



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2021 – 02:12 pm BST

PDB ID : 7ORA
Title : Crystal structure of the T478K mutant receptor binding domain of SARS-CoV-2 Spike glycoprotein in complex with COVOX-45 and COVOX-253 Fabs
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-06-04
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	2.23.1
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)	:	2.23.1

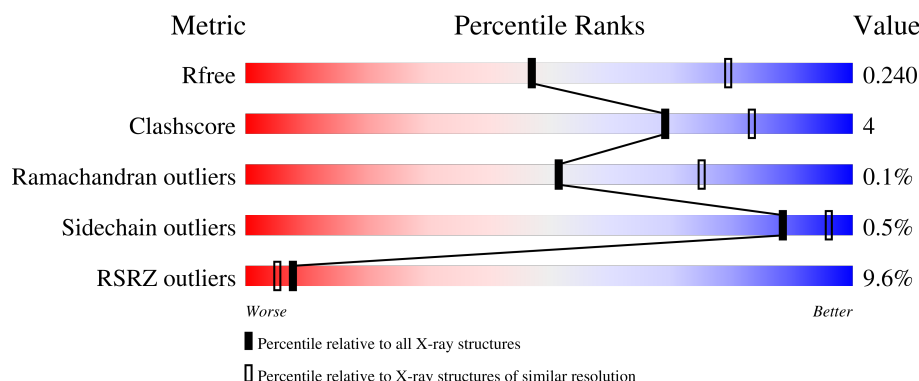
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



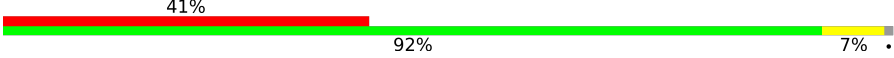





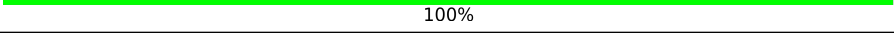

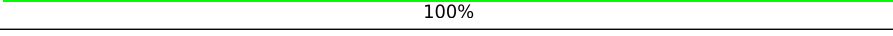
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	205	<div> <div>87%</div> <div>8%</div> <div>.</div> </div>
1	R	205	<div> <div>%</div> <div>88%</div> <div>7%</div> <div>.</div> </div>
2	A	226	<div> <div>9%</div> <div>83%</div> <div>12%</div> <div>.</div> </div>
2	D	226	<div> <div>31%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
3	B	214	<div> <div>10%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	214	
4	F	228	
4	H	228	
5	G	215	
5	L	215	
6	I	2	
7	J	3	
7	K	3	
7	M	3	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16719 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	R	197	Total	C	N	O	S	0	0	0
			1563	1001	264	290	8			
1	C	197	Total	C	N	O	S	0	0	0
			1563	1001	264	290	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	324	GLU	-	expression tag	UNP P0DTC2
R	325	THR	-	expression tag	UNP P0DTC2
R	326	GLY	-	expression tag	UNP P0DTC2
R	327	HIS	-	expression tag	UNP P0DTC2
R	328	HIS	-	expression tag	UNP P0DTC2
R	329	HIS	-	expression tag	UNP P0DTC2
R	330	HIS	-	expression tag	UNP P0DTC2
R	331	HIS	-	expression tag	UNP P0DTC2
R	332	HIS	-	expression tag	UNP P0DTC2
R	478	LYS	THR	engineered mutation	UNP P0DTC2
R	527	LYS	PRO	conflict	UNP P0DTC2
C	324	GLU	-	expression tag	UNP P0DTC2
C	325	THR	-	expression tag	UNP P0DTC2
C	326	GLY	-	expression tag	UNP P0DTC2
C	327	HIS	-	expression tag	UNP P0DTC2
C	328	HIS	-	expression tag	UNP P0DTC2
C	329	HIS	-	expression tag	UNP P0DTC2
C	330	HIS	-	expression tag	UNP P0DTC2
C	331	HIS	-	expression tag	UNP P0DTC2
C	332	HIS	-	expression tag	UNP P0DTC2
C	478	LYS	THR	engineered mutation	UNP P0DTC2
C	527	LYS	PRO	conflict	UNP P0DTC2

- Molecule 2 is a protein called COVOX-45 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	216	Total	C	N	O	S	0	0	0
			1631	1037	272	315	7			
2	D	216	Total	C	N	O	S	0	0	0
			1631	1037	272	315	7			

- Molecule 3 is a protein called COVOX-45 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	211	Total	C	N	O	S	0	0	0
			1623	1016	269	334	4			
3	E	211	Total	C	N	O	S	0	0	0
			1623	1016	269	334	4			

- Molecule 4 is a protein called COVOX-253 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	224	Total	C	N	O	S	0	0	0
			1681	1056	284	331	10			
4	H	224	Total	C	N	O	S	0	0	0
			1677	1053	283	331	10			

- Molecule 5 is a protein called COVOX-253 Fab light chain.

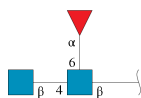
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	214	Total	C	N	O	S	0	0	0
			1628	1016	272	335	5			
5	L	214	Total	C	N	O	S	0	1	0
			1636	1021	275	335	5			

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



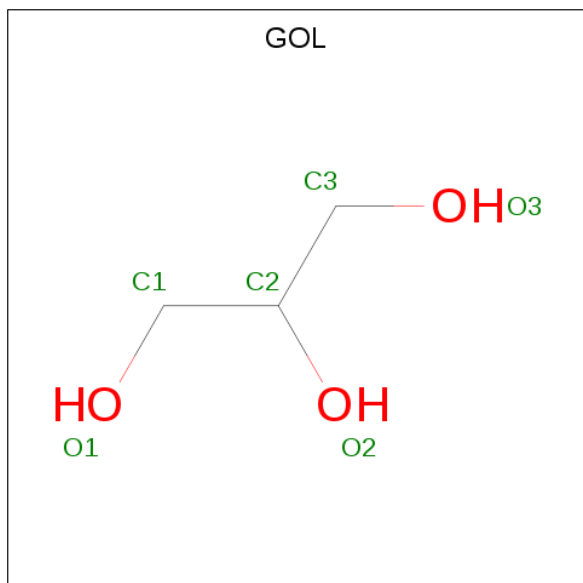
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
7	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
7	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	R	1	Total	C	O	0	0
			6	3	3		
8	R	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total 2	Cl 2	0	0
9	B	1	Total 1	Cl 1	0	0
9	F	2	Total 2	Cl 2	0	0
9	H	1	Total 1	Cl 1	0	0

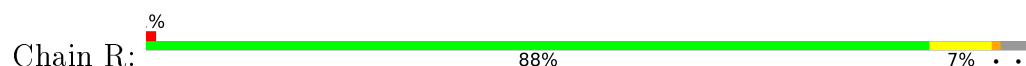
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	R	40	Total 40	O 40	0	0
10	A	31	Total 31	O 31	0	0
10	B	21	Total 21	O 21	0	0
10	F	32	Total 32	O 32	0	0
10	G	20	Total 20	O 20	0	0
10	C	33	Total 33	O 33	0	0
10	D	15	Total 15	O 15	0	0
10	E	19	Total 19	O 19	0	0
10	H	31	Total 31	O 31	0	0
10	L	41	Total 41	O 41	0	0

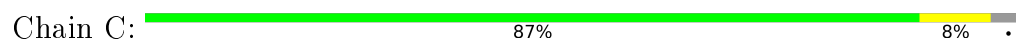
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

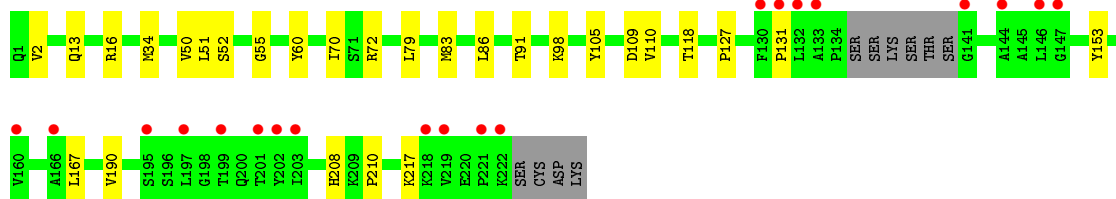
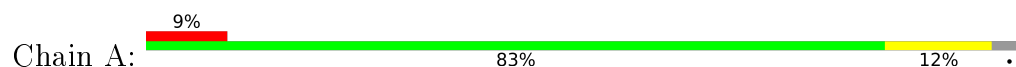
- Molecule 1: Spike protein S1



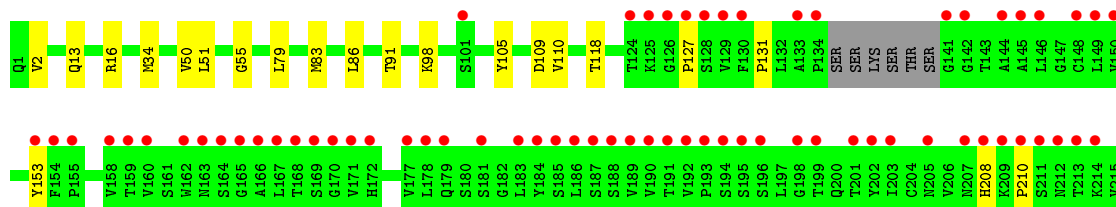
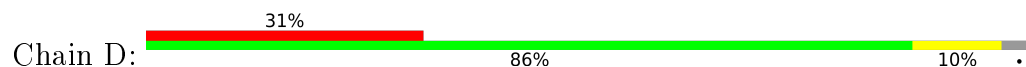
- Molecule 1: Spike protein S1



- Molecule 2: COVOX-45 Fab heavy chain



- Molecule 2: COVOX-45 Fab heavy chain



- Molecule 5: COVOX-253 Fab light chain

Chain L:  89% 10%



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

Chain I:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.57Å 182.38Å 142.41Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	51.50 – 2.60 60.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.2 (51.50-2.60) 90.2 (60.80-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.204 , 0.245 0.201 , 0.240	Depositor DCC
R_{free} test set	3637 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16719	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, NAG, 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	C	0.25	0/1608	0.48	0/2187
1	R	0.25	0/1608	0.48	0/2187
2	A	0.25	0/1672	0.48	0/2276
2	D	0.25	0/1672	0.48	0/2276
3	B	0.25	0/1657	0.47	0/2254
3	E	0.25	0/1657	0.47	0/2254
4	F	0.26	0/1719	0.50	0/2342
4	H	0.26	0/1715	0.51	0/2338
5	G	0.25	0/1664	0.48	0/2259
5	L	0.26	0/1675	0.50	0/2273
All	All	0.25	0/16647	0.49	0/22646

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	C	1563	0	1474	14	0
1	R	1563	0	1474	13	0
2	A	1631	0	1596	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1631	0	1596	11	0
3	B	1623	0	1572	16	0
3	E	1623	0	1572	11	0
4	F	1681	0	1652	14	0
4	H	1677	0	1641	11	0
5	G	1628	0	1566	12	0
5	L	1636	0	1579	13	0
6	I	24	0	22	1	0
7	J	38	0	34	0	0
7	K	38	0	34	0	0
7	M	38	0	34	0	0
8	C	12	0	16	0	0
8	F	6	0	8	0	0
8	L	6	0	8	1	0
8	R	12	0	16	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
9	F	2	0	0	1	0
9	H	1	0	0	0	0
10	A	31	0	0	0	0
10	B	21	0	0	1	0
10	C	33	0	0	3	0
10	D	15	0	0	0	0
10	E	19	0	0	2	0
10	F	32	0	0	0	0
10	G	20	0	0	0	0
10	H	31	0	0	1	0
10	L	41	0	0	1	0
10	R	40	0	0	0	0
All	All	16719	0	15894	120	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 4.

The worst 5 of 120 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:D:13:GLN:HB2	2:D:16:ARG:HD3	1.66	0.78
5:L:46:ARG:NH2	10:L:401:HOH:O	2.20	0.74
3:E:39:LYS:NZ	10:E:301:HOH:O	2.28	0.66
2:D:50:VAL:HG21	2:D:105:TYR:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:478:LYS:HG2	5:G:32:SER:HB3	1.80	0.62

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	C	195/205 (95%)	186 (95%)	9 (5%)	0	100	100
1	R	195/205 (95%)	186 (95%)	9 (5%)	0	100	100
2	A	212/226 (94%)	204 (96%)	7 (3%)	1 (0%)	29	52
2	D	212/226 (94%)	203 (96%)	8 (4%)	1 (0%)	29	52
3	B	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
3	E	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
4	F	220/228 (96%)	212 (96%)	8 (4%)	0	100	100
4	H	220/228 (96%)	211 (96%)	9 (4%)	0	100	100
5	G	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
5	L	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
All	All	2097/2176 (96%)	2013 (96%)	82 (4%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	109	ASP
2	D	109	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	169/177 (96%)	167 (99%)	2 (1%)	71	87
1	R	169/177 (96%)	167 (99%)	2 (1%)	71	87
2	A	179/189 (95%)	179 (100%)	0	100	100
2	D	179/189 (95%)	179 (100%)	0	100	100
3	B	186/188 (99%)	186 (100%)	0	100	100
3	E	186/188 (99%)	186 (100%)	0	100	100
4	F	193/196 (98%)	191 (99%)	2 (1%)	76	90
4	H	192/196 (98%)	190 (99%)	2 (1%)	76	90
5	G	183/184 (100%)	183 (100%)	0	100	100
5	L	184/184 (100%)	183 (100%)	1 (0%)	88	96
All	All	1820/1868 (97%)	1811 (100%)	9 (0%)	88	96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	72	ARG
5	L	101	GLN
4	F	72	ARG
1	C	332	HIS
1	C	518	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	360	ASN
2	A	172	HIS
4	F	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
6	NAG	I	1	6,1	14,14,15	0.33	0	17,19,21	0.68	1 (5%)
6	FUC	I	2	6	10,10,11	0.75	0	14,14,16	0.78	0
7	NAG	J	1	7,4	14,14,15	0.21	0	17,19,21	0.46	0
7	NAG	J	2	7	14,14,15	0.31	0	17,19,21	0.35	0
7	FUC	J	3	7	10,10,11	0.82	0	14,14,16	0.90	0
7	NAG	K	1	7,1	14,14,15	0.28	0	17,19,21	0.77	1 (5%)
7	NAG	K	2	7	14,14,15	0.31	0	17,19,21	0.39	0
7	FUC	K	3	7	10,10,11	0.78	0	14,14,16	0.75	0
7	NAG	M	1	7,4	14,14,15	0.33	0	17,19,21	0.58	0
7	NAG	M	2	7	14,14,15	0.28	0	17,19,21	0.36	0
7	FUC	M	3	7	10,10,11	0.76	0	14,14,16	0.89	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
6	NAG	I	1	6,1	-	2/6/23/26	0/1/1/1
6	FUC	I	2	6	-	-	0/1/1/1
7	NAG	J	1	7,4	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	FUC	J	3	7	-	-	0/1/1/1
7	NAG	K	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	FUC	K	3	7	-	-	0/1/1/1
7	NAG	M	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
7	FUC	M	3	7	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	1	NAG	C1-O5-C5	2.42	115.47	112.19
6	I	1	NAG	C1-O5-C5	2.40	115.45	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

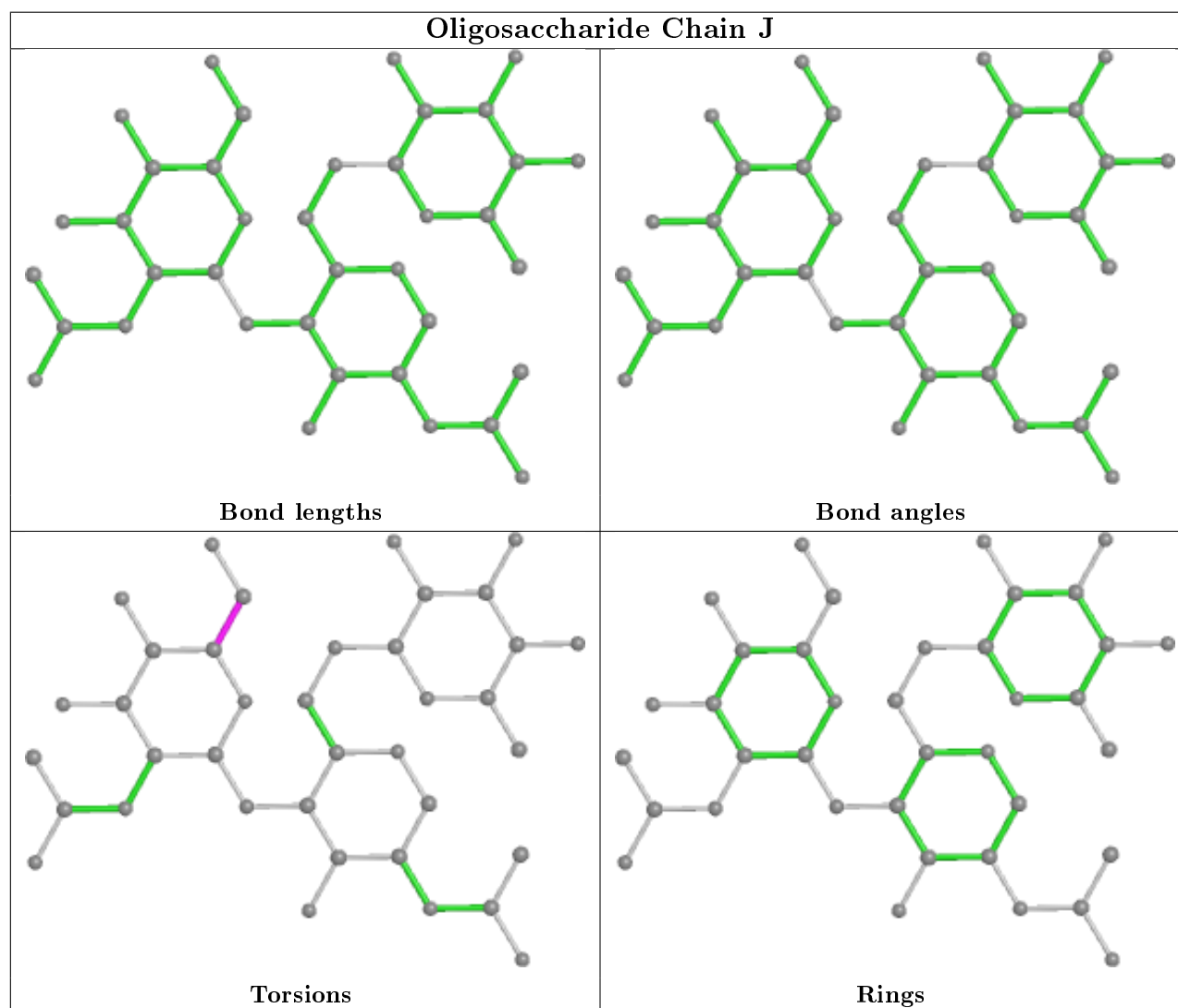
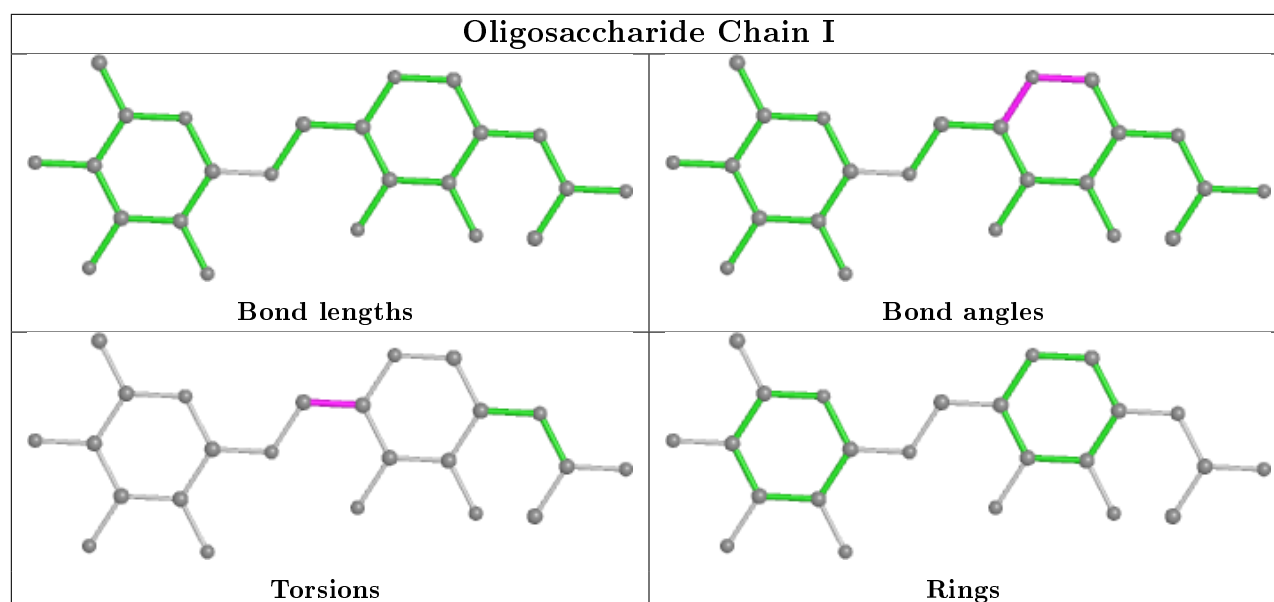
Mol	Chain	Res	Type	Atoms
7	J	2	NAG	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
7	M	2	NAG	C4-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6

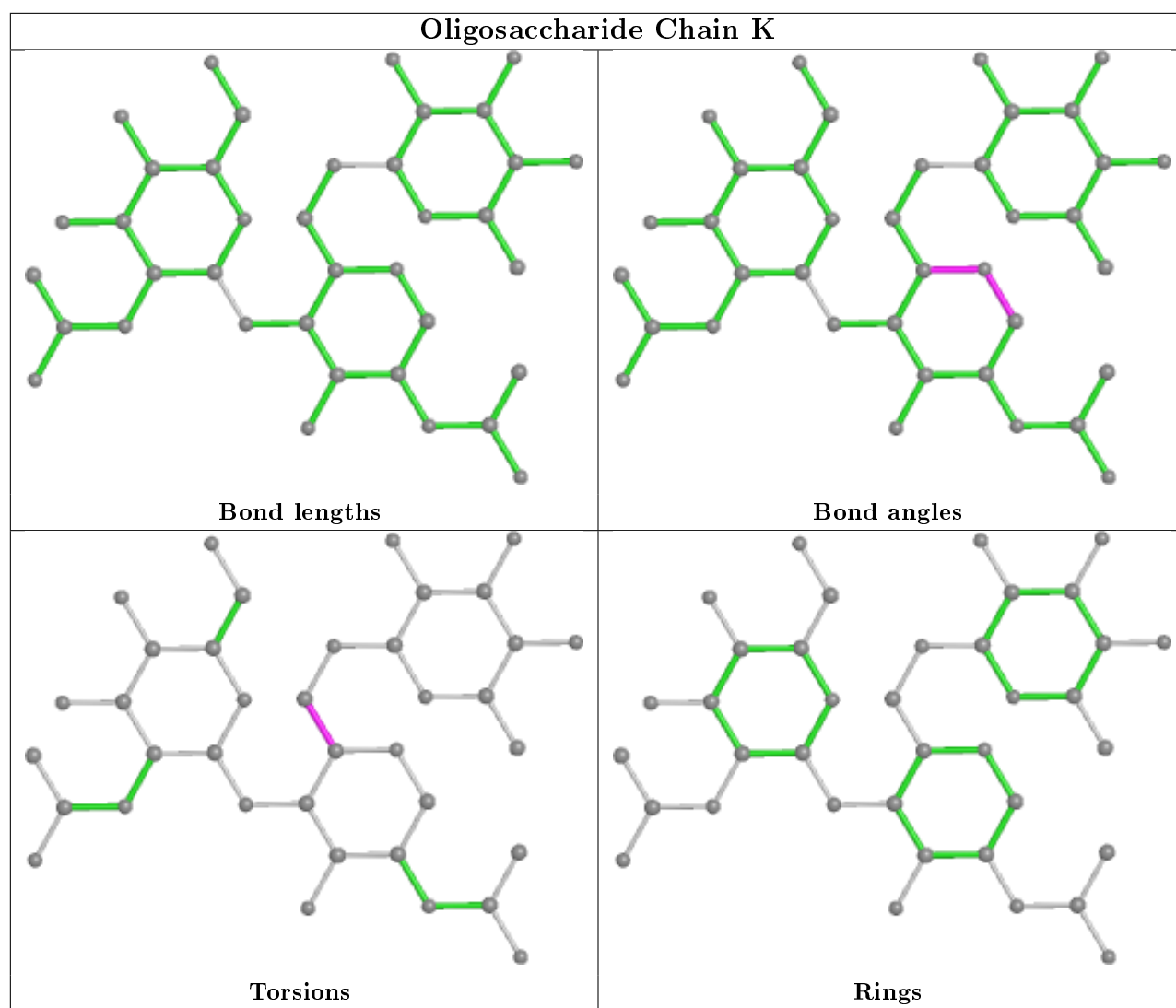
There are no ring outliers.

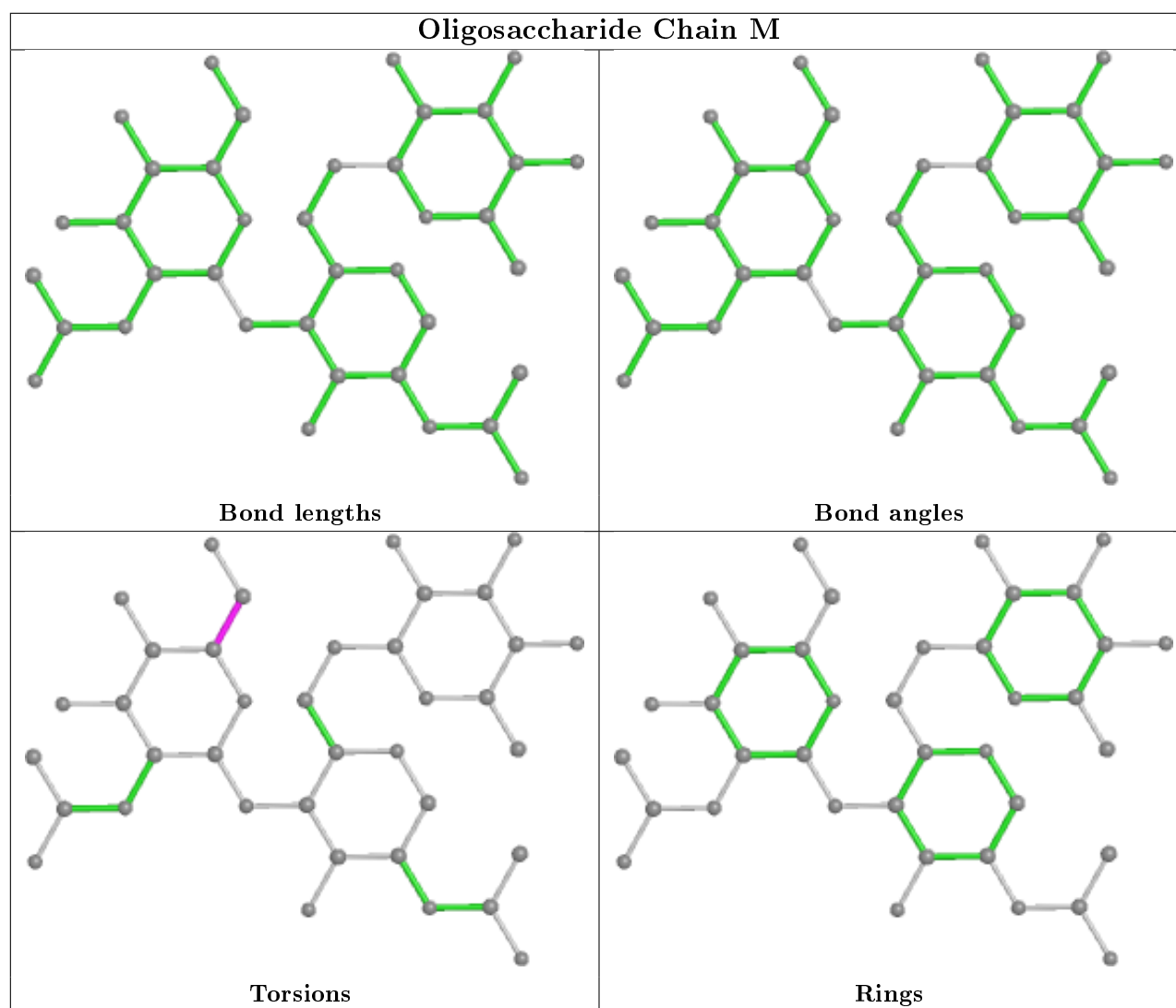
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
8	GOL	R	702	-	5,5,5	0.87	0	5,5,5	1.02	0
8	GOL	L	301	-	5,5,5	0.71	0	5,5,5	1.10	0
8	GOL	C	702	-	5,5,5	0.89	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	R	701	-	5,5,5	0.70	0	5,5,5	1.12	0
8	GOL	F	401	-	5,5,5	0.71	0	5,5,5	1.04	0
8	GOL	C	701	-	5,5,5	0.68	0	5,5,5	1.13	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
8	GOL	R	702	-	-	0/4/4/4	-
8	GOL	L	301	-	-	2/4/4/4	-
8	GOL	C	702	-	-	0/4/4/4	-
8	GOL	R	701	-	-	0/4/4/4	-
8	GOL	F	401	-	-	1/4/4/4	-
8	GOL	C	701	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	701	GOL	C1-C2-C3-O3
8	C	701	GOL	O1-C1-C2-C3
8	L	301	GOL	O1-C1-C2-C3
8	F	401	GOL	O2-C2-C3-O3
8	C	701	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	301	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	197/205 (96%)	0.03	0 100 100	28, 47, 81, 106	0
1	R	197/205 (96%)	0.04	3 (1%) 73 70	26, 43, 73, 126	0
2	A	216/226 (95%)	0.49	20 (9%) 8 6	29, 55, 149, 201	0
2	D	216/226 (95%)	1.50	71 (32%) 0 0	30, 68, 178, 231	0
3	B	211/214 (98%)	0.52	21 (9%) 7 4	30, 62, 141, 183	0
3	E	211/214 (98%)	2.10	87 (41%) 0 0	33, 102, 226, 250	0
4	F	224/228 (98%)	-0.01	1 (0%) 92 91	31, 51, 75, 121	0
4	H	224/228 (98%)	-0.02	0 100 100	29, 40, 70, 103	0
5	G	214/215 (99%)	-0.03	1 (0%) 91 89	33, 59, 95, 128	0
5	L	214/215 (99%)	-0.15	0 100 100	27, 43, 66, 90	0
All	All	2124/2176 (97%)	0.45	204 (9%) 8 5	26, 50, 167, 250	0

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	134	PRO	15.1
3	E	146	VAL	14.1
3	E	196	VAL	13.3
2	D	222	LYS	9.5
2	A	141	GLY	9.4

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	M	2	14/15	0.69	0.22	85,99,110,111	0
7	FUC	J	3	10/11	0.82	0.20	67,81,85,88	0
7	FUC	K	3	10/11	0.84	0.17	87,97,109,121	0
6	FUC	I	2	10/11	0.86	0.27	97,111,114,116	0
7	NAG	K	2	14/15	0.86	0.29	88,98,111,117	0
7	NAG	K	1	14/15	0.90	0.14	46,75,92,96	0
7	NAG	J	1	14/15	0.90	0.13	67,75,84,87	0
7	NAG	J	2	14/15	0.90	0.20	83,93,101,106	0
7	NAG	M	1	14/15	0.90	0.16	69,81,88,97	0
6	NAG	I	1	14/15	0.90	0.30	61,81,100,105	0
7	FUC	M	3	10/11	0.93	0.21	64,69,87,94	0

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	R	701	6/6	0.80	0.25	53,64,68,74	0
9	CL	B	301	1/1	0.89	0.12	61,61,61,61	0
8	GOL	L	301	6/6	0.90	0.28	44,46,50,59	0
8	GOL	F	401	6/6	0.90	0.34	53,57,62,65	0
8	GOL	C	701	6/6	0.91	0.28	60,66,70,70	0
9	CL	F	403	1/1	0.91	0.08	68,68,68,68	0
9	CL	A	301	1/1	0.92	0.08	62,62,62,62	0
9	CL	A	302	1/1	0.93	0.22	72,72,72,72	0
8	GOL	C	702	6/6	0.94	0.21	43,46,55,58	0
8	GOL	R	702	6/6	0.96	0.17	42,44,52,55	0
9	CL	F	402	1/1	0.97	0.11	41,41,41,41	0
9	CL	H	301	1/1	0.98	0.11	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.