wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 05:11 PM EDT

PDB ID	:	3NIG
Title	:	The Closed Headpiece of Integrin IIb 3 and its Complex with an IIb 3 -Specific Antagonist That Does Not Induce Opening
Authors	:	Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on	:	2010-06-15
Resolution	:	2.25 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 (i) 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 (i)) were used in the production of this report:

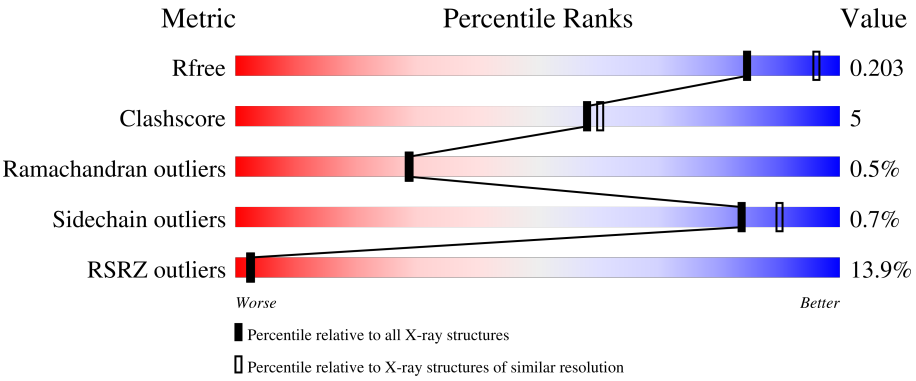
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	457	96%
1	C	457	92% 7%
2	B	471	16% 86% 12%
2	D	471	8% 88% 11%
3	E	221	49% 74% 22%

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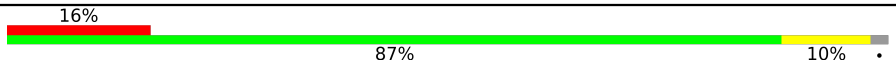
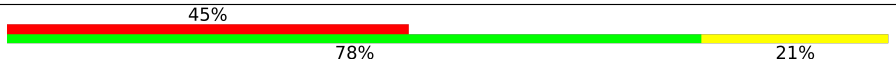
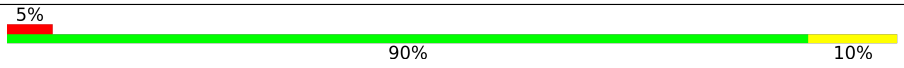
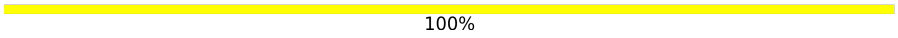
Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	3	
5	J	3	
6	I	2	
6	K	2	

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
5	MAN	G	3	X	-	-	-
5	MAN	J	3	X	-	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 22226 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	3	0
			3515	2235	605	667	8			
1	C	453	Total	C	N	O	S	0	3	0
			3489	2217	601	663	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	0	0	0
			3590	2236	613	708	33			
2	D	471	Total	C	N	O	S	0	1	0
			3634	2265	620	715	34			

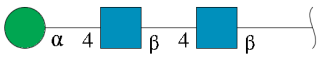
- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	G	3	Total C N O 39 22 2 15	0	0	0
5	J	3	Total C N O 39 22 2 15	0	0	0

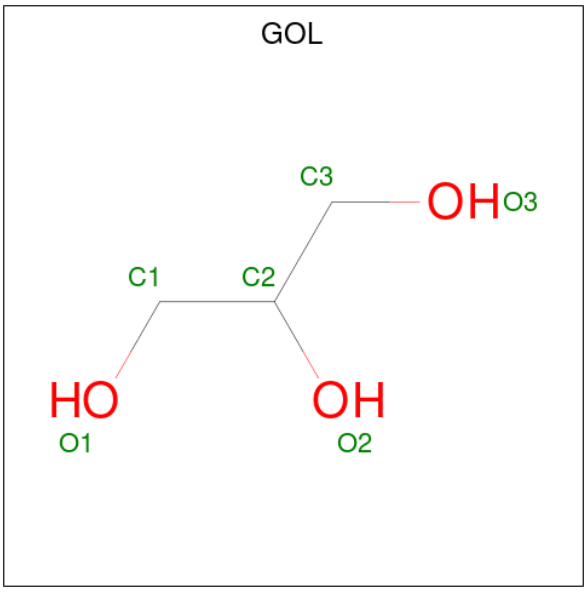
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	I	2	Total C N O 28 16 2 10	0	0	0
6	K	2	Total C N O 28 16 2 10	0	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

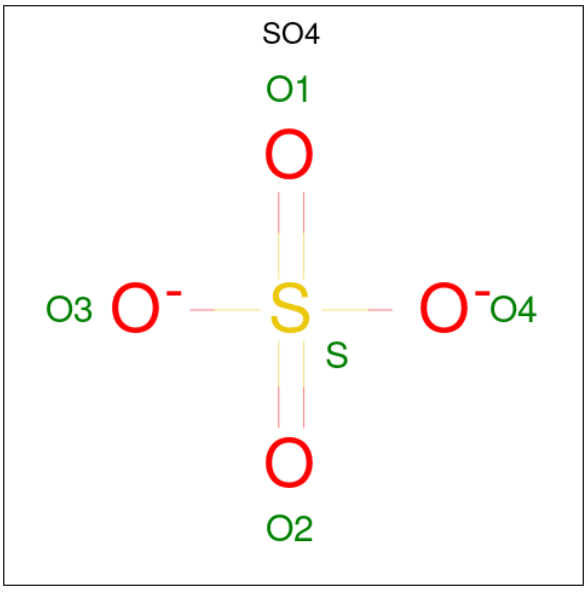
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total Ca 4 4	0	0
7	B	2	Total Ca 2 2	0	0
7	C	4	Total Ca 4 4	0	0
7	D	2	Total Ca 2 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

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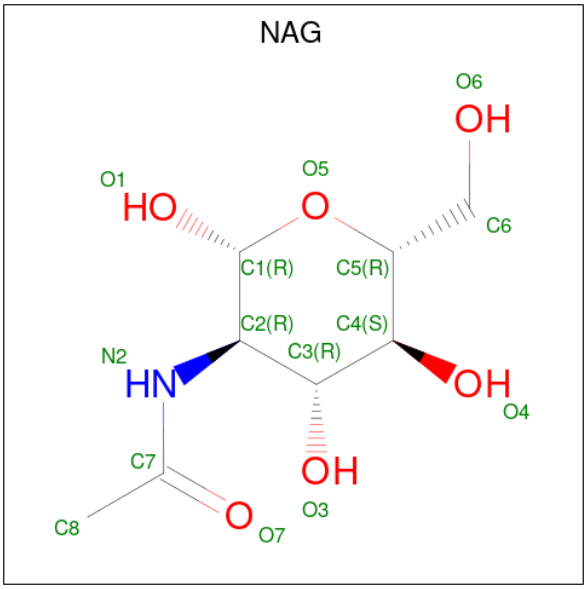
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	L	1	Total O S 5 4 1	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Mg 1 1	0	0
10	D	1	Total Mg 1 1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 12 is water.

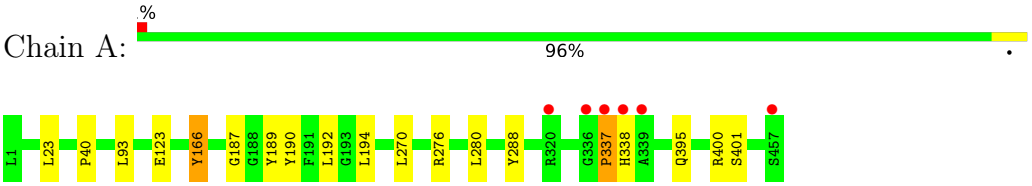
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	446	Total O 446 446	0	0
12	B	231	Total O 231 231	0	0
12	C	259	Total O 259 259	0	0
12	D	191	Total O 191 191	0	0
12	E	9	Total O 9 9	0	0
12	F	12	Total O 12 12	0	0
12	H	32	Total O 32 32	0	0
12	L	47	Total O 47 47	0	0

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.

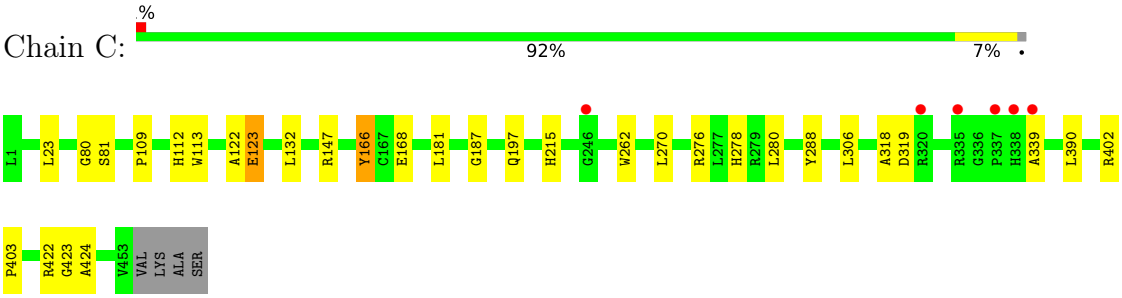
• Molecule 1: Integrin alpha-IIb

Chain A:



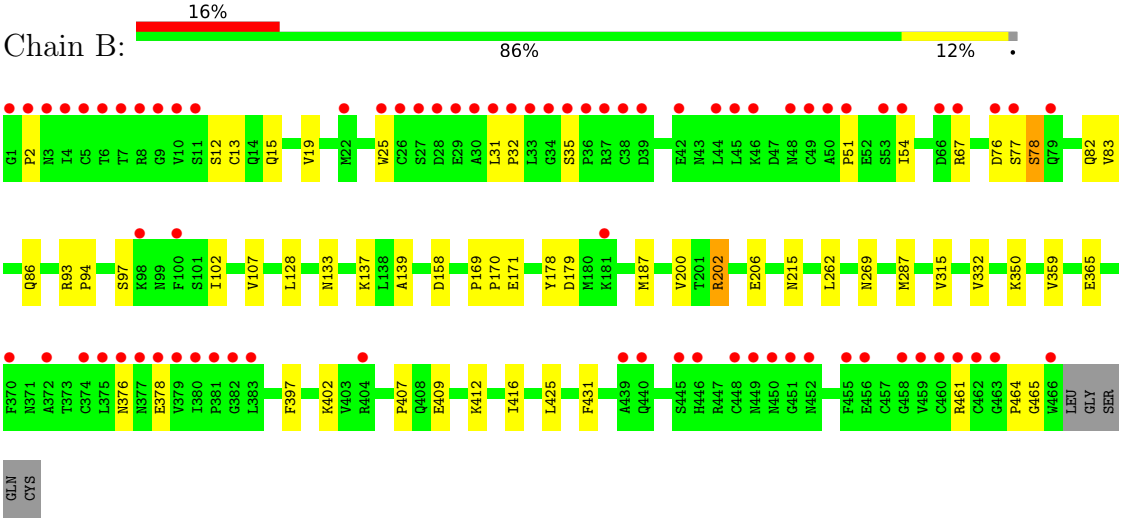
• Molecule 1: Integrin alpha-IIb

Chain C:



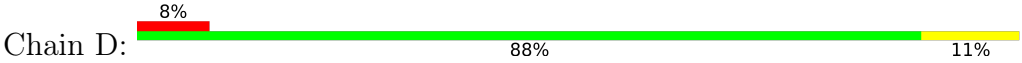
• Molecule 2: Integrin beta-3

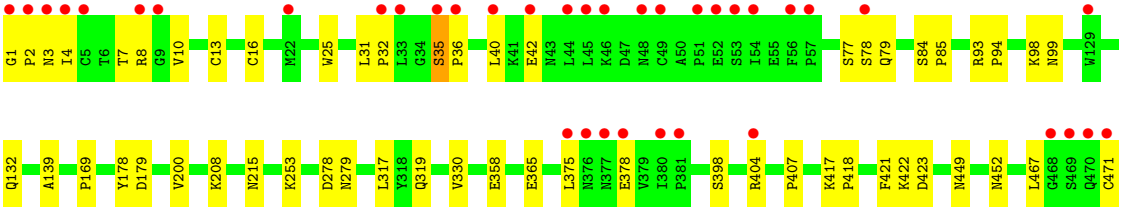
Chain B:



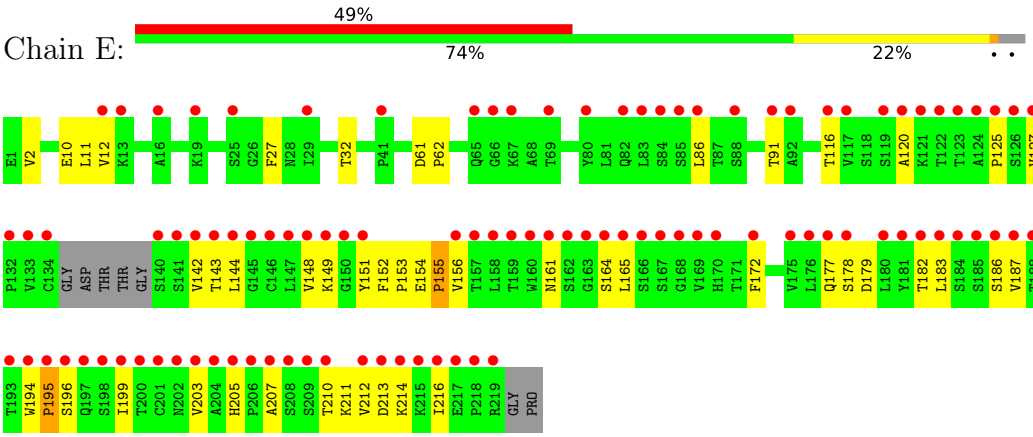
• Molecule 2: Integrin beta-3

Chain D:

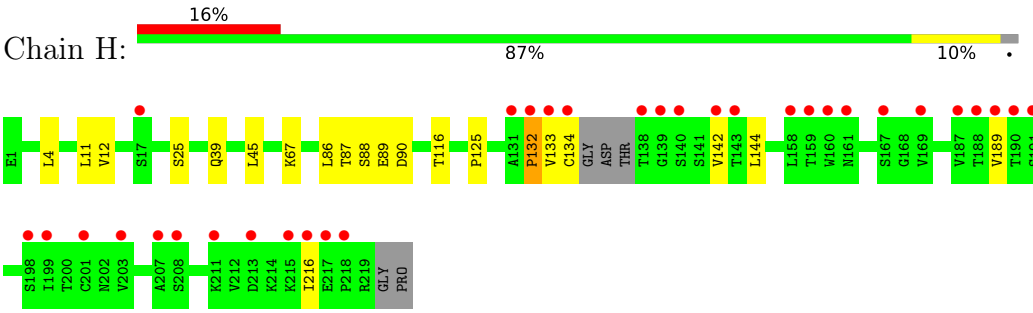




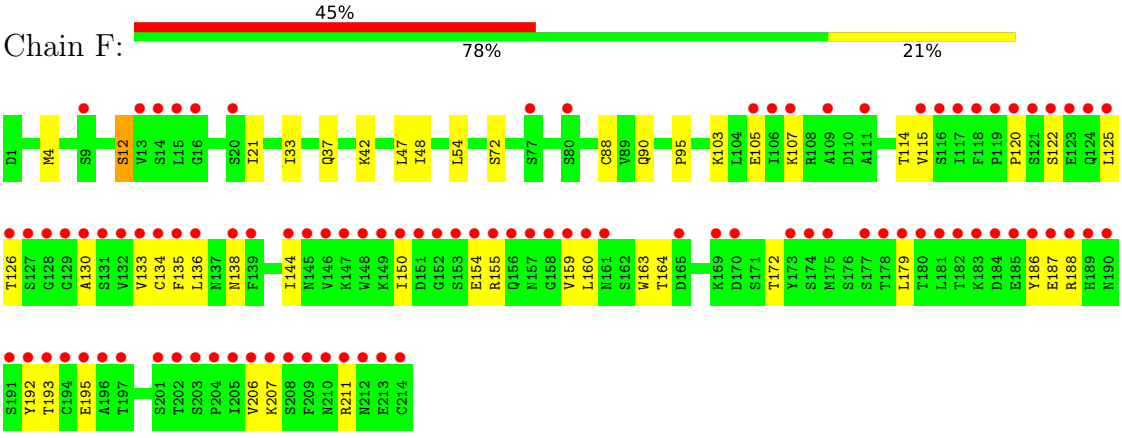
• Molecule 3: Monoclonal antibody 10E5 heavy chain



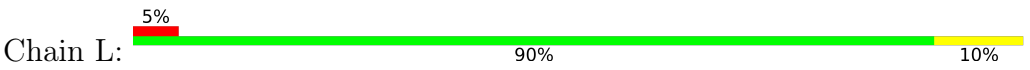
• Molecule 3: Monoclonal antibody 10E5 heavy chain

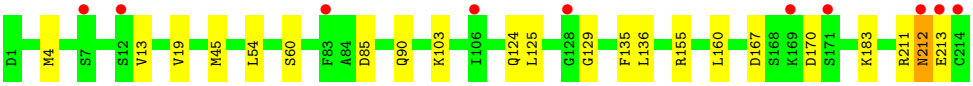


• Molecule 4: Monoclonal antibody 10E5 light chain



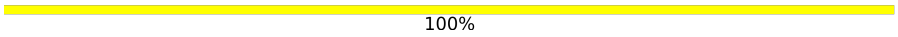
• Molecule 4: Monoclonal antibody 10E5 light chain





• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	260.67Å 145.17Å 104.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 2.25 48.49 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.49-2.25) 99.9 (48.49-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.172 , 0.212 0.161 , 0.203	Depositor DCC
R_{free} test set	1009 reflections (0.54%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22226	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: CA, NAG, MG, GOL, MAN, SO4

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	0.63	0/3621	0.68	1/4934 (0.0%)
1	C	0.49	0/3595	0.60	0/4899
2	B	0.50	0/3657	0.62	3/4959 (0.1%)
2	D	0.45	0/3706	0.55	0/5026
3	E	0.28	0/1673	0.46	0/2290
3	H	0.35	0/1684	0.51	0/2305
4	F	0.29	0/1673	0.46	0/2269
4	L	0.36	0/1673	0.54	0/2269
All	All	0.47	0/21282	0.58	4/28951 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	202	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	B	202	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	280	LEU	CA-CB-CG	-5.67	102.25	115.30
2	B	262	LEU	CA-CB-CG	-5.51	102.62	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	78	SER	Peptide

5.2 Too-close contacts (i)

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	3515	0	3361	9	0
1	C	3489	0	3327	23	0
2	B	3590	0	3511	36	0
2	D	3634	0	3551	34	0
3	E	1631	0	1590	36	0
3	H	1642	0	1600	14	0
4	F	1637	0	1553	32	0
4	L	1637	0	1553	13	0
5	G	39	0	34	0	0
5	J	39	0	34	2	0
6	I	28	0	25	1	0
6	K	28	0	25	1	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	C	4	0	0	0	0
7	D	2	0	0	0	0
8	A	12	0	16	3	0
8	C	6	0	8	2	0
9	A	10	0	0	1	0
9	C	10	0	0	0	0
9	D	5	0	0	0	0
9	L	5	0	0	1	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	A	446	0	0	1	0
12	B	231	0	0	1	0
12	C	259	0	0	2	0
12	D	191	0	0	2	0
12	E	9	0	0	1	0
12	F	12	0	0	0	0
12	H	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	47	0	0	1	0
All	All	22226	0	20214	197	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 197 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:365:GLU:HG3	2:D:407:PRO:HG3	1.66	0.76
2:D:78:SER:HB3	2:D:422:LYS:HE2	1.75	0.68
3:E:161:ASN:HB2	3:E:164:SER:HB2	1.77	0.66
2:D:375:LEU:O	2:D:378:GLU:HB2	1.95	0.65
1:C:402:ARG:HD2	12:C:574:HOH:O	1.98	0.64

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	458/457 (100%)	440 (96%)	16 (4%)	2 (0%)	34 37
1	C	454/457 (99%)	439 (97%)	14 (3%)	1 (0%)	47 55
2	B	464/471 (98%)	439 (95%)	22 (5%)	3 (1%)	25 25
2	D	470/471 (100%)	455 (97%)	14 (3%)	1 (0%)	47 55
3	E	210/221 (95%)	183 (87%)	24 (11%)	3 (1%)	11 7
3	H	212/221 (96%)	195 (92%)	16 (8%)	1 (0%)	29 29
4	F	212/214 (99%)	194 (92%)	18 (8%)	0	100 100
4	L	212/214 (99%)	204 (96%)	6 (3%)	2 (1%)	17 14
All	All	2692/2726 (99%)	2549 (95%)	130 (5%)	13 (0%)	29 29

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	GLU
3	E	178	SER
1	A	123	GLU
2	B	2	PRO
2	B	76	ASP

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	367/364 (101%)	362 (99%)	5 (1%)	67 76
1	C	364/364 (100%)	361 (99%)	3 (1%)	81 88
2	B	412/416 (99%)	410 (100%)	2 (0%)	88 92
2	D	417/416 (100%)	415 (100%)	2 (0%)	88 92
3	E	186/190 (98%)	186 (100%)	0	100 100
3	H	187/190 (98%)	185 (99%)	2 (1%)	73 82
4	F	188/188 (100%)	186 (99%)	2 (1%)	73 82
4	L	188/188 (100%)	188 (100%)	0	100 100
All	All	2309/2316 (100%)	2293 (99%)	16 (1%)	84 90

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	25	SER
4	F	95	PRO
1	C	166	TYR
4	F	12	SER
1	C	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	274	HIS
2	D	452	ASN
3	H	82	GLN
2	B	440	GLN
1	C	197	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 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	$\#\|Z\| > 2$
5	NAG	G	1	2,5	14,14,15	0.75	1 (7%)	17,19,21	0.97	0
5	NAG	G	2	5	14,14,15	0.64	0	17,19,21	3.20	6 (35%)
5	MAN	G	3	5	11,11,12	0.53	0	15,15,17	1.23	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.58	0	17,19,21	1.12	2 (11%)
6	NAG	I	2	6	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
5	NAG	J	1	2,5	14,14,15	0.49	0	17,19,21	1.28	2 (11%)
5	NAG	J	2	5	14,14,15	0.54	0	17,19,21	1.38	1 (5%)
5	MAN	J	3	5	11,11,12	0.52	0	15,15,17	1.38	3 (20%)
6	NAG	K	1	2,6	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
6	NAG	K	2	6	14,14,15	0.55	0	17,19,21	0.94	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	MAN	G	3	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
5	NAG	J	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	MAN	J	3	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	NAG	O5-C1	-2.04	1.40	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	2	NAG	C1-O5-C5	10.07	125.84	112.19
5	G	2	NAG	O5-C5-C6	-5.94	97.89	107.20
5	J	2	NAG	C1-O5-C5	4.76	118.64	112.19
5	G	3	MAN	C1-O5-C5	3.19	116.52	112.19
5	J	3	MAN	C1-O5-C5	3.13	116.44	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	3	MAN	C1
5	J	3	MAN	C1

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C8-C7-N2-C2
5	G	3	MAN	C4-C5-C6-O6
5	J	3	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	3	MAN	O5-C5-C6-O6

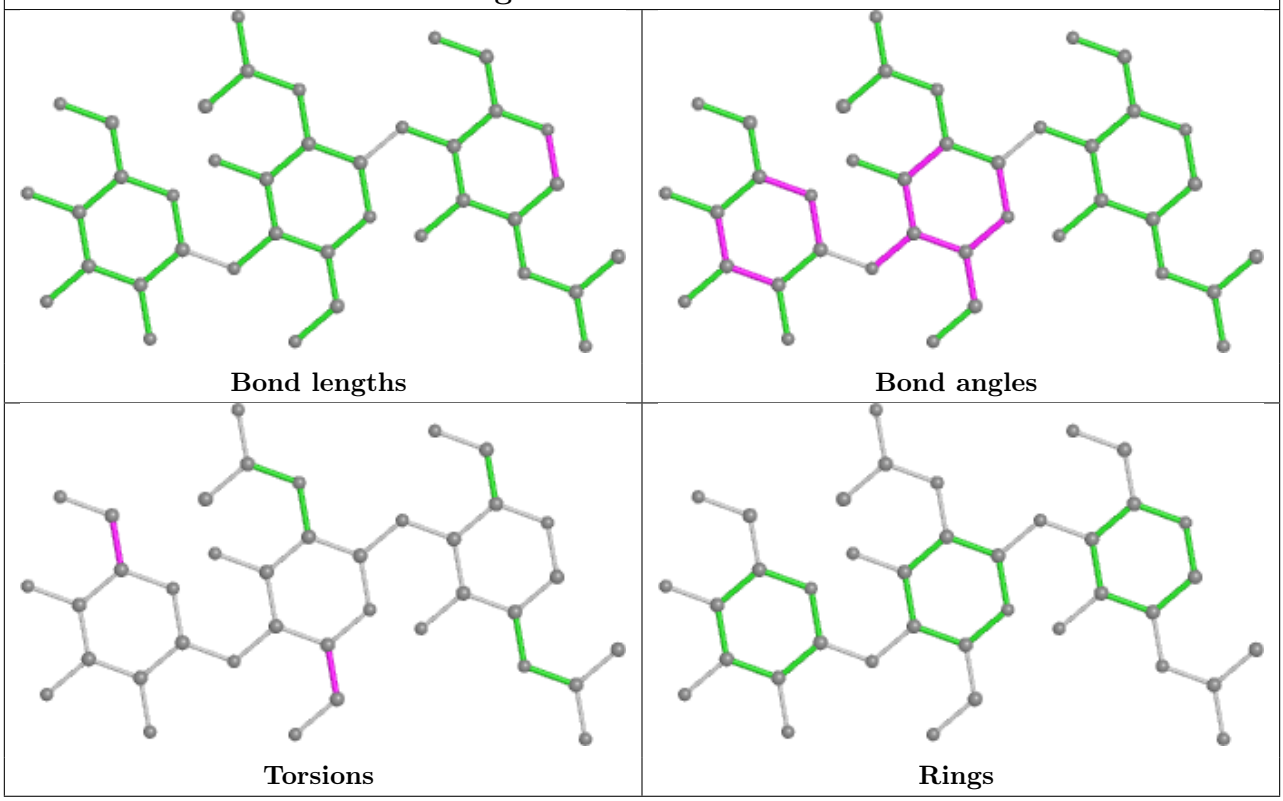
There are no ring outliers.

6 monomers are involved in 4 short contacts:

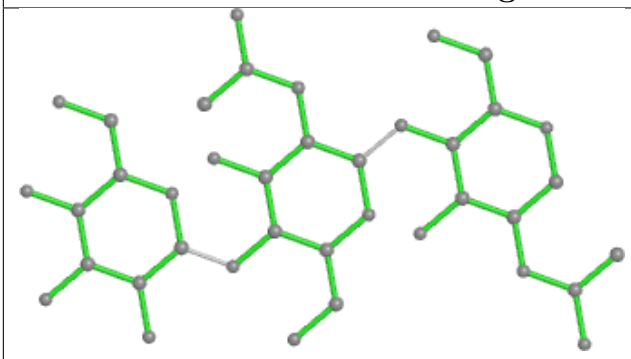
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0
6	I	1	NAG	1	0
5	J	2	NAG	2	0
5	J	3	MAN	1	0
6	I	2	NAG	1	0
5	J	1	NAG	1	0

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

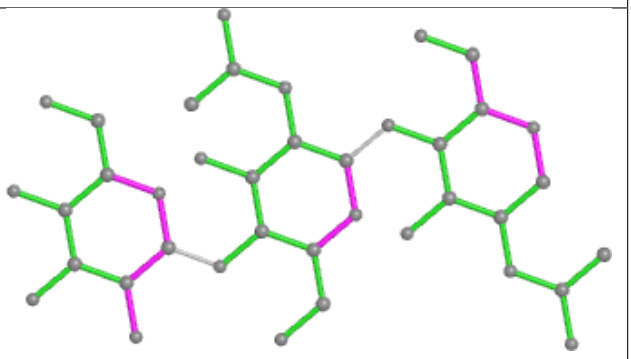
Oligosaccharide Chain G



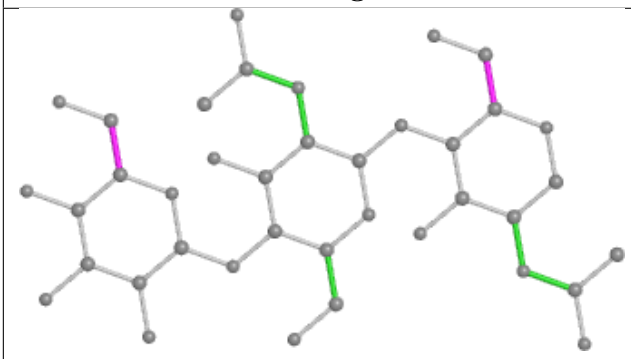
Oligosaccharide Chain J



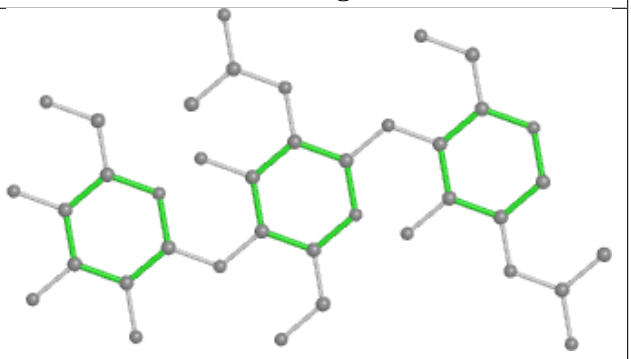
Bond lengths



Bond angles

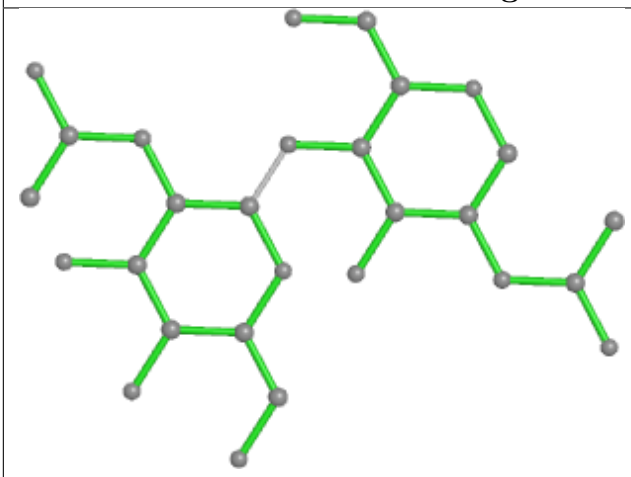


Torsions

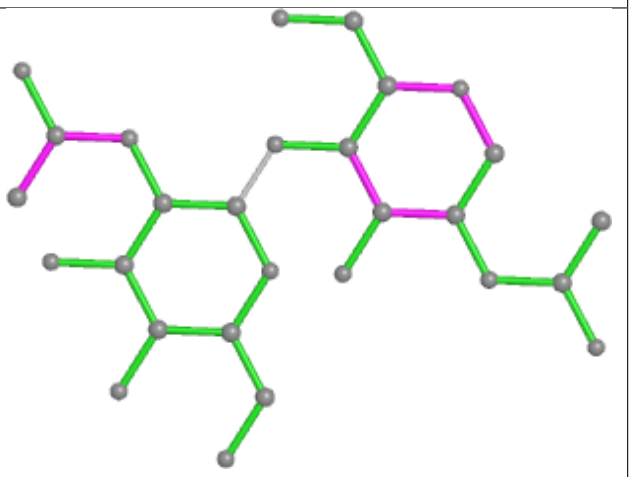


Rings

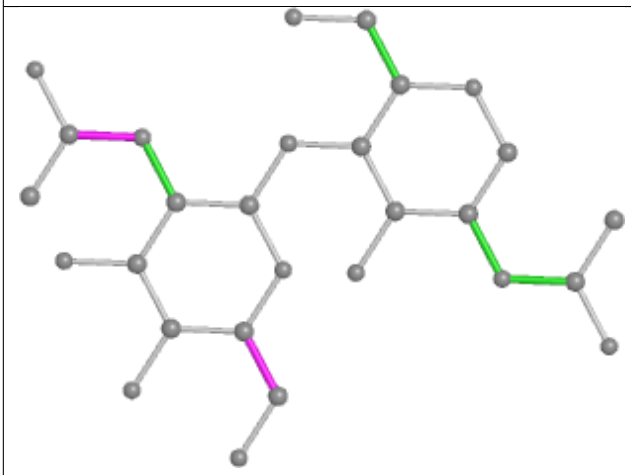
Oligosaccharide Chain I



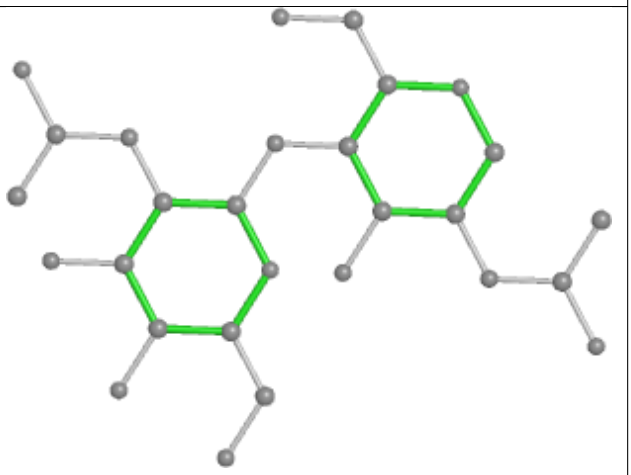
Bond lengths



Bond angles

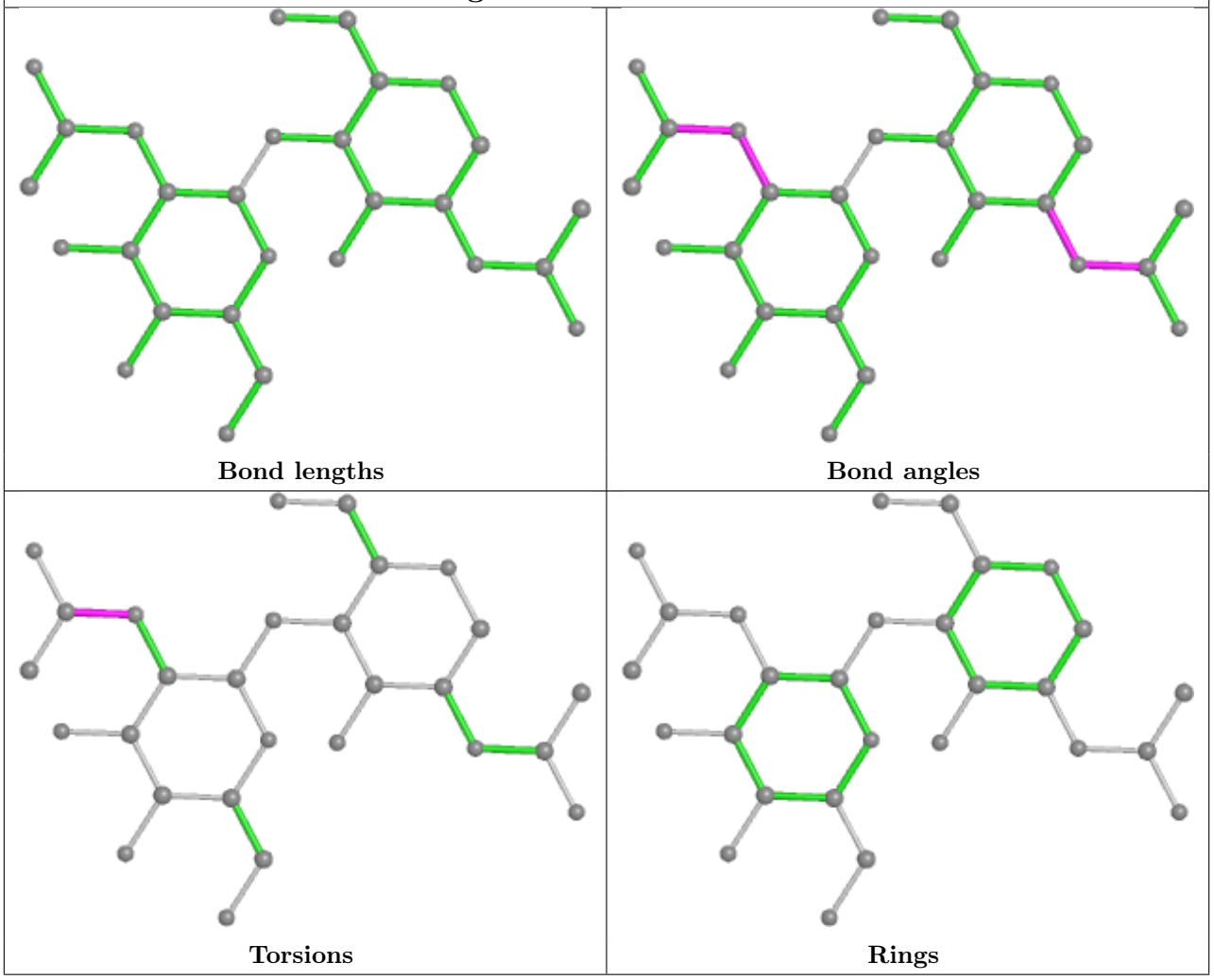


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
9	SO4	A	460	-	4,4,4	0.24	0	6,6,6	0.38	0
9	SO4	C	460	-	4,4,4	0.25	0	6,6,6	0.46	0
9	SO4	A	461	-	4,4,4	0.26	0	6,6,6	1.24	0
11	NAG	D	3099	2	14,14,15	0.60	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SO4	C	459	-	4,4,4	0.18	0	6,6,6	0.44	0
9	SO4	L	215	-	4,4,4	0.18	0	6,6,6	0.26	0
11	NAG	B	3099	2	14,14,15	0.55	0	17,19,21	0.64	0
8	GOL	A	458	-	5,5,5	0.23	0	5,5,5	0.47	0
8	GOL	C	458	-	5,5,5	0.25	0	5,5,5	0.79	0
8	GOL	A	459	-	5,5,5	0.44	0	5,5,5	0.34	0
9	SO4	D	472	-	4,4,4	0.24	0	6,6,6	0.54	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	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
11	NAG	B	3099	2	-	4/6/23/26	0/1/1/1
8	GOL	A	458	-	-	0/4/4/4	-
8	GOL	C	458	-	-	2/4/4/4	-
8	GOL	A	459	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	459	GOL	O1-C1-C2-C3
8	C	458	GOL	O1-C1-C2-O2
8	C	458	GOL	O1-C1-C2-C3
11	B	3099	NAG	O5-C5-C6-O6
8	A	459	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	461	SO4	1	0
9	L	215	SO4	1	0
8	C	458	GOL	2	0
8	A	459	GOL	3	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	457/457 (100%)	0.25	6 (1%) 77 79	15, 27, 61, 131	0
1	C	453/457 (99%)	0.12	6 (1%) 77 79	21, 42, 76, 121	0
2	B	466/471 (98%)	0.81	76 (16%) 1 1	18, 56, 134, 196	0
2	D	471/471 (100%)	0.33	38 (8%) 12 13	24, 54, 118, 159	0
3	E	214/221 (96%)	2.70	109 (50%) 0 0	47, 110, 196, 236	0
3	H	216/221 (97%)	0.50	35 (16%) 1 1	30, 77, 138, 181	0
4	F	214/214 (100%)	2.12	96 (44%) 0 0	49, 98, 187, 249	1 (0%)
4	L	214/214 (100%)	0.23	10 (4%) 31 34	36, 67, 102, 164	1 (0%)
All	All	2705/2726 (99%)	0.70	376 (13%) 2 2	15, 55, 142, 249	2 (0%)

The worst 5 of 376 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	216	ILE	15.7
3	E	199	ILE	13.9
3	E	198	SER	13.8
3	E	133	VAL	12.6
3	E	215	LYS	12.0

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,

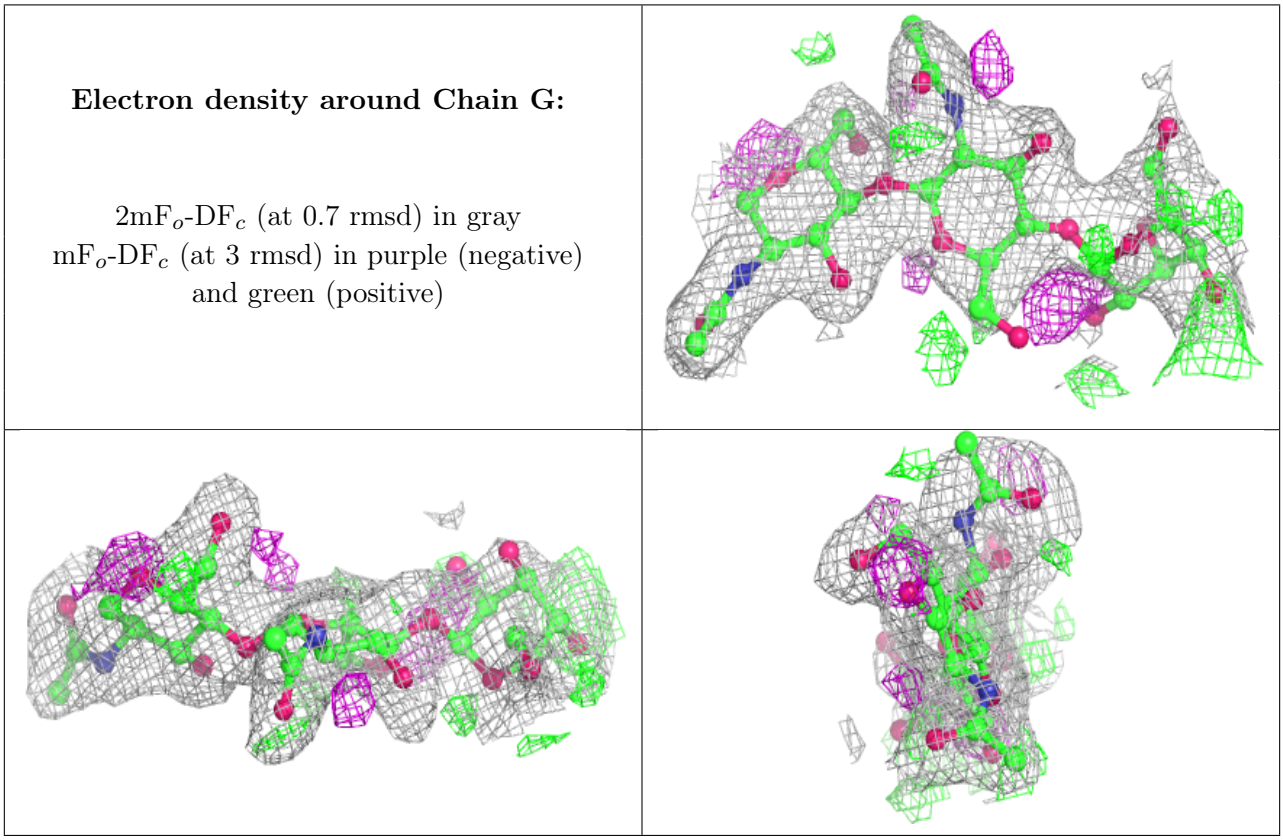
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	G	3	11/12	0.48	0.30	132,140,144,145	0
5	MAN	J	3	11/12	0.57	0.36	125,131,134,134	0
5	NAG	J	2	14/15	0.78	0.23	58,95,109,117	0
6	NAG	I	1	14/15	0.79	0.28	90,114,122,124	0
6	NAG	I	2	14/15	0.79	0.37	125,129,141,141	0
6	NAG	K	2	14/15	0.80	0.41	134,139,145,145	0
6	NAG	K	1	14/15	0.82	0.29	83,111,133,135	0
5	NAG	G	2	14/15	0.88	0.15	47,74,105,108	0
5	NAG	J	1	14/15	0.93	0.14	44,54,71,72	0
5	NAG	G	1	14/15	0.96	0.12	23,35,51,52	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.

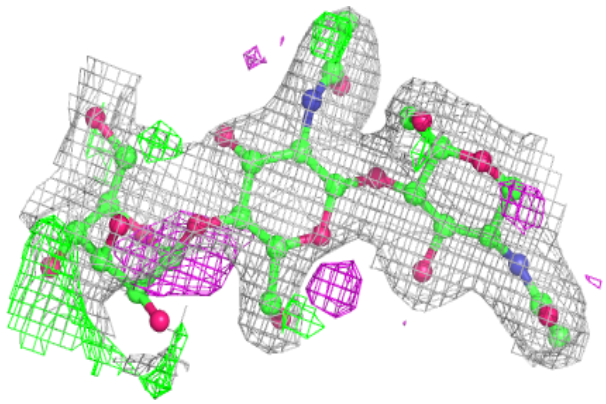
Electron density around Chain G:

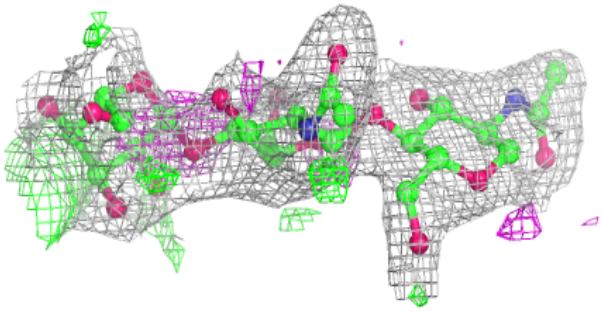
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

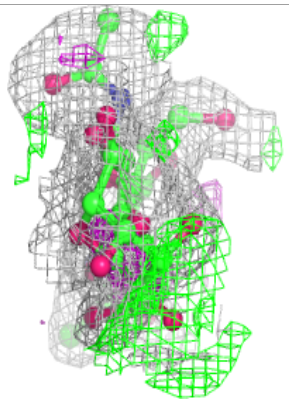


Electron density around Chain J:

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

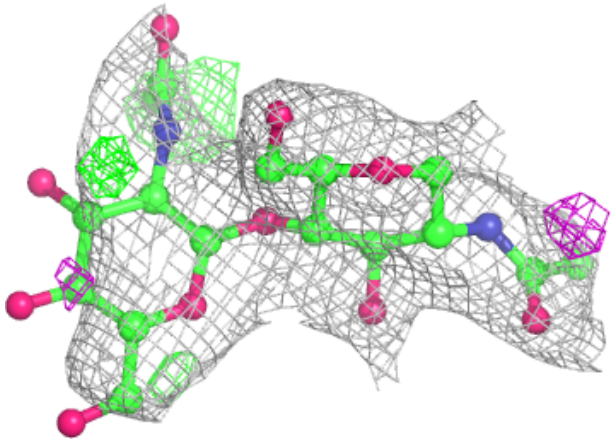


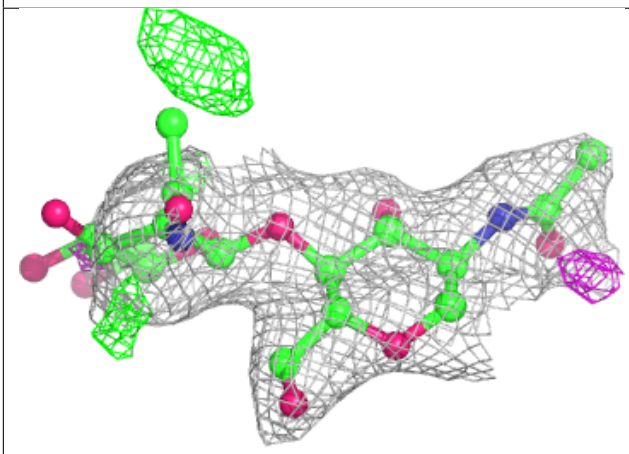


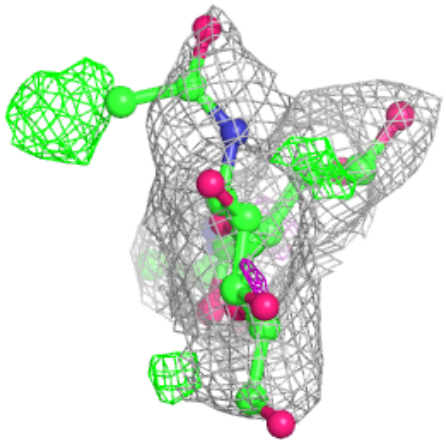


Electron density around Chain I:

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

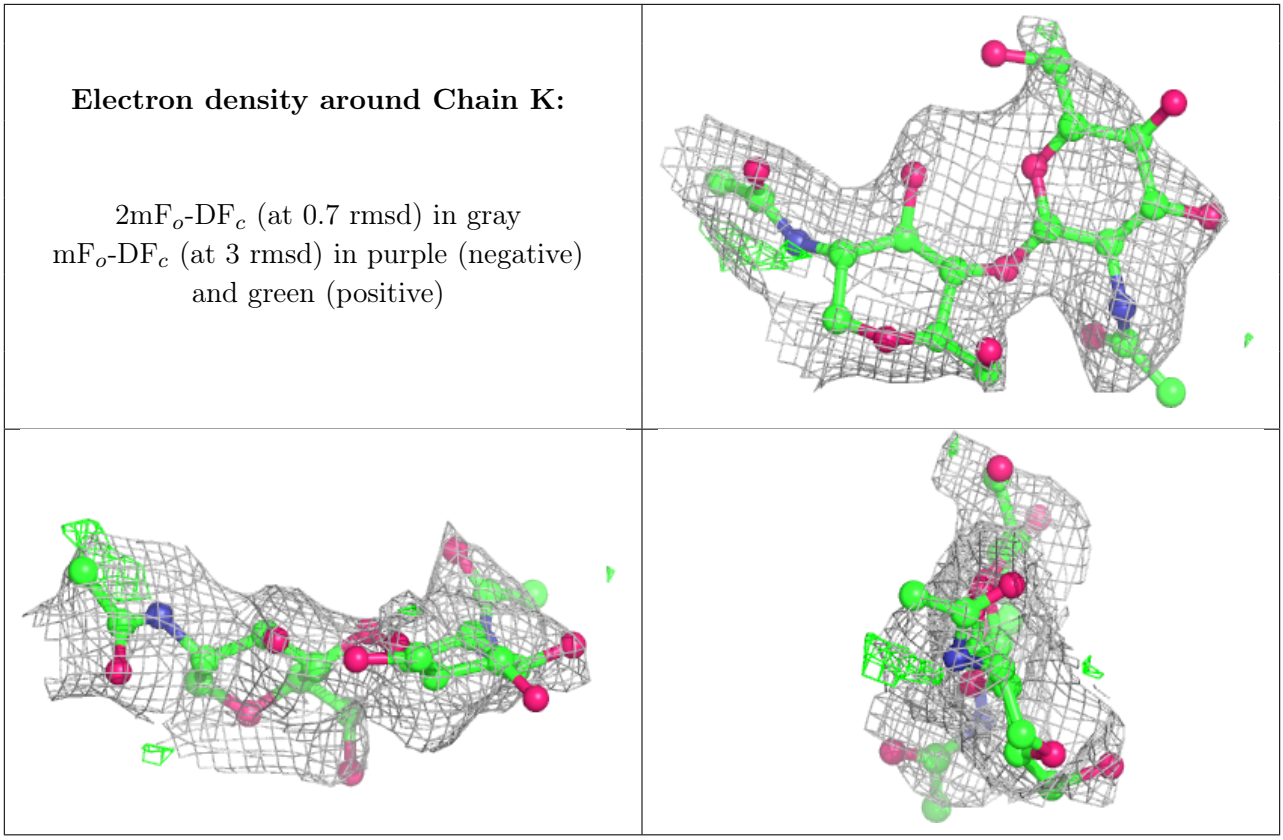






Electron density around Chain K:

$2mF_o$-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
11	NAG	D	3099	14/15	0.78	0.34	99,112,115,118	0
9	SO4	C	460	5/5	0.80	0.27	66,66,70,129	0
9	SO4	D	472	5/5	0.84	0.32	62,66,72,133	0
11	NAG	B	3099	14/15	0.89	0.29	108,118,123,123	0
8	GOL	A	459	6/6	0.90	0.19	34,51,67,74	0
9	SO4	A	461	5/5	0.90	0.14	48,49,63,70	0
9	SO4	A	460	5/5	0.91	0.22	57,67,89,90	0
9	SO4	L	215	5/5	0.91	0.23	81,82,86,95	0
8	GOL	A	458	6/6	0.93	0.20	44,55,69,77	0
9	SO4	C	459	5/5	0.94	0.17	56,71,86,96	0
8	GOL	C	458	6/6	0.94	0.13	43,61,65,68	0
10	MG	B	2001	1/1	0.96	0.16	38,38,38,38	0
7	CA	C	2005	1/1	0.96	0.06	44,44,44,44	0
7	CA	C	2004	1/1	0.96	0.05	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	C	2007	1/1	0.98	0.12	47,47,47,47	0
7	CA	C	2006	1/1	0.99	0.13	41,41,41,41	0
7	CA	B	2002	1/1	0.99	0.06	39,39,39,39	0
7	CA	D	2003	1/1	0.99	0.16	29,29,29,29	0
10	MG	D	2001	1/1	0.99	0.07	42,42,42,42	0
7	CA	A	2004	1/1	0.99	0.08	35,35,35,35	0
7	CA	A	2005	1/1	0.99	0.12	28,28,28,28	0
7	CA	A	2007	1/1	1.00	0.13	23,23,23,23	0
7	CA	D	2002	1/1	1.00	0.11	37,37,37,37	0
7	CA	A	2006	1/1	1.00	0.16	24,24,24,24	0
7	CA	B	2003	1/1	1.00	0.17	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.