



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:56 AM UTC

PDB ID : 3NID / pdb_00003nid
Title : The Closed Headpiece of Integrin α IIB β 3 and its Complex with an α IIB β 3-Specific Antagonist That Does Not Induce Opening
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on : 2010-06-15
Resolution : 2.30 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 types of validation reports are described at

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

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

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

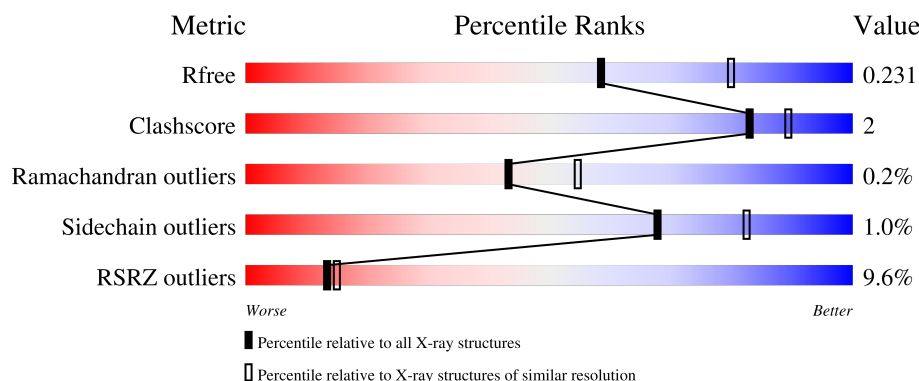
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	457	2% 95% 5%
1	C	457	2% 94% 5%
2	B	471	10% 91% 7%
2	D	471	6% 94% 6%
3	E	221	33% 86% 10%

Continued on next page...

Continued from previous page...

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

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	-	-	-
7	MAN	J	3	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22131 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	454	Total	C	N	O	S	0	5	0
			3504	2229	602	665	8			
1	C	453	Total	C	N	O	S	0	2	0
			3484	2214	600	662	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	4	2	0
			3601	2243	615	710	33			
2	D	471	Total	C	N	O	S	3	1	0
			3634	2265	620	715	34			

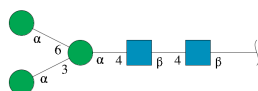
- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

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-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



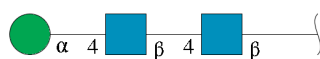
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 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.

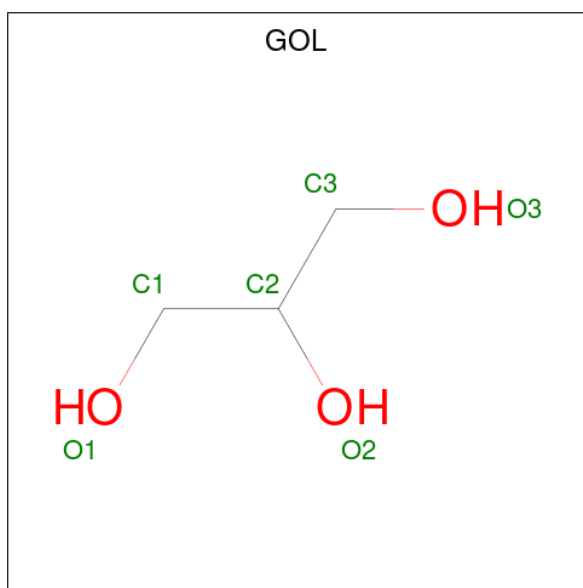


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

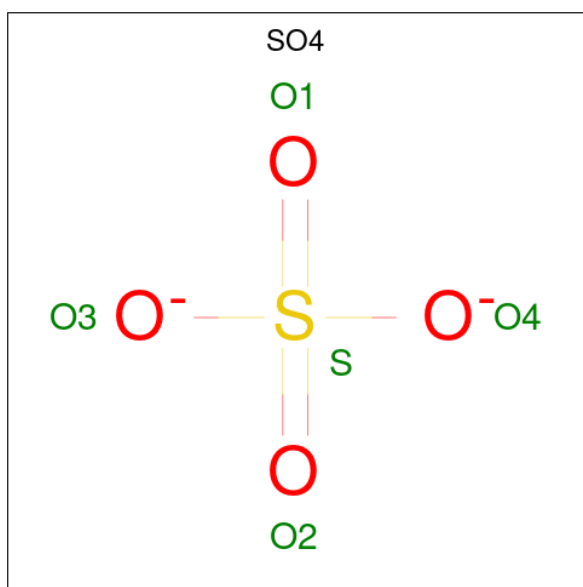
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	Ca	0	0
			4	4		
8	B	2	Total	Ca	0	0
			2	2		
8	C	4	Total	Ca	0	0
			4	4		
8	D	2	Total	Ca	0	0
			2	2		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

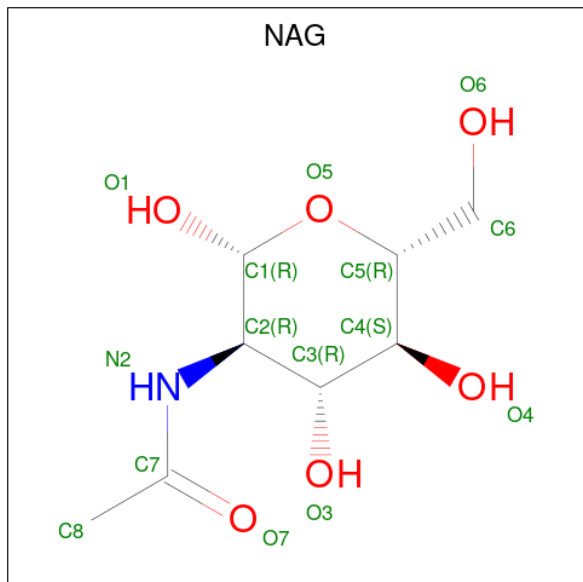


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10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

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	386	Total	O	0	0
			386	386		
13	B	192	Total	O	0	0
			192	192		
13	C	205	Total	O	0	0
			205	205		
13	D	182	Total	O	0	0
			182	182		
13	E	12	Total	O	0	0
			12	12		
13	F	12	Total	O	0	0
			12	12		
13	H	32	Total	O	0	0
			32	32		
13	L	38	Total	O	0	0
			38	38		

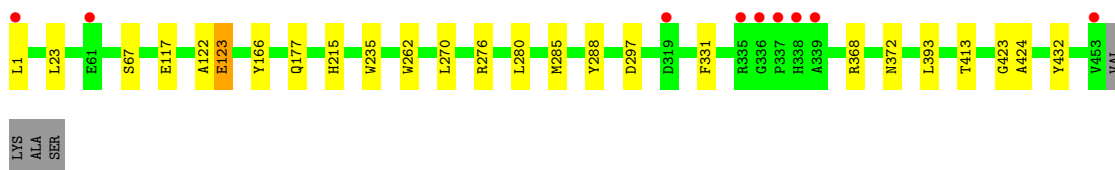
3 Residue-property plots [i](#)

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.

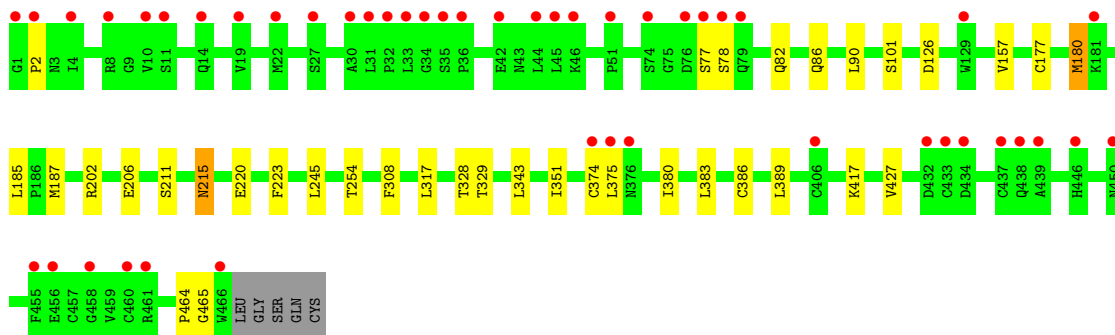
- Molecule 1: Integrin alpha-IIb



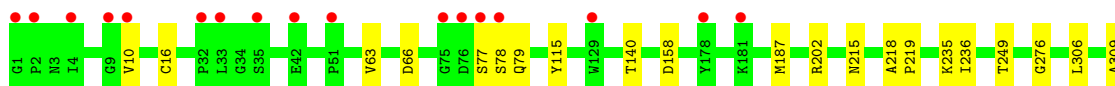
- Molecule 1: Integrin alpha-IIb



- Molecule 2: Integrin beta-3

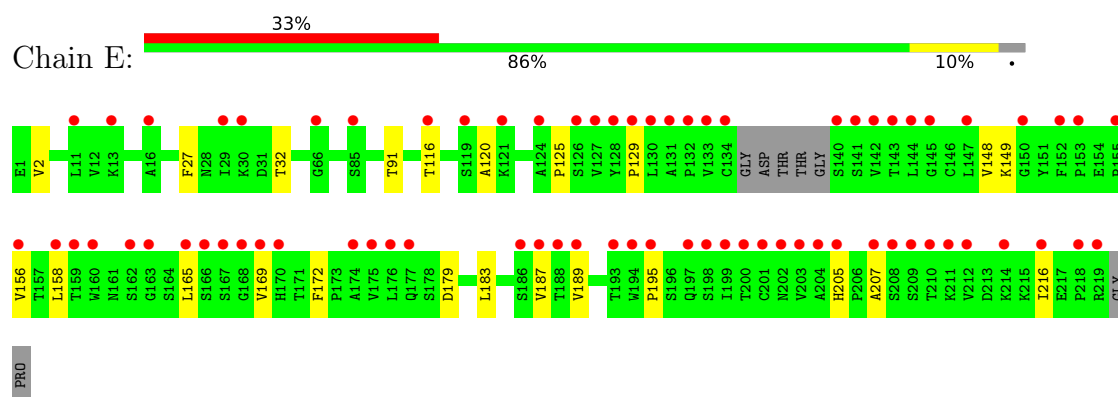


- Molecule 2: Integrin beta-3

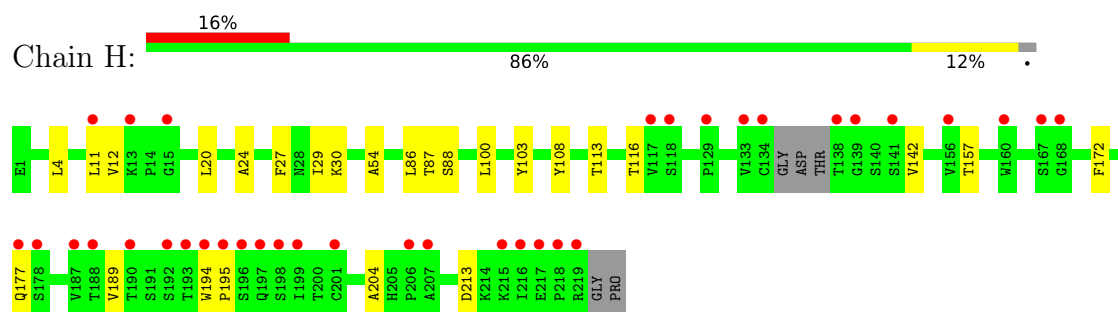




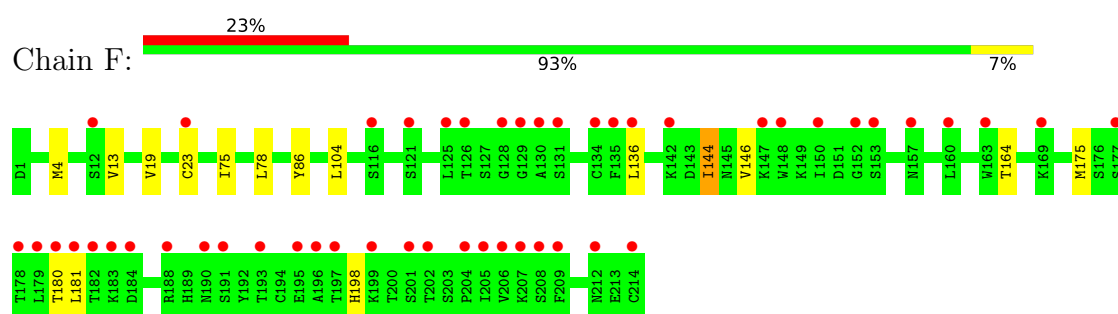
- Molecule 3: Monoclonal antibody 10E5 heavy chain



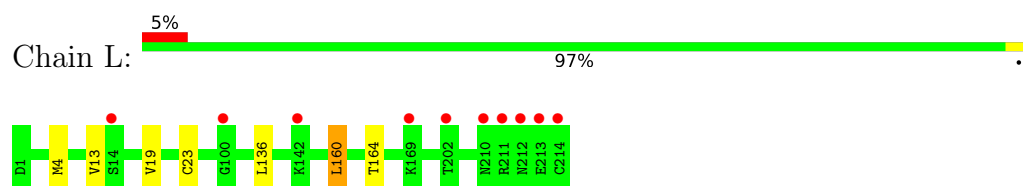
- Molecule 3: Monoclonal antibody 10E5 heavy chain



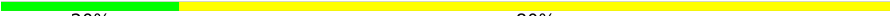
- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  20% 80%


MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain I:  100%


MAG1
MAG2

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

Chain K:  50% 50%


MAG1
MAG2

- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 67%


MAG1
MAG2
MAN3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	258.97Å 144.49Å 104.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 2.30 48.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.21-2.30) 97.8 (48.21-2.30)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.179 , 0.215 0.192 , 0.231	Depositor DCC
R_{free} test set	1029 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22131	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MAN, CA, NAG, GOL, 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	0.56	0/3616	0.70	0/4929
1	C	0.49	0/3587	0.67	0/4888
2	B	0.51	0/3674	0.72	1/4982 (0.0%)
2	D	0.48	0/3706	0.69	1/5026 (0.0%)
3	E	0.46	0/1673	0.62	0/2290
3	H	0.42	0/1684	0.61	0/2305
4	F	0.45	0/1673	0.60	0/2269
4	L	0.41	0/1673	0.61	0/2269
All	All	0.49	0/21286	0.67	2/28958 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	180	MET	N-CA-C	-6.01	100.54	109.86
2	D	79	GLN	N-CA-C	-5.23	106.75	112.72

There are no chirality outliers.

There are no planarity outliers.

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	3504	0	3351	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3484	0	3320	12	0
2	B	3601	0	3525	20	0
2	D	3634	0	3551	17	0
3	E	1631	0	1590	16	0
3	H	1642	0	1600	16	0
4	F	1637	0	1553	10	0
4	L	1637	0	1553	6	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	1	0
7	J	39	0	34	0	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	4	0	0	0	0
8	D	2	0	0	0	0
9	A	36	0	48	1	0
9	B	6	0	8	0	0
9	C	12	0	16	0	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
10	C	20	0	0	0	0
10	D	10	0	0	0	0
10	H	5	0	0	0	0
10	L	5	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	14	0	13	0	0
12	D	14	0	13	0	0
13	A	386	0	0	1	0
13	B	192	0	0	1	0
13	C	205	0	0	1	0
13	D	182	0	0	1	0
13	E	12	0	0	0	0
13	F	12	0	0	0	0
13	H	32	0	0	0	0
13	L	38	0	0	0	0
All	All	22131	0	20277	99	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 2.

The worst 5 of 99 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)
4:F:4:MET:HE3	4:F:23:CYS:SG	2.18	0.82
4:L:13:VAL:HG11	4:L:19:VAL:HG11	1.73	0.70
3:E:165:LEU:HD23	3:E:187:VAL:HG21	1.74	0.69
2:B:90:LEU:HD13	2:B:427:VAL:HG13	1.78	0.64
4:L:4:MET:HE3	4:L:23:CYS:SG	2.39	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	A	457/457 (100%)	444 (97%)	12 (3%)	1 (0%)	43	55
1	C	453/457 (99%)	440 (97%)	12 (3%)	1 (0%)	43	55
2	B	466/471 (99%)	451 (97%)	13 (3%)	2 (0%)	30	38
2	D	470/471 (100%)	457 (97%)	13 (3%)	0	100	100
3	E	210/221 (95%)	200 (95%)	9 (4%)	1 (0%)	24	31
3	H	212/221 (96%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
4	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	2692/2726 (99%)	2608 (97%)	79 (3%)	5 (0%)	43	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	375	LEU
1	C	123	GLU
2	B	2	PRO
3	E	195	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/364 (101%)	363 (99%)	4 (1%)	65	81
1	C	363/364 (100%)	357 (98%)	6 (2%)	53	72
2	B	414/416 (100%)	408 (99%)	6 (1%)	59	76
2	D	417/416 (100%)	413 (99%)	4 (1%)	68	82
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	81	90
4	F	188/188 (100%)	186 (99%)	2 (1%)	65	81
4	L	188/188 (100%)	187 (100%)	1 (0%)	81	90
All	All	2310/2316 (100%)	2286 (99%)	24 (1%)	68	82

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	177	GLN
2	D	365	GLU
2	D	215	ASN
2	D	383	LEU
2	B	101	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	133	ASN
2	D	148	ASN
4	L	190	ASN
4	L	37	GLN
4	L	38	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 ⓘ

12 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	5,2	14,14,15	0.49	0	17,19,21	1.02	2 (11%)
5	NAG	G	2	5	14,14,15	0.58	0	17,19,21	1.09	2 (11%)
5	MAN	G	3	5	11,11,12	0.57	0	15,15,17	1.39	2 (13%)
5	MAN	G	4	5	11,11,12	0.54	0	15,15,17	0.55	0
5	MAN	G	5	5	11,11,12	0.62	0	15,15,17	1.05	1 (6%)
6	NAG	I	1	2,6	14,14,15	0.59	0	17,19,21	0.77	0
6	NAG	I	2	6	14,14,15	0.48	0	17,19,21	0.98	0
7	NAG	J	1	2,7	14,14,15	0.48	0	17,19,21	1.20	2 (11%)
7	NAG	J	2	7	14,14,15	0.57	0	17,19,21	0.80	0
7	MAN	J	3	7	11,11,12	0.47	0	15,15,17	1.56	1 (6%)
6	NAG	K	1	2,6	14,14,15	0.56	0	17,19,21	0.87	1 (5%)
6	NAG	K	2	6	14,14,15	0.49	0	17,19,21	0.84	0

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	MAN	J	3	7	1/1/4/5	1/2/19/22	1/1/1/1
6	NAG	K	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	3	MAN	C1-O5-C5	5.27	119.24	112.19
7	J	1	NAG	C1-O5-C5	3.55	116.95	112.19
5	G	3	MAN	C3-C4-C5	3.28	116.18	110.23
5	G	2	NAG	C4-C3-C2	2.93	115.31	111.02
5	G	2	NAG	C3-C4-C5	2.60	114.94	110.23

All (2) chirality outliers are listed below:

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

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	I	1	NAG	C4-C5-C6-O6

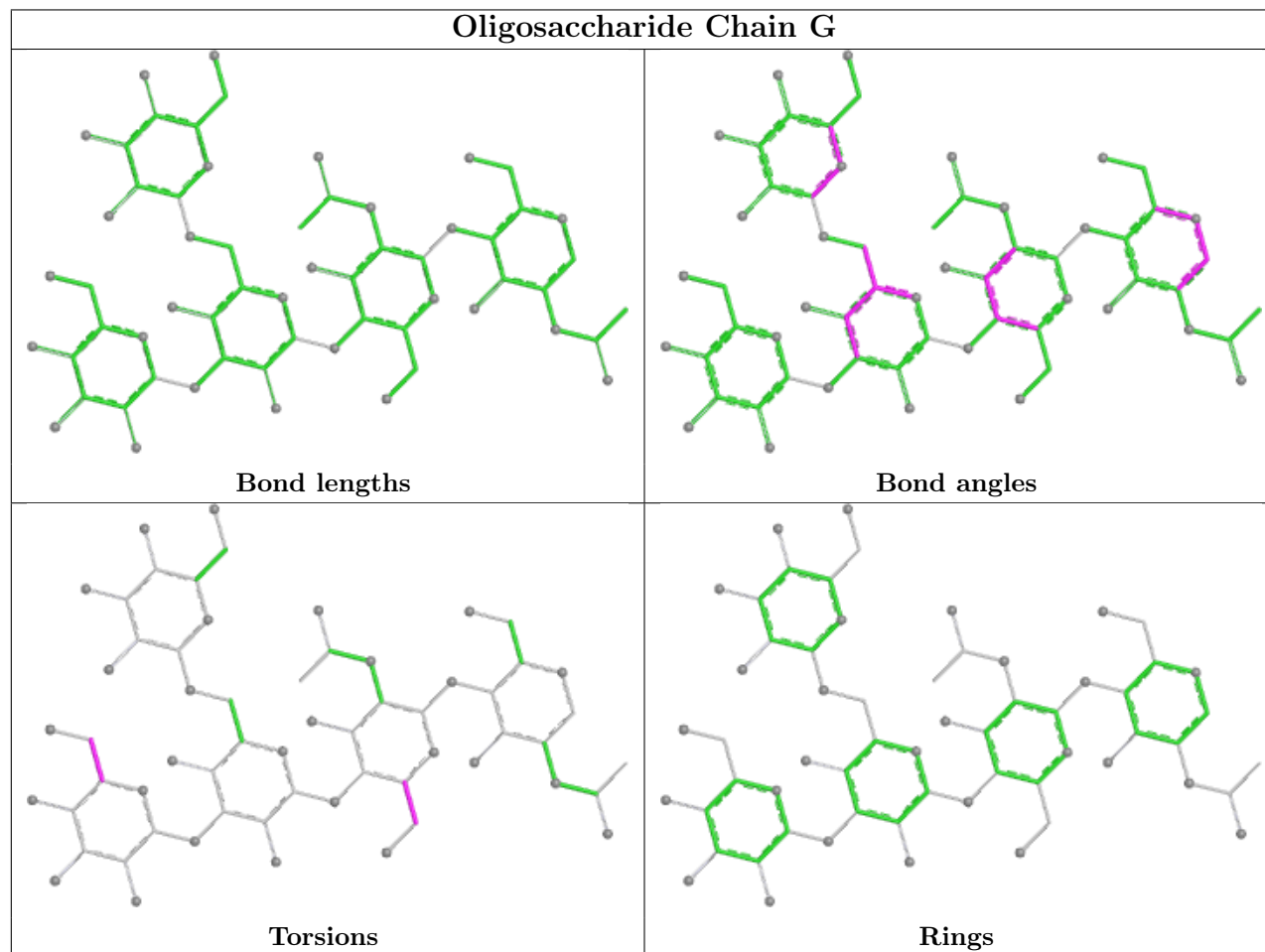
All (1) ring outliers are listed below:

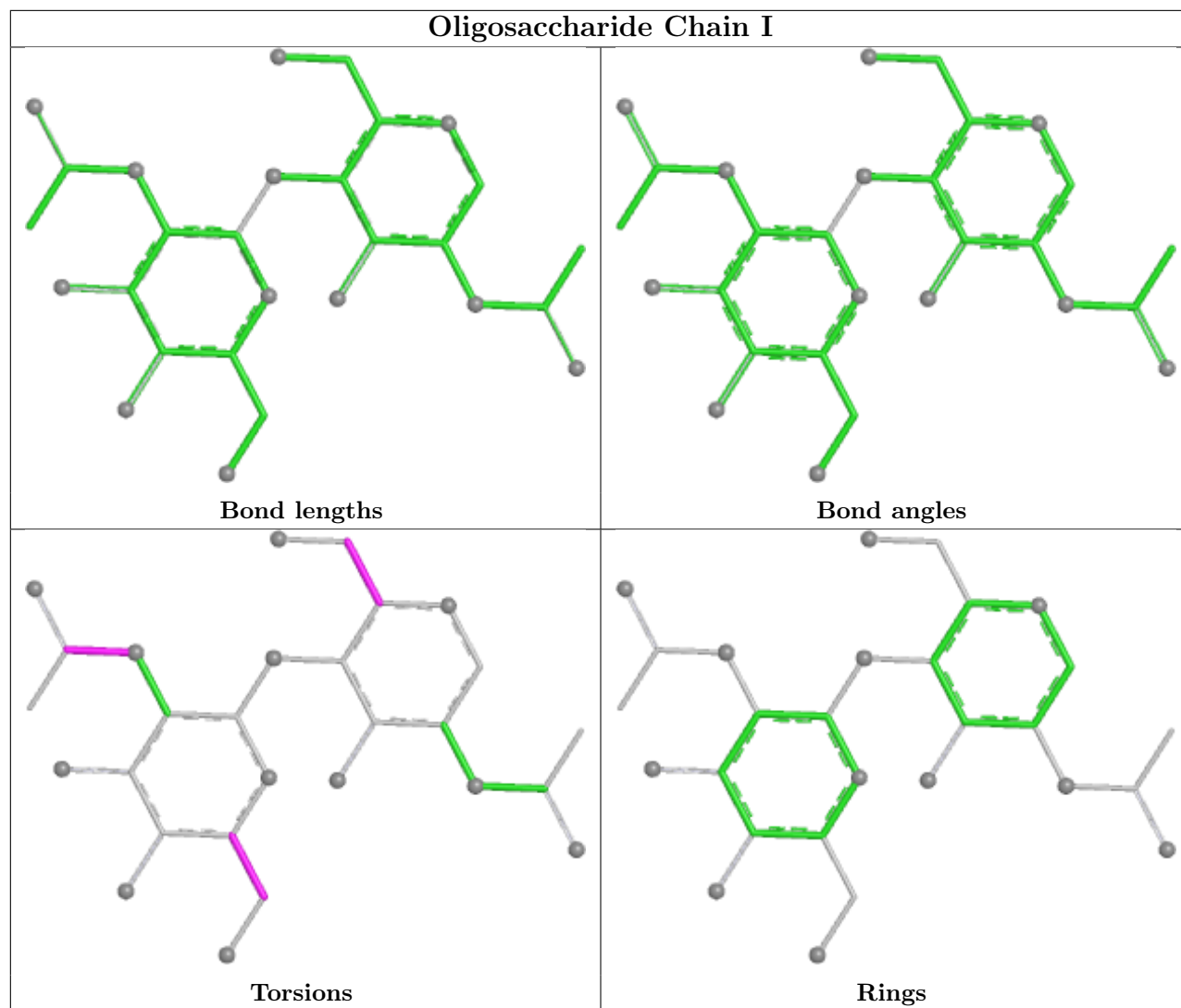
Mol	Chain	Res	Type	Atoms
7	J	3	MAN	C1-C2-C3-C4-C5-O5

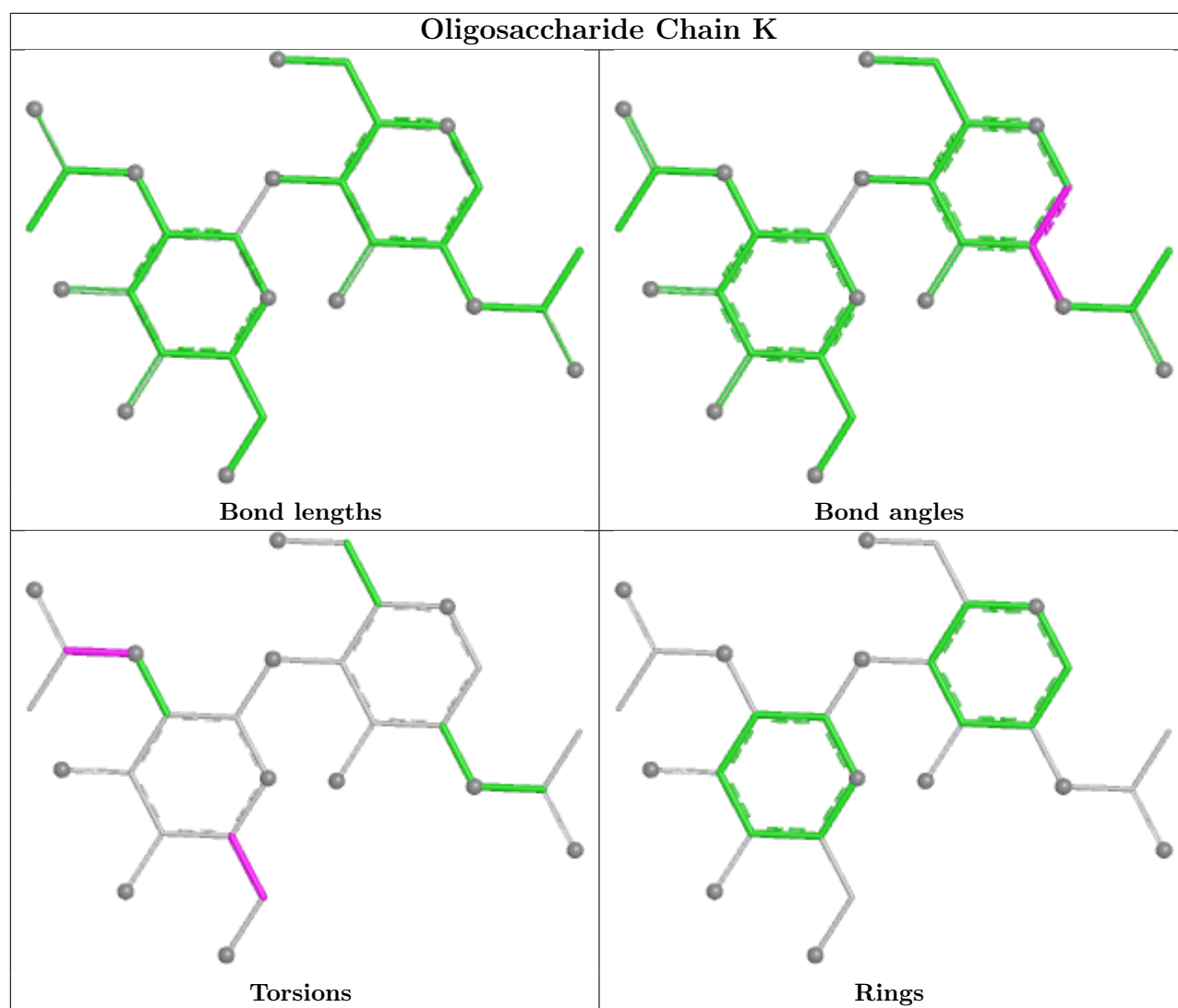
1 monomer is involved in 1 short contact:

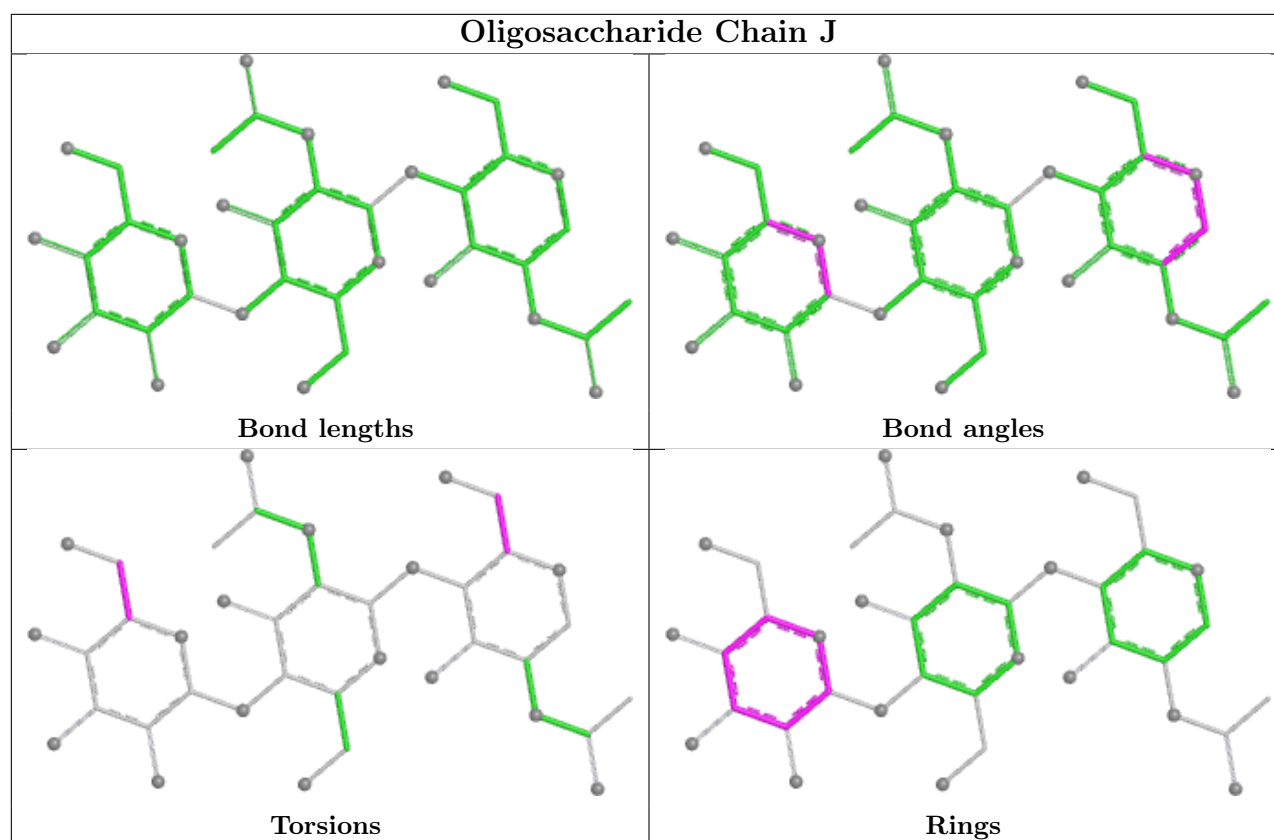
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0

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 35 ligands modelled in this entry, 14 are monoatomic - leaving 21 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	$\# Z > 2$
10	SO4	A	464	-	4,4,4	0.26	0	6,6,6	0.06	0
9	GOL	A	463	-	5,5,5	0.38	0	5,5,5	0.18	0
9	GOL	A	461	-	5,5,5	0.27	0	5,5,5	0.39	0
10	SO4	H	222	-	4,4,4	0.25	0	6,6,6	0.06	0
9	GOL	A	458	-	5,5,5	0.37	0	5,5,5	0.34	0
10	SO4	C	463	-	4,4,4	0.23	0	6,6,6	0.13	0
12	NAG	B	3099	2	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
10	SO4	C	462	-	4,4,4	0.25	0	6,6,6	0.06	0
10	SO4	C	460	-	4,4,4	0.25	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	D	3099	2	14,14,15	0.61	0	17,19,21	0.94	0
10	SO4	L	215	-	4,4,4	0.24	0	6,6,6	0.10	0
9	GOL	B	472	-	5,5,5	0.34	0	5,5,5	0.28	0
9	GOL	A	462	-	5,5,5	0.37	0	5,5,5	0.18	0
9	GOL	A	460	-	5,5,5	0.38	0	5,5,5	0.47	0
10	SO4	B	473	-	4,4,4	0.25	0	6,6,6	0.18	0
9	GOL	C	459	-	5,5,5	0.42	0	5,5,5	0.23	0
9	GOL	A	459	-	5,5,5	0.42	0	5,5,5	0.21	0
10	SO4	C	461	-	4,4,4	0.23	0	6,6,6	0.26	0
9	GOL	C	458	-	5,5,5	0.27	0	5,5,5	0.36	0
10	SO4	D	472	-	4,4,4	0.25	0	6,6,6	0.14	0
10	SO4	D	473	-	4,4,4	0.24	0	6,6,6	0.12	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
9	GOL	A	462	-	-	2/4/4/4	-
9	GOL	A	460	-	-	2/4/4/4	-
12	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
9	GOL	A	463	-	-	2/4/4/4	-
9	GOL	C	458	-	-	2/4/4/4	-
9	GOL	C	459	-	-	2/4/4/4	-
12	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
9	GOL	A	461	-	-	2/4/4/4	-
9	GOL	A	459	-	-	2/4/4/4	-
9	GOL	A	458	-	-	2/4/4/4	-
9	GOL	B	472	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	3099	NAG	C1-O5-C5	2.23	115.17	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	460	GOL	C1-C2-C3-O3
9	A	461	GOL	O1-C1-C2-C3
9	A	463	GOL	C1-C2-C3-O3
9	B	472	GOL	O1-C1-C2-O2
9	B	472	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	458	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 [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	A	454/457 (99%)	-0.65	7 (1%) 72 73	9, 20, 49, 89	5 (1%)
1	C	453/457 (99%)	-0.31	9 (1%) 65 66	14, 32, 63, 106	2 (0%)
2	B	466/471 (98%)	0.27	47 (10%) 12 14	10, 44, 127, 170	3 (0%)
2	D	471/471 (100%)	0.10	29 (6%) 26 28	16, 41, 101, 142	2 (0%)
3	E	214/221 (96%)	1.59	73 (34%) 1 1	41, 96, 147, 161	0
3	H	216/221 (97%)	0.89	36 (16%) 4 5	24, 73, 143, 176	0
4	F	214/214 (100%)	1.22	49 (22%) 2 2	41, 91, 143, 170	1 (0%)
4	L	214/214 (100%)	0.35	10 (4%) 36 38	26, 57, 104, 194	1 (0%)
All	All	2702/2726 (99%)	0.22	260 (9%) 13 15	9, 44, 128, 194	14 (0%)

The worst 5 of 260 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	9.2
2	B	33	LEU	6.4
3	E	165	LEU	5.9
3	E	203	VAL	5.6
3	E	201	CYS	5.0

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

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

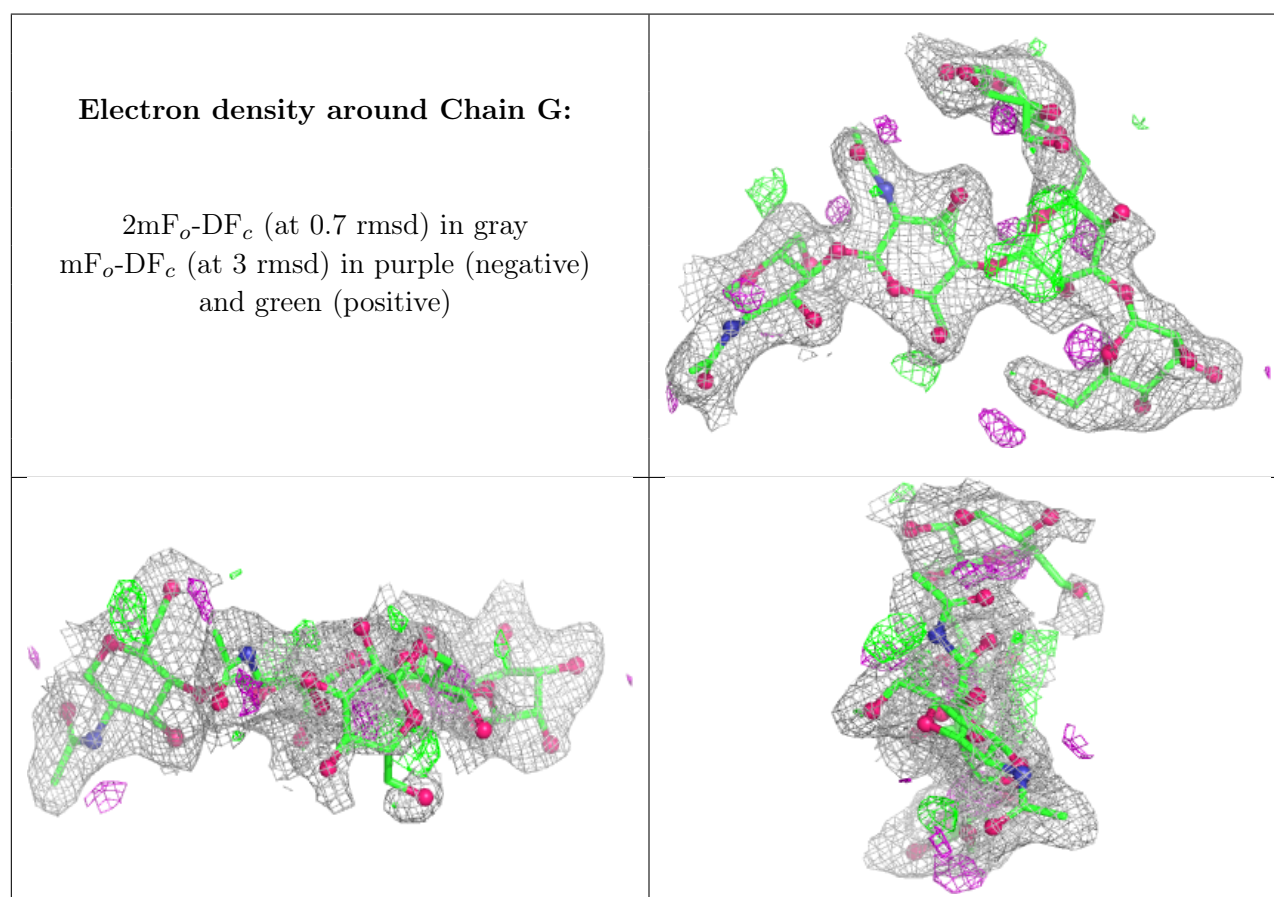
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

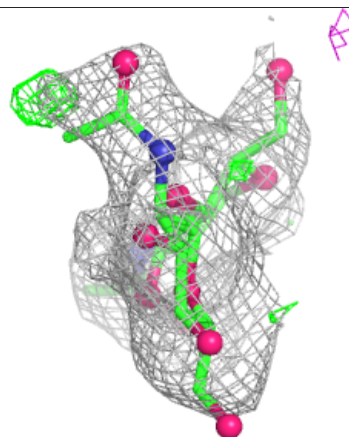
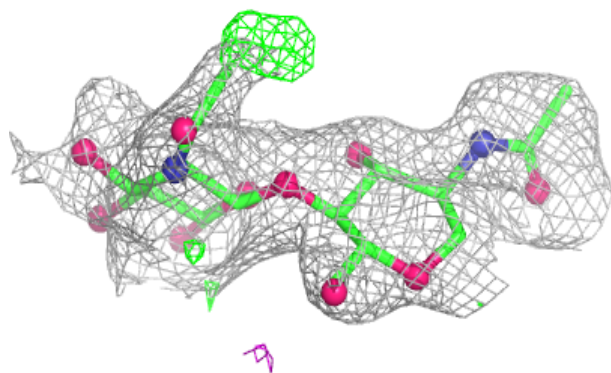
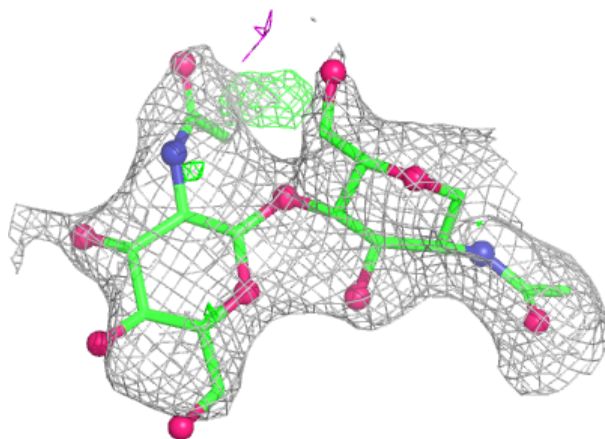
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	17,28,41,46	0
5	NAG	G	2	14/15	-	-	40,53,63,76	0
5	MAN	G	3	11/12	-	-	52,93,109,113	0
5	MAN	G	4	11/12	-	-	64,77,88,90	0
5	MAN	G	5	11/12	-	-	106,113,118,118	0
7	NAG	J	2	14/15	0.64	0.16	57,71,87,101	0
6	NAG	K	2	14/15	0.86	0.14	118,126,130,131	0
6	NAG	I	2	14/15	0.87	0.12	108,117,121,123	0
7	NAG	J	1	14/15	0.88	0.12	25,41,53,57	0
6	NAG	K	1	14/15	0.94	0.07	55,84,97,112	0
6	NAG	I	1	14/15	0.95	0.06	58,87,99,110	0
7	MAN	J	3	11/12	-	-	100,108,110,110	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.

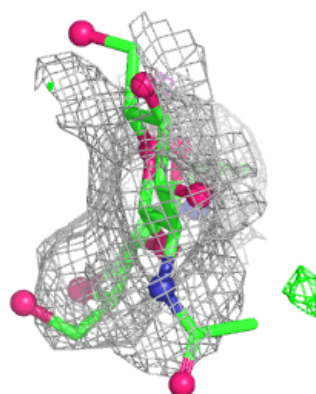
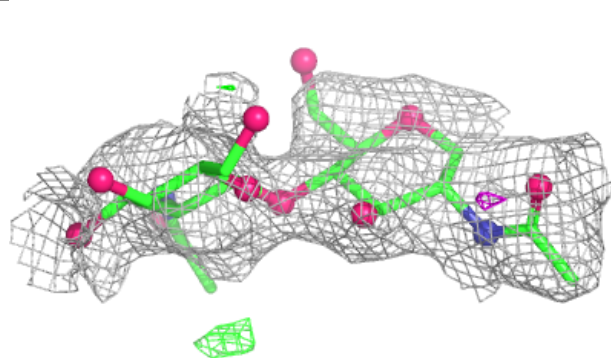
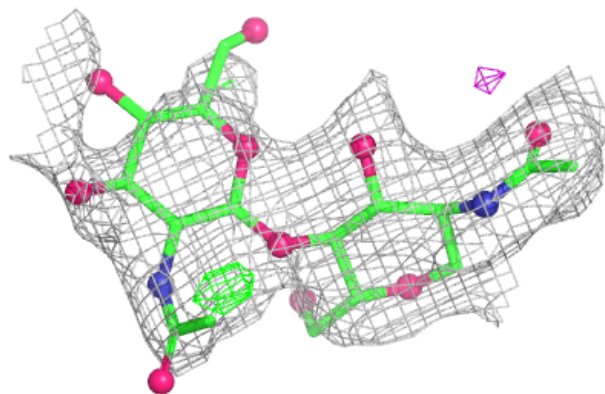


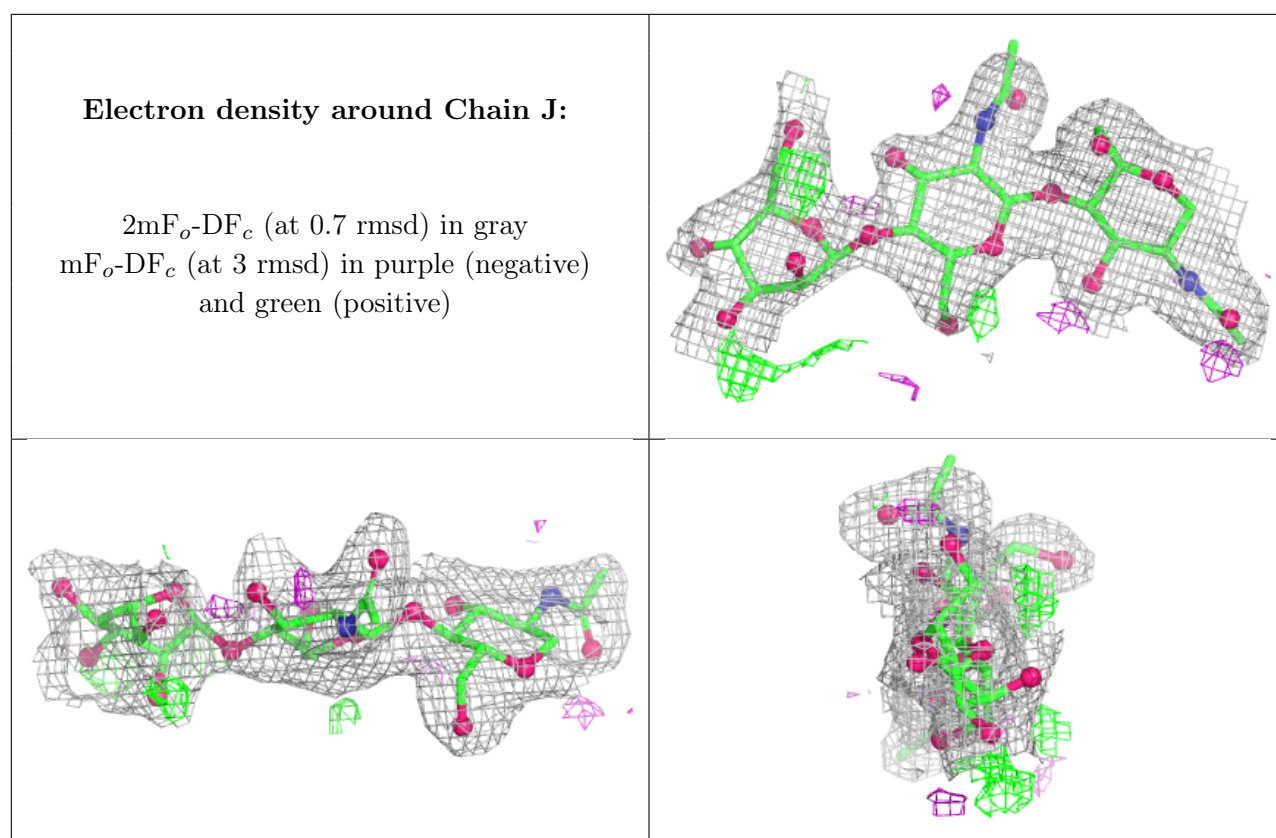
Electron density around Chain I:

$2mF_o-DF_c$ (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	MG	D	2001	1/1	0.53	0.32	41,41,41,41	1
12	NAG	D	3099	14/15	0.73	0.16	76,90,95,96	0
10	SO4	L	215	5/5	0.74	0.15	101,106,112,115	0
12	NAG	B	3099	14/15	0.77	0.13	85,98,104,106	0
10	SO4	D	472	5/5	0.77	0.17	73,92,98,108	0
10	SO4	B	473	5/5	0.79	0.19	90,98,103,108	0
10	SO4	H	222	5/5	0.79	0.13	112,116,118,123	0
9	GOL	A	463	6/6	0.80	0.25	77,79,83,84	0
9	GOL	B	472	6/6	0.81	0.18	65,70,72,77	0
10	SO4	C	461	5/5	0.81	0.14	55,75,85,87	0
9	GOL	C	458	6/6	0.84	0.19	45,61,71,79	0
10	SO4	C	462	5/5	0.84	0.12	110,113,117,118	0
10	SO4	D	473	5/5	0.85	0.21	131,133,136,137	0
10	SO4	C	463	5/5	0.85	0.10	84,91,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GOL	A	462	6/6	0.86	0.17	47,61,65,70	0
9	GOL	A	458	6/6	0.87	0.15	28,51,56,58	0
10	SO4	A	464	5/5	0.88	0.17	97,98,107,112	0
9	GOL	A	460	6/6	0.89	0.20	68,70,78,84	0
9	GOL	A	461	6/6	0.90	0.14	28,50,57,71	0
9	GOL	C	459	6/6	0.92	0.16	52,67,73,74	0
10	SO4	C	460	5/5	0.92	0.20	39,53,83,84	0
11	MG	B	2001	1/1	0.93	0.15	26,26,26,26	1
9	GOL	A	459	6/6	0.94	0.10	42,45,58,58	0
8	CA	D	2002	1/1	0.97	0.03	31,31,31,31	0
8	CA	B	2002	1/1	0.97	0.05	35,35,35,35	0
8	CA	C	2004	1/1	0.98	0.03	45,45,45,45	0
8	CA	C	2006	1/1	0.98	0.03	34,34,34,34	0
8	CA	C	2007	1/1	0.98	0.05	36,36,36,36	0
8	CA	A	2005	1/1	0.99	0.03	19,19,19,19	0
8	CA	D	2003	1/1	0.99	0.02	22,22,22,22	0
8	CA	C	2005	1/1	0.99	0.02	38,38,38,38	0
8	CA	A	2006	1/1	0.99	0.03	16,16,16,16	0
8	CA	A	2004	1/1	0.99	0.02	29,29,29,29	0
8	CA	B	2003	1/1	1.00	0.02	13,13,13,13	0
8	CA	A	2007	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.