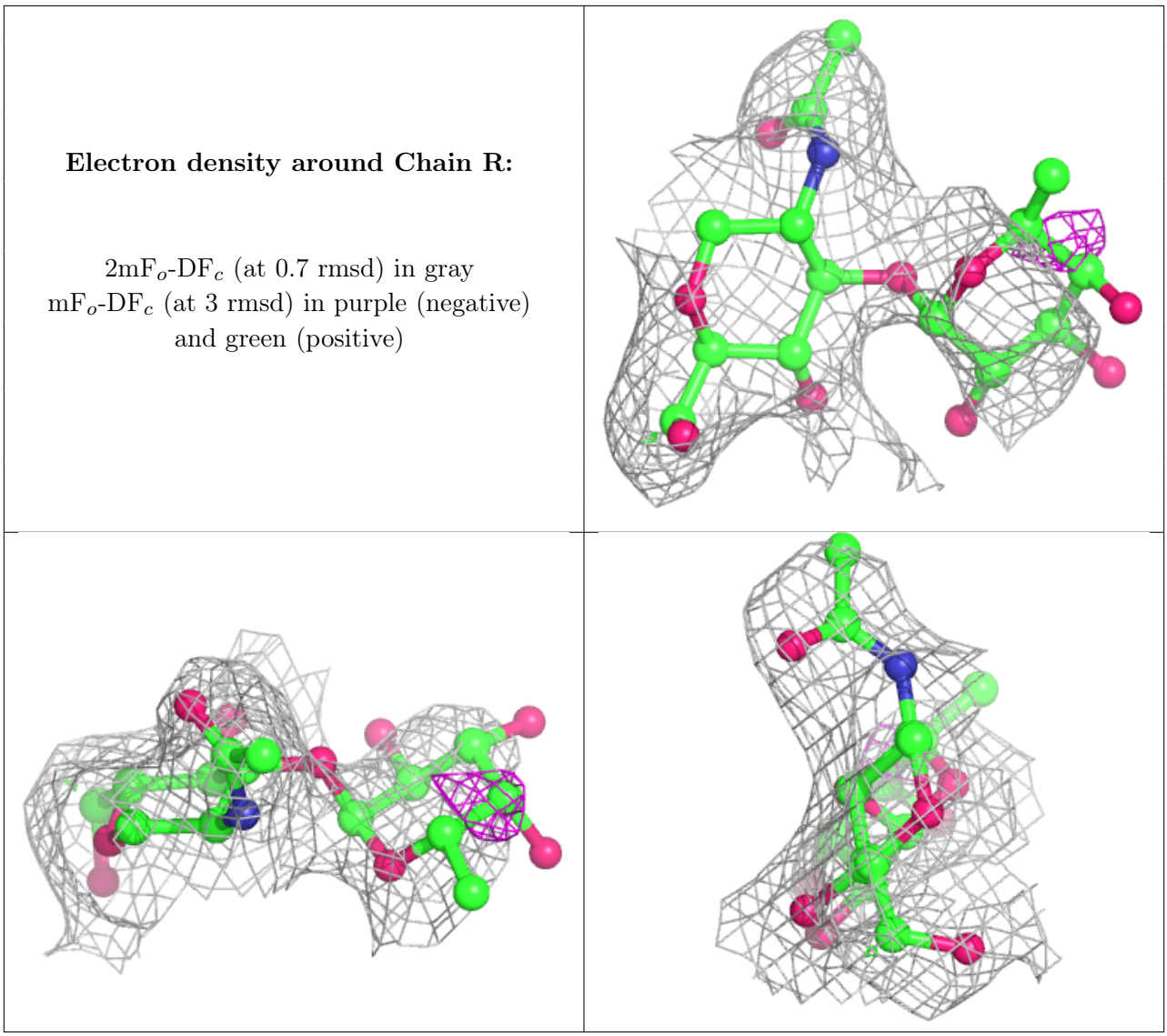






Electron density around Chain R:

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



6.4 Ligands

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, 95^{th} 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	MPD	B	1201	8/8	0.63	0.28	75,88,94,102	0
5	MPD	P	1201	8/8	0.64	0.27	71,82,87,91	0
6	CA	L	1201	1/1	0.64	0.23	43,43,43,43	0
5	MPD	O	602	8/8	0.69	0.49	89,92,100,102	0
8	NAG	O	601	14/15	0.69	0.26	95,112,117,119	0
5	MPD	A	702	8/8	0.70	0.25	81,88,89,91	0
6	CA	F	1201	1/1	0.70	0.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	B	1202	1/1	0.71	0.23	49,49,49,49	0
5	MPD	D	1201	8/8	0.71	0.31	83,91,97,100	0
8	NAG	C	601	14/15	0.73	0.26	133,142,146,147	0
5	MPD	I	601	8/8	0.76	0.46	82,86,92,97	0
5	MPD	H	1201	8/8	0.77	0.33	46,55,63,69	0
5	MPD	A	701	8/8	0.81	0.42	80,81,92,93	0
6	CA	D	1202	1/1	0.83	0.43	32,32,32,32	0
5	MPD	J	1202	8/8	0.84	0.26	52,56,59,61	0
5	MPD	I	602	8/8	0.86	0.29	76,83,85,85	0
5	MPD	J	1201	8/8	0.90	0.24	52,58,64,69	0
6	CA	P	1202	1/1	0.90	0.28	45,45,45,45	0
6	CA	N	1201	1/1	0.92	0.24	43,43,43,43	0
7	CL	G	601	1/1	0.96	0.08	44,44,44,44	0
7	CL	B	1203	1/1	0.97	0.21	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.