



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2021 – 02:15 pm BST

PDB ID : 7ORB
Title : Crystal structure of the L452R mutant receptor binding domain of SARS-CoV-2 Spike glycoprotein in complex with COVOX-75 and COVOX-253 Fabs
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-06-04
Resolution : 2.50 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

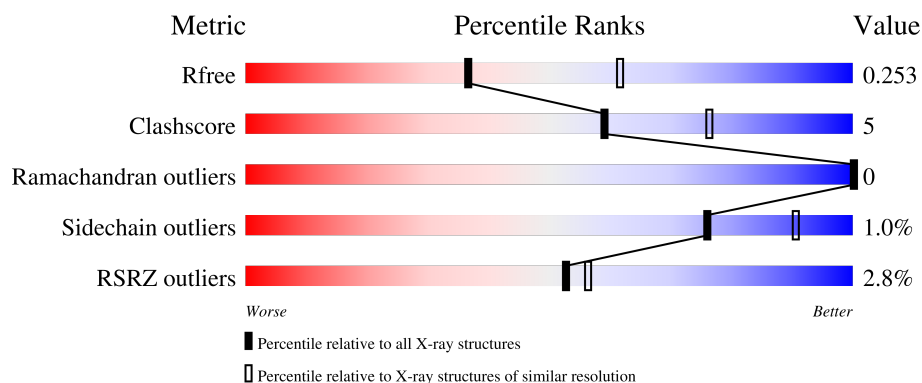
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	R	205	<div> <div>2%</div> <div>79% 11% 10%</div> </div>
1	X	205	<div> <div>3%</div> <div>77% 13% 10%</div> </div>
2	C	228	<div> <div>4%</div> <div>82% 14% .</div> </div>
2	H	228	<div> <div>5%</div> <div>84% 12% .</div> </div>
3	D	215	<div> <div>%</div> <div>85% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	215	
4	A	232	
4	E	232	
5	B	214	
5	F	214	
6	G	6	
7	I	3	
8	J	5	
9	K	4	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16964 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	185	Total	C	N	O	S	0	0	0
			1482	947	250	278	7			
1	X	184	Total	C	N	O	S	0	0	0
			1472	941	247	277	7			

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	452	ARG	LEU	engineered mutation	UNP P0DTC2
R	527	LYS	PRO	conflict	UNP P0DTC2
X	324	GLU	-	expression tag	UNP P0DTC2
X	325	THR	-	expression tag	UNP P0DTC2
X	326	GLY	-	expression tag	UNP P0DTC2
X	327	HIS	-	expression tag	UNP P0DTC2
X	328	HIS	-	expression tag	UNP P0DTC2
X	329	HIS	-	expression tag	UNP P0DTC2
X	330	HIS	-	expression tag	UNP P0DTC2
X	331	HIS	-	expression tag	UNP P0DTC2
X	332	HIS	-	expression tag	UNP P0DTC2
X	452	ARG	LEU	engineered mutation	UNP P0DTC2
X	527	LYS	PRO	conflict	UNP P0DTC2

- Molecule 2 is a protein called COVOX-253 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1639	1031	276	323	9			
2	C	219	Total	C	N	O	S	0	0	0
			1639	1031	276	323	9			

- Molecule 3 is a protein called COVOX-253 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	2	0
			1635	1022	272	335	6			
3	D	214	Total	C	N	O	S	0	2	0
			1635	1022	272	335	6			

- Molecule 4 is a protein called COVOX-75 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	224	Total	C	N	O	S	0	0	0
			1691	1066	293	326	6			
4	E	223	Total	C	N	O	S	0	0	0
			1685	1063	292	324	6			

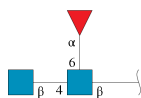
- Molecule 5 is a protein called COVOX-75 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	214	Total	C	N	O	S	0	1	0
			1639	1032	273	329	5			
5	F	214	Total	C	N	O	S	0	1	0
			1639	1032	273	329	5			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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
6	G	6	Total	C	N	O	0	0	0
			71	40	2	29			

- 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	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

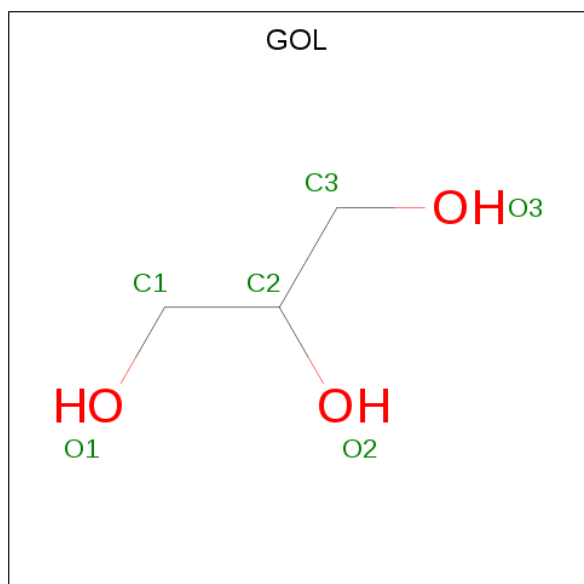
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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
9	K	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	R	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	X	1	Total	C	O	0	0
			6	3	3		
10	X	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	E	1	Total	C	O	0	0
			6	3	3		
10	E	1	Total	C	O	0	0
			6	3	3		
10	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

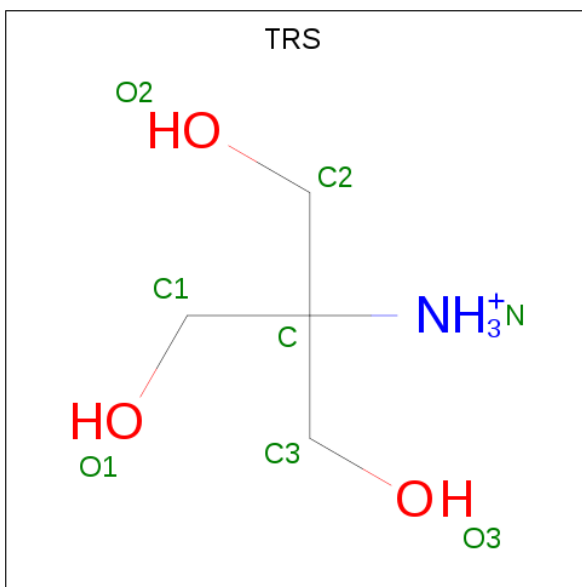


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	R	1	Total	C	O	0	0
			7	4	3		
11	X	1	Total	C	O	0	0
			7	4	3		
11	X	1	Total	C	O	0	0
			7	4	3		
11	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

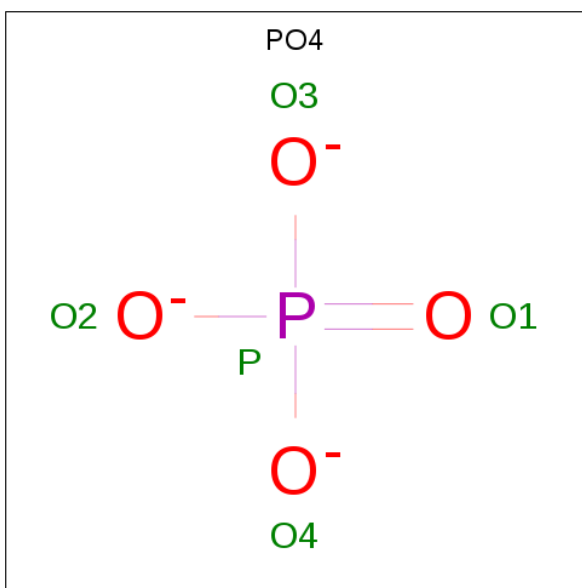
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	1	Total	Cl	0	0
			1	1		
12	C	1	Total	Cl	0	0
			1	1		
12	E	2	Total	Cl	0	0
			2	2		

- Molecule 13 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	L	1	Total	C	N	O	0	0
			8	4	1	3		
13	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



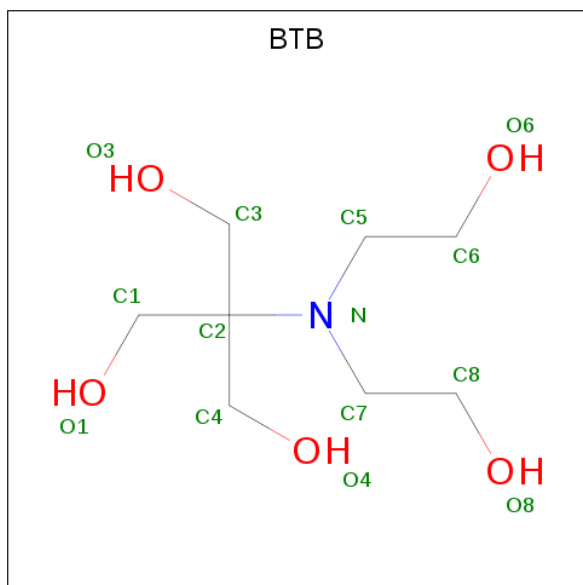
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	O	P	0	0
			5	4	1		
14	E	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 15 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	28	Total	O	0	0
			28	28		
16	H	43	Total	O	0	0
			43	43		
16	L	53	Total	O	0	0
			53	53		
16	A	44	Total	O	0	0
			44	44		
16	B	33	Total	O	0	0
			33	33		
16	X	32	Total	O	0	0
			32	32		
16	C	41	Total	O	0	0
			41	41		

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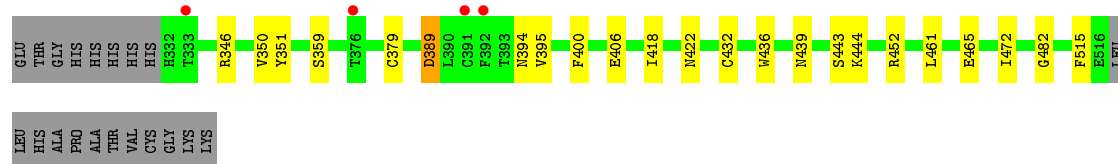
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	D	43	Total 43	O 43	0	0
16	E	56	Total 56	O 56	0	0
16	F	44	Total 44	O 44	0	0

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.

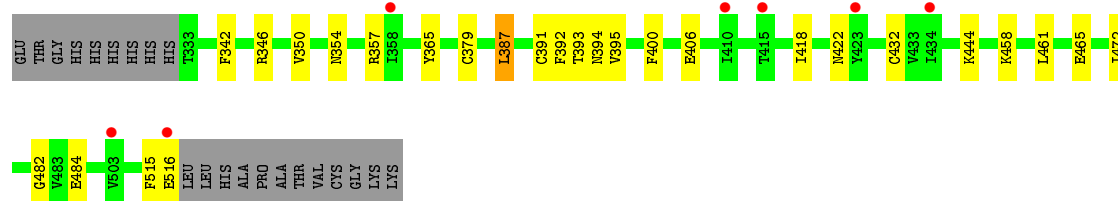
- Molecule 1: Spike protein S1

Chain R: 




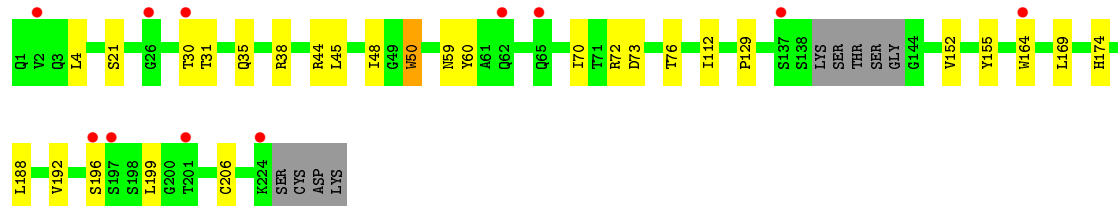
- Molecule 1: Spike protein S1

Chain X: 




- Molecule 2: COVOX-253 Fab heavy chain

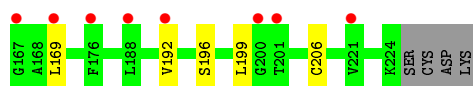
Chain H: 



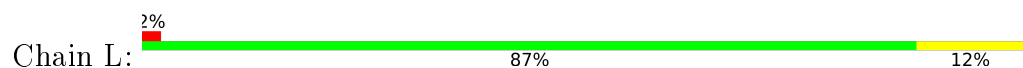
- Molecule 2: COVOX-253 Fab heavy chain

Chain C: 

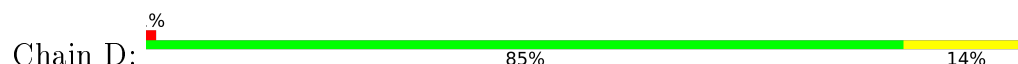




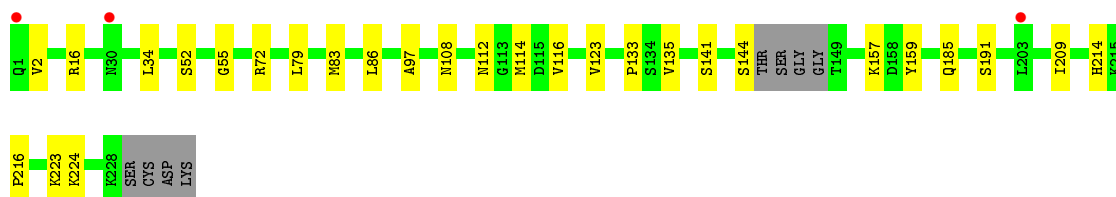
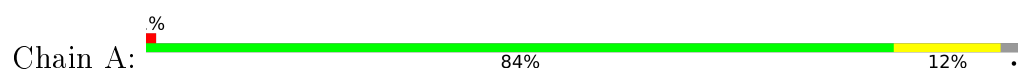
- Molecule 3: COVOX-253 Fab light chain



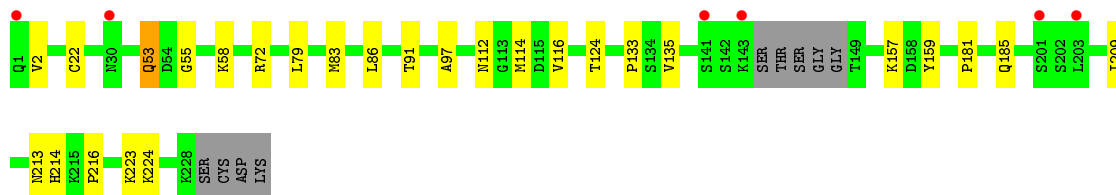
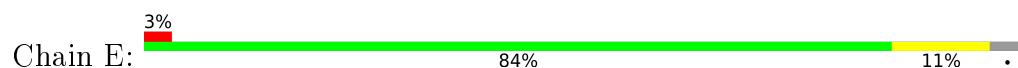
- Molecule 3: COVOX-253 Fab light chain



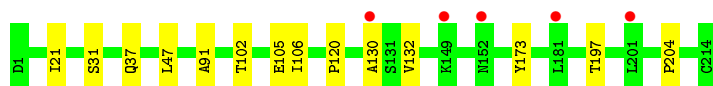
- Molecule 4: COVOX-75 Fab heavy chain



- Molecule 4: COVOX-75 Fab heavy chain

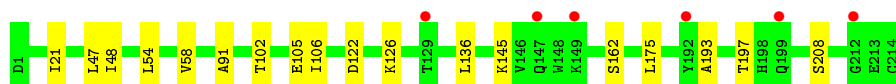


- Molecule 5: COVOX-75 Fab light chain



- Molecule 5: COVOX-75 Fab light chain





- Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain G:  50%




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

Chain I:  100%



- Molecule 8: α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  20%



- Molecule 9: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain K:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.24Å 149.43Å 115.04Å 90.00° 92.03° 90.00°	Depositor
Resolution (Å)	73.67 – 2.50 74.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (73.67-2.50) 99.3 (74.71-2.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.213 , 0.251 0.216 , 0.253	Depositor DCC
R_{free} test set	5504 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.089 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16964	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: FUC, BTB, BMA, TRS, CL, GOL, PEG, PO4, NAG, MAN

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	R	0.25	0/1524	0.48	0/2071
1	X	0.25	0/1513	0.49	0/2056
2	C	0.26	0/1677	0.50	0/2289
2	H	0.25	0/1677	0.49	0/2289
3	D	0.25	0/1677	0.50	0/2277
3	L	0.25	0/1677	0.50	0/2277
4	A	0.26	0/1731	0.51	0/2362
4	E	0.25	0/1725	0.51	0/2354
5	B	0.26	0/1679	0.49	0/2281
5	F	0.26	0/1679	0.48	0/2281
All	All	0.25	0/16559	0.50	0/22537

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	R	1482	0	1393	15	0
1	X	1472	0	1386	19	0
2	C	1639	0	1595	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1639	0	1595	14	0
3	D	1635	0	1579	20	0
3	L	1635	0	1579	22	0
4	A	1691	0	1657	15	0
4	E	1685	0	1652	17	0
5	B	1639	0	1606	9	0
5	F	1639	0	1606	10	0
6	G	71	0	61	0	0
7	I	38	0	34	0	0
8	J	60	0	52	1	0
9	K	49	0	43	0	0
10	A	18	0	24	1	0
10	B	12	0	16	0	0
10	C	6	0	8	0	0
10	D	6	0	8	0	0
10	E	12	0	16	3	0
10	F	6	0	8	0	0
10	H	18	0	24	0	0
10	R	6	0	8	1	0
10	X	12	0	16	1	0
11	E	7	0	10	0	0
11	R	7	0	10	0	0
11	X	14	0	20	0	0
12	C	1	0	0	0	0
12	E	2	0	0	1	0
12	H	1	0	0	0	0
13	D	8	0	12	2	0
13	L	8	0	12	1	0
14	A	5	0	0	1	0
14	E	10	0	0	1	0
15	E	14	0	19	3	0
16	A	44	0	0	0	0
16	B	33	0	0	0	0
16	C	41	0	0	0	0
16	D	43	0	0	0	0
16	E	56	0	0	2	0
16	F	44	0	0	1	0
16	H	43	0	0	1	0
16	L	53	0	0	2	0
16	R	28	0	0	0	0
16	X	32	0	0	1	0
All	All	16964	0	16049	152	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.

The worst 5 of 152 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:C:38:ARG:HB3	2:C:48:ILE:HD11	1.67	0.75
1:X:444:LYS:NZ	5:F:91:ALA:O	2.27	0.67
1:R:444:LYS:NZ	5:B:91:ALA:O	2.28	0.67
4:E:83:MET:HB3	4:E:86:LEU:HD21	1.77	0.66
12:E:407:CL:CL	16:F:437:HOH:O	2.50	0.66

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	R	183/205 (89%)	175 (96%)	8 (4%)	0	100	100
1	X	182/205 (89%)	175 (96%)	7 (4%)	0	100	100
2	C	215/228 (94%)	207 (96%)	8 (4%)	0	100	100
2	H	215/228 (94%)	206 (96%)	9 (4%)	0	100	100
3	D	214/215 (100%)	209 (98%)	5 (2%)	0	100	100
3	L	214/215 (100%)	208 (97%)	6 (3%)	0	100	100
4	A	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
4	E	219/232 (94%)	213 (97%)	6 (3%)	0	100	100
5	B	213/214 (100%)	208 (98%)	5 (2%)	0	100	100
5	F	213/214 (100%)	206 (97%)	7 (3%)	0	100	100
All	All	2088/2188 (95%)	2020 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	R	161/177 (91%)	159 (99%)	2 (1%)	71	88
1	X	160/177 (90%)	156 (98%)	4 (2%)	47	73
2	C	186/196 (95%)	183 (98%)	3 (2%)	62	84
2	H	186/196 (95%)	183 (98%)	3 (2%)	62	84
3	D	185/184 (100%)	183 (99%)	2 (1%)	73	89
3	L	185/184 (100%)	183 (99%)	2 (1%)	73	89
4	A	189/196 (96%)	187 (99%)	2 (1%)	73	89
4	E	188/196 (96%)	187 (100%)	1 (0%)	88	96
5	B	188/187 (100%)	188 (100%)	0	100	100
5	F	188/187 (100%)	188 (100%)	0	100	100
All	All	1816/1880 (97%)	1797 (99%)	19 (1%)	76	90

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	50	TRP
3	D	214	GLU
4	E	53	GLN
3	D	144	GLU
4	A	191	SER

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 ⓘ

18 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	G	1	6,1	14,14,15	0.41	0	17,19,21	0.48	0
6	NAG	G	2	6	14,14,15	0.22	0	17,19,21	0.34	0
6	BMA	G	3	6	11,11,12	0.99	0	15,15,17	1.44	3 (20%)
6	MAN	G	4	6	11,11,12	0.79	0	15,15,17	0.87	1 (6%)
6	MAN	G	5	6	11,11,12	1.50	3 (27%)	15,15,17	2.16	4 (26%)
6	FUC	G	6	6	10,10,11	0.69	0	14,14,16	0.92	0
7	NAG	I	1	7,2	14,14,15	0.29	0	17,19,21	0.56	0
7	NAG	I	2	7	14,14,15	0.27	0	17,19,21	0.39	0
7	FUC	I	3	7	10,10,11	0.80	0	14,14,16	0.74	0
8	NAG	J	1	8,1	14,14,15	0.37	0	17,19,21	0.48	0
8	NAG	J	2	8	14,14,15	0.21	0	17,19,21	0.43	0
8	BMA	J	3	8	11,11,12	0.70	0	15,15,17	1.14	1 (6%)
8	MAN	J	4	8	11,11,12	1.45	2 (18%)	15,15,17	2.10	4 (26%)
8	FUC	J	5	8	10,10,11	0.78	1 (10%)	14,14,16	0.99	0
9	NAG	K	1	9,2	14,14,15	0.34	0	17,19,21	0.62	0
9	NAG	K	2	9	14,14,15	0.26	0	17,19,21	0.43	0
9	BMA	K	3	9	11,11,12	0.69	0	15,15,17	0.80	0
9	FUC	K	4	9	10,10,11	0.82	0	14,14,16	0.70	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	G	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	1/2/19/22	0/1/1/1
6	FUC	G	6	6	-	-	0/1/1/1
7	NAG	I	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	FUC	I	3	7	-	-	0/1/1/1
8	NAG	J	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	BMA	J	3	8	-	2/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	FUC	J	5	8	-	-	0/1/1/1
9	NAG	K	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
9	BMA	K	3	9	-	0/2/19/22	0/1/1/1
9	FUC	K	4	9	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5	MAN	C1-C2	3.23	1.59	1.52
8	J	4	MAN	O5-C1	3.11	1.48	1.43
8	J	4	MAN	C1-C2	3.09	1.59	1.52
6	G	5	MAN	O5-C1	3.03	1.48	1.43
6	G	5	MAN	O5-C5	2.09	1.47	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	4	MAN	C1-O5-C5	6.95	121.61	112.19
6	G	5	MAN	C1-O5-C5	6.90	121.54	112.19
6	G	3	BMA	O3-C3-C2	4.02	117.68	109.99
8	J	3	BMA	C1-O5-C5	3.20	116.53	112.19
6	G	5	MAN	O5-C1-C2	2.83	115.14	110.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	1	NAG	C4-C5-C6-O6

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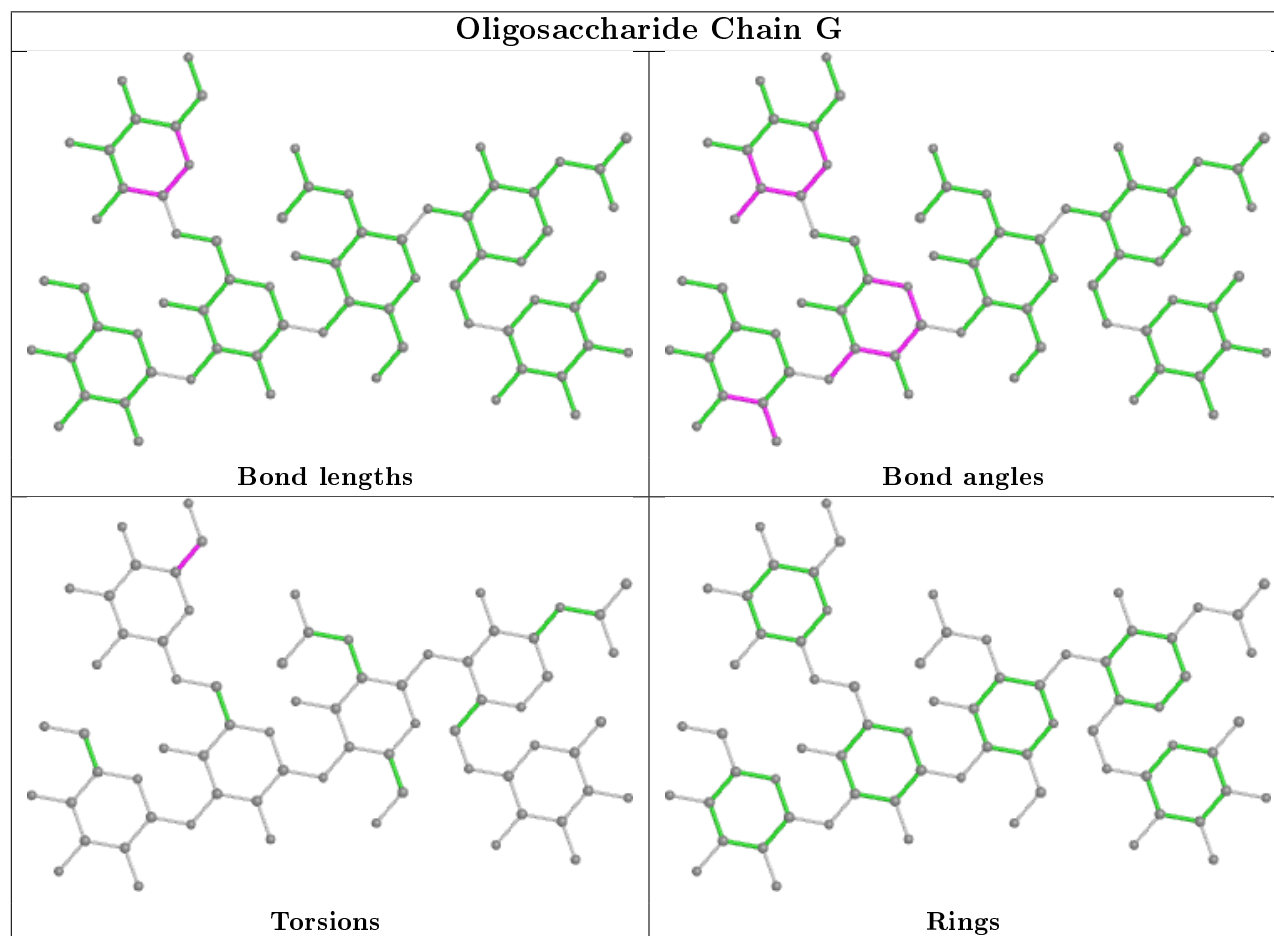
Mol	Chain	Res	Type	Atoms
9	K	1	NAG	O5-C5-C6-O6
6	G	5	MAN	O5-C5-C6-O6
8	J	3	BMA	O5-C5-C6-O6
8	J	3	BMA	C4-C5-C6-O6

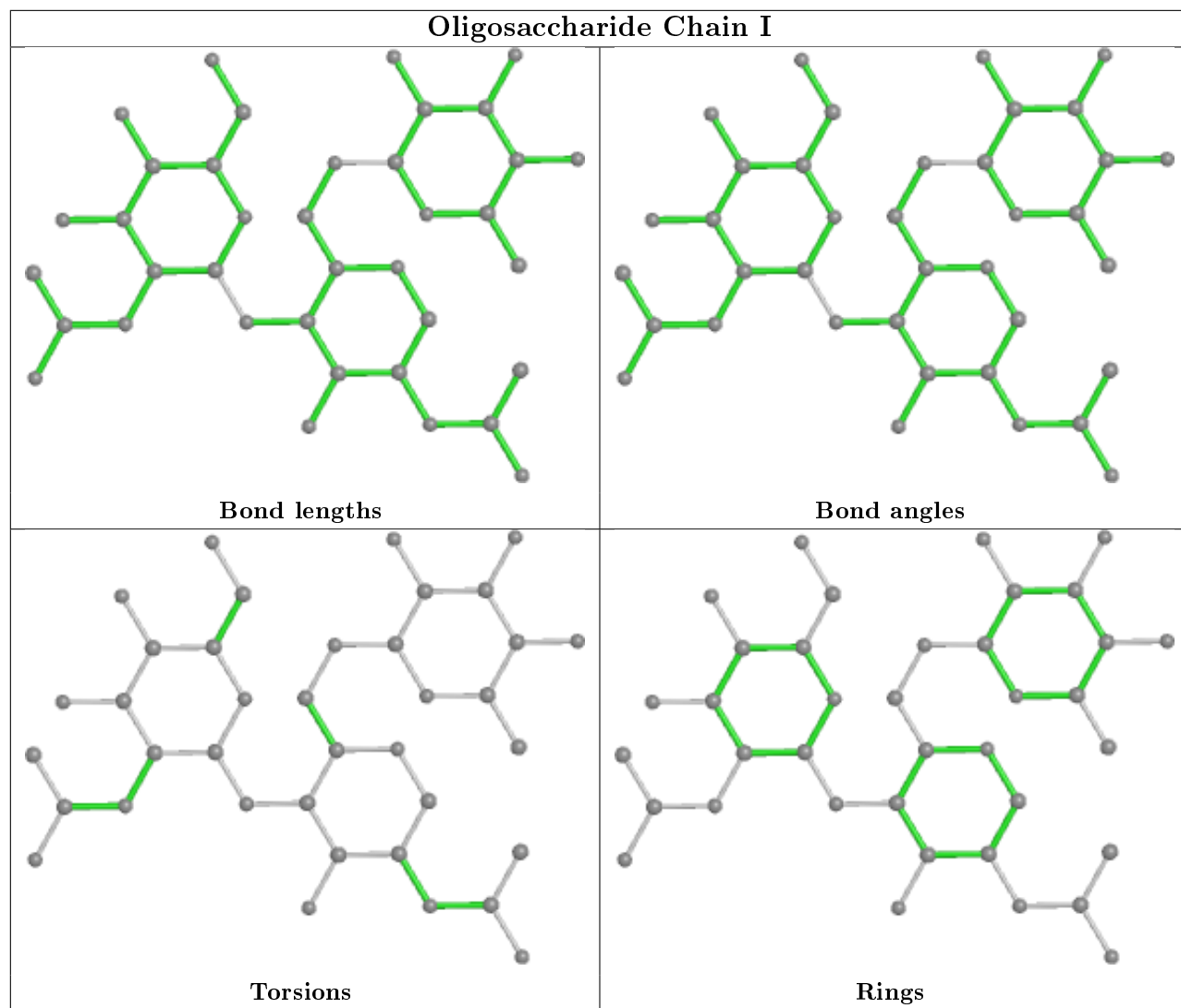
There are no ring outliers.

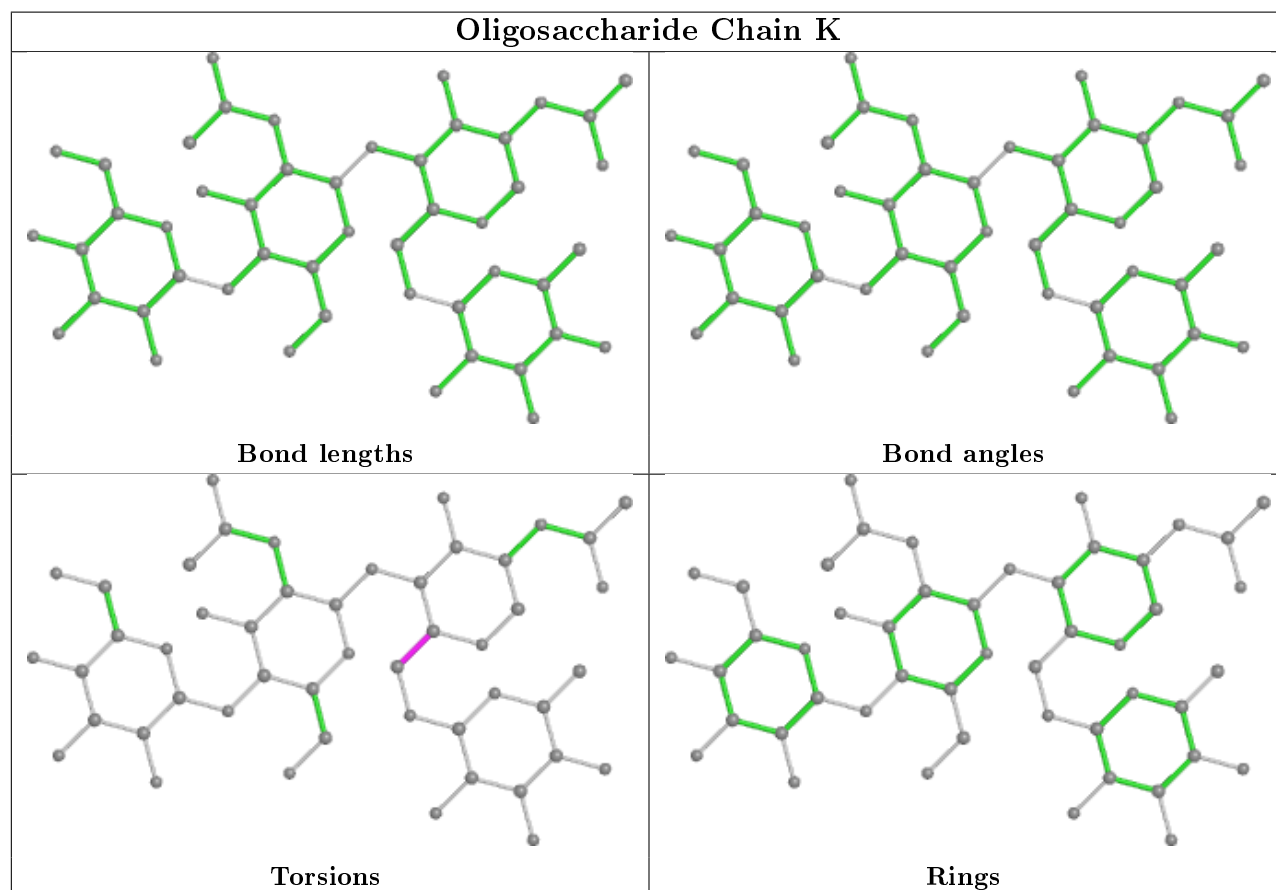
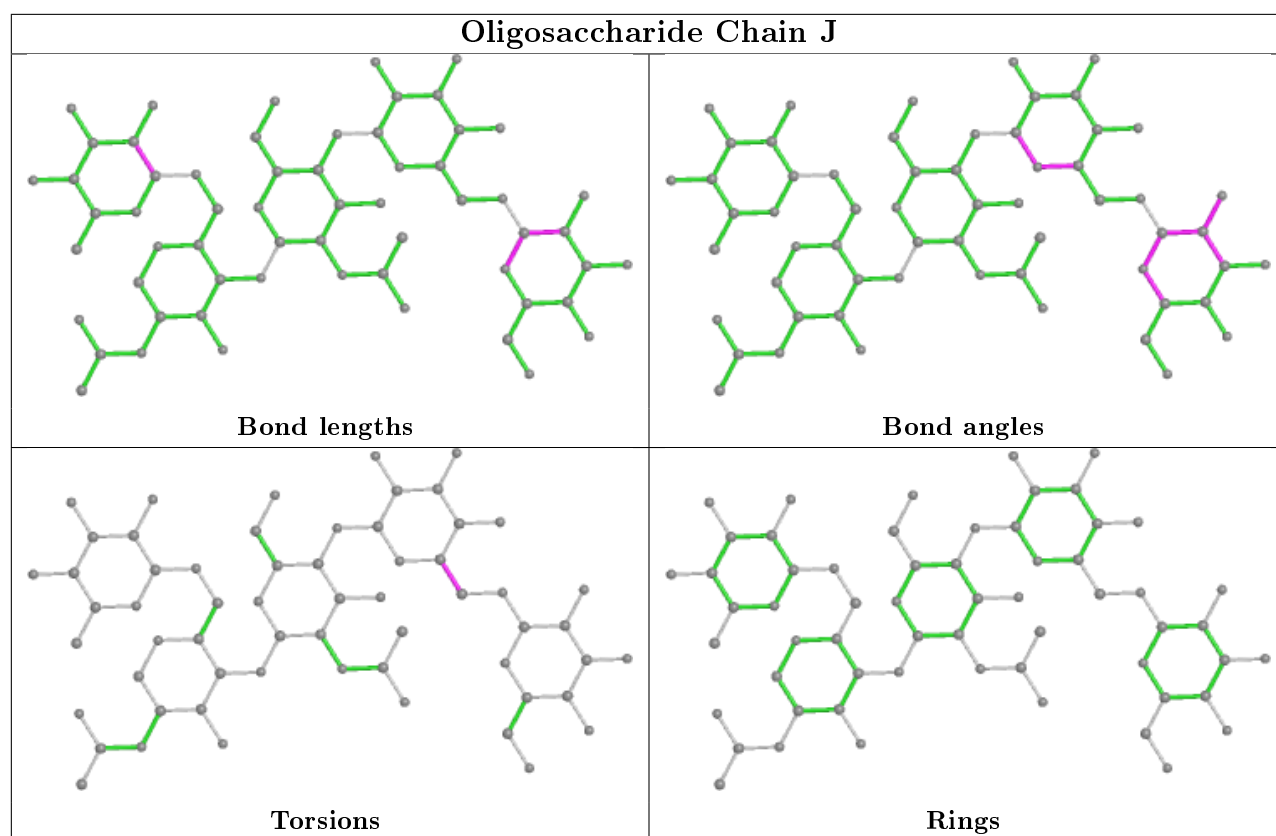
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	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

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 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	$\# Z > 2$
11	PEG	R	802	-	6,6,6	0.10	0	5,5,5	0.12	0
10	GOL	A	303	-	5,5,5	0.91	0	5,5,5	1.02	0
15	BTB	E	404	-	13,13,13	0.67	0	7,16,16	0.48	0
14	PO4	E	406	-	4,4,4	0.89	0	6,6,6	0.46	0
10	GOL	H	501	-	5,5,5	0.92	0	5,5,5	0.98	0
10	GOL	R	801	-	5,5,5	0.90	0	5,5,5	1.01	0
10	GOL	E	401	-	5,5,5	0.92	0	5,5,5	1.00	0
11	PEG	E	402	-	6,6,6	0.12	0	5,5,5	0.08	0
14	PO4	E	405	-	4,4,4	0.90	0	6,6,6	0.47	0
10	GOL	C	501	-	5,5,5	0.99	0	5,5,5	0.89	0
10	GOL	H	503	-	5,5,5	0.92	0	5,5,5	0.96	0
10	GOL	A	302	-	5,5,5	0.92	0	5,5,5	0.96	0
10	GOL	A	301	-	5,5,5	0.92	0	5,5,5	0.94	0
11	PEG	X	804	-	6,6,6	0.12	0	5,5,5	0.08	0
14	PO4	A	304	-	4,4,4	0.89	0	6,6,6	0.49	0
10	GOL	B	902	-	5,5,5	0.89	0	5,5,5	1.02	0
13	TRS	L	301	-	7,7,7	0.32	0	9,9,9	0.27	0
10	GOL	E	403	-	5,5,5	0.95	0	5,5,5	0.92	0
10	GOL	F	301	-	5,5,5	0.88	0	5,5,5	1.04	0
11	PEG	X	803	-	6,6,6	0.10	0	5,5,5	0.12	0
10	GOL	X	801	-	5,5,5	0.92	0	5,5,5	0.99	0
10	GOL	D	1202	-	5,5,5	0.88	0	5,5,5	0.97	0
13	TRS	D	1201	-	7,7,7	0.37	0	9,9,9	0.30	0
10	GOL	H	502	-	5,5,5	0.90	0	5,5,5	0.99	0
10	GOL	X	802	-	5,5,5	0.91	0	5,5,5	1.00	0
10	GOL	B	901	-	5,5,5	0.88	0	5,5,5	1.03	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
11	PEG	R	802	-	-	3/4/4/4	-
10	GOL	A	303	-	-	0/4/4/4	-
15	BTB	E	404	-	-	8/21/21/21	-
10	GOL	H	501	-	-	2/4/4/4	-
10	GOL	R	801	-	-	1/4/4/4	-
10	GOL	E	401	-	-	1/4/4/4	-
11	PEG	E	402	-	-	2/4/4/4	-
10	GOL	C	501	-	-	2/4/4/4	-
10	GOL	H	503	-	-	0/4/4/4	-
10	GOL	A	302	-	-	1/4/4/4	-
10	GOL	A	301	-	-	2/4/4/4	-
11	PEG	X	804	-	-	2/4/4/4	-
10	GOL	B	902	-	-	2/4/4/4	-
13	TRS	L	301	-	-	6/9/9/9	-
10	GOL	E	403	-	-	4/4/4/4	-
10	GOL	F	301	-	-	1/4/4/4	-
11	PEG	X	803	-	-	2/4/4/4	-
10	GOL	X	801	-	-	4/4/4/4	-
10	GOL	D	1202	-	-	4/4/4/4	-
13	TRS	D	1201	-	-	0/9/9/9	-
10	GOL	H	502	-	-	0/4/4/4	-
10	GOL	X	802	-	-	2/4/4/4	-
10	GOL	B	901	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	501	GOL	O1-C1-C2-C3
10	A	301	GOL	C1-C2-C3-O3
10	B	902	GOL	C1-C2-C3-O3
10	D	1202	GOL	O1-C1-C2-C3
10	D	1202	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	404	BTB	3	0
10	R	801	GOL	1	0
10	E	401	GOL	1	0
14	E	405	PO4	1	0
10	A	301	GOL	1	0
14	A	304	PO4	1	0
13	L	301	TRS	1	0
10	E	403	GOL	2	0
13	D	1201	TRS	2	0
10	X	802	GOL	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, 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	R	185/205 (90%)	0.52	4 (2%) 62 65	47, 62, 108, 160	0
1	X	184/205 (89%)	0.50	7 (3%) 40 43	43, 60, 100, 121	0
2	C	219/228 (96%)	0.44	10 (4%) 32 34	44, 68, 105, 134	0
2	H	219/228 (96%)	0.54	11 (5%) 28 30	46, 69, 100, 113	0
3	D	214/215 (99%)	0.42	2 (0%) 84 86	44, 66, 92, 128	0
3	L	214/215 (99%)	0.45	5 (2%) 60 63	42, 66, 95, 121	0
4	A	224/232 (96%)	0.39	3 (1%) 77 79	34, 52, 96, 128	0
4	E	223/232 (96%)	0.39	6 (2%) 54 58	34, 51, 85, 119	0
5	B	214/214 (100%)	0.33	5 (2%) 60 63	42, 61, 95, 132	0
5	F	214/214 (100%)	0.41	6 (2%) 53 56	41, 62, 93, 130	0
All	All	2110/2188 (96%)	0.44	59 (2%) 53 56	34, 62, 98, 160	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	141	SER	4.3
5	F	212	GLY	4.1
4	A	203	LEU	4.0
2	C	201	THR	3.7
5	F	129	THR	3.5

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

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

6.3 Carbohydrates ⓘ

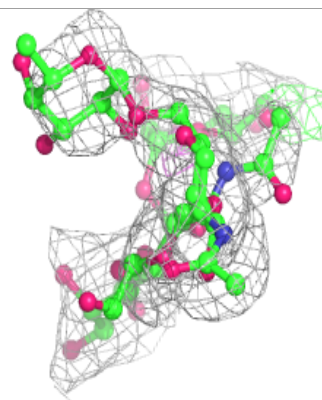
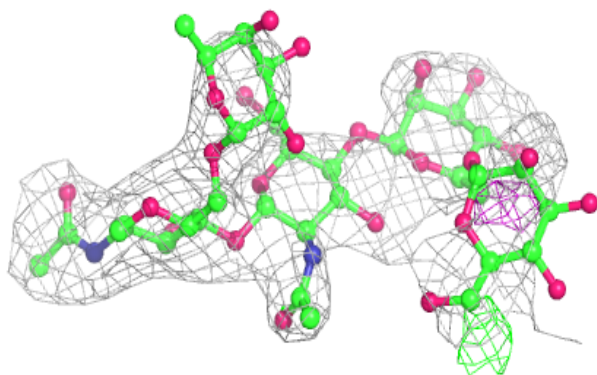
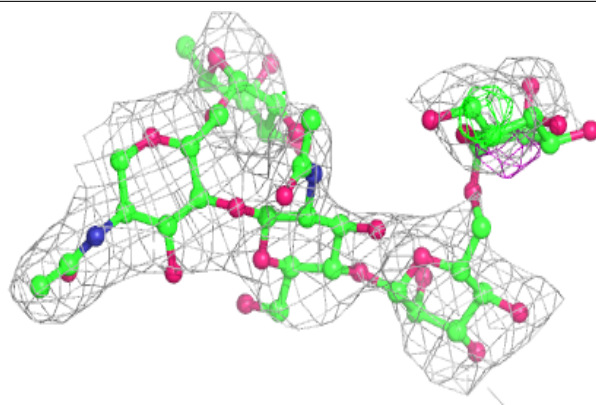
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

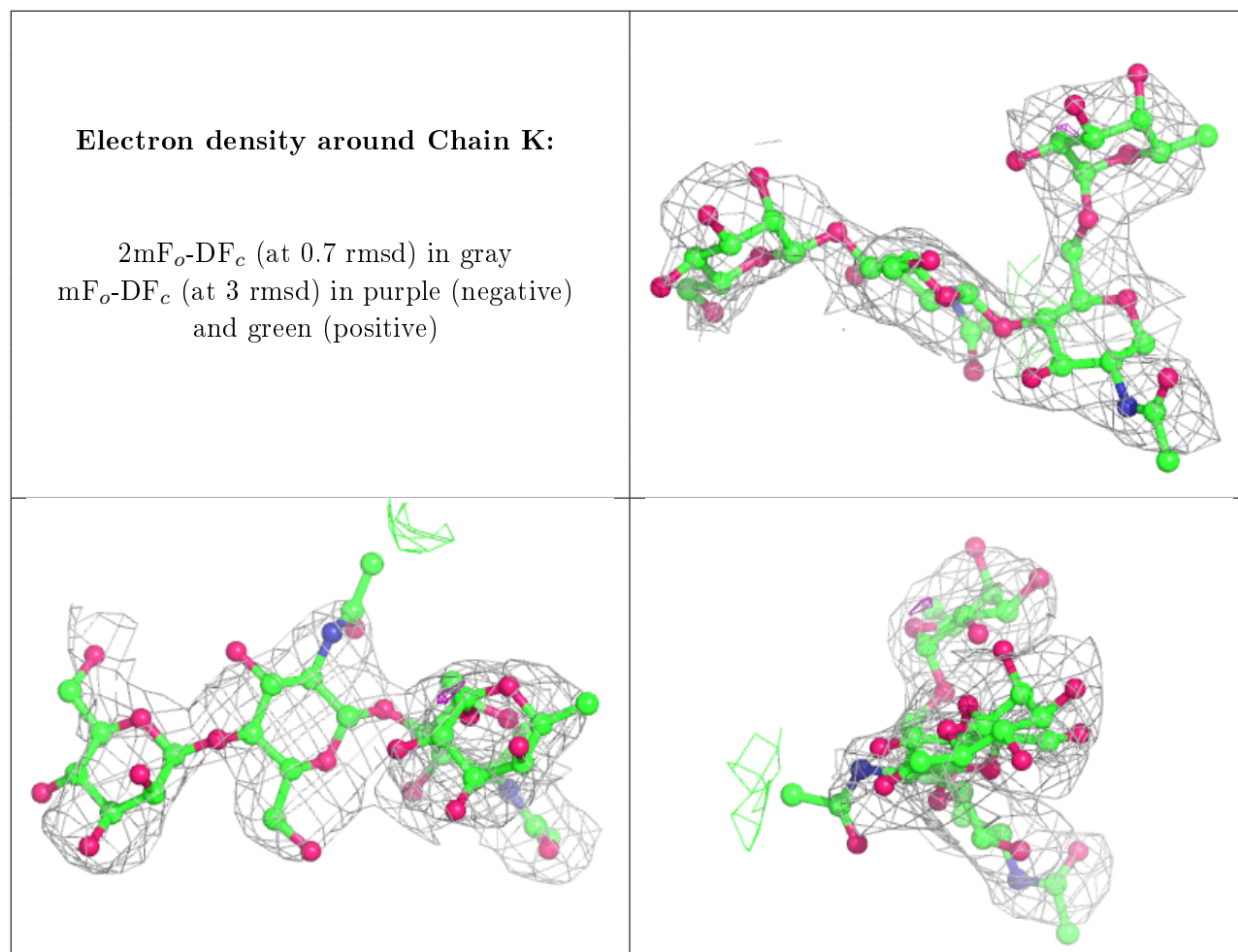
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MAN	J	4	11/12	0.32	0.40	115,135,145,146	0
6	MAN	G	4	11/12	0.55	0.28	106,133,146,152	0
6	BMA	G	3	11/12	0.62	0.28	137,140,145,148	0
9	BMA	K	3	11/12	0.65	0.24	120,131,141,142	0
8	BMA	J	3	11/12	0.69	0.24	107,125,136,140	0
6	MAN	G	5	11/12	0.70	0.25	116,130,142,144	0
6	NAG	G	1	14/15	0.74	0.19	59,100,127,127	0
6	NAG	G	2	14/15	0.79	0.28	99,124,135,143	0
7	NAG	I	2	14/15	0.80	0.24	100,109,117,120	0
9	NAG	K	2	14/15	0.82	0.28	99,103,117,125	0
8	NAG	J	2	14/15	0.82	0.25	92,120,127,138	0
7	FUC	I	3	10/11	0.83	0.20	79,89,93,95	0
8	NAG	J	1	14/15	0.85	0.16	62,90,107,113	0
6	FUC	G	6	10/11	0.86	0.36	110,128,131,132	0
8	FUC	J	5	10/11	0.86	0.47	120,127,135,142	0
9	FUC	K	4	10/11	0.86	0.29	74,83,92,95	0
9	NAG	K	1	14/15	0.90	0.19	64,78,93,100	0
7	NAG	I	1	14/15	0.92	0.16	67,81,95,101	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 J:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	PEG	E	402	7/7	0.70	0.30	60,71,80,86	0
10	GOL	C	501	6/6	0.73	0.27	66,75,83,89	0
10	GOL	E	403	6/6	0.74	0.19	56,73,75,81	0
10	GOL	H	502	6/6	0.74	0.17	72,82,91,93	0
13	TRS	D	1201	8/8	0.78	0.23	50,69,72,73	0
10	GOL	H	501	6/6	0.81	0.32	78,81,82,87	0
10	GOL	H	503	6/6	0.81	0.17	70,72,85,86	0
10	GOL	A	301	6/6	0.82	0.16	61,64,66,68	0
10	GOL	X	802	6/6	0.85	0.20	72,84,86,89	0
14	PO4	A	304	5/5	0.85	0.14	57,59,79,96	0
15	BTB	E	404	14/14	0.85	0.24	59,68,77,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	PEG	X	803	7/7	0.86	0.18	60,67,70,75	0
14	PO4	E	406	5/5	0.87	0.21	59,60,88,94	0
11	PEG	X	804	7/7	0.87	0.16	61,69,75,81	0
13	TRS	L	301	8/8	0.88	0.17	57,65,68,69	0
11	PEG	R	802	7/7	0.89	0.51	57,69,80,88	0
10	GOL	B	901	6/6	0.91	0.13	53,65,69,71	0
14	PO4	E	405	5/5	0.91	0.20	68,71,91,107	0
10	GOL	D	1202	6/6	0.93	0.27	66,68,76,78	0
10	GOL	X	801	6/6	0.93	0.17	63,65,67,70	0
12	CL	E	408	1/1	0.93	0.14	76,76,76,76	0
10	GOL	B	902	6/6	0.94	0.15	52,65,71,78	0
10	GOL	E	401	6/6	0.94	0.24	47,60,63,64	0
10	GOL	A	302	6/6	0.95	0.12	52,63,70,70	0
10	GOL	F	301	6/6	0.95	0.11	53,56,58,60	0
12	CL	E	407	1/1	0.95	0.10	72,72,72,72	0
10	GOL	A	303	6/6	0.95	0.28	51,61,65,66	0
10	GOL	R	801	6/6	0.95	0.11	63,68,73,74	0
12	CL	H	504	1/1	0.98	0.16	54,54,54,54	0
12	CL	C	502	1/1	0.99	0.14	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.